



Full wwPDB EM Validation Report ⓘ

Oct 13, 2024 – 05:40 am BST

PDB ID : 6SW9
EMDB ID : EMD-10320
Title : IC2A model of cryo-EM structure of a full archaeal ribosomal translation initiation complex devoid of aIF1 in *P. abyssi*
Authors : Coureux, P.-D.; Mechulam, Y.; Schmitt, E.
Deposited on : 2019-09-20
Resolution : 4.20 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

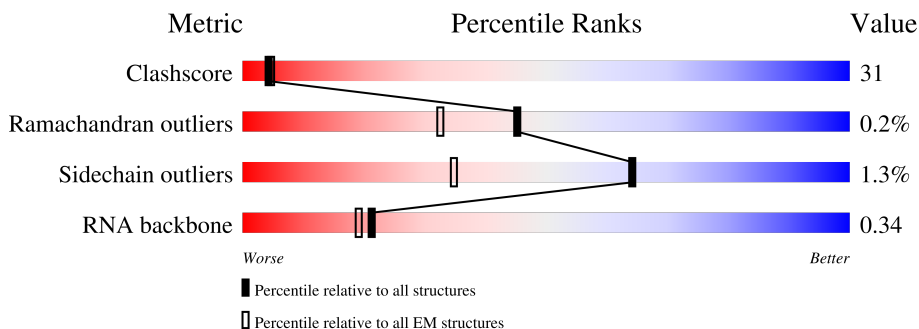
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 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.











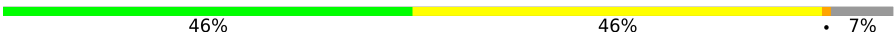
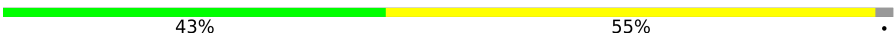



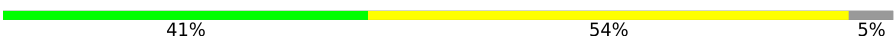











| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore | 210492 | 15764 |
| Ramachandran outliers | 207382 | 16835 |
| Sidechain outliers | 206894 | 16415 |
| RNA backbone | 6643 | 2191 |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | 2 | 1497 | |
| 2 | A | 199 | |
| 3 | B | 202 | |
| 4 | C | 63 | |
| 5 | D | 180 | |
| 6 | E | 243 | |
| 7 | F | 236 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 8 | G | 125 |  |
| 9 | H | 215 |  |
| 10 | I | 130 |  |
| 11 | J | 127 |  |
| 12 | K | 135 |  |
| 13 | L | 102 |  |
| 14 | M | 137 |  |
| 15 | N | 147 |  |
| 16 | O | 148 |  |
| 17 | P | 56 |  |
| 18 | Q | 158 |  |
| 19 | R | 113 |  |
| 20 | S | 67 |  |
| 21 | T | 132 |  |
| 22 | U | 150 |  |
| 23 | V | 99 |  |
| 24 | W | 65 |  |
| 25 | X | 71 |  |
| 26 | Y | 51 |  |
| 27 | Z | 210 |  |
| 28 | 0 | 36 |  |
| 29 | 3 | 123 |  |
| 30 | 5 | 20 |  |
| 31 | 4 | 76 |  |
| 32 | 6 | 113 |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 33 | 7 | 414 | <div><div></div><div>10%</div><div>36%</div><div>63%</div><div></div></div> |
| 34 | 8 | 129 | <div><div></div><div>71%</div><div>65%</div><div>33%</div><div></div></div> |
| 35 | 9 | 254 | <div><div></div><div>72%</div><div>66%</div><div>33%</div><div></div></div> |

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 70661 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 1 | 2 | 1497 | Total | C | N | O | P | 0 | 0 |
| | | | 32291 | 14394 | 5959 | 10441 | 1497 | | |

- Molecule 2 is a protein called 30S ribosomal protein S3Ae.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 2 | A | 188 | Total | C | N | O | S | 0 | 0 |
| | | | 1533 | 995 | 268 | 266 | 4 | | |

- Molecule 3 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 3 | B | 196 | Total | C | N | O | S | 0 | 0 |
| | | | 1571 | 1017 | 269 | 281 | 4 | | |

- Molecule 4 is a protein called Zn-ribbon RNA-binding protein involved in translation.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 4 | C | 61 | Total | C | N | O | S | 0 | 0 |
| | | | 482 | 304 | 85 | 85 | 8 | | |

- Molecule 5 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 5 | D | 175 | Total | C | N | O | S | 0 | 0 |
| | | | 1470 | 924 | 284 | 258 | 4 | | |

- Molecule 6 is a protein called 30S ribosomal protein S4e.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 6 | E | 242 | Total | C | N | O | S | 0 | 0 |
| | | | 1983 | 1281 | 358 | 339 | 5 | | |

- Molecule 7 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 7 | F | 229 | Total | C | N | O | S | 0 | 0 |
| | | | 1808 | 1147 | 334 | 320 | 7 | | |

- Molecule 8 is a protein called 30S ribosomal protein S6e.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8 | G | 124 | Total | C | N | O | S | 0 | 0 |
| | | | 977 | 621 | 178 | 176 | 2 | | |

- Molecule 9 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 9 | H | 213 | Total | C | N | O | S | 0 | 0 |
| | | | 1720 | 1092 | 322 | 299 | 7 | | |

- Molecule 10 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10 | I | 129 | Total | C | N | O | S | 0 | 0 |
| | | | 1034 | 668 | 184 | 180 | 2 | | |

- Molecule 11 is a protein called 30S ribosomal protein S8e.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11 | J | 126 | Total | C | N | O | S | 0 | 0 |
| | | | 996 | 617 | 206 | 173 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12 | K | 134 | Total | C | N | O | S | 0 | 0 |
| | | | 1065 | 668 | 206 | 188 | 3 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13 | L | 101 | Total | C | N | O | S | 0 | 0 |
| | | | 817 | 507 | 158 | 148 | 4 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14 | M | 128 | Total | C | N | O | S | 0 | 0 |
| | | | 964 | 597 | 192 | 173 | 2 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15 | N | 146 | Total | C | N | O | S | 0 | 0 |
| | | | 1148 | 727 | 224 | 194 | 3 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16 | O | 138 | Total | C | N | O | S | 0 | 0 |
| | | | 1116 | 700 | 221 | 190 | 5 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 17 | P | 55 | Total | C | N | O | S | 0 | 0 |
| | | | 455 | 288 | 95 | 67 | 5 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18 | Q | 152 | Total | C | N | O | S | 0 | 0 |
| | | | 1262 | 804 | 240 | 214 | 4 | | |

- Molecule 19 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19 | R | 109 | Total | C | N | O | S | 0 | 0 |
| | | | 900 | 572 | 174 | 151 | 3 | | |

- Molecule 20 is a protein called 30S ribosomal protein S17e.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 20 | S | 66 | Total | C | N | O | S | 0 | 0 |
| | | | 558 | 355 | 106 | 96 | 1 | | |

- Molecule 21 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21 | T | 125 | Total | C | N | O | S | 0 | 0 |
| | | | 1018 | 647 | 195 | 169 | 7 | | |

- Molecule 22 is a protein called 30S ribosomal protein S19e.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22 | U | 149 | Total | C | N | O | S | 0 | 0 |
| | | | 1223 | 790 | 221 | 212 | | | |

- Molecule 23 is a protein called 30S ribosomal protein S24e.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23 | V | 94 | Total | C | N | O | S | 0 | 0 |
| | | | 790 | 516 | 125 | 146 | 3 | | |

- Molecule 24 is a protein called 30S ribosomal protein S27e.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 24 | W | 63 | Total | C | N | O | S | 0 | 0 |
| | | | 481 | 303 | 93 | 80 | 5 | | |

- Molecule 25 is a protein called 30S ribosomal protein S28e.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 25 | X | 67 | Total | C | N | O | S | 0 | 0 |
| | | | 536 | 327 | 111 | 98 | | | |

- Molecule 26 is a protein called 30S ribosomal protein S27ae.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 26 | Y | 50 | Total | C | N | O | S | 0 | 0 |
| | | | 408 | 262 | 77 | 63 | 6 | | |

- Molecule 27 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27 | Z | 197 | Total | C | N | O | S | 0 | 0 |
| | | | 1550 | 989 | 286 | 271 | 4 | | |

- Molecule 28 is a protein called 50S ribosomal protein L41e.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 28 | 0 | 36 | Total | C | N | O | S | 0 | 0 |
| | | | 343 | 218 | 84 | 39 | 2 | | |

- Molecule 29 is a protein called 50S ribosomal protein L7Ae.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29 | 3 | 123 | Total | C | N | O | S | 0 | 0 |
| | | | 941 | 599 | 157 | 181 | 4 | | |

- Molecule 30 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|-------|
| 30 | 5 | 20 | Total | C | N | O | P | 0 | 0 |
| | | | 430 | 192 | 78 | 140 | 20 | | |

- Molecule 31 is a RNA chain called initiator Met-tRNA fMet from E. coli (A1U72 variant).

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|-------|
| 31 | 4 | 76 | Total | C | N | O | P | S | 0 | 0 |
| | | | 1622 | 724 | 291 | 530 | 76 | 1 | | |

- Molecule 32 is a protein called Translation initiation factor 1A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 32 | 6 | 95 | Total | C | N | O | S | 0 | 0 |
| | | | 777 | 496 | 148 | 130 | 3 | | |

- Molecule 33 is a protein called Translation initiation factor 2 subunit gamma.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 33 | 7 | 414 | Total | C | N | O | S | 0 | 0 |
| | | | 3213 | 2058 | 548 | 595 | 12 | | |

- Molecule 34 is a protein called Translation initiation factor 2 subunit beta.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 34 | 8 | 129 | Total | C | N | O | S | 0 | 0 |
| | | | 1032 | 659 | 171 | 192 | 10 | | |

There are 8 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| 8 | ? | - | GLU | deletion | UNP Q97W59 |
| 8 | ? | - | LYS | deletion | UNP Q97W59 |
| 8 | ? | - | GLY | deletion | UNP Q97W59 |
| 8 | ? | - | ARG | deletion | UNP Q97W59 |
| 8 | ? | - | LYS | deletion | UNP Q97W59 |
| 8 | ? | - | GLU | deletion | UNP Q97W59 |
| 8 | ? | - | GLY | deletion | UNP Q97W59 |
| 8 | ? | - | THR | deletion | UNP Q97W59 |

- Molecule 35 is a protein called Translation initiation factor 2 subunit alpha.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 35 | 9 | 253 | Total | C | N | O | S | 0 | 0 |
| | | | 2025 | 1296 | 345 | 383 | 1 | | |

There are 10 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| 9 | ? | - | SER | deletion | UNP Q97Z79 |
| 9 | ? | - | LYS | deletion | UNP Q97Z79 |
| 9 | ? | - | TRP | deletion | UNP Q97Z79 |
| 9 | ? | - | VAL | deletion | UNP Q97Z79 |
| 9 | ? | - | LYS | deletion | UNP Q97Z79 |
| 9 | ? | - | LYS | deletion | UNP Q97Z79 |
| 9 | ? | - | HIS | deletion | UNP Q97Z79 |
| 9 | ? | - | ALA | deletion | UNP Q97Z79 |
| 9 | ? | - | GLU | deletion | UNP Q97Z79 |
| 9 | ? | - | GLU | deletion | UNP Q97Z79 |

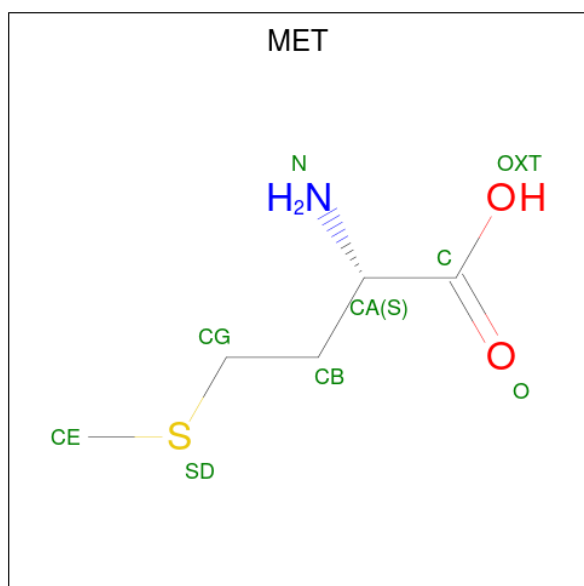
- Molecule 36 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 36 | 2 | 31 | Total | Mg | 0 |
| | | | 31 | 31 | |
| 36 | 5 | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 36 | 4 | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 36 | 7 | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |

- Molecule 37 is ZINC ION (three-letter code: ZN) (formula: Zn).

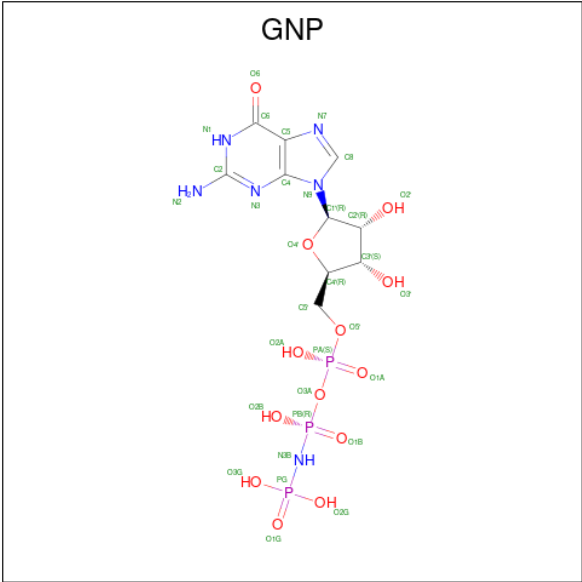
| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|------------|---------|---------|
| 37 | C | 2 | Total 2 | Zn 2 | 0 |
| 37 | F | 1 | Total 1 | Zn 1 | 0 |
| 37 | P | 1 | Total 1 | Zn 1 | 0 |
| 37 | R | 1 | Total 1 | Zn 1 | 0 |
| 37 | W | 1 | Total 1 | Zn 1 | 0 |

- Molecule 38 is METHIONINE (three-letter code: MET) (formula: $C_5H_{11}NO_2S$).



| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|------------|--------|--------|--------|--------|---------|
| 38 | 7 | 1 | Total 8 | C 5 | N 1 | O 1 | S 1 | 0 |

- Molecule 39 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 39 | 7 | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 6 | 13 | 3 | |

- Molecule 40 is water.

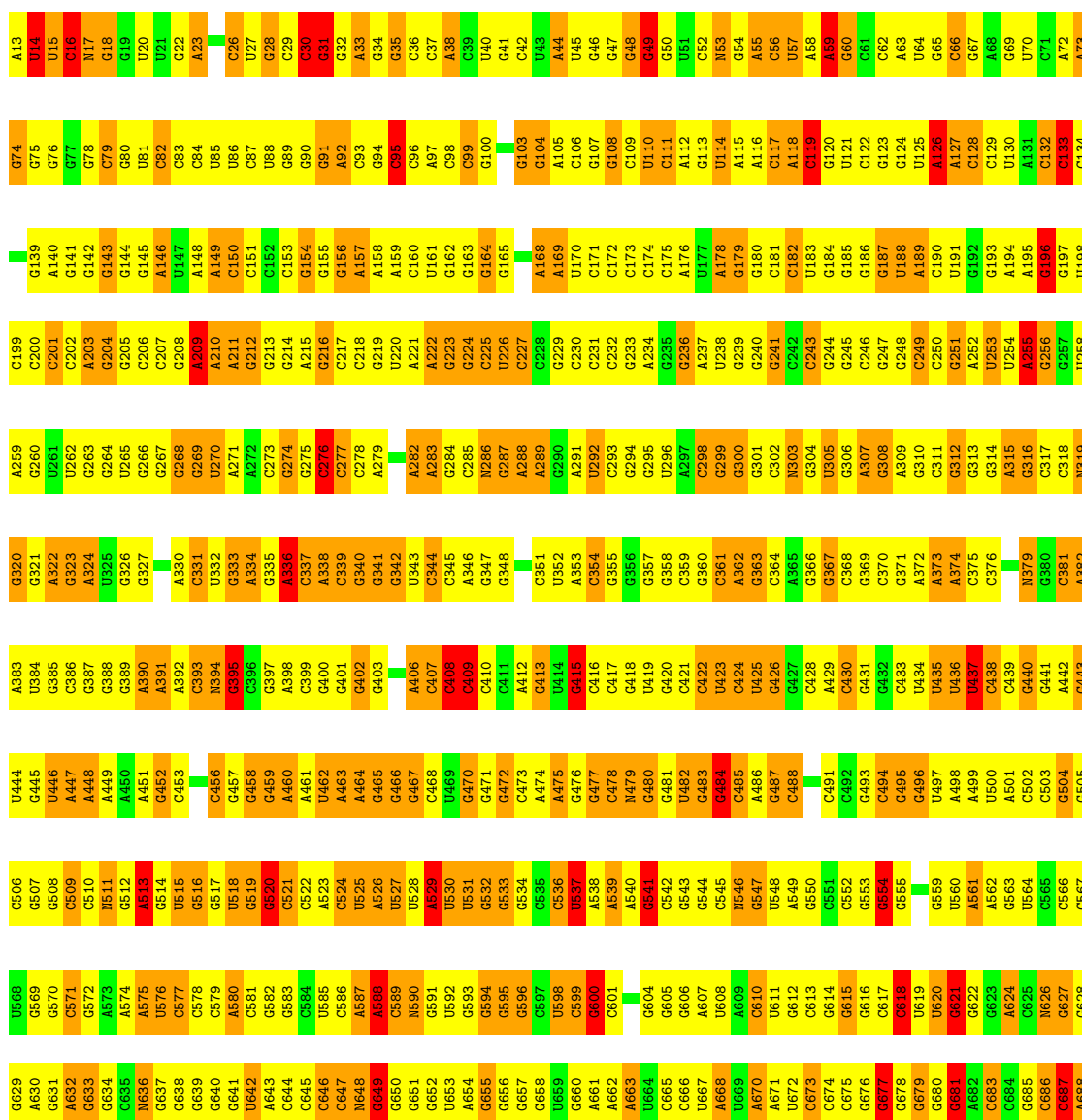
| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 40 | 2 | 40 | Total | O | 0 |
| | | | 40 | 40 | |
| 40 | K | 1 | Total | O | 0 |
| | | | 1 | 1 | |
| 40 | Q | 1 | Total | O | 0 |
| | | | 1 | 1 | |

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

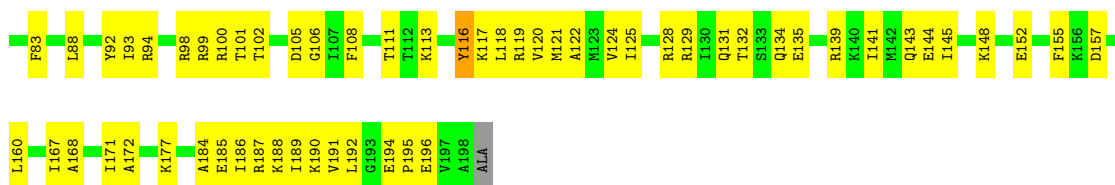
• Molecule 1: 16S ribosomal RNA

Chain 2: 



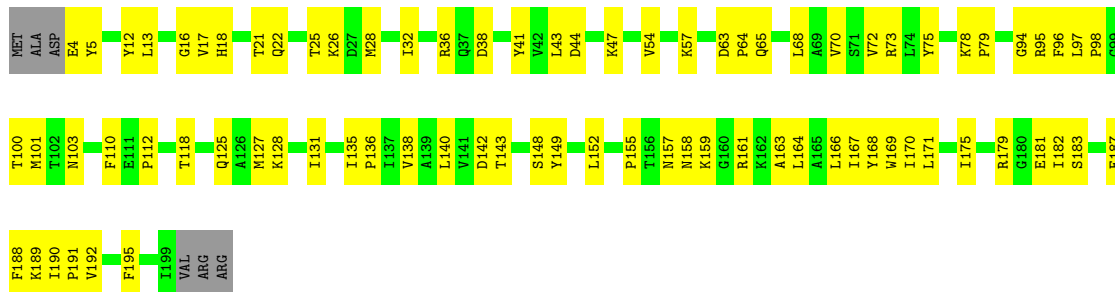
- Molecule 2: 30S ribosomal protein S3Ae

| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|--|--|-----|-----|-----|--|--|-----|--|-----|-----|-----|--|--|-----|-----|--|--|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|--|--|-----|-----|-----|--|--|-----|--|--|-----|-----|-----|--|-----|-----|-----|--|--|-----|
| MET | ALA | ALA | ALA | LYS | ARG | ARG | VAL | SER | ALA | ALA | K11 | D12 | K13 | W14 | K15 | L16 | K17 | Q18 | | | T22 | Y23 | A24 | | | F27 | | V31 | E32 | V33 | | | A38 | D39 | | | E42 | K43 | V44 | L45 | N46 | R47 | V48 | V49 | E50 | V51 | T52 | L53 | K54 | D55 | | | G58 | D59 | F60 | | | H64 | | | F69 | Q70 | V71 | | Y72 | D73 | V74 | | | W75 |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|--|--|-----|-----|-----|--|--|-----|--|-----|-----|-----|--|--|-----|-----|--|--|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|--|--|-----|-----|-----|--|--|-----|--|--|-----|-----|-----|--|-----|-----|-----|--|--|-----|



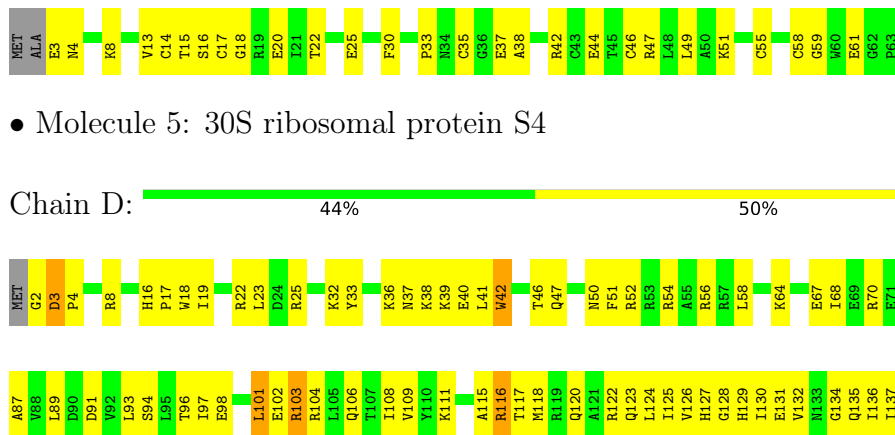
• Molecule 3: 30S ribosomal protein S2

Chain B: 57% 40%



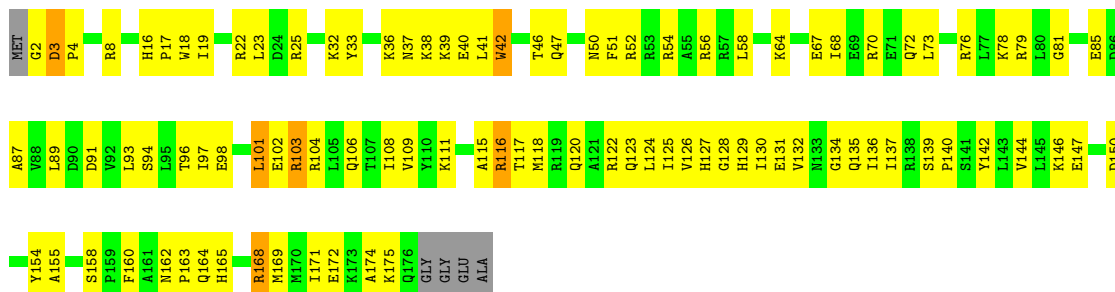
• Molecule 4: Zn-ribbon RNA-binding protein involved in translation

Chain C: 54% 43%



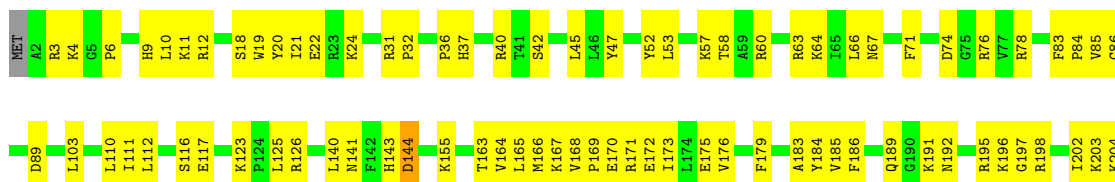
• Molecule 5: 30S ribosomal protein S4

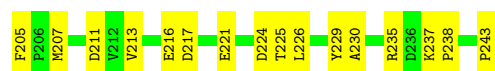
Chain D: 44% 50%



• Molecule 6: 30S ribosomal protein S4e

Chain E: 60% 40%





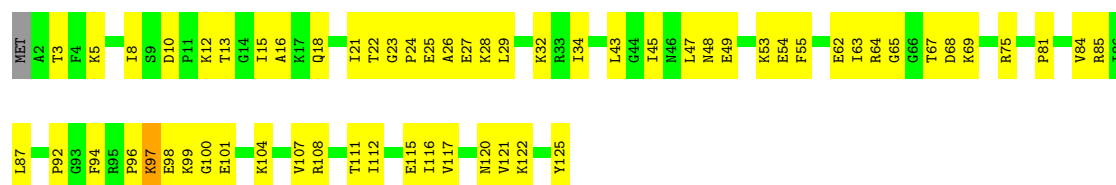
• Molecule 7: 30S ribosomal protein S5

Chain F: 53% 43% ..



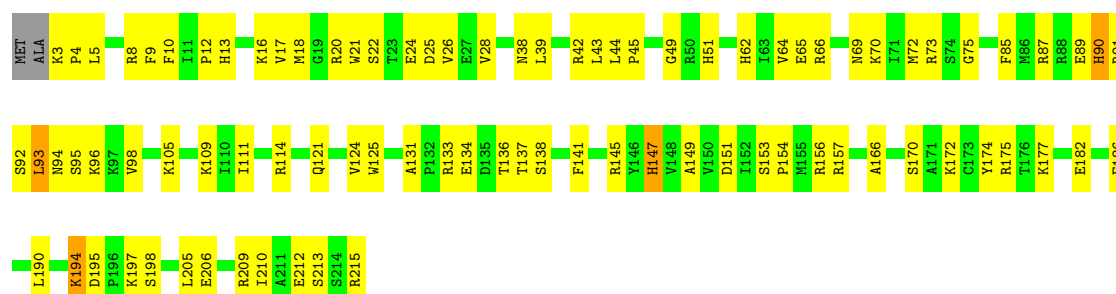
• Molecule 8: 30S ribosomal protein S6e

Chain G: 51% 47% ..



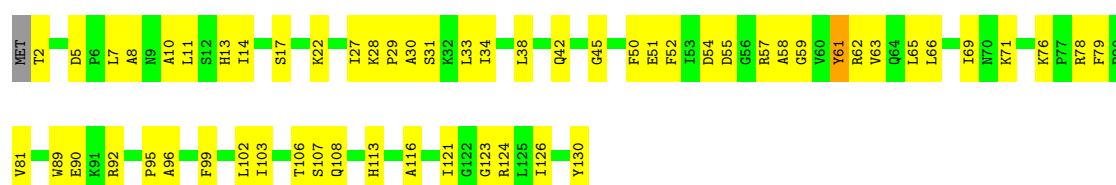
• Molecule 9: 30S ribosomal protein S7

Chain H: 58% 39% ..

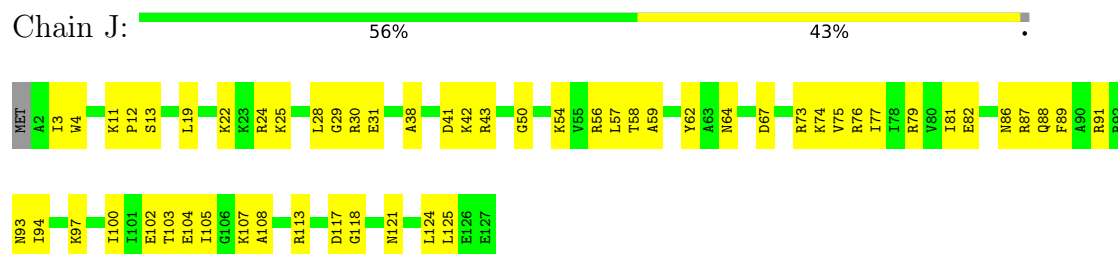


• Molecule 10: 30S ribosomal protein S8

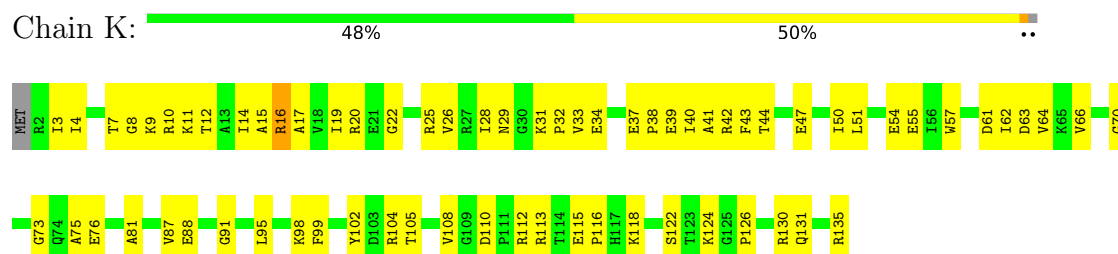
Chain I: 55% 43% ..



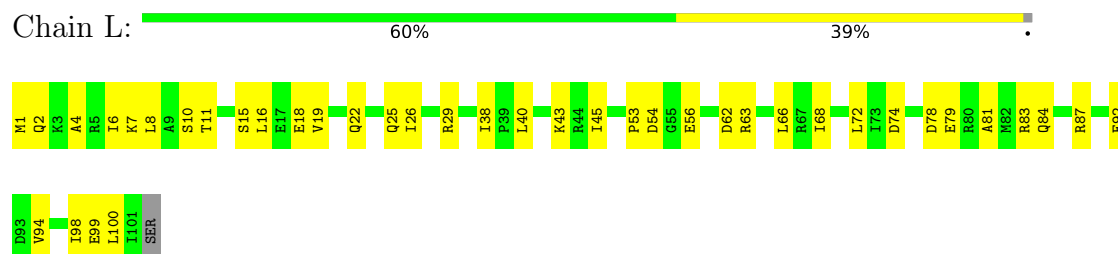
- Molecule 11: 30S ribosomal protein S8e



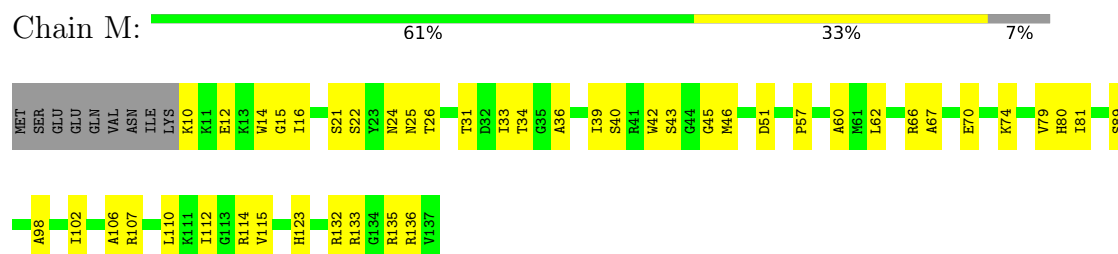
- Molecule 12: 30S ribosomal protein S9



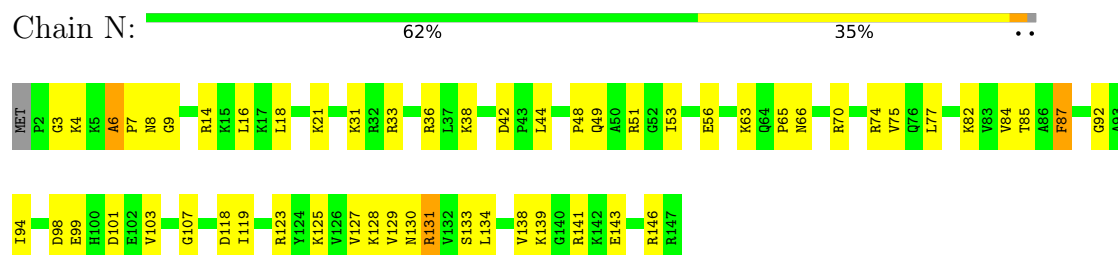
- Molecule 13: 30S ribosomal protein S10



- Molecule 14: 30S ribosomal protein S11

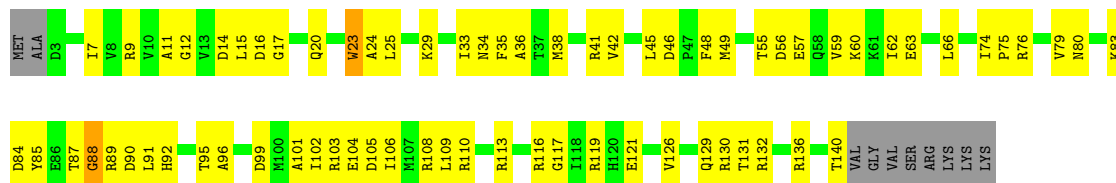


- Molecule 15: 30S ribosomal protein S12



- Molecule 16: 30S ribosomal protein S13

Chain O:  46% 46% 7%



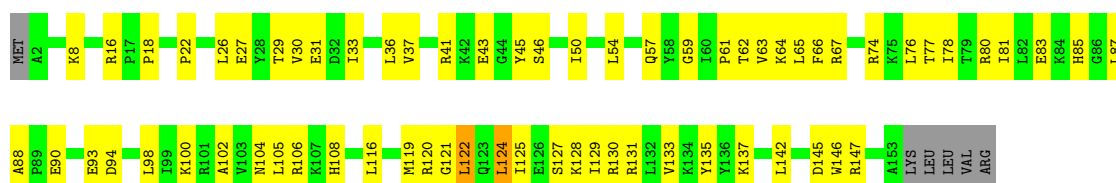
- Molecule 17: 30S ribosomal protein S14 type Z

Chain P:  43% 55%



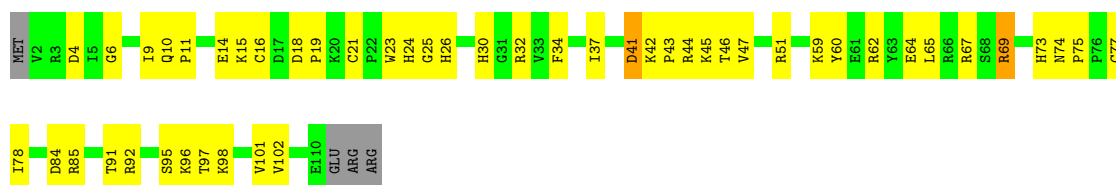
- Molecule 18: 30S ribosomal protein S15

Chain Q:  54% 41%



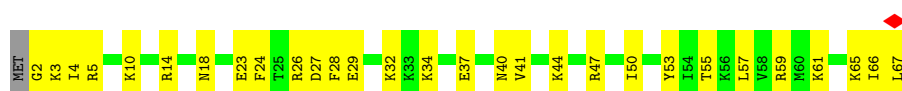
- Molecule 19: 30S ribosomal protein S17

Chain R:  53% 42%



- Molecule 20: 30S ribosomal protein S17e

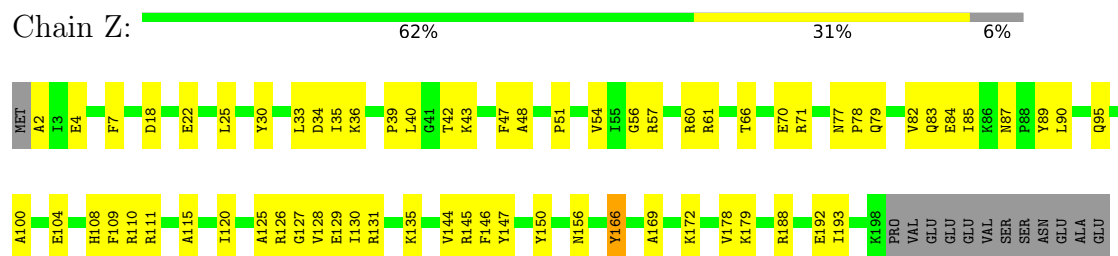
Chain S:  55% 43%



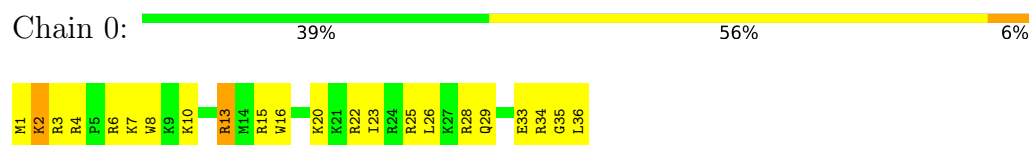
- Molecule 21: 30S ribosomal protein S19

Chain T:  41% 54% 5%

- Molecule 27: 30S ribosomal protein S3



- Molecule 28: 50S ribosomal protein L41e



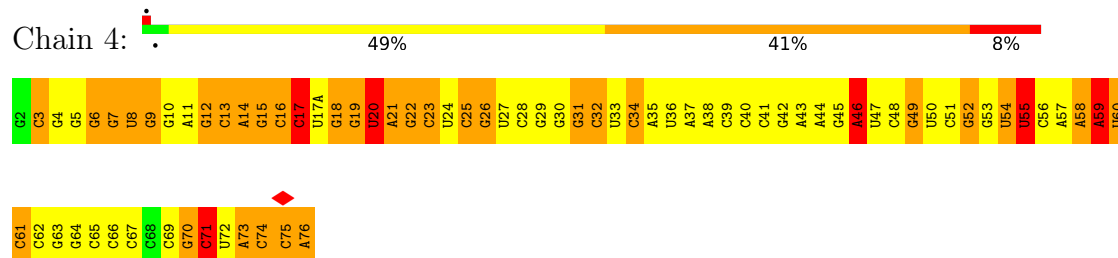
- Molecule 29: 50S ribosomal protein L7Ae



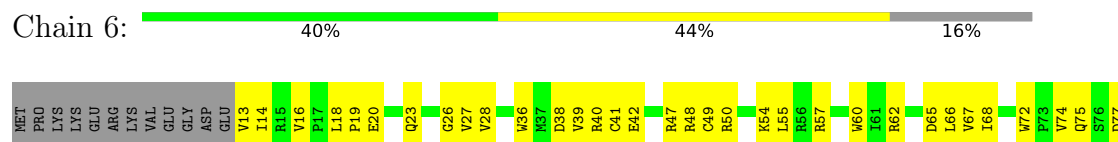
- Molecule 30: mRNA

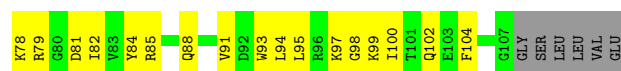


- Molecule 31: initiator Met-tRNA fMet from E. coli (A1U72 variant)

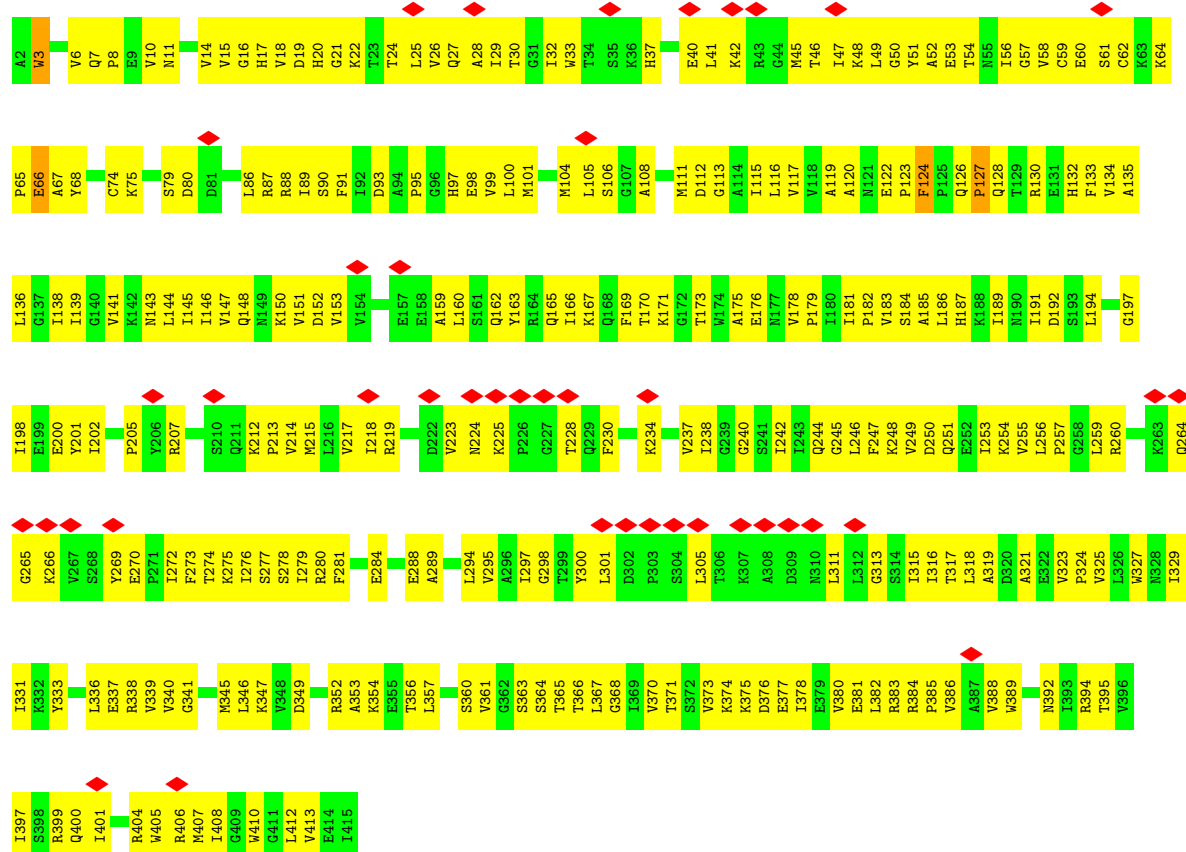


- Molecule 32: Translation initiation factor 1A

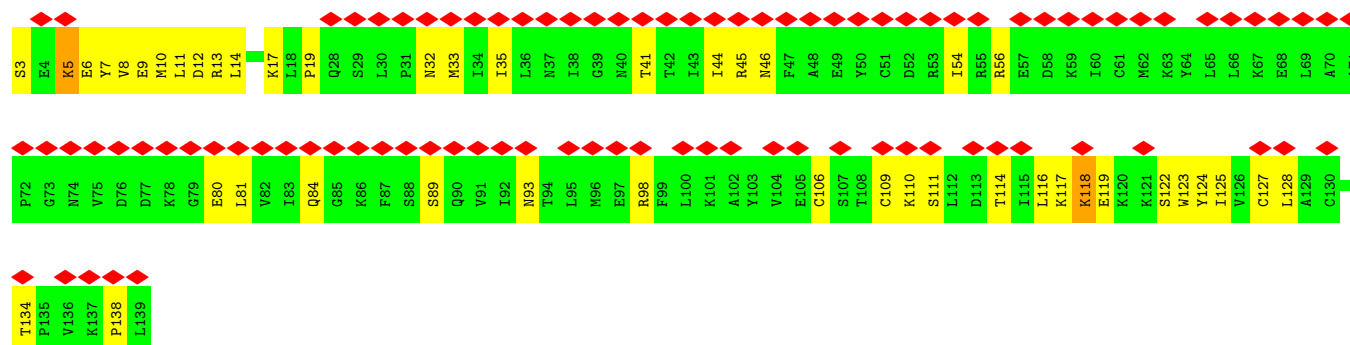




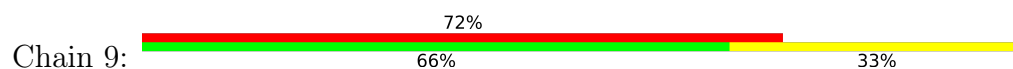
• Molecule 33: Translation initiation factor 2 subunit gamma



• Molecule 34: Translation initiation factor 2 subunit beta



• Molecule 35: Translation initiation factor 2 subunit alpha





4 Experimental information

| Property | Value | Source |
|--------------------------------------|---|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 34000 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 2 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | Not provided | |
| Image detector | GATAN K2 SUMMIT (4k x 4k) | Depositor |
| Maximum map value | 0.044 | Depositor |
| Minimum map value | -0.007 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 0.003 | Depositor |
| Recommended contour level | 0.004 | Depositor |
| Map size (Å) | 379.32, 379.32, 379.32 | wwPDB |
| Map dimensions | 348, 348, 348 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.09, 1.09, 1.09 | Depositor |

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A2M, UR3, B8H, MG, MA6, OMC, 4SU, 6MZ, 5MU, H2U, 5HM, PSU, LHH, 4AC, 5MC, ZN, GNP

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 | 2 | 1.32 | 33/35019 (0.1%) | 1.41 | 329/54586 (0.6%) |
| 2 | A | 0.61 | 0/1559 | 0.63 | 0/2090 |
| 3 | B | 0.56 | 0/1602 | 0.61 | 0/2165 |
| 4 | C | 0.57 | 0/496 | 0.60 | 0/673 |
| 5 | D | 0.63 | 1/1494 (0.1%) | 0.64 | 1/2003 (0.0%) |
| 6 | E | 0.62 | 0/2032 | 0.64 | 0/2742 |
| 7 | F | 0.67 | 0/1838 | 0.65 | 0/2478 |
| 8 | G | 0.46 | 0/993 | 0.56 | 0/1329 |
| 9 | H | 0.52 | 1/1757 (0.1%) | 0.61 | 1/2359 (0.0%) |
| 10 | I | 0.69 | 0/1055 | 0.72 | 0/1415 |
| 11 | J | 0.51 | 0/1005 | 0.65 | 0/1339 |
| 12 | K | 0.52 | 0/1081 | 0.61 | 0/1449 |
| 13 | L | 0.45 | 0/825 | 0.56 | 0/1107 |
| 14 | M | 0.51 | 0/982 | 0.61 | 0/1322 |
| 15 | N | 0.62 | 0/1165 | 0.67 | 1/1547 (0.1%) |
| 16 | O | 0.52 | 1/1135 (0.1%) | 0.60 | 0/1526 |
| 17 | P | 0.55 | 0/465 | 0.58 | 0/613 |
| 18 | Q | 0.54 | 0/1290 | 0.61 | 1/1734 (0.1%) |
| 19 | R | 0.68 | 1/923 (0.1%) | 0.64 | 0/1247 |
| 20 | S | 0.51 | 0/565 | 0.56 | 0/747 |
| 21 | T | 0.50 | 0/1037 | 0.63 | 0/1385 |
| 22 | U | 0.55 | 0/1253 | 0.60 | 0/1689 |
| 23 | V | 0.58 | 0/808 | 0.61 | 0/1086 |
| 24 | W | 0.45 | 0/488 | 0.60 | 0/659 |
| 25 | X | 0.49 | 0/538 | 0.62 | 0/719 |
| 26 | Y | 0.40 | 0/420 | 0.63 | 0/559 |
| 27 | Z | 0.50 | 0/1572 | 0.62 | 0/2110 |
| 28 | 0 | 0.62 | 0/349 | 0.65 | 0/451 |
| 29 | 3 | 0.37 | 0/953 | 0.59 | 0/1284 |
| 30 | 5 | 1.02 | 0/481 | 1.29 | 3/748 (0.4%) |
| 31 | 4 | 0.90 | 1/1699 (0.1%) | 1.29 | 15/2648 (0.6%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-----------------|-------------|-------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 32 | 6 | 0.43 | 0/793 | 0.68 | 0/1072 |
| 33 | 7 | 0.37 | 0/3272 | 0.62 | 1/4430 (0.0%) |
| 34 | 8 | 0.26 | 0/1045 | 0.48 | 0/1400 |
| 35 | 9 | 0.26 | 0/2050 | 0.44 | 0/2760 |
| All | All | 1.00 | 38/74039 (0.1%) | 1.11 | 352/107471 (0.3%) |

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 |
|-----|-------|---------------------|---------------------|
| 7 | F | 0 | 1 |
| 18 | Q | 0 | 1 |
| All | All | 0 | 2 |

All (38) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1 | 2 | 1453 | G | C8-N7 | -8.66 | 1.25 | 1.30 |
| 19 | R | 41 | ASP | CA-CB | -8.15 | 1.36 | 1.53 |
| 1 | 2 | 955 | A | N9-C4 | -7.73 | 1.33 | 1.37 |
| 1 | 2 | 795 | A | N9-C4 | -7.69 | 1.33 | 1.37 |
| 1 | 2 | 126 | A | N9-C4 | -7.46 | 1.33 | 1.37 |
| 1 | 2 | 1476 | A | N9-C4 | -6.20 | 1.34 | 1.37 |
| 9 | H | 194 | LYS | C-N | -6.04 | 1.20 | 1.34 |
| 1 | 2 | 209 | A | N9-C4 | -5.91 | 1.34 | 1.37 |
| 1 | 2 | 59 | A | N9-C4 | -5.80 | 1.34 | 1.37 |
| 1 | 2 | 1131 | A | N9-C4 | -5.76 | 1.34 | 1.37 |
| 1 | 2 | 781 | A | N9-C4 | -5.72 | 1.34 | 1.37 |
| 5 | D | 42 | TRP | CB-CG | -5.71 | 1.40 | 1.50 |
| 1 | 2 | 1470 | C | N1-C6 | -5.66 | 1.33 | 1.37 |
| 1 | 2 | 289 | A | N9-C4 | -5.65 | 1.34 | 1.37 |
| 1 | 2 | 796 | G | C5-C6 | -5.65 | 1.36 | 1.42 |
| 1 | 2 | 1203 | G | N7-C5 | -5.63 | 1.35 | 1.39 |
| 1 | 2 | 1476 | A | N3-C4 | -5.63 | 1.31 | 1.34 |
| 1 | 2 | 38 | A | N7-C5 | -5.62 | 1.35 | 1.39 |
| 1 | 2 | 773 | C | N1-C6 | -5.60 | 1.33 | 1.37 |
| 1 | 2 | 1495 | G | N1-C2 | -5.59 | 1.33 | 1.37 |
| 1 | 2 | 1337 | A | N9-C4 | -5.54 | 1.34 | 1.37 |
| 1 | 2 | 1032 | A | N7-C5 | -5.52 | 1.35 | 1.39 |
| 1 | 2 | 513 | A | N9-C4 | -5.52 | 1.34 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1 | 2 | 241 | G | C5-C4 | -5.51 | 1.34 | 1.38 |
| 1 | 2 | 529 | A | N7-C5 | -5.48 | 1.35 | 1.39 |
| 1 | 2 | 529 | A | N3-C4 | -5.40 | 1.31 | 1.34 |
| 31 | 4 | 46 | A | N9-C4 | -5.29 | 1.34 | 1.37 |
| 1 | 2 | 541 | G | C5-C4 | -5.28 | 1.34 | 1.38 |
| 16 | O | 23 | TRP | CB-CG | -5.25 | 1.40 | 1.50 |
| 1 | 2 | 1116 | A | N9-C4 | -5.24 | 1.34 | 1.37 |
| 1 | 2 | 49 | G | N9-C4 | -5.18 | 1.33 | 1.38 |
| 1 | 2 | 1483 | G | C5-C4 | -5.13 | 1.34 | 1.38 |
| 1 | 2 | 1495 | G | C5-C4 | -5.08 | 1.34 | 1.38 |
| 1 | 2 | 1349 | A | N3-C4 | -5.06 | 1.31 | 1.34 |
| 1 | 2 | 796 | G | N7-C5 | -5.06 | 1.36 | 1.39 |
| 1 | 2 | 1313 | A | N7-C5 | -5.06 | 1.36 | 1.39 |
| 1 | 2 | 901 | A | N9-C4 | -5.02 | 1.34 | 1.37 |
| 1 | 2 | 336 | A | N3-C4 | -5.01 | 1.31 | 1.34 |

All (352) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | 2 | 825 | U | N3-C2-O2 | -9.45 | 115.58 | 122.20 |
| 1 | 2 | 26 | C | C6-N1-C2 | -9.44 | 116.52 | 120.30 |
| 1 | 2 | 1383 | C | C2-N1-C1' | 9.44 | 129.18 | 118.80 |
| 1 | 2 | 494 | C | N3-C2-O2 | -9.26 | 115.42 | 121.90 |
| 1 | 2 | 683 | C | N3-C4-N4 | 8.90 | 124.23 | 118.00 |
| 1 | 2 | 494 | C | N1-C2-O2 | 8.78 | 124.17 | 118.90 |
| 1 | 2 | 129 | C | N3-C2-O2 | -8.67 | 115.83 | 121.90 |
| 1 | 2 | 683 | C | C5-C4-N4 | -8.54 | 114.22 | 120.20 |
| 1 | 2 | 1383 | C | N1-C2-O2 | 8.20 | 123.82 | 118.90 |
| 1 | 2 | 1077 | C | C2-N1-C1' | 8.15 | 127.77 | 118.80 |
| 1 | 2 | 618 | C | N3-C2-O2 | -7.92 | 116.36 | 121.90 |
| 1 | 2 | 1048 | C | C6-N1-C2 | -7.65 | 117.24 | 120.30 |
| 1 | 2 | 484 | G | N3-C4-C5 | -7.62 | 124.79 | 128.60 |
| 1 | 2 | 1191 | C | N3-C2-O2 | -7.52 | 116.64 | 121.90 |
| 31 | 4 | 56 | C | C2-N1-C1' | 7.49 | 127.04 | 118.80 |
| 1 | 2 | 796 | G | C6-C5-N7 | -7.46 | 125.93 | 130.40 |
| 1 | 2 | 577 | C | C2-N1-C1' | 7.38 | 126.92 | 118.80 |
| 1 | 2 | 1480 | G | C4-N9-C1' | 7.37 | 136.08 | 126.50 |
| 1 | 2 | 1383 | C | C6-N1-C1' | -7.35 | 111.98 | 120.80 |
| 1 | 2 | 129 | C | C6-N1-C2 | -7.32 | 117.37 | 120.30 |
| 1 | 2 | 576 | U | N3-C2-O2 | -7.32 | 117.08 | 122.20 |
| 1 | 2 | 362 | A | C8-N9-C4 | -7.32 | 102.87 | 105.80 |
| 1 | 2 | 894 | G | C6-C5-N7 | -7.31 | 126.02 | 130.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | 2 | 1094 | C | C2-N1-C1' | -7.29 | 110.78 | 118.80 |
| 1 | 2 | 1340 | G | C4-N9-C1' | 7.28 | 135.96 | 126.50 |
| 1 | 2 | 1357 | C | C6-N1-C2 | -7.21 | 117.42 | 120.30 |
| 1 | 2 | 1480 | G | C8-N9-C1' | -7.20 | 117.64 | 127.00 |
| 1 | 2 | 1366 | G | C8-N9-C1' | -7.20 | 117.64 | 127.00 |
| 1 | 2 | 1346 | C | C6-N1-C2 | -7.15 | 117.44 | 120.30 |
| 1 | 2 | 484 | G | N3-C4-N9 | 7.12 | 130.27 | 126.00 |
| 31 | 4 | 71 | C | N3-C4-C5 | 7.06 | 124.72 | 121.90 |
| 1 | 2 | 834 | G | C4-C5-N7 | 7.05 | 113.62 | 110.80 |
| 31 | 4 | 56 | C | N1-C2-O2 | 7.04 | 123.12 | 118.90 |
| 1 | 2 | 484 | G | C4-N9-C1' | 6.96 | 135.55 | 126.50 |
| 1 | 2 | 1117 | G | N3-C4-N9 | -6.96 | 121.83 | 126.00 |
| 1 | 2 | 610 | C | C2-N1-C1' | 6.92 | 126.41 | 118.80 |
| 1 | 2 | 887 | G | C4-N9-C1' | 6.92 | 135.50 | 126.50 |
| 1 | 2 | 1484 | G | N9-C4-C5 | -6.90 | 102.64 | 105.40 |
| 1 | 2 | 610 | C | C6-N1-C2 | -6.86 | 117.56 | 120.30 |
| 31 | 4 | 17 | C | C2-N1-C1' | 6.86 | 126.34 | 118.80 |
| 1 | 2 | 1340 | G | C8-N9-C1' | -6.82 | 118.14 | 127.00 |
| 1 | 2 | 796 | G | C4-C5-N7 | 6.82 | 113.53 | 110.80 |
| 1 | 2 | 1489 | C | N3-C2-O2 | -6.77 | 117.16 | 121.90 |
| 1 | 2 | 1094 | C | C6-N1-C1' | 6.73 | 128.87 | 120.80 |
| 1 | 2 | 932 | U | C2-N1-C1' | 6.69 | 125.73 | 117.70 |
| 1 | 2 | 747 | G | C4-N9-C1' | 6.69 | 135.19 | 126.50 |
| 1 | 2 | 1060 | U | N3-C2-O2 | -6.68 | 117.52 | 122.20 |
| 1 | 2 | 1366 | G | C6-C5-N7 | -6.67 | 126.40 | 130.40 |
| 1 | 2 | 1318 | C | N3-C2-O2 | -6.67 | 117.23 | 121.90 |
| 1 | 2 | 1480 | G | C6-C5-N7 | -6.67 | 126.40 | 130.40 |
| 1 | 2 | 829 | G | C2-N3-C4 | -6.66 | 108.57 | 111.90 |
| 1 | 2 | 1366 | G | C4-N9-C1' | 6.66 | 135.15 | 126.50 |
| 1 | 2 | 834 | G | C6-C5-N7 | -6.65 | 126.41 | 130.40 |
| 1 | 2 | 415 | G | C4-N9-C1' | 6.64 | 135.14 | 126.50 |
| 1 | 2 | 1443 | G | C6-C5-N7 | 6.64 | 134.39 | 130.40 |
| 1 | 2 | 752 | G | C4-C5-N7 | 6.62 | 113.45 | 110.80 |
| 1 | 2 | 588 | A | O5'-P-OP2 | -6.58 | 99.77 | 105.70 |
| 1 | 2 | 1077 | C | C6-N1-C1' | -6.58 | 112.90 | 120.80 |
| 1 | 2 | 838 | C | C2-N1-C1' | 6.56 | 126.01 | 118.80 |
| 1 | 2 | 114 | U | N3-C2-O2 | -6.54 | 117.62 | 122.20 |
| 18 | Q | 122 | LEU | CA-CB-CG | -6.53 | 100.27 | 115.30 |
| 1 | 2 | 615 | G | N3-C4-N9 | 6.53 | 129.92 | 126.00 |
| 1 | 2 | 1171 | G | C4-N9-C1' | 6.50 | 134.96 | 126.50 |
| 1 | 2 | 16 | C | C6-N1-C2 | 6.50 | 122.90 | 120.30 |
| 1 | 2 | 1048 | C | C2-N1-C1' | 6.50 | 125.95 | 118.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | 2 | 618 | C | N1-C2-O2 | 6.49 | 122.80 | 118.90 |
| 1 | 2 | 439 | C | C2-N1-C1' | 6.49 | 125.94 | 118.80 |
| 1 | 2 | 747 | G | C8-N9-C1' | -6.46 | 118.60 | 127.00 |
| 1 | 2 | 66 | C | N3-C4-C5 | 6.45 | 124.48 | 121.90 |
| 1 | 2 | 133 | C | N3-C2-O2 | -6.45 | 117.39 | 121.90 |
| 1 | 2 | 520 | G | C6-C5-N7 | -6.44 | 126.53 | 130.40 |
| 1 | 2 | 723 | G | C6-C5-N7 | -6.43 | 126.54 | 130.40 |
| 1 | 2 | 837 | G | N9-C4-C5 | -6.40 | 102.84 | 105.40 |
| 1 | 2 | 1087 | C | C6-N1-C2 | -6.38 | 117.75 | 120.30 |
| 1 | 2 | 824 | G | C4-N9-C1' | 6.35 | 134.75 | 126.50 |
| 1 | 2 | 1086 | C | C2-N1-C1' | 6.34 | 125.78 | 118.80 |
| 1 | 2 | 615 | G | C6-C5-N7 | -6.34 | 126.60 | 130.40 |
| 1 | 2 | 824 | G | C8-N9-C1' | -6.33 | 118.77 | 127.00 |
| 1 | 2 | 1114 | G | N3-C4-N9 | 6.29 | 129.77 | 126.00 |
| 1 | 2 | 747 | G | C6-C5-N7 | -6.29 | 126.63 | 130.40 |
| 1 | 2 | 1453 | G | C8-N9-C4 | -6.29 | 103.89 | 106.40 |
| 1 | 2 | 415 | G | C8-N9-C1' | -6.28 | 118.84 | 127.00 |
| 1 | 2 | 415 | G | C6-C5-N7 | -6.27 | 126.64 | 130.40 |
| 1 | 2 | 832 | G | C6-C5-N7 | -6.26 | 126.65 | 130.40 |
| 1 | 2 | 819 | G | C4-C5-N7 | 6.25 | 113.30 | 110.80 |
| 1 | 2 | 212 | G | C4-N9-C1' | 6.24 | 134.61 | 126.50 |
| 1 | 2 | 1060 | U | C6-N1-C2 | -6.24 | 117.26 | 121.00 |
| 1 | 2 | 1318 | C | N1-C2-O2 | 6.24 | 122.64 | 118.90 |
| 1 | 2 | 1443 | G | C4-N9-C1' | -6.24 | 118.39 | 126.50 |
| 1 | 2 | 1473 | G | N3-C4-N9 | 6.21 | 129.72 | 126.00 |
| 1 | 2 | 114 | U | C2-N1-C1' | 6.17 | 125.10 | 117.70 |
| 1 | 2 | 1117 | G | N3-C4-C5 | 6.16 | 131.68 | 128.60 |
| 1 | 2 | 526 | A | O4'-C1'-N9 | -6.15 | 103.28 | 108.20 |
| 1 | 2 | 955 | A | C2-N3-C4 | -6.14 | 107.53 | 110.60 |
| 1 | 2 | 520 | G | C4-C5-N7 | 6.13 | 113.25 | 110.80 |
| 1 | 2 | 1508 | C | N1-C2-O2 | 6.13 | 122.58 | 118.90 |
| 1 | 2 | 243 | C | N3-C2-O2 | -6.12 | 117.61 | 121.90 |
| 1 | 2 | 615 | G | C4-N9-C1' | 6.12 | 134.45 | 126.50 |
| 1 | 2 | 1493 | C | N3-C2-O2 | -6.08 | 117.64 | 121.90 |
| 1 | 2 | 693 | C | C6-N1-C2 | 6.07 | 122.73 | 120.30 |
| 1 | 2 | 437 | U | N3-C2-O2 | -6.06 | 117.96 | 122.20 |
| 1 | 2 | 1114 | G | N9-C4-C5 | -6.05 | 102.98 | 105.40 |
| 1 | 2 | 298 | C | C2-N1-C1' | 6.05 | 125.45 | 118.80 |
| 1 | 2 | 28 | G | C6-C5-N7 | -6.04 | 126.78 | 130.40 |
| 1 | 2 | 1330 | C | C2-N1-C1' | 6.04 | 125.44 | 118.80 |
| 1 | 2 | 576 | U | N1-C2-O2 | 6.03 | 127.02 | 122.80 |
| 1 | 2 | 364 | C | N3-C2-O2 | -6.02 | 117.69 | 121.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | 2 | 1114 | G | C6-C5-N7 | -6.01 | 126.79 | 130.40 |
| 1 | 2 | 1480 | G | N3-C4-N9 | 6.01 | 129.61 | 126.00 |
| 1 | 2 | 14 | U | C5-C6-N1 | -6.00 | 119.70 | 122.70 |
| 1 | 2 | 1383 | C | N3-C2-O2 | -6.00 | 117.70 | 121.90 |
| 1 | 2 | 1109 | G | C6-C5-N7 | -5.99 | 126.81 | 130.40 |
| 1 | 2 | 1114 | G | C4-C5-N7 | 5.98 | 113.19 | 110.80 |
| 1 | 2 | 312 | G | C6-C5-N7 | -5.97 | 126.81 | 130.40 |
| 1 | 2 | 749 | A | C8-N9-C4 | -5.97 | 103.41 | 105.80 |
| 1 | 2 | 767 | G | C6-C5-N7 | -5.96 | 126.82 | 130.40 |
| 1 | 2 | 677 | G | N3-C2-N2 | 5.96 | 124.07 | 119.90 |
| 1 | 2 | 1418 | C | C5-C6-N1 | 5.95 | 123.97 | 121.00 |
| 1 | 2 | 439 | C | N1-C2-O2 | 5.94 | 122.47 | 118.90 |
| 1 | 2 | 735 | G | C8-N9-C4 | -5.93 | 104.03 | 106.40 |
| 1 | 2 | 894 | G | C4-N9-C1' | 5.92 | 134.20 | 126.50 |
| 1 | 2 | 31 | G | C6-C5-N7 | -5.91 | 126.86 | 130.40 |
| 1 | 2 | 488 | C | N3-C4-N4 | -5.91 | 113.87 | 118.00 |
| 1 | 2 | 992 | U | C2-N1-C1' | 5.91 | 124.79 | 117.70 |
| 1 | 2 | 687 | C | N3-C4-C5 | 5.90 | 124.26 | 121.90 |
| 1 | 2 | 615 | G | C8-N9-C1' | -5.90 | 119.33 | 127.00 |
| 1 | 2 | 819 | G | C6-C5-N7 | -5.90 | 126.86 | 130.40 |
| 1 | 2 | 699 | C | C6-N1-C2 | -5.90 | 117.94 | 120.30 |
| 1 | 2 | 683 | C | C2-N1-C1' | 5.89 | 125.28 | 118.80 |
| 1 | 2 | 894 | G | N3-C4-N9 | 5.87 | 129.52 | 126.00 |
| 1 | 2 | 1484 | G | C8-N9-C4 | 5.87 | 108.75 | 106.40 |
| 31 | 4 | 19 | G | N3-C4-N9 | 5.85 | 129.51 | 126.00 |
| 1 | 2 | 484 | G | C6-C5-N7 | -5.84 | 126.89 | 130.40 |
| 1 | 2 | 894 | G | C4-C5-C6 | 5.84 | 122.31 | 118.80 |
| 1 | 2 | 887 | G | C8-N9-C1' | -5.84 | 119.41 | 127.00 |
| 1 | 2 | 577 | C | C6-N1-C1' | -5.83 | 113.80 | 120.80 |
| 1 | 2 | 1489 | C | N1-C2-O2 | 5.83 | 122.40 | 118.90 |
| 1 | 2 | 1357 | C | N3-C2-O2 | -5.83 | 117.82 | 121.90 |
| 1 | 2 | 1199 | A | C4-N9-C1' | 5.82 | 136.77 | 126.30 |
| 1 | 2 | 1369 | C | N3-C2-O2 | -5.82 | 117.83 | 121.90 |
| 1 | 2 | 1203 | G | C6-C5-N7 | -5.81 | 126.91 | 130.40 |
| 1 | 2 | 766 | G | N3-C4-N9 | 5.81 | 129.48 | 126.00 |
| 1 | 2 | 1489 | C | N3-C4-C5 | 5.81 | 124.22 | 121.90 |
| 1 | 2 | 872 | A | C8-N9-C4 | -5.80 | 103.48 | 105.80 |
| 1 | 2 | 1139 | C | C6-N1-C1' | -5.80 | 113.84 | 120.80 |
| 15 | N | 143 | GLU | C-N-CA | -5.80 | 107.21 | 121.70 |
| 1 | 2 | 488 | C | N3-C4-C5 | 5.79 | 124.22 | 121.90 |
| 1 | 2 | 914 | G | N1-C6-O6 | -5.75 | 116.45 | 119.90 |
| 1 | 2 | 554 | G | N1-C6-O6 | -5.75 | 116.45 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 33 | 7 | 41 | LEU | CA-CB-CG | 5.75 | 128.52 | 115.30 |
| 1 | 2 | 1191 | C | N1-C2-O2 | 5.74 | 122.34 | 118.90 |
| 1 | 2 | 1490 | C | C2-N1-C1' | 5.74 | 125.11 | 118.80 |
| 1 | 2 | 693 | C | N3-C4-C5 | 5.74 | 124.19 | 121.90 |
| 1 | 2 | 894 | G | N3-C4-C5 | -5.74 | 125.73 | 128.60 |
| 1 | 2 | 1447 | C | C2-N1-C1' | 5.73 | 125.11 | 118.80 |
| 1 | 2 | 276 | C | C6-N1-C1' | -5.73 | 113.93 | 120.80 |
| 1 | 2 | 1104 | C | C6-N1-C2 | 5.73 | 122.59 | 120.30 |
| 1 | 2 | 1493 | C | C6-N1-C2 | -5.72 | 118.01 | 120.30 |
| 1 | 2 | 1366 | G | N3-C4-N9 | 5.72 | 129.43 | 126.00 |
| 1 | 2 | 300 | G | C6-C5-N7 | -5.71 | 126.97 | 130.40 |
| 1 | 2 | 1109 | G | C4-N9-C1' | 5.70 | 133.91 | 126.50 |
| 1 | 2 | 415 | G | N3-C4-N9 | 5.70 | 129.42 | 126.00 |
| 1 | 2 | 730 | C | C2-N1-C1' | 5.70 | 125.07 | 118.80 |
| 1 | 2 | 484 | G | C8-N9-C1' | -5.69 | 119.60 | 127.00 |
| 1 | 2 | 18 | G | C6-C5-N7 | -5.69 | 126.98 | 130.40 |
| 1 | 2 | 1203 | G | C4-N9-C1' | 5.69 | 133.90 | 126.50 |
| 1 | 2 | 413 | G | N3-C4-N9 | 5.68 | 129.41 | 126.00 |
| 1 | 2 | 824 | G | N3-C4-N9 | 5.67 | 129.41 | 126.00 |
| 1 | 2 | 196 | G | N3-C4-N9 | 5.67 | 129.40 | 126.00 |
| 31 | 4 | 17 | C | C6-N1-C1' | -5.67 | 114.00 | 120.80 |
| 1 | 2 | 833 | G | C6-C5-N7 | -5.66 | 127.00 | 130.40 |
| 1 | 2 | 1453 | G | N7-C8-N9 | 5.66 | 115.93 | 113.10 |
| 1 | 2 | 600 | G | C6-C5-N7 | -5.66 | 127.00 | 130.40 |
| 1 | 2 | 837 | G | C4-C5-N7 | 5.65 | 113.06 | 110.80 |
| 31 | 4 | 61 | C | N1-C2-O2 | 5.64 | 122.29 | 118.90 |
| 1 | 2 | 888 | G | C4-C5-N7 | 5.64 | 113.06 | 110.80 |
| 1 | 2 | 914 | G | N3-C4-C5 | -5.64 | 125.78 | 128.60 |
| 1 | 2 | 1382 | A | N9-C1'-C2' | -5.64 | 105.80 | 112.00 |
| 1 | 2 | 1063 | G | N9-C4-C5 | -5.62 | 103.15 | 105.40 |
| 1 | 2 | 26 | C | C2-N1-C1' | 5.62 | 124.98 | 118.80 |
| 1 | 2 | 1493 | C | N1-C2-O2 | 5.62 | 122.27 | 118.90 |
| 1 | 2 | 1357 | C | C2-N1-C1' | 5.62 | 124.98 | 118.80 |
| 1 | 2 | 529 | A | N1-C2-N3 | 5.60 | 132.10 | 129.30 |
| 1 | 2 | 316 | G | C4-N9-C1' | 5.60 | 133.78 | 126.50 |
| 1 | 2 | 236 | G | N9-C4-C5 | 5.59 | 107.64 | 105.40 |
| 1 | 2 | 520 | G | C4-N9-C1' | 5.59 | 133.76 | 126.50 |
| 1 | 2 | 1167 | G | C6-C5-N7 | -5.58 | 127.05 | 130.40 |
| 1 | 2 | 1484 | G | C4-C5-N7 | 5.58 | 113.03 | 110.80 |
| 1 | 2 | 888 | G | N3-C4-N9 | 5.58 | 129.35 | 126.00 |
| 1 | 2 | 49 | G | N3-C4-C5 | 5.57 | 131.38 | 128.60 |
| 1 | 2 | 236 | G | N1-C6-O6 | -5.57 | 116.56 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | 2 | 537 | U | C2-N1-C1' | 5.56 | 124.38 | 117.70 |
| 1 | 2 | 212 | G | C8-N9-C4 | -5.56 | 104.18 | 106.40 |
| 1 | 2 | 819 | G | C4-N9-C1' | 5.56 | 133.72 | 126.50 |
| 1 | 2 | 564 | U | C2-N1-C1' | 5.55 | 124.36 | 117.70 |
| 5 | D | 101 | LEU | CA-CB-CG | -5.54 | 102.55 | 115.30 |
| 1 | 2 | 894 | G | N1-C2-N2 | -5.54 | 111.22 | 116.20 |
| 1 | 2 | 932 | U | C5-C6-N1 | 5.53 | 125.46 | 122.70 |
| 1 | 2 | 1139 | C | N1-C2-O2 | 5.53 | 122.22 | 118.90 |
| 1 | 2 | 838 | C | C6-N1-C1' | -5.52 | 114.18 | 120.80 |
| 31 | 4 | 56 | C | C5-C6-N1 | 5.52 | 123.76 | 121.00 |
| 1 | 2 | 723 | G | C8-N9-C1' | -5.51 | 119.84 | 127.00 |
| 1 | 2 | 114 | U | N1-C2-O2 | 5.50 | 126.65 | 122.80 |
| 1 | 2 | 1285 | G | N3-C4-C5 | 5.50 | 131.35 | 128.60 |
| 1 | 2 | 749 | A | N7-C8-N9 | 5.50 | 116.55 | 113.80 |
| 1 | 2 | 788 | G | C4-N9-C1' | 5.50 | 133.65 | 126.50 |
| 1 | 2 | 467 | G | N9-C4-C5 | 5.49 | 107.60 | 105.40 |
| 1 | 2 | 799 | G | C6-N1-C2 | -5.49 | 121.81 | 125.10 |
| 1 | 2 | 852 | G | C6-C5-N7 | -5.48 | 127.11 | 130.40 |
| 1 | 2 | 1205 | G | C8-N9-C4 | -5.48 | 104.21 | 106.40 |
| 1 | 2 | 236 | G | C8-N9-C4 | -5.48 | 104.21 | 106.40 |
| 1 | 2 | 673 | C | C2-N1-C1' | 5.48 | 124.82 | 118.80 |
| 1 | 2 | 649 | G | C4-C5-N7 | 5.47 | 112.99 | 110.80 |
| 1 | 2 | 484 | G | C4-C5-C6 | 5.47 | 122.08 | 118.80 |
| 1 | 2 | 853 | C | C6-N1-C1' | -5.45 | 114.26 | 120.80 |
| 1 | 2 | 824 | G | N3-C4-C5 | -5.45 | 125.88 | 128.60 |
| 1 | 2 | 1099 | C | N1-C2-O2 | 5.45 | 122.17 | 118.90 |
| 1 | 2 | 422 | C | N1-C2-O2 | 5.45 | 122.17 | 118.90 |
| 1 | 2 | 26 | C | C5-C6-N1 | 5.43 | 123.72 | 121.00 |
| 1 | 2 | 627 | G | C8-N9-C1' | -5.43 | 119.94 | 127.00 |
| 1 | 2 | 312 | G | C4-C5-N7 | 5.41 | 112.97 | 110.80 |
| 1 | 2 | 627 | G | C4-N9-C1' | 5.41 | 133.54 | 126.50 |
| 1 | 2 | 1317 | C | C6-N1-C2 | -5.41 | 118.14 | 120.30 |
| 1 | 2 | 663 | A | C6-C5-N7 | -5.41 | 128.51 | 132.30 |
| 1 | 2 | 1484 | G | N3-C4-N9 | 5.41 | 129.25 | 126.00 |
| 1 | 2 | 316 | G | N3-C4-N9 | 5.41 | 129.24 | 126.00 |
| 31 | 4 | 17 | C | N1-C2-O2 | 5.40 | 122.14 | 118.90 |
| 1 | 2 | 1180 | G | C8-N9-C1' | -5.40 | 119.98 | 127.00 |
| 1 | 2 | 825 | U | N1-C2-N3 | 5.39 | 118.14 | 114.90 |
| 1 | 2 | 18 | G | N3-C4-N9 | 5.39 | 129.23 | 126.00 |
| 1 | 2 | 31 | G | C4-C5-N7 | 5.39 | 112.95 | 110.80 |
| 1 | 2 | 647 | C | N1-C2-O2 | 5.38 | 122.13 | 118.90 |
| 1 | 2 | 1473 | G | N3-C4-C5 | -5.38 | 125.91 | 128.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | 2 | 663 | A | N1-C6-N6 | 5.37 | 121.82 | 118.60 |
| 1 | 2 | 767 | G | C8-N9-C4 | -5.37 | 104.25 | 106.40 |
| 1 | 2 | 837 | G | C6-C5-N7 | -5.37 | 127.18 | 130.40 |
| 1 | 2 | 276 | C | C2-N1-C1' | 5.37 | 124.70 | 118.80 |
| 1 | 2 | 1400 | C | N1-C2-O2 | 5.37 | 122.12 | 118.90 |
| 1 | 2 | 1063 | G | N3-C4-N9 | 5.36 | 129.22 | 126.00 |
| 1 | 2 | 824 | G | C6-C5-N7 | -5.34 | 127.19 | 130.40 |
| 1 | 2 | 1360 | C | C6-N1-C2 | -5.34 | 118.16 | 120.30 |
| 1 | 2 | 1478 | C | N1-C2-O2 | -5.33 | 115.70 | 118.90 |
| 1 | 2 | 1480 | G | N3-C4-C5 | -5.33 | 125.93 | 128.60 |
| 1 | 2 | 494 | C | C2-N1-C1' | 5.33 | 124.66 | 118.80 |
| 1 | 2 | 923 | G | C6-C5-N7 | -5.33 | 127.20 | 130.40 |
| 1 | 2 | 223 | G | N9-C4-C5 | -5.33 | 103.27 | 105.40 |
| 1 | 2 | 48 | G | C6-N1-C2 | -5.33 | 121.91 | 125.10 |
| 1 | 2 | 1086 | C | C6-N1-C1' | -5.32 | 114.41 | 120.80 |
| 1 | 2 | 992 | U | C5-C6-N1 | 5.32 | 125.36 | 122.70 |
| 1 | 2 | 320 | G | C4-N9-C1' | 5.31 | 133.41 | 126.50 |
| 1 | 2 | 1390 | C | C6-N1-C2 | -5.31 | 118.17 | 120.30 |
| 1 | 2 | 339 | C | C2-N1-C1' | 5.31 | 124.64 | 118.80 |
| 1 | 2 | 594 | G | C4-N9-C1' | -5.31 | 119.60 | 126.50 |
| 9 | H | 93 | LEU | CA-CB-CG | 5.30 | 127.49 | 115.30 |
| 1 | 2 | 723 | G | C4-N9-C1' | 5.30 | 133.39 | 126.50 |
| 31 | 4 | 70 | G | C6-C5-N7 | -5.30 | 127.22 | 130.40 |
| 1 | 2 | 1205 | G | N3-C4-C5 | -5.29 | 125.95 | 128.60 |
| 1 | 2 | 282 | A | C8-N9-C4 | 5.29 | 107.92 | 105.80 |
| 1 | 2 | 298 | C | C6-N1-C2 | -5.29 | 118.19 | 120.30 |
| 1 | 2 | 456 | C | N1-C2-O2 | 5.28 | 122.06 | 118.90 |
| 1 | 2 | 342 | G | N3-C4-N9 | 5.27 | 129.16 | 126.00 |
| 1 | 2 | 320 | G | C6-C5-N7 | -5.27 | 127.24 | 130.40 |
| 1 | 2 | 862 | U | N3-C2-O2 | -5.27 | 118.51 | 122.20 |
| 1 | 2 | 182 | C | N1-C2-O2 | 5.26 | 122.06 | 118.90 |
| 1 | 2 | 813 | G | N3-C4-C5 | -5.26 | 125.97 | 128.60 |
| 1 | 2 | 1470 | C | C6-N1-C2 | 5.26 | 122.40 | 120.30 |
| 1 | 2 | 681 | G | C4-C5-N7 | 5.25 | 112.90 | 110.80 |
| 1 | 2 | 1171 | G | C8-N9-C1' | -5.25 | 120.17 | 127.00 |
| 1 | 2 | 1294 | C | C6-N1-C2 | -5.25 | 118.20 | 120.30 |
| 1 | 2 | 270 | U | C2-N1-C1' | -5.24 | 111.41 | 117.70 |
| 1 | 2 | 1114 | G | C8-N9-C1' | -5.24 | 120.19 | 127.00 |
| 1 | 2 | 952 | C | C6-N1-C2 | -5.24 | 118.20 | 120.30 |
| 1 | 2 | 649 | G | C6-C5-N7 | -5.23 | 127.26 | 130.40 |
| 1 | 2 | 663 | A | N7-C8-N9 | 5.23 | 116.42 | 113.80 |
| 1 | 2 | 600 | G | C4-N9-C1' | 5.23 | 133.29 | 126.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | 2 | 1375 | G | N3-C4-N9 | 5.23 | 129.13 | 126.00 |
| 1 | 2 | 1324 | C | C2-N1-C1' | 5.21 | 124.53 | 118.80 |
| 1 | 2 | 1478 | C | C6-N1-C2 | -5.20 | 118.22 | 120.30 |
| 1 | 2 | 1059 | G | N9-C4-C5 | 5.20 | 107.48 | 105.40 |
| 1 | 2 | 60 | G | C6-C5-N7 | -5.19 | 127.28 | 130.40 |
| 1 | 2 | 1477 | G | C6-C5-N7 | -5.19 | 127.29 | 130.40 |
| 1 | 2 | 255 | A | C6-N1-C2 | -5.18 | 115.49 | 118.60 |
| 1 | 2 | 1040 | C | C2-N1-C1' | -5.18 | 113.10 | 118.80 |
| 1 | 2 | 35 | G | C6-C5-N7 | -5.18 | 127.29 | 130.40 |
| 1 | 2 | 95 | C | N3-C2-O2 | -5.18 | 118.28 | 121.90 |
| 1 | 2 | 340 | G | N1-C6-O6 | 5.18 | 123.01 | 119.90 |
| 1 | 2 | 1443 | G | C8-N9-C1' | 5.18 | 133.73 | 127.00 |
| 1 | 2 | 458 | G | N9-C4-C5 | -5.17 | 103.33 | 105.40 |
| 1 | 2 | 1077 | C | N1-C2-O2 | 5.17 | 122.00 | 118.90 |
| 1 | 2 | 986 | U | C5-C6-N1 | 5.17 | 125.29 | 122.70 |
| 1 | 2 | 789 | C | C2-N3-C4 | -5.17 | 117.31 | 119.90 |
| 1 | 2 | 600 | G | C4-C5-N7 | 5.17 | 112.87 | 110.80 |
| 1 | 2 | 903 | C | C2-N1-C1' | 5.16 | 124.48 | 118.80 |
| 30 | 5 | 816 | U | N3-C2-O2 | -5.16 | 118.58 | 122.20 |
| 30 | 5 | 810 | G | N3-C4-N9 | -5.16 | 122.91 | 126.00 |
| 1 | 2 | 621 | G | C6-C5-N7 | -5.15 | 127.31 | 130.40 |
| 31 | 4 | 56 | C | C6-N1-C1' | -5.15 | 114.61 | 120.80 |
| 1 | 2 | 830 | U | N3-C2-O2 | -5.15 | 118.59 | 122.20 |
| 1 | 2 | 1183 | C | C2-N1-C1' | 5.14 | 124.46 | 118.80 |
| 1 | 2 | 30 | C | N3-C4-C5 | 5.14 | 123.96 | 121.90 |
| 1 | 2 | 331 | C | C6-N1-C2 | -5.14 | 118.25 | 120.30 |
| 1 | 2 | 395 | G | N3-C2-N2 | 5.13 | 123.50 | 119.90 |
| 1 | 2 | 767 | G | C4-C5-N7 | 5.13 | 112.85 | 110.80 |
| 1 | 2 | 108 | G | C4-C5-N7 | 5.13 | 112.85 | 110.80 |
| 1 | 2 | 1059 | G | C4-C5-N7 | -5.13 | 108.75 | 110.80 |
| 1 | 2 | 615 | G | C4-C5-N7 | 5.13 | 112.85 | 110.80 |
| 1 | 2 | 1463 | G | C4-N9-C1' | 5.13 | 133.17 | 126.50 |
| 1 | 2 | 1199 | A | C8-N9-C1' | -5.12 | 118.48 | 127.70 |
| 1 | 2 | 1199 | A | C6-C5-N7 | -5.12 | 128.72 | 132.30 |
| 1 | 2 | 1048 | C | N3-C2-O2 | -5.11 | 118.32 | 121.90 |
| 1 | 2 | 1364 | U | C2-N1-C1' | 5.11 | 123.83 | 117.70 |
| 31 | 4 | 34 | C | C6-N1-C2 | 5.11 | 122.34 | 120.30 |
| 1 | 2 | 663 | A | C5-N7-C8 | -5.10 | 101.35 | 103.90 |
| 1 | 2 | 438 | C | C2-N1-C1' | 5.10 | 124.41 | 118.80 |
| 1 | 2 | 647 | C | N3-C2-O2 | -5.10 | 118.33 | 121.90 |
| 31 | 4 | 56 | C | C6-N1-C2 | -5.10 | 118.26 | 120.30 |
| 1 | 2 | 853 | C | C2-N1-C1' | 5.10 | 124.41 | 118.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | 2 | 1366 | G | N9-C4-C5 | -5.10 | 103.36 | 105.40 |
| 1 | 2 | 766 | G | N3-C4-C5 | -5.09 | 126.05 | 128.60 |
| 1 | 2 | 212 | G | N3-C4-C5 | -5.09 | 126.06 | 128.60 |
| 1 | 2 | 408 | C | C6-N1-C2 | -5.09 | 118.26 | 120.30 |
| 1 | 2 | 948 | G | OP1-P-O3' | 5.08 | 116.38 | 105.20 |
| 1 | 2 | 1375 | G | C6-C5-N7 | -5.07 | 127.36 | 130.40 |
| 1 | 2 | 1051 | C | C2-N1-C1' | 5.07 | 124.37 | 118.80 |
| 1 | 2 | 1109 | G | C8-N9-C1' | -5.06 | 120.42 | 127.00 |
| 31 | 4 | 19 | G | C8-N9-C1' | -5.06 | 120.42 | 127.00 |
| 1 | 2 | 342 | G | N3-C4-C5 | -5.05 | 126.07 | 128.60 |
| 1 | 2 | 104 | G | N1-C6-O6 | 5.05 | 122.93 | 119.90 |
| 1 | 2 | 413 | G | C6-C5-N7 | -5.05 | 127.37 | 130.40 |
| 1 | 2 | 900 | G | C4-C5-N7 | 5.05 | 112.82 | 110.80 |
| 1 | 2 | 944 | C | N3-C4-C5 | 5.04 | 123.92 | 121.90 |
| 1 | 2 | 216 | G | N9-C4-C5 | -5.03 | 103.39 | 105.40 |
| 1 | 2 | 487 | G | N1-C6-O6 | -5.03 | 116.88 | 119.90 |
| 1 | 2 | 119 | C | C2-N1-C1' | 5.03 | 124.33 | 118.80 |
| 1 | 2 | 1048 | C | C5-C6-N1 | 5.03 | 123.52 | 121.00 |
| 1 | 2 | 79 | C | N3-C4-C5 | 5.03 | 123.91 | 121.90 |
| 1 | 2 | 409 | C | C6-N1-C2 | -5.03 | 118.29 | 120.30 |
| 1 | 2 | 40 | U | C2-N1-C1' | 5.03 | 123.73 | 117.70 |
| 1 | 2 | 133 | C | N1-C2-O2 | 5.02 | 121.92 | 118.90 |
| 1 | 2 | 1117 | G | C2-N3-C4 | -5.02 | 109.39 | 111.90 |
| 1 | 2 | 30 | C | N1-C2-O2 | 5.02 | 121.91 | 118.90 |
| 1 | 2 | 849 | G | N3-C4-C5 | -5.02 | 126.09 | 128.60 |
| 1 | 2 | 1059 | G | N1-C6-O6 | -5.02 | 116.89 | 119.90 |
| 31 | 4 | 59 | A | O4'-C1'-N9 | -5.02 | 104.18 | 108.20 |
| 1 | 2 | 819 | G | C8-N9-C1' | -5.02 | 120.48 | 127.00 |
| 1 | 2 | 900 | G | C6-C5-N7 | -5.02 | 127.39 | 130.40 |
| 1 | 2 | 701 | C | C2-N1-C1' | 5.01 | 124.31 | 118.80 |
| 1 | 2 | 103 | G | N3-C4-C5 | 5.01 | 131.10 | 128.60 |
| 30 | 5 | 814 | U | N3-C2-O2 | -5.01 | 118.69 | 122.20 |
| 1 | 2 | 600 | G | N3-C4-N9 | 5.01 | 129.01 | 126.00 |
| 1 | 2 | 600 | G | C8-N9-C1' | -5.00 | 120.49 | 127.00 |
| 1 | 2 | 1360 | C | O4'-C1'-N1 | 5.00 | 112.20 | 108.20 |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 7 | F | 5 | TRP | Peptide |
| 18 | Q | 106 | ARG | Peptide |

5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | 2 | 32291 | 0 | 16316 | 2022 | 0 |
| 2 | A | 1533 | 0 | 1627 | 96 | 0 |
| 3 | B | 1571 | 0 | 1630 | 68 | 0 |
| 4 | C | 482 | 0 | 461 | 24 | 0 |
| 5 | D | 1470 | 0 | 1542 | 90 | 0 |
| 6 | E | 1983 | 0 | 2060 | 75 | 0 |
| 7 | F | 1808 | 0 | 1879 | 91 | 0 |
| 8 | G | 977 | 0 | 1037 | 59 | 0 |
| 9 | H | 1720 | 0 | 1775 | 87 | 0 |
| 10 | I | 1034 | 0 | 1069 | 57 | 0 |
| 11 | J | 996 | 0 | 1076 | 53 | 0 |
| 12 | K | 1065 | 0 | 1121 | 73 | 0 |
| 13 | L | 817 | 0 | 871 | 32 | 0 |
| 14 | M | 964 | 0 | 994 | 43 | 0 |
| 15 | N | 1148 | 0 | 1248 | 43 | 0 |
| 16 | O | 1116 | 0 | 1152 | 72 | 0 |
| 17 | P | 455 | 0 | 475 | 29 | 0 |
| 18 | Q | 1262 | 0 | 1331 | 53 | 0 |
| 19 | R | 900 | 0 | 921 | 52 | 0 |
| 20 | S | 558 | 0 | 595 | 31 | 0 |
| 21 | T | 1018 | 0 | 1086 | 72 | 0 |
| 22 | U | 1223 | 0 | 1263 | 64 | 0 |
| 23 | V | 790 | 0 | 806 | 35 | 0 |
| 24 | W | 481 | 0 | 512 | 20 | 0 |
| 25 | X | 536 | 0 | 571 | 43 | 0 |
| 26 | Y | 408 | 0 | 413 | 33 | 0 |
| 27 | Z | 1550 | 0 | 1637 | 55 | 0 |
| 28 | 0 | 343 | 0 | 407 | 24 | 0 |
| 29 | 3 | 941 | 0 | 994 | 86 | 0 |
| 30 | 5 | 430 | 0 | 215 | 41 | 0 |
| 31 | 4 | 1622 | 0 | 830 | 133 | 0 |
| 32 | 6 | 777 | 0 | 806 | 52 | 0 |
| 33 | 7 | 3213 | 0 | 3331 | 336 | 0 |
| 34 | 8 | 1032 | 0 | 1073 | 39 | 0 |
| 35 | 9 | 2025 | 0 | 2133 | 76 | 0 |
| 36 | 2 | 31 | 0 | 0 | 0 | 0 |
| 36 | 4 | 1 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 36 | 5 | 1 | 0 | 0 | 0 | 0 |
| 36 | 7 | 1 | 0 | 0 | 0 | 0 |
| 37 | C | 2 | 0 | 0 | 0 | 0 |
| 37 | F | 1 | 0 | 0 | 0 | 0 |
| 37 | P | 1 | 0 | 0 | 0 | 0 |
| 37 | R | 1 | 0 | 0 | 0 | 0 |
| 37 | W | 1 | 0 | 0 | 0 | 0 |
| 38 | 7 | 8 | 0 | 8 | 2 | 0 |
| 39 | 7 | 32 | 0 | 13 | 4 | 0 |
| 40 | 2 | 40 | 0 | 0 | 18 | 0 |
| 40 | K | 1 | 0 | 0 | 0 | 0 |
| 40 | Q | 1 | 0 | 0 | 1 | 0 |
| All | All | 70661 | 0 | 55278 | 3872 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 31.

All (3872) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:2:140:A:N6 | 1:2:229:G:H1 | 1.36 | 1.23 |
| 33:7:213:PRO:HA | 33:7:244:GLN:O | 1.39 | 1.22 |
| 33:7:240:GLY:O | 33:7:294:LEU:HA | 1.57 | 1.04 |
| 1:2:1300:C:OP1 | 22:U:39:ARG:NH2 | 1.96 | 0.97 |
| 1:2:465:G:O6 | 1:2:512:G:N2 | 1.99 | 0.95 |
| 31:4:21:A:O2' | 31:4:22:G:N7 | 2.01 | 0.92 |
| 1:2:337:C:N3 | 11:J:25:LYS:NZ | 2.18 | 0.92 |
| 1:2:1262:A:H2' | 1:2:1263:A:H8 | 1.36 | 0.91 |
| 1:2:17:4AC:O7 | 7:F:192:ARG:NH2 | 2.04 | 0.91 |
| 1:2:520:G:OP1 | 15:N:38:LYS:NZ | 2.04 | 0.91 |
| 1:2:321:G:H2' | 1:2:322:A:H8 | 1.37 | 0.90 |
| 1:2:1229:G:N2 | 1:2:1233:4AC:O2 | 2.04 | 0.89 |
| 1:2:46:G:H2' | 1:2:47:G:H8 | 1.36 | 0.89 |
| 31:4:3:C:O2 | 31:4:71:C:N4 | 2.05 | 0.89 |
| 1:2:849:G:OP2 | 15:N:4:LYS:NZ | 2.06 | 0.89 |
| 1:2:1134:G:OP1 | 20:S:5:ARG:NH2 | 2.06 | 0.88 |
| 1:2:1020:A:N3 | 27:Z:135:LYS:NZ | 2.20 | 0.88 |
| 7:F:133:CYS:SG | 7:F:139:HIS:CE1 | 2.60 | 0.88 |
| 1:2:17:4AC:H5 | 7:F:192:ARG:HH21 | 1.39 | 0.87 |
| 1:2:651:G:OP1 | 2:A:43:LYS:NZ | 2.07 | 0.86 |
| 23:V:23:ILE:HD13 | 23:V:31:PRO:HG2 | 1.57 | 0.86 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:2:262:U:H2' | 1:2:263:G:H8 | 1.38 | 0.86 |
| 1:2:1342:G:OP2 | 13:L:63:ARG:NH1 | 2.09 | 0.86 |
| 23:V:43:MET:HG2 | 23:V:44:LEU:HD12 | 1.56 | 0.86 |
| 33:7:325:VAL:HB | 33:7:385:PRO:HB2 | 1.58 | 0.86 |
| 29:3:27:ARG:HH11 | 29:3:90:ALA:HA | 1.41 | 0.85 |
| 1:2:1400:C:O2 | 1:2:1443:G:N2 | 2.09 | 0.85 |
| 1:2:300:G:N2 | 1:2:319:4AC:N3 | 2.25 | 0.85 |
| 33:7:98:GLU:HA | 33:7:101:MET:HB2 | 1.58 | 0.85 |
| 1:2:333:G:N2 | 1:2:336:A:OP2 | 2.08 | 0.84 |
| 9:H:131:ALA:HB1 | 9:H:157:ARG:HB3 | 1.59 | 0.84 |
| 33:7:152:ASP:OD2 | 33:7:187:HIS:ND1 | 2.10 | 0.84 |
| 1:2:1271:U:H4' | 1:2:1273:A:H2 | 1.43 | 0.84 |
| 1:2:1417:U:H2' | 1:2:1418:C:C6 | 2.13 | 0.83 |
| 1:2:1453:G:N7 | 33:7:352:ARG:NH1 | 2.26 | 0.83 |
| 20:S:5:ARG:O | 20:S:10:LYS:NZ | 2.10 | 0.83 |
| 15:N:77:LEU:HD12 | 15:N:82:LYS:HB2 | 1.61 | 0.83 |
| 34:8:8:VAL:HA | 34:8:11:LEU:HB3 | 1.61 | 0.83 |
| 33:7:59:CYS:H | 33:7:67:ALA:HB1 | 1.44 | 0.83 |
| 9:H:26:VAL:HG12 | 9:H:121:GLN:HB2 | 1.58 | 0.82 |
| 26:Y:47:GLU:O | 26:Y:50:LYS:NZ | 2.12 | 0.82 |
| 1:2:1480:G:OP1 | 28:0:20:LYS:NZ | 2.11 | 0.82 |
| 29:3:56:ASP:HB3 | 29:3:83:LYS:HE3 | 1.61 | 0.82 |
| 1:2:1425:G:H2' | 1:2:1426:A:H8 | 1.44 | 0.82 |
| 4:C:17:CYS:SG | 4:C:18:GLY:N | 2.52 | 0.82 |
| 13:L:83:ARG:HG2 | 13:L:87:ARG:HH12 | 1.45 | 0.82 |
| 31:4:18:G:N1 | 31:4:55:PSU:O2' | 2.11 | 0.82 |
| 1:2:1453:G:C5 | 33:7:352:ARG:HD2 | 2.14 | 0.82 |
| 1:2:1389:C:N3 | 1:2:1454:G:N1 | 2.27 | 0.81 |
| 33:7:27:GLN:HE21 | 33:7:33:TRP:HB3 | 1.45 | 0.81 |
| 1:2:702:C:H2' | 1:2:703:4AC:H6 | 1.59 | 0.81 |
| 29:3:18:LYS:HB3 | 29:3:110:LEU:HD22 | 1.62 | 0.81 |
| 33:7:339:VAL:HB | 33:7:345:MET:HA | 1.62 | 0.81 |
| 1:2:784:G:O6 | 1:2:1498:C:N4 | 2.14 | 0.81 |
| 33:7:365:THR:H | 33:7:384:ARG:HH11 | 1.28 | 0.81 |
| 1:2:1233:4AC:N3 | 1:2:1251:G:N1 | 2.29 | 0.81 |
| 33:7:48:LYS:NZ | 33:7:49:LEU:O | 2.14 | 0.81 |
| 33:7:277:SER:N | 33:7:298:GLY:O | 2.13 | 0.81 |
| 1:2:478:C:H2' | 1:2:479:4AC:H6 | 1.61 | 0.81 |
| 1:2:998:C:H2' | 1:2:999:G:H8 | 1.46 | 0.81 |
| 7:F:153:ARG:HB2 | 7:F:188:LEU:HD12 | 1.62 | 0.81 |
| 13:L:62:ASP:OD1 | 17:P:54:LYS:NZ | 2.14 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:2:126:A:N6 | 1:2:194:A:N7 | 2.29 | 0.81 |
| 1:2:1389:C:N4 | 1:2:1454:G:O6 | 2.12 | 0.81 |
| 33:7:361:VAL:HB | 33:7:364:SER:HB2 | 1.60 | 0.81 |
| 1:2:1204:C:O2' | 21:T:124:ARG:NH1 | 2.13 | 0.81 |
| 1:2:641:G:OP1 | 2:A:119:ARG:NH1 | 2.14 | 0.80 |
| 18:Q:137:LYS:NZ | 18:Q:146:TRP:O | 2.14 | 0.80 |
| 1:2:1400:C:N3 | 1:2:1443:G:N1 | 2.25 | 0.80 |
| 1:2:1034:C:OP2 | 40:2:1701:HOH:O | 1.98 | 0.80 |
| 22:U:27:LYS:NZ | 22:U:28:PRO:O | 2.14 | 0.80 |
| 1:2:1219:G:OP2 | 22:U:41:LYS:NZ | 2.14 | 0.80 |
| 4:C:22:THR:N | 4:C:25:GLU:OE2 | 2.13 | 0.80 |
| 2:A:52:THR:H | 14:M:114:ARG:HH22 | 1.30 | 0.80 |
| 1:2:869:G:O2' | 1:2:871:A:N6 | 2.13 | 0.80 |
| 25:X:16:GLY:O | 25:X:26:GLN:N | 2.14 | 0.80 |
| 1:2:423:U:OP2 | 1:2:424:C:N4 | 2.13 | 0.80 |
| 15:N:65:PRO:O | 15:N:66:ASN:ND2 | 2.15 | 0.80 |
| 33:7:17:HIS:HE1 | 33:7:97:HIS:HD2 | 1.30 | 0.80 |
| 29:3:104:PRO:O | 29:3:108:ARG:NH1 | 2.13 | 0.80 |
| 1:2:1290:G:N2 | 1:2:1293:A:OP2 | 2.15 | 0.79 |
| 1:2:49:G:N2 | 1:2:409:C:O2 | 2.15 | 0.79 |
| 1:2:1395:G:H1' | 1:2:1449:G:H22 | 1.47 | 0.79 |
| 19:R:75:PRO:HD2 | 19:R:78:ILE:HD11 | 1.62 | 0.79 |
| 5:D:155:ALA:HB3 | 5:D:158:SER:HB2 | 1.65 | 0.79 |
| 18:Q:26:LEU:HD11 | 18:Q:61:PRO:HD2 | 1.63 | 0.79 |
| 25:X:42:ARG:NH1 | 25:X:66:GLU:OE1 | 2.15 | 0.79 |
| 1:2:311:C:H2' | 1:2:312:G:H8 | 1.48 | 0.79 |
| 1:2:1083:C:H2' | 1:2:1084:C:H6 | 1.47 | 0.79 |
| 1:2:1262:A:H2' | 1:2:1263:A:C8 | 2.17 | 0.79 |
| 1:2:1191:C:OP1 | 17:P:9:ARG:NH2 | 2.15 | 0.79 |
| 1:2:581:C:H2' | 1:2:582:G:H8 | 1.47 | 0.79 |
| 1:2:627:G:H2' | 1:2:628:G:C8 | 2.18 | 0.79 |
| 1:2:16:C:N4 | 1:2:32:G:O6 | 2.16 | 0.79 |
| 1:2:26:C:OP1 | 7:F:151:SER:OG | 1.99 | 0.79 |
| 1:2:1137:G:O6 | 1:2:1147:4AC:N4 | 2.15 | 0.79 |
| 21:T:19:MET:HG2 | 21:T:20:SER:H | 1.46 | 0.79 |
| 1:2:695:A:H2' | 1:2:696:A:C8 | 2.18 | 0.79 |
| 10:I:5:ASP:OD2 | 10:I:8:ALA:N | 2.16 | 0.79 |
| 33:7:74:CYS:HB3 | 33:7:79:SER:HB3 | 1.64 | 0.79 |
| 1:2:782:A:OP1 | 28:0:3:ARG:NH2 | 2.16 | 0.78 |
| 1:2:817:U:OP1 | 2:A:128:ARG:NH2 | 2.15 | 0.78 |
| 1:2:1460:G:H21 | 32:6:36:TRP:HE1 | 1.28 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 31:4:22:G:O2' | 31:4:23:C:O4' | 2.02 | 0.78 |
| 1:2:93:C:H2' | 1:2:94:G:H8 | 1.47 | 0.78 |
| 1:2:372:A:OP2 | 15:N:51:ARG:NH1 | 2.16 | 0.78 |
| 1:2:381:C:H42 | 1:2:398:A:H62 | 1.30 | 0.78 |
| 1:2:547:G:N7 | 40:2:1711:HOH:O | 2.16 | 0.78 |
| 1:2:1415:U:O2 | 1:2:1428:G:N2 | 2.15 | 0.78 |
| 16:O:9:ARG:NH1 | 16:O:12:GLY:O | 2.15 | 0.78 |
| 1:2:46:G:H2' | 1:2:47:G:C8 | 2.18 | 0.78 |
| 1:2:303:4AC:H2' | 1:2:304:G:H8 | 1.48 | 0.78 |
| 1:2:1131:A:H62 | 1:2:1151:G:H22 | 1.29 | 0.78 |
| 22:U:14:GLU:OE1 | 22:U:53:TYR:OH | 2.01 | 0.78 |
| 1:2:879:A:H2' | 1:2:880:A:H8 | 1.48 | 0.78 |
| 1:2:1197:C:OP1 | 21:T:110:ARG:NH1 | 2.16 | 0.78 |
| 23:V:72:TYR:OH | 23:V:82:GLU:OE2 | 2.01 | 0.78 |
| 1:2:187:G:O6 | 1:2:200:C:N4 | 2.17 | 0.78 |
| 1:2:321:G:H2' | 1:2:322:A:C8 | 2.18 | 0.78 |
| 29:3:118:VAL:HA | 29:3:121:LEU:HB2 | 1.66 | 0.78 |
| 20:S:32:LYS:O | 20:S:47:ARG:NH1 | 2.16 | 0.78 |
| 31:4:29:G:H2' | 31:4:30:G:H8 | 1.49 | 0.78 |
| 16:O:105:ASP:OD1 | 16:O:108:ARG:NH1 | 2.16 | 0.77 |
| 31:4:5:G:H2' | 31:4:6:G:C8 | 2.19 | 0.77 |
| 1:2:359:C:H3' | 1:2:360:G:H21 | 1.49 | 0.77 |
| 1:2:876:U:OP2 | 28:0:2:LYS:NZ | 2.13 | 0.77 |
| 1:2:1311:G:OP2 | 9:H:85:PHE:N | 2.15 | 0.77 |
| 1:2:1358:U:N3 | 1:2:1359:G:N7 | 2.32 | 0.77 |
| 29:3:3:LYS:HD3 | 29:3:4:PRO:HD2 | 1.65 | 0.77 |
| 34:8:5:LYS:O | 34:8:9:GLU:HB2 | 1.84 | 0.77 |
| 1:2:1488:MA6:OP1 | 28:0:22:ARG:NH1 | 2.17 | 0.77 |
| 27:Z:144:VAL:HG12 | 27:Z:145:ARG:H | 1.49 | 0.77 |
| 33:7:66:GLU:OE1 | 34:8:17:LYS:NZ | 2.18 | 0.77 |
| 33:7:75:LYS:HG2 | 34:8:124:TYR:HB2 | 1.67 | 0.77 |
| 1:2:372:A:H2' | 1:2:373:A2M:H8 | 1.65 | 0.77 |
| 1:2:1211:C:OP2 | 9:H:91:ARG:NH1 | 2.18 | 0.77 |
| 16:O:16:ASP:OD1 | 16:O:17:GLY:N | 2.16 | 0.77 |
| 2:A:54:LYS:HA | 2:A:58:GLY:HA3 | 1.67 | 0.76 |
| 33:7:51:TYR:CZ | 33:7:294:LEU:HB3 | 2.21 | 0.76 |
| 35:9:235:ASN:ND2 | 35:9:238:GLU:OE2 | 2.17 | 0.76 |
| 26:Y:29:VAL:HG12 | 29:3:41:LYS:HD3 | 1.66 | 0.76 |
| 7:F:93:ASP:O | 7:F:126:ARG:NH2 | 2.19 | 0.76 |
| 9:H:72:MET:HA | 9:H:93:LEU:HD12 | 1.66 | 0.76 |
| 32:6:48:ARG:HG3 | 32:6:78:LYS:HG2 | 1.67 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:2:119:C:O3' | 1:2:299:G:N2 | 2.18 | 0.76 |
| 1:2:869:G:HO2' | 1:2:871:A:H62 | 1.33 | 0.76 |
| 33:7:74:CYS:O | 33:7:79:SER:N | 2.18 | 0.76 |
| 1:2:1349:A:O3' | 9:H:70:LYS:NZ | 2.18 | 0.76 |
| 35:9:180:SER:OG | 35:9:230:ASP:OD1 | 2.04 | 0.76 |
| 19:R:95:SER:OG | 19:R:96:LYS:N | 2.19 | 0.76 |
| 1:2:906:U:H5'' | 1:2:907:A:H5'' | 1.67 | 0.75 |
| 1:2:948:G:OP1 | 40:2:1702:HOH:O | 2.04 | 0.75 |
| 30:5:823:C:O2' | 32:6:57:ARG:NH1 | 2.18 | 0.75 |
| 1:2:263:G:H4' | 19:R:46:THR:HG21 | 1.68 | 0.75 |
| 10:I:31:SER:H | 10:I:34:ILE:HD12 | 1.51 | 0.75 |
| 33:7:98:GLU:HB2 | 33:7:128:GLN:HE21 | 1.51 | 0.75 |
| 1:2:1399:C:N4 | 1:2:1444:G:O6 | 2.15 | 0.75 |
| 5:D:36:LYS:N | 5:D:40:GLU:OE1 | 2.19 | 0.75 |
| 1:2:1136:C:N4 | 1:2:1148:G:O6 | 2.15 | 0.75 |
| 33:7:260:ARG:NH2 | 33:7:269:TYR:OH | 2.19 | 0.75 |
| 9:H:43:LEU:N | 12:K:102:TYR:OH | 2.20 | 0.75 |
| 19:R:37:ILE:HG22 | 19:R:85:ARG:HG2 | 1.69 | 0.75 |
| 1:2:632:A:H62 | 1:2:691:G:H1 | 1.32 | 0.75 |
| 1:2:1206:C:O2' | 12:K:130:ARG:NH2 | 2.19 | 0.75 |
| 8:G:75:ARG:HD2 | 8:G:92:PRO:HG2 | 1.69 | 0.75 |
| 1:2:203:A:H2' | 1:2:204:G:H8 | 1.51 | 0.74 |
| 1:2:1415:U:H3 | 1:2:1428:G:H1 | 1.35 | 0.74 |
| 11:J:104:GLU:HG3 | 11:J:105:ILE:HG23 | 1.70 | 0.74 |
| 27:Z:2:ALA:N | 27:Z:4:GLU:OE1 | 2.20 | 0.74 |
| 5:D:78:LYS:O | 5:D:146:LYS:NZ | 2.17 | 0.74 |
| 29:3:12:PRO:HD2 | 29:3:15:LEU:HD22 | 1.68 | 0.74 |
| 1:2:185:G:H2' | 1:2:186:G:H8 | 1.52 | 0.74 |
| 6:E:3:ARG:HE | 6:E:4:LYS:HZ3 | 1.34 | 0.74 |
| 1:2:1010:G:H2' | 1:2:1011:A:H8 | 1.53 | 0.74 |
| 1:2:1425:G:H2' | 1:2:1426:A:C8 | 2.21 | 0.74 |
| 33:7:182:PRO:HB2 | 34:8:14:LEU:HD22 | 1.69 | 0.74 |
| 1:2:1378:5HM:H8 | 1:2:1379:G:H8 | 1.52 | 0.74 |
| 1:2:295:G:H2' | 1:2:296:U:C6 | 2.23 | 0.74 |
| 1:2:428:C:H2' | 1:2:429:A:H8 | 1.52 | 0.74 |
| 1:2:531:U:O2' | 10:I:92:ARG:NH1 | 2.20 | 0.74 |
| 1:2:576:U:OP1 | 6:E:24:LYS:NZ | 2.20 | 0.74 |
| 19:R:24:HIS:HE1 | 19:R:77:CYS:SG | 2.03 | 0.74 |
| 33:7:248:LYS:HD3 | 33:7:288:GLU:HB2 | 1.68 | 0.74 |
| 1:2:140:A:N1 | 1:2:229:G:N2 | 2.34 | 0.74 |
| 1:2:1013:G:N2 | 1:2:1184:4AC:N3 | 2.35 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:G:85:ARG:NH1 | 8:G:104:LYS:O | 2.21 | 0.74 |
| 20:S:14:ARG:O | 20:S:18:ASN:ND2 | 2.19 | 0.74 |
| 33:7:106:SER:HA | 33:7:363:SER:HA | 1.69 | 0.74 |
| 16:O:57:GLU:HA | 16:O:60:LYS:HD3 | 1.70 | 0.74 |
| 19:R:18:ASP:OD2 | 19:R:45:LYS:NZ | 2.20 | 0.74 |
| 6:E:19:TRP:O | 6:E:52:TYR:OH | 2.04 | 0.73 |
| 8:G:32:LYS:HB2 | 8:G:112:ILE:HD12 | 1.71 | 0.73 |
| 1:2:992:U:OP1 | 17:P:3:LYS:NZ | 2.18 | 0.73 |
| 1:2:1481:U:H2' | 1:2:1482:A:H8 | 1.53 | 0.73 |
| 7:F:105:GLU:OE2 | 27:Z:110:ARG:NE | 2.21 | 0.73 |
| 1:2:643:A:H2' | 1:2:644:C:H6 | 1.54 | 0.73 |
| 1:2:1316:C:O2' | 12:K:131:GLN:HG3 | 1.87 | 0.73 |
| 27:Z:131:ARG:HH21 | 27:Z:145:ARG:HB2 | 1.53 | 0.73 |
| 5:D:171:ILE:HG22 | 5:D:175:LYS:HZ1 | 1.54 | 0.73 |
| 6:E:144:ASP:N | 6:E:144:ASP:OD1 | 2.21 | 0.73 |
| 1:2:253:U:O4' | 1:2:865:G:N2 | 2.22 | 0.73 |
| 1:2:725:G:N7 | 40:2:1711:HOH:O | 2.21 | 0.73 |
| 23:V:9:LYS:HB3 | 23:V:18:GLU:HB2 | 1.71 | 0.73 |
| 1:2:1010:G:H2' | 1:2:1011:A:C8 | 2.23 | 0.73 |
| 3:B:149:TYR:OH | 4:C:44:GLU:OE2 | 2.04 | 0.73 |
| 3:B:73:ARG:HH12 | 3:B:159:LYS:HE3 | 1.54 | 0.72 |
| 11:J:103:THR:HG23 | 11:J:105:ILE:H | 1.54 | 0.72 |
| 27:Z:42:THR:OG1 | 27:Z:77:ASN:O | 2.07 | 0.72 |
| 1:2:476:G:O6 | 1:2:506:C:N4 | 2.18 | 0.72 |
| 21:T:83:VAL:HG12 | 21:T:84:HIS:H | 1.54 | 0.72 |
| 23:V:6:THR:OG1 | 23:V:22:GLU:OE1 | 2.06 | 0.72 |
| 33:7:134:VAL:HG11 | 33:7:340:VAL:HG21 | 1.71 | 0.72 |
| 1:2:1214:U:O2' | 9:H:91:ARG:O | 2.07 | 0.72 |
| 31:4:18:G:OP2 | 31:4:60:U:O2' | 2.07 | 0.72 |
| 32:6:60:TRP:O | 32:6:85:ARG:NH1 | 2.22 | 0.72 |
| 1:2:262:U:H2' | 1:2:263:G:C8 | 2.24 | 0.72 |
| 1:2:1508:C:O2 | 30:5:807:G:N2 | 2.22 | 0.72 |
| 1:2:735:G:H2' | 1:2:736:G:H8 | 1.54 | 0.72 |
| 1:2:1219:G:H2' | 1:2:1220:G:H8 | 1.54 | 0.72 |
| 8:G:68:ASP:OD2 | 8:G:69:LYS:N | 2.23 | 0.72 |
| 17:P:21:CYS:SG | 17:P:22:ILE:N | 2.62 | 0.72 |
| 27:Z:56:GLY:HA2 | 27:Z:61:ARG:HD3 | 1.71 | 0.72 |
| 1:2:930:A:C2 | 21:T:87:LYS:HB3 | 2.25 | 0.72 |
| 1:2:1458:G:H2' | 1:2:1459:A:H8 | 1.55 | 0.72 |
| 12:K:17:ALA:HB2 | 12:K:81:ALA:HB1 | 1.69 | 0.72 |
| 27:Z:100:ALA:HB1 | 27:Z:169:ALA:HB2 | 1.69 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 29:3:50:LEU:HD13 | 29:3:104:PRO:HG3 | 1.70 | 0.72 |
| 1:2:972:G:O2' | 1:2:1001:A:N1 | 2.23 | 0.72 |
| 1:2:1396:G:H1 | 1:2:1448:C:H1' | 1.55 | 0.72 |
| 33:7:184:SER:OG | 39:7:502:GNP:O6 | 2.07 | 0.72 |
| 33:7:197:GLY:HA2 | 33:7:200:GLU:HG2 | 1.72 | 0.72 |
| 1:2:333:G:H21 | 1:2:335:G:H3' | 1.54 | 0.72 |
| 1:2:353:A:OP2 | 1:2:354:C:N4 | 2.23 | 0.72 |
| 1:2:859:G:N2 | 1:2:881:C:N3 | 2.38 | 0.72 |
| 2:A:52:THR:OG1 | 2:A:53:LEU:N | 2.23 | 0.72 |
| 16:O:11:ALA:N | 16:O:63:GLU:OE2 | 2.23 | 0.72 |
| 23:V:6:THR:N | 23:V:20:TYR:O | 2.22 | 0.72 |
| 34:8:6:GLU:HA | 34:8:9:GLU:HB3 | 1.72 | 0.72 |
| 1:2:1491:U:OP1 | 14:M:136:ARG:NH2 | 2.23 | 0.71 |
| 4:C:3:GLU:HB2 | 7:F:230:PRO:HD2 | 1.70 | 0.71 |
| 1:2:361:C:O2' | 1:2:363:G:OP1 | 2.09 | 0.71 |
| 1:2:1400:C:N4 | 1:2:1443:G:O6 | 2.20 | 0.71 |
| 3:B:169:TRP:HD1 | 3:B:195:PHE:HE2 | 1.37 | 0.71 |
| 14:M:25:ASN:OD1 | 14:M:26:THR:N | 2.20 | 0.71 |
| 1:2:267:G:H2' | 1:2:268:G:C8 | 2.25 | 0.71 |
| 1:2:287:G:OP2 | 19:R:69:ARG:NH2 | 2.23 | 0.71 |
| 1:2:955:A:O2' | 1:2:1015:G:OP2 | 2.07 | 0.71 |
| 33:7:144:LEU:HB3 | 33:7:178:VAL:HG11 | 1.72 | 0.71 |
| 1:2:834:G:OP1 | 7:F:153:ARG:NH2 | 2.21 | 0.71 |
| 1:2:1234:G:H21 | 1:2:1249:A:H62 | 1.36 | 0.71 |
| 33:7:191:ILE:HG23 | 33:7:194:LEU:HD23 | 1.71 | 0.71 |
| 1:2:1274:G:N2 | 40:2:1717:HOH:O | 2.24 | 0.71 |
| 33:7:56:ILE:HG22 | 33:7:86:LEU:HD13 | 1.73 | 0.71 |
| 1:2:112:A:H2' | 1:2:113:G:O4' | 1.89 | 0.71 |
| 1:2:1273:A:N7 | 1:2:1275:U:N3 | 2.39 | 0.71 |
| 6:E:175:GLU:OE2 | 6:E:235:ARG:NH2 | 2.23 | 0.71 |
| 33:7:249:VAL:HA | 33:7:276:ILE:HB | 1.73 | 0.71 |
| 35:9:19:VAL:HA | 35:9:29:VAL:HG12 | 1.71 | 0.71 |
| 1:2:1112:A:H2' | 1:2:1113:G:H8 | 1.55 | 0.71 |
| 3:B:163:ALA:O | 3:B:166:LEU:N | 2.22 | 0.71 |
| 4:C:14:CYS:HB3 | 4:C:17:CYS:SG | 2.30 | 0.71 |
| 15:N:101:ASP:OD1 | 15:N:146:ARG:NH1 | 2.24 | 0.71 |
| 1:2:1182:C:H2' | 1:2:1183:C:C6 | 2.26 | 0.70 |
| 1:2:1260:U:H3 | 22:U:61:ARG:HH21 | 1.39 | 0.70 |
| 3:B:70:VAL:O | 3:B:118:THR:OG1 | 2.08 | 0.70 |
| 23:V:74:ASP:OD1 | 23:V:75:LYS:N | 2.24 | 0.70 |
| 28:0:10:LYS:NZ | 28:0:13:ARG:O | 2.23 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:X:15:ILE:HD12 | 25:X:26:GLN:HG3 | 1.73 | 0.70 |
| 26:Y:31:MET:HA | 26:Y:40:CYS:HA | 1.71 | 0.70 |
| 1:2:1169:U:H2' | 1:2:1171:G:C8 | 2.26 | 0.70 |
| 35:9:239:ALA:HA | 35:9:242:ALA:HB3 | 1.72 | 0.70 |
| 1:2:222:A:C5 | 1:2:223:G:H1' | 2.27 | 0.70 |
| 2:A:196:GLU:OE1 | 2:A:196:GLU:N | 2.24 | 0.70 |
| 1:2:144:G:O6 | 1:2:173:C:N4 | 2.25 | 0.70 |
| 1:2:183:U:H2' | 1:2:184:G:H8 | 1.57 | 0.70 |
| 1:2:930:A:HO2' | 1:2:957:4AC:HO2' | 1.39 | 0.70 |
| 1:2:973:A:C6 | 29:3:92:ILE:HG21 | 2.27 | 0.70 |
| 1:2:1480:G:H1 | 1:2:1493:C:H42 | 1.36 | 0.70 |
| 6:E:196:LYS:NZ | 6:E:243:PRO:O | 2.24 | 0.70 |
| 1:2:93:C:H2' | 1:2:94:G:C8 | 2.26 | 0.70 |
| 1:2:451:A:H3' | 1:2:452:G:H8 | 1.55 | 0.70 |
| 1:2:938:B8H:C2 | 1:2:939:5MC:HM52 | 2.22 | 0.70 |
| 31:4:74:C:N4 | 33:7:33:TRP:CD1 | 2.57 | 0.70 |
| 31:4:76:A:H5'' | 33:7:223:VAL:HG22 | 1.74 | 0.70 |
| 33:7:49:LEU:HD21 | 33:7:104:MET:HA | 1.74 | 0.70 |
| 1:2:825:U:O4 | 40:2:1703:HOH:O | 2.07 | 0.70 |
| 1:2:926:G:H2' | 1:2:927:U:C6 | 2.27 | 0.70 |
| 1:2:991:G:OP1 | 17:P:2:ALA:N | 2.24 | 0.70 |
| 17:P:41:HIS:O | 17:P:44:ARG:N | 2.24 | 0.70 |
| 16:O:46:ASP:OD2 | 16:O:49:MET:N | 2.25 | 0.70 |
| 1:2:642:U:OP2 | 2:A:190:LYS:NZ | 2.24 | 0.69 |
| 16:O:119:ARG:HB2 | 16:O:126:VAL:HG22 | 1.74 | 0.69 |
| 21:T:79:LEU:HG | 21:T:80:THR:H | 1.57 | 0.69 |
| 8:G:10:ASP:OD1 | 8:G:12:LYS:N | 2.25 | 0.69 |
| 12:K:15:ALA:HA | 12:K:66:VAL:HG12 | 1.73 | 0.69 |
| 13:L:43:LYS:HB3 | 13:L:68:ILE:HB | 1.73 | 0.69 |
| 19:R:21:CYS:HB3 | 19:R:24:HIS:HB2 | 1.73 | 0.69 |
| 33:7:183:VAL:HG21 | 33:7:194:LEU:HD22 | 1.74 | 0.69 |
| 1:2:148:A:C2 | 1:2:149:A:H1' | 2.28 | 0.69 |
| 1:2:903:C:H2' | 1:2:904:A:C8 | 2.27 | 0.69 |
| 1:2:1312:G:H2' | 1:2:1313:A:C8 | 2.27 | 0.69 |
| 1:2:1321:G:H22 | 1:2:1347:G:H2' | 1.56 | 0.69 |
| 1:2:1479:4AC:N3 | 1:2:1495:G:N2 | 2.39 | 0.69 |
| 1:2:1494:G:OP2 | 14:M:132:ARG:NH2 | 2.26 | 0.69 |
| 11:J:88:GLN:OE1 | 11:J:91:ARG:NH2 | 2.25 | 0.69 |
| 12:K:17:ALA:HA | 12:K:64:VAL:HG12 | 1.74 | 0.69 |
| 21:T:32:GLN:N | 21:T:32:GLN:OE1 | 2.25 | 0.69 |
| 14:M:107:ARG:O | 25:X:35:ARG:NH2 | 2.25 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:4:47:U:H5'' | 31:4:48:C:H5' | 1.74 | 0.69 |
| 31:4:74:C:H5 | 33:7:33:TRP:HE1 | 1.39 | 0.69 |
| 1:2:580:A:OP1 | 5:D:54:ARG:NH2 | 2.25 | 0.69 |
| 1:2:1334:A:OP2 | 17:P:32:ARG:NH2 | 2.26 | 0.69 |
| 1:2:1417:U:H2' | 1:2:1418:C:H6 | 1.55 | 0.69 |
| 21:T:5:GLU:OE2 | 21:T:7:ARG:NE | 2.25 | 0.69 |
| 1:2:627:G:H2' | 1:2:628:G:H8 | 1.56 | 0.69 |
| 1:2:928:U:H1' | 21:T:113:VAL:HG23 | 1.74 | 0.69 |
| 29:3:32:ILE:HD11 | 29:3:34:LYS:HE3 | 1.73 | 0.69 |
| 31:4:44:A:H3' | 31:4:45:G:C8 | 2.28 | 0.69 |
| 1:2:1261:A:H2 | 1:2:1327:G:H1' | 1.57 | 0.69 |
| 8:G:75:ARG:HB2 | 8:G:107:VAL:HG21 | 1.74 | 0.69 |
| 33:7:331:ILE:HG12 | 33:7:413:VAL:HG12 | 1.74 | 0.69 |
| 20:S:47:ARG:HA | 20:S:50:ILE:HD12 | 1.75 | 0.69 |
| 1:2:205:G:O2' | 11:J:64:ASN:ND2 | 2.26 | 0.69 |
| 1:2:1239:4AC:OP2 | 22:U:99:ARG:NE | 2.24 | 0.69 |
| 1:2:1509:U:O2 | 30:5:806:G:N1 | 2.26 | 0.69 |
| 33:7:98:GLU:HG2 | 33:7:406:ARG:HH11 | 1.58 | 0.69 |
| 34:8:56:ARG:HH22 | 34:8:116:LEU:HB2 | 1.58 | 0.69 |
| 1:2:474:A:C4 | 5:D:18:TRP:NE1 | 2.61 | 0.68 |
| 9:H:133:ARG:HG3 | 25:X:58:ARG:HD2 | 1.75 | 0.68 |
| 16:O:63:GLU:HA | 16:O:66:LEU:HD12 | 1.73 | 0.68 |
| 1:2:966:C:H2' | 1:2:967:G:H8 | 1.59 | 0.68 |
| 2:A:52:THR:N | 14:M:114:ARG:HH22 | 1.90 | 0.68 |
| 34:8:109:CYS:SG | 34:8:111:SER:OG | 2.50 | 0.68 |
| 18:Q:63:VAL:O | 18:Q:65:LEU:N | 2.25 | 0.68 |
| 35:9:31:LEU:O | 35:9:36:GLY:HA2 | 1.94 | 0.68 |
| 1:2:466:G:N3 | 1:2:467:G:N2 | 2.42 | 0.68 |
| 1:2:731:4AC:C2 | 1:2:732:G:C8 | 2.76 | 0.68 |
| 6:E:202:ILE:HG12 | 6:E:213:VAL:HG12 | 1.73 | 0.68 |
| 1:2:344:C:H2' | 1:2:345:C:H6 | 1.58 | 0.68 |
| 1:2:554:G:H2' | 1:2:555:G:H8 | 1.57 | 0.68 |
| 1:2:1155:G:O2' | 1:2:1156:G:O5' | 2.10 | 0.68 |
| 5:D:171:ILE:O | 5:D:175:LYS:NZ | 2.24 | 0.68 |
| 10:I:27:ILE:HB | 10:I:61:TYR:HB2 | 1.75 | 0.68 |
| 33:7:30:THR:HG21 | 33:7:52:ALA:HB1 | 1.75 | 0.68 |
| 1:2:413:G:O2' | 1:2:463:A:N1 | 2.21 | 0.68 |
| 1:2:814:A:H1' | 2:A:134:GLN:HE21 | 1.57 | 0.68 |
| 1:2:957:4AC:O7 | 1:2:957:4AC:H5 | 1.91 | 0.68 |
| 7:F:122:ILE:HD13 | 7:F:206:TYR:HD1 | 1.59 | 0.68 |
| 1:2:154:G:OP1 | 8:G:18:GLN:NE2 | 2.23 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2:458:G:H3' | 1:2:459:G:H8 | 1.59 | 0.68 |
| 1:2:759:A:O2' | 1:2:761:A:N6 | 2.17 | 0.68 |
| 1:2:786:A:N6 | 1:2:1498:C:N3 | 2.42 | 0.68 |
| 31:4:43:A:H2' | 31:4:44:A:H8 | 1.59 | 0.68 |
| 1:2:299:G:OP1 | 40:2:1704:HOH:O | 2.11 | 0.68 |
| 18:Q:8:LYS:NZ | 40:Q:201:HOH:O | 2.26 | 0.68 |
| 35:9:183:ILE:HG13 | 35:9:227:TYR:HB2 | 1.75 | 0.68 |
| 1:2:163:G:H2' | 1:2:164:G:H8 | 1.59 | 0.68 |
| 1:2:529:A:O2' | 1:2:532:G:O2' | 2.12 | 0.68 |
| 1:2:930:A:H2 | 21:T:87:LYS:HB3 | 1.58 | 0.68 |
| 1:2:1083:C:H2' | 1:2:1084:C:C6 | 2.29 | 0.68 |
| 1:2:1240:G:OP2 | 22:U:99:ARG:NH2 | 2.27 | 0.68 |
| 6:E:42:SER:HA | 6:E:85:VAL:O | 1.93 | 0.68 |
| 19:R:15:LYS:HD2 | 19:R:24:HIS:HD2 | 1.59 | 0.68 |
| 1:2:926:G:H2' | 1:2:927:U:H6 | 1.59 | 0.68 |
| 5:D:168:ARG:NH1 | 5:D:172:GLU:OE2 | 2.27 | 0.68 |
| 12:K:12:THR:H | 12:K:113:ARG:HH22 | 1.41 | 0.68 |
| 33:7:150:LYS:HB3 | 33:7:153:VAL:HG12 | 1.75 | 0.68 |
| 1:2:89:G:H3' | 1:2:90:G:H8 | 1.59 | 0.67 |
| 1:2:925:G:H21 | 21:T:122:ALA:HB1 | 1.56 | 0.67 |
| 5:D:172:GLU:HA | 5:D:175:LYS:HE2 | 1.75 | 0.67 |
| 29:3:50:LEU:HB2 | 29:3:101:ILE:HG12 | 1.75 | 0.67 |
| 35:9:239:ALA:O | 35:9:243:LEU:N | 2.27 | 0.67 |
| 12:K:104:ARG:HE | 12:K:108:VAL:HG21 | 1.58 | 0.67 |
| 1:2:1279:G:N3 | 1:2:1305:G:N2 | 2.41 | 0.67 |
| 17:P:29:PRO:HB2 | 17:P:40:ARG:HB3 | 1.76 | 0.67 |
| 28:0:29:GLN:HB3 | 28:0:33:GLU:CD | 2.15 | 0.67 |
| 1:2:1183:C:O2' | 1:2:1188:A:N6 | 2.27 | 0.67 |
| 17:P:4:ALA:O | 17:P:8:LYS:NZ | 2.27 | 0.67 |
| 1:2:976:A:OP2 | 1:2:1000:G:N2 | 2.28 | 0.67 |
| 33:7:60:GLU:N | 33:7:60:GLU:OE2 | 2.26 | 0.67 |
| 12:K:55:GLU:OE1 | 12:K:55:GLU:N | 2.28 | 0.67 |
| 33:7:330:ARG:NH2 | 33:7:377:GLU:OE1 | 2.27 | 0.67 |
| 1:2:1261:A:C2 | 1:2:1327:G:H1' | 2.30 | 0.67 |
| 1:2:1378:5HM:H8 | 1:2:1379:G:C8 | 2.29 | 0.67 |
| 3:B:142:ASP:OD1 | 3:B:143:THR:N | 2.22 | 0.67 |
| 9:H:131:ALA:O | 9:H:157:ARG:NH2 | 2.28 | 0.67 |
| 30:5:807:G:H2' | 30:5:808:A:C8 | 2.30 | 0.67 |
| 32:6:41:CYS:SG | 32:6:42:GLU:N | 2.67 | 0.67 |
| 1:2:37:C:H2' | 1:2:38:A:H8 | 1.60 | 0.67 |
| 1:2:232:C:H2' | 1:2:233:G:H8 | 1.59 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2:278:C:H2' | 1:2:279:A:H8 | 1.59 | 0.67 |
| 8:G:26:ALA:HA | 8:G:29:LEU:HD21 | 1.76 | 0.67 |
| 32:6:74:VAL:O | 32:6:79:ARG:NH1 | 2.28 | 0.67 |
| 1:2:643:A:H2' | 1:2:644:C:C6 | 2.30 | 0.67 |
| 1:2:759:A:HO2' | 1:2:761:A:H62 | 1.40 | 0.67 |
| 1:2:843:A:O2' | 1:2:844:A:H3' | 1.95 | 0.66 |
| 1:2:916:G:OP1 | 40:2:1706:HOH:O | 2.12 | 0.66 |
| 1:2:1133:U:O4' | 1:2:1156:G:N2 | 2.28 | 0.66 |
| 18:Q:120:ARG:HH11 | 18:Q:124:LEU:HD21 | 1.59 | 0.66 |
| 24:W:55:ILE:HG22 | 24:W:57:ARG:HH12 | 1.59 | 0.66 |
| 1:2:337:C:H4' | 1:2:338:A:H5'' | 1.77 | 0.66 |
| 1:2:1147:4AC:O7 | 1:2:1147:4AC:H5 | 1.95 | 0.66 |
| 32:6:40:ARG:NH1 | 32:6:41:CYS:O | 2.29 | 0.66 |
| 1:2:1116:A:O2' | 1:2:1117:G:O5' | 2.12 | 0.66 |
| 1:2:1266:C:H2' | 1:2:1267:G:H8 | 1.59 | 0.66 |
| 16:O:83:LYS:HE2 | 21:T:9:ARG:HH12 | 1.61 | 0.66 |
| 22:U:137:LYS:NZ | 22:U:150:TYR:O | 2.26 | 0.66 |
| 1:2:50:G:N2 | 1:2:408:C:N3 | 2.43 | 0.66 |
| 1:2:848:4AC:O7 | 1:2:848:4AC:H5 | 1.95 | 0.66 |
| 1:2:972:G:N2 | 1:2:973:A:N1 | 2.43 | 0.66 |
| 1:2:1422:C:O2 | 1:2:1423:G:N1 | 2.28 | 0.66 |
| 2:A:118:LEU:HA | 2:A:192:LEU:HD13 | 1.77 | 0.66 |
| 5:D:56:ARG:HD3 | 7:F:160:PRO:HG3 | 1.76 | 0.66 |
| 26:Y:48:TRP:O | 26:Y:50:LYS:NZ | 2.22 | 0.66 |
| 1:2:718:4AC:O7 | 1:2:719:G:N1 | 2.27 | 0.66 |
| 1:2:848:4AC:O3' | 10:I:76:LYS:HG2 | 1.96 | 0.66 |
| 1:2:851:4AC:H2' | 1:2:852:G:H8 | 1.60 | 0.66 |
| 5:D:116:ARG:CZ | 5:D:174:ALA:HB2 | 2.26 | 0.66 |
| 33:7:248:LYS:N | 33:7:251:GLN:OE1 | 2.28 | 0.66 |
| 1:2:1391:G:N1 | 1:2:1451:G:N7 | 2.43 | 0.66 |
| 2:A:33:VAL:HG11 | 2:A:51:VAL:HG11 | 1.76 | 0.66 |
| 7:F:150:GLY:HA3 | 7:F:196:ASN:HD22 | 1.59 | 0.66 |
| 1:2:1193:4AC:O7 | 1:2:1193:4AC:H5 | 1.95 | 0.66 |
| 1:2:1209:U:OP1 | 40:2:1707:HOH:O | 2.13 | 0.66 |
| 1:2:1458:G:H2' | 1:2:1459:A:C8 | 2.30 | 0.66 |
| 5:D:104:ARG:NH2 | 5:D:140:PRO:O | 2.29 | 0.66 |
| 12:K:135:ARG:NH1 | 31:4:35:A:OP2 | 2.29 | 0.66 |
| 31:4:10:G:H22 | 31:4:26:G:H1' | 1.60 | 0.66 |
| 1:2:563:G:H21 | 10:I:124:ARG:HH21 | 1.43 | 0.66 |
| 1:2:860:A:O2' | 28:0:4:ARG:NH1 | 2.26 | 0.66 |
| 1:2:1381:C:H2' | 1:2:1382:A:C8 | 2.30 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:L:38:ILE:HB | 13:L:72:LEU:HB3 | 1.76 | 0.66 |
| 21:T:6:PHE:CD2 | 21:T:96:PRO:HB3 | 2.31 | 0.66 |
| 33:7:146:ILE:HG21 | 33:7:166:ILE:HG21 | 1.78 | 0.66 |
| 1:2:443:G:O2' | 23:V:30:THR:O | 2.14 | 0.66 |
| 1:2:1294:C:N4 | 21:T:69:ASP:OD1 | 2.29 | 0.66 |
| 2:A:102:THR:HG21 | 2:A:129:ARG:HA | 1.76 | 0.66 |
| 19:R:15:LYS:NZ | 19:R:16:CYS:O | 2.24 | 0.66 |
| 35:9:247:ILE:HG21 | 35:9:263:VAL:HB | 1.76 | 0.66 |
| 1:2:313:G:N2 | 5:D:3:ASP:OD2 | 2.29 | 0.66 |
| 1:2:251:G:C2 | 1:2:294:G:C2 | 2.85 | 0.65 |
| 1:2:390:A:H2' | 1:2:391:A:C8 | 2.31 | 0.65 |
| 1:2:446:U:O2' | 1:2:449:A:N7 | 2.23 | 0.65 |
| 1:2:903:C:H2' | 1:2:904:A:H8 | 1.61 | 0.65 |
| 1:2:993:C:H2' | 1:2:994:U:C6 | 2.30 | 0.65 |
| 1:2:1224:A:C5 | 1:2:1261:A:N7 | 2.64 | 0.65 |
| 1:2:1433:G:H2' | 1:2:1434:U:C6 | 2.32 | 0.65 |
| 1:2:1452:A:C2 | 33:7:373:VAL:HB | 2.31 | 0.65 |
| 29:3:40:THR:HG23 | 29:3:41:LYS:HG3 | 1.77 | 0.65 |
| 1:2:292:U:OP1 | 11:J:13:SER:OG | 2.15 | 0.65 |
| 1:2:553:G:N2 | 1:2:722:G:N7 | 2.45 | 0.65 |
| 5:D:46:THR:HG22 | 5:D:50:ASN:HD21 | 1.61 | 0.65 |
| 20:S:61:LYS:HB2 | 20:S:66:ILE:HD12 | 1.77 | 0.65 |
| 29:3:73:LYS:HZ3 | 29:3:75:ILE:HB | 1.60 | 0.65 |
| 33:7:269:TYR:CE1 | 33:7:385:PRO:HD2 | 2.31 | 0.65 |
| 1:2:638:G:H2' | 1:2:639:G:O4' | 1.96 | 0.65 |
| 13:L:8:LEU:HB3 | 13:L:16:LEU:HD11 | 1.78 | 0.65 |
| 1:2:703:4AC:OP1 | 2:A:139:ARG:NH1 | 2.29 | 0.65 |
| 1:2:1350:U:N3 | 1:2:1351:A:N1 | 2.44 | 0.65 |
| 10:I:51:GLU:OE2 | 10:I:62:ARG:NH1 | 2.29 | 0.65 |
| 33:7:108:ALA:HB1 | 33:7:139:ILE:HG13 | 1.78 | 0.65 |
| 33:7:260:ARG:HA | 33:7:269:TYR:HA | 1.77 | 0.65 |
| 33:7:333:TYR:CE1 | 33:7:378:ILE:HB | 2.31 | 0.65 |
| 33:7:365:THR:H | 33:7:384:ARG:NH1 | 1.94 | 0.65 |
| 1:2:168:A:O2' | 1:2:169:A:O4' | 2.15 | 0.65 |
| 1:2:203:A:H2' | 1:2:204:G:C8 | 2.30 | 0.65 |
| 1:2:1232:C:H2' | 1:2:1233:4AC:H6 | 1.79 | 0.65 |
| 2:A:12:ASP:OD2 | 2:A:13:LYS:N | 2.30 | 0.65 |
| 2:A:52:THR:HG23 | 2:A:55:ASP:H | 1.62 | 0.65 |
| 2:A:172:ALA:HB2 | 2:A:184:ALA:HB3 | 1.78 | 0.65 |
| 27:Z:4:GLU:OE2 | 27:Z:4:GLU:N | 2.25 | 0.65 |
| 27:Z:4:GLU:O | 27:Z:7:PHE:N | 2.30 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2:1328:C:H2' | 1:2:1329:G:H8 | 1.61 | 0.65 |
| 11:J:57:LEU:HG | 11:J:118:GLY:HA2 | 1.78 | 0.65 |
| 12:K:135:ARG:NH2 | 31:4:33:U:OP2 | 2.30 | 0.65 |
| 33:7:24:THR:HG21 | 33:7:186:LEU:HA | 1.77 | 0.65 |
| 33:7:364:SER:HB3 | 33:7:384:ARG:HH12 | 1.61 | 0.65 |
| 35:9:69:ILE:HG22 | 35:9:70:ARG:HG3 | 1.79 | 0.65 |
| 1:2:525:U:O4 | 40:2:1705:HOH:O | 2.11 | 0.65 |
| 1:2:1321:G:N2 | 1:2:1347:G:N3 | 2.45 | 0.65 |
| 5:D:46:THR:O | 5:D:50:ASN:ND2 | 2.29 | 0.65 |
| 5:D:94:SER:HG | 7:F:161:ARG:HH21 | 1.42 | 0.65 |
| 33:7:50:GLY:HA3 | 33:7:93:ASP:HB2 | 1.79 | 0.65 |
| 1:2:1198:U:H3 | 1:2:1296:C:H6 | 1.44 | 0.65 |
| 16:O:57:GLU:OE1 | 16:O:57:GLU:N | 2.20 | 0.65 |
| 27:Z:82:VAL:HG12 | 27:Z:83:GLN:H | 1.61 | 0.65 |
| 33:7:317:THR:HG22 | 33:7:318:LEU:H | 1.61 | 0.65 |
| 1:2:1386:C:H2' | 1:2:1387:A:C8 | 2.32 | 0.65 |
| 33:7:24:THR:HB | 33:7:185:ALA:HB1 | 1.78 | 0.65 |
| 6:E:57:LYS:HG3 | 6:E:58:THR:HG23 | 1.79 | 0.64 |
| 7:F:128:CYS:SG | 7:F:139:HIS:CE1 | 2.90 | 0.64 |
| 1:2:306:G:N2 | 1:2:309:A:OP2 | 2.30 | 0.64 |
| 1:2:344:C:H2' | 1:2:345:C:C6 | 2.32 | 0.64 |
| 1:2:1468:A:C4 | 1:2:1469:6MZ:H8 | 2.33 | 0.64 |
| 8:G:68:ASP:OD1 | 8:G:108:ARG:NE | 2.30 | 0.64 |
| 16:O:80:ASN:HB2 | 16:O:92:HIS:CG | 2.32 | 0.64 |
| 28:O:7:LYS:O | 28:O:13:ARG:NH1 | 2.28 | 0.64 |
| 32:6:77:ASP:H | 32:6:79:ARG:HH12 | 1.44 | 0.64 |
| 1:2:1287:G:OP2 | 21:T:33:ARG:NH2 | 2.30 | 0.64 |
| 21:T:109:THR:HG23 | 21:T:110:ARG:HG3 | 1.79 | 0.64 |
| 29:3:116:MET:O | 29:3:120:GLU:HG2 | 1.98 | 0.64 |
| 11:J:76:ARG:NH1 | 11:J:77:ILE:O | 2.30 | 0.64 |
| 1:2:379:4AC:N4 | 1:2:400:G:O6 | 2.29 | 0.64 |
| 1:2:582:G:C2 | 1:2:583:G:C8 | 2.84 | 0.64 |
| 1:2:949:A:OP1 | 40:2:1709:HOH:O | 2.14 | 0.64 |
| 13:L:6:ILE:HG22 | 13:L:98:ILE:HG12 | 1.79 | 0.64 |
| 19:R:34:PHE:HD1 | 19:R:51:ARG:HE | 1.43 | 0.64 |
| 33:7:130:ARG:HH21 | 33:7:340:VAL:HA | 1.63 | 0.64 |
| 1:2:224:G:O2' | 1:2:225:C:O5' | 2.15 | 0.64 |
| 1:2:543:G:OP1 | 40:2:1708:HOH:O | 2.14 | 0.64 |
| 1:2:632:A:N7 | 1:2:691:G:N2 | 2.34 | 0.64 |
| 1:2:710:A:H2' | 1:2:711:A:H8 | 1.61 | 0.64 |
| 1:2:1007:C:H2' | 1:2:1008:G:C8 | 2.31 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2:1309:C:O2' | 9:H:175:ARG:NH1 | 2.31 | 0.64 |
| 11:J:108:ALA:HA | 11:J:125:LEU:H | 1.62 | 0.64 |
| 13:L:53:PRO:O | 17:P:40:ARG:NH2 | 2.31 | 0.64 |
| 1:2:407:C:H2' | 1:2:408:C:H6 | 1.62 | 0.64 |
| 1:2:915:U:OP1 | 40:2:1710:HOH:O | 2.15 | 0.64 |
| 1:2:1086:C:H2' | 1:2:1087:C:C6 | 2.33 | 0.64 |
| 1:2:1347:G:O2' | 1:2:1348:A:O5' | 2.13 | 0.64 |
| 19:R:41:ASP:OD1 | 19:R:41:ASP:N | 2.24 | 0.64 |
| 21:T:12:THR:HG1 | 21:T:15:GLN:H | 1.46 | 0.64 |
| 21:T:32:GLN:HG3 | 21:T:71:ILE:HD13 | 1.79 | 0.64 |
| 33:7:65:PRO:O | 33:7:67:ALA:N | 2.30 | 0.64 |
| 1:2:128:C:O2' | 1:2:271:A:N3 | 2.24 | 0.64 |
| 1:2:833:G:H2' | 1:2:834:G:C8 | 2.33 | 0.64 |
| 1:2:1440:C:H2' | 1:2:1441:U:C6 | 2.32 | 0.64 |
| 1:2:1475:U:O2' | 1:2:1476:A:O5' | 2.10 | 0.64 |
| 9:H:195:ASP:OD1 | 9:H:197:LYS:N | 2.30 | 0.64 |
| 10:I:113:HIS:HA | 10:I:116:ALA:HB3 | 1.80 | 0.64 |
| 1:2:57:U:O2 | 1:2:370:C:O2' | 2.15 | 0.64 |
| 1:2:164:G:H2' | 1:2:165:G:H8 | 1.62 | 0.64 |
| 1:2:1041:4AC:O7 | 1:2:1041:4AC:H5 | 1.97 | 0.64 |
| 16:O:55:THR:OG1 | 16:O:56:ASP:N | 2.30 | 0.64 |
| 27:Z:57:ARG:O | 27:Z:60:ARG:NE | 2.30 | 0.64 |
| 35:9:196:ILE:O | 35:9:200:ILE:HG12 | 1.98 | 0.64 |
| 1:2:368:C:H2' | 1:2:369:G:C8 | 2.33 | 0.64 |
| 1:2:703:4AC:O7 | 1:2:703:4AC:H5 | 1.98 | 0.64 |
| 23:V:46:LEU:HB3 | 23:V:71:TYR:CE1 | 2.33 | 0.64 |
| 1:2:209:A:O2' | 1:2:210:A:O5' | 2.16 | 0.63 |
| 1:2:1236:C:OP2 | 22:U:71:GLU:HB2 | 1.97 | 0.63 |
| 9:H:141:PHE:CZ | 25:X:65:ARG:HD3 | 2.32 | 0.63 |
| 33:7:132:HIS:O | 33:7:136:LEU:HG | 1.98 | 0.63 |
| 33:7:254:LYS:NZ | 33:7:321:ALA:O | 2.31 | 0.63 |
| 33:7:279:ILE:HG21 | 33:7:289:ALA:HB2 | 1.80 | 0.63 |
| 1:2:268:G:P | 11:J:113:ARG:HE | 2.21 | 0.63 |
| 1:2:521:C:H2' | 1:2:522:C:C6 | 2.33 | 0.63 |
| 1:2:854:C:H2' | 1:2:855:U:H6 | 1.62 | 0.63 |
| 29:3:20:LEU:HD21 | 29:3:81:PRO:HD2 | 1.79 | 0.63 |
| 1:2:323:G:H2' | 1:2:324:A:C8 | 2.33 | 0.63 |
| 1:2:793:C:H4' | 10:I:13:HIS:ND1 | 2.13 | 0.63 |
| 2:A:120:VAL:HG12 | 2:A:189:ILE:HG12 | 1.80 | 0.63 |
| 21:T:40:LEU:HB2 | 21:T:45:LYS:HE3 | 1.79 | 0.63 |
| 24:W:15:PHE:HB2 | 24:W:64:LEU:HG | 1.80 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2:37:C:H2' | 1:2:38:A:C8 | 2.34 | 0.63 |
| 1:2:818:C:H2' | 1:2:819:G:H8 | 1.63 | 0.63 |
| 17:P:39:CYS:HB2 | 17:P:42:CYS:SG | 2.38 | 0.63 |
| 31:4:44:A:H3' | 31:4:45:G:H8 | 1.63 | 0.63 |
| 11:J:38:ALA:HB3 | 11:J:59:ALA:HB1 | 1.81 | 0.63 |
| 29:3:69:LEU:O | 29:3:73:LYS:NZ | 2.31 | 0.63 |
| 2:A:185:GLU:OE1 | 2:A:185:GLU:N | 2.32 | 0.63 |
| 7:F:56:GLU:N | 7:F:56:GLU:OE2 | 2.31 | 0.63 |
| 19:R:14:GLU:HG3 | 19:R:15:LYS:H | 1.62 | 0.63 |
| 26:Y:6:LYS:HG3 | 26:Y:7:LEU:HG | 1.81 | 0.63 |
| 33:7:97:HIS:HB3 | 33:7:99:VAL:HG12 | 1.80 | 0.63 |
| 33:7:167:LYS:O | 33:7:171:LYS:HG2 | 1.97 | 0.63 |
| 1:2:333:G:N2 | 1:2:335:G:H3' | 2.13 | 0.63 |
| 1:2:354:C:O2 | 1:2:355:G:N2 | 2.31 | 0.63 |
| 1:2:1131:A:N6 | 1:2:1154:A:N7 | 2.46 | 0.63 |
| 1:2:1402:A:H2' | 1:2:1403:G:H8 | 1.63 | 0.63 |
| 16:O:76:ARG:NH1 | 16:O:90:ASP:OD2 | 2.32 | 0.63 |
| 33:7:98:GLU:HB3 | 33:7:404:ARG:HG2 | 1.80 | 0.63 |
| 1:2:512:G:P | 5:D:37:ASN:HB2 | 2.39 | 0.63 |
| 1:2:1182:C:H2' | 1:2:1183:C:H6 | 1.63 | 0.63 |
| 2:A:48:VAL:O | 14:M:34:THR:OG1 | 2.16 | 0.63 |
| 1:2:66:C:H2' | 1:2:67:G:H8 | 1.62 | 0.63 |
| 1:2:1396:G:H22 | 1:2:1448:C:H1' | 1.63 | 0.63 |
| 5:D:78:LYS:NZ | 5:D:85:GLU:O | 2.23 | 0.63 |
| 5:D:171:ILE:HG22 | 5:D:175:LYS:NZ | 2.14 | 0.63 |
| 12:K:70:GLY:O | 12:K:73:GLY:N | 2.31 | 0.63 |
| 32:6:94:LEU:HG | 32:6:99:LYS:HB2 | 1.79 | 0.63 |
| 33:7:26:VAL:HA | 33:7:29:ILE:HG12 | 1.81 | 0.63 |
| 7:F:20:THR:HG22 | 7:F:21:LYS:H | 1.64 | 0.62 |
| 30:5:823:C:H4' | 32:6:57:ARG:HG3 | 1.80 | 0.62 |
| 33:7:163:TYR:OH | 34:8:3:SER:O | 2.14 | 0.62 |
| 3:B:44:ASP:OD2 | 3:B:47:LYS:NZ | 2.33 | 0.62 |
| 31:4:74:C:N4 | 33:7:33:TRP:NE1 | 2.44 | 0.62 |
| 33:7:162:GLN:O | 33:7:166:ILE:HG13 | 1.98 | 0.62 |
| 35:9:185:VAL:HG22 | 35:9:261:ILE:HG12 | 1.81 | 0.62 |
| 1:2:442:A:H2' | 1:2:443:G:H8 | 1.62 | 0.62 |
| 6:E:164:VAL:HG12 | 6:E:176:VAL:HG22 | 1.81 | 0.62 |
| 14:M:40:SER:OG | 14:M:70:GLU:OE1 | 2.13 | 0.62 |
| 18:Q:83:GLU:HG2 | 18:Q:88:ALA:HB2 | 1.80 | 0.62 |
| 31:4:10:G:N2 | 31:4:26:G:H1' | 2.15 | 0.62 |
| 32:6:28:VAL:HG22 | 32:6:39:VAL:HG12 | 1.80 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 33:7:360:SER:HA | 33:7:365:THR:HA | 1.80 | 0.62 |
| 1:2:872:A:O2' | 1:2:1482:A:OP1 | 2.18 | 0.62 |
| 1:2:1280:A:H3' | 1:2:1281:U:H6 | 1.64 | 0.62 |
| 17:P:31:ILE:HG22 | 17:P:33:ILE:H | 1.63 | 0.62 |
| 31:4:8:4SU:O2' | 31:4:13:C:N4 | 2.32 | 0.62 |
| 32:6:68:ILE:HG12 | 32:6:84:TYR:O | 2.00 | 0.62 |
| 33:7:130:ARG:NH2 | 33:7:340:VAL:HA | 2.15 | 0.62 |
| 33:7:256:LEU:HD12 | 33:7:257:PRO:HA | 1.81 | 0.62 |
| 1:2:582:G:C4 | 1:2:591:G:N2 | 2.67 | 0.62 |
| 1:2:1062:U:C2 | 1:2:1063:G:C8 | 2.86 | 0.62 |
| 1:2:1386:C:H2' | 1:2:1387:A:H8 | 1.65 | 0.62 |
| 1:2:1450:U:H2' | 1:2:1451:G:H5' | 1.80 | 0.62 |
| 7:F:150:GLY:HA3 | 7:F:196:ASN:ND2 | 2.15 | 0.62 |
| 9:H:18:MET:HE1 | 9:H:105:LYS:HB2 | 1.81 | 0.62 |
| 18:Q:27:GLU:OE1 | 18:Q:27:GLU:N | 2.32 | 0.62 |
| 35:9:254:GLY:HA3 | 35:9:261:ILE:HD12 | 1.80 | 0.62 |
| 1:2:263:G:C2 | 1:2:264:G:C8 | 2.88 | 0.62 |
| 1:2:343:U:H4' | 8:G:104:LYS:HE3 | 1.81 | 0.62 |
| 1:2:511:4AC:O7 | 1:2:511:4AC:H5 | 1.99 | 0.62 |
| 1:2:691:G:H2' | 1:2:692:G:H8 | 1.64 | 0.62 |
| 1:2:1453:G:OP2 | 33:7:352:ARG:NH1 | 2.33 | 0.62 |
| 5:D:123:GLN:HE21 | 5:D:127:HIS:CE1 | 2.17 | 0.62 |
| 27:Z:4:GLU:H | 27:Z:4:GLU:CD | 2.03 | 0.62 |
| 33:7:115:ILE:HG12 | 33:7:145:ILE:HB | 1.80 | 0.62 |
| 1:2:185:G:H2' | 1:2:186:G:C8 | 2.35 | 0.62 |
| 1:2:255:A:N1 | 1:2:287:G:O2' | 2.32 | 0.62 |
| 1:2:269:G:O2' | 1:2:270:U:O4' | 2.18 | 0.62 |
| 1:2:458:G:H3' | 1:2:459:G:C8 | 2.35 | 0.62 |
| 1:2:914:G:N2 | 12:K:131:GLN:HE22 | 1.98 | 0.62 |
| 1:2:991:G:H3' | 1:2:992:U:H6 | 1.64 | 0.62 |
| 1:2:1133:U:O5' | 20:S:5:ARG:NH2 | 2.28 | 0.62 |
| 1:2:1219:G:C4 | 1:2:1220:G:C8 | 2.88 | 0.62 |
| 7:F:20:THR:N | 7:F:46:GLU:OE2 | 2.33 | 0.62 |
| 1:2:82:C:H2' | 1:2:83:C:H6 | 1.64 | 0.62 |
| 1:2:485:C:OP1 | 32:6:54:LYS:NZ | 2.30 | 0.62 |
| 1:2:914:G:H21 | 12:K:131:GLN:HE22 | 1.47 | 0.62 |
| 8:G:98:GLU:HB3 | 8:G:101:GLU:OE2 | 2.00 | 0.62 |
| 15:N:84:VAL:HG12 | 15:N:85:THR:H | 1.64 | 0.62 |
| 29:3:101:ILE:HD11 | 29:3:104:PRO:HB3 | 1.80 | 0.62 |
| 33:7:183:VAL:HG11 | 33:7:194:LEU:HB2 | 1.80 | 0.62 |
| 1:2:55:A:C6 | 1:2:315:A:C5 | 2.88 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2:467:G:H2' | 1:2:468:C:O4' | 2.00 | 0.62 |
| 1:2:519:G:H2' | 1:2:520:G:H8 | 1.65 | 0.62 |
| 1:2:648:4AC:N3 | 1:2:677:G:N1 | 2.48 | 0.62 |
| 1:2:1395:G:N3 | 1:2:1449:G:N1 | 2.48 | 0.62 |
| 1:2:1419:C:OP1 | 8:G:64:ARG:NH1 | 2.33 | 0.62 |
| 2:A:132:THR:O | 2:A:135:GLU:N | 2.29 | 0.62 |
| 5:D:58:LEU:O | 5:D:70:ARG:NH2 | 2.29 | 0.62 |
| 33:7:144:LEU:HD23 | 33:7:178:VAL:HG21 | 1.81 | 0.62 |
| 5:D:139:SER:OG | 5:D:142:TYR:HB2 | 2.00 | 0.62 |
| 24:W:30:PHE:HD2 | 24:W:32:HIS:H | 1.47 | 0.62 |
| 1:2:636:4AC:O7 | 1:2:636:4AC:H5 | 2.00 | 0.61 |
| 1:2:1131:A:H62 | 1:2:1151:G:N2 | 1.97 | 0.61 |
| 6:E:86:GLY:N | 6:E:89:ASP:OD2 | 2.24 | 0.61 |
| 6:E:116:SER:OG | 6:E:117:GLU:N | 2.33 | 0.61 |
| 13:L:4:ALA:HA | 13:L:100:LEU:HA | 1.81 | 0.61 |
| 1:2:127:A:OP2 | 1:2:196:G:N2 | 2.30 | 0.61 |
| 1:2:981:C:N3 | 26:Y:37:ARG:NH2 | 2.46 | 0.61 |
| 1:2:1392:A:O2' | 1:2:1393:G:H8 | 1.83 | 0.61 |
| 2:A:11:LYS:O | 2:A:15:LYS:N | 2.28 | 0.61 |
| 19:R:15:LYS:HD2 | 19:R:24:HIS:CD2 | 2.34 | 0.61 |
| 1:2:96:C:H2' | 1:2:97:A:H8 | 1.65 | 0.61 |
| 1:2:718:4AC:C7 | 1:2:719:G:H1 | 2.12 | 0.61 |
| 1:2:996:G:O2' | 1:2:997:C:O4' | 2.18 | 0.61 |
| 1:2:1086:C:H2' | 1:2:1087:C:H6 | 1.65 | 0.61 |
| 3:B:36:ARG:NH2 | 3:B:38:ASP:OD2 | 2.33 | 0.61 |
| 8:G:34:ILE:HG23 | 8:G:63:ILE:HB | 1.83 | 0.61 |
| 16:O:99:ASP:OD1 | 16:O:99:ASP:N | 2.28 | 0.61 |
| 29:3:74:GLU:HG2 | 29:3:75:ILE:H | 1.66 | 0.61 |
| 29:3:85:GLU:N | 29:3:85:GLU:OE1 | 2.32 | 0.61 |
| 33:7:105:LEU:HD21 | 33:7:135:ALA:HB1 | 1.82 | 0.61 |
| 1:2:394:4AC:N4 | 1:2:395:G:O6 | 2.33 | 0.61 |
| 1:2:854:C:H2' | 1:2:855:U:C6 | 2.35 | 0.61 |
| 1:2:1392:A:O2' | 1:2:1393:G:O5' | 2.17 | 0.61 |
| 10:I:55:ASP:N | 10:I:55:ASP:OD1 | 2.32 | 0.61 |
| 33:7:353:ALA:HB1 | 33:7:370:VAL:HG13 | 1.83 | 0.61 |
| 1:2:1217:G:O2' | 22:U:43:ARG:HD2 | 2.00 | 0.61 |
| 2:A:47:ARG:HD3 | 14:M:34:THR:HG21 | 1.82 | 0.61 |
| 31:4:14:A:N6 | 31:4:15:G:N3 | 2.48 | 0.61 |
| 1:2:302:C:H1' | 5:D:2:GLY:N | 2.15 | 0.61 |
| 1:2:303:4AC:HM72 | 1:2:313:G:O6 | 1.99 | 0.61 |
| 1:2:1365:U:H2' | 1:2:1366:G:N7 | 2.15 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:D:135:GLN:OE1 | 5:D:136:ILE:N | 2.33 | 0.61 |
| 7:F:63:GLN:HA | 7:F:89:VAL:HG12 | 1.82 | 0.61 |
| 15:N:6:ALA:HB3 | 15:N:7:PRO:HD3 | 1.81 | 0.61 |
| 23:V:88:ILE:HG13 | 23:V:93:ILE:HD11 | 1.80 | 0.61 |
| 32:6:49:CYS:SG | 32:6:50:ARG:N | 2.74 | 0.61 |
| 1:2:946:G:O2' | 1:2:947:G:OP2 | 2.16 | 0.61 |
| 1:2:1085:C:H2' | 1:2:1086:C:H6 | 1.66 | 0.61 |
| 1:2:1217:G:H4' | 22:U:43:ARG:HE | 1.66 | 0.61 |
| 18:Q:102:ALA:HB2 | 18:Q:125:ILE:HG21 | 1.82 | 0.61 |
| 24:W:45:THR:OG1 | 24:W:47:VAL:O | 2.18 | 0.61 |
| 33:7:148:GLN:OE1 | 34:8:7:TYR:OH | 2.13 | 0.61 |
| 1:2:164:G:H2' | 1:2:165:G:C8 | 2.36 | 0.61 |
| 1:2:208:G:H2' | 1:2:208:G:N3 | 2.15 | 0.61 |
| 1:2:620:U:C5 | 10:I:57:ARG:HB2 | 2.36 | 0.61 |
| 23:V:46:LEU:HB3 | 23:V:71:TYR:CD1 | 2.35 | 0.61 |
| 33:7:325:VAL:HB | 33:7:385:PRO:CB | 2.27 | 0.61 |
| 33:7:382:LEU:HD23 | 33:7:384:ARG:O | 2.00 | 0.61 |
| 1:2:479:4AC:N4 | 1:2:504:G:O6 | 2.30 | 0.61 |
| 1:2:548:U:OP2 | 1:2:725:G:N1 | 2.32 | 0.61 |
| 1:2:790:G:C2 | 1:2:791:G:C8 | 2.88 | 0.61 |
| 1:2:1000:G:H2' | 29:3:38:GLU:OE2 | 2.01 | 0.61 |
| 25:X:67:ILE:HD13 | 25:X:70:ARG:HA | 1.82 | 0.61 |
| 1:2:714:G:N2 | 1:2:716:U:C4 | 2.69 | 0.61 |
| 1:2:1091:U:O2 | 1:2:1254:A:H2' | 2.00 | 0.61 |
| 1:2:1138:G:H1 | 1:2:1146:C:H42 | 1.49 | 0.61 |
| 5:D:17:PRO:HG2 | 5:D:18:TRP:CE3 | 2.36 | 0.61 |
| 7:F:149:GLU:OE2 | 7:F:150:GLY:N | 2.31 | 0.61 |
| 13:L:92:GLU:OE2 | 13:L:92:GLU:N | 2.29 | 0.61 |
| 16:O:33:ILE:O | 16:O:36:ALA:N | 2.31 | 0.61 |
| 17:P:10:LYS:HD3 | 17:P:11:PRO:HD2 | 1.83 | 0.61 |
| 21:T:84:HIS:CD2 | 21:T:86:GLY:H | 2.19 | 0.61 |
| 25:X:67:ILE:HG12 | 25:X:68:LYS:H | 1.66 | 0.61 |
| 29:3:71:GLU:OE1 | 29:3:71:GLU:N | 2.33 | 0.61 |
| 1:2:148:A:C5 | 1:2:149:A:C8 | 2.89 | 0.60 |
| 1:2:247:G:H2' | 1:2:248:G:C8 | 2.37 | 0.60 |
| 1:2:487:G:OP1 | 15:N:92:GLY:N | 2.30 | 0.60 |
| 1:2:1457:G:H2' | 1:2:1458:G:H8 | 1.66 | 0.60 |
| 2:A:73:ASP:OD1 | 2:A:74:VAL:N | 2.34 | 0.60 |
| 11:J:79:ARG:NH1 | 11:J:102:GLU:OE2 | 2.33 | 0.60 |
| 15:N:9:GLY:O | 19:R:62:ARG:NE | 2.33 | 0.60 |
| 31:4:9:G:O4' | 31:4:46:A:H1' | 2.00 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 31:4:76:A:H62 | 33:7:234:LYS:HE2 | 1.66 | 0.60 |
| 1:2:303:4AC:O7 | 1:2:303:4AC:H5 | 2.01 | 0.60 |
| 9:H:22:SER:OG | 9:H:24:GLU:OE1 | 2.19 | 0.60 |
| 13:L:7:LYS:NZ | 13:L:99:GLU:OE1 | 2.25 | 0.60 |
| 26:Y:47:GLU:OE1 | 26:Y:47:GLU:N | 2.33 | 0.60 |
| 1:2:315:A:OP2 | 40:2:1712:HOH:O | 2.16 | 0.60 |
| 1:2:1392:A:O2' | 1:2:1393:G:O4' | 2.19 | 0.60 |
| 10:I:28:LYS:HB3 | 10:I:29:PRO:HD3 | 1.84 | 0.60 |
| 25:X:18:THR:HG22 | 25:X:19:GLY:H | 1.65 | 0.60 |
| 29:3:37:ASN:HD21 | 29:3:62:ILE:HG21 | 1.63 | 0.60 |
| 33:7:19:ASP:H | 39:7:502:GNP:HNB3 | 1.49 | 0.60 |
| 1:2:627:G:C2 | 1:2:628:G:C5 | 2.89 | 0.60 |
| 1:2:666:C:C2 | 1:2:667:U:C5 | 2.90 | 0.60 |
| 1:2:1093:C:H42 | 1:2:1119:C:H41 | 1.48 | 0.60 |
| 1:2:1381:C:H2' | 1:2:1382:A:H8 | 1.65 | 0.60 |
| 1:2:1466:G:N1 | 1:2:1467:UR3:H3U2 | 2.16 | 0.60 |
| 26:Y:39:ALA:HA | 26:Y:45:TYR:O | 2.00 | 0.60 |
| 30:5:811:U:C2 | 30:5:812:G:C8 | 2.88 | 0.60 |
| 1:2:366:G:OP2 | 40:2:1713:HOH:O | 2.16 | 0.60 |
| 1:2:476:G:N1 | 1:2:506:C:N3 | 2.37 | 0.60 |
| 1:2:582:G:N1 | 1:2:583:G:N7 | 2.50 | 0.60 |
| 1:2:911:G:P | 9:H:156:ARG:HH22 | 2.24 | 0.60 |
| 6:E:216:GLU:HG2 | 6:E:217:ASP:O | 2.01 | 0.60 |
| 14:M:133:ARG:HB3 | 14:M:136:ARG:HH11 | 1.66 | 0.60 |
| 31:4:50:U:O2 | 31:4:64:G:O6 | 2.19 | 0.60 |
| 32:6:95:LEU:O | 32:6:98:GLY:N | 2.33 | 0.60 |
| 1:2:69:G:C6 | 1:2:103:G:N1 | 2.70 | 0.60 |
| 1:2:559:G:C6 | 1:2:614:G:C6 | 2.90 | 0.60 |
| 1:2:1279:G:H1 | 1:2:1305:G:HO2' | 1.48 | 0.60 |
| 1:2:1339:C:H2' | 1:2:1340:G:H8 | 1.67 | 0.60 |
| 2:A:23:TYR:HE1 | 2:A:32:GLU:HB2 | 1.67 | 0.60 |
| 14:M:22:SER:HG | 14:M:25:ASN:H | 1.47 | 0.60 |
| 29:3:70:CYS:HA | 29:3:75:ILE:HG21 | 1.82 | 0.60 |
| 1:2:69:G:C4 | 1:2:103:G:N2 | 2.70 | 0.60 |
| 1:2:817:U:P | 2:A:128:ARG:HH22 | 2.24 | 0.60 |
| 1:2:914:G:H2' | 1:2:915:U:C6 | 2.37 | 0.60 |
| 12:K:3:ILE:HG22 | 12:K:20:ARG:HB3 | 1.82 | 0.60 |
| 12:K:7:THR:OG1 | 12:K:8:GLY:N | 2.33 | 0.60 |
| 13:L:10:SER:OG | 13:L:11:THR:N | 2.35 | 0.60 |
| 23:V:86:ILE:HG23 | 23:V:87:LEU:HD12 | 1.82 | 0.60 |
| 28:0:34:ARG:HB3 | 33:7:371:THR:OG1 | 2.01 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2:1353:G:O2' | 1:2:1354:U:O4' | 2.19 | 0.60 |
| 5:D:165:HIS:O | 5:D:168:ARG:N | 2.35 | 0.60 |
| 33:7:240:GLY:O | 33:7:294:LEU:CA | 2.42 | 0.60 |
| 34:8:125:ILE:HD12 | 34:8:134:THR:HG23 | 1.84 | 0.60 |
| 1:2:1221:G:OP1 | 22:U:57:SER:OG | 2.16 | 0.60 |
| 1:2:1491:U:H2' | 1:2:1492:A:H8 | 1.66 | 0.60 |
| 9:H:66:ARG:HA | 9:H:69:ASN:HD21 | 1.66 | 0.60 |
| 15:N:139:LYS:HD2 | 15:N:141:ARG:HH11 | 1.67 | 0.60 |
| 18:Q:90:GLU:OE1 | 18:Q:90:GLU:N | 2.33 | 0.60 |
| 19:R:73:HIS:HA | 19:R:98:LYS:HZ2 | 1.67 | 0.60 |
| 33:7:329:ILE:HG21 | 33:7:386:VAL:HG11 | 1.83 | 0.60 |
| 1:2:886:A:C5 | 1:2:887:G:C8 | 2.89 | 0.60 |
| 1:2:1068:C:OP1 | 3:B:95:ARG:NH2 | 2.35 | 0.60 |
| 1:2:1391:G:H21 | 33:7:352:ARG:NE | 2.00 | 0.60 |
| 33:7:15:VAL:HB | 33:7:132:HIS:ND1 | 2.17 | 0.60 |
| 33:7:68:TYR:HB2 | 33:7:192:ASP:OD1 | 2.02 | 0.60 |
| 1:2:126:A:C6 | 1:2:194:A:N7 | 2.69 | 0.59 |
| 1:2:1316:C:H1' | 12:K:131:GLN:NE2 | 2.17 | 0.59 |
| 7:F:143:PHE:HB2 | 10:I:95:PRO:HB2 | 1.83 | 0.59 |
| 8:G:28:LYS:O | 8:G:32:LYS:NZ | 2.34 | 0.59 |
| 11:J:86:ASN:OD1 | 11:J:87:ARG:N | 2.35 | 0.59 |
| 29:3:23:VAL:HB | 29:3:89:ALA:HB1 | 1.84 | 0.59 |
| 31:4:34:C:C2 | 31:4:35:A:C8 | 2.90 | 0.59 |
| 33:7:58:VAL:HG23 | 33:7:86:LEU:HD11 | 1.83 | 0.59 |
| 33:7:163:TYR:HB2 | 34:8:7:TYR:CZ | 2.36 | 0.59 |
| 1:2:55:A:C6 | 1:2:315:A:C6 | 2.90 | 0.59 |
| 1:2:433:C:H2' | 1:2:434:U:C6 | 2.37 | 0.59 |
| 1:2:1114:G:C2 | 1:2:1115:G:C5 | 2.90 | 0.59 |
| 1:2:1148:G:H2' | 1:2:1149:G:C8 | 2.37 | 0.59 |
| 1:2:1211:C:C2 | 1:2:1310:U:H5 | 2.20 | 0.59 |
| 1:2:1283:G:OP1 | 16:O:116:ARG:NH2 | 2.35 | 0.59 |
| 1:2:1321:G:N7 | 12:K:112:ARG:NE | 2.50 | 0.59 |
| 33:7:327:TRP:NE1 | 33:7:382:LEU:O | 2.29 | 0.59 |
| 1:2:347:G:N1 | 1:2:348:G:N7 | 2.50 | 0.59 |
| 1:2:474:A:C2 | 5:D:18:TRP:NE1 | 2.69 | 0.59 |
| 1:2:648:4AC:O7 | 1:2:648:4AC:H5 | 2.03 | 0.59 |
| 1:2:991:G:C5 | 1:2:992:U:C4 | 2.91 | 0.59 |
| 1:2:1324:C:OP1 | 12:K:124:LYS:NZ | 2.34 | 0.59 |
| 1:2:1452:A:C8 | 33:7:352:ARG:NE | 2.66 | 0.59 |
| 35:9:61:ASN:HB2 | 35:9:62:ARG:HH21 | 1.67 | 0.59 |
| 1:2:666:C:H2' | 1:2:667:U:C6 | 2.37 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2:1171:G:C2 | 1:2:1172:G:C8 | 2.90 | 0.59 |
| 1:2:1235:A:H62 | 1:2:1248:G:H21 | 1.49 | 0.59 |
| 1:2:1453:G:H21 | 33:7:354:LYS:HG3 | 1.68 | 0.59 |
| 1:2:352:U:H3' | 1:2:354:C:N4 | 2.18 | 0.59 |
| 1:2:911:G:C2 | 1:2:912:G:N7 | 2.71 | 0.59 |
| 1:2:1476:A:C5 | 1:2:1499:G:C2 | 2.90 | 0.59 |
| 31:4:60:U:P | 31:4:61:C:H41 | 2.25 | 0.59 |
| 33:7:51:TYR:CE1 | 33:7:90:SER:HB2 | 2.38 | 0.59 |
| 1:2:85:U:H1' | 1:2:89:G:N2 | 2.18 | 0.59 |
| 1:2:637:G:N1 | 1:2:703:4AC:N3 | 2.40 | 0.59 |
| 1:2:825:U:H5 | 1:2:842:U:H5 | 1.49 | 0.59 |
| 1:2:873:G:H2' | 1:2:874:G:H8 | 1.67 | 0.59 |
| 1:2:966:C:H2' | 1:2:967:G:C8 | 2.37 | 0.59 |
| 5:D:130:ILE:HG22 | 5:D:131:GLU:H | 1.68 | 0.59 |
| 18:Q:145:ASP:O | 18:Q:147:ARG:NH1 | 2.35 | 0.59 |
| 1:2:116:A:C5 | 1:2:118:A:C5 | 2.89 | 0.59 |
| 1:2:337:C:OP2 | 11:J:25:LYS:N | 2.36 | 0.59 |
| 1:2:1036:C:H2' | 1:2:1037:G:H8 | 1.66 | 0.59 |
| 6:E:179:PHE:HE2 | 6:E:202:ILE:HD11 | 1.67 | 0.59 |
| 1:2:31:G:C2 | 1:2:32:G:C8 | 2.90 | 0.59 |
| 1:2:1140:G:N2 | 1:2:1143:A:OP2 | 2.32 | 0.59 |
| 1:2:1278:G:H21 | 1:2:1307:A:H62 | 1.48 | 0.59 |
| 1:2:1311:G:P | 9:H:85:PHE:H | 2.26 | 0.59 |
| 1:2:1331:G:N2 | 1:2:1340:G:C4 | 2.71 | 0.59 |
| 3:B:166:LEU:HG | 3:B:170:ILE:HD11 | 1.84 | 0.59 |
| 22:U:56:ALA:O | 22:U:59:LEU:N | 2.36 | 0.59 |
| 35:9:204:LEU:HG | 35:9:217:ILE:HG21 | 1.83 | 0.59 |
| 1:2:126:A:N7 | 1:2:194:A:N6 | 2.51 | 0.59 |
| 1:2:305:U:OP2 | 5:D:8:ARG:NH1 | 2.35 | 0.59 |
| 1:2:1148:G:H2' | 1:2:1149:G:H8 | 1.67 | 0.59 |
| 1:2:1509:U:N3 | 30:5:805:U:O4 | 2.35 | 0.59 |
| 2:A:24:ALA:HB3 | 2:A:31:VAL:H | 1.67 | 0.59 |
| 23:V:33:ARG:HH22 | 23:V:89:ARG:HE | 1.51 | 0.59 |
| 31:4:43:A:H2' | 31:4:44:A:C8 | 2.38 | 0.59 |
| 33:7:323:VAL:HG12 | 33:7:389:TRP:HA | 1.84 | 0.59 |
| 35:9:20:LYS:HD3 | 35:9:30:SER:OG | 2.02 | 0.59 |
| 1:2:162:G:H2' | 1:2:163:G:H8 | 1.67 | 0.59 |
| 1:2:163:G:H5' | 8:G:65:GLY:HA3 | 1.85 | 0.59 |
| 1:2:183:U:O4' | 11:J:121:ASN:ND2 | 2.35 | 0.59 |
| 1:2:437:U:N3 | 1:2:462:U:N3 | 2.50 | 0.59 |
| 1:2:1402:A:H2' | 1:2:1403:G:C8 | 2.37 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:I:90:GLU:OE2 | 10:I:113:HIS:NE2 | 2.36 | 0.59 |
| 21:T:12:THR:OG1 | 21:T:15:GLN:N | 2.23 | 0.59 |
| 25:X:8:PRO:HB2 | 25:X:32:LEU:HD21 | 1.83 | 0.59 |
| 1:2:337:C:H4' | 1:2:338:A:C5' | 2.33 | 0.58 |
| 1:2:1150:A:H3' | 1:2:1151:G:H8 | 1.68 | 0.58 |
| 1:2:1452:A:H2 | 33:7:373:VAL:HB | 1.65 | 0.58 |
| 8:G:87:LEU:HD12 | 8:G:104:LYS:HZ3 | 1.68 | 0.58 |
| 33:7:145:ILE:HD11 | 33:7:202:ILE:HG13 | 1.84 | 0.58 |
| 1:2:638:G:C5 | 1:2:639:G:C8 | 2.91 | 0.58 |
| 1:2:775:G:H8 | 1:2:775:G:OP2 | 1.87 | 0.58 |
| 1:2:955:A:H8 | 1:2:1175:A:C6 | 2.21 | 0.58 |
| 1:2:1505:C:N3 | 30:5:810:G:N1 | 2.51 | 0.58 |
| 3:B:169:TRP:HD1 | 3:B:195:PHE:CE2 | 2.18 | 0.58 |
| 35:9:31:LEU:O | 35:9:36:GLY:CA | 2.51 | 0.58 |
| 1:2:55:A:C5 | 1:2:315:A:C6 | 2.92 | 0.58 |
| 1:2:338:A:H2' | 1:2:341:G:O6 | 2.04 | 0.58 |
| 1:2:390:A:H2' | 1:2:391:A:H8 | 1.68 | 0.58 |
| 1:2:758:G:H2' | 1:2:759:A:H8 | 1.68 | 0.58 |
| 1:2:833:G:H2' | 1:2:834:G:H8 | 1.66 | 0.58 |
| 1:2:1239:4AC:N4 | 1:2:1244:G:O6 | 2.33 | 0.58 |
| 1:2:1279:G:O2' | 1:2:1305:G:N2 | 2.34 | 0.58 |
| 1:2:1396:G:N1 | 1:2:1448:C:H1' | 2.17 | 0.58 |
| 1:2:1481:U:H2' | 1:2:1482:A:C8 | 2.34 | 0.58 |
| 5:D:94:SER:OG | 7:F:161:ARG:NH2 | 2.21 | 0.58 |
| 13:L:83:ARG:O | 13:L:87:ARG:NH1 | 2.37 | 0.58 |
| 24:W:29:VAL:HG12 | 24:W:30:PHE:H | 1.67 | 0.58 |
| 31:4:17:C:H5'' | 31:4:17(A):U:H3' | 1.84 | 0.58 |
| 31:4:29:G:N3 | 31:4:30:G:C8 | 2.71 | 0.58 |
| 1:2:278:C:H2' | 1:2:279:A:C8 | 2.38 | 0.58 |
| 1:2:1117:G:C5 | 1:2:1118:G:N1 | 2.71 | 0.58 |
| 1:2:1492:A:H5'' | 1:2:1493:C:OP2 | 2.03 | 0.58 |
| 2:A:122:ALA:HB2 | 2:A:186:ILE:HG23 | 1.85 | 0.58 |
| 19:R:11:PRO:HB3 | 19:R:23:TRP:CZ3 | 2.37 | 0.58 |
| 27:Z:36:LYS:HB3 | 27:Z:43:LYS:HE3 | 1.84 | 0.58 |
| 33:7:133:PHE:HD1 | 33:7:136:LEU:HD12 | 1.68 | 0.58 |
| 1:2:620:U:O2' | 1:2:621:G:O5' | 2.19 | 0.58 |
| 1:2:803:G:H2' | 1:2:804:G:O4' | 2.03 | 0.58 |
| 1:2:838:C:H2' | 1:2:839:4AC:H5 | 1.84 | 0.58 |
| 1:2:1247:G:C4 | 1:2:1248:G:H1' | 2.38 | 0.58 |
| 1:2:1323:A:H62 | 1:2:1347:G:N2 | 2.01 | 0.58 |
| 1:2:1388:C:H2' | 1:2:1389:C:H6 | 1.67 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:T:93:GLU:N | 21:T:93:GLU:OE2 | 2.37 | 0.58 |
| 1:2:1131:A:N6 | 1:2:1151:G:H22 | 2.00 | 0.58 |
| 1:2:1321:G:O6 | 12:K:10:ARG:NH2 | 2.33 | 0.58 |
| 16:O:105:ASP:HA | 16:O:108:ARG:NH1 | 2.19 | 0.58 |
| 21:T:47:LEU:HD13 | 21:T:67:CYS:SG | 2.43 | 0.58 |
| 30:5:812:G:C2 | 30:5:813:A:C4 | 2.90 | 0.58 |
| 31:4:16:C:H4' | 31:4:60:U:H1' | 1.84 | 0.58 |
| 32:6:42:GLU:HB2 | 32:6:104:PHE:CZ | 2.39 | 0.58 |
| 33:7:28:ALA:HB1 | 33:7:191:ILE:HG13 | 1.86 | 0.58 |
| 33:7:179:PRO:HB3 | 33:7:201:TYR:CE2 | 2.39 | 0.58 |
| 1:2:163:G:H2' | 1:2:164:G:C8 | 2.39 | 0.58 |
| 1:2:1239:4AC:O7 | 1:2:1239:4AC:H5 | 2.03 | 0.58 |
| 9:H:12:PRO:HG3 | 12:K:43:PHE:HE1 | 1.68 | 0.58 |
| 12:K:12:THR:N | 12:K:113:ARG:HH12 | 2.01 | 0.58 |
| 15:N:63:LYS:HG2 | 15:N:118:ASP:O | 2.04 | 0.58 |
| 33:7:357:LEU:HD22 | 33:7:399:ARG:HA | 1.86 | 0.58 |
| 1:2:151:C:N3 | 1:2:165:G:N1 | 2.52 | 0.58 |
| 1:2:470:G:C2 | 1:2:471:G:N7 | 2.71 | 0.58 |
| 1:2:694:G:N2 | 1:2:698:G:C4 | 2.71 | 0.58 |
| 9:H:20:ARG:HB3 | 9:H:21:TRP:CE2 | 2.39 | 0.58 |
| 29:3:27:ARG:NH1 | 29:3:90:ALA:HA | 2.16 | 0.58 |
| 1:2:190:C:H5' | 6:E:155:LYS:HD2 | 1.85 | 0.58 |
| 1:2:488:C:H42 | 1:2:494:C:N4 | 2.01 | 0.58 |
| 1:2:1310:U:O2' | 9:H:85:PHE:O | 2.18 | 0.58 |
| 1:2:1359:G:C6 | 1:2:1360:C:C4 | 2.91 | 0.58 |
| 1:2:1398:G:O2' | 1:2:1399:C:O5' | 2.22 | 0.58 |
| 1:2:1453:G:H1' | 33:7:353:ALA:O | 2.04 | 0.58 |
| 2:A:14:TRP:CD1 | 2:A:15:LYS:HG2 | 2.39 | 0.58 |
| 27:Z:192:GLU:OE1 | 27:Z:192:GLU:N | 2.37 | 0.58 |
| 32:6:55:LEU:C | 32:6:57:ARG:H | 2.07 | 0.58 |
| 35:9:235:ASN:HB2 | 35:9:238:GLU:HB3 | 1.86 | 0.58 |
| 1:2:14:U:H5 | 7:F:184:TRP:CD2 | 2.22 | 0.58 |
| 1:2:81:U:H2' | 1:2:82:C:C6 | 2.39 | 0.58 |
| 1:2:407:C:H2' | 1:2:408:C:C6 | 2.39 | 0.58 |
| 1:2:828:4AC:O7 | 1:2:828:4AC:H5 | 2.04 | 0.58 |
| 1:2:1038:U:O2' | 3:B:103:ASN:OD1 | 2.21 | 0.58 |
| 1:2:1393:G:N3 | 33:7:375:LYS:HE3 | 2.19 | 0.58 |
| 33:7:135:ALA:O | 33:7:139:ILE:HG12 | 2.03 | 0.58 |
| 1:2:140:A:H61 | 1:2:229:G:H1 | 0.64 | 0.57 |
| 1:2:173:C:H2' | 1:2:174:C:H6 | 1.68 | 0.57 |
| 1:2:311:C:H2' | 1:2:312:G:C8 | 2.34 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2:705:G:H2' | 1:2:706:C:H6 | 1.69 | 0.57 |
| 1:2:1292:A:OP2 | 21:T:38:ARG:NH2 | 2.37 | 0.57 |
| 1:2:1446:U:H2' | 1:2:1447:C:C6 | 2.39 | 0.57 |
| 3:B:64:PRO:HB3 | 3:B:179:ARG:HH12 | 1.69 | 0.57 |
| 11:J:89:PHE:O | 11:J:93:ASN:N | 2.37 | 0.57 |
| 20:S:53:TYR:O | 20:S:57:LEU:HG | 2.04 | 0.57 |
| 27:Z:111:ARG:O | 27:Z:115:ALA:CB | 2.52 | 0.57 |
| 31:4:76:A:HO2' | 38:7:501:MET:N | 2.02 | 0.57 |
| 33:7:357:LEU:HD21 | 33:7:399:ARG:HG3 | 1.86 | 0.57 |
| 33:7:361:VAL:O | 33:7:364:SER:N | 2.28 | 0.57 |
| 34:8:3:SER:HB2 | 34:8:6:GLU:HB3 | 1.86 | 0.57 |
| 1:2:314:G:O2' | 5:D:3:ASP:OD1 | 2.22 | 0.57 |
| 1:2:581:C:H2' | 1:2:582:G:C8 | 2.34 | 0.57 |
| 1:2:731:4AC:H2' | 1:2:732:G:H8 | 1.69 | 0.57 |
| 1:2:1136:C:N3 | 1:2:1148:G:N1 | 2.51 | 0.57 |
| 1:2:1378:5HM:H6 | 1:2:1378:5HM:H11 | 1.86 | 0.57 |
| 12:K:104:ARG:NE | 12:K:108:VAL:HG21 | 2.18 | 0.57 |
| 1:2:144:G:N2 | 1:2:145:G:C4 | 2.72 | 0.57 |
| 1:2:336:A:O2' | 1:2:337:C:O5' | 2.21 | 0.57 |
| 1:2:838:C:H2' | 1:2:839:4AC:H6 | 1.86 | 0.57 |
| 1:2:1220:G:O2' | 22:U:10:ASP:OD1 | 2.21 | 0.57 |
| 2:A:46:ASN:HA | 2:A:70:GLN:HE21 | 1.68 | 0.57 |
| 5:D:17:PRO:HG2 | 5:D:18:TRP:CZ3 | 2.38 | 0.57 |
| 14:M:133:ARG:HG2 | 14:M:136:ARG:HD3 | 1.85 | 0.57 |
| 16:O:87:THR:O | 16:O:89:ARG:N | 2.37 | 0.57 |
| 35:9:175:ARG:NH2 | 35:9:234:THR:O | 2.37 | 0.57 |
| 1:2:389:G:N2 | 1:2:393:C:N3 | 2.53 | 0.57 |
| 1:2:474:A:N3 | 5:D:18:TRP:NE1 | 2.41 | 0.57 |
| 1:2:554:G:H1 | 1:2:619:U:H3 | 1.50 | 0.57 |
| 1:2:724:U:O4 | 1:2:725:G:N1 | 2.38 | 0.57 |
| 1:2:732:G:N2 | 1:2:779:G:H1' | 2.20 | 0.57 |
| 1:2:749:A:H5' | 1:2:750:C:OP2 | 2.05 | 0.57 |
| 1:2:1020:A:H62 | 1:2:1174:C:H42 | 1.50 | 0.57 |
| 1:2:1078:C:O2' | 27:Z:156:ASN:ND2 | 2.37 | 0.57 |
| 7:F:114:ILE:HG22 | 7:F:118:LYS:NZ | 2.19 | 0.57 |
| 12:K:28:ILE:O | 12:K:31:LYS:N | 2.29 | 0.57 |
| 21:T:8:TYR:HD2 | 21:T:9:ARG:HG2 | 1.69 | 0.57 |
| 33:7:367:LEU:HD12 | 33:7:368:GLY:H | 1.69 | 0.57 |
| 1:2:951:C:C2 | 1:2:952:C:C6 | 2.92 | 0.57 |
| 8:G:115:GLU:OE1 | 8:G:115:GLU:N | 2.38 | 0.57 |
| 1:2:170:U:O2 | 1:2:211:A:N6 | 2.38 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2:391:A:H4' | 6:E:67:ASN:HD22 | 1.69 | 0.57 |
| 1:2:480:G:C6 | 1:2:504:G:C6 | 2.93 | 0.57 |
| 1:2:1452:A:H2' | 33:7:352:ARG:HB2 | 1.87 | 0.57 |
| 1:2:1460:G:H2' | 1:2:1461:A:N3 | 2.19 | 0.57 |
| 1:2:633:G:O6 | 1:2:707:U:O2 | 2.22 | 0.57 |
| 9:H:215:ARG:OXT | 25:X:62:ARG:NH2 | 2.37 | 0.57 |
| 12:K:47:GLU:OE2 | 12:K:102:TYR:OH | 2.15 | 0.57 |
| 33:7:274:THR:OG1 | 33:7:275:LYS:N | 2.38 | 0.57 |
| 35:9:204:LEU:HD21 | 35:9:246:ILE:HG23 | 1.86 | 0.57 |
| 1:2:155:G:H5'' | 8:G:5:LYS:NZ | 2.20 | 0.57 |
| 1:2:372:A:C5 | 1:2:373:A2M:N7 | 2.72 | 0.57 |
| 1:2:424:C:O2 | 1:2:426:G:N2 | 2.38 | 0.57 |
| 1:2:484:G:H4' | 1:2:485:C:H5'' | 1.87 | 0.57 |
| 8:G:68:ASP:HA | 8:G:116:ILE:HD13 | 1.87 | 0.57 |
| 1:2:179:G:C2 | 1:2:180:G:C8 | 2.93 | 0.57 |
| 1:2:360:G:H4' | 1:2:361:C:OP2 | 2.05 | 0.57 |
| 1:2:735:G:H2' | 1:2:736:G:C8 | 2.38 | 0.57 |
| 1:2:934:G:C2 | 1:2:935:G:C8 | 2.93 | 0.57 |
| 1:2:1385:C:N4 | 1:2:1457:G:O6 | 2.37 | 0.57 |
| 1:2:1467:UR3:H5 | 30:5:820:U:H5' | 1.86 | 0.57 |
| 13:L:43:LYS:O | 13:L:68:ILE:N | 2.28 | 0.57 |
| 22:U:67:PRO:HA | 22:U:119:ARG:O | 2.04 | 0.57 |
| 1:2:64:U:H2' | 1:2:65:G:C8 | 2.39 | 0.57 |
| 5:D:129:HIS:ND1 | 5:D:158:SER:OG | 2.32 | 0.57 |
| 31:4:74:C:H41 | 33:7:33:TRP:HE1 | 1.51 | 0.57 |
| 32:6:55:LEU:HD12 | 32:6:82:ILE:HG22 | 1.87 | 0.57 |
| 33:7:361:VAL:N | 33:7:364:SER:O | 2.38 | 0.57 |
| 1:2:193:G:H21 | 6:E:207:MET:HA | 1.70 | 0.56 |
| 1:2:726:A:C8 | 1:2:727:G:C8 | 2.93 | 0.56 |
| 1:2:860:A:H2 | 1:2:861:G:N2 | 2.02 | 0.56 |
| 1:2:1342:G:P | 13:L:63:ARG:HH12 | 2.27 | 0.56 |
| 2:A:12:ASP:O | 2:A:16:LEU:N | 2.38 | 0.56 |
| 7:F:50:ILE:HD11 | 7:F:118:LYS:HB3 | 1.86 | 0.56 |
| 9:H:17:VAL:HG12 | 9:H:18:MET:HG3 | 1.87 | 0.56 |
| 11:J:75:VAL:HG11 | 11:J:105:ILE:HD13 | 1.87 | 0.56 |
| 20:S:32:LYS:HG3 | 20:S:47:ARG:HH12 | 1.70 | 0.56 |
| 27:Z:111:ARG:O | 27:Z:115:ALA:HB2 | 2.05 | 0.56 |
| 33:7:26:VAL:O | 33:7:30:THR:OG1 | 2.11 | 0.56 |
| 33:7:53:GLU:OE1 | 33:7:88:ARG:NH1 | 2.37 | 0.56 |
| 1:2:426:G:H8 | 1:2:426:G:O5' | 1.89 | 0.56 |
| 1:2:1195:G:C2 | 1:2:1196:G:C8 | 2.93 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2:1328:C:H2' | 1:2:1329:G:C8 | 2.38 | 0.56 |
| 7:F:50:ILE:HG13 | 7:F:51:ASP:N | 2.20 | 0.56 |
| 7:F:114:ILE:HG22 | 7:F:118:LYS:HZ1 | 1.70 | 0.56 |
| 16:O:80:ASN:HB2 | 16:O:92:HIS:ND1 | 2.20 | 0.56 |
| 33:7:364:SER:HB3 | 33:7:384:ARG:NH1 | 2.20 | 0.56 |
| 1:2:17:4AC:O7 | 1:2:17:4AC:H5 | 2.04 | 0.56 |
| 1:2:651:G:C6 | 1:2:652:G:C2 | 2.94 | 0.56 |
| 1:2:690:U:O4 | 30:5:808:A:O2' | 2.23 | 0.56 |
| 1:2:891:U:H2' | 1:2:892:U:H6 | 1.70 | 0.56 |
| 1:2:935:G:O2' | 1:2:1173:U:OP1 | 2.18 | 0.56 |
| 1:2:1002:C:H2' | 1:2:1003:G:C8 | 2.39 | 0.56 |
| 1:2:1411:C:O2' | 11:J:31:GLU:OE1 | 2.22 | 0.56 |
| 1:2:1443:G:H2' | 1:2:1444:G:C8 | 2.40 | 0.56 |
| 1:2:1466:G:C6 | 1:2:1467:UR3:H3U2 | 2.40 | 0.56 |
| 1:2:1493:C:N4 | 1:2:1494:G:O6 | 2.39 | 0.56 |
| 2:A:111:THR:HA | 2:A:117:LYS:HA | 1.86 | 0.56 |
| 7:F:144:THR:HG22 | 7:F:157:ILE:HA | 1.86 | 0.56 |
| 9:H:215:ARG:NH1 | 25:X:59:GLU:OE1 | 2.37 | 0.56 |
| 29:3:40:THR:HG23 | 29:3:41:LYS:H | 1.70 | 0.56 |
| 33:7:256:LEU:HD23 | 33:7:315:ILE:HD11 | 1.88 | 0.56 |
| 1:2:190:C:H2' | 1:2:191:U:C6 | 2.40 | 0.56 |
| 1:2:382:A:C2 | 1:2:383:A:C8 | 2.94 | 0.56 |
| 4:C:16:SER:OG | 4:C:46:CYS:HB3 | 2.05 | 0.56 |
| 7:F:166:VAL:HG11 | 7:F:184:TRP:HD1 | 1.71 | 0.56 |
| 12:K:10:ARG:NH1 | 12:K:110:ASP:OD2 | 2.38 | 0.56 |
| 12:K:26:VAL:HA | 12:K:62:ILE:O | 2.05 | 0.56 |
| 23:V:18:GLU:OE1 | 23:V:18:GLU:N | 2.34 | 0.56 |
| 33:7:318:LEU:HB2 | 33:7:321:ALA:HB2 | 1.87 | 0.56 |
| 1:2:79:C:H2' | 1:2:80:G:H8 | 1.69 | 0.56 |
| 1:2:240:G:C2 | 1:2:241:G:C8 | 2.93 | 0.56 |
| 1:2:267:G:C2 | 1:2:268:G:C6 | 2.94 | 0.56 |
| 1:2:323:G:H2' | 1:2:324:A:H8 | 1.69 | 0.56 |
| 1:2:338:A:C6 | 1:2:341:G:C2 | 2.93 | 0.56 |
| 2:A:12:ASP:CG | 35:9:22:VAL:HB | 2.26 | 0.56 |
| 6:E:20:TYR:HB2 | 6:E:52:TYR:OH | 2.06 | 0.56 |
| 9:H:137:THR:OG1 | 9:H:138:SER:N | 2.38 | 0.56 |
| 22:U:22:GLU:N | 22:U:22:GLU:OE1 | 2.38 | 0.56 |
| 24:W:17:ARG:HD2 | 24:W:28:ILE:HG12 | 1.88 | 0.56 |
| 27:Z:39:PRO:O | 27:Z:40:LEU:HG | 2.05 | 0.56 |
| 33:7:269:TYR:CD1 | 33:7:385:PRO:HD2 | 2.40 | 0.56 |
| 1:2:79:C:H2' | 1:2:80:G:C8 | 2.41 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:2:868:4AC:O7 | 1:2:868:4AC:H5 | 2.05 | 0.56 |
| 1:2:1290:G:O2' | 1:2:1292:A:N7 | 2.30 | 0.56 |
| 1:2:1345:G:C4 | 1:2:1346:C:C5 | 2.93 | 0.56 |
| 1:2:1506:U:H2' | 1:2:1507:C:C6 | 2.40 | 0.56 |
| 12:K:22:GLY:HA3 | 12:K:61:ASP:CG | 2.26 | 0.56 |
| 14:M:43:SER:HB2 | 14:M:46:MET:HG3 | 1.88 | 0.56 |
| 32:6:72:TRP:O | 32:6:74:VAL:N | 2.38 | 0.56 |
| 1:2:243:C:H2' | 1:2:244:G:H8 | 1.70 | 0.56 |
| 1:2:536:C:H2' | 1:2:537:U:C6 | 2.40 | 0.56 |
| 1:2:710:A:H2' | 1:2:711:A:C8 | 2.39 | 0.56 |
| 1:2:1065:U:OP2 | 3:B:95:ARG:HD3 | 2.06 | 0.56 |
| 1:2:1319:U:N3 | 1:2:1351:A:H2 | 2.04 | 0.56 |
| 3:B:138:VAL:HG23 | 3:B:152:LEU:HD23 | 1.87 | 0.56 |
| 31:4:76:A:N6 | 33:7:278:SER:HB2 | 2.20 | 0.56 |
| 35:9:15:LEU:HD11 | 35:9:31:LEU:HD22 | 1.87 | 0.56 |
| 1:2:145:G:N2 | 1:2:146:A:N1 | 2.53 | 0.56 |
| 1:2:286:4AC:O7 | 1:2:286:4AC:H5 | 2.04 | 0.56 |
| 1:2:441:G:H2' | 1:2:442:A:H8 | 1.71 | 0.56 |
| 1:2:442:A:H2' | 1:2:443:G:C8 | 2.41 | 0.56 |
| 1:2:445:G:OP2 | 23:V:33:ARG:NH1 | 2.38 | 0.56 |
| 1:2:691:G:H2' | 1:2:692:G:C8 | 2.41 | 0.56 |
| 1:2:695:A:H2' | 1:2:696:A:H8 | 1.70 | 0.56 |
| 1:2:717:C:OP2 | 18:Q:16:ARG:NH2 | 2.39 | 0.56 |
| 1:2:1121:C:O2 | 12:K:16:ARG:NH1 | 2.38 | 0.56 |
| 1:2:1234:G:HO2' | 1:2:1257:C:HO2' | 1.54 | 0.56 |
| 1:2:1323:A:H62 | 1:2:1347:G:H21 | 1.54 | 0.56 |
| 8:G:62:GLU:OE1 | 8:G:62:GLU:N | 2.39 | 0.56 |
| 9:H:44:LEU:HD12 | 9:H:45:PRO:HD2 | 1.88 | 0.56 |
| 12:K:34:GLU:OE1 | 22:U:150:TYR:OH | 2.24 | 0.56 |
| 22:U:21:LYS:HA | 22:U:52:TYR:HE1 | 1.71 | 0.56 |
| 33:7:194:LEU:O | 33:7:198:ILE:HG12 | 2.06 | 0.56 |
| 1:2:140:A:N6 | 1:2:229:G:N1 | 2.16 | 0.56 |
| 1:2:748:A:N6 | 1:2:769:A:N3 | 2.54 | 0.56 |
| 1:2:814:A:H1' | 2:A:134:GLN:NE2 | 2.20 | 0.56 |
| 1:2:1068:C:C4 | 1:2:1069:G:N7 | 2.74 | 0.56 |
| 1:2:1449:G:H2' | 1:2:1450:U:O4' | 2.06 | 0.56 |
| 7:F:66:LEU:HD11 | 7:F:174:ILE:HD11 | 1.88 | 0.56 |
| 12:K:41:ALA:O | 12:K:44:THR:N | 2.29 | 0.56 |
| 19:R:59:LYS:HG2 | 19:R:60:TYR:CE2 | 2.41 | 0.56 |
| 25:X:33:GLU:HA | 25:X:37:LYS:HG3 | 1.88 | 0.56 |
| 34:8:127:CYS:SG | 34:8:128:LEU:N | 2.78 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:2:516:G:C2 | 1:2:517:G:C8 | 2.94 | 0.56 |
| 1:2:1319:U:C2 | 1:2:1351:A:H2 | 2.24 | 0.56 |
| 12:K:10:ARG:HD3 | 12:K:76:GLU:HB3 | 1.86 | 0.56 |
| 25:X:12:ILE:HG12 | 25:X:29:VAL:HA | 1.88 | 0.56 |
| 26:Y:10:VAL:HG23 | 26:Y:15:VAL:HG12 | 1.88 | 0.56 |
| 31:4:3:C:H2' | 31:4:4:G:O4' | 2.05 | 0.56 |
| 33:7:275:LYS:HB2 | 33:7:300:TYR:CE2 | 2.40 | 0.56 |
| 35:9:123:GLU:HA | 35:9:127:TRP:HD1 | 1.71 | 0.56 |
| 1:2:185:G:C4 | 1:2:186:G:C8 | 2.94 | 0.55 |
| 1:2:437:U:O2 | 1:2:462:U:O2 | 2.23 | 0.55 |
| 1:2:1079:C:O2' | 17:P:56:GLU:OE2 | 2.11 | 0.55 |
| 1:2:1321:G:N2 | 1:2:1347:G:H2' | 2.20 | 0.55 |
| 1:2:1356:C:H2' | 1:2:1357:C:H6 | 1.71 | 0.55 |
| 9:H:98:VAL:HG22 | 12:K:40:ILE:HD11 | 1.87 | 0.55 |
| 33:7:14:VAL:HG12 | 33:7:115:ILE:HB | 1.89 | 0.55 |
| 1:2:868:4AC:H2' | 1:2:869:G:H8 | 1.71 | 0.55 |
| 1:2:1133:U:OP1 | 20:S:5:ARG:NE | 2.29 | 0.55 |
| 1:2:1453:G:C4 | 33:7:352:ARG:HD2 | 2.41 | 0.55 |
| 2:A:108:PHE:CE1 | 2:A:143:GLN:HB2 | 2.41 | 0.55 |
| 6:E:217:ASP:N | 6:E:217:ASP:OD1 | 2.38 | 0.55 |
| 9:H:28:VAL:HG12 | 9:H:124:VAL:HG13 | 1.88 | 0.55 |
| 11:J:88:GLN:HB2 | 11:J:91:ARG:NH2 | 2.20 | 0.55 |
| 31:4:10:G:H2' | 31:4:11:A:H8 | 1.70 | 0.55 |
| 1:2:838:C:H2' | 1:2:839:4AC:C5 | 2.37 | 0.55 |
| 1:2:845:G:C6 | 1:2:846:C:N4 | 2.75 | 0.55 |
| 1:2:1130:G:N7 | 20:S:44:LYS:NZ | 2.55 | 0.55 |
| 1:2:1334:A:P | 17:P:32:ARG:HH22 | 2.29 | 0.55 |
| 4:C:13:VAL:HG22 | 4:C:20:GLU:HB3 | 1.87 | 0.55 |
| 16:O:84:ASP:HB3 | 16:O:87:THR:O | 2.05 | 0.55 |
| 28:0:34:ARG:CZ | 33:7:381:GLU:HB2 | 2.35 | 0.55 |
| 29:3:4:PRO:HG3 | 29:3:55:GLU:HB3 | 1.87 | 0.55 |
| 33:7:6:VAL:HG11 | 33:7:87:ARG:HH21 | 1.71 | 0.55 |
| 33:7:50:GLY:N | 33:7:93:ASP:O | 2.25 | 0.55 |
| 33:7:130:ARG:HH12 | 33:7:338:ARG:HE | 1.54 | 0.55 |
| 1:2:56:C:OP2 | 1:2:374:A:N6 | 2.30 | 0.55 |
| 1:2:923:G:O2' | 1:2:942:C:O2' | 2.25 | 0.55 |
| 1:2:1396:G:N2 | 1:2:1448:C:H1' | 2.22 | 0.55 |
| 5:D:70:ARG:HD3 | 5:D:89:LEU:HD22 | 1.87 | 0.55 |
| 22:U:25:GLU:HG3 | 22:U:108:ALA:HA | 1.89 | 0.55 |
| 1:2:523:A:H2' | 1:2:524:C:O4' | 2.05 | 0.55 |
| 1:2:541:G:C2 | 1:2:788:G:C8 | 2.93 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2:832:G:H2' | 1:2:833:G:H8 | 1.72 | 0.55 |
| 1:2:1263:A:O2' | 9:H:96:LYS:HE3 | 2.07 | 0.55 |
| 1:2:1403:G:H2' | 1:2:1404:G:O4' | 2.07 | 0.55 |
| 5:D:163:PRO:HA | 5:D:168:ARG:HD2 | 1.87 | 0.55 |
| 11:J:42:LYS:O | 11:J:58:THR:OG1 | 2.23 | 0.55 |
| 13:L:10:SER:HB2 | 13:L:94:VAL:HG22 | 1.87 | 0.55 |
| 21:T:25:ALA:HB1 | 21:T:33:ARG:HG3 | 1.88 | 0.55 |
| 28:O:29:GLN:O | 28:O:33:GLU:N | 2.23 | 0.55 |
| 31:4:64:G:H2' | 31:4:65:C:O4' | 2.07 | 0.55 |
| 33:7:24:THR:HG23 | 33:7:27:GLN:OE1 | 2.06 | 0.55 |
| 1:2:178:A:C2 | 1:2:179:G:H1' | 2.41 | 0.55 |
| 1:2:237:A:H2' | 1:2:238:U:C6 | 2.42 | 0.55 |
| 1:2:607:A:C5 | 1:2:608:U:C4 | 2.95 | 0.55 |
| 1:2:1247:G:C2 | 1:2:1248:G:H1' | 2.41 | 0.55 |
| 33:7:255:VAL:HG12 | 33:7:272:ILE:HB | 1.89 | 0.55 |
| 33:7:259:LEU:O | 33:7:270:GLU:N | 2.39 | 0.55 |
| 1:2:1202:5MC:H3' | 16:O:136:ARG:HH12 | 1.71 | 0.55 |
| 1:2:1388:C:H2' | 1:2:1389:C:C6 | 2.42 | 0.55 |
| 1:2:1470:C:C4 | 1:2:1473:G:C6 | 2.94 | 0.55 |
| 6:E:168:VAL:HB | 6:E:169:PRO:HD3 | 1.87 | 0.55 |
| 10:I:52:PHE:HE1 | 10:I:54:ASP:HB2 | 1.72 | 0.55 |
| 21:T:83:VAL:HG12 | 21:T:84:HIS:N | 2.21 | 0.55 |
| 23:V:74:ASP:OD2 | 23:V:77:ARG:N | 2.26 | 0.55 |
| 27:Z:83:GLN:HG3 | 27:Z:84:GLU:H | 1.71 | 0.55 |
| 31:4:34:C:H2' | 31:4:35:A:H8 | 1.71 | 0.55 |
| 31:4:76:A:H61 | 33:7:278:SER:HB2 | 1.71 | 0.55 |
| 1:2:237:A:H2' | 1:2:238:U:H6 | 1.72 | 0.55 |
| 1:2:310:G:O3' | 19:R:59:LYS:NZ | 2.23 | 0.55 |
| 1:2:320:G:C2 | 1:2:321:G:C8 | 2.95 | 0.55 |
| 1:2:519:G:H2' | 1:2:520:G:C8 | 2.42 | 0.55 |
| 1:2:727:G:C6 | 1:2:728:G:H1' | 2.42 | 0.55 |
| 1:2:810:U:H3' | 1:2:812:C:N4 | 2.22 | 0.55 |
| 7:F:130:SER:HB2 | 7:F:158:PRO:HB2 | 1.89 | 0.55 |
| 8:G:3:THR:OG1 | 8:G:21:ILE:O | 2.16 | 0.55 |
| 8:G:54:GLU:N | 8:G:54:GLU:OE1 | 2.40 | 0.55 |
| 33:7:51:TYR:HE1 | 33:7:90:SER:HB2 | 1.70 | 0.55 |
| 34:8:12:ASP:OD1 | 34:8:13:ARG:N | 2.39 | 0.55 |
| 1:2:82:C:H2' | 1:2:83:C:C6 | 2.42 | 0.55 |
| 1:2:183:U:H2' | 1:2:184:G:C8 | 2.38 | 0.55 |
| 1:2:927:U:H2' | 1:2:928:U:C6 | 2.42 | 0.55 |
| 6:E:40:ARG:HH22 | 6:E:189:GLN:CD | 2.09 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:T:80:THR:OG1 | 21:T:93:GLU:HG3 | 2.07 | 0.55 |
| 25:X:63:GLU:N | 25:X:63:GLU:OE2 | 2.39 | 0.55 |
| 29:3:39:THR:HG21 | 29:3:100:ALA:HB3 | 1.88 | 0.55 |
| 33:7:276:ILE:HG23 | 33:7:297:ILE:HG23 | 1.89 | 0.55 |
| 1:2:162:G:O2' | 8:G:120:ASN:ND2 | 2.39 | 0.55 |
| 1:2:368:C:H2' | 1:2:369:G:H8 | 1.72 | 0.55 |
| 1:2:563:G:N2 | 10:I:124:ARG:HH21 | 2.05 | 0.55 |
| 1:2:1429:U:H2' | 1:2:1430:C:C6 | 2.42 | 0.55 |
| 1:2:1440:C:H2' | 1:2:1441:U:C5 | 2.41 | 0.55 |
| 31:4:9:G:H21 | 31:4:45:G:H2' | 1.71 | 0.55 |
| 32:6:38:ASP:OD1 | 32:6:48:ARG:HG2 | 2.06 | 0.55 |
| 1:2:236:G:C6 | 1:2:237:A:C5 | 2.95 | 0.54 |
| 1:2:512:G:OP2 | 5:D:38:LYS:N | 2.32 | 0.54 |
| 1:2:572:G:C2 | 1:2:598:U:C4 | 2.95 | 0.54 |
| 1:2:722:G:OP2 | 18:Q:131:ARG:NH1 | 2.32 | 0.54 |
| 1:2:867:C:H5 | 1:2:868:4AC:C7 | 2.21 | 0.54 |
| 1:2:869:G:N2 | 1:2:871:A:OP1 | 2.40 | 0.54 |
| 1:2:879:A:H2' | 1:2:880:A:C8 | 2.37 | 0.54 |
| 1:2:941:A:C5 | 1:2:942:C:N3 | 2.75 | 0.54 |
| 1:2:946:G:OP2 | 17:P:40:ARG:NE | 2.33 | 0.54 |
| 1:2:1035:U:OP1 | 7:F:80:ARG:NH1 | 2.40 | 0.54 |
| 3:B:13:LEU:HG | 3:B:18:HIS:HE1 | 1.71 | 0.54 |
| 6:E:179:PHE:CE2 | 6:E:202:ILE:HD11 | 2.42 | 0.54 |
| 1:2:858:G:H2' | 1:2:859:G:C8 | 2.42 | 0.54 |
| 1:2:1310:U:H4' | 1:2:1311:G:O5' | 2.07 | 0.54 |
| 1:2:1380:U:H2' | 1:2:1381:C:H6 | 1.71 | 0.54 |
| 9:H:10:PHE:H | 12:K:42:ARG:HH12 | 1.53 | 0.54 |
| 16:O:7:ILE:HD13 | 16:O:16:ASP:HA | 1.89 | 0.54 |
| 18:Q:120:ARG:NH1 | 18:Q:124:LEU:HD11 | 2.23 | 0.54 |
| 21:T:52:ARG:O | 21:T:56:LYS:N | 2.40 | 0.54 |
| 29:3:23:VAL:HG12 | 29:3:90:ALA:HB2 | 1.89 | 0.54 |
| 30:5:813:A:C6 | 30:5:814:U:C4 | 2.94 | 0.54 |
| 31:4:6:G:C2 | 31:4:7:G:H1' | 2.42 | 0.54 |
| 32:6:77:ASP:H | 32:6:79:ARG:NH1 | 2.06 | 0.54 |
| 33:7:17:HIS:HB3 | 33:7:20:HIS:CE1 | 2.43 | 0.54 |
| 33:7:213:PRO:HB3 | 33:7:246:LEU:H | 1.71 | 0.54 |
| 33:7:248:LYS:O | 33:7:251:GLN:HB2 | 2.07 | 0.54 |
| 1:2:22:G:H4' | 7:F:79:ARG:HH21 | 1.71 | 0.54 |
| 1:2:471:G:C6 | 1:2:472:G:C6 | 2.96 | 0.54 |
| 1:2:484:G:N2 | 1:2:495:G:O6 | 2.38 | 0.54 |
| 1:2:695:A:C2 | 1:2:696:A:C5 | 2.95 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:2:1022:G:C6 | 1:2:1178:A:N1 | 2.76 | 0.54 |
| 1:2:1113:G:C2 | 1:2:1114:G:C5 | 2.94 | 0.54 |
| 5:D:162:ASN:O | 5:D:164:GLN:N | 2.34 | 0.54 |
| 7:F:35:HIS:ND1 | 7:F:36:GLU:HG3 | 2.22 | 0.54 |
| 9:H:38:ASN:OD1 | 9:H:39:LEU:N | 2.40 | 0.54 |
| 1:2:546:4AC:O7 | 1:2:546:4AC:H5 | 2.07 | 0.54 |
| 1:2:657:G:O5' | 1:2:657:G:H8 | 1.91 | 0.54 |
| 1:2:738:C:C2 | 1:2:776:G:N2 | 2.75 | 0.54 |
| 1:2:1041:4AC:O2 | 1:2:1047:G:N2 | 2.40 | 0.54 |
| 7:F:179:GLY:O | 7:F:181:GLN:HG3 | 2.07 | 0.54 |
| 8:G:98:GLU:CD | 8:G:99:LYS:H | 2.10 | 0.54 |
| 14:M:98:ALA:O | 14:M:102:ILE:HG22 | 2.07 | 0.54 |
| 32:6:23:GLN:HE22 | 32:6:68:ILE:HD12 | 1.72 | 0.54 |
| 33:7:135:ALA:O | 33:7:138:ILE:HB | 2.08 | 0.54 |
| 1:2:69:G:C6 | 1:2:70:U:C4 | 2.96 | 0.54 |
| 1:2:1266:C:H2' | 1:2:1267:G:C8 | 2.41 | 0.54 |
| 1:2:1292:A:H5' | 21:T:41:THR:HG21 | 1.88 | 0.54 |
| 1:2:1448:C:O2' | 1:2:1449:G:O5' | 2.22 | 0.54 |
| 2:A:27:PHE:HZ | 2:A:83:PHE:HB2 | 1.73 | 0.54 |
| 3:B:54:VAL:HA | 3:B:57:LYS:HG2 | 1.90 | 0.54 |
| 18:Q:104:ASN:OD1 | 18:Q:104:ASN:N | 2.40 | 0.54 |
| 19:R:19:PRO:O | 19:R:26:HIS:N | 2.31 | 0.54 |
| 26:Y:8:TYR:HB3 | 26:Y:17:ARG:HG3 | 1.88 | 0.54 |
| 33:7:254:LYS:HB3 | 33:7:319:ALA:HA | 1.89 | 0.54 |
| 34:8:33:MET:HA | 34:8:46:ASN:HD21 | 1.72 | 0.54 |
| 35:9:245:GLN:OE1 | 35:9:249:ASN:ND2 | 2.40 | 0.54 |
| 1:2:123:G:C4' | 19:R:32:ARG:HH21 | 2.20 | 0.54 |
| 1:2:1419:C:C2' | 1:2:1420:U:H5' | 2.38 | 0.54 |
| 1:2:1506:U:O2 | 30:5:809:G:C2 | 2.61 | 0.54 |
| 33:7:162:GLN:NE2 | 33:7:165:GLN:OE1 | 2.41 | 0.54 |
| 1:2:346:A:H2' | 1:2:347:G:O4' | 2.08 | 0.54 |
| 1:2:624:A:O2' | 18:Q:94:ASP:OD1 | 2.17 | 0.54 |
| 1:2:687:C:O2' | 1:2:688:A:OP1 | 2.21 | 0.54 |
| 1:2:897:G:H22 | 30:5:818:A:H3' | 1.73 | 0.54 |
| 1:2:955:A:H8 | 1:2:1175:A:N1 | 2.06 | 0.54 |
| 16:O:80:ASN:HB2 | 16:O:92:HIS:CE1 | 2.42 | 0.54 |
| 20:S:27:ASP:OD1 | 20:S:29:GLU:N | 2.33 | 0.54 |
| 33:7:52:ALA:HB3 | 33:7:91:PHE:HB2 | 1.90 | 0.54 |
| 35:9:242:ALA:O | 35:9:245:GLN:NE2 | 2.40 | 0.54 |
| 1:2:643:A:C6 | 1:2:644:C:C4 | 2.96 | 0.54 |
| 1:2:839:4AC:H5 | 1:2:839:4AC:O7 | 2.08 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2:964:G:N1 | 1:2:1186:A:OP2 | 2.38 | 0.54 |
| 1:2:1212:A:N7 | 1:2:1275:U:N3 | 2.56 | 0.54 |
| 22:U:131:LYS:O | 22:U:134:THR:OG1 | 2.24 | 0.54 |
| 29:3:18:LYS:O | 29:3:110:LEU:HB3 | 2.08 | 0.54 |
| 31:4:75:C:H2' | 31:4:76:A:H5' | 1.90 | 0.54 |
| 33:7:15:VAL:HB | 33:7:132:HIS:CG | 2.43 | 0.54 |
| 1:2:98:C:H2' | 1:2:99:C:C6 | 2.43 | 0.54 |
| 1:2:1362:C:H2' | 1:2:1363:C:H6 | 1.72 | 0.54 |
| 1:2:1419:C:H2' | 1:2:1420:U:H5' | 1.90 | 0.54 |
| 6:E:10:LEU:HD12 | 6:E:11:LYS:H | 1.73 | 0.54 |
| 18:Q:105:LEU:HD23 | 18:Q:122:LEU:HD12 | 1.90 | 0.54 |
| 31:4:38:A:C5 | 31:4:39:C:C6 | 2.96 | 0.54 |
| 33:7:224:ASN:HB3 | 33:7:228:THR:HG21 | 1.89 | 0.54 |
| 35:9:194:GLU:OE2 | 35:9:197:LYS:NZ | 2.36 | 0.54 |
| 1:2:174:C:H2' | 1:2:175:C:H6 | 1.73 | 0.54 |
| 1:2:244:G:C2 | 1:2:245:G:N7 | 2.75 | 0.54 |
| 1:2:554:G:H2' | 1:2:555:G:C8 | 2.40 | 0.54 |
| 1:2:815:G:H2' | 1:2:816:C:H6 | 1.73 | 0.54 |
| 1:2:861:G:N7 | 28:0:2:LYS:HG2 | 2.23 | 0.54 |
| 1:2:924:C:H4' | 1:2:936:A:H61 | 1.72 | 0.54 |
| 1:2:1453:G:C6 | 33:7:352:ARG:HD2 | 2.42 | 0.54 |
| 1:2:1480:G:H2' | 1:2:1481:U:C6 | 2.42 | 0.54 |
| 3:B:75:TYR:CZ | 3:B:161:ARG:HD3 | 2.42 | 0.54 |
| 33:7:244:GLN:N | 33:7:244:GLN:OE1 | 2.41 | 0.54 |
| 1:2:632:A:H5' | 1:2:633:G:OP2 | 2.08 | 0.53 |
| 1:2:639:G:C6 | 1:2:640:G:N7 | 2.76 | 0.53 |
| 1:2:1048:C:O2 | 1:2:1048:C:H2' | 2.08 | 0.53 |
| 1:2:1479:4AC:OP2 | 28:0:15:ARG:NE | 2.39 | 0.53 |
| 1:2:1491:U:H5'' | 14:M:136:ARG:HH22 | 1.72 | 0.53 |
| 3:B:188:PHE:CE1 | 3:B:190:ILE:HD13 | 2.43 | 0.53 |
| 29:3:118:VAL:HA | 29:3:121:LEU:HD12 | 1.89 | 0.53 |
| 32:6:67:VAL:HG11 | 32:6:82:ILE:HG12 | 1.88 | 0.53 |
| 1:2:193:G:H2' | 1:2:194:A:O4' | 2.08 | 0.53 |
| 1:2:436:U:C4 | 1:2:437:U:C6 | 2.96 | 0.53 |
| 1:2:1393:G:O2' | 33:7:375:LYS:HD2 | 2.09 | 0.53 |
| 21:T:98:MET:HA | 21:T:101:HIS:CD2 | 2.43 | 0.53 |
| 26:Y:21:PHE:HB3 | 26:Y:28:GLY:H | 1.74 | 0.53 |
| 33:7:272:ILE:HD13 | 33:7:305:LEU:HD11 | 1.90 | 0.53 |
| 1:2:46:G:O6 | 1:2:412:A:N6 | 2.41 | 0.53 |
| 1:2:518:U:C2 | 1:2:519:G:C8 | 2.96 | 0.53 |
| 1:2:779:G:O6 | 40:2:1714:HOH:O | 2.18 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2:911:G:C2 | 1:2:912:G:C8 | 2.97 | 0.53 |
| 1:2:1184:4AC:O7 | 1:2:1184:4AC:H5 | 2.09 | 0.53 |
| 1:2:1333:C:OP1 | 17:P:19:ARG:NH2 | 2.41 | 0.53 |
| 1:2:1341:C:H3' | 12:K:122:SER:HB3 | 1.90 | 0.53 |
| 1:2:1459:A:N6 | 1:2:1460:G:O6 | 2.41 | 0.53 |
| 3:B:171:LEU:O | 3:B:175:ILE:N | 2.41 | 0.53 |
| 8:G:48:ASN:HD21 | 8:G:55:PHE:HB2 | 1.72 | 0.53 |
| 31:4:50:U:H2' | 31:4:51:C:C6 | 2.44 | 0.53 |
| 1:2:158:A:C5 | 1:2:159:A:C5 | 2.96 | 0.53 |
| 1:2:918:A:O2' | 1:2:1307:A:N3 | 2.38 | 0.53 |
| 1:2:923:G:OP2 | 16:O:130:ARG:NH1 | 2.42 | 0.53 |
| 1:2:1064:G:H2' | 1:2:1065:U:H6 | 1.73 | 0.53 |
| 1:2:1339:C:H2' | 1:2:1340:G:C8 | 2.43 | 0.53 |
| 3:B:142:ASP:HB2 | 3:B:158:ASN:ND2 | 2.24 | 0.53 |
| 33:7:98:GLU:HG2 | 33:7:406:ARG:NH1 | 2.24 | 0.53 |
| 33:7:122:GLU:HG2 | 33:7:126:GLN:HG3 | 1.90 | 0.53 |
| 1:2:182:C:H4' | 11:J:117:ASP:OD2 | 2.09 | 0.53 |
| 1:2:1014:A:H2 | 1:2:1175:A:N3 | 2.07 | 0.53 |
| 1:2:1020:A:N6 | 1:2:1180:G:C6 | 2.77 | 0.53 |
| 1:2:1406:G:O2' | 1:2:1437:A:N6 | 2.41 | 0.53 |
| 8:G:94:PHE:CZ | 8:G:96:PRO:HA | 2.44 | 0.53 |
| 10:I:106:THR:HG23 | 10:I:108:GLN:H | 1.72 | 0.53 |
| 18:Q:98:LEU:HB3 | 18:Q:129:ILE:HD11 | 1.90 | 0.53 |
| 24:W:17:ARG:HG2 | 24:W:64:LEU:CD2 | 2.39 | 0.53 |
| 33:7:392:ASN:N | 33:7:413:VAL:O | 2.33 | 0.53 |
| 1:2:50:G:N2 | 1:2:408:C:C2 | 2.77 | 0.53 |
| 1:2:64:U:H2' | 1:2:65:G:H8 | 1.73 | 0.53 |
| 1:2:246:C:H2' | 1:2:247:G:C8 | 2.43 | 0.53 |
| 1:2:330:A:C6 | 1:2:342:G:C6 | 2.96 | 0.53 |
| 1:2:394:4AC:O7 | 1:2:394:4AC:H5 | 2.09 | 0.53 |
| 1:2:614:G:C2 | 1:2:615:G:C8 | 2.97 | 0.53 |
| 1:2:851:4AC:O2' | 1:2:852:G:H5' | 2.08 | 0.53 |
| 1:2:937:U:C2 | 1:2:941:A:N1 | 2.77 | 0.53 |
| 1:2:1157:G:O2' | 1:2:1158:G:OP1 | 2.25 | 0.53 |
| 1:2:1389:C:O2 | 1:2:1454:G:N2 | 2.37 | 0.53 |
| 2:A:132:THR:HA | 2:A:135:GLU:HB3 | 1.89 | 0.53 |
| 12:K:115:GLU:CD | 12:K:126:PRO:HG2 | 2.29 | 0.53 |
| 26:Y:5:TRP:HH2 | 29:3:65:HIS:ND1 | 2.06 | 0.53 |
| 29:3:73:LYS:NZ | 29:3:75:ILE:HB | 2.22 | 0.53 |
| 1:2:955:A:C8 | 1:2:1175:A:N1 | 2.76 | 0.53 |
| 1:2:1023:G:O5' | 1:2:1023:G:H8 | 1.92 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2:1234:G:H21 | 1:2:1249:A:N6 | 2.06 | 0.53 |
| 1:2:1417:U:C2 | 1:2:1418:C:C5 | 2.97 | 0.53 |
| 3:B:131:ILE:HG12 | 3:B:149:TYR:CD1 | 2.43 | 0.53 |
| 6:E:224:ASP:N | 6:E:224:ASP:OD1 | 2.42 | 0.53 |
| 7:F:207:ASN:HA | 7:F:210:LYS:HG3 | 1.91 | 0.53 |
| 23:V:17:LYS:HD2 | 23:V:71:TYR:CD2 | 2.44 | 0.53 |
| 25:X:26:GLN:HE21 | 25:X:67:ILE:HB | 1.74 | 0.53 |
| 27:Z:70:GLU:HB3 | 27:Z:78:PRO:HG3 | 1.91 | 0.53 |
| 27:Z:109:PHE:CZ | 27:Z:110:ARG:HG3 | 2.43 | 0.53 |
| 31:4:59:A:H2' | 31:4:60:U:O4' | 2.09 | 0.53 |
| 1:2:181:C:H2' | 1:2:182:C:H6 | 1.73 | 0.53 |
| 1:2:304:G:O6 | 1:2:312:G:N1 | 2.42 | 0.53 |
| 1:2:1042:G:N1 | 1:2:1046:G:C6 | 2.77 | 0.53 |
| 1:2:1232:C:H2' | 1:2:1233:4AC:C6 | 2.39 | 0.53 |
| 1:2:1392:A:O2' | 1:2:1393:G:C8 | 2.61 | 0.53 |
| 8:G:84:VAL:HG12 | 8:G:85:ARG:H | 1.73 | 0.53 |
| 15:N:119:ILE:O | 15:N:119:ILE:HG13 | 2.09 | 0.53 |
| 19:R:30:HIS:ND1 | 19:R:30:HIS:O | 2.42 | 0.53 |
| 19:R:91:THR:OG1 | 19:R:92:ARG:N | 2.41 | 0.53 |
| 23:V:41:VAL:O | 23:V:45:ASP:HA | 2.09 | 0.53 |
| 23:V:52:VAL:HA | 23:V:90:ASP:OD2 | 2.09 | 0.53 |
| 30:5:806:G:C2 | 30:5:807:G:H1' | 2.44 | 0.53 |
| 31:4:12:G:O6 | 31:4:24:U:N3 | 2.42 | 0.53 |
| 31:4:53:G:C2 | 31:4:62:C:C2 | 2.97 | 0.53 |
| 1:2:1115:G:C5 | 1:2:1116:A:N6 | 2.76 | 0.53 |
| 1:2:1263:A:H2' | 1:2:1264:C:H5' | 1.89 | 0.53 |
| 21:T:54:ALA:HA | 21:T:58:LYS:O | 2.09 | 0.53 |
| 23:V:56:ILE:O | 23:V:56:ILE:HG13 | 2.08 | 0.53 |
| 35:9:22:VAL:HA | 35:9:27:SER:OG | 2.09 | 0.53 |
| 35:9:103:LEU:HD11 | 35:9:136:PRO:HB2 | 1.91 | 0.53 |
| 1:2:97:A:H2' | 1:2:98:C:H6 | 1.74 | 0.53 |
| 1:2:1241:A:C6 | 1:2:1242:A:C6 | 2.97 | 0.53 |
| 1:2:1395:G:N2 | 1:2:1448:C:O2 | 2.41 | 0.53 |
| 30:5:808:A:C6 | 30:5:809:G:N7 | 2.77 | 0.53 |
| 1:2:529:A:C2 | 1:2:533:G:C5 | 2.97 | 0.52 |
| 1:2:697:G:N2 | 1:2:733:A:OP1 | 2.42 | 0.52 |
| 1:2:838:C:H2' | 1:2:839:4AC:C6 | 2.39 | 0.52 |
| 1:2:1470:C:C5 | 1:2:1473:G:C5 | 2.98 | 0.52 |
| 5:D:123:GLN:HA | 5:D:126:VAL:HG12 | 1.91 | 0.52 |
| 8:G:23:GLY:O | 8:G:27:GLU:HG2 | 2.09 | 0.52 |
| 12:K:32:PRO:HB3 | 22:U:150:TYR:CE2 | 2.43 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 29:3:114:ILE:HA | 29:3:117:LYS:HB2 | 1.90 | 0.52 |
| 31:4:60:U:OP1 | 31:4:61:C:N4 | 2.42 | 0.52 |
| 32:6:23:GLN:HE21 | 32:6:68:ILE:HB | 1.75 | 0.52 |
| 32:6:27:VAL:O | 32:6:40:ARG:HB3 | 2.09 | 0.52 |
| 1:2:541:G:N1 | 1:2:788:G:N7 | 2.58 | 0.52 |
| 1:2:815:G:H2' | 1:2:816:C:C6 | 2.45 | 0.52 |
| 1:2:1449:G:H2' | 1:2:1450:U:C4' | 2.38 | 0.52 |
| 29:3:54:ALA:HA | 29:3:80:VAL:HB | 1.92 | 0.52 |
| 33:7:181:ILE:HD13 | 33:7:194:LEU:HA | 1.90 | 0.52 |
| 34:8:5:LYS:O | 34:8:9:GLU:CB | 2.56 | 0.52 |
| 1:2:236:G:H2' | 1:2:237:A:O4' | 2.10 | 0.52 |
| 1:2:386:C:H2' | 1:2:387:G:C8 | 2.45 | 0.52 |
| 1:2:387:G:C6 | 1:2:395:G:N1 | 2.77 | 0.52 |
| 1:2:561:A:O2' | 1:2:562:A:OP2 | 2.26 | 0.52 |
| 1:2:772:C:H2' | 1:2:772:C:O2 | 2.09 | 0.52 |
| 1:2:986:U:N3 | 1:2:988:A:OP2 | 2.42 | 0.52 |
| 1:2:1324:C:H2' | 1:2:1325:C:H6 | 1.74 | 0.52 |
| 1:2:1435:C:O2' | 1:2:1436:G:OP1 | 2.27 | 0.52 |
| 1:2:1479:4AC:C2 | 1:2:1495:G:N2 | 2.72 | 0.52 |
| 3:B:25:THR:O | 3:B:28:MET:N | 2.42 | 0.52 |
| 4:C:3:GLU:CB | 7:F:230:PRO:HD2 | 2.38 | 0.52 |
| 8:G:8:ILE:O | 8:G:16:ALA:HB1 | 2.09 | 0.52 |
| 9:H:182:GLU:O | 9:H:186:GLU:HG2 | 2.09 | 0.52 |
| 26:Y:38:TRP:HB2 | 26:Y:47:GLU:OE2 | 2.09 | 0.52 |
| 31:4:29:G:H2' | 31:4:30:G:C8 | 2.37 | 0.52 |
| 33:7:353:ALA:CB | 33:7:370:VAL:HG13 | 2.39 | 0.52 |
| 33:7:374:LYS:HE2 | 33:7:375:LYS:H | 1.74 | 0.52 |
| 1:2:393:C:H3' | 1:2:394:4AC:H6 | 1.92 | 0.52 |
| 1:2:417:C:H2' | 1:2:418:G:H8 | 1.75 | 0.52 |
| 1:2:466:G:C2 | 1:2:467:G:N2 | 2.69 | 0.52 |
| 1:2:479:4AC:O7 | 1:2:479:4AC:H5 | 2.09 | 0.52 |
| 1:2:652:G:H22 | 1:2:673:C:N4 | 2.08 | 0.52 |
| 1:2:1029:G:O2' | 1:2:1164:G:N2 | 2.43 | 0.52 |
| 1:2:1181:C:H2' | 1:2:1182:C:C6 | 2.45 | 0.52 |
| 1:2:1476:A:C2 | 1:2:1477:G:C5 | 2.97 | 0.52 |
| 2:A:11:LYS:HD2 | 35:9:21:GLN:HB3 | 1.91 | 0.52 |
| 3:B:187:GLU:O | 3:B:189:LYS:HG2 | 2.10 | 0.52 |
| 5:D:67:GLU:OE1 | 5:D:68:ILE:HG13 | 2.10 | 0.52 |
| 7:F:58:ASN:HA | 7:F:63:GLN:NE2 | 2.24 | 0.52 |
| 9:H:89:GLU:O | 9:H:90:HIS:ND1 | 2.42 | 0.52 |
| 13:L:100:LEU:HD23 | 13:L:100:LEU:H | 1.73 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:M:89:SER:O | 14:M:89:SER:OG | 2.17 | 0.52 |
| 21:T:79:LEU:O | 21:T:94:ILE:N | 2.39 | 0.52 |
| 21:T:101:HIS:HB3 | 21:T:105:GLU:OE1 | 2.09 | 0.52 |
| 29:3:18:LYS:HB2 | 29:3:114:ILE:HD11 | 1.92 | 0.52 |
| 33:7:95:PRO:HD2 | 33:7:104:MET:HB3 | 1.91 | 0.52 |
| 1:2:162:G:H2' | 1:2:163:G:C8 | 2.45 | 0.52 |
| 1:2:306:G:H4' | 1:2:523:A:H4' | 1.91 | 0.52 |
| 2:A:119:ARG:HB2 | 2:A:192:LEU:HD11 | 1.91 | 0.52 |
| 18:Q:46:SER:O | 18:Q:50:ILE:HG13 | 2.09 | 0.52 |
| 32:6:19:PRO:HB3 | 32:6:23:GLN:HB2 | 1.91 | 0.52 |
| 33:7:17:HIS:CG | 33:7:128:GLN:HB2 | 2.45 | 0.52 |
| 33:7:273:PHE:HB2 | 35:9:190:PRO:HG3 | 1.92 | 0.52 |
| 1:2:861:G:O2' | 1:2:877:G:O6 | 2.26 | 0.52 |
| 1:2:945:C:C5 | 1:2:947:G:C5 | 2.96 | 0.52 |
| 1:2:1194:G:N3 | 1:2:1195:G:C8 | 2.78 | 0.52 |
| 1:2:1320:A:C4 | 1:2:1322:U:C4 | 2.98 | 0.52 |
| 31:4:30:G:C2 | 31:4:31:G:C8 | 2.97 | 0.52 |
| 33:7:11:ASN:HA | 33:7:90:SER:OG | 2.09 | 0.52 |
| 33:7:101:MET:O | 33:7:104:MET:HG3 | 2.10 | 0.52 |
| 33:7:151:VAL:HG11 | 34:8:14:LEU:HD23 | 1.92 | 0.52 |
| 1:2:419:U:C2 | 1:2:420:G:C8 | 2.98 | 0.52 |
| 1:2:666:C:H2' | 1:2:667:U:H6 | 1.74 | 0.52 |
| 1:2:738:C:N3 | 1:2:776:G:C2 | 2.78 | 0.52 |
| 1:2:755:U:H2' | 1:2:756:U:O4' | 2.10 | 0.52 |
| 1:2:792:G:H2' | 1:2:793:C:H6 | 1.75 | 0.52 |
| 1:2:839:4AC:N3 | 1:2:840:G:C5 | 2.78 | 0.52 |
| 1:2:910:A:O3' | 9:H:156:ARG:NH2 | 2.39 | 0.52 |
| 1:2:982:A:H2' | 1:2:983:G:C8 | 2.43 | 0.52 |
| 1:2:1321:G:O2' | 1:2:1322:U:OP2 | 2.28 | 0.52 |
| 3:B:101:MET:SD | 3:B:112:PRO:HG2 | 2.50 | 0.52 |
| 5:D:125:ILE:O | 5:D:128:GLY:N | 2.26 | 0.52 |
| 6:E:12:ARG:HH21 | 6:E:22:GLU:HG3 | 1.75 | 0.52 |
| 10:I:50:PHE:CB | 10:I:63:VAL:HG22 | 2.40 | 0.52 |
| 12:K:4:ILE:HG21 | 12:K:88:GLU:OE1 | 2.09 | 0.52 |
| 13:L:25:GLN:O | 13:L:29:ARG:N | 2.39 | 0.52 |
| 31:4:7:G:H2' | 31:4:49:G:C8 | 2.45 | 0.52 |
| 35:9:194:GLU:HA | 35:9:197:LYS:HD2 | 1.91 | 0.52 |
| 1:2:97:A:H2' | 1:2:98:C:C6 | 2.45 | 0.52 |
| 1:2:274:G:H3' | 1:2:276:C:H41 | 1.75 | 0.52 |
| 1:2:300:G:H1 | 1:2:319:4AC:H4 | 1.58 | 0.52 |
| 1:2:514:G:H2' | 1:2:515:U:C6 | 2.44 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:2:796:G:H1 | 1:2:829:G:H21 | 1.58 | 0.52 |
| 1:2:1172:G:H2' | 1:2:1173:U:C6 | 2.44 | 0.52 |
| 3:B:13:LEU:O | 3:B:16:GLY:N | 2.37 | 0.52 |
| 6:E:66:LEU:HD21 | 6:E:71:PHE:CD2 | 2.45 | 0.52 |
| 8:G:97:LYS:HD2 | 8:G:97:LYS:O | 2.10 | 0.52 |
| 16:O:132:ARG:HG2 | 16:O:132:ARG:O | 2.09 | 0.52 |
| 17:P:23:ARG:HH11 | 17:P:42:CYS:HB3 | 1.75 | 0.52 |
| 29:3:82:SER:OG | 29:3:83:LYS:N | 2.41 | 0.52 |
| 33:7:248:LYS:HB3 | 33:7:251:GLN:CD | 2.30 | 0.52 |
| 35:9:183:ILE:O | 35:9:227:TYR:N | 2.39 | 0.52 |
| 1:2:231:C:H2' | 1:2:232:C:H6 | 1.75 | 0.52 |
| 1:2:712:C:H2' | 1:2:713:G:H8 | 1.75 | 0.52 |
| 1:2:793:C:H2' | 1:2:794:U:C6 | 2.45 | 0.52 |
| 1:2:894:G:N2 | 1:2:1369:C:C2 | 2.78 | 0.52 |
| 1:2:1233:4AC:O2 | 1:2:1251:G:N2 | 2.43 | 0.52 |
| 1:2:1379:G:C2 | 1:2:1380:U:C5 | 2.97 | 0.52 |
| 1:2:1494:G:N7 | 14:M:132:ARG:NH1 | 2.55 | 0.52 |
| 3:B:169:TRP:CD1 | 3:B:195:PHE:HE2 | 2.23 | 0.52 |
| 8:G:5:LYS:N | 8:G:117:VAL:O | 2.43 | 0.52 |
| 8:G:63:ILE:HA | 8:G:121:VAL:HG12 | 1.92 | 0.52 |
| 12:K:4:ILE:O | 12:K:19:ILE:HG22 | 2.10 | 0.52 |
| 15:N:134:LEU:O | 15:N:138:VAL:HG23 | 2.10 | 0.52 |
| 31:4:13:C:H2' | 31:4:14:A:H5'' | 1.90 | 0.52 |
| 1:2:143:G:O6 | 1:2:174:C:N4 | 2.43 | 0.52 |
| 1:2:158:A:H2' | 1:2:159:A:C8 | 2.45 | 0.52 |
| 1:2:379:4AC:O7 | 1:2:379:4AC:H5 | 2.10 | 0.52 |
| 1:2:424:C:O2' | 1:2:425:U:OP2 | 2.26 | 0.52 |
| 1:2:517:G:C2 | 1:2:518:U:C4 | 2.97 | 0.52 |
| 1:2:529:A:H5'' | 1:2:530:U:OP1 | 2.10 | 0.52 |
| 1:2:533:G:C6 | 1:2:534:G:C5 | 2.98 | 0.52 |
| 1:2:543:G:N2 | 1:2:544:G:C4 | 2.77 | 0.52 |
| 1:2:628:G:C4 | 1:2:629:G:C8 | 2.97 | 0.52 |
| 1:2:714:G:OP1 | 24:W:12:ARG:NH2 | 2.42 | 0.52 |
| 1:2:723:G:H2' | 1:2:724:U:O4' | 2.10 | 0.52 |
| 1:2:1049:G:C5 | 1:2:1050:U:C4 | 2.99 | 0.52 |
| 1:2:1141:A:C2 | 1:2:1143:A:C6 | 2.98 | 0.52 |
| 1:2:1196:G:H2' | 1:2:1197:C:C6 | 2.45 | 0.52 |
| 1:2:1224:A:C6 | 1:2:1261:A:C5 | 2.98 | 0.52 |
| 1:2:1241:A:H2' | 1:2:1242:A:H8 | 1.75 | 0.52 |
| 1:2:1310:U:O2 | 9:H:174:TYR:OH | 2.28 | 0.52 |
| 2:A:105:ASP:OD1 | 2:A:106:GLY:N | 2.43 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 7:F:173:LYS:O | 7:F:176:ARG:N | 2.42 | 0.52 |
| 10:I:81:VAL:HG22 | 10:I:123:GLY:O | 2.09 | 0.52 |
| 11:J:87:ARG:HE | 11:J:88:GLN:HB3 | 1.75 | 0.52 |
| 12:K:26:VAL:HG23 | 12:K:62:ILE:HG22 | 1.91 | 0.52 |
| 20:S:41:VAL:HG11 | 20:S:47:ARG:HB3 | 1.92 | 0.52 |
| 33:7:200:GLU:HG3 | 33:7:201:TYR:N | 2.25 | 0.52 |
| 34:8:114:THR:HG23 | 34:8:127:CYS:HA | 1.92 | 0.52 |
| 1:2:643:A:C4 | 1:2:644:C:C5 | 2.99 | 0.51 |
| 1:2:722:G:H2' | 1:2:723:G:C8 | 2.45 | 0.51 |
| 1:2:1194:G:C2 | 1:2:1195:G:C8 | 2.98 | 0.51 |
| 1:2:1241:A:C2 | 1:2:1242:A:C4 | 2.98 | 0.51 |
| 1:2:1396:G:N7 | 1:2:1397:G:H8 | 2.08 | 0.51 |
| 1:2:1474:G:H4' | 1:2:1475:U:H5'' | 1.92 | 0.51 |
| 6:E:103:LEU:O | 6:E:111:ILE:HG12 | 2.10 | 0.51 |
| 31:4:14:A:C6 | 31:4:15:G:H1' | 2.45 | 0.51 |
| 31:4:26:G:C2 | 31:4:27:U:C5 | 2.98 | 0.51 |
| 33:7:336:LEU:HD12 | 33:7:337:GLU:H | 1.74 | 0.51 |
| 1:2:423:U:O2' | 1:2:424:C:O5' | 2.26 | 0.51 |
| 1:2:705:G:H2' | 1:2:706:C:C6 | 2.44 | 0.51 |
| 1:2:1451:G:O2' | 1:2:1452:A:H5'' | 2.10 | 0.51 |
| 10:I:106:THR:OG1 | 10:I:107:SER:N | 2.44 | 0.51 |
| 20:S:26:ARG:NH2 | 20:S:59:ARG:HB2 | 2.25 | 0.51 |
| 33:7:89:ILE:HD12 | 33:7:91:PHE:CZ | 2.45 | 0.51 |
| 33:7:280:ARG:HG3 | 33:7:284:GLU:O | 2.10 | 0.51 |
| 1:2:106:C:C4 | 1:2:107:G:C5 | 2.97 | 0.51 |
| 1:2:549:A:H2' | 1:2:550:G:O4' | 2.10 | 0.51 |
| 1:2:641:G:H5'' | 1:2:642:U:OP2 | 2.11 | 0.51 |
| 1:2:802:G:C4 | 1:2:823:G:N2 | 2.77 | 0.51 |
| 1:2:1501:U:C2 | 1:2:1502:C:C5 | 2.98 | 0.51 |
| 9:H:13:HIS:CE1 | 12:K:54:GLU:HG3 | 2.44 | 0.51 |
| 9:H:25:ASP:OD1 | 9:H:25:ASP:N | 2.43 | 0.51 |
| 9:H:147:HIS:CD2 | 9:H:147:HIS:H | 2.21 | 0.51 |
| 19:R:84:ASP:N | 19:R:84:ASP:OD1 | 2.42 | 0.51 |
| 33:7:313:GLY:HA3 | 33:7:363:SER:O | 2.10 | 0.51 |
| 33:7:400:GLN:O | 33:7:400:GLN:NE2 | 2.43 | 0.51 |
| 34:8:122:SER:HA | 34:8:138:PRO:HD3 | 1.92 | 0.51 |
| 1:2:218:C:N4 | 1:2:219:G:C5 | 2.79 | 0.51 |
| 1:2:218:C:H2' | 1:2:219:G:O4' | 2.10 | 0.51 |
| 1:2:543:G:H2' | 1:2:544:G:C8 | 2.45 | 0.51 |
| 1:2:626:4AC:O7 | 1:2:626:4AC:H5 | 2.08 | 0.51 |
| 1:2:643:A:C4 | 1:2:644:C:C6 | 2.99 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2:643:A:C5 | 1:2:644:C:C5 | 2.98 | 0.51 |
| 1:2:795:A:H2' | 1:2:796:G:H8 | 1.76 | 0.51 |
| 1:2:875:C:N3 | 1:2:876:U:C5 | 2.78 | 0.51 |
| 1:2:911:G:C2 | 1:2:912:G:C5 | 2.97 | 0.51 |
| 1:2:1144:A:H8 | 1:2:1144:A:OP2 | 1.94 | 0.51 |
| 1:2:1338:U:P | 22:U:83:ARG:HH22 | 2.32 | 0.51 |
| 16:O:15:LEU:HD13 | 16:O:24:ALA:HB3 | 1.92 | 0.51 |
| 18:Q:67:ARG:HD3 | 18:Q:74:ARG:O | 2.10 | 0.51 |
| 25:X:18:THR:O | 25:X:24:VAL:HG22 | 2.11 | 0.51 |
| 27:Z:48:ALA:O | 27:Z:85:ILE:HG13 | 2.11 | 0.51 |
| 31:4:7:G:C2 | 31:4:67:C:C4 | 2.98 | 0.51 |
| 1:2:116:A:C4 | 1:2:118:A:C5 | 2.98 | 0.51 |
| 1:2:334:A:H4' | 11:J:50:GLY:O | 2.11 | 0.51 |
| 1:2:484:G:N2 | 1:2:495:G:C6 | 2.78 | 0.51 |
| 1:2:604:G:N3 | 1:2:605:G:C8 | 2.78 | 0.51 |
| 1:2:738:C:C2 | 1:2:776:G:C2 | 2.98 | 0.51 |
| 1:2:788:G:C2 | 1:2:789:C:C4 | 2.99 | 0.51 |
| 1:2:851:4AC:H5 | 1:2:851:4AC:O7 | 2.09 | 0.51 |
| 1:2:995:U:H2' | 1:2:996:G:O4' | 2.11 | 0.51 |
| 1:2:1131:A:C6 | 1:2:1154:A:N7 | 2.78 | 0.51 |
| 1:2:1242:A:P | 22:U:96:SER:HG | 2.34 | 0.51 |
| 1:2:1293:A:C4 | 1:2:1297:G:C8 | 2.99 | 0.51 |
| 1:2:1446:U:H2' | 1:2:1447:C:H6 | 1.76 | 0.51 |
| 1:2:1457:G:H2' | 1:2:1458:G:C8 | 2.46 | 0.51 |
| 7:F:163:LEU:HD11 | 7:F:184:TRP:HE1 | 1.75 | 0.51 |
| 11:J:41:ASP:HA | 11:J:59:ALA:HB3 | 1.93 | 0.51 |
| 16:O:20:GLN:HB2 | 16:O:23:TRP:HD1 | 1.75 | 0.51 |
| 17:P:21:CYS:SG | 17:P:24:CYS:N | 2.78 | 0.51 |
| 27:Z:70:GLU:CD | 27:Z:71:ARG:HG3 | 2.30 | 0.51 |
| 1:2:126:A:C2 | 1:2:195:A:N3 | 2.79 | 0.51 |
| 1:2:308:G:N1 | 1:2:309:A:C5 | 2.78 | 0.51 |
| 1:2:849:G:P | 10:I:76:LYS:HG2 | 2.51 | 0.51 |
| 1:2:1260:U:H3 | 22:U:61:ARG:NH2 | 2.06 | 0.51 |
| 6:E:140:LEU:O | 6:E:141:ASN:ND2 | 2.44 | 0.51 |
| 15:N:103:VAL:HG12 | 15:N:129:VAL:HG22 | 1.92 | 0.51 |
| 33:7:397:ILE:HG23 | 33:7:408:ILE:HG22 | 1.92 | 0.51 |
| 1:2:163:G:C2 | 1:2:164:G:C5 | 2.99 | 0.51 |
| 1:2:998:C:H2' | 1:2:999:G:C8 | 2.35 | 0.51 |
| 1:2:1000:G:O5' | 1:2:1000:G:H8 | 1.92 | 0.51 |
| 1:2:1279:G:C2 | 1:2:1305:G:N3 | 2.78 | 0.51 |
| 1:2:1393:G:OP1 | 33:7:374:LYS:HD3 | 2.11 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:2:1451:G:HO2' | 1:2:1452:A:H8 | 1.59 | 0.51 |
| 12:K:25:ARG:HB2 | 22:U:150:TYR:CD1 | 2.46 | 0.51 |
| 22:U:37:THR:HG23 | 22:U:41:LYS:HE3 | 1.93 | 0.51 |
| 27:Z:166:TYR:HB2 | 27:Z:179:LYS:HG2 | 1.93 | 0.51 |
| 28:0:25:ARG:O | 28:0:26:LEU:HD22 | 2.10 | 0.51 |
| 31:4:29:G:C2 | 31:4:30:G:C8 | 2.99 | 0.51 |
| 33:7:22:LYS:O | 33:7:26:VAL:HG22 | 2.09 | 0.51 |
| 34:8:54:ILE:HG13 | 34:8:56:ARG:HB2 | 1.91 | 0.51 |
| 1:2:32:G:H2' | 1:2:33:A:C8 | 2.45 | 0.51 |
| 1:2:78:G:H2' | 1:2:79:C:C6 | 2.46 | 0.51 |
| 1:2:173:C:C2 | 1:2:174:C:C5 | 2.99 | 0.51 |
| 1:2:276:C:H2' | 1:2:277:C:H6 | 1.76 | 0.51 |
| 1:2:299:G:O6 | 1:2:320:G:C5 | 2.63 | 0.51 |
| 1:2:733:A:C4 | 1:2:734:A:C8 | 2.99 | 0.51 |
| 1:2:1358:U:C2 | 1:2:1359:G:C8 | 2.99 | 0.51 |
| 2:A:88:LEU:HD13 | 2:A:187:ARG:O | 2.11 | 0.51 |
| 3:B:167:ILE:H | 3:B:167:ILE:HD12 | 1.75 | 0.51 |
| 9:H:65:GLU:O | 9:H:69:ASN:ND2 | 2.44 | 0.51 |
| 20:S:61:LYS:HA | 20:S:66:ILE:HB | 1.92 | 0.51 |
| 22:U:97:ILE:H | 22:U:97:ILE:HD12 | 1.75 | 0.51 |
| 1:2:75:G:H2' | 1:2:76:G:C8 | 2.46 | 0.51 |
| 1:2:83:C:H2' | 1:2:84:C:C6 | 2.46 | 0.51 |
| 1:2:98:C:H2' | 1:2:99:C:H6 | 1.75 | 0.51 |
| 1:2:373:A2M:HM'1 | 1:2:374:A:C4 | 2.45 | 0.51 |
| 1:2:647:C:H2' | 1:2:648:4AC:H6 | 1.92 | 0.51 |
| 1:2:647:C:N4 | 1:2:678:G:C6 | 2.79 | 0.51 |
| 1:2:745:G:C5 | 1:2:746:C:C5 | 2.99 | 0.51 |
| 1:2:772:C:C2 | 1:2:773:C:C5 | 2.98 | 0.51 |
| 1:2:795:A:H2' | 1:2:796:G:C8 | 2.45 | 0.51 |
| 1:2:952:C:O2' | 1:2:953:U:OP1 | 2.23 | 0.51 |
| 1:2:1026:G:C6 | 1:2:1027:C:C4 | 2.99 | 0.51 |
| 1:2:1194:G:H2' | 1:2:1195:G:H8 | 1.76 | 0.51 |
| 8:G:75:ARG:CD | 8:G:92:PRO:HG2 | 2.40 | 0.51 |
| 11:J:41:ASP:N | 11:J:41:ASP:OD1 | 2.36 | 0.51 |
| 29:3:73:LYS:HE2 | 29:3:75:ILE:HB | 1.92 | 0.51 |
| 1:2:423:U:H2' | 1:2:424:C:C2 | 2.46 | 0.51 |
| 1:2:742:G:H2' | 1:2:743:G:O4' | 2.11 | 0.51 |
| 1:2:806:G:C6 | 1:2:819:G:C6 | 2.99 | 0.51 |
| 1:2:883:U:O2' | 1:2:884:A:H5' | 2.11 | 0.51 |
| 1:2:1019:C:H4' | 1:2:1020:A:H5'' | 1.93 | 0.51 |
| 1:2:1361:U:H2' | 1:2:1362:C:C6 | 2.46 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2:1452:A:H8 | 33:7:352:ARG:HH21 | 1.57 | 0.51 |
| 1:2:1470:C:C4 | 1:2:1473:G:C5 | 2.99 | 0.51 |
| 2:A:117:LYS:HG3 | 2:A:192:LEU:HD22 | 1.91 | 0.51 |
| 3:B:182:ILE:HG22 | 3:B:183:SER:H | 1.76 | 0.51 |
| 5:D:56:ARG:HG2 | 7:F:132:GLU:HG2 | 1.92 | 0.51 |
| 7:F:122:ILE:HD13 | 7:F:206:TYR:CD1 | 2.44 | 0.51 |
| 9:H:49:GLY:HA2 | 9:H:51:HIS:CE1 | 2.46 | 0.51 |
| 10:I:107:SER:O | 10:I:107:SER:OG | 2.29 | 0.51 |
| 15:N:84:VAL:HG12 | 15:N:85:THR:N | 2.26 | 0.51 |
| 16:O:99:ASP:HB2 | 16:O:103:ARG:NH2 | 2.25 | 0.51 |
| 30:5:812:G:C4 | 30:5:813:A:C8 | 3.00 | 0.51 |
| 31:4:58:A:O2' | 31:4:60:U:OP2 | 2.18 | 0.51 |
| 33:7:64:LYS:HG3 | 33:7:65:PRO:HB3 | 1.91 | 0.51 |
| 33:7:247:PHE:O | 33:7:288:GLU:HG2 | 2.10 | 0.51 |
| 1:2:65:G:H2' | 1:2:66:C:C6 | 2.46 | 0.50 |
| 1:2:266:G:C6 | 1:2:267:G:N7 | 2.79 | 0.50 |
| 1:2:268:G:OP1 | 11:J:113:ARG:HG2 | 2.11 | 0.50 |
| 1:2:674:C:C2 | 1:2:675:C:C5 | 2.99 | 0.50 |
| 1:2:1114:G:N1 | 1:2:1115:G:C6 | 2.79 | 0.50 |
| 1:2:1132:C:C4 | 1:2:1134:G:C8 | 3.00 | 0.50 |
| 1:2:1366:G:H8 | 1:2:1366:G:O5' | 1.95 | 0.50 |
| 26:Y:37:ARG:HA | 26:Y:49:LYS:H | 1.75 | 0.50 |
| 30:5:806:G:N3 | 30:5:807:G:H1' | 2.25 | 0.50 |
| 32:6:20:GLU:O | 32:6:23:GLN:HG3 | 2.11 | 0.50 |
| 35:9:151:LEU:HD12 | 35:9:161:VAL:HG13 | 1.93 | 0.50 |
| 1:2:582:G:C2 | 1:2:583:G:N7 | 2.79 | 0.50 |
| 1:2:582:G:N1 | 1:2:583:G:C5 | 2.80 | 0.50 |
| 1:2:991:G:C6 | 1:2:992:U:C4 | 3.00 | 0.50 |
| 1:2:1176:G:O2' | 17:P:26:GLN:OE1 | 2.15 | 0.50 |
| 1:2:1190:C:O2' | 1:2:1191:C:O5' | 2.29 | 0.50 |
| 1:2:1346:C:C2 | 1:2:1347:G:C8 | 3.00 | 0.50 |
| 1:2:1396:G:H22 | 1:2:1448:C:C1' | 2.24 | 0.50 |
| 3:B:166:LEU:O | 3:B:169:TRP:N | 2.43 | 0.50 |
| 5:D:73:LEU:O | 5:D:76:ARG:N | 2.43 | 0.50 |
| 31:4:4:G:C2 | 31:4:70:G:C6 | 2.99 | 0.50 |
| 31:4:7:G:C2 | 31:4:49:G:C5 | 2.99 | 0.50 |
| 33:7:49:LEU:HD11 | 33:7:104:MET:HA | 1.93 | 0.50 |
| 1:2:580:A:N6 | 1:2:593:G:C6 | 2.80 | 0.50 |
| 1:2:685:G:N7 | 14:M:123:HIS:ND1 | 2.59 | 0.50 |
| 1:2:758:G:C8 | 1:2:759:A:C8 | 2.98 | 0.50 |
| 1:2:808:G:C6 | 1:2:809:C:C4 | 3.00 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2:1022:G:C6 | 1:2:1023:G:C5 | 2.98 | 0.50 |
| 1:2:1152:G:N2 | 1:2:1154:A:OP2 | 2.45 | 0.50 |
| 1:2:1180:G:C6 | 1:2:1181:C:C4 | 2.99 | 0.50 |
| 1:2:1353:G:H4' | 25:X:17:ARG:NE | 2.26 | 0.50 |
| 1:2:1380:U:H2' | 1:2:1381:C:O4' | 2.11 | 0.50 |
| 5:D:106:GLN:NE2 | 5:D:122:ARG:HB2 | 2.26 | 0.50 |
| 26:Y:22:CYS:HB2 | 26:Y:29:VAL:HG23 | 1.93 | 0.50 |
| 1:2:29:C:O2' | 1:2:884:A:N1 | 2.42 | 0.50 |
| 1:2:256:G:O6 | 1:2:287:G:N1 | 2.45 | 0.50 |
| 1:2:474:A:C6 | 1:2:475:A:N1 | 2.80 | 0.50 |
| 1:2:540:A:H5'' | 1:2:541:G:OP2 | 2.10 | 0.50 |
| 1:2:719:G:O6 | 18:Q:64:LYS:NZ | 2.44 | 0.50 |
| 1:2:759:A:N3 | 1:2:761:A:C5 | 2.80 | 0.50 |
| 2:A:11:LYS:HG3 | 35:9:22:VAL:O | 2.11 | 0.50 |
| 9:H:121:GLN:O | 9:H:124:VAL:HB | 2.11 | 0.50 |
| 10:I:71:LYS:HB3 | 10:I:130:TYR:CE2 | 2.46 | 0.50 |
| 15:N:31:LYS:O | 15:N:33:ARG:N | 2.45 | 0.50 |
| 29:3:76:PRO:HB3 | 29:3:119:ARG:HH21 | 1.77 | 0.50 |
| 33:7:27:GLN:NE2 | 33:7:33:TRP:HB3 | 2.20 | 0.50 |
| 33:7:175:ALA:O | 33:7:178:VAL:HG22 | 2.11 | 0.50 |
| 35:9:214:LEU:HD12 | 35:9:233:GLY:HA3 | 1.92 | 0.50 |
| 1:2:55:A:N6 | 1:2:315:A:N6 | 2.60 | 0.50 |
| 1:2:418:G:H2' | 1:2:419:U:H6 | 1.76 | 0.50 |
| 1:2:634:G:O6 | 1:2:707:U:N3 | 2.44 | 0.50 |
| 1:2:831:A:C6 | 1:2:832:G:C4 | 3.00 | 0.50 |
| 1:2:1053:A:C6 | 1:2:1054:C:C4 | 2.99 | 0.50 |
| 1:2:1207:G:C6 | 1:2:1208:C:N4 | 2.79 | 0.50 |
| 1:2:1208:C:H2' | 1:2:1209:U:C6 | 2.46 | 0.50 |
| 1:2:1376:OMC:HM22 | 1:2:1377:C:H5' | 1.94 | 0.50 |
| 16:O:129:GLN:OE1 | 16:O:129:GLN:N | 2.44 | 0.50 |
| 35:9:110:VAL:HG13 | 35:9:163:PRO:HB2 | 1.94 | 0.50 |
| 35:9:218:LYS:HG3 | 35:9:230:ASP:OD2 | 2.11 | 0.50 |
| 1:2:116:A:C6 | 1:2:118:A:C2 | 2.99 | 0.50 |
| 1:2:893:G:C2 | 1:2:1370:A:C2 | 3.00 | 0.50 |
| 1:2:951:C:H42 | 17:P:15:GLY:HA3 | 1.76 | 0.50 |
| 1:2:1028:4AC:O7 | 1:2:1028:4AC:H5 | 2.10 | 0.50 |
| 1:2:1044:G:H2' | 1:2:1045:A:C8 | 2.46 | 0.50 |
| 1:2:1101:U:H2' | 1:2:1102:C:C6 | 2.47 | 0.50 |
| 1:2:1125:G:C2 | 1:2:1126:G:C5 | 2.99 | 0.50 |
| 1:2:1202:5MC:H3' | 16:O:136:ARG:NH1 | 2.27 | 0.50 |
| 5:D:70:ARG:O | 5:D:73:LEU:HB3 | 2.12 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 21:T:72:VAL:HG23 | 21:T:76:MET:SD | 2.51 | 0.50 |
| 24:W:17:ARG:NH2 | 24:W:26:GLU:OE1 | 2.45 | 0.50 |
| 33:7:24:THR:HG21 | 33:7:186:LEU:HD12 | 1.93 | 0.50 |
| 1:2:531:U:H5'' | 1:2:532:G:H2' | 1.94 | 0.50 |
| 1:2:825:U:H5 | 1:2:842:U:C5 | 2.29 | 0.50 |
| 1:2:973:A:H8 | 29:3:34:LYS:HB2 | 1.75 | 0.50 |
| 1:2:1345:G:H2' | 1:2:1346:C:H6 | 1.76 | 0.50 |
| 2:A:99:ARG:HG2 | 2:A:100:ARG:HG3 | 1.93 | 0.50 |
| 5:D:32:LYS:HG3 | 5:D:33:TYR:CE2 | 2.47 | 0.50 |
| 8:G:22:THR:OG1 | 8:G:23:GLY:N | 2.44 | 0.50 |
| 9:H:190:LEU:HB3 | 9:H:198:SER:HB3 | 1.93 | 0.50 |
| 20:S:27:ASP:OD1 | 20:S:28:PHE:N | 2.44 | 0.50 |
| 27:Z:47:PHE:HD1 | 27:Z:84:GLU:O | 1.95 | 0.50 |
| 1:2:219:G:C2 | 1:2:223:G:C6 | 3.00 | 0.50 |
| 1:2:270:U:P | 11:J:54:LYS:HZ2 | 2.34 | 0.50 |
| 1:2:465:G:O2' | 1:2:466:G:H5' | 2.12 | 0.50 |
| 1:2:578:C:H2' | 1:2:579:C:C6 | 2.46 | 0.50 |
| 1:2:821:C:H5'' | 24:W:5:ARG:NH1 | 2.27 | 0.50 |
| 1:2:1039:A:N1 | 1:2:1067:A:C6 | 2.80 | 0.50 |
| 1:2:1241:A:C6 | 1:2:1242:A:C5 | 3.00 | 0.50 |
| 6:E:197:GLY:HA3 | 6:E:216:GLU:O | 2.11 | 0.50 |
| 23:V:44:LEU:HB3 | 23:V:46:LEU:HD21 | 1.94 | 0.50 |
| 30:5:816:U:H2' | 30:5:817:A:H8 | 1.77 | 0.50 |
| 33:7:339:VAL:O | 33:7:345:MET:HG2 | 2.11 | 0.50 |
| 1:2:545:C:N4 | 1:2:546:4AC:HM72 | 2.26 | 0.50 |
| 1:2:1002:C:H2' | 1:2:1003:G:H8 | 1.77 | 0.50 |
| 1:2:1242:A:H2' | 1:2:1243:A:H8 | 1.77 | 0.50 |
| 1:2:1265:C:C2 | 1:2:1266:C:C5 | 3.00 | 0.50 |
| 1:2:1469:6MZ:N3 | 1:2:1469:6MZ:H2' | 2.26 | 0.50 |
| 2:A:18:GLN:HB3 | 2:A:38:ALA:O | 2.12 | 0.50 |
| 8:G:47:LEU:HB3 | 8:G:49:GLU:HG2 | 1.93 | 0.50 |
| 8:G:55:PHE:HD2 | 8:G:125:TYR:HH | 1.59 | 0.50 |
| 29:3:14:GLU:HG3 | 29:3:15:LEU:HD12 | 1.94 | 0.50 |
| 29:3:74:GLU:HG2 | 29:3:75:ILE:N | 2.26 | 0.50 |
| 32:6:72:TRP:CH2 | 32:6:81:ASP:HB2 | 2.47 | 0.50 |
| 33:7:40:GLU:OE1 | 33:7:47:ILE:HB | 2.12 | 0.50 |
| 35:9:31:LEU:HD11 | 35:9:78:VAL:HG11 | 1.94 | 0.50 |
| 1:2:121:U:H2' | 1:2:122:C:C6 | 2.47 | 0.49 |
| 1:2:606:G:C2 | 1:2:607:A:C5 | 3.00 | 0.49 |
| 1:2:655:G:N1 | 1:2:656:G:C5 | 2.80 | 0.49 |
| 1:2:1039:A:O4' | 3:B:103:ASN:ND2 | 2.45 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:2:1465:C:C4 | 1:2:1466:G:N7 | 2.80 | 0.49 |
| 7:F:91:ASN:ND2 | 7:F:93:ASP:HB3 | 2.27 | 0.49 |
| 15:N:7:PRO:O | 15:N:9:GLY:N | 2.41 | 0.49 |
| 26:Y:40:CYS:O | 26:Y:42:ARG:N | 2.44 | 0.49 |
| 31:4:31:G:H2' | 31:4:32:OMC:H6 | 1.76 | 0.49 |
| 32:6:78:LYS:H | 32:6:79:ARG:CZ | 2.25 | 0.49 |
| 33:7:10:VAL:O | 33:7:90:SER:OG | 2.30 | 0.49 |
| 33:7:20:HIS:HB3 | 33:7:117:VAL:HG23 | 1.93 | 0.49 |
| 1:2:239:G:O2' | 6:E:6:PRO:HB3 | 2.11 | 0.49 |
| 1:2:319:4AC:O7 | 1:2:319:4AC:H5 | 2.11 | 0.49 |
| 1:2:347:G:C2 | 1:2:348:G:C8 | 3.00 | 0.49 |
| 1:2:369:G:C5 | 1:2:370:C:C4 | 3.00 | 0.49 |
| 1:2:865:G:N1 | 1:2:866:G:N2 | 2.60 | 0.49 |
| 1:2:866:G:N2 | 1:2:876:U:O2 | 2.26 | 0.49 |
| 1:2:876:U:P | 28:0:2:LYS:HZ2 | 2.27 | 0.49 |
| 1:2:1056:U:H2' | 1:2:1058:A:OP2 | 2.12 | 0.49 |
| 1:2:1062:U:N3 | 1:2:1063:G:N7 | 2.60 | 0.49 |
| 1:2:1093:C:H42 | 1:2:1119:C:N4 | 2.09 | 0.49 |
| 1:2:1505:C:C2 | 30:5:810:G:C2 | 3.00 | 0.49 |
| 6:E:185:VAL:HG21 | 6:E:230:ALA:HB1 | 1.94 | 0.49 |
| 8:G:67:THR:O | 8:G:116:ILE:HG23 | 2.12 | 0.49 |
| 31:4:20:H2U:H3' | 31:4:22:G:OP1 | 2.13 | 0.49 |
| 31:4:63:G:C2 | 31:4:64:G:C8 | 2.99 | 0.49 |
| 1:2:28:G:H1' | 1:2:885:A:H61 | 1.77 | 0.49 |
| 1:2:116:A:C5 | 1:2:118:A:C6 | 3.00 | 0.49 |
| 1:2:464:A:C2 | 1:2:513:A:C5 | 3.00 | 0.49 |
| 1:2:466:G:C4 | 1:2:467:G:N1 | 2.81 | 0.49 |
| 1:2:466:G:O2' | 1:2:467:G:H5' | 2.12 | 0.49 |
| 1:2:576:U:P | 6:E:24:LYS:HZ1 | 2.33 | 0.49 |
| 1:2:863:A:C6 | 1:2:864:C:N4 | 2.81 | 0.49 |
| 1:2:904:A:O2' | 1:2:906:U:OP1 | 2.20 | 0.49 |
| 1:2:1289:U:H2' | 1:2:1290:G:C8 | 2.47 | 0.49 |
| 1:2:1485:G:H22 | 1:2:1487:MA6:H3' | 1.77 | 0.49 |
| 6:E:10:LEU:HD12 | 6:E:11:LYS:N | 2.26 | 0.49 |
| 17:P:16:LYS:NZ | 17:P:28:GLY:O | 2.40 | 0.49 |
| 18:Q:29:THR:OG1 | 18:Q:30:VAL:N | 2.45 | 0.49 |
| 20:S:23:GLU:OE2 | 20:S:34:LYS:HD2 | 2.11 | 0.49 |
| 35:9:181:GLY:O | 35:9:229:VAL:N | 2.45 | 0.49 |
| 1:2:89:G:C2 | 1:2:90:G:C4 | 3.00 | 0.49 |
| 1:2:174:C:H2' | 1:2:175:C:C6 | 2.47 | 0.49 |
| 1:2:452:G:C6 | 1:2:453:C:C4 | 3.00 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2:974:U:HO2' | 26:Y:3:GLN:HE21 | 1.54 | 0.49 |
| 1:2:1013:G:N2 | 1:2:1184:4AC:C2 | 2.75 | 0.49 |
| 1:2:1085:C:H2' | 1:2:1086:C:C6 | 2.46 | 0.49 |
| 2:A:116:TYR:CD2 | 2:A:155:PHE:CG | 2.99 | 0.49 |
| 7:F:50:ILE:O | 7:F:54:LEU:N | 2.36 | 0.49 |
| 10:I:51:GLU:N | 10:I:51:GLU:OE1 | 2.46 | 0.49 |
| 28:0:28:ARG:HG2 | 28:0:29:GLN:NE2 | 2.27 | 0.49 |
| 29:3:16:ALA:O | 29:3:20:LEU:HB2 | 2.12 | 0.49 |
| 31:4:10:G:C2 | 31:4:11:A:C8 | 3.00 | 0.49 |
| 32:6:95:LEU:HD13 | 32:6:100:ILE:O | 2.12 | 0.49 |
| 33:7:113:GLY:HA2 | 33:7:143:ASN:HB2 | 1.95 | 0.49 |
| 35:9:68:VAL:HA | 35:9:80:VAL:HG12 | 1.95 | 0.49 |
| 1:2:32:G:H2' | 1:2:33:A:H8 | 1.77 | 0.49 |
| 1:2:117:C:OP2 | 11:J:11:LYS:HE2 | 2.13 | 0.49 |
| 1:2:418:G:H2' | 1:2:419:U:C6 | 2.47 | 0.49 |
| 1:2:636:4AC:N4 | 1:2:704:G:O6 | 2.46 | 0.49 |
| 1:2:990:G:N2 | 1:2:995:U:O4 | 2.40 | 0.49 |
| 1:2:1233:4AC:O7 | 1:2:1233:4AC:H5 | 2.11 | 0.49 |
| 1:2:1362:C:C2 | 1:2:1363:C:C5 | 3.01 | 0.49 |
| 1:2:1401:U:N3 | 1:2:1402:A:C5 | 2.80 | 0.49 |
| 9:H:38:ASN:HD22 | 9:H:62:HIS:N | 2.09 | 0.49 |
| 11:J:88:GLN:HB2 | 11:J:91:ARG:HH21 | 1.77 | 0.49 |
| 25:X:67:ILE:HG12 | 25:X:68:LYS:N | 2.26 | 0.49 |
| 27:Z:30:TYR:OH | 27:Z:33:LEU:HD23 | 2.13 | 0.49 |
| 33:7:366:THR:HG21 | 33:7:382:LEU:HD21 | 1.93 | 0.49 |
| 34:8:9:GLU:OE1 | 34:8:10:MET:HG3 | 2.12 | 0.49 |
| 35:9:69:ILE:HD11 | 35:9:81:SER:HB2 | 1.93 | 0.49 |
| 1:2:215:A:H2' | 1:2:216:G:C8 | 2.47 | 0.49 |
| 1:2:528:U:O4 | 1:2:855:U:O2' | 2.22 | 0.49 |
| 1:2:591:G:C2 | 1:2:592:U:N3 | 2.81 | 0.49 |
| 1:2:917:G:H2' | 1:2:917:G:N3 | 2.27 | 0.49 |
| 1:2:930:A:C5 | 1:2:931:A:C6 | 3.01 | 0.49 |
| 1:2:982:A:H2' | 1:2:983:G:H8 | 1.76 | 0.49 |
| 1:2:1115:G:N1 | 1:2:1116:A:N1 | 2.61 | 0.49 |
| 1:2:1115:G:C2 | 1:2:1116:A:C2 | 3.00 | 0.49 |
| 1:2:1234:G:N2 | 1:2:1249:A:H62 | 2.08 | 0.49 |
| 1:2:1271:U:H4' | 1:2:1273:A:C2 | 2.34 | 0.49 |
| 7:F:214:THR:HB | 7:F:215:PRO:HD2 | 1.94 | 0.49 |
| 9:H:10:PHE:HE2 | 9:H:12:PRO:HB3 | 1.78 | 0.49 |
| 9:H:73:ARG:NH2 | 9:H:75:GLY:O | 2.37 | 0.49 |
| 17:P:20:ARG:NH1 | 17:P:27:TYR:OH | 2.44 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 33:7:46:THR:HB | 33:7:95:PRO:HA | 1.95 | 0.49 |
| 1:2:245:G:C5 | 1:2:246:C:C5 | 3.01 | 0.49 |
| 1:2:267:G:C2 | 1:2:268:G:C5 | 3.01 | 0.49 |
| 1:2:689:G:C6 | 1:2:691:G:C4 | 2.99 | 0.49 |
| 1:2:964:G:O2' | 1:2:1009:A:N1 | 2.36 | 0.49 |
| 1:2:1112:A:C2 | 1:2:1113:G:C5 | 3.00 | 0.49 |
| 1:2:1476:A:C6 | 1:2:1499:G:C2 | 3.01 | 0.49 |
| 3:B:75:TYR:CE2 | 3:B:161:ARG:HD3 | 2.47 | 0.49 |
| 4:C:22:THR:O | 4:C:25:GLU:HG2 | 2.13 | 0.49 |
| 4:C:55:CYS:HB3 | 4:C:58:CYS:HB2 | 1.93 | 0.49 |
| 13:L:56:GLU:OE1 | 13:L:56:GLU:N | 2.46 | 0.49 |
| 18:Q:33:ILE:O | 18:Q:37:VAL:HG23 | 2.11 | 0.49 |
| 29:3:66:LEU:HB2 | 29:3:67:PRO:HD3 | 1.93 | 0.49 |
| 31:4:75:C:H1' | 33:7:225:LYS:HE3 | 1.94 | 0.49 |
| 34:8:35:ILE:HG12 | 34:8:44:ILE:HG12 | 1.94 | 0.49 |
| 1:2:206:C:O3' | 11:J:43:ARG:NH1 | 2.38 | 0.49 |
| 1:2:313:G:C2 | 1:2:314:G:H1' | 2.48 | 0.49 |
| 1:2:467:G:N7 | 1:2:468:C:C4 | 2.80 | 0.49 |
| 1:2:741:G:C4 | 1:2:742:G:C8 | 3.01 | 0.49 |
| 1:2:813:G:N1 | 1:2:815:G:C4 | 2.80 | 0.49 |
| 1:2:849:G:C6 | 1:2:850:C:N4 | 2.80 | 0.49 |
| 1:2:1013:G:H22 | 1:2:1184:4AC:C4 | 2.25 | 0.49 |
| 1:2:1192:C:H5'' | 1:2:1193:4AC:OP2 | 2.11 | 0.49 |
| 1:2:1437:A:C2 | 1:2:1438:G:H1' | 2.48 | 0.49 |
| 4:C:4:ASN:ND2 | 4:C:4:ASN:O | 2.45 | 0.49 |
| 4:C:16:SER:OG | 4:C:17:CYS:N | 2.45 | 0.49 |
| 14:M:106:ALA:HB2 | 14:M:112:ILE:HD11 | 1.95 | 0.49 |
| 18:Q:130:ARG:O | 18:Q:133:VAL:HG12 | 2.12 | 0.49 |
| 27:Z:56:GLY:CA | 27:Z:61:ARG:HB2 | 2.43 | 0.49 |
| 27:Z:109:PHE:CE1 | 27:Z:110:ARG:HG3 | 2.47 | 0.49 |
| 33:7:242:ILE:HG21 | 33:7:246:LEU:HA | 1.94 | 0.49 |
| 33:7:376:ASP:CG | 33:7:377:GLU:HG3 | 2.33 | 0.49 |
| 34:8:114:THR:HG21 | 34:8:125:ILE:HG23 | 1.93 | 0.49 |
| 1:2:49:G:N2 | 1:2:409:C:C2 | 2.80 | 0.49 |
| 1:2:263:G:C2 | 1:2:282:A:C2 | 3.00 | 0.49 |
| 1:2:593:G:N1 | 1:2:594:G:C5 | 2.81 | 0.49 |
| 1:2:638:G:C6 | 1:2:639:G:C5 | 3.00 | 0.49 |
| 1:2:739:A:N6 | 1:2:775:G:O6 | 2.45 | 0.49 |
| 1:2:832:G:C2 | 1:2:833:G:C5 | 3.01 | 0.49 |
| 1:2:1395:G:O2' | 1:2:1449:G:N2 | 2.46 | 0.49 |
| 1:2:1413:G:C6 | 1:2:1431:G:C6 | 3.01 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2:1482:A:O2' | 1:2:1483:G:H5' | 2.13 | 0.49 |
| 2:A:116:TYR:N | 2:A:116:TYR:CD1 | 2.81 | 0.49 |
| 7:F:53:LEU:O | 7:F:54:LEU:HD23 | 2.12 | 0.49 |
| 13:L:83:ARG:HG2 | 13:L:87:ARG:NH1 | 2.21 | 0.49 |
| 16:O:45:LEU:HD23 | 16:O:45:LEU:H | 1.78 | 0.49 |
| 18:Q:93:GLU:OE1 | 18:Q:93:GLU:N | 2.46 | 0.49 |
| 19:R:44:ARG:O | 19:R:46:THR:HG23 | 2.12 | 0.49 |
| 20:S:65:LYS:HE3 | 20:S:67:LEU:HD11 | 1.93 | 0.49 |
| 21:T:81:ILE:HD11 | 21:T:103:LEU:HD21 | 1.95 | 0.49 |
| 33:7:80:ASP:OD1 | 34:8:119:GLU:HA | 2.13 | 0.49 |
| 35:9:224:ALA:HB3 | 35:9:225:PRO:HD3 | 1.95 | 0.49 |
| 1:2:156:G:N2 | 1:2:158:A:H5'' | 2.28 | 0.49 |
| 1:2:171:C:H2' | 1:2:172:C:O4' | 2.12 | 0.49 |
| 1:2:485:C:H2' | 1:2:486:A:O4' | 2.13 | 0.49 |
| 1:2:588:A:H5' | 1:2:589:C:OP2 | 2.13 | 0.49 |
| 1:2:789:C:H2' | 1:2:790:G:H8 | 1.77 | 0.49 |
| 1:2:984:G:O6 | 1:2:993:C:N4 | 2.46 | 0.49 |
| 1:2:1127:G:C6 | 1:2:1128:G:N7 | 2.81 | 0.49 |
| 1:2:1324:C:H2' | 1:2:1325:C:C6 | 2.48 | 0.49 |
| 1:2:1380:U:C2 | 1:2:1381:C:C6 | 3.00 | 0.49 |
| 2:A:27:PHE:CZ | 2:A:83:PHE:HB2 | 2.48 | 0.49 |
| 2:A:100:ARG:HA | 2:A:129:ARG:HE | 1.78 | 0.49 |
| 12:K:25:ARG:HB2 | 22:U:150:TYR:HD1 | 1.78 | 0.49 |
| 25:X:59:GLU:C | 25:X:61:GLU:H | 2.16 | 0.49 |
| 33:7:273:PHE:HB2 | 35:9:190:PRO:CG | 2.43 | 0.49 |
| 33:7:289:ALA:HB2 | 33:7:295:VAL:HG21 | 1.95 | 0.49 |
| 33:7:324:PRO:HD2 | 33:7:388:VAL:HG13 | 1.94 | 0.49 |
| 34:8:116:LEU:HG | 34:8:123:TRP:CD1 | 2.48 | 0.49 |
| 1:2:179:G:C2 | 1:2:208:G:H1' | 2.47 | 0.48 |
| 1:2:606:G:H2' | 1:2:607:A:C8 | 2.48 | 0.48 |
| 1:2:610:C:O2' | 10:I:78:ARG:NH1 | 2.46 | 0.48 |
| 1:2:688:A:OP2 | 2:A:129:ARG:NH2 | 2.46 | 0.48 |
| 1:2:993:C:C2 | 1:2:994:U:C5 | 3.01 | 0.48 |
| 1:2:1160:G:C2 | 1:2:1161:G:C8 | 3.01 | 0.48 |
| 1:2:1241:A:H2' | 1:2:1242:A:C8 | 2.47 | 0.48 |
| 1:2:1279:G:N2 | 1:2:1305:G:N3 | 2.61 | 0.48 |
| 7:F:24:MET:O | 7:F:27:LYS:N | 2.46 | 0.48 |
| 16:O:117:GLY:O | 16:O:121:GLU:HG3 | 2.12 | 0.48 |
| 25:X:15:ILE:HD11 | 25:X:28:LYS:N | 2.28 | 0.48 |
| 27:Z:144:VAL:HG12 | 27:Z:145:ARG:N | 2.22 | 0.48 |
| 30:5:819:A:C6 | 31:4:37:A:C2 | 3.01 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 32:6:16:VAL:HG11 | 32:6:93:TRP:CZ3 | 2.47 | 0.48 |
| 1:2:157:A:H2' | 1:2:158:A:O4' | 2.13 | 0.48 |
| 1:2:193:G:C6 | 1:2:194:A:N1 | 2.81 | 0.48 |
| 1:2:255:A:N7 | 1:2:288:A:C5 | 2.81 | 0.48 |
| 1:2:268:G:O2' | 1:2:269:G:OP1 | 2.26 | 0.48 |
| 1:2:295:G:H2' | 1:2:296:U:C5 | 2.48 | 0.48 |
| 1:2:529:A:C2 | 1:2:533:G:N7 | 2.81 | 0.48 |
| 1:2:570:G:H2' | 1:2:571:C:O4' | 2.13 | 0.48 |
| 1:2:643:A:C2 | 1:2:644:C:C2 | 3.01 | 0.48 |
| 1:2:980:C:C4 | 1:2:990:G:C5 | 3.01 | 0.48 |
| 1:2:1133:U:C4 | 1:2:1156:G:C4 | 3.00 | 0.48 |
| 1:2:1272:C:N4 | 9:H:177:LYS:HA | 2.28 | 0.48 |
| 1:2:1476:A:N6 | 1:2:1499:G:C6 | 2.81 | 0.48 |
| 10:I:31:SER:OG | 10:I:33:LEU:N | 2.46 | 0.48 |
| 25:X:67:ILE:HG23 | 25:X:70:ARG:H | 1.78 | 0.48 |
| 32:6:16:VAL:HG21 | 32:6:93:TRP:HZ3 | 1.78 | 0.48 |
| 33:7:127:PRO:HB2 | 33:7:128:GLN:OE1 | 2.13 | 0.48 |
| 1:2:90:G:C4 | 1:2:91:G:C8 | 3.01 | 0.48 |
| 1:2:372:A:C4 | 1:2:373:A2M:N7 | 2.82 | 0.48 |
| 1:2:615:G:C2 | 1:2:616:G:C8 | 3.01 | 0.48 |
| 1:2:894:G:H2' | 1:2:895:C:O4' | 2.12 | 0.48 |
| 1:2:1112:A:N3 | 1:2:1113:G:C8 | 2.81 | 0.48 |
| 10:I:31:SER:OG | 10:I:34:ILE:HG13 | 2.13 | 0.48 |
| 25:X:18:THR:HG22 | 25:X:19:GLY:N | 2.27 | 0.48 |
| 27:Z:70:GLU:OE1 | 27:Z:71:ARG:HG3 | 2.13 | 0.48 |
| 27:Z:150:TYR:CD1 | 27:Z:150:TYR:N | 2.79 | 0.48 |
| 1:2:412:A:C2 | 1:2:413:G:C8 | 3.01 | 0.48 |
| 1:2:435:U:OP2 | 1:2:435:U:H6 | 1.95 | 0.48 |
| 1:2:981:C:O2 | 26:Y:37:ARG:NE | 2.47 | 0.48 |
| 1:2:1167:G:H2' | 1:2:1168:G:O4' | 2.13 | 0.48 |
| 1:2:1364:U:C2 | 1:2:1365:U:C5 | 3.02 | 0.48 |
| 1:2:1398:G:O2' | 1:2:1399:C:H6 | 1.96 | 0.48 |
| 1:2:1401:U:C2 | 1:2:1402:A:C8 | 3.01 | 0.48 |
| 1:2:1407:A:N7 | 1:2:1437:A:C6 | 2.81 | 0.48 |
| 2:A:11:LYS:NZ | 2:A:12:ASP:OD2 | 2.46 | 0.48 |
| 10:I:50:PHE:HB3 | 10:I:63:VAL:HG22 | 1.94 | 0.48 |
| 13:L:18:GLU:HG3 | 13:L:19:VAL:HG13 | 1.96 | 0.48 |
| 26:Y:27:PRO:O | 29:3:45:ARG:NE | 2.25 | 0.48 |
| 29:3:92:ILE:HG13 | 29:3:93:GLU:H | 1.79 | 0.48 |
| 31:4:54:5MU:H73 | 31:4:55:PSU:C2 | 2.49 | 0.48 |
| 33:7:8:PRO:HD2 | 33:7:281:PHE:CE1 | 2.48 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 34:8:44:ILE:HD12 | 34:8:81:LEU:HD23 | 1.94 | 0.48 |
| 35:9:123:GLU:HA | 35:9:127:TRP:CD1 | 2.48 | 0.48 |
| 1:2:22:G:C2 | 1:2:23:A:C4 | 3.01 | 0.48 |
| 1:2:465:G:H2' | 1:2:466:G:C8 | 2.49 | 0.48 |
| 1:2:1421:U:O2' | 1:2:1422:C:H5' | 2.14 | 0.48 |
| 7:F:62:ASN:CG | 7:F:91:ASN:HA | 2.34 | 0.48 |
| 7:F:142:PRO:HB2 | 7:F:143:PHE:HD2 | 1.78 | 0.48 |
| 8:G:3:THR:HB | 8:G:22:THR:HB | 1.95 | 0.48 |
| 8:G:87:LEU:HD12 | 8:G:104:LYS:NZ | 2.28 | 0.48 |
| 11:J:56:ARG:HD3 | 11:J:56:ARG:HA | 1.63 | 0.48 |
| 18:Q:74:ARG:HH11 | 18:Q:80:ARG:HD3 | 1.79 | 0.48 |
| 27:Z:104:GLU:HB3 | 27:Z:169:ALA:HB1 | 1.95 | 0.48 |
| 33:7:138:ILE:HG23 | 33:7:410:TRP:HB2 | 1.95 | 0.48 |
| 1:2:391:A:C2 | 1:2:392:A:C5 | 3.01 | 0.48 |
| 1:2:547:G:N2 | 1:2:728:G:C6 | 2.82 | 0.48 |
| 1:2:704:G:H2' | 1:2:705:G:H8 | 1.79 | 0.48 |
| 1:2:753:G:C2 | 1:2:764:C:C2 | 3.02 | 0.48 |
| 1:2:793:C:H2' | 1:2:794:U:H6 | 1.78 | 0.48 |
| 1:2:794:U:C4 | 1:2:841:U:C5 | 3.01 | 0.48 |
| 1:2:860:A:H2 | 1:2:861:G:H21 | 1.59 | 0.48 |
| 1:2:962:G:H5' | 17:P:3:LYS:HG2 | 1.95 | 0.48 |
| 1:2:1147:4AC:H5' | 1:2:1148:G:OP2 | 2.14 | 0.48 |
| 1:2:1484:G:C2 | 1:2:1485:G:C8 | 3.01 | 0.48 |
| 1:2:1502:C:C2 | 1:2:1503:A:C8 | 3.01 | 0.48 |
| 4:C:49:LEU:HD12 | 4:C:49:LEU:O | 2.14 | 0.48 |
| 8:G:21:ILE:HD12 | 8:G:25:GLU:HB3 | 1.95 | 0.48 |
| 12:K:38:PRO:O | 12:K:41:ALA:N | 2.43 | 0.48 |
| 16:O:80:ASN:N | 16:O:92:HIS:ND1 | 2.61 | 0.48 |
| 23:V:19:ILE:HB | 23:V:69:ALA:O | 2.14 | 0.48 |
| 31:4:8:4SU:H4' | 31:4:21:A:H61 | 1.78 | 0.48 |
| 1:2:80:G:C6 | 1:2:94:G:C6 | 3.02 | 0.48 |
| 1:2:323:G:H8 | 1:2:323:G:O5' | 1.96 | 0.48 |
| 1:2:425:U:O5' | 1:2:425:U:H6 | 1.96 | 0.48 |
| 1:2:595:G:C2 | 1:2:596:G:H1' | 2.48 | 0.48 |
| 1:2:687:C:N4 | 1:2:688:A:N1 | 2.62 | 0.48 |
| 1:2:813:G:C5 | 1:2:815:G:H1' | 2.49 | 0.48 |
| 1:2:1118:G:N7 | 1:2:1119:C:C4 | 2.81 | 0.48 |
| 1:2:1405:U:C2 | 1:2:1406:G:C8 | 3.01 | 0.48 |
| 1:2:1476:A:H2' | 1:2:1477:G:H8 | 1.79 | 0.48 |
| 3:B:128:LYS:O | 3:B:131:ILE:N | 2.47 | 0.48 |
| 9:H:10:PHE:H | 12:K:42:ARG:NH1 | 2.11 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:N:70:ARG:HH21 | 15:N:118:ASP:CG | 2.16 | 0.48 |
| 15:N:98:ASP:OD1 | 15:N:99:GLU:N | 2.46 | 0.48 |
| 16:O:101:ALA:HA | 16:O:104:GLU:HG2 | 1.95 | 0.48 |
| 21:T:49:ARG:O | 21:T:53:LEU:HG | 2.14 | 0.48 |
| 26:Y:17:ARG:HH12 | 29:3:44:GLU:CD | 2.17 | 0.48 |
| 33:7:51:TYR:CE2 | 33:7:294:LEU:HB3 | 2.48 | 0.48 |
| 1:2:120:G:C2 | 1:2:247:G:C2 | 3.02 | 0.48 |
| 1:2:141:G:C6 | 1:2:176:A:C6 | 3.02 | 0.48 |
| 1:2:466:G:N2 | 1:2:467:G:H22 | 2.12 | 0.48 |
| 1:2:930:A:C2 | 21:T:87:LYS:HE2 | 2.49 | 0.48 |
| 1:2:1025:C:H2' | 1:2:1026:G:H8 | 1.77 | 0.48 |
| 1:2:1061:G:N1 | 1:2:1062:U:C4 | 2.81 | 0.48 |
| 1:2:1444:G:C5 | 1:2:1445:C:C4 | 3.02 | 0.48 |
| 2:A:11:LYS:HZ2 | 2:A:13:LYS:H | 1.62 | 0.48 |
| 2:A:98:ARG:O | 2:A:101:THR:OG1 | 2.25 | 0.48 |
| 2:A:116:TYR:N | 2:A:116:TYR:HD1 | 2.11 | 0.48 |
| 5:D:22:ARG:HG3 | 5:D:25:ARG:NH2 | 2.29 | 0.48 |
| 7:F:70:LEU:HD23 | 7:F:70:LEU:H | 1.79 | 0.48 |
| 12:K:51:LEU:HD21 | 12:K:98:LYS:HB3 | 1.96 | 0.48 |
| 15:N:14:ARG:NH2 | 19:R:65:LEU:HB3 | 2.28 | 0.48 |
| 23:V:28:GLU:N | 23:V:28:GLU:OE1 | 2.47 | 0.48 |
| 23:V:62:SER:O | 23:V:62:SER:OG | 2.27 | 0.48 |
| 28:0:1:MET:HE3 | 28:0:23:ILE:HG21 | 1.96 | 0.48 |
| 33:7:58:VAL:HG23 | 33:7:86:LEU:CD1 | 2.43 | 0.48 |
| 33:7:289:ALA:CB | 33:7:295:VAL:HG21 | 2.44 | 0.48 |
| 1:2:486:A:N6 | 1:2:487:G:C4 | 2.81 | 0.48 |
| 1:2:781:A:C8 | 1:2:783:A:C8 | 3.02 | 0.48 |
| 1:2:925:G:H2' | 1:2:926:G:O4' | 2.14 | 0.48 |
| 1:2:1219:G:O2' | 1:2:1220:G:O4' | 2.31 | 0.48 |
| 1:2:1239:4AC:O2 | 1:2:1245:G:N2 | 2.47 | 0.48 |
| 1:2:1437:A:C4 | 1:2:1438:G:C8 | 3.02 | 0.48 |
| 3:B:78:LYS:HB3 | 3:B:79:PRO:HD3 | 1.95 | 0.48 |
| 7:F:122:ILE:HD11 | 7:F:202:PHE:CE1 | 2.48 | 0.48 |
| 29:3:75:ILE:HG12 | 29:3:77:TYR:HB3 | 1.94 | 0.48 |
| 33:7:127:PRO:O | 33:7:341:GLY:HA2 | 2.14 | 0.48 |
| 33:7:130:ARG:HH22 | 33:7:338:ARG:HG3 | 1.78 | 0.48 |
| 1:2:316:G:N2 | 5:D:4:PRO:HD2 | 2.29 | 0.48 |
| 1:2:504:G:C6 | 1:2:505:G:C5 | 3.02 | 0.48 |
| 1:2:680:G:H3' | 1:2:681:G:H8 | 1.77 | 0.48 |
| 1:2:886:A:H2' | 1:2:886:A:N3 | 2.29 | 0.48 |
| 1:2:958:G:C2 | 1:2:959:G:C8 | 3.01 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2:1197:C:H5'' | 1:2:1198:U:H5'' | 1.96 | 0.48 |
| 1:2:1331:G:OP2 | 1:2:1333:C:N4 | 2.47 | 0.48 |
| 1:2:1337:A:C6 | 1:2:1339:C:C2 | 3.02 | 0.48 |
| 3:B:118:THR:O | 3:B:140:LEU:HB2 | 2.13 | 0.48 |
| 6:E:3:ARG:HH21 | 6:E:4:LYS:NZ | 2.12 | 0.48 |
| 6:E:37:HIS:CD2 | 6:E:144:ASP:HB3 | 2.49 | 0.48 |
| 6:E:74:ASP:OD2 | 6:E:123:LYS:NZ | 2.28 | 0.48 |
| 10:I:42:GLN:O | 10:I:45:GLY:N | 2.39 | 0.48 |
| 14:M:133:ARG:CG | 14:M:136:ARG:HD3 | 2.44 | 0.48 |
| 15:N:48:PRO:O | 15:N:49:GLN:HG3 | 2.14 | 0.48 |
| 15:N:87:PHE:O | 15:N:125:LYS:HA | 2.14 | 0.48 |
| 27:Z:25:LEU:O | 27:Z:25:LEU:HD23 | 2.13 | 0.48 |
| 29:3:73:LYS:CE | 29:3:75:ILE:HB | 2.43 | 0.48 |
| 32:6:13:VAL:HG12 | 32:6:14:ILE:H | 1.79 | 0.48 |
| 33:7:217:VAL:HG11 | 33:7:238:ILE:HG23 | 1.96 | 0.48 |
| 1:2:188:U:H1' | 1:2:189:A:N7 | 2.29 | 0.47 |
| 1:2:263:G:C6 | 1:2:282:A:N1 | 2.82 | 0.47 |
| 1:2:481:G:C4 | 1:2:482:U:C5 | 3.02 | 0.47 |
| 1:2:759:A:N3 | 1:2:761:A:C6 | 2.82 | 0.47 |
| 1:2:871:A:C5 | 1:2:872:A:N1 | 2.81 | 0.47 |
| 1:2:1039:A:C2 | 1:2:1067:A:C2 | 3.02 | 0.47 |
| 3:B:13:LEU:HG | 3:B:18:HIS:CE1 | 2.48 | 0.47 |
| 9:H:24:GLU:OE2 | 9:H:24:GLU:N | 2.47 | 0.47 |
| 23:V:33:ARG:NH2 | 23:V:89:ARG:HG2 | 2.29 | 0.47 |
| 31:4:29:G:C4 | 31:4:30:G:C8 | 3.02 | 0.47 |
| 35:9:113:LYS:HD3 | 35:9:113:LYS:HA | 1.65 | 0.47 |
| 1:2:273:C:N4 | 1:2:274:G:C6 | 2.82 | 0.47 |
| 1:2:402:G:N3 | 1:2:403:G:C8 | 2.82 | 0.47 |
| 1:2:412:A:O2' | 1:2:413:G:H5' | 2.14 | 0.47 |
| 1:2:451:A:N3 | 1:2:452:G:H1' | 2.29 | 0.47 |
| 1:2:891:U:C2 | 1:2:892:U:C5 | 3.02 | 0.47 |
| 1:2:919:G:N2 | 1:2:1209:U:O2 | 2.47 | 0.47 |
| 1:2:986:U:H6 | 1:2:986:U:O5' | 1.98 | 0.47 |
| 1:2:1453:G:C5 | 1:2:1454:G:C8 | 3.03 | 0.47 |
| 2:A:15:LYS:O | 2:A:16:LEU:HD23 | 2.14 | 0.47 |
| 9:H:85:PHE:CD2 | 9:H:87:ARG:NH2 | 2.82 | 0.47 |
| 10:I:31:SER:N | 10:I:34:ILE:HD12 | 2.26 | 0.47 |
| 16:O:109:LEU:HD13 | 16:O:116:ARG:HB3 | 1.96 | 0.47 |
| 19:R:64:GLU:HG2 | 19:R:65:LEU:N | 2.29 | 0.47 |
| 24:W:16:LEU:O | 24:W:28:ILE:HA | 2.14 | 0.47 |
| 27:Z:130:ILE:HG23 | 27:Z:146:PHE:HD2 | 1.79 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 33:7:360:SER:O | 33:7:395:THR:HA | 2.14 | 0.47 |
| 1:2:226:U:HO2' | 1:2:227:C:H6 | 1.60 | 0.47 |
| 1:2:236:G:C4 | 1:2:237:A:C8 | 3.02 | 0.47 |
| 1:2:321:G:C2 | 1:2:322:A:C5 | 3.03 | 0.47 |
| 1:2:465:G:C6 | 1:2:466:G:N1 | 2.82 | 0.47 |
| 1:2:513:A:H4' | 1:2:514:G:O5' | 2.14 | 0.47 |
| 1:2:655:G:C2 | 1:2:656:G:C4 | 3.02 | 0.47 |
| 1:2:1028:4AC:H5'' | 1:2:1029:G:OP2 | 2.13 | 0.47 |
| 1:2:1083:C:C2 | 1:2:1084:C:C5 | 3.02 | 0.47 |
| 1:2:1434:U:O5' | 1:2:1434:U:H6 | 1.98 | 0.47 |
| 2:A:42:GLU:OE2 | 2:A:42:GLU:N | 2.45 | 0.47 |
| 5:D:32:LYS:HG3 | 5:D:33:TYR:CD2 | 2.49 | 0.47 |
| 5:D:129:HIS:CG | 5:D:158:SER:HG | 2.29 | 0.47 |
| 11:J:11:LYS:HB3 | 11:J:12:PRO:HD2 | 1.96 | 0.47 |
| 14:M:39:ILE:O | 14:M:74:LYS:NZ | 2.48 | 0.47 |
| 16:O:95:THR:OG1 | 16:O:96:ALA:N | 2.48 | 0.47 |
| 18:Q:100:LYS:HE3 | 18:Q:100:LYS:HB3 | 1.76 | 0.47 |
| 19:R:34:PHE:HE1 | 19:R:51:ARG:HH21 | 1.63 | 0.47 |
| 29:3:16:ALA:HA | 29:3:20:LEU:HD13 | 1.97 | 0.47 |
| 29:3:77:TYR:HE1 | 29:3:123:LYS:HA | 1.80 | 0.47 |
| 30:5:811:U:N3 | 30:5:812:G:N7 | 2.62 | 0.47 |
| 33:7:138:ILE:HG12 | 33:7:410:TRP:HB3 | 1.96 | 0.47 |
| 1:2:46:G:C6 | 1:2:412:A:C6 | 3.02 | 0.47 |
| 1:2:444:U:H2' | 1:2:445:G:C8 | 2.48 | 0.47 |
| 1:2:539:A:N7 | 1:2:540:A:C6 | 2.82 | 0.47 |
| 1:2:886:A:C6 | 1:2:887:G:C8 | 3.02 | 0.47 |
| 1:2:1235:A:C6 | 1:2:1236:C:C2 | 3.01 | 0.47 |
| 1:2:1272:C:C4 | 9:H:177:LYS:HA | 2.49 | 0.47 |
| 1:2:1302:C:C2 | 1:2:1303:G:C8 | 3.02 | 0.47 |
| 2:A:177:LYS:O | 2:A:177:LYS:HD3 | 2.15 | 0.47 |
| 7:F:175:LEU:HD21 | 7:F:205:LEU:HD11 | 1.95 | 0.47 |
| 18:Q:16:ARG:HH21 | 18:Q:62:THR:HG21 | 1.78 | 0.47 |
| 25:X:25:THR:O | 25:X:44:ASN:HA | 2.14 | 0.47 |
| 33:7:14:VAL:CG2 | 33:7:93:ASP:HA | 2.44 | 0.47 |
| 33:7:357:LEU:O | 33:7:367:LEU:HD12 | 2.14 | 0.47 |
| 1:2:46:G:C2 | 1:2:47:G:C5 | 3.03 | 0.47 |
| 1:2:401:G:H2' | 1:2:402:G:C8 | 2.48 | 0.47 |
| 1:2:831:A:C5 | 1:2:832:G:C8 | 3.02 | 0.47 |
| 1:2:1022:G:C5 | 1:2:1178:A:N1 | 2.83 | 0.47 |
| 1:2:1046:G:C2 | 1:2:1047:G:C8 | 3.03 | 0.47 |
| 1:2:1220:G:C2 | 1:2:1221:G:C8 | 3.02 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:2:1303:G:C2 | 1:2:1304:U:C6 | 3.02 | 0.47 |
| 1:2:1408:G:O6 | 1:2:1436:G:N2 | 2.47 | 0.47 |
| 1:2:1452:A:C5 | 33:7:352:ARG:HG3 | 2.50 | 0.47 |
| 5:D:23:LEU:HD23 | 5:D:23:LEU:HA | 1.63 | 0.47 |
| 5:D:169:MET:HA | 5:D:172:GLU:OE1 | 2.14 | 0.47 |
| 8:G:87:LEU:HA | 8:G:104:LYS:HD3 | 1.96 | 0.47 |
| 9:H:206:GLU:O | 9:H:210:ILE:HG12 | 2.15 | 0.47 |
| 10:I:57:ARG:O | 10:I:59:GLY:N | 2.47 | 0.47 |
| 13:L:19:VAL:HA | 13:L:22:GLN:HB2 | 1.96 | 0.47 |
| 20:S:40:ASN:OD1 | 27:Z:193:ILE:HG23 | 2.14 | 0.47 |
| 31:4:21:A:C8 | 31:4:46:A:C2 | 3.02 | 0.47 |
| 32:6:39:VAL:HG23 | 32:6:47:ARG:HB2 | 1.96 | 0.47 |
| 1:2:604:G:C2 | 1:2:605:G:C5 | 3.03 | 0.47 |
| 1:2:863:A:C6 | 1:2:878:A:N7 | 2.83 | 0.47 |
| 1:2:970:A:C2 | 1:2:1005:G:C4 | 3.02 | 0.47 |
| 1:2:993:C:H2' | 1:2:994:U:H6 | 1.75 | 0.47 |
| 1:2:1066:A:C8 | 3:B:125:GLN:NE2 | 2.83 | 0.47 |
| 1:2:1224:A:C5 | 1:2:1261:A:C5 | 3.02 | 0.47 |
| 1:2:1244:G:C6 | 1:2:1245:G:C5 | 3.03 | 0.47 |
| 1:2:1346:C:N4 | 1:2:1347:G:C6 | 2.83 | 0.47 |
| 1:2:1361:U:H2' | 1:2:1362:C:H6 | 1.80 | 0.47 |
| 1:2:1378:5HM:O2 | 1:2:1468:A:C6 | 2.67 | 0.47 |
| 10:I:79:PHE:O | 10:I:124:ARG:HA | 2.14 | 0.47 |
| 18:Q:121:GLY:O | 18:Q:125:ILE:HG13 | 2.14 | 0.47 |
| 22:U:21:LYS:HA | 22:U:52:TYR:CE1 | 2.48 | 0.47 |
| 29:3:113:GLU:OE1 | 29:3:114:ILE:HG12 | 2.14 | 0.47 |
| 30:5:812:G:C6 | 30:5:813:A:C5 | 3.03 | 0.47 |
| 31:4:4:G:O2' | 31:4:5:G:H5' | 2.14 | 0.47 |
| 33:7:269:TYR:HE1 | 33:7:385:PRO:HD2 | 1.77 | 0.47 |
| 1:2:41:G:O6 | 1:2:516:G:C5 | 2.68 | 0.47 |
| 1:2:186:G:C2 | 1:2:187:G:N7 | 2.83 | 0.47 |
| 1:2:373:A2M:HM'1 | 1:2:374:A:N3 | 2.29 | 0.47 |
| 1:2:429:A:C6 | 1:2:430:C:C4 | 3.02 | 0.47 |
| 1:2:525:U:C2 | 1:2:527:U:C4 | 3.02 | 0.47 |
| 1:2:588:A:H8 | 1:2:589:C:C5 | 2.33 | 0.47 |
| 1:2:616:G:C2 | 1:2:617:C:C6 | 3.02 | 0.47 |
| 1:2:618:C:C4 | 1:2:619:U:O4 | 2.68 | 0.47 |
| 1:2:665:C:C2 | 1:2:666:C:C5 | 3.03 | 0.47 |
| 1:2:691:G:OP2 | 1:2:799:G:N2 | 2.47 | 0.47 |
| 1:2:917:G:N1 | 1:2:1311:G:C6 | 2.83 | 0.47 |
| 1:2:1082:G:H5' | 12:K:113:ARG:HG3 | 1.97 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2:1094:C:H4' | 1:2:1095:A:H8 | 1.79 | 0.47 |
| 1:2:1112:A:H2' | 1:2:1113:G:C8 | 2.44 | 0.47 |
| 1:2:1141:A:C5 | 1:2:1143:A:C5 | 3.03 | 0.47 |
| 1:2:1148:G:C2 | 1:2:1149:G:C4 | 3.03 | 0.47 |
| 1:2:1180:G:C6 | 1:2:1181:C:N4 | 2.82 | 0.47 |
| 1:2:1252:U:H5'' | 1:2:1253:A:H5' | 1.96 | 0.47 |
| 1:2:1404:G:H2' | 1:2:1405:U:O4' | 2.15 | 0.47 |
| 3:B:166:LEU:O | 3:B:170:ILE:HG13 | 2.15 | 0.47 |
| 9:H:5:LEU:HA | 9:H:8:ARG:HB3 | 1.97 | 0.47 |
| 10:I:95:PRO:HG2 | 10:I:99:PHE:HB3 | 1.97 | 0.47 |
| 12:K:95:LEU:HD12 | 12:K:95:LEU:HA | 1.75 | 0.47 |
| 14:M:10:LYS:NZ | 14:M:12:GLU:HB2 | 2.30 | 0.47 |
| 20:S:23:GLU:HB3 | 20:S:24:PHE:CE1 | 2.49 | 0.47 |
| 21:T:65:THR:OG1 | 21:T:66:HIS:N | 2.47 | 0.47 |
| 27:Z:82:VAL:HG12 | 27:Z:83:GLN:N | 2.29 | 0.47 |
| 29:3:23:VAL:HA | 29:3:26:ALA:HB3 | 1.96 | 0.47 |
| 33:7:249:VAL:HG23 | 33:7:279:ILE:HG13 | 1.97 | 0.47 |
| 33:7:269:TYR:HE1 | 33:7:384:ARG:HB2 | 1.80 | 0.47 |
| 35:9:180:SER:HA | 35:9:230:ASP:HA | 1.95 | 0.47 |
| 1:2:145:G:H2' | 1:2:146:A:C8 | 2.50 | 0.47 |
| 1:2:312:G:O2' | 1:2:313:G:H5' | 2.15 | 0.47 |
| 1:2:424:C:H4' | 1:2:425:U:H5 | 1.80 | 0.47 |
| 1:2:494:C:H2' | 1:2:495:G:H5' | 1.96 | 0.47 |
| 1:2:519:G:N3 | 1:2:520:G:C8 | 2.82 | 0.47 |
| 1:2:590:4AC:O7 | 1:2:590:4AC:H5 | 2.15 | 0.47 |
| 1:2:637:G:C2 | 1:2:704:G:C5 | 3.03 | 0.47 |
| 1:2:793:C:H4' | 10:I:13:HIS:CE1 | 2.49 | 0.47 |
| 1:2:891:U:H2' | 1:2:892:U:C6 | 2.50 | 0.47 |
| 1:2:989:A:H2' | 1:2:991:G:N7 | 2.30 | 0.47 |
| 1:2:1109:G:C2 | 1:2:1110:G:C8 | 3.03 | 0.47 |
| 1:2:1116:A:C6 | 1:2:1117:G:N2 | 2.83 | 0.47 |
| 1:2:1479:4AC:O7 | 1:2:1479:4AC:H5 | 2.14 | 0.47 |
| 4:C:55:CYS:SG | 4:C:58:CYS:N | 2.73 | 0.47 |
| 11:J:89:PHE:CG | 11:J:94:ILE:HB | 2.50 | 0.47 |
| 23:V:11:ASN:O | 23:V:15:GLY:N | 2.46 | 0.47 |
| 35:9:215:LEU:HG | 35:9:233:GLY:HA2 | 1.97 | 0.47 |
| 1:2:94:G:H2' | 1:2:95:C:C6 | 2.50 | 0.47 |
| 1:2:205:G:C6 | 1:2:206:C:C4 | 3.03 | 0.47 |
| 1:2:645:C:H2' | 1:2:646:C:C6 | 2.50 | 0.47 |
| 1:2:685:G:C6 | 1:2:686:C:C4 | 3.02 | 0.47 |
| 1:2:769:A:C2 | 1:2:770:G:H1' | 2.50 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:2:770:G:H2' | 1:2:771:U:C6 | 2.49 | 0.47 |
| 1:2:897:G:N1 | 1:2:1474:G:N7 | 2.63 | 0.47 |
| 1:2:1304:U:O2' | 16:O:29:LYS:NZ | 2.47 | 0.47 |
| 1:2:1329:G:C6 | 1:2:1342:G:N1 | 2.82 | 0.47 |
| 4:C:14:CYS:CB | 4:C:17:CYS:SG | 2.98 | 0.47 |
| 12:K:51:LEU:HD23 | 12:K:99:PHE:CD1 | 2.50 | 0.47 |
| 13:L:83:ARG:CZ | 13:L:83:ARG:HB2 | 2.44 | 0.47 |
| 16:O:38:MET:O | 16:O:42:VAL:HG22 | 2.15 | 0.47 |
| 21:T:8:TYR:HE2 | 21:T:9:ARG:HE | 1.63 | 0.47 |
| 22:U:68:VAL:O | 22:U:119:ARG:N | 2.44 | 0.47 |
| 23:V:81:ILE:HG13 | 23:V:82:GLU:N | 2.30 | 0.47 |
| 31:4:36:U:H2' | 31:4:37:A:C8 | 2.50 | 0.47 |
| 31:4:60:U:H5'' | 31:4:61:C:C5 | 2.50 | 0.47 |
| 33:7:248:LYS:O | 33:7:276:ILE:HD12 | 2.15 | 0.47 |
| 1:2:27:U:H2' | 1:2:28:G:C8 | 2.50 | 0.47 |
| 1:2:99:C:H2' | 1:2:100:G:O4' | 2.14 | 0.47 |
| 1:2:105:A:C2 | 1:2:336:A:N1 | 2.83 | 0.47 |
| 1:2:255:A:C2 | 1:2:291:A:C4 | 3.03 | 0.47 |
| 1:2:672:U:C5 | 1:2:673:C:C5 | 3.03 | 0.47 |
| 1:2:1261:A:H2' | 1:2:1262:A:C8 | 2.49 | 0.47 |
| 1:2:1398:G:C2 | 1:2:1399:C:C2 | 3.03 | 0.47 |
| 1:2:1409:G:C6 | 1:2:1435:C:N3 | 2.83 | 0.47 |
| 3:B:4:GLU:HG3 | 3:B:4:GLU:O | 2.15 | 0.47 |
| 5:D:124:LEU:HA | 5:D:124:LEU:HD23 | 1.61 | 0.47 |
| 6:E:126:ARG:HB3 | 6:E:143:HIS:HB3 | 1.96 | 0.47 |
| 7:F:77:SER:O | 7:F:77:SER:OG | 2.32 | 0.47 |
| 8:G:99:LYS:HD2 | 8:G:100:GLY:N | 2.30 | 0.47 |
| 9:H:3:LYS:HB3 | 9:H:4:PRO:HD3 | 1.97 | 0.47 |
| 19:R:4:ASP:OD1 | 19:R:6:GLY:N | 2.41 | 0.47 |
| 22:U:106:GLU:O | 22:U:109:GLY:N | 2.48 | 0.47 |
| 31:4:17:C:H4' | 31:4:61:C:H5' | 1.96 | 0.47 |
| 33:7:24:THR:HA | 33:7:27:GLN:HB2 | 1.96 | 0.47 |
| 1:2:66:C:H2' | 1:2:67:G:C8 | 2.48 | 0.46 |
| 1:2:203:A:C2 | 1:2:204:G:C5 | 3.03 | 0.46 |
| 1:2:223:G:H2' | 1:2:224:G:C8 | 2.50 | 0.46 |
| 1:2:605:G:C2 | 1:2:606:G:C8 | 3.02 | 0.46 |
| 1:2:751:4AC:H5 | 1:2:751:4AC:O7 | 2.15 | 0.46 |
| 1:2:991:G:H3' | 1:2:992:U:C6 | 2.48 | 0.46 |
| 1:2:1098:C:H2' | 1:2:1099:C:H6 | 1.80 | 0.46 |
| 1:2:1214:U:C2 | 9:H:93:LEU:HG | 2.50 | 0.46 |
| 1:2:1224:A:C5 | 1:2:1261:A:C8 | 3.03 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2:1349:A:C6 | 1:2:1350:U:C4 | 3.03 | 0.46 |
| 7:F:14:ASP:OD1 | 7:F:14:ASP:N | 2.48 | 0.46 |
| 9:H:209:ARG:O | 9:H:212:GLU:HG3 | 2.15 | 0.46 |
| 12:K:39:GLU:HG3 | 12:K:42:ARG:HH21 | 1.80 | 0.46 |
| 14:M:16:ILE:HD12 | 14:M:80:HIS:HB2 | 1.97 | 0.46 |
| 19:R:42:LYS:HD3 | 19:R:42:LYS:HA | 1.65 | 0.46 |
| 21:T:20:SER:OG | 21:T:24:LEU:N | 2.48 | 0.46 |
| 30:5:807:G:H2' | 30:5:808:A:H8 | 1.79 | 0.46 |
| 31:4:53:G:H3' | 31:4:54:5MU:H71 | 1.97 | 0.46 |
| 1:2:123:G:O4' | 19:R:32:ARG:NH2 | 2.43 | 0.46 |
| 1:2:296:U:H5' | 15:N:36:ARG:HH22 | 1.79 | 0.46 |
| 1:2:621:G:C4 | 1:2:720:A:C6 | 3.03 | 0.46 |
| 1:2:770:G:C4 | 1:2:771:U:C5 | 3.04 | 0.46 |
| 1:2:1022:G:C6 | 1:2:1178:A:C6 | 3.03 | 0.46 |
| 1:2:1162:G:H2' | 1:2:1163:C:O4' | 2.15 | 0.46 |
| 1:2:1168:G:H2' | 1:2:1169:U:O4' | 2.15 | 0.46 |
| 1:2:1324:C:C2 | 1:2:1325:C:C5 | 3.03 | 0.46 |
| 4:C:42:ARG:NH2 | 4:C:47:ARG:HA | 2.30 | 0.46 |
| 16:O:113:ARG:HH12 | 16:O:121:GLU:CD | 2.18 | 0.46 |
| 18:Q:30:VAL:HG23 | 18:Q:31:GLU:OE1 | 2.15 | 0.46 |
| 18:Q:127:SER:OG | 18:Q:128:LYS:N | 2.48 | 0.46 |
| 32:6:16:VAL:O | 32:6:18:LEU:N | 2.48 | 0.46 |
| 32:6:72:TRP:C | 32:6:74:VAL:H | 2.19 | 0.46 |
| 1:2:276:C:OP2 | 19:R:96:LYS:HD2 | 2.16 | 0.46 |
| 1:2:479:4AC:C2 | 1:2:505:G:N2 | 2.77 | 0.46 |
| 1:2:559:G:C5 | 1:2:560:U:C4 | 3.03 | 0.46 |
| 1:2:569:G:C6 | 1:2:570:G:C5 | 3.03 | 0.46 |
| 1:2:648:4AC:H2' | 1:2:649:G:O4' | 2.15 | 0.46 |
| 1:2:778:U:H5 | 1:2:779:G:C5 | 2.33 | 0.46 |
| 1:2:966:C:C2 | 1:2:967:G:C8 | 3.03 | 0.46 |
| 1:2:1115:G:C5 | 1:2:1116:A:C6 | 3.04 | 0.46 |
| 1:2:1147:4AC:H6 | 1:2:1147:4AC:H5'' | 1.96 | 0.46 |
| 1:2:1289:U:C4 | 1:2:1290:G:C5 | 3.04 | 0.46 |
| 1:2:1390:C:H5'' | 1:2:1391:G:OP2 | 2.16 | 0.46 |
| 1:2:1427:G:C4 | 1:2:1428:G:C8 | 3.04 | 0.46 |
| 1:2:1450:U:H2' | 1:2:1451:G:C5' | 2.45 | 0.46 |
| 1:2:1457:G:O2' | 1:2:1458:G:H5' | 2.15 | 0.46 |
| 2:A:145:ILE:HD11 | 2:A:171:ILE:HG22 | 1.97 | 0.46 |
| 3:B:167:ILE:O | 3:B:171:LEU:HB2 | 2.14 | 0.46 |
| 5:D:87:ALA:HB1 | 5:D:91:ASP:HB2 | 1.98 | 0.46 |
| 6:E:167:LYS:HE3 | 6:E:170:GLU:HB3 | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:U:40:HIS:CE1 | 22:U:78:GLY:HA2 | 2.50 | 0.46 |
| 23:V:17:LYS:HG3 | 23:V:71:TYR:HB3 | 1.97 | 0.46 |
| 33:7:144:LEU:HD21 | 33:7:146:ILE:HD11 | 1.98 | 0.46 |
| 33:7:146:ILE:HB | 33:7:179:PRO:O | 2.15 | 0.46 |
| 33:7:301:LEU:O | 35:9:193:VAL:HG13 | 2.15 | 0.46 |
| 35:9:178:LYS:NZ | 35:9:180:SER:HB2 | 2.30 | 0.46 |
| 1:2:89:G:C3' | 1:2:90:G:H8 | 2.27 | 0.46 |
| 1:2:173:C:H2' | 1:2:174:C:C6 | 2.50 | 0.46 |
| 1:2:185:G:C5 | 1:2:186:G:N7 | 2.84 | 0.46 |
| 1:2:196:G:N7 | 19:R:26:HIS:CG | 2.84 | 0.46 |
| 1:2:401:G:C2 | 1:2:402:G:C4 | 3.03 | 0.46 |
| 1:2:733:A:H62 | 1:2:780:U:H3 | 1.64 | 0.46 |
| 1:2:733:A:C6 | 1:2:734:A:C5 | 3.04 | 0.46 |
| 1:2:772:C:N3 | 1:2:773:C:C5 | 2.83 | 0.46 |
| 1:2:833:G:C2 | 1:2:834:G:C5 | 3.03 | 0.46 |
| 1:2:869:G:HO2' | 1:2:871:A:N6 | 2.03 | 0.46 |
| 1:2:894:G:N2 | 1:2:1369:C:O2 | 2.49 | 0.46 |
| 1:2:1006:C:O2' | 1:2:1007:C:H5' | 2.16 | 0.46 |
| 1:2:1224:A:N7 | 1:2:1261:A:C8 | 2.83 | 0.46 |
| 1:2:1252:U:OP1 | 1:2:1252:U:H3' | 2.16 | 0.46 |
| 1:2:1386:C:N3 | 1:2:1457:G:N2 | 2.57 | 0.46 |
| 3:B:187:GLU:HA | 3:B:189:LYS:HE3 | 1.96 | 0.46 |
| 7:F:132:GLU:O | 7:F:134:ARG:N | 2.49 | 0.46 |
| 19:R:18:ASP:N | 19:R:18:ASP:OD1 | 2.46 | 0.46 |
| 27:Z:18:ASP:O | 27:Z:22:GLU:HG3 | 2.15 | 0.46 |
| 1:2:26:C:C2 | 1:2:27:U:C5 | 3.04 | 0.46 |
| 1:2:168:A:C8 | 1:2:169:A:C6 | 3.04 | 0.46 |
| 1:2:262:U:OP1 | 19:R:96:LYS:HD3 | 2.16 | 0.46 |
| 1:2:369:G:C6 | 1:2:370:C:C4 | 3.03 | 0.46 |
| 1:2:392:A:H5'' | 6:E:64:LYS:HE2 | 1.98 | 0.46 |
| 1:2:709:G:N1 | 1:2:710:A:C5 | 2.83 | 0.46 |
| 1:2:973:A:C5 | 29:3:92:ILE:HG21 | 2.50 | 0.46 |
| 1:2:976:A:C5 | 1:2:1001:A:C4 | 3.04 | 0.46 |
| 4:C:59:GLY:O | 4:C:61:GLU:HG3 | 2.16 | 0.46 |
| 6:E:112:LEU:HA | 6:E:112:LEU:HD23 | 1.56 | 0.46 |
| 6:E:185:VAL:HG22 | 6:E:186:PHE:H | 1.81 | 0.46 |
| 7:F:175:LEU:HD23 | 7:F:175:LEU:HA | 1.45 | 0.46 |
| 9:H:121:GLN:HG3 | 9:H:125:TRP:CZ3 | 2.51 | 0.46 |
| 10:I:55:ASP:O | 18:Q:18:PRO:HB3 | 2.15 | 0.46 |
| 16:O:99:ASP:HB2 | 16:O:103:ARG:HH21 | 1.80 | 0.46 |
| 16:O:105:ASP:HA | 16:O:108:ARG:HH12 | 1.80 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 19:R:11:PRO:HA | 19:R:23:TRP:CH2 | 2.51 | 0.46 |
| 20:S:2:GLY:C | 20:S:4:ILE:H | 2.19 | 0.46 |
| 24:W:21:ILE:HG12 | 24:W:59:LYS:NZ | 2.30 | 0.46 |
| 31:4:25:C:C2 | 31:4:26:G:C8 | 3.04 | 0.46 |
| 32:6:97:LYS:HB3 | 32:6:99:LYS:HD3 | 1.97 | 0.46 |
| 33:7:191:ILE:O | 33:7:194:LEU:HB3 | 2.15 | 0.46 |
| 33:7:249:VAL:HG12 | 33:7:250:ASP:CG | 2.35 | 0.46 |
| 1:2:22:G:H2' | 1:2:23:A:H8 | 1.81 | 0.46 |
| 1:2:41:G:H2' | 1:2:42:C:C6 | 2.51 | 0.46 |
| 1:2:108:G:C2 | 1:2:109:C:C6 | 3.03 | 0.46 |
| 1:2:178:A:N3 | 1:2:209:A:N1 | 2.64 | 0.46 |
| 1:2:315:A:N6 | 1:2:316:G:O6 | 2.49 | 0.46 |
| 1:2:334:A:N6 | 1:2:335:G:C2 | 2.84 | 0.46 |
| 1:2:685:G:C5 | 1:2:686:C:C4 | 3.04 | 0.46 |
| 1:2:731:4AC:H2' | 1:2:732:G:C8 | 2.50 | 0.46 |
| 1:2:781:A:H5'' | 1:2:783:A:N7 | 2.30 | 0.46 |
| 1:2:851:4AC:CM7 | 15:N:3:GLY:H | 2.27 | 0.46 |
| 1:2:1306:A:C2 | 1:2:1307:A:C5 | 3.04 | 0.46 |
| 1:2:1404:G:C2 | 1:2:1440:C:N3 | 2.84 | 0.46 |
| 1:2:1431:G:H2' | 1:2:1432:G:H8 | 1.80 | 0.46 |
| 3:B:68:LEU:HD21 | 3:B:110:PHE:CE2 | 2.51 | 0.46 |
| 13:L:1:MET:HG3 | 13:L:2:GLN:H | 1.81 | 0.46 |
| 15:N:42:ASP:O | 15:N:44:LEU:N | 2.49 | 0.46 |
| 31:4:14:A:C8 | 31:4:22:G:C2 | 3.04 | 0.46 |
| 33:7:7:GLN:HB2 | 33:7:281:PHE:CE2 | 2.50 | 0.46 |
| 33:7:311:LEU:H | 33:7:311:LEU:HD23 | 1.81 | 0.46 |
| 1:2:44:A:C6 | 1:2:406:A:C8 | 3.04 | 0.46 |
| 1:2:157:A:O4' | 1:2:353:A:C8 | 2.69 | 0.46 |
| 1:2:193:G:N2 | 6:E:207:MET:HA | 2.31 | 0.46 |
| 1:2:331:C:C2 | 1:2:332:U:C5 | 3.04 | 0.46 |
| 1:2:451:A:C2 | 1:2:452:G:H1' | 2.51 | 0.46 |
| 1:2:465:G:C2 | 1:2:466:G:C2 | 3.03 | 0.46 |
| 1:2:641:G:C2 | 1:2:642:U:C4 | 3.04 | 0.46 |
| 1:2:651:G:N1 | 1:2:652:G:N2 | 2.63 | 0.46 |
| 1:2:1042:G:C2 | 1:2:1046:G:C2 | 3.04 | 0.46 |
| 1:2:1053:A:C5 | 1:2:1054:C:C4 | 3.03 | 0.46 |
| 1:2:1298:C:H4' | 1:2:1336:C:H4' | 1.98 | 0.46 |
| 1:2:1396:G:C2 | 1:2:1448:C:H1' | 2.51 | 0.46 |
| 1:2:1398:G:OP2 | 1:2:1398:G:H8 | 1.99 | 0.46 |
| 7:F:107:GLY:O | 7:F:110:ILE:N | 2.48 | 0.46 |
| 7:F:135:CYS:C | 7:F:136:ARG:HD3 | 2.36 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:X:53:ASP:O | 25:X:54:ILE:HD13 | 2.16 | 0.46 |
| 33:7:3:TRP:HZ2 | 33:7:57:GLY:HA3 | 1.81 | 0.46 |
| 33:7:353:ALA:HB2 | 33:7:373:VAL:HG23 | 1.97 | 0.46 |
| 33:7:356:THR:HB | 33:7:367:LEU:HD11 | 1.98 | 0.46 |
| 1:2:59:A:N6 | 1:2:112:A:C4 | 2.84 | 0.46 |
| 1:2:559:G:C2 | 1:2:560:U:C2 | 3.04 | 0.46 |
| 1:2:600:G:C2 | 1:2:601:C:C5 | 3.03 | 0.46 |
| 1:2:799:G:C4 | 1:2:800:U:C6 | 3.03 | 0.46 |
| 1:2:911:G:N3 | 1:2:912:G:C8 | 2.84 | 0.46 |
| 1:2:1031:C:H6 | 1:2:1031:C:O5' | 1.99 | 0.46 |
| 1:2:1140:G:N1 | 1:2:1143:A:OP2 | 2.46 | 0.46 |
| 1:2:1264:C:C2 | 1:2:1265:C:C5 | 3.04 | 0.46 |
| 1:2:1399:C:C2 | 1:2:1400:C:C6 | 3.04 | 0.46 |
| 1:2:1419:C:C4 | 1:2:1420:U:C4 | 3.04 | 0.46 |
| 1:2:1429:U:H2' | 1:2:1430:C:H6 | 1.80 | 0.46 |
| 5:D:33:TYR:HA | 5:D:118:MET:SD | 2.56 | 0.46 |
| 9:H:212:GLU:HA | 9:H:215:ARG:HG2 | 1.97 | 0.46 |
| 11:J:3:ILE:O | 11:J:29:GLY:N | 2.41 | 0.46 |
| 11:J:62:TYR:CG | 11:J:74:LYS:HE3 | 2.51 | 0.46 |
| 12:K:87:VAL:O | 12:K:91:GLY:HA2 | 2.16 | 0.46 |
| 20:S:27:ASP:OD2 | 20:S:29:GLU:HB3 | 2.16 | 0.46 |
| 22:U:47:GLN:OE1 | 22:U:47:GLN:N | 2.32 | 0.46 |
| 22:U:90:PHE:CD1 | 22:U:91:TYR:N | 2.84 | 0.46 |
| 25:X:66:GLU:CD | 25:X:67:ILE:H | 2.18 | 0.46 |
| 29:3:1:MET:H1 | 29:3:53:ILE:HD12 | 1.80 | 0.46 |
| 29:3:48:ALA:HB1 | 29:3:51:VAL:HB | 1.98 | 0.46 |
| 31:4:29:G:C2 | 31:4:30:G:C5 | 3.03 | 0.46 |
| 31:4:34:C:H2' | 31:4:35:A:C8 | 2.51 | 0.46 |
| 33:7:138:ILE:CD1 | 33:7:410:TRP:HB3 | 2.46 | 0.46 |
| 34:8:41:THR:HG22 | 34:8:84:GLN:HA | 1.96 | 0.46 |
| 35:9:247:ILE:HG22 | 35:9:251:ILE:HD11 | 1.97 | 0.46 |
| 1:2:566:C:H2' | 1:2:567:C:H6 | 1.81 | 0.46 |
| 1:2:745:G:C6 | 1:2:746:C:C4 | 3.04 | 0.46 |
| 1:2:831:A:C2 | 1:2:832:G:H1' | 2.50 | 0.46 |
| 1:2:871:A:N7 | 1:2:872:A:C6 | 2.84 | 0.46 |
| 1:2:892:U:C2 | 1:2:893:G:C8 | 3.04 | 0.46 |
| 1:2:1113:G:N1 | 1:2:1114:G:C5 | 2.84 | 0.46 |
| 1:2:1247:G:C5 | 1:2:1248:G:H1' | 2.51 | 0.46 |
| 1:2:1368:A:N6 | 1:2:1470:C:H5' | 2.31 | 0.46 |
| 1:2:1386:C:C2 | 1:2:1387:A:C8 | 3.04 | 0.46 |
| 1:2:1388:C:C2 | 1:2:1389:C:C5 | 3.04 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:D:102:GLU:O | 5:D:104:ARG:N | 2.49 | 0.46 |
| 5:D:111:LYS:HD2 | 5:D:111:LYS:HA | 1.76 | 0.46 |
| 6:E:172:GLU:OE2 | 6:E:173:ILE:N | 2.49 | 0.46 |
| 6:E:191:LYS:HB3 | 6:E:191:LYS:HE2 | 1.70 | 0.46 |
| 9:H:92:SER:OG | 9:H:94:ASN:ND2 | 2.48 | 0.46 |
| 18:Q:77:THR:OG1 | 18:Q:80:ARG:HB2 | 2.16 | 0.46 |
| 19:R:42:LYS:HB2 | 19:R:43:PRO:HD3 | 1.98 | 0.46 |
| 22:U:70:ILE:O | 22:U:73:LEU:N | 2.49 | 0.46 |
| 31:4:14:A:C6 | 31:4:22:G:O4' | 2.69 | 0.46 |
| 31:4:51:C:H2' | 31:4:52:G:O4' | 2.16 | 0.46 |
| 33:7:333:TYR:HE1 | 33:7:378:ILE:HB | 1.78 | 0.46 |
| 33:7:346:LEU:HD12 | 33:7:347:LYS:O | 2.16 | 0.46 |
| 34:8:11:LEU:HA | 34:8:14:LEU:HB2 | 1.98 | 0.46 |
| 34:8:89:SER:O | 34:8:93:ASN:ND2 | 2.37 | 0.46 |
| 1:2:196:G:H2' | 1:2:196:G:N3 | 2.31 | 0.46 |
| 1:2:252:A:C2 | 1:2:254:U:C4 | 3.04 | 0.46 |
| 1:2:582:G:H2' | 1:2:582:G:N3 | 2.30 | 0.46 |
| 1:2:702:C:C2 | 1:2:703:4AC:C5 | 2.98 | 0.46 |
| 1:2:711:A:H2' | 1:2:712:C:O4' | 2.16 | 0.46 |
| 1:2:782:A:N6 | 1:2:1478:C:H1' | 2.31 | 0.46 |
| 1:2:1321:G:N2 | 1:2:1347:G:C4 | 2.84 | 0.46 |
| 1:2:1323:A:N6 | 1:2:1347:G:N2 | 2.64 | 0.46 |
| 1:2:1392:A:H5' | 1:2:1452:A:H61 | 1.81 | 0.46 |
| 1:2:1395:G:C2 | 1:2:1449:G:C6 | 3.03 | 0.46 |
| 1:2:1407:A:H2' | 1:2:1407:A:N3 | 2.30 | 0.46 |
| 1:2:1508:C:C2 | 30:5:807:G:N2 | 2.83 | 0.46 |
| 2:A:100:ARG:HG2 | 2:A:129:ARG:HH21 | 1.81 | 0.46 |
| 2:A:167:ILE:HB | 2:A:186:ILE:HD11 | 1.97 | 0.46 |
| 3:B:135:ILE:HG13 | 3:B:136:PRO:O | 2.16 | 0.46 |
| 9:H:134:GLU:HA | 9:H:151:ASP:HA | 1.97 | 0.46 |
| 9:H:194:LYS:HB2 | 9:H:194:LYS:HE3 | 1.78 | 0.46 |
| 30:5:816:U:C2 | 30:5:817:A:C8 | 3.04 | 0.46 |
| 33:7:144:LEU:O | 33:7:145:ILE:HD13 | 2.16 | 0.46 |
| 33:7:214:VAL:HB | 33:7:244:GLN:NE2 | 2.31 | 0.46 |
| 33:7:329:ILE:HD12 | 33:7:331:ILE:HD11 | 1.98 | 0.46 |
| 1:2:164:G:C2 | 1:2:165:G:C5 | 3.03 | 0.45 |
| 1:2:336:A:C2 | 1:2:338:A:C8 | 3.04 | 0.45 |
| 1:2:496:G:OP1 | 1:2:496:G:H2' | 2.16 | 0.45 |
| 1:2:678:G:H2' | 1:2:679:G:C8 | 2.51 | 0.45 |
| 1:2:999:G:H3' | 1:2:1000:G:C8 | 2.51 | 0.45 |
| 1:2:1467:UR3:C5 | 30:5:820:U:H5' | 2.46 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-------------------|--------------------------|-------------------|
| 5:D:76:ARG:O | 5:D:79:ARG:N | 2.49 | 0.45 |
| 5:D:106:GLN:O | 5:D:109:VAL:HG12 | 2.16 | 0.45 |
| 6:E:47:TYR:HD1 | 6:E:47:TYR:HA | 1.57 | 0.45 |
| 6:E:205:PHE:CE2 | 6:E:211:ASP:HA | 2.51 | 0.45 |
| 7:F:50:ILE:HG13 | 7:F:51:ASP:H | 1.80 | 0.45 |
| 8:G:81:PRO:HG3 | 8:G:111:THR:HB | 1.98 | 0.45 |
| 21:T:34:ARG:O | 21:T:36:LEU:N | 2.49 | 0.45 |
| 21:T:53:LEU:O | 21:T:57:GLY:N | 2.48 | 0.45 |
| 29:3:34:LYS:NZ | 29:3:92:ILE:HG22 | 2.30 | 0.45 |
| 29:3:114:ILE:O | 29:3:118:VAL:HG22 | 2.16 | 0.45 |
| 31:4:26:G:C6 | 31:4:27:U:C4 | 3.04 | 0.45 |
| 33:7:11:ASN:H | 33:7:112:ASP:HB2 | 1.81 | 0.45 |
| 1:2:149:A:H5' | 1:2:150:C:OP2 | 2.16 | 0.45 |
| 1:2:205:G:C2 | 1:2:206:C:C2 | 3.05 | 0.45 |
| 1:2:359:C:C2 | 1:2:360:G:C2 | 3.04 | 0.45 |
| 1:2:402:G:C2 | 1:2:403:G:C8 | 3.04 | 0.45 |
| 1:2:705:G:C4 | 1:2:706:C:C5 | 3.04 | 0.45 |
| 1:2:709:G:C2 | 1:2:710:A:C5 | 3.04 | 0.45 |
| 1:2:734:A:N6 | 1:2:780:U:N3 | 2.64 | 0.45 |
| 1:2:738:C:H2' | 1:2:739:A:O4' | 2.15 | 0.45 |
| 1:2:862:U:C4 | 1:2:877:G:N2 | 2.85 | 0.45 |
| 1:2:999:G:H2' | 1:2:999:G:N3 | 2.31 | 0.45 |
| 1:2:1192:C:N4 | 1:2:1193:4AC:HM72 | 2.30 | 0.45 |
| 1:2:1329:G:C4 | 1:2:1342:G:N2 | 2.84 | 0.45 |
| 1:2:1480:G:H2' | 1:2:1481:U:H6 | 1.82 | 0.45 |
| 6:E:31:ARG:HG3 | 6:E:32:PRO:HD2 | 1.97 | 0.45 |
| 9:H:172:LYS:NZ | 9:H:186:GLU:HB2 | 2.31 | 0.45 |
| 25:X:62:ARG:HD2 | 25:X:62:ARG:HA | 1.77 | 0.45 |
| 29:3:48:ALA:HB1 | 29:3:100:ALA:HB1 | 1.98 | 0.45 |
| 30:5:808:A:N1 | 30:5:809:G:C5 | 2.85 | 0.45 |
| 31:4:37:A:C2 | 31:4:38:A:C4 | 3.03 | 0.45 |
| 32:6:88:GLN:NE2 | 32:6:91:VAL:HG11 | 2.31 | 0.45 |
| 33:7:45:MET:O | 33:7:47:ILE:HG13 | 2.17 | 0.45 |
| 33:7:53:GLU:OE2 | 33:7:281:PHE:HD1 | 2.00 | 0.45 |
| 33:7:234:LYS:NZ | 33:7:277:SER:HB3 | 2.30 | 0.45 |
| 1:2:67:G:C6 | 1:2:363:G:C5 | 3.04 | 0.45 |
| 1:2:124:G:H2' | 1:2:125:U:C6 | 2.51 | 0.45 |
| 1:2:124:G:H2' | 1:2:125:U:H6 | 1.80 | 0.45 |
| 1:2:157:A:H2' | 1:2:158:A:C8 | 2.52 | 0.45 |
| 1:2:383:A:C2 | 1:2:384:U:C4 | 3.05 | 0.45 |
| 1:2:671:A:C5 | 1:2:672:U:C5 | 3.04 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2:759:A:H1' | 1:2:761:A:N7 | 2.31 | 0.45 |
| 1:2:781:A:H8 | 1:2:783:A:C8 | 2.35 | 0.45 |
| 1:2:904:A:C6 | 1:2:907:A:C4 | 3.04 | 0.45 |
| 1:2:1126:G:C2 | 1:2:1127:G:C4 | 3.05 | 0.45 |
| 1:2:1142:U:O2' | 1:2:1143:A:O5' | 2.26 | 0.45 |
| 1:2:1157:G:H3' | 1:2:1158:G:H5'' | 1.97 | 0.45 |
| 3:B:26:LYS:O | 3:B:26:LYS:HD3 | 2.17 | 0.45 |
| 3:B:43:LEU:HD23 | 3:B:155:PRO:HB2 | 1.98 | 0.45 |
| 13:L:26:ILE:HG21 | 13:L:84:GLN:CB | 2.46 | 0.45 |
| 18:Q:22:PRO:HB3 | 18:Q:66:PHE:HE1 | 1.80 | 0.45 |
| 19:R:47:VAL:HG13 | 19:R:74:ASN:HB2 | 1.98 | 0.45 |
| 24:W:25:ASN:OD1 | 24:W:26:GLU:N | 2.49 | 0.45 |
| 29:3:15:LEU:O | 29:3:19:ALA:HB3 | 2.16 | 0.45 |
| 31:4:12:G:C6 | 31:4:24:U:C2 | 3.04 | 0.45 |
| 33:7:144:LEU:HD12 | 33:7:145:ILE:N | 2.31 | 0.45 |
| 33:7:378:ILE:HG12 | 33:7:380:VAL:HG23 | 1.98 | 0.45 |
| 1:2:30:C:H5'' | 1:2:31:G:OP2 | 2.16 | 0.45 |
| 1:2:144:G:H2' | 1:2:145:G:C8 | 2.52 | 0.45 |
| 1:2:464:A:O2' | 1:2:465:G:N7 | 2.43 | 0.45 |
| 1:2:604:G:H2' | 1:2:605:G:H8 | 1.82 | 0.45 |
| 1:2:793:C:C2 | 1:2:794:U:C5 | 3.03 | 0.45 |
| 1:2:1041:4AC:H3' | 1:2:1041:4AC:H6 | 1.98 | 0.45 |
| 1:2:1173:U:H2' | 1:2:1174:C:H5'' | 1.99 | 0.45 |
| 1:2:1236:C:P | 22:U:72:ARG:HE | 2.39 | 0.45 |
| 2:A:131:GLN:OE1 | 2:A:131:GLN:N | 2.38 | 0.45 |
| 6:E:110:LEU:HD23 | 6:E:110:LEU:HA | 1.76 | 0.45 |
| 6:E:183:ALA:O | 6:E:198:ARG:HG3 | 2.16 | 0.45 |
| 7:F:53:LEU:HD23 | 7:F:53:LEU:HA | 1.65 | 0.45 |
| 16:O:108:ARG:NH1 | 16:O:108:ARG:HB2 | 2.31 | 0.45 |
| 31:4:17:C:OP1 | 31:4:60:U:O2' | 2.33 | 0.45 |
| 31:4:25:C:C4 | 31:4:26:G:C8 | 3.04 | 0.45 |
| 33:7:374:LYS:HD2 | 33:7:374:LYS:HA | 1.82 | 0.45 |
| 1:2:80:G:C6 | 1:2:81:U:C4 | 3.04 | 0.45 |
| 1:2:90:G:C6 | 1:2:91:G:C5 | 3.05 | 0.45 |
| 1:2:470:G:C8 | 1:2:501:A:C4 | 3.04 | 0.45 |
| 1:2:520:G:H5'' | 1:2:521:C:OP2 | 2.17 | 0.45 |
| 1:2:595:G:C4 | 1:2:596:G:C8 | 3.05 | 0.45 |
| 1:2:945:C:C4 | 1:2:947:G:C5 | 3.05 | 0.45 |
| 1:2:1053:A:H2' | 1:2:1054:C:C6 | 2.52 | 0.45 |
| 1:2:1081:C:H2' | 1:2:1082:G:C8 | 2.52 | 0.45 |
| 1:2:1086:C:C2 | 1:2:1127:G:N2 | 2.85 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:2:1166:C:C5 | 1:2:1167:G:C5 | 3.05 | 0.45 |
| 1:2:1398:G:O2' | 1:2:1399:C:O4' | 2.33 | 0.45 |
| 1:2:1420:U:O2' | 1:2:1421:U:H2' | 2.17 | 0.45 |
| 1:2:1424:G:N1 | 1:2:1425:G:C5 | 2.84 | 0.45 |
| 1:2:1484:G:C4 | 1:2:1485:G:C8 | 3.05 | 0.45 |
| 7:F:44:ILE:HG22 | 7:F:119:LEU:HD23 | 1.98 | 0.45 |
| 16:O:33:ILE:HG23 | 16:O:34:ASN:H | 1.82 | 0.45 |
| 18:Q:116:LEU:O | 18:Q:119:MET:N | 2.50 | 0.45 |
| 19:R:101:VAL:HG22 | 19:R:102:VAL:O | 2.16 | 0.45 |
| 26:Y:42:ARG:NH2 | 26:Y:43:CYS:SG | 2.89 | 0.45 |
| 33:7:86:LEU:O | 33:7:87:ARG:HB2 | 2.15 | 0.45 |
| 1:2:63:A:C5 | 1:2:64:U:C5 | 3.05 | 0.45 |
| 1:2:142:G:N1 | 1:2:143:G:C5 | 2.85 | 0.45 |
| 1:2:218:C:C4 | 1:2:219:G:C8 | 3.04 | 0.45 |
| 1:2:314:G:H2' | 1:2:314:G:N3 | 2.31 | 0.45 |
| 1:2:359:C:H2' | 1:2:360:G:N3 | 2.32 | 0.45 |
| 1:2:470:G:C5 | 1:2:501:A:C2 | 3.04 | 0.45 |
| 1:2:582:G:O6 | 1:2:590:4AC:HM72 | 2.17 | 0.45 |
| 1:2:718:4AC:C7 | 1:2:719:G:N1 | 2.77 | 0.45 |
| 1:2:832:G:C2 | 1:2:833:G:C4 | 3.05 | 0.45 |
| 1:2:1451:G:O2' | 33:7:352:ARG:NH2 | 2.49 | 0.45 |
| 1:2:1471:A:N6 | 1:2:1473:G:C2 | 2.85 | 0.45 |
| 1:2:1481:U:C2 | 1:2:1482:A:C8 | 3.05 | 0.45 |
| 2:A:44:VAL:HG22 | 2:A:47:ARG:CZ | 2.46 | 0.45 |
| 6:E:76:ARG:HB2 | 6:E:78:ARG:NH2 | 2.32 | 0.45 |
| 9:H:153:SER:OG | 9:H:154:PRO:HD2 | 2.17 | 0.45 |
| 9:H:166:ALA:O | 9:H:170:SER:OG | 2.19 | 0.45 |
| 12:K:118:LYS:HA | 12:K:118:LYS:HD3 | 1.75 | 0.45 |
| 14:M:12:GLU:HB3 | 14:M:14:TRP:HE1 | 1.82 | 0.45 |
| 15:N:4:LYS:NZ | 15:N:8:ASN:HD22 | 2.14 | 0.45 |
| 16:O:57:GLU:H | 16:O:57:GLU:CD | 2.09 | 0.45 |
| 23:V:11:ASN:OD1 | 23:V:14:ILE:N | 2.46 | 0.45 |
| 24:W:29:VAL:HG12 | 24:W:30:PHE:N | 2.31 | 0.45 |
| 25:X:29:VAL:O | 25:X:40:VAL:HG13 | 2.16 | 0.45 |
| 27:Z:51:PRO:HA | 27:Z:54:VAL:HG12 | 1.97 | 0.45 |
| 1:2:67:G:C4 | 1:2:340:G:N2 | 2.85 | 0.45 |
| 1:2:809:C:H3' | 1:2:810:U:C6 | 2.51 | 0.45 |
| 1:2:951:C:C4 | 1:2:952:C:C5 | 3.05 | 0.45 |
| 1:2:1261:A:C6 | 1:2:1262:A:C6 | 3.05 | 0.45 |
| 5:D:131:GLU:OE2 | 5:D:134:GLY:HA2 | 2.17 | 0.45 |
| 13:L:78:ASP:O | 13:L:81:ALA:N | 2.43 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:M:33:ILE:HG23 | 14:M:34:THR:N | 2.31 | 0.45 |
| 16:O:9:ARG:HA | 16:O:14:ASP:HA | 1.98 | 0.45 |
| 18:Q:26:LEU:HD21 | 18:Q:59:GLY:O | 2.16 | 0.45 |
| 21:T:52:ARG:O | 21:T:56:LYS:HG2 | 2.17 | 0.45 |
| 25:X:59:GLU:O | 25:X:61:GLU:N | 2.50 | 0.45 |
| 26:Y:27:PRO:HG2 | 29:3:45:ARG:HG2 | 1.98 | 0.45 |
| 28:0:4:ARG:HD2 | 28:0:7:LYS:HE2 | 1.98 | 0.45 |
| 29:3:25:ILE:HA | 29:3:28:ASP:OD1 | 2.17 | 0.45 |
| 31:4:22:G:H2' | 31:4:23:C:C6 | 2.52 | 0.45 |
| 33:7:300:TYR:HB3 | 35:9:191:LEU:HD23 | 1.99 | 0.45 |
| 33:7:329:ILE:HG21 | 33:7:386:VAL:CG1 | 2.46 | 0.45 |
| 1:2:22:G:N3 | 1:2:23:A:C8 | 2.85 | 0.45 |
| 1:2:44:A:C2 | 1:2:406:A:C5 | 3.04 | 0.45 |
| 1:2:174:C:C2 | 1:2:175:C:C5 | 3.04 | 0.45 |
| 1:2:304:G:C6 | 1:2:312:G:N1 | 2.85 | 0.45 |
| 1:2:656:G:OP1 | 14:M:25:ASN:ND2 | 2.50 | 0.45 |
| 1:2:694:G:N1 | 1:2:698:G:C6 | 2.84 | 0.45 |
| 1:2:1196:G:C2 | 1:2:1197:C:C4 | 3.04 | 0.45 |
| 1:2:1397:G:C2 | 1:2:1398:G:N7 | 2.85 | 0.45 |
| 1:2:1424:G:C2 | 1:2:1425:G:C4 | 3.04 | 0.45 |
| 7:F:58:ASN:OD1 | 7:F:58:ASN:N | 2.45 | 0.45 |
| 7:F:120:ASN:O | 7:F:122:ILE:HG23 | 2.17 | 0.45 |
| 10:I:17:SER:O | 10:I:22:LYS:HB2 | 2.17 | 0.45 |
| 10:I:55:ASP:OD2 | 24:W:8:ILE:HG12 | 2.16 | 0.45 |
| 18:Q:45:TYR:HD1 | 18:Q:45:TYR:HA | 1.58 | 0.45 |
| 22:U:73:LEU:HA | 22:U:73:LEU:HD23 | 1.51 | 0.45 |
| 33:7:100:LEU:HA | 33:7:100:LEU:HD12 | 1.61 | 0.45 |
| 33:7:213:PRO:HG3 | 33:7:245:GLY:HA3 | 1.98 | 0.45 |
| 33:7:347:LYS:HG3 | 33:7:349:ASP:OD1 | 2.16 | 0.45 |
| 34:8:106:CYS:HB2 | 34:8:110:LYS:HA | 1.99 | 0.45 |
| 1:2:69:G:N3 | 1:2:103:G:N2 | 2.65 | 0.45 |
| 1:2:211:A:N1 | 1:2:229:G:O2' | 2.47 | 0.45 |
| 1:2:225:C:O2' | 1:2:226:U:H5' | 2.17 | 0.45 |
| 1:2:273:C:C4 | 1:2:274:G:C5 | 3.04 | 0.45 |
| 1:2:702:C:H2' | 1:2:703:4AC:C6 | 2.40 | 0.45 |
| 1:2:739:A:N1 | 1:2:775:G:C6 | 2.85 | 0.45 |
| 1:2:861:G:H3' | 28:0:1:MET:HE2 | 1.98 | 0.45 |
| 1:2:959:G:H2' | 1:2:960:G:H8 | 1.82 | 0.45 |
| 1:2:1020:A:N1 | 1:2:1180:G:C4 | 2.85 | 0.45 |
| 1:2:1135:C:H2' | 1:2:1136:C:C6 | 2.52 | 0.45 |
| 1:2:1238:C:N3 | 1:2:1246:G:C2 | 2.85 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2:1294:C:C2 | 1:2:1295:U:C5 | 3.04 | 0.45 |
| 1:2:1313:A:O2' | 31:4:40:C:O2' | 2.35 | 0.45 |
| 1:2:1430:C:H2' | 1:2:1431:G:H8 | 1.82 | 0.45 |
| 2:A:132:THR:C | 2:A:135:GLU:H | 2.18 | 0.45 |
| 8:G:94:PHE:CE2 | 8:G:96:PRO:HA | 2.51 | 0.45 |
| 18:Q:57:GLN:HG3 | 24:W:37:VAL:HG13 | 1.98 | 0.45 |
| 21:T:20:SER:OG | 21:T:23:GLU:HB3 | 2.17 | 0.45 |
| 21:T:61:LYS:HG3 | 21:T:62:PRO:HD2 | 1.98 | 0.45 |
| 27:Z:126:ARG:HH12 | 27:Z:188:ARG:NH1 | 2.15 | 0.45 |
| 27:Z:179:LYS:HB2 | 27:Z:179:LYS:HE3 | 1.84 | 0.45 |
| 31:4:52:G:C6 | 31:4:63:G:C6 | 3.05 | 0.45 |
| 31:4:52:G:C2 | 31:4:53:G:C8 | 3.05 | 0.45 |
| 1:2:55:A:C5 | 1:2:315:A:C5 | 3.05 | 0.45 |
| 1:2:69:G:C2 | 1:2:70:U:C2 | 3.05 | 0.45 |
| 1:2:133:C:H2' | 1:2:134:C:C6 | 2.51 | 0.45 |
| 1:2:186:G:H1 | 1:2:200:C:H42 | 1.64 | 0.45 |
| 1:2:470:G:C2 | 1:2:471:G:C5 | 3.05 | 0.45 |
| 1:2:631:G:OP1 | 2:A:132:THR:N | 2.50 | 0.45 |
| 1:2:726:A:H8 | 1:2:727:G:C8 | 2.34 | 0.45 |
| 1:2:741:G:N1 | 1:2:773:C:C4 | 2.85 | 0.45 |
| 1:2:770:G:C2 | 1:2:771:U:C2 | 3.05 | 0.45 |
| 1:2:950:A:N1 | 1:2:1293:A:C4 | 2.85 | 0.45 |
| 1:2:1092:G:H5' | 1:2:1254:A:O2' | 2.17 | 0.45 |
| 1:2:1098:C:H2' | 1:2:1099:C:C6 | 2.52 | 0.45 |
| 1:2:1147:4AC:H6 | 1:2:1147:4AC:C5' | 2.47 | 0.45 |
| 1:2:1466:G:H21 | 1:2:1488:MA6:C2 | 2.30 | 0.45 |
| 2:A:17:LYS:HD3 | 2:A:39:ASP:OD1 | 2.17 | 0.45 |
| 2:A:121:MET:SD | 2:A:188:LYS:HB3 | 2.57 | 0.45 |
| 5:D:46:THR:HG22 | 5:D:50:ASN:ND2 | 2.30 | 0.45 |
| 8:G:32:LYS:HA | 8:G:32:LYS:HD3 | 1.72 | 0.45 |
| 19:R:9:ILE:HG13 | 19:R:10:GLN:H | 1.82 | 0.45 |
| 19:R:60:TYR:O | 19:R:62:ARG:HG3 | 2.17 | 0.45 |
| 25:X:12:ILE:HD13 | 25:X:30:ARG:HB3 | 1.99 | 0.45 |
| 26:Y:5:TRP:HB3 | 29:3:37:ASN:ND2 | 2.31 | 0.45 |
| 26:Y:17:ARG:NH1 | 29:3:44:GLU:OE2 | 2.50 | 0.45 |
| 27:Z:188:ARG:HH11 | 27:Z:188:ARG:H | 1.65 | 0.45 |
| 29:3:40:THR:HG23 | 29:3:41:LYS:N | 2.32 | 0.45 |
| 30:5:821:G:N1 | 31:4:35:A:C6 | 2.85 | 0.45 |
| 31:4:19:G:N2 | 31:4:57:A:H1' | 2.32 | 0.45 |
| 33:7:26:VAL:HG21 | 33:7:93:ASP:OD1 | 2.16 | 0.45 |
| 35:9:219:ILE:HD12 | 35:9:229:VAL:HG23 | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:2:187:G:C6 | 1:2:200:C:C4 | 3.05 | 0.44 |
| 1:2:200:C:H2' | 1:2:201:C:C6 | 2.51 | 0.44 |
| 1:2:451:A:C4 | 1:2:452:G:C8 | 3.05 | 0.44 |
| 1:2:656:G:OP2 | 14:M:45:GLY:HA3 | 2.17 | 0.44 |
| 1:2:814:A:O3' | 2:A:134:GLN:NE2 | 2.44 | 0.44 |
| 1:2:975:G:N1 | 29:3:38:GLU:OE1 | 2.40 | 0.44 |
| 1:2:1153:A:H2' | 1:2:1154:A:O4' | 2.17 | 0.44 |
| 1:2:1391:G:C6 | 1:2:1451:G:N7 | 2.85 | 0.44 |
| 1:2:1479:4AC:N3 | 1:2:1495:G:C2 | 2.84 | 0.44 |
| 2:A:124:VAL:HG12 | 2:A:125:ILE:N | 2.33 | 0.44 |
| 5:D:78:LYS:HE2 | 5:D:78:LYS:HB3 | 1.74 | 0.44 |
| 5:D:154:TYR:HE1 | 5:D:160:PHE:HD2 | 1.64 | 0.44 |
| 7:F:143:PHE:HE1 | 7:F:211:VAL:HG21 | 1.81 | 0.44 |
| 10:I:102:LEU:HD12 | 10:I:102:LEU:HA | 1.71 | 0.44 |
| 14:M:10:LYS:CE | 14:M:12:GLU:HB2 | 2.47 | 0.44 |
| 15:N:94:ILE:HD12 | 15:N:94:ILE:HA | 1.85 | 0.44 |
| 26:Y:15:VAL:O | 26:Y:16:ILE:HD13 | 2.17 | 0.44 |
| 32:6:26:GLY:O | 32:6:66:LEU:HD12 | 2.16 | 0.44 |
| 35:9:19:VAL:HG12 | 35:9:29:VAL:HG12 | 1.99 | 0.44 |
| 35:9:20:LYS:HE2 | 35:9:28:TYR:HB3 | 1.99 | 0.44 |
| 1:2:22:G:N2 | 1:2:23:A:C4 | 2.85 | 0.44 |
| 1:2:54:G:C4 | 1:2:374:A:N7 | 2.86 | 0.44 |
| 1:2:115:A:C6 | 1:2:249:C:C4 | 3.06 | 0.44 |
| 1:2:317:C:H2' | 1:2:318:C:C6 | 2.52 | 0.44 |
| 1:2:428:C:H2' | 1:2:429:A:C8 | 2.42 | 0.44 |
| 1:2:652:G:C8 | 1:2:653:U:H5 | 2.34 | 0.44 |
| 1:2:685:G:C5 | 1:2:686:C:C5 | 3.06 | 0.44 |
| 1:2:724:U:N3 | 1:2:725:G:C4 | 2.85 | 0.44 |
| 1:2:768:U:C2 | 1:2:769:A:C8 | 3.05 | 0.44 |
| 1:2:771:U:H5'' | 1:2:772:C:OP2 | 2.17 | 0.44 |
| 1:2:804:G:H2' | 1:2:805:C:C6 | 2.52 | 0.44 |
| 1:2:1273:A:C8 | 1:2:1275:U:N3 | 2.85 | 0.44 |
| 1:2:1403:G:C2 | 1:2:1441:U:N3 | 2.85 | 0.44 |
| 1:2:1451:G:O2' | 1:2:1452:A:H8 | 1.99 | 0.44 |
| 1:2:1452:A:C8 | 33:7:352:ARG:NH2 | 2.84 | 0.44 |
| 1:2:1476:A:C2 | 1:2:1477:G:C4 | 3.05 | 0.44 |
| 3:B:21:THR:H | 3:B:143:THR:HG21 | 1.83 | 0.44 |
| 3:B:21:THR:HG22 | 3:B:22:GLN:N | 2.32 | 0.44 |
| 8:G:87:LEU:HB2 | 8:G:104:LYS:HZ2 | 1.80 | 0.44 |
| 9:H:42:ARG:HH21 | 9:H:45:PRO:HA | 1.81 | 0.44 |
| 9:H:136:THR:OG1 | 9:H:137:THR:N | 2.50 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:Q:120:ARG:NH1 | 18:Q:124:LEU:HD21 | 2.31 | 0.44 |
| 20:S:2:GLY:O | 20:S:4:ILE:N | 2.49 | 0.44 |
| 21:T:53:LEU:HA | 21:T:56:LYS:HB2 | 1.99 | 0.44 |
| 22:U:70:ILE:O | 22:U:72:ARG:N | 2.50 | 0.44 |
| 31:4:28:C:H42 | 31:4:42:G:H1 | 1.64 | 0.44 |
| 33:7:105:LEU:HD23 | 33:7:105:LEU:HA | 1.84 | 0.44 |
| 33:7:138:ILE:HG22 | 33:7:139:ILE:HD13 | 1.98 | 0.44 |
| 1:2:206:C:H4' | 11:J:43:ARG:HH22 | 1.82 | 0.44 |
| 1:2:259:A:H2 | 1:2:283:A:N6 | 2.14 | 0.44 |
| 1:2:295:G:H2' | 1:2:296:U:H6 | 1.77 | 0.44 |
| 1:2:366:G:C6 | 1:2:367:G:N7 | 2.86 | 0.44 |
| 1:2:662:A:C6 | 1:2:663:A:C5 | 3.05 | 0.44 |
| 1:2:711:A:H4' | 1:2:823:G:O2' | 2.17 | 0.44 |
| 1:2:713:G:N1 | 1:2:714:G:C5 | 2.85 | 0.44 |
| 1:2:843:A:HO2' | 1:2:844:A:H3' | 1.82 | 0.44 |
| 1:2:858:G:N2 | 1:2:882:U:O2 | 2.50 | 0.44 |
| 1:2:865:G:C2 | 1:2:866:G:N2 | 2.86 | 0.44 |
| 1:2:930:A:O2' | 1:2:957:4AC:O2' | 2.14 | 0.44 |
| 1:2:1046:G:C4 | 1:2:1047:G:C8 | 3.06 | 0.44 |
| 1:2:1064:G:C4 | 1:2:1065:U:C5 | 3.05 | 0.44 |
| 1:2:1237:C:H2' | 1:2:1238:C:C6 | 2.53 | 0.44 |
| 1:2:1242:A:OP2 | 22:U:96:SER:OG | 2.32 | 0.44 |
| 1:2:1268:C:H2' | 1:2:1269:C:H6 | 1.81 | 0.44 |
| 1:2:1289:U:C2 | 1:2:1290:G:C8 | 3.04 | 0.44 |
| 1:2:1365:U:H2' | 1:2:1366:G:C8 | 2.52 | 0.44 |
| 4:C:37:GLU:HG2 | 4:C:38:ALA:N | 2.32 | 0.44 |
| 7:F:20:THR:OG1 | 7:F:46:GLU:OE2 | 2.24 | 0.44 |
| 10:I:11:LEU:HA | 10:I:14:ILE:HG22 | 1.99 | 0.44 |
| 11:J:4:TRP:HB2 | 11:J:28:LEU:HD22 | 1.99 | 0.44 |
| 16:O:83:LYS:CE | 21:T:9:ARG:HH12 | 2.29 | 0.44 |
| 21:T:123:THR:OG1 | 31:4:30:G:OP1 | 2.35 | 0.44 |
| 1:2:106:C:C5 | 1:2:107:G:N7 | 2.86 | 0.44 |
| 1:2:195:A:C5 | 1:2:197:G:C5 | 3.06 | 0.44 |
| 1:2:322:A:H2' | 1:2:323:G:C8 | 2.52 | 0.44 |
| 1:2:334:A:H2' | 1:2:335:G:O4' | 2.18 | 0.44 |
| 1:2:470:G:C2 | 1:2:471:G:C8 | 3.06 | 0.44 |
| 1:2:662:A:C5 | 1:2:663:A:C5 | 3.05 | 0.44 |
| 1:2:975:G:H4' | 26:Y:1:MET:HE3 | 2.00 | 0.44 |
| 1:2:1037:G:H2' | 1:2:1038:U:C6 | 2.52 | 0.44 |
| 1:2:1046:G:N1 | 1:2:1047:G:C5 | 2.85 | 0.44 |
| 1:2:1085:C:C2 | 1:2:1128:G:C2 | 3.06 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:2:1272:C:C5 | 9:H:177:LYS:HD3 | 2.52 | 0.44 |
| 3:B:168:TYR:HD1 | 3:B:168:TYR:HA | 1.68 | 0.44 |
| 6:E:40:ARG:NH2 | 6:E:189:GLN:OE1 | 2.23 | 0.44 |
| 6:E:184:TYR:CE2 | 6:E:238:PRO:HD3 | 2.52 | 0.44 |
| 15:N:134:LEU:HD12 | 15:N:134:LEU:HA | 1.69 | 0.44 |
| 16:O:7:ILE:HD12 | 16:O:14:ASP:OD2 | 2.18 | 0.44 |
| 16:O:15:LEU:HD21 | 16:O:25:LEU:HD22 | 1.99 | 0.44 |
| 16:O:106:ILE:O | 16:O:110:ARG:HG3 | 2.18 | 0.44 |
| 22:U:25:GLU:HB2 | 22:U:26:ILE:HD12 | 2.00 | 0.44 |
| 25:X:31:ILE:HG23 | 25:X:38:GLY:H | 1.82 | 0.44 |
| 29:3:23:VAL:O | 29:3:27:ARG:N | 2.50 | 0.44 |
| 31:4:34:C:N3 | 31:4:35:A:N7 | 2.66 | 0.44 |
| 33:7:244:GLN:O | 33:7:244:GLN:HG2 | 2.17 | 0.44 |
| 1:2:22:G:C2 | 1:2:23:A:C5 | 3.06 | 0.44 |
| 1:2:155:G:H2' | 1:2:156:G:H8 | 1.81 | 0.44 |
| 1:2:211:A:N3 | 1:2:213:G:H1' | 2.33 | 0.44 |
| 1:2:517:G:C2 | 1:2:518:U:C5 | 3.06 | 0.44 |
| 1:2:563:G:C2 | 1:2:611:U:C2 | 3.05 | 0.44 |
| 1:2:688:A:H4' | 1:2:689:G:O4' | 2.18 | 0.44 |
| 1:2:761:A:C6 | 1:2:762:C:C4 | 3.05 | 0.44 |
| 1:2:945:C:C4 | 1:2:947:G:C6 | 3.05 | 0.44 |
| 1:2:1289:U:H2' | 1:2:1290:G:H8 | 1.81 | 0.44 |
| 4:C:42:ARG:NH1 | 4:C:47:ARG:HG3 | 2.32 | 0.44 |
| 11:J:4:TRP:HH2 | 11:J:19:LEU:HD11 | 1.82 | 0.44 |
| 15:N:128:LYS:HB3 | 15:N:128:LYS:HE2 | 1.60 | 0.44 |
| 16:O:79:VAL:HG12 | 16:O:91:LEU:O | 2.16 | 0.44 |
| 16:O:113:ARG:NH1 | 16:O:121:GLU:OE2 | 2.51 | 0.44 |
| 21:T:50:LYS:HD2 | 21:T:59:TYR:CZ | 2.52 | 0.44 |
| 30:5:823:C:HO2' | 32:6:57:ARG:HH11 | 1.58 | 0.44 |
| 32:6:75:GLN:HB3 | 32:6:79:ARG:HH12 | 1.82 | 0.44 |
| 33:7:27:GLN:HA | 33:7:32:ILE:O | 2.18 | 0.44 |
| 33:7:230:PHE:HD2 | 35:9:219:ILE:O | 2.00 | 0.44 |
| 33:7:251:GLN:O | 33:7:275:LYS:HA | 2.17 | 0.44 |
| 35:9:72:ASP:O | 35:9:76:GLY:N | 2.51 | 0.44 |
| 35:9:176:LYS:HZ3 | 35:9:178:LYS:HA | 1.82 | 0.44 |
| 1:2:99:C:C2 | 1:2:100:G:C8 | 3.06 | 0.44 |
| 1:2:253:U:C6 | 1:2:865:G:N2 | 2.86 | 0.44 |
| 1:2:373:A2M:HM'3 | 1:2:373:A2M:H1' | 1.53 | 0.44 |
| 1:2:391:A:H4' | 6:E:67:ASN:ND2 | 2.31 | 0.44 |
| 1:2:695:A:C6 | 1:2:696:A:C6 | 3.06 | 0.44 |
| 1:2:739:A:C6 | 1:2:775:G:C6 | 3.05 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:2:1071:G:C6 | 1:2:1072:C:N4 | 2.85 | 0.44 |
| 1:2:1180:G:C4 | 1:2:1181:C:C5 | 3.06 | 0.44 |
| 1:2:1242:A:H2' | 1:2:1243:A:C8 | 2.53 | 0.44 |
| 1:2:1351:A:N7 | 1:2:1352:C:N4 | 2.65 | 0.44 |
| 1:2:1373:C:C4 | 1:2:1375:G:C2 | 3.06 | 0.44 |
| 1:2:1386:C:N4 | 1:2:1457:G:H1 | 2.15 | 0.44 |
| 1:2:1452:A:H3' | 33:7:352:ARG:CZ | 2.47 | 0.44 |
| 2:A:59:ASP:OD1 | 2:A:59:ASP:N | 2.47 | 0.44 |
| 3:B:148:SER:O | 3:B:148:SER:OG | 2.31 | 0.44 |
| 5:D:56:ARG:CG | 7:F:132:GLU:HG2 | 2.47 | 0.44 |
| 9:H:16:LYS:HD2 | 9:H:22:SER:HB2 | 1.99 | 0.44 |
| 30:5:810:G:H2' | 30:5:811:U:H6 | 1.83 | 0.44 |
| 31:4:10:G:N3 | 31:4:11:A:C8 | 2.85 | 0.44 |
| 31:4:73:A:C8 | 31:4:73:A:O5' | 2.70 | 0.44 |
| 1:2:34:G:C6 | 1:2:523:A:C2 | 3.05 | 0.44 |
| 1:2:78:G:H2' | 1:2:79:C:H6 | 1.83 | 0.44 |
| 1:2:180:G:C6 | 1:2:181:C:C4 | 3.06 | 0.44 |
| 1:2:197:G:C4 | 1:2:198:U:C5 | 3.06 | 0.44 |
| 1:2:205:G:C4 | 1:2:206:C:C5 | 3.05 | 0.44 |
| 1:2:246:C:O2' | 1:2:247:G:H5' | 2.18 | 0.44 |
| 1:2:651:G:C6 | 1:2:652:G:N1 | 2.86 | 0.44 |
| 1:2:665:C:N3 | 1:2:666:C:C5 | 2.86 | 0.44 |
| 1:2:799:G:C4 | 1:2:800:U:C5 | 3.06 | 0.44 |
| 1:2:856:G:C2 | 1:2:857:G:C8 | 3.05 | 0.44 |
| 1:2:976:A:C8 | 1:2:977:A:H1' | 2.53 | 0.44 |
| 1:2:991:G:C4 | 1:2:992:U:C5 | 3.06 | 0.44 |
| 1:2:1015:G:N2 | 1:2:1016:G:C5 | 2.85 | 0.44 |
| 1:2:1022:G:C6 | 1:2:1023:G:C6 | 3.05 | 0.44 |
| 1:2:1453:G:N9 | 33:7:352:ARG:HB3 | 2.33 | 0.44 |
| 9:H:16:LYS:O | 9:H:43:LEU:HA | 2.18 | 0.44 |
| 11:J:104:GLU:CG | 11:J:105:ILE:HG23 | 2.44 | 0.44 |
| 21:T:12:THR:HG21 | 21:T:14:GLU:OE1 | 2.18 | 0.44 |
| 26:Y:15:VAL:HG13 | 29:3:68:PRO:HB2 | 1.99 | 0.44 |
| 29:3:40:THR:O | 29:3:44:GLU:HB2 | 2.18 | 0.44 |
| 31:4:25:C:C4 | 31:4:26:G:N7 | 2.85 | 0.44 |
| 31:4:31:G:C4 | 31:4:32:OMC:C5 | 3.05 | 0.44 |
| 33:7:21:GLY:H | 39:7:502:GNP:PB | 2.38 | 0.44 |
| 33:7:50:GLY:C | 33:7:93:ASP:H | 2.21 | 0.44 |
| 33:7:133:PHE:CE2 | 33:7:173:THR:HG21 | 2.53 | 0.44 |
| 33:7:259:LEU:N | 33:7:272:ILE:HD11 | 2.33 | 0.44 |
| 33:7:264:GLN:O | 33:7:266:LYS:N | 2.50 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:2:508:G:C2 | 1:2:509:C:C4 | 3.05 | 0.44 |
| 1:2:663:A:H8 | 1:2:663:A:O5' | 2.00 | 0.44 |
| 1:2:676:G:C6 | 1:2:677:G:C5 | 3.05 | 0.44 |
| 1:2:714:G:C2 | 1:2:716:U:C4 | 3.06 | 0.44 |
| 1:2:738:C:C4 | 1:2:776:G:N1 | 2.86 | 0.44 |
| 1:2:757:A:N1 | 1:2:758:G:N2 | 2.66 | 0.44 |
| 1:2:804:G:H2' | 1:2:805:C:H6 | 1.83 | 0.44 |
| 1:2:925:G:C6 | 1:2:926:G:C5 | 3.06 | 0.44 |
| 1:2:926:G:H22 | 21:T:115:HIS:CE1 | 2.36 | 0.44 |
| 1:2:957:4AC:HM72 | 1:2:1195:G:O6 | 2.17 | 0.44 |
| 1:2:1026:G:C2 | 1:2:1027:C:C2 | 3.06 | 0.44 |
| 1:2:1154:A:OP1 | 12:K:104:ARG:NH2 | 2.49 | 0.44 |
| 1:2:1219:G:N3 | 1:2:1220:G:C8 | 2.86 | 0.44 |
| 1:2:1272:C:O5' | 1:2:1272:C:H6 | 2.01 | 0.44 |
| 1:2:1316:C:O2' | 1:2:1317:C:H5' | 2.17 | 0.44 |
| 2:A:75:LYS:HE2 | 2:A:75:LYS:HB3 | 1.73 | 0.44 |
| 2:A:88:LEU:HD13 | 2:A:187:ARG:HA | 2.00 | 0.44 |
| 5:D:132:VAL:O | 5:D:135:GLN:N | 2.51 | 0.44 |
| 6:E:125:LEU:O | 6:E:163:THR:HG23 | 2.18 | 0.44 |
| 7:F:25:LEU:HD23 | 7:F:25:LEU:HA | 1.85 | 0.44 |
| 8:G:96:PRO:C | 8:G:98:GLU:H | 2.21 | 0.44 |
| 16:O:113:ARG:NH1 | 16:O:121:GLU:OE1 | 2.40 | 0.44 |
| 18:Q:90:GLU:H | 18:Q:90:GLU:CD | 2.19 | 0.44 |
| 33:7:120:ALA:HB2 | 33:7:148:GLN:HG2 | 2.00 | 0.44 |
| 1:2:289:A:H2 | 19:R:67:ARG:HG3 | 1.83 | 0.44 |
| 1:2:437:U:C4 | 1:2:438:C:C5 | 3.06 | 0.44 |
| 1:2:509:C:H2' | 1:2:510:C:H6 | 1.82 | 0.44 |
| 1:2:531:U:H4' | 10:I:92:ARG:NH2 | 2.33 | 0.44 |
| 1:2:627:G:C2 | 1:2:628:G:C6 | 3.06 | 0.44 |
| 1:2:791:G:C2 | 1:2:792:G:N7 | 2.85 | 0.44 |
| 1:2:878:A:C6 | 1:2:879:A:C5 | 3.05 | 0.44 |
| 1:2:898:G:OP2 | 1:2:1472:A:C8 | 2.71 | 0.44 |
| 1:2:963:C:C4 | 1:2:1186:A:C2 | 3.06 | 0.44 |
| 1:2:1066:A:O4' | 3:B:98:PRO:HG2 | 2.18 | 0.44 |
| 1:2:1071:G:N1 | 1:2:1072:C:C4 | 2.85 | 0.44 |
| 1:2:1083:C:C2 | 1:2:1153:A:N1 | 2.86 | 0.44 |
| 1:2:1098:C:C2 | 1:2:1116:A:H2 | 2.36 | 0.44 |
| 1:2:1106:C:C6 | 1:2:1107:U:C5 | 3.06 | 0.44 |
| 1:2:1133:U:OP2 | 20:S:3:LYS:NZ | 2.24 | 0.44 |
| 1:2:1182:C:C4 | 1:2:1183:C:C4 | 3.06 | 0.44 |
| 1:2:1331:G:C2 | 1:2:1340:G:C2 | 3.06 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2:1341:C:O2' | 1:2:1342:G:OP1 | 2.29 | 0.44 |
| 1:2:1425:G:C2 | 1:2:1426:A:C5 | 3.05 | 0.44 |
| 3:B:166:LEU:HD12 | 3:B:166:LEU:HA | 1.75 | 0.44 |
| 3:B:179:ARG:O | 3:B:181:GLU:N | 2.50 | 0.44 |
| 5:D:150:ASP:N | 5:D:150:ASP:OD1 | 2.37 | 0.44 |
| 10:I:106:THR:OG1 | 10:I:121:ILE:HD12 | 2.17 | 0.44 |
| 22:U:11:LEU:HB3 | 22:U:136:LEU:HD21 | 2.00 | 0.44 |
| 32:6:75:GLN:HB3 | 32:6:79:ARG:NH1 | 2.32 | 0.44 |
| 32:6:77:ASP:HB3 | 32:6:78:LYS:HD2 | 1.98 | 0.44 |
| 33:7:15:VAL:O | 33:7:116:LEU:HA | 2.18 | 0.44 |
| 33:7:171:LYS:HD3 | 33:7:176:GLU:HG2 | 2.00 | 0.44 |
| 33:7:237:VAL:HG13 | 38:7:501:MET:HE3 | 2.00 | 0.44 |
| 1:2:73:A:O2' | 1:2:74:G:OP2 | 2.34 | 0.43 |
| 1:2:91:G:H3' | 1:2:92:A:H8 | 1.83 | 0.43 |
| 1:2:151:C:C2 | 1:2:165:G:C2 | 3.06 | 0.43 |
| 1:2:168:A:C4 | 1:2:169:A:C2 | 3.06 | 0.43 |
| 1:2:196:G:C6 | 19:R:26:HIS:HB3 | 2.53 | 0.43 |
| 1:2:238:U:H2' | 1:2:239:G:O4' | 2.18 | 0.43 |
| 1:2:284:G:C2 | 1:2:285:C:C6 | 3.06 | 0.43 |
| 1:2:447:A:C6 | 1:2:448:A:C5 | 3.06 | 0.43 |
| 1:2:578:C:H2' | 1:2:579:C:H6 | 1.84 | 0.43 |
| 1:2:800:U:H2' | 1:2:801:C:C5 | 2.53 | 0.43 |
| 1:2:837:G:H5'' | 1:2:838:C:H6 | 1.83 | 0.43 |
| 1:2:859:G:O6 | 1:2:860:A:N6 | 2.50 | 0.43 |
| 1:2:962:G:N1 | 1:2:1190:C:N3 | 2.66 | 0.43 |
| 1:2:997:C:N3 | 1:2:998:C:C4 | 2.85 | 0.43 |
| 1:2:1042:G:N2 | 1:2:1046:G:N3 | 2.65 | 0.43 |
| 1:2:1061:G:C4 | 1:2:1062:U:C5 | 3.06 | 0.43 |
| 1:2:1158:G:C2 | 1:2:1159:C:C5 | 3.05 | 0.43 |
| 1:2:1341:C:H3' | 12:K:122:SER:CB | 2.48 | 0.43 |
| 1:2:1483:G:C4 | 1:2:1484:G:C8 | 3.06 | 0.43 |
| 3:B:96:PHE:CE2 | 3:B:100:THR:HG21 | 2.53 | 0.43 |
| 3:B:169:TRP:CG | 3:B:192:VAL:HG12 | 2.52 | 0.43 |
| 6:E:3:ARG:HH21 | 6:E:4:LYS:HZ1 | 1.66 | 0.43 |
| 6:E:205:PHE:CD2 | 6:E:211:ASP:HA | 2.53 | 0.43 |
| 10:I:76:LYS:O | 10:I:78:ARG:N | 2.51 | 0.43 |
| 16:O:34:ASN:HA | 22:U:44:LEU:HD11 | 1.99 | 0.43 |
| 24:W:38:ARG:HB2 | 24:W:43:GLY:O | 2.18 | 0.43 |
| 31:4:26:G:H2' | 31:4:26:G:N3 | 2.33 | 0.43 |
| 33:7:8:PRO:HD2 | 33:7:281:PHE:CZ | 2.52 | 0.43 |
| 33:7:47:ILE:HA | 33:7:100:LEU:HD23 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 33:7:87:ARG:HA | 33:7:87:ARG:HD3 | 1.67 | 0.43 |
| 33:7:122:GLU:HG3 | 33:7:123:PRO:HD2 | 1.99 | 0.43 |
| 33:7:160:LEU:HD11 | 34:8:8:VAL:CG2 | 2.48 | 0.43 |
| 33:7:256:LEU:HD11 | 33:7:325:VAL:HG11 | 1.99 | 0.43 |
| 35:9:178:LYS:HA | 35:9:178:LYS:HD2 | 1.83 | 0.43 |
| 1:2:175:C:C2 | 1:2:176:A:C8 | 3.06 | 0.43 |
| 1:2:246:C:H2' | 1:2:247:G:H8 | 1.83 | 0.43 |
| 1:2:391:A:H2' | 1:2:392:A:C8 | 2.53 | 0.43 |
| 1:2:393:C:N4 | 1:2:394:4AC:C7 | 2.81 | 0.43 |
| 1:2:452:G:H5'' | 1:2:453:C:OP2 | 2.18 | 0.43 |
| 1:2:539:A:C5 | 1:2:540:A:N1 | 2.86 | 0.43 |
| 1:2:827:C:H2' | 1:2:828:4AC:H6 | 1.99 | 0.43 |
| 1:2:1037:G:H2' | 1:2:1038:U:H6 | 1.83 | 0.43 |
| 1:2:1090:U:HO2' | 1:2:1091:U:P | 2.41 | 0.43 |
| 1:2:1113:G:N1 | 1:2:1114:G:C6 | 2.86 | 0.43 |
| 1:2:1300:C:H2' | 1:2:1301:G:H8 | 1.83 | 0.43 |
| 1:2:1337:A:C4 | 1:2:1339:C:C5 | 3.06 | 0.43 |
| 1:2:1348:A:C2 | 1:2:1349:A:C8 | 3.06 | 0.43 |
| 3:B:63:ASP:HB3 | 3:B:65:GLN:OE1 | 2.18 | 0.43 |
| 8:G:25:GLU:O | 8:G:43:LEU:HD11 | 2.18 | 0.43 |
| 9:H:156:ARG:HH21 | 25:X:46:ARG:HH21 | 1.66 | 0.43 |
| 9:H:174:TYR:HE2 | 9:H:175:ARG:CZ | 2.31 | 0.43 |
| 13:L:79:GLU:OE1 | 13:L:79:GLU:N | 2.45 | 0.43 |
| 15:N:56:GLU:OE2 | 15:N:74:ARG:HG3 | 2.18 | 0.43 |
| 21:T:12:THR:OG1 | 21:T:14:GLU:N | 2.51 | 0.43 |
| 24:W:20:CYS:SG | 24:W:23:CYS:N | 2.80 | 0.43 |
| 31:4:21:A:OP1 | 31:4:21:A:H3' | 2.18 | 0.43 |
| 1:2:53:4AC:O7 | 1:2:53:4AC:H5 | 2.18 | 0.43 |
| 1:2:94:G:C6 | 1:2:95:C:N4 | 2.87 | 0.43 |
| 1:2:607:A:H2' | 1:2:608:U:C6 | 2.52 | 0.43 |
| 1:2:694:G:N1 | 1:2:698:G:C5 | 2.86 | 0.43 |
| 1:2:696:A:N3 | 1:2:697:G:C8 | 2.87 | 0.43 |
| 1:2:732:G:H5'' | 1:2:733:A:OP1 | 2.17 | 0.43 |
| 1:2:832:G:N3 | 1:2:833:G:C8 | 2.87 | 0.43 |
| 1:2:904:A:N6 | 1:2:907:A:C2 | 2.87 | 0.43 |
| 1:2:1115:G:C6 | 1:2:1116:A:N1 | 2.86 | 0.43 |
| 1:2:1387:A:C6 | 1:2:1457:G:N2 | 2.86 | 0.43 |
| 1:2:1439:C:H2' | 1:2:1440:C:C6 | 2.53 | 0.43 |
| 1:2:1459:A:N1 | 1:2:1460:G:C6 | 2.85 | 0.43 |
| 1:2:1460:G:H5'' | 1:2:1461:A:OP1 | 2.18 | 0.43 |
| 2:A:113:LYS:HE2 | 2:A:152:GLU:O | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:E:18:SER:C | 6:E:19:TRP:HD1 | 2.20 | 0.43 |
| 7:F:149:GLU:HB3 | 7:F:200:ALA:HB2 | 2.01 | 0.43 |
| 18:Q:29:THR:O | 18:Q:33:ILE:N | 2.50 | 0.43 |
| 18:Q:108:HIS:C | 18:Q:108:HIS:CD2 | 2.92 | 0.43 |
| 22:U:4:VAL:HG22 | 22:U:63:TYR:HE1 | 1.84 | 0.43 |
| 22:U:63:TYR:HD2 | 22:U:121:ILE:HD13 | 1.83 | 0.43 |
| 22:U:146:GLU:OE1 | 22:U:146:GLU:N | 2.51 | 0.43 |
| 28:0:34:ARG:HD3 | 33:7:371:THR:OG1 | 2.18 | 0.43 |
| 31:4:36:U:H2' | 31:4:37:A:H8 | 1.83 | 0.43 |
| 35:9:203:ALA:HB2 | 35:9:250:LEU:HD23 | 1.98 | 0.43 |
| 1:2:326:G:C2 | 1:2:327:G:C4 | 3.06 | 0.43 |
| 1:2:391:A:H2' | 1:2:392:A:H8 | 1.83 | 0.43 |
| 1:2:440:G:C6 | 1:2:457:G:C6 | 3.06 | 0.43 |
| 1:2:633:G:N3 | 1:2:633:G:H2' | 2.33 | 0.43 |
| 1:2:795:A:N7 | 1:2:830:U:C2 | 2.87 | 0.43 |
| 1:2:797:G:O6 | 1:2:828:4AC:HM72 | 2.18 | 0.43 |
| 1:2:798:U:O2' | 1:2:1509:U:OP1 | 2.30 | 0.43 |
| 1:2:840:G:H5'' | 1:2:841:U:OP1 | 2.18 | 0.43 |
| 1:2:909:A:OP2 | 40:2:1715:HOH:O | 2.20 | 0.43 |
| 1:2:983:G:C2 | 1:2:994:U:N3 | 2.86 | 0.43 |
| 1:2:1022:G:C6 | 1:2:1178:A:N6 | 2.85 | 0.43 |
| 1:2:1252:U:H5' | 1:2:1253:A:C2 | 2.54 | 0.43 |
| 1:2:1433:G:C5 | 1:2:1434:U:C4 | 3.06 | 0.43 |
| 1:2:1508:C:H2' | 1:2:1509:U:O4' | 2.19 | 0.43 |
| 2:A:45:LEU:HD11 | 2:A:72:TYR:C | 2.38 | 0.43 |
| 2:A:49:VAL:HG12 | 2:A:69:PHE:O | 2.19 | 0.43 |
| 11:J:93:ASN:O | 11:J:94:ILE:HD13 | 2.18 | 0.43 |
| 15:N:123:ARG:NH1 | 15:N:123:ARG:HB2 | 2.33 | 0.43 |
| 16:O:56:ASP:O | 16:O:60:LYS:HG3 | 2.17 | 0.43 |
| 18:Q:85:HIS:C | 18:Q:87:LEU:H | 2.22 | 0.43 |
| 20:S:32:LYS:HG3 | 20:S:47:ARG:NH1 | 2.33 | 0.43 |
| 20:S:37:GLU:CD | 20:S:37:GLU:H | 2.22 | 0.43 |
| 22:U:34:PHE:N | 22:U:34:PHE:CD1 | 2.81 | 0.43 |
| 22:U:76:TYR:CD2 | 22:U:77:TYR:HE2 | 2.36 | 0.43 |
| 26:Y:14:LYS:HA | 26:Y:14:LYS:HD3 | 1.70 | 0.43 |
| 29:3:16:ALA:O | 29:3:20:LEU:HD13 | 2.18 | 0.43 |
| 31:4:4:G:H1' | 31:4:70:G:N2 | 2.32 | 0.43 |
| 33:7:17:HIS:CG | 33:7:18:VAL:N | 2.86 | 0.43 |
| 1:2:20:U:O4 | 1:2:28:G:C2 | 2.71 | 0.43 |
| 1:2:143:G:N3 | 1:2:144:G:C8 | 2.86 | 0.43 |
| 1:2:181:C:C2 | 1:2:182:C:C5 | 3.07 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2:366:G:C2 | 1:2:367:G:C8 | 3.07 | 0.43 |
| 1:2:367:G:H2' | 1:2:368:C:H6 | 1.84 | 0.43 |
| 1:2:385:G:C2 | 1:2:398:A:N1 | 2.87 | 0.43 |
| 1:2:483:G:O2' | 1:2:484:G:OP2 | 2.30 | 0.43 |
| 1:2:633:G:C6 | 1:2:708:G:C6 | 3.07 | 0.43 |
| 1:2:838:C:C2 | 1:2:839:4AC:O7 | 2.72 | 0.43 |
| 1:2:964:G:N7 | 1:2:1186:A:N6 | 2.66 | 0.43 |
| 1:2:978:G:N1 | 1:2:979:G:C5 | 2.87 | 0.43 |
| 1:2:1134:G:H2' | 1:2:1135:C:H6 | 1.83 | 0.43 |
| 1:2:1274:G:C2 | 1:2:1309:C:C2 | 3.07 | 0.43 |
| 1:2:1289:U:H2' | 1:2:1290:G:O4' | 2.18 | 0.43 |
| 1:2:1322:U:H5 | 1:2:1347:G:N2 | 2.16 | 0.43 |
| 1:2:1340:G:C6 | 1:2:1341:C:C4 | 3.07 | 0.43 |
| 1:2:1351:A:C8 | 1:2:1352:C:C4 | 3.07 | 0.43 |
| 1:2:1412:C:H2' | 1:2:1413:G:O4' | 2.18 | 0.43 |
| 5:D:115:ALA:HB1 | 5:D:120:GLN:OE1 | 2.18 | 0.43 |
| 7:F:195:VAL:O | 7:F:198:ALA:N | 2.51 | 0.43 |
| 9:H:73:ARG:HE | 9:H:75:GLY:CA | 2.32 | 0.43 |
| 11:J:107:LYS:O | 11:J:125:LEU:N | 2.51 | 0.43 |
| 12:K:116:PRO:O | 12:K:126:PRO:HG3 | 2.19 | 0.43 |
| 14:M:31:THR:HA | 14:M:39:ILE:HG13 | 1.99 | 0.43 |
| 22:U:143:ILE:HG13 | 22:U:144:ILE:HD12 | 2.00 | 0.43 |
| 27:Z:87:ASN:O | 27:Z:89:TYR:N | 2.51 | 0.43 |
| 30:5:807:G:C2 | 30:5:808:A:C4 | 3.07 | 0.43 |
| 31:4:3:C:C2 | 31:4:71:C:N4 | 2.83 | 0.43 |
| 31:4:25:C:N3 | 31:4:26:G:C8 | 2.86 | 0.43 |
| 33:7:119:ALA:HB3 | 33:7:122:GLU:HB3 | 1.99 | 0.43 |
| 35:9:19:VAL:O | 35:9:61:ASN:HA | 2.19 | 0.43 |
| 1:2:41:G:H4' | 15:N:133:SER:OG | 2.19 | 0.43 |
| 1:2:148:A:C6 | 1:2:149:A:C4 | 3.06 | 0.43 |
| 1:2:222:A:N7 | 1:2:223:G:H1' | 2.34 | 0.43 |
| 1:2:255:A:C5 | 1:2:288:A:C6 | 3.06 | 0.43 |
| 1:2:270:U:H5'' | 11:J:30:ARG:NH1 | 2.33 | 0.43 |
| 1:2:336:A:HO2' | 1:2:337:C:P | 2.42 | 0.43 |
| 1:2:383:A:H2' | 1:2:384:U:C6 | 2.54 | 0.43 |
| 1:2:673:C:C2 | 1:2:674:C:C5 | 3.07 | 0.43 |
| 1:2:776:G:H5' | 1:2:777:C:OP2 | 2.19 | 0.43 |
| 1:2:1099:C:C2 | 1:2:1115:G:N2 | 2.87 | 0.43 |
| 1:2:1224:A:C2 | 1:2:1261:A:C6 | 3.07 | 0.43 |
| 2:A:196:GLU:H | 2:A:196:GLU:CD | 2.16 | 0.43 |
| 8:G:24:PRO:HA | 8:G:27:GLU:HB2 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 9:H:93:LEU:HD12 | 9:H:93:LEU:O | 2.19 | 0.43 |
| 16:O:41:ARG:NH2 | 22:U:45:PRO:O | 2.51 | 0.43 |
| 29:3:83:LYS:HD3 | 29:3:95:ALA:CB | 2.49 | 0.43 |
| 29:3:84:LYS:H | 29:3:84:LYS:HD3 | 1.83 | 0.43 |
| 1:2:146:A:H8 | 1:2:146:A:OP2 | 2.01 | 0.43 |
| 1:2:179:G:N1 | 1:2:208:G:H1' | 2.33 | 0.43 |
| 1:2:790:G:N3 | 1:2:790:G:H2' | 2.33 | 0.43 |
| 1:2:862:U:C5 | 1:2:877:G:N2 | 2.87 | 0.43 |
| 1:2:1101:U:H2' | 1:2:1102:C:H6 | 1.84 | 0.43 |
| 1:2:1196:G:H2' | 1:2:1197:C:H6 | 1.84 | 0.43 |
| 1:2:1320:A:C4 | 1:2:1322:U:N3 | 2.87 | 0.43 |
| 1:2:1323:A:N6 | 1:2:1347:G:H21 | 2.16 | 0.43 |
| 1:2:1387:A:C6 | 1:2:1457:G:C2 | 3.07 | 0.43 |
| 1:2:1387:A:N1 | 1:2:1456:G:O6 | 2.51 | 0.43 |
| 1:2:1397:G:C2 | 1:2:1398:G:C8 | 3.06 | 0.43 |
| 3:B:21:THR:O | 3:B:41:TYR:HB2 | 2.18 | 0.43 |
| 4:C:35:CYS:HB3 | 4:C:37:GLU:OE2 | 2.18 | 0.43 |
| 7:F:102:HIS:O | 7:F:109:ALA:HA | 2.18 | 0.43 |
| 9:H:186:GLU:O | 9:H:190:LEU:HG | 2.18 | 0.43 |
| 12:K:37:GLU:N | 12:K:38:PRO:HD2 | 2.34 | 0.43 |
| 12:K:63:ASP:N | 12:K:63:ASP:OD1 | 2.50 | 0.43 |
| 16:O:35:PHE:CE1 | 16:O:92:HIS:CE1 | 3.07 | 0.43 |
| 16:O:121:GLU:HG3 | 16:O:121:GLU:H | 1.65 | 0.43 |
| 22:U:7:VAL:HG21 | 22:U:12:LEU:HD12 | 2.01 | 0.43 |
| 24:W:30:PHE:HE2 | 24:W:32:HIS:HB2 | 1.84 | 0.43 |
| 29:3:53:ILE:O | 29:3:80:VAL:HG23 | 2.19 | 0.43 |
| 30:5:813:A:N3 | 30:5:813:A:H2' | 2.34 | 0.43 |
| 31:4:74:C:N4 | 33:7:33:TRP:HE1 | 2.11 | 0.43 |
| 33:7:144:LEU:O | 33:7:179:PRO:HD2 | 2.19 | 0.43 |
| 33:7:264:GLN:O | 33:7:266:LYS:HG2 | 2.18 | 0.43 |
| 33:7:400:GLN:HB3 | 33:7:405:TRP:NE1 | 2.34 | 0.43 |
| 35:9:238:GLU:O | 35:9:242:ALA:N | 2.50 | 0.43 |
| 1:2:141:G:C5 | 1:2:142:G:C8 | 3.06 | 0.43 |
| 1:2:143:G:C2 | 1:2:144:G:C8 | 3.07 | 0.43 |
| 1:2:308:G:C2 | 1:2:309:A:C8 | 3.06 | 0.43 |
| 1:2:384:U:N3 | 1:2:385:G:C8 | 2.87 | 0.43 |
| 1:2:415:G:C6 | 1:2:416:C:C4 | 3.06 | 0.43 |
| 1:2:647:C:H2' | 1:2:648:4AC:C6 | 2.47 | 0.43 |
| 1:2:660:G:OP1 | 14:M:135:ARG:NH1 | 2.50 | 0.43 |
| 1:2:662:A:OP2 | 14:M:51:ASP:HB2 | 2.19 | 0.43 |
| 1:2:695:A:N7 | 18:Q:120:ARG:NE | 2.45 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:2:740:G:N1 | 1:2:774:U:O4 | 2.52 | 0.43 |
| 1:2:755:U:C2 | 1:2:756:U:C6 | 3.07 | 0.43 |
| 1:2:778:U:O4 | 1:2:779:G:C2 | 2.71 | 0.43 |
| 1:2:913:G:O2' | 1:2:914:G:OP1 | 2.31 | 0.43 |
| 1:2:930:A:C5 | 1:2:931:A:N1 | 2.87 | 0.43 |
| 1:2:1037:G:C4 | 1:2:1038:U:C5 | 3.07 | 0.43 |
| 1:2:1046:G:C6 | 1:2:1047:G:N7 | 2.87 | 0.43 |
| 1:2:1134:G:C2 | 1:2:1135:C:C5 | 3.06 | 0.43 |
| 1:2:1141:A:C8 | 1:2:1143:A:C8 | 3.07 | 0.43 |
| 1:2:1207:G:C2 | 1:2:1208:C:C4 | 3.07 | 0.43 |
| 1:2:1211:C:C2 | 1:2:1310:U:C5 | 3.05 | 0.43 |
| 1:2:1220:G:N1 | 1:2:1221:G:C5 | 2.87 | 0.43 |
| 1:2:1241:A:C4 | 1:2:1242:A:C8 | 3.07 | 0.43 |
| 1:2:1274:G:N1 | 1:2:1309:C:C2 | 2.87 | 0.43 |
| 1:2:1285:G:C2 | 1:2:1301:G:C6 | 3.07 | 0.43 |
| 1:2:1485:G:N2 | 1:2:1487:MA6:H3' | 2.34 | 0.43 |
| 2:A:64:HIS:CE1 | 2:A:92:TYR:CZ | 3.07 | 0.43 |
| 2:A:194:GLU:OE1 | 2:A:195:PRO:HD3 | 2.19 | 0.43 |
| 3:B:136:PRO:HG3 | 4:C:30:PHE:HB3 | 2.00 | 0.43 |
| 4:C:33:PRO:C | 4:C:35:CYS:H | 2.22 | 0.43 |
| 4:C:49:LEU:CD1 | 4:C:51:LYS:HE2 | 2.49 | 0.43 |
| 5:D:162:ASN:HD22 | 5:D:164:GLN:HB2 | 1.84 | 0.43 |
| 6:E:66:LEU:HD21 | 6:E:71:PHE:HD2 | 1.84 | 0.43 |
| 12:K:47:GLU:HA | 12:K:50:ILE:HG22 | 2.00 | 0.43 |
| 13:L:40:LEU:HD23 | 13:L:40:LEU:HA | 1.63 | 0.43 |
| 23:V:81:ILE:HG13 | 23:V:82:GLU:HG2 | 2.00 | 0.43 |
| 29:3:27:ARG:HD3 | 29:3:90:ALA:HB1 | 2.00 | 0.43 |
| 31:4:51:C:C2 | 31:4:64:G:C6 | 3.07 | 0.43 |
| 33:7:352:ARG:HG2 | 33:7:353:ALA:H | 1.82 | 0.43 |
| 34:8:45:ARG:HA | 34:8:80:GLU:HG2 | 2.00 | 0.43 |
| 1:2:155:G:H2' | 1:2:156:G:C8 | 2.54 | 0.43 |
| 1:2:204:G:C2 | 1:2:205:G:C4 | 3.07 | 0.43 |
| 1:2:575:A:C5 | 1:2:576:U:C6 | 3.07 | 0.43 |
| 1:2:580:A:C4 | 1:2:581:C:C5 | 3.07 | 0.43 |
| 1:2:788:G:N1 | 1:2:851:4AC:N3 | 2.67 | 0.43 |
| 1:2:863:A:C6 | 1:2:878:A:C8 | 3.07 | 0.43 |
| 1:2:1078:C:H1' | 1:2:1162:G:N2 | 2.34 | 0.43 |
| 1:2:1327:G:C2 | 1:2:1344:G:C2 | 3.07 | 0.43 |
| 1:2:1446:U:O5' | 1:2:1446:U:H6 | 2.01 | 0.43 |
| 3:B:157:ASN:O | 3:B:159:LYS:N | 2.52 | 0.43 |
| 6:E:192:ASN:HB3 | 6:E:195:ARG:HD3 | 2.01 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 7:F:93:ASP:OD1 | 7:F:227:ARG:HA | 2.18 | 0.43 |
| 12:K:57:TRP:O | 12:K:57:TRP:CD1 | 2.72 | 0.43 |
| 17:P:26:GLN:NE2 | 17:P:39:CYS:SG | 2.91 | 0.43 |
| 21:T:66:HIS:O | 21:T:68:ARG:N | 2.52 | 0.43 |
| 21:T:70:MET:SD | 21:T:71:ILE:N | 2.91 | 0.43 |
| 25:X:15:ILE:HG22 | 25:X:70:ARG:HG2 | 2.00 | 0.43 |
| 27:Z:18:ASP:OD1 | 27:Z:30:TYR:OH | 2.22 | 0.43 |
| 29:3:8:LYS:HD2 | 29:3:79:TYR:OH | 2.19 | 0.43 |
| 33:7:124:PHE:HZ | 33:7:169:PHE:HB2 | 1.84 | 0.43 |
| 33:7:144:LEU:O | 33:7:178:VAL:HB | 2.18 | 0.43 |
| 33:7:212:LYS:O | 33:7:214:VAL:HG23 | 2.18 | 0.43 |
| 35:9:69:ILE:N | 35:9:79:ASP:O | 2.39 | 0.43 |
| 1:2:92:A:C6 | 1:2:93:C:C4 | 3.06 | 0.43 |
| 1:2:155:G:H5'' | 8:G:5:LYS:HZ2 | 1.82 | 0.43 |
| 1:2:263:G:N3 | 1:2:264:G:C8 | 2.87 | 0.43 |
| 1:2:323:G:OP1 | 11:J:22:LYS:HE2 | 2.19 | 0.43 |
| 1:2:388:G:O2' | 1:2:389:G:H5' | 2.18 | 0.43 |
| 1:2:695:A:C2 | 1:2:696:A:C4 | 3.06 | 0.43 |
| 1:2:722:G:N3 | 1:2:723:G:N7 | 2.67 | 0.43 |
| 1:2:778:U:H5 | 1:2:779:G:C4 | 2.37 | 0.43 |
| 1:2:808:G:C2 | 1:2:809:C:C2 | 3.06 | 0.43 |
| 1:2:898:G:O6 | 1:2:1365:U:N3 | 2.52 | 0.43 |
| 1:2:1061:G:C6 | 1:2:1062:U:C4 | 3.07 | 0.43 |
| 2:A:11:LYS:NZ | 2:A:13:LYS:HG3 | 2.33 | 0.43 |
| 7:F:12:VAL:HA | 7:F:15:GLU:HG2 | 2.00 | 0.43 |
| 8:G:13:THR:CG2 | 8:G:15:ILE:HG22 | 2.49 | 0.43 |
| 12:K:7:THR:HA | 12:K:15:ALA:O | 2.19 | 0.43 |
| 18:Q:41:ARG:C | 18:Q:43:GLU:H | 2.23 | 0.43 |
| 22:U:16:VAL:HG12 | 22:U:132:ILE:HG21 | 2.01 | 0.43 |
| 22:U:98:ILE:H | 22:U:98:ILE:HG13 | 1.56 | 0.43 |
| 27:Z:147:TYR:N | 27:Z:147:TYR:CD1 | 2.86 | 0.43 |
| 29:3:6:TYR:O | 29:3:8:LYS:NZ | 2.52 | 0.43 |
| 29:3:32:ILE:HG13 | 29:3:34:LYS:HG2 | 1.99 | 0.43 |
| 33:7:281:PHE:CZ | 33:7:295:VAL:HB | 2.54 | 0.43 |
| 34:8:6:GLU:HG3 | 34:8:9:GLU:OE1 | 2.18 | 0.43 |
| 35:9:124:GLN:OE1 | 35:9:160:TRP:NE1 | 2.52 | 0.43 |
| 1:2:531:U:C4 | 1:2:532:G:C5 | 3.07 | 0.42 |
| 1:2:668:A:H5'' | 1:2:670:A:H5' | 2.02 | 0.42 |
| 1:2:790:G:C5 | 1:2:849:G:N2 | 2.87 | 0.42 |
| 1:2:1007:C:H2' | 1:2:1008:G:H8 | 1.78 | 0.42 |
| 1:2:1016:G:H2' | 1:2:1017:U:C6 | 2.54 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:2:1040:C:O2' | 1:2:1041:4AC:H5' | 2.19 | 0.42 |
| 1:2:1083:C:C2 | 1:2:1153:A:C2 | 3.07 | 0.42 |
| 1:2:1285:G:N1 | 1:2:1301:G:C6 | 2.87 | 0.42 |
| 1:2:1386:C:H42 | 1:2:1457:G:H1 | 1.65 | 0.42 |
| 1:2:1437:A:C5 | 1:2:1438:G:C8 | 3.07 | 0.42 |
| 2:A:168:ALA:HB1 | 2:A:184:ALA:O | 2.19 | 0.42 |
| 5:D:96:THR:OG1 | 5:D:98:GLU:N | 2.52 | 0.42 |
| 5:D:97:ILE:HG13 | 5:D:101:LEU:HD12 | 2.01 | 0.42 |
| 5:D:146:LYS:HE3 | 5:D:146:LYS:HB2 | 1.37 | 0.42 |
| 10:I:38:LEU:HD23 | 10:I:38:LEU:HA | 1.75 | 0.42 |
| 15:N:18:LEU:HD23 | 15:N:18:LEU:HA | 1.85 | 0.42 |
| 16:O:59:VAL:HA | 16:O:62:ILE:HB | 2.01 | 0.42 |
| 18:Q:76:LEU:HB3 | 18:Q:81:ILE:HD11 | 2.01 | 0.42 |
| 20:S:23:GLU:HB3 | 20:S:24:PHE:CZ | 2.54 | 0.42 |
| 21:T:81:ILE:HG13 | 21:T:82:TYR:N | 2.30 | 0.42 |
| 22:U:81:LYS:HG2 | 22:U:82:ASN:N | 2.34 | 0.42 |
| 31:4:3:C:C2 | 31:4:4:G:C8 | 3.07 | 0.42 |
| 31:4:53:G:N2 | 31:4:54:5MU:H1' | 2.34 | 0.42 |
| 32:6:74:VAL:O | 32:6:79:ARG:HD2 | 2.18 | 0.42 |
| 32:6:102:GLN:OE1 | 32:6:102:GLN:N | 2.52 | 0.42 |
| 1:2:105:A:N7 | 1:2:335:G:C5 | 2.87 | 0.42 |
| 1:2:267:G:N1 | 1:2:268:G:O6 | 2.52 | 0.42 |
| 1:2:484:G:N7 | 1:2:496:G:C5 | 2.87 | 0.42 |
| 1:2:524:C:C5 | 1:2:525:U:C6 | 3.06 | 0.42 |
| 1:2:631:G:OP1 | 2:A:131:GLN:HB2 | 2.19 | 0.42 |
| 1:2:950:A:C4 | 1:2:1293:A:C2 | 3.06 | 0.42 |
| 1:2:961:G:C2 | 1:2:1191:C:N3 | 2.87 | 0.42 |
| 1:2:1070:A:C2 | 1:2:1071:G:C5 | 3.07 | 0.42 |
| 1:2:1098:C:N3 | 1:2:1116:A:C2 | 2.87 | 0.42 |
| 1:2:1169:U:H2' | 1:2:1171:G:H8 | 1.79 | 0.42 |
| 1:2:1312:G:C6 | 1:2:1313:A:C6 | 3.08 | 0.42 |
| 1:2:1413:G:N1 | 1:2:1414:A:C5 | 2.88 | 0.42 |
| 1:2:1424:G:C2 | 1:2:1425:G:C5 | 3.06 | 0.42 |
| 1:2:1486:G:O6 | 1:2:1487:MA6:H92 | 2.20 | 0.42 |
| 5:D:39:LYS:HA | 5:D:42:TRP:CE3 | 2.53 | 0.42 |
| 5:D:162:ASN:C | 5:D:164:GLN:H | 2.20 | 0.42 |
| 7:F:94:GLY:O | 7:F:124:ILE:HG12 | 2.19 | 0.42 |
| 8:G:48:ASN:O | 8:G:53:LYS:HD3 | 2.19 | 0.42 |
| 9:H:205:LEU:HD23 | 9:H:205:LEU:HA | 1.91 | 0.42 |
| 12:K:44:THR:HB | 12:K:75:ALA:HB1 | 2.00 | 0.42 |
| 21:T:103:LEU:HD12 | 21:T:103:LEU:HA | 1.65 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 29:3:32:ILE:HD12 | 29:3:99:VAL:HG13 | 2.01 | 0.42 |
| 29:3:76:PRO:HG3 | 29:3:119:ARG:NH2 | 2.34 | 0.42 |
| 30:5:813:A:C5 | 30:5:814:U:C5 | 3.07 | 0.42 |
| 32:6:23:GLN:NE2 | 32:6:68:ILE:HD12 | 2.33 | 0.42 |
| 32:6:62:ARG:N | 32:6:65:ASP:OD2 | 2.51 | 0.42 |
| 33:7:54:THR:HB | 33:7:89:ILE:HD11 | 1.99 | 0.42 |
| 1:2:13:A:N3 | 7:F:166:VAL:HG23 | 2.34 | 0.42 |
| 1:2:67:G:C6 | 1:2:363:G:C6 | 3.07 | 0.42 |
| 1:2:89:G:H3' | 1:2:90:G:C8 | 2.47 | 0.42 |
| 1:2:187:G:C5 | 1:2:188:U:C4 | 3.07 | 0.42 |
| 1:2:207:C:H6 | 1:2:207:C:O5' | 2.02 | 0.42 |
| 1:2:209:A:O2' | 1:2:210:A:O4' | 2.35 | 0.42 |
| 1:2:539:A:C6 | 1:2:540:A:N1 | 2.87 | 0.42 |
| 1:2:576:U:O2 | 1:2:576:U:H2' | 2.19 | 0.42 |
| 1:2:637:G:N2 | 1:2:704:G:C5 | 2.87 | 0.42 |
| 1:2:817:U:N3 | 1:2:818:C:C5 | 2.87 | 0.42 |
| 1:2:819:G:C6 | 1:2:820:C:C4 | 3.07 | 0.42 |
| 1:2:1095:A:H2' | 1:2:1096:G:H8 | 1.82 | 0.42 |
| 1:2:1279:G:C4 | 1:2:1305:G:N2 | 2.87 | 0.42 |
| 1:2:1397:G:H2' | 1:2:1397:G:N3 | 2.35 | 0.42 |
| 1:2:1444:G:N7 | 1:2:1445:C:N4 | 2.67 | 0.42 |
| 3:B:28:MET:O | 3:B:32:ILE:HG12 | 2.20 | 0.42 |
| 5:D:47:GLN:O | 5:D:51:PHE:CD2 | 2.72 | 0.42 |
| 6:E:237:LYS:HD3 | 6:E:237:LYS:HA | 1.51 | 0.42 |
| 9:H:111:ILE:HD13 | 9:H:111:ILE:HA | 1.84 | 0.42 |
| 15:N:21:LYS:HB3 | 15:N:21:LYS:HE2 | 1.84 | 0.42 |
| 16:O:83:LYS:HA | 16:O:88:GLY:O | 2.18 | 0.42 |
| 22:U:40:HIS:CD2 | 22:U:79:GLY:N | 2.88 | 0.42 |
| 23:V:49:GLU:OE1 | 23:V:49:GLU:N | 2.52 | 0.42 |
| 25:X:43:ARG:HA | 25:X:64:ALA:HB3 | 2.01 | 0.42 |
| 25:X:66:GLU:OE2 | 25:X:67:ILE:HG22 | 2.19 | 0.42 |
| 26:Y:5:TRP:HH2 | 29:3:65:HIS:HD1 | 1.65 | 0.42 |
| 26:Y:22:CYS:HB2 | 26:Y:29:VAL:O | 2.19 | 0.42 |
| 30:5:807:G:C5 | 30:5:808:A:C5 | 3.07 | 0.42 |
| 31:4:28:C:N4 | 31:4:43:A:C6 | 2.88 | 0.42 |
| 33:7:27:GLN:HE21 | 33:7:33:TRP:CB | 2.25 | 0.42 |
| 33:7:64:LYS:HA | 33:7:65:PRO:HA | 1.87 | 0.42 |
| 33:7:106:SER:CA | 33:7:363:SER:HA | 2.45 | 0.42 |
| 33:7:256:LEU:HB3 | 33:7:315:ILE:HD11 | 2.01 | 0.42 |
| 1:2:110:U:H2' | 1:2:111:C:C6 | 2.54 | 0.42 |
| 1:2:440:G:C6 | 1:2:441:G:N7 | 2.87 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:2:509:C:C2 | 1:2:510:C:C5 | 3.07 | 0.42 |
| 1:2:533:G:C5 | 1:2:534:G:C8 | 3.08 | 0.42 |
| 1:2:559:G:C6 | 1:2:560:U:C4 | 3.08 | 0.42 |
| 1:2:605:G:N3 | 1:2:606:G:C8 | 2.87 | 0.42 |
| 1:2:614:G:C6 | 1:2:615:G:N7 | 2.87 | 0.42 |
| 1:2:671:A:C6 | 1:2:672:U:C4 | 3.06 | 0.42 |
| 1:2:698:G:C2 | 1:2:699:C:C2 | 3.07 | 0.42 |
| 1:2:718:4AC:C7 | 1:2:719:G:H22 | 2.33 | 0.42 |
| 1:2:996:G:O2' | 1:2:997:C:O5' | 2.26 | 0.42 |
| 1:2:1084:C:C2 | 1:2:1129:G:C2 | 3.08 | 0.42 |
| 1:2:1120:A:H2' | 1:2:1120:A:N3 | 2.35 | 0.42 |
| 1:2:1321:G:HO2' | 1:2:1322:U:P | 2.43 | 0.42 |
| 1:2:1453:G:C8 | 33:7:352:ARG:NH1 | 2.87 | 0.42 |
| 1:2:1503:A:C6 | 1:2:1504:C:C4 | 3.08 | 0.42 |
| 2:A:13:LYS:O | 2:A:17:LYS:NZ | 2.34 | 0.42 |
| 2:A:45:LEU:HD12 | 2:A:45:LEU:HA | 1.76 | 0.42 |
| 4:C:4:ASN:HB3 | 4:C:8:LYS:HZ3 | 1.85 | 0.42 |
| 9:H:141:PHE:CE2 | 25:X:65:ARG:HD3 | 2.54 | 0.42 |
| 13:L:15:SER:OG | 13:L:18:GLU:OE2 | 2.31 | 0.42 |
| 14:M:110:LEU:H | 14:M:110:LEU:HD12 | 1.84 | 0.42 |
| 17:P:28:GLY:O | 17:P:30:ILE:N | 2.52 | 0.42 |
| 18:Q:74:ARG:CZ | 18:Q:74:ARG:HB2 | 2.49 | 0.42 |
| 25:X:50:ARG:HD3 | 25:X:51:VAL:H | 1.84 | 0.42 |
| 27:Z:108:HIS:CE1 | 27:Z:109:PHE:HD1 | 2.36 | 0.42 |
| 33:7:223:VAL:O | 33:7:225:LYS:HD2 | 2.18 | 0.42 |
| 35:9:20:LYS:N | 35:9:28:TYR:O | 2.42 | 0.42 |
| 35:9:23:PHE:HZ | 35:9:28:TYR:CE1 | 2.38 | 0.42 |
| 35:9:216:ASN:OD1 | 35:9:217:ILE:N | 2.52 | 0.42 |
| 1:2:13:A:C6 | 1:2:15:U:N3 | 2.87 | 0.42 |
| 1:2:76:G:O6 | 1:2:97:A:N1 | 2.53 | 0.42 |
| 1:2:141:G:C6 | 1:2:142:G:C5 | 3.07 | 0.42 |
| 1:2:313:G:H21 | 5:D:3:ASP:CG | 2.21 | 0.42 |
| 1:2:632:A:H1' | 1:2:700:G:O4' | 2.20 | 0.42 |
| 1:2:649:G:C2 | 1:2:676:G:C6 | 3.08 | 0.42 |
| 1:2:813:G:C2 | 1:2:815:G:C8 | 3.07 | 0.42 |
| 1:2:950:A:C6 | 1:2:1293:A:C4 | 3.07 | 0.42 |
| 1:2:991:G:C2 | 1:2:992:U:C2 | 3.07 | 0.42 |
| 1:2:1068:C:N4 | 1:2:1069:G:N7 | 2.68 | 0.42 |
| 1:2:1373:C:C5 | 1:2:1375:G:C2 | 3.08 | 0.42 |
| 6:E:40:ARG:CZ | 6:E:40:ARG:HB3 | 2.49 | 0.42 |
| 6:E:60:ARG:O | 6:E:63:ARG:HB3 | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:H:20:ARG:HG2 | 9:H:109:LYS:NZ | 2.35 | 0.42 |
| 14:M:81:ILE:HB | 14:M:115:VAL:HG23 | 2.01 | 0.42 |
| 19:R:73:HIS:HA | 19:R:98:LYS:NZ | 2.33 | 0.42 |
| 24:W:20:CYS:SG | 24:W:23:CYS:HB2 | 2.59 | 0.42 |
| 25:X:57:LEU:HD13 | 25:X:60:THR:H | 1.83 | 0.42 |
| 31:4:22:G:C2 | 31:4:23:C:C4 | 3.07 | 0.42 |
| 32:6:94:LEU:HD12 | 32:6:94:LEU:HA | 1.78 | 0.42 |
| 33:7:130:ARG:NH1 | 33:7:338:ARG:HE | 2.16 | 0.42 |
| 33:7:215:MET:HE3 | 33:7:240:GLY:N | 2.35 | 0.42 |
| 33:7:247:PHE:CE2 | 33:7:316:ILE:HG22 | 2.55 | 0.42 |
| 33:7:340:VAL:HG23 | 33:7:341:GLY:N | 2.34 | 0.42 |
| 1:2:46:G:C6 | 1:2:412:A:N6 | 2.88 | 0.42 |
| 1:2:74:G:C6 | 1:2:75:G:C5 | 3.07 | 0.42 |
| 1:2:244:G:N2 | 1:2:245:G:C5 | 2.87 | 0.42 |
| 1:2:503:C:H2' | 1:2:504:G:O4' | 2.19 | 0.42 |
| 1:2:650:G:N1 | 1:2:675:C:C4 | 2.87 | 0.42 |
| 1:2:754:A:C5 | 1:2:755:U:C5 | 3.07 | 0.42 |
| 1:2:788:G:O6 | 1:2:851:4AC:N4 | 2.51 | 0.42 |
| 1:2:964:G:H8 | 1:2:964:G:O5' | 2.03 | 0.42 |
| 1:2:1032:A:N6 | 1:2:1074:A:H5' | 2.34 | 0.42 |
| 1:2:1061:G:C2 | 1:2:1062:U:C4 | 3.06 | 0.42 |
| 1:2:1097:U:H2' | 1:2:1098:C:H5' | 2.00 | 0.42 |
| 1:2:1202:5MC:H4' | 16:O:140:THR:HA | 2.00 | 0.42 |
| 1:2:1299:C:H2' | 1:2:1300:C:C6 | 2.55 | 0.42 |
| 1:2:1411:C:N3 | 1:2:1433:G:N1 | 2.68 | 0.42 |
| 2:A:15:LYS:HD3 | 2:A:15:LYS:HA | 1.85 | 0.42 |
| 2:A:23:TYR:HD1 | 2:A:23:TYR:HA | 1.63 | 0.42 |
| 6:E:229:TYR:HD1 | 6:E:229:TYR:HA | 1.71 | 0.42 |
| 7:F:66:LEU:HD12 | 7:F:86:LEU:HD23 | 2.01 | 0.42 |
| 7:F:165:LEU:HG | 7:F:181:GLN:O | 2.20 | 0.42 |
| 10:I:130:TYR:O | 10:I:130:TYR:CG | 2.72 | 0.42 |
| 14:M:79:VAL:HG22 | 14:M:80:HIS:O | 2.19 | 0.42 |
| 16:O:102:ILE:HG13 | 16:O:103:ARG:N | 2.33 | 0.42 |
| 23:V:20:TYR:CZ | 23:V:68:TYR:CD1 | 3.07 | 0.42 |
| 27:Z:34:ASP:O | 27:Z:35:ILE:HD13 | 2.19 | 0.42 |
| 31:4:9:G:N2 | 31:4:45:G:N3 | 2.68 | 0.42 |
| 31:4:58:A:O2' | 31:4:59:A:O5' | 2.38 | 0.42 |
| 33:7:65:PRO:C | 33:7:67:ALA:H | 2.21 | 0.42 |
| 33:7:175:ALA:HB1 | 33:7:178:VAL:CG2 | 2.49 | 0.42 |
| 33:7:249:VAL:CG2 | 33:7:279:ILE:HG13 | 2.49 | 0.42 |
| 34:8:116:LEU:HD11 | 34:8:123:TRP:HB3 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 35:9:23:PHE:HB2 | 35:9:26:GLY:O | 2.19 | 0.42 |
| 35:9:189:GLU:OE1 | 35:9:191:LEU:HB2 | 2.19 | 0.42 |
| 1:2:116:A:C2 | 1:2:118:A:C4 | 3.07 | 0.42 |
| 1:2:193:G:H8 | 1:2:193:G:H3' | 1.85 | 0.42 |
| 1:2:219:G:N2 | 1:2:222:A:C8 | 2.88 | 0.42 |
| 1:2:265:U:H2' | 1:2:266:G:O4' | 2.19 | 0.42 |
| 1:2:322:A:H5'' | 11:J:24:ARG:NH2 | 2.34 | 0.42 |
| 1:2:466:G:C5 | 1:2:467:G:N1 | 2.88 | 0.42 |
| 1:2:656:G:P | 14:M:45:GLY:HA3 | 2.60 | 0.42 |
| 1:2:778:U:C5 | 1:2:779:G:C2 | 3.07 | 0.42 |
| 1:2:1115:G:O2' | 1:2:1116:A:C8 | 2.60 | 0.42 |
| 1:2:1143:A:H2' | 1:2:1144:A:C8 | 2.55 | 0.42 |
| 1:2:1145:G:O5' | 20:S:4:ILE:HD13 | 2.20 | 0.42 |
| 1:2:1244:G:C2 | 1:2:1245:G:C4 | 3.07 | 0.42 |
| 1:2:1252:U:H5' | 1:2:1253:A:N3 | 2.34 | 0.42 |
| 1:2:1310:U:C2 | 9:H:174:TYR:OH | 2.73 | 0.42 |
| 1:2:1322:U:H5 | 1:2:1347:G:H21 | 1.68 | 0.42 |
| 1:2:1345:G:N3 | 1:2:1346:C:C6 | 2.88 | 0.42 |
| 1:2:1414:A:N1 | 1:2:1430:C:C4 | 2.88 | 0.42 |
| 1:2:1427:G:C2 | 1:2:1428:G:C8 | 3.07 | 0.42 |
| 1:2:1446:U:H2' | 1:2:1447:C:C5 | 2.54 | 0.42 |
| 2:A:53:LEU:HA | 2:A:53:LEU:HD12 | 1.79 | 0.42 |
| 2:A:93:ILE:HG13 | 2:A:94:ARG:N | 2.35 | 0.42 |
| 3:B:97:LEU:O | 3:B:97:LEU:HD12 | 2.20 | 0.42 |
| 5:D:147:GLU:HG3 | 5:D:147:GLU:O | 2.19 | 0.42 |
| 9:H:62:HIS:HE1 | 9:H:64:VAL:HG23 | 1.85 | 0.42 |
| 12:K:9:LYS:HB2 | 12:K:9:LYS:HE3 | 1.79 | 0.42 |
| 18:Q:50:ILE:HG22 | 18:Q:54:LEU:HD13 | 2.02 | 0.42 |
| 19:R:37:ILE:CG2 | 19:R:85:ARG:HG2 | 2.45 | 0.42 |
| 23:V:11:ASN:O | 23:V:15:GLY:CA | 2.68 | 0.42 |
| 31:4:23:C:C4 | 31:4:24:U:C5 | 3.08 | 0.42 |
| 31:4:41:C:H2' | 31:4:42:G:H8 | 1.83 | 0.42 |
| 33:7:143:ASN:HB3 | 33:7:202:ILE:HG12 | 2.01 | 0.42 |
| 35:9:185:VAL:HB | 35:9:227:TYR:CE1 | 2.55 | 0.42 |
| 35:9:191:LEU:HD23 | 35:9:191:LEU:HA | 1.78 | 0.42 |
| 1:2:78:G:C4 | 1:2:79:C:C5 | 3.08 | 0.42 |
| 1:2:139:G:H2' | 1:2:140:A:O4' | 2.20 | 0.42 |
| 1:2:268:G:OP1 | 11:J:97:LYS:HB2 | 2.19 | 0.42 |
| 1:2:372:A:C4 | 1:2:373:A2M:C8 | 3.03 | 0.42 |
| 1:2:559:G:N1 | 1:2:614:G:C5 | 2.88 | 0.42 |
| 1:2:859:G:C6 | 1:2:860:A:N6 | 2.88 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:2:937:U:OP1 | 40:2:1716:HOH:O | 2.22 | 0.42 |
| 1:2:962:G:C2 | 1:2:1190:C:C2 | 3.07 | 0.42 |
| 1:2:1068:C:N4 | 1:2:1069:G:C5 | 2.88 | 0.42 |
| 1:2:1285:G:C6 | 1:2:1301:G:O6 | 2.73 | 0.42 |
| 6:E:225:THR:HG22 | 6:E:226:LEU:N | 2.35 | 0.42 |
| 7:F:206:TYR:O | 7:F:208:THR:N | 2.53 | 0.42 |
| 9:H:136:THR:HA | 9:H:149:ALA:HA | 2.02 | 0.42 |
| 14:M:21:SER:OG | 14:M:22:SER:N | 2.53 | 0.42 |
| 16:O:83:LYS:HB3 | 21:T:9:ARG:HH12 | 1.85 | 0.42 |
| 22:U:15:ARG:NE | 22:U:136:LEU:HD13 | 2.34 | 0.42 |
| 25:X:10:GLU:O | 25:X:29:VAL:HB | 2.20 | 0.42 |
| 25:X:18:THR:C | 25:X:24:VAL:HG22 | 2.40 | 0.42 |
| 29:3:14:GLU:HG3 | 29:3:15:LEU:N | 2.34 | 0.42 |
| 32:6:94:LEU:HG | 32:6:94:LEU:O | 2.20 | 0.42 |
| 33:7:48:LYS:HZ3 | 33:7:49:LEU:HB2 | 1.85 | 0.42 |
| 35:9:57:VAL:HG13 | 35:9:58:LEU:HD23 | 2.02 | 0.42 |
| 1:2:14:U:O2 | 1:2:307:A:C4 | 2.73 | 0.42 |
| 1:2:22:G:H2' | 1:2:23:A:C8 | 2.55 | 0.42 |
| 1:2:55:A:C2 | 1:2:315:A:C8 | 3.07 | 0.42 |
| 1:2:173:C:N3 | 1:2:174:C:C5 | 2.88 | 0.42 |
| 1:2:223:G:H2' | 1:2:224:G:O4' | 2.19 | 0.42 |
| 1:2:255:A:O2' | 1:2:288:A:N6 | 2.53 | 0.42 |
| 1:2:267:G:H5' | 11:J:97:LYS:HD2 | 2.02 | 0.42 |
| 1:2:268:G:N1 | 1:2:277:C:C2 | 2.87 | 0.42 |
| 1:2:403:G:H2' | 1:2:403:G:N3 | 2.35 | 0.42 |
| 1:2:477:G:N2 | 1:2:500:U:C6 | 2.88 | 0.42 |
| 1:2:658:G:H8 | 14:M:24:ASN:ND2 | 2.18 | 0.42 |
| 1:2:863:A:C5 | 1:2:864:C:N4 | 2.88 | 0.42 |
| 1:2:964:G:OP2 | 1:2:1186:A:N6 | 2.53 | 0.42 |
| 1:2:1244:G:C4 | 1:2:1245:G:C8 | 3.08 | 0.42 |
| 1:2:1392:A:C8 | 1:2:1451:G:N2 | 2.88 | 0.42 |
| 1:2:1416:C:H2' | 1:2:1417:U:C6 | 2.55 | 0.42 |
| 7:F:141:VAL:HG13 | 7:F:142:PRO:HD2 | 2.00 | 0.42 |
| 14:M:62:LEU:O | 14:M:66:ARG:HG3 | 2.20 | 0.42 |
| 20:S:50:ILE:H | 20:S:50:ILE:HG13 | 1.72 | 0.42 |
| 21:T:55:LYS:HE2 | 21:T:75:GLU:O | 2.20 | 0.42 |
| 26:Y:45:TYR:CE1 | 26:Y:47:GLU:HB3 | 2.55 | 0.42 |
| 27:Z:95:GLN:HG3 | 27:Z:120:ILE:HD11 | 2.01 | 0.42 |
| 30:5:807:G:C6 | 30:5:808:A:C6 | 3.08 | 0.42 |
| 33:7:49:LEU:HD22 | 33:7:95:PRO:HD3 | 2.01 | 0.42 |
| 33:7:274:THR:HA | 35:9:190:PRO:HB3 | 2.02 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 33:7:356:THR:O | 33:7:357:LEU:HD23 | 2.19 | 0.42 |
| 1:2:28:G:H8 | 1:2:28:G:O5' | 2.02 | 0.42 |
| 1:2:185:G:N3 | 1:2:186:G:C8 | 2.88 | 0.42 |
| 1:2:321:G:C4 | 1:2:322:A:N7 | 2.88 | 0.42 |
| 1:2:604:G:C2 | 1:2:605:G:C8 | 3.07 | 0.42 |
| 1:2:662:A:C6 | 1:2:663:A:C4 | 3.08 | 0.42 |
| 1:2:679:G:H2' | 1:2:680:G:C8 | 2.55 | 0.42 |
| 1:2:738:C:O4' | 1:2:870:C:N4 | 2.51 | 0.42 |
| 1:2:962:G:N2 | 1:2:1190:C:C2 | 2.88 | 0.42 |
| 1:2:989:A:C4 | 1:2:991:G:N7 | 2.88 | 0.42 |
| 1:2:1141:A:C4 | 1:2:1143:A:C5 | 3.08 | 0.42 |
| 1:2:1142:U:HO2' | 1:2:1143:A:P | 2.43 | 0.42 |
| 7:F:62:ASN:OD1 | 7:F:91:ASN:HA | 2.20 | 0.42 |
| 7:F:144:THR:HA | 7:F:156:LEU:O | 2.20 | 0.42 |
| 10:I:61:TYR:HD1 | 10:I:61:TYR:HA | 1.75 | 0.42 |
| 18:Q:74:ARG:HD2 | 18:Q:80:ARG:NE | 2.34 | 0.42 |
| 22:U:80:ARG:HD2 | 22:U:88:GLU:HG2 | 2.01 | 0.42 |
| 28:0:35:GLY:N | 28:0:36:LEU:HD12 | 2.35 | 0.42 |
| 33:7:17:HIS:CE1 | 33:7:97:HIS:HD2 | 2.21 | 0.42 |
| 33:7:138:ILE:HD11 | 33:7:407:MET:SD | 2.60 | 0.42 |
| 33:7:218:ILE:HG23 | 33:7:219:ARG:HG3 | 2.02 | 0.42 |
| 33:7:300:TYR:O | 35:9:193:VAL:HG22 | 2.20 | 0.42 |
| 33:7:401:ILE:HD12 | 33:7:406:ARG:CD | 2.50 | 0.42 |
| 35:9:235:ASN:OD1 | 35:9:239:ALA:HB2 | 2.19 | 0.42 |
| 1:2:148:A:N3 | 1:2:149:A:H1' | 2.34 | 0.41 |
| 1:2:632:A:C2 | 1:2:699:C:C4 | 3.08 | 0.41 |
| 1:2:644:C:H2' | 1:2:645:C:H6 | 1.85 | 0.41 |
| 1:2:722:G:N2 | 1:2:723:G:C5 | 2.88 | 0.41 |
| 1:2:819:G:C6 | 1:2:820:C:N4 | 2.88 | 0.41 |
| 1:2:1126:G:C4 | 1:2:1127:G:C8 | 3.08 | 0.41 |
| 1:2:1509:U:O2 | 30:5:806:G:C2 | 2.72 | 0.41 |
| 5:D:137:ILE:HG22 | 5:D:139:SER:H | 1.84 | 0.41 |
| 7:F:21:LYS:HB3 | 7:F:21:LYS:HE3 | 1.67 | 0.41 |
| 7:F:62:ASN:HB3 | 7:F:90:GLY:O | 2.19 | 0.41 |
| 7:F:132:GLU:OE1 | 7:F:132:GLU:N | 2.53 | 0.41 |
| 10:I:50:PHE:HB2 | 10:I:63:VAL:HG22 | 2.02 | 0.41 |
| 12:K:29:ASN:OD1 | 12:K:66:VAL:HG22 | 2.20 | 0.41 |
| 14:M:42:TRP:CD1 | 14:M:67:ALA:HA | 2.55 | 0.41 |
| 15:N:84:VAL:CG1 | 15:N:85:THR:H | 2.32 | 0.41 |
| 16:O:62:ILE:HD13 | 16:O:62:ILE:HA | 1.82 | 0.41 |
| 16:O:74:ILE:HA | 16:O:75:PRO:HD3 | 1.86 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:O:108:ARG:HB2 | 16:O:108:ARG:CZ | 2.50 | 0.41 |
| 19:R:97:THR:O | 19:R:97:THR:HG22 | 2.20 | 0.41 |
| 21:T:94:ILE:HA | 21:T:98:MET:SD | 2.60 | 0.41 |
| 26:Y:42:ARG:HG3 | 26:Y:43:CYS:N | 2.35 | 0.41 |
| 31:4:14:A:N6 | 31:4:22:G:O4' | 2.53 | 0.41 |
| 31:4:26:G:C2 | 31:4:27:U:C6 | 3.08 | 0.41 |
| 31:4:34:C:C2 | 31:4:35:A:N7 | 2.87 | 0.41 |
| 31:4:63:G:N2 | 31:4:64:G:C8 | 2.88 | 0.41 |
| 32:6:94:LEU:HD23 | 32:6:100:ILE:HG23 | 2.02 | 0.41 |
| 33:7:144:LEU:HD12 | 33:7:145:ILE:H | 1.85 | 0.41 |
| 33:7:340:VAL:HG23 | 33:7:341:GLY:H | 1.85 | 0.41 |
| 34:8:3:SER:O | 34:8:3:SER:OG | 2.28 | 0.41 |
| 1:2:32:G:C4 | 1:2:33:A:N7 | 2.88 | 0.41 |
| 1:2:155:G:H5'' | 8:G:5:LYS:HZ1 | 1.85 | 0.41 |
| 1:2:181:C:H2' | 1:2:182:C:C6 | 2.54 | 0.41 |
| 1:2:230:C:C2 | 1:2:231:C:C5 | 3.08 | 0.41 |
| 1:2:231:C:H2' | 1:2:232:C:C6 | 2.53 | 0.41 |
| 1:2:344:C:C2 | 1:2:345:C:C5 | 3.08 | 0.41 |
| 1:2:574:A:C6 | 1:2:575:A:C4 | 3.07 | 0.41 |
| 1:2:574:A:H8 | 1:2:574:A:O5' | 2.03 | 0.41 |
| 1:2:831:A:C4 | 1:2:832:G:C8 | 3.08 | 0.41 |
| 1:2:832:G:H2' | 1:2:833:G:C8 | 2.51 | 0.41 |
| 1:2:863:A:C5 | 1:2:878:A:N7 | 2.88 | 0.41 |
| 1:2:911:G:OP1 | 9:H:156:ARG:NH2 | 2.53 | 0.41 |
| 1:2:1070:A:C2 | 1:2:1071:G:C8 | 3.08 | 0.41 |
| 1:2:1234:G:C2 | 1:2:1250:G:O6 | 2.73 | 0.41 |
| 1:2:1452:A:H3' | 33:7:352:ARG:NH2 | 2.34 | 0.41 |
| 2:A:157:ASP:O | 2:A:160:LEU:HB3 | 2.19 | 0.41 |
| 3:B:190:ILE:HG23 | 3:B:191:PRO:HD2 | 2.02 | 0.41 |
| 6:E:9:HIS:O | 6:E:31:ARG:HD2 | 2.19 | 0.41 |
| 8:G:48:ASN:ND2 | 8:G:55:PHE:HB2 | 2.35 | 0.41 |
| 10:I:7:LEU:O | 10:I:10:ALA:N | 2.51 | 0.41 |
| 11:J:67:ASP:OD1 | 11:J:124:LEU:HB2 | 2.20 | 0.41 |
| 14:M:57:PRO:O | 14:M:60:ALA:HB3 | 2.19 | 0.41 |
| 17:P:28:GLY:O | 17:P:30:ILE:HG13 | 2.20 | 0.41 |
| 18:Q:36:LEU:HD23 | 18:Q:36:LEU:HA | 1.87 | 0.41 |
| 21:T:8:TYR:O | 21:T:9:ARG:HD3 | 2.19 | 0.41 |
| 27:Z:78:PRO:O | 27:Z:79:GLN:HG3 | 2.20 | 0.41 |
| 27:Z:128:VAL:HG22 | 27:Z:129:GLU:N | 2.35 | 0.41 |
| 31:4:7:G:H2' | 31:4:49:G:H8 | 1.84 | 0.41 |
| 31:4:14:A:H2' | 31:4:14:A:N3 | 2.35 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 31:4:19:G:N2 | 31:4:57:A:O2' | 2.52 | 0.41 |
| 31:4:48:C:N3 | 31:4:59:A:C4 | 2.87 | 0.41 |
| 33:7:111:MET:O | 33:7:141:VAL:HG21 | 2.19 | 0.41 |
| 33:7:148:GLN:NE2 | 33:7:159:ALA:HA | 2.35 | 0.41 |
| 35:9:195:LYS:O | 35:9:199:VAL:HG13 | 2.19 | 0.41 |
| 1:2:112:A:C6 | 1:2:113:G:C4 | 3.08 | 0.41 |
| 1:2:268:G:N1 | 1:2:277:C:O2 | 2.54 | 0.41 |
| 1:2:333:G:O5' | 1:2:333:G:H8 | 2.03 | 0.41 |
| 1:2:517:G:H2' | 1:2:518:U:C6 | 2.56 | 0.41 |
| 1:2:791:G:C2 | 1:2:792:G:C5 | 3.09 | 0.41 |
| 1:2:808:G:H2' | 1:2:809:C:C6 | 2.55 | 0.41 |
| 1:2:1042:G:C6 | 1:2:1046:G:C6 | 3.08 | 0.41 |
| 1:2:1172:G:O2' | 13:L:54:ASP:OD2 | 2.38 | 0.41 |
| 1:2:1379:G:C2 | 1:2:1380:U:C4 | 3.08 | 0.41 |
| 3:B:17:VAL:HG22 | 3:B:163:ALA:HB1 | 2.01 | 0.41 |
| 5:D:81:GLY:HA3 | 5:D:103:ARG:NH2 | 2.35 | 0.41 |
| 16:O:113:ARG:HA | 16:O:113:ARG:HD2 | 1.50 | 0.41 |
| 19:R:21:CYS:O | 19:R:25:GLY:N | 2.50 | 0.41 |
| 21:T:23:GLU:O | 21:T:23:GLU:HG2 | 2.21 | 0.41 |
| 26:Y:15:VAL:CG1 | 29:3:68:PRO:HB2 | 2.51 | 0.41 |
| 27:Z:90:LEU:HD21 | 27:Z:125:ALA:HB2 | 2.02 | 0.41 |
| 30:5:810:G:H2' | 30:5:811:U:C6 | 2.55 | 0.41 |
| 31:4:11:A:C2 | 31:4:25:C:C2 | 3.08 | 0.41 |
| 33:7:24:THR:CG2 | 33:7:186:LEU:HA | 2.49 | 0.41 |
| 33:7:25:LEU:HD23 | 33:7:25:LEU:HA | 1.83 | 0.41 |
| 33:7:51:TYR:CG | 33:7:294:LEU:HD13 | 2.55 | 0.41 |
| 1:2:55:A:C8 | 1:2:315:A:C2 | 3.08 | 0.41 |
| 1:2:91:G:N3 | 1:2:91:G:H2' | 2.34 | 0.41 |
| 1:2:201:C:H2' | 1:2:202:C:H6 | 1.85 | 0.41 |
| 1:2:252:A:C2 | 1:2:254:U:N3 | 2.88 | 0.41 |
| 1:2:276:C:OP1 | 19:R:96:LYS:HB2 | 2.20 | 0.41 |
| 1:2:386:C:H2' | 1:2:387:G:H8 | 1.84 | 0.41 |
| 1:2:529:A:C2 | 1:2:533:G:C8 | 3.08 | 0.41 |
| 1:2:643:A:C5 | 1:2:644:C:C4 | 3.08 | 0.41 |
| 1:2:818:C:C2 | 1:2:819:G:C8 | 3.08 | 0.41 |
| 1:2:975:G:H2' | 1:2:1000:G:N2 | 2.36 | 0.41 |
| 1:2:1015:G:O2' | 1:2:1016:G:H5' | 2.20 | 0.41 |
| 1:2:1203:G:N2 | 1:2:1204:C:C2 | 2.89 | 0.41 |
| 1:2:1271:U:O2' | 1:2:1272:C:OP2 | 2.36 | 0.41 |
| 1:2:1401:U:H2' | 1:2:1402:A:C8 | 2.55 | 0.41 |
| 1:2:1488:MA6:H3' | 1:2:1488:MA6:H8 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:A:152:GLU:OE1 | 2:A:152:GLU:N | 2.53 | 0.41 |
| 5:D:135:GLN:HG3 | 5:D:136:ILE:O | 2.20 | 0.41 |
| 6:E:166:MET:CE | 6:E:171:ARG:HG3 | 2.51 | 0.41 |
| 7:F:137:ARG:HA | 7:F:138:PRO:HD3 | 1.79 | 0.41 |
| 10:I:69:ILE:HD13 | 10:I:69:ILE:HG21 | 1.86 | 0.41 |
| 15:N:107:GLY:O | 15:N:125:LYS:HG2 | 2.20 | 0.41 |
| 17:P:23:ARG:NH1 | 17:P:42:CYS:HB3 | 2.35 | 0.41 |
| 21:T:79:LEU:HA | 21:T:79:LEU:HD12 | 1.72 | 0.41 |
| 22:U:41:LYS:HA | 22:U:41:LYS:HD3 | 1.84 | 0.41 |
| 22:U:144:ILE:HA | 22:U:145:PRO:HD3 | 1.87 | 0.41 |
| 25:X:15:ILE:HD11 | 25:X:28:LYS:HB2 | 2.02 | 0.41 |
| 33:7:133:PHE:HA | 33:7:136:LEU:HD12 | 2.03 | 0.41 |
| 33:7:260:ARG:HB2 | 33:7:269:TYR:CE2 | 2.56 | 0.41 |
| 1:2:65:G:C6 | 1:2:66:C:C4 | 3.09 | 0.41 |
| 1:2:130:U:O2 | 1:2:239:G:C2 | 2.74 | 0.41 |
| 1:2:149:A:H2' | 1:2:149:A:N3 | 2.35 | 0.41 |
| 1:2:330:A:H2' | 1:2:331:C:H6 | 1.85 | 0.41 |
| 1:2:436:U:O2 | 1:2:436:U:H2' | 2.20 | 0.41 |
| 1:2:465:G:C5 | 1:2:466:G:C6 | 3.07 | 0.41 |
| 1:2:467:G:C8 | 1:2:468:C:C2 | 3.09 | 0.41 |
| 1:2:599:C:H4' | 1:2:600:G:O5' | 2.20 | 0.41 |
| 1:2:679:G:H2' | 1:2:680:G:O4' | 2.19 | 0.41 |
| 1:2:790:G:C5 | 1:2:849:G:C2 | 3.08 | 0.41 |
| 1:2:896:G:C6 | 1:2:1366:G:N1 | 2.88 | 0.41 |
| 1:2:1022:G:H8 | 1:2:1022:G:O5' | 2.04 | 0.41 |
| 1:2:1116:A:C5 | 1:2:1117:G:C2 | 3.09 | 0.41 |
| 1:2:1201:A:C2 | 21:T:115:HIS:CD2 | 3.08 | 0.41 |
| 1:2:1239:4AC:H5'' | 1:2:1240:G:OP2 | 2.21 | 0.41 |
| 3:B:4:GLU:HB2 | 3:B:5:TYR:CD2 | 2.55 | 0.41 |
| 5:D:16:HIS:ND1 | 5:D:17:PRO:HD2 | 2.35 | 0.41 |
| 5:D:39:LYS:O | 5:D:41:LEU:N | 2.53 | 0.41 |
| 5:D:117:THR:OG1 | 5:D:118:MET:N | 2.53 | 0.41 |
| 6:E:12:ARG:CZ | 6:E:21:ILE:HD11 | 2.51 | 0.41 |
| 7:F:91:ASN:HD21 | 7:F:93:ASP:HB3 | 1.85 | 0.41 |
| 12:K:22:GLY:HA3 | 12:K:61:ASP:OD2 | 2.20 | 0.41 |
| 15:N:127:VAL:HG23 | 15:N:128:LYS:N | 2.35 | 0.41 |
| 18:Q:78:ILE:H | 18:Q:78:ILE:HG13 | 1.61 | 0.41 |
| 18:Q:142:LEU:HD23 | 18:Q:142:LEU:HA | 1.73 | 0.41 |
| 19:R:64:GLU:HG2 | 19:R:65:LEU:H | 1.86 | 0.41 |
| 27:Z:57:ARG:HB3 | 27:Z:60:ARG:HD2 | 2.02 | 0.41 |
| 31:4:43:A:O2' | 31:4:44:A:H5' | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 33:7:17:HIS:CG | 33:7:18:VAL:H | 2.38 | 0.41 |
| 33:7:105:LEU:HD22 | 33:7:139:ILE:HD11 | 2.02 | 0.41 |
| 33:7:138:ILE:HD13 | 33:7:410:TRP:HB3 | 2.01 | 0.41 |
| 33:7:147:VAL:HG11 | 33:7:183:VAL:HG22 | 2.02 | 0.41 |
| 1:2:139:G:C6 | 1:2:140:A:N7 | 2.89 | 0.41 |
| 1:2:485:C:C2 | 1:2:486:A:C8 | 3.08 | 0.41 |
| 1:2:621:G:N3 | 1:2:720:A:C2 | 2.89 | 0.41 |
| 1:2:652:G:OP1 | 2:A:13:LYS:HE2 | 2.20 | 0.41 |
| 1:2:671:A:C4 | 1:2:672:U:C6 | 3.09 | 0.41 |
| 1:2:731:4AC:O7 | 1:2:731:4AC:H5 | 2.18 | 0.41 |
| 1:2:886:A:C2 | 28:0:6:ARG:NH2 | 2.88 | 0.41 |
| 1:2:1037:G:C6 | 1:2:1038:U:C4 | 3.08 | 0.41 |
| 1:2:1218:C:H5' | 22:U:43:ARG:HB2 | 2.03 | 0.41 |
| 1:2:1262:A:C2 | 1:2:1263:A:C5 | 3.08 | 0.41 |
| 1:2:1337:A:C5 | 1:2:1339:C:C4 | 3.09 | 0.41 |
| 1:2:1346:C:N4 | 1:2:1347:G:O6 | 2.54 | 0.41 |
| 1:2:1380:U:O4' | 1:2:1487:MA6:H4' | 2.21 | 0.41 |
| 1:2:1395:G:N2 | 1:2:1449:G:C6 | 2.89 | 0.41 |
| 5:D:19:ILE:HD13 | 5:D:19:ILE:HA | 1.85 | 0.41 |
| 14:M:34:THR:HG23 | 14:M:36:ALA:H | 1.86 | 0.41 |
| 15:N:31:LYS:HB2 | 15:N:31:LYS:HE3 | 1.62 | 0.41 |
| 16:O:85:TYR:O | 16:O:85:TYR:CG | 2.73 | 0.41 |
| 18:Q:31:GLU:OE1 | 18:Q:31:GLU:N | 2.54 | 0.41 |
| 27:Z:66:THR:O | 27:Z:70:GLU:HG3 | 2.21 | 0.41 |
| 29:3:83:LYS:HD3 | 29:3:95:ALA:HB1 | 2.03 | 0.41 |
| 31:4:31:G:H2' | 31:4:32:OMC:C6 | 2.55 | 0.41 |
| 31:4:47:U:HO2' | 31:4:48:C:H5 | 1.68 | 0.41 |
| 31:4:55:PSU:O2' | 31:4:57:A:N7 | 2.40 | 0.41 |
| 32:6:20:GLU:H | 32:6:23:GLN:CD | 2.19 | 0.41 |
| 33:7:62:CYS:SG | 33:7:79:SER:HB2 | 2.60 | 0.41 |
| 33:7:205:PRO:HB2 | 33:7:207:ARG:HH11 | 1.86 | 0.41 |
| 33:7:276:ILE:CG2 | 33:7:297:ILE:HG23 | 2.49 | 0.41 |
| 34:8:106:CYS:SG | 34:8:127:CYS:HB2 | 2.60 | 0.41 |
| 1:2:160:C:H2' | 1:2:161:U:O4' | 2.21 | 0.41 |
| 1:2:229:G:N3 | 1:2:229:G:H2' | 2.34 | 0.41 |
| 1:2:367:G:N2 | 1:2:368:C:C2 | 2.89 | 0.41 |
| 1:2:417:C:H2' | 1:2:418:G:C8 | 2.56 | 0.41 |
| 1:2:544:G:C2 | 1:2:545:C:C6 | 3.09 | 0.41 |
| 1:2:607:A:H1' | 10:I:107:SER:OG | 2.20 | 0.41 |
| 1:2:640:G:C2 | 1:2:701:C:C2 | 3.08 | 0.41 |
| 1:2:676:G:C4 | 1:2:677:G:C8 | 3.08 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:2:959:G:H2' | 1:2:960:G:C8 | 2.55 | 0.41 |
| 1:2:1056:U:O2 | 1:2:1060:U:N3 | 2.54 | 0.41 |
| 1:2:1079:C:C2 | 1:2:1080:G:C8 | 3.09 | 0.41 |
| 1:2:1088:A:C6 | 1:2:1125:G:O6 | 2.73 | 0.41 |
| 1:2:1096:G:H4' | 12:K:3:ILE:HD13 | 2.02 | 0.41 |
| 1:2:1125:G:H4' | 1:2:1126:G:OP1 | 2.21 | 0.41 |
| 1:2:1131:A:C6 | 1:2:1154:A:C5 | 3.09 | 0.41 |
| 1:2:1166:C:N4 | 1:2:1167:G:C4 | 2.89 | 0.41 |
| 1:2:1181:C:C4 | 1:2:1182:C:N4 | 2.89 | 0.41 |
| 1:2:1200:C:H2' | 16:O:131:THR:OG1 | 2.20 | 0.41 |
| 1:2:1304:U:C4 | 1:2:1305:G:C5 | 3.09 | 0.41 |
| 1:2:1316:C:H1' | 12:K:131:GLN:HE21 | 1.84 | 0.41 |
| 1:2:1362:C:H2' | 1:2:1363:C:C6 | 2.55 | 0.41 |
| 1:2:1401:U:H2' | 1:2:1402:A:O4' | 2.21 | 0.41 |
| 2:A:121:MET:O | 2:A:187:ARG:NH2 | 2.46 | 0.41 |
| 5:D:129:HIS:CE1 | 5:D:158:SER:HG | 2.28 | 0.41 |
| 6:E:53:LEU:HD23 | 6:E:53:LEU:HA | 1.91 | 0.41 |
| 14:M:15:GLY:O | 14:M:16:ILE:HD13 | 2.20 | 0.41 |
| 23:V:24:TYR:CE1 | 23:V:26:PRO:HG3 | 2.55 | 0.41 |
| 25:X:32:LEU:O | 25:X:37:LYS:HG3 | 2.21 | 0.41 |
| 28:O:8:TRP:NE1 | 28:O:16:TRP:CD1 | 2.88 | 0.41 |
| 34:8:117:LYS:HG2 | 34:8:118:LYS:N | 2.36 | 0.41 |
| 35:9:180:SER:O | 35:9:243:LEU:HD21 | 2.21 | 0.41 |
| 1:2:48:G:H2' | 1:2:49:G:C8 | 2.56 | 0.41 |
| 1:2:103:G:O2' | 1:2:104:G:O5' | 2.30 | 0.41 |
| 1:2:196:G:C5 | 19:R:26:HIS:HB3 | 2.56 | 0.41 |
| 1:2:229:G:C2 | 1:2:230:C:C5 | 3.09 | 0.41 |
| 1:2:236:G:C5 | 1:2:237:A:N7 | 2.89 | 0.41 |
| 1:2:259:A:H2 | 1:2:283:A:C6 | 2.38 | 0.41 |
| 1:2:274:G:C4 | 1:2:276:C:C5 | 3.09 | 0.41 |
| 1:2:415:G:C4 | 1:2:460:A:C6 | 3.08 | 0.41 |
| 1:2:505:G:H2' | 1:2:506:C:C6 | 2.55 | 0.41 |
| 1:2:554:G:N3 | 1:2:555:G:C8 | 2.88 | 0.41 |
| 1:2:655:G:C4 | 1:2:656:G:C8 | 3.08 | 0.41 |
| 1:2:803:G:C4 | 1:2:804:G:C8 | 3.09 | 0.41 |
| 1:2:917:G:C2 | 1:2:918:A:C8 | 3.09 | 0.41 |
| 1:2:1169:U:H5'' | 1:2:1170:A:OP2 | 2.21 | 0.41 |
| 1:2:1312:G:C2 | 1:2:1313:A:C4 | 3.09 | 0.41 |
| 1:2:1332:U:H3' | 1:2:1333:C:C6 | 2.55 | 0.41 |
| 3:B:96:PHE:HE2 | 3:B:100:THR:HG21 | 1.85 | 0.41 |
| 7:F:84:ARG:NH1 | 7:F:195:VAL:HG21 | 2.36 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-------------------|--------------------------|-------------------|
| 7:F:148:LYS:HE2 | 7:F:148:LYS:HB3 | 1.73 | 0.41 |
| 7:F:162:GLY:N | 7:F:182:ASP:OD2 | 2.29 | 0.41 |
| 11:J:25:LYS:HG2 | 11:J:25:LYS:O | 2.21 | 0.41 |
| 12:K:12:THR:H | 12:K:113:ARG:NH2 | 2.12 | 0.41 |
| 16:O:80:ASN:HB2 | 16:O:92:HIS:CD2 | 2.56 | 0.41 |
| 21:T:84:HIS:CD2 | 21:T:84:HIS:C | 2.94 | 0.41 |
| 22:U:20:LEU:HA | 22:U:20:LEU:HD23 | 1.82 | 0.41 |
| 31:4:52:G:N3 | 31:4:53:G:C8 | 2.89 | 0.41 |
| 33:7:16:GLY:H | 33:7:132:HIS:CD2 | 2.38 | 0.41 |
| 33:7:183:VAL:HB | 33:7:191:ILE:HD13 | 2.01 | 0.41 |
| 33:7:253:ILE:O | 33:7:273:PHE:HA | 2.20 | 0.41 |
| 1:2:18:G:C6 | 1:2:31:G:C6 | 3.09 | 0.41 |
| 1:2:73:A:HO2' | 1:2:74:G:P | 2.43 | 0.41 |
| 1:2:154:G:C4 | 1:2:162:G:C6 | 3.09 | 0.41 |
| 1:2:195:A:N7 | 1:2:197:G:C6 | 2.89 | 0.41 |
| 1:2:198:U:N3 | 1:2:199:C:C5 | 2.88 | 0.41 |
| 1:2:289:A:C2 | 19:R:67:ARG:HG3 | 2.56 | 0.41 |
| 1:2:294:G:C6 | 1:2:295:G:N7 | 2.88 | 0.41 |
| 1:2:322:A:C2 | 1:2:323:G:C5 | 3.09 | 0.41 |
| 1:2:351:C:N3 | 1:2:357:G:N1 | 2.68 | 0.41 |
| 1:2:572:G:C2 | 1:2:600:G:C6 | 3.09 | 0.41 |
| 1:2:580:A:C6 | 1:2:581:C:C4 | 3.09 | 0.41 |
| 1:2:612:G:C5 | 1:2:613:C:C5 | 3.09 | 0.41 |
| 1:2:754:A:N3 | 1:2:754:A:H2' | 2.36 | 0.41 |
| 1:2:778:U:O4 | 1:2:779:G:N2 | 2.54 | 0.41 |
| 1:2:790:G:H21 | 10:I:2:THR:N | 2.18 | 0.41 |
| 1:2:819:G:C4 | 1:2:820:C:C5 | 3.09 | 0.41 |
| 1:2:897:G:N2 | 30:5:818:A:C4 | 2.89 | 0.41 |
| 1:2:950:A:C6 | 1:2:1293:A:C5 | 3.09 | 0.41 |
| 1:2:1118:G:H2' | 1:2:1119:C:O4' | 2.21 | 0.41 |
| 1:2:1139:C:C4 | 1:2:1140:G:C5 | 3.08 | 0.41 |
| 1:2:1149:G:C4 | 1:2:1150:A:C8 | 3.09 | 0.41 |
| 1:2:1242:A:C4 | 1:2:1243:A:C8 | 3.09 | 0.41 |
| 1:2:1267:G:H2' | 1:2:1268:C:H6 | 1.85 | 0.41 |
| 1:2:1324:C:O2 | 9:H:95:SER:OG | 2.38 | 0.41 |
| 1:2:1402:A:N1 | 1:2:1441:U:C4 | 2.89 | 0.41 |
| 1:2:1437:A:C6 | 1:2:1438:G:C5 | 3.09 | 0.41 |
| 1:2:1441:U:H2' | 1:2:1442:A:C8 | 2.56 | 0.41 |
| 2:A:60:PHE:N | 2:A:60:PHE:CD1 | 2.88 | 0.41 |
| 3:B:21:THR:HG22 | 3:B:22:GLN:H | 1.86 | 0.41 |
| 3:B:127:MET:O | 3:B:131:ILE:HG13 | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:D:108:ILE:HD13 | 5:D:108:ILE:HA | 1.84 | 0.41 |
| 5:D:135:GLN:HE22 | 23:V:62:SER:HB2 | 1.85 | 0.41 |
| 5:D:142:TYR:HE2 | 5:D:144:VAL:HA | 1.85 | 0.41 |
| 6:E:45:LEU:HD12 | 6:E:45:LEU:HA | 1.72 | 0.41 |
| 6:E:203:LYS:HG2 | 6:E:204:LYS:N | 2.36 | 0.41 |
| 8:G:10:ASP:OD2 | 8:G:13:THR:HG22 | 2.21 | 0.41 |
| 8:G:12:LYS:HD3 | 8:G:12:LYS:HA | 1.75 | 0.41 |
| 9:H:114:ARG:HH12 | 9:H:186:GLU:CD | 2.24 | 0.41 |
| 10:I:103:ILE:HG21 | 10:I:126:ILE:HD11 | 2.03 | 0.41 |
| 12:K:10:ARG:HG2 | 12:K:11:LYS:HG2 | 2.03 | 0.41 |
| 12:K:105:THR:HG22 | 12:K:105:THR:O | 2.20 | 0.41 |
| 15:N:53:ILE:O | 15:N:75:VAL:HA | 2.21 | 0.41 |
| 19:R:10:GLN:OE1 | 19:R:11:PRO:HD2 | 2.21 | 0.41 |
| 25:X:60:THR:O | 25:X:60:THR:HG22 | 2.21 | 0.41 |
| 29:3:75:ILE:HG23 | 29:3:75:ILE:O | 2.21 | 0.41 |
| 30:5:819:A:N6 | 31:4:37:A:C2 | 2.88 | 0.41 |
| 30:5:823:C:H4' | 32:6:57:ARG:CG | 2.47 | 0.41 |
| 33:7:15:VAL:HG21 | 33:7:136:LEU:HD21 | 2.01 | 0.41 |
| 33:7:52:ALA:O | 33:7:90:SER:HA | 2.21 | 0.41 |
| 33:7:170:THR:HB | 33:7:175:ALA:O | 2.21 | 0.41 |
| 33:7:269:TYR:CE1 | 33:7:384:ARG:HB2 | 2.55 | 0.41 |
| 1:2:116:A:C4 | 1:2:118:A:C8 | 3.09 | 0.41 |
| 1:2:132:C:HO2' | 1:2:133:C:P | 2.39 | 0.41 |
| 1:2:141:G:C6 | 1:2:142:G:N7 | 2.89 | 0.41 |
| 1:2:158:A:C6 | 1:2:159:A:C6 | 3.09 | 0.41 |
| 1:2:172:C:H2' | 1:2:173:C:H6 | 1.86 | 0.41 |
| 1:2:293:C:H2' | 1:2:294:G:H8 | 1.86 | 0.41 |
| 1:2:320:G:N1 | 1:2:321:G:C5 | 2.89 | 0.41 |
| 1:2:428:C:C2 | 1:2:429:A:C8 | 3.09 | 0.41 |
| 1:2:525:U:N3 | 1:2:527:U:C4 | 2.89 | 0.41 |
| 1:2:566:C:H2' | 1:2:567:C:C6 | 2.56 | 0.41 |
| 1:2:686:C:H3' | 1:2:687:C:C5 | 2.56 | 0.41 |
| 1:2:778:U:H5 | 1:2:779:G:C6 | 2.39 | 0.41 |
| 1:2:1053:A:C6 | 1:2:1063:G:N1 | 2.89 | 0.41 |
| 1:2:1117:G:C5 | 1:2:1118:G:C6 | 3.09 | 0.41 |
| 1:2:1166:C:C4 | 1:2:1167:G:C4 | 3.09 | 0.41 |
| 1:2:1300:C:H2' | 1:2:1301:G:C8 | 2.56 | 0.41 |
| 1:2:1360:C:O2' | 1:2:1361:U:H5' | 2.20 | 0.41 |
| 1:2:1484:G:N3 | 1:2:1485:G:C8 | 2.89 | 0.41 |
| 9:H:9:PHE:HD1 | 12:K:34:GLU:O | 2.04 | 0.41 |
| 10:I:76:LYS:HD2 | 10:I:76:LYS:HA | 1.74 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:I:81:VAL:HG12 | 10:I:89:TRP:HE1 | 1.86 | 0.41 |
| 16:O:46:ASP:CG | 16:O:48:PHE:H | 2.25 | 0.41 |
| 20:S:55:THR:O | 20:S:59:ARG:HG2 | 2.21 | 0.41 |
| 22:U:57:SER:O | 22:U:61:ARG:HG2 | 2.21 | 0.41 |
| 29:3:4:PRO:C | 29:3:6:TYR:H | 2.24 | 0.41 |
| 31:4:71:C:O3' | 33:7:42:LYS:HE3 | 2.21 | 0.41 |
| 33:7:61:SER:OG | 33:7:79:SER:OG | 2.37 | 0.41 |
| 33:7:357:LEU:CD2 | 33:7:399:ARG:HA | 2.50 | 0.41 |
| 1:2:114:U:O2 | 1:2:114:U:H2' | 2.20 | 0.40 |
| 1:2:162:G:C2 | 1:2:163:G:C5 | 3.09 | 0.40 |
| 1:2:185:G:N1 | 1:2:202:C:N3 | 2.69 | 0.40 |
| 1:2:229:G:C2 | 1:2:230:C:C6 | 3.09 | 0.40 |
| 1:2:255:A:C6 | 1:2:288:A:C2 | 3.09 | 0.40 |
| 1:2:311:C:N4 | 1:2:312:G:O6 | 2.54 | 0.40 |
| 1:2:367:G:N1 | 1:2:368:C:C4 | 2.90 | 0.40 |
| 1:2:575:A:N7 | 1:2:576:U:C5 | 2.89 | 0.40 |
| 1:2:576:U:N3 | 1:2:577:C:C5 | 2.89 | 0.40 |
| 1:2:642:U:C2 | 1:2:643:A:C8 | 3.10 | 0.40 |
| 1:2:686:C:C5 | 1:2:687:C:N4 | 2.89 | 0.40 |
| 1:2:782:A:C6 | 1:2:1498:C:H5 | 2.39 | 0.40 |
| 1:2:925:G:H21 | 21:T:122:ALA:CB | 2.28 | 0.40 |
| 1:2:987:G:OP2 | 21:T:64:ARG:NH2 | 2.21 | 0.40 |
| 1:2:1166:C:N4 | 1:2:1167:G:C2 | 2.89 | 0.40 |
| 1:2:1358:U:C4 | 1:2:1359:G:N7 | 2.87 | 0.40 |
| 1:2:1375:G:C2 | 1:2:1376:OMC:O2 | 2.74 | 0.40 |
| 2:A:22:ILE:HB | 2:A:33:VAL:O | 2.21 | 0.40 |
| 11:J:100:ILE:HG12 | 11:J:125:LEU:HD13 | 2.03 | 0.40 |
| 18:Q:41:ARG:O | 18:Q:43:GLU:N | 2.54 | 0.40 |
| 33:7:255:VAL:HG23 | 33:7:316:ILE:HG12 | 2.03 | 0.40 |
| 33:7:357:LEU:HD23 | 33:7:357:LEU:HA | 1.73 | 0.40 |
| 34:8:32:ASN:O | 34:8:46:ASN:ND2 | 2.54 | 0.40 |
| 1:2:108:G:H21 | 1:2:363:G:H5' | 1.86 | 0.40 |
| 1:2:124:G:N1 | 1:2:243:C:N3 | 2.69 | 0.40 |
| 1:2:200:C:O2' | 1:2:201:C:H5' | 2.21 | 0.40 |
| 1:2:220:U:C4 | 1:2:221:A:C4 | 3.08 | 0.40 |
| 1:2:326:G:C4 | 1:2:327:G:C8 | 3.08 | 0.40 |
| 1:2:410:C:O2' | 1:2:587:A:N3 | 2.53 | 0.40 |
| 1:2:476:G:C2 | 1:2:478:C:C4 | 3.10 | 0.40 |
| 1:2:539:A:C5 | 1:2:540:A:C6 | 3.09 | 0.40 |
| 1:2:666:C:N3 | 1:2:667:U:C4 | 2.89 | 0.40 |
| 1:2:852:G:H2' | 1:2:853:C:H6 | 1.86 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:2:946:G:N3 | 1:2:946:G:H2' | 2.36 | 0.40 |
| 1:2:1003:G:H8 | 1:2:1003:G:OP2 | 2.04 | 0.40 |
| 1:2:1122:U:O2' | 12:K:14:ILE:HD13 | 2.21 | 0.40 |
| 1:2:1133:U:H3' | 20:S:5:ARG:HH22 | 1.85 | 0.40 |
| 1:2:1137:G:N2 | 1:2:1148:G:H1' | 2.36 | 0.40 |
| 2:A:17:LYS:HD3 | 2:A:17:LYS:HA | 1.90 | 0.40 |
| 2:A:148:LYS:HD3 | 2:A:148:LYS:C | 2.42 | 0.40 |
| 3:B:164:LEU:HD23 | 3:B:164:LEU:HA | 1.93 | 0.40 |
| 5:D:52:ARG:NH2 | 5:D:93:LEU:HD22 | 2.36 | 0.40 |
| 5:D:56:ARG:HB3 | 7:F:132:GLU:HG2 | 2.03 | 0.40 |
| 6:E:83:PHE:HA | 6:E:84:PRO:HD3 | 1.88 | 0.40 |
| 6:E:123:LYS:O | 6:E:165:LEU:HD13 | 2.21 | 0.40 |
| 6:E:217:ASP:OD1 | 6:E:221:GLU:HB2 | 2.20 | 0.40 |
| 7:F:13:LEU:O | 7:F:13:LEU:HD23 | 2.22 | 0.40 |
| 7:F:131:TRP:CZ2 | 10:I:96:ALA:O | 2.74 | 0.40 |
| 8:G:29:LEU:O | 8:G:32:LYS:HG2 | 2.22 | 0.40 |
| 8:G:122:LYS:HE3 | 8:G:122:LYS:HB2 | 1.68 | 0.40 |
| 9:H:210:ILE:HA | 9:H:213:SER:OG | 2.21 | 0.40 |
| 10:I:65:LEU:C | 10:I:66:LEU:HD12 | 2.42 | 0.40 |
| 12:K:108:VAL:O | 12:K:108:VAL:HG12 | 2.21 | 0.40 |
| 15:N:130:ASN:O | 15:N:131:ARG:HB2 | 2.20 | 0.40 |
| 16:O:99:ASP:O | 16:O:102:ILE:HG12 | 2.21 | 0.40 |
| 21:T:60:ASN:OD1 | 21:T:60:ASN:N | 2.37 | 0.40 |
| 21:T:121:GLY:O | 21:T:123:THR:N | 2.53 | 0.40 |
| 33:7:313:GLY:HA2 | 33:7:363:SER:HB3 | 2.03 | 0.40 |
| 33:7:392:ASN:HB3 | 33:7:412:LEU:HB3 | 2.02 | 0.40 |
| 1:2:35:G:C6 | 1:2:36:C:C5 | 3.09 | 0.40 |
| 1:2:154:G:C6 | 1:2:155:G:C5 | 3.09 | 0.40 |
| 1:2:187:G:H2' | 1:2:188:U:C6 | 2.56 | 0.40 |
| 1:2:200:C:H2' | 1:2:201:C:H6 | 1.87 | 0.40 |
| 1:2:202:C:C2 | 1:2:203:A:C8 | 3.09 | 0.40 |
| 1:2:233:G:C2 | 1:2:234:A:C5 | 3.09 | 0.40 |
| 1:2:269:G:N7 | 11:J:113:ARG:NH2 | 2.69 | 0.40 |
| 1:2:331:C:C2 | 1:2:332:U:C6 | 3.09 | 0.40 |
| 1:2:547:G:O2' | 1:2:548:U:H5' | 2.21 | 0.40 |
| 1:2:733:A:C5 | 1:2:781:A:C6 | 3.10 | 0.40 |
| 1:2:773:C:C2 | 1:2:774:U:C5 | 3.09 | 0.40 |
| 1:2:896:G:C2 | 1:2:898:G:C8 | 3.09 | 0.40 |
| 1:2:950:A:C2 | 1:2:1293:A:N3 | 2.90 | 0.40 |
| 1:2:992:U:C2 | 1:2:993:C:C5 | 3.09 | 0.40 |
| 1:2:1062:U:H2' | 1:2:1063:G:O4' | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2:1214:U:O2 | 9:H:93:LEU:N | 2.54 | 0.40 |
| 1:2:1241:A:N3 | 1:2:1242:A:C8 | 2.89 | 0.40 |
| 1:2:1268:C:C2 | 1:2:1269:C:C5 | 3.09 | 0.40 |
| 1:2:1273:A:H5'' | 1:2:1274:G:OP2 | 2.21 | 0.40 |
| 1:2:1294:C:N3 | 1:2:1295:U:C5 | 2.89 | 0.40 |
| 1:2:1298:C:H2' | 1:2:1299:C:H6 | 1.85 | 0.40 |
| 10:I:81:VAL:HG23 | 10:I:81:VAL:O | 2.22 | 0.40 |
| 11:J:42:LYS:H | 11:J:59:ALA:HB3 | 1.86 | 0.40 |
| 11:J:75:VAL:HB | 11:J:104:GLU:OE2 | 2.21 | 0.40 |
| 13:L:45:ILE:HD11 | 13:L:66:LEU:HD23 | 2.04 | 0.40 |
| 21:T:111:LYS:HG2 | 21:T:112:ARG:O | 2.20 | 0.40 |
| 22:U:140:LEU:HD12 | 22:U:140:LEU:HA | 1.91 | 0.40 |
| 27:Z:127:GLY:HA3 | 27:Z:150:TYR:O | 2.21 | 0.40 |
| 27:Z:172:LYS:HD2 | 27:Z:172:LYS:HA | 1.81 | 0.40 |
| 28:O:20:LYS:HE3 | 28:O:20:LYS:HB2 | 1.57 | 0.40 |
| 33:7:259:LEU:HD21 | 35:9:188:ASN:HD21 | 1.85 | 0.40 |
| 1:2:121:U:H2' | 1:2:122:C:O4' | 2.21 | 0.40 |
| 1:2:628:G:C2 | 1:2:629:G:C4 | 3.09 | 0.40 |
| 1:2:638:G:C6 | 1:2:639:G:N7 | 2.89 | 0.40 |
| 1:2:689:G:N7 | 1:2:691:G:H1' | 2.36 | 0.40 |
| 1:2:709:G:C2 | 1:2:710:A:C4 | 3.10 | 0.40 |
| 1:2:955:A:C8 | 1:2:1175:A:C6 | 3.07 | 0.40 |
| 1:2:989:A:C5 | 1:2:991:G:C5 | 3.10 | 0.40 |
| 1:2:1104:C:N3 | 1:2:1110:G:C6 | 2.89 | 0.40 |
| 1:2:1152:G:H21 | 1:2:1154:A:H5'' | 1.85 | 0.40 |
| 1:2:1249:A:N3 | 1:2:1249:A:H2' | 2.36 | 0.40 |
| 1:2:1261:A:H2' | 1:2:1262:A:H8 | 1.86 | 0.40 |
| 1:2:1300:C:P | 22:U:39:ARG:HH22 | 2.39 | 0.40 |
| 1:2:1359:G:C5 | 1:2:1360:C:C5 | 3.08 | 0.40 |
| 2:A:118:LEU:HD21 | 2:A:191:VAL:HG12 | 2.03 | 0.40 |
| 3:B:72:VAL:HG23 | 3:B:94:GLY:O | 2.21 | 0.40 |
| 5:D:68:ILE:O | 5:D:72:GLN:N | 2.48 | 0.40 |
| 6:E:86:GLY:O | 6:E:89:ASP:HB2 | 2.22 | 0.40 |
| 9:H:154:PRO:O | 9:H:157:ARG:HB2 | 2.21 | 0.40 |
| 10:I:30:ALA:HB3 | 10:I:58:ALA:O | 2.21 | 0.40 |
| 11:J:81:ILE:HD12 | 11:J:82:GLU:OE2 | 2.21 | 0.40 |
| 15:N:77:LEU:HA | 15:N:77:LEU:HD23 | 1.77 | 0.40 |
| 17:P:16:LYS:HE3 | 17:P:16:LYS:HB3 | 1.96 | 0.40 |
| 22:U:3:THR:HG22 | 22:U:130:ASP:OD2 | 2.22 | 0.40 |
| 31:4:50:U:H2' | 31:4:51:C:C5 | 2.56 | 0.40 |
| 33:7:49:LEU:HB3 | 33:7:218:ILE:HD11 | 2.03 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 33:7:134:VAL:CG1 | 33:7:340:VAL:HG21 | 2.48 | 0.40 |
| 33:7:152:ASP:OD2 | 33:7:189:ILE:HD11 | 2.21 | 0.40 |
| 39:7:502:GNP:O1A | 39:7:502:GNP:H2' | 2.21 | 0.40 |
| 1:2:56:C:O2' | 1:2:57:U:OP1 | 2.38 | 0.40 |
| 1:2:346:A:C4 | 1:2:347:G:C8 | 3.09 | 0.40 |
| 1:2:398:A:H3' | 1:2:399:C:C6 | 2.56 | 0.40 |
| 1:2:520:G:C2 | 1:2:521:C:C5 | 3.10 | 0.40 |
| 1:2:618:C:H2' | 1:2:619:U:C6 | 2.56 | 0.40 |
| 1:2:738:C:C4 | 1:2:739:A:N7 | 2.90 | 0.40 |
| 1:2:925:G:C5 | 1:2:926:G:C8 | 3.10 | 0.40 |
| 1:2:980:C:O5' | 1:2:980:C:H6 | 2.04 | 0.40 |
| 1:2:1062:U:N3 | 1:2:1063:G:C5 | 2.89 | 0.40 |
| 1:2:1070:A:N1 | 1:2:1071:G:C5 | 2.90 | 0.40 |
| 1:2:1097:U:H2' | 1:2:1097:U:O2 | 2.21 | 0.40 |
| 1:2:1107:U:C2 | 1:2:1109:G:C6 | 3.09 | 0.40 |
| 1:2:1128:G:C2 | 1:2:1129:G:C5 | 3.10 | 0.40 |
| 1:2:1150:A:C4 | 1:2:1151:G:C8 | 3.09 | 0.40 |
| 1:2:1211:C:H4' | 1:2:1308:G:N2 | 2.36 | 0.40 |
| 1:2:1215:G:C2 | 1:2:1216:G:C5 | 3.09 | 0.40 |
| 1:2:1278:G:C6 | 1:2:1279:G:C6 | 3.09 | 0.40 |
| 1:2:1390:C:O5' | 1:2:1390:C:H6 | 2.04 | 0.40 |
| 1:2:1411:C:C2 | 1:2:1433:G:C2 | 3.09 | 0.40 |
| 1:2:1480:G:C2 | 1:2:1481:U:C4 | 3.10 | 0.40 |
| 2:A:141:ILE:HA | 2:A:144:GLU:OE1 | 2.22 | 0.40 |
| 6:E:167:LYS:HE3 | 6:E:170:GLU:CB | 2.51 | 0.40 |
| 8:G:25:GLU:OE1 | 8:G:45:ILE:HG22 | 2.21 | 0.40 |
| 12:K:26:VAL:O | 12:K:33:VAL:HG23 | 2.21 | 0.40 |
| 13:L:45:ILE:HG13 | 13:L:45:ILE:O | 2.21 | 0.40 |
| 14:M:22:SER:OG | 14:M:24:ASN:N | 2.51 | 0.40 |
| 15:N:7:PRO:CG | 15:N:16:LEU:HD13 | 2.52 | 0.40 |
| 16:O:83:LYS:HB3 | 21:T:9:ARG:NH1 | 2.37 | 0.40 |
| 21:T:55:LYS:NZ | 21:T:79:LEU:HB2 | 2.36 | 0.40 |
| 31:4:15:G:H1 | 31:4:21:A:H2 | 1.63 | 0.40 |
| 31:4:46:A:H8 | 31:4:46:A:OP2 | 2.04 | 0.40 |
| 31:4:63:G:C2 | 31:4:64:G:N7 | 2.89 | 0.40 |
| 33:7:37:HIS:CD2 | 33:7:48:LYS:HB2 | 2.57 | 0.40 |
| 33:7:88:ARG:HG3 | 33:7:88:ARG:HH21 | 1.87 | 0.40 |
| 33:7:330:ARG:HG3 | 33:7:330:ARG:O | 2.21 | 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 PDB entries followed by that with respect to all EM entries.

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 2 | A | 186/199 (94%) | 157 (84%) | 29 (16%) | 0 | 100 | 100 |
| 3 | B | 194/202 (96%) | 162 (84%) | 32 (16%) | 0 | 100 | 100 |
| 4 | C | 59/63 (94%) | 43 (73%) | 16 (27%) | 0 | 100 | 100 |
| 5 | D | 173/180 (96%) | 140 (81%) | 32 (18%) | 1 (1%) | 22 | 59 |
| 6 | E | 240/243 (99%) | 179 (75%) | 60 (25%) | 1 (0%) | 30 | 67 |
| 7 | F | 227/236 (96%) | 172 (76%) | 55 (24%) | 0 | 100 | 100 |
| 8 | G | 122/125 (98%) | 97 (80%) | 25 (20%) | 0 | 100 | 100 |
| 9 | H | 211/215 (98%) | 171 (81%) | 40 (19%) | 0 | 100 | 100 |
| 10 | I | 127/130 (98%) | 96 (76%) | 31 (24%) | 0 | 100 | 100 |
| 11 | J | 124/127 (98%) | 91 (73%) | 33 (27%) | 0 | 100 | 100 |
| 12 | K | 132/135 (98%) | 107 (81%) | 25 (19%) | 0 | 100 | 100 |
| 13 | L | 99/102 (97%) | 86 (87%) | 13 (13%) | 0 | 100 | 100 |
| 14 | M | 126/137 (92%) | 105 (83%) | 21 (17%) | 0 | 100 | 100 |
| 15 | N | 144/147 (98%) | 104 (72%) | 39 (27%) | 1 (1%) | 19 | 56 |
| 16 | O | 136/148 (92%) | 107 (79%) | 28 (21%) | 1 (1%) | 19 | 56 |
| 17 | P | 53/56 (95%) | 40 (76%) | 13 (24%) | 0 | 100 | 100 |
| 18 | Q | 150/158 (95%) | 127 (85%) | 23 (15%) | 0 | 100 | 100 |
| 19 | R | 107/113 (95%) | 80 (75%) | 27 (25%) | 0 | 100 | 100 |
| 20 | S | 64/67 (96%) | 54 (84%) | 10 (16%) | 0 | 100 | 100 |
| 21 | T | 123/132 (93%) | 94 (76%) | 29 (24%) | 0 | 100 | 100 |
| 22 | U | 147/150 (98%) | 125 (85%) | 22 (15%) | 0 | 100 | 100 |
| 23 | V | 92/99 (93%) | 69 (75%) | 23 (25%) | 0 | 100 | 100 |
| 24 | W | 61/65 (94%) | 45 (74%) | 16 (26%) | 0 | 100 | 100 |
| 25 | X | 65/71 (92%) | 48 (74%) | 17 (26%) | 0 | 100 | 100 |
| 26 | Y | 48/51 (94%) | 28 (58%) | 20 (42%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|----------|-------------|-----|
| 27 | Z | 195/210 (93%) | 152 (78%) | 43 (22%) | 0 | 100 | 100 |
| 28 | 0 | 34/36 (94%) | 22 (65%) | 12 (35%) | 0 | 100 | 100 |
| 29 | 3 | 121/123 (98%) | 96 (79%) | 25 (21%) | 0 | 100 | 100 |
| 32 | 6 | 93/113 (82%) | 78 (84%) | 15 (16%) | 0 | 100 | 100 |
| 33 | 7 | 412/414 (100%) | 363 (88%) | 46 (11%) | 3 (1%) | 19 | 56 |
| 34 | 8 | 125/129 (97%) | 113 (90%) | 12 (10%) | 0 | 100 | 100 |
| 35 | 9 | 247/254 (97%) | 234 (95%) | 13 (5%) | 0 | 100 | 100 |
| All | All | 4437/4630 (96%) | 3585 (81%) | 845 (19%) | 7 (0%) | 45 | 77 |

All (7) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 16 | O | 88 | GLY |
| 33 | 7 | 66 | GLU |
| 5 | D | 103 | ARG |
| 33 | 7 | 265 | GLY |
| 15 | N | 6 | ALA |
| 6 | E | 36 | PRO |
| 33 | 7 | 127 | PRO |

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 PDB entries followed by that with respect to all EM entries.

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|------------|----------|-------------|----|
| 2 | A | 161/167 (96%) | 159 (99%) | 2 (1%) | 67 | 78 |
| 3 | B | 168/173 (97%) | 167 (99%) | 1 (1%) | 84 | 88 |
| 4 | C | 54/55 (98%) | 53 (98%) | 1 (2%) | 52 | 69 |
| 5 | D | 158/160 (99%) | 154 (98%) | 4 (2%) | 42 | 62 |
| 6 | E | 213/214 (100%) | 212 (100%) | 1 (0%) | 86 | 90 |
| 7 | F | 192/198 (97%) | 187 (97%) | 5 (3%) | 41 | 61 |
| 8 | G | 107/108 (99%) | 106 (99%) | 1 (1%) | 75 | 83 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 9 | H | 183/184 (100%) | 180 (98%) | 3 (2%) | 58 | 73 |
| 10 | I | 106/107 (99%) | 105 (99%) | 1 (1%) | 75 | 83 |
| 11 | J | 102/103 (99%) | 101 (99%) | 1 (1%) | 73 | 81 |
| 12 | K | 110/111 (99%) | 109 (99%) | 1 (1%) | 75 | 83 |
| 13 | L | 90/91 (99%) | 89 (99%) | 1 (1%) | 70 | 79 |
| 14 | M | 95/104 (91%) | 95 (100%) | 0 | 100 | 100 |
| 15 | N | 120/121 (99%) | 118 (98%) | 2 (2%) | 56 | 72 |
| 16 | O | 115/123 (94%) | 115 (100%) | 0 | 100 | 100 |
| 17 | P | 45/46 (98%) | 44 (98%) | 1 (2%) | 47 | 65 |
| 18 | Q | 137/143 (96%) | 135 (98%) | 2 (2%) | 60 | 74 |
| 19 | R | 98/102 (96%) | 97 (99%) | 1 (1%) | 73 | 81 |
| 20 | S | 60/61 (98%) | 60 (100%) | 0 | 100 | 100 |
| 21 | T | 109/114 (96%) | 109 (100%) | 0 | 100 | 100 |
| 22 | U | 126/127 (99%) | 124 (98%) | 2 (2%) | 58 | 73 |
| 23 | V | 86/90 (96%) | 86 (100%) | 0 | 100 | 100 |
| 24 | W | 54/56 (96%) | 54 (100%) | 0 | 100 | 100 |
| 25 | X | 57/60 (95%) | 56 (98%) | 1 (2%) | 54 | 71 |
| 26 | Y | 41/42 (98%) | 38 (93%) | 3 (7%) | 11 | 34 |
| 27 | Z | 156/168 (93%) | 154 (99%) | 2 (1%) | 65 | 76 |
| 28 | 0 | 34/34 (100%) | 32 (94%) | 2 (6%) | 16 | 40 |
| 29 | 3 | 99/99 (100%) | 97 (98%) | 2 (2%) | 50 | 68 |
| 32 | 6 | 83/99 (84%) | 83 (100%) | 0 | 100 | 100 |
| 33 | 7 | 356/356 (100%) | 352 (99%) | 4 (1%) | 70 | 79 |
| 34 | 8 | 117/118 (99%) | 113 (97%) | 4 (3%) | 32 | 53 |
| 35 | 9 | 226/228 (99%) | 225 (100%) | 1 (0%) | 89 | 91 |
| All | All | 3858/3962 (97%) | 3809 (99%) | 49 (1%) | 64 | 76 |

All (49) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | A | 23 | TYR |
| 2 | A | 116 | TYR |
| 3 | B | 12 | TYR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | C | 15 | THR |
| 5 | D | 3 | ASP |
| 5 | D | 64 | LYS |
| 5 | D | 116 | ARG |
| 5 | D | 168 | ARG |
| 6 | E | 144 | ASP |
| 7 | F | 8 | TYR |
| 7 | F | 21 | LYS |
| 7 | F | 37 | ILE |
| 7 | F | 82 | ARG |
| 7 | F | 136 | ARG |
| 8 | G | 97 | LYS |
| 9 | H | 90 | HIS |
| 9 | H | 145 | ARG |
| 9 | H | 147 | HIS |
| 10 | I | 61 | TYR |
| 11 | J | 73 | ARG |
| 12 | K | 16 | ARG |
| 13 | L | 74 | ASP |
| 15 | N | 87 | PHE |
| 15 | N | 131 | ARG |
| 17 | P | 14 | PHE |
| 18 | Q | 124 | LEU |
| 18 | Q | 135 | TYR |
| 19 | R | 69 | ARG |
| 22 | U | 71 | GLU |
| 22 | U | 85 | HIS |
| 25 | X | 71 | ARG |
| 26 | Y | 15 | VAL |
| 26 | Y | 37 | ARG |
| 26 | Y | 49 | LYS |
| 27 | Z | 166 | TYR |
| 27 | Z | 178 | VAL |
| 28 | 0 | 2 | LYS |
| 28 | 0 | 13 | ARG |
| 29 | 3 | 9 | PHE |
| 29 | 3 | 122 | MET |
| 33 | 7 | 3 | TRP |
| 33 | 7 | 124 | PHE |
| 33 | 7 | 383 | ARG |
| 33 | 7 | 394 | ARG |
| 34 | 8 | 5 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34 | 8 | 19 | PRO |
| 34 | 8 | 98 | ARG |
| 34 | 8 | 118 | LYS |
| 35 | 9 | 241 | GLU |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | A | 64 | HIS |
| 2 | A | 70 | GLN |
| 2 | A | 134 | GLN |
| 2 | A | 164 | ASN |
| 3 | B | 18 | HIS |
| 3 | B | 178 | ASN |
| 4 | C | 4 | ASN |
| 5 | D | 50 | ASN |
| 5 | D | 123 | GLN |
| 5 | D | 162 | ASN |
| 6 | E | 9 | HIS |
| 7 | F | 181 | GLN |
| 7 | F | 196 | ASN |
| 7 | F | 203 | ASN |
| 8 | G | 120 | ASN |
| 9 | H | 13 | HIS |
| 9 | H | 46 | HIS |
| 9 | H | 51 | HIS |
| 9 | H | 94 | ASN |
| 9 | H | 147 | HIS |
| 9 | H | 164 | ASN |
| 9 | H | 193 | ASN |
| 10 | I | 9 | ASN |
| 11 | J | 64 | ASN |
| 12 | K | 117 | HIS |
| 12 | K | 131 | GLN |
| 14 | M | 18 | HIS |
| 15 | N | 8 | ASN |
| 15 | N | 66 | ASN |
| 16 | O | 6 | HIS |
| 16 | O | 18 | ASN |
| 18 | Q | 112 | HIS |
| 19 | R | 26 | HIS |
| 19 | R | 71 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20 | S | 22 | ASN |
| 21 | T | 66 | HIS |
| 21 | T | 84 | HIS |
| 21 | T | 115 | HIS |
| 22 | U | 40 | HIS |
| 24 | W | 27 | GLN |
| 25 | X | 26 | GLN |
| 27 | Z | 77 | ASN |
| 27 | Z | 95 | GLN |
| 27 | Z | 123 | ASN |
| 27 | Z | 156 | ASN |
| 29 | 3 | 37 | ASN |
| 33 | 7 | 97 | HIS |
| 33 | 7 | 143 | ASN |
| 33 | 7 | 162 | GLN |
| 33 | 7 | 224 | ASN |
| 33 | 7 | 400 | GLN |
| 34 | 8 | 84 | GLN |
| 35 | 9 | 53 | ASN |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | 2 | 1458/1497 (97%) | 501 (34%) | 19 (1%) |
| 30 | 5 | 19/20 (95%) | 9 (47%) | 0 |
| 31 | 4 | 75/76 (98%) | 32 (42%) | 1 (1%) |
| All | All | 1552/1593 (97%) | 542 (34%) | 20 (1%) |

All (542) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 2 | 14 | U |
| 1 | 2 | 15 | U |
| 1 | 2 | 16 | C |
| 1 | 2 | 23 | A |
| 1 | 2 | 30 | C |
| 1 | 2 | 31 | G |
| 1 | 2 | 33 | A |
| 1 | 2 | 44 | A |
| 1 | 2 | 45 | U |
| 1 | 2 | 49 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 2 | 52 | C |
| 1 | 2 | 55 | A |
| 1 | 2 | 56 | C |
| 1 | 2 | 57 | U |
| 1 | 2 | 58 | A |
| 1 | 2 | 59 | A |
| 1 | 2 | 60 | G |
| 1 | 2 | 62 | C |
| 1 | 2 | 72 | A |
| 1 | 2 | 73 | A |
| 1 | 2 | 74 | G |
| 1 | 2 | 82 | C |
| 1 | 2 | 86 | U |
| 1 | 2 | 87 | C |
| 1 | 2 | 88 | U |
| 1 | 2 | 91 | G |
| 1 | 2 | 92 | A |
| 1 | 2 | 95 | C |
| 1 | 2 | 99 | C |
| 1 | 2 | 110 | U |
| 1 | 2 | 111 | C |
| 1 | 2 | 117 | C |
| 1 | 2 | 118 | A |
| 1 | 2 | 119 | C |
| 1 | 2 | 126 | A |
| 1 | 2 | 127 | A |
| 1 | 2 | 128 | C |
| 1 | 2 | 132 | C |
| 1 | 2 | 133 | C |
| 1 | 2 | 143 | G |
| 1 | 2 | 146 | A |
| 1 | 2 | 149 | A |
| 1 | 2 | 150 | C |
| 1 | 2 | 153 | C |
| 1 | 2 | 154 | G |
| 1 | 2 | 156 | G |
| 1 | 2 | 157 | A |
| 1 | 2 | 164 | G |
| 1 | 2 | 168 | A |
| 1 | 2 | 169 | A |
| 1 | 2 | 178 | A |
| 1 | 2 | 179 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 2 | 187 | G |
| 1 | 2 | 188 | U |
| 1 | 2 | 189 | A |
| 1 | 2 | 196 | G |
| 1 | 2 | 201 | C |
| 1 | 2 | 203 | A |
| 1 | 2 | 204 | G |
| 1 | 2 | 209 | A |
| 1 | 2 | 210 | A |
| 1 | 2 | 211 | A |
| 1 | 2 | 212 | G |
| 1 | 2 | 214 | G |
| 1 | 2 | 217 | C |
| 1 | 2 | 222 | A |
| 1 | 2 | 224 | G |
| 1 | 2 | 225 | C |
| 1 | 2 | 226 | U |
| 1 | 2 | 227 | C |
| 1 | 2 | 249 | C |
| 1 | 2 | 251 | G |
| 1 | 2 | 253 | U |
| 1 | 2 | 255 | A |
| 1 | 2 | 256 | G |
| 1 | 2 | 258 | U |
| 1 | 2 | 260 | G |
| 1 | 2 | 268 | G |
| 1 | 2 | 269 | G |
| 1 | 2 | 274 | G |
| 1 | 2 | 275 | G |
| 1 | 2 | 276 | C |
| 1 | 2 | 277 | C |
| 1 | 2 | 283 | A |
| 1 | 2 | 287 | G |
| 1 | 2 | 288 | A |
| 1 | 2 | 292 | U |
| 1 | 2 | 298 | C |
| 1 | 2 | 299 | G |
| 1 | 2 | 301 | G |
| 1 | 2 | 305 | U |
| 1 | 2 | 307 | A |
| 1 | 2 | 308 | G |
| 1 | 2 | 315 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 2 | 322 | A |
| 1 | 2 | 323 | G |
| 1 | 2 | 324 | A |
| 1 | 2 | 333 | G |
| 1 | 2 | 334 | A |
| 1 | 2 | 336 | A |
| 1 | 2 | 337 | C |
| 1 | 2 | 338 | A |
| 1 | 2 | 339 | C |
| 1 | 2 | 341 | G |
| 1 | 2 | 344 | C |
| 1 | 2 | 354 | C |
| 1 | 2 | 358 | G |
| 1 | 2 | 361 | C |
| 1 | 2 | 362 | A |
| 1 | 2 | 363 | G |
| 1 | 2 | 367 | G |
| 1 | 2 | 371 | G |
| 1 | 2 | 374 | A |
| 1 | 2 | 375 | C |
| 1 | 2 | 376 | C |
| 1 | 2 | 381 | C |
| 1 | 2 | 382 | A |
| 1 | 2 | 390 | A |
| 1 | 2 | 391 | A |
| 1 | 2 | 393 | C |
| 1 | 2 | 395 | G |
| 1 | 2 | 397 | G |
| 1 | 2 | 402 | G |
| 1 | 2 | 406 | A |
| 1 | 2 | 407 | C |
| 1 | 2 | 408 | C |
| 1 | 2 | 409 | C |
| 1 | 2 | 415 | G |
| 1 | 2 | 421 | C |
| 1 | 2 | 422 | C |
| 1 | 2 | 423 | U |
| 1 | 2 | 424 | C |
| 1 | 2 | 425 | U |
| 1 | 2 | 426 | G |
| 1 | 2 | 430 | C |
| 1 | 2 | 431 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 2 | 435 | U |
| 1 | 2 | 436 | U |
| 1 | 2 | 437 | U |
| 1 | 2 | 440 | G |
| 1 | 2 | 443 | G |
| 1 | 2 | 446 | U |
| 1 | 2 | 447 | A |
| 1 | 2 | 448 | A |
| 1 | 2 | 452 | G |
| 1 | 2 | 456 | C |
| 1 | 2 | 459 | G |
| 1 | 2 | 460 | A |
| 1 | 2 | 462 | U |
| 1 | 2 | 463 | A |
| 1 | 2 | 464 | A |
| 1 | 2 | 465 | G |
| 1 | 2 | 466 | G |
| 1 | 2 | 470 | G |
| 1 | 2 | 472 | G |
| 1 | 2 | 473 | C |
| 1 | 2 | 475 | A |
| 1 | 2 | 477 | G |
| 1 | 2 | 478 | C |
| 1 | 2 | 480 | G |
| 1 | 2 | 482 | U |
| 1 | 2 | 483 | G |
| 1 | 2 | 484 | G |
| 1 | 2 | 485 | C |
| 1 | 2 | 491 | C |
| 1 | 2 | 493 | G |
| 1 | 2 | 495 | G |
| 1 | 2 | 496 | G |
| 1 | 2 | 497 | U |
| 1 | 2 | 498 | A |
| 1 | 2 | 499 | A |
| 1 | 2 | 502 | C |
| 1 | 2 | 504 | G |
| 1 | 2 | 507 | G |
| 1 | 2 | 509 | C |
| 1 | 2 | 513 | A |
| 1 | 2 | 515 | U |
| 1 | 2 | 516 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 2 | 518 | U |
| 1 | 2 | 519 | G |
| 1 | 2 | 520 | G |
| 1 | 2 | 521 | C |
| 1 | 2 | 524 | C |
| 1 | 2 | 525 | U |
| 1 | 2 | 526 | A |
| 1 | 2 | 527 | U |
| 1 | 2 | 529 | A |
| 1 | 2 | 530 | U |
| 1 | 2 | 531 | U |
| 1 | 2 | 532 | G |
| 1 | 2 | 533 | G |
| 1 | 2 | 536 | C |
| 1 | 2 | 537 | U |
| 1 | 2 | 538 | A |
| 1 | 2 | 539 | A |
| 1 | 2 | 541 | G |
| 1 | 2 | 542 | C |
| 1 | 2 | 547 | G |
| 1 | 2 | 552 | C |
| 1 | 2 | 554 | G |
| 1 | 2 | 561 | A |
| 1 | 2 | 571 | C |
| 1 | 2 | 575 | A |
| 1 | 2 | 580 | A |
| 1 | 2 | 585 | U |
| 1 | 2 | 586 | C |
| 1 | 2 | 587 | A |
| 1 | 2 | 588 | A |
| 1 | 2 | 589 | C |
| 1 | 2 | 595 | G |
| 1 | 2 | 596 | G |
| 1 | 2 | 598 | U |
| 1 | 2 | 600 | G |
| 1 | 2 | 620 | U |
| 1 | 2 | 621 | G |
| 1 | 2 | 622 | G |
| 1 | 2 | 624 | A |
| 1 | 2 | 630 | A |
| 1 | 2 | 632 | A |
| 1 | 2 | 633 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 2 | 642 | U |
| 1 | 2 | 646 | C |
| 1 | 2 | 649 | G |
| 1 | 2 | 654 | A |
| 1 | 2 | 655 | G |
| 1 | 2 | 661 | A |
| 1 | 2 | 668 | A |
| 1 | 2 | 670 | A |
| 1 | 2 | 677 | G |
| 1 | 2 | 679 | G |
| 1 | 2 | 681 | G |
| 1 | 2 | 683 | C |
| 1 | 2 | 686 | C |
| 1 | 2 | 687 | C |
| 1 | 2 | 688 | A |
| 1 | 2 | 690 | U |
| 1 | 2 | 691 | G |
| 1 | 2 | 694 | G |
| 1 | 2 | 698 | G |
| 1 | 2 | 701 | C |
| 1 | 2 | 715 | G |
| 1 | 2 | 716 | U |
| 1 | 2 | 722 | G |
| 1 | 2 | 727 | G |
| 1 | 2 | 733 | A |
| 1 | 2 | 739 | A |
| 1 | 2 | 740 | G |
| 1 | 2 | 743 | G |
| 1 | 2 | 744 | A |
| 1 | 2 | 748 | A |
| 1 | 2 | 749 | A |
| 1 | 2 | 759 | A |
| 1 | 2 | 760 | U |
| 1 | 2 | 761 | A |
| 1 | 2 | 767 | G |
| 1 | 2 | 770 | G |
| 1 | 2 | 775 | G |
| 1 | 2 | 776 | G |
| 1 | 2 | 777 | C |
| 1 | 2 | 778 | U |
| 1 | 2 | 782 | A |
| 1 | 2 | 784 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 2 | 785 | G |
| 1 | 2 | 786 | A |
| 1 | 2 | 787 | U |
| 1 | 2 | 788 | G |
| 1 | 2 | 789 | C |
| 1 | 2 | 795 | A |
| 1 | 2 | 796 | G |
| 1 | 2 | 809 | C |
| 1 | 2 | 812 | C |
| 1 | 2 | 813 | G |
| 1 | 2 | 819 | G |
| 1 | 2 | 823 | G |
| 1 | 2 | 824 | G |
| 1 | 2 | 829 | G |
| 1 | 2 | 835 | A |
| 1 | 2 | 836 | A |
| 1 | 2 | 837 | G |
| 1 | 2 | 838 | C |
| 1 | 2 | 841 | U |
| 1 | 2 | 843 | A |
| 1 | 2 | 844 | A |
| 1 | 2 | 853 | C |
| 1 | 2 | 856 | G |
| 1 | 2 | 870 | C |
| 1 | 2 | 873 | G |
| 1 | 2 | 875 | C |
| 1 | 2 | 885 | A |
| 1 | 2 | 886 | A |
| 1 | 2 | 892 | U |
| 1 | 2 | 897 | G |
| 1 | 2 | 905 | C |
| 1 | 2 | 906 | U |
| 1 | 2 | 914 | G |
| 1 | 2 | 915 | U |
| 1 | 2 | 926 | G |
| 1 | 2 | 928 | U |
| 1 | 2 | 932 | U |
| 1 | 2 | 936 | A |
| 1 | 2 | 939 | 5MC |
| 1 | 2 | 940 | A |
| 1 | 2 | 941 | A |
| 1 | 2 | 943 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 2 | 946 | G |
| 1 | 2 | 947 | G |
| 1 | 2 | 950 | A |
| 1 | 2 | 953 | U |
| 1 | 2 | 962 | G |
| 1 | 2 | 965 | A |
| 1 | 2 | 966 | C |
| 1 | 2 | 968 | G |
| 1 | 2 | 969 | C |
| 1 | 2 | 970 | A |
| 1 | 2 | 971 | G |
| 1 | 2 | 974 | U |
| 1 | 2 | 975 | G |
| 1 | 2 | 976 | A |
| 1 | 2 | 977 | A |
| 1 | 2 | 978 | G |
| 1 | 2 | 980 | C |
| 1 | 2 | 986 | U |
| 1 | 2 | 990 | G |
| 1 | 2 | 991 | G |
| 1 | 2 | 992 | U |
| 1 | 2 | 996 | G |
| 1 | 2 | 997 | C |
| 1 | 2 | 999 | G |
| 1 | 2 | 1000 | G |
| 1 | 2 | 1001 | A |
| 1 | 2 | 1002 | C |
| 1 | 2 | 1003 | G |
| 1 | 2 | 1004 | C |
| 1 | 2 | 1005 | G |
| 1 | 2 | 1011 | A |
| 1 | 2 | 1018 | G |
| 1 | 2 | 1019 | C |
| 1 | 2 | 1029 | G |
| 1 | 2 | 1032 | A |
| 1 | 2 | 1040 | C |
| 1 | 2 | 1043 | U |
| 1 | 2 | 1047 | G |
| 1 | 2 | 1049 | G |
| 1 | 2 | 1051 | C |
| 1 | 2 | 1055 | U |
| 1 | 2 | 1057 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 2 | 1058 | A |
| 1 | 2 | 1059 | G |
| 1 | 2 | 1060 | U |
| 1 | 2 | 1065 | U |
| 1 | 2 | 1066 | A |
| 1 | 2 | 1067 | A |
| 1 | 2 | 1068 | C |
| 1 | 2 | 1071 | G |
| 1 | 2 | 1078 | C |
| 1 | 2 | 1090 | U |
| 1 | 2 | 1098 | C |
| 1 | 2 | 1105 | G |
| 1 | 2 | 1106 | C |
| 1 | 2 | 1107 | U |
| 1 | 2 | 1108 | C |
| 1 | 2 | 1109 | G |
| 1 | 2 | 1114 | G |
| 1 | 2 | 1116 | A |
| 1 | 2 | 1117 | G |
| 1 | 2 | 1119 | C |
| 1 | 2 | 1123 | C |
| 1 | 2 | 1126 | G |
| 1 | 2 | 1131 | A |
| 1 | 2 | 1133 | U |
| 1 | 2 | 1134 | G |
| 1 | 2 | 1136 | C |
| 1 | 2 | 1141 | A |
| 1 | 2 | 1142 | U |
| 1 | 2 | 1143 | A |
| 1 | 2 | 1144 | A |
| 1 | 2 | 1155 | G |
| 1 | 2 | 1156 | G |
| 1 | 2 | 1157 | G |
| 1 | 2 | 1158 | G |
| 1 | 2 | 1161 | G |
| 1 | 2 | 1163 | C |
| 1 | 2 | 1170 | A |
| 1 | 2 | 1171 | G |
| 1 | 2 | 1174 | C |
| 1 | 2 | 1175 | A |
| 1 | 2 | 1185 | G |
| 1 | 2 | 1186 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 2 | 1187 | A |
| 1 | 2 | 1189 | C |
| 1 | 2 | 1190 | C |
| 1 | 2 | 1192 | C |
| 1 | 2 | 1195 | G |
| 1 | 2 | 1197 | C |
| 1 | 2 | 1199 | A |
| 1 | 2 | 1200 | C |
| 1 | 2 | 1201 | A |
| 1 | 2 | 1203 | G |
| 1 | 2 | 1211 | C |
| 1 | 2 | 1212 | A |
| 1 | 2 | 1214 | U |
| 1 | 2 | 1215 | G |
| 1 | 2 | 1221 | G |
| 1 | 2 | 1229 | G |
| 1 | 2 | 1230 | U |
| 1 | 2 | 1232 | C |
| 1 | 2 | 1234 | G |
| 1 | 2 | 1236 | C |
| 1 | 2 | 1244 | G |
| 1 | 2 | 1245 | G |
| 1 | 2 | 1248 | G |
| 1 | 2 | 1249 | A |
| 1 | 2 | 1254 | A |
| 1 | 2 | 1260 | U |
| 1 | 2 | 1264 | C |
| 1 | 2 | 1273 | A |
| 1 | 2 | 1274 | G |
| 1 | 2 | 1276 | U |
| 1 | 2 | 1277 | C |
| 1 | 2 | 1279 | G |
| 1 | 2 | 1284 | C |
| 1 | 2 | 1294 | C |
| 1 | 2 | 1303 | G |
| 1 | 2 | 1309 | C |
| 1 | 2 | 1310 | U |
| 1 | 2 | 1311 | G |
| 1 | 2 | 1312 | G |
| 1 | 2 | 1313 | A |
| 1 | 2 | 1319 | U |
| 1 | 2 | 1322 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 2 | 1327 | G |
| 1 | 2 | 1333 | C |
| 1 | 2 | 1338 | U |
| 1 | 2 | 1340 | G |
| 1 | 2 | 1342 | G |
| 1 | 2 | 1344 | G |
| 1 | 2 | 1347 | G |
| 1 | 2 | 1348 | A |
| 1 | 2 | 1350 | U |
| 1 | 2 | 1354 | U |
| 1 | 2 | 1356 | C |
| 1 | 2 | 1361 | U |
| 1 | 2 | 1364 | U |
| 1 | 2 | 1366 | G |
| 1 | 2 | 1368 | A |
| 1 | 2 | 1369 | C |
| 1 | 2 | 1371 | C |
| 1 | 2 | 1372 | A |
| 1 | 2 | 1383 | C |
| 1 | 2 | 1385 | C |
| 1 | 2 | 1386 | C |
| 1 | 2 | 1388 | C |
| 1 | 2 | 1391 | G |
| 1 | 2 | 1393 | G |
| 1 | 2 | 1394 | C |
| 1 | 2 | 1395 | G |
| 1 | 2 | 1397 | G |
| 1 | 2 | 1398 | G |
| 1 | 2 | 1399 | C |
| 1 | 2 | 1401 | U |
| 1 | 2 | 1404 | G |
| 1 | 2 | 1412 | C |
| 1 | 2 | 1416 | C |
| 1 | 2 | 1419 | C |
| 1 | 2 | 1420 | U |
| 1 | 2 | 1424 | G |
| 1 | 2 | 1436 | G |
| 1 | 2 | 1437 | A |
| 1 | 2 | 1440 | C |
| 1 | 2 | 1441 | U |
| 1 | 2 | 1444 | G |
| 1 | 2 | 1445 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 2 | 1449 | G |
| 1 | 2 | 1450 | U |
| 1 | 2 | 1451 | G |
| 1 | 2 | 1452 | A |
| 1 | 2 | 1453 | G |
| 1 | 2 | 1454 | G |
| 1 | 2 | 1456 | G |
| 1 | 2 | 1457 | G |
| 1 | 2 | 1459 | A |
| 1 | 2 | 1461 | A |
| 1 | 2 | 1462 | A |
| 1 | 2 | 1463 | G |
| 1 | 2 | 1466 | G |
| 1 | 2 | 1467 | UR3 |
| 1 | 2 | 1471 | A |
| 1 | 2 | 1472 | A |
| 1 | 2 | 1473 | G |
| 1 | 2 | 1475 | U |
| 1 | 2 | 1476 | A |
| 1 | 2 | 1480 | G |
| 1 | 2 | 1486 | G |
| 1 | 2 | 1492 | A |
| 1 | 2 | 1493 | C |
| 1 | 2 | 1494 | G |
| 1 | 2 | 1497 | U |
| 1 | 2 | 1498 | C |
| 1 | 2 | 1499 | G |
| 1 | 2 | 1505 | C |
| 1 | 2 | 1508 | C |
| 30 | 5 | 806 | G |
| 30 | 5 | 807 | G |
| 30 | 5 | 813 | A |
| 30 | 5 | 814 | U |
| 30 | 5 | 815 | U |
| 30 | 5 | 816 | U |
| 30 | 5 | 817 | A |
| 30 | 5 | 822 | C |
| 30 | 5 | 823 | C |
| 31 | 4 | 3 | C |
| 31 | 4 | 6 | G |
| 31 | 4 | 7 | G |
| 31 | 4 | 9 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 31 | 4 | 12 | G |
| 31 | 4 | 13 | C |
| 31 | 4 | 14 | A |
| 31 | 4 | 15 | G |
| 31 | 4 | 16 | C |
| 31 | 4 | 17 | C |
| 31 | 4 | 18 | G |
| 31 | 4 | 20 | H2U |
| 31 | 4 | 21 | A |
| 31 | 4 | 22 | G |
| 31 | 4 | 23 | C |
| 31 | 4 | 25 | C |
| 31 | 4 | 26 | G |
| 31 | 4 | 31 | G |
| 31 | 4 | 46 | A |
| 31 | 4 | 49 | G |
| 31 | 4 | 52 | G |
| 31 | 4 | 55 | PSU |
| 31 | 4 | 58 | A |
| 31 | 4 | 59 | A |
| 31 | 4 | 60 | U |
| 31 | 4 | 66 | C |
| 31 | 4 | 69 | C |
| 31 | 4 | 71 | C |
| 31 | 4 | 72 | U |
| 31 | 4 | 74 | C |
| 31 | 4 | 75 | C |
| 31 | 4 | 76 | A |

All (20) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 2 | 87 | C |
| 1 | 2 | 132 | C |
| 1 | 2 | 168 | A |
| 1 | 2 | 209 | A |
| 1 | 2 | 268 | G |
| 1 | 2 | 461 | A |
| 1 | 2 | 599 | C |
| 1 | 2 | 618 | C |
| 1 | 2 | 632 | A |
| 1 | 2 | 687 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 2 | 913 | G |
| 1 | 2 | 952 | C |
| 1 | 2 | 998 | C |
| 1 | 2 | 1106 | C |
| 1 | 2 | 1155 | G |
| 1 | 2 | 1341 | C |
| 1 | 2 | 1347 | G |
| 1 | 2 | 1435 | C |
| 1 | 2 | 1448 | C |
| 31 | 4 | 73 | A |

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

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

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 1 | 4AC | 2 | 868 | 1 | 21,24,25 | 1.23 | 3 (14%) | 29,34,37 | 1.37 | 4 (13%) |
| 1 | 4AC | 2 | 1479 | 1 | 21,24,25 | 1.10 | 3 (14%) | 29,34,37 | 1.50 | 4 (13%) |
| 1 | LHH | 2 | 250 | 1 | 22,25,26 | 2.45 | 8 (36%) | 29,35,38 | 1.20 | 2 (6%) |
| 1 | 5HM | 2 | 1378 | 1 | 19,23,24 | 2.94 | 7 (36%) | 25,33,36 | 0.64 | 0 |
| 1 | MA6 | 2 | 1488 | 1 | 18,26,27 | 0.95 | 1 (5%) | 19,38,41 | 1.18 | 2 (10%) |
| 1 | B8H | 2 | 938 | 1 | 19,22,23 | 0.82 | 0 | 22,32,35 | 1.52 | 3 (13%) |
| 1 | 4AC | 2 | 17 | 1 | 21,24,25 | 1.06 | 2 (9%) | 29,34,37 | 1.77 | 5 (17%) |
| 1 | 4AC | 2 | 479 | 1 | 21,24,25 | 1.13 | 3 (14%) | 29,34,37 | 1.59 | 5 (17%) |
| 1 | 4AC | 2 | 1028 | 1 | 21,24,25 | 1.05 | 3 (14%) | 29,34,37 | 1.62 | 4 (13%) |
| 1 | 4AC | 2 | 1239 | 1 | 21,24,25 | 1.15 | 2 (9%) | 29,34,37 | 1.87 | 4 (13%) |
| 1 | OMC | 2 | 1376 | 1 | 19,22,23 | 0.90 | 2 (10%) | 26,31,34 | 0.76 | 0 |
| 1 | 4AC | 2 | 751 | 1 | 21,24,25 | 1.13 | 3 (14%) | 29,34,37 | 1.26 | 4 (13%) |
| 1 | UR3 | 2 | 1467 | 1 | 19,22,23 | 1.10 | 2 (10%) | 26,32,35 | 1.50 | 5 (19%) |
| 1 | 4AC | 2 | 303 | 1 | 21,24,25 | 1.16 | 3 (14%) | 29,34,37 | 1.44 | 3 (10%) |
| 1 | 4AC | 2 | 703 | 1 | 21,24,25 | 1.07 | 2 (9%) | 29,34,37 | 1.82 | 6 (20%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 1 | 5MC | 2 | 939 | 1 | 18,22,23 | 1.05 | 2 (11%) | 26,32,35 | 1.25 | 3 (11%) |
| 1 | 4AC | 2 | 546 | 1 | 21,24,25 | 1.03 | 2 (9%) | 29,34,37 | 1.44 | 3 (10%) |
| 31 | H2U | 4 | 20 | 31 | 18,21,22 | 1.10 | 2 (11%) | 21,30,33 | 2.24 | 1 (4%) |
| 1 | 4AC | 2 | 394 | 1 | 21,24,25 | 1.02 | 2 (9%) | 29,34,37 | 1.66 | 5 (17%) |
| 1 | 5MC | 2 | 1202 | 1 | 18,22,23 | 1.00 | 1 (5%) | 26,32,35 | 1.21 | 1 (3%) |
| 1 | 4AC | 2 | 718 | 1 | 21,24,25 | 1.08 | 2 (9%) | 29,34,37 | 1.18 | 3 (10%) |
| 1 | 4AC | 2 | 731 | 1 | 21,24,25 | 1.16 | 3 (14%) | 29,34,37 | 1.37 | 5 (17%) |
| 1 | 4AC | 2 | 1147 | 1 | 21,24,25 | 1.12 | 3 (14%) | 29,34,37 | 2.24 | 6 (20%) |
| 1 | 4AC | 2 | 957 | 1 | 21,24,25 | 1.12 | 1 (4%) | 29,34,37 | 2.29 | 7 (24%) |
| 31 | OMC | 4 | 32 | 31 | 19,22,23 | 0.99 | 2 (10%) | 26,31,34 | 1.13 | 2 (7%) |
| 1 | 4AC | 2 | 828 | 1 | 21,24,25 | 1.01 | 1 (4%) | 29,34,37 | 1.64 | 4 (13%) |
| 1 | 4AC | 2 | 1233 | 1 | 21,24,25 | 1.09 | 2 (9%) | 29,34,37 | 1.53 | 4 (13%) |
| 1 | 4AC | 2 | 286 | 1 | 21,24,25 | 1.11 | 2 (9%) | 29,34,37 | 1.64 | 7 (24%) |
| 1 | 4AC | 2 | 636 | 1 | 21,24,25 | 1.12 | 3 (14%) | 29,34,37 | 1.60 | 4 (13%) |
| 1 | 4AC | 2 | 1184 | 1 | 21,24,25 | 1.06 | 3 (14%) | 29,34,37 | 1.39 | 4 (13%) |
| 1 | 4AC | 2 | 851 | 1 | 21,24,25 | 1.24 | 3 (14%) | 29,34,37 | 1.57 | 4 (13%) |
| 31 | 4SU | 4 | 8 | 31 | 18,21,22 | 1.79 | 5 (27%) | 26,30,33 | 2.15 | 4 (15%) |
| 31 | 5MU | 4 | 54 | 31 | 19,22,23 | 1.44 | 6 (31%) | 28,32,35 | 2.05 | 8 (28%) |
| 1 | 4AC | 2 | 648 | 1 | 21,24,25 | 1.20 | 3 (14%) | 29,34,37 | 1.85 | 7 (24%) |
| 1 | 4AC | 2 | 848 | 1 | 21,24,25 | 1.12 | 2 (9%) | 29,34,37 | 1.75 | 4 (13%) |
| 1 | 4AC | 2 | 53 | 1 | 21,24,25 | 1.06 | 2 (9%) | 29,34,37 | 1.48 | 5 (17%) |
| 1 | 6MZ | 2 | 1469 | 36,1 | 18,25,26 | 0.76 | 1 (5%) | 16,36,39 | 2.10 | 3 (18%) |
| 1 | A2M | 2 | 373 | 1 | 18,25,26 | 1.06 | 1 (5%) | 18,36,39 | 1.39 | 4 (22%) |
| 1 | 4AC | 2 | 511 | 1 | 21,24,25 | 1.15 | 3 (14%) | 29,34,37 | 1.87 | 6 (20%) |
| 1 | 4AC | 2 | 590 | 36,1 | 21,24,25 | 1.15 | 3 (14%) | 29,34,37 | 1.47 | 4 (13%) |
| 1 | MA6 | 2 | 1487 | 1 | 18,26,27 | 0.92 | 1 (5%) | 19,38,41 | 1.28 | 3 (15%) |
| 31 | PSU | 4 | 55 | 31 | 18,21,22 | 1.38 | 2 (11%) | 22,30,33 | 1.85 | 3 (13%) |
| 1 | 4AC | 2 | 626 | 1 | 21,24,25 | 1.05 | 3 (14%) | 29,34,37 | 1.41 | 4 (13%) |
| 1 | 4AC | 2 | 1041 | 1 | 21,24,25 | 1.01 | 2 (9%) | 29,34,37 | 1.98 | 4 (13%) |
| 1 | 4AC | 2 | 319 | 1 | 21,24,25 | 1.20 | 3 (14%) | 29,34,37 | 1.48 | 4 (13%) |
| 1 | 4AC | 2 | 379 | 1 | 21,24,25 | 1.08 | 3 (14%) | 29,34,37 | 1.55 | 5 (17%) |
| 1 | 4AC | 2 | 1193 | 1 | 21,24,25 | 1.13 | 2 (9%) | 29,34,37 | 2.00 | 5 (17%) |
| 1 | 4AC | 2 | 839 | 1 | 21,24,25 | 1.13 | 2 (9%) | 29,34,37 | 1.80 | 6 (20%) |

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 |
|-----|------|-------|------|------|---------|------------|---------|
| 1 | 4AC | 2 | 868 | 1 | - | 2/11/29/30 | 0/2/2/2 |
| 1 | 4AC | 2 | 1479 | 1 | - | 0/11/29/30 | 0/2/2/2 |
| 1 | LHH | 2 | 250 | 1 | - | 1/13/31/32 | 0/2/2/2 |
| 1 | 5HM | 2 | 1378 | 1 | - | 2/9/27/28 | 0/2/2/2 |
| 1 | MA6 | 2 | 1488 | 1 | - | 0/7/29/30 | 0/3/3/3 |
| 1 | B8H | 2 | 938 | 1 | - | 3/7/25/26 | 0/2/2/2 |
| 1 | 4AC | 2 | 17 | 1 | - | 0/11/29/30 | 0/2/2/2 |
| 1 | 4AC | 2 | 479 | 1 | - | 3/11/29/30 | 0/2/2/2 |
| 1 | 4AC | 2 | 1028 | 1 | - | 2/11/29/30 | 0/2/2/2 |
| 1 | 4AC | 2 | 1239 | 1 | - | 2/11/29/30 | 0/2/2/2 |
| 1 | OMC | 2 | 1376 | 1 | - | 2/9/27/28 | 0/2/2/2 |
| 1 | 4AC | 2 | 751 | 1 | - | 0/11/29/30 | 0/2/2/2 |
| 1 | UR3 | 2 | 1467 | 1 | - | 6/7/25/26 | 0/2/2/2 |
| 1 | 4AC | 2 | 303 | 1 | - | 0/11/29/30 | 0/2/2/2 |
| 1 | 4AC | 2 | 703 | 1 | - | 0/11/29/30 | 0/2/2/2 |
| 1 | 5MC | 2 | 939 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 4AC | 2 | 546 | 1 | - | 2/11/29/30 | 0/2/2/2 |
| 31 | H2U | 4 | 20 | 31 | - | 4/7/38/39 | 0/2/2/2 |
| 1 | 4AC | 2 | 394 | 1 | - | 2/11/29/30 | 0/2/2/2 |
| 1 | 5MC | 2 | 1202 | 1 | - | 2/7/25/26 | 0/2/2/2 |
| 1 | 4AC | 2 | 718 | 1 | - | 0/11/29/30 | 0/2/2/2 |
| 1 | 4AC | 2 | 731 | 1 | - | 3/11/29/30 | 0/2/2/2 |
| 1 | 4AC | 2 | 1147 | 1 | - | 2/11/29/30 | 0/2/2/2 |
| 1 | 4AC | 2 | 957 | 1 | - | 1/11/29/30 | 0/2/2/2 |
| 31 | OMC | 4 | 32 | 31 | - | 2/9/27/28 | 0/2/2/2 |
| 1 | 4AC | 2 | 828 | 1 | - | 0/11/29/30 | 0/2/2/2 |
| 1 | 4AC | 2 | 1233 | 1 | - | 0/11/29/30 | 0/2/2/2 |
| 1 | 4AC | 2 | 286 | 1 | - | 5/11/29/30 | 0/2/2/2 |
| 1 | 4AC | 2 | 636 | 1 | - | 0/11/29/30 | 0/2/2/2 |
| 1 | 4AC | 2 | 1184 | 1 | - | 2/11/29/30 | 0/2/2/2 |
| 1 | 4AC | 2 | 851 | 1 | - | 4/11/29/30 | 0/2/2/2 |
| 31 | 4SU | 4 | 8 | 31 | - | 5/7/25/26 | 0/2/2/2 |
| 31 | 5MU | 4 | 54 | 31 | - | 1/7/25/26 | 0/2/2/2 |
| 1 | 4AC | 2 | 648 | 1 | - | 2/11/29/30 | 0/2/2/2 |
| 1 | 4AC | 2 | 848 | 1 | - | 2/11/29/30 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|------------|---------|
| 1 | 4AC | 2 | 53 | 1 | - | 0/11/29/30 | 0/2/2/2 |
| 1 | 6MZ | 2 | 1469 | 36,1 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | A2M | 2 | 373 | 1 | - | 1/5/27/28 | 0/3/3/3 |
| 1 | 4AC | 2 | 511 | 1 | - | 2/11/29/30 | 0/2/2/2 |
| 1 | 4AC | 2 | 590 | 36,1 | - | 2/11/29/30 | 0/2/2/2 |
| 1 | MA6 | 2 | 1487 | 1 | - | 0/7/29/30 | 0/3/3/3 |
| 31 | PSU | 4 | 55 | 31 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 4AC | 2 | 626 | 1 | - | 2/11/29/30 | 0/2/2/2 |
| 1 | 4AC | 2 | 1041 | 1 | - | 0/11/29/30 | 0/2/2/2 |
| 1 | 4AC | 2 | 319 | 1 | - | 4/11/29/30 | 0/2/2/2 |
| 1 | 4AC | 2 | 379 | 1 | - | 2/11/29/30 | 0/2/2/2 |
| 1 | 4AC | 2 | 1193 | 1 | - | 0/11/29/30 | 0/2/2/2 |
| 1 | 4AC | 2 | 839 | 1 | - | 1/11/29/30 | 0/2/2/2 |

All (122) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1 | 2 | 1378 | 5HM | C4-N3 | 6.29 | 1.44 | 1.34 |
| 1 | 2 | 250 | LHH | C4-N4 | 6.05 | 1.48 | 1.39 |
| 1 | 2 | 250 | LHH | C7-N4 | 5.67 | 1.47 | 1.37 |
| 1 | 2 | 1378 | 5HM | C2-N3 | 5.46 | 1.47 | 1.36 |
| 1 | 2 | 1378 | 5HM | C4-N4 | 5.36 | 1.48 | 1.34 |
| 1 | 2 | 1378 | 5HM | C6-C5 | 4.88 | 1.48 | 1.34 |
| 31 | 4 | 8 | 4SU | C4-S4 | -4.50 | 1.59 | 1.68 |
| 1 | 2 | 250 | LHH | O2-C2 | -4.33 | 1.15 | 1.23 |
| 1 | 2 | 1378 | 5HM | C6-N1 | 3.83 | 1.44 | 1.38 |
| 1 | 2 | 1378 | 5HM | O2-C2 | -3.63 | 1.17 | 1.23 |
| 1 | 2 | 319 | 4AC | C4-N3 | -3.50 | 1.26 | 1.32 |
| 31 | 4 | 55 | PSU | C6-C5 | 3.50 | 1.39 | 1.35 |
| 31 | 4 | 8 | 4SU | C4-N3 | -3.48 | 1.33 | 1.37 |
| 1 | 2 | 851 | 4AC | C4-N3 | -3.41 | 1.26 | 1.32 |
| 1 | 2 | 731 | 4AC | C4-N3 | -3.37 | 1.27 | 1.32 |
| 1 | 2 | 250 | LHH | C2-N1 | -3.26 | 1.32 | 1.40 |
| 1 | 2 | 868 | 4AC | C4-N3 | -3.23 | 1.27 | 1.32 |
| 1 | 2 | 303 | 4AC | C4-N3 | -3.21 | 1.27 | 1.32 |
| 1 | 2 | 1233 | 4AC | C4-N3 | -3.13 | 1.27 | 1.32 |
| 1 | 2 | 868 | 4AC | C4-N4 | -3.12 | 1.35 | 1.39 |
| 1 | 2 | 839 | 4AC | C4-N3 | -3.12 | 1.27 | 1.32 |
| 1 | 2 | 648 | 4AC | C4-N3 | -3.11 | 1.27 | 1.32 |
| 1 | 2 | 1202 | 5MC | C6-N1 | -3.09 | 1.32 | 1.38 |
| 1 | 2 | 1378 | 5HM | C2-N1 | 3.03 | 1.46 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1 | 2 | 590 | 4AC | C4-N3 | -3.02 | 1.27 | 1.32 |
| 1 | 2 | 479 | 4AC | C4-N3 | -2.99 | 1.27 | 1.32 |
| 1 | 2 | 636 | 4AC | C4-N3 | -2.97 | 1.27 | 1.32 |
| 1 | 2 | 751 | 4AC | C4-N3 | -2.91 | 1.27 | 1.32 |
| 1 | 2 | 250 | LHH | C6-N1 | -2.87 | 1.31 | 1.38 |
| 1 | 2 | 1479 | 4AC | C4-N3 | -2.86 | 1.27 | 1.32 |
| 1 | 2 | 939 | 5MC | C6-C5 | 2.83 | 1.39 | 1.34 |
| 1 | 2 | 1193 | 4AC | C4-N3 | -2.82 | 1.27 | 1.32 |
| 1 | 2 | 53 | 4AC | C5-C4 | 2.81 | 1.46 | 1.40 |
| 31 | 4 | 20 | H2U | C4-N3 | -2.80 | 1.32 | 1.37 |
| 1 | 2 | 379 | 4AC | C4-N3 | -2.80 | 1.27 | 1.32 |
| 1 | 2 | 1028 | 4AC | C4-N3 | -2.79 | 1.28 | 1.32 |
| 31 | 4 | 20 | H2U | C2-N3 | -2.77 | 1.33 | 1.38 |
| 1 | 2 | 1184 | 4AC | C4-N3 | -2.76 | 1.28 | 1.32 |
| 1 | 2 | 511 | 4AC | C4-N3 | -2.74 | 1.28 | 1.32 |
| 1 | 2 | 718 | 4AC | C5-C4 | 2.72 | 1.46 | 1.40 |
| 1 | 2 | 250 | LHH | C2-N3 | -2.71 | 1.30 | 1.36 |
| 31 | 4 | 54 | 5MU | C2-N1 | 2.70 | 1.42 | 1.38 |
| 1 | 2 | 828 | 4AC | C5-C4 | 2.69 | 1.46 | 1.40 |
| 1 | 2 | 590 | 4AC | C5-C4 | 2.68 | 1.46 | 1.40 |
| 1 | 2 | 626 | 4AC | C4-N3 | -2.63 | 1.28 | 1.32 |
| 1 | 2 | 319 | 4AC | C4-N4 | -2.62 | 1.35 | 1.39 |
| 1 | 2 | 939 | 5MC | C6-N1 | -2.62 | 1.33 | 1.38 |
| 1 | 2 | 1239 | 4AC | C4-N3 | -2.61 | 1.28 | 1.32 |
| 1 | 2 | 751 | 4AC | C5-C4 | 2.59 | 1.46 | 1.40 |
| 1 | 2 | 479 | 4AC | C5-C4 | 2.59 | 1.46 | 1.40 |
| 1 | 2 | 286 | 4AC | C5-C4 | 2.59 | 1.46 | 1.40 |
| 1 | 2 | 53 | 4AC | C4-N3 | -2.56 | 1.28 | 1.32 |
| 31 | 4 | 54 | 5MU | C4-N3 | -2.55 | 1.34 | 1.38 |
| 1 | 2 | 648 | 4AC | C4-N4 | -2.55 | 1.36 | 1.39 |
| 1 | 2 | 1467 | UR3 | C5-C4 | -2.54 | 1.37 | 1.43 |
| 1 | 2 | 286 | 4AC | C4-N3 | -2.53 | 1.28 | 1.32 |
| 1 | 2 | 546 | 4AC | C4-N3 | -2.53 | 1.28 | 1.32 |
| 1 | 2 | 1147 | 4AC | C6-C5 | -2.50 | 1.29 | 1.35 |
| 31 | 4 | 55 | PSU | C4-N3 | -2.49 | 1.34 | 1.38 |
| 1 | 2 | 703 | 4AC | C4-N3 | -2.49 | 1.28 | 1.32 |
| 1 | 2 | 718 | 4AC | C4-N3 | -2.48 | 1.28 | 1.32 |
| 1 | 2 | 957 | 4AC | C4-N3 | -2.48 | 1.28 | 1.32 |
| 31 | 4 | 8 | 4SU | C2-N1 | 2.45 | 1.42 | 1.38 |
| 31 | 4 | 54 | 5MU | C6-C5 | 2.45 | 1.38 | 1.34 |
| 1 | 2 | 17 | 4AC | C4-N3 | -2.44 | 1.28 | 1.32 |
| 1 | 2 | 394 | 4AC | C4-N3 | -2.44 | 1.28 | 1.32 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1 | 2 | 848 | 4AC | C4-N3 | -2.40 | 1.28 | 1.32 |
| 31 | 4 | 32 | OMC | C5-C4 | -2.40 | 1.37 | 1.42 |
| 1 | 2 | 1184 | 4AC | C5-C4 | 2.38 | 1.45 | 1.40 |
| 1 | 2 | 731 | 4AC | C4-N4 | -2.35 | 1.36 | 1.39 |
| 1 | 2 | 479 | 4AC | C4-N4 | -2.33 | 1.36 | 1.39 |
| 1 | 2 | 839 | 4AC | C4-N4 | -2.32 | 1.36 | 1.39 |
| 1 | 2 | 17 | 4AC | C4-N4 | -2.31 | 1.36 | 1.39 |
| 31 | 4 | 32 | OMC | C6-N1 | -2.30 | 1.32 | 1.38 |
| 1 | 2 | 1239 | 4AC | C4-N4 | -2.30 | 1.36 | 1.39 |
| 1 | 2 | 626 | 4AC | C4-N4 | -2.27 | 1.36 | 1.39 |
| 31 | 4 | 8 | 4SU | C5-C4 | -2.26 | 1.39 | 1.42 |
| 31 | 4 | 54 | 5MU | C6-N1 | -2.26 | 1.34 | 1.38 |
| 1 | 2 | 379 | 4AC | C4-N4 | -2.25 | 1.36 | 1.39 |
| 1 | 2 | 851 | 4AC | C5-C4 | 2.24 | 1.45 | 1.40 |
| 31 | 4 | 54 | 5MU | C2-N3 | -2.23 | 1.34 | 1.38 |
| 31 | 4 | 54 | 5MU | C4-C5 | 2.21 | 1.48 | 1.44 |
| 1 | 2 | 1147 | 4AC | C4-N3 | -2.21 | 1.29 | 1.32 |
| 1 | 2 | 848 | 4AC | C4-N4 | -2.20 | 1.36 | 1.39 |
| 1 | 2 | 868 | 4AC | C5-C4 | 2.19 | 1.45 | 1.40 |
| 1 | 2 | 1469 | 6MZ | C5-C4 | 2.19 | 1.46 | 1.40 |
| 1 | 2 | 379 | 4AC | C5-C4 | 2.19 | 1.45 | 1.40 |
| 1 | 2 | 648 | 4AC | C5-C4 | 2.19 | 1.45 | 1.40 |
| 1 | 2 | 1147 | 4AC | C4-N4 | -2.19 | 1.36 | 1.39 |
| 1 | 2 | 303 | 4AC | C5-C4 | 2.19 | 1.45 | 1.40 |
| 1 | 2 | 1233 | 4AC | C5-C4 | 2.18 | 1.45 | 1.40 |
| 1 | 2 | 636 | 4AC | C5-C4 | 2.18 | 1.45 | 1.40 |
| 1 | 2 | 250 | LHH | O7-C7 | -2.17 | 1.18 | 1.23 |
| 1 | 2 | 1184 | 4AC | C4-N4 | -2.16 | 1.36 | 1.39 |
| 1 | 2 | 511 | 4AC | C4-N4 | -2.15 | 1.36 | 1.39 |
| 1 | 2 | 1479 | 4AC | C4-N4 | -2.15 | 1.36 | 1.39 |
| 1 | 2 | 303 | 4AC | C4-N4 | -2.14 | 1.36 | 1.39 |
| 1 | 2 | 1376 | OMC | C5-C4 | -2.14 | 1.38 | 1.42 |
| 1 | 2 | 636 | 4AC | C4-N4 | -2.14 | 1.36 | 1.39 |
| 1 | 2 | 626 | 4AC | C5-C4 | 2.13 | 1.45 | 1.40 |
| 31 | 4 | 8 | 4SU | C6-C5 | 2.12 | 1.40 | 1.35 |
| 1 | 2 | 1028 | 4AC | C5-C4 | 2.12 | 1.45 | 1.40 |
| 1 | 2 | 751 | 4AC | C4-N4 | -2.12 | 1.36 | 1.39 |
| 1 | 2 | 1487 | MA6 | C4-N3 | -2.11 | 1.32 | 1.35 |
| 1 | 2 | 546 | 4AC | C5-C4 | 2.11 | 1.45 | 1.40 |
| 1 | 2 | 1028 | 4AC | C4-N4 | -2.10 | 1.36 | 1.39 |
| 1 | 2 | 590 | 4AC | C4-N4 | -2.10 | 1.36 | 1.39 |
| 1 | 2 | 1193 | 4AC | C4-N4 | -2.09 | 1.36 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1 | 2 | 1488 | MA6 | C5-C4 | 2.09 | 1.46 | 1.40 |
| 1 | 2 | 511 | 4AC | C5-C4 | 2.09 | 1.45 | 1.40 |
| 1 | 2 | 250 | LHH | C6-C5 | 2.08 | 1.39 | 1.35 |
| 1 | 2 | 1467 | UR3 | C6-N1 | -2.08 | 1.33 | 1.38 |
| 1 | 2 | 1041 | 4AC | C5-C4 | 2.08 | 1.45 | 1.40 |
| 1 | 2 | 703 | 4AC | C5-C4 | 2.07 | 1.45 | 1.40 |
| 1 | 2 | 731 | 4AC | C5-C4 | 2.06 | 1.45 | 1.40 |
| 1 | 2 | 394 | 4AC | C5-C4 | 2.05 | 1.45 | 1.40 |
| 1 | 2 | 851 | 4AC | C4-N4 | -2.05 | 1.36 | 1.39 |
| 1 | 2 | 319 | 4AC | C5-C4 | 2.04 | 1.45 | 1.40 |
| 1 | 2 | 373 | A2M | C5-N7 | -2.04 | 1.32 | 1.39 |
| 1 | 2 | 1479 | 4AC | C5-C4 | 2.03 | 1.45 | 1.40 |
| 1 | 2 | 1376 | OMC | C6-N1 | -2.03 | 1.33 | 1.38 |
| 1 | 2 | 1041 | 4AC | C4-N3 | -2.01 | 1.29 | 1.32 |

All (193) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 31 | 4 | 20 | H2U | C4-N3-C2 | -9.61 | 117.82 | 125.79 |
| 31 | 4 | 8 | 4SU | C4-N3-C2 | -6.85 | 120.68 | 127.34 |
| 1 | 2 | 1469 | 6MZ | C2-N1-C6 | 6.51 | 122.17 | 116.59 |
| 1 | 2 | 1147 | 4AC | C5-C4-N4 | -6.34 | 111.91 | 122.92 |
| 1 | 2 | 957 | 4AC | N4-C4-N3 | 6.19 | 124.24 | 113.85 |
| 1 | 2 | 1193 | 4AC | O7-C7-N4 | 5.84 | 131.27 | 121.82 |
| 31 | 4 | 55 | PSU | N1-C2-N3 | 5.76 | 121.65 | 115.13 |
| 1 | 2 | 1041 | 4AC | C5-C4-N4 | -5.69 | 113.04 | 122.92 |
| 1 | 2 | 957 | 4AC | O7-C7-N4 | 5.64 | 130.95 | 121.82 |
| 1 | 2 | 1041 | 4AC | O7-C7-N4 | 5.64 | 130.95 | 121.82 |
| 1 | 2 | 957 | 4AC | C5-C4-N4 | -5.59 | 113.22 | 122.92 |
| 1 | 2 | 648 | 4AC | O7-C7-N4 | 5.56 | 130.82 | 121.82 |
| 1 | 2 | 1147 | 4AC | O7-C7-N4 | 5.55 | 130.80 | 121.82 |
| 1 | 2 | 1147 | 4AC | N4-C4-N3 | 5.53 | 123.13 | 113.85 |
| 1 | 2 | 1239 | 4AC | O7-C7-N4 | 5.41 | 130.58 | 121.82 |
| 1 | 2 | 938 | B8H | C4-N3-C2 | -5.41 | 120.35 | 127.35 |
| 1 | 2 | 839 | 4AC | O7-C7-N4 | 5.35 | 130.48 | 121.82 |
| 31 | 4 | 8 | 4SU | C5-C4-N3 | 5.29 | 119.59 | 114.69 |
| 1 | 2 | 848 | 4AC | O7-C7-N4 | 5.26 | 130.34 | 121.82 |
| 1 | 2 | 1041 | 4AC | N4-C4-N3 | 5.26 | 122.68 | 113.85 |
| 1 | 2 | 1193 | 4AC | C5-C4-N4 | -5.17 | 113.94 | 122.92 |
| 1 | 2 | 17 | 4AC | O7-C7-N4 | 5.14 | 130.14 | 121.82 |
| 1 | 2 | 319 | 4AC | O7-C7-N4 | 5.04 | 129.98 | 121.82 |
| 1 | 2 | 1028 | 4AC | O7-C7-N4 | 5.01 | 129.93 | 121.82 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | 2 | 511 | 4AC | O7-C7-N4 | 5.01 | 129.92 | 121.82 |
| 1 | 2 | 1193 | 4AC | N4-C4-N3 | 4.99 | 122.23 | 113.85 |
| 1 | 2 | 479 | 4AC | O7-C7-N4 | 4.93 | 129.79 | 121.82 |
| 1 | 2 | 1467 | UR3 | C4-N3-C2 | -4.88 | 119.97 | 124.56 |
| 1 | 2 | 1233 | 4AC | O7-C7-N4 | 4.84 | 129.66 | 121.82 |
| 1 | 2 | 636 | 4AC | O7-C7-N4 | 4.83 | 129.63 | 121.82 |
| 1 | 2 | 1202 | 5MC | C5-C6-N1 | -4.79 | 118.41 | 123.34 |
| 31 | 4 | 54 | 5MU | C4-N3-C2 | -4.79 | 121.15 | 127.35 |
| 1 | 2 | 511 | 4AC | C5-C4-N4 | -4.79 | 114.61 | 122.92 |
| 1 | 2 | 53 | 4AC | O7-C7-N4 | 4.78 | 129.55 | 121.82 |
| 1 | 2 | 703 | 4AC | O7-C7-N4 | 4.77 | 129.54 | 121.82 |
| 31 | 4 | 54 | 5MU | C5-C4-N3 | 4.76 | 119.37 | 115.31 |
| 1 | 2 | 848 | 4AC | N4-C4-N3 | 4.75 | 121.82 | 113.85 |
| 1 | 2 | 1479 | 4AC | O7-C7-N4 | 4.73 | 129.47 | 121.82 |
| 1 | 2 | 394 | 4AC | N4-C4-N3 | 4.72 | 121.78 | 113.85 |
| 1 | 2 | 379 | 4AC | O7-C7-N4 | 4.72 | 129.46 | 121.82 |
| 1 | 2 | 848 | 4AC | C5-C4-N4 | -4.71 | 114.74 | 122.92 |
| 1 | 2 | 703 | 4AC | C5-C4-N4 | -4.65 | 114.85 | 122.92 |
| 31 | 4 | 8 | 4SU | N3-C2-N1 | 4.61 | 121.02 | 114.89 |
| 1 | 2 | 703 | 4AC | N4-C4-N3 | 4.60 | 121.58 | 113.85 |
| 1 | 2 | 731 | 4AC | O7-C7-N4 | 4.58 | 129.23 | 121.82 |
| 1 | 2 | 1239 | 4AC | C5-C4-N4 | -4.53 | 115.05 | 122.92 |
| 1 | 2 | 626 | 4AC | O7-C7-N4 | 4.49 | 129.08 | 121.82 |
| 1 | 2 | 851 | 4AC | O7-C7-N4 | 4.48 | 129.07 | 121.82 |
| 1 | 2 | 17 | 4AC | C5-C4-N4 | -4.47 | 115.15 | 122.92 |
| 1 | 2 | 286 | 4AC | O7-C7-N4 | 4.44 | 129.00 | 121.82 |
| 1 | 2 | 828 | 4AC | O7-C7-N4 | 4.43 | 128.98 | 121.82 |
| 1 | 2 | 394 | 4AC | O7-C7-N4 | 4.42 | 128.96 | 121.82 |
| 1 | 2 | 828 | 4AC | C5-C4-N4 | -4.40 | 115.27 | 122.92 |
| 1 | 2 | 511 | 4AC | N4-C4-N3 | 4.39 | 121.22 | 113.85 |
| 1 | 2 | 868 | 4AC | O7-C7-N4 | 4.38 | 128.91 | 121.82 |
| 31 | 4 | 54 | 5MU | N3-C2-N1 | 4.30 | 120.60 | 114.89 |
| 1 | 2 | 303 | 4AC | O7-C7-N4 | 4.30 | 128.77 | 121.82 |
| 1 | 2 | 1184 | 4AC | O7-C7-N4 | 4.24 | 128.68 | 121.82 |
| 1 | 2 | 1239 | 4AC | N4-C4-N3 | 4.23 | 120.95 | 113.85 |
| 1 | 2 | 17 | 4AC | N4-C4-N3 | 4.21 | 120.92 | 113.85 |
| 1 | 2 | 648 | 4AC | C5-C4-N4 | -4.19 | 115.64 | 122.92 |
| 1 | 2 | 839 | 4AC | N4-C4-N3 | 4.14 | 120.80 | 113.85 |
| 1 | 2 | 546 | 4AC | N4-C4-N3 | 4.05 | 120.66 | 113.85 |
| 1 | 2 | 590 | 4AC | O2-C2-N3 | -4.03 | 115.77 | 122.33 |
| 1 | 2 | 751 | 4AC | O7-C7-N4 | 4.03 | 128.34 | 121.82 |
| 1 | 2 | 1479 | 4AC | CM7-C7-N4 | -4.01 | 108.36 | 115.29 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 31 | 4 | 55 | PSU | O2-C2-N1 | -4.00 | 118.39 | 122.79 |
| 1 | 2 | 828 | 4AC | N4-C4-N3 | 3.99 | 120.55 | 113.85 |
| 1 | 2 | 546 | 4AC | O7-C7-N4 | 3.98 | 128.26 | 121.82 |
| 1 | 2 | 718 | 4AC | O7-C7-N4 | 3.96 | 128.23 | 121.82 |
| 1 | 2 | 636 | 4AC | C5-C4-N4 | -3.94 | 116.08 | 122.92 |
| 31 | 4 | 54 | 5MU | O4-C4-C5 | -3.82 | 120.47 | 124.90 |
| 1 | 2 | 957 | 4AC | C1'-N1-C2 | 3.78 | 126.85 | 118.42 |
| 1 | 2 | 839 | 4AC | C5-C4-N4 | -3.78 | 116.36 | 122.92 |
| 1 | 2 | 53 | 4AC | CM7-C7-N4 | -3.76 | 108.79 | 115.29 |
| 1 | 2 | 1469 | 6MZ | N3-C2-N1 | -3.73 | 122.85 | 128.68 |
| 1 | 2 | 636 | 4AC | N4-C4-N3 | 3.70 | 120.06 | 113.85 |
| 1 | 2 | 939 | 5MC | C5-C6-N1 | -3.69 | 119.54 | 123.34 |
| 1 | 2 | 1028 | 4AC | C5-C4-N4 | -3.69 | 116.51 | 122.92 |
| 1 | 2 | 590 | 4AC | O7-C7-N4 | 3.66 | 127.74 | 121.82 |
| 1 | 2 | 546 | 4AC | C5-C4-N4 | -3.66 | 116.57 | 122.92 |
| 1 | 2 | 479 | 4AC | CM7-C7-N4 | -3.65 | 108.98 | 115.29 |
| 1 | 2 | 394 | 4AC | C5-C4-N4 | -3.59 | 116.69 | 122.92 |
| 1 | 2 | 648 | 4AC | N4-C4-N3 | 3.56 | 119.83 | 113.85 |
| 1 | 2 | 379 | 4AC | C5-C4-N4 | -3.54 | 116.76 | 122.92 |
| 1 | 2 | 1028 | 4AC | N4-C4-N3 | 3.51 | 119.75 | 113.85 |
| 1 | 2 | 626 | 4AC | C5-C4-N4 | -3.51 | 116.82 | 122.92 |
| 1 | 2 | 1233 | 4AC | C5-C4-N4 | -3.50 | 116.83 | 122.92 |
| 1 | 2 | 286 | 4AC | C5-C4-N4 | -3.50 | 116.84 | 122.92 |
| 1 | 2 | 303 | 4AC | N4-C4-N3 | 3.46 | 119.66 | 113.85 |
| 31 | 4 | 55 | PSU | C4-N3-C2 | -3.44 | 121.38 | 126.34 |
| 1 | 2 | 286 | 4AC | N4-C4-N3 | 3.42 | 119.59 | 113.85 |
| 1 | 2 | 303 | 4AC | C5-C4-N4 | -3.41 | 117.00 | 122.92 |
| 1 | 2 | 1233 | 4AC | N4-C4-N3 | 3.41 | 119.57 | 113.85 |
| 1 | 2 | 868 | 4AC | CM7-C7-N4 | -3.40 | 109.41 | 115.29 |
| 1 | 2 | 1479 | 4AC | N4-C4-N3 | 3.40 | 119.56 | 113.85 |
| 1 | 2 | 839 | 4AC | CM7-C7-N4 | -3.34 | 109.52 | 115.29 |
| 1 | 2 | 1184 | 4AC | C5-C4-N4 | -3.33 | 117.14 | 122.92 |
| 1 | 2 | 851 | 4AC | C5-C4-N4 | -3.31 | 117.17 | 122.92 |
| 1 | 2 | 1028 | 4AC | CM7-C7-N4 | -3.30 | 109.58 | 115.29 |
| 1 | 2 | 1479 | 4AC | C5-C4-N4 | -3.23 | 117.30 | 122.92 |
| 31 | 4 | 32 | OMC | O2-C2-N3 | -3.22 | 117.10 | 122.33 |
| 31 | 4 | 54 | 5MU | C5-C6-N1 | -3.17 | 120.07 | 123.34 |
| 1 | 2 | 379 | 4AC | CM7-C7-N4 | -3.13 | 109.88 | 115.29 |
| 1 | 2 | 626 | 4AC | N4-C4-N3 | 3.10 | 119.06 | 113.85 |
| 1 | 2 | 1239 | 4AC | CM7-C7-N4 | -3.09 | 109.94 | 115.29 |
| 1 | 2 | 1147 | 4AC | C1'-N1-C2 | 3.09 | 125.31 | 118.42 |
| 1 | 2 | 250 | LHH | N4-C4-N3 | 3.05 | 118.97 | 113.85 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | 2 | 479 | 4AC | C5-C4-N4 | -3.05 | 117.63 | 122.92 |
| 1 | 2 | 1467 | UR3 | C3U-N3-C2 | 3.04 | 122.64 | 117.31 |
| 1 | 2 | 17 | 4AC | CM7-C7-N4 | -3.04 | 110.03 | 115.29 |
| 31 | 4 | 8 | 4SU | C5-C4-S4 | -3.01 | 120.58 | 124.47 |
| 1 | 2 | 648 | 4AC | CM7-C7-N4 | -3.01 | 110.09 | 115.29 |
| 1 | 2 | 379 | 4AC | N4-C4-N3 | 3.00 | 118.89 | 113.85 |
| 1 | 2 | 1147 | 4AC | CM7-C7-N4 | -2.99 | 110.11 | 115.29 |
| 1 | 2 | 851 | 4AC | O2-C2-N3 | -2.95 | 117.53 | 122.33 |
| 1 | 2 | 1487 | MA6 | C4-C5-N7 | -2.95 | 106.32 | 109.40 |
| 1 | 2 | 319 | 4AC | CM7-C7-N4 | -2.95 | 110.20 | 115.29 |
| 1 | 2 | 373 | A2M | C4-C5-N7 | -2.95 | 106.33 | 109.40 |
| 1 | 2 | 851 | 4AC | N4-C4-N3 | 2.94 | 118.79 | 113.85 |
| 1 | 2 | 319 | 4AC | C5-C4-N4 | -2.93 | 117.83 | 122.92 |
| 1 | 2 | 319 | 4AC | N4-C4-N3 | 2.92 | 118.75 | 113.85 |
| 1 | 2 | 286 | 4AC | C1'-N1-C2 | 2.91 | 124.92 | 118.42 |
| 1 | 2 | 957 | 4AC | C1'-N1-C6 | -2.91 | 114.49 | 120.84 |
| 1 | 2 | 731 | 4AC | CM7-C7-N4 | -2.91 | 110.27 | 115.29 |
| 1 | 2 | 718 | 4AC | CM7-C7-N4 | -2.90 | 110.28 | 115.29 |
| 1 | 2 | 1467 | UR3 | C1'-N1-C2 | 2.88 | 121.85 | 116.99 |
| 1 | 2 | 511 | 4AC | CM7-C7-N4 | -2.84 | 110.37 | 115.29 |
| 1 | 2 | 626 | 4AC | CM7-C7-N4 | -2.81 | 110.43 | 115.29 |
| 1 | 2 | 1233 | 4AC | CM7-C7-N4 | -2.80 | 110.45 | 115.29 |
| 1 | 2 | 1487 | MA6 | N3-C2-N1 | -2.79 | 124.31 | 128.68 |
| 1 | 2 | 1488 | MA6 | C4-C5-N7 | -2.79 | 106.49 | 109.40 |
| 1 | 2 | 868 | 4AC | C5-C4-N4 | -2.79 | 118.08 | 122.92 |
| 1 | 2 | 1488 | MA6 | N3-C2-N1 | -2.77 | 124.35 | 128.68 |
| 1 | 2 | 1041 | 4AC | CM7-C7-N4 | -2.76 | 110.52 | 115.29 |
| 1 | 2 | 590 | 4AC | O2-C2-N1 | 2.75 | 124.56 | 118.89 |
| 1 | 2 | 1469 | 6MZ | C4-C5-N7 | -2.74 | 106.54 | 109.40 |
| 1 | 2 | 839 | 4AC | C1'-N1-C2 | 2.69 | 124.42 | 118.42 |
| 1 | 2 | 479 | 4AC | O2-C2-N3 | -2.68 | 117.98 | 122.33 |
| 1 | 2 | 1184 | 4AC | N4-C4-N3 | 2.67 | 118.34 | 113.85 |
| 1 | 2 | 53 | 4AC | C5-C4-N4 | -2.65 | 118.31 | 122.92 |
| 1 | 2 | 1487 | MA6 | N1-C6-N6 | 2.65 | 119.84 | 117.06 |
| 1 | 2 | 648 | 4AC | O2-C2-N3 | -2.64 | 118.04 | 122.33 |
| 1 | 2 | 1184 | 4AC | CM7-C7-N4 | -2.62 | 110.75 | 115.29 |
| 1 | 2 | 394 | 4AC | C1'-N1-C2 | 2.62 | 124.26 | 118.42 |
| 1 | 2 | 751 | 4AC | CM7-C7-N4 | -2.61 | 110.78 | 115.29 |
| 1 | 2 | 939 | 5MC | C5-C4-N3 | -2.60 | 118.87 | 121.67 |
| 1 | 2 | 1193 | 4AC | CM7-C7-N4 | -2.58 | 110.82 | 115.29 |
| 1 | 2 | 479 | 4AC | N4-C4-N3 | 2.53 | 118.09 | 113.85 |
| 1 | 2 | 751 | 4AC | C5-C4-N4 | -2.51 | 118.56 | 122.92 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | 2 | 286 | 4AC | O2-C2-N3 | -2.50 | 118.26 | 122.33 |
| 31 | 4 | 32 | OMC | C1'-N1-C2 | 2.50 | 124.00 | 118.42 |
| 1 | 2 | 590 | 4AC | CM7-C7-N4 | -2.49 | 110.98 | 115.29 |
| 1 | 2 | 848 | 4AC | CM7-C7-N4 | -2.46 | 111.03 | 115.29 |
| 31 | 4 | 54 | 5MU | C5M-C5-C4 | 2.46 | 121.47 | 118.77 |
| 1 | 2 | 938 | B8H | N3-C2-N1 | 2.46 | 117.80 | 115.14 |
| 1 | 2 | 731 | 4AC | N4-C4-N3 | 2.46 | 117.98 | 113.85 |
| 1 | 2 | 286 | 4AC | CM7-C7-N4 | -2.44 | 111.08 | 115.29 |
| 1 | 2 | 250 | LHH | C5-C6-N1 | -2.42 | 117.76 | 121.81 |
| 1 | 2 | 1467 | UR3 | C6-N1-C2 | -2.41 | 119.63 | 121.79 |
| 1 | 2 | 373 | A2M | C5'-C4'-C3' | -2.39 | 106.21 | 115.18 |
| 1 | 2 | 373 | A2M | N3-C2-N1 | -2.38 | 124.96 | 128.68 |
| 1 | 2 | 53 | 4AC | N4-C4-N3 | 2.37 | 117.84 | 113.85 |
| 1 | 2 | 957 | 4AC | O7-C7-CM7 | -2.34 | 117.71 | 122.06 |
| 31 | 4 | 54 | 5MU | C1'-N1-C2 | 2.32 | 121.76 | 117.57 |
| 1 | 2 | 703 | 4AC | C1'-N1-C2 | 2.31 | 123.58 | 118.42 |
| 1 | 2 | 731 | 4AC | C5-C4-N4 | -2.30 | 118.92 | 122.92 |
| 1 | 2 | 511 | 4AC | C1'-N1-C2 | 2.29 | 123.53 | 118.42 |
| 1 | 2 | 957 | 4AC | CM7-C7-N4 | -2.29 | 111.33 | 115.29 |
| 1 | 2 | 511 | 4AC | O2-C2-N3 | -2.26 | 118.65 | 122.33 |
| 1 | 2 | 1193 | 4AC | O7-C7-CM7 | -2.23 | 117.91 | 122.06 |
| 1 | 2 | 938 | B8H | O4'-C1'-C2' | 2.23 | 108.29 | 105.14 |
| 1 | 2 | 286 | 4AC | C1'-N1-C6 | -2.22 | 116.01 | 120.84 |
| 1 | 2 | 53 | 4AC | O2-C2-N3 | -2.21 | 118.74 | 122.33 |
| 1 | 2 | 703 | 4AC | C1'-N1-C6 | -2.17 | 116.11 | 120.84 |
| 31 | 4 | 54 | 5MU | C1'-N1-C6 | -2.17 | 117.51 | 121.12 |
| 1 | 2 | 636 | 4AC | CM7-C7-N4 | -2.16 | 111.56 | 115.29 |
| 1 | 2 | 703 | 4AC | CM7-C7-N4 | -2.15 | 111.58 | 115.29 |
| 1 | 2 | 868 | 4AC | N4-C4-N3 | 2.15 | 117.46 | 113.85 |
| 1 | 2 | 648 | 4AC | C1'-N1-C2 | 2.14 | 123.20 | 118.42 |
| 1 | 2 | 939 | 5MC | N4-C4-N3 | 2.13 | 122.36 | 118.48 |
| 1 | 2 | 828 | 4AC | CM7-C7-N4 | -2.12 | 111.62 | 115.29 |
| 1 | 2 | 751 | 4AC | N4-C4-N3 | 2.11 | 117.39 | 113.85 |
| 1 | 2 | 648 | 4AC | C4-N3-C2 | -2.11 | 117.25 | 120.12 |
| 1 | 2 | 373 | A2M | C3'-C2'-C1' | 2.09 | 106.81 | 102.89 |
| 1 | 2 | 731 | 4AC | O2-C2-N3 | -2.08 | 118.95 | 122.33 |
| 1 | 2 | 394 | 4AC | O7-C7-CM7 | -2.07 | 118.22 | 122.06 |
| 1 | 2 | 839 | 4AC | O2-C2-N3 | -2.04 | 119.01 | 122.33 |
| 1 | 2 | 1467 | UR3 | O3'-C3'-C2' | -2.04 | 105.22 | 111.82 |
| 1 | 2 | 718 | 4AC | C5-C4-N4 | -2.04 | 119.38 | 122.92 |
| 1 | 2 | 1147 | 4AC | C1'-N1-C6 | -2.01 | 116.45 | 120.84 |
| 1 | 2 | 17 | 4AC | O2-C2-N3 | -2.00 | 119.07 | 122.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1 | 2 | 379 | 4AC | O2-C2-N3 | -2.00 | 119.07 | 122.33 |

There are no chirality outliers.

All (76) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 1 | 2 | 250 | LHH | C1'-C2'-O2'-C1 |
| 1 | 2 | 286 | 4AC | C3'-C4'-C5'-O5' |
| 1 | 2 | 373 | A2M | C1'-C2'-O2'-CM' |
| 1 | 2 | 379 | 4AC | C3'-C4'-C5'-O5' |
| 1 | 2 | 511 | 4AC | O4'-C4'-C5'-O5' |
| 1 | 2 | 511 | 4AC | C3'-C4'-C5'-O5' |
| 1 | 2 | 546 | 4AC | C3'-C4'-C5'-O5' |
| 1 | 2 | 648 | 4AC | O4'-C4'-C5'-O5' |
| 1 | 2 | 848 | 4AC | O4'-C4'-C5'-O5' |
| 1 | 2 | 868 | 4AC | C3'-C4'-C5'-O5' |
| 1 | 2 | 1028 | 4AC | O4'-C4'-C5'-O5' |
| 1 | 2 | 1147 | 4AC | C3'-C4'-C5'-O5' |
| 1 | 2 | 1239 | 4AC | C3'-C4'-C5'-O5' |
| 1 | 2 | 1467 | UR3 | C2'-C1'-N1-C6 |
| 31 | 4 | 8 | 4SU | C2'-C1'-N1-C2 |
| 31 | 4 | 8 | 4SU | C2'-C1'-N1-C6 |
| 31 | 4 | 20 | H2U | O4'-C1'-N1-C6 |
| 1 | 2 | 379 | 4AC | O4'-C4'-C5'-O5' |
| 1 | 2 | 546 | 4AC | O4'-C4'-C5'-O5' |
| 1 | 2 | 648 | 4AC | C3'-C4'-C5'-O5' |
| 1 | 2 | 731 | 4AC | O4'-C4'-C5'-O5' |
| 1 | 2 | 731 | 4AC | C3'-C4'-C5'-O5' |
| 1 | 2 | 848 | 4AC | C3'-C4'-C5'-O5' |
| 1 | 2 | 868 | 4AC | O4'-C4'-C5'-O5' |
| 1 | 2 | 1028 | 4AC | C3'-C4'-C5'-O5' |
| 1 | 2 | 1202 | 5MC | C3'-C4'-C5'-O5' |
| 1 | 2 | 1239 | 4AC | O4'-C4'-C5'-O5' |
| 1 | 2 | 1467 | UR3 | O4'-C4'-C5'-O5' |
| 31 | 4 | 8 | 4SU | O4'-C1'-N1-C2 |
| 1 | 2 | 479 | 4AC | O4'-C4'-C5'-O5' |
| 1 | 2 | 1147 | 4AC | O4'-C4'-C5'-O5' |
| 1 | 2 | 1202 | 5MC | O4'-C4'-C5'-O5' |
| 1 | 2 | 1376 | OMC | C3'-C4'-C5'-O5' |
| 1 | 2 | 1376 | OMC | O4'-C4'-C5'-O5' |
| 1 | 2 | 1467 | UR3 | C3'-C4'-C5'-O5' |
| 1 | 2 | 1467 | UR3 | C2'-C1'-N1-C2 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 1 | 2 | 286 | 4AC | O4'-C4'-C5'-O5' |
| 31 | 4 | 8 | 4SU | O4'-C1'-N1-C6 |
| 1 | 2 | 1184 | 4AC | O4'-C4'-C5'-O5' |
| 1 | 2 | 626 | 4AC | O4'-C4'-C5'-O5' |
| 1 | 2 | 1184 | 4AC | C3'-C4'-C5'-O5' |
| 1 | 2 | 938 | B8H | O4'-C4'-C5'-O5' |
| 1 | 2 | 851 | 4AC | C2'-C1'-N1-C6 |
| 1 | 2 | 319 | 4AC | O4'-C4'-C5'-O5' |
| 1 | 2 | 938 | B8H | C3'-C4'-C5'-O5' |
| 1 | 2 | 1378 | 5HM | C4-C5-CM5-OM5 |
| 31 | 4 | 32 | OMC | C2'-C1'-N1-C2 |
| 1 | 2 | 479 | 4AC | C3'-C4'-C5'-O5' |
| 1 | 2 | 851 | 4AC | O4'-C1'-N1-C6 |
| 1 | 2 | 1467 | UR3 | O4'-C1'-N1-C6 |
| 1 | 2 | 394 | 4AC | C4'-C5'-O5'-P |
| 31 | 4 | 32 | OMC | C2'-C1'-N1-C6 |
| 31 | 4 | 20 | H2U | C2'-C1'-N1-C2 |
| 31 | 4 | 20 | H2U | C2'-C1'-N1-C6 |
| 1 | 2 | 1467 | UR3 | O4'-C1'-N1-C2 |
| 31 | 4 | 20 | H2U | O4'-C1'-N1-C2 |
| 1 | 2 | 286 | 4AC | C2'-C1'-N1-C6 |
| 1 | 2 | 851 | 4AC | O4'-C1'-N1-C2 |
| 1 | 2 | 286 | 4AC | C2'-C1'-N1-C2 |
| 1 | 2 | 590 | 4AC | C2'-C1'-N1-C6 |
| 1 | 2 | 626 | 4AC | C3'-C4'-C5'-O5' |
| 1 | 2 | 319 | 4AC | O4'-C1'-N1-C6 |
| 1 | 2 | 590 | 4AC | C2'-C1'-N1-C2 |
| 1 | 2 | 938 | B8H | O4'-C1'-C5-C6 |
| 1 | 2 | 394 | 4AC | C2'-C1'-N1-C2 |
| 1 | 2 | 479 | 4AC | C2'-C1'-N1-C2 |
| 1 | 2 | 839 | 4AC | C2'-C1'-N1-C2 |
| 1 | 2 | 851 | 4AC | C2'-C1'-N1-C2 |
| 31 | 4 | 8 | 4SU | C4'-C5'-O5'-P |
| 1 | 2 | 319 | 4AC | C2'-C1'-N1-C6 |
| 1 | 2 | 957 | 4AC | C2'-C1'-N1-C2 |
| 31 | 4 | 54 | 5MU | C2'-C1'-N1-C2 |
| 1 | 2 | 319 | 4AC | C3'-C4'-C5'-O5' |
| 1 | 2 | 1378 | 5HM | C6-C5-CM5-OM5 |
| 1 | 2 | 731 | 4AC | C2'-C1'-N1-C2 |
| 1 | 2 | 286 | 4AC | C4'-C5'-O5'-P |

There are no ring outliers.

47 monomers are involved in 149 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 1 | 2 | 868 | 4AC | 3 | 0 |
| 1 | 2 | 1479 | 4AC | 5 | 0 |
| 1 | 2 | 1378 | 5HM | 4 | 0 |
| 1 | 2 | 1488 | MA6 | 3 | 0 |
| 1 | 2 | 938 | B8H | 1 | 0 |
| 1 | 2 | 17 | 4AC | 3 | 0 |
| 1 | 2 | 479 | 4AC | 4 | 0 |
| 1 | 2 | 1028 | 4AC | 2 | 0 |
| 1 | 2 | 1239 | 4AC | 5 | 0 |
| 1 | 2 | 1376 | OMC | 2 | 0 |
| 1 | 2 | 751 | 4AC | 1 | 0 |
| 1 | 2 | 1467 | UR3 | 4 | 0 |
| 1 | 2 | 303 | 4AC | 3 | 0 |
| 1 | 2 | 703 | 4AC | 6 | 0 |
| 1 | 2 | 939 | 5MC | 1 | 0 |
| 1 | 2 | 546 | 4AC | 2 | 0 |
| 31 | 4 | 20 | H2U | 1 | 0 |
| 1 | 2 | 394 | 4AC | 4 | 0 |
| 1 | 2 | 1202 | 5MC | 3 | 0 |
| 1 | 2 | 718 | 4AC | 4 | 0 |
| 1 | 2 | 731 | 4AC | 4 | 0 |
| 1 | 2 | 1147 | 4AC | 5 | 0 |
| 1 | 2 | 957 | 4AC | 4 | 0 |
| 31 | 4 | 32 | OMC | 3 | 0 |
| 1 | 2 | 828 | 4AC | 3 | 0 |
| 1 | 2 | 1233 | 4AC | 6 | 0 |
| 1 | 2 | 286 | 4AC | 1 | 0 |
| 1 | 2 | 636 | 4AC | 2 | 0 |
| 1 | 2 | 1184 | 4AC | 4 | 0 |
| 1 | 2 | 851 | 4AC | 6 | 0 |
| 31 | 4 | 8 | 4SU | 2 | 0 |
| 31 | 4 | 54 | 5MU | 3 | 0 |
| 1 | 2 | 648 | 4AC | 5 | 0 |
| 1 | 2 | 848 | 4AC | 2 | 0 |
| 1 | 2 | 53 | 4AC | 1 | 0 |
| 1 | 2 | 1469 | 6MZ | 2 | 0 |
| 1 | 2 | 373 | A2M | 7 | 0 |
| 1 | 2 | 511 | 4AC | 1 | 0 |
| 1 | 2 | 590 | 4AC | 2 | 0 |
| 1 | 2 | 1487 | MA6 | 4 | 0 |
| 31 | 4 | 55 | PSU | 3 | 0 |
| 1 | 2 | 626 | 4AC | 1 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 1 | 2 | 1041 | 4AC | 4 | 0 |
| 1 | 2 | 319 | 4AC | 3 | 0 |
| 1 | 2 | 379 | 4AC | 2 | 0 |
| 1 | 2 | 1193 | 4AC | 3 | 0 |
| 1 | 2 | 839 | 4AC | 7 | 0 |

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 42 ligands modelled in this entry, 40 are monoatomic - leaving 2 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 |
| 38 | MET | 7 | 501 | - | 6,7,8 | 0.50 | 0 | 2,7,9 | 0.39 | 0 |
| 39 | GNP | 7 | 502 | 36 | 29,34,34 | 1.58 | 7 (24%) | 33,54,54 | 2.14 | 7 (21%) |

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 |
|-----|------|-------|-----|------|---------|------------|---------|
| 38 | MET | 7 | 501 | - | - | 2/5/6/8 | - |
| 39 | GNP | 7 | 502 | 36 | - | 7/14/38/38 | 0/3/3/3 |

All (7) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 39 | 7 | 502 | GNP | PB-O3A | 4.26 | 1.64 | 1.59 |
| 39 | 7 | 502 | GNP | PB-O1B | 3.18 | 1.51 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 39 | 7 | 502 | GNP | C6-N1 | 2.97 | 1.38 | 1.33 |
| 39 | 7 | 502 | GNP | PG-N3B | 2.80 | 1.70 | 1.63 |
| 39 | 7 | 502 | GNP | PG-O1G | 2.60 | 1.50 | 1.46 |
| 39 | 7 | 502 | GNP | C5-C6 | 2.08 | 1.44 | 1.41 |
| 39 | 7 | 502 | GNP | PB-O2B | -2.07 | 1.51 | 1.56 |

All (7) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 39 | 7 | 502 | GNP | C5-C6-N1 | -8.34 | 112.03 | 123.43 |
| 39 | 7 | 502 | GNP | C2-N1-C6 | 5.83 | 125.19 | 115.93 |
| 39 | 7 | 502 | GNP | PB-O3A-PA | -2.95 | 122.22 | 132.62 |
| 39 | 7 | 502 | GNP | N3-C2-N1 | -2.85 | 123.42 | 127.22 |
| 39 | 7 | 502 | GNP | C4-C5-C6 | -2.70 | 118.22 | 120.80 |
| 39 | 7 | 502 | GNP | O3G-PG-O1G | -2.32 | 107.63 | 113.45 |
| 39 | 7 | 502 | GNP | C2-N3-C4 | -2.08 | 112.98 | 115.36 |

There are no chirality outliers.

All (9) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 39 | 7 | 502 | GNP | PB-N3B-PG-O1G |
| 39 | 7 | 502 | GNP | PG-N3B-PB-O1B |
| 39 | 7 | 502 | GNP | C5'-O5'-PA-O3A |
| 39 | 7 | 502 | GNP | O4'-C4'-C5'-O5' |
| 38 | 7 | 501 | MET | CA-CB-CG-SD |
| 38 | 7 | 501 | MET | N-CA-CB-CG |
| 39 | 7 | 502 | GNP | C5'-O5'-PA-O1A |
| 39 | 7 | 502 | GNP | C3'-C4'-C5'-O5' |
| 39 | 7 | 502 | GNP | C4'-C5'-O5'-PA |

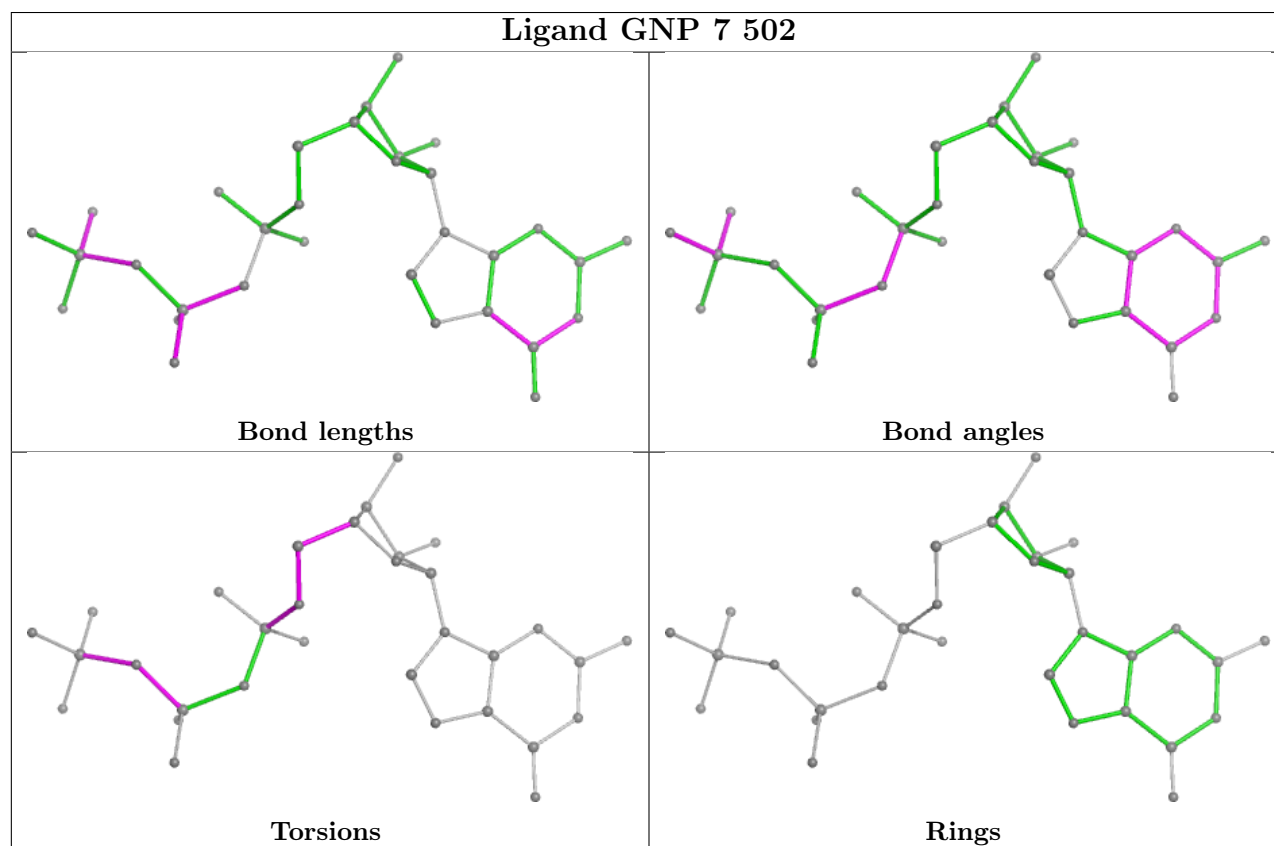
There are no ring outliers.

2 monomers are involved in 6 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 38 | 7 | 501 | MET | 2 | 0 |
| 39 | 7 | 502 | GNP | 4 | 0 |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 35 | 9 | 2 |
| 34 | 8 | 1 |
| 9 | H | 1 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | 8 | 19:PRO | C | 28:GLN | N | 14.63 |
| 1 | 9 | 47:SER | C | 53:ASN | N | 11.57 |
| 1 | 9 | 169:SER | C | 175:ARG | N | 8.00 |
| 1 | H | 194:LYS | C | 195:ASP | N | 1.20 |

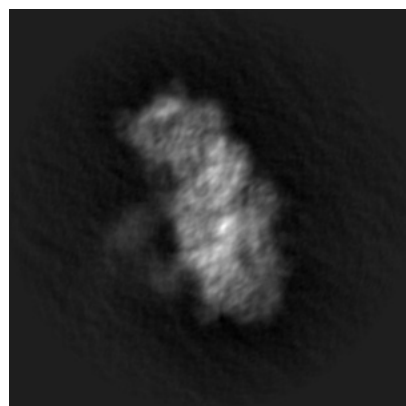
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10320. These allow visual inspection of the internal detail of the map and identification of artifacts.

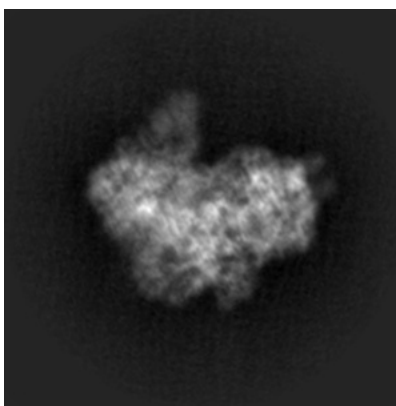
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

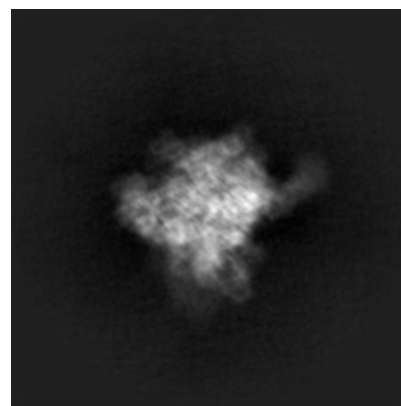
6.1.1 Primary map



X

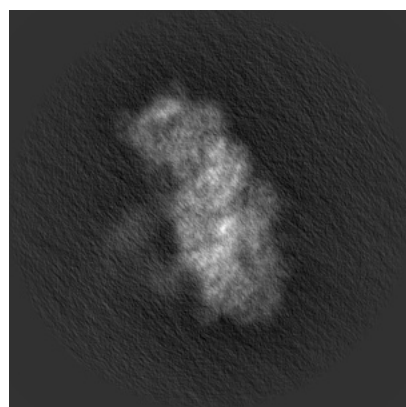


Y

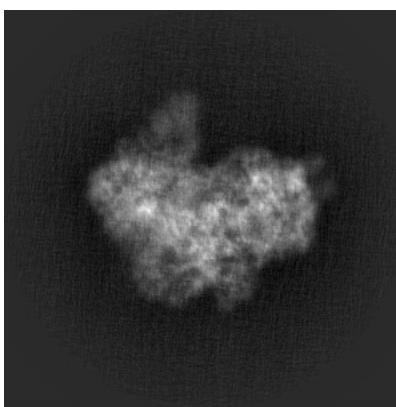


Z

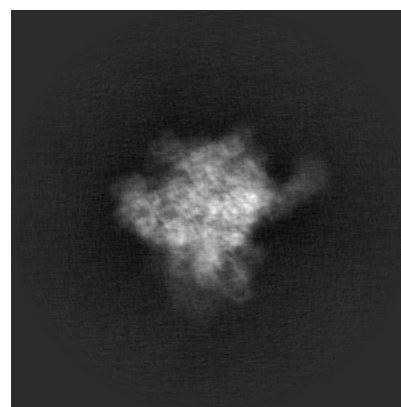
6.1.2 Raw map



X



Y

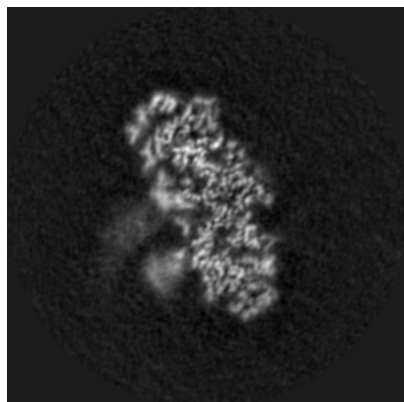


Z

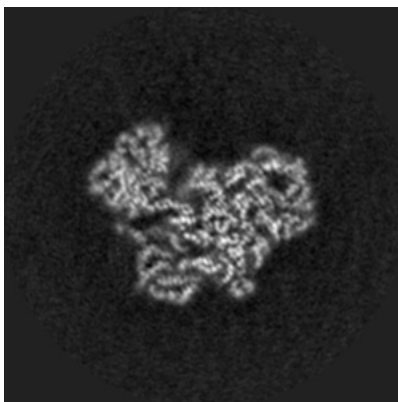
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

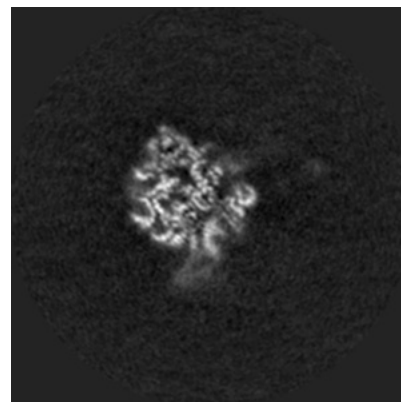
6.2.1 Primary map



X Index: 174

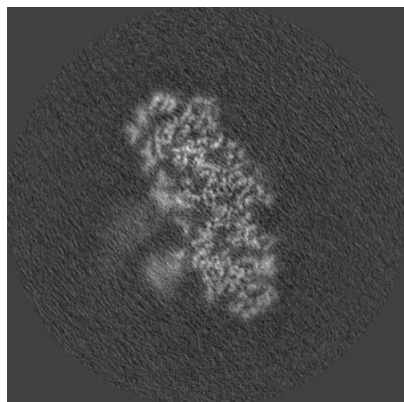


Y Index: 174

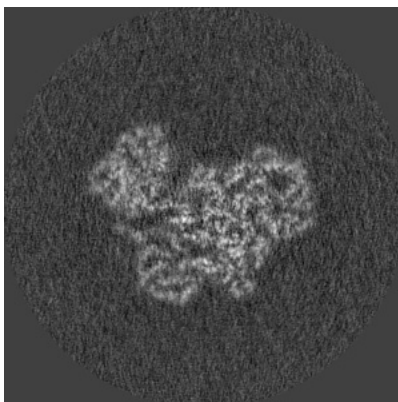


Z Index: 174

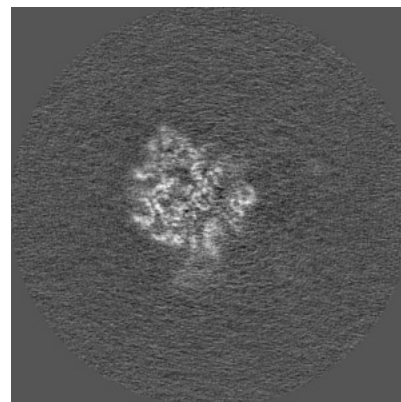
6.2.2 Raw map



X Index: 174



Y Index: 174

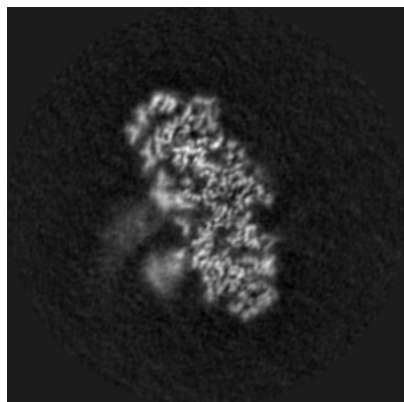


Z Index: 174

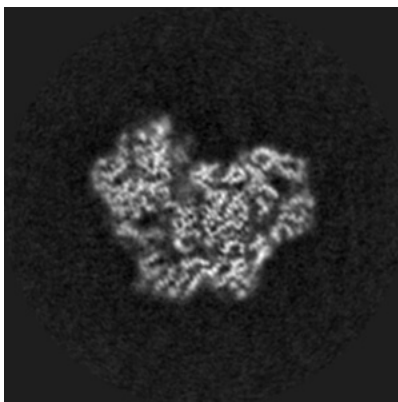
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

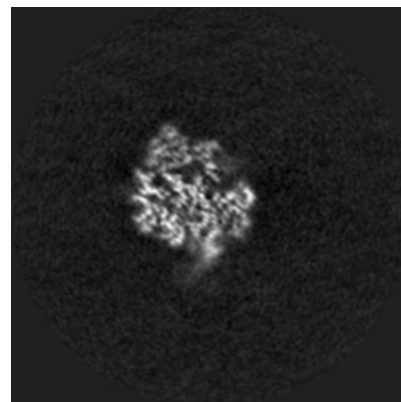
6.3.1 Primary map



X Index: 174

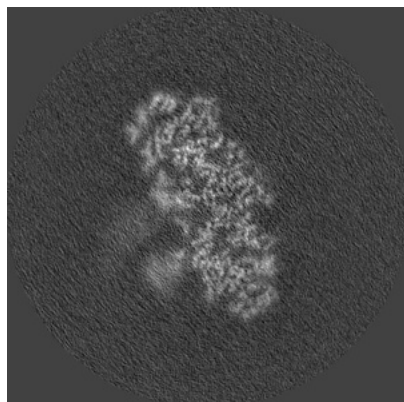


Y Index: 178

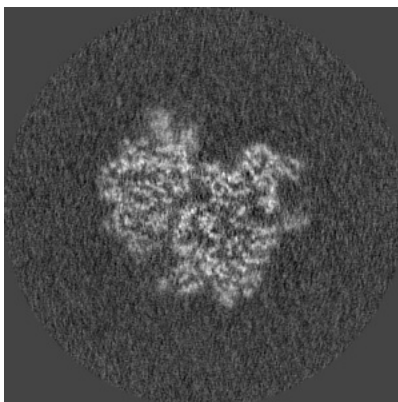


Z Index: 180

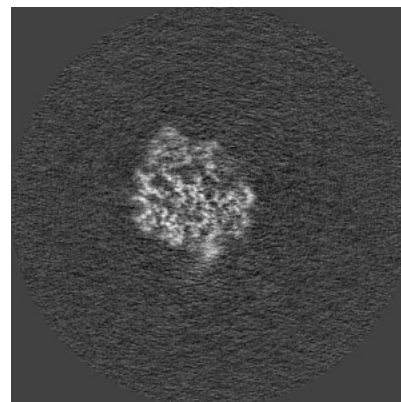
6.3.2 Raw map



X Index: 174



Y Index: 185

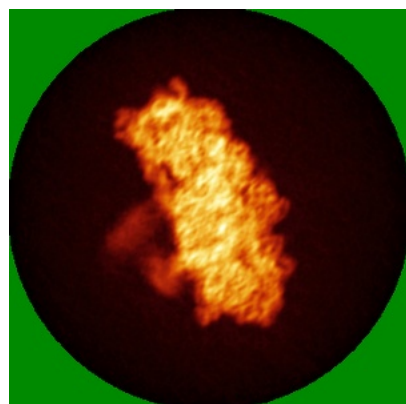


Z Index: 180

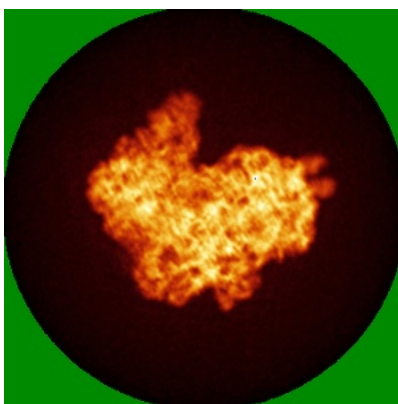
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

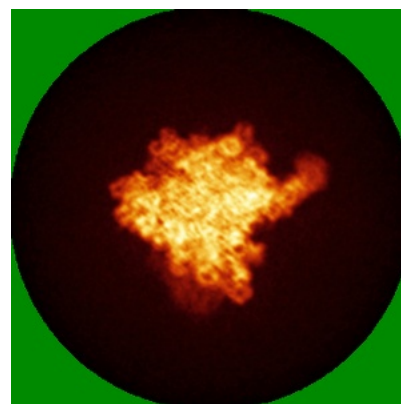
6.4.1 Primary map



X

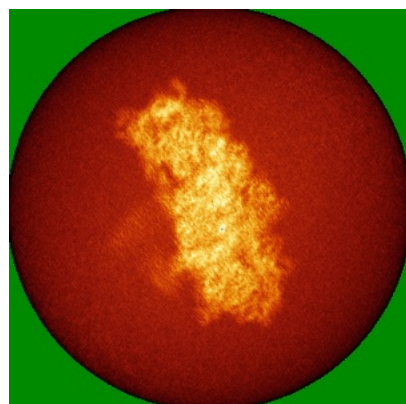


Y

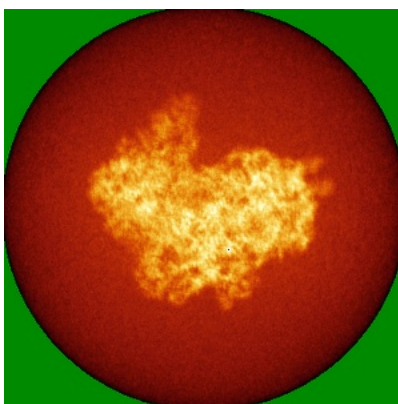


Z

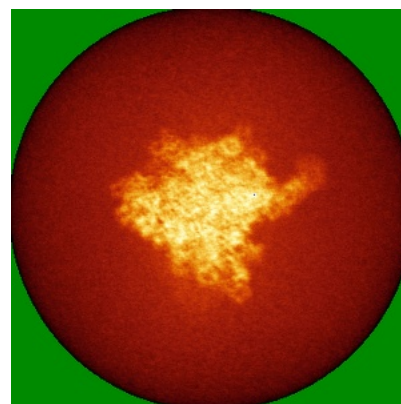
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



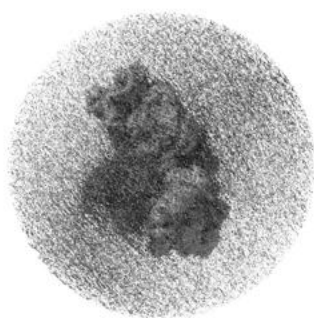
Y



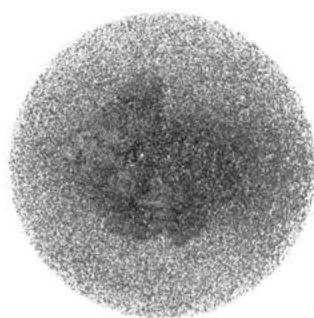
Z

The images above show the 3D surface view of the map at the recommended contour level 0.004. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

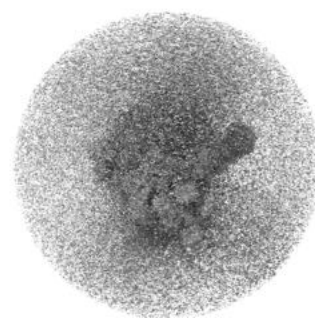
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

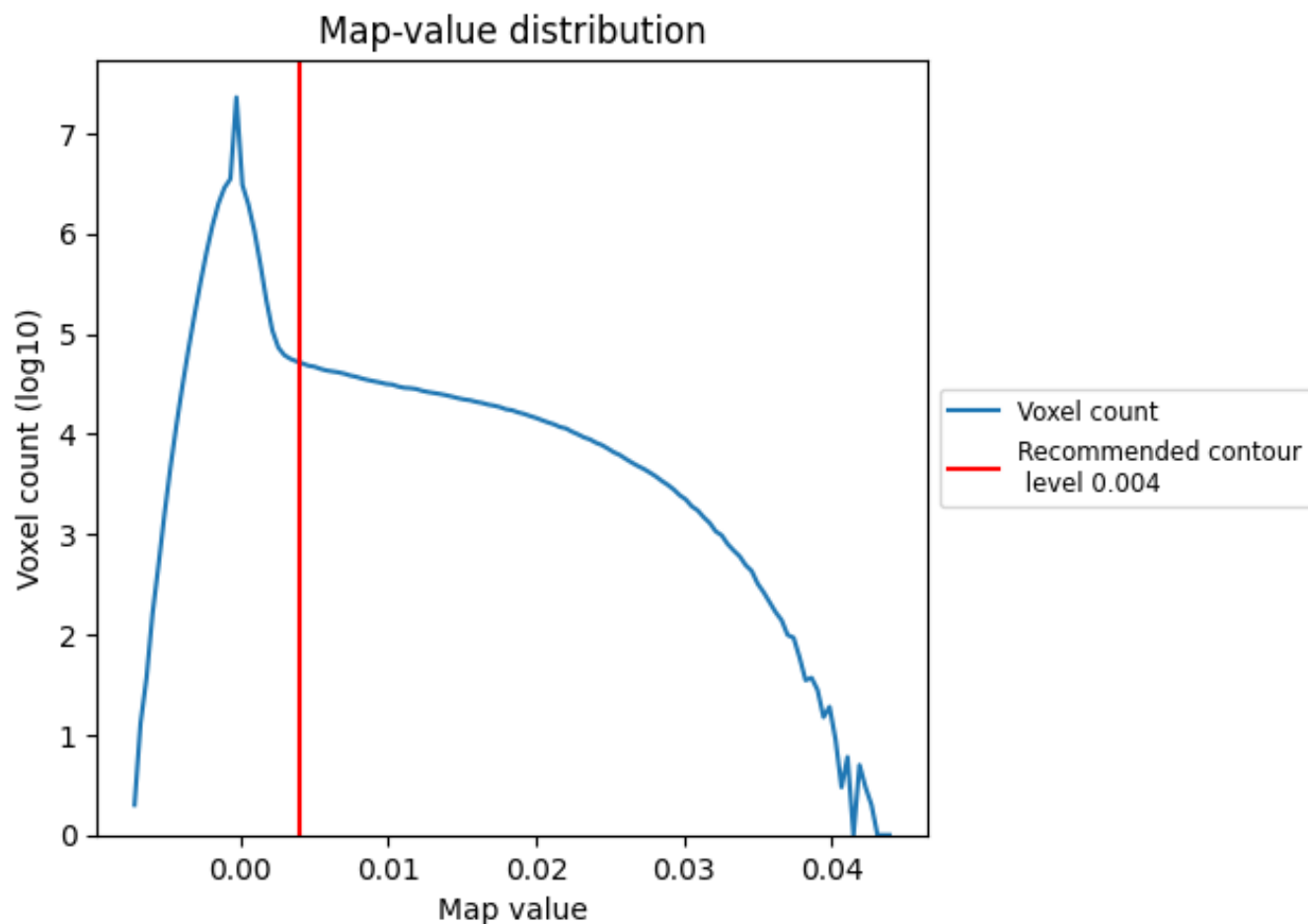
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

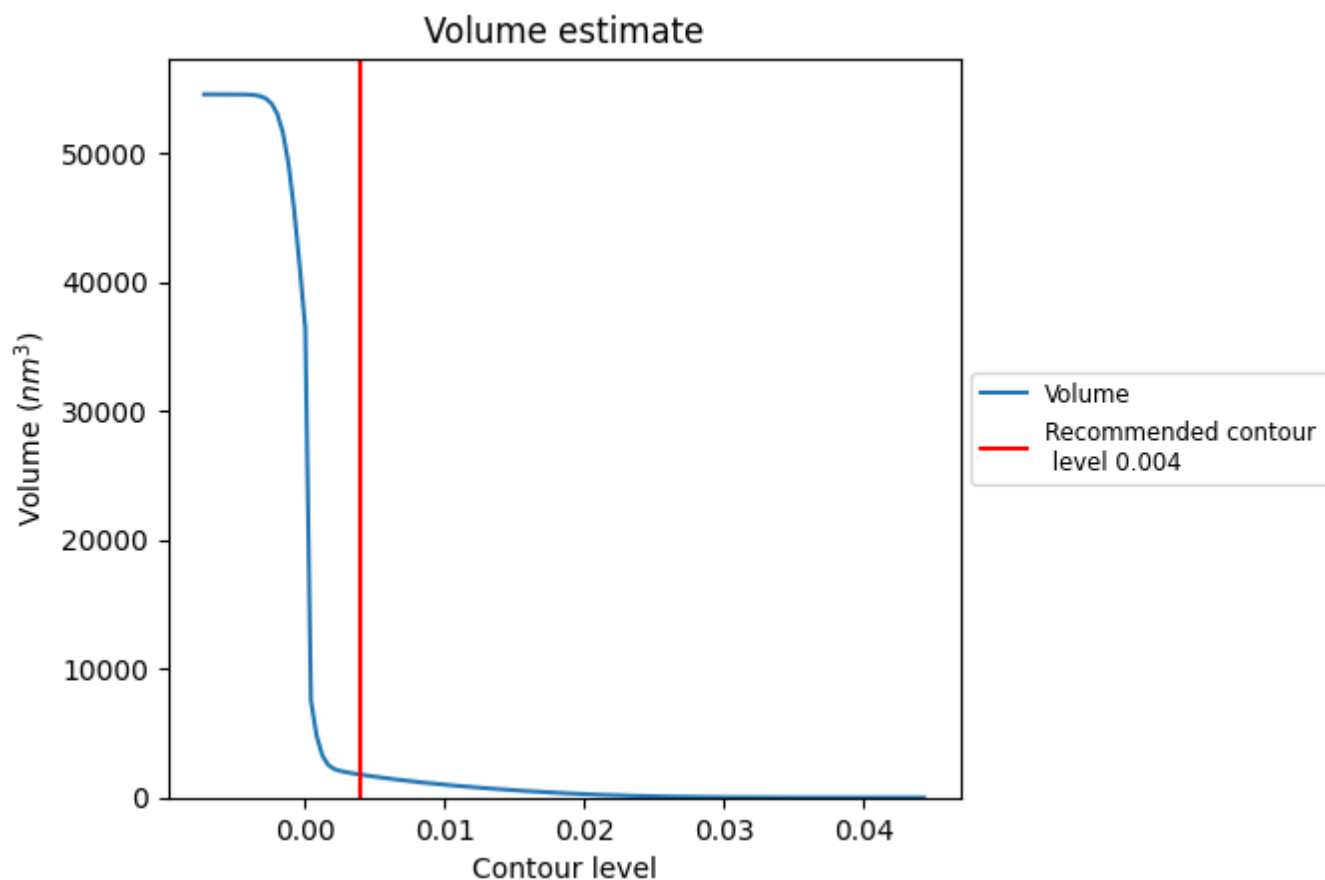
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

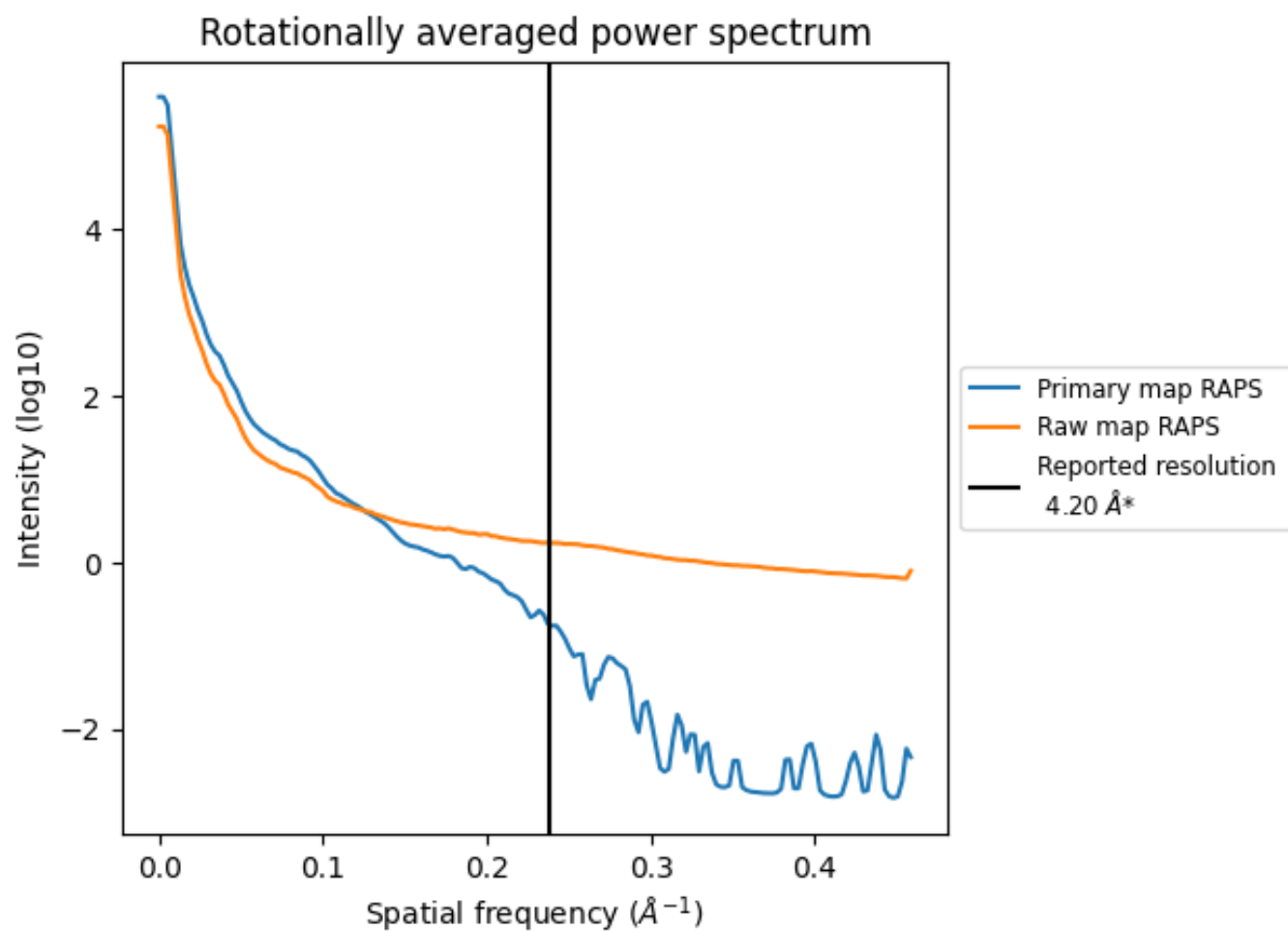
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1784 nm^3 ; this corresponds to an approximate mass of 1611 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

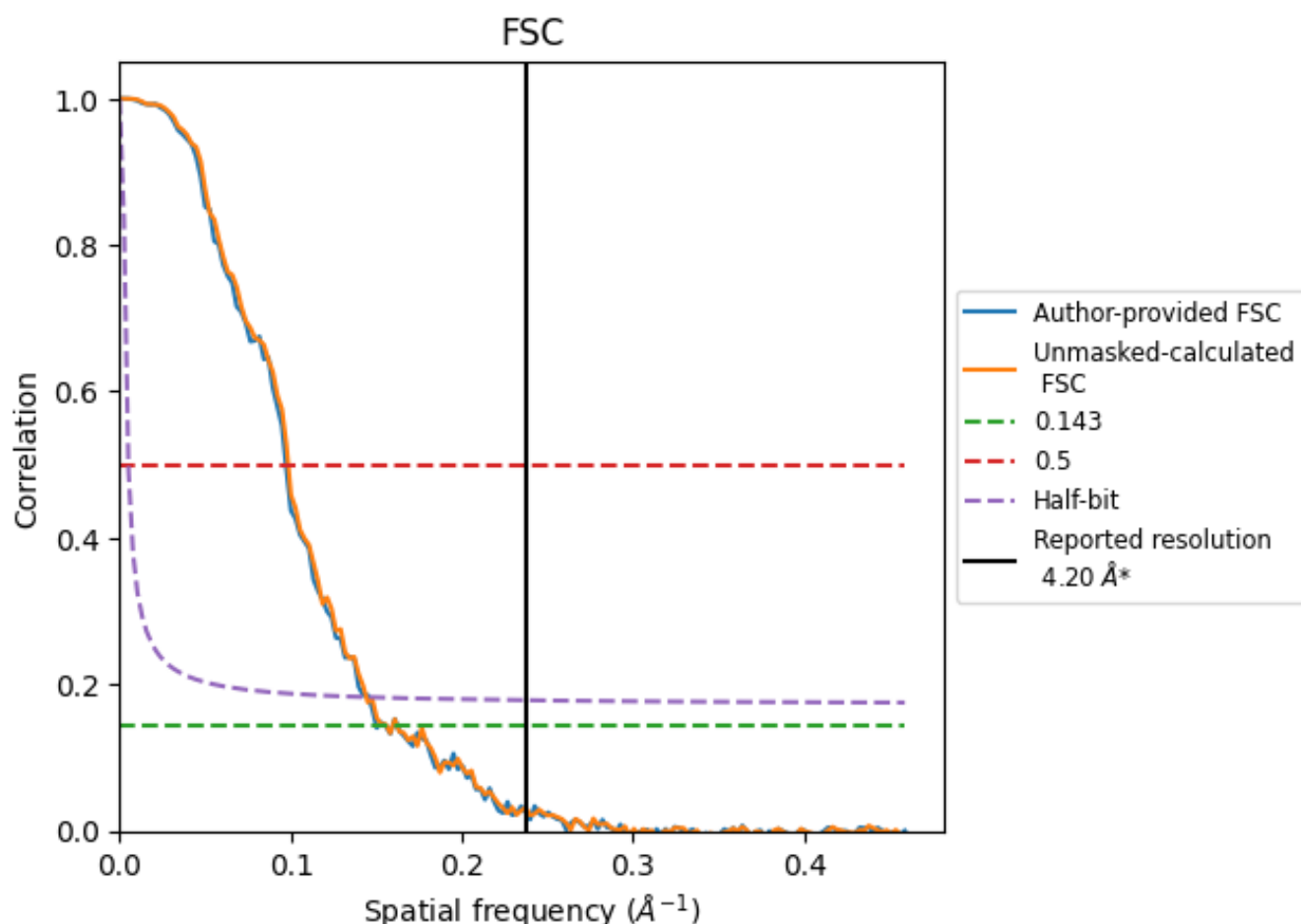


*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

8.2 Resolution estimates [i](#)

| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---------------------------|------------------------------------|-------|----------|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 4.20 | - | - |
| Author-provided FSC curve | 6.67 | 10.29 | 6.87 |
| Unmasked-calculated* | 6.41 | 10.14 | 6.93 |

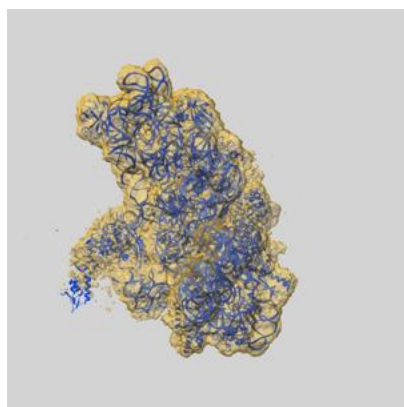
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 6.67 differs from the reported value 4.2 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.41 differs from the reported value 4.2 by more than 10 %

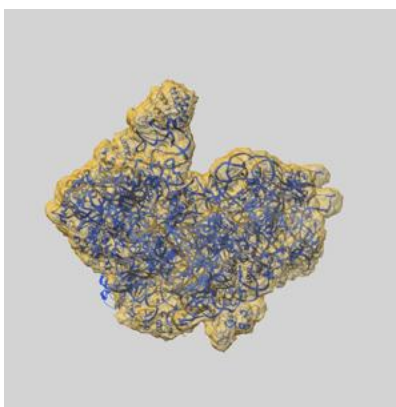
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10320 and PDB model 6SW9. Per-residue inclusion information can be found in section [3](#) on page [13](#).

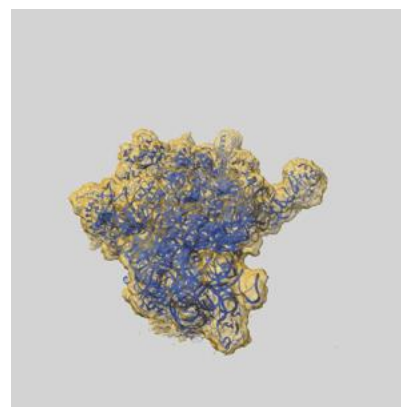
9.1 Map-model overlay [i](#)



X



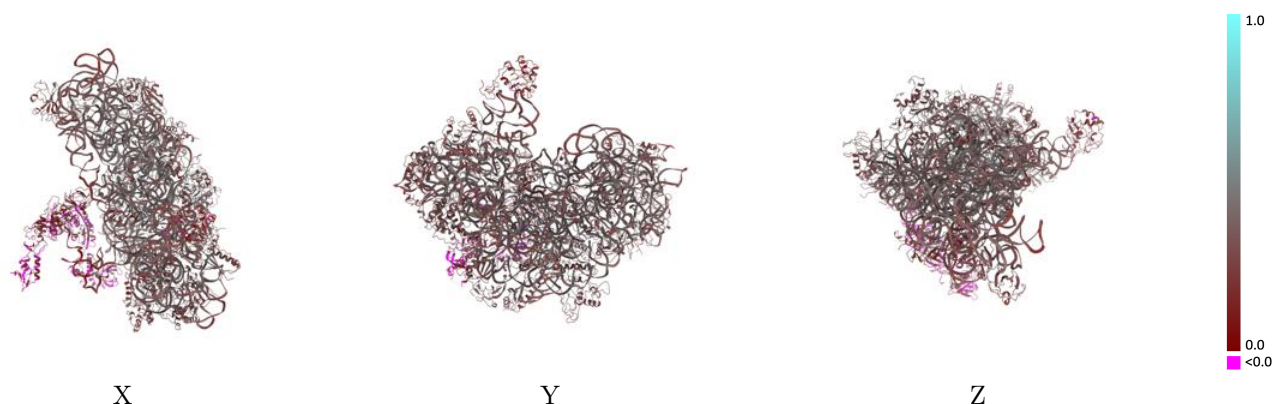
Y



Z

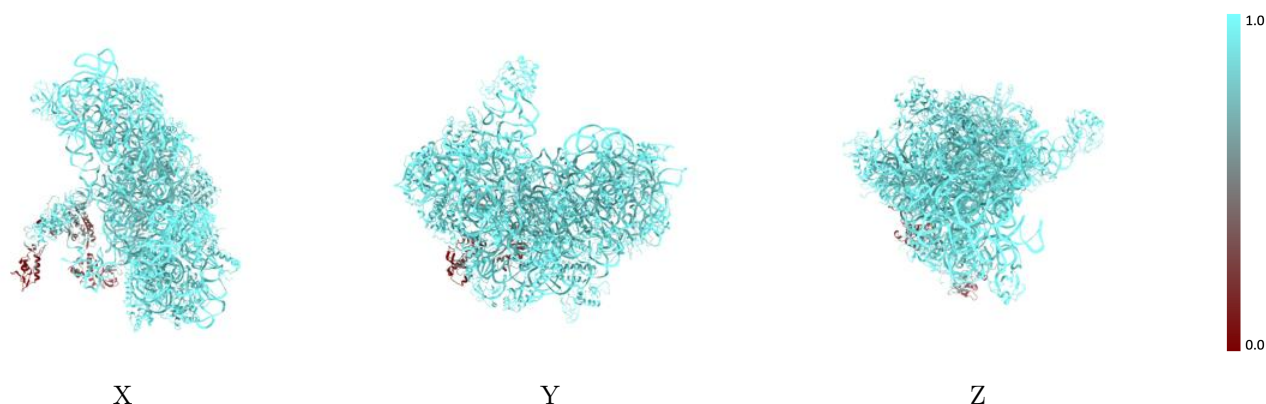
The images above show the 3D surface view of the map at the recommended contour level 0.004 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



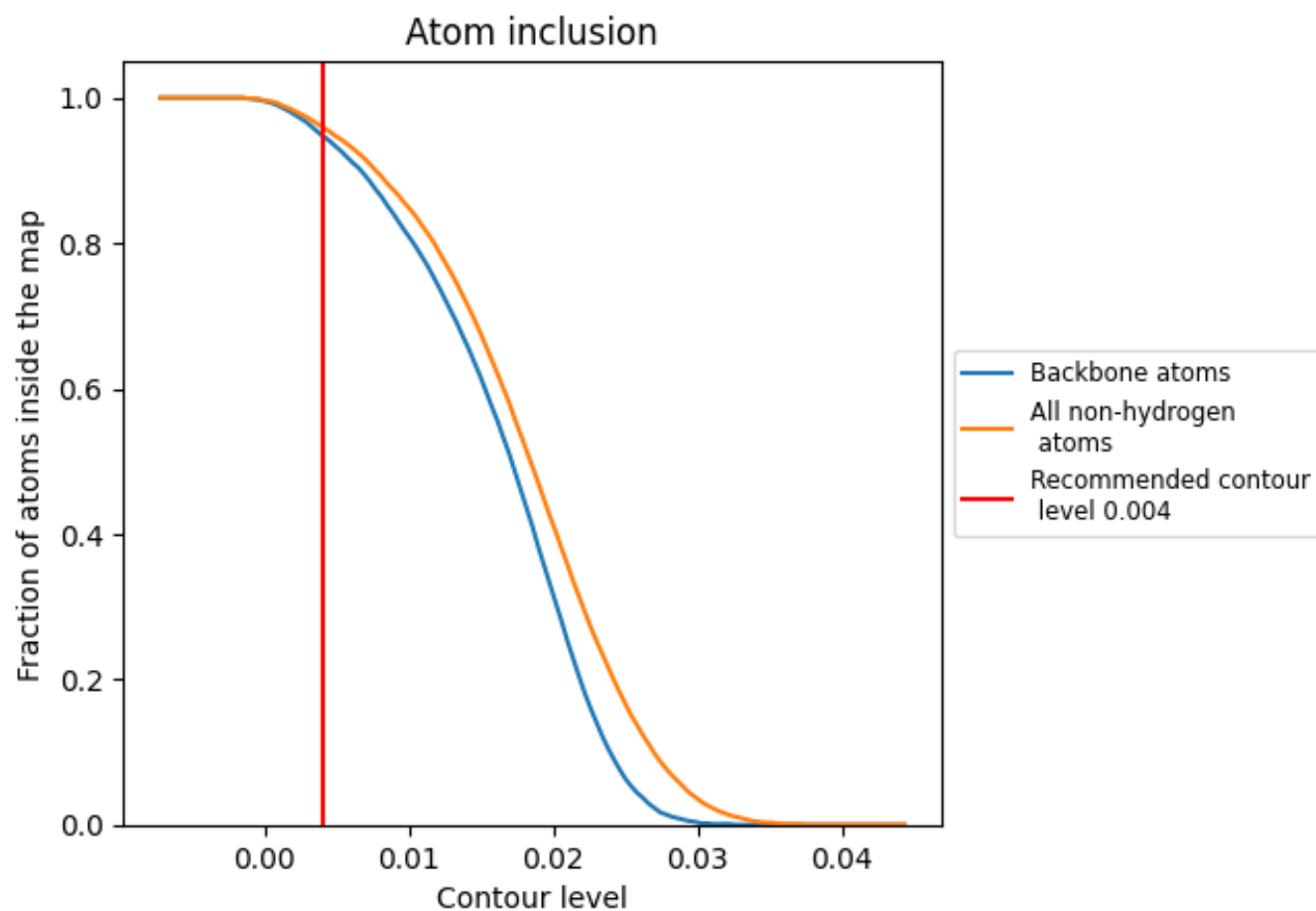
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.004).









































































9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.004) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|--|--|
| All |  0.9600 |  0.3370 |
| 0 |  0.9970 |  0.3730 |
| 2 |  1.0000 |  0.3830 |
| 3 |  1.0000 |  0.2200 |
| 4 |  0.9870 |  0.2310 |
| 5 |  0.9980 |  0.3390 |
| 6 |  1.0000 |  0.2490 |
| 7 |  0.8600 |  0.1420 |
| 8 |  0.2740 |  0.0540 |
| 9 |  0.2580 |  0.0380 |
| A |  0.9960 |  0.3430 |
| B |  0.9970 |  0.3580 |
| C |  0.9940 |  0.3660 |
| D |  1.0000 |  0.3580 |
| E |  0.9990 |  0.3700 |
| F |  0.9930 |  0.3750 |
| G |  0.9980 |  0.3170 |
| H |  0.9960 |  0.3410 |
| I |  0.9980 |  0.3770 |
| J |  0.9980 |  0.3550 |
| K |  0.9980 |  0.3510 |
| L |  0.9980 |  0.3520 |
| M |  1.0000 |  0.3570 |
| N |  0.9980 |  0.3830 |
| O |  0.9980 |  0.3280 |
| P |  1.0000 |  0.3630 |
| Q |  0.9980 |  0.3450 |
| R |  0.9990 |  0.3900 |
| S |  0.9850 |  0.3060 |
| T |  0.9930 |  0.3340 |
| U |  0.9980 |  0.3410 |
| V |  0.9990 |  0.3440 |
| W |  0.9960 |  0.3620 |
| X |  1.0000 |  0.3480 |
| Y |  0.9900 |  0.2050 |
| Z |  0.9950 |  0.3530 |

