



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 04:00 PM GMT

PDB ID : 4IO9
Title : Crystal structure of compound 4d bound to large ribosomal subunit (50S) from *Deinococcus radiodurans*
Authors : Han, S.; Marr, E.S.
Deposited on : 2013-01-07
Resolution : 3.20 Å(reported)

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

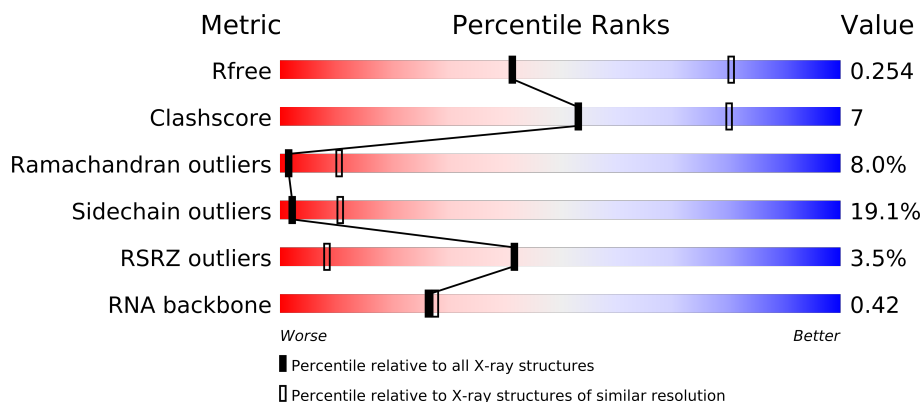
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.20 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) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 66092 | 1824 (3.30-3.10) |
| Clashscore | 79885 | 1078 (3.26-3.14) |
| Ramachandran outliers | 78287 | 1059 (3.26-3.14) |
| Sidechain outliers | 78261 | 1058 (3.26-3.14) |
| RSRZ outliers | 66119 | 1825 (3.30-3.10) |
| RNA backbone | 1838 | 1002 (3.72-2.68) |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | X | 2880 | |
| 2 | Y | 123 | |
| 3 | A | 274 | |
| 4 | B | 211 | |
| 5 | C | 205 | |
| 6 | D | 180 | |
| 7 | E | 185 | |
| 8 | F | 144 | |
| 9 | G | 174 | |
| 10 | H | 134 | |
| 11 | I | 156 | |
| 12 | J | 141 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 13 | K | 116 | |
| 14 | L | 114 | |
| 15 | M | 166 | |
| 16 | N | 118 | |
| 17 | O | 100 | |
| 18 | P | 134 | |
| 19 | Q | 95 | |
| 20 | R | 115 | |
| 21 | S | 237 | |
| 22 | T | 91 | |
| 23 | U | 81 | |
| 24 | V | 67 | |
| 25 | W | 55 | |
| 26 | Z | 60 | |
| 27 | 1 | 55 | |
| 28 | 2 | 47 | |
| 29 | 3 | 66 | |
| 30 | 4 | 37 | |

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Geometry | Electron density |
|-----|------|-------|------|----------|------------------|
| 31 | MG | J | 201 | - | X |
| 31 | MG | M | 201 | - | X |
| 31 | MG | X | 2901 | - | X |
| 31 | MG | X | 2902 | - | X |
| 31 | MG | X | 2903 | - | X |
| 31 | MG | X | 2904 | - | X |
| 31 | MG | X | 2905 | - | X |
| 31 | MG | X | 2906 | - | X |
| 31 | MG | X | 2907 | - | X |
| 31 | MG | X | 2908 | - | X |
| 31 | MG | X | 2909 | - | X |
| 31 | MG | X | 2910 | - | X |
| 31 | MG | X | 2911 | - | X |
| 31 | MG | X | 2912 | - | X |
| 31 | MG | X | 2913 | - | X |
| 31 | MG | X | 2915 | - | X |
| 31 | MG | X | 2916 | - | X |
| 31 | MG | X | 2917 | - | X |
| 31 | MG | X | 2918 | - | X |

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| Mol | Type | Chain | Res | Geometry | Electron density |
|-----|------|-------|------|----------|------------------|
| 31 | MG | X | 2919 | - | X |
| 31 | MG | X | 2920 | - | X |
| 31 | MG | X | 2921 | - | X |
| 31 | MG | X | 2922 | - | X |
| 31 | MG | X | 2923 | - | X |
| 31 | MG | X | 2924 | - | X |
| 31 | MG | X | 2925 | - | X |
| 31 | MG | X | 2926 | - | X |
| 31 | MG | X | 2927 | - | X |
| 31 | MG | X | 2928 | - | X |
| 31 | MG | Y | 201 | - | X |
| 31 | MG | Y | 202 | - | X |
| 31 | MG | Y | 203 | - | X |
| 31 | MG | Y | 204 | - | X |
| 31 | MG | Y | 205 | - | X |

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 83875 atoms, of which 0 are hydrogen and 0 are deuterium.

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

- Molecule 1 is a RNA chain called 23S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 1 | X | 2686 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 57651 | 25718 | 10642 | 18606 | 2685 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 2 | Y | 122 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2598 | 1161 | 476 | 840 | 121 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3 | A | 240 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1826 | 1137 | 366 | 321 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 4 | B | 205 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1539 | 965 | 295 | 271 | 8 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5 | C | 197 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1506 | 935 | 287 | 282 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6 | D | 177 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1400 | 892 | 247 | 254 | 7 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7 | E | 171 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1286 | 812 | 237 | 236 | 1 | | | |

- Molecule 8 is a protein called 50S ribosomal protein L11.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 8 | F | 71 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 503 | 310 | 91 | 99 | 3 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 9 | G | 142 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1114 | 704 | 209 | 198 | 3 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10 | H | 134 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 997 | 614 | 198 | 180 | 5 | | | |

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

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 11 | I | 141 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1067 | 655 | 216 | 196 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12 | J | 136 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1090 | 696 | 202 | 185 | 7 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13 | K | 113 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 878 | 541 | 178 | 157 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 14 | L | 104 | Total | C | N | O | 0 | 0 | 0 |
| | | | 779 | 476 | 161 | 142 | | | |

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

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 15 | M | 108 | Total | C | N | O | 0 | 0 | 0 |
| | | | 871 | 543 | 172 | 156 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16 | N | 117 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 978 | 608 | 210 | 159 | 1 | | | |

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

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 17 | O | 94 | Total | C | N | O | 0 | 0 | 0 |
| | | | 741 | 465 | 139 | 137 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 18 | P | 127 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1014 | 639 | 199 | 174 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19 | Q | 93 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 726 | 458 | 136 | 130 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20 | R | 110 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 825 | 513 | 160 | 151 | 1 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 21 | S | 175 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1345 | 849 | 236 | 254 | 6 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 22 | T | 84 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 625 | 393 | 122 | 109 | 1 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|--|---------|---------|-------|
| 23 | U | 72 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 552 | 341 | 116 | 95 | | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 24 | V | 66 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 533 | 327 | 107 | 96 | 3 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 25 | W | 55 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 424 | 264 | 82 | 76 | 2 | | | |

- Molecule 26 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 26 | Z | 58 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 457 | 281 | 94 | 77 | 5 | | | |

- Molecule 27 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------|---------|---------|-------|
| 27 | 1 | 53 | Total C | 0 | 0 | 53 |
| | | | 53 53 | | | |

- Molecule 28 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf | Trace |
|-----|-------|----------|------------------|---------|---------|-------|
| 28 | 2 | 46 | Total C 46 46 | 0 | 0 | 46 |

- Molecule 29 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf | Trace |
|-----|-------|----------|------------------|---------|---------|-------|
| 29 | 3 | 63 | Total C 63 63 | 0 | 0 | 63 |

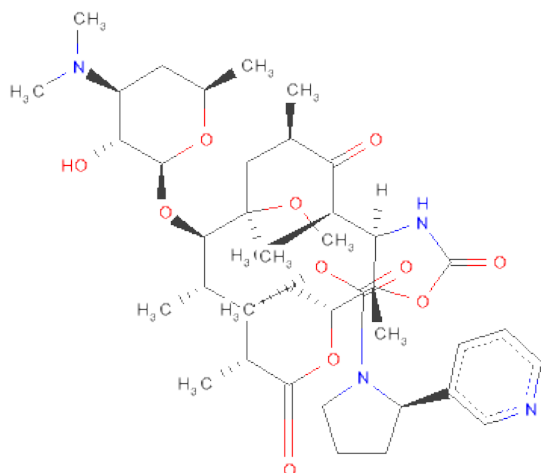
- Molecule 30 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf | Trace |
|-----|-------|----------|----------------------------------|---------|---------|-------|
| 30 | 4 | 37 | Total C N O S 297 179 66 47 5 | 0 | 0 | 0 |

- Molecule 31 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-------------------|---------|---------|
| 31 | X | 28 | Total Mg 28 28 | 0 | 0 |
| 31 | J | 1 | Total Mg 1 1 | 0 | 0 |
| 31 | Y | 5 | Total Mg 5 5 | 0 | 0 |
| 31 | M | 1 | Total Mg 1 1 | 0 | 0 |

- Molecule 32 is (3AS,4R,7R,8S,9S,10R,11R,13R,15R,15AR)-4-ETHYL-11-METHOXY-3A,7,9,11,13,15-HEXAMETHYL-2,6,14-TRIOXO-10-{[3,4,6-TRIDEOXY-3-(DIMETHYLAMINO)-BETA-D-XYLO-HEXOPYRANOSYL]OXY}TETRADECAHYDRO-2H-OXACYCLO TETRADECINO[4,3-D][1,3]OXAZOL-8-YL(2R)-2-(PYRIDIN-3-YL)PYRROLIDINE-1-CARBOXYLATE (three-letter code: 1F2) (formula: C₄₁H₆₄N₄O₁₁).



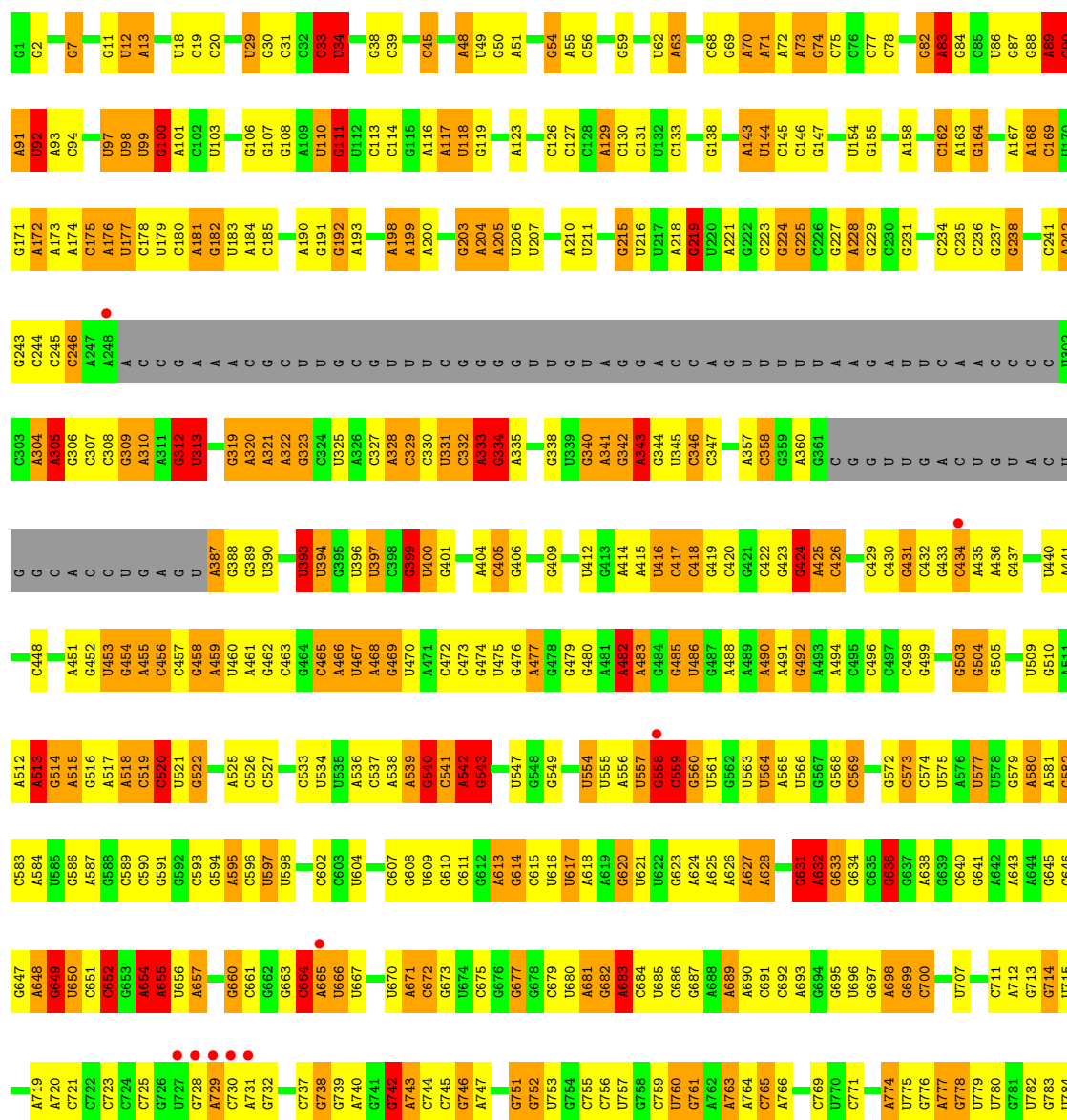
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---------|---------|
| | | | Total | C | N | O | | |
| 32 | X | 1 | 56 | 41 | 4 | 11 | 0 | 0 |

3 Residue-property plots

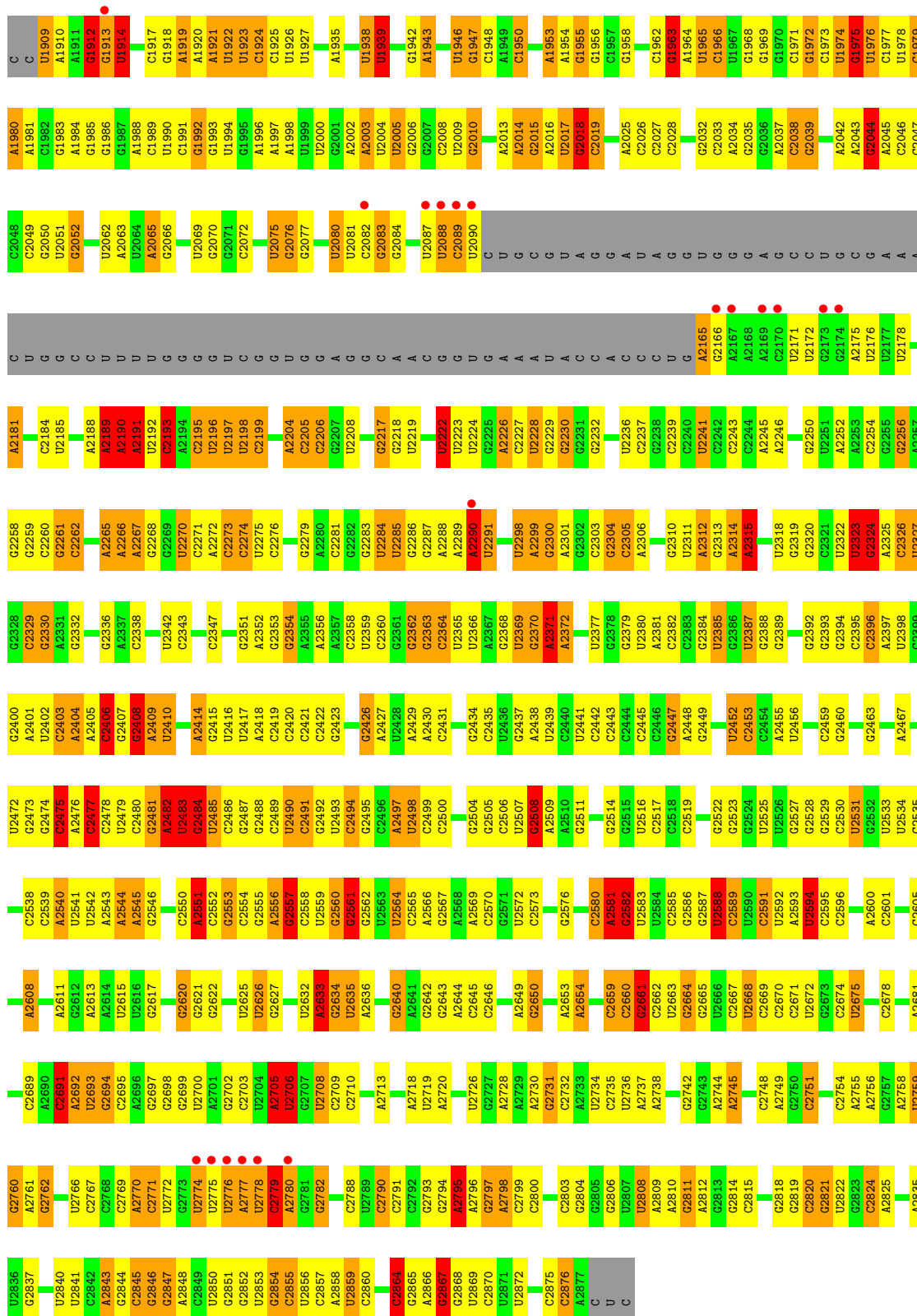
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

• Molecule 1: 23S ribosomal RNA

Chain X: 



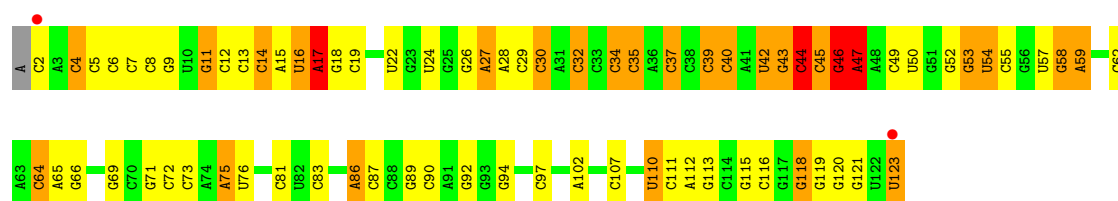




• Molecule 2: 5S ribosomal RNA

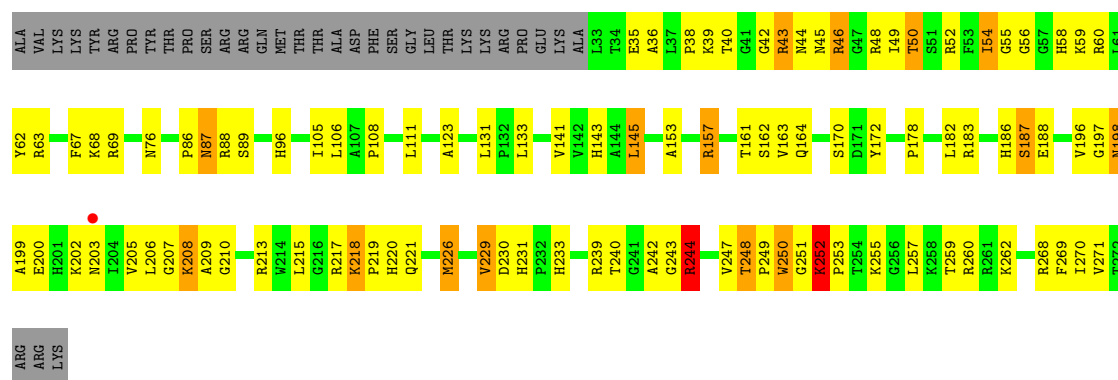
Chain Y:





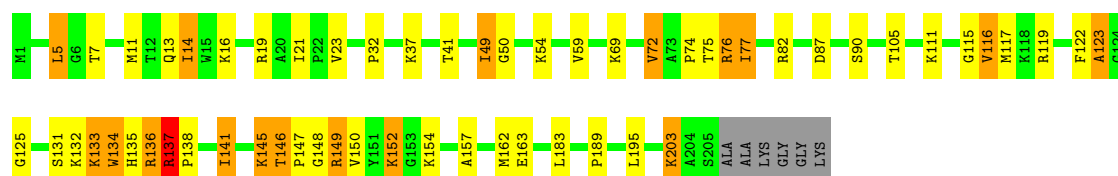
• Molecule 3: 50S ribosomal protein L2

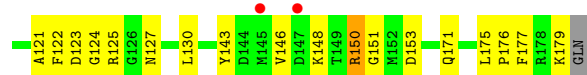
Chain A:



• Molecule 4: 50S ribosomal protein L3

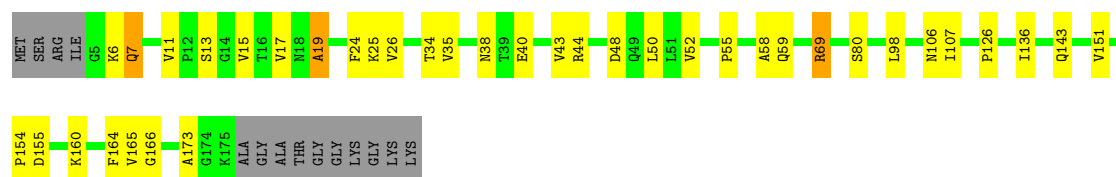
Chain B:





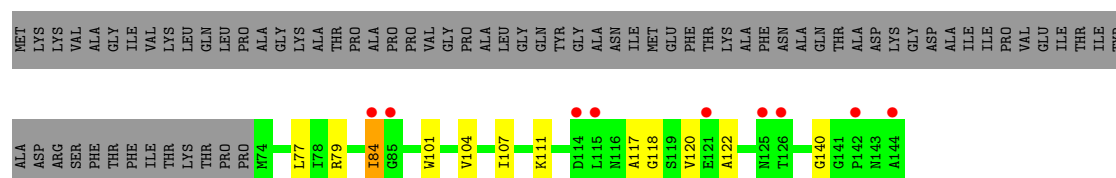
- Molecule 7: 50S ribosomal protein L6

Chain E:



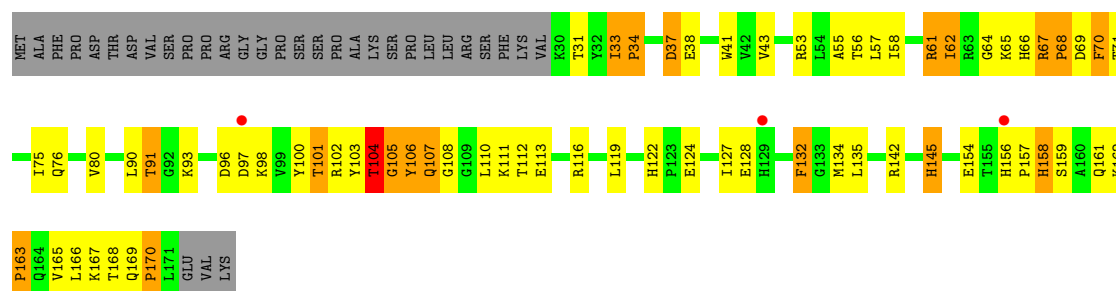
- Molecule 8: 50S ribosomal protein L11

Chain F:



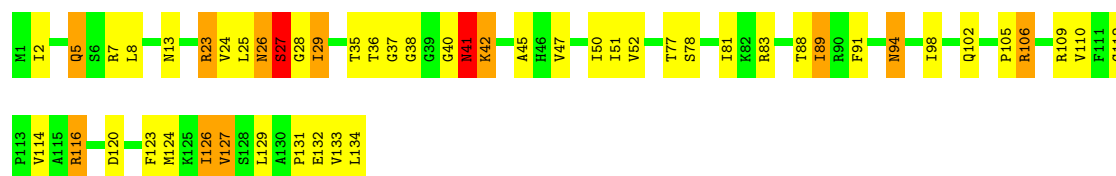
- Molecule 9: 50S ribosomal protein L13

Chain G:



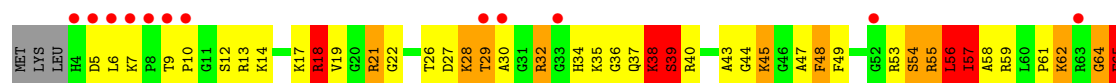
- Molecule 10: 50S ribosomal protein L14

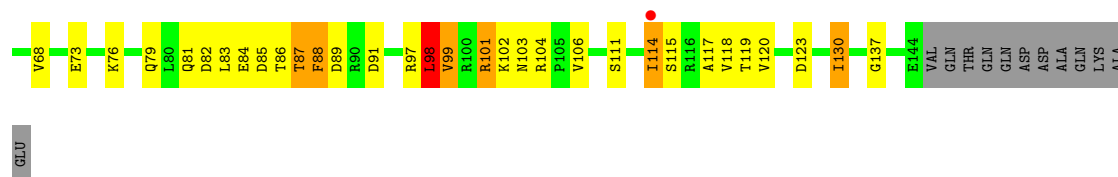
Chain H:



- Molecule 11: 50S ribosomal protein L15

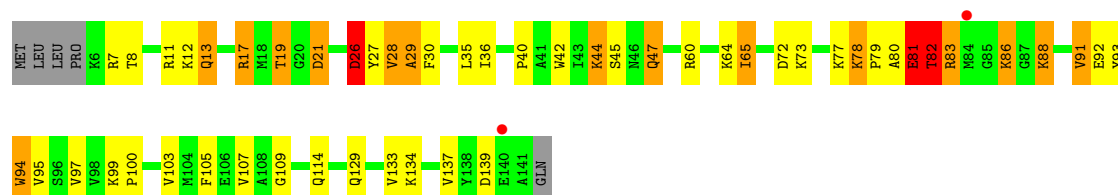
Chain I:





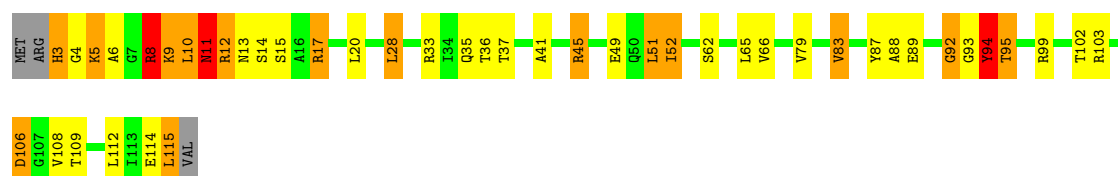
- Molecule 12: 50S ribosomal protein L16

Chain J:



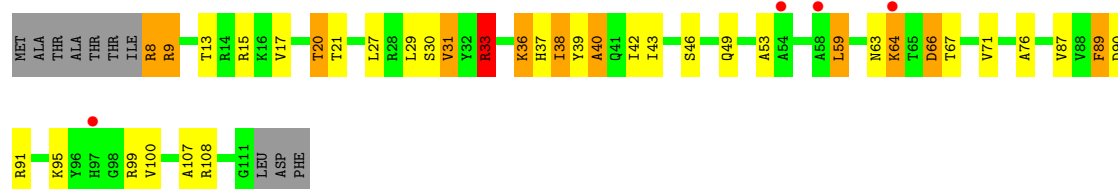
- Molecule 13: 50S ribosomal protein L17

Chain K:



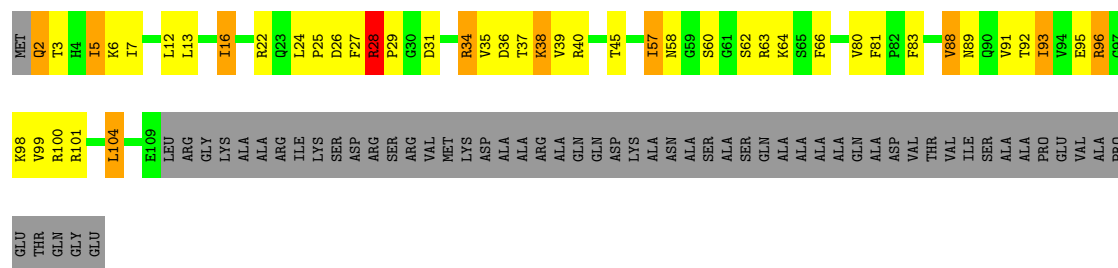
- Molecule 14: 50S ribosomal protein L18

Chain L:



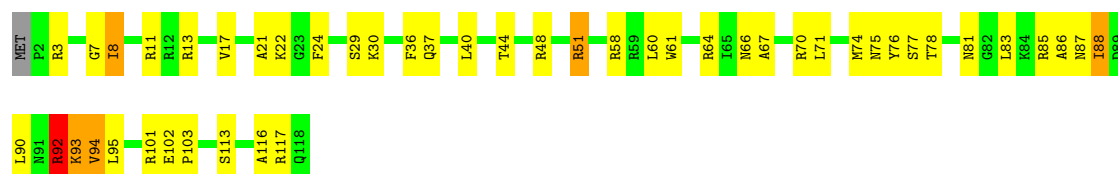
- Molecule 15: 50S ribosomal protein L19

Chain M:



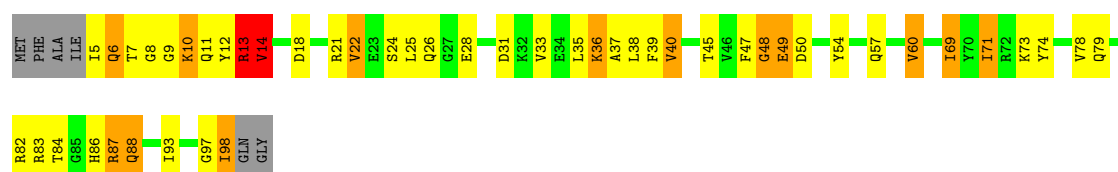
- Molecule 16: 50S ribosomal protein L20

Chain N:



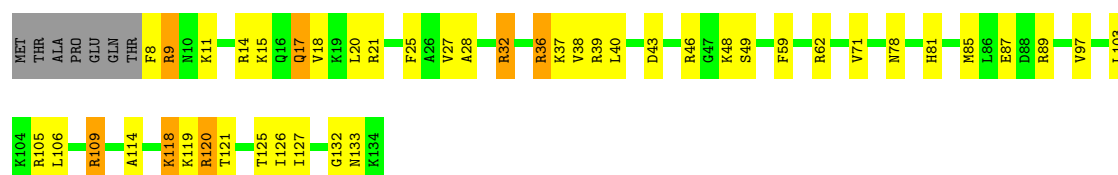
- Molecule 17: 50S ribosomal protein L21

Chain O:



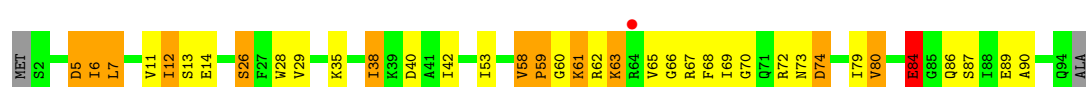
- Molecule 18: 50S ribosomal protein L22

Chain P:



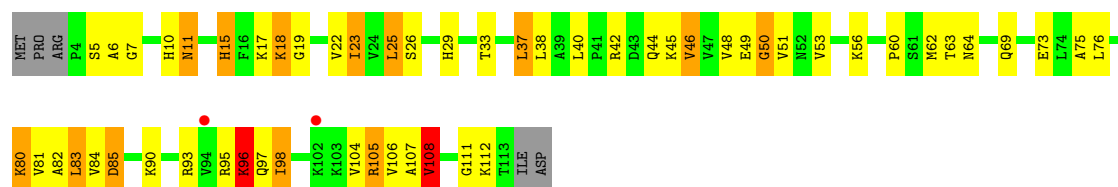
- Molecule 19: 50S ribosomal protein L23

Chain Q:



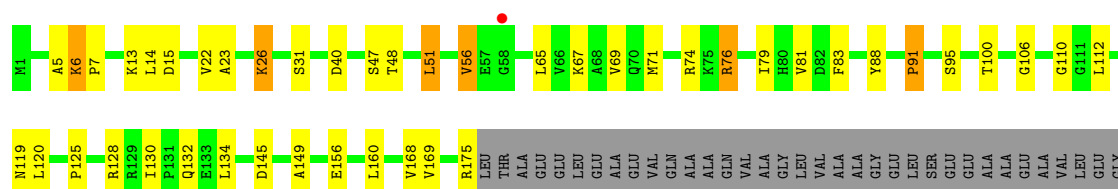
- Molecule 20: 50S ribosomal protein L24

Chain R:



- Molecule 21: 50S ribosomal protein L25

Chain S:



ASP
ALA
SER
LEU
GLU
GLU
VAL
LYS
ALA
GLU
ALA
ALA
SER
GLU
ASP
ASN
ALA
GLY
THR
ASP
SER
GLU
ASP
ASN
SER
ASP
ALA
GLN

- Molecule 22: 50S ribosomal protein L27

Chain T:

MET A2 H3 K4 K5 G8 S9 S10 M11 M12 G13 S16 M17 P18 P19 Y20 Y21 L21 L22 G23 G27 L37 L38 V38 R39 Q40 R41 G42 T43 K46 Q49 Q50 L62 S63 D64 G73 K74 F78 Q85 THR GLU VAL ALA ASP

- Molecule 23: 50S ribosomal protein L28

Chain U:

MET SER ARG GLU CYS TYR LEU T8 G9 K10 K11 V14 V15 M16 M17 S17 S18 V19 V20 R21 G22 G23 D27 G28 G29 Y30 G31 G32 R33 K34 T35 G36 G37 I37 K39 R40 R41 V41 Q42 R43 A44 N45 L46 H47 K48 K49 A50 I51 R52 E53 Q56 T59 V60 W61 L62 S63 N65
A66 L67 P74 Y75 I78 E79 LEU ILE

- Molecule 24: 50S ribosomal protein L29

Chain V:

M1 K2 P3 R7 F14 D19 A20 R21 L25 L28 Q36 L37 R44 R47 L53 V56 R57 A58 E59 L60 E65 Q66 GLN

- Molecule 25: 50S ribosomal protein L30

Chain W:

M1 K2 I3 K4 V9 I10 G11 R12 R26 D30 S31 R32 E33 V34 T37 V40 M43 V44 K45 T46 V47 L50 L51 E55

- Molecule 26: 50S ribosomal protein L32

Chain Z:

MET A2 K3 H4 P5 V6 P7 K8 T11 R16 D17 M18 R19 R20 L25 Q35 C36 H37 K40 L41 S42 H43 H44 T45 C49 D53 G54 R55 Q56 V57 L58 A59 VAL

- Molecule 27: 50S ribosomal protein L33

Chain 1:

MET A2 R7 K26 Y40 D41 P42 V43 A44 K54 VAL

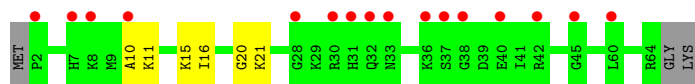
- Molecule 28: 50S ribosomal protein L34

Chain 2:

M1 K2 R3 T4 Y5 Q6 P7 N8 N9 R10 R11 K11 K14 T15 H16 A20 R21 M22 K23 T24 K25 S26 G27 R28 N29 I30 L31 A32 R33 R34 R35 A36 K37 G38 R39 H40 Q41 D46 GLU

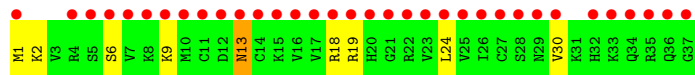
- Molecule 29: 50S ribosomal protein L35

Chain 3: 



- Molecule 30: 50S ribosomal protein L36

Chain 4: 



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | I 2 2 2 | Depositor |
| Cell constants a, b, c, α , β , γ | 169.94Å 409.69Å 694.79Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 30.00 – 3.20 30.20 – 3.21 | Depositor EDS |
| % Data completeness (in resolution range) | (Not available) (30.00-3.20) 94.1 (30.20-3.21) | Depositor EDS |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 3.63 (at 3.24Å) | Xtriage |
| Refinement program | autobuster | Depositor |
| R, R_{free} | 0.199 , 0.235 0.215 , 0.254 | Depositor DCC |
| R_{free} test set | 18481 reflections (5.30%) | DCC |
| Wilson B-factor (Å ²) | 81.2 | Xtriage |
| Anisotropy | 0.747 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.22 , 56.0 | EDS |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| L-test for twinning | $\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$ | Xtriage |
| Outliers | 0 of 367392 reflections | Xtriage |
| F_o, F_c correlation | 0.93 | EDS |
| Total number of atoms | 83875 | wwPDB-VP |
| Average B, all atoms (Å ²) | 107.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.92% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 1F2

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 | X | 1.00 | 46/64561 (0.1%) | 1.87 | 1961/100708 (1.9%) |
| 2 | Y | 1.05 | 0/2904 | 1.78 | 84/4525 (1.9%) |
| 3 | A | 0.61 | 0/1862 | 0.92 | 1/2510 (0.0%) |
| 4 | B | 0.57 | 0/1567 | 0.94 | 1/2105 (0.0%) |
| 5 | C | 0.62 | 0/1529 | 0.98 | 2/2070 (0.1%) |
| 6 | D | 0.45 | 0/1419 | 0.66 | 0/1903 |
| 7 | E | 0.45 | 0/1308 | 0.67 | 0/1771 |
| 8 | F | 0.46 | 0/508 | 0.64 | 0/683 |
| 9 | G | 0.58 | 0/1138 | 0.94 | 1/1539 (0.1%) |
| 10 | H | 0.55 | 0/1007 | 0.88 | 1/1352 (0.1%) |
| 11 | I | 0.73 | 1/1081 (0.1%) | 1.12 | 6/1448 (0.4%) |
| 12 | J | 0.68 | 1/1113 (0.1%) | 0.95 | 1/1486 (0.1%) |
| 13 | K | 0.77 | 2/886 (0.2%) | 1.02 | 3/1188 (0.3%) |
| 14 | L | 0.53 | 0/785 | 0.88 | 1/1048 (0.1%) |
| 15 | M | 0.64 | 0/884 | 0.98 | 1/1186 (0.1%) |
| 16 | N | 0.51 | 0/994 | 0.77 | 0/1323 |
| 17 | O | 0.52 | 0/750 | 0.95 | 1/1000 (0.1%) |
| 18 | P | 0.56 | 0/1027 | 0.85 | 0/1373 |
| 19 | Q | 0.60 | 0/737 | 1.03 | 5/988 (0.5%) |
| 20 | R | 0.61 | 0/835 | 0.99 | 0/1121 |
| 21 | S | 0.48 | 0/1370 | 0.73 | 0/1862 |
| 22 | T | 0.55 | 0/633 | 0.82 | 0/838 |
| 23 | U | 0.75 | 0/556 | 1.10 | 1/741 (0.1%) |
| 24 | V | 0.47 | 0/537 | 0.71 | 0/714 |
| 25 | W | 0.48 | 0/426 | 0.81 | 0/568 |
| 26 | Z | 0.62 | 0/469 | 0.97 | 0/629 |
| 30 | 4 | 0.44 | 0/298 | 0.62 | 0/390 |
| All | All | 0.91 | 50/91184 (0.1%) | 1.69 | 2070/137069 (1.5%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is

detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | X | 0 | 6 |

All (50) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1 | X | 1688 | U | C4-O4 | 9.12 | 1.30 | 1.23 |
| 1 | X | 774 | A | C5-C4 | 8.90 | 1.45 | 1.38 |
| 1 | X | 1685 | A | C3'-O3' | 7.74 | 1.52 | 1.42 |
| 1 | X | 1468 | A | N9-C4 | 7.70 | 1.42 | 1.37 |
| 1 | X | 1333 | G | N9-C4 | -7.09 | 1.32 | 1.38 |
| 1 | X | 1688 | U | N3-C4 | 6.99 | 1.44 | 1.38 |
| 1 | X | 1688 | U | C2-N3 | 6.89 | 1.42 | 1.37 |
| 1 | X | 2189 | A | C3'-O3' | 6.77 | 1.51 | 1.42 |
| 13 | K | 52 | ILE | CG1-CD1 | 6.46 | 1.95 | 1.50 |
| 1 | X | 1980 | A | N7-C5 | -6.44 | 1.35 | 1.39 |
| 1 | X | 1467 | U | C1'-N1 | 6.42 | 1.58 | 1.48 |
| 1 | X | 774 | A | N7-C5 | -6.38 | 1.35 | 1.39 |
| 1 | X | 774 | A | C6-N1 | 6.35 | 1.40 | 1.35 |
| 1 | X | 346 | C | C1'-N1 | 6.33 | 1.58 | 1.48 |
| 1 | X | 2018 | G | N9-C8 | 6.33 | 1.42 | 1.37 |
| 1 | X | 559 | C | C3'-O3' | 6.18 | 1.50 | 1.42 |
| 1 | X | 1946 | U | C1'-N1 | 6.16 | 1.57 | 1.48 |
| 1 | X | 1288 | A | C4'-C3' | -6.11 | 1.46 | 1.53 |
| 1 | X | 1975 | G | C3'-O3' | 6.11 | 1.50 | 1.42 |
| 11 | I | 57 | ILE | CG1-CD1 | 6.08 | 1.92 | 1.50 |
| 1 | X | 774 | A | N1-C2 | 6.08 | 1.39 | 1.34 |
| 1 | X | 1223 | G | C2-N3 | 5.85 | 1.37 | 1.32 |
| 1 | X | 699 | G | N9-C4 | -5.84 | 1.33 | 1.38 |
| 1 | X | 796 | A | N9-C4 | -5.64 | 1.34 | 1.37 |
| 1 | X | 759 | C | N3-C4 | 5.62 | 1.37 | 1.33 |
| 1 | X | 838 | A | C3'-O3' | 5.59 | 1.50 | 1.42 |
| 1 | X | 661 | C | C1'-N1 | 5.59 | 1.57 | 1.48 |
| 1 | X | 646 | C | C1'-N1 | 5.57 | 1.57 | 1.48 |
| 1 | X | 343 | A | N9-C4 | 5.56 | 1.41 | 1.37 |
| 1 | X | 540 | G | C2-N3 | 5.52 | 1.37 | 1.32 |
| 1 | X | 393 | U | C1'-N1 | 5.50 | 1.57 | 1.48 |
| 1 | X | 656 | U | P-O5' | 5.49 | 1.65 | 1.59 |
| 1 | X | 559 | C | C1'-N1 | 5.47 | 1.56 | 1.48 |
| 12 | J | 19 | THR | CA-C | 5.42 | 1.67 | 1.52 |
| 13 | K | 3 | HIS | CA-C | 5.41 | 1.67 | 1.52 |
| 1 | X | 2735 | C | C1'-N1 | 5.39 | 1.56 | 1.48 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1 | X | 796 | A | N7-C5 | -5.39 | 1.36 | 1.39 |
| 1 | X | 540 | G | C5-C6 | 5.37 | 1.47 | 1.42 |
| 1 | X | 462 | G | C6-O6 | 5.26 | 1.28 | 1.24 |
| 1 | X | 2015 | G | N7-C5 | 5.25 | 1.42 | 1.39 |
| 1 | X | 2668 | U | C4-C5 | 5.22 | 1.48 | 1.43 |
| 1 | X | 577 | U | C4-C5 | 5.18 | 1.48 | 1.43 |
| 1 | X | 927 | C | C1'-N1 | 5.16 | 1.56 | 1.48 |
| 1 | X | 2582 | G | P-O5' | 5.13 | 1.64 | 1.59 |
| 1 | X | 774 | A | N3-C4 | 5.13 | 1.38 | 1.34 |
| 1 | X | 1688 | U | C1'-N1 | 5.12 | 1.56 | 1.48 |
| 1 | X | 2697 | G | C5-C4 | -5.09 | 1.34 | 1.38 |
| 1 | X | 661 | C | N1-C2 | 5.06 | 1.45 | 1.40 |
| 1 | X | 757 | U | C3'-O3' | -5.03 | 1.35 | 1.42 |
| 1 | X | 2800 | C | C3'-O3' | -5.00 | 1.35 | 1.42 |

All (2070) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 1 | X | 1631 | C | C1'-O4'-C4' | -33.72 | 82.92 | 109.90 |
| 1 | X | 1288 | A | C1'-O4'-C4' | -32.93 | 83.55 | 109.90 |
| 1 | X | 1288 | A | C5'-C4'-O4' | 20.68 | 133.91 | 109.10 |
| 1 | X | 1288 | A | O4'-C1'-N9 | 20.52 | 124.61 | 108.20 |
| 1 | X | 1019 | U | P-O3'-C3' | 19.59 | 143.21 | 119.70 |
| 1 | X | 774 | A | N1-C6-N6 | 19.05 | 130.03 | 118.60 |
| 1 | X | 1631 | C | C5'-C4'-O4' | 18.47 | 131.26 | 109.10 |
| 1 | X | 2808 | U | O4'-C1'-N1 | 17.97 | 122.57 | 108.20 |
| 1 | X | 774 | A | N7-C8-N9 | 17.08 | 122.34 | 113.80 |
| 1 | X | 2705 | A | P-O3'-C3' | 17.01 | 140.11 | 119.70 |
| 1 | X | 1278 | A | O4'-C1'-N9 | 16.77 | 121.61 | 108.20 |
| 1 | X | 1963 | G | P-O3'-C3' | 16.73 | 139.78 | 119.70 |
| 1 | X | 1716 | G | P-O3'-C3' | 16.57 | 139.58 | 119.70 |
| 1 | X | 1631 | C | C4'-C3'-C2' | -16.28 | 86.32 | 102.60 |
| 1 | X | 1775 | A | P-O3'-C3' | 16.21 | 139.15 | 119.70 |
| 1 | X | 1333 | G | N3-C4-N9 | -16.10 | 116.34 | 126.00 |
| 1 | X | 343 | A | O4'-C1'-N9 | 15.89 | 120.92 | 108.20 |
| 1 | X | 994 | A | P-O3'-C3' | 15.83 | 138.70 | 119.70 |
| 1 | X | 788 | G | P-O3'-C3' | 15.71 | 138.55 | 119.70 |
| 1 | X | 1634 | A | P-O3'-C3' | 15.64 | 138.47 | 119.70 |
| 1 | X | 2189 | A | P-O3'-C3' | 15.53 | 138.34 | 119.70 |
| 1 | X | 1475 | U | P-O3'-C3' | 15.44 | 138.22 | 119.70 |
| 1 | X | 1473 | U | P-O3'-C3' | 15.14 | 137.87 | 119.70 |
| 1 | X | 774 | A | C5-N7-C8 | -15.10 | 96.35 | 103.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 1 | X | 2497 | A | P-O3'-C3' | 14.90 | 137.58 | 119.70 |
| 1 | X | 2564 | U | P-O3'-C3' | 14.53 | 137.13 | 119.70 |
| 1 | X | 774 | A | C6-C5-N7 | -14.30 | 122.29 | 132.30 |
| 1 | X | 1333 | G | O4'-C1'-N9 | 14.26 | 119.61 | 108.20 |
| 1 | X | 594 | G | P-O3'-C3' | 14.24 | 136.79 | 119.70 |
| 1 | X | 399 | G | P-O3'-C3' | 14.02 | 136.53 | 119.70 |
| 1 | X | 469 | G | P-O3'-C3' | 13.93 | 136.41 | 119.70 |
| 1 | X | 1574 | A | O4'-C1'-N9 | 13.91 | 119.33 | 108.20 |
| 1 | X | 1355 | A | P-O3'-C3' | 13.80 | 136.26 | 119.70 |
| 1 | X | 558 | G | P-O3'-C3' | 13.72 | 136.16 | 119.70 |
| 1 | X | 73 | A | P-O3'-C3' | 13.62 | 136.04 | 119.70 |
| 1 | X | 1249 | G | P-O3'-C3' | 13.61 | 136.03 | 119.70 |
| 1 | X | 176 | A | P-O3'-C3' | 13.39 | 135.77 | 119.70 |
| 1 | X | 540 | G | N1-C6-O6 | -13.38 | 111.87 | 119.90 |
| 1 | X | 204 | A | P-O3'-C3' | 13.37 | 135.74 | 119.70 |
| 1 | X | 1261 | G | P-O3'-C3' | 13.07 | 135.39 | 119.70 |
| 1 | X | 467 | U | P-O3'-C3' | 12.91 | 135.20 | 119.70 |
| 1 | X | 1938 | U | P-O3'-C3' | 12.82 | 135.09 | 119.70 |
| 1 | X | 2769 | C | O4'-C1'-N1 | 12.79 | 118.43 | 108.20 |
| 1 | X | 242 | A | O4'-C1'-N9 | 12.78 | 118.42 | 108.20 |
| 1 | X | 2312 | A | P-O3'-C3' | 12.72 | 134.96 | 119.70 |
| 1 | X | 2551 | A | P-O3'-C3' | 12.67 | 134.91 | 119.70 |
| 1 | X | 2018 | G | P-O3'-C3' | 12.66 | 134.90 | 119.70 |
| 1 | X | 2014 | A | P-O3'-C3' | 12.60 | 134.82 | 119.70 |
| 2 | Y | 58 | G | P-O3'-C3' | 12.56 | 134.78 | 119.70 |
| 1 | X | 181 | A | P-O3'-C3' | 12.54 | 134.75 | 119.70 |
| 1 | X | 1036 | G | P-O3'-C3' | 12.54 | 134.75 | 119.70 |
| 1 | X | 100 | G | P-O3'-C3' | 12.53 | 134.74 | 119.70 |
| 1 | X | 99 | U | P-O3'-C3' | 12.52 | 134.73 | 119.70 |
| 1 | X | 71 | A | P-O3'-C3' | 12.46 | 134.66 | 119.70 |
| 1 | X | 1820 | G | P-O3'-C3' | 12.44 | 134.63 | 119.70 |
| 2 | Y | 16 | U | P-O3'-C3' | 12.29 | 134.45 | 119.70 |
| 1 | X | 334 | G | P-O3'-C3' | 12.27 | 134.42 | 119.70 |
| 1 | X | 33 | C | O4'-C1'-N1 | 12.23 | 117.98 | 108.20 |
| 1 | X | 2088 | U | P-O3'-C3' | 12.23 | 134.37 | 119.70 |
| 1 | X | 342 | G | P-O3'-C3' | 12.19 | 134.33 | 119.70 |
| 1 | X | 559 | C | O4'-C1'-N1 | 12.09 | 117.87 | 108.20 |
| 1 | X | 774 | A | C4-C5-N7 | 12.09 | 116.74 | 110.70 |
| 1 | X | 1288 | A | C4'-C3'-C2' | -12.04 | 90.56 | 102.60 |
| 1 | X | 1688 | U | N3-C4-O4 | 12.02 | 127.81 | 119.40 |
| 1 | X | 33 | C | P-O3'-C3' | 11.96 | 134.06 | 119.70 |
| 1 | X | 1790 | G | P-O3'-C3' | 11.79 | 133.85 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 1 | X | 1142 | G | C5'-C4'-O4' | 11.74 | 123.19 | 109.10 |
| 1 | X | 664 | C | P-O3'-C3' | 11.72 | 133.76 | 119.70 |
| 1 | X | 2298 | U | P-O3'-C3' | 11.70 | 133.74 | 119.70 |
| 1 | X | 537 | C | N1-C2-O2 | 11.68 | 125.91 | 118.90 |
| 1 | X | 1333 | G | N3-C4-C5 | 11.66 | 134.43 | 128.60 |
| 1 | X | 2190 | A | O4'-C1'-N9 | 11.63 | 117.50 | 108.20 |
| 1 | X | 1688 | U | N3-C4-C5 | -11.60 | 107.64 | 114.60 |
| 1 | X | 218 | A | P-O3'-C3' | 11.56 | 133.57 | 119.70 |
| 1 | X | 2736 | U | P-O3'-C3' | 11.55 | 133.56 | 119.70 |
| 1 | X | 454 | G | P-O3'-C3' | 11.53 | 133.53 | 119.70 |
| 1 | X | 2769 | C | C1'-O4'-C4' | -11.49 | 100.70 | 109.90 |
| 1 | X | 1442 | C | P-O3'-C3' | 11.48 | 133.48 | 119.70 |
| 1 | X | 559 | C | C4'-C3'-C2' | -11.37 | 91.23 | 102.60 |
| 1 | X | 1467 | U | P-O3'-C3' | -11.29 | 106.15 | 119.70 |
| 1 | X | 1574 | A | C1'-O4'-C4' | -11.15 | 100.98 | 109.90 |
| 1 | X | 2668 | U | C5-C4-O4 | 11.13 | 132.58 | 125.90 |
| 1 | X | 943 | U | O4'-C1'-N1 | 11.08 | 117.06 | 108.20 |
| 1 | X | 2669 | C | N1-C2-O2 | 11.05 | 125.53 | 118.90 |
| 1 | X | 518 | A | P-O3'-C3' | 11.03 | 132.93 | 119.70 |
| 1 | X | 774 | A | C5-C6-N1 | -11.02 | 112.19 | 117.70 |
| 1 | X | 969 | U | P-O3'-C3' | 10.98 | 132.88 | 119.70 |
| 1 | X | 1152 | C | P-O3'-C3' | 10.96 | 132.86 | 119.70 |
| 1 | X | 1468 | A | O4'-C1'-N9 | 10.96 | 116.97 | 108.20 |
| 1 | X | 774 | A | C8-N9-C4 | -10.94 | 101.42 | 105.80 |
| 1 | X | 1799 | A | C1'-O4'-C4' | -10.92 | 101.17 | 109.90 |
| 1 | X | 814 | G | P-O3'-C3' | 10.89 | 132.76 | 119.70 |
| 1 | X | 341 | A | P-O3'-C3' | 10.85 | 132.72 | 119.70 |
| 1 | X | 2261 | G | P-O3'-C3' | 10.85 | 132.72 | 119.70 |
| 1 | X | 1467 | U | C5-C6-N1 | 10.85 | 128.12 | 122.70 |
| 1 | X | 2691 | C | O4'-C1'-N1 | 10.80 | 116.84 | 108.20 |
| 1 | X | 1122 | A | P-O3'-C3' | 10.79 | 132.64 | 119.70 |
| 1 | X | 2204 | A | P-O3'-C3' | 10.78 | 132.63 | 119.70 |
| 1 | X | 683 | A | P-O3'-C3' | 10.73 | 132.58 | 119.70 |
| 1 | X | 48 | A | P-O3'-C3' | 10.69 | 132.53 | 119.70 |
| 1 | X | 1552 | C | P-O3'-C3' | 10.69 | 132.53 | 119.70 |
| 1 | X | 198 | A | P-O3'-C3' | 10.63 | 132.46 | 119.70 |
| 1 | X | 469 | G | O4'-C1'-N9 | 10.60 | 116.68 | 108.20 |
| 1 | X | 1429 | A | O4'-C1'-N9 | 10.57 | 116.66 | 108.20 |
| 1 | X | 1632 | A | P-O3'-C3' | 10.57 | 132.38 | 119.70 |
| 1 | X | 1850 | G | P-O3'-C3' | 10.55 | 132.36 | 119.70 |
| 1 | X | 1096 | A | P-O3'-C3' | 10.52 | 132.32 | 119.70 |
| 1 | X | 699 | G | C5-N7-C8 | -10.51 | 99.05 | 104.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 1 | X | 803 | C | P-O3'-C3' | 10.47 | 132.26 | 119.70 |
| 1 | X | 2770 | A | P-O3'-C3' | 10.45 | 132.24 | 119.70 |
| 1 | X | 182 | G | P-O3'-C3' | 10.40 | 132.18 | 119.70 |
| 1 | X | 655 | A | P-O3'-C3' | 10.37 | 132.14 | 119.70 |
| 1 | X | 2190 | A | P-O5'-C5' | 10.35 | 137.45 | 120.90 |
| 1 | X | 1053 | G | P-O3'-C3' | 10.34 | 132.10 | 119.70 |
| 1 | X | 1923 | U | P-O3'-C3' | 10.32 | 132.09 | 119.70 |
| 1 | X | 1142 | G | O4'-C1'-C2' | -10.30 | 95.50 | 105.80 |
| 1 | X | 1186 | G | P-O3'-C3' | 10.27 | 132.03 | 119.70 |
| 1 | X | 638 | A | P-O3'-C3' | 10.27 | 132.02 | 119.70 |
| 1 | X | 1631 | C | N1-C1'-C2' | 10.22 | 127.28 | 114.00 |
| 1 | X | 1574 | A | C4'-C3'-C2' | -10.20 | 92.40 | 102.60 |
| 1 | X | 2371 | A | O4'-C1'-N9 | 10.16 | 116.33 | 108.20 |
| 1 | X | 98 | U | P-O3'-C3' | 10.16 | 131.89 | 119.70 |
| 1 | X | 469 | G | C5'-C4'-C3' | -10.15 | 99.76 | 116.00 |
| 2 | Y | 54 | U | O4'-C1'-N1 | 10.14 | 116.31 | 108.20 |
| 1 | X | 1613 | G | C1'-O4'-C4' | -10.14 | 101.79 | 109.90 |
| 1 | X | 2018 | G | C5'-C4'-O4' | -10.11 | 96.97 | 109.10 |
| 1 | X | 34 | U | O4'-C1'-N1 | 10.08 | 116.27 | 108.20 |
| 1 | X | 559 | C | P-O3'-C3' | 10.06 | 131.77 | 119.70 |
| 1 | X | 1710 | U | P-O3'-C3' | 10.01 | 131.71 | 119.70 |
| 1 | X | 2498 | U | P-O3'-C3' | 9.98 | 131.68 | 119.70 |
| 1 | X | 418 | C | C1'-O4'-C4' | -9.97 | 101.92 | 109.90 |
| 1 | X | 1333 | G | N3-C2-N2 | -9.96 | 112.93 | 119.90 |
| 1 | X | 1468 | A | C8-N9-C4 | -9.96 | 101.82 | 105.80 |
| 1 | X | 89 | A | P-O3'-C3' | 9.94 | 131.63 | 119.70 |
| 1 | X | 1631 | C | O4'-C4'-C3' | -9.94 | 94.06 | 104.00 |
| 1 | X | 1142 | G | P-O3'-C3' | 9.92 | 131.60 | 119.70 |
| 1 | X | 2475 | C | O4'-C1'-N1 | 9.91 | 116.13 | 108.20 |
| 1 | X | 1496 | G | P-O3'-C3' | 9.89 | 131.57 | 119.70 |
| 1 | X | 2323 | U | O4'-C1'-N1 | 9.89 | 116.11 | 108.20 |
| 1 | X | 1770 | U | O4'-C4'-C3' | -9.88 | 94.12 | 104.00 |
| 1 | X | 765 | C | P-O3'-C3' | 9.87 | 131.54 | 119.70 |
| 1 | X | 2795 | A | P-O3'-C3' | 9.85 | 131.52 | 119.70 |
| 1 | X | 841 | G | O4'-C4'-C3' | -9.84 | 94.16 | 104.00 |
| 1 | X | 1223 | G | C3'-C2'-C1' | 9.78 | 109.33 | 101.50 |
| 1 | X | 2016 | A | P-O3'-C3' | 9.77 | 131.43 | 119.70 |
| 1 | X | 1523 | A | P-O3'-C3' | 9.76 | 131.41 | 119.70 |
| 1 | X | 2596 | C | O4'-C1'-N1 | 9.76 | 116.01 | 108.20 |
| 1 | X | 242 | A | C1'-O4'-C4' | -9.74 | 102.11 | 109.90 |
| 1 | X | 1811 | A | P-O3'-C3' | 9.71 | 131.35 | 119.70 |
| 1 | X | 1333 | G | C8-N9-C1' | 9.70 | 139.61 | 127.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | X | 938 | G | O4'-C1'-N9 | 9.68 | 115.94 | 108.20 |
| 1 | X | 1266 | G | P-O3'-C3' | 9.68 | 131.31 | 119.70 |
| 1 | X | 1288 | A | C3'-C2'-C1' | -9.65 | 93.78 | 101.50 |
| 1 | X | 515 | A | P-O3'-C3' | 9.65 | 131.28 | 119.70 |
| 1 | X | 1975 | G | C2'-C3'-O3' | 9.64 | 130.71 | 109.50 |
| 1 | X | 1391 | A | P-O3'-C3' | 9.60 | 131.22 | 119.70 |
| 1 | X | 1055 | A | P-O3'-C3' | 9.59 | 131.21 | 119.70 |
| 1 | X | 1469 | U | P-O3'-C3' | 9.57 | 131.19 | 119.70 |
| 1 | X | 1575 | C | P-O3'-C3' | 9.57 | 131.18 | 119.70 |
| 1 | X | 650 | U | O4'-C1'-N1 | 9.56 | 115.84 | 108.20 |
| 1 | X | 2323 | U | P-O3'-C3' | 9.56 | 131.17 | 119.70 |
| 1 | X | 655 | A | O4'-C1'-N9 | 9.55 | 115.84 | 108.20 |
| 1 | X | 805 | G | O4'-C1'-N9 | -9.54 | 100.56 | 108.20 |
| 1 | X | 2426 | G | P-O3'-C3' | 9.54 | 131.15 | 119.70 |
| 1 | X | 581 | A | P-O3'-C3' | -9.51 | 108.29 | 119.70 |
| 1 | X | 1409 | U | P-O3'-C3' | 9.49 | 131.09 | 119.70 |
| 1 | X | 1141 | U | P-O3'-C3' | 9.48 | 131.08 | 119.70 |
| 1 | X | 1753 | A | O4'-C1'-N9 | 9.45 | 115.76 | 108.20 |
| 1 | X | 1333 | G | N9-C4-C5 | 9.36 | 109.14 | 105.40 |
| 2 | Y | 11 | G | C1'-O4'-C4' | -9.36 | 102.41 | 109.90 |
| 1 | X | 777 | A | P-O3'-C3' | 9.35 | 130.92 | 119.70 |
| 1 | X | 1732 | U | P-O3'-C3' | 9.32 | 130.88 | 119.70 |
| 1 | X | 1468 | A | O4'-C1'-C2' | -9.27 | 96.53 | 105.80 |
| 1 | X | 1288 | A | O4'-C4'-C3' | -9.25 | 94.75 | 104.00 |
| 1 | X | 1412 | C | C3'-C2'-C1' | -9.24 | 94.11 | 101.50 |
| 1 | X | 2437 | G | P-O3'-C3' | 9.23 | 130.77 | 119.70 |
| 1 | X | 514 | G | P-O3'-C3' | 9.22 | 130.76 | 119.70 |
| 1 | X | 699 | G | N3-C4-C5 | 9.21 | 133.21 | 128.60 |
| 1 | X | 1086 | C | P-O3'-C3' | 9.21 | 130.75 | 119.70 |
| 1 | X | 1469 | U | N1-C1'-C2' | 9.21 | 125.97 | 114.00 |
| 1 | X | 540 | G | C5-C6-O6 | 9.20 | 134.12 | 128.60 |
| 1 | X | 580 | A | P-O3'-C3' | 9.16 | 130.70 | 119.70 |
| 1 | X | 1345 | G | C1'-O4'-C4' | -9.16 | 102.57 | 109.90 |
| 1 | X | 1601 | U | P-O3'-C3' | 9.16 | 130.69 | 119.70 |
| 1 | X | 1674 | C | O4'-C1'-N1 | 9.14 | 115.51 | 108.20 |
| 1 | X | 68 | C | O4'-C1'-N1 | 9.13 | 115.50 | 108.20 |
| 1 | X | 563 | U | O4'-C1'-N1 | 9.12 | 115.49 | 108.20 |
| 1 | X | 686 | C | O4'-C1'-N1 | 9.11 | 115.49 | 108.20 |
| 1 | X | 2589 | C | P-O3'-C3' | 9.09 | 130.61 | 119.70 |
| 1 | X | 1790 | G | O4'-C1'-N9 | 9.07 | 115.45 | 108.20 |
| 1 | X | 175 | C | P-O3'-C3' | 9.05 | 130.56 | 119.70 |
| 1 | X | 2018 | G | N3-C4-C5 | 9.04 | 133.12 | 128.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | X | 2481 | G | P-O3'-C3' | 9.02 | 130.52 | 119.70 |
| 1 | X | 632 | A | O4'-C1'-N9 | 9.01 | 115.41 | 108.20 |
| 1 | X | 1770 | U | C1'-O4'-C4' | -9.00 | 102.70 | 109.90 |
| 1 | X | 731 | A | P-O3'-C3' | 8.98 | 130.48 | 119.70 |
| 1 | X | 1975 | G | P-O3'-C3' | 8.98 | 130.47 | 119.70 |
| 1 | X | 957 | G | P-O3'-C3' | 8.96 | 130.45 | 119.70 |
| 1 | X | 2703 | C | O4'-C1'-N1 | 8.94 | 115.36 | 108.20 |
| 1 | X | 1233 | A | P-O3'-C3' | 8.94 | 130.42 | 119.70 |
| 1 | X | 346 | C | O4'-C1'-N1 | 8.93 | 115.35 | 108.20 |
| 1 | X | 2229 | G | P-O3'-C3' | 8.92 | 130.40 | 119.70 |
| 1 | X | 2491 | C | O5'-P-OP2 | -8.91 | 97.68 | 105.70 |
| 1 | X | 554 | U | P-O3'-C3' | 8.88 | 130.36 | 119.70 |
| 1 | X | 841 | G | N9-C1'-C2' | 8.88 | 125.55 | 114.00 |
| 1 | X | 522 | G | O4'-C1'-N9 | 8.87 | 115.30 | 108.20 |
| 1 | X | 579 | G | C4-C5-N7 | -8.85 | 107.26 | 110.80 |
| 1 | X | 2324 | G | P-O3'-C3' | 8.81 | 130.28 | 119.70 |
| 1 | X | 1283 | C | P-O3'-C3' | 8.80 | 130.26 | 119.70 |
| 1 | X | 714 | G | O4'-C4'-C3' | -8.78 | 95.22 | 104.00 |
| 1 | X | 2530 | C | O5'-P-OP2 | -8.78 | 97.80 | 105.70 |
| 1 | X | 333 | A | P-O3'-C3' | 8.76 | 130.21 | 119.70 |
| 1 | X | 1474 | A | P-O3'-C3' | 8.74 | 130.19 | 119.70 |
| 1 | X | 774 | A | C5-C6-N6 | -8.73 | 116.71 | 123.70 |
| 1 | X | 387 | A | P-O3'-C3' | 8.73 | 130.17 | 119.70 |
| 1 | X | 939 | C | P-O3'-C3' | 8.69 | 130.13 | 119.70 |
| 1 | X | 2493 | U | O4'-C1'-N1 | 8.67 | 115.14 | 108.20 |
| 1 | X | 656 | U | O4'-C1'-N1 | 8.66 | 115.13 | 108.20 |
| 1 | X | 2044 | G | O4'-C1'-C2' | -8.66 | 97.14 | 105.80 |
| 1 | X | 2487 | G | O4'-C1'-N9 | 8.64 | 115.11 | 108.20 |
| 1 | X | 689 | A | C5-N7-C8 | -8.63 | 99.58 | 103.90 |
| 1 | X | 172 | A | P-O3'-C3' | 8.62 | 130.04 | 119.70 |
| 1 | X | 2633 | A | P-O3'-C3' | 8.61 | 130.03 | 119.70 |
| 1 | X | 2808 | U | C1'-O4'-C4' | -8.55 | 103.06 | 109.90 |
| 1 | X | 2554 | C | N1-C2-O2 | 8.55 | 124.03 | 118.90 |
| 1 | X | 540 | G | O4'-C1'-N9 | 8.54 | 115.03 | 108.20 |
| 1 | X | 841 | G | C8-N9-C4 | -8.52 | 102.99 | 106.40 |
| 1 | X | 2671 | C | O4'-C1'-N1 | 8.52 | 115.02 | 108.20 |
| 1 | X | 346 | C | C6-N1-C2 | -8.51 | 116.89 | 120.30 |
| 1 | X | 1524 | C | P-O3'-C3' | 8.49 | 129.89 | 119.70 |
| 1 | X | 2018 | G | N9-C1'-C2' | 8.49 | 125.04 | 114.00 |
| 1 | X | 976 | C | O4'-C1'-N1 | 8.49 | 114.99 | 108.20 |
| 1 | X | 1359 | G | C8-N9-C4 | -8.47 | 103.01 | 106.40 |
| 1 | X | 574 | C | O4'-C1'-N1 | 8.46 | 114.97 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | X | 1409 | U | C1'-O4'-C4' | -8.45 | 103.14 | 109.90 |
| 1 | X | 742 | G | P-O3'-C3' | 8.44 | 129.83 | 119.70 |
| 2 | Y | 17 | A | O4'-C1'-N9 | 8.44 | 114.95 | 108.20 |
| 1 | X | 2404 | A | P-O3'-C3' | 8.44 | 129.83 | 119.70 |
| 1 | X | 2477 | C | O4'-C1'-N1 | 8.44 | 114.95 | 108.20 |
| 1 | X | 699 | G | N3-C4-N9 | -8.43 | 120.94 | 126.00 |
| 1 | X | 636 | G | C8-N9-C4 | -8.43 | 103.03 | 106.40 |
| 1 | X | 2479 | U | P-O3'-C3' | 8.42 | 129.81 | 119.70 |
| 1 | X | 2691 | C | C1'-O4'-C4' | -8.39 | 103.19 | 109.90 |
| 1 | X | 804 | C | O4'-C1'-N1 | 8.38 | 114.90 | 108.20 |
| 1 | X | 2265 | A | P-O3'-C3' | 8.37 | 129.75 | 119.70 |
| 1 | X | 2847 | G | C8-N9-C4 | -8.35 | 103.06 | 106.40 |
| 1 | X | 394 | U | O4'-C1'-N1 | 8.34 | 114.88 | 108.20 |
| 1 | X | 2456 | U | O4'-C1'-N1 | 8.34 | 114.87 | 108.20 |
| 1 | X | 1006 | C | P-O3'-C3' | 8.31 | 129.67 | 119.70 |
| 1 | X | 2672 | U | O4'-C1'-N1 | 8.30 | 114.84 | 108.20 |
| 1 | X | 2812 | A | O4'-C1'-N9 | 8.30 | 114.84 | 108.20 |
| 1 | X | 1200 | G | O4'-C1'-N9 | 8.28 | 114.83 | 108.20 |
| 1 | X | 1656 | U | P-O3'-C3' | 8.28 | 129.63 | 119.70 |
| 1 | X | 838 | A | OP1-P-O3' | 8.26 | 123.37 | 105.20 |
| 1 | X | 1286 | U | O4'-C1'-N1 | 8.24 | 114.80 | 108.20 |
| 1 | X | 2706 | U | O4'-C1'-N1 | 8.24 | 114.79 | 108.20 |
| 1 | X | 2854 | G | N9-C1'-C2' | 8.24 | 124.72 | 114.00 |
| 1 | X | 801 | A | P-O3'-C3' | 8.23 | 129.57 | 119.70 |
| 1 | X | 1468 | A | P-O3'-C3' | 8.21 | 129.55 | 119.70 |
| 1 | X | 2744 | A | P-O3'-C3' | 8.21 | 129.55 | 119.70 |
| 1 | X | 2660 | C | O4'-C1'-N1 | 8.20 | 114.76 | 108.20 |
| 1 | X | 184 | A | O4'-C1'-N9 | 8.20 | 114.76 | 108.20 |
| 1 | X | 2854 | G | P-O3'-C3' | 8.20 | 129.53 | 119.70 |
| 1 | X | 2853 | U | O4'-C1'-N1 | 8.17 | 114.74 | 108.20 |
| 1 | X | 490 | A | P-O3'-C3' | 8.16 | 129.50 | 119.70 |
| 1 | X | 2667 | C | P-O3'-C3' | 8.16 | 129.50 | 119.70 |
| 1 | X | 814 | G | O4'-C1'-N9 | -8.14 | 101.68 | 108.20 |
| 1 | X | 1953 | A | P-O5'-C5' | -8.14 | 107.87 | 120.90 |
| 1 | X | 332 | C | O4'-C1'-N1 | 8.14 | 114.71 | 108.20 |
| 1 | X | 953 | G | O4'-C1'-N9 | 8.13 | 114.71 | 108.20 |
| 1 | X | 483 | A | P-O3'-C3' | -8.13 | 109.95 | 119.70 |
| 1 | X | 308 | C | O4'-C1'-N1 | 8.12 | 114.70 | 108.20 |
| 1 | X | 1468 | A | C3'-C2'-C1' | -8.12 | 95.01 | 101.50 |
| 1 | X | 1278 | A | C1'-O4'-C4' | -8.11 | 103.41 | 109.90 |
| 1 | X | 1333 | G | C8-N9-C4 | -8.11 | 103.16 | 106.40 |
| 1 | X | 2480 | C | O4'-C1'-N1 | 8.10 | 114.68 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | X | 1310 | C | O4'-C1'-N1 | 8.09 | 114.67 | 108.20 |
| 1 | X | 1631 | C | C5'-C4'-C3' | 8.09 | 128.94 | 116.00 |
| 1 | X | 1459 | U | P-O3'-C3' | 8.08 | 129.39 | 119.70 |
| 1 | X | 1984 | A | P-O5'-C5' | -8.08 | 107.97 | 120.90 |
| 1 | X | 1122 | A | O4'-C1'-N9 | 8.08 | 114.66 | 108.20 |
| 1 | X | 1250 | A | O4'-C1'-N9 | -8.07 | 101.74 | 108.20 |
| 1 | X | 83 | A | P-O3'-C3' | 8.07 | 129.38 | 119.70 |
| 1 | X | 1199 | U | O4'-C1'-N1 | 8.07 | 114.65 | 108.20 |
| 1 | X | 1313 | U | O4'-C1'-N1 | 8.06 | 114.65 | 108.20 |
| 1 | X | 2044 | G | O4'-C1'-N9 | -8.06 | 101.75 | 108.20 |
| 1 | X | 656 | U | P-O3'-C3' | 8.05 | 129.37 | 119.70 |
| 1 | X | 2051 | U | O4'-C1'-N1 | 8.05 | 114.64 | 108.20 |
| 1 | X | 2032 | G | P-O3'-C3' | -8.04 | 110.05 | 119.70 |
| 1 | X | 1574 | A | C5'-C4'-O4' | 8.03 | 118.74 | 109.10 |
| 1 | X | 1674 | C | C5'-C4'-O4' | -8.03 | 99.47 | 109.10 |
| 1 | X | 63 | A | C5'-C4'-C3' | -8.01 | 103.18 | 116.00 |
| 1 | X | 843 | G | P-O3'-C3' | 8.00 | 129.30 | 119.70 |
| 1 | X | 1278 | A | C3'-C2'-C1' | -8.00 | 95.10 | 101.50 |
| 1 | X | 990 | A | O4'-C4'-C3' | -8.00 | 96.00 | 104.00 |
| 1 | X | 2477 | C | C5'-C4'-O4' | -8.00 | 99.50 | 109.10 |
| 1 | X | 699 | G | N7-C8-N9 | 7.99 | 117.10 | 113.10 |
| 1 | X | 1441 | A | P-O3'-C3' | 7.99 | 129.29 | 119.70 |
| 1 | X | 2323 | U | N1-C1'-C2' | 7.98 | 124.38 | 114.00 |
| 1 | X | 514 | G | O4'-C1'-N9 | -7.98 | 101.81 | 108.20 |
| 1 | X | 1938 | U | C4'-C3'-C2' | 7.97 | 110.57 | 102.60 |
| 1 | X | 2481 | G | O5'-P-OP1 | -7.97 | 98.53 | 105.70 |
| 1 | X | 480 | G | C5-C6-O6 | -7.96 | 123.83 | 128.60 |
| 1 | X | 1358 | C | O4'-C1'-N1 | 7.95 | 114.56 | 108.20 |
| 1 | X | 1526 | U | O4'-C1'-N1 | 7.95 | 114.56 | 108.20 |
| 1 | X | 957 | G | N1-C6-O6 | -7.94 | 115.14 | 119.90 |
| 1 | X | 1250 | A | P-O3'-C3' | 7.94 | 129.23 | 119.70 |
| 1 | X | 2756 | A | P-O3'-C3' | 7.94 | 129.22 | 119.70 |
| 1 | X | 1338 | G | P-O3'-C3' | 7.93 | 129.22 | 119.70 |
| 1 | X | 2237 | C | P-O3'-C3' | 7.92 | 129.21 | 119.70 |
| 1 | X | 343 | A | C8-N9-C4 | -7.92 | 102.63 | 105.80 |
| 1 | X | 1467 | U | N1-C2-O2 | 7.92 | 128.35 | 122.80 |
| 1 | X | 2447 | G | P-O3'-C3' | 7.92 | 129.21 | 119.70 |
| 1 | X | 2487 | G | C8-N9-C4 | -7.91 | 103.23 | 106.40 |
| 2 | Y | 26 | G | P-O3'-C3' | 7.91 | 129.19 | 119.70 |
| 1 | X | 1792 | C | P-O3'-C3' | 7.90 | 129.18 | 119.70 |
| 1 | X | 169 | C | N1-C2-O2 | 7.90 | 123.64 | 118.90 |
| 1 | X | 1684 | G | P-O3'-C3' | 7.90 | 129.18 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | X | 774 | A | C4-C5-C6 | 7.89 | 120.95 | 117.00 |
| 1 | X | 2018 | G | N3-C4-N9 | -7.89 | 121.27 | 126.00 |
| 1 | X | 1072 | U | P-O3'-C3' | 7.88 | 129.16 | 119.70 |
| 1 | X | 689 | A | N7-C8-N9 | 7.88 | 117.74 | 113.80 |
| 1 | X | 1980 | A | C4'-C3'-C2' | -7.87 | 94.73 | 102.60 |
| 1 | X | 2013 | A | O4'-C1'-N9 | -7.87 | 101.90 | 108.20 |
| 1 | X | 169 | C | O4'-C1'-N1 | 7.87 | 114.49 | 108.20 |
| 1 | X | 2408 | G | N3-C4-C5 | -7.87 | 124.67 | 128.60 |
| 1 | X | 796 | A | C5-N7-C8 | -7.86 | 99.97 | 103.90 |
| 1 | X | 1291 | G | O4'-C4'-C3' | -7.86 | 96.14 | 104.00 |
| 1 | X | 1607 | A | P-O3'-C3' | 7.86 | 129.13 | 119.70 |
| 2 | Y | 92 | G | O4'-C4'-C3' | -7.86 | 96.14 | 104.00 |
| 1 | X | 2554 | C | O4'-C1'-N1 | 7.86 | 114.48 | 108.20 |
| 1 | X | 975 | C | O4'-C1'-N1 | 7.85 | 114.48 | 108.20 |
| 1 | X | 2500 | C | O4'-C1'-N1 | 7.83 | 114.47 | 108.20 |
| 1 | X | 2692 | A | P-O3'-C3' | 7.83 | 129.10 | 119.70 |
| 19 | Q | 60 | GLY | C-N-CA | 7.83 | 141.28 | 121.70 |
| 1 | X | 825 | C | P-O3'-C3' | -7.83 | 110.30 | 119.70 |
| 1 | X | 2481 | G | P-O5'-C5' | 7.82 | 133.41 | 120.90 |
| 1 | X | 2824 | C | C2'-C3'-O3' | 7.80 | 126.67 | 109.50 |
| 1 | X | 1333 | G | C4-N9-C1' | -7.79 | 116.37 | 126.50 |
| 1 | X | 1631 | C | C3'-C2'-C1' | -7.79 | 95.27 | 101.50 |
| 1 | X | 1680 | U | C2'-C3'-O3' | 7.79 | 126.63 | 109.50 |
| 1 | X | 2019 | C | O5'-P-OP2 | -7.78 | 98.70 | 105.70 |
| 1 | X | 1509 | A | O4'-C1'-N9 | 7.78 | 114.42 | 108.20 |
| 1 | X | 1313 | U | C1'-O4'-C4' | -7.77 | 103.68 | 109.90 |
| 1 | X | 1665 | C | O5'-P-OP2 | -7.77 | 98.70 | 105.70 |
| 1 | X | 1792 | C | N1-C1'-C2' | 7.77 | 124.10 | 114.00 |
| 1 | X | 2667 | C | N1-C2-O2 | 7.76 | 123.56 | 118.90 |
| 1 | X | 2196 | U | P-O3'-C3' | 7.76 | 129.01 | 119.70 |
| 2 | Y | 30 | C | O4'-C1'-N1 | 7.76 | 114.41 | 108.20 |
| 1 | X | 1458 | A | P-O3'-C3' | 7.75 | 129.01 | 119.70 |
| 1 | X | 203 | G | O4'-C1'-N9 | 7.75 | 114.40 | 108.20 |
| 1 | X | 1559 | G | P-O3'-C3' | 7.74 | 128.98 | 119.70 |
| 1 | X | 2525 | U | O4'-C1'-N1 | 7.72 | 114.37 | 108.20 |
| 1 | X | 540 | G | C8-N9-C4 | -7.71 | 103.31 | 106.40 |
| 1 | X | 2859 | U | O4'-C1'-N1 | 7.71 | 114.37 | 108.20 |
| 1 | X | 1664 | G | O5'-P-OP2 | 7.70 | 119.94 | 110.70 |
| 1 | X | 1142 | G | N3-C4-C5 | -7.70 | 124.75 | 128.60 |
| 1 | X | 1142 | G | N3-C4-N9 | 7.70 | 130.62 | 126.00 |
| 1 | X | 738 | G | C8-N9-C4 | -7.69 | 103.32 | 106.40 |
| 1 | X | 1223 | G | P-O3'-C3' | 7.69 | 128.92 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | X | 1843 | U | O4'-C1'-N1 | 7.69 | 114.35 | 108.20 |
| 1 | X | 617 | U | N3-C2-O2 | -7.69 | 116.82 | 122.20 |
| 1 | X | 518 | A | N9-C1'-C2' | 7.68 | 123.98 | 114.00 |
| 1 | X | 864 | C | O4'-C1'-N1 | 7.67 | 114.34 | 108.20 |
| 1 | X | 1509 | A | C1'-O4'-C4' | -7.67 | 103.77 | 109.90 |
| 1 | X | 564 | U | O4'-C1'-N1 | 7.67 | 114.33 | 108.20 |
| 1 | X | 1795 | C | O4'-C1'-N1 | 7.66 | 114.33 | 108.20 |
| 1 | X | 972 | C | C1'-O4'-C4' | -7.66 | 103.77 | 109.90 |
| 1 | X | 2867 | G | C5-N7-C8 | -7.66 | 100.47 | 104.30 |
| 1 | X | 1439 | G | P-O3'-C3' | 7.65 | 128.88 | 119.70 |
| 1 | X | 1981 | A | N1-C6-N6 | 7.64 | 123.19 | 118.60 |
| 1 | X | 2778 | U | P-O3'-C3' | 7.64 | 128.87 | 119.70 |
| 1 | X | 1770 | U | O4'-C1'-N1 | 7.64 | 114.31 | 108.20 |
| 1 | X | 176 | A | N9-C1'-C2' | 7.62 | 123.91 | 114.00 |
| 1 | X | 223 | C | O4'-C1'-N1 | 7.62 | 114.30 | 108.20 |
| 1 | X | 516 | G | O4'-C1'-N9 | 7.62 | 114.30 | 108.20 |
| 2 | Y | 37 | C | O4'-C1'-N1 | 7.62 | 114.30 | 108.20 |
| 1 | X | 636 | G | N7-C8-N9 | 7.62 | 116.91 | 113.10 |
| 1 | X | 74 | G | O4'-C4'-C3' | -7.61 | 96.39 | 104.00 |
| 1 | X | 2018 | G | C5-N7-C8 | -7.61 | 100.49 | 104.30 |
| 1 | X | 809 | C | O4'-C1'-N1 | 7.61 | 114.29 | 108.20 |
| 1 | X | 577 | U | C4'-C3'-C2' | -7.58 | 95.02 | 102.60 |
| 1 | X | 1006 | C | P-O5'-C5' | 7.58 | 133.03 | 120.90 |
| 1 | X | 12 | U | N3-C2-O2 | -7.57 | 116.90 | 122.20 |
| 1 | X | 751 | G | O4'-C4'-C3' | -7.57 | 96.43 | 104.00 |
| 1 | X | 672 | C | O4'-C4'-C3' | -7.57 | 96.43 | 104.00 |
| 1 | X | 1791 | C | O4'-C1'-N1 | 7.57 | 114.25 | 108.20 |
| 1 | X | 168 | A | O4'-C1'-N9 | 7.56 | 114.25 | 108.20 |
| 1 | X | 774 | A | N9-C4-C5 | -7.55 | 102.78 | 105.80 |
| 1 | X | 2439 | U | O4'-C1'-N1 | 7.55 | 114.24 | 108.20 |
| 1 | X | 2759 | U | P-O3'-C3' | 7.54 | 128.75 | 119.70 |
| 1 | X | 661 | C | N1-C2-O2 | 7.54 | 123.43 | 118.90 |
| 1 | X | 699 | G | C4-C5-N7 | 7.54 | 113.82 | 110.80 |
| 1 | X | 542 | A | C5-N7-C8 | -7.54 | 100.13 | 103.90 |
| 1 | X | 1333 | G | C2-N3-C4 | -7.53 | 108.14 | 111.90 |
| 1 | X | 1467 | U | N1-C1'-C2' | 7.53 | 123.79 | 114.00 |
| 1 | X | 1251 | G | O4'-C1'-N9 | 7.52 | 114.21 | 108.20 |
| 1 | X | 1184 | G | P-O3'-C3' | 7.51 | 128.72 | 119.70 |
| 1 | X | 661 | C | O4'-C1'-N1 | 7.51 | 114.21 | 108.20 |
| 1 | X | 685 | U | O4'-C1'-N1 | 7.51 | 114.21 | 108.20 |
| 1 | X | 847 | C | O4'-C1'-N1 | 7.51 | 114.21 | 108.20 |
| 1 | X | 1467 | U | C4-C5-C6 | -7.49 | 115.20 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | X | 1663 | C | N1-C2-O2 | 7.49 | 123.39 | 118.90 |
| 1 | X | 1631 | C | C2'-C3'-O3' | 7.49 | 125.97 | 109.50 |
| 1 | X | 2697 | G | C5-C6-O6 | -7.49 | 124.11 | 128.60 |
| 1 | X | 343 | A | P-O3'-C3' | 7.47 | 128.67 | 119.70 |
| 1 | X | 334 | G | O4'-C1'-N9 | 7.47 | 114.17 | 108.20 |
| 11 | I | 38 | LYS | C-N-CA | 7.46 | 140.36 | 121.70 |
| 1 | X | 192 | G | P-O3'-C3' | 7.45 | 128.64 | 119.70 |
| 1 | X | 2492 | G | O4'-C1'-N9 | 7.45 | 114.16 | 108.20 |
| 1 | X | 661 | C | N3-C2-O2 | -7.45 | 116.69 | 121.90 |
| 1 | X | 1031 | C | P-O3'-C3' | 7.44 | 128.63 | 119.70 |
| 1 | X | 1289 | A | P-O5'-C5' | 7.44 | 132.81 | 120.90 |
| 2 | Y | 11 | G | O4'-C1'-N9 | 7.44 | 114.15 | 108.20 |
| 1 | X | 2867 | G | C4-C5-N7 | 7.44 | 113.78 | 110.80 |
| 1 | X | 818 | G | O4'-C1'-C2' | -7.44 | 98.36 | 105.80 |
| 1 | X | 1150 | C | P-O3'-C3' | 7.44 | 128.63 | 119.70 |
| 1 | X | 2274 | C | O4'-C1'-N1 | 7.43 | 114.15 | 108.20 |
| 1 | X | 540 | G | P-O3'-C3' | 7.41 | 128.59 | 119.70 |
| 1 | X | 2330 | G | P-O3'-C3' | 7.41 | 128.59 | 119.70 |
| 1 | X | 2668 | U | N3-C2-O2 | -7.40 | 117.02 | 122.20 |
| 1 | X | 725 | C | O4'-C1'-N1 | 7.40 | 114.12 | 108.20 |
| 1 | X | 1071 | U | P-O3'-C3' | 7.40 | 128.58 | 119.70 |
| 1 | X | 19 | C | O4'-C1'-N1 | 7.40 | 114.12 | 108.20 |
| 1 | X | 579 | G | C5-C6-O6 | 7.40 | 133.04 | 128.60 |
| 1 | X | 577 | U | N3-C4-C5 | -7.39 | 110.16 | 114.60 |
| 1 | X | 841 | G | N7-C8-N9 | 7.39 | 116.80 | 113.10 |
| 1 | X | 126 | C | O4'-C1'-N1 | 7.39 | 114.11 | 108.20 |
| 1 | X | 2347 | C | O4'-C1'-N1 | 7.38 | 114.10 | 108.20 |
| 1 | X | 1830 | C | P-O3'-C3' | 7.37 | 128.55 | 119.70 |
| 1 | X | 199 | A | P-O3'-C3' | 7.36 | 128.54 | 119.70 |
| 1 | X | 921 | A | P-O3'-C3' | 7.36 | 128.53 | 119.70 |
| 1 | X | 1038 | U | O4'-C1'-N1 | 7.35 | 114.08 | 108.20 |
| 1 | X | 1302 | C | O4'-C1'-N1 | 7.35 | 114.08 | 108.20 |
| 1 | X | 2299 | A | O4'-C1'-N9 | 7.35 | 114.08 | 108.20 |
| 1 | X | 2190 | A | P-O3'-C3' | 7.34 | 128.51 | 119.70 |
| 1 | X | 2573 | C | O4'-C1'-N1 | 7.34 | 114.08 | 108.20 |
| 1 | X | 472 | C | O4'-C1'-N1 | 7.34 | 114.07 | 108.20 |
| 1 | X | 788 | G | C1'-O4'-C4' | -7.34 | 104.03 | 109.90 |
| 1 | X | 1496 | G | C3'-C2'-C1' | -7.34 | 95.63 | 101.50 |
| 2 | Y | 75 | A | P-O3'-C3' | 7.34 | 128.51 | 119.70 |
| 1 | X | 1137 | A | P-O3'-C3' | 7.33 | 128.50 | 119.70 |
| 1 | X | 2876 | C | O4'-C1'-N1 | 7.33 | 114.06 | 108.20 |
| 1 | X | 1991 | C | N3-C4-C5 | 7.32 | 124.83 | 121.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | X | 1976 | U | O4'-C1'-N1 | 7.32 | 114.06 | 108.20 |
| 1 | X | 2541 | U | O4'-C1'-N1 | 7.32 | 114.05 | 108.20 |
| 1 | X | 2841 | U | O4'-C1'-N1 | 7.31 | 114.05 | 108.20 |
| 1 | X | 1804 | U | O4'-C1'-N1 | 7.31 | 114.05 | 108.20 |
| 1 | X | 541 | C | P-O3'-C3' | 7.30 | 128.47 | 119.70 |
| 1 | X | 2615 | U | O4'-C1'-N1 | 7.30 | 114.04 | 108.20 |
| 1 | X | 2814 | G | O4'-C1'-N9 | 7.30 | 114.04 | 108.20 |
| 1 | X | 2824 | C | P-O3'-C3' | 7.30 | 128.46 | 119.70 |
| 1 | X | 1627 | C | O4'-C1'-N1 | 7.30 | 114.04 | 108.20 |
| 1 | X | 2408 | G | C8-N9-C4 | -7.30 | 103.48 | 106.40 |
| 1 | X | 2697 | G | C2-N3-C4 | 7.29 | 115.55 | 111.90 |
| 1 | X | 331 | U | O4'-C1'-N1 | 7.29 | 114.03 | 108.20 |
| 1 | X | 559 | C | C5'-C4'-O4' | 7.28 | 117.84 | 109.10 |
| 1 | X | 2222 | U | O4'-C1'-N1 | 7.28 | 114.03 | 108.20 |
| 1 | X | 802 | A | P-O3'-C3' | 7.28 | 128.43 | 119.70 |
| 1 | X | 2587 | G | C5-C6-O6 | -7.27 | 124.24 | 128.60 |
| 1 | X | 114 | C | O4'-C1'-N1 | 7.27 | 114.01 | 108.20 |
| 1 | X | 959 | C | P-O3'-C3' | -7.27 | 110.98 | 119.70 |
| 1 | X | 2529 | G | O5'-P-OP2 | -7.26 | 99.17 | 105.70 |
| 1 | X | 2860 | C | O4'-C1'-N1 | 7.26 | 114.01 | 108.20 |
| 1 | X | 1153 | A | P-O5'-C5' | 7.26 | 132.51 | 120.90 |
| 2 | Y | 32 | C | C6-N1-C2 | -7.26 | 117.40 | 120.30 |
| 1 | X | 2854 | G | N7-C8-N9 | 7.25 | 116.72 | 113.10 |
| 1 | X | 774 | A | C6-N1-C2 | 7.25 | 122.95 | 118.60 |
| 1 | X | 978 | U | O4'-C1'-N1 | 7.24 | 113.99 | 108.20 |
| 1 | X | 343 | A | P-O5'-C5' | 7.24 | 132.48 | 120.90 |
| 1 | X | 1489 | C | P-O3'-C3' | 7.23 | 128.38 | 119.70 |
| 1 | X | 1731 | C | O4'-C1'-N1 | 7.23 | 113.98 | 108.20 |
| 1 | X | 946 | U | O4'-C1'-N1 | 7.22 | 113.98 | 108.20 |
| 1 | X | 711 | C | O4'-C1'-N1 | 7.21 | 113.97 | 108.20 |
| 1 | X | 558 | G | N9-C1'-C2' | 7.21 | 123.37 | 114.00 |
| 1 | X | 2290 | A | P-O3'-C3' | 7.21 | 128.35 | 119.70 |
| 1 | X | 696 | U | O4'-C1'-N1 | 7.20 | 113.96 | 108.20 |
| 1 | X | 610 | G | C3'-C2'-C1' | -7.20 | 95.74 | 101.50 |
| 2 | Y | 52 | G | P-O5'-C5' | 7.20 | 132.42 | 120.90 |
| 1 | X | 870 | C | O4'-C1'-N1 | 7.20 | 113.96 | 108.20 |
| 1 | X | 358 | C | O4'-C1'-N1 | 7.20 | 113.96 | 108.20 |
| 1 | X | 2472 | U | O4'-C1'-N1 | 7.19 | 113.95 | 108.20 |
| 1 | X | 2015 | G | N9-C1'-C2' | 7.19 | 123.35 | 114.00 |
| 1 | X | 2343 | C | O4'-C1'-N1 | 7.19 | 113.95 | 108.20 |
| 1 | X | 2790 | C | P-O3'-C3' | -7.19 | 111.08 | 119.70 |
| 1 | X | 853 | C | C3'-C2'-C1' | -7.18 | 95.75 | 101.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | X | 1985 | G | O4'-C1'-N9 | 7.18 | 113.94 | 108.20 |
| 1 | X | 1505 | U | P-O3'-C3' | 7.18 | 128.31 | 119.70 |
| 1 | X | 691 | C | O4'-C1'-N1 | 7.18 | 113.94 | 108.20 |
| 1 | X | 2019 | C | O4'-C1'-N1 | 7.18 | 113.94 | 108.20 |
| 1 | X | 2691 | C | O3'-P-O5' | -7.17 | 90.37 | 104.00 |
| 1 | X | 1986 | G | O4'-C4'-C3' | -7.17 | 96.83 | 104.00 |
| 1 | X | 1202 | U | O4'-C1'-N1 | 7.17 | 113.93 | 108.20 |
| 1 | X | 542 | A | C2-N3-C4 | -7.17 | 107.02 | 110.60 |
| 2 | Y | 81 | C | O4'-C1'-N1 | 7.17 | 113.93 | 108.20 |
| 1 | X | 117 | A | C1'-O4'-C4' | -7.16 | 104.17 | 109.90 |
| 1 | X | 1800 | A | P-O3'-C3' | 7.16 | 128.29 | 119.70 |
| 1 | X | 2587 | G | O4'-C1'-N9 | 7.15 | 113.92 | 108.20 |
| 1 | X | 751 | G | C2'-C3'-O3' | 7.14 | 125.22 | 109.50 |
| 1 | X | 617 | U | O4'-C1'-N1 | 7.14 | 113.91 | 108.20 |
| 1 | X | 2032 | G | C5-C6-O6 | -7.14 | 124.32 | 128.60 |
| 1 | X | 2400 | G | P-O3'-C3' | 7.14 | 128.26 | 119.70 |
| 1 | X | 738 | G | N7-C8-N9 | 7.13 | 116.67 | 113.10 |
| 1 | X | 2735 | C | O4'-C1'-N1 | 7.13 | 113.91 | 108.20 |
| 1 | X | 1633 | C | O4'-C1'-N1 | 7.13 | 113.90 | 108.20 |
| 1 | X | 1339 | U | OP2-P-O3' | 7.12 | 120.88 | 105.20 |
| 1 | X | 796 | A | N7-C8-N9 | 7.12 | 117.36 | 113.80 |
| 1 | X | 955 | G | N9-C1'-C2' | 7.12 | 123.25 | 114.00 |
| 1 | X | 2062 | U | O4'-C1'-N1 | 7.12 | 113.89 | 108.20 |
| 1 | X | 2544 | A | O4'-C1'-N9 | 7.11 | 113.89 | 108.20 |
| 1 | X | 689 | A | O4'-C1'-N9 | 7.11 | 113.88 | 108.20 |
| 1 | X | 2270 | U | O4'-C1'-N1 | 7.11 | 113.88 | 108.20 |
| 1 | X | 2314 | A | O4'-C1'-N9 | 7.10 | 113.88 | 108.20 |
| 1 | X | 2414 | A | P-O3'-C3' | 7.10 | 128.22 | 119.70 |
| 1 | X | 645 | G | P-O3'-C3' | 7.10 | 128.22 | 119.70 |
| 1 | X | 2567 | G | C6-N1-C2 | -7.10 | 120.84 | 125.10 |
| 1 | X | 2258 | G | C4'-C3'-C2' | -7.09 | 95.51 | 102.60 |
| 1 | X | 312 | G | C1'-O4'-C4' | -7.09 | 104.23 | 109.90 |
| 1 | X | 1708 | C | O4'-C1'-N1 | 7.09 | 113.87 | 108.20 |
| 1 | X | 2429 | A | P-O3'-C3' | -7.09 | 111.19 | 119.70 |
| 1 | X | 2564 | U | N1-C1'-C2' | 7.09 | 123.22 | 114.00 |
| 1 | X | 1634 | A | C4'-C3'-C2' | 7.09 | 109.69 | 102.60 |
| 1 | X | 1656 | U | O4'-C1'-N1 | 7.08 | 113.87 | 108.20 |
| 1 | X | 1357 | U | C1'-O4'-C4' | -7.08 | 104.24 | 109.90 |
| 1 | X | 1161 | U | O4'-C1'-N1 | 7.08 | 113.86 | 108.20 |
| 1 | X | 1914 | U | O4'-C1'-N1 | 7.08 | 113.86 | 108.20 |
| 1 | X | 2705 | A | C4'-C3'-C2' | 7.08 | 109.67 | 102.60 |
| 1 | X | 2372 | A | O4'-C1'-N9 | 7.07 | 113.86 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | X | 1679 | U | O4'-C4'-C3' | -7.07 | 96.93 | 104.00 |
| 1 | X | 2050 | G | P-O3'-C3' | 7.07 | 128.19 | 119.70 |
| 1 | X | 1621 | C | O4'-C1'-N1 | 7.07 | 113.85 | 108.20 |
| 1 | X | 1278 | A | N1-C2-N3 | 7.06 | 132.83 | 129.30 |
| 1 | X | 1602 | G | P-O3'-C3' | 7.06 | 128.17 | 119.70 |
| 1 | X | 537 | C | P-O3'-C3' | 7.05 | 128.16 | 119.70 |
| 1 | X | 966 | A | P-O3'-C3' | -7.05 | 111.24 | 119.70 |
| 1 | X | 483 | A | C5'-C4'-O4' | 7.05 | 117.56 | 109.10 |
| 1 | X | 1412 | C | P-O3'-C3' | 7.05 | 128.16 | 119.70 |
| 1 | X | 1689 | U | O4'-C1'-N1 | 7.04 | 113.84 | 108.20 |
| 1 | X | 2478 | C | P-O3'-C3' | -7.04 | 111.25 | 119.70 |
| 1 | X | 2305 | C | P-O3'-C3' | 7.04 | 128.15 | 119.70 |
| 1 | X | 2018 | G | C1'-O4'-C4' | -7.04 | 104.27 | 109.90 |
| 1 | X | 1775 | A | C4'-C3'-C2' | 7.03 | 109.63 | 102.60 |
| 1 | X | 59 | G | P-O3'-C3' | 7.02 | 128.12 | 119.70 |
| 1 | X | 683 | A | N9-C1'-C2' | 7.02 | 123.13 | 114.00 |
| 1 | X | 814 | G | N9-C1'-C2' | 7.02 | 123.12 | 114.00 |
| 1 | X | 1467 | U | N1-C2-N3 | -7.01 | 110.69 | 114.90 |
| 1 | X | 393 | U | O4'-C1'-N1 | 7.01 | 113.81 | 108.20 |
| 1 | X | 1974 | U | O4'-C1'-N1 | 7.01 | 113.81 | 108.20 |
| 1 | X | 2620 | G | C4'-C3'-C2' | -7.00 | 95.60 | 102.60 |
| 1 | X | 558 | G | O4'-C1'-N9 | 7.00 | 113.80 | 108.20 |
| 1 | X | 652 | C | P-O5'-C5' | -7.00 | 109.70 | 120.90 |
| 1 | X | 1745 | C | O4'-C1'-N1 | 7.00 | 113.80 | 108.20 |
| 1 | X | 224 | G | C3'-C2'-C1' | 7.00 | 107.10 | 101.50 |
| 1 | X | 739 | G | O4'-C1'-N9 | 7.00 | 113.80 | 108.20 |
| 1 | X | 813 | A | P-O3'-C3' | 6.99 | 128.09 | 119.70 |
| 1 | X | 2311 | U | O4'-C1'-N1 | 6.99 | 113.79 | 108.20 |
| 1 | X | 587 | A | O4'-C1'-N9 | 6.99 | 113.79 | 108.20 |
| 1 | X | 480 | G | C4-C5-N7 | 6.98 | 113.59 | 110.80 |
| 1 | X | 2845 | C | O4'-C1'-N1 | 6.98 | 113.78 | 108.20 |
| 1 | X | 575 | U | O4'-C1'-N1 | 6.97 | 113.78 | 108.20 |
| 1 | X | 2267 | A | P-O3'-C3' | 6.97 | 128.06 | 119.70 |
| 1 | X | 1963 | G | C2'-C3'-O3' | 6.96 | 124.83 | 113.70 |
| 1 | X | 2478 | C | O4'-C1'-N1 | 6.95 | 113.76 | 108.20 |
| 1 | X | 2857 | C | O4'-C1'-N1 | 6.95 | 113.76 | 108.20 |
| 1 | X | 2478 | C | C6-N1-C2 | -6.95 | 117.52 | 120.30 |
| 1 | X | 698 | A | P-O3'-C3' | 6.94 | 128.03 | 119.70 |
| 1 | X | 1678 | G | O4'-C4'-C3' | -6.93 | 97.07 | 104.00 |
| 1 | X | 2291 | U | O4'-C1'-N1 | 6.93 | 113.74 | 108.20 |
| 1 | X | 2393 | G | O4'-C1'-N9 | 6.93 | 113.74 | 108.20 |
| 1 | X | 2820 | C | O4'-C1'-N1 | 6.92 | 113.74 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | X | 1172 | U | O4'-C1'-N1 | 6.92 | 113.74 | 108.20 |
| 1 | X | 2561 | G | O4'-C1'-N9 | 6.92 | 113.73 | 108.20 |
| 1 | X | 646 | C | O4'-C1'-N1 | 6.91 | 113.73 | 108.20 |
| 1 | X | 422 | C | O4'-C1'-N1 | 6.91 | 113.72 | 108.20 |
| 1 | X | 1668 | G | P-O3'-C3' | -6.90 | 111.42 | 119.70 |
| 1 | X | 2322 | U | O4'-C1'-N1 | 6.90 | 113.72 | 108.20 |
| 1 | X | 1489 | C | N1-C2-O2 | 6.89 | 123.04 | 118.90 |
| 1 | X | 1980 | A | C5'-C4'-O4' | 6.89 | 117.37 | 109.10 |
| 1 | X | 2366 | U | O4'-C1'-N1 | 6.89 | 113.71 | 108.20 |
| 1 | X | 859 | U | O4'-C1'-N1 | 6.88 | 113.71 | 108.20 |
| 1 | X | 1151 | U | O4'-C1'-N1 | 6.88 | 113.70 | 108.20 |
| 1 | X | 1250 | A | C5'-C4'-O4' | 6.88 | 117.36 | 109.10 |
| 2 | Y | 34 | C | O4'-C1'-N1 | 6.88 | 113.70 | 108.20 |
| 1 | X | 1655 | C | O4'-C1'-N1 | 6.87 | 113.70 | 108.20 |
| 1 | X | 2208 | U | O4'-C1'-N1 | 6.87 | 113.70 | 108.20 |
| 1 | X | 2622 | G | C5-C6-O6 | -6.86 | 124.48 | 128.60 |
| 1 | X | 305 | A | O4'-C1'-N9 | 6.85 | 113.68 | 108.20 |
| 1 | X | 526 | C | O4'-C1'-N1 | 6.85 | 113.68 | 108.20 |
| 1 | X | 2329 | C | O4'-C1'-N1 | 6.83 | 113.67 | 108.20 |
| 1 | X | 1663 | C | OP1-P-O3' | 6.83 | 120.23 | 105.20 |
| 1 | X | 2854 | G | O4'-C1'-N9 | 6.83 | 113.67 | 108.20 |
| 2 | Y | 123 | U | C2-N1-C1' | 6.83 | 125.89 | 117.70 |
| 1 | X | 968 | C | N1-C2-O2 | 6.83 | 123.00 | 118.90 |
| 1 | X | 1980 | A | O4'-C4'-C3' | -6.83 | 97.17 | 104.00 |
| 1 | X | 675 | C | O4'-C1'-N1 | 6.82 | 113.66 | 108.20 |
| 1 | X | 2605 | C | O4'-C1'-N1 | 6.82 | 113.66 | 108.20 |
| 1 | X | 761 | G | O5'-P-OP2 | -6.81 | 99.57 | 105.70 |
| 1 | X | 1279 | G | C3'-C2'-C1' | -6.81 | 96.05 | 101.50 |
| 1 | X | 1726 | C | O4'-C1'-N1 | 6.80 | 113.64 | 108.20 |
| 1 | X | 763 | A | P-O3'-C3' | 6.80 | 127.86 | 119.70 |
| 1 | X | 2080 | U | O4'-C1'-N1 | 6.80 | 113.64 | 108.20 |
| 1 | X | 1343 | C | O4'-C1'-N1 | 6.80 | 113.64 | 108.20 |
| 1 | X | 2808 | U | P-O5'-C5' | 6.79 | 131.77 | 120.90 |
| 1 | X | 542 | A | C3'-C2'-C1' | 6.79 | 106.93 | 101.50 |
| 1 | X | 1593 | C | O4'-C1'-N1 | 6.79 | 113.63 | 108.20 |
| 1 | X | 1770 | U | N3-C2-O2 | -6.79 | 117.45 | 122.20 |
| 1 | X | 2258 | G | O4'-C1'-N9 | 6.79 | 113.63 | 108.20 |
| 1 | X | 559 | C | N3-C2-O2 | -6.78 | 117.15 | 121.90 |
| 1 | X | 2303 | C | P-O3'-C3' | 6.78 | 127.83 | 119.70 |
| 1 | X | 2039 | G | C8-N9-C4 | -6.78 | 103.69 | 106.40 |
| 1 | X | 92 | U | O4'-C1'-N1 | 6.77 | 113.61 | 108.20 |
| 1 | X | 321 | A | P-O3'-C3' | 6.77 | 127.82 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | X | 2668 | U | N3-C4-O4 | -6.76 | 114.67 | 119.40 |
| 1 | X | 1882 | G | P-O3'-C3' | 6.76 | 127.81 | 119.70 |
| 1 | X | 689 | A | C4-C5-N7 | 6.75 | 114.08 | 110.70 |
| 19 | Q | 61 | LYS | N-CA-C | 6.75 | 129.23 | 111.00 |
| 1 | X | 1218 | C | O4'-C1'-N1 | 6.75 | 113.60 | 108.20 |
| 1 | X | 1820 | G | C4'-C3'-C2' | 6.75 | 109.35 | 102.60 |
| 1 | X | 2627 | G | C5-C6-O6 | -6.75 | 124.55 | 128.60 |
| 1 | X | 540 | G | N9-C4-C5 | 6.74 | 108.09 | 105.40 |
| 1 | X | 1067 | G | P-O3'-C3' | 6.74 | 127.78 | 119.70 |
| 1 | X | 117 | A | P-O3'-C3' | 6.73 | 127.78 | 119.70 |
| 1 | X | 2032 | G | O4'-C4'-C3' | -6.73 | 97.27 | 104.00 |
| 1 | X | 2771 | C | O4'-C1'-N1 | 6.73 | 113.58 | 108.20 |
| 1 | X | 2482 | A | O5'-P-OP1 | 6.73 | 118.77 | 110.70 |
| 1 | X | 322 | A | P-O3'-C3' | 6.73 | 127.77 | 119.70 |
| 1 | X | 1992 | G | C5'-C4'-O4' | -6.72 | 101.04 | 109.10 |
| 1 | X | 2560 | G | C5'-C4'-O4' | 6.71 | 117.16 | 109.10 |
| 1 | X | 2206 | C | O4'-C1'-N1 | 6.71 | 113.57 | 108.20 |
| 1 | X | 466 | A | P-O3'-C3' | 6.71 | 127.75 | 119.70 |
| 1 | X | 1001 | A | O4'-C1'-N9 | 6.71 | 113.57 | 108.20 |
| 1 | X | 1631 | C | O4'-C1'-N1 | 6.71 | 113.57 | 108.20 |
| 1 | X | 1289 | A | O4'-C4'-C3' | -6.71 | 97.29 | 104.00 |
| 1 | X | 1530 | U | O4'-C1'-N1 | 6.71 | 113.57 | 108.20 |
| 1 | X | 981 | C | O4'-C1'-N1 | 6.71 | 113.56 | 108.20 |
| 1 | X | 1679 | U | N3-C2-O2 | -6.71 | 117.51 | 122.20 |
| 1 | X | 2018 | G | O5'-P-OP1 | -6.71 | 99.67 | 105.70 |
| 1 | X | 1340 | C | O4'-C1'-N1 | 6.70 | 113.56 | 108.20 |
| 1 | X | 2047 | C | O4'-C1'-N1 | 6.70 | 113.56 | 108.20 |
| 1 | X | 2708 | U | N3-C2-O2 | -6.70 | 117.51 | 122.20 |
| 1 | X | 1250 | A | O5'-P-OP1 | 6.69 | 118.73 | 110.70 |
| 1 | X | 2476 | A | P-O3'-C3' | 6.69 | 127.73 | 119.70 |
| 1 | X | 2534 | U | C1'-O4'-C4' | -6.69 | 104.55 | 109.90 |
| 1 | X | 527 | C | N1-C2-O2 | 6.69 | 122.91 | 118.90 |
| 1 | X | 387 | A | C5'-C4'-O4' | 6.68 | 117.12 | 109.10 |
| 1 | X | 649 | G | O4'-C1'-N9 | 6.68 | 113.55 | 108.20 |
| 1 | X | 313 | U | O4'-C1'-N1 | 6.68 | 113.54 | 108.20 |
| 1 | X | 1032 | A | C3'-C2'-C1' | -6.68 | 96.16 | 101.50 |
| 1 | X | 1439 | G | C2'-C3'-O3' | 6.68 | 124.39 | 113.70 |
| 1 | X | 841 | G | O4'-C1'-N9 | 6.67 | 113.54 | 108.20 |
| 1 | X | 2634 | G | C1'-O4'-C4' | -6.67 | 104.56 | 109.90 |
| 1 | X | 456 | C | O4'-C1'-N1 | 6.67 | 113.54 | 108.20 |
| 1 | X | 811 | G | O4'-C1'-N9 | 6.67 | 113.54 | 108.20 |
| 1 | X | 796 | A | N1-C6-N6 | 6.67 | 122.60 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | X | 1404 | C | C1'-O4'-C4' | -6.67 | 104.56 | 109.90 |
| 1 | X | 1324 | G | O4'-C1'-N9 | 6.67 | 113.53 | 108.20 |
| 1 | X | 1562 | G | O4'-C1'-N9 | 6.67 | 113.53 | 108.20 |
| 1 | X | 1771 | A | P-O3'-C3' | 6.67 | 127.70 | 119.70 |
| 1 | X | 1762 | C | O4'-C1'-N1 | 6.66 | 113.53 | 108.20 |
| 1 | X | 1716 | G | C4'-C3'-C2' | 6.66 | 109.26 | 102.60 |
| 1 | X | 1319 | C | C6-N1-C2 | -6.66 | 117.64 | 120.30 |
| 1 | X | 13 | A | P-O3'-C3' | 6.66 | 127.69 | 119.70 |
| 1 | X | 31 | C | O4'-C1'-N1 | 6.66 | 113.52 | 108.20 |
| 1 | X | 2776 | U | P-O3'-C3' | 6.66 | 127.69 | 119.70 |
| 1 | X | 1469 | U | C5'-C4'-O4' | 6.65 | 117.08 | 109.10 |
| 1 | X | 789 | G | P-O3'-C3' | 6.65 | 127.68 | 119.70 |
| 1 | X | 2441 | U | O4'-C1'-N1 | 6.65 | 113.52 | 108.20 |
| 1 | X | 12 | U | N1-C2-O2 | 6.65 | 127.45 | 122.80 |
| 9 | G | 106 | TYR | N-CA-CB | 6.64 | 122.56 | 110.60 |
| 1 | X | 2437 | G | O4'-C1'-N9 | 6.64 | 113.51 | 108.20 |
| 1 | X | 2794 | G | P-O3'-C3' | 6.64 | 127.67 | 119.70 |
| 1 | X | 1339 | U | P-O3'-C3' | 6.64 | 127.67 | 119.70 |
| 1 | X | 1434 | U | C1'-O4'-C4' | -6.64 | 104.59 | 109.90 |
| 1 | X | 30 | G | C8-N9-C4 | -6.64 | 103.75 | 106.40 |
| 1 | X | 1470 | G | P-O5'-C5' | -6.63 | 110.29 | 120.90 |
| 1 | X | 2033 | C | P-O3'-C3' | 6.63 | 127.65 | 119.70 |
| 1 | X | 1712 | G | N3-C4-N9 | 6.62 | 129.97 | 126.00 |
| 2 | Y | 72 | C | O4'-C1'-N1 | 6.62 | 113.50 | 108.20 |
| 1 | X | 485 | G | P-O5'-C5' | 6.62 | 131.49 | 120.90 |
| 1 | X | 1792 | C | N1-C2-O2 | 6.62 | 122.87 | 118.90 |
| 1 | X | 2588 | U | O4'-C1'-N1 | 6.62 | 113.49 | 108.20 |
| 1 | X | 2409 | A | P-O3'-C3' | 6.61 | 127.64 | 119.70 |
| 1 | X | 1468 | A | N9-C1'-C2' | 6.61 | 122.59 | 114.00 |
| 1 | X | 1622 | G | P-O3'-C3' | 6.61 | 127.63 | 119.70 |
| 1 | X | 2539 | C | O4'-C1'-N1 | 6.61 | 113.49 | 108.20 |
| 1 | X | 1466 | C | O4'-C1'-N1 | 6.61 | 113.49 | 108.20 |
| 2 | Y | 9 | G | C3'-C2'-C1' | -6.61 | 96.21 | 101.50 |
| 1 | X | 700 | C | O4'-C1'-N1 | 6.61 | 113.48 | 108.20 |
| 1 | X | 100 | G | O4'-C1'-N9 | 6.60 | 113.48 | 108.20 |
| 1 | X | 1249 | G | O4'-C1'-N9 | 6.60 | 113.48 | 108.20 |
| 1 | X | 2315 | A | P-O5'-C5' | 6.60 | 131.47 | 120.90 |
| 1 | X | 788 | G | O4'-C1'-N9 | 6.60 | 113.48 | 108.20 |
| 1 | X | 955 | G | P-O5'-C5' | -6.60 | 110.34 | 120.90 |
| 1 | X | 2490 | U | O4'-C1'-N1 | 6.60 | 113.48 | 108.20 |
| 1 | X | 1805 | G | O4'-C1'-N9 | 6.59 | 113.47 | 108.20 |
| 1 | X | 2804 | G | C5-C6-O6 | -6.59 | 124.64 | 128.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | X | 1469 | U | N3-C2-O2 | -6.59 | 117.59 | 122.20 |
| 1 | X | 1711 | C | C1'-O4'-C4' | -6.59 | 104.63 | 109.90 |
| 1 | X | 2867 | G | N7-C8-N9 | 6.58 | 116.39 | 113.10 |
| 1 | X | 2338 | C | O4'-C1'-N1 | 6.58 | 113.46 | 108.20 |
| 1 | X | 2719 | U | P-O5'-C5' | 6.58 | 131.42 | 120.90 |
| 1 | X | 794 | A | O4'-C1'-N9 | -6.57 | 102.95 | 108.20 |
| 1 | X | 2669 | C | N3-C2-O2 | -6.57 | 117.30 | 121.90 |
| 1 | X | 2766 | U | O4'-C1'-N1 | 6.57 | 113.45 | 108.20 |
| 1 | X | 2846 | G | P-O3'-C3' | 6.57 | 127.58 | 119.70 |
| 1 | X | 467 | U | N3-C2-O2 | -6.56 | 117.61 | 122.20 |
| 1 | X | 540 | G | N9-C1'-C2' | 6.56 | 122.52 | 114.00 |
| 1 | X | 1446 | U | O4'-C1'-N1 | 6.55 | 113.44 | 108.20 |
| 1 | X | 1694 | A | O4'-C1'-N9 | 6.55 | 113.44 | 108.20 |
| 1 | X | 308 | C | P-O3'-C3' | -6.55 | 111.84 | 119.70 |
| 1 | X | 429 | C | O4'-C1'-N1 | 6.55 | 113.44 | 108.20 |
| 1 | X | 2081 | U | O4'-C1'-N1 | 6.55 | 113.44 | 108.20 |
| 1 | X | 1359 | G | N7-C8-N9 | 6.55 | 116.37 | 113.10 |
| 1 | X | 1690 | U | O4'-C1'-N1 | 6.55 | 113.44 | 108.20 |
| 1 | X | 399 | G | C4'-C3'-C2' | 6.54 | 109.14 | 102.60 |
| 1 | X | 440 | U | P-O3'-C3' | 6.54 | 127.55 | 119.70 |
| 1 | X | 1652 | G | O4'-C1'-N9 | -6.54 | 102.97 | 108.20 |
| 1 | X | 967 | G | P-O5'-C5' | 6.54 | 131.36 | 120.90 |
| 1 | X | 1647 | U | O4'-C1'-N1 | 6.54 | 113.43 | 108.20 |
| 1 | X | 2406 | C | O4'-C1'-N1 | 6.54 | 113.43 | 108.20 |
| 1 | X | 2481 | G | O3'-P-O5' | -6.54 | 91.58 | 104.00 |
| 1 | X | 322 | A | O4'-C1'-N9 | 6.54 | 113.43 | 108.20 |
| 1 | X | 2691 | C | O4'-C1'-C2' | -6.53 | 99.27 | 105.80 |
| 1 | X | 517 | A | P-O3'-C3' | 6.53 | 127.53 | 119.70 |
| 23 | U | 18 | VAL | C-N-CA | 6.53 | 138.02 | 121.70 |
| 1 | X | 1776 | A | P-O3'-C3' | 6.52 | 127.53 | 119.70 |
| 1 | X | 2669 | C | O4'-C1'-C2' | -6.52 | 99.28 | 105.80 |
| 1 | X | 513 | A | P-O3'-C3' | 6.52 | 127.52 | 119.70 |
| 1 | X | 784 | U | O4'-C1'-N1 | 6.52 | 113.42 | 108.20 |
| 1 | X | 2417 | U | N3-C2-O2 | -6.51 | 117.64 | 122.20 |
| 1 | X | 2561 | G | C5'-C4'-O4' | -6.51 | 101.28 | 109.10 |
| 1 | X | 2437 | G | N3-C4-C5 | -6.51 | 125.34 | 128.60 |
| 1 | X | 241 | C | O4'-C4'-C3' | -6.51 | 97.49 | 104.00 |
| 1 | X | 242 | A | C4'-C3'-C2' | -6.51 | 96.09 | 102.60 |
| 1 | X | 1439 | G | C3'-C2'-C1' | -6.51 | 96.29 | 101.50 |
| 1 | X | 859 | U | C5'-C4'-O4' | 6.51 | 116.91 | 109.10 |
| 1 | X | 1994 | U | O4'-C1'-N1 | 6.51 | 113.41 | 108.20 |
| 1 | X | 2384 | G | P-O3'-C3' | 6.50 | 127.50 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | X | 1749 | G | P-O3'-C3' | 6.50 | 127.50 | 119.70 |
| 1 | X | 320 | A | P-O3'-C3' | 6.49 | 127.49 | 119.70 |
| 1 | X | 424 | G | P-O3'-C3' | 6.49 | 127.48 | 119.70 |
| 1 | X | 631 | G | P-O3'-C3' | 6.49 | 127.49 | 119.70 |
| 1 | X | 1044 | U | P-O3'-C3' | 6.49 | 127.49 | 119.70 |
| 1 | X | 1912 | G | P-O3'-C3' | 6.49 | 127.48 | 119.70 |
| 1 | X | 543 | G | C3'-C2'-C1' | -6.49 | 96.31 | 101.50 |
| 2 | Y | 47 | A | N7-C8-N9 | 6.49 | 117.04 | 113.80 |
| 1 | X | 467 | U | N1-C2-O2 | 6.47 | 127.33 | 122.80 |
| 1 | X | 1170 | U | O4'-C1'-N1 | 6.47 | 113.37 | 108.20 |
| 1 | X | 2591 | C | C2-N3-C4 | 6.47 | 123.13 | 119.90 |
| 1 | X | 2488 | G | C5-C6-N1 | 6.46 | 114.73 | 111.50 |
| 1 | X | 312 | G | P-O3'-C3' | 6.46 | 127.45 | 119.70 |
| 1 | X | 2486 | C | N1-C2-O2 | 6.46 | 122.78 | 118.90 |
| 1 | X | 1670 | G | P-O3'-C3' | 6.46 | 127.45 | 119.70 |
| 1 | X | 2852 | G | O4'-C4'-C3' | -6.46 | 97.54 | 104.00 |
| 1 | X | 1925 | C | O4'-C1'-N1 | 6.46 | 113.36 | 108.20 |
| 1 | X | 2185 | U | O4'-C1'-N1 | 6.46 | 113.36 | 108.20 |
| 1 | X | 580 | A | P-O5'-C5' | -6.45 | 110.58 | 120.90 |
| 1 | X | 2556 | A | P-O3'-C3' | 6.45 | 127.44 | 119.70 |
| 1 | X | 453 | U | O4'-C1'-N1 | 6.45 | 113.36 | 108.20 |
| 1 | X | 2256 | G | C8-N9-C4 | -6.45 | 103.82 | 106.40 |
| 1 | X | 307 | C | O4'-C1'-N1 | 6.44 | 113.36 | 108.20 |
| 1 | X | 1200 | G | P-O5'-C5' | 6.44 | 131.21 | 120.90 |
| 1 | X | 2039 | G | C5-C6-O6 | -6.44 | 124.73 | 128.60 |
| 1 | X | 1758 | C | O4'-C1'-N1 | 6.43 | 113.35 | 108.20 |
| 1 | X | 1732 | U | O4'-C1'-N1 | 6.43 | 113.34 | 108.20 |
| 1 | X | 460 | U | P-O3'-C3' | 6.43 | 127.41 | 119.70 |
| 1 | X | 1685 | A | OP1-P-O3' | 6.43 | 119.34 | 105.20 |
| 1 | X | 469 | G | C1'-O4'-C4' | -6.42 | 104.76 | 109.90 |
| 1 | X | 2779 | C | P-O3'-C3' | 6.42 | 127.41 | 119.70 |
| 1 | X | 1667 | A | O4'-C1'-N9 | 6.42 | 113.34 | 108.20 |
| 1 | X | 608 | G | O4'-C4'-C3' | -6.42 | 97.58 | 104.00 |
| 1 | X | 1468 | A | C5-C6-N1 | 6.42 | 120.91 | 117.70 |
| 1 | X | 2659 | C | O4'-C1'-N1 | 6.42 | 113.34 | 108.20 |
| 1 | X | 661 | C | C4'-C3'-C2' | -6.42 | 96.18 | 102.60 |
| 1 | X | 925 | U | P-O3'-C3' | 6.41 | 127.39 | 119.70 |
| 1 | X | 2044 | G | N3-C4-N9 | 6.41 | 129.85 | 126.00 |
| 1 | X | 330 | C | O4'-C1'-N1 | 6.41 | 113.33 | 108.20 |
| 1 | X | 1922 | U | N3-C2-O2 | -6.41 | 117.71 | 122.20 |
| 1 | X | 1037 | U | C1'-O4'-C4' | -6.41 | 104.78 | 109.90 |
| 1 | X | 1031 | C | O4'-C1'-N1 | 6.41 | 113.33 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | X | 2667 | C | N3-C2-O2 | -6.41 | 117.42 | 121.90 |
| 1 | X | 2581 | A | P-O3'-C3' | 6.40 | 127.39 | 119.70 |
| 1 | X | 338 | G | O4'-C1'-N9 | 6.40 | 113.32 | 108.20 |
| 1 | X | 458 | G | P-O3'-C3' | 6.40 | 127.38 | 119.70 |
| 1 | X | 1669 | A | O4'-C4'-C3' | -6.39 | 97.61 | 104.00 |
| 1 | X | 308 | C | P-O5'-C5' | 6.38 | 131.11 | 120.90 |
| 1 | X | 595 | A | P-O3'-C3' | 6.38 | 127.36 | 119.70 |
| 1 | X | 2246 | A | N9-C1'-C2' | 6.38 | 122.30 | 114.00 |
| 2 | Y | 110 | U | N3-C2-O2 | -6.38 | 117.73 | 122.20 |
| 19 | Q | 62 | ARG | C-N-CA | 6.38 | 137.66 | 121.70 |
| 1 | X | 2527 | G | O4'-C1'-N9 | 6.38 | 113.30 | 108.20 |
| 1 | X | 2551 | A | O3'-P-O5' | -6.38 | 91.88 | 104.00 |
| 1 | X | 2691 | C | P-O3'-C3' | 6.38 | 127.35 | 119.70 |
| 1 | X | 1696 | C | O4'-C1'-N1 | 6.37 | 113.30 | 108.20 |
| 1 | X | 56 | C | O4'-C1'-N1 | 6.37 | 113.29 | 108.20 |
| 1 | X | 1467 | U | C4'-C3'-O3' | 6.37 | 125.73 | 113.00 |
| 1 | X | 2678 | C | O4'-C1'-N1 | 6.37 | 113.29 | 108.20 |
| 2 | Y | 6 | C | O4'-C1'-N1 | 6.37 | 113.29 | 108.20 |
| 1 | X | 1429 | A | C1'-O4'-C4' | -6.36 | 104.81 | 109.90 |
| 1 | X | 645 | G | O4'-C1'-N9 | 6.36 | 113.29 | 108.20 |
| 1 | X | 1339 | U | O4'-C1'-N1 | 6.36 | 113.29 | 108.20 |
| 2 | Y | 53 | G | N3-C4-C5 | -6.36 | 125.42 | 128.60 |
| 1 | X | 2774 | U | P-O3'-C3' | 6.36 | 127.33 | 119.70 |
| 1 | X | 1885 | C | N1-C2-O2 | 6.35 | 122.71 | 118.90 |
| 1 | X | 325 | U | O4'-C1'-N1 | 6.35 | 113.28 | 108.20 |
| 1 | X | 1679 | U | N3-C4-C5 | 6.35 | 118.41 | 114.60 |
| 1 | X | 990 | A | C3'-C2'-C1' | -6.35 | 96.42 | 101.50 |
| 1 | X | 2523 | G | O4'-C1'-N9 | 6.35 | 113.28 | 108.20 |
| 1 | X | 18 | U | O4'-C1'-N1 | 6.35 | 113.28 | 108.20 |
| 1 | X | 1979 | C | P-O3'-C3' | 6.34 | 127.31 | 119.70 |
| 1 | X | 618 | A | O4'-C1'-N9 | 6.34 | 113.27 | 108.20 |
| 2 | Y | 86 | A | C1'-O4'-C4' | -6.34 | 104.83 | 109.90 |
| 1 | X | 742 | G | C1'-O4'-C4' | -6.34 | 104.83 | 109.90 |
| 1 | X | 1882 | G | C3'-C2'-C1' | 6.34 | 106.57 | 101.50 |
| 1 | X | 1664 | G | O5'-P-OP1 | -6.34 | 100.00 | 105.70 |
| 1 | X | 689 | A | N1-C6-N6 | 6.34 | 122.40 | 118.60 |
| 1 | X | 593 | C | O4'-C1'-N1 | 6.33 | 113.26 | 108.20 |
| 1 | X | 632 | A | P-O3'-C3' | 6.32 | 127.29 | 119.70 |
| 1 | X | 2538 | C | O4'-C1'-N1 | 6.32 | 113.26 | 108.20 |
| 1 | X | 2735 | C | C6-N1-C2 | -6.32 | 117.77 | 120.30 |
| 10 | H | 26 | ASN | C-N-CA | 6.32 | 137.50 | 121.70 |
| 1 | X | 1673 | C | O4'-C1'-N1 | 6.31 | 113.25 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | X | 1017 | C | O4'-C1'-N1 | 6.31 | 113.25 | 108.20 |
| 1 | X | 1649 | A | C2-N3-C4 | 6.31 | 113.75 | 110.60 |
| 1 | X | 1664 | G | N9-C1'-C2' | 6.30 | 122.20 | 114.00 |
| 1 | X | 1716 | G | C2'-C3'-O3' | 6.30 | 123.79 | 113.70 |
| 1 | X | 2217 | G | C1'-O4'-C4' | -6.30 | 104.86 | 109.90 |
| 1 | X | 566 | U | O4'-C1'-N1 | 6.30 | 113.24 | 108.20 |
| 1 | X | 1023 | U | O4'-C1'-N1 | 6.30 | 113.24 | 108.20 |
| 1 | X | 1671 | A | OP1-P-OP2 | 6.30 | 129.05 | 119.60 |
| 1 | X | 2627 | G | N1-C6-O6 | 6.30 | 123.68 | 119.90 |
| 1 | X | 2359 | U | P-O3'-C3' | 6.30 | 127.26 | 119.70 |
| 1 | X | 682 | G | C5-C6-N1 | 6.29 | 114.65 | 111.50 |
| 1 | X | 884 | C | O4'-C1'-N1 | 6.29 | 113.23 | 108.20 |
| 1 | X | 542 | A | N7-C8-N9 | 6.29 | 116.94 | 113.80 |
| 1 | X | 1764 | A | N1-C6-N6 | 6.29 | 122.37 | 118.60 |
| 2 | Y | 4 | C | O4'-C1'-N1 | 6.29 | 113.23 | 108.20 |
| 1 | X | 2566 | A | P-O3'-C3' | 6.29 | 127.25 | 119.70 |
| 1 | X | 1749 | G | C1'-O4'-C4' | -6.29 | 104.87 | 109.90 |
| 1 | X | 98 | U | O4'-C1'-N1 | 6.28 | 113.22 | 108.20 |
| 1 | X | 467 | U | C2-N1-C1' | 6.28 | 125.24 | 117.70 |
| 1 | X | 2710 | C | N1-C2-O2 | 6.28 | 122.67 | 118.90 |
| 1 | X | 1748 | U | P-O3'-C3' | 6.28 | 127.23 | 119.70 |
| 1 | X | 2419 | C | O4'-C1'-N1 | 6.28 | 113.22 | 108.20 |
| 1 | X | 2485 | U | N1-C2-O2 | 6.28 | 127.19 | 122.80 |
| 1 | X | 2668 | U | C5-C6-N1 | -6.27 | 119.56 | 122.70 |
| 1 | X | 430 | C | O4'-C1'-N1 | 6.27 | 113.21 | 108.20 |
| 1 | X | 1142 | G | O5'-C5'-C4' | 6.27 | 123.61 | 111.70 |
| 1 | X | 117 | A | O4'-C1'-N9 | 6.27 | 113.21 | 108.20 |
| 1 | X | 926 | C | O4'-C1'-N1 | 6.26 | 113.21 | 108.20 |
| 1 | X | 1224 | A | P-O3'-C3' | 6.26 | 127.21 | 119.70 |
| 1 | X | 2593 | A | O3'-P-O5' | -6.26 | 92.11 | 104.00 |
| 1 | X | 426 | C | O4'-C1'-N1 | 6.26 | 113.20 | 108.20 |
| 1 | X | 2760 | G | P-O3'-C3' | 6.26 | 127.21 | 119.70 |
| 1 | X | 2811 | G | O4'-C1'-N9 | 6.25 | 113.20 | 108.20 |
| 1 | X | 2582 | G | P-O5'-C5' | 6.25 | 130.91 | 120.90 |
| 1 | X | 2782 | G | C6-C5-N7 | -6.25 | 126.65 | 130.40 |
| 1 | X | 609 | U | C3'-C2'-C1' | -6.24 | 96.50 | 101.50 |
| 1 | X | 941 | U | O4'-C1'-N1 | 6.24 | 113.19 | 108.20 |
| 1 | X | 2875 | C | O4'-C1'-N1 | 6.24 | 113.19 | 108.20 |
| 1 | X | 780 | U | O4'-C1'-N1 | 6.24 | 113.19 | 108.20 |
| 1 | X | 1558 | C | N1-C2-O2 | 6.24 | 122.64 | 118.90 |
| 1 | X | 2645 | C | O4'-C1'-N1 | 6.24 | 113.19 | 108.20 |
| 1 | X | 656 | U | P-O5'-C5' | 6.24 | 130.88 | 120.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | X | 1468 | A | N3-C4-C5 | -6.24 | 122.44 | 126.80 |
| 1 | X | 1222 | G | N3-C4-C5 | -6.23 | 125.48 | 128.60 |
| 1 | X | 2745 | A | P-O3'-C3' | 6.23 | 127.18 | 119.70 |
| 1 | X | 242 | A | P-O3'-C3' | 6.23 | 127.18 | 119.70 |
| 1 | X | 2506 | C | O4'-C1'-N1 | 6.23 | 113.19 | 108.20 |
| 1 | X | 88 | G | P-O3'-C3' | 6.23 | 127.17 | 119.70 |
| 1 | X | 346 | C | N1-C1'-C2' | 6.23 | 122.10 | 114.00 |
| 1 | X | 431 | G | O4'-C1'-N9 | 6.22 | 113.18 | 108.20 |
| 1 | X | 917 | U | O4'-C1'-N1 | 6.22 | 113.18 | 108.20 |
| 1 | X | 2559 | U | C5-C4-O4 | -6.22 | 122.17 | 125.90 |
| 1 | X | 2359 | U | O4'-C1'-N1 | 6.22 | 113.17 | 108.20 |
| 1 | X | 113 | C | O4'-C1'-N1 | 6.21 | 113.17 | 108.20 |
| 1 | X | 632 | A | C1'-O4'-C4' | -6.21 | 104.93 | 109.90 |
| 1 | X | 604 | U | O4'-C1'-N1 | 6.21 | 113.17 | 108.20 |
| 1 | X | 1487 | C | O4'-C1'-N1 | 6.21 | 113.17 | 108.20 |
| 1 | X | 1551 | U | O4'-C1'-N1 | 6.21 | 113.17 | 108.20 |
| 1 | X | 221 | A | O4'-C1'-N9 | 6.21 | 113.17 | 108.20 |
| 1 | X | 1746 | A | O4'-C1'-N9 | 6.21 | 113.17 | 108.20 |
| 1 | X | 2665 | G | C5-C6-O6 | -6.21 | 124.88 | 128.60 |
| 1 | X | 1652 | G | C4-C5-N7 | 6.21 | 113.28 | 110.80 |
| 1 | X | 1675 | C | O5'-P-OP1 | -6.21 | 100.11 | 105.70 |
| 1 | X | 2239 | C | O4'-C1'-N1 | 6.20 | 113.16 | 108.20 |
| 1 | X | 526 | C | C3'-C2'-C1' | -6.20 | 96.54 | 101.50 |
| 1 | X | 2492 | G | C3'-C2'-C1' | -6.20 | 96.54 | 101.50 |
| 2 | Y | 62 | C | O4'-C1'-N1 | 6.20 | 113.16 | 108.20 |
| 1 | X | 577 | U | O4'-C1'-N1 | 6.19 | 113.15 | 108.20 |
| 1 | X | 1338 | G | N3-C4-C5 | -6.19 | 125.51 | 128.60 |
| 1 | X | 1016 | C | O4'-C1'-N1 | 6.18 | 113.15 | 108.20 |
| 1 | X | 580 | A | C5'-C4'-O4' | 6.18 | 116.52 | 109.10 |
| 1 | X | 2459 | C | O4'-C1'-N1 | 6.18 | 113.14 | 108.20 |
| 1 | X | 626 | A | P-O3'-C3' | 6.18 | 127.12 | 119.70 |
| 1 | X | 665 | A | O4'-C1'-N9 | 6.18 | 113.14 | 108.20 |
| 1 | X | 1455 | C | O4'-C1'-N1 | 6.17 | 113.14 | 108.20 |
| 1 | X | 1279 | G | C1'-O4'-C4' | -6.17 | 104.97 | 109.90 |
| 1 | X | 2043 | A | P-O5'-C5' | -6.17 | 111.03 | 120.90 |
| 1 | X | 97 | U | O4'-C1'-N1 | 6.17 | 113.13 | 108.20 |
| 1 | X | 175 | C | C5-C6-N1 | 6.17 | 124.08 | 121.00 |
| 1 | X | 1328 | C | O4'-C1'-N1 | 6.16 | 113.13 | 108.20 |
| 1 | X | 1679 | U | N3-C4-O4 | -6.16 | 115.09 | 119.40 |
| 1 | X | 1865 | C | O4'-C1'-N1 | 6.16 | 113.13 | 108.20 |
| 1 | X | 2697 | G | P-O3'-C3' | -6.16 | 112.31 | 119.70 |
| 1 | X | 1434 | U | N1-C1'-C2' | 6.16 | 122.01 | 114.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | X | 2708 | U | O4'-C1'-N1 | 6.16 | 113.13 | 108.20 |
| 2 | Y | 92 | G | C3'-C2'-C1' | -6.16 | 96.57 | 101.50 |
| 1 | X | 90 | G | P-O3'-C3' | 6.16 | 127.09 | 119.70 |
| 1 | X | 677 | G | C4'-C3'-C2' | -6.15 | 96.45 | 102.60 |
| 1 | X | 2478 | C | C5-C6-N1 | 6.15 | 124.08 | 121.00 |
| 1 | X | 672 | C | C3'-C2'-C1' | -6.15 | 96.58 | 101.50 |
| 1 | X | 1652 | G | C5-C6-O6 | -6.15 | 124.91 | 128.60 |
| 1 | X | 547 | U | O4'-C1'-N1 | 6.15 | 113.12 | 108.20 |
| 1 | X | 774 | A | C2-N3-C4 | -6.15 | 107.53 | 110.60 |
| 1 | X | 1540 | C | O4'-C1'-N1 | 6.15 | 113.12 | 108.20 |
| 1 | X | 345 | U | O4'-C1'-N1 | 6.14 | 113.12 | 108.20 |
| 1 | X | 1269 | G | O4'-C1'-N9 | 6.14 | 113.11 | 108.20 |
| 1 | X | 499 | G | P-O3'-C3' | -6.14 | 112.33 | 119.70 |
| 1 | X | 1030 | U | O4'-C1'-N1 | 6.14 | 113.11 | 108.20 |
| 1 | X | 1171 | A | O4'-C1'-N9 | 6.14 | 113.11 | 108.20 |
| 1 | X | 2039 | G | N3-C2-N2 | -6.14 | 115.60 | 119.90 |
| 1 | X | 2821 | G | O4'-C1'-N9 | 6.14 | 113.11 | 108.20 |
| 1 | X | 928 | G | C5-C6-O6 | -6.13 | 124.92 | 128.60 |
| 1 | X | 1820 | G | P-O5'-C5' | 6.13 | 130.71 | 120.90 |
| 1 | X | 416 | U | O4'-C1'-N1 | 6.13 | 113.10 | 108.20 |
| 1 | X | 1950 | C | O4'-C1'-N1 | 6.13 | 113.11 | 108.20 |
| 1 | X | 2246 | A | C2-N3-C4 | 6.13 | 113.67 | 110.60 |
| 2 | Y | 24 | U | O4'-C1'-N1 | 6.13 | 113.11 | 108.20 |
| 1 | X | 1788 | C | O4'-C1'-N1 | 6.13 | 113.10 | 108.20 |
| 1 | X | 1938 | U | N1-C1'-C2' | 6.12 | 121.96 | 114.00 |
| 1 | X | 2840 | U | P-O3'-C3' | 6.12 | 127.05 | 119.70 |
| 1 | X | 483 | A | O4'-C1'-N9 | 6.12 | 113.09 | 108.20 |
| 1 | X | 2038 | C | OP2-P-O3' | 6.11 | 118.65 | 105.20 |
| 1 | X | 2371 | A | C3'-C2'-C1' | -6.11 | 96.61 | 101.50 |
| 1 | X | 1341 | G | N3-C4-C5 | -6.11 | 125.55 | 128.60 |
| 1 | X | 1792 | C | N3-C2-O2 | -6.11 | 117.62 | 121.90 |
| 1 | X | 2540 | A | O4'-C1'-N9 | 6.11 | 113.09 | 108.20 |
| 1 | X | 2594 | U | C5-C6-N1 | 6.11 | 125.75 | 122.70 |
| 1 | X | 343 | A | N7-C8-N9 | 6.11 | 116.85 | 113.80 |
| 2 | Y | 13 | C | O4'-C1'-N1 | 6.11 | 113.08 | 108.20 |
| 1 | X | 589 | C | O4'-C1'-N1 | 6.10 | 113.08 | 108.20 |
| 1 | X | 1938 | U | P-O5'-C5' | 6.10 | 130.66 | 120.90 |
| 1 | X | 2363 | G | C5'-C4'-O4' | 6.10 | 116.42 | 109.10 |
| 1 | X | 2246 | A | P-O3'-C3' | 6.09 | 127.01 | 119.70 |
| 1 | X | 2431 | C | O4'-C1'-N1 | 6.09 | 113.08 | 108.20 |
| 1 | X | 2691 | C | C5'-C4'-C3' | -6.09 | 106.25 | 116.00 |
| 1 | X | 968 | C | C5-C6-N1 | 6.09 | 124.05 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | X | 1336 | G | C4-C5-N7 | 6.09 | 113.24 | 110.80 |
| 2 | Y | 123 | U | N1-C1'-C2' | 6.09 | 121.92 | 114.00 |
| 1 | X | 12 | U | C2-N1-C1' | 6.09 | 125.01 | 117.70 |
| 1 | X | 1412 | C | O4'-C4'-C3' | -6.09 | 97.91 | 104.00 |
| 1 | X | 2558 | C | O4'-C1'-N1 | 6.09 | 113.07 | 108.20 |
| 1 | X | 1993 | G | O4'-C1'-N9 | 6.08 | 113.07 | 108.20 |
| 1 | X | 2489 | C | O4'-C1'-N1 | 6.08 | 113.07 | 108.20 |
| 1 | X | 2581 | A | O4'-C1'-N9 | 6.08 | 113.07 | 108.20 |
| 1 | X | 1086 | C | O4'-C1'-N1 | 6.08 | 113.06 | 108.20 |
| 1 | X | 1631 | C | C6-N1-C1' | -6.08 | 113.50 | 120.80 |
| 2 | Y | 83 | C | N1-C2-O2 | 6.08 | 122.55 | 118.90 |
| 1 | X | 557 | U | O4'-C1'-N1 | 6.07 | 113.06 | 108.20 |
| 2 | Y | 30 | C | P-O5'-C5' | 6.07 | 130.62 | 120.90 |
| 1 | X | 432 | C | O4'-C1'-N1 | 6.07 | 113.06 | 108.20 |
| 1 | X | 480 | G | C5-C6-N1 | 6.07 | 114.53 | 111.50 |
| 1 | X | 2230 | G | C5-C6-O6 | -6.07 | 124.96 | 128.60 |
| 1 | X | 2767 | C | O4'-C1'-N1 | 6.07 | 113.06 | 108.20 |
| 1 | X | 1468 | A | C2-N3-C4 | 6.07 | 113.63 | 110.60 |
| 1 | X | 2661 | G | O4'-C1'-N9 | 6.07 | 113.05 | 108.20 |
| 1 | X | 2018 | G | C5'-C4'-C3' | -6.07 | 106.29 | 116.00 |
| 1 | X | 1717 | A | O4'-C1'-N9 | 6.06 | 113.05 | 108.20 |
| 1 | X | 2354 | G | O4'-C4'-C3' | -6.06 | 97.94 | 104.00 |
| 1 | X | 74 | G | C1'-O4'-C4' | -6.06 | 105.05 | 109.90 |
| 1 | X | 632 | A | C4'-C3'-C2' | -6.06 | 96.54 | 102.60 |
| 1 | X | 660 | G | N3-C2-N2 | -6.06 | 115.66 | 119.90 |
| 1 | X | 1442 | C | N1-C2-O2 | 6.05 | 122.53 | 118.90 |
| 2 | Y | 35 | C | O4'-C1'-N1 | 6.05 | 113.04 | 108.20 |
| 1 | X | 537 | C | C6-N1-C1' | -6.05 | 113.54 | 120.80 |
| 1 | X | 579 | G | N9-C4-C5 | 6.05 | 107.82 | 105.40 |
| 1 | X | 1006 | C | N1-C2-O2 | 6.05 | 122.53 | 118.90 |
| 2 | Y | 44 | C | O4'-C1'-N1 | 6.05 | 113.04 | 108.20 |
| 2 | Y | 111 | C | P-O3'-C3' | 6.05 | 126.96 | 119.70 |
| 1 | X | 2189 | A | O3'-P-O5' | 6.05 | 115.49 | 104.00 |
| 1 | X | 2245 | A | P-O3'-C3' | 6.05 | 126.96 | 119.70 |
| 2 | Y | 32 | C | O4'-C1'-N1 | 6.05 | 113.04 | 108.20 |
| 1 | X | 1981 | A | C5-C6-N6 | -6.05 | 118.86 | 123.70 |
| 1 | X | 455 | A | P-O3'-C3' | 6.04 | 126.95 | 119.70 |
| 1 | X | 63 | A | C4'-C3'-C2' | 6.04 | 108.64 | 102.60 |
| 1 | X | 956 | A | C5-C6-N6 | -6.04 | 118.87 | 123.70 |
| 1 | X | 769 | C | O4'-C1'-N1 | 6.04 | 113.03 | 108.20 |
| 1 | X | 1105 | U | O4'-C1'-N1 | 6.03 | 113.03 | 108.20 |
| 1 | X | 2484 | G | N3-C2-N2 | 6.03 | 124.12 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | X | 526 | C | O5'-P-OP2 | -6.03 | 100.28 | 105.70 |
| 1 | X | 236 | C | O4'-C1'-N1 | 6.03 | 113.02 | 108.20 |
| 1 | X | 965 | G | P-O3'-C3' | -6.03 | 112.47 | 119.70 |
| 1 | X | 1191 | G | P-O3'-C3' | 6.02 | 126.93 | 119.70 |
| 1 | X | 2689 | C | P-O3'-C3' | 6.02 | 126.93 | 119.70 |
| 1 | X | 1392 | U | P-O3'-C3' | 6.02 | 126.92 | 119.70 |
| 1 | X | 590 | C | O4'-C1'-N1 | 6.02 | 113.01 | 108.20 |
| 1 | X | 1076 | U | O4'-C1'-N1 | 6.02 | 113.02 | 108.20 |
| 1 | X | 1154 | A | P-O3'-C3' | 6.02 | 126.92 | 119.70 |
| 1 | X | 1829 | C | O4'-C1'-N1 | 6.02 | 113.01 | 108.20 |
| 1 | X | 2645 | C | N1-C2-O2 | 6.02 | 122.51 | 118.90 |
| 1 | X | 2854 | G | C8-N9-C4 | -6.02 | 103.99 | 106.40 |
| 1 | X | 652 | C | C5'-C4'-C3' | -6.01 | 106.38 | 116.00 |
| 1 | X | 1942 | G | O4'-C4'-C3' | -6.01 | 97.99 | 104.00 |
| 1 | X | 2417 | U | O4'-C1'-N1 | 6.01 | 113.01 | 108.20 |
| 1 | X | 2560 | G | N3-C4-C5 | -6.01 | 125.59 | 128.60 |
| 1 | X | 1183 | C | O4'-C1'-N1 | 6.01 | 113.01 | 108.20 |
| 2 | Y | 55 | C | P-O3'-C3' | 6.01 | 126.91 | 119.70 |
| 1 | X | 873 | U | O4'-C1'-N1 | 6.01 | 113.01 | 108.20 |
| 1 | X | 2395 | C | O4'-C1'-N1 | 6.01 | 113.01 | 108.20 |
| 1 | X | 2591 | C | N1-C2-O2 | 6.01 | 122.50 | 118.90 |
| 1 | X | 2482 | A | P-O5'-C5' | 6.00 | 130.50 | 120.90 |
| 1 | X | 2695 | C | O4'-C1'-N1 | 6.00 | 113.00 | 108.20 |
| 1 | X | 1277 | G | N3-C4-C5 | -6.00 | 125.60 | 128.60 |
| 1 | X | 2314 | A | P-O3'-C3' | 6.00 | 126.90 | 119.70 |
| 1 | X | 1645 | U | N3-C2-O2 | -6.00 | 118.00 | 122.20 |
| 1 | X | 2804 | G | C5-C6-N1 | 6.00 | 114.50 | 111.50 |
| 1 | X | 1749 | G | O4'-C1'-C2' | -5.99 | 99.81 | 105.80 |
| 1 | X | 2193 | C | O4'-C1'-N1 | 5.99 | 112.99 | 108.20 |
| 1 | X | 2314 | A | P-O5'-C5' | 5.99 | 130.49 | 120.90 |
| 1 | X | 1268 | U | P-O5'-C5' | 5.99 | 130.48 | 120.90 |
| 1 | X | 2797 | G | N3-C4-N9 | 5.99 | 129.59 | 126.00 |
| 1 | X | 2519 | C | O4'-C1'-N1 | 5.98 | 112.99 | 108.20 |
| 1 | X | 2591 | C | C5-C6-N1 | 5.98 | 123.99 | 121.00 |
| 1 | X | 304 | A | P-O5'-C5' | 5.98 | 130.47 | 120.90 |
| 1 | X | 646 | C | C6-N1-C2 | -5.98 | 117.91 | 120.30 |
| 1 | X | 1515 | U | O4'-C1'-N1 | 5.97 | 112.98 | 108.20 |
| 1 | X | 621 | U | O4'-C1'-N1 | 5.97 | 112.98 | 108.20 |
| 1 | X | 2258 | G | C1'-O4'-C4' | -5.97 | 105.12 | 109.90 |
| 1 | X | 2600 | A | O4'-C1'-N9 | 5.97 | 112.98 | 108.20 |
| 2 | Y | 14 | C | P-O3'-C3' | 5.97 | 126.87 | 119.70 |
| 1 | X | 611 | C | O4'-C1'-N1 | 5.97 | 112.98 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | X | 824 | U | N1-C1'-C2' | 5.97 | 121.76 | 114.00 |
| 1 | X | 2284 | U | O4'-C1'-N1 | 5.97 | 112.97 | 108.20 |
| 1 | X | 2477 | C | C6-N1-C2 | -5.97 | 117.91 | 120.30 |
| 1 | X | 879 | A | C5'-C4'-C3' | -5.97 | 106.45 | 116.00 |
| 1 | X | 1288 | A | P-O3'-C3' | -5.97 | 112.54 | 119.70 |
| 1 | X | 826 | U | O4'-C1'-N1 | 5.96 | 112.97 | 108.20 |
| 1 | X | 2435 | C | N1-C2-O2 | 5.96 | 122.48 | 118.90 |
| 1 | X | 490 | A | C5'-C4'-O4' | 5.96 | 116.25 | 109.10 |
| 1 | X | 1223 | G | N7-C8-N9 | 5.96 | 116.08 | 113.10 |
| 1 | X | 1111 | C | O4'-C1'-N1 | 5.96 | 112.97 | 108.20 |
| 1 | X | 1746 | A | N1-C6-N6 | -5.96 | 115.03 | 118.60 |
| 1 | X | 2226 | A | N1-C6-N6 | 5.96 | 122.17 | 118.60 |
| 1 | X | 30 | G | O4'-C1'-N9 | 5.96 | 112.97 | 108.20 |
| 1 | X | 647 | G | P-O3'-C3' | 5.96 | 126.85 | 119.70 |
| 1 | X | 2791 | C | O4'-C1'-N1 | 5.96 | 112.97 | 108.20 |
| 1 | X | 1496 | G | C2'-C3'-O3' | 5.96 | 123.23 | 113.70 |
| 4 | B | 132 | LYS | C-N-CA | 5.96 | 136.59 | 121.70 |
| 1 | X | 1396 | C | O4'-C1'-N1 | 5.95 | 112.96 | 108.20 |
| 1 | X | 1680 | U | O4'-C4'-C3' | -5.95 | 98.05 | 104.00 |
| 1 | X | 1787 | U | O4'-C1'-N1 | 5.95 | 112.96 | 108.20 |
| 1 | X | 1778 | U | O4'-C1'-N1 | 5.95 | 112.96 | 108.20 |
| 1 | X | 162 | C | O4'-C1'-N1 | 5.95 | 112.96 | 108.20 |
| 1 | X | 1201 | G | N3-C2-N2 | -5.95 | 115.73 | 119.90 |
| 1 | X | 2392 | G | O4'-C1'-N9 | 5.95 | 112.96 | 108.20 |
| 1 | X | 2782 | G | O4'-C1'-N9 | 5.95 | 112.96 | 108.20 |
| 1 | X | 448 | C | N1-C2-O2 | 5.95 | 122.47 | 118.90 |
| 1 | X | 505 | G | N9-C1'-C2' | 5.95 | 121.73 | 114.00 |
| 1 | X | 1711 | C | P-O3'-C3' | 5.95 | 126.83 | 119.70 |
| 1 | X | 609 | U | O4'-C4'-C3' | -5.94 | 98.06 | 104.00 |
| 1 | X | 2511 | G | P-O5'-C5' | 5.94 | 130.40 | 120.90 |
| 1 | X | 2855 | C | O4'-C1'-N1 | 5.94 | 112.95 | 108.20 |
| 1 | X | 1051 | U | O4'-C1'-N1 | 5.94 | 112.95 | 108.20 |
| 1 | X | 437 | G | O4'-C1'-N9 | 5.93 | 112.95 | 108.20 |
| 1 | X | 969 | U | C4'-C3'-C2' | 5.93 | 108.53 | 102.60 |
| 1 | X | 2567 | G | N3-C4-C5 | -5.93 | 125.63 | 128.60 |
| 1 | X | 2662 | C | N1-C2-O2 | 5.93 | 122.46 | 118.90 |
| 1 | X | 483 | A | C4'-C3'-C2' | 5.93 | 108.53 | 102.60 |
| 1 | X | 397 | U | O4'-C1'-N1 | 5.93 | 112.94 | 108.20 |
| 1 | X | 1272 | G | O4'-C4'-C3' | -5.93 | 98.07 | 104.00 |
| 1 | X | 1221 | C | O4'-C1'-N1 | 5.93 | 112.94 | 108.20 |
| 1 | X | 683 | A | C2'-C3'-O3' | 5.93 | 123.18 | 113.70 |
| 1 | X | 456 | C | C5'-C4'-O4' | -5.92 | 102.00 | 109.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | X | 1688 | U | N1-C2-O2 | -5.92 | 118.65 | 122.80 |
| 1 | X | 582 | G | OP2-P-O3' | 5.92 | 118.22 | 105.20 |
| 1 | X | 2844 | G | O4'-C1'-N9 | 5.92 | 112.94 | 108.20 |
| 1 | X | 2668 | U | N1-C2-N3 | 5.92 | 118.45 | 114.90 |
| 1 | X | 2698 | G | C4'-C3'-C2' | -5.92 | 96.68 | 102.60 |
| 1 | X | 980 | G | O4'-C1'-N9 | 5.92 | 112.93 | 108.20 |
| 1 | X | 1411 | C | O4'-C1'-N1 | 5.92 | 112.93 | 108.20 |
| 1 | X | 1706 | A | P-O3'-C3' | 5.92 | 126.80 | 119.70 |
| 1 | X | 1034 | U | O4'-C1'-N1 | 5.91 | 112.93 | 108.20 |
| 1 | X | 2072 | C | O4'-C1'-N1 | 5.91 | 112.93 | 108.20 |
| 1 | X | 78 | C | O4'-C1'-N1 | 5.91 | 112.93 | 108.20 |
| 1 | X | 751 | G | P-O3'-C3' | 5.91 | 126.79 | 119.70 |
| 1 | X | 788 | G | N9-C1'-C2' | 5.91 | 121.68 | 114.00 |
| 1 | X | 1262 | U | C5'-C4'-O4' | -5.91 | 102.01 | 109.10 |
| 1 | X | 1415 | C | O4'-C1'-N1 | 5.91 | 112.93 | 108.20 |
| 1 | X | 2018 | G | C4-C5-N7 | 5.91 | 113.16 | 110.80 |
| 1 | X | 959 | C | C5-C6-N1 | 5.91 | 123.95 | 121.00 |
| 1 | X | 1349 | A | P-O5'-C5' | 5.90 | 130.34 | 120.90 |
| 2 | Y | 55 | C | O4'-C1'-N1 | 5.90 | 112.92 | 108.20 |
| 1 | X | 1624 | A | C1'-O4'-C4' | -5.90 | 105.18 | 109.90 |
| 2 | Y | 50 | U | O4'-C1'-N1 | 5.90 | 112.92 | 108.20 |
| 13 | K | 93 | GLY | C-N-CA | -5.90 | 106.96 | 121.70 |
| 1 | X | 1664 | G | O4'-C1'-N9 | -5.89 | 103.48 | 108.20 |
| 1 | X | 858 | G | C3'-C2'-C1' | 5.89 | 106.21 | 101.50 |
| 1 | X | 1099 | A | P-O3'-C3' | 5.89 | 126.77 | 119.70 |
| 1 | X | 1214 | C | C3'-C2'-C1' | -5.89 | 96.79 | 101.50 |
| 1 | X | 1858 | C | O4'-C1'-N1 | 5.89 | 112.91 | 108.20 |
| 1 | X | 2487 | G | N9-C4-C5 | 5.89 | 107.76 | 105.40 |
| 1 | X | 2377 | U | O4'-C1'-N1 | 5.89 | 112.91 | 108.20 |
| 17 | O | 6 | GLN | C-N-CA | 5.88 | 136.41 | 121.70 |
| 1 | X | 2681 | A | C4'-C3'-C2' | -5.88 | 96.72 | 102.60 |
| 1 | X | 540 | G | C3'-C2'-C1' | 5.88 | 106.20 | 101.50 |
| 1 | X | 1252 | C | O4'-C1'-N1 | 5.88 | 112.90 | 108.20 |
| 1 | X | 110 | U | O4'-C1'-N1 | 5.88 | 112.90 | 108.20 |
| 1 | X | 1004 | A | C2-N3-C4 | 5.88 | 113.54 | 110.60 |
| 1 | X | 1210 | C | O4'-C1'-N1 | 5.88 | 112.90 | 108.20 |
| 1 | X | 1263 | G | P-O3'-C3' | 5.88 | 126.75 | 119.70 |
| 1 | X | 1858 | C | N1-C2-O2 | 5.87 | 122.42 | 118.90 |
| 1 | X | 2782 | G | C5-C6-O6 | -5.87 | 125.08 | 128.60 |
| 1 | X | 111 | G | C5'-C4'-C3' | -5.87 | 106.61 | 116.00 |
| 2 | Y | 57 | U | O4'-C1'-N1 | 5.87 | 112.89 | 108.20 |
| 1 | X | 731 | A | C3'-C2'-C1' | 5.86 | 106.19 | 101.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | X | 2488 | G | O4'-C1'-N9 | 5.86 | 112.89 | 108.20 |
| 1 | X | 2671 | C | O5'-P-OP2 | -5.86 | 100.42 | 105.70 |
| 2 | Y | 71 | G | C8-N9-C4 | -5.86 | 104.06 | 106.40 |
| 1 | X | 957 | G | N3-C4-C5 | -5.86 | 125.67 | 128.60 |
| 1 | X | 525 | A | O4'-C1'-N9 | 5.86 | 112.89 | 108.20 |
| 1 | X | 469 | G | O4'-C1'-C2' | -5.86 | 99.94 | 105.80 |
| 1 | X | 1522 | C | N1-C2-O2 | 5.86 | 122.41 | 118.90 |
| 2 | Y | 110 | U | O4'-C1'-N1 | 5.86 | 112.89 | 108.20 |
| 1 | X | 479 | G | C5-C6-O6 | -5.86 | 125.09 | 128.60 |
| 1 | X | 2082 | C | O4'-C1'-N1 | 5.86 | 112.89 | 108.20 |
| 13 | K | 11 | ASN | C-N-CA | 5.86 | 136.34 | 121.70 |
| 1 | X | 2795 | A | C3'-C2'-C1' | 5.85 | 106.18 | 101.50 |
| 1 | X | 960 | U | O4'-C1'-N1 | 5.85 | 112.88 | 108.20 |
| 1 | X | 1326 | U | N1-C2-O2 | 5.85 | 126.89 | 122.80 |
| 1 | X | 2193 | C | O4'-C4'-C3' | -5.85 | 98.15 | 104.00 |
| 1 | X | 68 | C | N1-C2-O2 | 5.85 | 122.41 | 118.90 |
| 1 | X | 204 | A | C2'-C3'-O3' | 5.84 | 123.05 | 113.70 |
| 1 | X | 1015 | U | O4'-C1'-N1 | 5.84 | 112.88 | 108.20 |
| 1 | X | 234 | C | O4'-C1'-N1 | 5.84 | 112.88 | 108.20 |
| 1 | X | 2382 | C | O4'-C1'-N1 | 5.84 | 112.87 | 108.20 |
| 1 | X | 2668 | U | O4'-C1'-N1 | 5.84 | 112.87 | 108.20 |
| 1 | X | 559 | C | C1'-O4'-C4' | -5.84 | 105.23 | 109.90 |
| 1 | X | 1128 | G | P-O3'-C3' | 5.84 | 126.70 | 119.70 |
| 1 | X | 1663 | C | P-O3'-C3' | 5.84 | 126.70 | 119.70 |
| 1 | X | 2236 | U | O4'-C1'-N1 | 5.84 | 112.87 | 108.20 |
| 2 | Y | 53 | G | O4'-C1'-N9 | 5.83 | 112.87 | 108.20 |
| 1 | X | 1333 | G | N1-C2-N2 | 5.83 | 121.45 | 116.20 |
| 1 | X | 540 | G | C4-C5-N7 | -5.83 | 108.47 | 110.80 |
| 1 | X | 2720 | A | P-O3'-C3' | 5.83 | 126.69 | 119.70 |
| 1 | X | 2742 | G | O4'-C4'-C3' | -5.83 | 98.17 | 104.00 |
| 1 | X | 1765 | C | N1-C2-O2 | 5.83 | 122.40 | 118.90 |
| 1 | X | 509 | U | O4'-C1'-N1 | 5.82 | 112.86 | 108.20 |
| 1 | X | 520 | C | P-O3'-C3' | 5.82 | 126.69 | 119.70 |
| 1 | X | 799 | C | O4'-C1'-N1 | 5.82 | 112.86 | 108.20 |
| 1 | X | 1010 | U | P-O5'-C5' | 5.82 | 130.21 | 120.90 |
| 1 | X | 93 | A | O4'-C1'-N9 | 5.82 | 112.86 | 108.20 |
| 1 | X | 1168 | G | P-O5'-C5' | 5.82 | 130.21 | 120.90 |
| 1 | X | 2808 | U | P-O3'-C3' | 5.82 | 126.68 | 119.70 |
| 1 | X | 1972 | G | C5'-C4'-O4' | 5.82 | 116.08 | 109.10 |
| 1 | X | 1447 | U | O4'-C1'-N1 | 5.82 | 112.85 | 108.20 |
| 1 | X | 2051 | U | P-O3'-C3' | 5.82 | 126.68 | 119.70 |
| 1 | X | 2243 | C | O4'-C1'-N1 | 5.82 | 112.85 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | X | 20 | C | O4'-C1'-N1 | 5.81 | 112.85 | 108.20 |
| 1 | X | 1077 | U | P-O3'-C3' | 5.81 | 126.67 | 119.70 |
| 1 | X | 1149 | G | P-O3'-C3' | 5.81 | 126.67 | 119.70 |
| 1 | X | 1336 | G | C5-C6-O6 | -5.81 | 125.11 | 128.60 |
| 1 | X | 1783 | G | O4'-C4'-C3' | -5.81 | 98.19 | 104.00 |
| 1 | X | 2492 | G | N3-C4-C5 | -5.81 | 125.70 | 128.60 |
| 1 | X | 2852 | G | C5-C6-O6 | -5.81 | 125.11 | 128.60 |
| 1 | X | 729 | A | P-O3'-C3' | 5.81 | 126.67 | 119.70 |
| 1 | X | 1607 | A | C2'-C3'-O3' | 5.80 | 122.99 | 113.70 |
| 1 | X | 1983 | G | O4'-C4'-C3' | -5.80 | 98.19 | 104.00 |
| 1 | X | 2250 | G | P-O5'-C5' | 5.80 | 130.19 | 120.90 |
| 1 | X | 1353 | A | O4'-C1'-N9 | 5.80 | 112.84 | 108.20 |
| 1 | X | 1412 | C | C2'-C3'-O3' | 5.80 | 122.98 | 113.70 |
| 1 | X | 1767 | G | C5-C6-O6 | -5.80 | 125.12 | 128.60 |
| 1 | X | 1811 | A | C4'-C3'-C2' | 5.80 | 108.40 | 102.60 |
| 1 | X | 2015 | G | P-O3'-C3' | 5.80 | 126.66 | 119.70 |
| 1 | X | 1091 | C | O4'-C1'-N1 | 5.80 | 112.84 | 108.20 |
| 1 | X | 1935 | A | P-O3'-C3' | 5.79 | 126.65 | 119.70 |
| 1 | X | 2426 | G | O4'-C1'-N9 | 5.79 | 112.83 | 108.20 |
| 19 | Q | 60 | GLY | N-CA-C | 5.79 | 127.58 | 113.10 |
| 1 | X | 1314 | A | O4'-C1'-C2' | -5.79 | 100.01 | 105.80 |
| 1 | X | 2588 | U | N3-C2-O2 | -5.79 | 118.15 | 122.20 |
| 1 | X | 219 | G | P-O3'-C3' | 5.78 | 126.64 | 119.70 |
| 1 | X | 1790 | G | C1'-O4'-C4' | -5.78 | 105.27 | 109.90 |
| 1 | X | 2198 | U | P-O3'-C3' | 5.78 | 126.64 | 119.70 |
| 1 | X | 1337 | G | O4'-C1'-N9 | 5.78 | 112.82 | 108.20 |
| 1 | X | 1232 | U | O4'-C1'-N1 | 5.78 | 112.82 | 108.20 |
| 1 | X | 2025 | A | O5'-P-OP2 | -5.78 | 100.50 | 105.70 |
| 1 | X | 2482 | A | N1-C2-N3 | -5.78 | 126.41 | 129.30 |
| 1 | X | 2403 | C | N1-C2-O2 | 5.78 | 122.36 | 118.90 |
| 2 | Y | 32 | C | C5-C6-N1 | 5.78 | 123.89 | 121.00 |
| 1 | X | 416 | U | C1'-O4'-C4' | -5.77 | 105.28 | 109.90 |
| 1 | X | 2627 | G | C6-C5-N7 | -5.77 | 126.94 | 130.40 |
| 1 | X | 183 | U | O4'-C1'-N1 | 5.77 | 112.82 | 108.20 |
| 1 | X | 707 | U | O4'-C1'-N1 | 5.77 | 112.82 | 108.20 |
| 1 | X | 796 | A | C8-N9-C4 | -5.77 | 103.49 | 105.80 |
| 1 | X | 864 | C | C6-N1-C2 | -5.77 | 117.99 | 120.30 |
| 1 | X | 1148 | G | O4'-C1'-N9 | 5.77 | 112.82 | 108.20 |
| 1 | X | 2416 | U | C3'-C2'-C1' | -5.77 | 96.89 | 101.50 |
| 1 | X | 2601 | C | C4'-C3'-C2' | -5.77 | 96.83 | 102.60 |
| 1 | X | 477 | A | P-O3'-C3' | 5.77 | 126.62 | 119.70 |
| 1 | X | 2710 | C | N3-C2-O2 | -5.77 | 117.86 | 121.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | X | 860 | U | C1'-O4'-C4' | -5.77 | 105.29 | 109.90 |
| 1 | X | 216 | U | O4'-C1'-N1 | 5.76 | 112.81 | 108.20 |
| 1 | X | 1036 | G | C4'-C3'-C2' | 5.76 | 108.36 | 102.60 |
| 1 | X | 1090 | C | O4'-C1'-N1 | 5.76 | 112.81 | 108.20 |
| 1 | X | 1140 | A | O5'-P-OP1 | -5.76 | 100.52 | 105.70 |
| 1 | X | 2731 | G | P-O3'-C3' | 5.76 | 126.61 | 119.70 |
| 11 | I | 28 | LYS | C-N-CA | 5.76 | 136.10 | 121.70 |
| 1 | X | 835 | U | N3-C2-O2 | -5.76 | 118.17 | 122.20 |
| 1 | X | 1313 | U | C3'-C2'-C1' | -5.76 | 96.90 | 101.50 |
| 1 | X | 1380 | C | O4'-C1'-N1 | 5.76 | 112.81 | 108.20 |
| 1 | X | 1850 | G | O4'-C1'-N9 | 5.76 | 112.80 | 108.20 |
| 1 | X | 482 | A | C8-N9-C4 | -5.75 | 103.50 | 105.80 |
| 1 | X | 357 | A | P-O3'-C3' | 5.75 | 126.61 | 119.70 |
| 1 | X | 1958 | G | C5-C6-O6 | -5.75 | 125.15 | 128.60 |
| 1 | X | 2749 | A | O4'-C1'-N9 | 5.75 | 112.80 | 108.20 |
| 1 | X | 1142 | G | N1-C2-N2 | -5.75 | 111.02 | 116.20 |
| 1 | X | 2481 | G | C3'-C2'-C1' | 5.75 | 106.10 | 101.50 |
| 11 | I | 35 | LYS | N-CA-C | -5.75 | 95.49 | 111.00 |
| 1 | X | 2327 | U | N1-C2-O2 | 5.74 | 126.82 | 122.80 |
| 1 | X | 2195 | C | O4'-C1'-N1 | 5.74 | 112.79 | 108.20 |
| 1 | X | 2406 | C | P-O5'-C5' | 5.74 | 130.08 | 120.90 |
| 1 | X | 1770 | U | C5-C6-N1 | -5.74 | 119.83 | 122.70 |
| 1 | X | 1833 | U | O4'-C1'-N1 | 5.74 | 112.79 | 108.20 |
| 1 | X | 2256 | G | O4'-C1'-N9 | 5.74 | 112.79 | 108.20 |
| 1 | X | 796 | A | C6-C5-N7 | -5.73 | 128.29 | 132.30 |
| 1 | X | 2421 | C | O4'-C1'-N1 | 5.73 | 112.79 | 108.20 |
| 1 | X | 1075 | C | O4'-C1'-N1 | 5.73 | 112.79 | 108.20 |
| 1 | X | 488 | A | O4'-C1'-N9 | 5.73 | 112.78 | 108.20 |
| 1 | X | 943 | U | C1'-O4'-C4' | -5.73 | 105.31 | 109.90 |
| 1 | X | 771 | C | O4'-C1'-N1 | 5.73 | 112.78 | 108.20 |
| 1 | X | 309 | G | C8-N9-C4 | -5.72 | 104.11 | 106.40 |
| 1 | X | 1652 | G | C6-C5-N7 | -5.72 | 126.97 | 130.40 |
| 1 | X | 559 | C | N1-C2-O2 | 5.72 | 122.33 | 118.90 |
| 1 | X | 2228 | U | N3-C4-C5 | -5.72 | 111.17 | 114.60 |
| 1 | X | 2038 | C | N1-C2-O2 | 5.72 | 122.33 | 118.90 |
| 1 | X | 1625 | A | P-O3'-C3' | 5.71 | 126.56 | 119.70 |
| 1 | X | 2437 | G | C3'-C2'-C1' | 5.71 | 106.07 | 101.50 |
| 1 | X | 957 | G | O4'-C1'-N9 | 5.71 | 112.77 | 108.20 |
| 1 | X | 2841 | U | P-O3'-C3' | 5.71 | 126.56 | 119.70 |
| 1 | X | 332 | C | P-O3'-C3' | 5.71 | 126.55 | 119.70 |
| 2 | Y | 45 | C | N1-C2-O2 | 5.71 | 122.33 | 118.90 |
| 1 | X | 405 | C | N1-C2-O2 | 5.71 | 122.33 | 118.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | X | 2847 | G | N9-C1'-C2' | 5.71 | 121.42 | 114.00 |
| 1 | X | 846 | A | O4'-C1'-N9 | 5.71 | 112.77 | 108.20 |
| 1 | X | 1333 | G | C5-N7-C8 | -5.71 | 101.45 | 104.30 |
| 1 | X | 2442 | C | P-O3'-C3' | -5.71 | 112.85 | 119.70 |
| 1 | X | 2709 | C | O4'-C1'-N1 | 5.71 | 112.77 | 108.20 |
| 1 | X | 2846 | G | O4'-C1'-N9 | 5.71 | 112.77 | 108.20 |
| 1 | X | 418 | C | O4'-C1'-N1 | 5.71 | 112.76 | 108.20 |
| 1 | X | 845 | U | O4'-C1'-N1 | 5.71 | 112.76 | 108.20 |
| 1 | X | 2847 | G | N9-C4-C5 | 5.71 | 107.68 | 105.40 |
| 1 | X | 615 | C | O4'-C1'-N1 | 5.70 | 112.76 | 108.20 |
| 1 | X | 2706 | U | P-O3'-C3' | 5.70 | 126.54 | 119.70 |
| 1 | X | 983 | G | P-O3'-C3' | 5.70 | 126.54 | 119.70 |
| 2 | Y | 29 | C | O4'-C1'-N1 | 5.70 | 112.76 | 108.20 |
| 1 | X | 7 | G | C5'-C4'-C3' | -5.70 | 106.89 | 116.00 |
| 1 | X | 468 | A | P-O3'-C3' | 5.70 | 126.53 | 119.70 |
| 1 | X | 862 | A | O4'-C1'-N9 | 5.70 | 112.76 | 108.20 |
| 1 | X | 1466 | C | C4'-C3'-C2' | -5.70 | 96.90 | 102.60 |
| 1 | X | 1115 | C | O4'-C1'-N1 | 5.69 | 112.75 | 108.20 |
| 1 | X | 1459 | U | C4'-C3'-C2' | 5.69 | 108.29 | 102.60 |
| 1 | X | 2276 | C | O4'-C1'-N1 | 5.69 | 112.75 | 108.20 |
| 1 | X | 242 | A | C5'-C4'-O4' | 5.69 | 115.92 | 109.10 |
| 1 | X | 1032 | A | C5-N7-C8 | -5.69 | 101.06 | 103.90 |
| 1 | X | 490 | A | O4'-C1'-N9 | 5.69 | 112.75 | 108.20 |
| 1 | X | 542 | A | C4-C5-N7 | 5.69 | 113.54 | 110.70 |
| 1 | X | 1550 | C | O4'-C1'-N1 | 5.69 | 112.75 | 108.20 |
| 1 | X | 2730 | A | P-O3'-C3' | 5.69 | 126.52 | 119.70 |
| 1 | X | 1245 | G | C4'-C3'-C2' | -5.68 | 96.92 | 102.60 |
| 1 | X | 1278 | A | C2-N3-C4 | -5.68 | 107.76 | 110.60 |
| 1 | X | 1652 | G | N9-C4-C5 | -5.68 | 103.13 | 105.40 |
| 1 | X | 1133 | G | O4'-C1'-N9 | 5.67 | 112.74 | 108.20 |
| 1 | X | 1295 | U | O4'-C1'-N1 | 5.67 | 112.74 | 108.20 |
| 1 | X | 1412 | C | C6-N1-C2 | -5.67 | 118.03 | 120.30 |
| 1 | X | 1598 | C | O4'-C1'-N1 | 5.67 | 112.74 | 108.20 |
| 1 | X | 788 | G | C2'-C3'-O3' | 5.67 | 122.78 | 113.70 |
| 1 | X | 1412 | C | O4'-C1'-N1 | 5.67 | 112.74 | 108.20 |
| 1 | X | 1978 | U | O4'-C1'-N1 | 5.67 | 112.74 | 108.20 |
| 1 | X | 744 | C | O4'-C1'-N1 | 5.67 | 112.74 | 108.20 |
| 1 | X | 837 | U | O4'-C1'-N1 | 5.67 | 112.74 | 108.20 |
| 1 | X | 942 | U | O4'-C1'-N1 | 5.67 | 112.74 | 108.20 |
| 1 | X | 2037 | A | O4'-C1'-N9 | 5.67 | 112.74 | 108.20 |
| 1 | X | 1683 | G | P-O3'-C3' | -5.67 | 112.90 | 119.70 |
| 1 | X | 1971 | C | P-O3'-C3' | -5.67 | 112.90 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | X | 418 | C | C4'-C3'-C2' | -5.67 | 96.93 | 102.60 |
| 1 | X | 569 | C | N1-C2-O2 | 5.66 | 122.30 | 118.90 |
| 1 | X | 1108 | U | O4'-C1'-N1 | 5.66 | 112.73 | 108.20 |
| 1 | X | 2477 | C | P-O5'-C5' | 5.66 | 129.96 | 120.90 |
| 1 | X | 814 | G | C5-C6-N1 | 5.66 | 114.33 | 111.50 |
| 1 | X | 1508 | G | P-O3'-C3' | 5.66 | 126.49 | 119.70 |
| 1 | X | 2260 | C | O4'-C1'-N1 | 5.66 | 112.73 | 108.20 |
| 1 | X | 796 | A | C4-C5-N7 | 5.66 | 113.53 | 110.70 |
| 1 | X | 878 | C | N1-C2-O2 | 5.66 | 122.29 | 118.90 |
| 1 | X | 2008 | C | C5-C6-N1 | 5.66 | 123.83 | 121.00 |
| 1 | X | 1181 | C | O4'-C1'-N1 | 5.65 | 112.72 | 108.20 |
| 1 | X | 805 | G | P-O5'-C5' | 5.65 | 129.94 | 120.90 |
| 1 | X | 2199 | C | P-O5'-C5' | 5.65 | 129.94 | 120.90 |
| 1 | X | 39 | C | O4'-C1'-N1 | 5.65 | 112.72 | 108.20 |
| 1 | X | 937 | C | O4'-C1'-N1 | 5.65 | 112.72 | 108.20 |
| 1 | X | 2443 | C | O4'-C1'-N1 | 5.65 | 112.72 | 108.20 |
| 1 | X | 2449 | G | O4'-C1'-N9 | 5.65 | 112.72 | 108.20 |
| 2 | Y | 53 | G | C8-N9-C4 | -5.65 | 104.14 | 106.40 |
| 1 | X | 462 | G | C4-C5-C6 | 5.65 | 122.19 | 118.80 |
| 1 | X | 607 | C | O4'-C4'-C3' | -5.65 | 98.35 | 104.00 |
| 1 | X | 751 | G | O4'-C1'-N9 | 5.65 | 112.72 | 108.20 |
| 1 | X | 1513 | U | P-O3'-C3' | 5.65 | 126.48 | 119.70 |
| 1 | X | 1607 | A | C3'-C2'-C1' | -5.65 | 96.98 | 101.50 |
| 1 | X | 1341 | G | P-O3'-C3' | -5.64 | 112.93 | 119.70 |
| 1 | X | 2854 | G | C5-N7-C8 | -5.64 | 101.48 | 104.30 |
| 1 | X | 569 | C | N3-C2-O2 | -5.64 | 117.95 | 121.90 |
| 1 | X | 2557 | G | C3'-C2'-C1' | 5.64 | 106.02 | 101.50 |
| 1 | X | 1434 | U | O4'-C1'-N1 | 5.64 | 112.71 | 108.20 |
| 1 | X | 817 | A | C1'-O4'-C4' | -5.64 | 105.39 | 109.90 |
| 1 | X | 1770 | U | N1-C2-N3 | 5.64 | 118.28 | 114.90 |
| 1 | X | 2002 | A | P-O5'-C5' | 5.64 | 129.92 | 120.90 |
| 1 | X | 860 | U | C5'-C4'-O4' | 5.64 | 115.87 | 109.10 |
| 1 | X | 2797 | G | C6-C5-N7 | -5.64 | 127.02 | 130.40 |
| 1 | X | 1594 | U | O4'-C1'-N1 | 5.63 | 112.71 | 108.20 |
| 1 | X | 868 | U | O4'-C1'-N1 | 5.63 | 112.70 | 108.20 |
| 1 | X | 549 | G | O4'-C1'-N9 | 5.63 | 112.70 | 108.20 |
| 1 | X | 2483 | U | O4'-C1'-N1 | 5.63 | 112.70 | 108.20 |
| 1 | X | 1087 | C | O4'-C1'-N1 | 5.63 | 112.70 | 108.20 |
| 1 | X | 1966 | C | P-O3'-C3' | -5.63 | 112.94 | 119.70 |
| 1 | X | 2219 | U | O4'-C1'-N1 | 5.63 | 112.70 | 108.20 |
| 1 | X | 2274 | C | N1-C2-O2 | 5.63 | 122.28 | 118.90 |
| 1 | X | 2636 | A | P-O3'-C3' | 5.63 | 126.45 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | X | 746 | G | N3-C4-C5 | -5.63 | 125.79 | 128.60 |
| 1 | X | 1142 | G | N3-C2-N2 | 5.63 | 123.84 | 119.90 |
| 1 | X | 2726 | U | O4'-C1'-N1 | 5.63 | 112.70 | 108.20 |
| 2 | Y | 90 | C | N1-C2-O2 | 5.63 | 122.28 | 118.90 |
| 1 | X | 1715 | A | P-O3'-C3' | 5.62 | 126.45 | 119.70 |
| 1 | X | 537 | C | N1-C2-N3 | -5.62 | 115.26 | 119.20 |
| 2 | Y | 118 | G | C3'-C2'-C1' | -5.62 | 97.00 | 101.50 |
| 1 | X | 2300 | G | C2-N3-C4 | 5.62 | 114.71 | 111.90 |
| 1 | X | 103 | U | C5-C6-N1 | 5.62 | 125.51 | 122.70 |
| 1 | X | 1245 | G | O4'-C1'-N9 | 5.62 | 112.69 | 108.20 |
| 1 | X | 2217 | G | P-O3'-C3' | 5.61 | 126.44 | 119.70 |
| 1 | X | 1683 | G | C4-C5-N7 | -5.61 | 108.56 | 110.80 |
| 1 | X | 327 | C | N1-C2-O2 | 5.61 | 122.27 | 118.90 |
| 1 | X | 594 | G | C4'-C3'-C2' | -5.61 | 96.99 | 102.60 |
| 1 | X | 2362 | G | P-O3'-C3' | 5.61 | 126.43 | 119.70 |
| 1 | X | 956 | A | N1-C6-N6 | 5.61 | 121.96 | 118.60 |
| 11 | I | 55 | ARG | C-N-CA | 5.61 | 135.72 | 121.70 |
| 1 | X | 1688 | U | O4'-C1'-N1 | 5.60 | 112.68 | 108.20 |
| 1 | X | 2692 | A | C3'-C2'-C1' | 5.60 | 105.98 | 101.50 |
| 1 | X | 2793 | G | O4'-C4'-C3' | -5.60 | 98.40 | 104.00 |
| 1 | X | 689 | A | C8-N9-C4 | -5.60 | 103.56 | 105.80 |
| 1 | X | 816 | U | O4'-C1'-N1 | 5.60 | 112.68 | 108.20 |
| 1 | X | 1753 | A | C8-N9-C4 | -5.60 | 103.56 | 105.80 |
| 1 | X | 465 | C | P-O5'-C5' | -5.60 | 111.94 | 120.90 |
| 1 | X | 2803 | C | P-O5'-C5' | -5.60 | 111.94 | 120.90 |
| 1 | X | 2452 | U | O4'-C1'-N1 | 5.60 | 112.68 | 108.20 |
| 1 | X | 616 | U | O4'-C1'-N1 | 5.59 | 112.68 | 108.20 |
| 1 | X | 940 | G | P-O5'-C5' | 5.59 | 129.85 | 120.90 |
| 1 | X | 2797 | G | N3-C4-C5 | -5.59 | 125.80 | 128.60 |
| 1 | X | 126 | C | N1-C1'-C2' | 5.59 | 121.27 | 114.00 |
| 1 | X | 1288 | A | C5'-C4'-C3' | 5.59 | 124.94 | 116.00 |
| 1 | X | 1490 | U | O4'-C1'-N1 | 5.59 | 112.67 | 108.20 |
| 1 | X | 1913 | G | O4'-C1'-N9 | -5.59 | 103.73 | 108.20 |
| 1 | X | 1924 | C | N1-C2-O2 | 5.59 | 122.25 | 118.90 |
| 1 | X | 2205 | C | O4'-C1'-N1 | 5.59 | 112.67 | 108.20 |
| 1 | X | 1337 | G | C8-N9-C4 | -5.58 | 104.17 | 106.40 |
| 1 | X | 1981 | A | C6-C5-N7 | -5.58 | 128.39 | 132.30 |
| 1 | X | 498 | C | N1-C2-O2 | 5.58 | 122.25 | 118.90 |
| 1 | X | 1089 | C | P-O3'-C3' | 5.58 | 126.40 | 119.70 |
| 1 | X | 2252 | A | N1-C6-N6 | -5.58 | 115.25 | 118.60 |
| 1 | X | 2640 | G | O4'-C1'-N9 | 5.58 | 112.66 | 108.20 |
| 1 | X | 1712 | G | N3-C4-C5 | -5.58 | 125.81 | 128.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | X | 2410 | U | O4'-C1'-N1 | 5.58 | 112.66 | 108.20 |
| 2 | Y | 89 | G | O4'-C1'-N9 | 5.58 | 112.66 | 108.20 |
| 1 | X | 462 | G | C5-C6-N1 | -5.57 | 108.71 | 111.50 |
| 1 | X | 1539 | U | O4'-C1'-N1 | 5.57 | 112.66 | 108.20 |
| 1 | X | 1977 | C | O4'-C1'-N1 | 5.57 | 112.66 | 108.20 |
| 1 | X | 2576 | G | C5-C6-O6 | -5.57 | 125.26 | 128.60 |
| 1 | X | 1150 | C | O4'-C1'-N1 | 5.57 | 112.65 | 108.20 |
| 1 | X | 1469 | U | O3'-P-O5' | 5.57 | 114.58 | 104.00 |
| 1 | X | 237 | G | O4'-C1'-N9 | 5.57 | 112.65 | 108.20 |
| 1 | X | 465 | C | O3'-P-O5' | -5.56 | 93.43 | 104.00 |
| 1 | X | 2418 | A | P-O3'-C3' | 5.56 | 126.38 | 119.70 |
| 1 | X | 434 | C | C3'-C2'-C1' | 5.56 | 105.95 | 101.50 |
| 1 | X | 699 | G | C8-N9-C4 | -5.56 | 104.17 | 106.40 |
| 1 | X | 764 | A | N9-C1'-C2' | 5.56 | 121.23 | 114.00 |
| 1 | X | 2479 | U | C4'-C3'-C2' | -5.56 | 97.04 | 102.60 |
| 1 | X | 737 | C | C5-C6-N1 | 5.56 | 123.78 | 121.00 |
| 13 | K | 94 | TYR | N-CA-CB | 5.56 | 120.61 | 110.60 |
| 1 | X | 1237 | G | O4'-C1'-N9 | 5.56 | 112.65 | 108.20 |
| 1 | X | 2483 | U | C5-C6-N1 | 5.56 | 125.48 | 122.70 |
| 1 | X | 2305 | C | O4'-C1'-N1 | 5.56 | 112.65 | 108.20 |
| 1 | X | 2370 | G | C1'-O4'-C4' | -5.56 | 105.45 | 109.90 |
| 1 | X | 1223 | G | C4-C5-N7 | 5.55 | 113.02 | 110.80 |
| 1 | X | 1853 | C | O4'-C1'-N1 | 5.55 | 112.64 | 108.20 |
| 1 | X | 2049 | C | O4'-C1'-N1 | 5.55 | 112.64 | 108.20 |
| 1 | X | 2050 | G | C5-C6-O6 | -5.55 | 125.27 | 128.60 |
| 1 | X | 1277 | G | O4'-C1'-N9 | 5.55 | 112.64 | 108.20 |
| 1 | X | 1398 | G | N9-C1'-C2' | 5.55 | 121.21 | 114.00 |
| 1 | X | 475 | U | O4'-C1'-N1 | 5.54 | 112.64 | 108.20 |
| 1 | X | 2564 | U | C1'-O4'-C4' | -5.54 | 105.46 | 109.90 |
| 1 | X | 2853 | U | P-O3'-C3' | 5.54 | 126.35 | 119.70 |
| 1 | X | 1968 | G | O4'-C1'-N9 | 5.54 | 112.64 | 108.20 |
| 2 | Y | 11 | G | O4'-C4'-C3' | -5.54 | 98.46 | 104.00 |
| 1 | X | 1153 | A | P-O3'-C3' | 5.54 | 126.35 | 119.70 |
| 1 | X | 537 | C | C5'-C4'-O4' | 5.54 | 115.75 | 109.10 |
| 1 | X | 755 | C | O4'-C1'-N1 | 5.54 | 112.63 | 108.20 |
| 1 | X | 1056 | U | O4'-C1'-N1 | 5.54 | 112.63 | 108.20 |
| 1 | X | 1399 | C | O4'-C1'-N1 | 5.54 | 112.63 | 108.20 |
| 1 | X | 1969 | G | P-O3'-C3' | -5.54 | 113.05 | 119.70 |
| 1 | X | 1514 | C | O4'-C1'-N1 | 5.54 | 112.63 | 108.20 |
| 1 | X | 1644 | G | O4'-C1'-N9 | 5.54 | 112.63 | 108.20 |
| 1 | X | 1688 | U | C4-C5-C6 | 5.53 | 123.02 | 119.70 |
| 1 | X | 2232 | G | C5-C6-O6 | -5.53 | 125.28 | 128.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | X | 2312 | A | O4'-C1'-N9 | 5.53 | 112.63 | 108.20 |
| 1 | X | 2799 | C | O4'-C1'-N1 | 5.53 | 112.63 | 108.20 |
| 1 | X | 2870 | C | C6-N1-C2 | -5.53 | 118.09 | 120.30 |
| 1 | X | 185 | C | O4'-C1'-N1 | 5.53 | 112.62 | 108.20 |
| 1 | X | 423 | G | C8-N9-C4 | -5.52 | 104.19 | 106.40 |
| 1 | X | 634 | G | P-O5'-C5' | 5.52 | 129.74 | 120.90 |
| 1 | X | 1608 | U | O4'-C1'-N1 | 5.52 | 112.62 | 108.20 |
| 1 | X | 2191 | A | O4'-C1'-N9 | 5.52 | 112.62 | 108.20 |
| 1 | X | 1326 | U | N3-C2-O2 | -5.52 | 118.33 | 122.20 |
| 1 | X | 794 | A | O4'-C4'-C3' | -5.52 | 98.48 | 104.00 |
| 1 | X | 883 | A | O4'-C1'-N9 | 5.52 | 112.62 | 108.20 |
| 1 | X | 1249 | G | C4'-C3'-C2' | 5.52 | 108.12 | 102.60 |
| 1 | X | 1662 | G | N9-C1'-C2' | 5.52 | 121.17 | 114.00 |
| 1 | X | 1217 | U | O4'-C1'-N1 | 5.52 | 112.61 | 108.20 |
| 1 | X | 820 | U | P-O3'-C3' | -5.51 | 113.08 | 119.70 |
| 1 | X | 1434 | U | P-O3'-C3' | 5.51 | 126.31 | 119.70 |
| 1 | X | 1863 | U | O4'-C1'-N1 | 5.51 | 112.61 | 108.20 |
| 1 | X | 2010 | G | O4'-C1'-N9 | 5.51 | 112.61 | 108.20 |
| 1 | X | 522 | G | N7-C8-N9 | 5.51 | 115.85 | 113.10 |
| 1 | X | 1992 | G | OP1-P-OP2 | -5.50 | 111.34 | 119.60 |
| 1 | X | 2819 | G | N3-C4-C5 | -5.50 | 125.85 | 128.60 |
| 1 | X | 2835 | A | O4'-C1'-N9 | 5.50 | 112.60 | 108.20 |
| 1 | X | 1623 | C | N1-C2-O2 | 5.50 | 122.20 | 118.90 |
| 1 | X | 2782 | G | C4-C5-N7 | 5.50 | 113.00 | 110.80 |
| 1 | X | 1990 | U | O4'-C1'-N1 | 5.50 | 112.60 | 108.20 |
| 1 | X | 1201 | G | C8-N9-C4 | -5.50 | 104.20 | 106.40 |
| 1 | X | 1432 | G | C3'-C2'-C1' | 5.50 | 105.90 | 101.50 |
| 1 | X | 2580 | C | P-O3'-C3' | 5.50 | 126.30 | 119.70 |
| 1 | X | 596 | C | P-O5'-C5' | -5.50 | 112.11 | 120.90 |
| 1 | X | 1270 | C | C6-N1-C2 | -5.49 | 118.10 | 120.30 |
| 1 | X | 1081 | A | P-O3'-C3' | 5.49 | 126.29 | 119.70 |
| 1 | X | 841 | G | C5-N7-C8 | -5.49 | 101.56 | 104.30 |
| 1 | X | 1468 | A | N1-C6-N6 | -5.49 | 115.31 | 118.60 |
| 1 | X | 1947 | G | O4'-C1'-N9 | -5.49 | 103.81 | 108.20 |
| 1 | X | 633 | G | O4'-C1'-N9 | 5.49 | 112.59 | 108.20 |
| 1 | X | 666 | U | P-O3'-C3' | 5.49 | 126.28 | 119.70 |
| 1 | X | 1201 | G | P-O3'-C3' | 5.48 | 126.28 | 119.70 |
| 1 | X | 1792 | C | C6-N1-C2 | -5.48 | 118.11 | 120.30 |
| 1 | X | 308 | C | C4'-C3'-C2' | 5.48 | 108.08 | 102.60 |
| 1 | X | 1341 | G | P-O5'-C5' | 5.48 | 129.67 | 120.90 |
| 1 | X | 1754 | G | P-O5'-C5' | 5.48 | 129.67 | 120.90 |
| 1 | X | 1103 | C | O4'-C1'-N1 | 5.48 | 112.58 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | X | 45 | C | O4'-C1'-N1 | 5.48 | 112.58 | 108.20 |
| 1 | X | 167 | A | P-O5'-C5' | 5.48 | 129.66 | 120.90 |
| 1 | X | 1319 | C | C5-C6-N1 | 5.48 | 123.74 | 121.00 |
| 2 | Y | 81 | C | C6-N1-C2 | -5.48 | 118.11 | 120.30 |
| 1 | X | 327 | C | O4'-C1'-N1 | 5.47 | 112.58 | 108.20 |
| 1 | X | 818 | G | C6-C5-N7 | -5.47 | 127.12 | 130.40 |
| 1 | X | 1467 | U | C4'-C3'-C2' | 5.47 | 108.07 | 102.60 |
| 1 | X | 2087 | U | O4'-C1'-N1 | 5.47 | 112.58 | 108.20 |
| 1 | X | 346 | C | C5-C6-N1 | 5.47 | 123.74 | 121.00 |
| 1 | X | 1275 | A | P-O3'-C3' | -5.47 | 113.13 | 119.70 |
| 1 | X | 1876 | C | N1-C2-O2 | 5.47 | 122.18 | 118.90 |
| 1 | X | 2315 | A | O4'-C1'-N9 | -5.47 | 103.82 | 108.20 |
| 1 | X | 2555 | G | O4'-C4'-C3' | -5.47 | 98.53 | 104.00 |
| 1 | X | 2778 | U | N1-C1'-C2' | 5.47 | 121.11 | 114.00 |
| 1 | X | 503 | G | C5-C6-N1 | 5.47 | 114.23 | 111.50 |
| 1 | X | 1725 | C | O4'-C1'-N1 | 5.47 | 112.58 | 108.20 |
| 1 | X | 94 | C | O4'-C1'-N1 | 5.47 | 112.57 | 108.20 |
| 1 | X | 176 | A | C1'-O4'-C4' | -5.47 | 105.53 | 109.90 |
| 1 | X | 1341 | G | N3-C4-N9 | 5.46 | 129.28 | 126.00 |
| 1 | X | 2224 | U | O4'-C1'-N1 | 5.46 | 112.57 | 108.20 |
| 1 | X | 2437 | G | C8-N9-C4 | -5.46 | 104.22 | 106.40 |
| 1 | X | 857 | U | O4'-C1'-N1 | 5.46 | 112.57 | 108.20 |
| 1 | X | 1948 | C | O4'-C1'-N1 | 5.46 | 112.57 | 108.20 |
| 1 | X | 133 | C | O4'-C1'-N1 | 5.46 | 112.57 | 108.20 |
| 1 | X | 1775 | A | C2'-C3'-O3' | 5.46 | 122.44 | 113.70 |
| 1 | X | 765 | C | C4'-C3'-C2' | 5.46 | 108.06 | 102.60 |
| 1 | X | 878 | C | O4'-C1'-N1 | 5.46 | 112.57 | 108.20 |
| 1 | X | 1336 | G | C5-C6-N1 | 5.46 | 114.23 | 111.50 |
| 1 | X | 2089 | C | O4'-C1'-N1 | 5.46 | 112.56 | 108.20 |
| 1 | X | 2342 | U | C3'-C2'-C1' | -5.46 | 97.14 | 101.50 |
| 1 | X | 2705 | A | C4'-C3'-O3' | 5.46 | 123.91 | 113.00 |
| 1 | X | 1566 | G | O4'-C1'-N9 | 5.46 | 112.56 | 108.20 |
| 1 | X | 2032 | G | N3-C4-C5 | -5.45 | 125.87 | 128.60 |
| 1 | X | 2495 | G | C5-C6-N1 | 5.45 | 114.23 | 111.50 |
| 1 | X | 309 | G | N7-C8-N9 | 5.45 | 115.83 | 113.10 |
| 1 | X | 1142 | G | C1'-O4'-C4' | -5.45 | 105.54 | 109.90 |
| 1 | X | 1143 | A | C3'-C2'-C1' | -5.45 | 97.14 | 101.50 |
| 1 | X | 1651 | U | O4'-C1'-N1 | 5.45 | 112.56 | 108.20 |
| 1 | X | 1712 | G | C4-N9-C1' | 5.45 | 133.59 | 126.50 |
| 1 | X | 1049 | C | O4'-C1'-N1 | 5.45 | 112.56 | 108.20 |
| 1 | X | 1301 | U | N3-C2-O2 | -5.45 | 118.39 | 122.20 |
| 2 | Y | 110 | U | N1-C2-O2 | 5.45 | 126.61 | 122.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | X | 832 | A | C5'-C4'-O4' | -5.45 | 102.56 | 109.10 |
| 1 | X | 1340 | C | O3'-P-O5' | -5.45 | 93.65 | 104.00 |
| 1 | X | 2016 | A | N1-C2-N3 | -5.45 | 126.58 | 129.30 |
| 1 | X | 533 | C | O4'-C1'-N1 | 5.44 | 112.56 | 108.20 |
| 1 | X | 721 | C | O4'-C1'-N1 | 5.44 | 112.55 | 108.20 |
| 1 | X | 2336 | G | O5'-P-OP2 | -5.44 | 100.80 | 105.70 |
| 1 | X | 179 | U | O4'-C1'-N1 | 5.44 | 112.55 | 108.20 |
| 1 | X | 2013 | A | C1'-O4'-C4' | -5.44 | 105.55 | 109.90 |
| 1 | X | 2482 | A | C5-C6-N6 | -5.44 | 119.35 | 123.70 |
| 1 | X | 2646 | C | C5-C6-N1 | 5.44 | 123.72 | 121.00 |
| 1 | X | 2808 | U | C5'-C4'-O4' | 5.44 | 115.63 | 109.10 |
| 1 | X | 2407 | G | P-O3'-C3' | 5.44 | 126.23 | 119.70 |
| 1 | X | 1814 | G | O4'-C1'-N9 | 5.44 | 112.55 | 108.20 |
| 1 | X | 2675 | U | O4'-C1'-N1 | 5.44 | 112.55 | 108.20 |
| 1 | X | 871 | U | P-O5'-C5' | 5.43 | 129.60 | 120.90 |
| 1 | X | 1917 | C | O4'-C1'-N1 | 5.43 | 112.55 | 108.20 |
| 1 | X | 1396 | C | C6-N1-C2 | -5.43 | 118.13 | 120.30 |
| 1 | X | 1652 | G | N1-C6-O6 | 5.43 | 123.16 | 119.90 |
| 1 | X | 70 | A | P-O3'-C3' | 5.43 | 126.22 | 119.70 |
| 1 | X | 573 | C | O4'-C1'-N1 | 5.43 | 112.54 | 108.20 |
| 1 | X | 1015 | U | P-O3'-C3' | 5.43 | 126.21 | 119.70 |
| 1 | X | 1163 | C | O4'-C1'-N1 | 5.43 | 112.54 | 108.20 |
| 1 | X | 1278 | A | N9-C1'-C2' | 5.43 | 121.06 | 114.00 |
| 1 | X | 1285 | A | P-O3'-C3' | 5.43 | 126.22 | 119.70 |
| 1 | X | 29 | U | O4'-C1'-N1 | 5.43 | 112.54 | 108.20 |
| 1 | X | 2731 | G | C3'-C2'-C1' | 5.43 | 105.84 | 101.50 |
| 1 | X | 840 | U | C1'-O4'-C4' | -5.42 | 105.56 | 109.90 |
| 1 | X | 2626 | U | O4'-C1'-N1 | 5.42 | 112.54 | 108.20 |
| 1 | X | 319 | G | N9-C1'-C2' | 5.42 | 121.05 | 114.00 |
| 1 | X | 2550 | C | O4'-C1'-N1 | 5.42 | 112.54 | 108.20 |
| 1 | X | 236 | C | N1-C2-O2 | 5.42 | 122.15 | 118.90 |
| 2 | Y | 86 | A | O4'-C4'-C3' | -5.42 | 98.58 | 104.00 |
| 1 | X | 235 | C | N1-C2-O2 | 5.42 | 122.15 | 118.90 |
| 1 | X | 882 | C | O4'-C1'-N1 | 5.42 | 112.53 | 108.20 |
| 1 | X | 1364 | C | O4'-C1'-N1 | 5.42 | 112.53 | 108.20 |
| 1 | X | 215 | G | O4'-C1'-N9 | 5.42 | 112.53 | 108.20 |
| 1 | X | 329 | C | C6-N1-C2 | -5.42 | 118.13 | 120.30 |
| 1 | X | 2076 | G | C8-N9-C4 | -5.42 | 104.23 | 106.40 |
| 1 | X | 1162 | A | P-O3'-C3' | 5.41 | 126.20 | 119.70 |
| 1 | X | 1683 | G | N3-C2-N2 | -5.41 | 116.11 | 119.90 |
| 2 | Y | 49 | C | N1-C2-O2 | 5.41 | 122.15 | 118.90 |
| 2 | Y | 7 | C | O4'-C1'-N1 | 5.41 | 112.53 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | X | 473 | C | OP2-P-O3' | 5.41 | 117.10 | 105.20 |
| 1 | X | 2000 | U | O5'-P-OP2 | -5.41 | 100.83 | 105.70 |
| 1 | X | 2872 | U | O4'-C1'-N1 | 5.41 | 112.53 | 108.20 |
| 2 | Y | 5 | C | O4'-C1'-N1 | 5.41 | 112.53 | 108.20 |
| 1 | X | 617 | U | C2-N1-C1' | 5.41 | 124.19 | 117.70 |
| 1 | X | 211 | U | O4'-C1'-N1 | 5.41 | 112.53 | 108.20 |
| 1 | X | 2229 | G | C5'-C4'-O4' | 5.41 | 115.59 | 109.10 |
| 1 | X | 2323 | U | P-O5'-C5' | 5.41 | 129.55 | 120.90 |
| 1 | X | 2864 | C | O4'-C1'-N1 | 5.41 | 112.52 | 108.20 |
| 1 | X | 467 | U | N1-C1'-C2' | 5.40 | 121.02 | 114.00 |
| 1 | X | 1573 | G | P-O3'-C3' | 5.40 | 126.18 | 119.70 |
| 1 | X | 1618 | U | P-O3'-C3' | 5.40 | 126.18 | 119.70 |
| 1 | X | 2285 | U | O4'-C1'-N1 | 5.40 | 112.52 | 108.20 |
| 1 | X | 338 | G | C8-N9-C4 | -5.40 | 104.24 | 106.40 |
| 1 | X | 964 | A | O4'-C1'-N9 | 5.40 | 112.52 | 108.20 |
| 1 | X | 2273 | C | O4'-C1'-N1 | 5.40 | 112.52 | 108.20 |
| 1 | X | 1923 | U | C2'-C3'-O3' | 5.40 | 122.34 | 113.70 |
| 1 | X | 2009 | U | P-O3'-C3' | -5.40 | 113.22 | 119.70 |
| 1 | X | 178 | C | O4'-C1'-N1 | 5.40 | 112.52 | 108.20 |
| 1 | X | 561 | U | C3'-C2'-C1' | -5.40 | 97.18 | 101.50 |
| 1 | X | 699 | G | C8-N9-C1' | 5.40 | 134.02 | 127.00 |
| 1 | X | 1338 | G | N3-C4-N9 | 5.40 | 129.24 | 126.00 |
| 1 | X | 1796 | A | P-O3'-C3' | 5.40 | 126.18 | 119.70 |
| 1 | X | 1939 | U | N3-C2-O2 | -5.40 | 118.42 | 122.20 |
| 1 | X | 2699 | G | OP1-P-O3' | 5.40 | 117.08 | 105.20 |
| 1 | X | 998 | C | O4'-C1'-N1 | 5.40 | 112.52 | 108.20 |
| 1 | X | 1325 | U | P-O3'-C3' | 5.40 | 126.17 | 119.70 |
| 1 | X | 175 | C | C6-N1-C2 | -5.39 | 118.14 | 120.30 |
| 1 | X | 537 | C | C2-N1-C1' | 5.39 | 124.73 | 118.80 |
| 1 | X | 2778 | U | C3'-C2'-C1' | 5.39 | 105.82 | 101.50 |
| 1 | X | 90 | G | N3-C4-C5 | -5.39 | 125.90 | 128.60 |
| 1 | X | 346 | C | C3'-C2'-C1' | 5.39 | 105.81 | 101.50 |
| 1 | X | 2586 | G | C8-N9-C4 | -5.39 | 104.24 | 106.40 |
| 1 | X | 753 | U | O4'-C1'-N1 | 5.39 | 112.51 | 108.20 |
| 1 | X | 1141 | U | O4'-C1'-N1 | 5.39 | 112.51 | 108.20 |
| 1 | X | 1984 | A | N1-C6-N6 | -5.39 | 115.36 | 118.60 |
| 1 | X | 2699 | G | C2-N3-C4 | 5.39 | 114.59 | 111.90 |
| 1 | X | 1471 | G | O4'-C1'-N9 | 5.39 | 112.51 | 108.20 |
| 1 | X | 145 | C | O4'-C1'-N1 | 5.39 | 112.51 | 108.20 |
| 1 | X | 2363 | G | O4'-C1'-N9 | 5.39 | 112.51 | 108.20 |
| 2 | Y | 19 | C | N1-C2-O2 | 5.39 | 122.13 | 118.90 |
| 1 | X | 1992 | G | C2-N3-C4 | 5.39 | 114.59 | 111.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | X | 2018 | G | O4'-C1'-N9 | 5.39 | 112.51 | 108.20 |
| 1 | X | 2774 | U | O4'-C1'-N1 | 5.39 | 112.51 | 108.20 |
| 1 | X | 2772 | U | O4'-C1'-N1 | 5.38 | 112.51 | 108.20 |
| 1 | X | 591 | G | O4'-C1'-N9 | 5.38 | 112.51 | 108.20 |
| 1 | X | 820 | U | N3-C2-O2 | -5.38 | 118.43 | 122.20 |
| 1 | X | 1743 | C | P-O3'-C3' | -5.38 | 113.24 | 119.70 |
| 1 | X | 675 | C | C3'-C2'-C1' | -5.38 | 97.20 | 101.50 |
| 1 | X | 715 | U | O4'-C1'-N1 | 5.38 | 112.50 | 108.20 |
| 1 | X | 1247 | U | O4'-C1'-N1 | 5.38 | 112.50 | 108.20 |
| 1 | X | 2533 | U | O4'-C1'-N1 | 5.38 | 112.50 | 108.20 |
| 1 | X | 417 | C | N1-C2-O2 | 5.38 | 122.12 | 118.90 |
| 1 | X | 1766 | U | P-O5'-C5' | -5.38 | 112.30 | 120.90 |
| 1 | X | 2176 | U | O4'-C1'-N1 | 5.38 | 112.50 | 108.20 |
| 1 | X | 689 | A | C1'-O4'-C4' | -5.38 | 105.60 | 109.90 |
| 1 | X | 1093 | U | O4'-C1'-N1 | 5.38 | 112.50 | 108.20 |
| 1 | X | 2551 | A | OP1-P-O3' | 5.38 | 117.03 | 105.20 |
| 1 | X | 1097 | A | P-O3'-C3' | 5.37 | 126.15 | 119.70 |
| 1 | X | 1274 | C | O4'-C1'-N1 | 5.37 | 112.50 | 108.20 |
| 2 | Y | 47 | A | C8-N9-C4 | -5.37 | 103.65 | 105.80 |
| 1 | X | 541 | C | O5'-P-OP1 | -5.37 | 100.87 | 105.70 |
| 1 | X | 1627 | C | N1-C2-O2 | 5.37 | 122.12 | 118.90 |
| 1 | X | 660 | G | C3'-C2'-C1' | -5.37 | 97.20 | 101.50 |
| 1 | X | 613 | A | O4'-C1'-N9 | 5.37 | 112.50 | 108.20 |
| 1 | X | 2854 | G | P-O5'-C5' | 5.37 | 129.49 | 120.90 |
| 1 | X | 1752 | U | O4'-C1'-N1 | 5.37 | 112.49 | 108.20 |
| 1 | X | 1825 | C | O4'-C1'-N1 | 5.37 | 112.49 | 108.20 |
| 1 | X | 2028 | C | C5-C6-N1 | 5.36 | 123.68 | 121.00 |
| 1 | X | 2665 | G | N3-C4-N9 | 5.36 | 129.22 | 126.00 |
| 15 | M | 28 | ARG | N-CA-C | -5.36 | 96.52 | 111.00 |
| 1 | X | 2531 | U | N3-C2-O2 | -5.36 | 118.45 | 122.20 |
| 1 | X | 1080 | A | C1'-O4'-C4' | -5.36 | 105.61 | 109.90 |
| 1 | X | 2275 | U | P-O5'-C5' | 5.36 | 129.47 | 120.90 |
| 1 | X | 238 | G | C4'-C3'-C2' | -5.36 | 97.24 | 102.60 |
| 1 | X | 697 | G | O4'-C1'-N9 | 5.36 | 112.49 | 108.20 |
| 1 | X | 2480 | C | N3-C4-C5 | 5.36 | 124.04 | 121.90 |
| 1 | X | 2697 | G | C5-C6-N1 | 5.36 | 114.18 | 111.50 |
| 1 | X | 925 | U | O4'-C1'-N1 | 5.36 | 112.48 | 108.20 |
| 1 | X | 2840 | U | O4'-C1'-N1 | 5.36 | 112.48 | 108.20 |
| 2 | Y | 81 | C | C5-C6-N1 | 5.36 | 123.68 | 121.00 |
| 1 | X | 522 | G | C5-C6-N1 | 5.35 | 114.18 | 111.50 |
| 1 | X | 652 | C | C5-C6-N1 | 5.35 | 123.68 | 121.00 |
| 1 | X | 1262 | U | O4'-C1'-N1 | 5.35 | 112.48 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | X | 2323 | U | C5-C6-N1 | 5.35 | 125.38 | 122.70 |
| 3 | A | 242 | ALA | N-CA-C | 5.35 | 125.46 | 111.00 |
| 1 | X | 78 | C | C6-N1-C2 | -5.35 | 118.16 | 120.30 |
| 1 | X | 2788 | C | O4'-C1'-N1 | 5.35 | 112.48 | 108.20 |
| 1 | X | 146 | C | O4'-C1'-N1 | 5.35 | 112.48 | 108.20 |
| 1 | X | 2008 | C | N3-C4-N4 | 5.35 | 121.75 | 118.00 |
| 1 | X | 2815 | C | C3'-C2'-C1' | -5.35 | 97.22 | 101.50 |
| 1 | X | 1306 | U | P-O3'-C3' | -5.35 | 113.28 | 119.70 |
| 1 | X | 1270 | C | N3-C4-C5 | -5.35 | 119.76 | 121.90 |
| 1 | X | 1776 | A | C4'-C3'-C2' | -5.34 | 97.25 | 102.60 |
| 1 | X | 2650 | G | P-O3'-C3' | -5.34 | 113.29 | 119.70 |
| 1 | X | 2165 | A | P-O3'-C3' | 5.34 | 126.11 | 119.70 |
| 1 | X | 1691 | G | C5-C6-O6 | -5.34 | 125.40 | 128.60 |
| 1 | X | 1828 | C | O4'-C1'-N1 | 5.34 | 112.47 | 108.20 |
| 1 | X | 2477 | C | O5'-P-OP1 | -5.34 | 100.89 | 105.70 |
| 1 | X | 2754 | C | N1-C2-O2 | 5.34 | 122.10 | 118.90 |
| 1 | X | 2837 | G | O4'-C1'-N9 | 5.34 | 112.47 | 108.20 |
| 1 | X | 2088 | U | O4'-C1'-N1 | 5.34 | 112.47 | 108.20 |
| 1 | X | 611 | C | C6-N1-C2 | -5.34 | 118.17 | 120.30 |
| 1 | X | 1716 | G | C1'-O4'-C4' | 5.34 | 114.17 | 109.90 |
| 1 | X | 2430 | A | O4'-C1'-N9 | 5.34 | 112.47 | 108.20 |
| 1 | X | 129 | A | P-O5'-C5' | 5.33 | 129.44 | 120.90 |
| 1 | X | 1054 | C | O4'-C1'-N1 | 5.33 | 112.47 | 108.20 |
| 1 | X | 1315 | A | O5'-P-OP2 | -5.33 | 100.90 | 105.70 |
| 1 | X | 2017 | U | P-O3'-C3' | 5.33 | 126.10 | 119.70 |
| 1 | X | 677 | G | P-O3'-C3' | 5.33 | 126.10 | 119.70 |
| 1 | X | 1092 | U | O4'-C1'-N1 | 5.33 | 112.47 | 108.20 |
| 1 | X | 1686 | A | OP1-P-OP2 | -5.33 | 111.60 | 119.60 |
| 1 | X | 2467 | A | O4'-C1'-N9 | 5.33 | 112.47 | 108.20 |
| 1 | X | 827 | C | O4'-C1'-N1 | 5.33 | 112.46 | 108.20 |
| 2 | Y | 123 | U | N1-C2-O2 | 5.33 | 126.53 | 122.80 |
| 1 | X | 579 | G | C5-C6-N1 | -5.33 | 108.84 | 111.50 |
| 1 | X | 190 | A | C1'-O4'-C4' | -5.33 | 105.64 | 109.90 |
| 1 | X | 1188 | A | P-O3'-C3' | 5.33 | 126.09 | 119.70 |
| 1 | X | 1409 | U | O4'-C1'-N1 | 5.33 | 112.46 | 108.20 |
| 1 | X | 440 | U | O3'-P-O5' | -5.32 | 93.89 | 104.00 |
| 1 | X | 596 | C | N3-C4-C5 | -5.32 | 119.77 | 121.90 |
| 1 | X | 1296 | G | P-O3'-C3' | 5.32 | 126.09 | 119.70 |
| 1 | X | 2559 | U | N3-C4-C5 | 5.32 | 117.80 | 114.60 |
| 1 | X | 2856 | U | N3-C2-O2 | -5.32 | 118.47 | 122.20 |
| 1 | X | 696 | U | P-O5'-C5' | 5.32 | 129.42 | 120.90 |
| 1 | X | 54 | G | P-O3'-C3' | 5.32 | 126.08 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | X | 144 | U | O4'-C1'-N1 | 5.32 | 112.46 | 108.20 |
| 1 | X | 687 | G | N3-C4-C5 | -5.32 | 125.94 | 128.60 |
| 1 | X | 1009 | C | N1-C2-O2 | 5.32 | 122.09 | 118.90 |
| 1 | X | 1564 | U | O4'-C1'-N1 | 5.32 | 112.46 | 108.20 |
| 1 | X | 2075 | U | P-O3'-C3' | 5.32 | 126.08 | 119.70 |
| 1 | X | 2632 | U | O4'-C1'-N1 | 5.32 | 112.46 | 108.20 |
| 1 | X | 1871 | G | O4'-C1'-N9 | 5.32 | 112.46 | 108.20 |
| 1 | X | 103 | U | O4'-C1'-N1 | 5.32 | 112.45 | 108.20 |
| 1 | X | 429 | C | C5-C6-N1 | 5.32 | 123.66 | 121.00 |
| 1 | X | 967 | G | P-O3'-C3' | 5.32 | 126.08 | 119.70 |
| 1 | X | 1219 | C | O4'-C1'-N1 | 5.32 | 112.45 | 108.20 |
| 1 | X | 1355 | A | C4'-C3'-C2' | 5.32 | 107.92 | 102.60 |
| 1 | X | 1439 | G | O4'-C4'-C3' | -5.32 | 98.69 | 104.00 |
| 1 | X | 2474 | G | C5-C6-N1 | 5.32 | 114.16 | 111.50 |
| 1 | X | 2554 | C | N3-C2-O2 | -5.32 | 118.18 | 121.90 |
| 1 | X | 2844 | G | C8-N9-C4 | -5.32 | 104.27 | 106.40 |
| 2 | Y | 42 | U | P-O3'-C3' | 5.31 | 126.08 | 119.70 |
| 1 | X | 1489 | C | C2-N1-C1' | 5.31 | 124.64 | 118.80 |
| 2 | Y | 64 | C | O4'-C1'-N1 | 5.31 | 112.45 | 108.20 |
| 1 | X | 246 | C | O4'-C1'-N1 | 5.31 | 112.44 | 108.20 |
| 1 | X | 682 | G | C3'-C2'-C1' | 5.31 | 105.75 | 101.50 |
| 1 | X | 2027 | C | C3'-C2'-C1' | -5.31 | 97.25 | 101.50 |
| 1 | X | 586 | G | O4'-C4'-C3' | -5.30 | 98.69 | 104.00 |
| 1 | X | 756 | C | O4'-C1'-N1 | 5.30 | 112.44 | 108.20 |
| 1 | X | 2507 | U | O4'-C1'-N1 | 5.30 | 112.44 | 108.20 |
| 1 | X | 536 | A | P-O3'-C3' | 5.30 | 126.06 | 119.70 |
| 19 | Q | 73 | ASN | C-N-CA | 5.30 | 134.95 | 121.70 |
| 1 | X | 747 | A | N1-C6-N6 | 5.30 | 121.78 | 118.60 |
| 1 | X | 1506 | C | O4'-C1'-N1 | 5.30 | 112.44 | 108.20 |
| 1 | X | 2281 | C | O4'-C1'-N1 | 5.30 | 112.44 | 108.20 |
| 1 | X | 580 | A | N9-C1'-C2' | 5.30 | 120.89 | 114.00 |
| 1 | X | 650 | U | P-O5'-C5' | 5.30 | 129.38 | 120.90 |
| 1 | X | 1275 | A | C2-N3-C4 | 5.30 | 113.25 | 110.60 |
| 1 | X | 1400 | A | P-O3'-C3' | -5.30 | 113.34 | 119.70 |
| 1 | X | 2299 | A | C1'-O4'-C4' | -5.30 | 105.66 | 109.90 |
| 1 | X | 1069 | G | C3'-C2'-C1' | 5.29 | 105.73 | 101.50 |
| 1 | X | 2195 | C | C6-N1-C2 | -5.29 | 118.18 | 120.30 |
| 1 | X | 2662 | C | O4'-C1'-N1 | 5.29 | 112.43 | 108.20 |
| 12 | J | 82 | THR | C-N-CA | 5.29 | 134.93 | 121.70 |
| 1 | X | 1336 | G | C6-C5-N7 | -5.29 | 127.23 | 130.40 |
| 1 | X | 1349 | A | C2-N3-C4 | 5.29 | 113.25 | 110.60 |
| 1 | X | 75 | C | O4'-C1'-N1 | 5.29 | 112.43 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | X | 2625 | U | C5-C4-O4 | -5.29 | 122.73 | 125.90 |
| 2 | Y | 2 | C | O4'-C1'-N1 | 5.29 | 112.43 | 108.20 |
| 2 | Y | 87 | C | O4'-C1'-N1 | 5.29 | 112.43 | 108.20 |
| 1 | X | 2528 | G | O4'-C1'-N9 | -5.29 | 103.97 | 108.20 |
| 1 | X | 2594 | U | C4-C5-C6 | -5.29 | 116.53 | 119.70 |
| 1 | X | 70 | A | P-O5'-C5' | -5.28 | 112.45 | 120.90 |
| 1 | X | 1147 | G | O4'-C1'-N9 | 5.28 | 112.43 | 108.20 |
| 1 | X | 1489 | C | N3-C2-O2 | -5.28 | 118.20 | 121.90 |
| 1 | X | 2434 | G | N3-C4-C5 | -5.28 | 125.96 | 128.60 |
| 1 | X | 2484 | G | C8-N9-C4 | -5.28 | 104.29 | 106.40 |
| 1 | X | 943 | U | N3-C2-O2 | -5.28 | 118.50 | 122.20 |
| 1 | X | 1712 | G | O4'-C1'-N9 | 5.28 | 112.42 | 108.20 |
| 1 | X | 2044 | G | N3-C4-C5 | -5.28 | 125.96 | 128.60 |
| 1 | X | 1467 | U | C5-C4-O4 | -5.28 | 122.73 | 125.90 |
| 1 | X | 2522 | G | O4'-C1'-N9 | 5.28 | 112.42 | 108.20 |
| 1 | X | 2702 | G | P-O3'-C3' | 5.28 | 126.03 | 119.70 |
| 1 | X | 2642 | G | P-O5'-C5' | 5.27 | 129.34 | 120.90 |
| 1 | X | 574 | C | OP2-P-O3' | 5.27 | 116.80 | 105.20 |
| 1 | X | 660 | G | C8-N9-C4 | -5.27 | 104.29 | 106.40 |
| 1 | X | 2776 | U | O4'-C1'-N1 | 5.27 | 112.42 | 108.20 |
| 1 | X | 2304 | G | P-O3'-C3' | 5.27 | 126.03 | 119.70 |
| 1 | X | 1055 | A | O4'-C1'-N9 | 5.27 | 112.42 | 108.20 |
| 1 | X | 527 | C | O4'-C1'-N1 | 5.27 | 112.41 | 108.20 |
| 1 | X | 2228 | U | N3-C4-O4 | 5.27 | 123.09 | 119.40 |
| 1 | X | 2556 | A | C5'-C4'-O4' | 5.27 | 115.42 | 109.10 |
| 1 | X | 549 | G | C3'-C2'-C1' | -5.27 | 97.29 | 101.50 |
| 1 | X | 434 | C | O4'-C1'-N1 | 5.26 | 112.41 | 108.20 |
| 1 | X | 687 | G | N3-C4-N9 | 5.26 | 129.16 | 126.00 |
| 1 | X | 11 | G | C8-N9-C4 | -5.26 | 104.30 | 106.40 |
| 1 | X | 1022 | A | P-O3'-C3' | -5.26 | 113.39 | 119.70 |
| 1 | X | 1162 | A | C4'-C3'-C2' | -5.26 | 97.34 | 102.60 |
| 1 | X | 859 | U | N3-C2-O2 | -5.26 | 118.52 | 122.20 |
| 1 | X | 1306 | U | O4'-C1'-N1 | 5.26 | 112.41 | 108.20 |
| 1 | X | 2858 | A | C5-C6-N6 | -5.26 | 119.49 | 123.70 |
| 1 | X | 514 | G | N9-C1'-C2' | 5.26 | 120.83 | 114.00 |
| 11 | I | 32 | ARG | N-CA-C | -5.26 | 96.81 | 111.00 |
| 1 | X | 1032 | A | N7-C8-N9 | 5.25 | 116.43 | 113.80 |
| 1 | X | 1375 | C | O4'-C1'-N1 | 5.25 | 112.40 | 108.20 |
| 1 | X | 1524 | C | N1-C2-O2 | 5.25 | 122.05 | 118.90 |
| 1 | X | 1767 | G | C5-C6-N1 | 5.25 | 114.13 | 111.50 |
| 1 | X | 759 | C | N3-C4-C5 | -5.25 | 119.80 | 121.90 |
| 1 | X | 828 | C | N1-C2-O2 | 5.25 | 122.05 | 118.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | X | 522 | G | C5-N7-C8 | -5.25 | 101.68 | 104.30 |
| 1 | X | 579 | G | O4'-C1'-N9 | 5.25 | 112.40 | 108.20 |
| 1 | X | 2332 | G | O4'-C1'-N9 | 5.25 | 112.40 | 108.20 |
| 2 | Y | 12 | C | O4'-C4'-C3' | -5.25 | 98.75 | 104.00 |
| 1 | X | 607 | C | C3'-C2'-C1' | -5.25 | 97.30 | 101.50 |
| 1 | X | 2528 | G | OP1-P-O3' | 5.25 | 116.74 | 105.20 |
| 1 | X | 2275 | U | P-O3'-C3' | 5.24 | 125.99 | 119.70 |
| 1 | X | 2649 | A | P-O3'-C3' | -5.24 | 113.41 | 119.70 |
| 1 | X | 1642 | G | O4'-C1'-N9 | -5.24 | 104.01 | 108.20 |
| 1 | X | 2522 | G | C8-N9-C4 | -5.24 | 104.30 | 106.40 |
| 1 | X | 597 | U | O4'-C4'-C3' | -5.24 | 98.76 | 104.00 |
| 11 | I | 48 | PHE | C-N-CA | 5.24 | 134.80 | 121.70 |
| 1 | X | 1277 | G | C5-C6-N1 | 5.24 | 114.12 | 111.50 |
| 1 | X | 1729 | C | C6-N1-C2 | -5.24 | 118.20 | 120.30 |
| 1 | X | 2570 | C | O4'-C1'-N1 | 5.24 | 112.39 | 108.20 |
| 1 | X | 1303 | U | N1-C2-O2 | 5.23 | 126.46 | 122.80 |
| 1 | X | 2491 | C | C3'-C2'-C1' | -5.23 | 97.31 | 101.50 |
| 1 | X | 344 | G | N9-C1'-C2' | 5.23 | 120.80 | 114.00 |
| 1 | X | 2241 | U | N3-C4-O4 | 5.23 | 123.06 | 119.40 |
| 1 | X | 787 | A | P-O3'-C3' | 5.23 | 125.98 | 119.70 |
| 1 | X | 1319 | C | O4'-C1'-N1 | 5.23 | 112.38 | 108.20 |
| 1 | X | 542 | A | P-O3'-C3' | 5.23 | 125.97 | 119.70 |
| 1 | X | 1635 | G | C8-N9-C4 | -5.23 | 104.31 | 106.40 |
| 1 | X | 1733 | U | P-O3'-C3' | 5.23 | 125.97 | 119.70 |
| 1 | X | 2489 | C | P-O3'-C3' | -5.23 | 113.43 | 119.70 |
| 2 | Y | 46 | G | C3'-C2'-C1' | 5.23 | 105.68 | 101.50 |
| 2 | Y | 44 | C | P-O3'-C3' | 5.23 | 125.97 | 119.70 |
| 1 | X | 620 | G | P-O3'-C3' | 5.22 | 125.97 | 119.70 |
| 1 | X | 982 | C | O4'-C1'-N1 | 5.22 | 112.38 | 108.20 |
| 1 | X | 2184 | C | O4'-C1'-N1 | 5.22 | 112.38 | 108.20 |
| 1 | X | 1562 | G | C4'-C3'-C2' | 5.22 | 107.82 | 102.60 |
| 1 | X | 1918 | G | P-O3'-C3' | 5.22 | 125.97 | 119.70 |
| 1 | X | 698 | A | C1'-O4'-C4' | -5.22 | 105.72 | 109.90 |
| 1 | X | 795 | A | N1-C6-N6 | 5.22 | 121.73 | 118.60 |
| 1 | X | 1407 | G | C4-N9-C1' | 5.22 | 133.28 | 126.50 |
| 1 | X | 1986 | G | N3-C4-C5 | -5.22 | 125.99 | 128.60 |
| 1 | X | 1148 | G | C5-C6-O6 | -5.21 | 125.47 | 128.60 |
| 1 | X | 542 | A | N1-C6-N6 | 5.21 | 121.73 | 118.60 |
| 1 | X | 652 | C | C4'-C3'-C2' | 5.21 | 107.81 | 102.60 |
| 1 | X | 1249 | G | N1-C6-O6 | -5.21 | 116.77 | 119.90 |
| 1 | X | 1363 | C | O4'-C1'-N1 | 5.21 | 112.37 | 108.20 |
| 1 | X | 1721 | G | O4'-C4'-C3' | -5.21 | 98.79 | 104.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | X | 859 | U | P-O3'-C3' | 5.21 | 125.95 | 119.70 |
| 1 | X | 2812 | A | C8-N9-C4 | -5.21 | 103.72 | 105.80 |
| 1 | X | 1501 | C | O4'-C1'-N1 | 5.21 | 112.37 | 108.20 |
| 2 | Y | 22 | U | O4'-C1'-N1 | 5.21 | 112.37 | 108.20 |
| 1 | X | 200 | A | P-O3'-C3' | 5.21 | 125.95 | 119.70 |
| 1 | X | 661 | C | C6-N1-C2 | -5.21 | 118.22 | 120.30 |
| 1 | X | 746 | G | N3-C4-N9 | 5.21 | 129.12 | 126.00 |
| 1 | X | 1529 | C | O4'-C1'-N1 | 5.21 | 112.37 | 108.20 |
| 1 | X | 2646 | C | O4'-C1'-N1 | 5.21 | 112.36 | 108.20 |
| 2 | Y | 14 | C | C3'-C2'-C1' | 5.21 | 105.67 | 101.50 |
| 1 | X | 1123 | G | P-O3'-C3' | 5.20 | 125.94 | 119.70 |
| 1 | X | 2669 | C | C2-N1-C1' | 5.20 | 124.52 | 118.80 |
| 1 | X | 2748 | C | P-O3'-C3' | -5.20 | 113.46 | 119.70 |
| 2 | Y | 50 | U | C3'-C2'-C1' | -5.20 | 97.34 | 101.50 |
| 1 | X | 841 | G | C1'-O4'-C4' | -5.20 | 105.74 | 109.90 |
| 1 | X | 503 | G | O4'-C4'-C3' | -5.20 | 98.80 | 104.00 |
| 1 | X | 786 | U | O4'-C1'-N1 | 5.20 | 112.36 | 108.20 |
| 1 | X | 1470 | G | C8-N9-C4 | -5.20 | 104.32 | 106.40 |
| 1 | X | 1679 | U | C2-N3-C4 | -5.20 | 123.88 | 127.00 |
| 1 | X | 1774 | A | P-O3'-C3' | 5.20 | 125.94 | 119.70 |
| 1 | X | 2065 | A | O4'-C1'-N9 | 5.20 | 112.36 | 108.20 |
| 1 | X | 1351 | G | O4'-C1'-N9 | 5.20 | 112.36 | 108.20 |
| 1 | X | 2380 | U | O4'-C1'-N1 | 5.20 | 112.36 | 108.20 |
| 1 | X | 89 | A | N9-C1'-C2' | 5.20 | 120.75 | 114.00 |
| 1 | X | 943 | U | N1-C1'-C2' | 5.20 | 120.75 | 114.00 |
| 1 | X | 2692 | A | O3'-P-O5' | -5.20 | 94.13 | 104.00 |
| 1 | X | 623 | G | O4'-C1'-N9 | 5.19 | 112.36 | 108.20 |
| 1 | X | 518 | A | P-O5'-C5' | 5.19 | 129.21 | 120.90 |
| 1 | X | 991 | A | N9-C1'-C2' | 5.19 | 120.75 | 114.00 |
| 1 | X | 2541 | U | N3-C2-O2 | -5.19 | 118.57 | 122.20 |
| 1 | X | 420 | C | O4'-C1'-N1 | 5.19 | 112.35 | 108.20 |
| 1 | X | 594 | G | O4'-C1'-N9 | 5.18 | 112.35 | 108.20 |
| 1 | X | 1277 | G | N1-C6-O6 | -5.18 | 116.79 | 119.90 |
| 1 | X | 1467 | U | C2-N3-C4 | 5.18 | 130.11 | 127.00 |
| 1 | X | 71 | A | C4'-C3'-C2' | 5.18 | 107.78 | 102.60 |
| 1 | X | 2533 | U | N1-C2-O2 | 5.18 | 126.43 | 122.80 |
| 1 | X | 1819 | U | N3-C2-O2 | -5.18 | 118.58 | 122.20 |
| 1 | X | 2032 | G | C2'-C3'-O3' | 5.18 | 121.99 | 113.70 |
| 1 | X | 521 | U | C2-N1-C1' | 5.17 | 123.91 | 117.70 |
| 1 | X | 1006 | C | C1'-O4'-C4' | -5.17 | 105.76 | 109.90 |
| 1 | X | 2421 | C | P-O5'-C5' | 5.17 | 129.18 | 120.90 |
| 1 | X | 1219 | C | N1-C2-O2 | 5.17 | 122.00 | 118.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | X | 1770 | U | C4-C5-C6 | 5.17 | 122.80 | 119.70 |
| 1 | X | 422 | C | C6-N1-C2 | -5.17 | 118.23 | 120.30 |
| 1 | X | 1685 | A | P-O3'-C3' | 5.17 | 125.90 | 119.70 |
| 1 | X | 2569 | A | P-O5'-C5' | -5.17 | 112.63 | 120.90 |
| 1 | X | 683 | A | C4'-C3'-C2' | 5.17 | 107.77 | 102.60 |
| 1 | X | 1132 | C | C5-C6-N1 | 5.16 | 123.58 | 121.00 |
| 2 | Y | 73 | C | O4'-C1'-N1 | 5.16 | 112.33 | 108.20 |
| 1 | X | 2226 | A | C5-C6-N6 | -5.16 | 119.57 | 123.70 |
| 2 | Y | 119 | G | C3'-C2'-C1' | -5.16 | 97.37 | 101.50 |
| 1 | X | 1799 | A | O4'-C1'-N9 | 5.16 | 112.33 | 108.20 |
| 1 | X | 1222 | G | P-O3'-C3' | 5.16 | 125.89 | 119.70 |
| 1 | X | 2018 | G | C3'-C2'-C1' | -5.16 | 97.37 | 101.50 |
| 2 | Y | 53 | G | N3-C4-N9 | 5.16 | 129.09 | 126.00 |
| 1 | X | 460 | U | O5'-P-OP1 | -5.16 | 101.06 | 105.70 |
| 1 | X | 1482 | U | C1'-O4'-C4' | -5.16 | 105.77 | 109.90 |
| 1 | X | 2731 | G | O4'-C1'-N9 | 5.16 | 112.33 | 108.20 |
| 1 | X | 822 | G | C4'-C3'-C2' | -5.16 | 97.44 | 102.60 |
| 1 | X | 1312 | G | N7-C8-N9 | 5.16 | 115.68 | 113.10 |
| 2 | Y | 107 | C | P-O3'-C3' | 5.16 | 125.89 | 119.70 |
| 1 | X | 2751 | C | O4'-C1'-N1 | 5.15 | 112.32 | 108.20 |
| 2 | Y | 92 | G | C5-C6-N1 | 5.15 | 114.08 | 111.50 |
| 1 | X | 1152 | C | O4'-C1'-N1 | 5.15 | 112.32 | 108.20 |
| 1 | X | 1223 | G | N3-C2-N2 | 5.15 | 123.51 | 119.90 |
| 1 | X | 1244 | U | C5-C6-N1 | 5.15 | 125.28 | 122.70 |
| 1 | X | 1628 | C | C6-N1-C2 | -5.15 | 118.24 | 120.30 |
| 1 | X | 2525 | U | N3-C2-O2 | -5.15 | 118.60 | 122.20 |
| 1 | X | 1294 | G | O4'-C1'-N9 | 5.15 | 112.32 | 108.20 |
| 1 | X | 1327 | C | C5-C6-N1 | 5.15 | 123.57 | 121.00 |
| 1 | X | 1677 | C | C4'-C3'-C2' | -5.15 | 97.45 | 102.60 |
| 1 | X | 2782 | G | N1-C6-O6 | 5.14 | 122.99 | 119.90 |
| 1 | X | 2500 | C | N1-C2-O2 | 5.14 | 121.98 | 118.90 |
| 1 | X | 2700 | U | OP1-P-OP2 | -5.14 | 111.89 | 119.60 |
| 1 | X | 1674 | C | OP1-P-O3' | 5.14 | 116.51 | 105.20 |
| 1 | X | 927 | C | N1-C2-O2 | 5.14 | 121.98 | 118.90 |
| 1 | X | 983 | G | C8-N9-C4 | -5.14 | 104.34 | 106.40 |
| 1 | X | 1764 | A | C5-C6-N6 | -5.14 | 119.59 | 123.70 |
| 1 | X | 2699 | G | N3-C4-C5 | -5.14 | 126.03 | 128.60 |
| 1 | X | 1383 | C | N1-C2-O2 | 5.14 | 121.98 | 118.90 |
| 1 | X | 2460 | G | O4'-C1'-N9 | 5.14 | 112.31 | 108.20 |
| 1 | X | 779 | U | O4'-C1'-N1 | 5.14 | 112.31 | 108.20 |
| 1 | X | 1574 | A | P-O5'-C5' | 5.14 | 129.12 | 120.90 |
| 1 | X | 2858 | A | O4'-C1'-N9 | 5.14 | 112.31 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | X | 761 | G | C1'-O4'-C4' | -5.13 | 105.79 | 109.90 |
| 1 | X | 1988 | A | N9-C4-C5 | -5.13 | 103.75 | 105.80 |
| 1 | X | 2523 | G | C6-C5-N7 | -5.13 | 127.32 | 130.40 |
| 1 | X | 1709 | U | P-O3'-C3' | 5.13 | 125.86 | 119.70 |
| 1 | X | 1705 | U | O4'-C1'-N1 | 5.13 | 112.31 | 108.20 |
| 1 | X | 1805 | G | N3-C4-C5 | -5.13 | 126.03 | 128.60 |
| 1 | X | 1547 | U | O4'-C1'-N1 | 5.13 | 112.30 | 108.20 |
| 1 | X | 2077 | G | O4'-C1'-N9 | 5.13 | 112.30 | 108.20 |
| 1 | X | 1801 | C | P-O3'-C3' | 5.13 | 125.85 | 119.70 |
| 1 | X | 2430 | A | N1-C6-N6 | -5.13 | 115.52 | 118.60 |
| 1 | X | 957 | G | C4-C5-N7 | -5.12 | 108.75 | 110.80 |
| 1 | X | 191 | G | O4'-C1'-N9 | 5.12 | 112.30 | 108.20 |
| 1 | X | 2165 | A | C3'-C2'-C1' | 5.12 | 105.60 | 101.50 |
| 1 | X | 30 | G | N3-C4-C5 | -5.12 | 126.04 | 128.60 |
| 1 | X | 509 | U | P-O3'-C3' | 5.12 | 125.85 | 119.70 |
| 1 | X | 540 | G | N3-C4-C5 | -5.12 | 126.04 | 128.60 |
| 1 | X | 1223 | G | N3-C4-N9 | 5.12 | 129.07 | 126.00 |
| 1 | X | 459 | A | P-O3'-C3' | 5.12 | 125.84 | 119.70 |
| 1 | X | 1631 | C | O5'-C5'-C4' | -5.12 | 101.97 | 111.70 |
| 1 | X | 2847 | G | N7-C8-N9 | 5.12 | 115.66 | 113.10 |
| 1 | X | 776 | G | N9-C1'-C2' | 5.12 | 120.65 | 114.00 |
| 1 | X | 2535 | C | O4'-C1'-N1 | 5.12 | 112.29 | 108.20 |
| 1 | X | 2621 | G | OP2-P-O3' | 5.12 | 116.45 | 105.20 |
| 1 | X | 825 | C | P-O5'-C5' | 5.11 | 129.08 | 120.90 |
| 1 | X | 1245 | G | P-O3'-C3' | 5.11 | 125.84 | 119.70 |
| 1 | X | 1306 | U | C3'-C2'-C1' | -5.11 | 97.41 | 101.50 |
| 1 | X | 1094 | C | O4'-C1'-N1 | 5.11 | 112.29 | 108.20 |
| 1 | X | 1711 | C | C5'-C4'-O4' | 5.11 | 115.23 | 109.10 |
| 1 | X | 2408 | G | C2-N3-C4 | 5.11 | 114.45 | 111.90 |
| 1 | X | 2635 | U | O4'-C1'-N1 | 5.11 | 112.29 | 108.20 |
| 1 | X | 729 | A | C1'-O4'-C4' | -5.11 | 105.81 | 109.90 |
| 1 | X | 1312 | G | P-O3'-C3' | 5.11 | 125.83 | 119.70 |
| 1 | X | 538 | A | P-O3'-C3' | 5.11 | 125.83 | 119.70 |
| 1 | X | 559 | C | C6-N1-C2 | -5.11 | 118.26 | 120.30 |
| 1 | X | 2851 | G | C5-C6-O6 | -5.11 | 125.54 | 128.60 |
| 1 | X | 328 | A | C5'-C4'-O4' | 5.10 | 115.22 | 109.10 |
| 2 | Y | 54 | U | N3-C2-O2 | -5.10 | 118.63 | 122.20 |
| 2 | Y | 120 | G | O4'-C1'-N9 | 5.10 | 112.28 | 108.20 |
| 1 | X | 89 | A | C5'-C4'-O4' | 5.10 | 115.22 | 109.10 |
| 1 | X | 1149 | G | C4'-C3'-C2' | -5.10 | 97.50 | 102.60 |
| 2 | Y | 27 | A | P-O3'-C3' | 5.10 | 125.82 | 119.70 |
| 1 | X | 1012 | A | O4'-C1'-N9 | 5.10 | 112.28 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | X | 1946 | U | N3-C2-O2 | -5.10 | 118.63 | 122.20 |
| 1 | X | 2806 | G | O4'-C1'-N9 | 5.10 | 112.28 | 108.20 |
| 1 | X | 2850 | U | P-O5'-C5' | 5.10 | 129.06 | 120.90 |
| 1 | X | 2867 | G | C6-C5-N7 | -5.10 | 127.34 | 130.40 |
| 1 | X | 1682 | A | C8-N9-C4 | -5.10 | 103.76 | 105.80 |
| 1 | X | 2508 | G | N9-C1'-C2' | 5.10 | 120.63 | 114.00 |
| 1 | X | 743 | A | C3'-C2'-C1' | -5.10 | 97.42 | 101.50 |
| 1 | X | 858 | G | N7-C8-N9 | 5.10 | 115.65 | 113.10 |
| 1 | X | 1083 | C | O4'-C1'-N1 | 5.10 | 112.28 | 108.20 |
| 1 | X | 2385 | U | O4'-C1'-N1 | 5.09 | 112.28 | 108.20 |
| 1 | X | 1690 | U | N1-C1'-C2' | -5.09 | 106.40 | 112.00 |
| 1 | X | 2033 | C | O4'-C1'-N1 | 5.09 | 112.28 | 108.20 |
| 1 | X | 312 | G | O4'-C1'-N9 | 5.09 | 112.27 | 108.20 |
| 1 | X | 473 | C | O4'-C1'-N1 | 5.09 | 112.27 | 108.20 |
| 1 | X | 830 | C | N3-C2-O2 | -5.09 | 118.34 | 121.90 |
| 1 | X | 430 | C | C5-C6-N1 | 5.09 | 123.54 | 121.00 |
| 1 | X | 1980 | A | N1-C6-N6 | 5.09 | 121.65 | 118.60 |
| 1 | X | 2279 | G | C8-N9-C4 | -5.09 | 104.37 | 106.40 |
| 1 | X | 2369 | U | O4'-C1'-N1 | 5.09 | 112.27 | 108.20 |
| 1 | X | 2654 | A | P-O3'-C3' | -5.09 | 113.59 | 119.70 |
| 5 | C | 194 | GLU | C-N-CA | 5.09 | 134.42 | 121.70 |
| 1 | X | 971 | A | C2-N3-C4 | 5.08 | 113.14 | 110.60 |
| 1 | X | 1805 | G | C2-N3-C4 | 5.08 | 114.44 | 111.90 |
| 1 | X | 2033 | C | N1-C1'-C2' | 5.08 | 120.61 | 114.00 |
| 1 | X | 2463 | G | O4'-C1'-N9 | 5.08 | 112.27 | 108.20 |
| 1 | X | 745 | C | N1-C2-O2 | 5.08 | 121.95 | 118.90 |
| 1 | X | 820 | U | O4'-C1'-N1 | 5.08 | 112.27 | 108.20 |
| 1 | X | 2178 | U | O4'-C1'-N1 | 5.08 | 112.27 | 108.20 |
| 2 | Y | 123 | U | N3-C2-O2 | -5.08 | 118.64 | 122.20 |
| 1 | X | 1681 | A | C2-N3-C4 | -5.08 | 108.06 | 110.60 |
| 1 | X | 2396 | C | P-O3'-C3' | -5.08 | 113.61 | 119.70 |
| 1 | X | 2720 | A | O4'-C4'-C3' | -5.08 | 98.92 | 104.00 |
| 1 | X | 2843 | A | P-O5'-C5' | -5.08 | 112.77 | 120.90 |
| 2 | Y | 113 | G | O4'-C1'-N9 | 5.08 | 112.26 | 108.20 |
| 1 | X | 496 | C | P-O3'-C3' | -5.08 | 113.61 | 119.70 |
| 1 | X | 1504 | G | P-O3'-C3' | 5.08 | 125.79 | 119.70 |
| 1 | X | 2003 | A | C2-N3-C4 | 5.08 | 113.14 | 110.60 |
| 1 | X | 1518 | C | O4'-C1'-N1 | 5.08 | 112.26 | 108.20 |
| 1 | X | 1578 | U | O4'-C1'-N1 | 5.08 | 112.26 | 108.20 |
| 1 | X | 2818 | G | C4'-C3'-C2' | -5.08 | 97.52 | 102.60 |
| 1 | X | 855 | G | O4'-C1'-N9 | 5.07 | 112.26 | 108.20 |
| 1 | X | 2181 | A | O4'-C1'-N9 | 5.07 | 112.26 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | X | 180 | C | O4'-C1'-N1 | 5.07 | 112.26 | 108.20 |
| 1 | X | 177 | U | O4'-C1'-N1 | 5.07 | 112.26 | 108.20 |
| 1 | X | 1253 | C | O4'-C1'-N1 | 5.07 | 112.26 | 108.20 |
| 1 | X | 2777 | A | P-O3'-C3' | 5.07 | 125.78 | 119.70 |
| 1 | X | 1796 | A | O4'-C1'-N9 | 5.07 | 112.25 | 108.20 |
| 1 | X | 164 | G | C8-N9-C4 | -5.07 | 104.37 | 106.40 |
| 1 | X | 2734 | U | O4'-C1'-N1 | 5.07 | 112.25 | 108.20 |
| 1 | X | 2365 | U | O4'-C1'-N1 | 5.07 | 112.25 | 108.20 |
| 1 | X | 2482 | A | C5'-C4'-O4' | 5.07 | 115.18 | 109.10 |
| 1 | X | 2560 | G | C8-N9-C4 | -5.07 | 104.37 | 106.40 |
| 1 | X | 2858 | A | N1-C6-N6 | 5.07 | 121.64 | 118.60 |
| 1 | X | 991 | A | N1-C2-N3 | -5.06 | 126.77 | 129.30 |
| 5 | C | 171 | PRO | C-N-CA | 5.06 | 134.36 | 121.70 |
| 1 | X | 244 | C | N1-C2-O2 | 5.06 | 121.94 | 118.90 |
| 1 | X | 430 | C | C6-N1-C2 | -5.06 | 118.28 | 120.30 |
| 1 | X | 1753 | A | N7-C8-N9 | 5.06 | 116.33 | 113.80 |
| 1 | X | 756 | C | C3'-C2'-C1' | -5.06 | 97.45 | 101.50 |
| 1 | X | 1120 | C | P-O3'-C3' | 5.06 | 125.77 | 119.70 |
| 1 | X | 1753 | A | C2-N3-C4 | 5.06 | 113.13 | 110.60 |
| 1 | X | 1006 | C | O4'-C1'-N1 | 5.06 | 112.25 | 108.20 |
| 1 | X | 598 | U | C3'-C2'-C1' | -5.05 | 97.46 | 101.50 |
| 1 | X | 740 | A | N9-C1'-C2' | 5.05 | 120.57 | 114.00 |
| 1 | X | 1688 | U | C5-C6-N1 | 5.05 | 125.23 | 122.70 |
| 1 | X | 172 | A | P-O5'-C5' | 5.05 | 128.99 | 120.90 |
| 1 | X | 611 | C | C3'-C2'-C1' | -5.05 | 97.46 | 101.50 |
| 1 | X | 738 | G | N3-C4-C5 | -5.05 | 126.07 | 128.60 |
| 1 | X | 1124 | U | O4'-C1'-N1 | 5.05 | 112.24 | 108.20 |
| 1 | X | 174 | A | O5'-P-OP2 | -5.05 | 101.15 | 105.70 |
| 1 | X | 1159 | U | O4'-C1'-N1 | 5.05 | 112.24 | 108.20 |
| 1 | X | 2002 | A | C5-C6-N6 | -5.05 | 119.66 | 123.70 |
| 1 | X | 2229 | G | C2-N3-C4 | 5.05 | 114.43 | 111.90 |
| 1 | X | 2869 | U | O4'-C1'-N1 | 5.05 | 112.24 | 108.20 |
| 1 | X | 131 | C | O4'-C1'-N1 | 5.05 | 112.24 | 108.20 |
| 1 | X | 223 | C | C6-N1-C2 | -5.05 | 118.28 | 120.30 |
| 1 | X | 2762 | G | C6-C5-N7 | -5.05 | 127.37 | 130.40 |
| 1 | X | 542 | A | N1-C2-N3 | 5.05 | 131.82 | 129.30 |
| 1 | X | 972 | C | N1-C1'-C2' | 5.05 | 120.56 | 114.00 |
| 1 | X | 1712 | G | C6-C5-N7 | -5.05 | 127.37 | 130.40 |
| 1 | X | 2002 | A | N1-C6-N6 | 5.05 | 121.63 | 118.60 |
| 1 | X | 2608 | A | C1'-O4'-C4' | -5.05 | 105.86 | 109.90 |
| 1 | X | 203 | G | C4'-C3'-C2' | -5.05 | 97.55 | 102.60 |
| 1 | X | 654 | A | O4'-C1'-N9 | 5.05 | 112.24 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | X | 778 | G | C4'-C3'-C2' | -5.05 | 97.55 | 102.60 |
| 1 | X | 1764 | A | C4-C5-N7 | 5.05 | 113.22 | 110.70 |
| 1 | X | 334 | G | N3-C4-C5 | -5.04 | 126.08 | 128.60 |
| 1 | X | 1467 | U | O4'-C1'-C2' | -5.04 | 100.75 | 105.80 |
| 1 | X | 469 | G | N3-C4-C5 | -5.04 | 126.08 | 128.60 |
| 1 | X | 1613 | G | C5'-C4'-O4' | 5.04 | 115.15 | 109.10 |
| 1 | X | 2371 | A | N7-C8-N9 | 5.04 | 116.32 | 113.80 |
| 1 | X | 2670 | C | N3-C2-O2 | -5.04 | 118.37 | 121.90 |
| 1 | X | 2422 | C | O4'-C1'-N1 | 5.04 | 112.23 | 108.20 |
| 1 | X | 539 | A | P-O3'-C3' | 5.04 | 125.75 | 119.70 |
| 1 | X | 699 | G | C2-N3-C4 | -5.04 | 109.38 | 111.90 |
| 1 | X | 1570 | C | N1-C2-O2 | 5.04 | 121.92 | 118.90 |
| 1 | X | 1592 | U | O4'-C1'-N1 | 5.04 | 112.23 | 108.20 |
| 1 | X | 2387 | U | O4'-C1'-N1 | 5.04 | 112.23 | 108.20 |
| 1 | X | 1229 | C | O4'-C1'-N1 | 5.04 | 112.23 | 108.20 |
| 1 | X | 774 | A | C5'-C4'-O4' | 5.04 | 115.14 | 109.10 |
| 1 | X | 1407 | G | N9-C1'-C2' | 5.04 | 120.55 | 114.00 |
| 1 | X | 1541 | G | C4'-C3'-C2' | -5.04 | 97.56 | 102.60 |
| 2 | Y | 97 | C | N1-C2-O2 | 5.04 | 121.92 | 118.90 |
| 1 | X | 1280 | U | P-O3'-C3' | 5.03 | 125.74 | 119.70 |
| 1 | X | 2261 | G | C5-C6-N1 | 5.03 | 114.02 | 111.50 |
| 1 | X | 1716 | G | C8-N9-C4 | -5.03 | 104.39 | 106.40 |
| 1 | X | 344 | G | C8-N9-C4 | -5.03 | 104.39 | 106.40 |
| 1 | X | 1304 | U | O4'-C1'-N1 | 5.03 | 112.22 | 108.20 |
| 1 | X | 469 | G | C2'-C3'-O3' | 5.03 | 121.75 | 113.70 |
| 1 | X | 1376 | C | N1-C2-O2 | 5.03 | 121.92 | 118.90 |
| 1 | X | 2299 | A | P-O3'-C3' | 5.03 | 125.73 | 119.70 |
| 1 | X | 2347 | C | C3'-C2'-C1' | -5.03 | 97.48 | 101.50 |
| 1 | X | 2044 | G | C6-C5-N7 | -5.03 | 127.38 | 130.40 |
| 1 | X | 2069 | U | O4'-C1'-N1 | 5.03 | 112.22 | 108.20 |
| 1 | X | 2592 | U | O4'-C1'-N1 | 5.03 | 112.22 | 108.20 |
| 1 | X | 2090 | U | O4'-C1'-N1 | 5.03 | 112.22 | 108.20 |
| 1 | X | 2230 | G | C3'-C2'-C1' | -5.03 | 97.48 | 101.50 |
| 1 | X | 2453 | C | N1-C2-O2 | 5.03 | 121.92 | 118.90 |
| 1 | X | 2553 | G | C5-N7-C8 | -5.02 | 101.79 | 104.30 |
| 1 | X | 2800 | C | C5'-C4'-C3' | -5.02 | 107.97 | 116.00 |
| 1 | X | 404 | A | O4'-C1'-N9 | 5.02 | 112.22 | 108.20 |
| 1 | X | 2587 | G | N1-C6-O6 | 5.02 | 122.91 | 119.90 |
| 2 | Y | 39 | C | N1-C2-O2 | 5.02 | 121.91 | 118.90 |
| 1 | X | 1244 | U | O4'-C1'-N1 | 5.02 | 112.21 | 108.20 |
| 1 | X | 1347 | C | OP2-P-O3' | 5.02 | 116.24 | 105.20 |
| 1 | X | 1828 | C | N1-C2-O2 | 5.02 | 121.91 | 118.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | X | 2032 | G | N3-C4-N9 | 5.02 | 129.01 | 126.00 |
| 1 | X | 2222 | U | N3-C2-O2 | -5.02 | 118.69 | 122.20 |
| 1 | X | 2567 | G | O4'-C1'-N9 | 5.02 | 112.21 | 108.20 |
| 1 | X | 2572 | U | N3-C4-O4 | 5.02 | 122.91 | 119.40 |
| 1 | X | 823 | U | OP1-P-O3' | 5.01 | 116.23 | 105.20 |
| 1 | X | 1201 | G | N1-C6-O6 | 5.01 | 122.91 | 119.90 |
| 2 | Y | 14 | C | N1-C2-O2 | 5.01 | 121.91 | 118.90 |
| 1 | X | 7 | G | C4'-C3'-C2' | 5.01 | 107.61 | 102.60 |
| 1 | X | 2327 | U | N3-C2-O2 | -5.01 | 118.69 | 122.20 |
| 1 | X | 610 | G | O3'-P-O5' | -5.01 | 94.48 | 104.00 |
| 1 | X | 752 | G | O3'-P-O5' | -5.01 | 94.48 | 104.00 |
| 1 | X | 1665 | C | P-O5'-C5' | 5.01 | 128.91 | 120.90 |
| 1 | X | 1956 | G | C5-C6-O6 | -5.01 | 125.59 | 128.60 |
| 1 | X | 130 | C | O4'-C1'-N1 | 5.01 | 112.21 | 108.20 |
| 1 | X | 1333 | G | C6-C5-N7 | 5.01 | 133.41 | 130.40 |
| 1 | X | 1729 | C | O4'-C1'-N1 | 5.01 | 112.21 | 108.20 |
| 1 | X | 2239 | C | N1-C2-O2 | 5.01 | 121.91 | 118.90 |
| 1 | X | 462 | G | C4-C5-N7 | -5.01 | 108.80 | 110.80 |
| 1 | X | 1683 | G | N9-C4-C5 | 5.01 | 107.40 | 105.40 |
| 1 | X | 2423 | G | O5'-P-OP2 | -5.01 | 101.19 | 105.70 |
| 1 | X | 2561 | G | C4-C5-N7 | 5.01 | 112.80 | 110.80 |
| 1 | X | 614 | G | O4'-C1'-N9 | 5.00 | 112.20 | 108.20 |
| 1 | X | 2621 | G | N3-C4-C5 | -5.00 | 126.10 | 128.60 |
| 14 | L | 20 | THR | C-N-CA | 5.00 | 134.21 | 121.70 |
| 1 | X | 225 | G | O4'-C1'-N9 | 5.00 | 112.20 | 108.20 |
| 1 | X | 2039 | G | N7-C8-N9 | 5.00 | 115.60 | 113.10 |
| 1 | X | 2075 | U | O4'-C1'-N1 | 5.00 | 112.20 | 108.20 |
| 1 | X | 2188 | A | O4'-C1'-N9 | 5.00 | 112.20 | 108.20 |
| 1 | X | 2193 | C | N1-C2-O2 | 5.00 | 121.90 | 118.90 |
| 1 | X | 454 | G | C2'-C3'-O3' | 5.00 | 121.70 | 113.70 |

There are no chirality outliers.

All (6) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|------|------|-----------|
| 1 | X | 1143 | A | Sidechain |
| 1 | X | 1337 | G | Sidechain |
| 1 | X | 474 | G | Sidechain |
| 1 | X | 671 | A | Sidechain |
| 1 | X | 683 | A | Sidechain |
| 1 | X | 805 | G | Sidechain |

5.2 Close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | X | 57651 | 0 | 29049 | 404 | 0 |
| 2 | Y | 2598 | 0 | 1328 | 17 | 0 |
| 3 | A | 1826 | 0 | 1885 | 61 | 0 |
| 4 | B | 1539 | 0 | 1600 | 61 | 0 |
| 5 | C | 1506 | 0 | 1525 | 49 | 0 |
| 6 | D | 1400 | 0 | 1481 | 22 | 0 |
| 7 | E | 1286 | 0 | 1336 | 10 | 0 |
| 8 | F | 503 | 0 | 520 | 5 | 0 |
| 9 | G | 1114 | 0 | 1144 | 68 | 0 |
| 10 | H | 997 | 0 | 1046 | 31 | 0 |
| 11 | I | 1067 | 0 | 1103 | 37 | 0 |
| 12 | J | 1090 | 0 | 1125 | 36 | 0 |
| 13 | K | 878 | 0 | 930 | 36 | 0 |
| 14 | L | 779 | 0 | 820 | 25 | 0 |
| 15 | M | 871 | 0 | 894 | 25 | 0 |
| 16 | N | 978 | 0 | 1020 | 33 | 0 |
| 17 | O | 741 | 0 | 756 | 34 | 0 |
| 18 | P | 1014 | 0 | 1096 | 20 | 0 |
| 19 | Q | 726 | 0 | 753 | 15 | 0 |
| 20 | R | 825 | 0 | 881 | 27 | 0 |
| 21 | S | 1345 | 0 | 1372 | 18 | 0 |
| 22 | T | 625 | 0 | 655 | 11 | 0 |
| 23 | U | 552 | 0 | 604 | 26 | 0 |
| 24 | V | 533 | 0 | 558 | 5 | 0 |
| 25 | W | 424 | 0 | 470 | 8 | 0 |
| 26 | Z | 457 | 0 | 462 | 12 | 0 |
| 27 | 1 | 53 | 0 | 0 | 1 | 0 |
| 28 | 2 | 46 | 0 | 0 | 2 | 0 |
| 29 | 3 | 63 | 0 | 0 | 3 | 0 |
| 30 | 4 | 297 | 0 | 330 | 5 | 0 |
| 31 | J | 1 | 0 | 0 | 0 | 0 |
| 31 | M | 1 | 0 | 0 | 0 | 0 |
| 31 | X | 28 | 0 | 0 | 0 | 0 |
| 31 | Y | 5 | 0 | 0 | 0 | 0 |
| 32 | X | 56 | 0 | 64 | 3 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| All | All | 83875 | 0 | 54807 | 954 | 0 |

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (954) close contacts within the same asymmetric unit are listed below.

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 15:M:57:ILE:CD1 | 15:M:57:ILE:CG1 | 1.79 | 1.58 |
| 13:K:52:ILE:CD1 | 13:K:52:ILE:CG1 | 1.95 | 1.45 |
| 11:I:57:ILE:CD1 | 11:I:57:ILE:CG1 | 1.92 | 1.45 |
| 9:G:100:TYR:HB2 | 9:G:116:ARG:NH1 | 1.66 | 1.08 |
| 11:I:62:LYS:HE2 | 11:I:64:GLY:HA2 | 1.34 | 1.03 |
| 1:X:787:A:H2 | 1:X:800:U:HO2' | 1.06 | 1.03 |
| 1:X:1333:G:N2 | 1:X:1344:C:H41 | 1.55 | 1.03 |
| 1:X:1882:G:N2 | 1:X:1885:C:H41 | 1.55 | 1.03 |
| 23:U:31:GLY:HA2 | 23:U:32:ARG:HH11 | 1.18 | 1.02 |
| 4:B:152:LYS:HB2 | 9:G:106:TYR:HB3 | 1.42 | 1.01 |
| 1:X:617:U:H5 | 1:X:632:A:C2 | 1.82 | 0.97 |
| 11:I:62:LYS:CE | 11:I:64:GLY:HA2 | 1.97 | 0.95 |
| 3:A:43:ARG:N | 3:A:43:ARG:HD2 | 1.82 | 0.95 |
| 1:X:1919:A:H2 | 1:X:1926:U:H3 | 0.97 | 0.94 |
| 26:Z:4:HIS:HB3 | 26:Z:5:PRO:HD3 | 1.49 | 0.94 |
| 17:O:87:ARG:HG2 | 17:O:87:ARG:HH11 | 1.32 | 0.94 |
| 1:X:1030:U:H3 | 1:X:1153:A:H62 | 1.12 | 0.91 |
| 3:A:247:VAL:HG23 | 3:A:248:THR:HG23 | 1.52 | 0.91 |
| 1:X:1033:G:H22 | 1:X:1153:A:H2 | 1.20 | 0.90 |
| 1:X:2371:A:H2 | 1:X:2403:C:H42 | 1.19 | 0.90 |
| 1:X:1466:C:H2' | 1:X:1467:U:O4' | 1.73 | 0.89 |
| 9:G:61:ARG:HH11 | 9:G:66:HIS:H | 1.15 | 0.89 |
| 9:G:100:TYR:HB2 | 9:G:116:ARG:HH12 | 1.35 | 0.89 |
| 4:B:116:VAL:HG22 | 4:B:136:ARG:HE | 1.36 | 0.88 |
| 14:L:38:ILE:HG13 | 14:L:39:TYR:H | 1.37 | 0.87 |
| 17:O:5:ILE:HD12 | 17:O:6:GLN:H | 1.41 | 0.86 |
| 1:X:1542:G:H22 | 1:X:1562:G:H1 | 0.92 | 0.86 |
| 3:A:43:ARG:HD2 | 3:A:43:ARG:H | 1.39 | 0.85 |
| 4:B:32:PRO:HB3 | 4:B:72:VAL:HG11 | 1.55 | 0.85 |
| 13:K:17:ARG:NH1 | 13:K:20:LEU:HD23 | 1.91 | 0.85 |
| 32:X:2929:1F2:H9 | 32:X:2929:1F2:H54 | 1.58 | 0.85 |
| 3:A:231:HIS:HD2 | 3:A:233:HIS:H | 1.24 | 0.85 |
| 1:X:1030:U:H3 | 1:X:1153:A:N6 | 1.75 | 0.84 |
| 3:A:210:GLY:HA2 | 3:A:213:ARG:HB2 | 1.59 | 0.84 |
| 1:X:1919:A:H2 | 1:X:1926:U:N3 | 1.74 | 0.84 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 19:Q:61:LYS:H | 19:Q:72:ARG:HA | 1.42 | 0.83 |
| 1:X:559:C:H2' | 1:X:560:G:C1' | 2.08 | 0.83 |
| 1:X:215:G:H21 | 1:X:632:A:H8 | 1.25 | 0.83 |
| 1:X:1468:A:H5' | 1:X:1472:C:N4 | 1.94 | 0.83 |
| 1:X:1007:A:H1' | 17:O:6:GLN:HG2 | 1.61 | 0.83 |
| 1:X:1333:G:H22 | 1:X:1344:C:H41 | 1.26 | 0.82 |
| 1:X:1494:G:HO2' | 1:X:1574:A:H2 | 1.26 | 0.82 |
| 9:G:33:ILE:HB | 9:G:34:PRO:HD3 | 1.61 | 0.82 |
| 9:G:108:GLY:H | 9:G:110:LEU:HG | 1.45 | 0.82 |
| 1:X:1333:G:H22 | 1:X:1344:C:N4 | 1.78 | 0.82 |
| 13:K:17:ARG:HH11 | 13:K:20:LEU:HD23 | 1.41 | 0.81 |
| 4:B:116:VAL:HG22 | 4:B:136:ARG:NE | 1.95 | 0.81 |
| 1:X:1333:G:N2 | 1:X:1344:C:N4 | 2.28 | 0.81 |
| 13:K:3:HIS:HB3 | 13:K:5:LYS:HD2 | 1.62 | 0.79 |
| 1:X:774:A:H8 | 1:X:774:A:O5' | 1.65 | 0.78 |
| 1:X:559:C:H2' | 1:X:560:G:H1' | 1.66 | 0.78 |
| 9:G:93:LYS:HG2 | 9:G:96:ASP:HB3 | 1.65 | 0.78 |
| 1:X:2266:A:H62 | 1:X:2323:U:H3 | 1.29 | 0.77 |
| 3:A:244:ARG:HB3 | 3:A:252:LYS:HZ1 | 1.49 | 0.77 |
| 9:G:106:TYR:O | 9:G:110:LEU:HG | 1.85 | 0.77 |
| 3:A:231:HIS:CD2 | 3:A:233:HIS:H | 2.03 | 0.77 |
| 1:X:1142:G:H21 | 9:G:101:THR:CG2 | 1.99 | 0.76 |
| 10:H:13:ASN:HD21 | 10:H:109:ARG:HG2 | 1.50 | 0.76 |
| 23:U:48:LYS:HG2 | 23:U:49:LYS:H | 1.50 | 0.76 |
| 9:G:61:ARG:NH1 | 9:G:66:HIS:H | 1.84 | 0.76 |
| 5:C:148:VAL:HG13 | 5:C:185:ARG:HB2 | 1.66 | 0.76 |
| 13:K:11:ASN:OD1 | 13:K:17:ARG:NH2 | 2.18 | 0.76 |
| 1:X:2797:G:OP2 | 13:K:3:HIS:NE2 | 2.18 | 0.76 |
| 4:B:147:PRO:C | 4:B:149:ARG:H | 1.88 | 0.75 |
| 12:J:78:LYS:HA | 12:J:88:LYS:HZ3 | 1.49 | 0.75 |
| 20:R:107:ALA:HB1 | 20:R:111:GLY:HA2 | 1.68 | 0.75 |
| 23:U:31:GLY:HA2 | 23:U:32:ARG:NH1 | 1.99 | 0.74 |
| 1:X:2042:A:H5'' | 5:C:65:GLY:HA2 | 1.70 | 0.74 |
| 1:X:83:A:H5'' | 20:R:17:LYS:HG2 | 1.70 | 0.74 |
| 9:G:132:PHE:CZ | 9:G:145:HIS:HB2 | 2.23 | 0.74 |
| 4:B:54:LYS:HB2 | 4:B:75:THR:O | 1.88 | 0.74 |
| 1:X:1882:G:H22 | 1:X:1885:C:H41 | 1.31 | 0.73 |
| 1:X:631:G:H4' | 1:X:632:A:H5' | 1.70 | 0.73 |
| 4:B:152:LYS:CB | 9:G:106:TYR:HB3 | 2.18 | 0.73 |
| 16:N:61:TRP:HH2 | 16:N:94:VAL:H | 1.37 | 0.73 |
| 25:W:12:ARG:CG | 25:W:12:ARG:HH11 | 2.01 | 0.73 |
| 16:N:66:ASN:HB3 | 16:N:76:TYR:HB2 | 1.70 | 0.73 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:X:1770:U:H5 | 1:X:1775:A:N7 | 1.86 | 0.72 |
| 12:J:40:PRO:HB3 | 12:J:99:LYS:HD2 | 1.71 | 0.72 |
| 1:X:1373:G:H22 | 1:X:2192:U:H3 | 1.37 | 0.72 |
| 9:G:100:TYR:HB2 | 9:G:116:ARG:HH11 | 1.52 | 0.72 |
| 1:X:1266:G:N7 | 11:I:32:ARG:NH1 | 2.38 | 0.71 |
| 17:O:87:ARG:NH1 | 17:O:87:ARG:HG2 | 2.01 | 0.71 |
| 1:X:1142:G:H21 | 9:G:101:THR:HG22 | 1.54 | 0.71 |
| 5:C:43:ALA:HB1 | 5:C:86:PRO:HB2 | 1.72 | 0.71 |
| 1:X:2691:C:OP1 | 1:X:2694:G:H4' | 1.90 | 0.71 |
| 12:J:27:TYR:HB2 | 12:J:137:VAL:HG21 | 1.72 | 0.71 |
| 1:X:1542:G:N2 | 1:X:1562:G:H1 | 1.78 | 0.70 |
| 14:L:8:ARG:HG3 | 14:L:9:ARG:N | 2.06 | 0.70 |
| 1:X:823:U:OP1 | 11:I:32:ARG:NH1 | 2.24 | 0.70 |
| 6:D:4:LEU:HG | 6:D:5:LYS:H | 1.57 | 0.70 |
| 1:X:512:A:H4' | 18:P:15:LYS:HB3 | 1.73 | 0.70 |
| 1:X:1448:A:H61 | 1:X:1574:A:H61 | 1.37 | 0.70 |
| 29:3:15:LYS:CA | 29:3:16:ILE:CA | 2.70 | 0.70 |
| 1:X:2241:U:H5 | 22:T:17:ASN:OD1 | 1.75 | 0.70 |
| 4:B:7:THR:HG21 | 15:M:5:ILE:HD11 | 1.74 | 0.70 |
| 1:X:542:A:C2 | 1:X:2004:U:H2' | 2.27 | 0.69 |
| 1:X:227:G:H2' | 1:X:228:A:C8 | 2.27 | 0.69 |
| 4:B:152:LYS:HB2 | 9:G:106:TYR:CB | 2.22 | 0.69 |
| 9:G:104:THR:OG1 | 9:G:110:LEU:HB3 | 1.93 | 0.69 |
| 1:X:2561:G:H8 | 1:X:2561:G:H5' | 1.55 | 0.69 |
| 3:A:172:TYR:HA | 3:A:186:HIS:HA | 1.73 | 0.69 |
| 7:E:107:ILE:HD11 | 7:E:151:VAL:HG12 | 1.74 | 0.69 |
| 25:W:12:ARG:HG2 | 25:W:12:ARG:HH11 | 1.57 | 0.69 |
| 1:X:2368:G:H5'' | 1:X:2369:U:H5' | 1.72 | 0.69 |
| 12:J:27:TYR:CB | 12:J:137:VAL:HG21 | 2.22 | 0.69 |
| 14:L:8:ARG:HG3 | 14:L:9:ARG:H | 1.57 | 0.69 |
| 1:X:558:G:H4' | 1:X:559:C:H5' | 1.76 | 0.68 |
| 1:X:1673:C:H5'' | 4:B:136:ARG:HD3 | 1.76 | 0.68 |
| 17:O:88:GLN:HE21 | 17:O:88:GLN:HA | 1.58 | 0.68 |
| 15:M:34:ARG:NH2 | 15:M:88:VAL:HG13 | 2.08 | 0.68 |
| 17:O:12:TYR:HB2 | 17:O:40:VAL:H | 1.58 | 0.68 |
| 22:T:23:VAL:HA | 22:T:38:VAL:HG23 | 1.74 | 0.68 |
| 1:X:1745:C:P | 15:M:101:ARG:HH22 | 2.16 | 0.68 |
| 26:Z:4:HIS:HB3 | 26:Z:5:PRO:CD | 2.24 | 0.68 |
| 11:I:62:LYS:NZ | 11:I:64:GLY:HA2 | 2.09 | 0.68 |
| 23:U:32:ARG:HG2 | 23:U:33:LYS:H | 1.58 | 0.68 |
| 1:X:1675:C:OP1 | 4:B:134:TRP:CE2 | 2.46 | 0.68 |
| 1:X:2653:A:O2' | 10:H:41:ASN:ND2 | 2.27 | 0.68 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:X:2561:G:H5' | 1:X:2561:G:C8 | 2.29 | 0.67 |
| 20:R:23:ILE:HG22 | 20:R:33:THR:HB | 1.75 | 0.67 |
| 1:X:504:G:H21 | 18:P:78:ASN:HD21 | 1.42 | 0.67 |
| 10:H:13:ASN:ND2 | 10:H:109:ARG:HG2 | 2.09 | 0.67 |
| 5:C:45:THR:HG21 | 5:C:85:GLY:HA3 | 1.75 | 0.67 |
| 11:I:32:ARG:HD2 | 17:O:79:GLN:NE2 | 2.09 | 0.67 |
| 1:X:652:C:H42 | 1:X:657:A:H61 | 1.42 | 0.67 |
| 1:X:2387:U:H2' | 1:X:2388:G:H8 | 1.58 | 0.67 |
| 9:G:67:ARG:HG2 | 9:G:70:PHE:HA | 1.77 | 0.67 |
| 4:B:16:LYS:HB2 | 4:B:21:ILE:HD11 | 1.77 | 0.66 |
| 1:X:1882:G:H21 | 1:X:1885:C:H41 | 1.43 | 0.66 |
| 1:X:1257:U:H5'' | 11:I:17:LYS:HG3 | 1.77 | 0.66 |
| 1:X:1673:C:H5'' | 4:B:136:ARG:CD | 2.26 | 0.66 |
| 1:X:1673:C:C5' | 4:B:136:ARG:HD2 | 2.25 | 0.66 |
| 3:A:218:LYS:HE3 | 3:A:221:GLN:HB2 | 1.76 | 0.66 |
| 1:X:323:G:OP1 | 1:X:343:A:H5'' | 1.94 | 0.66 |
| 5:C:137:ALA:HB1 | 5:C:142:LEU:HB2 | 1.77 | 0.66 |
| 5:C:112:GLN:HA | 5:C:116:LYS:HD3 | 1.78 | 0.66 |
| 17:O:57:GLN:H | 17:O:97:GLY:HA3 | 1.61 | 0.66 |
| 1:X:1673:C:C5' | 4:B:136:ARG:CD | 2.74 | 0.66 |
| 1:X:1744:G:OP1 | 15:M:100:ARG:HD2 | 1.96 | 0.66 |
| 1:X:1770:U:C5 | 1:X:1775:A:N7 | 2.64 | 0.65 |
| 1:X:617:U:C5 | 1:X:632:A:C2 | 2.74 | 0.65 |
| 1:X:1673:C:H5' | 4:B:136:ARG:HD2 | 1.79 | 0.65 |
| 1:X:2594:U:H2' | 1:X:2595:C:H6 | 1.61 | 0.65 |
| 1:X:2319:G:H2' | 1:X:2320:G:H8 | 1.61 | 0.65 |
| 20:R:90:LYS:HB2 | 20:R:108:VAL:HG21 | 1.78 | 0.65 |
| 1:X:640:C:H4' | 1:X:660:G:H21 | 1.62 | 0.65 |
| 1:X:320:A:N3 | 1:X:340:G:O2' | 2.29 | 0.64 |
| 14:L:38:ILE:HG13 | 14:L:39:TYR:N | 2.11 | 0.64 |
| 1:X:1753:A:O5' | 1:X:1753:A:H8 | 1.81 | 0.64 |
| 4:B:134:TRP:H | 4:B:134:TRP:HD1 | 1.45 | 0.64 |
| 9:G:33:ILE:HB | 9:G:34:PRO:CD | 2.27 | 0.64 |
| 20:R:10:HIS:HD2 | 20:R:44:GLN:NE2 | 1.96 | 0.64 |
| 3:A:200:GLU:HG3 | 3:A:202:LYS:HB2 | 1.80 | 0.64 |
| 3:A:86:PRO:O | 3:A:87:ASN:HB2 | 1.97 | 0.64 |
| 6:D:80:ARG:HD3 | 6:D:83:MET:HB2 | 1.80 | 0.63 |
| 23:U:52:ARG:HG3 | 23:U:79:GLU:HA | 1.80 | 0.63 |
| 1:X:1468:A:H5' | 1:X:1472:C:H42 | 1.64 | 0.63 |
| 1:X:482:A:H2' | 1:X:483:A:O4' | 1.98 | 0.63 |
| 13:K:3:HIS:CG | 13:K:5:LYS:HZ2 | 2.15 | 0.63 |
| 1:X:564:U:H2' | 1:X:565:A:C8 | 2.34 | 0.63 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:X:1113:C:H2' | 1:X:1114:A:H8 | 1.64 | 0.63 |
| 17:O:87:ARG:CG | 17:O:87:ARG:HH11 | 2.10 | 0.62 |
| 5:C:148:VAL:O | 5:C:167:VAL:HA | 2.00 | 0.62 |
| 13:K:11:ASN:ND2 | 13:K:12:ARG:HE | 1.97 | 0.62 |
| 23:U:22:GLY:HA3 | 23:U:39:LYS:HD2 | 1.82 | 0.62 |
| 9:G:107:GLN:HA | 9:G:110:LEU:HB2 | 1.81 | 0.62 |
| 1:X:2477:C:H5' | 1:X:2477:C:H6 | 1.65 | 0.62 |
| 1:X:2042:A:H5'' | 5:C:65:GLY:CA | 2.30 | 0.62 |
| 11:I:18:ARG:HB3 | 11:I:21:ARG:HB2 | 1.81 | 0.62 |
| 2:Y:30:C:OP1 | 14:L:37:HIS:HB3 | 2.00 | 0.62 |
| 1:X:504:G:H4' | 18:P:27:VAL:HG13 | 1.81 | 0.62 |
| 10:H:98:ILE:HG22 | 10:H:106:ARG:HG3 | 1.81 | 0.62 |
| 1:X:971:A:H61 | 12:J:83:ARG:HH22 | 1.47 | 0.62 |
| 13:K:79:VAL:HA | 13:K:83:VAL:HG13 | 1.81 | 0.62 |
| 19:Q:53:ILE:HD13 | 19:Q:80:VAL:HG13 | 1.80 | 0.62 |
| 1:X:1737:G:H2' | 1:X:1738:U:C6 | 2.36 | 0.61 |
| 1:X:2790:C:O2' | 26:Z:43:HIS:HD2 | 1.83 | 0.61 |
| 1:X:2659:C:H5' | 4:B:189:PRO:HA | 1.82 | 0.61 |
| 11:I:17:LYS:O | 11:I:18:ARG:HB2 | 2.00 | 0.61 |
| 1:X:2779:C:H2' | 1:X:2780:A:C8 | 2.36 | 0.61 |
| 11:I:62:LYS:HG2 | 11:I:64:GLY:H | 1.66 | 0.61 |
| 1:X:2222:U:H2' | 1:X:2223:U:C6 | 2.35 | 0.61 |
| 4:B:152:LYS:H | 9:G:106:TYR:HB3 | 1.65 | 0.60 |
| 1:X:559:C:H2' | 1:X:560:G:O4' | 2.01 | 0.60 |
| 17:O:73:LYS:HB2 | 17:O:82:ARG:HB2 | 1.82 | 0.60 |
| 16:N:93:LYS:HD3 | 17:O:5:ILE:HB | 1.84 | 0.60 |
| 23:U:22:GLY:HA3 | 23:U:39:LYS:CD | 2.31 | 0.60 |
| 3:A:226:MET:HG2 | 3:A:230:ASP:HB2 | 1.84 | 0.60 |
| 2:Y:45:C:H2' | 6:D:92:ARG:NH1 | 2.17 | 0.60 |
| 32:X:2929:1F2:H9 | 32:X:2929:1F2:C43 | 2.29 | 0.60 |
| 4:B:75:THR:O | 4:B:76:ARG:HB2 | 2.00 | 0.60 |
| 1:X:857:U:H3' | 1:X:858:G:C8 | 2.37 | 0.60 |
| 3:A:58:HIS:O | 3:A:58:HIS:ND1 | 2.35 | 0.60 |
| 14:L:38:ILE:HG21 | 14:L:71:VAL:HG21 | 1.84 | 0.60 |
| 1:X:954:U:OP2 | 11:I:38:LYS:HG2 | 2.01 | 0.60 |
| 10:H:83:ARG:HH21 | 10:H:89:ILE:HD11 | 1.67 | 0.59 |
| 1:X:689:A:H8 | 1:X:2052:G:H21 | 1.50 | 0.59 |
| 1:X:636:G:H8 | 1:X:636:G:H5'' | 1.67 | 0.59 |
| 1:X:2845:C:H5'' | 13:K:65:LEU:HD11 | 1.84 | 0.59 |
| 1:X:2044:G:OP1 | 5:C:62:LYS:NZ | 2.36 | 0.59 |
| 3:A:45:ASN:CG | 3:A:46:ARG:H | 2.05 | 0.59 |
| 12:J:19:THR:HG23 | 12:J:99:LYS:HD3 | 1.84 | 0.59 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:X:1811:A:H5'' | 3:A:161:THR:HG21 | 1.83 | 0.59 |
| 1:X:2795:A:H4' | 13:K:5:LYS:HG2 | 1.83 | 0.59 |
| 4:B:122:PHE:O | 4:B:123:ALA:HB2 | 2.02 | 0.59 |
| 6:D:75:SER:HB2 | 6:D:79:LEU:HD13 | 1.82 | 0.59 |
| 1:X:793:G:H21 | 1:X:796:A:H62 | 1.50 | 0.59 |
| 14:L:33:ARG:CZ | 14:L:38:ILE:HB | 2.33 | 0.59 |
| 1:X:1173:G:H21 | 17:O:88:GLN:HE22 | 1.50 | 0.59 |
| 1:X:172:A:H61 | 1:X:175:C:H3' | 1.68 | 0.59 |
| 1:X:1466:C:C2' | 1:X:1467:U:O4' | 2.47 | 0.59 |
| 13:K:3:HIS:CG | 13:K:5:LYS:NZ | 2.70 | 0.59 |
| 5:C:164:VAL:C | 5:C:166:TRP:H | 2.05 | 0.59 |
| 1:X:2310:G:H4' | 22:T:43:THR:H | 1.68 | 0.59 |
| 16:N:37:GLN:HA | 16:N:40:LEU:HD12 | 1.85 | 0.59 |
| 14:L:38:ILE:HG13 | 14:L:40:ALA:H | 1.67 | 0.59 |
| 1:X:1448:A:H61 | 1:X:1574:A:N6 | 2.01 | 0.59 |
| 23:U:27:ASP:H | 23:U:32:ARG:HH21 | 1.51 | 0.58 |
| 1:X:692:C:H2' | 1:X:693:A:H8 | 1.68 | 0.58 |
| 1:X:1142:G:OP1 | 9:G:107:GLN:O | 2.21 | 0.58 |
| 1:X:746:G:N7 | 1:X:774:A:C6 | 2.71 | 0.58 |
| 1:X:333:A:H2' | 5:C:162:ARG:HH12 | 1.68 | 0.58 |
| 16:N:93:LYS:CE | 17:O:5:ILE:HD13 | 2.34 | 0.58 |
| 16:N:93:LYS:HE3 | 17:O:5:ILE:HD13 | 1.85 | 0.58 |
| 20:R:105:ARG:HH12 | 20:R:112:LYS:HA | 1.69 | 0.58 |
| 9:G:132:PHE:HB2 | 9:G:145:HIS:CE1 | 2.38 | 0.58 |
| 19:Q:29:VAL:HG11 | 19:Q:38:ILE:HD11 | 1.85 | 0.58 |
| 10:H:132:GLU:HG2 | 10:H:134:LEU:HG | 1.84 | 0.58 |
| 3:A:133:LEU:HB2 | 3:A:187:SER:HA | 1.86 | 0.58 |
| 1:X:1675:C:OP1 | 4:B:134:TRP:NE1 | 2.36 | 0.58 |
| 11:I:38:LYS:HD2 | 11:I:40:ARG:O | 2.04 | 0.58 |
| 12:J:36:ILE:HD11 | 12:J:103:VAL:HG22 | 1.86 | 0.57 |
| 1:X:2594:U:H2' | 1:X:2595:C:C6 | 2.39 | 0.57 |
| 23:U:17:SER:HB2 | 23:U:44:ALA:HA | 1.86 | 0.57 |
| 1:X:405:C:H2' | 1:X:406:G:H8 | 1.69 | 0.57 |
| 16:N:66:ASN:HB3 | 16:N:76:TYR:CB | 2.35 | 0.57 |
| 1:X:2387:U:H2' | 1:X:2388:G:C8 | 2.39 | 0.57 |
| 13:K:87:TYR:HE1 | 13:K:94:TYR:HD2 | 1.51 | 0.57 |
| 12:J:44:LYS:HD2 | 12:J:47:GLN:HE22 | 1.68 | 0.57 |
| 1:X:1342:U:H5'' | 1:X:1343:C:H5 | 1.68 | 0.57 |
| 1:X:1467:U:H2' | 1:X:1468:A:OP1 | 2.05 | 0.57 |
| 1:X:1773:C:H1' | 1:X:2588:U:H5'' | 1.87 | 0.57 |
| 1:X:692:C:H2' | 1:X:693:A:C8 | 2.40 | 0.57 |
| 1:X:939:C:H6 | 1:X:939:C:H5' | 1.70 | 0.57 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 9:G:67:ARG:CG | 9:G:70:PHE:HA | 2.35 | 0.57 |
| 11:I:97:ARG:O | 11:I:98:LEU:HB2 | 2.05 | 0.56 |
| 18:P:28:ALA:HB2 | 18:P:71:VAL:HG22 | 1.87 | 0.56 |
| 1:X:1142:G:C1' | 9:G:103:TYR:HD2 | 2.18 | 0.56 |
| 1:X:794:A:H5' | 3:A:218:LYS:HZ2 | 1.71 | 0.56 |
| 18:P:14:ARG:HA | 18:P:17:GLN:HG2 | 1.87 | 0.56 |
| 21:S:95:SER:HB3 | 21:S:119:ASN:HB3 | 1.87 | 0.56 |
| 23:U:31:GLY:C | 23:U:32:ARG:HE | 2.08 | 0.56 |
| 1:X:333:A:H2' | 5:C:162:ARG:NH1 | 2.20 | 0.56 |
| 20:R:25:LEU:HD12 | 20:R:81:VAL:N | 2.20 | 0.56 |
| 13:K:13:ASN:ND2 | 13:K:15:SER:OG | 2.38 | 0.56 |
| 26:Z:35:GLN:O | 26:Z:37:HIS:N | 2.39 | 0.56 |
| 6:D:150:ARG:HE | 6:D:151:GLY:H | 1.54 | 0.56 |
| 8:F:117:ALA:HB1 | 8:F:122:ALA:HB1 | 1.87 | 0.56 |
| 1:X:1805:G:H1' | 3:A:50:THR:CG2 | 2.36 | 0.56 |
| 1:X:1673:C:H5' | 4:B:136:ARG:CD | 2.36 | 0.56 |
| 9:G:103:TYR:CG | 9:G:111:LYS:HA | 2.40 | 0.56 |
| 21:S:6:LYS:H | 21:S:7:PRO:HD3 | 1.71 | 0.56 |
| 1:X:485:G:C6 | 1:X:520:C:N4 | 2.74 | 0.56 |
| 1:X:794:A:H2 | 1:X:1767:G:N3 | 2.04 | 0.56 |
| 1:X:38:G:H21 | 5:C:42:THR:HG21 | 1.71 | 0.56 |
| 9:G:162:LYS:H | 9:G:163:PRO:HD3 | 1.71 | 0.56 |
| 4:B:147:PRO:HB2 | 4:B:149:ARG:HD2 | 1.87 | 0.55 |
| 9:G:105:GLY:O | 9:G:106:TYR:C | 2.42 | 0.55 |
| 1:X:794:A:H5' | 3:A:218:LYS:NZ | 2.21 | 0.55 |
| 1:X:2490:U:H2' | 1:X:2491:C:O4' | 2.06 | 0.55 |
| 4:B:149:ARG:NH2 | 9:G:106:TYR:HD1 | 2.04 | 0.55 |
| 1:X:2319:G:H2' | 1:X:2320:G:C8 | 2.42 | 0.55 |
| 1:X:2620:G:H5'' | 9:G:104:THR:HB | 1.89 | 0.55 |
| 1:X:1673:C:C5' | 4:B:136:ARG:HD3 | 2.36 | 0.55 |
| 23:U:62:LEU:HD23 | 23:U:67:LEU:HD12 | 1.89 | 0.55 |
| 11:I:10:PRO:HA | 11:I:14:LYS:HB2 | 1.89 | 0.55 |
| 3:A:86:PRO:O | 3:A:87:ASN:CB | 2.54 | 0.55 |
| 25:W:1:MET:HB3 | 25:W:34:VAL:HG12 | 1.89 | 0.55 |
| 30:4:19:ARG:HD2 | 30:4:24:LEU:HD22 | 1.89 | 0.55 |
| 1:X:1122:A:O2' | 1:X:1123:G:H4' | 2.07 | 0.55 |
| 9:G:68:PRO:HD2 | 9:G:76:GLN:HB3 | 1.88 | 0.55 |
| 1:X:38:G:H1 | 1:X:453:U:H3 | 1.53 | 0.55 |
| 3:A:43:ARG:HB3 | 3:A:54:ILE:HG13 | 1.89 | 0.55 |
| 16:N:66:ASN:HB3 | 16:N:76:TYR:H | 1.71 | 0.55 |
| 1:X:2516:U:H2' | 1:X:2517:C:C6 | 2.42 | 0.55 |
| 1:X:1268:U:C2 | 5:C:66:ASN:HA | 2.42 | 0.54 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:X:1008:G:H5'' | 16:N:92:ARG:HB3 | 1.89 | 0.54 |
| 2:Y:53:G:H21 | 2:Y:54:U:H5'' | 1.72 | 0.54 |
| 1:X:1278:A:H61 | 1:X:1996:A:H5'' | 1.72 | 0.54 |
| 9:G:157:PRO:C | 9:G:159:SER:H | 2.10 | 0.54 |
| 16:N:101:ARG:O | 16:N:103:PRO:HD3 | 2.08 | 0.54 |
| 3:A:243:GLY:C | 3:A:244:ARG:HD3 | 2.28 | 0.54 |
| 17:O:10:LYS:HG3 | 17:O:11:GLN:HG2 | 1.90 | 0.54 |
| 1:X:742:G:N1 | 3:A:208:LYS:HD3 | 2.23 | 0.54 |
| 1:X:654:A:H2' | 1:X:655:A:H5' | 1.89 | 0.54 |
| 5:C:158:ARG:HA | 5:C:169:VAL:HG21 | 1.90 | 0.54 |
| 1:X:1962:C:H2' | 1:X:1963:G:H5' | 1.90 | 0.54 |
| 1:X:494:A:C8 | 20:R:56:LYS:HD2 | 2.43 | 0.54 |
| 8:F:79:ARG:HG2 | 8:F:84:ILE:HB | 1.89 | 0.54 |
| 9:G:106:TYR:O | 9:G:110:LEU:CG | 2.56 | 0.54 |
| 1:X:1337:G:OP2 | 18:P:105:ARG:NH1 | 2.41 | 0.54 |
| 24:V:25:LEU:HD21 | 24:V:47:ARG:HG2 | 1.90 | 0.54 |
| 1:X:219:G:N2 | 1:X:231:G:H2' | 2.22 | 0.54 |
| 4:B:116:VAL:HG13 | 4:B:136:ARG:HH21 | 1.73 | 0.53 |
| 1:X:797:A:C5 | 3:A:229:VAL:HG21 | 2.43 | 0.53 |
| 1:X:224:G:H4' | 1:X:399:G:C5 | 2.42 | 0.53 |
| 1:X:969:U:C4 | 12:J:17:ARG:HB2 | 2.43 | 0.53 |
| 13:K:49:GLU:O | 13:K:52:ILE:HG12 | 2.08 | 0.53 |
| 23:U:53:GLU:HB2 | 23:U:56:GLN:O | 2.09 | 0.53 |
| 5:C:133:PHE:HB2 | 5:C:160:ALA:HB1 | 1.89 | 0.53 |
| 11:I:58:ALA:O | 11:I:59:ARG:HB3 | 2.08 | 0.53 |
| 1:X:2761:A:H5'' | 1:X:2762:G:H5' | 1.89 | 0.53 |
| 4:B:149:ARG:CZ | 9:G:106:TYR:HD1 | 2.21 | 0.53 |
| 1:X:617:U:H5 | 1:X:632:A:N1 | 2.04 | 0.53 |
| 1:X:1033:G:N2 | 1:X:1153:A:H2 | 1.98 | 0.53 |
| 12:J:28:VAL:HG12 | 12:J:29:ALA:H | 1.72 | 0.53 |
| 1:X:1810:U:H2' | 3:A:157:ARG:HD3 | 1.90 | 0.53 |
| 5:C:41:GLY:HA3 | 5:C:89:ARG:O | 2.09 | 0.53 |
| 16:N:21:ALA:HB1 | 16:N:29:SER:HA | 1.91 | 0.53 |
| 12:J:28:VAL:HG23 | 12:J:137:VAL:HB | 1.91 | 0.53 |
| 1:X:2241:U:C5 | 22:T:17:ASN:OD1 | 2.59 | 0.53 |
| 6:D:40:LEU:HD21 | 6:D:87:ILE:HD12 | 1.91 | 0.53 |
| 1:X:617:U:H5 | 1:X:632:A:H2 | 1.50 | 0.53 |
| 17:O:69:ILE:HG22 | 17:O:86:HIS:HB3 | 1.90 | 0.53 |
| 18:P:38:VAL:HG12 | 18:P:97:VAL:HG21 | 1.90 | 0.53 |
| 21:S:91:PRO:HG2 | 21:S:125:PRO:HD2 | 1.90 | 0.53 |
| 4:B:152:LYS:H | 9:G:106:TYR:CB | 2.22 | 0.53 |
| 1:X:1373:G:N2 | 1:X:2192:U:H3 | 2.04 | 0.53 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 14:L:76:ALA:HB2 | 14:L:107:ALA:HA | 1.91 | 0.53 |
| 2:Y:32:C:H1' | 2:Y:59:A:H61 | 1.73 | 0.53 |
| 16:N:66:ASN:HB2 | 16:N:70:ARG:HH11 | 1.73 | 0.52 |
| 12:J:109:GLY:HA3 | 21:S:112:LEU:HD21 | 1.90 | 0.52 |
| 3:A:42:GLY:C | 3:A:43:ARG:HH11 | 2.12 | 0.52 |
| 1:X:1033:G:N2 | 1:X:1153:A:C2 | 2.75 | 0.52 |
| 4:B:183:LEU:HD11 | 15:M:16:ILE:HG21 | 1.90 | 0.52 |
| 1:X:760:U:C6 | 26:Z:3:LYS:HG3 | 2.44 | 0.52 |
| 1:X:2545:A:H61 | 10:H:40:GLY:HA3 | 1.74 | 0.52 |
| 1:X:1468:A:H5' | 1:X:1472:C:H41 | 1.73 | 0.52 |
| 10:H:41:ASN:H | 10:H:41:ASN:ND2 | 2.08 | 0.52 |
| 1:X:1765:C:N3 | 3:A:208:LYS:HE2 | 2.24 | 0.52 |
| 2:Y:16:U:H3' | 2:Y:17:A:H5'' | 1.90 | 0.52 |
| 19:Q:5:ASP:O | 19:Q:7:LEU:N | 2.43 | 0.52 |
| 17:O:38:LEU:HD23 | 17:O:47:PHE:HB3 | 1.91 | 0.52 |
| 10:H:27:SER:HA | 10:H:50:ILE:HD12 | 1.91 | 0.52 |
| 22:T:50:GLY:O | 22:T:62:LEU:HB2 | 2.10 | 0.52 |
| 1:X:2397:A:H2' | 1:X:2398:U:O4' | 2.10 | 0.52 |
| 15:M:99:VAL:HG11 | 15:M:104:LEU:HD22 | 1.90 | 0.52 |
| 1:X:879:A:H2' | 1:X:879:A:N3 | 2.25 | 0.52 |
| 12:J:12:LYS:O | 12:J:13:GLN:HB2 | 2.08 | 0.52 |
| 12:J:100:PRO:HB2 | 21:S:74:ARG:HG2 | 1.91 | 0.52 |
| 9:G:62:ILE:HG22 | 9:G:135:LEU:HD21 | 1.90 | 0.52 |
| 18:P:25:PHE:HD1 | 18:P:127:ILE:HD11 | 1.74 | 0.52 |
| 1:X:1845:A:N1 | 1:X:2070:G:H1' | 2.25 | 0.52 |
| 5:C:30:VAL:HG11 | 5:C:177:VAL:HG21 | 1.92 | 0.52 |
| 10:H:2:ILE:HB | 10:H:45:ALA:HB3 | 1.92 | 0.52 |
| 1:X:415:A:H61 | 1:X:436:A:H61 | 1.58 | 0.52 |
| 14:L:29:LEU:HB3 | 14:L:89:PHE:HA | 1.92 | 0.52 |
| 1:X:1939:U:H1' | 1:X:2531:U:OP1 | 2.10 | 0.52 |
| 10:H:24:VAL:HA | 10:H:51:ILE:HG22 | 1.92 | 0.52 |
| 1:X:1943:A:H5'' | 1:X:1943:A:H8 | 1.74 | 0.52 |
| 9:G:98:LYS:HB3 | 9:G:116:ARG:HB2 | 1.92 | 0.52 |
| 19:Q:66:GLY:O | 19:Q:68:PHE:N | 2.30 | 0.52 |
| 1:X:1686:A:H5'' | 1:X:1687:C:OP2 | 2.09 | 0.52 |
| 1:X:2368:G:H5'' | 1:X:2369:U:C5' | 2.39 | 0.51 |
| 1:X:1805:G:H1' | 3:A:50:THR:HG21 | 1.90 | 0.51 |
| 16:N:24:PHE:O | 16:N:29:SER:HB3 | 2.11 | 0.51 |
| 1:X:1630:A:N1 | 18:P:114:ALA:HB2 | 2.26 | 0.51 |
| 1:X:1643:A:H61 | 1:X:1656:U:H3 | 1.59 | 0.51 |
| 1:X:118:U:H4' | 1:X:119:G:H5'' | 1.93 | 0.51 |
| 4:B:147:PRO:C | 4:B:149:ARG:N | 2.58 | 0.51 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 14:L:33:ARG:NH1 | 14:L:38:ILE:HB | 2.25 | 0.51 |
| 13:K:10:LEU:HA | 13:K:17:ARG:HG2 | 1.93 | 0.51 |
| 1:X:1342:U:H5'' | 1:X:1343:C:C5 | 2.46 | 0.51 |
| 1:X:1586:A:H2' | 1:X:1587:A:C8 | 2.45 | 0.51 |
| 1:X:305:A:H8 | 1:X:305:A:H5' | 1.75 | 0.51 |
| 1:X:2551:A:H62 | 4:B:145:LYS:HG3 | 1.74 | 0.51 |
| 6:D:123:ASP:HB3 | 6:D:127:ASN:HB2 | 1.92 | 0.51 |
| 3:A:182:LEU:HB2 | 3:A:268:ARG:O | 2.10 | 0.51 |
| 6:D:8:TYR:O | 6:D:12:VAL:HB | 2.11 | 0.51 |
| 16:N:81:ASN:HD22 | 16:N:117:ARG:HH21 | 1.58 | 0.51 |
| 14:L:36:LYS:HB3 | 14:L:64:LYS:HB2 | 1.93 | 0.51 |
| 9:G:57:LEU:HD22 | 9:G:170:PRO:HA | 1.92 | 0.51 |
| 21:S:51:LEU:HB3 | 21:S:65:LEU:HD12 | 1.92 | 0.51 |
| 20:R:51:VAL:HG21 | 20:R:76:LEU:HD21 | 1.92 | 0.51 |
| 1:X:486:U:H4' | 1:X:519:C:H2' | 1.92 | 0.51 |
| 1:X:504:G:N2 | 18:P:78:ASN:HD21 | 2.08 | 0.51 |
| 11:I:21:ARG:HH11 | 11:I:22:GLY:HA3 | 1.76 | 0.51 |
| 13:K:45:ARG:HD2 | 13:K:95:THR:HG22 | 1.92 | 0.51 |
| 14:L:8:ARG:CG | 14:L:9:ARG:H | 2.22 | 0.51 |
| 9:G:70:PHE:HB2 | 16:N:64:ARG:HG2 | 1.93 | 0.51 |
| 1:X:1737:G:H2' | 1:X:1738:U:H6 | 1.75 | 0.51 |
| 9:G:103:TYR:HB3 | 9:G:107:GLN:HE21 | 1.76 | 0.50 |
| 1:X:2475:C:OP1 | 12:J:83:ARG:HB3 | 2.11 | 0.50 |
| 24:V:7:ARG:HB2 | 24:V:60:LEU:HD11 | 1.92 | 0.50 |
| 5:C:8:GLY:HA3 | 5:C:120:VAL:HB | 1.93 | 0.50 |
| 3:A:43:ARG:N | 3:A:43:ARG:CD | 2.64 | 0.50 |
| 6:D:78:LYS:HG2 | 6:D:80:ARG:HH11 | 1.76 | 0.50 |
| 23:U:48:LYS:HG2 | 23:U:49:LYS:N | 2.21 | 0.50 |
| 23:U:49:LYS:HA | 23:U:62:LEU:H | 1.75 | 0.50 |
| 9:G:162:LYS:N | 9:G:163:PRO:CD | 2.74 | 0.50 |
| 1:X:2083:G:H1 | 1:X:2172:U:H3 | 1.58 | 0.50 |
| 5:C:148:VAL:HB | 5:C:167:VAL:HG12 | 1.94 | 0.50 |
| 19:Q:66:GLY:C | 19:Q:68:PHE:H | 2.10 | 0.50 |
| 3:A:36:ALA:HB1 | 3:A:62:TYR:O | 2.12 | 0.50 |
| 10:H:25:LEU:HD11 | 10:H:52:VAL:HG23 | 1.93 | 0.50 |
| 1:X:954:U:P | 11:I:38:LYS:HG2 | 2.52 | 0.50 |
| 18:P:17:GLN:HG3 | 18:P:18:VAL:HG23 | 1.94 | 0.50 |
| 12:J:92:GLU:HG3 | 12:J:93:TYR:CD2 | 2.46 | 0.50 |
| 13:K:17:ARG:NH1 | 13:K:20:LEU:CD2 | 2.71 | 0.50 |
| 20:R:29:HIS:CD2 | 20:R:51:VAL:HG22 | 2.47 | 0.50 |
| 9:G:124:GLU:O | 9:G:128:GLU:HB2 | 2.11 | 0.50 |
| 6:D:143:TYR:HA | 6:D:146:VAL:HG22 | 1.94 | 0.50 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:X:1142:G:N2 | 9:G:101:THR:HG22 | 2.22 | 0.50 |
| 1:X:670:U:H2' | 1:X:671:A:C8 | 2.46 | 0.50 |
| 1:X:490:A:N3 | 1:X:492:G:H5'' | 2.27 | 0.50 |
| 1:X:654:A:H2' | 1:X:655:A:C5' | 2.42 | 0.50 |
| 16:N:44:THR:O | 16:N:48:ARG:HG3 | 2.12 | 0.50 |
| 21:S:69:VAL:HG22 | 21:S:81:VAL:HG13 | 1.93 | 0.50 |
| 4:B:146:THR:OG1 | 4:B:147:PRO:HD3 | 2.12 | 0.50 |
| 4:B:50:GLY:HA3 | 4:B:75:THR:HG21 | 1.94 | 0.50 |
| 12:J:65:ILE:HG23 | 12:J:107:VAL:HG12 | 1.94 | 0.50 |
| 1:X:2034:A:O4' | 4:B:141:ILE:HD12 | 2.12 | 0.50 |
| 7:E:154:PRO:HA | 7:E:160:LYS:O | 2.11 | 0.50 |
| 11:I:28:LYS:NZ | 11:I:36:GLY:HA3 | 2.27 | 0.50 |
| 1:X:922:A:N1 | 1:X:2256:G:H1' | 2.27 | 0.50 |
| 4:B:147:PRO:O | 4:B:149:ARG:N | 2.45 | 0.49 |
| 2:Y:45:C:H2' | 6:D:92:ARG:HH11 | 1.77 | 0.49 |
| 21:S:6:LYS:HB2 | 21:S:31:SER:HB3 | 1.94 | 0.49 |
| 1:X:2272:A:H5'' | 14:L:15:ARG:HH21 | 1.77 | 0.49 |
| 23:U:14:VAL:O | 23:U:15:VAL:HG22 | 2.12 | 0.49 |
| 5:C:22:VAL:HG13 | 5:C:106:MET:HG2 | 1.94 | 0.49 |
| 1:X:2508:G:C8 | 1:X:2508:G:H5' | 2.47 | 0.49 |
| 1:X:1467:U:H3' | 1:X:1467:U:H6 | 1.77 | 0.49 |
| 1:X:1493:A:H2' | 1:X:1494:G:O4' | 2.12 | 0.49 |
| 9:G:132:PHE:HZ | 9:G:142:ARG:HA | 1.77 | 0.49 |
| 1:X:742:G:N7 | 3:A:209:ALA:O | 2.45 | 0.49 |
| 14:L:31:VAL:HG21 | 14:L:100:VAL:HG23 | 1.93 | 0.49 |
| 1:X:1134:C:H1' | 30:4:18:ARG:HH12 | 1.77 | 0.49 |
| 4:B:5:LEU:HG | 4:B:195:LEU:HD11 | 1.94 | 0.49 |
| 17:O:12:TYR:CB | 17:O:40:VAL:H | 2.23 | 0.49 |
| 17:O:71:ILE:HD11 | 17:O:86:HIS:HB2 | 1.94 | 0.49 |
| 7:E:6:LYS:HB3 | 7:E:69:ARG:HD3 | 1.92 | 0.49 |
| 23:U:51:ILE:HG23 | 23:U:59:THR:HA | 1.94 | 0.49 |
| 7:E:11:VAL:HB | 7:E:15:VAL:HG21 | 1.93 | 0.49 |
| 1:X:2352:A:H2' | 1:X:2353:G:C8 | 2.46 | 0.49 |
| 1:X:2266:A:H2 | 1:X:2325:A:H62 | 1.58 | 0.49 |
| 11:I:117:ALA:HA | 11:I:137:GLY:O | 2.13 | 0.49 |
| 23:U:49:LYS:HB2 | 23:U:61:TRP:CE3 | 2.48 | 0.49 |
| 23:U:48:LYS:CG | 23:U:49:LYS:H | 2.24 | 0.49 |
| 1:X:649:G:H1 | 1:X:660:G:H1 | 1.60 | 0.49 |
| 10:H:78:SER:HA | 10:H:91:PHE:O | 2.11 | 0.49 |
| 13:K:11:ASN:HD22 | 13:K:12:ARG:HE | 1.60 | 0.49 |
| 12:J:77:LYS:O | 12:J:79:PRO:HD3 | 2.12 | 0.49 |
| 1:X:2867:G:O5' | 1:X:2867:G:H8 | 1.95 | 0.49 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 18:P:36:ARG:HA | 18:P:39:ARG:HD2 | 1.93 | 0.49 |
| 1:X:426:C:HO2' | 1:X:1863:U:HO2' | 1.59 | 0.49 |
| 10:H:110:VAL:HG23 | 10:H:129:LEU:HB2 | 1.94 | 0.49 |
| 16:N:88:ILE:HG12 | 17:O:49:GLU:HB2 | 1.94 | 0.49 |
| 1:X:29:U:H4' | 16:N:11:ARG:HH22 | 1.78 | 0.49 |
| 1:X:2017:U:H2' | 1:X:2018:G:H5'' | 1.95 | 0.49 |
| 18:P:32:ARG:HA | 18:P:121:THR:HG22 | 1.94 | 0.49 |
| 23:U:23:LYS:HD2 | 23:U:35:THR:HG21 | 1.95 | 0.49 |
| 12:J:27:TYR:HB3 | 12:J:137:VAL:HG21 | 1.93 | 0.49 |
| 1:X:389:G:H2' | 1:X:390:U:C6 | 2.47 | 0.49 |
| 10:H:28:GLY:HA3 | 10:H:35:THR:OG1 | 2.13 | 0.49 |
| 1:X:2661:G:O6 | 1:X:2708:U:H1' | 2.13 | 0.49 |
| 1:X:2080:U:H3 | 1:X:2175:A:H61 | 1.60 | 0.49 |
| 1:X:649:G:N2 | 1:X:660:G:N2 | 2.60 | 0.48 |
| 14:L:15:ARG:HA | 14:L:15:ARG:HH11 | 1.78 | 0.48 |
| 1:X:818:G:H1' | 1:X:844:G:O2' | 2.13 | 0.48 |
| 1:X:91:A:H2' | 1:X:92:U:C6 | 2.48 | 0.48 |
| 11:I:54:SER:C | 11:I:56:LEU:H | 2.17 | 0.48 |
| 13:K:10:LEU:HD23 | 13:K:17:ARG:HB2 | 1.95 | 0.48 |
| 21:S:6:LYS:N | 21:S:7:PRO:HD3 | 2.27 | 0.48 |
| 4:B:195:LEU:H | 15:M:2:GLN:HG2 | 1.78 | 0.48 |
| 18:P:103:LEU:HB2 | 18:P:119:LYS:HB2 | 1.96 | 0.48 |
| 16:N:83:LEU:HD12 | 16:N:113:SER:HB2 | 1.93 | 0.48 |
| 4:B:13:GLN:O | 4:B:14:ILE:HD12 | 2.13 | 0.48 |
| 1:X:2505:G:H1' | 30:4:1:MET:HB2 | 1.93 | 0.48 |
| 7:E:38:ASN:HB3 | 7:E:40:GLU:HG2 | 1.95 | 0.48 |
| 6:D:72:LYS:HE2 | 6:D:81:GLN:HE21 | 1.79 | 0.48 |
| 1:X:12:U:H2' | 1:X:12:U:O2 | 2.13 | 0.48 |
| 1:X:2352:A:H2' | 1:X:2353:G:H8 | 1.78 | 0.48 |
| 1:X:2484:G:HO2' | 1:X:2485:U:H6 | 1.59 | 0.48 |
| 14:L:27:LEU:HB2 | 14:L:87:VAL:HG22 | 1.95 | 0.48 |
| 5:C:164:VAL:O | 5:C:166:TRP:N | 2.40 | 0.48 |
| 1:X:89:A:H4' | 1:X:90:G:H5'' | 1.96 | 0.48 |
| 27:1:40:TYR:CA | 27:1:41:ASP:CA | 2.91 | 0.48 |
| 1:X:1562:G:H5'' | 1:X:1563:U:H5' | 1.94 | 0.48 |
| 11:I:32:ARG:HD2 | 17:O:79:GLN:HE22 | 1.77 | 0.48 |
| 9:G:157:PRO:O | 9:G:159:SER:N | 2.46 | 0.48 |
| 1:X:1705:U:O2 | 1:X:1717:A:H8 | 1.97 | 0.48 |
| 1:X:1278:A:H2 | 1:X:1997:A:H62 | 1.61 | 0.48 |
| 17:O:10:LYS:HD2 | 17:O:37:ALA:HB3 | 1.95 | 0.48 |
| 1:X:2270:U:H2' | 1:X:2271:C:C6 | 2.47 | 0.48 |
| 10:H:116:ARG:HH11 | 15:M:38:LYS:HD3 | 1.78 | 0.48 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 5:C:5:ASN:HB2 | 5:C:10:ASN:HA | 1.95 | 0.48 |
| 1:X:617:U:C5 | 1:X:632:A:N1 | 2.81 | 0.48 |
| 17:O:33:VAL:HG12 | 17:O:57:GLN:HE21 | 1.79 | 0.48 |
| 1:X:627:A:H2' | 1:X:628:A:C8 | 2.49 | 0.48 |
| 1:X:1685:A:H5'' | 10:H:5:GLN:HG2 | 1.96 | 0.48 |
| 1:X:1997:A:H2' | 1:X:1998:A:C8 | 2.49 | 0.48 |
| 23:U:51:ILE:HA | 23:U:59:THR:O | 2.13 | 0.48 |
| 4:B:133:LYS:HD2 | 4:B:137:ARG:HB3 | 1.96 | 0.48 |
| 3:A:43:ARG:CD | 3:A:43:ARG:H | 2.18 | 0.48 |
| 30:4:19:ARG:HB2 | 30:4:24:LEU:HD13 | 1.96 | 0.48 |
| 1:X:1833:U:H2' | 1:X:1834:G:C8 | 2.49 | 0.48 |
| 1:X:2289:A:H3' | 1:X:2290:A:H8 | 1.78 | 0.48 |
| 4:B:117:MET:H | 4:B:136:ARG:HG3 | 1.79 | 0.47 |
| 20:R:105:ARG:HH21 | 20:R:107:ALA:HB2 | 1.77 | 0.47 |
| 1:X:1777:A:H1' | 1:X:1921:A:N6 | 2.28 | 0.47 |
| 9:G:55:ALA:C | 9:G:134:MET:HE1 | 2.35 | 0.47 |
| 1:X:712:A:H2' | 1:X:713:G:O4' | 2.15 | 0.47 |
| 1:X:1820:G:OP2 | 3:A:239:ARG:NH1 | 2.47 | 0.47 |
| 8:F:101:TRP:HZ3 | 8:F:140:GLY:HA3 | 1.78 | 0.47 |
| 3:A:45:ASN:CG | 3:A:46:ARG:N | 2.67 | 0.47 |
| 11:I:88:PHE:HE2 | 11:I:119:THR:HB | 1.79 | 0.47 |
| 1:X:1776:A:OP1 | 1:X:1965:U:H5' | 2.15 | 0.47 |
| 18:P:40:LEU:HB3 | 26:Z:25:LEU:HD13 | 1.96 | 0.47 |
| 12:J:81:GLU:HG2 | 12:J:82:THR:H | 1.79 | 0.47 |
| 1:X:1787:U:H2' | 1:X:1788:C:C6 | 2.49 | 0.47 |
| 1:X:738:G:H8 | 1:X:738:G:O5' | 1.98 | 0.47 |
| 1:X:1992:G:H1' | 13:K:106:ASP:O | 2.13 | 0.47 |
| 26:Z:16:ARG:HD3 | 26:Z:20:ARG:CZ | 2.44 | 0.47 |
| 23:U:27:ASP:N | 23:U:32:ARG:HH21 | 2.12 | 0.47 |
| 1:X:334:G:C8 | 5:C:164:VAL:HG13 | 2.49 | 0.47 |
| 4:B:137:ARG:HG3 | 4:B:138:PRO:HD2 | 1.97 | 0.47 |
| 18:P:59:PHE:HD2 | 26:Z:41:LEU:HD22 | 1.79 | 0.47 |
| 5:C:149:LEU:HD23 | 5:C:180:ILE:HG22 | 1.96 | 0.47 |
| 1:X:1859:A:H2' | 1:X:1860:A:C8 | 2.50 | 0.47 |
| 5:C:118:VAL:HG22 | 5:C:188:ILE:HD12 | 1.97 | 0.47 |
| 4:B:59:VAL:HG21 | 4:B:74:PRO:HB2 | 1.96 | 0.47 |
| 9:G:106:TYR:O | 9:G:110:LEU:CD1 | 2.62 | 0.47 |
| 24:V:56:VAL:C | 24:V:58:ALA:H | 2.18 | 0.47 |
| 1:X:143:A:H2' | 1:X:144:U:C6 | 2.49 | 0.47 |
| 1:X:2189:A:C2 | 1:X:2190:A:C4 | 3.02 | 0.47 |
| 1:X:33:C:O2' | 1:X:34:U:H5'' | 2.14 | 0.47 |
| 1:X:1137:A:H4' | 1:X:1138:A:O5' | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 11:I:62:LYS:NZ | 11:I:64:GLY:CA | 2.76 | 0.47 |
| 16:N:61:TRP:CZ3 | 16:N:94:VAL:N | 2.82 | 0.47 |
| 1:X:774:A:C8 | 1:X:774:A:O5' | 2.56 | 0.47 |
| 1:X:879:A:H5' | 1:X:880:C:OP2 | 2.14 | 0.47 |
| 1:X:86:U:H5'' | 1:X:87:G:H5' | 1.95 | 0.47 |
| 1:X:1586:A:H5' | 3:A:38:PRO:HG3 | 1.95 | 0.47 |
| 1:X:2654:A:H5' | 10:H:42:LYS:H | 1.80 | 0.47 |
| 1:X:203:G:H21 | 1:X:205:A:H62 | 1.62 | 0.47 |
| 23:U:19:ILE:HA | 23:U:42:GLN:HA | 1.95 | 0.47 |
| 22:T:3:HIS:CD2 | 22:T:5:LYS:HB2 | 2.50 | 0.47 |
| 20:R:105:ARG:HH22 | 20:R:111:GLY:C | 2.17 | 0.47 |
| 1:X:1173:G:H4' | 17:O:22:VAL:HG23 | 1.97 | 0.47 |
| 10:H:83:ARG:NH2 | 10:H:89:ILE:HD11 | 2.28 | 0.47 |
| 4:B:122:PHE:O | 4:B:123:ALA:CB | 2.63 | 0.47 |
| 10:H:77:THR:HA | 10:H:94:ASN:HB3 | 1.96 | 0.47 |
| 1:X:935:C:H2' | 1:X:936:A:C8 | 2.50 | 0.47 |
| 1:X:577:U:OP1 | 11:I:40:ARG:NH2 | 2.48 | 0.46 |
| 5:C:186:LEU:HG | 5:C:188:ILE:HG12 | 1.95 | 0.46 |
| 6:D:35:VAL:HG22 | 6:D:90:THR:HG23 | 1.97 | 0.46 |
| 3:A:106:LEU:H | 3:A:106:LEU:HD12 | 1.79 | 0.46 |
| 9:G:103:TYR:CZ | 9:G:111:LYS:HB2 | 2.51 | 0.46 |
| 12:J:26:ASP:O | 12:J:27:TYR:HD1 | 1.97 | 0.46 |
| 1:X:2289:A:H3' | 1:X:2290:A:C8 | 2.49 | 0.46 |
| 10:H:112:GLY:O | 10:H:131:PRO:HD2 | 2.15 | 0.46 |
| 20:R:23:ILE:HG23 | 20:R:84:VAL:HG21 | 1.96 | 0.46 |
| 1:X:923:A:C6 | 12:J:12:LYS:HG2 | 2.50 | 0.46 |
| 20:R:40:LEU:HB2 | 20:R:45:LYS:HB2 | 1.97 | 0.46 |
| 6:D:72:LYS:HG2 | 6:D:81:GLN:HG2 | 1.98 | 0.46 |
| 18:P:118:LYS:HD2 | 18:P:120:ARG:HH21 | 1.80 | 0.46 |
| 1:X:2581:A:H2' | 1:X:2582:G:C4' | 2.46 | 0.46 |
| 1:X:1469:U:OP2 | 1:X:1471:G:OP2 | 2.33 | 0.46 |
| 1:X:650:U:H2' | 1:X:651:C:C6 | 2.50 | 0.46 |
| 1:X:1030:U:N3 | 1:X:1153:A:N6 | 2.54 | 0.46 |
| 1:X:542:A:C2 | 1:X:2004:U:C2' | 2.97 | 0.46 |
| 12:J:77:LYS:HG3 | 12:J:78:LYS:H | 1.80 | 0.46 |
| 11:I:76:LYS:HB3 | 11:I:79:GLN:HG2 | 1.98 | 0.46 |
| 25:W:46:THR:HG22 | 25:W:47:VAL:HG13 | 1.97 | 0.46 |
| 1:X:1142:G:O5' | 9:G:107:GLN:HB3 | 2.15 | 0.46 |
| 12:J:27:TYR:HB2 | 12:J:137:VAL:HG11 | 1.98 | 0.46 |
| 9:G:67:ARG:HE | 9:G:70:PHE:HA | 1.80 | 0.46 |
| 13:K:87:TYR:CE1 | 13:K:94:TYR:HD2 | 2.30 | 0.46 |
| 9:G:69:ASP:H | 9:G:76:GLN:HE21 | 1.62 | 0.46 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 8:F:77:LEU:HD13 | 8:F:107:ILE:HG23 | 1.98 | 0.46 |
| 1:X:2705:A:H1' | 1:X:2706:U:H2' | 1.97 | 0.46 |
| 7:E:164:PHE:O | 7:E:166:GLY:N | 2.48 | 0.46 |
| 10:H:28:GLY:O | 10:H:29:ILE:HB | 2.16 | 0.46 |
| 3:A:270:ILE:HG13 | 3:A:271:VAL:H | 1.81 | 0.46 |
| 1:X:334:G:H5' | 5:C:162:ARG:NH2 | 2.31 | 0.46 |
| 1:X:719:A:H2' | 1:X:720:A:O4' | 2.16 | 0.46 |
| 1:X:673:G:H5' | 5:C:93:TYR:CD1 | 2.51 | 0.46 |
| 16:N:74:MET:HB3 | 16:N:75:ASN:H | 1.59 | 0.46 |
| 13:K:3:HIS:HB3 | 13:K:5:LYS:CD | 2.42 | 0.46 |
| 9:G:156:HIS:N | 9:G:157:PRO:CD | 2.79 | 0.46 |
| 1:X:641:G:N2 | 1:X:643:A:H3' | 2.31 | 0.46 |
| 13:K:3:HIS:ND1 | 13:K:5:LYS:NZ | 2.47 | 0.45 |
| 20:R:105:ARG:HH22 | 20:R:112:LYS:HA | 1.80 | 0.45 |
| 1:X:1469:U:P | 1:X:1471:G:OP2 | 2.74 | 0.45 |
| 8:F:104:VAL:HA | 8:F:107:ILE:HD12 | 1.98 | 0.45 |
| 1:X:510:G:N1 | 1:X:513:A:OP2 | 2.45 | 0.45 |
| 13:K:36:THR:HG23 | 13:K:41:ALA:HB2 | 1.98 | 0.45 |
| 1:X:2326:C:H2' | 1:X:2327:U:H6 | 1.81 | 0.45 |
| 1:X:652:C:H6 | 1:X:652:C:H5'' | 1.81 | 0.45 |
| 1:X:1744:G:H5'' | 15:M:100:ARG:HD3 | 1.98 | 0.45 |
| 3:A:182:LEU:HD12 | 3:A:269:PHE:HB2 | 1.97 | 0.45 |
| 20:R:45:LYS:HA | 20:R:76:LEU:O | 2.16 | 0.45 |
| 28:2:39:ARG:CA | 28:2:40:HIS:CA | 2.95 | 0.45 |
| 1:X:834:A:H5' | 1:X:835:U:H6 | 1.81 | 0.45 |
| 1:X:568:G:H2' | 1:X:569:C:O4' | 2.15 | 0.45 |
| 12:J:42:TRP:CG | 12:J:95:VAL:HG11 | 2.52 | 0.45 |
| 5:C:4:ILE:HG23 | 5:C:13:ARG:HH22 | 1.80 | 0.45 |
| 2:Y:46:G:H4' | 6:D:92:ARG:HH12 | 1.82 | 0.45 |
| 1:X:2372:A:H5'' | 11:I:61:PRO:HB3 | 1.98 | 0.45 |
| 5:C:74:VAL:HB | 5:C:75:PRO:HD2 | 1.97 | 0.45 |
| 1:X:597:U:O4 | 1:X:683:A:H1' | 2.16 | 0.45 |
| 5:C:170:LEU:HA | 5:C:171:PRO:HD3 | 1.84 | 0.45 |
| 24:V:21:ARG:HH11 | 24:V:53:LEU:HD11 | 1.81 | 0.45 |
| 1:X:2790:C:O2' | 26:Z:43:HIS:CD2 | 2.65 | 0.45 |
| 20:R:22:VAL:HG11 | 20:R:80:LYS:HZ3 | 1.80 | 0.45 |
| 10:H:123:PHE:HB3 | 10:H:126:ILE:HG13 | 1.98 | 0.45 |
| 12:J:26:ASP:O | 12:J:27:TYR:CD1 | 2.70 | 0.45 |
| 5:C:127:ASP:HB2 | 5:C:129:LYS:HG3 | 1.99 | 0.45 |
| 1:X:2273:C:H2' | 1:X:2274:C:H6 | 1.82 | 0.45 |
| 1:X:312:G:HO2' | 1:X:313:U:H6 | 1.63 | 0.45 |
| 1:X:1974:U:H2' | 1:X:1975:G:H5'' | 1.99 | 0.45 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 26:Z:16:ARG:O | 26:Z:20:ARG:HD2 | 2.17 | 0.45 |
| 4:B:59:VAL:HG21 | 4:B:74:PRO:CB | 2.46 | 0.45 |
| 25:W:3:ILE:HD12 | 25:W:51:LEU:HD13 | 1.99 | 0.45 |
| 1:X:2226:A:H2' | 1:X:2227:C:H6 | 1.81 | 0.45 |
| 1:X:1012:A:H2' | 1:X:1013:G:O4' | 2.16 | 0.45 |
| 1:X:2821:G:H2' | 1:X:2822:U:C6 | 2.51 | 0.45 |
| 1:X:347:C:H4' | 20:R:15:HIS:CD2 | 2.52 | 0.45 |
| 1:X:1882:G:H22 | 1:X:1885:C:N4 | 2.08 | 0.45 |
| 25:W:47:VAL:HB | 25:W:50:LEU:HD12 | 1.99 | 0.45 |
| 15:M:93:ILE:HG21 | 15:M:96:ARG:HG2 | 1.99 | 0.45 |
| 9:G:66:HIS:HA | 16:N:67:ALA:HB1 | 1.98 | 0.45 |
| 3:A:252:LYS:HD2 | 3:A:253:PRO:HD3 | 1.98 | 0.45 |
| 1:X:2691:C:O2' | 1:X:2693:U:H5' | 2.17 | 0.45 |
| 12:J:27:TYR:CZ | 21:S:76:ARG:HB3 | 2.52 | 0.45 |
| 4:B:23:VAL:HG21 | 4:B:183:LEU:HD13 | 1.98 | 0.45 |
| 1:X:2189:A:H2 | 1:X:2190:A:C5 | 2.35 | 0.45 |
| 1:X:1922:U:OP1 | 1:X:2583:U:O2' | 2.33 | 0.45 |
| 4:B:146:THR:CB | 4:B:147:PRO:HD3 | 2.47 | 0.45 |
| 14:L:38:ILE:CG1 | 14:L:39:TYR:H | 2.18 | 0.45 |
| 15:M:5:ILE:H | 15:M:5:ILE:HG13 | 1.62 | 0.44 |
| 1:X:649:G:H22 | 1:X:660:G:N2 | 2.15 | 0.44 |
| 1:X:310:A:N1 | 1:X:333:A:O2' | 2.42 | 0.44 |
| 13:K:33:ARG:HD3 | 13:K:112:LEU:HD22 | 2.00 | 0.44 |
| 1:X:763:A:OP1 | 1:X:1631:C:N4 | 2.43 | 0.44 |
| 1:X:1688:U:HO2' | 1:X:1690:U:H5 | 1.63 | 0.44 |
| 1:X:1474:A:H2' | 1:X:1474:A:N3 | 2.32 | 0.44 |
| 1:X:1167:A:C8 | 16:N:51:ARG:HG3 | 2.52 | 0.44 |
| 1:X:1142:G:O4' | 9:G:107:GLN:HG2 | 2.17 | 0.44 |
| 12:J:77:LYS:HG3 | 12:J:78:LYS:N | 2.32 | 0.44 |
| 5:C:45:THR:HG22 | 5:C:47:THR:OG1 | 2.17 | 0.44 |
| 2:Y:40:C:H42 | 2:Y:46:G:H1 | 1.65 | 0.44 |
| 17:O:36:LYS:HD2 | 17:O:54:TYR:HB2 | 1.99 | 0.44 |
| 7:E:25:LYS:HG3 | 7:E:34:THR:HG22 | 1.98 | 0.44 |
| 20:R:96:LYS:CG | 20:R:97:GLN:H | 2.31 | 0.44 |
| 25:W:12:ARG:CG | 25:W:12:ARG:NH1 | 2.72 | 0.44 |
| 1:X:1833:U:H2' | 1:X:1834:G:H8 | 1.80 | 0.44 |
| 16:N:75:ASN:ND2 | 16:N:77:SER:HB3 | 2.33 | 0.44 |
| 7:E:43:VAL:HB | 7:E:52:VAL:HG13 | 1.99 | 0.44 |
| 1:X:679:C:H2' | 1:X:680:U:C6 | 2.52 | 0.44 |
| 9:G:58:ILE:HG12 | 9:G:80:VAL:HG11 | 1.99 | 0.44 |
| 4:B:115:GLY:HA2 | 4:B:157:ALA:CB | 2.47 | 0.44 |
| 6:D:116:GLY:HA2 | 6:D:176:PRO:HB2 | 1.99 | 0.44 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:X:857:U:H3' | 1:X:858:G:H8 | 1.79 | 0.44 |
| 1:X:577:U:H5'' | 1:X:956:A:N6 | 2.32 | 0.44 |
| 1:X:2751:C:H5' | 4:B:203:LYS:HD3 | 1.98 | 0.44 |
| 19:Q:11:VAL:HB | 19:Q:26:SER:HB2 | 1.98 | 0.44 |
| 3:A:67:PHE:HD2 | 3:A:153:ALA:HB3 | 1.83 | 0.44 |
| 1:X:680:U:H2' | 1:X:681:A:H5'' | 1.99 | 0.44 |
| 3:A:145:LEU:HD13 | 3:A:163:VAL:HG11 | 2.00 | 0.44 |
| 1:X:1032:A:H3' | 1:X:1032:A:C8 | 2.52 | 0.44 |
| 1:X:573:C:HO2' | 1:X:1266:G:H1 | 1.65 | 0.44 |
| 2:Y:47:A:H8 | 6:D:92:ARG:CZ | 2.30 | 0.44 |
| 3:A:123:ALA:HB3 | 3:A:131:LEU:HB3 | 2.00 | 0.44 |
| 9:G:158:HIS:HA | 9:G:161:GLN:HB2 | 2.00 | 0.44 |
| 1:X:1827:G:H1' | 1:X:1914:U:C2 | 2.53 | 0.44 |
| 1:X:1509:A:H8 | 1:X:1510:A:C8 | 2.36 | 0.44 |
| 1:X:1465:G:H2' | 1:X:1466:C:C6 | 2.53 | 0.44 |
| 1:X:1007:A:H4' | 16:N:93:LYS:HB3 | 2.00 | 0.44 |
| 22:T:38:VAL:HG13 | 22:T:40:GLN:HG2 | 1.98 | 0.44 |
| 5:C:164:VAL:HB | 5:C:165:SER:H | 1.42 | 0.44 |
| 1:X:2445:C:H5'' | 30:4:6:SER:HB3 | 2.00 | 0.44 |
| 1:X:1385:C:H2' | 1:X:1386:A:O4' | 2.17 | 0.44 |
| 1:X:400:U:H5 | 23:U:21:ARG:HH12 | 1.64 | 0.44 |
| 1:X:1050:G:H1 | 1:X:1127:C:H42 | 1.65 | 0.44 |
| 1:X:168:A:H2' | 1:X:169:C:C6 | 2.53 | 0.44 |
| 4:B:32:PRO:CB | 4:B:72:VAL:HG11 | 2.38 | 0.44 |
| 1:X:1583:A:H3' | 3:A:86:PRO:HG3 | 2.00 | 0.44 |
| 4:B:11:MET:HA | 4:B:23:VAL:O | 2.17 | 0.44 |
| 3:A:67:PHE:CE2 | 3:A:106:LEU:HD11 | 2.53 | 0.44 |
| 3:A:67:PHE:HB3 | 3:A:153:ALA:H | 1.83 | 0.44 |
| 20:R:22:VAL:HG13 | 20:R:82:ALA:HA | 2.00 | 0.44 |
| 10:H:105:PRO:HG3 | 10:H:126:ILE:HD13 | 1.99 | 0.44 |
| 1:X:457:C:H5'' | 16:N:3:ARG:HB3 | 1.99 | 0.44 |
| 1:X:663:G:C5 | 1:X:664:C:H1' | 2.52 | 0.44 |
| 2:Y:116:C:H4' | 14:L:49:GLN:HG2 | 2.00 | 0.44 |
| 14:L:42:ILE:HD12 | 14:L:87:VAL:HG21 | 2.00 | 0.43 |
| 2:Y:118:G:H21 | 14:L:39:TYR:HH | 1.66 | 0.43 |
| 1:X:1811:A:H3' | 3:A:178:PRO:HB2 | 1.99 | 0.43 |
| 1:X:834:A:H5' | 1:X:835:U:C6 | 2.53 | 0.43 |
| 12:J:73:LYS:H | 12:J:94:TRP:HD1 | 1.66 | 0.43 |
| 5:C:47:THR:HG23 | 5:C:84:PHE:H | 1.83 | 0.43 |
| 1:X:465:C:O2' | 1:X:483:A:N6 | 2.52 | 0.43 |
| 5:C:154:ASP:HB2 | 5:C:157:THR:OG1 | 2.17 | 0.43 |
| 12:J:86:LYS:HG2 | 12:J:86:LYS:H | 1.68 | 0.43 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:X:800:U:H5'' | 1:X:801:A:H5' | 2.01 | 0.43 |
| 13:K:11:ASN:OD1 | 13:K:17:ARG:CZ | 2.66 | 0.43 |
| 1:X:1745:C:OP1 | 15:M:101:ARG:NH2 | 2.51 | 0.43 |
| 1:X:1113:C:H2' | 1:X:1114:A:C8 | 2.48 | 0.43 |
| 20:R:56:LYS:HD3 | 20:R:69:GLN:HG2 | 1.99 | 0.43 |
| 1:X:1630:A:C2 | 18:P:114:ALA:HB2 | 2.54 | 0.43 |
| 10:H:28:GLY:HA3 | 10:H:35:THR:H | 1.84 | 0.43 |
| 1:X:1955:G:OP2 | 3:A:239:ARG:NH1 | 2.49 | 0.43 |
| 1:X:1973:C:H2' | 1:X:1974:U:O4' | 2.18 | 0.43 |
| 11:I:81:GLN:HG2 | 11:I:114:ILE:HG22 | 1.99 | 0.43 |
| 23:U:33:LYS:O | 23:U:34:THR:HB | 2.18 | 0.43 |
| 9:G:103:TYR:CB | 9:G:107:GLN:HE21 | 2.32 | 0.43 |
| 1:X:534:U:H4' | 1:X:564:U:H4' | 2.00 | 0.43 |
| 11:I:38:LYS:HB3 | 11:I:39:SER:H | 1.65 | 0.43 |
| 1:X:1731:C:H2' | 1:X:1732:U:H3' | 1.98 | 0.43 |
| 22:T:20:TYR:HB3 | 22:T:21:LEU:H | 1.72 | 0.43 |
| 5:C:58:MET:HB2 | 5:C:70:GLY:O | 2.18 | 0.43 |
| 1:X:1674:C:H2' | 1:X:1675:C:C6 | 2.54 | 0.43 |
| 1:X:224:G:H4' | 1:X:399:G:C6 | 2.53 | 0.43 |
| 29:3:20:GLY:CA | 29:3:21:LYS:CA | 2.97 | 0.43 |
| 1:X:841:G:H2' | 1:X:842:A:C8 | 2.53 | 0.43 |
| 1:X:82:G:N2 | 1:X:100:G:O2' | 2.51 | 0.43 |
| 1:X:2197:U:H2' | 1:X:2198:U:C6 | 2.54 | 0.43 |
| 1:X:163:A:H2' | 1:X:164:G:C8 | 2.54 | 0.43 |
| 1:X:1674:C:H2' | 1:X:1675:C:H6 | 1.84 | 0.43 |
| 9:G:67:ARG:HB3 | 9:G:70:PHE:HA | 2.01 | 0.43 |
| 1:X:2543:A:C2 | 1:X:2626:U:H4' | 2.54 | 0.43 |
| 1:X:1314:A:H2 | 1:X:1642:G:N3 | 2.16 | 0.43 |
| 20:R:37:LEU:HD21 | 20:R:49:GLU:HG3 | 2.01 | 0.43 |
| 1:X:1223:G:H5' | 1:X:1225:G:O4' | 2.18 | 0.43 |
| 14:L:89:PHE:CD1 | 14:L:89:PHE:N | 2.71 | 0.43 |
| 1:X:2356:A:H1' | 14:L:89:PHE:CZ | 2.54 | 0.43 |
| 1:X:2189:A:H2 | 1:X:2190:A:C4 | 2.37 | 0.43 |
| 3:A:250:TRP:HB3 | 3:A:251:GLY:H | 1.61 | 0.43 |
| 13:K:8:ARG:O | 13:K:9:LYS:HB3 | 2.19 | 0.43 |
| 1:X:476:G:H2' | 1:X:477:A:C8 | 2.54 | 0.43 |
| 28:2:22:MET:CA | 28:2:23:LYS:CA | 2.97 | 0.43 |
| 9:G:70:PHE:CB | 16:N:64:ARG:HG2 | 2.49 | 0.43 |
| 19:Q:68:PHE:O | 19:Q:70:GLY:N | 2.51 | 0.43 |
| 1:X:1966:C:H4' | 1:X:2585:C:H4' | 2.01 | 0.43 |
| 19:Q:58:VAL:HA | 19:Q:59:PRO:HD3 | 1.81 | 0.43 |
| 2:Y:43:G:H5' | 2:Y:44:C:H5' | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 7:E:17:VAL:HG22 | 7:E:26:VAL:HG22 | 2.00 | 0.43 |
| 1:X:2633:A:N1 | 1:X:2644:A:H5'' | 2.34 | 0.43 |
| 4:B:115:GLY:HA2 | 4:B:157:ALA:HB2 | 2.00 | 0.42 |
| 10:H:124:MET:O | 10:H:127:VAL:HG12 | 2.18 | 0.42 |
| 1:X:807:A:H2' | 1:X:808:C:C6 | 2.53 | 0.42 |
| 1:X:1699:A:H61 | 1:X:1723:U:H3 | 1.66 | 0.42 |
| 1:X:77:C:H42 | 1:X:106:G:H1 | 1.66 | 0.42 |
| 1:X:331:U:O2' | 5:C:162:ARG:NH1 | 2.52 | 0.42 |
| 17:O:36:LYS:HD3 | 17:O:39:PHE:HB3 | 2.01 | 0.42 |
| 1:X:1623:C:H4' | 1:X:1624:A:O5' | 2.19 | 0.42 |
| 10:H:88:THR:HB | 15:M:80:VAL:HB | 2.00 | 0.42 |
| 4:B:125:GLY:H | 4:B:135:HIS:HA | 1.84 | 0.42 |
| 1:X:1367:A:H2' | 1:X:1368:G:O4' | 2.19 | 0.42 |
| 1:X:830:C:O2' | 1:X:852:U:H5'' | 2.19 | 0.42 |
| 1:X:2581:A:H2' | 1:X:2582:G:H4' | 2.00 | 0.42 |
| 1:X:540:G:C5 | 1:X:2005:U:H5'' | 2.54 | 0.42 |
| 1:X:2394:G:H4' | 11:I:65:PHE:HB3 | 2.02 | 0.42 |
| 1:X:2324:G:N3 | 1:X:2360:C:H2' | 2.35 | 0.42 |
| 19:Q:84:GLU:HA | 19:Q:86:GLN:HE21 | 1.84 | 0.42 |
| 17:O:13:ARG:HB3 | 17:O:14:VAL:H | 1.71 | 0.42 |
| 2:Y:65:A:H2' | 2:Y:66:G:H8 | 1.84 | 0.42 |
| 1:X:1989:C:O2' | 1:X:2798:A:N3 | 2.49 | 0.42 |
| 17:O:98:ILE:H | 17:O:98:ILE:HG13 | 1.75 | 0.42 |
| 1:X:1142:G:H5' | 9:G:111:LYS:HB3 | 2.02 | 0.42 |
| 12:J:27:TYR:CE2 | 21:S:76:ARG:HB3 | 2.55 | 0.42 |
| 12:J:27:TYR:HE2 | 21:S:76:ARG:HD3 | 1.84 | 0.42 |
| 4:B:16:LYS:HB2 | 4:B:21:ILE:CD1 | 2.46 | 0.42 |
| 1:X:334:G:H8 | 5:C:164:VAL:HG13 | 1.83 | 0.42 |
| 10:H:27:SER:HB3 | 10:H:50:ILE:HG13 | 2.01 | 0.42 |
| 2:Y:94:G:H5' | 21:S:74:ARG:HH12 | 1.84 | 0.42 |
| 1:X:1658:A:H2' | 1:X:1659:G:O4' | 2.19 | 0.42 |
| 2:Y:34:C:H2' | 2:Y:35:C:C6 | 2.54 | 0.42 |
| 11:I:130:ILE:HG13 | 11:I:130:ILE:H | 1.65 | 0.42 |
| 9:G:106:TYR:CE2 | 9:G:108:GLY:CA | 3.03 | 0.42 |
| 1:X:1030:U:C4 | 1:X:1031:C:H5 | 2.37 | 0.42 |
| 3:A:247:VAL:HG23 | 3:A:248:THR:N | 2.34 | 0.42 |
| 3:A:186:HIS:HB2 | 3:A:188:GLU:HG3 | 2.01 | 0.42 |
| 1:X:636:G:C5' | 1:X:636:G:H8 | 2.33 | 0.42 |
| 9:G:69:ASP:H | 9:G:76:GLN:NE2 | 2.17 | 0.42 |
| 5:C:150:LEU:HB3 | 5:C:169:VAL:HG23 | 2.00 | 0.42 |
| 20:R:46:VAL:HG21 | 20:R:80:LYS:HE3 | 2.02 | 0.42 |
| 1:X:82:G:N1 | 1:X:100:G:H2' | 2.34 | 0.42 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 19:Q:28:TRP:HZ3 | 19:Q:58:VAL:HG21 | 1.84 | 0.42 |
| 5:C:194:GLU:O | 5:C:195:ILE:HG12 | 2.20 | 0.42 |
| 21:S:23:ALA:HA | 21:S:83:PHE:O | 2.18 | 0.42 |
| 10:H:26:ASN:HB3 | 10:H:38:GLY:H | 1.84 | 0.42 |
| 5:C:27:LEU:O | 5:C:31:VAL:HG22 | 2.19 | 0.42 |
| 11:I:43:ALA:C | 11:I:45:LYS:H | 2.23 | 0.42 |
| 1:X:2191:A:OP1 | 1:X:2193:C:N4 | 2.52 | 0.42 |
| 13:K:28:LEU:HD13 | 13:K:115:LEU:HD23 | 2.00 | 0.42 |
| 3:A:43:ARG:HH11 | 3:A:43:ARG:N | 2.17 | 0.42 |
| 9:G:65:LYS:HD2 | 9:G:66:HIS:CD2 | 2.54 | 0.42 |
| 20:R:105:ARG:HH22 | 20:R:112:LYS:CA | 2.33 | 0.42 |
| 1:X:2663:U:C4 | 1:X:2664:G:N7 | 2.88 | 0.42 |
| 1:X:451:A:H2' | 1:X:452:G:C8 | 2.55 | 0.42 |
| 1:X:1909:U:P | 1:X:1912:G:H1 | 2.42 | 0.42 |
| 5:C:95:LEU:HD23 | 5:C:96:PRO:HD2 | 2.00 | 0.42 |
| 1:X:2540:A:O2' | 10:H:23:ARG:HG3 | 2.19 | 0.42 |
| 15:M:39:VAL:HA | 15:M:45:THR:HA | 2.02 | 0.42 |
| 1:X:110:U:H3' | 1:X:111:G:H5'' | 2.01 | 0.42 |
| 26:Z:36:CYS:HB3 | 26:Z:49:CYS:HB3 | 1.91 | 0.42 |
| 14:L:63:ASN:HB3 | 14:L:66:ASP:HB2 | 2.01 | 0.42 |
| 3:A:108:PRO:HB3 | 3:A:143:HIS:HE1 | 1.84 | 0.42 |
| 6:D:17:MET:HG2 | 6:D:22:TYR:HB2 | 2.01 | 0.42 |
| 29:3:10:ALA:CA | 29:3:11:LYS:CA | 2.98 | 0.42 |
| 7:E:19:ALA:HB1 | 7:E:24:PHE:HD2 | 1.84 | 0.42 |
| 1:X:503:G:H2' | 1:X:504:G:O4' | 2.20 | 0.42 |
| 1:X:648:A:H4' | 1:X:649:G:O4' | 2.20 | 0.42 |
| 19:Q:59:PRO:HA | 19:Q:74:ASP:OD1 | 2.19 | 0.42 |
| 1:X:1441:A:H4' | 1:X:1442:C:O5' | 2.19 | 0.42 |
| 1:X:2617:G:O2' | 1:X:2755:A:N1 | 2.45 | 0.42 |
| 1:X:1766:U:O4 | 1:X:1780:A:H2 | 2.02 | 0.42 |
| 3:A:231:HIS:HD2 | 3:A:233:HIS:N | 2.04 | 0.42 |
| 19:Q:35:LYS:HA | 19:Q:38:ILE:HG22 | 2.01 | 0.42 |
| 20:R:80:LYS:O | 20:R:80:LYS:NZ | 2.45 | 0.42 |
| 1:X:2542:U:O2 | 1:X:2544:A:H8 | 2.03 | 0.42 |
| 1:X:760:U:O2 | 1:X:1997:A:H1' | 2.20 | 0.42 |
| 1:X:543:G:H5' | 16:N:24:PHE:CE1 | 2.55 | 0.42 |
| 9:G:43:VAL:HB | 9:G:167:LYS:HG2 | 2.02 | 0.42 |
| 1:X:2674:C:H2' | 1:X:2675:U:H6 | 1.85 | 0.42 |
| 1:X:1151:U:H3' | 9:G:91:THR:HG21 | 2.01 | 0.41 |
| 12:J:36:ILE:HD12 | 12:J:133:VAL:HG21 | 2.01 | 0.41 |
| 15:M:34:ARG:HB2 | 15:M:91:VAL:HG23 | 2.02 | 0.41 |
| 2:Y:8:C:H4' | 2:Y:30:C:H5' | 2.01 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 3:A:208:LYS:HE3 | 3:A:208:LYS:HA | 2.01 | 0.41 |
| 4:B:183:LEU:HD11 | 15:M:16:ILE:CG2 | 2.50 | 0.41 |
| 1:X:1939:U:H2' | 1:X:1939:U:O2 | 2.18 | 0.41 |
| 1:X:2315:A:H2 | 1:X:2364:C:O2 | 2.03 | 0.41 |
| 21:S:168:VAL:HG12 | 21:S:169:VAL:HG23 | 2.01 | 0.41 |
| 1:X:1378:A:H3' | 1:X:1379:A:H8 | 1.85 | 0.41 |
| 1:X:171:G:H2' | 1:X:172:A:O4' | 2.20 | 0.41 |
| 1:X:2326:C:H2' | 1:X:2327:U:C6 | 2.55 | 0.41 |
| 1:X:2326:C:C2 | 1:X:2327:U:C5 | 3.08 | 0.41 |
| 1:X:1300:A:H5' | 13:K:103:ARG:HD2 | 2.01 | 0.41 |
| 1:X:2065:A:H2' | 1:X:2066:G:O4' | 2.20 | 0.41 |
| 15:M:66:PHE:CE2 | 15:M:81:PHE:HB2 | 2.55 | 0.41 |
| 23:U:49:LYS:HB2 | 23:U:61:TRP:CD2 | 2.56 | 0.41 |
| 4:B:134:TRP:CD1 | 4:B:134:TRP:N | 2.83 | 0.41 |
| 1:X:577:U:C5' | 1:X:956:A:N6 | 2.84 | 0.41 |
| 9:G:162:LYS:H | 9:G:163:PRO:CD | 2.33 | 0.41 |
| 6:D:38:GLU:HG3 | 6:D:40:LEU:HD23 | 2.01 | 0.41 |
| 22:T:46:LYS:HB2 | 22:T:78:PHE:CE2 | 2.56 | 0.41 |
| 14:L:30:SER:O | 14:L:40:ALA:HA | 2.21 | 0.41 |
| 5:C:62:LYS:HB3 | 5:C:62:LYS:HE2 | 1.72 | 0.41 |
| 17:O:60:VAL:HA | 17:O:93:ILE:HG22 | 2.03 | 0.41 |
| 1:X:2820:C:H5'' | 15:M:60:SER:HB3 | 2.02 | 0.41 |
| 1:X:1231:A:H2' | 1:X:1232:U:C6 | 2.55 | 0.41 |
| 11:I:87:THR:HB | 11:I:97:ARG:HD3 | 2.02 | 0.41 |
| 4:B:5:LEU:HD22 | 4:B:49:ILE:HG22 | 2.02 | 0.41 |
| 24:V:2:LYS:H | 24:V:3:PRO:CD | 2.34 | 0.41 |
| 6:D:48:LYS:HG3 | 6:D:48:LYS:H | 1.67 | 0.41 |
| 1:X:558:G:H4' | 1:X:559:C:C5' | 2.48 | 0.41 |
| 1:X:636:G:C5' | 1:X:636:G:C8 | 3.04 | 0.41 |
| 15:M:39:VAL:HG12 | 15:M:45:THR:HG23 | 2.01 | 0.41 |
| 1:X:1442:C:O2' | 1:X:1443:G:H5' | 2.19 | 0.41 |
| 3:A:141:VAL:HG13 | 3:A:162:SER:HB3 | 2.02 | 0.41 |
| 13:K:51:LEU:HD12 | 13:K:66:VAL:HG22 | 2.02 | 0.41 |
| 1:X:2406:C:C5' | 1:X:2408:G:H5' | 2.50 | 0.41 |
| 5:C:12:GLY:O | 5:C:14:THR:N | 2.49 | 0.41 |
| 4:B:149:ARG:CZ | 9:G:106:TYR:CD1 | 3.03 | 0.41 |
| 16:N:93:LYS:HE2 | 17:O:5:ILE:HD13 | 2.03 | 0.41 |
| 1:X:564:U:H2' | 1:X:565:A:H8 | 1.83 | 0.41 |
| 1:X:346:C:O2 | 1:X:347:C:C5 | 2.73 | 0.41 |
| 6:D:104:ILE:HA | 6:D:108:LEU:HD12 | 2.03 | 0.41 |
| 1:X:1283:C:H5'' | 1:X:1284:G:O5' | 2.21 | 0.41 |
| 15:M:24:LEU:HD12 | 15:M:83:PHE:CG | 2.56 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 21:S:47:SER:OG | 21:S:48:THR:N | 2.51 | 0.41 |
| 1:X:1813:A:O5' | 1:X:1813:A:H8 | 2.04 | 0.41 |
| 15:M:58:ASN:HD22 | 15:M:58:ASN:H | 1.67 | 0.41 |
| 18:P:43:ASP:OD2 | 18:P:46:ARG:NH2 | 2.54 | 0.41 |
| 1:X:1919:A:C2 | 1:X:1926:U:N3 | 2.67 | 0.41 |
| 4:B:183:LEU:HD21 | 15:M:16:ILE:HD13 | 2.02 | 0.41 |
| 5:C:173:ALA:HB1 | 5:C:193:LEU:HD13 | 2.02 | 0.41 |
| 1:X:393:U:H2' | 1:X:394:U:H6 | 1.85 | 0.41 |
| 23:U:10:LYS:HD2 | 23:U:60:VAL:HG11 | 2.02 | 0.41 |
| 17:O:40:VAL:HG13 | 17:O:45:THR:HG22 | 2.01 | 0.41 |
| 1:X:172:A:N6 | 1:X:175:C:H3' | 2.34 | 0.41 |
| 1:X:405:C:H2' | 1:X:406:G:C8 | 2.53 | 0.41 |
| 1:X:1687:C:H6 | 1:X:1687:C:O5' | 2.03 | 0.41 |
| 13:K:106:ASP:OD1 | 13:K:108:VAL:HB | 2.21 | 0.41 |
| 1:X:1032:A:H2' | 1:X:1034:U:H5'' | 2.03 | 0.41 |
| 1:X:162:C:H2' | 1:X:163:A:H8 | 1.85 | 0.41 |
| 1:X:1179:A:H2' | 1:X:1180:A:C8 | 2.56 | 0.41 |
| 21:S:149:ALA:HB1 | 21:S:160:LEU:HD13 | 2.02 | 0.41 |
| 1:X:2206:C:H1' | 3:A:262:LYS:HE2 | 2.03 | 0.41 |
| 10:H:114:VAL:HG22 | 10:H:133:VAL:HG22 | 2.02 | 0.41 |
| 5:C:117:LEU:HB3 | 5:C:187:VAL:HA | 2.02 | 0.41 |
| 11:I:102:LYS:O | 11:I:104:ARG:N | 2.37 | 0.41 |
| 1:X:1467:U:C5' | 1:X:1467:U:C6 | 3.04 | 0.41 |
| 19:Q:72:ARG:HG2 | 19:Q:72:ARG:H | 1.65 | 0.41 |
| 13:K:3:HIS:CE1 | 13:K:5:LYS:HZ2 | 2.31 | 0.41 |
| 11:I:54:SER:O | 11:I:56:LEU:N | 2.50 | 0.41 |
| 1:X:2189:A:C2 | 1:X:2190:A:C5 | 3.09 | 0.41 |
| 22:T:21:LEU:HD11 | 22:T:41:ARG:CZ | 2.51 | 0.41 |
| 16:N:17:VAL:HG11 | 16:N:36:PHE:HB2 | 2.02 | 0.41 |
| 17:O:48:GLY:C | 17:O:50:ASP:H | 2.24 | 0.41 |
| 11:I:30:ALA:HB3 | 11:I:34:HIS:CE1 | 2.56 | 0.41 |
| 1:X:1795:C:H5' | 3:A:257:LEU:HD13 | 2.02 | 0.41 |
| 13:K:49:GLU:OE1 | 13:K:95:THR:HB | 2.21 | 0.40 |
| 16:N:93:LYS:H | 16:N:93:LYS:HG3 | 1.69 | 0.40 |
| 1:X:573:C:H5'' | 17:O:74:TYR:OH | 2.21 | 0.40 |
| 12:J:133:VAL:HG12 | 21:S:76:ARG:CZ | 2.51 | 0.40 |
| 1:X:2262:C:C2 | 1:X:2368:G:C2 | 3.10 | 0.40 |
| 20:R:93:ARG:HE | 20:R:108:VAL:HG12 | 1.86 | 0.40 |
| 1:X:689:A:H2 | 1:X:815:A:H61 | 1.68 | 0.40 |
| 22:T:3:HIS:HD2 | 22:T:5:LYS:HB2 | 1.85 | 0.40 |
| 11:I:76:LYS:HG2 | 11:I:111:SER:HB2 | 2.03 | 0.40 |
| 1:X:82:G:H1 | 1:X:100:G:H2' | 1.86 | 0.40 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 12:J:35:LEU:HD23 | 12:J:105:PHE:HD2 | 1.86 | 0.40 |
| 3:A:205:VAL:O | 3:A:207:GLY:N | 2.54 | 0.40 |
| 1:X:1467:U:C2' | 1:X:1468:A:OP1 | 2.68 | 0.40 |
| 12:J:26:ASP:HB3 | 12:J:27:TYR:H | 1.60 | 0.40 |
| 2:Y:64:C:H2' | 2:Y:65:A:H8 | 1.85 | 0.40 |
| 16:N:86:ALA:HB2 | 16:N:116:ALA:HB2 | 2.03 | 0.40 |
| 1:X:2855:C:H1' | 13:K:92:GLY:O | 2.22 | 0.40 |
| 1:X:2864:C:H2' | 1:X:2865:G:C8 | 2.57 | 0.40 |
| 9:G:119:LEU:HD23 | 9:G:122:HIS:HD2 | 1.85 | 0.40 |
| 1:X:1235:C:H2' | 1:X:1236:G:C8 | 2.57 | 0.40 |
| 4:B:77:ILE:HD13 | 15:M:3:THR:HG22 | 2.02 | 0.40 |
| 1:X:1142:G:OP2 | 1:X:2494:C:H5'' | 2.21 | 0.40 |
| 15:M:27:PHE:CE2 | 15:M:91:VAL:HG11 | 2.56 | 0.40 |
| 1:X:636:G:C8 | 1:X:636:G:H5'' | 2.53 | 0.40 |
| 1:X:2551:A:N7 | 4:B:145:LYS:HB2 | 2.37 | 0.40 |
| 1:X:424:G:H4' | 1:X:425:A:O5' | 2.21 | 0.40 |
| 16:N:93:LYS:O | 16:N:94:VAL:HB | 2.21 | 0.40 |
| 3:A:217:ARG:O | 3:A:218:LYS:C | 2.60 | 0.40 |
| 1:X:309:G:H5'' | 1:X:310:A:OP1 | 2.21 | 0.40 |
| 17:O:10:LYS:HA | 17:O:36:LYS:HA | 2.03 | 0.40 |
| 9:G:62:ILE:CG2 | 9:G:135:LEU:HD21 | 2.50 | 0.40 |
| 1:X:2556:A:H5'' | 1:X:2557:G:H5' | 2.04 | 0.40 |
| 6:D:177:PHE:HB2 | 6:D:179:LYS:HE3 | 2.02 | 0.40 |
| 1:X:1151:U:H4' | 1:X:1153:A:H5'' | 2.04 | 0.40 |
| 13:K:17:ARG:HA | 13:K:17:ARG:HD3 | 2.00 | 0.40 |
| 32:X:2929:1F2:H46 | 32:X:2929:1F2:O41 | 2.21 | 0.40 |
| 3:A:60:ARG:HD3 | 3:A:86:PRO:HB2 | 2.04 | 0.40 |
| 19:Q:6:ILE:HG22 | 19:Q:7:LEU:HD23 | 2.01 | 0.40 |
| 1:X:89:A:C4' | 1:X:90:G:H5'' | 2.52 | 0.40 |
| 1:X:393:U:H2' | 1:X:394:U:C6 | 2.57 | 0.40 |
| 25:W:40:VAL:HG22 | 25:W:43:MET:HE3 | 2.04 | 0.40 |
| 1:X:761:G:OP2 | 18:P:109:ARG:HG3 | 2.21 | 0.40 |
| 1:X:2482:A:H4' | 1:X:2483:U:OP1 | 2.21 | 0.40 |
| 1:X:1287:A:H2' | 1:X:1288:A:H5'' | 2.03 | 0.40 |
| 20:R:48:VAL:HG12 | 20:R:50:GLY:H | 1.86 | 0.40 |
| 26:Z:45:ILE:HG21 | 26:Z:57:VAL:HG23 | 2.03 | 0.40 |
| 5:C:48:ARG:HB2 | 5:C:51:VAL:HG22 | 2.02 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|----------|-------------|-----|
| 3 | A | 238/274 (87%) | 178 (75%) | 39 (16%) | 21 (9%) | 1 | 8 |
| 4 | B | 203/211 (96%) | 171 (84%) | 24 (12%) | 8 (4%) | 5 | 33 |
| 5 | C | 195/205 (95%) | 129 (66%) | 45 (23%) | 21 (11%) | 1 | 5 |
| 6 | D | 175/180 (97%) | 141 (81%) | 27 (15%) | 7 (4%) | 5 | 32 |
| 7 | E | 169/185 (91%) | 139 (82%) | 20 (12%) | 10 (6%) | 2 | 20 |
| 8 | F | 69/144 (48%) | 57 (83%) | 10 (14%) | 2 (3%) | 7 | 43 |
| 9 | G | 140/174 (80%) | 105 (75%) | 21 (15%) | 14 (10%) | 1 | 6 |
| 10 | H | 132/134 (98%) | 115 (87%) | 11 (8%) | 6 (4%) | 4 | 29 |
| 11 | I | 139/156 (89%) | 85 (61%) | 28 (20%) | 26 (19%) | 0 | 0 |
| 12 | J | 134/141 (95%) | 101 (75%) | 19 (14%) | 14 (10%) | 1 | 5 |
| 13 | K | 111/116 (96%) | 92 (83%) | 11 (10%) | 8 (7%) | 2 | 13 |
| 14 | L | 102/114 (90%) | 75 (74%) | 19 (19%) | 8 (8%) | 1 | 11 |
| 15 | M | 106/166 (64%) | 89 (84%) | 13 (12%) | 4 (4%) | 5 | 34 |
| 16 | N | 115/118 (98%) | 92 (80%) | 17 (15%) | 6 (5%) | 3 | 25 |
| 17 | O | 92/100 (92%) | 67 (73%) | 13 (14%) | 12 (13%) | 0 | 3 |
| 18 | P | 125/134 (93%) | 108 (86%) | 12 (10%) | 5 (4%) | 5 | 32 |
| 19 | Q | 91/95 (96%) | 64 (70%) | 14 (15%) | 13 (14%) | 0 | 2 |
| 20 | R | 108/115 (94%) | 66 (61%) | 24 (22%) | 18 (17%) | 0 | 1 |
| 21 | S | 173/237 (73%) | 135 (78%) | 28 (16%) | 10 (6%) | 3 | 21 |
| 22 | T | 82/91 (90%) | 64 (78%) | 11 (13%) | 7 (8%) | 1 | 9 |
| 23 | U | 70/81 (86%) | 43 (61%) | 16 (23%) | 11 (16%) | 0 | 1 |
| 24 | V | 64/67 (96%) | 58 (91%) | 4 (6%) | 2 (3%) | 7 | 41 |
| 25 | W | 53/55 (96%) | 50 (94%) | 3 (6%) | 0 | 100 | 100 |
| 26 | Z | 56/60 (93%) | 48 (86%) | 5 (9%) | 3 (5%) | 3 | 24 |
| 30 | 4 | 35/37 (95%) | 31 (89%) | 3 (9%) | 1 (3%) | 7 | 43 |
| All | All | 2977/3390 (88%) | 2303 (77%) | 437 (15%) | 237 (8%) | 1 | 10 |

All (237) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | A | 56 | GLY |
| 3 | A | 89 | SER |
| 3 | A | 198 | ASN |
| 3 | A | 199 | ALA |
| 3 | A | 249 | PRO |
| 3 | A | 250 | TRP |
| 4 | B | 116 | VAL |
| 4 | B | 146 | THR |
| 5 | C | 13 | ARG |
| 5 | C | 20 | PRO |
| 5 | C | 60 | GLY |
| 5 | C | 67 | ALA |
| 5 | C | 121 | ASP |
| 5 | C | 129 | LYS |
| 5 | C | 164 | VAL |
| 5 | C | 165 | SER |
| 5 | C | 172 | VAL |
| 5 | C | 195 | ILE |
| 6 | D | 81 | GLN |
| 7 | E | 55 | PRO |
| 7 | E | 126 | PRO |
| 7 | E | 165 | VAL |
| 9 | G | 34 | PRO |
| 9 | G | 67 | ARG |
| 9 | G | 91 | THR |
| 9 | G | 104 | THR |
| 9 | G | 107 | GLN |
| 9 | G | 158 | HIS |
| 10 | H | 27 | SER |
| 10 | H | 29 | ILE |
| 11 | I | 18 | ARG |
| 11 | I | 37 | GLN |
| 11 | I | 39 | SER |
| 11 | I | 55 | ARG |
| 11 | I | 62 | LYS |
| 11 | I | 98 | LEU |
| 11 | I | 99 | VAL |
| 11 | I | 103 | ASN |
| 12 | J | 13 | GLN |
| 12 | J | 21 | ASP |
| 12 | J | 26 | ASP |
| 13 | K | 6 | ALA |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13 | K | 9 | LYS |
| 14 | L | 21 | THR |
| 15 | M | 26 | ASP |
| 15 | M | 29 | PRO |
| 16 | N | 7 | GLY |
| 16 | N | 87 | ASN |
| 17 | O | 7 | THR |
| 17 | O | 9 | GLY |
| 17 | O | 10 | LYS |
| 17 | O | 14 | VAL |
| 17 | O | 31 | ASP |
| 17 | O | 48 | GLY |
| 19 | Q | 6 | ILE |
| 19 | Q | 12 | ILE |
| 19 | Q | 67 | ARG |
| 19 | Q | 69 | ILE |
| 19 | Q | 90 | ALA |
| 20 | R | 5 | SER |
| 20 | R | 11 | ASN |
| 21 | S | 26 | LYS |
| 22 | T | 19 | LYS |
| 23 | U | 15 | VAL |
| 23 | U | 19 | ILE |
| 23 | U | 29 | GLY |
| 23 | U | 60 | VAL |
| 24 | V | 2 | LYS |
| 26 | Z | 4 | HIS |
| 26 | Z | 36 | CYS |
| 26 | Z | 53 | ASP |
| 3 | A | 87 | ASN |
| 3 | A | 206 | LEU |
| 3 | A | 248 | THR |
| 4 | B | 76 | ARG |
| 4 | B | 123 | ALA |
| 4 | B | 148 | GLY |
| 5 | C | 22 | VAL |
| 5 | C | 84 | PHE |
| 6 | D | 124 | GLY |
| 7 | E | 13 | SER |
| 9 | G | 64 | GLY |
| 9 | G | 97 | ASP |
| 9 | G | 170 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11 | I | 47 | ALA |
| 11 | I | 49 | PHE |
| 11 | I | 54 | SER |
| 11 | I | 56 | LEU |
| 11 | I | 64 | GLY |
| 11 | I | 86 | THR |
| 12 | J | 11 | ARG |
| 12 | J | 80 | ALA |
| 12 | J | 83 | ARG |
| 13 | K | 4 | GLY |
| 13 | K | 92 | GLY |
| 14 | L | 33 | ARG |
| 14 | L | 40 | ALA |
| 14 | L | 46 | SER |
| 17 | O | 8 | GLY |
| 17 | O | 60 | VAL |
| 18 | P | 9 | ARG |
| 19 | Q | 74 | ASP |
| 19 | Q | 84 | GLU |
| 19 | Q | 87 | SER |
| 19 | Q | 89 | GLU |
| 20 | R | 7 | GLY |
| 20 | R | 60 | PRO |
| 20 | R | 83 | LEU |
| 20 | R | 85 | ASP |
| 20 | R | 98 | ILE |
| 20 | R | 108 | VAL |
| 21 | S | 5 | ALA |
| 21 | S | 88 | TYR |
| 21 | S | 91 | PRO |
| 21 | S | 156 | GLU |
| 22 | T | 21 | LEU |
| 22 | T | 74 | LYS |
| 23 | U | 27 | ASP |
| 23 | U | 32 | ARG |
| 23 | U | 41 | VAL |
| 23 | U | 56 | GLN |
| 24 | V | 57 | LYS |
| 3 | A | 170 | SER |
| 3 | A | 220 | HIS |
| 3 | A | 244 | ARG |
| 4 | B | 90 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | C | 15 | ILE |
| 5 | C | 190 | ALA |
| 6 | D | 122 | PHE |
| 7 | E | 19 | ALA |
| 7 | E | 58 | ALA |
| 7 | E | 173 | ALA |
| 8 | F | 120 | VAL |
| 9 | G | 33 | ILE |
| 9 | G | 37 | ASP |
| 10 | H | 5 | GLN |
| 10 | H | 37 | GLY |
| 11 | I | 29 | THR |
| 11 | I | 65 | PHE |
| 11 | I | 82 | ASP |
| 11 | I | 88 | PHE |
| 11 | I | 115 | SER |
| 12 | J | 60 | ARG |
| 12 | J | 81 | GLU |
| 13 | K | 11 | ASN |
| 14 | L | 20 | THR |
| 16 | N | 92 | ARG |
| 16 | N | 95 | LEU |
| 17 | O | 13 | ARG |
| 17 | O | 36 | LYS |
| 17 | O | 49 | GLU |
| 18 | P | 132 | GLY |
| 19 | Q | 5 | ASP |
| 19 | Q | 59 | PRO |
| 19 | Q | 63 | LYS |
| 20 | R | 6 | ALA |
| 20 | R | 18 | LYS |
| 20 | R | 26 | SER |
| 20 | R | 50 | GLY |
| 20 | R | 62 | MET |
| 20 | R | 63 | THR |
| 20 | R | 96 | LYS |
| 21 | S | 76 | ARG |
| 21 | S | 106 | GLY |
| 3 | A | 59 | LYS |
| 4 | B | 137 | ARG |
| 5 | C | 72 | ARG |
| 5 | C | 196 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6 | D | 42 | SER |
| 7 | E | 7 | GLN |
| 9 | G | 163 | PRO |
| 11 | I | 91 | ASP |
| 13 | K | 8 | ARG |
| 13 | K | 14 | SER |
| 13 | K | 88 | ALA |
| 14 | L | 59 | LEU |
| 15 | M | 25 | PRO |
| 16 | N | 94 | VAL |
| 19 | Q | 13 | SER |
| 21 | S | 6 | LYS |
| 22 | T | 13 | GLY |
| 22 | T | 73 | GLY |
| 23 | U | 34 | THR |
| 23 | U | 48 | LYS |
| 3 | A | 35 | GLU |
| 3 | A | 54 | ILE |
| 3 | A | 55 | GLY |
| 3 | A | 187 | SER |
| 3 | A | 219 | PRO |
| 5 | C | 4 | ILE |
| 5 | C | 11 | GLY |
| 5 | C | 66 | ASN |
| 5 | C | 126 | ALA |
| 6 | D | 10 | ASP |
| 6 | D | 40 | LEU |
| 7 | E | 80 | SER |
| 9 | G | 68 | PRO |
| 10 | H | 41 | ASN |
| 10 | H | 42 | LYS |
| 11 | I | 19 | VAL |
| 11 | I | 101 | ARG |
| 12 | J | 29 | ALA |
| 12 | J | 30 | PHE |
| 12 | J | 78 | LYS |
| 14 | L | 53 | ALA |
| 16 | N | 8 | ILE |
| 18 | P | 20 | LEU |
| 18 | P | 81 | HIS |
| 18 | P | 85 | MET |
| 21 | S | 56 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22 | T | 11 | LYS |
| 22 | T | 27 | GLY |
| 30 | 4 | 13 | ASN |
| 3 | A | 252 | LYS |
| 3 | A | 255 | LYS |
| 5 | C | 171 | PRO |
| 6 | D | 121 | ALA |
| 9 | G | 105 | GLY |
| 11 | I | 9 | THR |
| 11 | I | 84 | GLU |
| 12 | J | 28 | VAL |
| 12 | J | 82 | THR |
| 20 | R | 75 | ALA |
| 21 | S | 110 | GLY |
| 23 | U | 74 | PRO |
| 4 | B | 72 | VAL |
| 8 | F | 118 | GLY |
| 11 | I | 44 | GLY |
| 11 | I | 68 | VAL |
| 12 | J | 91 | VAL |
| 20 | R | 19 | GLY |
| 14 | L | 38 | ILE |
| 15 | M | 28 | ARG |
| 17 | O | 22 | VAL |
| 20 | R | 64 | ASN |
| 3 | A | 197 | GLY |
| 7 | E | 136 | ILE |

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|-------------|----|
| 3 | A | 185/215 (86%) | 151 (82%) | 34 (18%) | 2 | 11 |
| 4 | B | 155/157 (99%) | 128 (83%) | 27 (17%) | 3 | 13 |
| 5 | C | 157/163 (96%) | 120 (76%) | 37 (24%) | 1 | 4 |
| 6 | D | 153/156 (98%) | 133 (87%) | 20 (13%) | 6 | 28 |

Continued on next page...

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 7 | E | 136/144 (94%) | 125 (92%) | 11 (8%) | 17 | 56 |
| 8 | F | 51/107 (48%) | 49 (96%) | 2 (4%) | 43 | 84 |
| 9 | G | 118/146 (81%) | 93 (79%) | 25 (21%) | 1 | 8 |
| 10 | H | 103/103 (100%) | 87 (84%) | 16 (16%) | 4 | 17 |
| 11 | I | 108/121 (89%) | 76 (70%) | 32 (30%) | 0 | 1 |
| 12 | J | 110/115 (96%) | 88 (80%) | 22 (20%) | 2 | 9 |
| 13 | K | 90/93 (97%) | 68 (76%) | 22 (24%) | 1 | 3 |
| 14 | L | 74/82 (90%) | 56 (76%) | 18 (24%) | 1 | 3 |
| 15 | M | 94/134 (70%) | 66 (70%) | 28 (30%) | 0 | 1 |
| 16 | N | 96/97 (99%) | 81 (84%) | 15 (16%) | 4 | 17 |
| 17 | O | 75/79 (95%) | 57 (76%) | 18 (24%) | 1 | 4 |
| 18 | P | 109/115 (95%) | 89 (82%) | 20 (18%) | 2 | 12 |
| 19 | Q | 75/76 (99%) | 62 (83%) | 13 (17%) | 3 | 13 |
| 20 | R | 91/96 (95%) | 70 (77%) | 21 (23%) | 1 | 5 |
| 21 | S | 149/192 (78%) | 130 (87%) | 19 (13%) | 6 | 28 |
| 22 | T | 62/67 (92%) | 53 (86%) | 9 (14%) | 5 | 22 |
| 23 | U | 57/66 (86%) | 37 (65%) | 20 (35%) | 0 | 0 |
| 24 | V | 54/55 (98%) | 46 (85%) | 8 (15%) | 4 | 20 |
| 25 | W | 48/48 (100%) | 35 (73%) | 13 (27%) | 1 | 2 |
| 26 | Z | 51/53 (96%) | 39 (76%) | 12 (24%) | 1 | 5 |
| 30 | 4 | 35/35 (100%) | 31 (89%) | 4 (11%) | 8 | 35 |
| All | All | 2436/2715 (90%) | 1970 (81%) | 466 (19%) | 2 | 11 |

All (466) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | A | 39 | LYS |
| 3 | A | 40 | THR |
| 3 | A | 43 | ARG |
| 3 | A | 44 | ASN |
| 3 | A | 46 | ARG |
| 3 | A | 48 | ARG |
| 3 | A | 49 | ILE |
| 3 | A | 50 | THR |
| 3 | A | 52 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | A | 63 | ARG |
| 3 | A | 68 | LYS |
| 3 | A | 69 | ARG |
| 3 | A | 76 | ASN |
| 3 | A | 88 | ARG |
| 3 | A | 96 | HIS |
| 3 | A | 105 | ILE |
| 3 | A | 111 | LEU |
| 3 | A | 145 | LEU |
| 3 | A | 157 | ARG |
| 3 | A | 164 | GLN |
| 3 | A | 183 | ARG |
| 3 | A | 196 | VAL |
| 3 | A | 198 | ASN |
| 3 | A | 203 | ASN |
| 3 | A | 208 | LYS |
| 3 | A | 215 | LEU |
| 3 | A | 218 | LYS |
| 3 | A | 226 | MET |
| 3 | A | 229 | VAL |
| 3 | A | 240 | THR |
| 3 | A | 244 | ARG |
| 3 | A | 252 | LYS |
| 3 | A | 259 | THR |
| 3 | A | 260 | ARG |
| 4 | B | 5 | LEU |
| 4 | B | 14 | ILE |
| 4 | B | 19 | ARG |
| 4 | B | 37 | LYS |
| 4 | B | 41 | THR |
| 4 | B | 49 | ILE |
| 4 | B | 69 | LYS |
| 4 | B | 77 | ILE |
| 4 | B | 82 | ARG |
| 4 | B | 87 | ASP |
| 4 | B | 105 | THR |
| 4 | B | 111 | LYS |
| 4 | B | 119 | ARG |
| 4 | B | 131 | SER |
| 4 | B | 133 | LYS |
| 4 | B | 134 | TRP |
| 4 | B | 136 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | B | 137 | ARG |
| 4 | B | 141 | ILE |
| 4 | B | 145 | LYS |
| 4 | B | 149 | ARG |
| 4 | B | 150 | VAL |
| 4 | B | 152 | LYS |
| 4 | B | 154 | LYS |
| 4 | B | 162 | MET |
| 4 | B | 163 | GLU |
| 4 | B | 203 | LYS |
| 5 | C | 4 | ILE |
| 5 | C | 5 | ASN |
| 5 | C | 10 | ASN |
| 5 | C | 13 | ARG |
| 5 | C | 14 | THR |
| 5 | C | 15 | ILE |
| 5 | C | 31 | VAL |
| 5 | C | 45 | THR |
| 5 | C | 48 | ARG |
| 5 | C | 51 | VAL |
| 5 | C | 62 | LYS |
| 5 | C | 72 | ARG |
| 5 | C | 90 | SER |
| 5 | C | 91 | TYR |
| 5 | C | 95 | LEU |
| 5 | C | 97 | ARG |
| 5 | C | 102 | LEU |
| 5 | C | 104 | LEU |
| 5 | C | 117 | LEU |
| 5 | C | 121 | ASP |
| 5 | C | 124 | ASP |
| 5 | C | 127 | ASP |
| 5 | C | 130 | THR |
| 5 | C | 143 | ASP |
| 5 | C | 148 | VAL |
| 5 | C | 150 | LEU |
| 5 | C | 153 | ASP |
| 5 | C | 154 | ASP |
| 5 | C | 162 | ARG |
| 5 | C | 164 | VAL |
| 5 | C | 168 | SER |
| 5 | C | 175 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | C | 176 | ASN |
| 5 | C | 180 | ILE |
| 5 | C | 188 | ILE |
| 5 | C | 193 | LEU |
| 5 | C | 194 | GLU |
| 6 | D | 10 | ASP |
| 6 | D | 40 | LEU |
| 6 | D | 48 | LYS |
| 6 | D | 51 | ASP |
| 6 | D | 74 | ILE |
| 6 | D | 80 | ARG |
| 6 | D | 81 | GLN |
| 6 | D | 83 | MET |
| 6 | D | 89 | VAL |
| 6 | D | 100 | LEU |
| 6 | D | 112 | ARG |
| 6 | D | 115 | ARG |
| 6 | D | 117 | ILE |
| 6 | D | 125 | ARG |
| 6 | D | 130 | LEU |
| 6 | D | 148 | LYS |
| 6 | D | 150 | ARG |
| 6 | D | 153 | ASP |
| 6 | D | 171 | GLN |
| 6 | D | 175 | LEU |
| 7 | E | 7 | GLN |
| 7 | E | 35 | VAL |
| 7 | E | 44 | ARG |
| 7 | E | 48 | ASP |
| 7 | E | 50 | LEU |
| 7 | E | 59 | GLN |
| 7 | E | 69 | ARG |
| 7 | E | 98 | LEU |
| 7 | E | 106 | ASN |
| 7 | E | 143 | GLN |
| 7 | E | 155 | ASP |
| 8 | F | 84 | ILE |
| 8 | F | 111 | LYS |
| 9 | G | 31 | THR |
| 9 | G | 37 | ASP |
| 9 | G | 38 | GLU |
| 9 | G | 41 | TRP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9 | G | 53 | ARG |
| 9 | G | 56 | THR |
| 9 | G | 61 | ARG |
| 9 | G | 62 | ILE |
| 9 | G | 70 | PHE |
| 9 | G | 71 | THR |
| 9 | G | 75 | ILE |
| 9 | G | 90 | LEU |
| 9 | G | 101 | THR |
| 9 | G | 102 | ARG |
| 9 | G | 104 | THR |
| 9 | G | 112 | THR |
| 9 | G | 113 | GLU |
| 9 | G | 127 | ILE |
| 9 | G | 132 | PHE |
| 9 | G | 145 | HIS |
| 9 | G | 154 | GLU |
| 9 | G | 165 | VAL |
| 9 | G | 166 | LEU |
| 9 | G | 168 | THR |
| 9 | G | 169 | GLN |
| 10 | H | 7 | ARG |
| 10 | H | 8 | LEU |
| 10 | H | 23 | ARG |
| 10 | H | 27 | SER |
| 10 | H | 36 | THR |
| 10 | H | 41 | ASN |
| 10 | H | 47 | VAL |
| 10 | H | 81 | ILE |
| 10 | H | 89 | ILE |
| 10 | H | 94 | ASN |
| 10 | H | 102 | GLN |
| 10 | H | 106 | ARG |
| 10 | H | 116 | ARG |
| 10 | H | 120 | ASP |
| 10 | H | 126 | ILE |
| 10 | H | 127 | VAL |
| 11 | I | 5 | ASP |
| 11 | I | 6 | LEU |
| 11 | I | 7 | LYS |
| 11 | I | 12 | SER |
| 11 | I | 13 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11 | I | 18 | ARG |
| 11 | I | 21 | ARG |
| 11 | I | 26 | THR |
| 11 | I | 27 | ASP |
| 11 | I | 29 | THR |
| 11 | I | 38 | LYS |
| 11 | I | 39 | SER |
| 11 | I | 45 | LYS |
| 11 | I | 48 | PHE |
| 11 | I | 53 | ARG |
| 11 | I | 56 | LEU |
| 11 | I | 57 | ILE |
| 11 | I | 65 | PHE |
| 11 | I | 73 | GLU |
| 11 | I | 83 | LEU |
| 11 | I | 85 | ASP |
| 11 | I | 87 | THR |
| 11 | I | 89 | ASP |
| 11 | I | 98 | LEU |
| 11 | I | 99 | VAL |
| 11 | I | 101 | ARG |
| 11 | I | 106 | VAL |
| 11 | I | 114 | ILE |
| 11 | I | 118 | VAL |
| 11 | I | 120 | VAL |
| 11 | I | 123 | ASP |
| 11 | I | 130 | ILE |
| 12 | J | 7 | ARG |
| 12 | J | 8 | THR |
| 12 | J | 17 | ARG |
| 12 | J | 21 | ASP |
| 12 | J | 26 | ASP |
| 12 | J | 44 | LYS |
| 12 | J | 45 | SER |
| 12 | J | 47 | GLN |
| 12 | J | 64 | LYS |
| 12 | J | 65 | ILE |
| 12 | J | 72 | ASP |
| 12 | J | 81 | GLU |
| 12 | J | 82 | THR |
| 12 | J | 86 | LYS |
| 12 | J | 88 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12 | J | 91 | VAL |
| 12 | J | 94 | TRP |
| 12 | J | 97 | VAL |
| 12 | J | 114 | GLN |
| 12 | J | 129 | GLN |
| 12 | J | 134 | LYS |
| 12 | J | 139 | ASP |
| 13 | K | 5 | LYS |
| 13 | K | 8 | ARG |
| 13 | K | 10 | LEU |
| 13 | K | 11 | ASN |
| 13 | K | 12 | ARG |
| 13 | K | 17 | ARG |
| 13 | K | 28 | LEU |
| 13 | K | 35 | GLN |
| 13 | K | 37 | THR |
| 13 | K | 45 | ARG |
| 13 | K | 51 | LEU |
| 13 | K | 62 | SER |
| 13 | K | 83 | VAL |
| 13 | K | 89 | GLU |
| 13 | K | 94 | TYR |
| 13 | K | 95 | THR |
| 13 | K | 99 | ARG |
| 13 | K | 102 | THR |
| 13 | K | 106 | ASP |
| 13 | K | 109 | THR |
| 13 | K | 114 | GLU |
| 13 | K | 115 | LEU |
| 14 | L | 8 | ARG |
| 14 | L | 9 | ARG |
| 14 | L | 13 | THR |
| 14 | L | 17 | VAL |
| 14 | L | 31 | VAL |
| 14 | L | 33 | ARG |
| 14 | L | 36 | LYS |
| 14 | L | 43 | ILE |
| 14 | L | 59 | LEU |
| 14 | L | 64 | LYS |
| 14 | L | 66 | ASP |
| 14 | L | 67 | THR |
| 14 | L | 89 | PHE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14 | L | 90 | ASP |
| 14 | L | 91 | ARG |
| 14 | L | 95 | LYS |
| 14 | L | 99 | ARG |
| 14 | L | 108 | ARG |
| 15 | M | 2 | GLN |
| 15 | M | 5 | ILE |
| 15 | M | 6 | LYS |
| 15 | M | 7 | ILE |
| 15 | M | 12 | LEU |
| 15 | M | 13 | LEU |
| 15 | M | 16 | ILE |
| 15 | M | 22 | ARG |
| 15 | M | 28 | ARG |
| 15 | M | 31 | ASP |
| 15 | M | 34 | ARG |
| 15 | M | 35 | VAL |
| 15 | M | 36 | ASP |
| 15 | M | 37 | THR |
| 15 | M | 38 | LYS |
| 15 | M | 40 | ARG |
| 15 | M | 57 | ILE |
| 15 | M | 62 | SER |
| 15 | M | 63 | ARG |
| 15 | M | 64 | LYS |
| 15 | M | 88 | VAL |
| 15 | M | 89 | ASN |
| 15 | M | 92 | THR |
| 15 | M | 93 | ILE |
| 15 | M | 95 | GLU |
| 15 | M | 96 | ARG |
| 15 | M | 98 | LYS |
| 15 | M | 104 | LEU |
| 16 | N | 8 | ILE |
| 16 | N | 13 | ARG |
| 16 | N | 22 | LYS |
| 16 | N | 30 | LYS |
| 16 | N | 51 | ARG |
| 16 | N | 58 | ARG |
| 16 | N | 60 | LEU |
| 16 | N | 71 | LEU |
| 16 | N | 78 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 16 | N | 85 | ARG |
| 16 | N | 88 | ILE |
| 16 | N | 90 | LEU |
| 16 | N | 92 | ARG |
| 16 | N | 93 | LYS |
| 16 | N | 102 | GLU |
| 17 | O | 13 | ARG |
| 17 | O | 14 | VAL |
| 17 | O | 18 | ASP |
| 17 | O | 21 | ARG |
| 17 | O | 24 | SER |
| 17 | O | 25 | LEU |
| 17 | O | 26 | GLN |
| 17 | O | 28 | GLU |
| 17 | O | 35 | LEU |
| 17 | O | 40 | VAL |
| 17 | O | 69 | ILE |
| 17 | O | 71 | ILE |
| 17 | O | 78 | VAL |
| 17 | O | 83 | ARG |
| 17 | O | 84 | THR |
| 17 | O | 87 | ARG |
| 17 | O | 88 | GLN |
| 17 | O | 98 | ILE |
| 18 | P | 8 | PHE |
| 18 | P | 9 | ARG |
| 18 | P | 11 | LYS |
| 18 | P | 17 | GLN |
| 18 | P | 21 | ARG |
| 18 | P | 32 | ARG |
| 18 | P | 36 | ARG |
| 18 | P | 37 | LYS |
| 18 | P | 48 | LYS |
| 18 | P | 49 | SER |
| 18 | P | 62 | ARG |
| 18 | P | 87 | GLU |
| 18 | P | 89 | ARG |
| 18 | P | 106 | LEU |
| 18 | P | 109 | ARG |
| 18 | P | 118 | LYS |
| 18 | P | 120 | ARG |
| 18 | P | 125 | THR |

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Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 18 | P | 126 | ILE |
| 18 | P | 133 | ASN |
| 19 | Q | 7 | LEU |
| 19 | Q | 12 | ILE |
| 19 | Q | 14 | GLU |
| 19 | Q | 26 | SER |
| 19 | Q | 38 | ILE |
| 19 | Q | 40 | ASP |
| 19 | Q | 42 | ILE |
| 19 | Q | 58 | VAL |
| 19 | Q | 63 | LYS |
| 19 | Q | 65 | VAL |
| 19 | Q | 79 | ILE |
| 19 | Q | 80 | VAL |
| 19 | Q | 84 | GLU |
| 20 | R | 11 | ASN |
| 20 | R | 15 | HIS |
| 20 | R | 18 | LYS |
| 20 | R | 23 | ILE |
| 20 | R | 25 | LEU |
| 20 | R | 37 | LEU |
| 20 | R | 38 | LEU |
| 20 | R | 42 | ARG |
| 20 | R | 46 | VAL |
| 20 | R | 53 | VAL |
| 20 | R | 73 | GLU |
| 20 | R | 80 | LYS |
| 20 | R | 83 | LEU |
| 20 | R | 85 | ASP |
| 20 | R | 95 | ARG |
| 20 | R | 96 | LYS |
| 20 | R | 98 | ILE |
| 20 | R | 104 | VAL |
| 20 | R | 105 | ARG |
| 20 | R | 106 | VAL |
| 20 | R | 108 | VAL |
| 21 | S | 13 | LYS |
| 21 | S | 14 | LEU |
| 21 | S | 15 | ASP |
| 21 | S | 22 | VAL |
| 21 | S | 26 | LYS |
| 21 | S | 40 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21 | S | 51 | LEU |
| 21 | S | 56 | VAL |
| 21 | S | 67 | LYS |
| 21 | S | 71 | MET |
| 21 | S | 79 | ILE |
| 21 | S | 100 | THR |
| 21 | S | 120 | LEU |
| 21 | S | 128 | ARG |
| 21 | S | 130 | ILE |
| 21 | S | 132 | GLN |
| 21 | S | 134 | LEU |
| 21 | S | 145 | ASP |
| 21 | S | 175 | ARG |
| 22 | T | 16 | SER |
| 22 | T | 17 | ASN |
| 22 | T | 37 | LEU |
| 22 | T | 38 | VAL |
| 22 | T | 46 | LYS |
| 22 | T | 49 | GLN |
| 22 | T | 62 | LEU |
| 22 | T | 64 | ASP |
| 22 | T | 85 | GLN |
| 23 | U | 8 | THR |
| 23 | U | 10 | LYS |
| 23 | U | 11 | LYS |
| 23 | U | 17 | SER |
| 23 | U | 19 | ILE |
| 23 | U | 23 | LYS |
| 23 | U | 32 | ARG |
| 23 | U | 35 | THR |
| 23 | U | 37 | ILE |
| 23 | U | 40 | ARG |
| 23 | U | 42 | GLN |
| 23 | U | 43 | ARG |
| 23 | U | 45 | ASN |
| 23 | U | 47 | HIS |
| 23 | U | 52 | ARG |
| 23 | U | 63 | SER |
| 23 | U | 65 | ASN |
| 23 | U | 75 | TYR |
| 23 | U | 78 | ILE |
| 23 | U | 79 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24 | V | 1 | MET |
| 24 | V | 7 | ARG |
| 24 | V | 14 | PHE |
| 24 | V | 19 | ASP |
| 24 | V | 28 | LEU |
| 24 | V | 37 | LEU |
| 24 | V | 44 | ARG |
| 24 | V | 65 | GLU |
| 25 | W | 2 | LYS |
| 25 | W | 3 | ILE |
| 25 | W | 4 | LYS |
| 25 | W | 9 | VAL |
| 25 | W | 10 | ILE |
| 25 | W | 12 | ARG |
| 25 | W | 26 | ARG |
| 25 | W | 30 | ASP |
| 25 | W | 32 | ARG |
| 25 | W | 34 | VAL |
| 25 | W | 37 | THR |
| 25 | W | 45 | LYS |
| 25 | W | 46 | THR |
| 26 | Z | 3 | LYS |
| 26 | Z | 4 | HIS |
| 26 | Z | 6 | VAL |
| 26 | Z | 8 | LYS |
| 26 | Z | 11 | THR |
| 26 | Z | 18 | MET |
| 26 | Z | 35 | GLN |
| 26 | Z | 40 | LYS |
| 26 | Z | 41 | LEU |
| 26 | Z | 53 | ASP |
| 26 | Z | 55 | ARG |
| 26 | Z | 58 | LEU |
| 30 | 4 | 2 | LYS |
| 30 | 4 | 9 | LYS |
| 30 | 4 | 13 | ASN |
| 30 | 4 | 30 | VAL |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | A | 231 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | B | 129 | HIS |
| 4 | B | 180 | ASN |
| 5 | C | 61 | GLN |
| 6 | D | 9 | ASN |
| 6 | D | 81 | GLN |
| 6 | D | 129 | ASN |
| 7 | E | 20 | GLN |
| 7 | E | 106 | ASN |
| 7 | E | 143 | GLN |
| 9 | G | 76 | GLN |
| 9 | G | 122 | HIS |
| 10 | H | 41 | ASN |
| 11 | I | 66 | ASN |
| 12 | J | 47 | GLN |
| 12 | J | 58 | HIS |
| 13 | K | 13 | ASN |
| 14 | L | 41 | GLN |
| 14 | L | 49 | GLN |
| 15 | M | 58 | ASN |
| 16 | N | 31 | GLN |
| 16 | N | 72 | HIS |
| 16 | N | 91 | ASN |
| 17 | O | 11 | GLN |
| 17 | O | 79 | GLN |
| 17 | O | 88 | GLN |
| 18 | P | 78 | ASN |
| 18 | P | 81 | HIS |
| 18 | P | 115 | ASN |
| 19 | Q | 8 | GLN |
| 19 | Q | 73 | ASN |
| 19 | Q | 86 | GLN |
| 20 | R | 10 | HIS |
| 20 | R | 29 | HIS |
| 20 | R | 44 | GLN |
| 22 | T | 3 | HIS |
| 22 | T | 17 | ASN |
| 22 | T | 49 | GLN |
| 22 | T | 57 | HIS |
| 25 | W | 49 | HIS |
| 25 | W | 54 | GLN |
| 26 | Z | 29 | ASN |
| 26 | Z | 43 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26 | Z | 44 | HIS |
| 30 | 4 | 36 | GLN |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | X | 2683/2880 (93%) | 672 (25%) | 252 (9%) |
| 2 | Y | 121/123 (98%) | 26 (21%) | 7 (5%) |
| All | All | 2804/3003 (93%) | 698 (24%) | 259 (9%) |

All (698) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | X | 2 | G |
| 1 | X | 7 | G |
| 1 | X | 34 | U |
| 1 | X | 45 | C |
| 1 | X | 48 | A |
| 1 | X | 49 | U |
| 1 | X | 50 | G |
| 1 | X | 51 | A |
| 1 | X | 54 | G |
| 1 | X | 55 | A |
| 1 | X | 63 | A |
| 1 | X | 69 | G |
| 1 | X | 70 | A |
| 1 | X | 71 | A |
| 1 | X | 72 | A |
| 1 | X | 74 | G |
| 1 | X | 82 | G |
| 1 | X | 83 | A |
| 1 | X | 84 | G |
| 1 | X | 89 | A |
| 1 | X | 90 | G |
| 1 | X | 91 | A |
| 1 | X | 92 | U |
| 1 | X | 97 | U |
| 1 | X | 98 | U |
| 1 | X | 99 | U |
| 1 | X | 100 | G |
| 1 | X | 101 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | X | 107 | G |
| 1 | X | 108 | G |
| 1 | X | 111 | G |
| 1 | X | 116 | A |
| 1 | X | 117 | A |
| 1 | X | 118 | U |
| 1 | X | 123 | A |
| 1 | X | 127 | C |
| 1 | X | 129 | A |
| 1 | X | 138 | G |
| 1 | X | 143 | A |
| 1 | X | 147 | G |
| 1 | X | 154 | U |
| 1 | X | 155 | G |
| 1 | X | 158 | A |
| 1 | X | 173 | A |
| 1 | X | 176 | A |
| 1 | X | 177 | U |
| 1 | X | 181 | A |
| 1 | X | 182 | G |
| 1 | X | 192 | G |
| 1 | X | 193 | A |
| 1 | X | 198 | A |
| 1 | X | 199 | A |
| 1 | X | 204 | A |
| 1 | X | 205 | A |
| 1 | X | 206 | U |
| 1 | X | 207 | U |
| 1 | X | 210 | A |
| 1 | X | 219 | G |
| 1 | X | 225 | G |
| 1 | X | 228 | A |
| 1 | X | 229 | G |
| 1 | X | 238 | G |
| 1 | X | 242 | A |
| 1 | X | 243 | G |
| 1 | X | 245 | C |
| 1 | X | 246 | C |
| 1 | X | 304 | A |
| 1 | X | 305 | A |
| 1 | X | 306 | G |
| 1 | X | 310 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | X | 312 | G |
| 1 | X | 313 | U |
| 1 | X | 319 | G |
| 1 | X | 321 | A |
| 1 | X | 322 | A |
| 1 | X | 323 | G |
| 1 | X | 329 | C |
| 1 | X | 332 | C |
| 1 | X | 333 | A |
| 1 | X | 334 | G |
| 1 | X | 335 | A |
| 1 | X | 340 | G |
| 1 | X | 341 | A |
| 1 | X | 342 | G |
| 1 | X | 343 | A |
| 1 | X | 358 | C |
| 1 | X | 360 | A |
| 1 | X | 388 | G |
| 1 | X | 393 | U |
| 1 | X | 396 | U |
| 1 | X | 397 | U |
| 1 | X | 399 | G |
| 1 | X | 400 | U |
| 1 | X | 401 | G |
| 1 | X | 409 | G |
| 1 | X | 412 | U |
| 1 | X | 414 | A |
| 1 | X | 416 | U |
| 1 | X | 418 | C |
| 1 | X | 419 | G |
| 1 | X | 424 | G |
| 1 | X | 425 | A |
| 1 | X | 431 | G |
| 1 | X | 433 | G |
| 1 | X | 435 | A |
| 1 | X | 441 | A |
| 1 | X | 454 | G |
| 1 | X | 455 | A |
| 1 | X | 456 | C |
| 1 | X | 458 | G |
| 1 | X | 459 | A |
| 1 | X | 461 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | X | 463 | C |
| 1 | X | 467 | U |
| 1 | X | 468 | A |
| 1 | X | 469 | G |
| 1 | X | 470 | U |
| 1 | X | 482 | A |
| 1 | X | 486 | U |
| 1 | X | 491 | A |
| 1 | X | 492 | G |
| 1 | X | 504 | G |
| 1 | X | 514 | G |
| 1 | X | 515 | A |
| 1 | X | 518 | A |
| 1 | X | 519 | C |
| 1 | X | 520 | C |
| 1 | X | 539 | A |
| 1 | X | 540 | G |
| 1 | X | 541 | C |
| 1 | X | 542 | A |
| 1 | X | 543 | G |
| 1 | X | 554 | U |
| 1 | X | 555 | U |
| 1 | X | 556 | A |
| 1 | X | 557 | U |
| 1 | X | 558 | G |
| 1 | X | 559 | C |
| 1 | X | 560 | G |
| 1 | X | 572 | G |
| 1 | X | 580 | A |
| 1 | X | 582 | G |
| 1 | X | 583 | C |
| 1 | X | 584 | A |
| 1 | X | 595 | A |
| 1 | X | 602 | C |
| 1 | X | 613 | A |
| 1 | X | 614 | G |
| 1 | X | 620 | G |
| 1 | X | 624 | A |
| 1 | X | 625 | A |
| 1 | X | 627 | A |
| 1 | X | 628 | A |
| 1 | X | 631 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | X | 632 | A |
| 1 | X | 633 | G |
| 1 | X | 636 | G |
| 1 | X | 648 | A |
| 1 | X | 649 | G |
| 1 | X | 652 | C |
| 1 | X | 654 | A |
| 1 | X | 655 | A |
| 1 | X | 657 | A |
| 1 | X | 664 | C |
| 1 | X | 665 | A |
| 1 | X | 666 | U |
| 1 | X | 667 | U |
| 1 | X | 681 | A |
| 1 | X | 682 | G |
| 1 | X | 683 | A |
| 1 | X | 684 | C |
| 1 | X | 690 | A |
| 1 | X | 695 | G |
| 1 | X | 698 | A |
| 1 | X | 699 | G |
| 1 | X | 700 | C |
| 1 | X | 723 | C |
| 1 | X | 728 | G |
| 1 | X | 729 | A |
| 1 | X | 730 | C |
| 1 | X | 732 | G |
| 1 | X | 742 | G |
| 1 | X | 743 | A |
| 1 | X | 751 | G |
| 1 | X | 752 | G |
| 1 | X | 760 | U |
| 1 | X | 766 | A |
| 1 | X | 778 | G |
| 1 | X | 782 | U |
| 1 | X | 783 | G |
| 1 | X | 788 | G |
| 1 | X | 789 | G |
| 1 | X | 790 | A |
| 1 | X | 795 | A |
| 1 | X | 797 | A |
| 1 | X | 798 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | X | 801 | A |
| 1 | X | 802 | A |
| 1 | X | 803 | C |
| 1 | X | 804 | C |
| 1 | X | 805 | G |
| 1 | X | 806 | A |
| 1 | X | 807 | A |
| 1 | X | 814 | G |
| 1 | X | 815 | A |
| 1 | X | 816 | U |
| 1 | X | 818 | G |
| 1 | X | 824 | U |
| 1 | X | 825 | C |
| 1 | X | 832 | A |
| 1 | X | 840 | U |
| 1 | X | 841 | G |
| 1 | X | 859 | U |
| 1 | X | 860 | U |
| 1 | X | 871 | U |
| 1 | X | 872 | G |
| 1 | X | 878 | C |
| 1 | X | 879 | A |
| 1 | X | 880 | C |
| 1 | X | 919 | U |
| 1 | X | 922 | A |
| 1 | X | 926 | C |
| 1 | X | 931 | G |
| 1 | X | 938 | G |
| 1 | X | 939 | C |
| 1 | X | 940 | G |
| 1 | X | 941 | U |
| 1 | X | 943 | U |
| 1 | X | 944 | A |
| 1 | X | 952 | A |
| 1 | X | 955 | G |
| 1 | X | 956 | A |
| 1 | X | 957 | G |
| 1 | X | 964 | A |
| 1 | X | 968 | C |
| 1 | X | 969 | U |
| 1 | X | 970 | A |
| 1 | X | 972 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | X | 973 | U |
| 1 | X | 985 | G |
| 1 | X | 994 | A |
| 1 | X | 995 | A |
| 1 | X | 996 | C |
| 1 | X | 1000 | G |
| 1 | X | 1001 | A |
| 1 | X | 1006 | C |
| 1 | X | 1007 | A |
| 1 | X | 1010 | U |
| 1 | X | 1014 | G |
| 1 | X | 1016 | C |
| 1 | X | 1019 | U |
| 1 | X | 1020 | A |
| 1 | X | 1022 | A |
| 1 | X | 1023 | U |
| 1 | X | 1024 | G |
| 1 | X | 1033 | G |
| 1 | X | 1034 | U |
| 1 | X | 1035 | G |
| 1 | X | 1036 | G |
| 1 | X | 1037 | U |
| 1 | X | 1038 | U |
| 1 | X | 1044 | U |
| 1 | X | 1052 | C |
| 1 | X | 1053 | G |
| 1 | X | 1054 | C |
| 1 | X | 1055 | A |
| 1 | X | 1056 | U |
| 1 | X | 1057 | A |
| 1 | X | 1058 | G |
| 1 | X | 1059 | A |
| 1 | X | 1068 | A |
| 1 | X | 1069 | G |
| 1 | X | 1070 | G |
| 1 | X | 1072 | U |
| 1 | X | 1073 | G |
| 1 | X | 1077 | U |
| 1 | X | 1078 | A |
| 1 | X | 1079 | G |
| 1 | X | 1081 | A |
| 1 | X | 1082 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | X | 1086 | C |
| 1 | X | 1087 | C |
| 1 | X | 1090 | C |
| 1 | X | 1094 | C |
| 1 | X | 1097 | A |
| 1 | X | 1098 | G |
| 1 | X | 1099 | A |
| 1 | X | 1100 | G |
| 1 | X | 1107 | A |
| 1 | X | 1108 | U |
| 1 | X | 1121 | G |
| 1 | X | 1122 | A |
| 1 | X | 1123 | G |
| 1 | X | 1124 | U |
| 1 | X | 1128 | G |
| 1 | X | 1129 | A |
| 1 | X | 1139 | A |
| 1 | X | 1140 | A |
| 1 | X | 1141 | U |
| 1 | X | 1142 | G |
| 1 | X | 1143 | A |
| 1 | X | 1145 | C |
| 1 | X | 1146 | G |
| 1 | X | 1152 | C |
| 1 | X | 1153 | A |
| 1 | X | 1161 | U |
| 1 | X | 1162 | A |
| 1 | X | 1182 | U |
| 1 | X | 1185 | C |
| 1 | X | 1187 | A |
| 1 | X | 1189 | G |
| 1 | X | 1192 | A |
| 1 | X | 1194 | U |
| 1 | X | 1224 | A |
| 1 | X | 1233 | A |
| 1 | X | 1234 | C |
| 1 | X | 1250 | A |
| 1 | X | 1251 | G |
| 1 | X | 1262 | U |
| 1 | X | 1264 | C |
| 1 | X | 1266 | G |
| 1 | X | 1269 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | X | 1275 | A |
| 1 | X | 1281 | A |
| 1 | X | 1282 | A |
| 1 | X | 1284 | G |
| 1 | X | 1285 | A |
| 1 | X | 1286 | U |
| 1 | X | 1288 | A |
| 1 | X | 1289 | A |
| 1 | X | 1302 | C |
| 1 | X | 1313 | U |
| 1 | X | 1314 | A |
| 1 | X | 1315 | A |
| 1 | X | 1316 | G |
| 1 | X | 1319 | C |
| 1 | X | 1334 | A |
| 1 | X | 1342 | U |
| 1 | X | 1345 | G |
| 1 | X | 1356 | G |
| 1 | X | 1357 | U |
| 1 | X | 1358 | C |
| 1 | X | 1359 | G |
| 1 | X | 1365 | U |
| 1 | X | 1370 | U |
| 1 | X | 1378 | A |
| 1 | X | 1379 | A |
| 1 | X | 1381 | G |
| 1 | X | 1392 | U |
| 1 | X | 1404 | C |
| 1 | X | 1409 | U |
| 1 | X | 1410 | U |
| 1 | X | 1412 | C |
| 1 | X | 1413 | U |
| 1 | X | 1425 | G |
| 1 | X | 1428 | G |
| 1 | X | 1429 | A |
| 1 | X | 1432 | G |
| 1 | X | 1433 | A |
| 1 | X | 1434 | U |
| 1 | X | 1435 | G |
| 1 | X | 1440 | G |
| 1 | X | 1441 | A |
| 1 | X | 1442 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | X | 1443 | G |
| 1 | X | 1451 | C |
| 1 | X | 1459 | U |
| 1 | X | 1460 | G |
| 1 | X | 1465 | G |
| 1 | X | 1467 | U |
| 1 | X | 1468 | A |
| 1 | X | 1469 | U |
| 1 | X | 1470 | G |
| 1 | X | 1474 | A |
| 1 | X | 1475 | U |
| 1 | X | 1476 | G |
| 1 | X | 1483 | G |
| 1 | X | 1489 | C |
| 1 | X | 1490 | U |
| 1 | X | 1497 | C |
| 1 | X | 1498 | G |
| 1 | X | 1505 | U |
| 1 | X | 1506 | C |
| 1 | X | 1508 | G |
| 1 | X | 1509 | A |
| 1 | X | 1513 | U |
| 1 | X | 1514 | C |
| 1 | X | 1523 | A |
| 1 | X | 1524 | C |
| 1 | X | 1525 | A |
| 1 | X | 1528 | C |
| 1 | X | 1531 | C |
| 1 | X | 1545 | G |
| 1 | X | 1551 | U |
| 1 | X | 1552 | C |
| 1 | X | 1553 | G |
| 1 | X | 1554 | G |
| 1 | X | 1562 | G |
| 1 | X | 1563 | U |
| 1 | X | 1570 | C |
| 1 | X | 1571 | G |
| 1 | X | 1574 | A |
| 1 | X | 1575 | C |
| 1 | X | 1576 | G |
| 1 | X | 1582 | A |
| 1 | X | 1585 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | X | 1594 | U |
| 1 | X | 1600 | U |
| 1 | X | 1601 | U |
| 1 | X | 1602 | G |
| 1 | X | 1603 | A |
| 1 | X | 1607 | A |
| 1 | X | 1608 | U |
| 1 | X | 1613 | G |
| 1 | X | 1624 | A |
| 1 | X | 1625 | A |
| 1 | X | 1626 | A |
| 1 | X | 1631 | C |
| 1 | X | 1632 | A |
| 1 | X | 1634 | A |
| 1 | X | 1635 | G |
| 1 | X | 1648 | C |
| 1 | X | 1651 | U |
| 1 | X | 1657 | A |
| 1 | X | 1661 | C |
| 1 | X | 1665 | C |
| 1 | X | 1681 | A |
| 1 | X | 1685 | A |
| 1 | X | 1686 | A |
| 1 | X | 1691 | G |
| 1 | X | 1710 | U |
| 1 | X | 1711 | C |
| 1 | X | 1712 | G |
| 1 | X | 1713 | G |
| 1 | X | 1716 | G |
| 1 | X | 1717 | A |
| 1 | X | 1724 | C |
| 1 | X | 1732 | U |
| 1 | X | 1733 | U |
| 1 | X | 1734 | C |
| 1 | X | 1747 | G |
| 1 | X | 1749 | G |
| 1 | X | 1754 | G |
| 1 | X | 1755 | G |
| 1 | X | 1760 | G |
| 1 | X | 1764 | A |
| 1 | X | 1775 | A |
| 1 | X | 1776 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | X | 1777 | A |
| 1 | X | 1782 | A |
| 1 | X | 1790 | G |
| 1 | X | 1791 | C |
| 1 | X | 1792 | C |
| 1 | X | 1793 | A |
| 1 | X | 1799 | A |
| 1 | X | 1800 | A |
| 1 | X | 1801 | C |
| 1 | X | 1808 | C |
| 1 | X | 1810 | U |
| 1 | X | 1811 | A |
| 1 | X | 1812 | U |
| 1 | X | 1819 | U |
| 1 | X | 1821 | A |
| 1 | X | 1825 | C |
| 1 | X | 1840 | A |
| 1 | X | 1850 | G |
| 1 | X | 1861 | G |
| 1 | X | 1867 | A |
| 1 | X | 1883 | A |
| 1 | X | 1886 | G |
| 1 | X | 1910 | A |
| 1 | X | 1912 | G |
| 1 | X | 1913 | G |
| 1 | X | 1914 | U |
| 1 | X | 1919 | A |
| 1 | X | 1920 | A |
| 1 | X | 1921 | A |
| 1 | X | 1923 | U |
| 1 | X | 1924 | C |
| 1 | X | 1927 | U |
| 1 | X | 1938 | U |
| 1 | X | 1939 | U |
| 1 | X | 1943 | A |
| 1 | X | 1946 | U |
| 1 | X | 1947 | G |
| 1 | X | 1950 | C |
| 1 | X | 1953 | A |
| 1 | X | 1954 | A |
| 1 | X | 1955 | G |
| 1 | X | 1964 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | X | 1965 | U |
| 1 | X | 1972 | G |
| 1 | X | 1976 | U |
| 1 | X | 1979 | C |
| 1 | X | 1980 | A |
| 1 | X | 2003 | A |
| 1 | X | 2005 | U |
| 1 | X | 2006 | G |
| 1 | X | 2010 | G |
| 1 | X | 2014 | A |
| 1 | X | 2015 | G |
| 1 | X | 2018 | G |
| 1 | X | 2019 | C |
| 1 | X | 2026 | C |
| 1 | X | 2035 | G |
| 1 | X | 2038 | C |
| 1 | X | 2039 | G |
| 1 | X | 2044 | G |
| 1 | X | 2045 | A |
| 1 | X | 2046 | C |
| 1 | X | 2052 | G |
| 1 | X | 2063 | A |
| 1 | X | 2076 | G |
| 1 | X | 2084 | G |
| 1 | X | 2089 | C |
| 1 | X | 2166 | G |
| 1 | X | 2171 | U |
| 1 | X | 2181 | A |
| 1 | X | 2189 | A |
| 1 | X | 2190 | A |
| 1 | X | 2191 | A |
| 1 | X | 2195 | C |
| 1 | X | 2196 | U |
| 1 | X | 2197 | U |
| 1 | X | 2199 | C |
| 1 | X | 2204 | A |
| 1 | X | 2205 | C |
| 1 | X | 2217 | G |
| 1 | X | 2218 | G |
| 1 | X | 2222 | U |
| 1 | X | 2230 | G |
| 1 | X | 2259 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | X | 2262 | C |
| 1 | X | 2265 | A |
| 1 | X | 2266 | A |
| 1 | X | 2267 | A |
| 1 | X | 2268 | G |
| 1 | X | 2283 | G |
| 1 | X | 2284 | U |
| 1 | X | 2285 | U |
| 1 | X | 2286 | G |
| 1 | X | 2287 | G |
| 1 | X | 2288 | A |
| 1 | X | 2290 | A |
| 1 | X | 2291 | U |
| 1 | X | 2298 | U |
| 1 | X | 2299 | A |
| 1 | X | 2300 | G |
| 1 | X | 2301 | A |
| 1 | X | 2304 | G |
| 1 | X | 2305 | C |
| 1 | X | 2306 | A |
| 1 | X | 2313 | G |
| 1 | X | 2314 | A |
| 1 | X | 2315 | A |
| 1 | X | 2318 | U |
| 1 | X | 2323 | U |
| 1 | X | 2324 | G |
| 1 | X | 2326 | C |
| 1 | X | 2329 | C |
| 1 | X | 2330 | G |
| 1 | X | 2351 | G |
| 1 | X | 2358 | C |
| 1 | X | 2362 | G |
| 1 | X | 2363 | G |
| 1 | X | 2364 | C |
| 1 | X | 2371 | A |
| 1 | X | 2379 | G |
| 1 | X | 2381 | A |
| 1 | X | 2385 | U |
| 1 | X | 2389 | G |
| 1 | X | 2396 | C |
| 1 | X | 2401 | A |
| 1 | X | 2402 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | X | 2404 | A |
| 1 | X | 2405 | A |
| 1 | X | 2406 | C |
| 1 | X | 2408 | G |
| 1 | X | 2409 | A |
| 1 | X | 2410 | U |
| 1 | X | 2414 | A |
| 1 | X | 2415 | G |
| 1 | X | 2420 | C |
| 1 | X | 2426 | G |
| 1 | X | 2427 | A |
| 1 | X | 2438 | A |
| 1 | X | 2447 | G |
| 1 | X | 2448 | A |
| 1 | X | 2452 | U |
| 1 | X | 2453 | C |
| 1 | X | 2455 | A |
| 1 | X | 2473 | G |
| 1 | X | 2475 | C |
| 1 | X | 2477 | C |
| 1 | X | 2481 | G |
| 1 | X | 2482 | A |
| 1 | X | 2483 | U |
| 1 | X | 2484 | G |
| 1 | X | 2494 | C |
| 1 | X | 2497 | A |
| 1 | X | 2498 | U |
| 1 | X | 2499 | C |
| 1 | X | 2504 | G |
| 1 | X | 2508 | G |
| 1 | X | 2509 | A |
| 1 | X | 2514 | G |
| 1 | X | 2545 | A |
| 1 | X | 2546 | G |
| 1 | X | 2552 | C |
| 1 | X | 2553 | G |
| 1 | X | 2557 | G |
| 1 | X | 2561 | G |
| 1 | X | 2562 | G |
| 1 | X | 2565 | C |
| 1 | X | 2581 | A |
| 1 | X | 2582 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | X | 2588 | U |
| 1 | X | 2589 | C |
| 1 | X | 2591 | C |
| 1 | X | 2594 | U |
| 1 | X | 2608 | A |
| 1 | X | 2611 | A |
| 1 | X | 2613 | A |
| 1 | X | 2633 | A |
| 1 | X | 2635 | U |
| 1 | X | 2640 | G |
| 1 | X | 2643 | G |
| 1 | X | 2650 | G |
| 1 | X | 2661 | G |
| 1 | X | 2664 | G |
| 1 | X | 2668 | U |
| 1 | X | 2691 | C |
| 1 | X | 2692 | A |
| 1 | X | 2693 | U |
| 1 | X | 2694 | G |
| 1 | X | 2705 | A |
| 1 | X | 2706 | U |
| 1 | X | 2713 | A |
| 1 | X | 2718 | A |
| 1 | X | 2728 | A |
| 1 | X | 2731 | G |
| 1 | X | 2732 | C |
| 1 | X | 2737 | A |
| 1 | X | 2745 | A |
| 1 | X | 2758 | A |
| 1 | X | 2759 | U |
| 1 | X | 2760 | G |
| 1 | X | 2770 | A |
| 1 | X | 2771 | C |
| 1 | X | 2774 | U |
| 1 | X | 2775 | U |
| 1 | X | 2776 | U |
| 1 | X | 2777 | A |
| 1 | X | 2778 | U |
| 1 | X | 2779 | C |
| 1 | X | 2780 | A |
| 1 | X | 2782 | G |
| 1 | X | 2795 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | X | 2796 | A |
| 1 | X | 2798 | A |
| 1 | X | 2808 | U |
| 1 | X | 2809 | A |
| 1 | X | 2810 | A |
| 1 | X | 2811 | G |
| 1 | X | 2825 | A |
| 1 | X | 2843 | A |
| 1 | X | 2847 | G |
| 1 | X | 2854 | G |
| 1 | X | 2859 | U |
| 1 | X | 2864 | C |
| 1 | X | 2866 | A |
| 1 | X | 2868 | G |
| 2 | Y | 4 | C |
| 2 | Y | 11 | G |
| 2 | Y | 14 | C |
| 2 | Y | 15 | A |
| 2 | Y | 17 | A |
| 2 | Y | 18 | G |
| 2 | Y | 27 | A |
| 2 | Y | 28 | A |
| 2 | Y | 37 | C |
| 2 | Y | 39 | C |
| 2 | Y | 40 | C |
| 2 | Y | 42 | U |
| 2 | Y | 43 | G |
| 2 | Y | 44 | C |
| 2 | Y | 46 | G |
| 2 | Y | 47 | A |
| 2 | Y | 59 | A |
| 2 | Y | 69 | G |
| 2 | Y | 75 | A |
| 2 | Y | 76 | U |
| 2 | Y | 102 | A |
| 2 | Y | 110 | U |
| 2 | Y | 112 | A |
| 2 | Y | 115 | G |
| 2 | Y | 121 | G |
| 2 | Y | 123 | U |

All (259) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | X | 13 | A |
| 1 | X | 33 | C |
| 1 | X | 34 | U |
| 1 | X | 48 | A |
| 1 | X | 49 | U |
| 1 | X | 50 | G |
| 1 | X | 62 | U |
| 1 | X | 70 | A |
| 1 | X | 71 | A |
| 1 | X | 73 | A |
| 1 | X | 74 | G |
| 1 | X | 82 | G |
| 1 | X | 83 | A |
| 1 | X | 89 | A |
| 1 | X | 98 | U |
| 1 | X | 99 | U |
| 1 | X | 100 | G |
| 1 | X | 117 | A |
| 1 | X | 154 | U |
| 1 | X | 173 | A |
| 1 | X | 176 | A |
| 1 | X | 181 | A |
| 1 | X | 182 | G |
| 1 | X | 198 | A |
| 1 | X | 199 | A |
| 1 | X | 204 | A |
| 1 | X | 242 | A |
| 1 | X | 312 | G |
| 1 | X | 321 | A |
| 1 | X | 322 | A |
| 1 | X | 328 | A |
| 1 | X | 332 | C |
| 1 | X | 334 | G |
| 1 | X | 341 | A |
| 1 | X | 342 | G |
| 1 | X | 343 | A |
| 1 | X | 387 | A |
| 1 | X | 396 | U |
| 1 | X | 399 | G |
| 1 | X | 416 | U |
| 1 | X | 417 | C |
| 1 | X | 418 | C |
| 1 | X | 419 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | X | 434 | C |
| 1 | X | 454 | G |
| 1 | X | 458 | G |
| 1 | X | 466 | A |
| 1 | X | 467 | U |
| 1 | X | 469 | G |
| 1 | X | 504 | G |
| 1 | X | 513 | A |
| 1 | X | 522 | G |
| 1 | X | 539 | A |
| 1 | X | 540 | G |
| 1 | X | 542 | A |
| 1 | X | 557 | U |
| 1 | X | 558 | G |
| 1 | X | 559 | C |
| 1 | X | 580 | A |
| 1 | X | 631 | G |
| 1 | X | 648 | A |
| 1 | X | 652 | C |
| 1 | X | 664 | C |
| 1 | X | 672 | C |
| 1 | X | 677 | G |
| 1 | X | 681 | A |
| 1 | X | 682 | G |
| 1 | X | 683 | A |
| 1 | X | 698 | A |
| 1 | X | 714 | G |
| 1 | X | 751 | G |
| 1 | X | 765 | C |
| 1 | X | 775 | U |
| 1 | X | 777 | A |
| 1 | X | 788 | G |
| 1 | X | 803 | C |
| 1 | X | 806 | A |
| 1 | X | 813 | A |
| 1 | X | 814 | G |
| 1 | X | 818 | G |
| 1 | X | 824 | U |
| 1 | X | 840 | U |
| 1 | X | 842 | A |
| 1 | X | 858 | G |
| 1 | X | 859 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | X | 860 | U |
| 1 | X | 871 | U |
| 1 | X | 872 | G |
| 1 | X | 878 | C |
| 1 | X | 938 | G |
| 1 | X | 939 | C |
| 1 | X | 955 | G |
| 1 | X | 969 | U |
| 1 | X | 972 | C |
| 1 | X | 990 | A |
| 1 | X | 994 | A |
| 1 | X | 995 | A |
| 1 | X | 1000 | G |
| 1 | X | 1006 | C |
| 1 | X | 1007 | A |
| 1 | X | 1019 | U |
| 1 | X | 1032 | A |
| 1 | X | 1036 | G |
| 1 | X | 1038 | U |
| 1 | X | 1053 | G |
| 1 | X | 1055 | A |
| 1 | X | 1056 | U |
| 1 | X | 1057 | A |
| 1 | X | 1069 | G |
| 1 | X | 1072 | U |
| 1 | X | 1080 | A |
| 1 | X | 1081 | A |
| 1 | X | 1086 | C |
| 1 | X | 1096 | A |
| 1 | X | 1099 | A |
| 1 | X | 1122 | A |
| 1 | X | 1141 | U |
| 1 | X | 1142 | G |
| 1 | X | 1152 | C |
| 1 | X | 1185 | C |
| 1 | X | 1186 | G |
| 1 | X | 1223 | G |
| 1 | X | 1233 | A |
| 1 | X | 1249 | G |
| 1 | X | 1266 | G |
| 1 | X | 1288 | A |
| 1 | X | 1289 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | X | 1291 | G |
| 1 | X | 1299 | A |
| 1 | X | 1314 | A |
| 1 | X | 1315 | A |
| 1 | X | 1333 | G |
| 1 | X | 1345 | G |
| 1 | X | 1355 | A |
| 1 | X | 1357 | U |
| 1 | X | 1403 | U |
| 1 | X | 1404 | C |
| 1 | X | 1409 | U |
| 1 | X | 1412 | C |
| 1 | X | 1429 | A |
| 1 | X | 1433 | A |
| 1 | X | 1434 | U |
| 1 | X | 1439 | G |
| 1 | X | 1441 | A |
| 1 | X | 1442 | C |
| 1 | X | 1459 | U |
| 1 | X | 1473 | U |
| 1 | X | 1475 | U |
| 1 | X | 1482 | U |
| 1 | X | 1496 | G |
| 1 | X | 1508 | G |
| 1 | X | 1513 | U |
| 1 | X | 1552 | C |
| 1 | X | 1562 | G |
| 1 | X | 1570 | C |
| 1 | X | 1574 | A |
| 1 | X | 1575 | C |
| 1 | X | 1601 | U |
| 1 | X | 1602 | G |
| 1 | X | 1607 | A |
| 1 | X | 1613 | G |
| 1 | X | 1624 | A |
| 1 | X | 1631 | C |
| 1 | X | 1632 | A |
| 1 | X | 1634 | A |
| 1 | X | 1680 | U |
| 1 | X | 1684 | G |
| 1 | X | 1685 | A |
| 1 | X | 1710 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | X | 1711 | C |
| 1 | X | 1716 | G |
| 1 | X | 1732 | U |
| 1 | X | 1749 | G |
| 1 | X | 1770 | U |
| 1 | X | 1775 | A |
| 1 | X | 1777 | A |
| 1 | X | 1790 | G |
| 1 | X | 1799 | A |
| 1 | X | 1800 | A |
| 1 | X | 1810 | U |
| 1 | X | 1811 | A |
| 1 | X | 1820 | G |
| 1 | X | 1839 | A |
| 1 | X | 1871 | G |
| 1 | X | 1882 | G |
| 1 | X | 1883 | A |
| 1 | X | 1909 | U |
| 1 | X | 1920 | A |
| 1 | X | 1923 | U |
| 1 | X | 1938 | U |
| 1 | X | 1953 | A |
| 1 | X | 1963 | G |
| 1 | X | 1975 | G |
| 1 | X | 1980 | A |
| 1 | X | 2005 | U |
| 1 | X | 2014 | A |
| 1 | X | 2018 | G |
| 1 | X | 2045 | A |
| 1 | X | 2075 | U |
| 1 | X | 2083 | G |
| 1 | X | 2088 | U |
| 1 | X | 2165 | A |
| 1 | X | 2189 | A |
| 1 | X | 2193 | C |
| 1 | X | 2204 | A |
| 1 | X | 2217 | G |
| 1 | X | 2228 | U |
| 1 | X | 2254 | C |
| 1 | X | 2261 | G |
| 1 | X | 2265 | A |
| 1 | X | 2290 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | X | 2298 | U |
| 1 | X | 2299 | A |
| 1 | X | 2305 | C |
| 1 | X | 2312 | A |
| 1 | X | 2314 | A |
| 1 | X | 2323 | U |
| 1 | X | 2354 | G |
| 1 | X | 2363 | G |
| 1 | X | 2370 | G |
| 1 | X | 2381 | A |
| 1 | X | 2401 | A |
| 1 | X | 2447 | G |
| 1 | X | 2477 | C |
| 1 | X | 2482 | A |
| 1 | X | 2497 | A |
| 1 | X | 2498 | U |
| 1 | X | 2508 | G |
| 1 | X | 2551 | A |
| 1 | X | 2560 | G |
| 1 | X | 2561 | G |
| 1 | X | 2564 | U |
| 1 | X | 2565 | C |
| 1 | X | 2580 | C |
| 1 | X | 2634 | G |
| 1 | X | 2660 | C |
| 1 | X | 2691 | C |
| 1 | X | 2705 | A |
| 1 | X | 2731 | G |
| 1 | X | 2738 | A |
| 1 | X | 2758 | A |
| 1 | X | 2770 | A |
| 1 | X | 2777 | A |
| 1 | X | 2778 | U |
| 1 | X | 2808 | U |
| 1 | X | 2810 | A |
| 1 | X | 2824 | C |
| 1 | X | 2846 | G |
| 1 | X | 2848 | A |
| 1 | X | 2854 | G |
| 1 | X | 2867 | G |
| 1 | X | 2876 | C |
| 2 | Y | 4 | C |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | Y | 11 | G |
| 2 | Y | 14 | C |
| 2 | Y | 46 | G |
| 2 | Y | 58 | G |
| 2 | Y | 59 | A |
| 2 | Y | 86 | A |

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 36 ligands modelled in this entry, 35 are monoatomic - leaving 1 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | $\# Z > 2$ | Counts | RMSZ | $\# Z > 2$ |
| 32 | 1F2 | X | 2929 | - | 60,60,60 | 1.94 | 14 (23%) | 90,90,90 | 2.53 | 33 (36%) |

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 |
|-----|------|-------|------|------|---------|--------------|---------|
| 32 | 1F2 | X | 2929 | - | - | 0/74/115/115 | 0/3/5/5 |

All (14) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 32 | X | 2929 | 1F2 | C30-N29 | 8.88 | 1.46 | 1.33 |
| 32 | X | 2929 | 1F2 | C8-C10 | 4.10 | 1.59 | 1.52 |
| 32 | X | 2929 | 1F2 | O11-C12 | -3.56 | 1.26 | 1.34 |
| 32 | X | 2929 | 1F2 | C2-C5 | -3.35 | 1.50 | 1.54 |
| 32 | X | 2929 | 1F2 | C10-C9 | -3.24 | 1.46 | 1.55 |
| 32 | X | 2929 | 1F2 | C5-N29 | 3.14 | 1.52 | 1.45 |
| 32 | X | 2929 | 1F2 | C17-C2 | 3.00 | 1.60 | 1.53 |
| 32 | X | 2929 | 1F2 | C25-C6 | 2.77 | 1.57 | 1.51 |
| 32 | X | 2929 | 1F2 | O11-C7 | 2.71 | 1.51 | 1.46 |
| 32 | X | 2929 | 1F2 | O18-C6 | -2.65 | 1.43 | 1.47 |
| 32 | X | 2929 | 1F2 | C15-C14 | -2.56 | 1.48 | 1.54 |
| 32 | X | 2929 | 1F2 | C13-C12 | -2.44 | 1.45 | 1.51 |
| 32 | X | 2929 | 1F2 | C15-C9 | -2.41 | 1.49 | 1.55 |
| 32 | X | 2929 | 1F2 | O18-C30 | -2.18 | 1.33 | 1.36 |

All (33) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 32 | X | 2929 | 1F2 | C25-C6-C5 | -9.69 | 109.41 | 117.03 |
| 32 | X | 2929 | 1F2 | C5-N29-C30 | -9.13 | 103.55 | 112.50 |
| 32 | X | 2929 | 1F2 | O1-C44-N45 | 7.46 | 119.70 | 111.02 |
| 32 | X | 2929 | 1F2 | C24-C7-C6 | -5.59 | 107.76 | 115.53 |
| 32 | X | 2929 | 1F2 | C48-C47-N45 | 4.99 | 107.56 | 101.74 |
| 32 | X | 2929 | 1F2 | O31-C30-N29 | -4.12 | 124.25 | 129.22 |
| 32 | X | 2929 | 1F2 | O46-C44-N45 | -3.94 | 119.63 | 124.31 |
| 32 | X | 2929 | 1F2 | O16-C4-C2 | -3.92 | 114.51 | 120.62 |
| 32 | X | 2929 | 1F2 | C3-C4-C2 | 3.43 | 125.44 | 118.99 |
| 32 | X | 2929 | 1F2 | O11-C12-C13 | 3.42 | 119.57 | 111.64 |
| 32 | X | 2929 | 1F2 | C22-C15-C9 | 3.42 | 119.72 | 112.86 |
| 32 | X | 2929 | 1F2 | C22-C15-C14 | 3.27 | 117.73 | 111.46 |
| 32 | X | 2929 | 1F2 | O19-C10-C9 | 3.00 | 113.59 | 108.10 |
| 32 | X | 2929 | 1F2 | C8-C10-C9 | -2.91 | 106.72 | 110.03 |
| 32 | X | 2929 | 1F2 | C10-C9-C15 | 2.77 | 117.95 | 113.60 |
| 32 | X | 2929 | 1F2 | O1-C14-C13 | -2.58 | 103.12 | 107.90 |
| 32 | X | 2929 | 1F2 | C54-N55-C56 | 2.57 | 121.46 | 116.85 |
| 32 | X | 2929 | 1F2 | C32-O21-C9 | -2.56 | 111.82 | 116.28 |
| 32 | X | 2929 | 1F2 | C32-C37-C36 | 2.56 | 113.66 | 109.31 |
| 32 | X | 2929 | 1F2 | O18-C6-C5 | -2.50 | 100.53 | 103.28 |
| 32 | X | 2929 | 1F2 | C6-C5-N29 | 2.38 | 102.59 | 99.92 |
| 32 | X | 2929 | 1F2 | O18-C30-N29 | 2.32 | 111.22 | 109.39 |
| 32 | X | 2929 | 1F2 | C50-N45-C47 | -2.31 | 108.54 | 112.00 |
| 32 | X | 2929 | 1F2 | C7-O11-C12 | 2.29 | 122.38 | 118.17 |
| 32 | X | 2929 | 1F2 | O18-C30-O31 | 2.28 | 124.53 | 121.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 32 | X | 2929 | 1F2 | O19-C10-C8 | 2.26 | 110.72 | 105.76 |
| 32 | X | 2929 | 1F2 | O27-C12-C13 | -2.24 | 117.57 | 123.94 |
| 32 | X | 2929 | 1F2 | C7-C6-C5 | 2.13 | 112.70 | 110.30 |
| 32 | X | 2929 | 1F2 | O18-C6-C7 | 2.13 | 109.19 | 105.02 |
| 32 | X | 2929 | 1F2 | C14-O1-C44 | 2.06 | 119.56 | 116.74 |
| 32 | X | 2929 | 1F2 | O11-C7-C6 | 2.05 | 110.18 | 105.36 |
| 32 | X | 2929 | 1F2 | C28-C13-C14 | -2.05 | 108.12 | 112.84 |
| 32 | X | 2929 | 1F2 | C56-C51-C47 | -2.02 | 118.82 | 122.58 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1 | X | 2686/2880 (93%) | -0.31 | 71 (2%) 53 11 | 43, 92, 197, 276 | 0 |
| 2 | Y | 122/123 (99%) | -0.18 | 2 (1%) 68 20 | 83, 136, 170, 192 | 0 |
| 3 | A | 240/274 (87%) | -0.01 | 1 (0%) 90 51 | 69, 116, 146, 173 | 0 |
| 4 | B | 205/211 (97%) | -0.23 | 0 100 100 | 45, 73, 106, 154 | 0 |
| 5 | C | 197/205 (96%) | 0.04 | 5 (2%) 54 12 | 57, 114, 155, 187 | 0 |
| 6 | D | 177/180 (98%) | 0.24 | 5 (2%) 50 11 | 146, 183, 216, 227 | 0 |
| 7 | E | 171/185 (92%) | -0.16 | 0 100 100 | 92, 143, 192, 206 | 0 |
| 8 | F | 71/144 (49%) | 1.21 | 9 (12%) 4 1 | 211, 236, 252, 257 | 0 |
| 9 | G | 142/174 (81%) | -0.01 | 3 (2%) 60 15 | 73, 97, 145, 161 | 0 |
| 10 | H | 134/134 (100%) | -0.32 | 0 100 100 | 50, 70, 96, 120 | 0 |
| 11 | I | 141/156 (90%) | 0.42 | 13 (9%) 9 2 | 67, 129, 174, 204 | 0 |
| 12 | J | 136/141 (96%) | 0.02 | 2 (1%) 70 21 | 74, 103, 149, 184 | 0 |
| 13 | K | 113/116 (97%) | -0.31 | 0 100 100 | 35, 60, 79, 91 | 0 |
| 14 | L | 104/114 (91%) | 0.16 | 4 (3%) 38 7 | 98, 134, 156, 169 | 0 |
| 15 | M | 108/166 (65%) | -0.29 | 0 100 100 | 50, 73, 111, 144 | 0 |
| 16 | N | 117/118 (99%) | -0.23 | 0 100 100 | 60, 90, 127, 160 | 0 |
| 17 | O | 94/100 (94%) | -0.20 | 0 100 100 | 67, 115, 156, 173 | 0 |
| 18 | P | 127/134 (94%) | -0.28 | 0 100 100 | 50, 67, 108, 158 | 0 |
| 19 | Q | 93/95 (97%) | -0.06 | 1 (1%) 77 27 | 73, 106, 162, 195 | 0 |
| 20 | R | 110/115 (95%) | 0.05 | 2 (1%) 65 18 | 88, 117, 170, 178 | 0 |
| 21 | S | 175/237 (73%) | 0.04 | 1 (0%) 86 41 | 121, 155, 175, 190 | 0 |
| 22 | T | 84/91 (92%) | 0.22 | 5 (5%) 21 5 | 80, 108, 186, 199 | 0 |
| 23 | U | 72/81 (88%) | 0.24 | 3 (4%) 35 7 | 92, 128, 153, 162 | 0 |
| 24 | V | 66/67 (98%) | 0.28 | 4 (6%) 21 4 | 100, 132, 211, 216 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 25 | W | 55/55 (100%) | -0.29 | 0 100 100 | 81, 98, 126, 152 | 0 |
| 26 | Z | 58/60 (96%) | -0.18 | 1 (1%) 67 19 | 49, 71, 105, 113 | 0 |
| 27 | 1 | 53/55 (96%) | 0.38 | 5 (9%) 9 2 | 8, 32, 61, 96 | 0 |
| 28 | 2 | 46/47 (97%) | 2.13 | 25 (54%) 0 0 | 3, 16, 37, 59 | 0 |
| 29 | 3 | 63/66 (95%) | 1.30 | 16 (25%) 1 1 | 3, 25, 40, 60 | 0 |
| 30 | 4 | 37/37 (100%) | 4.29 | 34 (91%) 0 0 | 227, 254, 265, 269 | 0 |
| All | All | 5997/6561 (91%) | -0.08 | 212 (3%) 42 8 | 3, 100, 196, 276 | 0 |

All (212) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 30 | 4 | 24 | LEU | 12.1 |
| 27 | 1 | 7 | ARG | 9.0 |
| 30 | 4 | 25 | VAL | 8.9 |
| 30 | 4 | 17 | VAL | 8.7 |
| 24 | V | 1 | MET | 7.9 |
| 2 | Y | 123 | U | 7.8 |
| 1 | X | 731 | A | 7.4 |
| 30 | 4 | 35 | ARG | 7.0 |
| 30 | 4 | 11 | CYS | 6.7 |
| 30 | 4 | 34 | GLN | 6.6 |
| 1 | X | 1095 | A | 6.2 |
| 28 | 2 | 27 | GLY | 6.1 |
| 30 | 4 | 20 | HIS | 6.1 |
| 30 | 4 | 19 | ARG | 6.0 |
| 8 | F | 125 | ASN | 5.9 |
| 30 | 4 | 10 | MET | 5.8 |
| 30 | 4 | 22 | ARG | 5.3 |
| 1 | X | 248 | A | 5.1 |
| 24 | V | 2 | LYS | 5.0 |
| 1 | X | 1086 | C | 4.9 |
| 29 | 3 | 40 | GLU | 4.9 |
| 30 | 4 | 14 | CYS | 4.9 |
| 26 | Z | 2 | ALA | 4.8 |
| 30 | 4 | 26 | ILE | 4.7 |
| 30 | 4 | 12 | ASP | 4.6 |
| 28 | 2 | 32 | ALA | 4.5 |
| 30 | 4 | 21 | GLY | 4.5 |
| 11 | I | 6 | LEU | 4.5 |
| 30 | 4 | 16 | VAL | 4.4 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 1 | X | 2169 | A | 4.3 |
| 1 | X | 1085 | G | 4.3 |
| 1 | X | 1080 | A | 4.2 |
| 11 | I | 8 | PRO | 4.2 |
| 23 | U | 27 | ASP | 4.1 |
| 30 | 4 | 29 | ASN | 4.1 |
| 1 | X | 665 | A | 4.1 |
| 1 | X | 1090 | C | 4.1 |
| 29 | 3 | 31 | HIS | 4.0 |
| 8 | F | 114 | ASP | 4.0 |
| 1 | X | 1089 | C | 4.0 |
| 1 | X | 1077 | U | 4.0 |
| 24 | V | 3 | PRO | 3.9 |
| 1 | X | 1523 | A | 3.9 |
| 2 | Y | 2 | C | 3.9 |
| 1 | X | 1072 | U | 3.9 |
| 1 | X | 1524 | C | 3.8 |
| 1 | X | 1106 | A | 3.8 |
| 1 | X | 1068 | A | 3.8 |
| 1 | X | 2776 | U | 3.8 |
| 30 | 4 | 15 | LYS | 3.7 |
| 1 | X | 727 | U | 3.7 |
| 1 | X | 728 | G | 3.7 |
| 28 | 2 | 34 | ARG | 3.7 |
| 27 | 1 | 2 | ALA | 3.7 |
| 29 | 3 | 38 | GLY | 3.6 |
| 8 | F | 121 | GLU | 3.6 |
| 1 | X | 1081 | A | 3.6 |
| 30 | 4 | 6 | SER | 3.6 |
| 11 | I | 9 | THR | 3.6 |
| 23 | U | 28 | GLY | 3.6 |
| 1 | X | 1551 | U | 3.6 |
| 30 | 4 | 4 | ARG | 3.6 |
| 1 | X | 1552 | C | 3.5 |
| 30 | 4 | 23 | VAL | 3.5 |
| 22 | T | 8 | GLY | 3.5 |
| 1 | X | 1103 | C | 3.5 |
| 1 | X | 2166 | G | 3.5 |
| 30 | 4 | 1 | MET | 3.4 |
| 22 | T | 11 | LYS | 3.4 |
| 29 | 3 | 30 | ARG | 3.4 |
| 28 | 2 | 35 | ARG | 3.4 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 30 | 4 | 36 | GLN | 3.4 |
| 1 | X | 2170 | C | 3.4 |
| 29 | 3 | 33 | ASN | 3.4 |
| 30 | 4 | 28 | SER | 3.4 |
| 30 | 4 | 7 | VAL | 3.4 |
| 1 | X | 1066 | G | 3.3 |
| 3 | A | 203 | ASN | 3.3 |
| 1 | X | 1065 | A | 3.3 |
| 11 | I | 63 | ARG | 3.2 |
| 30 | 4 | 32 | HIS | 3.2 |
| 28 | 2 | 7 | PRO | 3.2 |
| 1 | X | 2774 | U | 3.2 |
| 28 | 2 | 36 | ALA | 3.2 |
| 1 | X | 730 | C | 3.2 |
| 5 | C | 19 | LEU | 3.2 |
| 22 | T | 9 | SER | 3.2 |
| 28 | 2 | 37 | LYS | 3.2 |
| 6 | D | 145 | MET | 3.1 |
| 1 | X | 1107 | A | 3.1 |
| 28 | 2 | 33 | ARG | 3.1 |
| 19 | Q | 64 | ARG | 3.1 |
| 11 | I | 114 | ILE | 3.0 |
| 30 | 4 | 27 | CYS | 3.0 |
| 28 | 2 | 22 | MET | 3.0 |
| 11 | I | 5 | ASP | 3.0 |
| 1 | X | 891 | A | 3.0 |
| 1 | X | 2088 | U | 2.9 |
| 28 | 2 | 11 | LYS | 2.9 |
| 1 | X | 1186 | G | 2.9 |
| 30 | 4 | 33 | LYS | 2.9 |
| 12 | J | 84 | MET | 2.9 |
| 11 | I | 4 | HIS | 2.8 |
| 1 | X | 1734 | C | 2.8 |
| 8 | F | 126 | THR | 2.8 |
| 8 | F | 115 | LEU | 2.8 |
| 1 | X | 1188 | A | 2.7 |
| 20 | R | 102 | LYS | 2.7 |
| 11 | I | 29 | THR | 2.7 |
| 28 | 2 | 25 | LYS | 2.7 |
| 1 | X | 2777 | A | 2.7 |
| 29 | 3 | 42 | ARG | 2.7 |
| 1 | X | 1084 | A | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 11 | I | 52 | GLY | 2.7 |
| 29 | 3 | 60 | LEU | 2.7 |
| 1 | X | 1104 | G | 2.7 |
| 1 | X | 1093 | U | 2.7 |
| 1 | X | 1189 | G | 2.7 |
| 14 | L | 64 | LYS | 2.7 |
| 28 | 2 | 9 | ASN | 2.7 |
| 29 | 3 | 37 | SER | 2.6 |
| 1 | X | 1187 | A | 2.6 |
| 30 | 4 | 30 | VAL | 2.6 |
| 1 | X | 1091 | C | 2.6 |
| 14 | L | 97 | HIS | 2.6 |
| 12 | J | 140 | GLU | 2.6 |
| 1 | X | 2082 | C | 2.6 |
| 8 | F | 85 | GLY | 2.6 |
| 5 | C | 197 | GLU | 2.6 |
| 29 | 3 | 8 | LYS | 2.6 |
| 1 | X | 1120 | C | 2.6 |
| 11 | I | 33 | GLY | 2.6 |
| 28 | 2 | 30 | ILE | 2.6 |
| 1 | X | 558 | G | 2.6 |
| 28 | 2 | 24 | THR | 2.6 |
| 1 | X | 2775 | U | 2.6 |
| 28 | 2 | 6 | GLN | 2.6 |
| 29 | 3 | 7 | HIS | 2.5 |
| 1 | X | 2780 | A | 2.5 |
| 9 | G | 97 | ASP | 2.5 |
| 1 | X | 2290 | A | 2.5 |
| 5 | C | 47 | THR | 2.5 |
| 1 | X | 2778 | U | 2.5 |
| 30 | 4 | 18 | ARG | 2.5 |
| 1 | X | 1067 | G | 2.5 |
| 1 | X | 1109 | A | 2.5 |
| 1 | X | 2174 | G | 2.5 |
| 1 | X | 1094 | C | 2.5 |
| 28 | 2 | 8 | ASN | 2.4 |
| 28 | 2 | 2 | LYS | 2.4 |
| 1 | X | 1108 | U | 2.4 |
| 30 | 4 | 5 | SER | 2.4 |
| 5 | C | 198 | GLU | 2.4 |
| 1 | X | 1098 | G | 2.4 |
| 11 | I | 7 | LYS | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 6 | D | 22 | TYR | 2.4 |
| 28 | 2 | 16 | HIS | 2.4 |
| 30 | 4 | 8 | LYS | 2.4 |
| 14 | L | 58 | ALA | 2.4 |
| 11 | I | 30 | ALA | 2.4 |
| 28 | 2 | 41 | GLN | 2.4 |
| 1 | X | 434 | C | 2.4 |
| 28 | 2 | 26 | SER | 2.3 |
| 27 | 1 | 44 | ALA | 2.3 |
| 1 | X | 1913 | G | 2.3 |
| 23 | U | 47 | HIS | 2.3 |
| 9 | G | 156 | HIS | 2.3 |
| 1 | X | 2167 | A | 2.3 |
| 6 | D | 147 | ASP | 2.3 |
| 28 | 2 | 14 | LYS | 2.3 |
| 8 | F | 142 | PRO | 2.3 |
| 1 | X | 1071 | U | 2.3 |
| 1 | X | 2089 | C | 2.3 |
| 8 | F | 84 | ILE | 2.3 |
| 30 | 4 | 37 | GLY | 2.2 |
| 21 | S | 58 | GLY | 2.2 |
| 1 | X | 1050 | G | 2.2 |
| 1 | X | 2090 | U | 2.2 |
| 28 | 2 | 4 | THR | 2.2 |
| 28 | 2 | 20 | ALA | 2.2 |
| 29 | 3 | 10 | ALA | 2.2 |
| 1 | X | 2173 | G | 2.2 |
| 27 | 1 | 26 | LYS | 2.2 |
| 9 | G | 129 | HIS | 2.2 |
| 1 | X | 1073 | G | 2.1 |
| 6 | D | 74 | ILE | 2.1 |
| 11 | I | 10 | PRO | 2.1 |
| 29 | 3 | 45 | GLY | 2.1 |
| 1 | X | 2087 | U | 2.1 |
| 1 | X | 729 | A | 2.1 |
| 1 | X | 1114 | A | 2.1 |
| 1 | X | 1052 | C | 2.1 |
| 27 | 1 | 43 | VAL | 2.1 |
| 1 | X | 1051 | U | 2.1 |
| 30 | 4 | 13 | ASN | 2.1 |
| 29 | 3 | 28 | GLY | 2.1 |
| 14 | L | 54 | ALA | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | X | 1190 | C | 2.1 |
| 8 | F | 144 | ALA | 2.1 |
| 29 | 3 | 2 | PRO | 2.1 |
| 22 | T | 73 | GLY | 2.1 |
| 29 | 3 | 36 | LYS | 2.1 |
| 30 | 4 | 9 | LYS | 2.1 |
| 6 | D | 20 | PHE | 2.1 |
| 20 | R | 94 | VAL | 2.1 |
| 28 | 2 | 1 | MET | 2.0 |
| 1 | X | 1553 | G | 2.0 |
| 24 | V | 36 | GLN | 2.0 |
| 29 | 3 | 32 | GLN | 2.0 |
| 5 | C | 44 | SER | 2.0 |
| 22 | T | 74 | LYS | 2.0 |
| 28 | 2 | 29 | ASN | 2.0 |

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|--------|----------------------------|-------|
| 31 | MG | X | 2908 | 1/1 | 0.87 | 111.52 | 37,37,37,37 | 0 |
| 31 | MG | X | 2921 | 1/1 | 0.40 | 58.00 | 81,81,81,81 | 0 |
| 31 | MG | X | 2926 | 1/1 | 0.92 | 32.92 | 45,45,45,45 | 0 |
| 31 | MG | Y | 203 | 1/1 | 0.70 | 30.49 | 87,87,87,87 | 0 |
| 31 | MG | X | 2918 | 1/1 | 0.66 | 28.04 | 42,42,42,42 | 0 |
| 31 | MG | X | 2924 | 1/1 | 1.19 | 25.73 | 69,69,69,69 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|-------|----------------------------|-------|
| 31 | MG | X | 2922 | 1/1 | 0.66 | 23.81 | 44,44,44,44 | 0 |
| 31 | MG | X | 2919 | 1/1 | 0.43 | 23.69 | 30,30,30,30 | 0 |
| 31 | MG | X | 2903 | 1/1 | 0.69 | 22.35 | 89,89,89,89 | 0 |
| 31 | MG | X | 2912 | 1/1 | 0.49 | 22.16 | 71,71,71,71 | 0 |
| 31 | MG | X | 2911 | 1/1 | 0.22 | 21.86 | 68,68,68,68 | 0 |
| 31 | MG | X | 2907 | 1/1 | 0.63 | 21.46 | 51,51,51,51 | 0 |
| 31 | MG | Y | 204 | 1/1 | 0.25 | 19.50 | 82,82,82,82 | 0 |
| 31 | MG | X | 2909 | 1/1 | 0.54 | 18.56 | 96,96,96,96 | 0 |
| 31 | MG | X | 2923 | 1/1 | 0.33 | 18.18 | 34,34,34,34 | 0 |
| 31 | MG | M | 201 | 1/1 | 0.51 | 18.17 | 23,23,23,23 | 0 |
| 31 | MG | X | 2928 | 1/1 | 0.47 | 17.77 | 62,62,62,62 | 0 |
| 31 | MG | X | 2913 | 1/1 | 0.57 | 17.22 | 61,61,61,61 | 0 |
| 31 | MG | X | 2915 | 1/1 | 0.59 | 17.16 | 57,57,57,57 | 0 |
| 31 | MG | X | 2917 | 1/1 | 0.52 | 16.51 | 55,55,55,55 | 0 |
| 31 | MG | X | 2916 | 1/1 | 0.60 | 16.49 | 37,37,37,37 | 0 |
| 31 | MG | Y | 202 | 1/1 | 0.51 | 16.30 | 58,58,58,58 | 0 |
| 31 | MG | Y | 201 | 1/1 | 0.77 | 13.50 | 89,89,89,89 | 0 |
| 31 | MG | X | 2910 | 1/1 | 0.44 | 13.08 | 42,42,42,42 | 0 |
| 31 | MG | Y | 205 | 1/1 | 0.35 | 12.06 | 79,79,79,79 | 0 |
| 31 | MG | X | 2901 | 1/1 | 0.36 | 11.30 | 50,50,50,50 | 0 |
| 31 | MG | X | 2927 | 1/1 | 0.53 | 11.22 | 62,62,62,62 | 0 |
| 31 | MG | X | 2902 | 1/1 | 0.70 | 10.73 | 94,94,94,94 | 0 |
| 31 | MG | X | 2906 | 1/1 | 0.37 | 9.00 | 58,58,58,58 | 0 |
| 31 | MG | X | 2925 | 1/1 | 0.45 | 7.65 | 122,122,122,122 | 0 |
| 31 | MG | X | 2904 | 1/1 | 0.30 | 7.37 | 107,107,107,107 | 0 |
| 31 | MG | X | 2905 | 1/1 | 0.25 | 6.78 | 65,65,65,65 | 0 |
| 31 | MG | J | 201 | 1/1 | 0.31 | 5.34 | 100,100,100,100 | 0 |
| 31 | MG | X | 2920 | 1/1 | 0.21 | 3.58 | 115,115,115,115 | 0 |
| 31 | MG | X | 2914 | 1/1 | 0.37 | 1.32 | 27,27,27,27 | 0 |
| 32 | 1F2 | X | 2929 | 56/56 | 0.19 | -0.26 | 42,68,77,83 | 0 |

6.5 Other polymers ⓘ

There are no such residues in this entry.