



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 04:01 PM GMT

PDB ID : 3V25
Title : Crystal structure of RMF bound to the 70S ribosome. This PDB entry contains coordinates for the 50S subunit of the 2nd ribosome in the ASU
Authors : Polikanov, Y.S.; Blaha, G.M.; Steitz, T.A.
Deposited on : 2011-12-11
Resolution : 3.00 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>

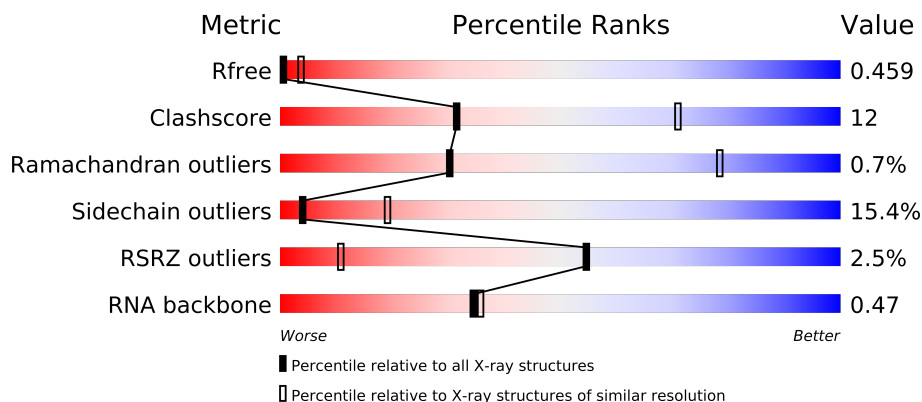
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.00 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 | 1216 (3.00-3.00) |
| Clashscore | 79885 | 1594 (3.00-3.00) |
| Ramachandran outliers | 78287 | 1537 (3.00-3.00) |
| Sidechain outliers | 78261 | 1540 (3.00-3.00) |
| RSRZ outliers | 66119 | 1217 (3.00-3.00) |
| RNA backbone | 1838 | 1070 (3.50-2.50) |

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 | A | 2915 | |
| 2 | B | 122 | |
| 3 | D | 276 | |
| 4 | E | 206 | |
| 5 | F | 210 | |
| 6 | G | 182 | |
| 7 | H | 180 | |
| 8 | I | 148 | |
| 9 | N | 140 | |
| 10 | O | 122 | |
| 11 | P | 150 | |
| 12 | Q | 141 | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 13 | R | 118 | |
| 14 | S | 112 | |
| 15 | T | 146 | |
| 16 | U | 118 | |
| 17 | V | 101 | |
| 18 | W | 113 | |
| 19 | X | 96 | |
| 20 | Y | 110 | |
| 21 | Z | 206 | |
| 22 | 0 | 85 | |
| 23 | 1 | 98 | |
| 24 | 2 | 72 | |
| 25 | 3 | 60 | |
| 26 | 4 | 71 | |
| 27 | 5 | 60 | |
| 28 | 6 | 54 | |
| 29 | 7 | 49 | |
| 30 | 8 | 65 | |
| 31 | 9 | 37 | |

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 91067 atoms, of which 0 are hydrogen and 0 are deuterium.

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 1 | A | 2814 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 60620 | 26978 | 11348 | 19481 | 2813 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 2 | B | 120 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2573 | 1146 | 476 | 832 | 119 | | | |

- Molecule 3 is a protein called 50S Ribosomal Protein L2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3 | D | 275 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2136 | 1349 | 423 | 361 | 3 | | | |

- Molecule 4 is a protein called 50S Ribosomal Protein L3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 4 | E | 204 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1555 | 982 | 297 | 270 | 6 | | | |

- Molecule 5 is a protein called 50S Ribosomal Protein L4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 5 | F | 203 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1580 | 1007 | 298 | 273 | 2 | | | |

- Molecule 6 is a protein called 50S Ribosomal Protein L5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6 | G | 181 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1368 | 879 | 242 | 244 | 3 | | | |

- Molecule 7 is a protein called 50S Ribosomal Protein L6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7 | H | 174 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1317 | 837 | 243 | 236 | 1 | | | |

- Molecule 8 is a protein called 50S Ribosomal Protein L9.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8 | I | 146 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1038 | 668 | 180 | 189 | 1 | | | |

- Molecule 9 is a protein called 50S Ribosomal Protein L13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 9 | N | 140 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1112 | 717 | 207 | 184 | 4 | | | |

- Molecule 10 is a protein called 50S Ribosomal Protein L14.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10 | O | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 923 | 583 | 168 | 168 | 4 | | | |

- Molecule 11 is a protein called 50S Ribosomal Protein L15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11 | P | 149 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1131 | 703 | 229 | 196 | 3 | | | |

- Molecule 12 is a protein called 50S Ribosomal Protein L16.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12 | Q | 141 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1122 | 715 | 212 | 188 | 7 | | | |

- Molecule 13 is a protein called 50S Ribosomal Protein L17.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13 | R | 118 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 968 | 604 | 203 | 160 | 1 | | | |

- Molecule 14 is a protein called 50S Ribosomal Protein L18.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 14 | S | 110 | Total | C | N | O | | | |
| | | | 865 | 544 | 172 | 149 | 0 | 0 | 0 |

- Molecule 15 is a protein called 50S Ribosomal Protein L19.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 15 | T | 131 | Total | C | N | O | S | | |
| | | | 1063 | 666 | 213 | 183 | 1 | 0 | 0 |

- Molecule 16 is a protein called 50S Ribosomal Protein L20.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 16 | U | 116 | Total | C | N | O | S | | |
| | | | 959 | 608 | 201 | 149 | 1 | 0 | 0 |

- Molecule 17 is a protein called 50S Ribosomal Protein L21.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 17 | V | 101 | Total | C | N | O | S | | |
| | | | 771 | 495 | 140 | 135 | 1 | 0 | 0 |

- Molecule 18 is a protein called 50S Ribosomal Protein L22.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 18 | W | 112 | Total | C | N | O | S | | |
| | | | 881 | 554 | 172 | 153 | 2 | 0 | 0 |

- Molecule 19 is a protein called 50S Ribosomal Protein L23.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 19 | X | 95 | Total | C | N | O | S | | |
| | | | 742 | 483 | 134 | 124 | 1 | 0 | 0 |

- Molecule 20 is a protein called 50S Ribosomal Protein L24.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 20 | Y | 107 | Total | C | N | O | S | | |
| | | | 785 | 503 | 145 | 131 | 6 | 0 | 0 |

- Molecule 21 is a protein called 50S Ribosomal Protein L25.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 21 | Z | 198 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1522 | 972 | 269 | 279 | 2 | | | |

- Molecule 22 is a protein called 50S Ribosomal Protein L27.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 22 | 0 | 76 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 594 | 368 | 125 | 100 | 1 | | | |

- Molecule 23 is a protein called 50S Ribosomal Protein L28.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 23 | 1 | 97 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 745 | 469 | 144 | 131 | 1 | | | |

- Molecule 24 is a protein called 50S Ribosomal Protein L29.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 24 | 2 | 70 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 588 | 365 | 118 | 103 | 2 | | | |

- Molecule 25 is a protein called 50S Ribosomal Protein L30.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 25 | 3 | 59 | Total | C | N | O | 0 | 0 | 0 |
| | | | 458 | 293 | 87 | 78 | | | |

- Molecule 26 is a protein called 50S Ribosomal Protein L31.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 26 | 4 | 46 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 349 | 223 | 57 | 64 | 5 | | | |

- Molecule 27 is a protein called 50S Ribosomal Protein L32.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 27 | 5 | 59 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 455 | 286 | 90 | 74 | 5 | | | |

- Molecule 28 is a protein called 50S Ribosomal Protein L33.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 28 | 6 | 53 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 449 | 278 | 90 | 77 | 4 | | | |

- Molecule 29 is a protein called 50S Ribosomal Protein L34.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 29 | 7 | 48 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 418 | 257 | 104 | 55 | 2 | | | |

- Molecule 30 is a protein called 50S Ribosomal Protein L35.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 30 | 8 | 64 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 509 | 326 | 99 | 82 | 2 | | | |

- Molecule 31 is a protein called 50S Ribosomal Protein L36.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 31 | 9 | 36 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 297 | 182 | 66 | 46 | 3 | | | |

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

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 32 | P | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 32 | D | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 32 | E | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 32 | B | 5 | Total | Mg | 0 | 0 |
| | | | 5 | 5 | | |
| 32 | 6 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 32 | 7 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 32 | A | 428 | Total | Mg | 0 | 0 |
| | | | 428 | 428 | | |
| 32 | 8 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 32 | F | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |

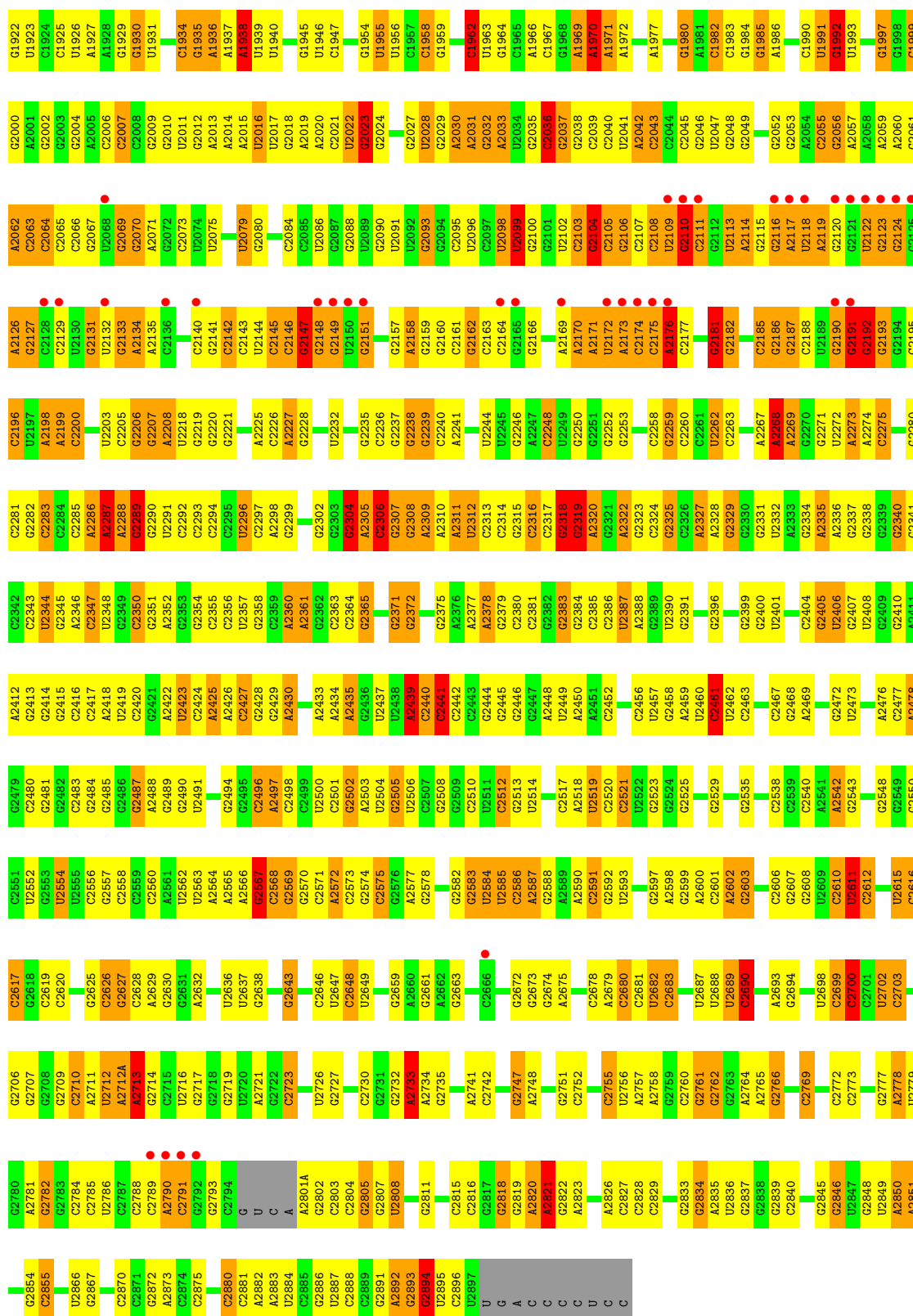
- Molecule 33 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 33 | 9 | 1 | Total 1 | Zn 1 | 0 | 0 |
| 33 | Y | 1 | Total 1 | Zn 1 | 0 | 0 |
| 33 | 4 | 1 | Total 1 | Zn 1 | 0 | 0 |
| 33 | 6 | 1 | Total 1 | Zn 1 | 0 | 0 |
| 33 | 5 | 1 | Total 1 | Zn 1 | 0 | 0 |

- Molecule 34 is water.

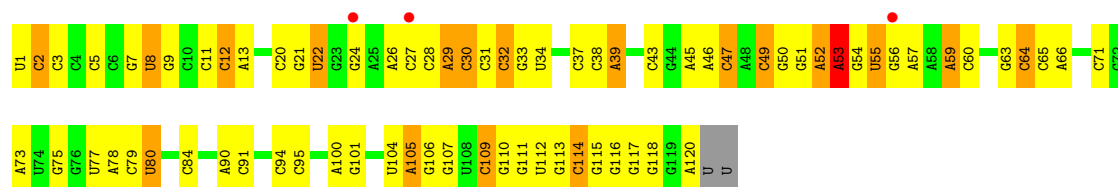
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 34 | A | 696 | Total 696 | O 696 | 0 | 0 |
| 34 | B | 9 | Total 9 | O 9 | 0 | 0 |
| 34 | D | 3 | Total 3 | O 3 | 0 | 0 |
| 34 | E | 1 | Total 1 | O 1 | 0 | 0 |
| 34 | F | 5 | Total 5 | O 5 | 0 | 0 |
| 34 | P | 5 | Total 5 | O 5 | 0 | 0 |
| 34 | Q | 2 | Total 2 | O 2 | 0 | 0 |
| 34 | R | 1 | Total 1 | O 1 | 0 | 0 |
| 34 | V | 1 | Total 1 | O 1 | 0 | 0 |
| 34 | X | 1 | Total 1 | O 1 | 0 | 0 |
| 34 | Y | 1 | Total 1 | O 1 | 0 | 0 |
| 34 | 0 | 1 | Total 1 | O 1 | 0 | 0 |
| 34 | 1 | 2 | Total 2 | O 2 | 0 | 0 |

WORLDWIDE
PDB
PROTEIN DATA BANK



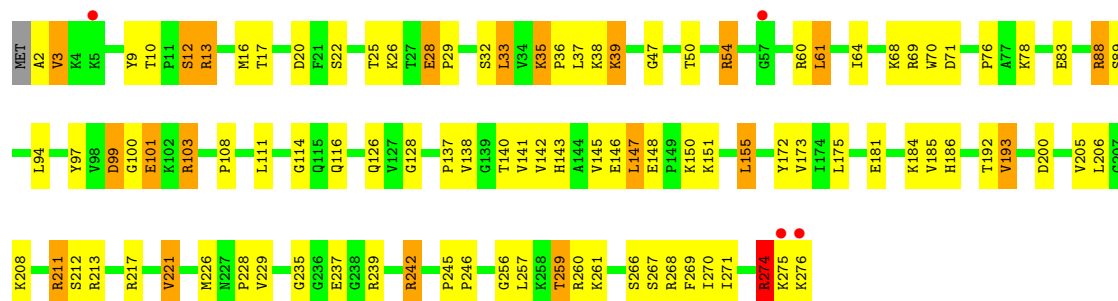
• Molecule 2: 5S Ribosomal RNA

Chain B:



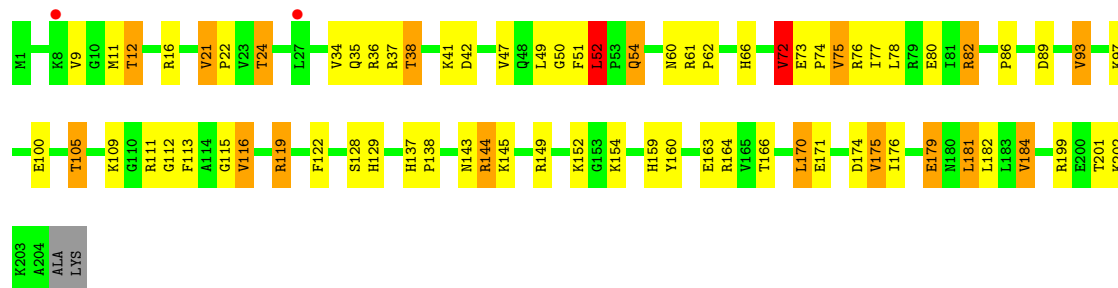
• Molecule 3: 50S Ribosomal Protein L2

Chain D:



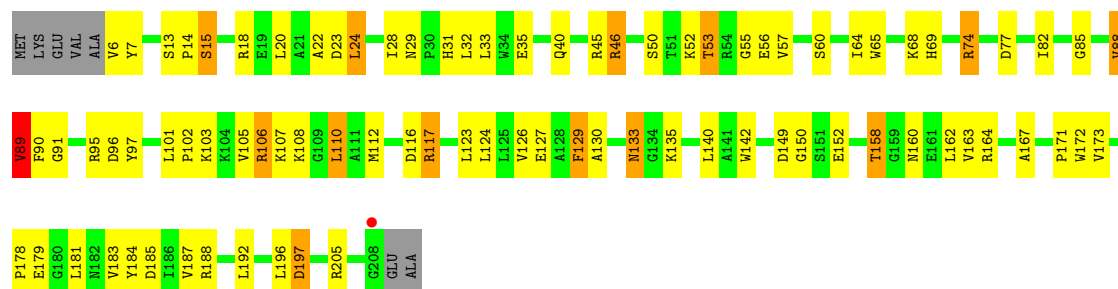
• Molecule 4: 50S Ribosomal Protein L3

Chain E:



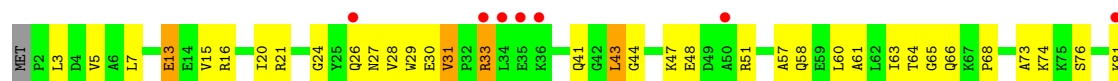
• Molecule 5: 50S Ribosomal Protein L4

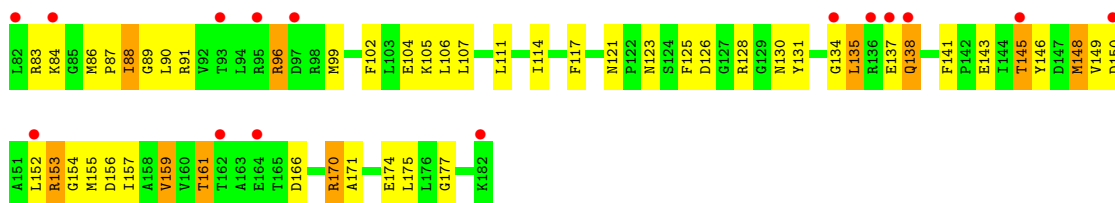
Chain F:



• Molecule 6: 50S Ribosomal Protein L5

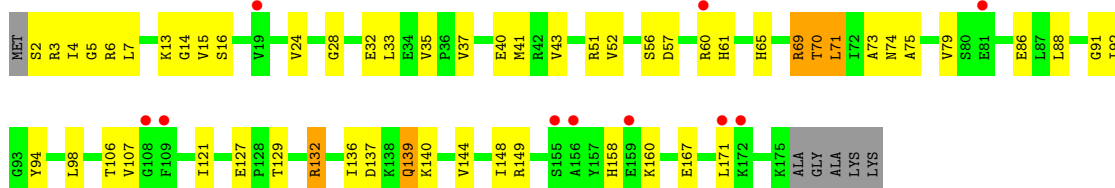
Chain G:





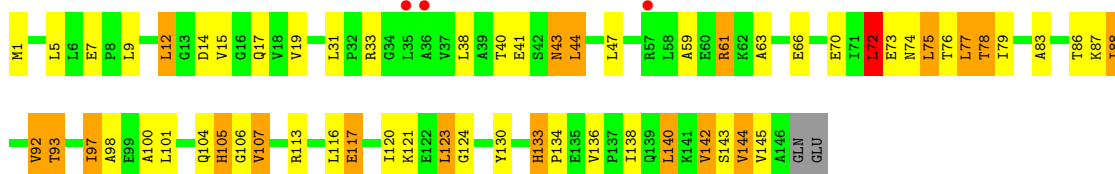
• Molecule 7: 50S Ribosomal Protein L6

Chain H:



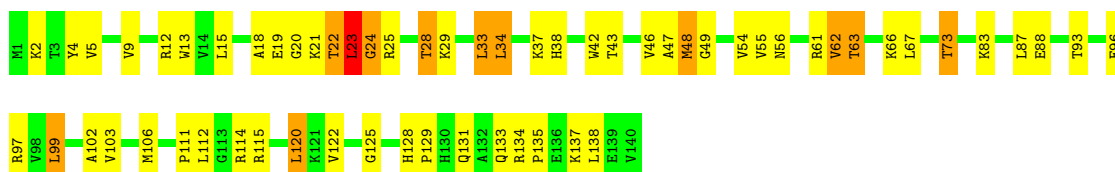
• Molecule 8: 50S Ribosomal Protein L9

Chain I:



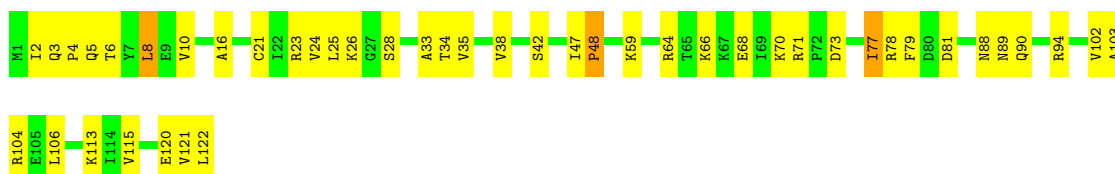
• Molecule 9: 50S Ribosomal Protein L13

Chain N:



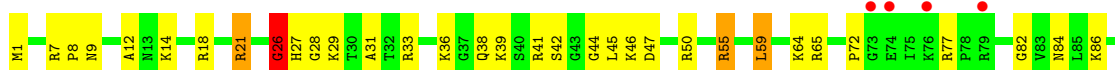
• Molecule 10: 50S Ribosomal Protein L14

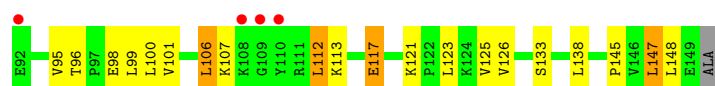
Chain O:



• Molecule 11: 50S Ribosomal Protein L15

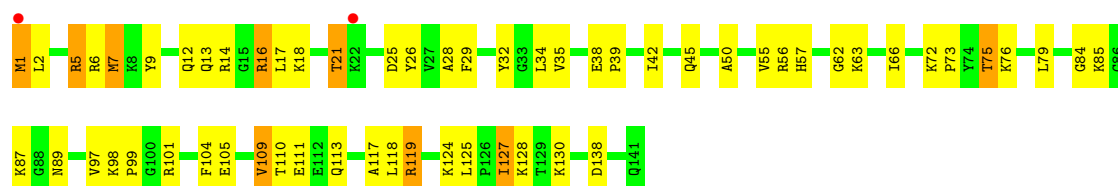
Chain P:





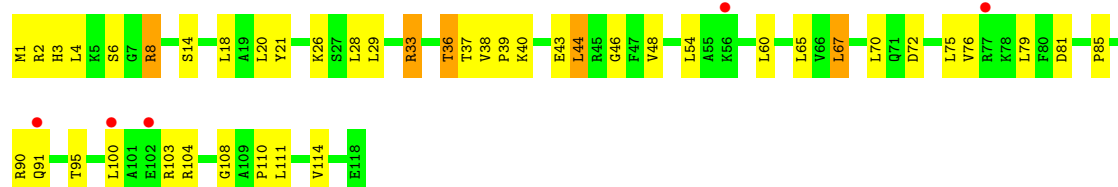
• Molecule 12: 50S Ribosomal Protein L16

Chain Q:



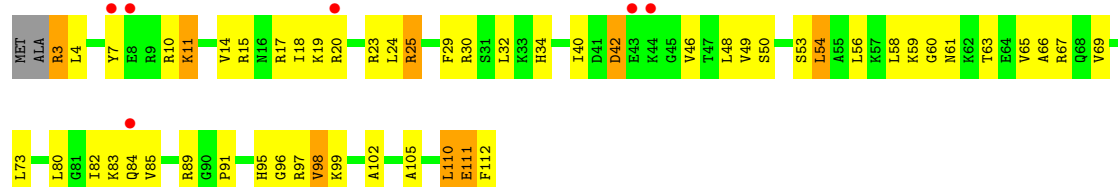
• Molecule 13: 50S Ribosomal Protein L17

Chain R:



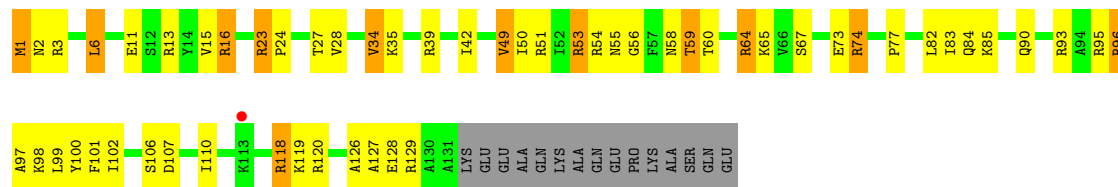
• Molecule 14: 50S Ribosomal Protein L18

Chain S:



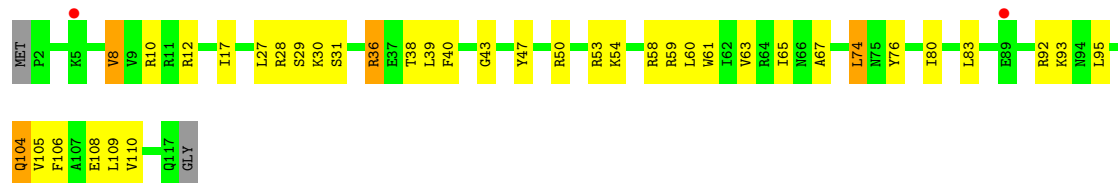
• Molecule 15: 50S Ribosomal Protein L19

Chain T:



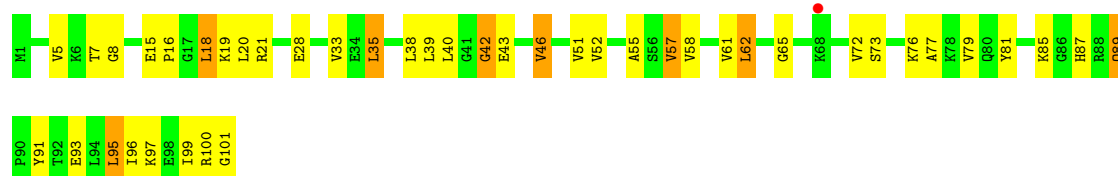
• Molecule 16: 50S Ribosomal Protein L20

Chain U:



- Molecule 17: 50S Ribosomal Protein L21

Chain V:



- Molecule 18: 50S Ribosomal Protein L22

Chain W:



- Molecule 19: 50S Ribosomal Protein L23

Chain X:



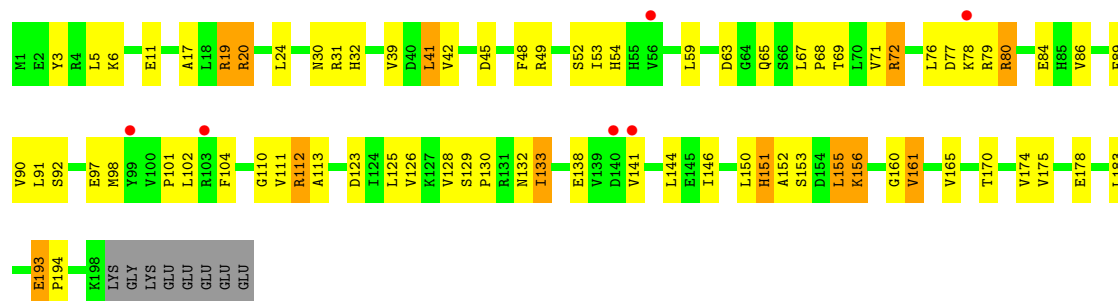
- Molecule 20: 50S Ribosomal Protein L24

Chain Y:



- Molecule 21: 50S Ribosomal Protein L25

Chain Z:



- Molecule 22: 50S Ribosomal Protein L27

Chain 0:





• Molecule 23: 50S Ribosomal Protein L28

Chain 1:



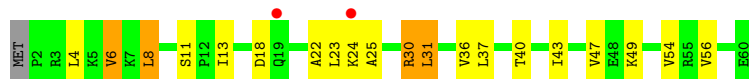
• Molecule 24: 50S Ribosomal Protein L29

Chain 2:



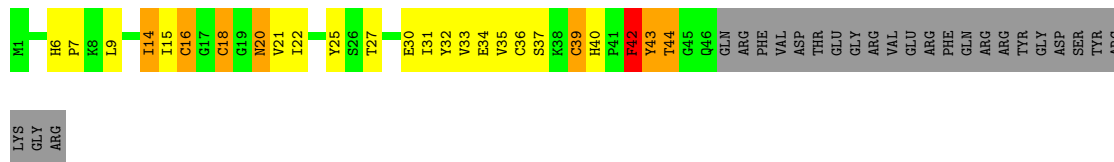
• Molecule 25: 50S Ribosomal Protein L30

Chain 3:



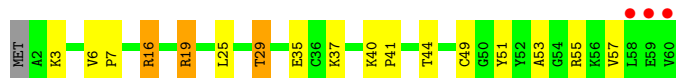
• Molecule 26: 50S Ribosomal Protein L31

Chain 4:



• Molecule 27: 50S Ribosomal Protein L32

Chain 5:



• Molecule 28: 50S Ribosomal Protein L33

Chain 6:



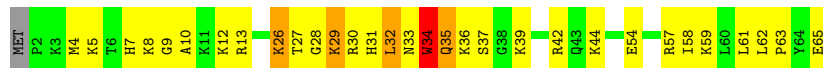
• Molecule 29: 50S Ribosomal Protein L34

Chain 7:



- Molecule 30: 50S Ribosomal Protein L35

Chain 8: 



- Molecule 31: 50S Ribosomal Protein L36

Chain 9: 



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 210.24Å 451.44Å 621.64Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 49.75 – 3.00 49.75 – 3.00 | Depositor EDS |
| % Data completeness (in resolution range) | 97.9 (49.75-3.00) 98.0 (49.75-3.00) | Depositor EDS |
| R_{merge} | 0.27 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.34 (at 3.01Å) | Xtriage |
| Refinement program | PHENIX (phenix.refine: 1.7.2_869) | Depositor |
| R, R_{free} | 0.218 , 0.254 0.457 , 0.459 | Depositor DCC |
| R_{free} test set | 57194 reflections (5.27%) | DCC |
| Wilson B-factor (Å ²) | 68.3 | Xtriage |
| Anisotropy | 0.254 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.25 , 41.0 | EDS |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| L-test for twinning | $\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$ | Xtriage |
| Outliers | 0 of 1142037 reflections | Xtriage |
| F_o, F_c correlation | 0.60 | EDS |
| Total number of atoms | 91067 | wwPDB-VP |
| Average B, all atoms (Å ²) | 68.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.58% 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: ZN, MG

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|------------------|-------------|--------------------|
| | | RMSZ | # $ Z > 5$ | RMSZ | # $ Z > 5$ |
| 1 | A | 1.16 | 149/67893 (0.2%) | 1.60 | 1664/105982 (1.6%) |
| 2 | B | 0.97 | 4/2878 (0.1%) | 1.46 | 37/4490 (0.8%) |
| 3 | D | 0.80 | 2/2186 (0.1%) | 0.91 | 1/2944 (0.0%) |
| 4 | E | 0.75 | 0/1588 | 0.92 | 0/2145 |
| 5 | F | 0.70 | 0/1615 | 0.90 | 2/2188 (0.1%) |
| 6 | G | 0.59 | 0/1393 | 0.71 | 0/1892 |
| 7 | H | 0.60 | 0/1343 | 0.77 | 2/1820 (0.1%) |
| 8 | I | 0.65 | 0/1053 | 0.84 | 1/1442 (0.1%) |
| 9 | N | 0.65 | 0/1139 | 0.87 | 1/1538 (0.1%) |
| 10 | O | 0.70 | 0/933 | 0.86 | 1/1257 (0.1%) |
| 11 | P | 0.67 | 0/1148 | 0.93 | 2/1529 (0.1%) |
| 12 | Q | 0.70 | 0/1143 | 0.86 | 0/1527 |
| 13 | R | 0.74 | 0/982 | 0.93 | 2/1312 (0.2%) |
| 14 | S | 0.66 | 0/875 | 0.84 | 0/1168 |
| 15 | T | 0.66 | 0/1077 | 0.85 | 0/1444 |
| 16 | U | 0.79 | 0/977 | 0.88 | 0/1301 |
| 17 | V | 0.70 | 0/782 | 0.84 | 1/1049 (0.1%) |
| 18 | W | 0.87 | 0/891 | 0.91 | 0/1197 |
| 19 | X | 0.78 | 0/756 | 0.84 | 1/1016 (0.1%) |
| 20 | Y | 0.72 | 1/798 (0.1%) | 0.87 | 1/1073 (0.1%) |
| 21 | Z | 0.63 | 0/1555 | 0.80 | 1/2118 (0.0%) |
| 22 | 0 | 0.73 | 0/602 | 0.81 | 0/804 |
| 23 | 1 | 0.77 | 0/752 | 0.99 | 2/1003 (0.2%) |
| 24 | 2 | 0.71 | 0/590 | 0.83 | 0/781 |
| 25 | 3 | 0.64 | 0/463 | 0.82 | 0/623 |
| 26 | 4 | 0.70 | 0/358 | 0.82 | 1/487 (0.2%) |
| 27 | 5 | 0.75 | 0/469 | 0.95 | 1/634 (0.2%) |
| 28 | 6 | 0.92 | 2/456 (0.4%) | 0.89 | 2/609 (0.3%) |
| 29 | 7 | 0.92 | 0/426 | 1.00 | 0/561 |
| 30 | 8 | 0.73 | 1/516 (0.2%) | 0.92 | 1/679 (0.1%) |
| 31 | 9 | 0.68 | 0/300 | 0.83 | 0/395 |
| All | All | 1.05 | 159/97937 (0.2%) | 1.45 | 1724/147008 (1.2%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 3 | D | 0 | 1 |
| 4 | E | 0 | 1 |
| 5 | F | 0 | 3 |
| 6 | G | 0 | 1 |
| 8 | I | 0 | 1 |
| 9 | N | 0 | 2 |
| 10 | O | 0 | 1 |
| 11 | P | 0 | 2 |
| 14 | S | 0 | 1 |
| 15 | T | 0 | 1 |
| 19 | X | 0 | 1 |
| 20 | Y | 0 | 1 |
| 23 | 1 | 0 | 1 |
| 26 | 4 | 0 | 2 |
| 30 | 8 | 0 | 2 |
| All | All | 0 | 21 |

All (159) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|---------|------|-------|--------|-------------|----------|
| 1 | A | 528 | A | N9-C4 | -14.88 | 1.28 | 1.37 |
| 2 | B | 120 | A | C6-N6 | -11.72 | 1.24 | 1.33 |
| 28 | 6 | 13 | CYS | CB-SG | -10.86 | 1.63 | 1.82 |
| 1 | A | 2296 | U | C4-C5 | 10.51 | 1.53 | 1.43 |
| 1 | A | 2335 | A | C6-N6 | -9.99 | 1.25 | 1.33 |
| 1 | A | 530 | G | C2-N3 | -9.04 | 1.25 | 1.32 |
| 1 | A | 530 | G | N9-C8 | 8.33 | 1.43 | 1.37 |
| 1 | A | 1142(A) | A | N9-C4 | -8.10 | 1.32 | 1.37 |
| 1 | A | 2296 | U | C4-O4 | 8.06 | 1.30 | 1.23 |
| 1 | A | 1762 | A | N9-C4 | 8.02 | 1.42 | 1.37 |
| 1 | A | 2296 | U | N1-C2 | 7.81 | 1.45 | 1.38 |
| 28 | 6 | 40 | CYS | CB-SG | 7.76 | 1.95 | 1.82 |
| 1 | A | 1605 | C | N1-C6 | -7.71 | 1.32 | 1.37 |
| 1 | A | 1817 | G | N7-C5 | -7.31 | 1.34 | 1.39 |
| 1 | A | 194 | G | N7-C5 | -7.24 | 1.34 | 1.39 |
| 1 | A | 530 | G | C8-N7 | 7.21 | 1.35 | 1.30 |
| 1 | A | 2104 | G | N1-C2 | -7.19 | 1.31 | 1.37 |
| 1 | A | 2104 | G | C6-N1 | -7.17 | 1.34 | 1.39 |
| 1 | A | 2031 | A | C5-C6 | -7.14 | 1.34 | 1.41 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|---------|------|--------|-------|-------------|----------|
| 1 | A | 310 | A | N9-C4 | -7.07 | 1.33 | 1.37 |
| 1 | A | 687 | C | N1-C6 | -7.01 | 1.32 | 1.37 |
| 1 | A | 1638 | C | N1-C6 | -6.92 | 1.32 | 1.37 |
| 2 | B | 120 | A | C6-N1 | 6.91 | 1.40 | 1.35 |
| 1 | A | 1204 | A | N9-C4 | -6.89 | 1.33 | 1.37 |
| 1 | A | 1127 | A | N7-C5 | -6.82 | 1.35 | 1.39 |
| 1 | A | 272(A) | U | C1'-N1 | 6.74 | 1.58 | 1.48 |
| 1 | A | 686 | G | N7-C5 | -6.72 | 1.35 | 1.39 |
| 1 | A | 528 | A | N3-C4 | -6.66 | 1.30 | 1.34 |
| 1 | A | 1142(A) | A | N3-C4 | -6.64 | 1.30 | 1.34 |
| 1 | A | 2287 | A | N9-C4 | -6.52 | 1.33 | 1.37 |
| 1 | A | 139(A) | G | N9-C8 | 6.46 | 1.42 | 1.37 |
| 1 | A | 2572 | A | N3-C4 | -6.41 | 1.31 | 1.34 |
| 1 | A | 1289 | C | N1-C6 | -6.40 | 1.33 | 1.37 |
| 1 | A | 2607 | G | N7-C5 | -6.37 | 1.35 | 1.39 |
| 1 | A | 2322 | A | C5-C6 | 6.32 | 1.46 | 1.41 |
| 1 | A | 2617 | C | N1-C6 | -6.24 | 1.33 | 1.37 |
| 1 | A | 2335 | A | C5-C6 | -6.23 | 1.35 | 1.41 |
| 1 | A | 793 | A | N3-C4 | -6.23 | 1.31 | 1.34 |
| 1 | A | 2017 | U | N1-C6 | -6.22 | 1.32 | 1.38 |
| 1 | A | 27 | G | N3-C4 | -6.21 | 1.31 | 1.35 |
| 1 | A | 2821 | A | C5-C6 | -6.17 | 1.35 | 1.41 |
| 1 | A | 1785 | A | N7-C5 | -6.16 | 1.35 | 1.39 |
| 1 | A | 1660 | C | N1-C6 | -6.13 | 1.33 | 1.37 |
| 1 | A | 1635 | G | N7-C5 | -6.12 | 1.35 | 1.39 |
| 1 | A | 205 | G | N9-C4 | 6.12 | 1.42 | 1.38 |
| 1 | A | 697 | C | N1-C6 | -6.07 | 1.33 | 1.37 |
| 1 | A | 2252 | G | C5-C4 | -6.06 | 1.34 | 1.38 |
| 1 | A | 2430 | A | N9-C4 | -6.04 | 1.34 | 1.37 |
| 1 | A | 2625 | G | N3-C4 | -6.02 | 1.31 | 1.35 |
| 1 | A | 2430 | A | N3-C4 | -6.01 | 1.31 | 1.34 |
| 1 | A | 506 | G | N9-C4 | -6.01 | 1.33 | 1.38 |
| 1 | A | 2070 | G | N9-C8 | -6.01 | 1.33 | 1.37 |
| 1 | A | 1614 | A | N9-C4 | -5.98 | 1.34 | 1.37 |
| 1 | A | 1571 | A | N9-C4 | -5.96 | 1.34 | 1.37 |
| 1 | A | 462 | C | N3-C4 | -5.95 | 1.29 | 1.33 |
| 1 | A | 1569 | A | C6-N1 | -5.92 | 1.31 | 1.35 |
| 1 | A | 1698 | A | C5-C4 | 5.90 | 1.42 | 1.38 |
| 1 | A | 933 | A | N3-C4 | -5.89 | 1.31 | 1.34 |
| 1 | A | 2288 | A | N9-C4 | 5.87 | 1.41 | 1.37 |
| 20 | Y | 79 | CYS | CB-SG | -5.86 | 1.72 | 1.81 |
| 1 | A | 990 | A | N3-C4 | -5.85 | 1.31 | 1.34 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1 | A | 2503 | A | N7-C5 | -5.85 | 1.35 | 1.39 |
| 1 | A | 1786 | A | N9-C4 | -5.83 | 1.34 | 1.37 |
| 1 | A | 1535 | A | N9-C4 | 5.80 | 1.41 | 1.37 |
| 1 | A | 1779 | U | C2-N3 | -5.80 | 1.33 | 1.37 |
| 1 | A | 330 | A | N9-C4 | -5.79 | 1.34 | 1.37 |
| 1 | A | 788 | A | N7-C5 | -5.77 | 1.35 | 1.39 |
| 3 | D | 237 | GLU | CD-OE1 | 5.76 | 1.31 | 1.25 |
| 1 | A | 777 | A | N7-C5 | -5.76 | 1.35 | 1.39 |
| 1 | A | 463 | G | C6-N1 | -5.76 | 1.35 | 1.39 |
| 1 | A | 1325 | G | C2-N3 | 5.74 | 1.37 | 1.32 |
| 1 | A | 2512 | C | C4-C5 | 5.74 | 1.47 | 1.43 |
| 1 | A | 191 | A | N7-C5 | -5.74 | 1.35 | 1.39 |
| 1 | A | 463 | G | N1-C2 | -5.72 | 1.33 | 1.37 |
| 1 | A | 2016 | U | C2-O2 | 5.70 | 1.27 | 1.22 |
| 1 | A | 1829 | A | N9-C4 | -5.70 | 1.34 | 1.37 |
| 3 | D | 28 | GLU | CG-CD | 5.68 | 1.60 | 1.51 |
| 1 | A | 2513 | G | C8-N7 | 5.67 | 1.34 | 1.30 |
| 1 | A | 2287 | A | C5-C6 | -5.67 | 1.35 | 1.41 |
| 1 | A | 2689 | U | C3'-O3' | 5.67 | 1.50 | 1.42 |
| 1 | A | 2335 | A | N9-C4 | -5.66 | 1.34 | 1.37 |
| 1 | A | 506 | G | N3-C4 | -5.65 | 1.31 | 1.35 |
| 1 | A | 741 | G | N1-C2 | -5.60 | 1.33 | 1.37 |
| 1 | A | 1308 | A | N7-C5 | -5.60 | 1.35 | 1.39 |
| 1 | A | 805 | G | N9-C8 | -5.58 | 1.33 | 1.37 |
| 1 | A | 1854 | A | N7-C5 | -5.58 | 1.35 | 1.39 |
| 1 | A | 832 | G | C6-N1 | -5.57 | 1.35 | 1.39 |
| 1 | A | 2587 | A | N7-C5 | -5.57 | 1.35 | 1.39 |
| 1 | A | 2597 | G | N7-C5 | -5.54 | 1.35 | 1.39 |
| 1 | A | 1613 | G | N7-C5 | -5.54 | 1.35 | 1.39 |
| 1 | A | 2084 | C | N1-C6 | -5.53 | 1.33 | 1.37 |
| 1 | A | 1665 | A | N3-C4 | -5.50 | 1.31 | 1.34 |
| 1 | A | 2017 | U | N3-C4 | -5.50 | 1.33 | 1.38 |
| 2 | B | 54 | G | N9-C8 | 5.50 | 1.41 | 1.37 |
| 1 | A | 2851 | A | N9-C4 | -5.49 | 1.34 | 1.37 |
| 1 | A | 1296 | G | N7-C5 | -5.49 | 1.35 | 1.39 |
| 1 | A | 70 | G | C6-N1 | -5.49 | 1.35 | 1.39 |
| 1 | A | 1308 | A | N9-C4 | -5.49 | 1.34 | 1.37 |
| 1 | A | 463 | G | N7-C5 | -5.48 | 1.35 | 1.39 |
| 1 | A | 1779 | U | N3-C4 | -5.46 | 1.33 | 1.38 |
| 1 | A | 1605 | C | N3-C4 | -5.45 | 1.30 | 1.33 |
| 1 | A | 2883 | A | N7-C5 | -5.44 | 1.35 | 1.39 |
| 1 | A | 2790 | A | N9-C4 | 5.44 | 1.41 | 1.37 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1 | A | 2071 | A | P-O5' | -5.41 | 1.54 | 1.59 |
| 1 | A | 118 | A | N9-C4 | -5.41 | 1.34 | 1.37 |
| 1 | A | 471 | A | N3-C4 | -5.40 | 1.31 | 1.34 |
| 1 | A | 2296 | U | C5-C6 | 5.39 | 1.39 | 1.34 |
| 1 | A | 775 | G | C6-N1 | -5.38 | 1.35 | 1.39 |
| 1 | A | 298 | G | N7-C5 | -5.38 | 1.36 | 1.39 |
| 1 | A | 2335 | A | C5-C4 | -5.38 | 1.34 | 1.38 |
| 1 | A | 1612 | C | N1-C6 | -5.36 | 1.33 | 1.37 |
| 1 | A | 671 | C | N1-C6 | -5.35 | 1.33 | 1.37 |
| 1 | A | 2689 | U | C2-N3 | -5.35 | 1.34 | 1.37 |
| 1 | A | 959 | A | N9-C4 | 5.35 | 1.41 | 1.37 |
| 1 | A | 532 | A | P-O5' | -5.34 | 1.54 | 1.59 |
| 1 | A | 2322 | A | N9-C4 | 5.33 | 1.41 | 1.37 |
| 1 | A | 2823 | A | N7-C5 | -5.32 | 1.36 | 1.39 |
| 1 | A | 780 | G | N9-C8 | -5.30 | 1.34 | 1.37 |
| 1 | A | 2177 | C | N1-C6 | 5.30 | 1.40 | 1.37 |
| 1 | A | 2053 | G | N7-C5 | -5.28 | 1.36 | 1.39 |
| 1 | A | 1284 | A | N3-C4 | 5.27 | 1.38 | 1.34 |
| 1 | A | 1209 | G | C6-N1 | -5.26 | 1.35 | 1.39 |
| 1 | A | 2322 | A | C6-N1 | 5.25 | 1.39 | 1.35 |
| 1 | A | 529 | A | N9-C4 | -5.24 | 1.34 | 1.37 |
| 1 | A | 761 | A | P-O5' | -5.23 | 1.54 | 1.59 |
| 1 | A | 2826 | A | C6-N1 | -5.23 | 1.31 | 1.35 |
| 1 | A | 450 | G | N7-C5 | -5.23 | 1.36 | 1.39 |
| 1 | A | 1780 | A | C6-N1 | -5.22 | 1.31 | 1.35 |
| 1 | A | 1210 | A | N9-C4 | -5.21 | 1.34 | 1.37 |
| 1 | A | 784 | A | N9-C8 | -5.21 | 1.33 | 1.37 |
| 1 | A | 677 | A | N7-C5 | -5.21 | 1.36 | 1.39 |
| 1 | A | 1617 | C | N1-C6 | -5.20 | 1.34 | 1.37 |
| 1 | A | 2502 | G | C2-N3 | 5.20 | 1.36 | 1.32 |
| 1 | A | 249 | C | N3-C4 | -5.19 | 1.30 | 1.33 |
| 1 | A | 783 | A | N3-C4 | -5.18 | 1.31 | 1.34 |
| 1 | A | 2444 | G | P-O5' | -5.17 | 1.54 | 1.59 |
| 30 | 8 | 34 | TRP | CB-CG | -5.13 | 1.41 | 1.50 |
| 1 | A | 513 | A | C5-C4 | -5.12 | 1.35 | 1.38 |
| 1 | A | 933 | A | N9-C8 | 5.12 | 1.41 | 1.37 |
| 1 | A | 1823 | G | C2-N3 | -5.12 | 1.28 | 1.32 |
| 1 | A | 2286 | A | C5-C4 | 5.12 | 1.42 | 1.38 |
| 2 | B | 53 | A | N9-C4 | 5.11 | 1.41 | 1.37 |
| 1 | A | 780 | G | C5-C4 | -5.10 | 1.34 | 1.38 |
| 1 | A | 1788 | C | N1-C6 | -5.10 | 1.34 | 1.37 |
| 1 | A | 1954 | G | N3-C4 | -5.10 | 1.31 | 1.35 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1 | A | 2607 | G | N9-C8 | -5.10 | 1.34 | 1.37 |
| 1 | A | 1309 | G | C8-N7 | -5.08 | 1.27 | 1.30 |
| 1 | A | 675 | A | C6-N6 | -5.08 | 1.29 | 1.33 |
| 1 | A | 1191 | G | N9-C8 | -5.08 | 1.34 | 1.37 |
| 1 | A | 1660 | C | N3-C4 | -5.08 | 1.30 | 1.33 |
| 1 | A | 1383 | C | C2-N3 | 5.06 | 1.39 | 1.35 |
| 1 | A | 746 | A | N9-C4 | -5.05 | 1.34 | 1.37 |
| 1 | A | 687 | C | C4-C5 | -5.05 | 1.39 | 1.43 |
| 1 | A | 1899 | G | N7-C5 | -5.05 | 1.36 | 1.39 |
| 1 | A | 687 | C | N3-C4 | -5.04 | 1.30 | 1.33 |
| 1 | A | 523 | C | N1-C6 | -5.04 | 1.34 | 1.37 |
| 1 | A | 195 | A | N7-C5 | -5.03 | 1.36 | 1.39 |
| 1 | A | 472 | A | N3-C4 | -5.02 | 1.31 | 1.34 |
| 1 | A | 573 | G | N3-C4 | -5.02 | 1.31 | 1.35 |

All (1724) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 1 | A | 1779 | U | C5-C6-N1 | -22.12 | 111.64 | 122.70 |
| 1 | A | 2296 | U | C5-C6-N1 | -19.00 | 113.20 | 122.70 |
| 1 | A | 2104 | G | N3-C2-N2 | 17.67 | 132.27 | 119.90 |
| 1 | A | 2296 | U | N1-C2-N3 | 17.55 | 125.43 | 114.90 |
| 1 | A | 2296 | U | C2-N3-C4 | -17.29 | 116.62 | 127.00 |
| 1 | A | 130 | C | C6-N1-C2 | 16.32 | 126.83 | 120.30 |
| 1 | A | 2296 | U | C2-N1-C1' | -15.87 | 98.66 | 117.70 |
| 1 | A | 528 | A | C2-N3-C4 | -15.78 | 102.71 | 110.60 |
| 1 | A | 528 | A | N3-C4-N9 | -15.63 | 114.90 | 127.40 |
| 1 | A | 528 | A | N3-C4-C5 | 15.39 | 137.57 | 126.80 |
| 1 | A | 530 | G | N3-C2-N2 | -15.35 | 109.16 | 119.90 |
| 1 | A | 2296 | U | N3-C4-O4 | -14.77 | 109.06 | 119.40 |
| 1 | A | 2296 | U | C5-C4-O4 | 14.09 | 134.35 | 125.90 |
| 1 | A | 2104 | G | N1-C2-N2 | -13.86 | 103.73 | 116.20 |
| 1 | A | 2296 | U | N3-C2-O2 | -13.73 | 112.59 | 122.20 |
| 1 | A | 2322 | A | C6-N1-C2 | -13.72 | 110.37 | 118.60 |
| 1 | A | 2296 | U | C6-N1-C1' | 13.49 | 140.08 | 121.20 |
| 1 | A | 2335 | A | C5-C6-N1 | 13.43 | 124.42 | 117.70 |
| 1 | A | 2104 | G | C5-C6-O6 | 13.38 | 136.62 | 128.60 |
| 1 | A | 2185 | C | N1-C2-O2 | 13.12 | 126.77 | 118.90 |
| 1 | A | 2104 | G | N1-C6-O6 | -13.10 | 112.04 | 119.90 |
| 1 | A | 1779 | U | C2-N3-C4 | -13.07 | 119.16 | 127.00 |
| 2 | B | 120 | A | C5-C6-N1 | -13.03 | 111.18 | 117.70 |
| 1 | A | 330 | A | C2-N3-C4 | -12.73 | 104.23 | 110.60 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|--------|-------------|----------|
| 1 | A | 1107 | G | C4-N9-C1' | 12.60 | 142.88 | 126.50 |
| 1 | A | 2322 | A | N1-C6-N6 | -12.41 | 111.15 | 118.60 |
| 1 | A | 1142(A) | A | C2-N3-C4 | -12.25 | 104.48 | 110.60 |
| 1 | A | 2296 | U | C4-C5-C6 | 12.06 | 126.94 | 119.70 |
| 1 | A | 1107 | G | C8-N9-C1' | -12.05 | 111.34 | 127.00 |
| 1 | A | 409 | C | C6-N1-C2 | 12.04 | 125.12 | 120.30 |
| 1 | A | 148 | C | C6-N1-C2 | 11.80 | 125.02 | 120.30 |
| 1 | A | 1779 | U | N3-C4-O4 | -11.68 | 111.22 | 119.40 |
| 1 | A | 141 | A | N7-C8-N9 | 11.61 | 119.61 | 113.80 |
| 2 | B | 120 | A | C6-N1-C2 | 11.56 | 125.54 | 118.60 |
| 1 | A | 1108 | U | N3-C2-O2 | -11.54 | 114.12 | 122.20 |
| 1 | A | 1359 | A | N1-C6-N6 | -11.51 | 111.69 | 118.60 |
| 1 | A | 1210 | A | C5-N7-C8 | -11.47 | 98.17 | 103.90 |
| 1 | A | 2322 | A | C5-C6-N1 | 11.41 | 123.41 | 117.70 |
| 1 | A | 530 | G | N1-C2-N2 | 11.37 | 126.44 | 116.20 |
| 1 | A | 777 | A | N9-C4-C5 | 11.34 | 110.34 | 105.80 |
| 1 | A | 530 | G | N3-C4-N9 | -11.28 | 119.23 | 126.00 |
| 1 | A | 141 | A | N1-C6-N6 | 11.26 | 125.35 | 118.60 |
| 1 | A | 1204 | A | N1-C6-N6 | 11.21 | 125.33 | 118.60 |
| 1 | A | 933 | A | C5-N7-C8 | -11.19 | 98.30 | 103.90 |
| 1 | A | 1779 | U | N1-C2-N3 | 11.15 | 121.59 | 114.90 |
| 1 | A | 1698 | A | N1-C6-N6 | 11.11 | 125.27 | 118.60 |
| 1 | A | 1698 | A | C5-N7-C8 | -11.00 | 98.40 | 103.90 |
| 1 | A | 1107 | G | C6-C5-N7 | -10.87 | 123.88 | 130.40 |
| 1 | A | 2253 | G | N1-C6-O6 | 10.78 | 126.37 | 119.90 |
| 1 | A | 1698 | A | C2-N3-C4 | -10.73 | 105.24 | 110.60 |
| 1 | A | 2322 | A | N9-C4-C5 | 10.64 | 110.05 | 105.80 |
| 1 | A | 839 | U | C5-C4-O4 | 10.61 | 132.27 | 125.90 |
| 1 | A | 530 | G | N9-C4-C5 | 10.55 | 109.62 | 105.40 |
| 1 | A | 1779 | U | C4-C5-C6 | 10.54 | 126.03 | 119.70 |
| 2 | B | 120 | A | N1-C2-N3 | -10.47 | 124.06 | 129.30 |
| 1 | A | 2287 | A | C2-N3-C4 | -10.45 | 105.38 | 110.60 |
| 1 | A | 27 | G | N3-C2-N2 | -10.43 | 112.60 | 119.90 |
| 1 | A | 456 | C | C6-N1-C2 | 10.39 | 124.46 | 120.30 |
| 1 | A | 1204 | A | C5-N7-C8 | -10.24 | 98.78 | 103.90 |
| 1 | A | 141 | A | C5-N7-C8 | -10.20 | 98.80 | 103.90 |
| 1 | A | 528 | A | C5-C6-N1 | -10.20 | 112.60 | 117.70 |
| 1 | A | 530 | G | C8-N9-C4 | -10.19 | 102.32 | 106.40 |
| 1 | A | 1762 | A | C8-N9-C4 | -10.14 | 101.74 | 105.80 |
| 1 | A | 1779 | U | C5-C4-O4 | 10.06 | 131.94 | 125.90 |
| 1 | A | 1328 | G | C5-C6-O6 | -10.03 | 122.58 | 128.60 |
| 1 | A | 933 | A | N7-C8-N9 | 10.01 | 118.81 | 113.80 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 1 | A | 208 | C | C6-N1-C2 | 10.00 | 124.30 | 120.30 |
| 1 | A | 1107 | G | N3-C4-N9 | 9.98 | 131.99 | 126.00 |
| 1 | A | 652(T) | C | C2-N3-C4 | 9.91 | 124.86 | 119.90 |
| 1 | A | 1204 | A | C6-C5-N7 | -9.91 | 125.36 | 132.30 |
| 1 | A | 1107 | G | N1-C6-O6 | 9.85 | 125.81 | 119.90 |
| 1 | A | 1779 | U | C2-N1-C1' | -9.85 | 105.88 | 117.70 |
| 1 | A | 1698 | A | C4-C5-N7 | 9.85 | 115.63 | 110.70 |
| 1 | A | 210 | C | C6-N1-C2 | 9.83 | 124.23 | 120.30 |
| 1 | A | 1108 | U | N1-C2-O2 | 9.74 | 129.62 | 122.80 |
| 1 | A | 2286 | A | C6-C5-N7 | -9.73 | 125.49 | 132.30 |
| 1 | A | 777 | A | N1-C6-N6 | -9.68 | 112.79 | 118.60 |
| 1 | A | 1210 | A | N7-C8-N9 | 9.66 | 118.63 | 113.80 |
| 1 | A | 2067 | G | C8-N9-C4 | -9.65 | 102.54 | 106.40 |
| 2 | B | 115 | G | C8-N9-C4 | 9.64 | 110.26 | 106.40 |
| 1 | A | 2286 | A | N7-C8-N9 | 9.63 | 118.61 | 113.80 |
| 1 | A | 1997 | G | N1-C6-O6 | -9.49 | 114.21 | 119.90 |
| 1 | A | 1109 | C | C4-C5-C6 | 9.46 | 122.13 | 117.40 |
| 1 | A | 802 | A | C8-N9-C4 | -9.38 | 102.05 | 105.80 |
| 1 | A | 139(A) | G | N7-C8-N9 | 9.36 | 117.78 | 113.10 |
| 1 | A | 141 | A | C8-N9-C4 | -9.35 | 102.06 | 105.80 |
| 1 | A | 2185 | C | C2-N3-C4 | 9.35 | 124.57 | 119.90 |
| 1 | A | 2446 | G | N3-C2-N2 | 9.31 | 126.42 | 119.90 |
| 1 | A | 528 | A | C6-N1-C2 | 9.27 | 124.16 | 118.60 |
| 1 | A | 1210 | A | N1-C6-N6 | 9.26 | 124.16 | 118.60 |
| 1 | A | 139(A) | G | C4-C5-N7 | 9.17 | 114.47 | 110.80 |
| 1 | A | 1107 | G | C5-C6-O6 | -9.16 | 123.11 | 128.60 |
| 1 | A | 645 | C | N1-C2-O2 | 9.14 | 124.38 | 118.90 |
| 2 | B | 30 | C | C6-N1-C2 | -9.11 | 116.66 | 120.30 |
| 1 | A | 2322 | A | C2-N3-C4 | 9.11 | 115.16 | 110.60 |
| 1 | A | 1333 | C | N3-C4-C5 | 9.05 | 125.52 | 121.90 |
| 1 | A | 1698 | A | C6-C5-N7 | -9.04 | 125.97 | 132.30 |
| 1 | A | 2286 | A | N1-C6-N6 | 9.04 | 124.03 | 118.60 |
| 1 | A | 139(A) | G | C5-N7-C8 | -9.04 | 99.78 | 104.30 |
| 1 | A | 2283 | C | N1-C2-O2 | -9.04 | 113.47 | 118.90 |
| 1 | A | 2473 | U | C2-N1-C1' | 9.03 | 128.54 | 117.70 |
| 1 | A | 1153 | C | N1-C2-O2 | -9.03 | 113.48 | 118.90 |
| 1 | A | 2741 | A | C8-N9-C4 | 9.02 | 109.41 | 105.80 |
| 1 | A | 2286 | A | C5-N7-C8 | -8.98 | 99.41 | 103.90 |
| 1 | A | 1784 | A | C8-N9-C4 | 8.93 | 109.37 | 105.80 |
| 1 | A | 1661 | G | C8-N9-C4 | 8.92 | 109.97 | 106.40 |
| 1 | A | 1204 | A | C4-C5-N7 | 8.91 | 115.16 | 110.70 |
| 1 | A | 1248 | G | C8-N9-C4 | 8.90 | 109.96 | 106.40 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | A | 1107 | G | C4-C5-N7 | 8.88 | 114.35 | 110.80 |
| 1 | A | 195 | A | N1-C6-N6 | 8.88 | 123.93 | 118.60 |
| 1 | A | 2440 | C | C5-C6-N1 | -8.86 | 116.57 | 121.00 |
| 1 | A | 1204 | A | C2-N3-C4 | -8.86 | 106.17 | 110.60 |
| 1 | A | 2335 | A | C5-C6-N6 | -8.82 | 116.64 | 123.70 |
| 1 | A | 141 | A | C6-C5-N7 | -8.78 | 126.16 | 132.30 |
| 1 | A | 2182 | G | C5-C6-O6 | 8.73 | 133.84 | 128.60 |
| 1 | A | 2440 | C | N3-C4-N4 | -8.73 | 111.89 | 118.00 |
| 1 | A | 2346 | A | N1-C6-N6 | -8.72 | 113.37 | 118.60 |
| 1 | A | 1210 | A | C4-C5-N7 | 8.71 | 115.06 | 110.70 |
| 1 | A | 847 | U | C5-C4-O4 | 8.70 | 131.12 | 125.90 |
| 1 | A | 2689 | U | N3-C4-O4 | -8.68 | 113.32 | 119.40 |
| 1 | A | 2286 | A | C2-N3-C4 | -8.68 | 106.26 | 110.60 |
| 1 | A | 130 | C | C5-C6-N1 | -8.66 | 116.67 | 121.00 |
| 11 | P | 26 | GLY | N-CA-C | -8.62 | 91.55 | 113.10 |
| 1 | A | 1210 | A | C6-C5-N7 | -8.61 | 126.28 | 132.30 |
| 1 | A | 2322 | A | C4-C5-N7 | -8.60 | 106.40 | 110.70 |
| 1 | A | 12 | U | N3-C2-O2 | -8.57 | 116.20 | 122.20 |
| 1 | A | 1123 | C | C6-N1-C2 | 8.56 | 123.72 | 120.30 |
| 1 | A | 2568 | C | C6-N1-C2 | 8.54 | 123.72 | 120.30 |
| 1 | A | 1180 | C | C6-N1-C2 | 8.53 | 123.71 | 120.30 |
| 1 | A | 2828 | C | N1-C2-O2 | -8.53 | 113.78 | 118.90 |
| 1 | A | 1829 | A | N1-C6-N6 | -8.52 | 113.49 | 118.60 |
| 1 | A | 2463 | C | C6-N1-C2 | 8.51 | 123.70 | 120.30 |
| 23 | 1 | 21 | ARG | NE-CZ-NH1 | 8.48 | 124.54 | 120.30 |
| 1 | A | 2441 | C | C5-C6-N1 | -8.47 | 116.77 | 121.00 |
| 1 | A | 2312 | U | N3-C2-O2 | -8.47 | 116.27 | 122.20 |
| 1 | A | 2017 | U | C5-C6-N1 | -8.44 | 118.48 | 122.70 |
| 1 | A | 1558 | A | C2-N3-C4 | -8.43 | 106.38 | 110.60 |
| 1 | A | 752 | A | C8-N9-C4 | -8.42 | 102.43 | 105.80 |
| 1 | A | 2446 | G | N1-C2-N2 | -8.41 | 108.63 | 116.20 |
| 1 | A | 1125 | G | N1-C6-O6 | 8.41 | 124.95 | 119.90 |
| 1 | A | 1826 | G | C5-N7-C8 | 8.41 | 108.50 | 104.30 |
| 1 | A | 1304 | C | N3-C4-C5 | 8.40 | 125.26 | 121.90 |
| 1 | A | 2440 | C | C5-C4-N4 | 8.40 | 126.08 | 120.20 |
| 1 | A | 1698 | A | N7-C8-N9 | 8.39 | 118.00 | 113.80 |
| 2 | B | 114 | C | C6-N1-C2 | 8.35 | 123.64 | 120.30 |
| 1 | A | 1605 | C | C4-C5-C6 | 8.34 | 121.57 | 117.40 |
| 1 | A | 860 | U | N3-C2-O2 | -8.33 | 116.37 | 122.20 |
| 1 | A | 2007 | C | C6-N1-C2 | -8.32 | 116.97 | 120.30 |
| 1 | A | 2473 | U | N3-C2-O2 | -8.31 | 116.39 | 122.20 |
| 1 | A | 1382 | G | N1-C6-O6 | 8.29 | 124.87 | 119.90 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 28 | 6 | 40 | CYS | CA-CB-SG | 8.25 | 128.84 | 114.00 |
| 1 | A | 777 | A | C4-C5-N7 | -8.23 | 106.58 | 110.70 |
| 1 | A | 2346 | A | N9-C4-C5 | 8.23 | 109.09 | 105.80 |
| 1 | A | 2617 | C | N3-C4-C5 | 8.22 | 125.19 | 121.90 |
| 1 | A | 1022 | G | N3-C4-N9 | -8.22 | 121.07 | 126.00 |
| 1 | A | 729 | G | N3-C2-N2 | -8.22 | 114.15 | 119.90 |
| 2 | B | 49 | C | N1-C2-O2 | -8.21 | 113.98 | 118.90 |
| 1 | A | 1142(A) | A | N3-C4-N9 | -8.20 | 120.84 | 127.40 |
| 1 | A | 2473 | U | N1-C2-O2 | 8.19 | 128.53 | 122.80 |
| 1 | A | 1210 | A | C2-N3-C4 | -8.16 | 106.52 | 110.60 |
| 1 | A | 933 | A | C8-N9-C4 | -8.16 | 102.54 | 105.80 |
| 1 | A | 221 | A | C8-N9-C4 | -8.15 | 102.54 | 105.80 |
| 1 | A | 2191 | G | C5-C6-O6 | -8.13 | 123.72 | 128.60 |
| 1 | A | 488 | G | C5-N7-C8 | 8.11 | 108.35 | 104.30 |
| 1 | A | 130 | C | N3-C4-C5 | 8.09 | 125.14 | 121.90 |
| 1 | A | 2441 | C | C6-N1-C2 | 8.08 | 123.53 | 120.30 |
| 1 | A | 694 | U | N1-C2-O2 | 8.07 | 128.45 | 122.80 |
| 1 | A | 2742 | C | C5-C6-N1 | -8.06 | 116.97 | 121.00 |
| 1 | A | 1826 | G | N7-C8-N9 | -8.05 | 109.07 | 113.10 |
| 1 | A | 2674 | G | C8-N9-C4 | -8.05 | 103.18 | 106.40 |
| 1 | A | 2791 | C | N1-C2-O2 | 8.04 | 123.72 | 118.90 |
| 1 | A | 444 | C | N3-C4-C5 | 8.01 | 125.11 | 121.90 |
| 1 | A | 1017 | G | N1-C6-O6 | 8.01 | 124.71 | 119.90 |
| 1 | A | 2501 | C | N3-C4-C5 | 8.01 | 125.10 | 121.90 |
| 1 | A | 2182 | G | C6-N1-C2 | 7.99 | 129.89 | 125.10 |
| 1 | A | 236 | C | C6-N1-C2 | 7.96 | 123.49 | 120.30 |
| 2 | B | 104 | U | C5-C6-N1 | -7.94 | 118.73 | 122.70 |
| 1 | A | 1128 | A | C8-N9-C4 | 7.92 | 108.97 | 105.80 |
| 1 | A | 1493 | C | C2-N1-C1' | 7.91 | 127.50 | 118.80 |
| 1 | A | 949 | C | N3-C4-C5 | 7.90 | 125.06 | 121.90 |
| 1 | A | 1107 | G | N9-C4-C5 | -7.89 | 102.24 | 105.40 |
| 1 | A | 1108 | U | C2-N1-C1' | 7.88 | 127.15 | 117.70 |
| 1 | A | 1820 | U | C6-N1-C2 | 7.86 | 125.72 | 121.00 |
| 1 | A | 139(A) | G | C5-C6-O6 | -7.86 | 123.88 | 128.60 |
| 1 | A | 775 | G | N1-C6-O6 | -7.86 | 115.19 | 119.90 |
| 1 | A | 194 | G | C8-N9-C4 | -7.86 | 103.26 | 106.40 |
| 1 | A | 2424 | C | N1-C2-O2 | -7.85 | 114.19 | 118.90 |
| 1 | A | 772 | C | N3-C2-O2 | 7.85 | 127.39 | 121.90 |
| 1 | A | 2446 | G | N1-C6-O6 | -7.85 | 115.19 | 119.90 |
| 1 | A | 2440 | C | C6-N1-C2 | 7.84 | 123.44 | 120.30 |
| 1 | A | 614 | U | C5-C4-O4 | 7.83 | 130.60 | 125.90 |
| 1 | A | 2040 | C | N3-C4-N4 | 7.83 | 123.48 | 118.00 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 1 | A | 940 | G | C8-N9-C4 | -7.82 | 103.27 | 106.40 |
| 1 | A | 2500 | U | N3-C4-C5 | 7.81 | 119.29 | 114.60 |
| 1 | A | 768 | G | N3-C4-C5 | -7.81 | 124.70 | 128.60 |
| 1 | A | 2332 | U | N3-C2-O2 | -7.80 | 116.74 | 122.20 |
| 1 | A | 2036 | C | N1-C2-O2 | -7.80 | 114.22 | 118.90 |
| 1 | A | 2103 | C | C2-N3-C4 | 7.80 | 123.80 | 119.90 |
| 1 | A | 2500 | U | N3-C4-O4 | -7.79 | 113.94 | 119.40 |
| 1 | A | 856 | C | C6-N1-C2 | -7.76 | 117.20 | 120.30 |
| 1 | A | 1997 | G | C5-C6-O6 | 7.75 | 133.25 | 128.60 |
| 1 | A | 2791 | C | C2-N1-C1' | 7.75 | 127.32 | 118.80 |
| 1 | A | 1142(A) | A | N1-C2-N3 | 7.75 | 133.17 | 129.30 |
| 1 | A | 128 | C | N3-C4-C5 | 7.74 | 125.00 | 121.90 |
| 1 | A | 781 | A | C8-N9-C4 | 7.74 | 108.89 | 105.80 |
| 1 | A | 1142(A) | A | C5-N7-C8 | -7.72 | 100.04 | 103.90 |
| 1 | A | 2689 | U | C5-C4-O4 | 7.72 | 130.53 | 125.90 |
| 1 | A | 27 | G | N3-C4-N9 | -7.71 | 121.37 | 126.00 |
| 1 | A | 1651 | G | C5-C6-O6 | -7.71 | 123.97 | 128.60 |
| 1 | A | 1204 | A | N7-C8-N9 | 7.69 | 117.65 | 113.80 |
| 1 | A | 2821 | A | N1-C6-N6 | 7.69 | 123.21 | 118.60 |
| 1 | A | 2375 | G | C8-N9-C4 | 7.67 | 109.47 | 106.40 |
| 1 | A | 2463 | C | N1-C2-O2 | -7.65 | 114.31 | 118.90 |
| 1 | A | 194 | G | C6-N1-C2 | -7.64 | 120.52 | 125.10 |
| 1 | A | 784 | A | C4-C5-N7 | -7.62 | 106.89 | 110.70 |
| 1 | A | 2185 | C | N3-C2-O2 | -7.62 | 116.57 | 121.90 |
| 1 | A | 978 | G | C8-N9-C4 | 7.61 | 109.44 | 106.40 |
| 1 | A | 1047 | G | N3-C4-N9 | 7.61 | 130.57 | 126.00 |
| 1 | A | 394 | A | C8-N9-C4 | 7.60 | 108.84 | 105.80 |
| 1 | A | 847 | U | C5-C6-N1 | -7.60 | 118.90 | 122.70 |
| 1 | A | 1497 | U | C5-C4-O4 | 7.60 | 130.46 | 125.90 |
| 1 | A | 2823 | A | N1-C6-N6 | 7.60 | 123.16 | 118.60 |
| 1 | A | 777 | A | C8-N9-C4 | -7.59 | 102.76 | 105.80 |
| 1 | A | 2070 | G | C5-N7-C8 | 7.59 | 108.10 | 104.30 |
| 1 | A | 1786 | A | N1-C6-N6 | -7.59 | 114.05 | 118.60 |
| 1 | A | 2591 | C | C2-N3-C4 | -7.59 | 116.11 | 119.90 |
| 1 | A | 1497 | U | N3-C4-O4 | -7.58 | 114.09 | 119.40 |
| 1 | A | 154(A) | C | N1-C2-O2 | 7.58 | 123.45 | 118.90 |
| 1 | A | 2423 | U | C5-C6-N1 | -7.58 | 118.91 | 122.70 |
| 1 | A | 1997 | G | C4-C5-N7 | -7.57 | 107.77 | 110.80 |
| 1 | A | 672 | C | C5-C6-N1 | -7.57 | 117.22 | 121.00 |
| 1 | A | 2498 | C | C5-C6-N1 | -7.56 | 117.22 | 121.00 |
| 1 | A | 2022 | U | N1-C2-O2 | -7.56 | 117.51 | 122.80 |
| 1 | A | 267 | C | C6-N1-C2 | 7.55 | 123.32 | 120.30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 1 | A | 1047 | G | N3-C4-C5 | -7.55 | 124.83 | 128.60 |
| 1 | A | 2755 | C | C5-C6-N1 | 7.54 | 124.77 | 121.00 |
| 1 | A | 933 | A | C4-C5-N7 | 7.54 | 114.47 | 110.70 |
| 1 | A | 729 | G | N1-C2-N2 | 7.53 | 122.98 | 116.20 |
| 1 | A | 1382 | G | C5-C6-O6 | -7.53 | 124.08 | 128.60 |
| 1 | A | 530 | G | C8-N9-C1' | 7.52 | 136.78 | 127.00 |
| 1 | A | 686 | G | C6-C5-N7 | -7.52 | 125.89 | 130.40 |
| 1 | A | 1605 | C | C6-N1-C2 | -7.51 | 117.30 | 120.30 |
| 1 | A | 2512 | C | C2-N3-C4 | -7.50 | 116.15 | 119.90 |
| 1 | A | 139(A) | G | C8-N9-C4 | -7.48 | 103.41 | 106.40 |
| 1 | A | 530 | G | C4-C5-C6 | -7.48 | 114.31 | 118.80 |
| 1 | A | 1049 | C | C6-N1-C2 | -7.47 | 117.31 | 120.30 |
| 1 | A | 2742 | C | C6-N1-C2 | 7.47 | 123.29 | 120.30 |
| 1 | A | 2283 | C | N3-C2-O2 | 7.46 | 127.12 | 121.90 |
| 1 | A | 1827 | C | N3-C2-O2 | -7.46 | 116.68 | 121.90 |
| 1 | A | 1977 | A | C8-N9-C4 | 7.46 | 108.78 | 105.80 |
| 1 | A | 2407 | G | C4-N9-C1' | 7.46 | 136.19 | 126.50 |
| 1 | A | 2031 | A | N1-C6-N6 | 7.44 | 123.06 | 118.60 |
| 1 | A | 34 | C | C6-N1-C2 | -7.43 | 117.33 | 120.30 |
| 1 | A | 2069 | G | N7-C8-N9 | -7.43 | 109.39 | 113.10 |
| 1 | A | 129 | C | C6-N1-C2 | 7.43 | 123.27 | 120.30 |
| 1 | A | 2741 | A | N7-C8-N9 | -7.42 | 110.09 | 113.80 |
| 1 | A | 468 | G | C8-N9-C4 | 7.42 | 109.37 | 106.40 |
| 1 | A | 2325 | G | N1-C6-O6 | 7.42 | 124.35 | 119.90 |
| 1 | A | 330 | A | N3-C4-C5 | 7.41 | 131.99 | 126.80 |
| 2 | B | 22 | U | C2-N1-C1' | 7.40 | 126.58 | 117.70 |
| 1 | A | 2329 | G | C8-N9-C4 | 7.38 | 109.35 | 106.40 |
| 1 | A | 2591 | C | N1-C2-O2 | -7.38 | 114.47 | 118.90 |
| 1 | A | 2458 | G | N1-C6-O6 | 7.38 | 124.33 | 119.90 |
| 1 | A | 1760 | A | N1-C6-N6 | -7.38 | 114.17 | 118.60 |
| 1 | A | 2491 | U | C5-C4-O4 | -7.37 | 121.48 | 125.90 |
| 1 | A | 1125 | G | C2-N3-C4 | -7.37 | 108.22 | 111.90 |
| 1 | A | 1468 | C | C6-N1-C2 | -7.35 | 117.36 | 120.30 |
| 1 | A | 1272 | A | N1-C6-N6 | -7.34 | 114.20 | 118.60 |
| 1 | A | 113 | G | N3-C4-C5 | 7.34 | 132.27 | 128.60 |
| 1 | A | 2598 | A | N1-C6-N6 | 7.34 | 123.00 | 118.60 |
| 1 | A | 1325 | G | C5-C6-O6 | -7.33 | 124.20 | 128.60 |
| 1 | A | 2457 | U | N3-C2-O2 | -7.33 | 117.07 | 122.20 |
| 1 | A | 1959 | G | N9-C4-C5 | 7.33 | 108.33 | 105.40 |
| 1 | A | 2286 | A | C4-C5-C6 | 7.32 | 120.66 | 117.00 |
| 7 | H | 71 | LEU | CA-CB-CG | 7.32 | 132.14 | 115.30 |
| 1 | A | 1488 | G | C8-N9-C4 | -7.32 | 103.47 | 106.40 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | A | 1611 | C | C6-N1-C2 | -7.32 | 117.37 | 120.30 |
| 1 | A | 2028 | U | C2-N3-C4 | -7.31 | 122.61 | 127.00 |
| 1 | A | 456 | C | N3-C4-C5 | 7.31 | 124.82 | 121.90 |
| 1 | A | 1652 | A | C8-N9-C4 | -7.31 | 102.88 | 105.80 |
| 1 | A | 2114 | A | C8-N9-C4 | -7.31 | 102.88 | 105.80 |
| 1 | A | 1661 | G | N7-C8-N9 | -7.30 | 109.45 | 113.10 |
| 1 | A | 1775 | U | N1-C2-O2 | -7.30 | 117.69 | 122.80 |
| 1 | A | 2271 | G | N3-C4-C5 | -7.30 | 124.95 | 128.60 |
| 1 | A | 2296 | U | O4'-C1'-N1 | 7.30 | 114.04 | 108.20 |
| 1 | A | 616 | G | C8-N9-C4 | 7.30 | 109.32 | 106.40 |
| 1 | A | 1637 | A | N1-C6-N6 | -7.29 | 114.22 | 118.60 |
| 1 | A | 1977 | A | N7-C8-N9 | -7.29 | 110.16 | 113.80 |
| 1 | A | 530 | G | C6-C5-N7 | 7.29 | 134.77 | 130.40 |
| 1 | A | 982 | C | C5-C6-N1 | 7.28 | 124.64 | 121.00 |
| 1 | A | 1028 | A | C8-N9-C4 | 7.28 | 108.71 | 105.80 |
| 1 | A | 374 | A | C2-N3-C4 | -7.28 | 106.96 | 110.60 |
| 1 | A | 563 | G | C5-C6-O6 | -7.26 | 124.24 | 128.60 |
| 1 | A | 780 | G | C6-N1-C2 | -7.26 | 120.74 | 125.10 |
| 1 | A | 467 | G | C8-N9-C4 | 7.26 | 109.30 | 106.40 |
| 1 | A | 125 | G | N3-C4-C5 | -7.25 | 124.97 | 128.60 |
| 1 | A | 2010 | G | N1-C6-O6 | 7.25 | 124.25 | 119.90 |
| 1 | A | 45 | C | C2-N3-C4 | -7.24 | 116.28 | 119.90 |
| 1 | A | 58 | G | C5-C6-O6 | 7.23 | 132.94 | 128.60 |
| 1 | A | 236 | C | C5-C6-N1 | -7.22 | 117.39 | 121.00 |
| 1 | A | 39 | C | N3-C4-C5 | 7.22 | 124.79 | 121.90 |
| 1 | A | 2575 | C | C6-N1-C2 | 7.22 | 123.19 | 120.30 |
| 1 | A | 2386 | C | C5-C6-N1 | -7.21 | 117.39 | 121.00 |
| 1 | A | 2312 | U | N1-C2-O2 | 7.21 | 127.84 | 122.80 |
| 1 | A | 1305 | C | N3-C4-C5 | 7.20 | 124.78 | 121.90 |
| 1 | A | 801 | G | C5-C6-O6 | 7.20 | 132.92 | 128.60 |
| 1 | A | 802 | A | N7-C8-N9 | 7.19 | 117.40 | 113.80 |
| 1 | A | 847 | U | N3-C4-O4 | -7.19 | 114.37 | 119.40 |
| 1 | A | 2498 | C | C6-N1-C2 | 7.19 | 123.18 | 120.30 |
| 1 | A | 784 | A | N1-C6-N6 | -7.19 | 114.29 | 118.60 |
| 1 | A | 205 | G | N3-C2-N2 | 7.19 | 124.93 | 119.90 |
| 1 | A | 2433 | A | N1-C6-N6 | 7.18 | 122.91 | 118.60 |
| 2 | B | 104 | U | C6-N1-C2 | 7.16 | 125.30 | 121.00 |
| 1 | A | 2377 | A | C2-N3-C4 | -7.16 | 107.02 | 110.60 |
| 1 | A | 936 | C | C6-N1-C2 | 7.16 | 123.16 | 120.30 |
| 1 | A | 310 | A | C8-N9-C4 | 7.15 | 108.66 | 105.80 |
| 1 | A | 2569 | G | C5-C6-N1 | 7.15 | 115.07 | 111.50 |
| 1 | A | 1959 | G | C8-N9-C4 | -7.14 | 103.54 | 106.40 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 1 | A | 1295 | C | N1-C2-O2 | -7.14 | 114.62 | 118.90 |
| 1 | A | 826 | U | C5-C6-N1 | -7.14 | 119.13 | 122.70 |
| 1 | A | 2593 | U | C4-C5-C6 | 7.12 | 123.97 | 119.70 |
| 1 | A | 784 | A | C5-C6-N6 | 7.12 | 129.40 | 123.70 |
| 1 | A | 265 | A | N1-C6-N6 | 7.12 | 122.87 | 118.60 |
| 1 | A | 729 | G | C8-N9-C4 | -7.11 | 103.56 | 106.40 |
| 1 | A | 419 | C | N3-C4-C5 | 7.11 | 124.75 | 121.90 |
| 1 | A | 103 | A | C8-N9-C4 | 7.11 | 108.64 | 105.80 |
| 1 | A | 1826 | G | C8-N9-C4 | 7.10 | 109.24 | 106.40 |
| 1 | A | 2176 | A | C6-N1-C2 | 7.10 | 122.86 | 118.60 |
| 1 | A | 1610 | A | C5-N7-C8 | -7.10 | 100.35 | 103.90 |
| 1 | A | 1820 | U | N3-C4-C5 | 7.10 | 118.86 | 114.60 |
| 1 | A | 1336 | A | N1-C6-N6 | -7.09 | 114.34 | 118.60 |
| 1 | A | 2508 | G | N1-C6-O6 | -7.09 | 115.65 | 119.90 |
| 1 | A | 1365 | A | N1-C6-N6 | 7.08 | 122.85 | 118.60 |
| 1 | A | 1784 | A | N9-C4-C5 | -7.06 | 102.97 | 105.80 |
| 1 | A | 2287 | A | N3-C4-C5 | 7.06 | 131.74 | 126.80 |
| 1 | A | 488 | G | N7-C8-N9 | -7.05 | 109.58 | 113.10 |
| 1 | A | 330 | A | C5-N7-C8 | -7.05 | 100.38 | 103.90 |
| 1 | A | 1109 | C | N3-C4-C5 | -7.05 | 119.08 | 121.90 |
| 2 | B | 101 | G | C8-N9-C4 | 7.04 | 109.22 | 106.40 |
| 1 | A | 148 | C | C5-C6-N1 | -7.04 | 117.48 | 121.00 |
| 1 | A | 1142(A) | A | N3-C4-C5 | 7.04 | 131.72 | 126.80 |
| 1 | A | 764 | A | N1-C2-N3 | -7.03 | 125.78 | 129.30 |
| 1 | A | 772 | C | N1-C2-O2 | -7.03 | 114.68 | 118.90 |
| 1 | A | 2030 | A | N1-C6-N6 | 7.03 | 122.82 | 118.60 |
| 1 | A | 652(T) | C | C5-C4-N4 | 7.03 | 125.12 | 120.20 |
| 1 | A | 807 | U | N3-C4-O4 | 7.03 | 124.32 | 119.40 |
| 1 | A | 1817 | G | N9-C4-C5 | -7.03 | 102.59 | 105.40 |
| 1 | A | 1955 | U | C5-C6-N1 | -7.03 | 119.19 | 122.70 |
| 1 | A | 847 | U | C2-N1-C1' | -7.02 | 109.28 | 117.70 |
| 1 | A | 841 | A | C2-N3-C4 | -7.02 | 107.09 | 110.60 |
| 1 | A | 2286 | A | C5-C6-N1 | -7.01 | 114.19 | 117.70 |
| 1 | A | 2620 | C | N3-C4-C5 | 7.01 | 124.70 | 121.90 |
| 1 | A | 62 | C | C2-N3-C4 | -7.01 | 116.39 | 119.90 |
| 1 | A | 546 | C | C6-N1-C2 | -7.01 | 117.50 | 120.30 |
| 1 | A | 2626 | C | C6-N1-C2 | 7.01 | 123.10 | 120.30 |
| 1 | A | 1042 | G | N1-C6-O6 | 6.99 | 124.10 | 119.90 |
| 1 | A | 2681 | C | N3-C2-O2 | -6.99 | 117.01 | 121.90 |
| 1 | A | 528 | A | C5-N7-C8 | -6.98 | 100.41 | 103.90 |
| 1 | A | 1786 | A | N1-C2-N3 | 6.98 | 132.79 | 129.30 |
| 1 | A | 801 | G | N9-C4-C5 | 6.98 | 108.19 | 105.40 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2 | B | 101 | G | N9-C4-C5 | -6.97 | 102.61 | 105.40 |
| 1 | A | 2040 | C | C5-C4-N4 | -6.97 | 115.32 | 120.20 |
| 1 | A | 62 | C | C5-C6-N1 | -6.97 | 117.52 | 121.00 |
| 1 | A | 1271 | G | N1-C6-O6 | 6.97 | 124.08 | 119.90 |
| 1 | A | 2244 | U | C2-N3-C4 | -6.97 | 122.82 | 127.00 |
| 1 | A | 2361 | A | N1-C6-N6 | 6.97 | 122.78 | 118.60 |
| 1 | A | 2296 | U | C3'-C2'-C1' | -6.96 | 95.93 | 101.50 |
| 1 | A | 2312 | U | C2-N1-C1' | 6.95 | 126.04 | 117.70 |
| 1 | A | 2221 | G | C8-N9-C4 | -6.94 | 103.62 | 106.40 |
| 1 | A | 1568 | G | N1-C6-O6 | -6.94 | 115.73 | 119.90 |
| 1 | A | 2017 | U | C4-C5-C6 | 6.94 | 123.87 | 119.70 |
| 1 | A | 1825 | A | C5-C6-N1 | 6.94 | 121.17 | 117.70 |
| 1 | A | 12 | U | C2-N1-C1' | 6.93 | 126.01 | 117.70 |
| 1 | A | 2713 | A | C8-N9-C4 | 6.93 | 108.57 | 105.80 |
| 1 | A | 195 | A | C4-C5-C6 | 6.92 | 120.46 | 117.00 |
| 1 | A | 2268 | A | N1-C6-N6 | 6.92 | 122.75 | 118.60 |
| 1 | A | 140 | G | C8-N9-C4 | 6.91 | 109.16 | 106.40 |
| 1 | A | 115 | C | N1-C2-O2 | -6.91 | 114.76 | 118.90 |
| 1 | A | 2114 | A | N7-C8-N9 | 6.90 | 117.25 | 113.80 |
| 1 | A | 2181 | G | C5-C6-O6 | 6.90 | 132.74 | 128.60 |
| 1 | A | 2415 | G | C5-C6-O6 | -6.90 | 124.46 | 128.60 |
| 2 | B | 71 | C | N1-C2-O2 | 6.90 | 123.04 | 118.90 |
| 1 | A | 679 | C | N3-C2-O2 | 6.90 | 126.73 | 121.90 |
| 1 | A | 27 | G | N9-C4-C5 | 6.90 | 108.16 | 105.40 |
| 1 | A | 2069 | G | C5-N7-C8 | 6.89 | 107.75 | 104.30 |
| 1 | A | 2124 | G | C5-C6-O6 | 6.89 | 132.74 | 128.60 |
| 1 | A | 819 | A | C8-N9-C4 | -6.89 | 103.05 | 105.80 |
| 1 | A | 2855 | C | C6-N1-C2 | -6.89 | 117.55 | 120.30 |
| 1 | A | 141 | A | C4-C5-N7 | 6.88 | 114.14 | 110.70 |
| 1 | A | 1207 | C | C6-N1-C2 | 6.88 | 123.05 | 120.30 |
| 1 | A | 488 | G | C4-C5-N7 | -6.88 | 108.05 | 110.80 |
| 1 | A | 97 | C | C5-C4-N4 | 6.88 | 125.01 | 120.20 |
| 1 | A | 1354 | A | C5-C6-N1 | 6.87 | 121.14 | 117.70 |
| 1 | A | 802 | A | N1-C6-N6 | -6.87 | 114.48 | 118.60 |
| 1 | A | 1616 | A | N1-C6-N6 | 6.87 | 122.72 | 118.60 |
| 1 | A | 2260 | C | C5-C6-N1 | -6.87 | 117.57 | 121.00 |
| 1 | A | 2360 | A | C8-N9-C4 | 6.86 | 108.55 | 105.80 |
| 1 | A | 379 | G | N1-C6-O6 | 6.86 | 124.01 | 119.90 |
| 1 | A | 1900 | A | N3-C4-C5 | -6.86 | 122.00 | 126.80 |
| 1 | A | 24 | G | N1-C6-O6 | 6.85 | 124.01 | 119.90 |
| 1 | A | 478 | A | C8-N9-C4 | -6.85 | 103.06 | 105.80 |
| 1 | A | 73 | A | N9-C4-C5 | 6.85 | 108.54 | 105.80 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | A | 201 | C | C2-N3-C4 | -6.85 | 116.47 | 119.90 |
| 1 | A | 695 | G | N3-C2-N2 | 6.84 | 124.69 | 119.90 |
| 2 | B | 120 | A | C5-C6-N6 | 6.84 | 129.18 | 123.70 |
| 1 | A | 1201 | C | N1-C2-O2 | -6.84 | 114.80 | 118.90 |
| 1 | A | 1638 | C | C4-C5-C6 | 6.84 | 120.82 | 117.40 |
| 1 | A | 528 | A | C8-N9-C1' | 6.84 | 140.00 | 127.70 |
| 1 | A | 2181 | G | C6-N1-C2 | 6.83 | 129.20 | 125.10 |
| 1 | A | 297 | C | C6-N1-C2 | -6.83 | 117.57 | 120.30 |
| 1 | A | 645 | C | C2-N1-C1' | 6.83 | 126.31 | 118.80 |
| 1 | A | 1408 | C | N1-C2-O2 | -6.83 | 114.80 | 118.90 |
| 1 | A | 12 | U | N1-C2-O2 | 6.83 | 127.58 | 122.80 |
| 1 | A | 1244 | G | N1-C6-O6 | 6.82 | 123.99 | 119.90 |
| 1 | A | 1775 | U | C2-N3-C4 | -6.82 | 122.91 | 127.00 |
| 1 | A | 1959 | G | C5-C6-O6 | 6.82 | 132.69 | 128.60 |
| 1 | A | 2067 | G | N9-C4-C5 | 6.82 | 108.13 | 105.40 |
| 1 | A | 1007 | C | N3-C4-C5 | 6.81 | 124.63 | 121.90 |
| 1 | A | 2766 | G | N1-C6-O6 | -6.81 | 115.81 | 119.90 |
| 1 | A | 912 | C | C6-N1-C2 | -6.81 | 117.58 | 120.30 |
| 1 | A | 2122 | U | C5-C4-O4 | 6.80 | 129.98 | 125.90 |
| 1 | A | 769 | G | C8-N9-C4 | 6.80 | 109.12 | 106.40 |
| 1 | A | 2417 | C | N3-C2-O2 | -6.80 | 117.14 | 121.90 |
| 1 | A | 1954 | G | N3-C2-N2 | -6.79 | 115.15 | 119.90 |
| 1 | A | 915 | C | C6-N1-C2 | -6.78 | 117.59 | 120.30 |
| 1 | A | 2193 | G | C5-C6-N1 | -6.78 | 108.11 | 111.50 |
| 1 | A | 183 | C | N3-C4-C5 | 6.78 | 124.61 | 121.90 |
| 1 | A | 2335 | A | C6-N1-C2 | -6.78 | 114.53 | 118.60 |
| 1 | A | 2335 | A | C4-C5-N7 | 6.78 | 114.09 | 110.70 |
| 1 | A | 1834 | U | N3-C2-O2 | -6.77 | 117.46 | 122.20 |
| 1 | A | 830 | G | N1-C6-O6 | -6.77 | 115.84 | 119.90 |
| 1 | A | 1325 | G | C5-C6-N1 | 6.77 | 114.88 | 111.50 |
| 1 | A | 2821 | A | C4-C5-N7 | 6.76 | 114.08 | 110.70 |
| 1 | A | 2063 | C | N3-C4-N4 | 6.76 | 122.73 | 118.00 |
| 1 | A | 2123 | G | C6-C5-N7 | 6.76 | 134.46 | 130.40 |
| 1 | A | 1660 | C | C5-C6-N1 | -6.75 | 117.62 | 121.00 |
| 1 | A | 801 | G | N3-C4-N9 | -6.75 | 121.95 | 126.00 |
| 1 | A | 2407 | G | C8-N9-C1' | -6.75 | 118.23 | 127.00 |
| 1 | A | 2260 | C | C2-N3-C4 | -6.74 | 116.53 | 119.90 |
| 1 | A | 2318 | G | N3-C4-C5 | -6.74 | 125.23 | 128.60 |
| 1 | A | 2575 | C | C5-C6-N1 | -6.74 | 117.63 | 121.00 |
| 1 | A | 645 | C | N3-C2-O2 | -6.73 | 117.19 | 121.90 |
| 1 | A | 768 | G | C6-N1-C2 | -6.73 | 121.06 | 125.10 |
| 1 | A | 1937 | A | N1-C6-N6 | 6.73 | 122.64 | 118.60 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 1 | A | 463 | G | C8-N9-C4 | -6.72 | 103.71 | 106.40 |
| 1 | A | 2332 | U | N1-C2-O2 | 6.72 | 127.50 | 122.80 |
| 1 | A | 652(T) | C | N1-C2-O2 | 6.72 | 122.93 | 118.90 |
| 1 | A | 2306 | C | C2-N1-C1' | 6.72 | 126.19 | 118.80 |
| 1 | A | 484 | C | N3-C4-C5 | 6.71 | 124.58 | 121.90 |
| 23 | 1 | 21 | ARG | NE-CZ-NH2 | -6.71 | 116.94 | 120.30 |
| 1 | A | 2123 | G | C8-N9-C1' | 6.71 | 135.72 | 127.00 |
| 1 | A | 154(A) | C | C6-N1-C1' | -6.71 | 112.75 | 120.80 |
| 1 | A | 1397 | U | N3-C2-O2 | -6.70 | 117.51 | 122.20 |
| 1 | A | 1211 | U | C5-C4-O4 | -6.70 | 121.88 | 125.90 |
| 1 | A | 2733 | A | N1-C6-N6 | 6.70 | 122.62 | 118.60 |
| 1 | A | 121 | G | C5-C6-O6 | -6.69 | 124.58 | 128.60 |
| 1 | A | 154(A) | C | C2-N1-C1' | 6.69 | 126.16 | 118.80 |
| 1 | A | 1128 | A | N1-C6-N6 | 6.69 | 122.61 | 118.60 |
| 1 | A | 453 | C | C6-N1-C2 | 6.69 | 122.98 | 120.30 |
| 1 | A | 1359 | A | C5-C6-N6 | 6.69 | 129.05 | 123.70 |
| 1 | A | 2821 | A | C5-C6-N6 | -6.69 | 118.35 | 123.70 |
| 1 | A | 2322 | A | N3-C4-C5 | -6.68 | 122.12 | 126.80 |
| 1 | A | 1026 | U | N1-C2-O2 | 6.68 | 127.47 | 122.80 |
| 1 | A | 12 | U | C6-N1-C2 | -6.66 | 117.00 | 121.00 |
| 1 | A | 2347 | C | N3-C2-O2 | -6.66 | 117.24 | 121.90 |
| 1 | A | 652(E) | G | N3-C2-N2 | 6.66 | 124.56 | 119.90 |
| 1 | A | 2346 | A | C8-N9-C4 | -6.65 | 103.14 | 105.80 |
| 1 | A | 1210 | A | C8-N9-C4 | -6.65 | 103.14 | 105.80 |
| 1 | A | 429 | A | N1-C6-N6 | 6.65 | 122.59 | 118.60 |
| 1 | A | 728 | G | C8-N9-C4 | 6.64 | 109.06 | 106.40 |
| 1 | A | 2024 | G | N9-C4-C5 | -6.64 | 102.74 | 105.40 |
| 1 | A | 1247 | A | C8-N9-C4 | 6.64 | 108.46 | 105.80 |
| 1 | A | 1597 | A | N9-C4-C5 | 6.64 | 108.45 | 105.80 |
| 1 | A | 528 | A | C4-N9-C1' | -6.64 | 114.36 | 126.30 |
| 1 | A | 362 | U | C5-C4-O4 | -6.63 | 121.92 | 125.90 |
| 1 | A | 2444 | G | C4-C5-N7 | -6.63 | 108.15 | 110.80 |
| 1 | A | 2762 | G | C8-N9-C4 | -6.62 | 103.75 | 106.40 |
| 1 | A | 2084 | C | C4-C5-C6 | 6.62 | 120.71 | 117.40 |
| 1 | A | 2244 | U | C5-C6-N1 | -6.62 | 119.39 | 122.70 |
| 1 | A | 2407 | G | C6-C5-N7 | -6.62 | 126.43 | 130.40 |
| 1 | A | 1826 | G | C4-C5-N7 | -6.61 | 108.16 | 110.80 |
| 1 | A | 1578 | U | N3-C2-O2 | -6.60 | 117.58 | 122.20 |
| 1 | A | 2307 | G | N7-C8-N9 | 6.60 | 116.40 | 113.10 |
| 1 | A | 1471 | A | N7-C8-N9 | 6.59 | 117.09 | 113.80 |
| 1 | A | 784 | A | C5-N7-C8 | 6.58 | 107.19 | 103.90 |
| 1 | A | 798 | G | C2-N3-C4 | -6.58 | 108.61 | 111.90 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 1 | A | 409 | C | N3-C4-C5 | 6.58 | 124.53 | 121.90 |
| 1 | A | 1471 | A | C8-N9-C4 | -6.57 | 103.17 | 105.80 |
| 1 | A | 2090 | G | C4-C5-N7 | -6.57 | 108.17 | 110.80 |
| 1 | A | 39 | C | N3-C4-N4 | -6.56 | 113.41 | 118.00 |
| 1 | A | 1377 | G | N3-C4-C5 | -6.56 | 125.32 | 128.60 |
| 1 | A | 678 | C | C6-N1-C2 | 6.56 | 122.92 | 120.30 |
| 1 | A | 1384 | A | N1-C6-N6 | -6.56 | 114.66 | 118.60 |
| 1 | A | 2174 | C | C5-C6-N1 | 6.56 | 124.28 | 121.00 |
| 19 | X | 57 | LEU | CA-CB-CG | 6.56 | 130.38 | 115.30 |
| 1 | A | 1355 | G | N3-C2-N2 | -6.55 | 115.32 | 119.90 |
| 1 | A | 2030 | A | C5-C6-N6 | -6.55 | 118.46 | 123.70 |
| 1 | A | 143 | G | C8-N9-C4 | 6.54 | 109.02 | 106.40 |
| 1 | A | 2027 | G | N1-C2-N3 | 6.54 | 127.83 | 123.90 |
| 1 | A | 728 | G | N7-C8-N9 | -6.54 | 109.83 | 113.10 |
| 1 | A | 2075 | U | C5-C6-N1 | -6.54 | 119.43 | 122.70 |
| 1 | A | 2456 | C | C6-N1-C2 | 6.54 | 122.92 | 120.30 |
| 1 | A | 2067 | G | N7-C8-N9 | 6.54 | 116.37 | 113.10 |
| 1 | A | 271(S) | G | N1-C6-O6 | 6.54 | 123.82 | 119.90 |
| 1 | A | 465 | G | C8-N9-C4 | -6.53 | 103.79 | 106.40 |
| 1 | A | 756 | C | N3-C2-O2 | -6.52 | 117.33 | 121.90 |
| 1 | A | 1758 | G | C5-C6-O6 | -6.52 | 124.69 | 128.60 |
| 1 | A | 1204 | A | C3'-C2'-C1' | -6.51 | 96.29 | 101.50 |
| 1 | A | 1826 | G | N1-C6-O6 | -6.51 | 115.99 | 119.90 |
| 1 | A | 2021 | C | C2-N3-C4 | -6.51 | 116.64 | 119.90 |
| 1 | A | 1758 | G | C6-C5-N7 | -6.51 | 126.50 | 130.40 |
| 1 | A | 2312 | U | C6-N1-C2 | -6.51 | 117.10 | 121.00 |
| 1 | A | 1602 | U | C5-C4-O4 | 6.50 | 129.80 | 125.90 |
| 1 | A | 210 | C | C5-C6-N1 | -6.50 | 117.75 | 121.00 |
| 1 | A | 54 | G | N1-C6-O6 | 6.50 | 123.80 | 119.90 |
| 11 | P | 147 | LEU | CA-CB-CG | 6.50 | 130.24 | 115.30 |
| 1 | A | 975 | C | N1-C2-O2 | 6.49 | 122.80 | 118.90 |
| 1 | A | 2047 | U | N3-C4-C5 | 6.49 | 118.49 | 114.60 |
| 1 | A | 2306 | C | C5-C6-N1 | 6.49 | 124.24 | 121.00 |
| 1 | A | 945 | A | N1-C6-N6 | 6.49 | 122.49 | 118.60 |
| 1 | A | 1244 | G | C4-C5-N7 | 6.48 | 113.39 | 110.80 |
| 1 | A | 1327 | C | N1-C2-O2 | -6.48 | 115.01 | 118.90 |
| 1 | A | 1997 | G | N9-C4-C5 | 6.48 | 107.99 | 105.40 |
| 1 | A | 737 | C | C6-N1-C2 | 6.47 | 122.89 | 120.30 |
| 1 | A | 2569 | G | N3-C4-C5 | -6.47 | 125.36 | 128.60 |
| 1 | A | 2070 | G | C6-N1-C2 | -6.47 | 121.22 | 125.10 |
| 1 | A | 2070 | G | N7-C8-N9 | -6.46 | 109.87 | 113.10 |
| 2 | B | 22 | U | C5-C6-N1 | 6.46 | 125.93 | 122.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | A | 1007 | C | C2-N3-C4 | -6.46 | 116.67 | 119.90 |
| 1 | A | 1022 | G | N9-C4-C5 | 6.46 | 107.98 | 105.40 |
| 2 | B | 115 | G | N7-C8-N9 | -6.46 | 109.87 | 113.10 |
| 1 | A | 945 | A | C8-N9-C4 | 6.46 | 108.38 | 105.80 |
| 1 | A | 2262 | U | N1-C2-O2 | -6.46 | 118.28 | 122.80 |
| 1 | A | 773 | U | C5-C4-O4 | 6.45 | 129.77 | 125.90 |
| 1 | A | 1992 | G | N3-C4-C5 | -6.45 | 125.37 | 128.60 |
| 1 | A | 2182 | G | N3-C4-N9 | -6.45 | 122.13 | 126.00 |
| 1 | A | 2045 | C | C5-C6-N1 | -6.45 | 117.78 | 121.00 |
| 1 | A | 1374 | G | C5-C6-N1 | -6.44 | 108.28 | 111.50 |
| 1 | A | 2344 | U | C5-C4-O4 | 6.44 | 129.77 | 125.90 |
| 1 | A | 512 | G | O4'-C1'-N9 | 6.44 | 113.35 | 108.20 |
| 1 | A | 1022 | G | C8-N9-C1' | 6.43 | 135.37 | 127.00 |
| 1 | A | 2607 | G | N3-C4-C5 | -6.43 | 125.38 | 128.60 |
| 1 | A | 2519 | U | N3-C2-O2 | 6.43 | 126.70 | 122.20 |
| 1 | A | 1610 | A | C4-C5-N7 | 6.43 | 113.91 | 110.70 |
| 1 | A | 2322 | A | C6-C5-N7 | 6.42 | 136.79 | 132.30 |
| 1 | A | 2104 | G | C6-N1-C2 | 6.42 | 128.95 | 125.10 |
| 1 | A | 1817 | G | C4-C5-N7 | 6.41 | 113.37 | 110.80 |
| 1 | A | 1794 | U | C2-N3-C4 | -6.41 | 123.15 | 127.00 |
| 1 | A | 860 | U | C6-N1-C2 | -6.41 | 117.15 | 121.00 |
| 1 | A | 1762 | A | C2-N3-C4 | 6.41 | 113.81 | 110.60 |
| 1 | A | 2062 | A | N7-C8-N9 | 6.41 | 117.00 | 113.80 |
| 1 | A | 2519 | U | C6-N1-C2 | 6.41 | 124.85 | 121.00 |
| 1 | A | 2440 | C | C2-N1-C1' | -6.41 | 111.75 | 118.80 |
| 1 | A | 2286 | A | C8-N9-C4 | -6.40 | 103.24 | 105.80 |
| 1 | A | 1789 | A | C8-N9-C4 | 6.39 | 108.36 | 105.80 |
| 1 | A | 2386 | C | C6-N1-C2 | 6.39 | 122.86 | 120.30 |
| 1 | A | 791 | C | C5-C6-N1 | -6.39 | 117.80 | 121.00 |
| 1 | A | 2286 | A | N1-C2-N3 | 6.39 | 132.49 | 129.30 |
| 1 | A | 2325 | G | C5-C6-O6 | -6.39 | 124.77 | 128.60 |
| 1 | A | 780 | G | N3-C2-N2 | -6.38 | 115.43 | 119.90 |
| 1 | A | 1605 | C | N3-C4-C5 | -6.38 | 119.35 | 121.90 |
| 1 | A | 2672 | G | C6-C5-N7 | -6.37 | 126.58 | 130.40 |
| 1 | A | 2423 | U | C6-N1-C2 | 6.37 | 124.82 | 121.00 |
| 1 | A | 860 | U | C5-C4-O4 | 6.37 | 129.72 | 125.90 |
| 1 | A | 985 | C | N3-C4-C5 | 6.37 | 124.45 | 121.90 |
| 1 | A | 394 | A | N7-C8-N9 | -6.36 | 110.62 | 113.80 |
| 1 | A | 1616 | A | C6-C5-N7 | -6.36 | 127.85 | 132.30 |
| 1 | A | 1966 | A | C8-N9-C4 | 6.36 | 108.34 | 105.80 |
| 1 | A | 1397 | U | N3-C4-O4 | -6.36 | 114.95 | 119.40 |
| 1 | A | 1955 | U | C2-N1-C1' | -6.36 | 110.07 | 117.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | A | 2426 | A | N7-C8-N9 | 6.36 | 116.98 | 113.80 |
| 1 | A | 2567 | G | C8-N9-C4 | 6.36 | 108.94 | 106.40 |
| 1 | A | 1128 | A | N9-C4-C5 | -6.35 | 103.26 | 105.80 |
| 1 | A | 1368 | G | C2-N3-C4 | 6.35 | 115.08 | 111.90 |
| 1 | A | 2570 | G | C4-C5-N7 | -6.35 | 108.26 | 110.80 |
| 1 | A | 1042 | G | C5-C6-O6 | -6.35 | 124.79 | 128.60 |
| 1 | A | 1565 | C | N3-C4-C5 | 6.35 | 124.44 | 121.90 |
| 1 | A | 2343 | C | N1-C2-O2 | -6.35 | 115.09 | 118.90 |
| 1 | A | 933 | A | N1-C6-N6 | 6.35 | 122.41 | 118.60 |
| 1 | A | 148 | C | N3-C4-C5 | 6.34 | 124.44 | 121.90 |
| 1 | A | 2069 | G | C8-N9-C4 | 6.34 | 108.94 | 106.40 |
| 1 | A | 1254 | A | C6-N1-C2 | -6.34 | 114.80 | 118.60 |
| 1 | A | 1305 | C | C5-C4-N4 | -6.34 | 115.76 | 120.20 |
| 1 | A | 2028 | U | C5-C6-N1 | -6.34 | 119.53 | 122.70 |
| 1 | A | 1956 | U | N1-C2-N3 | 6.33 | 118.70 | 114.90 |
| 1 | A | 768 | G | C4-C5-C6 | 6.33 | 122.60 | 118.80 |
| 1 | A | 2383 | G | C8-N9-C1' | -6.33 | 118.77 | 127.00 |
| 1 | A | 2501 | C | C2-N1-C1' | -6.32 | 111.85 | 118.80 |
| 1 | A | 1827 | C | C6-N1-C2 | -6.32 | 117.77 | 120.30 |
| 1 | A | 2312 | U | C5-C6-N1 | 6.32 | 125.86 | 122.70 |
| 1 | A | 1248 | G | N7-C8-N9 | -6.32 | 109.94 | 113.10 |
| 1 | A | 2823 | A | C6-C5-N7 | -6.31 | 127.88 | 132.30 |
| 1 | A | 804 | A | C6-N1-C2 | -6.31 | 114.81 | 118.60 |
| 1 | A | 205 | G | N3-C4-N9 | 6.30 | 129.78 | 126.00 |
| 1 | A | 744 | G | C4-C5-N7 | -6.30 | 108.28 | 110.80 |
| 1 | A | 2286 | A | C4-C5-N7 | 6.30 | 113.85 | 110.70 |
| 1 | A | 194 | G | N7-C8-N9 | 6.30 | 116.25 | 113.10 |
| 1 | A | 1244 | G | C5-C6-O6 | -6.30 | 124.82 | 128.60 |
| 1 | A | 2463 | C | C5-C6-N1 | -6.30 | 117.85 | 121.00 |
| 2 | B | 54 | G | C8-N9-C4 | -6.30 | 103.88 | 106.40 |
| 1 | A | 1660 | C | C4-C5-C6 | 6.30 | 120.55 | 117.40 |
| 1 | A | 2719 | G | C8-N9-C4 | 6.30 | 108.92 | 106.40 |
| 1 | A | 1834 | U | N1-C2-O2 | 6.29 | 127.21 | 122.80 |
| 1 | A | 330 | A | C4-C5-N7 | 6.29 | 113.85 | 110.70 |
| 1 | A | 371 | A | N1-C6-N6 | 6.29 | 122.37 | 118.60 |
| 1 | A | 2191 | G | C6-C5-N7 | -6.29 | 126.63 | 130.40 |
| 1 | A | 933 | A | C6-C5-N7 | -6.29 | 127.90 | 132.30 |
| 1 | A | 1284 | A | N9-C4-C5 | -6.29 | 103.29 | 105.80 |
| 1 | A | 1782 | C | C6-N1-C2 | 6.29 | 122.81 | 120.30 |
| 1 | A | 19 | C | N1-C2-O2 | -6.28 | 115.13 | 118.90 |
| 1 | A | 1955 | U | N3-C4-O4 | -6.28 | 115.00 | 119.40 |
| 1 | A | 513 | A | C5-C6-N1 | 6.28 | 120.84 | 117.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 1 | A | 2075 | U | N3-C2-O2 | -6.28 | 117.81 | 122.20 |
| 1 | A | 2123 | G | N3-C4-N9 | -6.28 | 122.23 | 126.00 |
| 1 | A | 2446 | G | C5-C6-O6 | 6.28 | 132.37 | 128.60 |
| 1 | A | 2110 | G | N3-C4-N9 | 6.27 | 129.76 | 126.00 |
| 1 | A | 1125 | G | N3-C4-C5 | 6.27 | 131.74 | 128.60 |
| 1 | A | 569 | U | C5-C6-N1 | -6.27 | 119.57 | 122.70 |
| 1 | A | 1023 | U | N1-C2-N3 | 6.27 | 118.66 | 114.90 |
| 1 | A | 1489 | U | C5-C4-O4 | 6.27 | 129.66 | 125.90 |
| 1 | A | 272(C) | G | C8-N9-C4 | 6.26 | 108.90 | 106.40 |
| 1 | A | 418 | G | C6-C5-N7 | -6.26 | 126.64 | 130.40 |
| 1 | A | 1205 | U | C5-C6-N1 | -6.26 | 119.57 | 122.70 |
| 1 | A | 24 | G | C5-C6-O6 | -6.26 | 124.85 | 128.60 |
| 1 | A | 2502 | G | N1-C2-N2 | -6.25 | 110.57 | 116.20 |
| 1 | A | 2648 | C | C6-N1-C2 | 6.25 | 122.80 | 120.30 |
| 1 | A | 194 | G | N1-C2-N3 | 6.25 | 127.65 | 123.90 |
| 1 | A | 686 | G | N1-C2-N2 | -6.24 | 110.58 | 116.20 |
| 1 | A | 546 | C | C5-C6-N1 | 6.24 | 124.12 | 121.00 |
| 1 | A | 777 | A | C4-C5-C6 | 6.24 | 120.12 | 117.00 |
| 1 | A | 802 | A | N9-C4-C5 | 6.24 | 108.30 | 105.80 |
| 1 | A | 1204 | A | C1'-O4'-C4' | -6.24 | 104.91 | 109.90 |
| 1 | A | 1637 | A | N9-C4-C5 | 6.23 | 108.29 | 105.80 |
| 1 | A | 1125 | G | C5-C6-N1 | -6.23 | 108.39 | 111.50 |
| 1 | A | 2675 | A | C2-N3-C4 | -6.22 | 107.49 | 110.60 |
| 1 | A | 271(S) | G | C5-C6-N1 | -6.22 | 108.39 | 111.50 |
| 1 | A | 791 | C | C4-C5-C6 | 6.22 | 120.51 | 117.40 |
| 1 | A | 1779 | U | C6-N1-C2 | 6.21 | 124.73 | 121.00 |
| 1 | A | 528 | A | C4-C5-C6 | -6.21 | 113.89 | 117.00 |
| 1 | A | 1022 | G | C4-N9-C1' | -6.21 | 118.43 | 126.50 |
| 1 | A | 1602 | U | C4-C5-C6 | 6.20 | 123.42 | 119.70 |
| 1 | A | 1638 | C | C5-C6-N1 | -6.20 | 117.90 | 121.00 |
| 1 | A | 234 | C | C6-N1-C2 | -6.20 | 117.82 | 120.30 |
| 1 | A | 1782 | C | C5-C6-N1 | -6.20 | 117.90 | 121.00 |
| 1 | A | 2822 | G | C8-N9-C4 | 6.20 | 108.88 | 106.40 |
| 1 | A | 39 | C | C5-C6-N1 | -6.19 | 117.90 | 121.00 |
| 1 | A | 1238 | G | C5-C6-O6 | -6.19 | 124.88 | 128.60 |
| 1 | A | 1628 | G | C8-N9-C1' | -6.19 | 118.95 | 127.00 |
| 1 | A | 2894 | G | C8-N9-C4 | -6.19 | 103.92 | 106.40 |
| 1 | A | 19 | C | C2-N3-C4 | -6.19 | 116.81 | 119.90 |
| 2 | B | 63 | G | C8-N9-C4 | 6.19 | 108.88 | 106.40 |
| 1 | A | 2124 | G | C6-N1-C2 | 6.19 | 128.81 | 125.10 |
| 1 | A | 2322 | A | C5-N7-C8 | 6.19 | 106.99 | 103.90 |
| 1 | A | 209 | C | C6-N1-C2 | 6.18 | 122.77 | 120.30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 1 | A | 567 | A | N1-C6-N6 | 6.18 | 122.31 | 118.60 |
| 1 | A | 2433 | A | N9-C4-C5 | -6.18 | 103.33 | 105.80 |
| 2 | B | 30 | C | C2-N1-C1' | 6.18 | 125.60 | 118.80 |
| 1 | A | 527 | C | N3-C2-O2 | -6.18 | 117.58 | 121.90 |
| 1 | A | 1762 | A | N7-C8-N9 | 6.17 | 116.89 | 113.80 |
| 1 | A | 595 | C | C6-N1-C2 | 6.17 | 122.77 | 120.30 |
| 1 | A | 2497 | A | C6-N1-C2 | -6.17 | 114.90 | 118.60 |
| 1 | A | 463 | G | N9-C4-C5 | 6.16 | 107.86 | 105.40 |
| 1 | A | 491 | G | N1-C6-O6 | -6.16 | 116.20 | 119.90 |
| 1 | A | 1204 | A | C4-N9-C1' | 6.16 | 137.38 | 126.30 |
| 1 | A | 2033 | A | C6-N1-C2 | -6.16 | 114.91 | 118.60 |
| 1 | A | 1954 | G | N3-C4-N9 | -6.15 | 122.31 | 126.00 |
| 1 | A | 2287 | A | N1-C6-N6 | 6.15 | 122.29 | 118.60 |
| 7 | H | 127 | GLU | C-N-CD | 6.15 | 141.32 | 128.40 |
| 1 | A | 527 | C | C6-N1-C2 | -6.15 | 117.84 | 120.30 |
| 1 | A | 2123 | G | C4-N9-C1' | -6.15 | 118.50 | 126.50 |
| 1 | A | 272(H) | C | C2-N1-C1' | 6.15 | 125.56 | 118.80 |
| 1 | A | 815 | C | C2-N3-C4 | -6.15 | 116.83 | 119.90 |
| 1 | A | 1254 | A | N1-C2-N3 | 6.15 | 132.38 | 129.30 |
| 1 | A | 131 | G | C8-N9-C4 | 6.15 | 108.86 | 106.40 |
| 1 | A | 183 | C | C6-N1-C2 | 6.15 | 122.76 | 120.30 |
| 1 | A | 2062 | A | N1-C6-N6 | 6.15 | 122.29 | 118.60 |
| 1 | A | 2473 | U | C6-N1-C1' | -6.15 | 112.59 | 121.20 |
| 1 | A | 764 | A | C5-N7-C8 | -6.15 | 100.83 | 103.90 |
| 1 | A | 1823 | G | C8-N9-C4 | -6.14 | 103.94 | 106.40 |
| 1 | A | 2031 | A | C4-C5-N7 | 6.14 | 113.77 | 110.70 |
| 1 | A | 1493 | C | C6-N1-C1' | -6.14 | 113.43 | 120.80 |
| 1 | A | 128 | C | C6-N1-C2 | 6.14 | 122.75 | 120.30 |
| 1 | A | 2823 | A | C5-N7-C8 | -6.14 | 100.83 | 103.90 |
| 1 | A | 1488 | G | C4-N9-C1' | 6.13 | 134.47 | 126.50 |
| 1 | A | 1429 | G | C8-N9-C1' | -6.13 | 119.03 | 127.00 |
| 1 | A | 2186 | G | C5-C6-O6 | 6.13 | 132.28 | 128.60 |
| 1 | A | 1142(A) | A | C5-C6-N1 | -6.13 | 114.63 | 117.70 |
| 1 | A | 683 | C | N3-C4-C5 | 6.13 | 124.35 | 121.90 |
| 5 | F | 89 | VAL | O-C-N | -6.13 | 112.90 | 122.70 |
| 1 | A | 1445(A) | C | C6-N1-C2 | -6.13 | 117.85 | 120.30 |
| 1 | A | 1637 | A | C5-C6-N6 | 6.13 | 128.60 | 123.70 |
| 1 | A | 2015 | A | C8-N9-C4 | 6.12 | 108.25 | 105.80 |
| 1 | A | 987 | G | N9-C4-C5 | 6.12 | 107.85 | 105.40 |
| 1 | A | 2540 | C | C6-N1-C2 | 6.12 | 122.75 | 120.30 |
| 1 | A | 669 | G | C5-N7-C8 | 6.11 | 107.36 | 104.30 |
| 1 | A | 684 | G | C8-N9-C4 | -6.11 | 103.96 | 106.40 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1 | A | 1966 | A | N9-C4-C5 | -6.11 | 103.36 | 105.80 |
| 1 | A | 1128 | A | C5-C6-N6 | -6.11 | 118.81 | 123.70 |
| 1 | A | 1575 | C | C6-N1-C2 | 6.11 | 122.74 | 120.30 |
| 1 | A | 1325 | G | C6-N1-C2 | -6.10 | 121.44 | 125.10 |
| 1 | A | 1339 | G | C8-N9-C4 | -6.10 | 103.96 | 106.40 |
| 1 | A | 2505 | G | N3-C2-N2 | 6.10 | 124.17 | 119.90 |
| 21 | Z | 151 | HIS | N-CA-C | 6.10 | 127.47 | 111.00 |
| 1 | A | 187 | G | C4-C5-N7 | 6.10 | 113.24 | 110.80 |
| 1 | A | 351 | G | C8-N9-C4 | 6.10 | 108.84 | 106.40 |
| 1 | A | 2151 | G | C5-C6-O6 | -6.10 | 124.94 | 128.60 |
| 1 | A | 836 | G | N1-C6-O6 | -6.10 | 116.24 | 119.90 |
| 1 | A | 1025 | G | C8-N9-C4 | -6.09 | 103.96 | 106.40 |
| 1 | A | 2064 | C | C6-N1-C2 | 6.09 | 122.74 | 120.30 |
| 1 | A | 2174 | C | C2-N3-C4 | 6.09 | 122.95 | 119.90 |
| 1 | A | 2472 | G | C8-N9-C4 | -6.09 | 103.97 | 106.40 |
| 1 | A | 2244 | U | N1-C2-N3 | 6.08 | 118.55 | 114.90 |
| 1 | A | 2452 | C | N3-C4-N4 | 6.07 | 122.25 | 118.00 |
| 1 | A | 512 | G | N1-C6-O6 | -6.07 | 116.26 | 119.90 |
| 1 | A | 2091 | U | C5-C4-O4 | 6.07 | 129.54 | 125.90 |
| 1 | A | 743 | G | N1-C6-O6 | -6.06 | 116.26 | 119.90 |
| 1 | A | 2619 | C | C6-N1-C2 | 6.06 | 122.72 | 120.30 |
| 1 | A | 2683 | C | C6-N1-C2 | -6.06 | 117.88 | 120.30 |
| 1 | A | 823 | G | C8-N9-C4 | -6.06 | 103.98 | 106.40 |
| 1 | A | 2463 | C | N3-C2-O2 | 6.06 | 126.14 | 121.90 |
| 1 | A | 2458 | G | N3-C2-N2 | -6.05 | 115.67 | 119.90 |
| 1 | A | 1790 | C | C5-C4-N4 | -6.05 | 115.97 | 120.20 |
| 1 | A | 2444 | G | N3-C2-N2 | -6.05 | 115.67 | 119.90 |
| 1 | A | 2335 | A | C4-C5-C6 | -6.04 | 113.98 | 117.00 |
| 1 | A | 1222 | C | N1-C2-O2 | -6.04 | 115.27 | 118.90 |
| 1 | A | 241 | A | C2-N3-C4 | -6.04 | 107.58 | 110.60 |
| 1 | A | 1830 | C | N3-C4-C5 | 6.04 | 124.32 | 121.90 |
| 1 | A | 2195 | C | N1-C2-O2 | -6.04 | 115.28 | 118.90 |
| 1 | A | 143 | G | N3-C4-C5 | 6.04 | 131.62 | 128.60 |
| 1 | A | 2253 | G | C5-C6-N1 | -6.04 | 108.48 | 111.50 |
| 1 | A | 1605 | C | N1-C2-N3 | 6.03 | 123.42 | 119.20 |
| 5 | F | 89 | VAL | CA-C-N | 6.03 | 130.47 | 117.20 |
| 1 | A | 92 | A | N7-C8-N9 | 6.03 | 116.82 | 113.80 |
| 1 | A | 463 | G | C5-C6-O6 | 6.03 | 132.22 | 128.60 |
| 1 | A | 1926 | U | N1-C2-N3 | 6.03 | 118.52 | 114.90 |
| 1 | A | 2607 | G | N3-C4-N9 | 6.03 | 129.62 | 126.00 |
| 1 | A | 1934 | C | C5-C6-N1 | -6.03 | 117.98 | 121.00 |
| 1 | A | 1488 | G | N3-C4-C5 | -6.03 | 125.59 | 128.60 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | A | 248 | G | C8-N9-C4 | -6.02 | 103.99 | 106.40 |
| 1 | A | 1049 | C | C5-C6-N1 | 6.02 | 124.01 | 121.00 |
| 1 | A | 141 | A | C2-N3-C4 | -6.01 | 107.59 | 110.60 |
| 1 | A | 2607 | G | C4-C5-C6 | 6.01 | 122.41 | 118.80 |
| 1 | A | 2710 | C | C4-C5-C6 | 6.01 | 120.41 | 117.40 |
| 1 | A | 265 | A | C5-N7-C8 | -6.01 | 100.89 | 103.90 |
| 1 | A | 1352 | U | N3-C2-O2 | -6.01 | 117.99 | 122.20 |
| 1 | A | 2253 | G | C6-C5-N7 | -6.01 | 126.79 | 130.40 |
| 1 | A | 1786 | A | C5-C6-N6 | 6.01 | 128.51 | 123.70 |
| 1 | A | 62 | C | C6-N1-C2 | 6.01 | 122.70 | 120.30 |
| 1 | A | 398 | G | N1-C6-O6 | 6.01 | 123.50 | 119.90 |
| 1 | A | 2052 | G | N3-C2-N2 | -6.01 | 115.69 | 119.90 |
| 1 | A | 141 | A | C5-C6-N1 | -6.00 | 114.70 | 117.70 |
| 1 | A | 673 | C | C6-N1-C2 | 6.00 | 122.70 | 120.30 |
| 1 | A | 1200 | C | N1-C2-O2 | -6.00 | 115.30 | 118.90 |
| 1 | A | 583 | G | C2-N3-C4 | -6.00 | 108.90 | 111.90 |
| 1 | A | 2031 | A | C5-C6-N6 | -6.00 | 118.90 | 123.70 |
| 1 | A | 1992 | G | C2-N3-C4 | 6.00 | 114.90 | 111.90 |
| 1 | A | 2504 | U | N3-C4-C5 | 6.00 | 118.20 | 114.60 |
| 1 | A | 31 | C | C5-C4-N4 | -5.99 | 116.01 | 120.20 |
| 2 | B | 55 | U | C6-N1-C2 | -5.99 | 117.41 | 121.00 |
| 1 | A | 839 | U | C2-N3-C4 | 5.99 | 130.59 | 127.00 |
| 1 | A | 2110 | G | C4-N9-C1' | 5.99 | 134.29 | 126.50 |
| 1 | A | 1539 | G | C4-N9-C1' | 5.99 | 134.28 | 126.50 |
| 1 | A | 179 | G | C8-N9-C4 | 5.99 | 108.79 | 106.40 |
| 1 | A | 2252 | G | N7-C8-N9 | -5.99 | 110.11 | 113.10 |
| 1 | A | 679 | C | N1-C2-O2 | -5.98 | 115.31 | 118.90 |
| 1 | A | 2332 | U | C5-C6-N1 | -5.98 | 119.71 | 122.70 |
| 1 | A | 2424 | C | N1-C2-N3 | 5.98 | 123.39 | 119.20 |
| 1 | A | 73 | A | C8-N9-C4 | -5.98 | 103.41 | 105.80 |
| 1 | A | 1616 | A | C2-N3-C4 | -5.98 | 107.61 | 110.60 |
| 1 | A | 2569 | G | C6-N1-C2 | -5.98 | 121.51 | 125.10 |
| 1 | A | 2324 | C | C2-N3-C4 | -5.98 | 116.91 | 119.90 |
| 1 | A | 1665 | A | N1-C6-N6 | -5.98 | 115.02 | 118.60 |
| 1 | A | 1022 | G | C6-C5-N7 | 5.97 | 133.99 | 130.40 |
| 1 | A | 2886 | G | N3-C4-C5 | -5.97 | 125.61 | 128.60 |
| 1 | A | 41 | C | C6-N1-C2 | 5.97 | 122.69 | 120.30 |
| 1 | A | 1782 | C | C2-N3-C4 | -5.97 | 116.91 | 119.90 |
| 1 | A | 53 | A | C4-C5-C6 | 5.97 | 119.98 | 117.00 |
| 1 | A | 1617 | C | C5-C6-N1 | -5.97 | 118.02 | 121.00 |
| 1 | A | 133 | C | C6-N1-C2 | 5.97 | 122.69 | 120.30 |
| 1 | A | 27 | G | N1-C2-N2 | 5.96 | 121.57 | 116.20 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | A | 269 | U | C2-N1-C1' | 5.96 | 124.86 | 117.70 |
| 1 | A | 2024 | G | C8-N9-C4 | 5.96 | 108.78 | 106.40 |
| 1 | A | 2248 | C | N3-C4-N4 | -5.96 | 113.83 | 118.00 |
| 1 | A | 474 | G | C8-N9-C4 | -5.96 | 104.02 | 106.40 |
| 1 | A | 847 | U | N1-C2-N3 | 5.95 | 118.47 | 114.90 |
| 1 | A | 1609 | A | N1-C6-N6 | 5.95 | 122.17 | 118.60 |
| 1 | A | 2782 | G | N1-C6-O6 | -5.94 | 116.33 | 119.90 |
| 1 | A | 808 | G | N3-C4-C5 | -5.94 | 125.63 | 128.60 |
| 1 | A | 1758 | G | N1-C6-O6 | 5.94 | 123.47 | 119.90 |
| 1 | A | 2259 | G | N1-C6-O6 | 5.94 | 123.47 | 119.90 |
| 1 | A | 777 | A | N3-C4-C5 | -5.94 | 122.64 | 126.80 |
| 1 | A | 2103 | C | C5-C4-N4 | 5.94 | 124.36 | 120.20 |
| 1 | A | 2069 | G | C5-C6-O6 | -5.94 | 125.04 | 128.60 |
| 1 | A | 2828 | C | N3-C2-O2 | 5.94 | 126.06 | 121.90 |
| 1 | A | 2723 | C | N3-C2-O2 | -5.93 | 117.75 | 121.90 |
| 1 | A | 205 | G | N9-C4-C5 | -5.93 | 103.03 | 105.40 |
| 1 | A | 1789 | A | N7-C8-N9 | -5.93 | 110.83 | 113.80 |
| 1 | A | 2290 | G | C2-N3-C4 | -5.93 | 108.93 | 111.90 |
| 1 | A | 191 | A | C6-N1-C2 | -5.93 | 115.04 | 118.60 |
| 1 | A | 616 | G | N9-C4-C5 | -5.93 | 103.03 | 105.40 |
| 1 | A | 2079 | U | C4-C5-C6 | 5.93 | 123.26 | 119.70 |
| 1 | A | 2329 | G | N7-C8-N9 | -5.93 | 110.14 | 113.10 |
| 1 | A | 2514 | U | C5-C6-N1 | -5.93 | 119.74 | 122.70 |
| 1 | A | 1571 | A | N1-C6-N6 | -5.92 | 115.05 | 118.60 |
| 1 | A | 546 | C | C2-N1-C1' | 5.92 | 125.31 | 118.80 |
| 1 | A | 2028 | U | N3-C4-C5 | 5.92 | 118.15 | 114.60 |
| 1 | A | 2823 | A | C4-C5-N7 | 5.92 | 113.66 | 110.70 |
| 1 | A | 799 | G | N1-C6-O6 | -5.92 | 116.35 | 119.90 |
| 1 | A | 2260 | C | N1-C2-O2 | -5.92 | 115.35 | 118.90 |
| 1 | A | 2585 | U | N3-C2-O2 | -5.92 | 118.06 | 122.20 |
| 1 | A | 766 | C | N3-C4-C5 | -5.92 | 119.53 | 121.90 |
| 1 | A | 1027 | A | C5-C6-N6 | -5.92 | 118.97 | 123.70 |
| 1 | A | 2110 | G | C8-N9-C1' | -5.92 | 119.31 | 127.00 |
| 1 | A | 2191 | G | C4-C5-N7 | 5.91 | 113.16 | 110.80 |
| 1 | A | 329 | G | C8-N9-C4 | 5.91 | 108.76 | 106.40 |
| 1 | A | 1778 | U | C4-C5-C6 | 5.91 | 123.25 | 119.70 |
| 1 | A | 463 | G | C8-N9-C1' | 5.90 | 134.68 | 127.00 |
| 1 | A | 330 | A | N1-C2-N3 | 5.90 | 132.25 | 129.30 |
| 1 | A | 2346 | A | C5-C6-N6 | 5.89 | 128.41 | 123.70 |
| 1 | A | 1566 | A | C8-N9-C4 | -5.89 | 103.44 | 105.80 |
| 1 | A | 1835 | G | N3-C4-C5 | -5.89 | 125.65 | 128.60 |
| 1 | A | 2319 | G | C5-N7-C8 | -5.89 | 101.35 | 104.30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 1 | A | 462 | C | N3-C4-N4 | -5.89 | 113.88 | 118.00 |
| 1 | A | 1488 | G | N7-C8-N9 | 5.89 | 116.05 | 113.10 |
| 1 | A | 2042 | A | C8-N9-C4 | 5.89 | 108.16 | 105.80 |
| 1 | A | 2606 | C | C6-N1-C2 | 5.89 | 122.66 | 120.30 |
| 1 | A | 56 | A | N1-C6-N6 | -5.89 | 115.07 | 118.60 |
| 1 | A | 2098 | U | C2-N3-C4 | 5.89 | 130.53 | 127.00 |
| 1 | A | 1275 | A | C2-N3-C4 | -5.89 | 107.66 | 110.60 |
| 1 | A | 2569 | G | N3-C4-N9 | 5.88 | 129.53 | 126.00 |
| 1 | A | 2035 | G | N9-C4-C5 | 5.88 | 107.75 | 105.40 |
| 1 | A | 2203 | U | C5-C6-N1 | -5.88 | 119.76 | 122.70 |
| 1 | A | 2733 | A | C4-C5-N7 | 5.88 | 113.64 | 110.70 |
| 1 | A | 509 | C | C4-C5-C6 | 5.88 | 120.34 | 117.40 |
| 1 | A | 1190 | G | N1-C2-N3 | 5.88 | 127.43 | 123.90 |
| 1 | A | 272(C) | G | N1-C6-O6 | 5.88 | 123.43 | 119.90 |
| 1 | A | 768 | G | C4-C5-N7 | -5.88 | 108.45 | 110.80 |
| 1 | A | 2719 | G | N9-C4-C5 | -5.88 | 103.05 | 105.40 |
| 1 | A | 981 | A | N7-C8-N9 | -5.87 | 110.86 | 113.80 |
| 1 | A | 1962 | C | C5-C6-N1 | 5.87 | 123.94 | 121.00 |
| 1 | A | 1980 | G | C8-N9-C4 | -5.87 | 104.05 | 106.40 |
| 1 | A | 2346 | A | C4-C5-N7 | -5.87 | 107.76 | 110.70 |
| 1 | A | 2023 | G | C5-C6-N1 | 5.87 | 114.44 | 111.50 |
| 1 | A | 2755 | C | N3-C4-N4 | 5.87 | 122.11 | 118.00 |
| 1 | A | 125 | G | N3-C2-N2 | 5.87 | 124.00 | 119.90 |
| 1 | A | 1983 | C | N1-C2-O2 | -5.87 | 115.38 | 118.90 |
| 1 | A | 2682 | U | C2-N1-C1' | 5.86 | 124.73 | 117.70 |
| 1 | A | 56 | A | C4-C5-C6 | -5.86 | 114.07 | 117.00 |
| 1 | A | 1602 | U | N1-C2-N3 | 5.86 | 118.41 | 114.90 |
| 1 | A | 333 | G | C5-C6-O6 | -5.85 | 125.09 | 128.60 |
| 1 | A | 1124 | C | C6-N1-C2 | 5.85 | 122.64 | 120.30 |
| 1 | A | 513 | A | C6-N1-C2 | -5.85 | 115.09 | 118.60 |
| 1 | A | 847 | U | C6-N1-C1' | 5.85 | 129.39 | 121.20 |
| 1 | A | 914 | C | N1-C2-O2 | 5.85 | 122.41 | 118.90 |
| 1 | A | 2496 | C | N3-C4-C5 | 5.85 | 124.24 | 121.90 |
| 1 | A | 2599 | G | C4-C5-N7 | -5.85 | 108.46 | 110.80 |
| 1 | A | 117 | G | C8-N9-C4 | 5.84 | 108.74 | 106.40 |
| 1 | A | 1286 | A | C8-N9-C4 | -5.84 | 103.46 | 105.80 |
| 1 | A | 1493 | C | N1-C2-O2 | 5.84 | 122.41 | 118.90 |
| 1 | A | 271(M) | G | N3-C4-C5 | -5.84 | 125.68 | 128.60 |
| 1 | A | 1665 | A | N9-C4-C5 | 5.84 | 108.14 | 105.80 |
| 1 | A | 2046 | G | C5-C6-O6 | -5.84 | 125.10 | 128.60 |
| 1 | A | 2318 | G | C2-N3-C4 | 5.83 | 114.82 | 111.90 |
| 1 | A | 1640 | C | C5-C6-N1 | 5.83 | 123.92 | 121.00 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 1 | A | 2306 | C | C6-N1-C1' | -5.83 | 113.80 | 120.80 |
| 1 | A | 768 | G | N1-C2-N3 | 5.83 | 127.40 | 123.90 |
| 1 | A | 2088 | G | C2-N3-C4 | -5.83 | 108.98 | 111.90 |
| 1 | A | 801 | G | N1-C6-O6 | -5.83 | 116.40 | 119.90 |
| 1 | A | 2628 | C | C6-N1-C2 | 5.83 | 122.63 | 120.30 |
| 1 | A | 772 | C | N3-C4-N4 | 5.82 | 122.08 | 118.00 |
| 1 | A | 1954 | G | N1-C2-N2 | 5.82 | 121.44 | 116.20 |
| 1 | A | 2818 | G | N1-C2-N3 | 5.82 | 127.39 | 123.90 |
| 1 | A | 2387 | U | C5-C6-N1 | -5.82 | 119.79 | 122.70 |
| 1 | A | 1779 | U | C6-N1-C1' | 5.82 | 129.35 | 121.20 |
| 1 | A | 2174 | C | C6-N1-C2 | -5.82 | 117.97 | 120.30 |
| 1 | A | 2439 | A | N1-C6-N6 | -5.82 | 115.11 | 118.60 |
| 1 | A | 1275 | A | C8-N9-C4 | 5.81 | 108.12 | 105.80 |
| 1 | A | 1328 | G | C5-C6-N1 | 5.81 | 114.41 | 111.50 |
| 1 | A | 1997 | G | C5-N7-C8 | 5.81 | 107.20 | 104.30 |
| 1 | A | 2719 | G | N3-C2-N2 | 5.81 | 123.97 | 119.90 |
| 1 | A | 271(K) | U | N1-C2-O2 | 5.80 | 126.86 | 122.80 |
| 1 | A | 2599 | G | N1-C6-O6 | -5.80 | 116.42 | 119.90 |
| 1 | A | 2017 | U | N1-C2-N3 | 5.80 | 118.38 | 114.90 |
| 1 | A | 2031 | A | C6-C5-N7 | -5.80 | 128.24 | 132.30 |
| 1 | A | 2383 | G | N3-C4-N9 | 5.80 | 129.48 | 126.00 |
| 1 | A | 1124 | C | N3-C2-O2 | 5.80 | 125.96 | 121.90 |
| 2 | B | 55 | U | N3-C4-C5 | -5.80 | 111.12 | 114.60 |
| 1 | A | 2062 | A | C8-N9-C4 | -5.79 | 103.48 | 105.80 |
| 2 | B | 115 | G | N9-C4-C5 | -5.79 | 103.08 | 105.40 |
| 1 | A | 1329 | U | N1-C2-N3 | 5.79 | 118.38 | 114.90 |
| 1 | A | 2519 | U | C5-C6-N1 | -5.79 | 119.81 | 122.70 |
| 1 | A | 1112 | G | N3-C4-C5 | 5.79 | 131.49 | 128.60 |
| 1 | A | 2021 | C | N1-C2-O2 | -5.79 | 115.43 | 118.90 |
| 1 | A | 2434 | A | C2-N3-C4 | -5.79 | 107.71 | 110.60 |
| 1 | A | 2840 | C | N3-C4-C5 | 5.79 | 124.21 | 121.90 |
| 1 | A | 1259 | G | C5-C6-O6 | 5.78 | 132.07 | 128.60 |
| 1 | A | 698 | C | C5-C4-N4 | -5.78 | 116.15 | 120.20 |
| 1 | A | 2070 | G | N1-C6-O6 | -5.78 | 116.43 | 119.90 |
| 1 | A | 23 | G | N1-C6-O6 | -5.78 | 116.43 | 119.90 |
| 1 | A | 1328 | G | N9-C4-C5 | -5.78 | 103.09 | 105.40 |
| 1 | A | 664 | C | C5-C6-N1 | -5.78 | 118.11 | 121.00 |
| 1 | A | 1597 | A | C8-N9-C4 | -5.78 | 103.49 | 105.80 |
| 1 | A | 1678 | G | C8-N9-C4 | -5.78 | 104.09 | 106.40 |
| 1 | A | 2296 | U | C1'-O4'-C4' | -5.78 | 105.28 | 109.90 |
| 1 | A | 74 | A | C8-N9-C4 | -5.78 | 103.49 | 105.80 |
| 1 | A | 253 | C | N1-C2-O2 | -5.78 | 115.44 | 118.90 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 1 | A | 2682 | U | N3-C2-O2 | -5.78 | 118.16 | 122.20 |
| 1 | A | 669 | G | N7-C8-N9 | -5.77 | 110.21 | 113.10 |
| 1 | A | 864 | G | C8-N9-C4 | -5.77 | 104.09 | 106.40 |
| 1 | A | 1813 | G | N3-C4-C5 | -5.77 | 125.71 | 128.60 |
| 1 | A | 2191 | G | N1-C6-O6 | 5.77 | 123.36 | 119.90 |
| 1 | A | 2441 | C | C2-N3-C4 | -5.77 | 117.01 | 119.90 |
| 1 | A | 2607 | G | C6-C5-N7 | -5.77 | 126.94 | 130.40 |
| 1 | A | 194 | G | C6-C5-N7 | -5.77 | 126.94 | 130.40 |
| 1 | A | 197 | A | C5-C6-N6 | -5.77 | 119.08 | 123.70 |
| 2 | B | 49 | C | N3-C2-O2 | 5.77 | 125.94 | 121.90 |
| 1 | A | 272(B) | G | C8-N9-C4 | 5.76 | 108.71 | 106.40 |
| 1 | A | 672 | C | C4-C5-C6 | 5.76 | 120.28 | 117.40 |
| 1 | A | 27 | G | C4-C5-N7 | -5.76 | 108.50 | 110.80 |
| 1 | A | 1775 | U | C5-C6-N1 | -5.76 | 119.82 | 122.70 |
| 1 | A | 260 | G | C2-N3-C4 | -5.76 | 109.02 | 111.90 |
| 1 | A | 391 | G | C8-N9-C1' | -5.76 | 119.52 | 127.00 |
| 1 | A | 1429 | G | C4-N9-C1' | 5.76 | 133.98 | 126.50 |
| 1 | A | 2028 | U | N3-C4-O4 | -5.76 | 115.37 | 119.40 |
| 1 | A | 185 | U | C2-N3-C4 | -5.75 | 123.55 | 127.00 |
| 1 | A | 85 | G | N1-C2-N3 | 5.75 | 127.35 | 123.90 |
| 1 | A | 1128 | A | N7-C8-N9 | -5.75 | 110.92 | 113.80 |
| 1 | A | 1327 | C | C6-N1-C2 | -5.75 | 118.00 | 120.30 |
| 1 | A | 2079 | U | C5-C6-N1 | -5.75 | 119.82 | 122.70 |
| 1 | A | 2253 | G | C5-C6-O6 | -5.75 | 125.15 | 128.60 |
| 1 | A | 2563 | U | C5-C6-N1 | -5.75 | 119.82 | 122.70 |
| 1 | A | 2700 | C | C5-C4-N4 | -5.75 | 116.17 | 120.20 |
| 1 | A | 658 | C | N3-C2-O2 | -5.75 | 117.88 | 121.90 |
| 1 | A | 1204 | A | N9-C4-C5 | -5.75 | 103.50 | 105.80 |
| 1 | A | 2075 | U | N1-C2-N3 | 5.75 | 118.35 | 114.90 |
| 1 | A | 2123 | G | N9-C4-C5 | 5.75 | 107.70 | 105.40 |
| 1 | A | 2271 | G | N3-C4-N9 | 5.74 | 129.44 | 126.00 |
| 1 | A | 2690 | C | N1-C2-O2 | -5.74 | 115.45 | 118.90 |
| 1 | A | 472 | A | N9-C4-C5 | 5.74 | 108.10 | 105.80 |
| 1 | A | 1760 | A | C5-C6-N6 | 5.74 | 128.29 | 123.70 |
| 1 | A | 1938 | A | N1-C6-N6 | 5.74 | 122.04 | 118.60 |
| 27 | 5 | 19 | ARG | NE-CZ-NH1 | -5.74 | 117.43 | 120.30 |
| 1 | A | 2062 | A | C5-N7-C8 | -5.73 | 101.03 | 103.90 |
| 1 | A | 2307 | G | C8-N9-C4 | -5.73 | 104.11 | 106.40 |
| 1 | A | 1558 | A | C5-C6-N1 | -5.73 | 114.84 | 117.70 |
| 1 | A | 2262 | U | N3-C2-O2 | 5.73 | 126.21 | 122.20 |
| 1 | A | 2570 | G | N3-C4-N9 | -5.73 | 122.56 | 126.00 |
| 1 | A | 751 | A | C4-C5-C6 | 5.72 | 119.86 | 117.00 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | A | 2113 | U | C5-C6-N1 | 5.72 | 125.56 | 122.70 |
| 1 | A | 2808 | U | C6-N1-C2 | 5.72 | 124.44 | 121.00 |
| 1 | A | 176 | G | C8-N9-C4 | -5.72 | 104.11 | 106.40 |
| 2 | B | 101 | G | C4-C5-N7 | 5.72 | 113.09 | 110.80 |
| 1 | A | 1365 | A | C4-C5-N7 | 5.72 | 113.56 | 110.70 |
| 1 | A | 741 | G | N3-C2-N2 | 5.72 | 123.90 | 119.90 |
| 1 | A | 777 | A | C6-N1-C2 | -5.72 | 115.17 | 118.60 |
| 1 | A | 2556 | C | N1-C2-O2 | -5.72 | 115.47 | 118.90 |
| 1 | A | 2611 | U | N1-C2-N3 | 5.72 | 118.33 | 114.90 |
| 1 | A | 777 | A | C5-C6-N6 | 5.71 | 128.27 | 123.70 |
| 1 | A | 1030 | G | C4-C5-N7 | 5.71 | 113.08 | 110.80 |
| 1 | A | 2088 | G | N1-C2-N3 | 5.71 | 127.33 | 123.90 |
| 2 | B | 54 | G | C8-N9-C1' | 5.71 | 134.43 | 127.00 |
| 1 | A | 1939 | U | N3-C4-C5 | 5.71 | 118.03 | 114.60 |
| 1 | A | 2239 | G | C5-N7-C8 | 5.71 | 107.16 | 104.30 |
| 1 | A | 1825 | A | C6-N1-C2 | -5.71 | 115.18 | 118.60 |
| 1 | A | 2590 | A | N1-C6-N6 | -5.71 | 115.18 | 118.60 |
| 1 | A | 2791 | C | C6-N1-C2 | -5.70 | 118.02 | 120.30 |
| 1 | A | 1204 | A | O4'-C1'-N9 | 5.70 | 112.76 | 108.20 |
| 1 | A | 2104 | G | N3-C4-N9 | 5.70 | 129.42 | 126.00 |
| 1 | A | 2560 | C | N3-C4-C5 | 5.70 | 124.18 | 121.90 |
| 1 | A | 97 | C | N3-C4-N4 | -5.70 | 114.01 | 118.00 |
| 1 | A | 2894 | G | N7-C8-N9 | 5.70 | 115.95 | 113.10 |
| 1 | A | 1047 | G | C6-C5-N7 | -5.69 | 126.98 | 130.40 |
| 1 | A | 1315 | C | C2-N3-C4 | -5.69 | 117.05 | 119.90 |
| 1 | A | 1563 | G | N9-C4-C5 | -5.69 | 103.12 | 105.40 |
| 1 | A | 794 | G | C4-C5-N7 | -5.69 | 108.52 | 110.80 |
| 1 | A | 2490 | G | C8-N9-C4 | 5.69 | 108.68 | 106.40 |
| 1 | A | 444 | C | C6-N1-C2 | 5.69 | 122.58 | 120.30 |
| 1 | A | 788 | A | C4-C5-C6 | 5.69 | 119.84 | 117.00 |
| 1 | A | 985 | C | C6-N1-C2 | 5.69 | 122.58 | 120.30 |
| 1 | A | 2012 | G | C4-C5-N7 | 5.69 | 113.08 | 110.80 |
| 1 | A | 2306 | C | C2-N3-C4 | 5.69 | 122.74 | 119.90 |
| 1 | A | 2427 | C | N1-C2-O2 | -5.69 | 115.49 | 118.90 |
| 1 | A | 45 | C | C5-C6-N1 | -5.69 | 118.16 | 121.00 |
| 1 | A | 1107 | G | N3-C4-C5 | -5.68 | 125.76 | 128.60 |
| 1 | A | 2883 | A | N1-C6-N6 | 5.68 | 122.01 | 118.60 |
| 1 | A | 154 | G | C5-C6-O6 | -5.68 | 125.19 | 128.60 |
| 1 | A | 2383 | G | C4-N9-C1' | 5.68 | 133.88 | 126.50 |
| 1 | A | 267 | C | C5-C6-N1 | -5.68 | 118.16 | 121.00 |
| 1 | A | 1966 | A | N1-C2-N3 | -5.68 | 126.46 | 129.30 |
| 1 | A | 2365 | G | C5-C6-N1 | 5.68 | 114.34 | 111.50 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | A | 788 | A | N1-C6-N6 | 5.67 | 122.00 | 118.60 |
| 1 | A | 2508 | G | C6-C5-N7 | 5.67 | 133.81 | 130.40 |
| 1 | A | 1307 | A | C8-N9-C4 | 5.67 | 108.07 | 105.80 |
| 1 | A | 1022 | G | N3-C2-N2 | -5.67 | 115.93 | 119.90 |
| 1 | A | 1313 | U | C2-N1-C1' | 5.67 | 124.50 | 117.70 |
| 1 | A | 2191 | G | N3-C4-N9 | 5.67 | 129.40 | 126.00 |
| 1 | A | 1023 | U | N3-C4-O4 | -5.66 | 115.44 | 119.40 |
| 1 | A | 2789 | C | C6-N1-C2 | 5.66 | 122.56 | 120.30 |
| 1 | A | 2287 | A | C4-C5-N7 | 5.66 | 113.53 | 110.70 |
| 1 | A | 2151 | G | N1-C6-O6 | 5.66 | 123.29 | 119.90 |
| 1 | A | 1329 | U | N1-C2-O2 | -5.66 | 118.84 | 122.80 |
| 1 | A | 2503 | A | C6-C5-N7 | -5.66 | 128.34 | 132.30 |
| 1 | A | 2435 | A | N1-C6-N6 | -5.65 | 115.21 | 118.60 |
| 1 | A | 774 | A | N7-C8-N9 | 5.65 | 116.62 | 113.80 |
| 1 | A | 1328 | G | C8-N9-C4 | 5.65 | 108.66 | 106.40 |
| 1 | A | 2487 | G | C6-C5-N7 | -5.65 | 127.01 | 130.40 |
| 1 | A | 36 | G | C4-C5-N7 | -5.65 | 108.54 | 110.80 |
| 1 | A | 1112 | G | C8-N9-C4 | 5.65 | 108.66 | 106.40 |
| 1 | A | 1112 | G | C4-N9-C1' | -5.65 | 119.16 | 126.50 |
| 1 | A | 2147 | G | C8-N9-C4 | -5.65 | 104.14 | 106.40 |
| 1 | A | 981 | A | C8-N9-C4 | 5.64 | 108.06 | 105.80 |
| 1 | A | 959 | A | C8-N9-C4 | -5.64 | 103.54 | 105.80 |
| 1 | A | 1372 | U | C5-C6-N1 | -5.64 | 119.88 | 122.70 |
| 1 | A | 1825 | A | C5-C6-N6 | -5.64 | 119.19 | 123.70 |
| 1 | A | 2456 | C | N1-C2-N3 | -5.64 | 115.25 | 119.20 |
| 1 | A | 1647 | G | C8-N9-C4 | 5.64 | 108.66 | 106.40 |
| 1 | A | 1790 | C | C2-N3-C4 | -5.64 | 117.08 | 119.90 |
| 1 | A | 2828 | C | C6-N1-C2 | 5.64 | 122.56 | 120.30 |
| 1 | A | 781 | A | N7-C8-N9 | -5.63 | 110.98 | 113.80 |
| 1 | A | 2894 | G | C4-N9-C1' | 5.63 | 133.82 | 126.50 |
| 1 | A | 453 | C | C5-C6-N1 | -5.63 | 118.19 | 121.00 |
| 1 | A | 1257 | C | C6-N1-C2 | -5.63 | 118.05 | 120.30 |
| 1 | A | 2627 | G | C8-N9-C4 | 5.63 | 108.65 | 106.40 |
| 1 | A | 26 | G | C8-N9-C4 | -5.62 | 104.15 | 106.40 |
| 1 | A | 1258 | C | N3-C4-C5 | 5.62 | 124.15 | 121.90 |
| 1 | A | 1318 | C | N3-C4-C5 | 5.62 | 124.15 | 121.90 |
| 1 | A | 1653 | G | N1-C2-N3 | 5.62 | 127.27 | 123.90 |
| 1 | A | 2548 | G | N3-C2-N2 | -5.62 | 115.96 | 119.90 |
| 1 | A | 125 | G | C2-N3-C4 | 5.62 | 114.71 | 111.90 |
| 1 | A | 187 | G | C5-N7-C8 | -5.62 | 101.49 | 104.30 |
| 1 | A | 2027 | G | N1-C6-O6 | -5.62 | 116.53 | 119.90 |
| 1 | A | 2583 | G | C5-C6-O6 | -5.62 | 125.23 | 128.60 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | A | 686 | G | N9-C4-C5 | -5.62 | 103.15 | 105.40 |
| 1 | A | 2488 | A | N1-C2-N3 | 5.62 | 132.11 | 129.30 |
| 1 | A | 41 | C | C2-N3-C4 | -5.62 | 117.09 | 119.90 |
| 1 | A | 1382 | G | C6-C5-N7 | -5.62 | 127.03 | 130.40 |
| 1 | A | 2124 | G | N3-C4-N9 | -5.62 | 122.63 | 126.00 |
| 1 | A | 1668 | A | N1-C6-N6 | -5.61 | 115.23 | 118.60 |
| 1 | A | 1779 | U | N3-C2-O2 | -5.61 | 118.27 | 122.20 |
| 1 | A | 2297 | C | N1-C2-O2 | -5.61 | 115.53 | 118.90 |
| 1 | A | 1835 | G | N3-C4-N9 | 5.61 | 129.37 | 126.00 |
| 1 | A | 1958 | C | N1-C2-O2 | -5.61 | 115.53 | 118.90 |
| 2 | B | 26 | A | C8-N9-C4 | 5.61 | 108.04 | 105.80 |
| 1 | A | 2002 | G | N3-C4-C5 | -5.61 | 125.80 | 128.60 |
| 1 | A | 26 | G | N3-C4-C5 | -5.61 | 125.80 | 128.60 |
| 1 | A | 1271 | G | C6-C5-N7 | -5.61 | 127.04 | 130.40 |
| 1 | A | 1614 | A | N9-C4-C5 | 5.61 | 108.04 | 105.80 |
| 1 | A | 1121 | C | C5-C6-N1 | -5.60 | 118.20 | 121.00 |
| 1 | A | 766 | C | C6-N1-C2 | -5.60 | 118.06 | 120.30 |
| 1 | A | 989 | G | C8-N9-C4 | 5.60 | 108.64 | 106.40 |
| 1 | A | 2822 | G | N7-C8-N9 | -5.60 | 110.30 | 113.10 |
| 1 | A | 494 | G | C5-C6-O6 | 5.60 | 131.96 | 128.60 |
| 1 | A | 2037 | G | N1-C6-O6 | -5.60 | 116.54 | 119.90 |
| 1 | A | 1628 | G | C4-N9-C1' | 5.60 | 133.78 | 126.50 |
| 1 | A | 1638 | C | C2-N3-C4 | -5.60 | 117.10 | 119.90 |
| 1 | A | 2870 | C | C6-N1-C2 | -5.60 | 118.06 | 120.30 |
| 1 | A | 1274 | A | N1-C6-N6 | 5.60 | 121.96 | 118.60 |
| 1 | A | 2710 | C | C5-C6-N1 | -5.59 | 118.20 | 121.00 |
| 1 | A | 1940 | U | N1-C2-O2 | -5.59 | 118.89 | 122.80 |
| 1 | A | 2048 | G | C8-N9-C4 | -5.59 | 104.16 | 106.40 |
| 1 | A | 2823 | A | C5-C6-N6 | -5.59 | 119.23 | 123.70 |
| 1 | A | 1351 | C | N1-C2-O2 | -5.59 | 115.55 | 118.90 |
| 1 | A | 1611 | C | N1-C2-O2 | -5.59 | 115.55 | 118.90 |
| 1 | A | 1773 | A | C8-N9-C4 | 5.59 | 108.03 | 105.80 |
| 1 | A | 563 | G | N1-C6-O6 | 5.58 | 123.25 | 119.90 |
| 1 | A | 1954 | G | C5-C6-N1 | -5.58 | 108.71 | 111.50 |
| 1 | A | 54 | G | C5-C6-O6 | -5.58 | 125.25 | 128.60 |
| 1 | A | 690 | G | C2-N3-C4 | 5.58 | 114.69 | 111.90 |
| 1 | A | 933 | A | C2-N3-C4 | -5.58 | 107.81 | 110.60 |
| 1 | A | 2324 | C | N3-C4-C5 | 5.58 | 124.13 | 121.90 |
| 1 | A | 2446 | G | C8-N9-C4 | 5.58 | 108.63 | 106.40 |
| 1 | A | 195 | A | C2-N3-C4 | -5.58 | 107.81 | 110.60 |
| 1 | A | 2258 | C | N3-C4-N4 | 5.58 | 121.91 | 118.00 |
| 1 | A | 2508 | G | C5-C6-N1 | 5.58 | 114.29 | 111.50 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | A | 1786 | A | C2-N3-C4 | -5.58 | 107.81 | 110.60 |
| 1 | A | 209 | C | N3-C4-C5 | 5.58 | 124.13 | 121.90 |
| 1 | A | 1374 | G | C6-C5-N7 | -5.58 | 127.05 | 130.40 |
| 1 | A | 1204 | A | C8-N9-C1' | -5.58 | 117.66 | 127.70 |
| 1 | A | 2638 | G | N3-C2-N2 | 5.57 | 123.80 | 119.90 |
| 1 | A | 478 | A | N9-C4-C5 | 5.57 | 108.03 | 105.80 |
| 1 | A | 542 | C | C3'-C2'-C1' | -5.57 | 97.04 | 101.50 |
| 1 | A | 1204 | A | C5-C6-N1 | -5.57 | 114.92 | 117.70 |
| 1 | A | 1374 | G | N1-C6-O6 | 5.57 | 123.24 | 119.90 |
| 1 | A | 1675 | C | N3-C4-C5 | -5.57 | 119.67 | 121.90 |
| 1 | A | 97 | C | N3-C2-O2 | -5.57 | 118.00 | 121.90 |
| 1 | A | 774 | A | C8-N9-C4 | -5.57 | 103.57 | 105.80 |
| 1 | A | 1647 | G | N1-C6-O6 | 5.57 | 123.24 | 119.90 |
| 1 | A | 2022 | U | N3-C4-O4 | 5.57 | 123.30 | 119.40 |
| 1 | A | 2755 | C | C2-N1-C1' | 5.57 | 124.92 | 118.80 |
| 1 | A | 487 | C | N3-C4-C5 | -5.57 | 119.67 | 121.90 |
| 1 | A | 741 | G | N1-C2-N2 | -5.56 | 111.19 | 116.20 |
| 1 | A | 1984 | G | N1-C6-O6 | -5.56 | 116.56 | 119.90 |
| 1 | A | 2347 | C | N1-C2-O2 | 5.56 | 122.24 | 118.90 |
| 10 | O | 8 | LEU | CA-CB-CG | 5.56 | 128.09 | 115.30 |
| 1 | A | 1762 | A | N3-C4-C5 | -5.56 | 122.91 | 126.80 |
| 1 | A | 1939 | U | C2-N3-C4 | -5.56 | 123.66 | 127.00 |
| 1 | A | 133 | C | C5-C6-N1 | -5.56 | 118.22 | 121.00 |
| 1 | A | 1359 | A | N9-C4-C5 | 5.56 | 108.02 | 105.80 |
| 1 | A | 2055 | C | C6-N1-C2 | 5.56 | 122.52 | 120.30 |
| 1 | A | 202 | U | C5-C6-N1 | -5.56 | 119.92 | 122.70 |
| 1 | A | 791 | C | N1-C2-N3 | 5.56 | 123.09 | 119.20 |
| 1 | A | 245 | G | N1-C6-O6 | 5.55 | 123.23 | 119.90 |
| 1 | A | 763 | G | N1-C6-O6 | -5.55 | 116.57 | 119.90 |
| 1 | A | 2103 | C | N3-C4-C5 | -5.55 | 119.68 | 121.90 |
| 1 | A | 2585 | U | C2-N1-C1' | 5.55 | 124.36 | 117.70 |
| 1 | A | 1794 | U | N1-C2-N3 | 5.55 | 118.23 | 114.90 |
| 1 | A | 215 | G | C8-N9-C4 | 5.54 | 108.62 | 106.40 |
| 1 | A | 992 | C | N1-C2-O2 | -5.54 | 115.57 | 118.90 |
| 1 | A | 1708 | C | C6-N1-C2 | 5.54 | 122.52 | 120.30 |
| 2 | B | 47 | C | C6-N1-C2 | 5.54 | 122.52 | 120.30 |
| 1 | A | 2437 | U | C5-C6-N1 | -5.54 | 119.93 | 122.70 |
| 1 | A | 218 | A | C5-C6-N6 | 5.54 | 128.13 | 123.70 |
| 1 | A | 311 | A | N1-C6-N6 | 5.54 | 121.92 | 118.60 |
| 1 | A | 804 | A | N1-C2-N3 | 5.54 | 132.07 | 129.30 |
| 1 | A | 1990 | C | N3-C2-O2 | -5.53 | 118.03 | 121.90 |
| 1 | A | 2006 | C | C6-N1-C2 | -5.53 | 118.09 | 120.30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 1 | A | 2489 | G | C2-N3-C4 | -5.53 | 109.13 | 111.90 |
| 1 | A | 2730 | C | N3-C4-C5 | 5.53 | 124.11 | 121.90 |
| 1 | A | 2322 | A | N1-C2-N3 | 5.53 | 132.06 | 129.30 |
| 1 | A | 74 | A | C5-N7-C8 | -5.53 | 101.14 | 103.90 |
| 1 | A | 45 | C | N1-C2-N3 | 5.53 | 123.07 | 119.20 |
| 1 | A | 195 | A | N1-C2-N3 | 5.53 | 132.06 | 129.30 |
| 1 | A | 2325 | G | C8-N9-C1' | -5.53 | 119.82 | 127.00 |
| 1 | A | 1252 | G | C4-N9-C1' | -5.52 | 119.32 | 126.50 |
| 1 | A | 1370 | C | N1-C2-O2 | -5.52 | 115.59 | 118.90 |
| 1 | A | 2689 | U | N3-C2-O2 | -5.52 | 118.34 | 122.20 |
| 1 | A | 54 | G | C8-N9-C4 | -5.52 | 104.19 | 106.40 |
| 1 | A | 249 | C | C5-C4-N4 | 5.52 | 124.06 | 120.20 |
| 1 | A | 113 | G | C2-N3-C4 | -5.51 | 109.14 | 111.90 |
| 1 | A | 286 | C | N3-C2-O2 | -5.51 | 118.04 | 121.90 |
| 1 | A | 1393 | A | N1-C6-N6 | -5.51 | 115.29 | 118.60 |
| 1 | A | 2306 | C | N1-C2-O2 | 5.51 | 122.21 | 118.90 |
| 1 | A | 425 | G | N3-C4-N9 | 5.51 | 129.31 | 126.00 |
| 1 | A | 1955 | U | C2-N3-C4 | -5.51 | 123.69 | 127.00 |
| 1 | A | 2481 | G | N1-C6-O6 | 5.51 | 123.21 | 119.90 |
| 1 | A | 652(E) | G | C6-N1-C2 | 5.51 | 128.41 | 125.10 |
| 2 | B | 75 | G | C5-C6-O6 | -5.51 | 125.29 | 128.60 |
| 1 | A | 1289 | C | C6-N1-C2 | 5.51 | 122.50 | 120.30 |
| 1 | A | 1383 | C | N1-C2-O2 | -5.51 | 115.60 | 118.90 |
| 1 | A | 580 | C | N3-C4-C5 | 5.50 | 124.10 | 121.90 |
| 1 | A | 1539 | G | C8-N9-C1' | -5.50 | 119.84 | 127.00 |
| 1 | A | 1558 | A | N1-C6-N6 | 5.50 | 121.90 | 118.60 |
| 1 | A | 672 | C | C2-N3-C4 | -5.50 | 117.15 | 119.90 |
| 1 | A | 1616 | A | C4-C5-N7 | 5.50 | 113.45 | 110.70 |
| 1 | A | 2791 | C | N3-C2-O2 | -5.50 | 118.05 | 121.90 |
| 1 | A | 2004 | G | C8-N9-C4 | 5.50 | 108.60 | 106.40 |
| 1 | A | 2104 | G | N9-C4-C5 | -5.50 | 103.20 | 105.40 |
| 1 | A | 2503 | A | C8-N9-C4 | -5.50 | 103.60 | 105.80 |
| 1 | A | 143 | G | N1-C6-O6 | 5.49 | 123.20 | 119.90 |
| 1 | A | 1022 | G | C4-C5-N7 | -5.49 | 108.60 | 110.80 |
| 1 | A | 23 | G | C5-C6-N1 | 5.49 | 114.24 | 111.50 |
| 1 | A | 434 | U | C6-N1-C2 | 5.49 | 124.29 | 121.00 |
| 1 | A | 1397 | U | N1-C2-O2 | 5.49 | 126.64 | 122.80 |
| 1 | A | 1613 | G | C8-N9-C4 | -5.49 | 104.21 | 106.40 |
| 1 | A | 1962 | C | C4-C5-C6 | -5.49 | 114.66 | 117.40 |
| 1 | A | 1493 | C | N3-C2-O2 | -5.48 | 118.06 | 121.90 |
| 1 | A | 1990 | C | N1-C2-N3 | 5.48 | 123.04 | 119.20 |
| 1 | A | 2307 | G | C4-N9-C1' | 5.48 | 133.63 | 126.50 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | A | 452 | G | C5-C6-N1 | 5.48 | 114.24 | 111.50 |
| 1 | A | 509 | C | N3-C2-O2 | -5.48 | 118.06 | 121.90 |
| 1 | A | 2147 | G | N7-C8-N9 | 5.48 | 115.84 | 113.10 |
| 1 | A | 2467 | C | C6-N1-C2 | -5.48 | 118.11 | 120.30 |
| 1 | A | 783 | A | C2-N3-C4 | 5.48 | 113.34 | 110.60 |
| 1 | A | 2742 | C | C4-C5-C6 | 5.48 | 120.14 | 117.40 |
| 1 | A | 605 | C | C2-N3-C4 | -5.48 | 117.16 | 119.90 |
| 1 | A | 2570 | G | C5-C6-N1 | -5.48 | 108.76 | 111.50 |
| 1 | A | 1108 | U | C6-N1-C2 | -5.47 | 117.72 | 121.00 |
| 1 | A | 2100 | G | N3-C4-N9 | 5.47 | 129.28 | 126.00 |
| 1 | A | 567 | A | C2-N3-C4 | -5.47 | 107.86 | 110.60 |
| 1 | A | 2002 | G | C5-C6-N1 | 5.47 | 114.23 | 111.50 |
| 1 | A | 2461 | C | C5-C4-N4 | 5.47 | 124.03 | 120.20 |
| 1 | A | 265 | A | C6-C5-N7 | -5.47 | 128.47 | 132.30 |
| 1 | A | 749 | C | C6-N1-C1' | -5.46 | 114.24 | 120.80 |
| 1 | A | 1339 | G | N7-C8-N9 | 5.46 | 115.83 | 113.10 |
| 1 | A | 482 | A | C6-N1-C2 | -5.46 | 115.32 | 118.60 |
| 1 | A | 2426 | A | C5-N7-C8 | -5.46 | 101.17 | 103.90 |
| 1 | A | 1788 | C | C6-N1-C2 | -5.46 | 118.11 | 120.30 |
| 1 | A | 2007 | C | N3-C2-O2 | -5.46 | 118.08 | 121.90 |
| 1 | A | 279 | C | C6-N1-C2 | -5.46 | 118.12 | 120.30 |
| 1 | A | 785 | G | N1-C6-O6 | -5.46 | 116.62 | 119.90 |
| 1 | A | 800 | A | C6-N1-C2 | -5.46 | 115.32 | 118.60 |
| 1 | A | 2239 | G | C4-C5-N7 | -5.46 | 108.62 | 110.80 |
| 1 | A | 1823 | G | N3-C2-N2 | -5.46 | 116.08 | 119.90 |
| 1 | A | 2552 | U | N1-C2-O2 | -5.46 | 118.98 | 122.80 |
| 13 | R | 114 | VAL | CB-CA-C | -5.46 | 101.03 | 111.40 |
| 1 | A | 1642 | G | C6-N1-C2 | -5.45 | 121.83 | 125.10 |
| 1 | A | 2585 | U | N1-C2-O2 | 5.45 | 126.62 | 122.80 |
| 1 | A | 1581 | G | C5-C6-O6 | -5.45 | 125.33 | 128.60 |
| 1 | A | 1616 | A | C5-N7-C8 | -5.45 | 101.17 | 103.90 |
| 1 | A | 1747 | G | C8-N9-C4 | 5.45 | 108.58 | 106.40 |
| 1 | A | 2002 | G | N1-C6-O6 | -5.45 | 116.63 | 119.90 |
| 1 | A | 197 | A | C5-C6-N1 | 5.45 | 120.42 | 117.70 |
| 1 | A | 774 | A | N1-C2-N3 | 5.44 | 132.02 | 129.30 |
| 1 | A | 2616 | C | C5-C4-N4 | 5.44 | 124.01 | 120.20 |
| 1 | A | 1127 | A | C6-C5-N7 | -5.44 | 128.49 | 132.30 |
| 1 | A | 2145 | C | C5-C6-N1 | 5.44 | 123.72 | 121.00 |
| 3 | D | 33 | LEU | CA-CB-CG | -5.44 | 102.79 | 115.30 |
| 1 | A | 2458 | G | C5-C6-O6 | -5.44 | 125.34 | 128.60 |
| 9 | N | 23 | LEU | O-C-N | -5.44 | 113.95 | 123.20 |
| 1 | A | 614 | U | N3-C4-O4 | -5.44 | 115.59 | 119.40 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 1 | A | 1286 | A | N9-C4-C5 | 5.43 | 107.97 | 105.80 |
| 1 | A | 2502 | G | N3-C2-N2 | 5.43 | 123.70 | 119.90 |
| 1 | A | 271(M) | G | N3-C4-N9 | 5.43 | 129.26 | 126.00 |
| 1 | A | 461 | C | C6-N1-C2 | 5.43 | 122.47 | 120.30 |
| 1 | A | 807 | U | C5-C4-O4 | -5.43 | 122.64 | 125.90 |
| 1 | A | 2444 | G | N1-C2-N3 | 5.43 | 127.16 | 123.90 |
| 1 | A | 2881 | C | N1-C2-O2 | -5.43 | 115.64 | 118.90 |
| 1 | A | 1332 | G | C4-C5-N7 | 5.43 | 112.97 | 110.80 |
| 1 | A | 512 | G | C5-C6-O6 | 5.43 | 131.86 | 128.60 |
| 1 | A | 1784 | A | N7-C8-N9 | -5.43 | 111.08 | 113.80 |
| 1 | A | 2617 | C | C2-N3-C4 | -5.43 | 117.19 | 119.90 |
| 1 | A | 2733 | A | C5-N7-C8 | -5.43 | 101.19 | 103.90 |
| 1 | A | 52 | A | C8-N9-C4 | -5.42 | 103.63 | 105.80 |
| 1 | A | 1618 | A | N1-C6-N6 | -5.42 | 115.35 | 118.60 |
| 1 | A | 411 | G | N3-C2-N2 | 5.42 | 123.69 | 119.90 |
| 1 | A | 775 | G | C5-C6-O6 | 5.42 | 131.85 | 128.60 |
| 1 | A | 949 | C | C2-N3-C4 | -5.42 | 117.19 | 119.90 |
| 1 | A | 2045 | C | C2-N3-C4 | -5.42 | 117.19 | 119.90 |
| 1 | A | 945 | A | N9-C4-C5 | -5.42 | 103.63 | 105.80 |
| 1 | A | 1190 | G | C2-N3-C4 | -5.42 | 109.19 | 111.90 |
| 1 | A | 311 | A | N9-C4-C5 | -5.41 | 103.64 | 105.80 |
| 1 | A | 797 | C | C4-C5-C6 | 5.41 | 120.11 | 117.40 |
| 1 | A | 1990 | C | C6-N1-C2 | -5.41 | 118.14 | 120.30 |
| 1 | A | 2408 | U | N3-C4-O4 | 5.41 | 123.19 | 119.40 |
| 1 | A | 2423 | U | C2-N1-C1' | -5.41 | 111.21 | 117.70 |
| 1 | A | 107 | C | C5-C4-N4 | -5.41 | 116.41 | 120.20 |
| 1 | A | 1597 | A | N1-C6-N6 | -5.41 | 115.35 | 118.60 |
| 1 | A | 2098 | U | N1-C2-O2 | 5.41 | 126.58 | 122.80 |
| 1 | A | 141 | A | C4-C5-C6 | 5.41 | 119.70 | 117.00 |
| 1 | A | 1252 | G | C8-N9-C1' | 5.41 | 134.03 | 127.00 |
| 1 | A | 1534 | U | C5-C4-O4 | -5.41 | 122.66 | 125.90 |
| 1 | A | 1602 | U | N3-C4-C5 | -5.41 | 111.36 | 114.60 |
| 1 | A | 1117 | G | C5-C6-O6 | -5.40 | 125.36 | 128.60 |
| 1 | A | 2361 | A | N9-C4-C5 | -5.40 | 103.64 | 105.80 |
| 1 | A | 438 | G | C8-N9-C4 | -5.40 | 104.24 | 106.40 |
| 1 | A | 444 | C | N3-C4-N4 | -5.40 | 114.22 | 118.00 |
| 1 | A | 1568 | G | C5-C6-N1 | 5.40 | 114.20 | 111.50 |
| 1 | A | 1600 | C | C5-C6-N1 | -5.40 | 118.30 | 121.00 |
| 1 | A | 2779 | U | N3-C4-C5 | 5.40 | 117.84 | 114.60 |
| 1 | A | 389 | G | C8-N9-C4 | 5.40 | 108.56 | 106.40 |
| 1 | A | 1004 | C | N1-C2-O2 | -5.40 | 115.66 | 118.90 |
| 1 | A | 2099 | U | C5-C6-N1 | 5.40 | 125.40 | 122.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | A | 2848 | G | N3-C4-C5 | -5.40 | 125.90 | 128.60 |
| 1 | A | 1653 | G | P-O3'-C3' | 5.40 | 126.18 | 119.70 |
| 1 | A | 2185 | C | C5-C4-N4 | 5.40 | 123.98 | 120.20 |
| 1 | A | 265 | A | C2-N3-C4 | -5.39 | 107.90 | 110.60 |
| 1 | A | 750 | A | C8-N9-C4 | -5.39 | 103.64 | 105.80 |
| 1 | A | 1831 | G | C8-N9-C4 | -5.39 | 104.24 | 106.40 |
| 1 | A | 1792 | G | C5-N7-C8 | 5.39 | 107.00 | 104.30 |
| 1 | A | 2567 | G | C6-N1-C2 | -5.39 | 121.87 | 125.10 |
| 1 | A | 335 | C | N1-C2-O2 | -5.39 | 115.67 | 118.90 |
| 1 | A | 2021 | C | C5-C6-N1 | -5.39 | 118.31 | 121.00 |
| 1 | A | 2450 | A | N7-C8-N9 | -5.39 | 111.11 | 113.80 |
| 1 | A | 286 | C | N1-C2-O2 | 5.38 | 122.13 | 118.90 |
| 1 | A | 1284 | A | N1-C6-N6 | 5.38 | 121.83 | 118.60 |
| 1 | A | 1615 | C | C5-C6-N1 | 5.38 | 123.69 | 121.00 |
| 1 | A | 1758 | G | C4-C5-N7 | 5.38 | 112.95 | 110.80 |
| 1 | A | 2075 | U | C2-N3-C4 | -5.38 | 123.77 | 127.00 |
| 1 | A | 2122 | U | C2-N3-C4 | 5.38 | 130.23 | 127.00 |
| 1 | A | 191 | A | C5-C6-N1 | 5.38 | 120.39 | 117.70 |
| 1 | A | 2304 | G | C8-N9-C4 | -5.38 | 104.25 | 106.40 |
| 1 | A | 154 | G | N1-C6-O6 | 5.38 | 123.13 | 119.90 |
| 1 | A | 419 | C | C6-N1-C2 | 5.38 | 122.45 | 120.30 |
| 1 | A | 1365 | A | C5-C6-N6 | -5.38 | 119.40 | 123.70 |
| 1 | A | 1845 | G | N1-C6-O6 | -5.38 | 116.67 | 119.90 |
| 1 | A | 2010 | G | C8-N9-C4 | -5.37 | 104.25 | 106.40 |
| 1 | A | 2450 | A | C8-N9-C4 | 5.37 | 107.95 | 105.80 |
| 2 | B | 54 | G | N3-C4-N9 | -5.37 | 122.78 | 126.00 |
| 1 | A | 276 | A | C8-N9-C4 | -5.37 | 103.65 | 105.80 |
| 1 | A | 463 | G | N3-C4-N9 | -5.37 | 122.78 | 126.00 |
| 1 | A | 291 | C | N3-C2-O2 | 5.37 | 125.66 | 121.90 |
| 1 | A | 827 | U | N3-C2-O2 | 5.37 | 125.96 | 122.20 |
| 1 | A | 1780 | A | N1-C2-N3 | 5.37 | 131.98 | 129.30 |
| 1 | A | 602 | G | C5-C6-O6 | -5.37 | 125.38 | 128.60 |
| 1 | A | 1017 | G | C5-C6-O6 | -5.37 | 125.38 | 128.60 |
| 1 | A | 2042 | A | C2-N3-C4 | -5.37 | 107.92 | 110.60 |
| 1 | A | 978 | G | N7-C8-N9 | -5.36 | 110.42 | 113.10 |
| 1 | A | 2244 | U | N3-C2-O2 | -5.36 | 118.44 | 122.20 |
| 1 | A | 2542 | A | C8-N9-C4 | 5.36 | 107.94 | 105.80 |
| 1 | A | 1617 | C | C2-N3-C4 | -5.36 | 117.22 | 119.90 |
| 1 | A | 2322 | A | C8-N9-C4 | -5.36 | 103.66 | 105.80 |
| 1 | A | 788 | A | C6-C5-N7 | -5.36 | 128.55 | 132.30 |
| 1 | A | 1614 | A | N1-C6-N6 | -5.36 | 115.38 | 118.60 |
| 1 | A | 1773 | A | C5-C6-N1 | 5.36 | 120.38 | 117.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | A | 1792 | G | C4-C5-N7 | -5.36 | 108.66 | 110.80 |
| 1 | A | 534 | U | C5-C6-N1 | -5.36 | 120.02 | 122.70 |
| 1 | A | 398 | G | C2-N3-C4 | -5.35 | 109.22 | 111.90 |
| 1 | A | 2063 | C | N3-C2-O2 | 5.35 | 125.65 | 121.90 |
| 1 | A | 2379 | G | C4-C5-N7 | 5.35 | 112.94 | 110.80 |
| 1 | A | 2449 | U | C2-N3-C4 | -5.35 | 123.79 | 127.00 |
| 20 | Y | 76 | CYS | CA-CB-SG | 5.35 | 123.63 | 114.00 |
| 1 | A | 784 | A | C4-N9-C1' | -5.35 | 116.67 | 126.30 |
| 1 | A | 1582 | C | C6-N1-C2 | 5.35 | 122.44 | 120.30 |
| 1 | A | 1320 | C | N3-C4-N4 | 5.34 | 121.74 | 118.00 |
| 1 | A | 1381 | G | C5-C6-O6 | 5.34 | 131.81 | 128.60 |
| 1 | A | 1338 | G | C2-N3-C4 | 5.34 | 114.57 | 111.90 |
| 1 | A | 1671 | U | N3-C4-C5 | 5.34 | 117.81 | 114.60 |
| 1 | A | 76 | C | C2-N3-C4 | -5.34 | 117.23 | 119.90 |
| 1 | A | 1581 | G | C4-C5-N7 | 5.34 | 112.94 | 110.80 |
| 26 | 4 | 42 | PHE | C-N-CA | 5.34 | 135.05 | 121.70 |
| 1 | A | 2709 | G | N3-C4-C5 | -5.34 | 125.93 | 128.60 |
| 1 | A | 2142 | C | C5-C6-N1 | 5.34 | 123.67 | 121.00 |
| 1 | A | 2661 | G | N9-C4-C5 | -5.34 | 103.27 | 105.40 |
| 1 | A | 799 | G | C4-C5-N7 | -5.33 | 108.67 | 110.80 |
| 1 | A | 2449 | U | C5-C4-O4 | -5.33 | 122.70 | 125.90 |
| 1 | A | 1331 | A | N7-C8-N9 | -5.33 | 111.13 | 113.80 |
| 1 | A | 1651 | G | N1-C6-O6 | 5.33 | 123.10 | 119.90 |
| 1 | A | 143 | G | C4-N9-C1' | -5.33 | 119.57 | 126.50 |
| 1 | A | 375 | C | C5-C6-N1 | -5.33 | 118.34 | 121.00 |
| 1 | A | 1325 | G | C8-N9-C4 | 5.33 | 108.53 | 106.40 |
| 1 | A | 1925 | C | N1-C2-O2 | -5.33 | 115.70 | 118.90 |
| 13 | R | 72 | ASP | CB-CG-OD2 | 5.33 | 123.09 | 118.30 |
| 2 | B | 101 | G | N3-C2-N2 | 5.32 | 123.63 | 119.90 |
| 1 | A | 2699 | C | C6-N1-C2 | 5.32 | 122.43 | 120.30 |
| 1 | A | 140 | G | N9-C4-C5 | -5.32 | 103.27 | 105.40 |
| 1 | A | 2332 | U | N3-C4-O4 | -5.32 | 115.68 | 119.40 |
| 1 | A | 2593 | U | N1-C2-N3 | 5.32 | 118.09 | 114.90 |
| 1 | A | 1010 | A | C8-N9-C4 | 5.32 | 107.93 | 105.80 |
| 1 | A | 2070 | G | N1-C2-N2 | -5.32 | 111.41 | 116.20 |
| 1 | A | 987 | G | N3-C4-N9 | -5.32 | 122.81 | 126.00 |
| 1 | A | 1272 | A | C5-C6-N6 | 5.32 | 127.95 | 123.70 |
| 1 | A | 1381 | G | N1-C6-O6 | -5.32 | 116.71 | 119.90 |
| 1 | A | 203 | C | C5-C4-N4 | -5.32 | 116.48 | 120.20 |
| 1 | A | 2680 | C | N3-C4-C5 | 5.32 | 124.03 | 121.90 |
| 1 | A | 2344 | U | N1-C2-O2 | 5.31 | 126.52 | 122.80 |
| 1 | A | 1207 | C | C5-C4-N4 | -5.31 | 116.48 | 120.20 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | A | 2010 | G | C5-C6-N1 | -5.31 | 108.84 | 111.50 |
| 1 | A | 2195 | C | C2-N1-C1' | -5.31 | 112.96 | 118.80 |
| 1 | A | 1374 | G | C2-N3-C4 | -5.31 | 109.25 | 111.90 |
| 1 | A | 275 | G | C4-N9-C1' | 5.31 | 133.40 | 126.50 |
| 1 | A | 333 | G | C6-C5-N7 | -5.31 | 127.22 | 130.40 |
| 1 | A | 1681 | G | N1-C6-O6 | 5.31 | 123.08 | 119.90 |
| 1 | A | 1763 | G | N7-C8-N9 | -5.31 | 110.45 | 113.10 |
| 1 | A | 121 | G | C4-C5-N7 | 5.30 | 112.92 | 110.80 |
| 1 | A | 1800 | C | C4-C5-C6 | 5.30 | 120.05 | 117.40 |
| 1 | A | 978 | G | N9-C4-C5 | -5.30 | 103.28 | 105.40 |
| 1 | A | 2643 | G | N1-C6-O6 | 5.30 | 123.08 | 119.90 |
| 1 | A | 39 | C | N3-C2-O2 | -5.30 | 118.19 | 121.90 |
| 1 | A | 74 | A | N7-C8-N9 | 5.30 | 116.45 | 113.80 |
| 1 | A | 574 | C | C5-C4-N4 | 5.30 | 123.91 | 120.20 |
| 1 | A | 1970 | A | N9-C4-C5 | -5.30 | 103.68 | 105.80 |
| 8 | I | 72 | LEU | CA-CB-CG | 5.30 | 127.49 | 115.30 |
| 1 | A | 511 | U | C2-N1-C1' | 5.30 | 124.06 | 117.70 |
| 1 | A | 844 | C | C6-N1-C2 | 5.30 | 122.42 | 120.30 |
| 1 | A | 2181 | G | N3-C2-N2 | 5.30 | 123.61 | 119.90 |
| 1 | A | 2591 | C | N3-C4-C5 | 5.30 | 124.02 | 121.90 |
| 1 | A | 860 | U | N1-C2-N3 | 5.29 | 118.08 | 114.90 |
| 1 | A | 2380 | C | N3-C4-C5 | 5.29 | 124.02 | 121.90 |
| 1 | A | 1247 | A | N7-C8-N9 | -5.29 | 111.15 | 113.80 |
| 1 | A | 252 | G | N1-C2-N3 | 5.29 | 127.08 | 123.90 |
| 1 | A | 1831 | G | N1-C2-N2 | -5.29 | 111.44 | 116.20 |
| 1 | A | 305 | U | C6-N1-C2 | 5.29 | 124.17 | 121.00 |
| 1 | A | 1415 | U | C5-C4-O4 | 5.29 | 129.07 | 125.90 |
| 1 | A | 103 | A | N7-C8-N9 | -5.29 | 111.16 | 113.80 |
| 1 | A | 377 | C | C5-C4-N4 | -5.29 | 116.50 | 120.20 |
| 1 | A | 953 | A | N1-C6-N6 | -5.29 | 115.43 | 118.60 |
| 1 | A | 2883 | A | C5-C6-N6 | -5.29 | 119.47 | 123.70 |
| 1 | A | 178 | G | N1-C6-O6 | -5.29 | 116.73 | 119.90 |
| 1 | A | 1382 | G | N9-C4-C5 | -5.29 | 103.29 | 105.40 |
| 1 | A | 1794 | U | N3-C4-C5 | 5.29 | 117.77 | 114.60 |
| 1 | A | 2383 | G | N3-C4-C5 | -5.29 | 125.96 | 128.60 |
| 1 | A | 440 | G | N1-C6-O6 | -5.28 | 116.73 | 119.90 |
| 1 | A | 682 | G | C2-N3-C4 | -5.28 | 109.26 | 111.90 |
| 1 | A | 2587 | A | N7-C8-N9 | 5.28 | 116.44 | 113.80 |
| 1 | A | 1788 | C | C2-N1-C1' | 5.28 | 124.61 | 118.80 |
| 1 | A | 2027 | G | C6-N1-C2 | -5.28 | 121.93 | 125.10 |
| 1 | A | 2513 | G | C8-N9-C4 | -5.28 | 104.29 | 106.40 |
| 1 | A | 995 | C | N3-C4-C5 | -5.28 | 119.79 | 121.90 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | A | 1227 | G | N1-C6-O6 | 5.28 | 123.07 | 119.90 |
| 1 | A | 2826 | A | N1-C6-N6 | -5.28 | 115.43 | 118.60 |
| 1 | A | 1389 | G | N3-C4-C5 | -5.28 | 125.96 | 128.60 |
| 1 | A | 1698 | A | N1-C2-N3 | 5.27 | 131.94 | 129.30 |
| 1 | A | 337 | C | C6-N1-C2 | 5.27 | 122.41 | 120.30 |
| 1 | A | 570 | G | C4-C5-N7 | 5.27 | 112.91 | 110.80 |
| 1 | A | 602 | G | N9-C4-C5 | -5.27 | 103.29 | 105.40 |
| 1 | A | 764 | A | C4-C5-C6 | -5.27 | 114.36 | 117.00 |
| 1 | A | 1118 | C | C6-N1-C2 | -5.27 | 118.19 | 120.30 |
| 1 | A | 2678 | C | C5-C6-N1 | -5.27 | 118.36 | 121.00 |
| 1 | A | 386 | G | N1-C2-N2 | -5.27 | 111.46 | 116.20 |
| 1 | A | 602 | G | C8-N9-C4 | 5.27 | 108.51 | 106.40 |
| 1 | A | 949 | C | C5-C4-N4 | -5.27 | 116.51 | 120.20 |
| 1 | A | 221 | A | N7-C8-N9 | 5.26 | 116.43 | 113.80 |
| 1 | A | 686 | G | C4-C5-N7 | 5.26 | 112.91 | 110.80 |
| 1 | A | 756 | C | C6-N1-C2 | -5.26 | 118.19 | 120.30 |
| 1 | A | 1153 | C | N3-C2-O2 | 5.26 | 125.58 | 121.90 |
| 1 | A | 2193 | G | N3-C4-C5 | 5.26 | 131.23 | 128.60 |
| 1 | A | 2568 | C | C5-C6-N1 | -5.26 | 118.37 | 121.00 |
| 1 | A | 686 | G | N3-C2-N2 | 5.26 | 123.58 | 119.90 |
| 1 | A | 1977 | A | C5-N7-C8 | 5.26 | 106.53 | 103.90 |
| 1 | A | 14 | A | N7-C8-N9 | 5.26 | 116.43 | 113.80 |
| 1 | A | 2252 | G | C8-N9-C4 | 5.26 | 108.50 | 106.40 |
| 2 | B | 84 | C | C2-N1-C1' | -5.26 | 113.02 | 118.80 |
| 1 | A | 303 | U | N3-C4-O4 | -5.25 | 115.72 | 119.40 |
| 1 | A | 1617 | C | C6-N1-C2 | 5.25 | 122.40 | 120.30 |
| 1 | A | 1703 | G | C4-N9-C1' | 5.25 | 133.33 | 126.50 |
| 1 | A | 2383 | G | N1-C2-N2 | -5.25 | 111.47 | 116.20 |
| 1 | A | 866 | A | C5-N7-C8 | -5.25 | 101.27 | 103.90 |
| 1 | A | 1049 | C | N1-C2-O2 | 5.25 | 122.05 | 118.90 |
| 1 | A | 1962 | C | N3-C2-O2 | 5.25 | 125.58 | 121.90 |
| 1 | A | 1992 | G | P-O3'-C3' | 5.25 | 126.00 | 119.70 |
| 1 | A | 2033 | A | C2-N3-C4 | 5.25 | 113.23 | 110.60 |
| 1 | A | 1569 | A | N1-C6-N6 | -5.25 | 115.45 | 118.60 |
| 1 | A | 791 | C | C2-N3-C4 | -5.25 | 117.28 | 119.90 |
| 1 | A | 1348 | G | C4-C5-N7 | 5.25 | 112.90 | 110.80 |
| 1 | A | 1698 | A | C5-C6-N1 | -5.25 | 115.08 | 117.70 |
| 1 | A | 334 | C | C6-N1-C2 | 5.25 | 122.40 | 120.30 |
| 1 | A | 221 | A | N9-C4-C5 | 5.24 | 107.90 | 105.80 |
| 1 | A | 834 | C | C6-N1-C2 | -5.24 | 118.20 | 120.30 |
| 1 | A | 928 | G | C8-N9-C1' | -5.24 | 120.18 | 127.00 |
| 1 | A | 1120 | G | N1-C6-O6 | 5.24 | 123.05 | 119.90 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | A | 1244 | G | N3-C4-C5 | 5.24 | 131.22 | 128.60 |
| 1 | A | 2325 | G | C4-N9-C1' | 5.24 | 133.32 | 126.50 |
| 1 | A | 1389 | G | N1-C2-N2 | -5.24 | 111.48 | 116.20 |
| 1 | A | 192 | C | C2-N1-C1' | -5.24 | 113.04 | 118.80 |
| 1 | A | 946 | G | C8-N9-C4 | 5.24 | 108.49 | 106.40 |
| 1 | A | 1319 | G | C4-N9-C1' | 5.23 | 133.30 | 126.50 |
| 1 | A | 2452 | C | N3-C4-C5 | -5.23 | 119.81 | 121.90 |
| 1 | A | 261 | G | C5-C6-N1 | 5.23 | 114.12 | 111.50 |
| 1 | A | 1544 | A | N1-C6-N6 | -5.23 | 115.46 | 118.60 |
| 1 | A | 2052 | G | N7-C8-N9 | -5.23 | 110.48 | 113.10 |
| 1 | A | 671 | C | C2-N3-C4 | -5.23 | 117.29 | 119.90 |
| 1 | A | 673 | C | C5-C6-N1 | -5.23 | 118.39 | 121.00 |
| 1 | A | 1168 | G | C5-C6-O6 | -5.23 | 125.46 | 128.60 |
| 1 | A | 2619 | C | N3-C4-C5 | 5.23 | 123.99 | 121.90 |
| 1 | A | 72 | U | C5-C6-N1 | -5.22 | 120.09 | 122.70 |
| 1 | A | 777 | A | C5-N7-C8 | 5.22 | 106.51 | 103.90 |
| 1 | A | 2543 | G | C5-C6-N1 | -5.22 | 108.89 | 111.50 |
| 2 | B | 109 | C | C6-N1-C2 | 5.22 | 122.39 | 120.30 |
| 1 | A | 1259 | G | C5-N7-C8 | 5.22 | 106.91 | 104.30 |
| 1 | A | 2047 | U | C5-C4-O4 | -5.22 | 122.77 | 125.90 |
| 1 | A | 738 | G | N1-C6-O6 | -5.22 | 116.77 | 119.90 |
| 1 | A | 2340 | G | C8-N9-C4 | 5.22 | 108.49 | 106.40 |
| 1 | A | 2538 | C | C2-N1-C1' | -5.22 | 113.06 | 118.80 |
| 1 | A | 303 | U | C5-C4-O4 | 5.22 | 129.03 | 125.90 |
| 1 | A | 84 | A | C5-C6-N1 | 5.21 | 120.31 | 117.70 |
| 1 | A | 495 | G | C8-N9-C4 | 5.21 | 108.49 | 106.40 |
| 1 | A | 571 | A | N1-C6-N6 | 5.21 | 121.73 | 118.60 |
| 1 | A | 1605 | C | N3-C2-O2 | -5.21 | 118.25 | 121.90 |
| 1 | A | 1631 | C | N1-C2-O2 | -5.21 | 115.77 | 118.90 |
| 1 | A | 2084 | C | C5-C6-N1 | -5.21 | 118.39 | 121.00 |
| 1 | A | 2523 | G | C8-N9-C4 | -5.21 | 104.32 | 106.40 |
| 1 | A | 2554 | U | N1-C2-O2 | -5.21 | 119.15 | 122.80 |
| 1 | A | 1576 | U | N3-C2-O2 | -5.21 | 118.55 | 122.20 |
| 1 | A | 398 | G | C5-C6-O6 | -5.21 | 125.47 | 128.60 |
| 1 | A | 665 | C | N3-C2-O2 | -5.21 | 118.25 | 121.90 |
| 1 | A | 734 | A | C2-N3-C4 | -5.21 | 108.00 | 110.60 |
| 1 | A | 768 | G | C5-N7-C8 | 5.21 | 106.90 | 104.30 |
| 1 | A | 2791 | C | C6-N1-C1' | -5.21 | 114.55 | 120.80 |
| 1 | A | 602 | G | N1-C6-O6 | 5.21 | 123.02 | 119.90 |
| 1 | A | 794 | G | C5-N7-C8 | 5.21 | 106.90 | 104.30 |
| 1 | A | 680 | G | C2-N3-C4 | -5.21 | 109.30 | 111.90 |
| 1 | A | 2512 | C | C6-N1-C2 | 5.21 | 122.38 | 120.30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 1 | A | 749 | C | C2-N1-C1' | 5.20 | 124.52 | 118.80 |
| 1 | A | 811 | U | N1-C2-N3 | 5.20 | 118.02 | 114.90 |
| 1 | A | 2501 | C | C6-N1-C2 | 5.20 | 122.38 | 120.30 |
| 1 | A | 645 | C | C6-N1-C2 | -5.20 | 118.22 | 120.30 |
| 1 | A | 1558 | A | N1-C2-N3 | 5.20 | 131.90 | 129.30 |
| 1 | A | 2504 | U | N3-C4-O4 | -5.20 | 115.76 | 119.40 |
| 1 | A | 195 | A | C6-C5-N7 | -5.20 | 128.66 | 132.30 |
| 1 | A | 2449 | U | C2-N1-C1' | 5.20 | 123.94 | 117.70 |
| 1 | A | 696 | G | C2-N3-C4 | 5.20 | 114.50 | 111.90 |
| 1 | A | 658 | C | C6-N1-C2 | -5.20 | 118.22 | 120.30 |
| 1 | A | 1544 | A | N9-C4-C5 | 5.20 | 107.88 | 105.80 |
| 1 | A | 2241 | A | N1-C2-N3 | 5.20 | 131.90 | 129.30 |
| 1 | A | 2378 | A | C8-N9-C4 | 5.20 | 107.88 | 105.80 |
| 1 | A | 271(J) | C | C6-N1-C2 | 5.19 | 122.38 | 120.30 |
| 1 | A | 1315 | C | N3-C2-O2 | -5.19 | 118.27 | 121.90 |
| 1 | A | 599 | G | N1-C6-O6 | 5.19 | 123.01 | 119.90 |
| 1 | A | 825 | C | N3-C4-C5 | -5.19 | 119.82 | 121.90 |
| 1 | A | 265 | A | C5-C6-N1 | -5.19 | 115.11 | 117.70 |
| 1 | A | 1200 | C | N3-C2-O2 | 5.19 | 125.53 | 121.90 |
| 1 | A | 391 | G | C4-N9-C1' | 5.19 | 133.24 | 126.50 |
| 1 | A | 252 | G | C6-N1-C2 | -5.18 | 121.99 | 125.10 |
| 1 | A | 2176 | A | N1-C2-N3 | -5.18 | 126.71 | 129.30 |
| 1 | A | 812 | C | N3-C4-C5 | -5.18 | 119.83 | 121.90 |
| 1 | A | 866 | A | N9-C4-C5 | -5.18 | 103.73 | 105.80 |
| 1 | A | 77 | C | N3-C4-C5 | 5.18 | 123.97 | 121.90 |
| 1 | A | 212 | G | C2-N3-C4 | -5.18 | 109.31 | 111.90 |
| 1 | A | 527 | C | C5-C4-N4 | 5.18 | 123.83 | 120.20 |
| 1 | A | 2638 | G | N1-C2-N2 | -5.18 | 111.54 | 116.20 |
| 1 | A | 1800 | C | N1-C2-N3 | 5.18 | 122.83 | 119.20 |
| 1 | A | 2045 | C | C6-N1-C2 | 5.18 | 122.37 | 120.30 |
| 1 | A | 272(H) | C | C6-N1-C1' | -5.18 | 114.59 | 120.80 |
| 1 | A | 333 | G | C4-C5-N7 | 5.18 | 112.87 | 110.80 |
| 1 | A | 1935 | G | C5-C6-N1 | 5.18 | 114.09 | 111.50 |
| 1 | A | 815 | C | C5-C4-N4 | -5.17 | 116.58 | 120.20 |
| 1 | A | 2319 | G | N7-C8-N9 | 5.17 | 115.69 | 113.10 |
| 1 | A | 1328 | G | N1-C6-O6 | 5.17 | 123.00 | 119.90 |
| 1 | A | 2073 | C | N3-C4-C5 | 5.17 | 123.97 | 121.90 |
| 1 | A | 2730 | C | N3-C4-N4 | -5.17 | 114.38 | 118.00 |
| 1 | A | 94 | C | C6-N1-C2 | -5.17 | 118.23 | 120.30 |
| 1 | A | 784 | A | C8-N9-C1' | 5.17 | 137.01 | 127.70 |
| 1 | A | 1607 | C | C5-C4-N4 | -5.17 | 116.58 | 120.20 |
| 1 | A | 2031 | A | C2-N3-C4 | -5.17 | 108.01 | 110.60 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 1 | A | 2325 | G | C6-C5-N7 | -5.17 | 127.30 | 130.40 |
| 1 | A | 1985 | G | C8-N9-C4 | 5.17 | 108.47 | 106.40 |
| 1 | A | 1142(A) | A | N7-C8-N9 | 5.17 | 116.38 | 113.80 |
| 1 | A | 1602 | U | N3-C2-O2 | -5.17 | 118.58 | 122.20 |
| 1 | A | 139(A) | G | C6-C5-N7 | -5.17 | 127.30 | 130.40 |
| 1 | A | 2607 | G | C4-N9-C1' | 5.17 | 133.22 | 126.50 |
| 1 | A | 474 | G | N3-C4-C5 | -5.17 | 126.02 | 128.60 |
| 1 | A | 2567 | G | C5-C6-O6 | -5.17 | 125.50 | 128.60 |
| 1 | A | 399 | G | N1-C2-N2 | -5.16 | 111.55 | 116.20 |
| 1 | A | 2439 | A | C8-N9-C4 | -5.16 | 103.73 | 105.80 |
| 1 | A | 194 | G | C5-C6-O6 | -5.16 | 125.50 | 128.60 |
| 1 | A | 1999 | C | C6-N1-C2 | 5.16 | 122.36 | 120.30 |
| 1 | A | 446 | G | N1-C6-O6 | 5.16 | 123.00 | 119.90 |
| 1 | A | 672 | C | C6-N1-C2 | 5.16 | 122.36 | 120.30 |
| 1 | A | 1023 | U | C2-N3-C4 | -5.16 | 123.90 | 127.00 |
| 1 | A | 2709 | G | N3-C4-N9 | 5.16 | 129.10 | 126.00 |
| 1 | A | 1125 | G | N3-C4-N9 | -5.16 | 122.91 | 126.00 |
| 1 | A | 1222 | C | C2-N1-C1' | -5.16 | 113.13 | 118.80 |
| 1 | A | 2226 | C | N3-C4-C5 | 5.16 | 123.96 | 121.90 |
| 1 | A | 1039 | G | C4-N9-C1' | -5.16 | 119.80 | 126.50 |
| 1 | A | 1219 | G | C8-N9-C4 | 5.16 | 108.46 | 106.40 |
| 1 | A | 1642 | G | N1-C2-N3 | 5.16 | 126.99 | 123.90 |
| 1 | A | 72 | U | C6-N1-C2 | 5.16 | 124.09 | 121.00 |
| 1 | A | 1142(A) | A | N1-C6-N6 | 5.16 | 121.69 | 118.60 |
| 1 | A | 2063 | C | C2-N3-C4 | 5.16 | 122.48 | 119.90 |
| 1 | A | 39 | C | N1-C2-O2 | 5.15 | 121.99 | 118.90 |
| 1 | A | 506 | G | N3-C4-C5 | 5.15 | 131.18 | 128.60 |
| 1 | A | 2565 | A | C8-N9-C4 | 5.15 | 107.86 | 105.80 |
| 1 | A | 2689 | U | P-O3'-C3' | 5.15 | 125.88 | 119.70 |
| 1 | A | 375 | C | N1-C2-O2 | -5.15 | 115.81 | 118.90 |
| 1 | A | 2147 | G | C5-C6-O6 | -5.15 | 125.51 | 128.60 |
| 1 | A | 269 | U | C6-N1-C1' | -5.15 | 114.00 | 121.20 |
| 1 | A | 1219 | G | N9-C4-C5 | -5.15 | 103.34 | 105.40 |
| 1 | A | 1524 | G | C5-C6-O6 | 5.15 | 131.69 | 128.60 |
| 1 | A | 1788 | C | N3-C2-O2 | -5.15 | 118.30 | 121.90 |
| 1 | A | 2015 | A | C6-N1-C2 | 5.15 | 121.69 | 118.60 |
| 1 | A | 2007 | C | N1-C2-N3 | 5.14 | 122.80 | 119.20 |
| 1 | A | 128 | C | C2-N1-C1' | -5.14 | 113.14 | 118.80 |
| 1 | A | 653 | A | N1-C6-N6 | 5.14 | 121.69 | 118.60 |
| 1 | A | 330 | A | N9-C4-C5 | -5.14 | 103.74 | 105.80 |
| 1 | A | 381 | G | N3-C4-C5 | -5.14 | 126.03 | 128.60 |
| 1 | A | 1333 | C | C4-C5-C6 | -5.14 | 114.83 | 117.40 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | A | 1674 | G | N1-C6-O6 | -5.14 | 116.81 | 119.90 |
| 1 | A | 1259 | G | N1-C2-N2 | -5.14 | 111.58 | 116.20 |
| 1 | A | 1681 | G | C4-C5-N7 | 5.14 | 112.86 | 110.80 |
| 1 | A | 2779 | U | N3-C4-O4 | -5.13 | 115.81 | 119.40 |
| 1 | A | 2399 | G | N1-C6-O6 | -5.13 | 116.82 | 119.90 |
| 1 | A | 1415 | U | C2-N1-C1' | -5.13 | 111.54 | 117.70 |
| 1 | A | 1210 | A | C5-C6-N6 | -5.13 | 119.60 | 123.70 |
| 1 | A | 1693 | U | C5-C6-N1 | -5.13 | 120.14 | 122.70 |
| 1 | A | 41 | C | N3-C4-C5 | 5.13 | 123.95 | 121.90 |
| 1 | A | 398 | G | C6-C5-N7 | -5.13 | 127.32 | 130.40 |
| 1 | A | 1999 | C | C5-C4-N4 | -5.13 | 116.61 | 120.20 |
| 1 | A | 2192 | G | N3-C4-C5 | -5.13 | 126.04 | 128.60 |
| 1 | A | 54 | G | C5-N7-C8 | -5.12 | 101.74 | 104.30 |
| 1 | A | 28 | A | N1-C6-N6 | 5.12 | 121.67 | 118.60 |
| 1 | A | 41 | C | C5-C6-N1 | -5.12 | 118.44 | 121.00 |
| 1 | A | 804 | A | N9-C4-C5 | 5.12 | 107.85 | 105.80 |
| 1 | A | 2319 | G | C4-C5-N7 | 5.12 | 112.85 | 110.80 |
| 1 | A | 131 | G | N9-C4-C5 | -5.12 | 103.35 | 105.40 |
| 1 | A | 192 | C | N1-C2-O2 | -5.12 | 115.83 | 118.90 |
| 1 | A | 1136 | G | C5-C6-O6 | -5.12 | 125.53 | 128.60 |
| 1 | A | 2599 | G | C5-N7-C8 | 5.12 | 106.86 | 104.30 |
| 1 | A | 154 | G | N9-C4-C5 | -5.12 | 103.35 | 105.40 |
| 1 | A | 2037 | G | N1-C2-N2 | -5.12 | 111.59 | 116.20 |
| 1 | A | 371 | A | C5-C6-N6 | -5.11 | 119.61 | 123.70 |
| 1 | A | 614 | U | N3-C2-O2 | -5.11 | 118.62 | 122.20 |
| 1 | A | 1010 | A | C4-C5-C6 | -5.11 | 114.44 | 117.00 |
| 1 | A | 45 | C | C4-C5-C6 | 5.11 | 119.95 | 117.40 |
| 1 | A | 809 | G | N1-C2-N3 | 5.11 | 126.97 | 123.90 |
| 1 | A | 1397 | U | N3-C4-C5 | 5.11 | 117.67 | 114.60 |
| 1 | A | 1703 | G | N7-C8-N9 | 5.11 | 115.65 | 113.10 |
| 1 | A | 2071 | A | C5-N7-C8 | 5.11 | 106.45 | 103.90 |
| 1 | A | 845 | G | C8-N9-C1' | -5.11 | 120.36 | 127.00 |
| 1 | A | 1817 | G | C2-N3-C4 | -5.11 | 109.35 | 111.90 |
| 1 | A | 2769 | C | C6-N1-C2 | -5.11 | 118.26 | 120.30 |
| 1 | A | 409 | C | N1-C2-N3 | -5.10 | 115.63 | 119.20 |
| 1 | A | 1204 | A | N1-C2-N3 | 5.10 | 131.85 | 129.30 |
| 1 | A | 1319 | G | C8-N9-C1' | -5.10 | 120.37 | 127.00 |
| 1 | A | 2307 | G | C6-C5-N7 | -5.10 | 127.34 | 130.40 |
| 1 | A | 208 | C | N3-C4-C5 | 5.10 | 123.94 | 121.90 |
| 1 | A | 2084 | C | C6-N1-C2 | 5.10 | 122.34 | 120.30 |
| 1 | A | 2408 | U | N1-C2-O2 | -5.10 | 119.23 | 122.80 |
| 1 | A | 2709 | G | C5-C6-N1 | 5.10 | 114.05 | 111.50 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 1 | A | 2829 | C | N1-C2-O2 | -5.10 | 115.84 | 118.90 |
| 1 | A | 311 | A | C8-N9-C4 | 5.10 | 107.84 | 105.80 |
| 1 | A | 1013 | C | N3-C4-C5 | 5.10 | 123.94 | 121.90 |
| 1 | A | 1783 | A | N9-C4-C5 | 5.10 | 107.84 | 105.80 |
| 2 | B | 53 | A | C4-N9-C1' | 5.10 | 135.48 | 126.30 |
| 1 | A | 1985 | G | N7-C8-N9 | -5.10 | 110.55 | 113.10 |
| 1 | A | 1298 | C | C2-N3-C4 | -5.09 | 117.35 | 119.90 |
| 1 | A | 429 | A | C5-C6-N6 | -5.09 | 119.63 | 123.70 |
| 1 | A | 1437 | C | N1-C2-O2 | 5.09 | 121.96 | 118.90 |
| 1 | A | 2379 | G | C6-C5-N7 | -5.09 | 127.34 | 130.40 |
| 1 | A | 809 | G | C4-C5-N7 | -5.09 | 108.76 | 110.80 |
| 1 | A | 991 | C | N3-C4-C5 | 5.09 | 123.94 | 121.90 |
| 1 | A | 1841 | U | C5-C6-N1 | -5.09 | 120.15 | 122.70 |
| 1 | A | 429 | A | C6-C5-N7 | -5.09 | 128.74 | 132.30 |
| 1 | A | 444 | C | C2-N1-C1' | -5.09 | 113.20 | 118.80 |
| 1 | A | 908 | C | C6-N1-C2 | -5.09 | 118.26 | 120.30 |
| 1 | A | 2719 | G | C5-C6-O6 | -5.09 | 125.55 | 128.60 |
| 1 | A | 25 | U | N1-C2-O2 | -5.09 | 119.24 | 122.80 |
| 1 | A | 2042 | A | N1-C6-N6 | 5.09 | 121.65 | 118.60 |
| 1 | A | 453 | C | C2-N3-C4 | -5.09 | 117.36 | 119.90 |
| 1 | A | 530 | G | N3-C4-C5 | 5.09 | 131.14 | 128.60 |
| 1 | A | 928 | G | C6-C5-N7 | -5.09 | 127.35 | 130.40 |
| 1 | A | 2032 | G | C5-N7-C8 | 5.09 | 106.84 | 104.30 |
| 1 | A | 2193 | G | C6-N1-C2 | 5.09 | 128.15 | 125.10 |
| 1 | A | 2239 | G | N7-C8-N9 | -5.09 | 110.56 | 113.10 |
| 1 | A | 272(C) | G | C5-C6-O6 | -5.08 | 125.55 | 128.60 |
| 1 | A | 1342 | A | N1-C6-N6 | 5.08 | 121.65 | 118.60 |
| 1 | A | 1937 | A | C8-N9-C4 | 5.08 | 107.83 | 105.80 |
| 1 | A | 1861 | G | C8-N9-C1' | 5.08 | 133.61 | 127.00 |
| 1 | A | 2086 | U | C5-C4-O4 | -5.08 | 122.85 | 125.90 |
| 1 | A | 2828 | C | C2-N3-C4 | -5.08 | 117.36 | 119.90 |
| 1 | A | 959 | A | N3-C4-C5 | -5.08 | 123.24 | 126.80 |
| 1 | A | 1899 | G | C8-N9-C4 | -5.08 | 104.37 | 106.40 |
| 1 | A | 2363 | C | C6-N1-C2 | 5.08 | 122.33 | 120.30 |
| 1 | A | 729 | G | C2-N3-C4 | 5.08 | 114.44 | 111.90 |
| 1 | A | 1576 | U | N1-C2-O2 | 5.08 | 126.36 | 122.80 |
| 1 | A | 1990 | C | C2-N3-C4 | -5.08 | 117.36 | 119.90 |
| 1 | A | 2059 | A | N1-C6-N6 | 5.08 | 121.65 | 118.60 |
| 1 | A | 2361 | A | C8-N9-C4 | 5.08 | 107.83 | 105.80 |
| 1 | A | 2747 | G | N1-C6-O6 | 5.08 | 122.95 | 119.90 |
| 1 | A | 2612 | C | C5-C6-N1 | -5.08 | 118.46 | 121.00 |
| 1 | A | 1877 | A | N1-C6-N6 | 5.08 | 121.65 | 118.60 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|------------|-------|-------------|----------|
| 1 | A | 1259 | G | C4-C5-N7 | -5.07 | 108.77 | 110.80 |
| 1 | A | 2042 | A | N7-C8-N9 | -5.07 | 111.26 | 113.80 |
| 1 | A | 2239 | G | N1-C2-N3 | 5.07 | 126.94 | 123.90 |
| 1 | A | 1820 | U | N3-C2-O2 | 5.07 | 125.75 | 122.20 |
| 1 | A | 2372 | G | C5-C6-O6 | -5.07 | 125.56 | 128.60 |
| 2 | B | 105 | A | C8-N9-C4 | 5.07 | 107.83 | 105.80 |
| 1 | A | 864 | G | C2-N3-C4 | 5.07 | 114.43 | 111.90 |
| 1 | A | 1858 | G | N3-C4-C5 | -5.07 | 126.07 | 128.60 |
| 1 | A | 1980 | G | N9-C4-C5 | 5.07 | 107.43 | 105.40 |
| 1 | A | 2031 | A | C5-N7-C8 | -5.07 | 101.37 | 103.90 |
| 1 | A | 2592 | G | C2-N3-C4 | 5.07 | 114.43 | 111.90 |
| 1 | A | 1405 | U | N3-C4-C5 | 5.07 | 117.64 | 114.60 |
| 1 | A | 142(A) | C | C6-N1-C2 | 5.06 | 122.33 | 120.30 |
| 1 | A | 2289 | G | N3-C2-N2 | -5.06 | 116.36 | 119.90 |
| 1 | A | 2480 | C | C6-N1-C2 | -5.06 | 118.28 | 120.30 |
| 1 | A | 1985 | G | C5-N7-C8 | 5.06 | 106.83 | 104.30 |
| 1 | A | 105 | C | N3-C4-C5 | 5.06 | 123.92 | 121.90 |
| 1 | A | 130 | C | C6-N1-C1' | -5.06 | 114.73 | 120.80 |
| 1 | A | 566 | U | N1-C2-N3 | -5.06 | 111.86 | 114.90 |
| 1 | A | 984 | A | C8-N9-C4 | 5.06 | 107.82 | 105.80 |
| 1 | A | 2070 | G | C5-C6-N1 | 5.06 | 114.03 | 111.50 |
| 1 | A | 2079 | U | N1-C2-O2 | -5.06 | 119.26 | 122.80 |
| 1 | A | 744 | G | N3-C4-C5 | -5.06 | 126.07 | 128.60 |
| 1 | A | 1203 | G | C4-C5-N7 | -5.06 | 108.78 | 110.80 |
| 1 | A | 1367 | A | C6-N1-C2 | -5.06 | 115.56 | 118.60 |
| 2 | B | 64 | C | C5-C6-N1 | -5.06 | 118.47 | 121.00 |
| 1 | A | 1607 | C | N3-C4-N4 | 5.05 | 121.54 | 118.00 |
| 1 | A | 1698 | A | C5-C6-N6 | -5.05 | 119.66 | 123.70 |
| 1 | A | 2158 | A | C5-N7-C8 | -5.05 | 101.37 | 103.90 |
| 1 | A | 493 | G | C5-N7-C8 | -5.05 | 101.77 | 104.30 |
| 1 | A | 915 | C | N3-C2-O2 | -5.05 | 118.36 | 121.90 |
| 1 | A | 2071 | A | C6-N1-C2 | -5.05 | 115.57 | 118.60 |
| 1 | A | 143 | G | N1-C2-N2 | 5.05 | 120.74 | 116.20 |
| 1 | A | 801 | G | C8-N9-C4 | -5.05 | 104.38 | 106.40 |
| 1 | A | 1415 | U | C5-C6-N1 | -5.05 | 120.17 | 122.70 |
| 1 | A | 2104 | G | C8-N9-C1' | -5.05 | 120.44 | 127.00 |
| 1 | A | 78 | A | N1-C6-N6 | 5.05 | 121.63 | 118.60 |
| 1 | A | 139(A) | G | C5-C6-N1 | 5.05 | 114.02 | 111.50 |
| 1 | A | 507 | A | N9-C4-C5 | -5.05 | 103.78 | 105.80 |
| 1 | A | 693 | C | C5-C6-N1 | -5.05 | 118.48 | 121.00 |
| 1 | A | 1827 | C | N1-C2-O2 | 5.05 | 121.93 | 118.90 |
| 1 | A | 2296 | U | N1-C1'-C2' | 5.05 | 120.56 | 114.00 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 1 | A | 530 | G | C5-N7-C8 | -5.04 | 101.78 | 104.30 |
| 1 | A | 995 | C | C2-N3-C4 | 5.04 | 122.42 | 119.90 |
| 1 | A | 195 | A | C5-C6-N1 | -5.04 | 115.18 | 117.70 |
| 1 | A | 1325 | G | N3-C4-N9 | 5.04 | 129.03 | 126.00 |
| 1 | A | 2053 | G | C5-N7-C8 | 5.04 | 106.82 | 104.30 |
| 1 | A | 52 | A | N7-C8-N9 | 5.04 | 116.32 | 113.80 |
| 1 | A | 784 | A | N9-C4-C5 | 5.04 | 107.81 | 105.80 |
| 1 | A | 741 | G | N1-C6-O6 | -5.04 | 116.88 | 119.90 |
| 1 | A | 349 | G | N7-C8-N9 | -5.04 | 110.58 | 113.10 |
| 28 | 6 | 13 | CYS | CA-CB-SG | -5.04 | 104.94 | 114.00 |
| 1 | A | 1302 | A | N1-C6-N6 | -5.03 | 115.58 | 118.60 |
| 1 | A | 2147 | G | N1-C6-O6 | 5.03 | 122.92 | 119.90 |
| 1 | A | 2293 | C | C2-N1-C1' | -5.03 | 113.26 | 118.80 |
| 1 | A | 2412 | A | C2-N3-C4 | 5.03 | 113.12 | 110.60 |
| 1 | A | 2571 | C | N3-C2-O2 | -5.03 | 118.38 | 121.90 |
| 1 | A | 2828 | C | C5-C6-N1 | -5.03 | 118.48 | 121.00 |
| 1 | A | 1807 | G | C8-N9-C4 | 5.03 | 108.41 | 106.40 |
| 1 | A | 1045 | A | N9-C4-C5 | -5.03 | 103.79 | 105.80 |
| 1 | A | 1328 | G | N3-C4-N9 | 5.03 | 129.02 | 126.00 |
| 1 | A | 2808 | U | N1-C2-N3 | -5.03 | 111.88 | 114.90 |
| 1 | A | 931 | G | C8-N9-C4 | -5.03 | 104.39 | 106.40 |
| 1 | A | 2011 | U | N3-C2-O2 | 5.03 | 125.72 | 122.20 |
| 1 | A | 139(A) | G | C4-N9-C1' | 5.03 | 133.03 | 126.50 |
| 1 | A | 499 | U | N1-C2-O2 | -5.03 | 119.28 | 122.80 |
| 1 | A | 986 | C | C5-C4-N4 | -5.03 | 116.68 | 120.20 |
| 1 | A | 2818 | G | C6-N1-C2 | -5.03 | 122.08 | 125.10 |
| 30 | 8 | 34 | TRP | O-C-N | -5.03 | 114.66 | 122.70 |
| 1 | A | 645 | C | C5-C6-N1 | 5.02 | 123.51 | 121.00 |
| 1 | A | 2433 | A | C5-C6-N6 | -5.02 | 119.68 | 123.70 |
| 1 | A | 1179 | C | C6-N1-C2 | 5.02 | 122.31 | 120.30 |
| 1 | A | 1429 | G | N3-C4-N9 | 5.02 | 129.01 | 126.00 |
| 1 | A | 2149 | G | N9-C4-C5 | -5.02 | 103.39 | 105.40 |
| 1 | A | 673 | C | C5-C4-N4 | -5.02 | 116.69 | 120.20 |
| 1 | A | 338 | G | C5-C6-O6 | -5.02 | 125.59 | 128.60 |
| 1 | A | 1353 | A | N9-C4-C5 | 5.02 | 107.81 | 105.80 |
| 1 | A | 2227 | A | C5-C6-N1 | -5.02 | 115.19 | 117.70 |
| 1 | A | 2719 | G | C5-C6-N1 | 5.02 | 114.01 | 111.50 |
| 1 | A | 1253 | A | C6-C5-N7 | 5.02 | 135.81 | 132.30 |
| 1 | A | 1558 | A | P-O3'-C3' | 5.01 | 125.72 | 119.70 |
| 1 | A | 62 | C | N1-C2-O2 | -5.01 | 115.89 | 118.90 |
| 1 | A | 784 | A | P-O3'-C3' | 5.01 | 125.72 | 119.70 |
| 1 | A | 1766 | U | N1-C2-N3 | 5.01 | 117.91 | 114.90 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 1 | A | 1653 | G | N3-C4-C5 | -5.01 | 126.09 | 128.60 |
| 1 | A | 1208 | C | N3-C2-O2 | -5.01 | 118.39 | 121.90 |
| 1 | A | 2067 | G | N3-C2-N2 | -5.01 | 116.39 | 119.90 |
| 1 | A | 2500 | U | C4-C5-C6 | -5.01 | 116.69 | 119.70 |
| 1 | A | 2672 | G | C4-N9-C1' | 5.01 | 133.01 | 126.50 |
| 1 | A | 2713 | A | N9-C4-C5 | -5.01 | 103.80 | 105.80 |
| 2 | B | 80 | U | C5-C4-O4 | 5.01 | 128.91 | 125.90 |
| 1 | A | 1162 | G | C4-C5-N7 | -5.01 | 108.80 | 110.80 |
| 1 | A | 2540 | C | N3-C4-C5 | 5.01 | 123.90 | 121.90 |
| 1 | A | 2755 | C | C5-C4-N4 | -5.01 | 116.69 | 120.20 |
| 2 | B | 1 | U | C2-N1-C1' | 5.01 | 123.71 | 117.70 |
| 1 | A | 483 | A | C2-N3-C4 | -5.00 | 108.10 | 110.60 |
| 1 | A | 408 | G | C5-C6-N1 | 5.00 | 114.00 | 111.50 |
| 1 | A | 2459 | A | N1-C6-N6 | -5.00 | 115.60 | 118.60 |
| 17 | V | 42 | GLY | N-CA-C | -5.00 | 100.59 | 113.10 |
| 1 | A | 271(J) | C | C5-C4-N4 | -5.00 | 116.70 | 120.20 |
| 1 | A | 2271 | G | C4-N9-C1' | 5.00 | 133.00 | 126.50 |
| 1 | A | 2510 | C | C5-C6-N1 | -5.00 | 118.50 | 121.00 |
| 1 | A | 2521 | C | C5-C6-N1 | -5.00 | 118.50 | 121.00 |
| 1 | A | 2827 | C | C2-N3-C4 | -5.00 | 117.40 | 119.90 |

There are no chirality outliers.

All (21) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-------------------|
| 23 | 1 | 83 | GLU | Peptide |
| 26 | 4 | 42 | PHE | Peptide |
| 26 | 4 | 44 | THR | Peptide |
| 30 | 8 | 34 | TRP | Mainchain,Peptide |
| 3 | D | 274 | ARG | Peptide |
| 4 | E | 72 | VAL | Peptide |
| 5 | F | 129 | PHE | Peptide |
| 5 | F | 85 | GLY | Peptide |
| 5 | F | 89 | VAL | Mainchain |
| 6 | G | 13 | GLU | Peptide |
| 8 | I | 113 | ARG | Peptide |
| 9 | N | 23 | LEU | Mainchain,Peptide |
| 10 | O | 48 | PRO | Peptide |
| 11 | P | 26 | GLY | Peptide |
| 11 | P | 44 | GLY | Peptide |
| 14 | S | 82 | ILE | Peptide |
| 15 | T | 126 | ALA | Peptide |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 19 | X | 93 | GLU | Peptide |
| 20 | Y | 102 | CYS | Peptide |

5.2 Close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 60620 | 0 | 30560 | 940 | 0 |
| 2 | B | 2573 | 0 | 1304 | 52 | 0 |
| 3 | D | 2136 | 0 | 2218 | 67 | 0 |
| 4 | E | 1555 | 0 | 1607 | 52 | 0 |
| 5 | F | 1580 | 0 | 1621 | 65 | 0 |
| 6 | G | 1368 | 0 | 1324 | 56 | 0 |
| 7 | H | 1317 | 0 | 1376 | 31 | 0 |
| 8 | I | 1038 | 0 | 1040 | 38 | 0 |
| 9 | N | 1112 | 0 | 1180 | 37 | 0 |
| 10 | O | 923 | 0 | 981 | 28 | 0 |
| 11 | P | 1131 | 0 | 1201 | 39 | 0 |
| 12 | Q | 1122 | 0 | 1179 | 45 | 0 |
| 13 | R | 968 | 0 | 1033 | 29 | 0 |
| 14 | S | 865 | 0 | 905 | 52 | 0 |
| 15 | T | 1063 | 0 | 1103 | 40 | 0 |
| 16 | U | 959 | 0 | 1019 | 29 | 0 |
| 17 | V | 771 | 0 | 830 | 24 | 0 |
| 18 | W | 881 | 0 | 935 | 21 | 0 |
| 19 | X | 742 | 0 | 799 | 18 | 0 |
| 20 | Y | 785 | 0 | 828 | 27 | 0 |
| 21 | Z | 1522 | 0 | 1511 | 52 | 0 |
| 22 | 0 | 594 | 0 | 604 | 31 | 0 |
| 23 | 1 | 745 | 0 | 804 | 31 | 0 |
| 24 | 2 | 588 | 0 | 643 | 24 | 0 |
| 25 | 3 | 458 | 0 | 503 | 13 | 0 |
| 26 | 4 | 349 | 0 | 336 | 19 | 0 |
| 27 | 5 | 455 | 0 | 472 | 17 | 0 |
| 28 | 6 | 449 | 0 | 462 | 18 | 0 |
| 29 | 7 | 418 | 0 | 467 | 15 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 30 | 8 | 509 | 0 | 565 | 28 | 0 |
| 31 | 9 | 297 | 0 | 316 | 10 | 0 |
| 32 | 6 | 1 | 0 | 0 | 0 | 0 |
| 32 | 7 | 1 | 0 | 0 | 0 | 0 |
| 32 | 8 | 1 | 0 | 0 | 0 | 0 |
| 32 | A | 428 | 0 | 0 | 0 | 0 |
| 32 | B | 5 | 0 | 0 | 0 | 0 |
| 32 | D | 1 | 0 | 0 | 0 | 0 |
| 32 | E | 1 | 0 | 0 | 0 | 0 |
| 32 | F | 2 | 0 | 0 | 0 | 0 |
| 32 | P | 1 | 0 | 0 | 0 | 0 |
| 33 | 4 | 1 | 0 | 0 | 0 | 0 |
| 33 | 5 | 1 | 0 | 0 | 0 | 0 |
| 33 | 6 | 1 | 0 | 0 | 0 | 0 |
| 33 | 9 | 1 | 0 | 0 | 0 | 0 |
| 33 | Y | 1 | 0 | 0 | 0 | 0 |
| 34 | 0 | 1 | 0 | 0 | 0 | 0 |
| 34 | 1 | 2 | 0 | 0 | 0 | 0 |
| 34 | A | 696 | 0 | 0 | 56 | 0 |
| 34 | B | 9 | 0 | 0 | 0 | 0 |
| 34 | D | 3 | 0 | 0 | 0 | 0 |
| 34 | E | 1 | 0 | 0 | 0 | 0 |
| 34 | F | 5 | 0 | 0 | 0 | 0 |
| 34 | P | 5 | 0 | 0 | 0 | 0 |
| 34 | Q | 2 | 0 | 0 | 0 | 0 |
| 34 | R | 1 | 0 | 0 | 0 | 0 |
| 34 | V | 1 | 0 | 0 | 0 | 0 |
| 34 | X | 1 | 0 | 0 | 0 | 0 |
| 34 | Y | 1 | 0 | 0 | 0 | 0 |
| All | All | 91067 | 0 | 59726 | 1702 | 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 12.

All (1702) close contacts within the same asymmetric unit are listed below.

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-----------------|-------------|----------|
| 1:A:2296:U:O4 | 1:A:2335:A:N6 | 1.79 | 1.15 |
| 23:1:21:ARG:HH11 | 23:1:21:ARG:HG2 | 1.27 | 0.99 |
| 1:A:2304:G:H1 | 1:A:2312:U:H3 | 1.12 | 0.97 |
| 1:A:1310:G:OP2 | 29:7:9:ARG:NH1 | 1.97 | 0.96 |
| 1:A:139(A):G:N2 | 19:X:44:GLU:OE1 | 1.99 | 0.96 |
| 1:A:1359:A:N6 | 1:A:1372:U:O4 | 1.99 | 0.96 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 20:Y:76:CYS:HB3 | 20:Y:79:CYS:HB2 | 1.47 | 0.95 |
| 11:P:39:LYS:HB2 | 11:P:45:LEU:HG | 1.49 | 0.95 |
| 1:A:2322:A:H61 | 1:A:2335:A:N6 | 1.65 | 0.94 |
| 6:G:61:ALA:HB1 | 26:4:7:PRO:HG3 | 1.51 | 0.93 |
| 1:A:1779:U:H5 | 1:A:1784:A:N7 | 1.67 | 0.92 |
| 1:A:197:A:OP1 | 34:A:3891:HOH:O | 1.88 | 0.92 |
| 1:A:2122:U:H3 | 1:A:2176:A:H61 | 1.12 | 0.90 |
| 1:A:2287:A:H62 | 1:A:2344:U:H3 | 1.19 | 0.90 |
| 1:A:2287:A:N6 | 1:A:2344:U:H3 | 1.69 | 0.89 |
| 1:A:2820:A:OP2 | 13:R:2:ARG:NH2 | 2.05 | 0.89 |
| 30:8:7:HIS:HD2 | 30:8:10:ALA:H | 1.20 | 0.88 |
| 1:A:287:C:O2 | 1:A:354:G:N2 | 2.05 | 0.88 |
| 1:A:27:G:N2 | 1:A:512:G:O2' | 2.07 | 0.87 |
| 31:9:11:CYS:SG | 31:9:32:HIS:HE1 | 1.97 | 0.87 |
| 1:A:2319:G:H22 | 14:S:3:ARG:HE | 1.23 | 0.86 |
| 1:A:882:G:H1 | 1:A:894:C:H42 | 1.23 | 0.86 |
| 1:A:1388:G:N7 | 34:A:4126:HOH:O | 2.08 | 0.86 |
| 1:A:2134:A:O2' | 1:A:2159:G:N2 | 2.08 | 0.86 |
| 1:A:1204:A:H2 | 1:A:1241:A:H62 | 1.24 | 0.86 |
| 1:A:631:A:OP1 | 11:P:65:ARG:NH1 | 2.08 | 0.85 |
| 1:A:1603:A:OP1 | 34:A:3879:HOH:O | 1.93 | 0.85 |
| 5:F:46:ARG:HG2 | 5:F:46:ARG:HH11 | 1.42 | 0.85 |
| 1:A:2777:G:H5'' | 1:A:2778:A:H5' | 1.58 | 0.84 |
| 1:A:27:G:N2 | 1:A:512:G:HO2' | 1.74 | 0.84 |
| 13:R:33:ARG:NH2 | 27:5:57:VAL:O | 2.11 | 0.84 |
| 1:A:571:A:H5' | 1:A:2030:A:H62 | 1.42 | 0.84 |
| 1:A:1689:A:H62 | 1:A:1698:A:H2 | 1.21 | 0.83 |
| 1:A:2306:C:H5' | 1:A:2307:G:H2' | 1.60 | 0.83 |
| 15:T:64:ARG:HB2 | 15:T:73:GLU:HG2 | 1.61 | 0.83 |
| 1:A:1109:C:H5 | 1:A:1110:G:C2 | 1.97 | 0.83 |
| 1:A:90:U:HO2' | 1:A:92:A:H8 | 0.87 | 0.82 |
| 1:A:2115:G:N2 | 1:A:2119:A:OP2 | 2.11 | 0.82 |
| 1:A:1403:C:H5'' | 1:A:1471:A:H1' | 1.62 | 0.82 |
| 4:E:54:GLN:HG3 | 4:E:76:ARG:HB3 | 1.61 | 0.81 |
| 8:I:40:THR:OG1 | 8:I:43:ASN:OD1 | 1.99 | 0.80 |
| 1:A:1017:G:N7 | 34:A:4000:HOH:O | 2.15 | 0.80 |
| 20:Y:30:VAL:HG22 | 20:Y:37:VAL:HG12 | 1.64 | 0.80 |
| 1:A:1366:A:OP1 | 23:1:3:LYS:NZ | 2.15 | 0.80 |
| 1:A:27:G:H22 | 1:A:512:G:HO2' | 1.29 | 0.80 |
| 1:A:90:U:O2' | 1:A:92:A:H8 | 1.64 | 0.80 |
| 28:6:23:THR:OG1 | 28:6:24:GLU:N | 2.14 | 0.80 |
| 1:A:240:G:O6 | 34:A:4022:HOH:O | 2.00 | 0.79 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:A:1449:A:OP1 | 34:A:4004:HOH:O | 2.01 | 0.79 |
| 1:A:271(I):G:H1 | 1:A:271(O):C:H42 | 1.29 | 0.79 |
| 1:A:1210:A:H5' | 1:A:1210:A:H8 | 1.46 | 0.79 |
| 1:A:548:A:H62 | 17:V:19:LYS:HB2 | 1.46 | 0.79 |
| 1:A:2322:A:N6 | 1:A:2335:A:N6 | 2.30 | 0.79 |
| 8:I:106:GLY:HA2 | 8:I:107:VAL:HB | 1.65 | 0.78 |
| 6:G:131:TYR:HB3 | 6:G:159:VAL:HG13 | 1.65 | 0.78 |
| 1:A:2562:U:H1' | 10:O:23:ARG:HH11 | 1.49 | 0.78 |
| 8:I:78:THR:O | 8:I:104:GLN:NE2 | 2.13 | 0.78 |
| 15:T:56:GLY:O | 15:T:59:THR:HG23 | 1.83 | 0.78 |
| 1:A:1013:C:OP2 | 34:A:3998:HOH:O | 2.01 | 0.78 |
| 1:A:2134:A:H61 | 1:A:2157:G:H1' | 1.49 | 0.77 |
| 21:Z:45:ASP:OD2 | 21:Z:49:ARG:NH1 | 2.17 | 0.77 |
| 1:A:1243:G:O2' | 11:P:7:ARG:NH2 | 2.17 | 0.77 |
| 15:T:60:THR:HG22 | 15:T:77:PRO:HA | 1.67 | 0.77 |
| 1:A:2405:G:H4' | 1:A:2406:U:OP2 | 1.83 | 0.77 |
| 1:A:1026:U:O2' | 1:A:1027:A:O5' | 2.02 | 0.76 |
| 1:A:1767:C:O2 | 1:A:1985:G:N2 | 2.17 | 0.76 |
| 11:P:59:LEU:HD11 | 30:8:10:ALA:HB2 | 1.65 | 0.76 |
| 8:I:92:VAL:HG23 | 8:I:97:ILE:HD11 | 1.68 | 0.76 |
| 1:A:221:A:H4' | 1:A:222:A:O5' | 1.85 | 0.75 |
| 7:H:70:THR:O | 7:H:71:LEU:HB2 | 1.86 | 0.75 |
| 24:2:35:LEU:HD12 | 24:2:53:LEU:HD12 | 1.68 | 0.75 |
| 23:1:54:ALA:HB1 | 23:1:83:GLU:HB2 | 1.67 | 0.75 |
| 1:A:300:A:P | 20:Y:86:ARG:HH22 | 2.09 | 0.75 |
| 24:2:51:ARG:HA | 24:2:54:LYS:HB2 | 1.68 | 0.75 |
| 1:A:2602:A:H4' | 1:A:2603:G:OP1 | 1.87 | 0.75 |
| 30:8:34:TRP:O | 30:8:36:LYS:N | 2.19 | 0.75 |
| 1:A:2291:U:O4 | 34:A:4090:HOH:O | 2.04 | 0.75 |
| 1:A:1019:U:H3 | 1:A:1142(A):A:H62 | 1.34 | 0.74 |
| 1:A:2134:A:N6 | 1:A:2157:G:H1' | 2.02 | 0.74 |
| 1:A:2588:G:OP1 | 34:A:3978:HOH:O | 2.05 | 0.74 |
| 1:A:2683:C:OP1 | 15:T:53:ARG:NH2 | 2.21 | 0.74 |
| 1:A:2108:C:H2' | 1:A:2109:U:O5' | 1.88 | 0.74 |
| 2:B:105:A:OP1 | 21:Z:72:ARG:NH1 | 2.21 | 0.74 |
| 1:A:2760:C:H2' | 1:A:2761:G:H5'' | 1.68 | 0.74 |
| 6:G:76:SER:HA | 6:G:83:ARG:HA | 1.70 | 0.74 |
| 1:A:226:G:H21 | 1:A:228:A:H62 | 1.34 | 0.74 |
| 1:A:1858:G:O2' | 1:A:1884:A:N6 | 2.20 | 0.74 |
| 5:F:53:THR:HG23 | 5:F:55:GLY:H | 1.52 | 0.74 |
| 2:B:117:G:H4' | 14:S:54:LEU:HD23 | 1.69 | 0.73 |
| 1:A:921:G:O6 | 34:A:3902:HOH:O | 2.05 | 0.73 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:1654:A:OP1 | 13:R:1:MET:N | 2.14 | 0.73 |
| 1:A:747:U:O2 | 1:A:2014:A:H1' | 1.88 | 0.73 |
| 17:V:40:LEU:HB2 | 17:V:46:VAL:HG13 | 1.69 | 0.73 |
| 12:Q:38:GLU:HB2 | 12:Q:127:ILE:HG22 | 1.69 | 0.73 |
| 26:4:18:CYS:HB2 | 26:4:39:CYS:SG | 2.29 | 0.73 |
| 1:A:1038:C:H42 | 1:A:1117:G:H1 | 1.36 | 0.73 |
| 23:1:3:LYS:HB2 | 23:1:61:ARG:NH1 | 2.04 | 0.72 |
| 1:A:1141:U:OP2 | 9:N:63:THR:OG1 | 2.06 | 0.72 |
| 1:A:2721:A:OP1 | 34:A:4046:HOH:O | 2.05 | 0.72 |
| 2:B:28:C:H2' | 2:B:29:A:H8 | 1.53 | 0.72 |
| 22:0:65:GLY:HA3 | 22:0:81:VAL:HG12 | 1.71 | 0.72 |
| 1:A:1828:G:OP1 | 34:A:3603:HOH:O | 2.07 | 0.72 |
| 1:A:1494:A:H2' | 1:A:1495:A:C8 | 2.24 | 0.72 |
| 1:A:639:U:H2' | 1:A:640:C:C6 | 2.25 | 0.72 |
| 1:A:615:G:OP1 | 5:F:40:GLN:NE2 | 2.23 | 0.72 |
| 14:S:102:ALA:HA | 14:S:105:ALA:HB3 | 1.70 | 0.72 |
| 1:A:2308:G:O2' | 1:A:2310:A:OP2 | 2.04 | 0.72 |
| 7:H:28:GLY:HA3 | 7:H:79:VAL:HB | 1.70 | 0.72 |
| 2:B:28:C:H2' | 2:B:29:A:C8 | 2.25 | 0.72 |
| 1:A:2122:U:H3 | 1:A:2176:A:N6 | 1.84 | 0.71 |
| 1:A:1250:G:N7 | 11:P:18:ARG:NH2 | 2.38 | 0.71 |
| 1:A:1980:G:O2' | 1:A:1982:C:OP2 | 2.07 | 0.71 |
| 1:A:2140:C:N3 | 1:A:2151:G:O6 | 2.24 | 0.71 |
| 1:A:1022:G:H22 | 1:A:1142(A):A:H2 | 1.38 | 0.71 |
| 15:T:95:ARG:HG2 | 15:T:95:ARG:HH11 | 1.56 | 0.71 |
| 1:A:1815:A:OP2 | 3:D:54:ARG:NH2 | 2.23 | 0.71 |
| 11:P:126:VAL:HG12 | 11:P:148:LEU:HD22 | 1.72 | 0.71 |
| 1:A:2104:G:N7 | 1:A:2186:G:N2 | 2.38 | 0.71 |
| 1:A:2296:U:C4 | 1:A:2335:A:N6 | 2.59 | 0.71 |
| 1:A:2036:C:H6 | 1:A:2036:C:H5' | 1.55 | 0.71 |
| 1:A:2181:G:H2' | 1:A:2182:G:C8 | 2.25 | 0.70 |
| 1:A:833:U:O2 | 11:P:55:ARG:NH2 | 2.25 | 0.70 |
| 15:T:51:ARG:HG3 | 15:T:98:LYS:HE3 | 1.74 | 0.70 |
| 1:A:1817:G:OP1 | 3:D:88:ARG:NH2 | 2.23 | 0.70 |
| 1:A:243:U:OP2 | 30:8:8:LYS:NZ | 2.22 | 0.70 |
| 23:1:21:ARG:NH1 | 23:1:21:ARG:HG2 | 1.98 | 0.70 |
| 1:A:301:G:OP2 | 20:Y:84:ARG:NH2 | 2.24 | 0.70 |
| 15:T:16:ARG:NH2 | 15:T:83:ILE:O | 2.25 | 0.70 |
| 1:A:2357:U:OP1 | 22:0:20:ARG:NH1 | 2.24 | 0.70 |
| 1:A:530:G:O4' | 1:A:530:G:N3 | 2.23 | 0.69 |
| 1:A:248:G:OP1 | 34:A:3740:HOH:O | 2.09 | 0.69 |
| 1:A:39:C:O2 | 5:F:46:ARG:NH2 | 2.25 | 0.69 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:141:A:C8 | 1:A:1408:C:O2' | 2.46 | 0.69 |
| 1:A:81:G:N7 | 34:A:4116:HOH:O | 2.24 | 0.69 |
| 6:G:16:ARG:HE | 6:G:31:VAL:HG11 | 1.57 | 0.69 |
| 1:A:2124:G:N2 | 1:A:2174:C:C2 | 2.61 | 0.69 |
| 1:A:1405:U:H2' | 1:A:1406:U:C6 | 2.28 | 0.69 |
| 1:A:2206:G:H5' | 1:A:2207:G:C5 | 2.28 | 0.69 |
| 18:W:60:ASN:N | 18:W:60:ASN:HD22 | 1.91 | 0.69 |
| 20:Y:79:CYS:HB3 | 20:Y:81:LYS:H | 1.58 | 0.69 |
| 7:H:149:ARG:NH1 | 7:H:167:GLU:OE1 | 2.26 | 0.69 |
| 1:A:1278:A:OP1 | 13:R:36:THR:HG23 | 1.91 | 0.69 |
| 22:O:27:GLU:HG3 | 22:O:68:GLU:HA | 1.74 | 0.69 |
| 25:3:8:LEU:HD13 | 25:3:31:LEU:HD23 | 1.75 | 0.69 |
| 1:A:1253:A:N7 | 34:A:4108:HOH:O | 2.26 | 0.69 |
| 1:A:1395:A:OP1 | 34:A:3879:HOH:O | 2.10 | 0.68 |
| 7:H:3:ARG:HG2 | 7:H:6:ARG:HE | 1.57 | 0.68 |
| 1:A:2445:G:OP1 | 5:F:74:ARG:NH2 | 2.25 | 0.68 |
| 1:A:2786:U:O2' | 4:E:62:PRO:O | 2.08 | 0.68 |
| 1:A:1798:U:H5' | 3:D:259:THR:HG22 | 1.74 | 0.68 |
| 26:4:16:CYS:HA | 26:4:33:VAL:HB | 1.74 | 0.68 |
| 1:A:2839:G:H5' | 13:R:46:GLY:HA2 | 1.74 | 0.68 |
| 13:R:20:LEU:HD21 | 13:R:40:LYS:HD3 | 1.74 | 0.68 |
| 5:F:7:TYR:H | 5:F:22:ALA:HB3 | 1.59 | 0.68 |
| 1:A:271(E):U:H2' | 1:A:271(F):C:C6 | 2.29 | 0.68 |
| 17:V:76:LYS:HB2 | 17:V:81:TYR:HB3 | 1.76 | 0.68 |
| 1:A:220:G:O2' | 1:A:233:A:N3 | 2.25 | 0.68 |
| 24:2:50:ILE:O | 24:2:51:ARG:HB3 | 1.94 | 0.67 |
| 5:F:185:ASP:OD1 | 5:F:188:ARG:NH1 | 2.27 | 0.67 |
| 21:Z:69:THR:HG22 | 21:Z:90:VAL:HA | 1.76 | 0.67 |
| 1:A:1653:G:H3' | 13:R:2:ARG:HD3 | 1.76 | 0.67 |
| 1:A:106:C:O4' | 20:Y:1:MET:HB2 | 1.95 | 0.67 |
| 1:A:2099:U:H3 | 1:A:2190:G:H1 | 1.42 | 0.67 |
| 14:S:34:HIS:CE1 | 14:S:54:LEU:HD12 | 2.29 | 0.67 |
| 1:A:818:G:OP2 | 34:A:4017:HOH:O | 2.13 | 0.67 |
| 12:Q:62:GLY:O | 21:Z:178:GLU:HG2 | 1.95 | 0.67 |
| 1:A:2887:U:H2' | 1:A:2888:C:C6 | 2.30 | 0.67 |
| 1:A:2682:U:OP2 | 34:A:4046:HOH:O | 2.12 | 0.67 |
| 1:A:1153:C:OP1 | 16:U:92:ARG:NH1 | 2.26 | 0.67 |
| 1:A:2361:A:N7 | 34:A:3908:HOH:O | 2.27 | 0.67 |
| 1:A:529:A:H62 | 1:A:2041:U:H3 | 1.42 | 0.67 |
| 3:D:275:LYS:HG3 | 3:D:276:LYS:HG2 | 1.77 | 0.67 |
| 7:H:137:ASP:HB3 | 7:H:140:LYS:HB3 | 1.77 | 0.67 |
| 6:G:15:VAL:HG13 | 6:G:175:LEU:HB3 | 1.77 | 0.67 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 16:U:92:ARG:HA | 16:U:95:LEU:HB2 | 1.75 | 0.67 |
| 1:A:2108:C:C2' | 1:A:2109:U:O5' | 2.42 | 0.66 |
| 11:P:95:VAL:HA | 11:P:99:LEU:HD12 | 1.77 | 0.66 |
| 1:A:993:G:OP1 | 16:U:50:ARG:NH2 | 2.29 | 0.66 |
| 27:5:49:CYS:SG | 27:5:51:TYR:HB2 | 2.36 | 0.66 |
| 13:R:67:LEU:HD13 | 13:R:76:VAL:HG21 | 1.75 | 0.66 |
| 1:A:574:C:OP1 | 34:A:3661:HOH:O | 2.14 | 0.66 |
| 18:W:79:GLY:HA3 | 18:W:100:THR:HG22 | 1.77 | 0.66 |
| 16:U:36:ARG:HD2 | 16:U:40:PHE:CZ | 2.31 | 0.66 |
| 20:Y:23:ARG:HG2 | 20:Y:42:VAL:HG22 | 1.78 | 0.65 |
| 3:D:33:LEU:O | 3:D:64:ILE:HG13 | 1.97 | 0.65 |
| 4:E:11:MET:HG2 | 4:E:24:THR:HB | 1.77 | 0.65 |
| 1:A:1796:U:H2' | 1:A:1797:C:C6 | 2.31 | 0.65 |
| 1:A:587:C:OP2 | 11:P:21:ARG:NH2 | 2.29 | 0.65 |
| 23:1:20:ARG:HG2 | 23:1:20:ARG:HH11 | 1.61 | 0.65 |
| 9:N:120:LEU:HD22 | 9:N:122:VAL:HG23 | 1.78 | 0.65 |
| 3:D:108:PRO:HB3 | 3:D:143:HIS:HE1 | 1.60 | 0.65 |
| 9:N:47:ALA:HB2 | 9:N:112:LEU:HD11 | 1.78 | 0.65 |
| 1:A:946:G:OP2 | 34:A:3959:HOH:O | 2.14 | 0.65 |
| 1:A:708:C:H42 | 1:A:723:G:H1 | 1.45 | 0.65 |
| 1:A:1031:G:H21 | 31:9:36:GLN:HE22 | 1.45 | 0.65 |
| 20:Y:92:ASN:N | 20:Y:93:GLY:HA2 | 2.12 | 0.65 |
| 1:A:796:C:H2' | 1:A:797:C:C6 | 2.32 | 0.64 |
| 1:A:1991:U:H2' | 1:A:1992:G:H5'' | 1.77 | 0.64 |
| 26:4:9:LEU:HD23 | 26:4:27:THR:HG23 | 1.77 | 0.64 |
| 1:A:2107:C:N4 | 1:A:2108:C:H42 | 1.95 | 0.64 |
| 12:Q:38:GLU:OE2 | 12:Q:128:LYS:N | 2.23 | 0.64 |
| 1:A:602:G:O2' | 1:A:655:A:N6 | 2.31 | 0.64 |
| 1:A:1430:C:H2' | 1:A:1431:U:C6 | 2.32 | 0.64 |
| 1:A:2123:G:H1 | 1:A:2175:C:H42 | 1.44 | 0.64 |
| 21:Z:111:VAL:C | 21:Z:113:ALA:H | 2.01 | 0.64 |
| 8:I:83:ALA:HB2 | 8:I:88:ILE:HA | 1.78 | 0.64 |
| 1:A:299:A:H5'' | 20:Y:86:ARG:HH21 | 1.63 | 0.64 |
| 1:A:2887:U:H2' | 1:A:2888:C:H6 | 1.63 | 0.64 |
| 8:I:5:LEU:HD11 | 8:I:19:VAL:HG22 | 1.79 | 0.64 |
| 1:A:2637:U:H5'' | 4:E:82:ARG:HH21 | 1.62 | 0.64 |
| 1:A:1778:U:H2' | 1:A:1784:A:N6 | 2.13 | 0.64 |
| 8:I:83:ALA:HB1 | 8:I:86:THR:O | 1.98 | 0.64 |
| 1:A:2269:A:OP1 | 34:A:4012:HOH:O | 2.15 | 0.64 |
| 1:A:546:C:H2' | 1:A:547:A:H5' | 1.80 | 0.63 |
| 2:B:27:C:H5'' | 14:S:54:LEU:HD11 | 1.79 | 0.63 |
| 4:E:47:VAL:HG21 | 4:E:86:PRO:HD2 | 1.80 | 0.63 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 16:U:29:SER:OG | 16:U:30:LYS:NZ | 2.30 | 0.63 |
| 1:A:2140:C:O2 | 1:A:2151:G:N1 | 2.23 | 0.63 |
| 1:A:1153:C:H2' | 1:A:1154:G:O4' | 1.98 | 0.63 |
| 1:A:879:G:H22 | 1:A:899:A:H1' | 1.63 | 0.63 |
| 1:A:2567:G:H2' | 1:A:2568:C:C6 | 2.33 | 0.63 |
| 1:A:1486:A:H2' | 1:A:1487:G:H8 | 1.62 | 0.63 |
| 7:H:56:SER:HB3 | 7:H:61:HIS:ND1 | 2.13 | 0.63 |
| 26:4:42:PHE:HB3 | 26:4:43:TYR:HB2 | 1.81 | 0.63 |
| 1:A:1494:A:H2' | 1:A:1495:A:H8 | 1.63 | 0.63 |
| 1:A:2331:G:O3' | 22:0:43:THR:HG22 | 1.99 | 0.63 |
| 1:A:2364:C:H2' | 1:A:2365:G:O4' | 1.99 | 0.63 |
| 30:8:4:MET:HE3 | 30:8:63:PRO:HG3 | 1.81 | 0.63 |
| 1:A:1866:C:H2' | 1:A:1876:A:O4' | 1.99 | 0.63 |
| 1:A:2646:C:OP2 | 1:A:2732:G:O2' | 2.13 | 0.63 |
| 1:A:1045:A:N3 | 1:A:1045:A:H2' | 2.14 | 0.63 |
| 1:A:271(M):G:H4' | 1:A:271(N):U:OP1 | 1.99 | 0.62 |
| 23:1:50:ARG:HG2 | 23:1:59:THR:HB | 1.80 | 0.62 |
| 1:A:277:C:H1' | 1:A:278:A:OP2 | 1.98 | 0.62 |
| 14:S:96:GLY:HA3 | 14:S:98:VAL:N | 2.14 | 0.62 |
| 1:A:1143:A:OP1 | 9:N:25:ARG:NH2 | 2.32 | 0.62 |
| 1:A:1495:A:H2' | 1:A:1496:A:C8 | 2.35 | 0.62 |
| 1:A:271(R):G:H2' | 1:A:271(S):G:H8 | 1.64 | 0.62 |
| 1:A:2250:G:O2' | 1:A:2496:C:OP1 | 2.15 | 0.62 |
| 3:D:108:PRO:HB3 | 3:D:143:HIS:CE1 | 2.35 | 0.62 |
| 1:A:11:G:H2' | 1:A:12:U:H5' | 1.81 | 0.62 |
| 23:1:80:LEU:HD23 | 23:1:82:LEU:HD21 | 1.82 | 0.62 |
| 1:A:1359:A:N6 | 1:A:1372:U:C4 | 2.59 | 0.62 |
| 1:A:574:C:N3 | 4:E:145:LYS:NZ | 2.37 | 0.62 |
| 1:A:1106:G:O2' | 1:A:1107:G:OP1 | 2.16 | 0.62 |
| 8:I:93:THR:O | 8:I:97:ILE:HD13 | 2.00 | 0.62 |
| 13:R:104:ARG:HG3 | 13:R:111:LEU:HD21 | 1.81 | 0.62 |
| 1:A:1488:G:H5' | 1:A:1489:U:OP2 | 1.98 | 0.62 |
| 1:A:873:G:N2 | 1:A:905:U:O2 | 2.32 | 0.62 |
| 1:A:1036:G:H1 | 1:A:1119:C:H42 | 1.47 | 0.62 |
| 1:A:271(I):G:H1 | 1:A:271(O):C:N4 | 1.98 | 0.61 |
| 12:Q:21:THR:HG21 | 12:Q:101:ARG:HB2 | 1.82 | 0.61 |
| 3:D:267:SER:O | 3:D:268:ARG:HB3 | 2.00 | 0.61 |
| 5:F:28:ILE:HG12 | 5:F:116:ASP:HB2 | 1.82 | 0.61 |
| 9:N:20:GLY:HA2 | 9:N:61:ARG:HG2 | 1.81 | 0.61 |
| 12:Q:29:PHE:N | 12:Q:105:GLU:OE2 | 2.33 | 0.61 |
| 4:E:111:ARG:HG3 | 4:E:160:TYR:CD1 | 2.35 | 0.61 |
| 1:A:548:A:N6 | 17:V:19:LYS:HB2 | 2.16 | 0.61 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:1533:G:H21 | 1:A:1536:C:H5 | 1.49 | 0.61 |
| 4:E:72:VAL:HA | 4:E:73:GLU:HB3 | 1.82 | 0.61 |
| 28:6:9:LEU:HD21 | 28:6:25:LYS:HB3 | 1.81 | 0.61 |
| 1:A:1798:U:C5' | 3:D:259:THR:HG22 | 2.30 | 0.61 |
| 1:A:90:U:O2' | 1:A:92:A:O5' | 2.17 | 0.61 |
| 2:B:11:C:H3' | 2:B:12:C:C6 | 2.36 | 0.61 |
| 1:A:207:A:H2' | 1:A:208:C:O4' | 2.00 | 0.61 |
| 31:9:14:CYS:HA | 31:9:27:CYS:HB2 | 1.82 | 0.61 |
| 11:P:47:ASP:OD2 | 11:P:50:ARG:NH2 | 2.33 | 0.61 |
| 1:A:2291:U:H2' | 1:A:2292:C:C6 | 2.36 | 0.61 |
| 1:A:607:U:OP1 | 5:F:102:PRO:HA | 2.01 | 0.61 |
| 11:P:38:GLN:O | 11:P:39:LYS:HB3 | 2.00 | 0.60 |
| 1:A:1107:G:N7 | 1:A:1108:U:N3 | 2.49 | 0.60 |
| 1:A:2272:U:H5'' | 1:A:2273:A:OP1 | 2.01 | 0.60 |
| 6:G:126:ASP:HB3 | 6:G:130:ASN:H | 1.66 | 0.60 |
| 13:R:36:THR:HG22 | 13:R:37:THR:H | 1.66 | 0.60 |
| 5:F:13:SER:HB3 | 5:F:15:SER:HB2 | 1.83 | 0.60 |
| 1:A:2315:G:H2' | 1:A:2316:C:C6 | 2.36 | 0.60 |
| 1:A:1311:G:O6 | 34:A:3780:HOH:O | 2.13 | 0.60 |
| 1:A:2319:G:N2 | 14:S:3:ARG:HE | 1.96 | 0.60 |
| 1:A:535:C:O3' | 16:U:53:ARG:NH1 | 2.34 | 0.60 |
| 21:Z:17:ALA:HA | 21:Z:20:ARG:HD2 | 1.82 | 0.60 |
| 1:A:8:A:H2' | 1:A:9:U:C6 | 2.35 | 0.60 |
| 1:A:546:C:H6 | 1:A:547:A:H5' | 1.65 | 0.60 |
| 1:A:185:U:H4' | 1:A:218:A:H4' | 1.83 | 0.60 |
| 1:A:1298:C:H5'' | 1:A:1299:G:OP2 | 2.02 | 0.60 |
| 21:Z:160:GLY:HA2 | 21:Z:161:VAL:HB | 1.83 | 0.60 |
| 1:A:141:A:H8 | 1:A:1408:C:O2' | 1.83 | 0.60 |
| 3:D:148:GLU:HB2 | 3:D:151:LYS:HD2 | 1.84 | 0.60 |
| 14:S:10:ARG:HH21 | 14:S:91:PRO:HB2 | 1.67 | 0.60 |
| 1:A:2104:G:N2 | 1:A:2105:C:C2 | 2.70 | 0.59 |
| 1:A:2306:C:C5' | 1:A:2307:G:H2' | 2.30 | 0.59 |
| 1:A:1803:A:O2' | 3:D:259:THR:HG21 | 2.02 | 0.59 |
| 1:A:528:A:O2' | 1:A:529:A:H5' | 2.02 | 0.59 |
| 1:A:2327:A:H2' | 1:A:2328:A:C8 | 2.37 | 0.59 |
| 1:A:2384:G:OP2 | 22:0:55:ARG:NH1 | 2.35 | 0.59 |
| 1:A:2118:U:OP1 | 1:A:2147:G:O2' | 2.21 | 0.59 |
| 23:1:85:LEU:HB3 | 23:1:89:GLU:HG3 | 1.84 | 0.59 |
| 1:A:1570:A:H5' | 3:D:36:PRO:HG3 | 1.84 | 0.59 |
| 1:A:528:A:N1 | 1:A:2042:A:H2' | 2.17 | 0.59 |
| 1:A:12:U:O2 | 1:A:12:U:H2' | 2.02 | 0.59 |
| 4:E:170:LEU:HB3 | 4:E:184:VAL:HG22 | 1.84 | 0.59 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 1:A:2706:G:O6 | 34:A:4038:HOH:O | 2.17 | 0.59 |
| 1:A:1962:C:O2' | 1:A:1964:G:OP2 | 2.20 | 0.59 |
| 1:A:2834:G:H8 | 1:A:2834:G:H5'' | 1.68 | 0.59 |
| 11:P:121:LYS:HG2 | 11:P:123:LEU:HG | 1.83 | 0.59 |
| 6:G:137:GLU:HG2 | 6:G:138:GLN:H | 1.68 | 0.59 |
| 1:A:2022:U:O2' | 1:A:2617:C:H5' | 2.02 | 0.59 |
| 1:A:751:A:H5' | 18:W:90:ARG:HA | 1.83 | 0.59 |
| 1:A:581:C:H2' | 1:A:582:G:C8 | 2.38 | 0.59 |
| 1:A:2602:A:H1' | 1:A:2603:G:H5'' | 1.85 | 0.59 |
| 23:1:3:LYS:HB2 | 23:1:61:ARG:HH12 | 1.68 | 0.58 |
| 1:A:330:A:H2 | 1:A:1210:A:H2' | 1.68 | 0.58 |
| 5:F:102:PRO:HB2 | 5:F:105:VAL:HG23 | 1.84 | 0.58 |
| 1:A:1530:C:O2' | 1:A:1531:C:O4' | 2.20 | 0.58 |
| 9:N:128:HIS:CE1 | 9:N:135:PRO:HG2 | 2.38 | 0.58 |
| 1:A:2113:U:H2' | 1:A:2114:A:C8 | 2.39 | 0.58 |
| 1:A:1038:C:N4 | 1:A:1117:G:H1 | 2.01 | 0.58 |
| 21:Z:92:SER:O | 21:Z:130:PRO:HG2 | 2.03 | 0.58 |
| 1:A:203:C:H3' | 1:A:204:A:H5'' | 1.85 | 0.58 |
| 24:2:13:ALA:HA | 24:2:16:LEU:HD12 | 1.84 | 0.58 |
| 1:A:652(D):C:H2' | 1:A:652(E):G:O4' | 2.03 | 0.58 |
| 1:A:271(L):U:H4' | 1:A:271(M):G:OP1 | 2.03 | 0.58 |
| 1:A:879:G:N2 | 1:A:899:A:H1' | 2.17 | 0.58 |
| 1:A:581:C:H2' | 1:A:582:G:H8 | 1.67 | 0.58 |
| 20:Y:99:CYS:SG | 20:Y:102:CYS:N | 2.77 | 0.58 |
| 21:Z:102:LEU:HD13 | 21:Z:123:ASP:HA | 1.85 | 0.58 |
| 18:W:43:GLY:O | 18:W:47:VAL:HG23 | 2.04 | 0.58 |
| 5:F:181:LEU:HB3 | 5:F:205:ARG:HH22 | 1.67 | 0.58 |
| 1:A:2134:A:N3 | 1:A:2159:G:H1' | 2.18 | 0.58 |
| 15:T:97:ALA:O | 15:T:98:LYS:HD2 | 2.03 | 0.58 |
| 14:S:25:ARG:NH1 | 14:S:42:ASP:OD2 | 2.37 | 0.58 |
| 1:A:579:G:H2' | 1:A:580:C:C6 | 2.38 | 0.58 |
| 1:A:1427:A:H4' | 1:A:1428:C:O5' | 2.04 | 0.58 |
| 9:N:67:LEU:O | 9:N:88:GLU:HG3 | 2.04 | 0.58 |
| 1:A:1722:A:C2 | 1:A:1740:G:C8 | 2.92 | 0.58 |
| 3:D:145:VAL:HG12 | 3:D:146:GLU:O | 2.04 | 0.58 |
| 26:4:15:ILE:HB | 26:4:32:TYR:CD2 | 2.38 | 0.58 |
| 1:A:154(A):C:N4 | 1:A:172:C:N3 | 2.51 | 0.58 |
| 3:D:206:LEU:HD22 | 3:D:211:ARG:HG2 | 1.85 | 0.58 |
| 1:A:1364:G:C8 | 23:1:3:LYS:HD3 | 2.39 | 0.57 |
| 26:4:14:ILE:HG13 | 26:4:22:ILE:HB | 1.85 | 0.57 |
| 1:A:1456:G:OP2 | 34:A:4007:HOH:O | 2.17 | 0.57 |
| 28:6:10:LEU:HD12 | 28:6:54:ILE:HA | 1.86 | 0.57 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 10:O:24:VAL:HB | 10:O:33:ALA:HB2 | 1.86 | 0.57 |
| 1:A:1109:C:C5 | 1:A:1110:G:C2 | 2.88 | 0.57 |
| 1:A:2849:U:OP2 | 15:T:95:ARG:NH1 | 2.36 | 0.57 |
| 8:I:5:LEU:HD21 | 8:I:12:LEU:HD13 | 1.86 | 0.57 |
| 20:Y:99:CYS:HB3 | 20:Y:104:GLY:H | 1.68 | 0.57 |
| 12:Q:16:ARG:HH11 | 12:Q:16:ARG:HG2 | 1.69 | 0.57 |
| 1:A:2773:C:H5'' | 4:E:164:ARG:HG2 | 1.85 | 0.57 |
| 1:A:2497:A:O3' | 34:A:3887:HOH:O | 2.17 | 0.57 |
| 1:A:1971:A:OP2 | 3:D:242:ARG:NH2 | 2.37 | 0.57 |
| 15:T:84:GLN:HE21 | 15:T:85:LYS:HG2 | 1.69 | 0.57 |
| 30:8:34:TRP:CG | 30:8:35:GLN:N | 2.71 | 0.57 |
| 16:U:76:TYR:CZ | 16:U:80:ILE:HG13 | 2.40 | 0.57 |
| 1:A:226:G:H21 | 1:A:228:A:N6 | 2.01 | 0.57 |
| 14:S:46:VAL:HG12 | 14:S:48:LEU:HD12 | 1.87 | 0.57 |
| 1:A:1614:A:C2 | 18:W:93:ALA:HB2 | 2.40 | 0.57 |
| 1:A:1359:A:N6 | 1:A:1372:U:C5 | 2.73 | 0.57 |
| 24:2:22:GLU:OE2 | 24:2:68:ARG:NH2 | 2.37 | 0.57 |
| 2:B:55:U:HO2' | 6:G:29:TRP:HD1 | 1.51 | 0.57 |
| 1:A:928:G:O6 | 34:A:3788:HOH:O | 2.16 | 0.57 |
| 1:A:547:A:H1' | 1:A:548:A:H4' | 1.87 | 0.57 |
| 5:F:23:ASP:O | 5:F:24:LEU:HD13 | 2.05 | 0.57 |
| 18:W:86:LEU:HD12 | 18:W:87:PRO:HD2 | 1.85 | 0.57 |
| 1:A:686:G:H5'' | 29:7:11:LYS:HE2 | 1.86 | 0.57 |
| 1:A:1007:C:OP1 | 9:N:37:LYS:NZ | 2.33 | 0.57 |
| 10:O:88:ASN:HD21 | 10:O:90:GLN:HB2 | 1.70 | 0.57 |
| 1:A:1786:A:H1' | 1:A:1938:A:N6 | 2.20 | 0.57 |
| 1:A:1945:G:H2' | 1:A:1946:U:C6 | 2.40 | 0.57 |
| 1:A:588:U:H2' | 1:A:589:C:C6 | 2.40 | 0.57 |
| 1:A:2790:A:N3 | 1:A:2790:A:H2' | 2.20 | 0.57 |
| 1:A:674:G:H1' | 5:F:74:ARG:HD3 | 1.87 | 0.56 |
| 1:A:2591:C:OP2 | 3:D:239:ARG:HB3 | 2.03 | 0.56 |
| 1:A:2308:G:H4' | 1:A:2309:A:OP2 | 2.04 | 0.56 |
| 1:A:2126:A:H4' | 1:A:2127:G:O5' | 2.05 | 0.56 |
| 17:V:15:GLU:O | 17:V:18:LEU:HB2 | 2.04 | 0.56 |
| 30:8:7:HIS:CD2 | 30:8:10:ALA:H | 2.12 | 0.56 |
| 1:A:1210:A:C8 | 1:A:1210:A:H5' | 2.35 | 0.56 |
| 26:4:18:CYS:SG | 26:4:39:CYS:HB2 | 2.44 | 0.56 |
| 1:A:2361:A:OP1 | 30:8:27:THR:HG23 | 2.05 | 0.56 |
| 3:D:16:MET:HG3 | 3:D:206:LEU:O | 2.05 | 0.56 |
| 1:A:453:C:H5'' | 34:A:3992:HOH:O | 2.05 | 0.56 |
| 26:4:18:CYS:CB | 26:4:39:CYS:SG | 2.91 | 0.56 |
| 5:F:6:VAL:HA | 5:F:23:ASP:H | 1.70 | 0.56 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 10:O:102:VAL:HB | 10:O:106:LEU:HD12 | 1.87 | 0.56 |
| 1:A:1506:C:H2' | 1:A:1507:A:H5' | 1.86 | 0.56 |
| 1:A:1378:A:OP1 | 29:7:10:ARG:NH2 | 2.38 | 0.56 |
| 12:Q:32:TYR:OH | 12:Q:111:GLU:OE1 | 2.19 | 0.56 |
| 7:H:86:GLU:HG2 | 7:H:132:ARG:HG3 | 1.87 | 0.56 |
| 6:G:48:GLU:O | 6:G:51:ARG:N | 2.39 | 0.56 |
| 21:Z:77:ASP:OD1 | 21:Z:80:ARG:HG2 | 2.06 | 0.56 |
| 7:H:3:ARG:HG3 | 7:H:4:ILE:N | 2.20 | 0.56 |
| 15:T:127:ALA:HA | 15:T:128:GLU:C | 2.26 | 0.56 |
| 1:A:975:C:H6 | 34:A:3869:HOH:O | 1.87 | 0.56 |
| 18:W:19:LEU:O | 27:5:25:LEU:HD12 | 2.06 | 0.56 |
| 1:A:2228:G:OP1 | 3:D:261:LYS:NZ | 2.27 | 0.56 |
| 15:T:118:ARG:HA | 15:T:118:ARG:HH11 | 1.71 | 0.56 |
| 10:O:115:VAL:HG13 | 10:O:121:VAL:HG21 | 1.88 | 0.56 |
| 1:A:566:U:H5'' | 11:P:29:LYS:HE3 | 1.87 | 0.56 |
| 1:A:1779:U:C5 | 1:A:1784:A:N7 | 2.60 | 0.56 |
| 1:A:2109:U:H3' | 1:A:2109:U:H6 | 1.71 | 0.56 |
| 18:W:60:ASN:HD22 | 18:W:60:ASN:H | 1.52 | 0.56 |
| 12:Q:16:ARG:HG2 | 12:Q:16:ARG:NH1 | 2.21 | 0.56 |
| 1:A:2805:G:H2' | 1:A:2807:G:H8 | 1.69 | 0.56 |
| 1:A:1509(B):A:H2' | 1:A:1510:G:C8 | 2.41 | 0.56 |
| 8:I:105:HIS:CD2 | 8:I:105:HIS:N | 2.74 | 0.56 |
| 1:A:1466:G:O2' | 1:A:1546:C:O2' | 2.23 | 0.56 |
| 5:F:53:THR:CG2 | 5:F:55:GLY:H | 2.18 | 0.55 |
| 15:T:42:ILE:HG12 | 15:T:84:GLN:OE1 | 2.06 | 0.55 |
| 20:Y:76:CYS:CB | 20:Y:79:CYS:HB2 | 2.29 | 0.55 |
| 1:A:2306:C:H3' | 1:A:2307:G:C8 | 2.41 | 0.55 |
| 1:A:1026:U:H2' | 1:A:1026:U:O2 | 2.05 | 0.55 |
| 1:A:907:U:O2' | 12:Q:101:ARG:NH2 | 2.39 | 0.55 |
| 6:G:41:GLN:NE2 | 6:G:154:GLY:O | 2.34 | 0.55 |
| 4:E:16:ARG:NH1 | 4:E:171:GLU:OE2 | 2.39 | 0.55 |
| 25:3:6:VAL:HG13 | 25:3:56:VAL:HG13 | 1.87 | 0.55 |
| 9:N:56:ASN:H | 9:N:125:GLY:HA3 | 1.71 | 0.55 |
| 25:3:18:ASP:OD1 | 25:3:18:ASP:N | 2.26 | 0.55 |
| 1:A:184:C:H2' | 1:A:185:U:C6 | 2.41 | 0.55 |
| 1:A:2023:G:H5' | 1:A:2617:C:H4' | 1.88 | 0.55 |
| 1:A:1514:U:H2' | 1:A:1515:G:H8 | 1.71 | 0.55 |
| 1:A:1288:U:C2 | 1:A:1327:C:O2 | 2.60 | 0.55 |
| 2:B:8:U:O2' | 14:S:40:ILE:HD13 | 2.07 | 0.55 |
| 24:2:9:GLN:HE22 | 24:2:56:GLN:HB3 | 1.70 | 0.55 |
| 1:A:247:G:H4' | 1:A:386:G:C5 | 2.42 | 0.55 |
| 9:N:42:TRP:HD1 | 9:N:48:MET:HE1 | 1.72 | 0.55 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-----------------|-------------------|-------------|----------|
| 1:A:2723:C:OP1 | 13:R:3:HIS:ND1 | 2.26 | 0.55 |
| 3:D:76:PRO:HB2 | 3:D:116:GLN:HE21 | 1.71 | 0.55 |
| 4:E:97:LYS:N | 4:E:100:GLU:OE1 | 2.39 | 0.55 |
| 1:A:272:G:N7 | 1:A:421:U:H2' | 2.22 | 0.55 |
| 9:N:28:THR:HG22 | 9:N:29:LYS:N | 2.22 | 0.55 |
| 2:B:32:C:C2 | 2:B:51:G:N2 | 2.74 | 0.55 |
| 1:A:2166:G:N2 | 1:A:2172:U:O4 | 2.40 | 0.55 |
| 1:A:1040:C:H2' | 1:A:1041:C:O4' | 2.07 | 0.55 |
| 5:F:129:PHE:CD2 | 5:F:163:VAL:HG21 | 2.41 | 0.55 |
| 14:S:59:LYS:HB3 | 14:S:60:GLY:CA | 2.37 | 0.55 |
| 22:O:29:GLN:O | 22:O:67:VAL:HG23 | 2.07 | 0.55 |
| 11:P:8:PRO:HB2 | 11:P:12:ALA:HB3 | 1.87 | 0.55 |
| 1:A:83:G:OP1 | 20:Y:95:LYS:NZ | 2.40 | 0.55 |
| 1:A:2036:C:C6 | 1:A:2036:C:H5' | 2.40 | 0.55 |
| 1:A:2328:A:H2' | 1:A:2329:G:C8 | 2.40 | 0.55 |
| 12:Q:34:LEU:HB2 | 12:Q:118:LEU:HD22 | 1.89 | 0.55 |
| 1:A:956:G:OP2 | 12:Q:14:ARG:NH2 | 2.40 | 0.55 |
| 1:A:1358:G:H2' | 1:A:1359:A:C2 | 2.42 | 0.55 |
| 14:S:102:ALA:HA | 14:S:105:ALA:CB | 2.37 | 0.55 |
| 5:F:184:TYR:CE2 | 5:F:188:ARG:HD2 | 2.42 | 0.55 |
| 16:U:74:LEU:H | 16:U:74:LEU:HD12 | 1.72 | 0.55 |
| 1:A:2557:G:H2' | 1:A:2558:C:C6 | 2.41 | 0.55 |
| 5:F:31:HIS:HB2 | 11:P:9:ASN:OD1 | 2.07 | 0.55 |
| 3:D:78:LYS:HE2 | 3:D:114:GLY:HA2 | 1.89 | 0.55 |
| 17:V:65:GLY:HA3 | 17:V:91:TYR:CZ | 2.42 | 0.55 |
| 1:A:1642:G:N7 | 34:A:4095:HOH:O | 2.33 | 0.55 |
| 1:A:2781:A:H5'' | 1:A:2782:G:H5' | 1.88 | 0.55 |
| 10:O:34:THR:OG1 | 10:O:35:VAL:N | 2.39 | 0.55 |
| 1:A:548:A:N6 | 17:V:19:LYS:H | 2.05 | 0.55 |
| 1:A:1022:G:N7 | 9:N:66:LYS:HE2 | 2.21 | 0.55 |
| 2:B:11:C:OP2 | 2:B:12:C:N4 | 2.30 | 0.55 |
| 5:F:89:VAL:HG12 | 5:F:90:PHE:N | 2.22 | 0.55 |
| 1:A:2712:U:O2' | 1:A:2713:A:H5' | 2.07 | 0.55 |
| 14:S:84:GLN:HB3 | 14:S:111:GLU:HB2 | 1.89 | 0.55 |
| 1:A:2575:C:H5' | 4:E:143:ASN:O | 2.06 | 0.55 |
| 1:A:646:A:H2' | 1:A:647:G:O4' | 2.07 | 0.55 |
| 2:B:2:C:H2' | 2:B:3:C:C6 | 2.42 | 0.55 |
| 1:A:2820:A:OP1 | 13:R:4:LEU:HD23 | 2.07 | 0.54 |
| 1:A:1048:A:O2' | 1:A:1049:C:OP2 | 2.24 | 0.54 |
| 7:H:94:TYR:CE2 | 7:H:107:VAL:HB | 2.42 | 0.54 |
| 1:A:733:G:N7 | 34:A:3616:HOH:O | 2.33 | 0.54 |
| 1:A:2037:G:O6 | 34:A:3649:HOH:O | 2.17 | 0.54 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:A:107:C:H2' | 1:A:108:U:H6 | 1.72 | 0.54 |
| 21:Z:146:ILE:HA | 21:Z:174:VAL:HG12 | 1.89 | 0.54 |
| 1:A:2784:C:H1' | 4:E:37:ARG:HH12 | 1.72 | 0.54 |
| 1:A:2133:G:H2' | 1:A:2157:G:H22 | 1.73 | 0.54 |
| 10:O:88:ASN:ND2 | 10:O:90:GLN:H | 2.06 | 0.54 |
| 1:A:720:C:H2' | 1:A:721:C:H6 | 1.72 | 0.54 |
| 12:Q:39:PRO:HD3 | 12:Q:99:PRO:HG3 | 1.89 | 0.54 |
| 8:I:31:LEU:HD21 | 8:I:38:LEU:HG | 1.88 | 0.54 |
| 6:G:121:ASN:HD21 | 6:G:123:ASN:HB2 | 1.72 | 0.54 |
| 8:I:72:LEU:O | 8:I:73:GLU:HB2 | 2.07 | 0.54 |
| 15:T:65:LYS:HE2 | 15:T:67:SER:HB2 | 1.90 | 0.54 |
| 1:A:2171:A:H4' | 1:A:2172:U:OP1 | 2.07 | 0.54 |
| 1:A:1212:G:N2 | 1:A:1236:G:O2' | 2.39 | 0.54 |
| 1:A:443:A:N7 | 5:F:45:ARG:HG2 | 2.22 | 0.54 |
| 1:A:1639:U:C2' | 1:A:1640:C:H5'' | 2.36 | 0.54 |
| 21:Z:68:PRO:O | 21:Z:91:LEU:HB2 | 2.07 | 0.54 |
| 6:G:58:GLN:HA | 6:G:61:ALA:HB3 | 1.90 | 0.54 |
| 1:A:188:G:H1 | 1:A:208:C:H42 | 1.55 | 0.54 |
| 1:A:641:C:O2' | 1:A:2350:C:OP1 | 2.19 | 0.54 |
| 1:A:1503:U:H2' | 1:A:1504:C:C6 | 2.43 | 0.54 |
| 17:V:35:LEU:HB2 | 17:V:57:VAL:HG13 | 1.88 | 0.54 |
| 2:B:107:G:OP1 | 21:Z:31:ARG:NH2 | 2.41 | 0.54 |
| 1:A:2577:A:H5' | 27:5:3:LYS:HD2 | 1.90 | 0.54 |
| 1:A:2131:G:H5'' | 1:A:2132:U:H5'' | 1.88 | 0.54 |
| 15:T:54:ARG:HA | 15:T:59:THR:HB | 1.89 | 0.54 |
| 1:A:1026:U:HO2' | 1:A:1027:A:P | 2.31 | 0.54 |
| 9:N:42:TRP:HA | 9:N:48:MET:SD | 2.48 | 0.54 |
| 1:A:2727:G:O2' | 10:O:70:LYS:HE2 | 2.08 | 0.54 |
| 19:X:2:LYS:HE2 | 19:X:38:GLU:OE2 | 2.07 | 0.54 |
| 7:H:24:VAL:HG13 | 7:H:37:VAL:HG21 | 1.89 | 0.54 |
| 1:A:1762:A:H8 | 1:A:1762:A:O5' | 1.91 | 0.54 |
| 1:A:1364:G:OP1 | 23:1:2:SER:HA | 2.08 | 0.54 |
| 1:A:2144:U:O2' | 1:A:2145:C:H2' | 2.08 | 0.54 |
| 1:A:784:A:H5' | 1:A:785:G:OP1 | 2.07 | 0.54 |
| 1:A:2477:C:O2 | 31:9:4:ARG:NH2 | 2.36 | 0.54 |
| 19:X:31:HIS:CD2 | 19:X:33:LYS:H | 2.26 | 0.54 |
| 1:A:628:G:H2' | 1:A:629:G:H8 | 1.72 | 0.54 |
| 1:A:861:A:C2 | 1:A:917:A:C4 | 2.95 | 0.54 |
| 1:A:2236:C:H2' | 1:A:2237:G:H5' | 1.90 | 0.54 |
| 9:N:102:ALA:O | 9:N:106:MET:HG3 | 2.07 | 0.54 |
| 1:A:1430:C:H2' | 1:A:1431:U:H6 | 1.73 | 0.54 |
| 1:A:2262:U:O2' | 1:A:2263:C:H5' | 2.08 | 0.54 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:2000:G:N7 | 34:A:4190:HOH:O | 2.33 | 0.54 |
| 1:A:277:C:H4' | 1:A:278:A:O5' | 2.08 | 0.53 |
| 6:G:27:ASN:HB3 | 6:G:30:GLU:HG3 | 1.90 | 0.53 |
| 15:T:1:MET:HE2 | 15:T:3:ARG:HG2 | 1.89 | 0.53 |
| 1:A:2108:C:H6 | 1:A:2108:C:H3' | 1.72 | 0.53 |
| 1:A:2815:C:H2' | 1:A:2816:C:H6 | 1.73 | 0.53 |
| 1:A:819:A:H2' | 1:A:820:A:H5' | 1.89 | 0.53 |
| 13:R:37:THR:OG1 | 13:R:40:LYS:HG3 | 2.08 | 0.53 |
| 1:A:1876:A:H2' | 1:A:1877:A:C8 | 2.44 | 0.53 |
| 21:Z:54:HIS:ND1 | 21:Z:101:PRO:HG3 | 2.23 | 0.53 |
| 1:A:154:G:H5' | 1:A:154(A):C:OP2 | 2.08 | 0.53 |
| 1:A:2690:C:OP2 | 13:R:14:SER:HB3 | 2.09 | 0.53 |
| 1:A:2129:C:N3 | 1:A:2160:G:C6 | 2.76 | 0.53 |
| 14:S:14:VAL:O | 14:S:18:ILE:HG12 | 2.09 | 0.53 |
| 1:A:2064:C:H2' | 1:A:2065:C:C6 | 2.44 | 0.53 |
| 20:Y:2:ARG:HH11 | 20:Y:2:ARG:HA | 1.73 | 0.53 |
| 6:G:156:ASP:O | 6:G:157:ILE:HG13 | 2.07 | 0.53 |
| 1:A:2305:A:H1' | 6:G:135:LEU:O | 2.09 | 0.53 |
| 30:8:28:GLY:O | 30:8:36:LYS:NZ | 2.41 | 0.53 |
| 6:G:16:ARG:HH21 | 6:G:31:VAL:HB | 1.74 | 0.53 |
| 1:A:244:A:C2 | 1:A:255:A:C4 | 2.96 | 0.53 |
| 1:A:2892:A:H2' | 1:A:2893:G:H5'' | 1.89 | 0.53 |
| 16:U:8:VAL:O | 16:U:12:ARG:HG3 | 2.07 | 0.53 |
| 6:G:111:LEU:HD22 | 6:G:114:ILE:HD11 | 1.91 | 0.53 |
| 1:A:1406:U:H2' | 1:A:1407:C:C6 | 2.42 | 0.53 |
| 1:A:271(F):C:H2' | 1:A:271(G):C:H6 | 1.73 | 0.53 |
| 9:N:62:VAL:HG12 | 9:N:67:LEU:HD22 | 1.91 | 0.53 |
| 1:A:386:G:H4' | 1:A:387:U:OP2 | 2.09 | 0.53 |
| 5:F:150:GLY:HA2 | 5:F:172:TRP:CD2 | 2.44 | 0.53 |
| 1:A:1108:U:O2' | 1:A:1109:C:O5' | 2.27 | 0.53 |
| 8:I:98:ALA:O | 8:I:101:LEU:N | 2.42 | 0.53 |
| 1:A:1899:G:H2' | 1:A:1899:G:N3 | 2.24 | 0.53 |
| 1:A:2115:G:O2' | 1:A:2166:G:N2 | 2.42 | 0.53 |
| 20:Y:23:ARG:HB2 | 20:Y:23:ARG:NH1 | 2.23 | 0.53 |
| 1:A:2144:U:H1' | 1:A:2147:G:H1 | 1.72 | 0.53 |
| 5:F:107:LYS:HE3 | 5:F:205:ARG:O | 2.08 | 0.53 |
| 3:D:20:ASP:OD2 | 3:D:22:SER:OG | 2.20 | 0.53 |
| 8:I:134:PRO:C | 8:I:136:VAL:H | 2.12 | 0.53 |
| 1:A:813:U:H2' | 1:A:814:C:C6 | 2.44 | 0.53 |
| 22:0:53:MET:HG3 | 22:0:59:LEU:CD2 | 2.38 | 0.53 |
| 20:Y:51:VAL:HG22 | 20:Y:58:GLY:H | 1.73 | 0.53 |
| 8:I:14:ASP:O | 8:I:17:GLN:HB3 | 2.09 | 0.53 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:A:1434:A:H61 | 1:A:1558:A:N6 | 2.06 | 0.53 |
| 6:G:134:GLY:HA2 | 6:G:156:ASP:HA | 1.91 | 0.53 |
| 1:A:638:G:H2' | 1:A:639:U:C6 | 2.43 | 0.53 |
| 1:A:271(E):U:H2' | 1:A:271(F):C:H6 | 1.72 | 0.53 |
| 25:3:4:LEU:O | 25:3:36:VAL:HA | 2.08 | 0.53 |
| 1:A:1593:G:H2' | 1:A:1594:G:C8 | 2.44 | 0.53 |
| 1:A:1507:A:O2' | 1:A:1508:A:O5' | 2.17 | 0.52 |
| 6:G:106:LEU:HG | 6:G:111:LEU:HG | 1.91 | 0.52 |
| 5:F:185:ASP:HA | 5:F:188:ARG:HD3 | 1.90 | 0.52 |
| 20:Y:28:LYS:CG | 20:Y:40:GLU:HG2 | 2.39 | 0.52 |
| 13:R:81:ASP:O | 13:R:85:PRO:HG2 | 2.09 | 0.52 |
| 1:A:1877:A:H5' | 1:A:1878:G:OP2 | 2.09 | 0.52 |
| 14:S:59:LYS:HB3 | 14:S:60:GLY:HA2 | 1.90 | 0.52 |
| 22:0:53:MET:HG3 | 22:0:59:LEU:HD23 | 1.92 | 0.52 |
| 1:A:1688:U:O2 | 1:A:1700:A:H5' | 2.09 | 0.52 |
| 21:Z:52:SER:OG | 21:Z:53:ILE:N | 2.42 | 0.52 |
| 1:A:2751:G:C5 | 7:H:2:SER:N | 2.77 | 0.52 |
| 1:A:2309:A:N6 | 1:A:2310:A:N1 | 2.57 | 0.52 |
| 1:A:2206:G:H5' | 1:A:2207:G:N7 | 2.24 | 0.52 |
| 1:A:1429:G:H2' | 1:A:1430:C:C6 | 2.44 | 0.52 |
| 5:F:108:LYS:O | 5:F:112:MET:HG3 | 2.09 | 0.52 |
| 1:A:1946:U:H2' | 1:A:1947:C:C6 | 2.44 | 0.52 |
| 3:D:10:THR:OG1 | 3:D:13:ARG:HB2 | 2.10 | 0.52 |
| 1:A:2198:A:O5' | 8:I:33:ARG:NH2 | 2.42 | 0.52 |
| 1:A:2227:A:OP2 | 34:A:3994:HOH:O | 2.18 | 0.52 |
| 22:0:51:VAL:N | 22:0:62:LEU:HD12 | 2.25 | 0.52 |
| 1:A:686:G:O6 | 29:7:12:ARG:HD2 | 2.09 | 0.52 |
| 14:S:56:LEU:O | 14:S:58:LEU:HD23 | 2.09 | 0.52 |
| 30:8:39:LYS:HA | 30:8:42:ARG:NH1 | 2.24 | 0.52 |
| 1:A:542:C:H2' | 1:A:543:C:C6 | 2.44 | 0.52 |
| 2:B:52:A:O2' | 2:B:53:A:N3 | 2.38 | 0.52 |
| 15:T:55:ASN:N | 15:T:59:THR:HG22 | 2.25 | 0.52 |
| 7:H:71:LEU:HA | 7:H:74:ASN:HB2 | 1.92 | 0.52 |
| 1:A:1858:G:H2' | 1:A:1883:G:H22 | 1.75 | 0.52 |
| 1:A:2206:G:H2' | 1:A:2207:G:C2 | 2.45 | 0.52 |
| 1:A:1531:C:H42 | 1:A:1538:G:H1 | 1.56 | 0.52 |
| 2:B:113:G:H2' | 2:B:114:C:C6 | 2.44 | 0.52 |
| 1:A:1607:C:H4' | 1:A:1608:A:O5' | 2.10 | 0.52 |
| 1:A:263:C:H2' | 1:A:264:C:O4' | 2.09 | 0.52 |
| 1:A:2238:G:N7 | 34:A:3621:HOH:O | 2.34 | 0.52 |
| 11:P:148:LEU:H | 11:P:148:LEU:HD23 | 1.74 | 0.52 |
| 1:A:1721:G:H5' | 1:A:1722:A:OP2 | 2.10 | 0.52 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 15:T:99:LEU:O | 15:T:101:PHE:N | 2.42 | 0.52 |
| 12:Q:57:HIS:HD2 | 12:Q:117:ALA:HB2 | 1.75 | 0.52 |
| 1:A:2298:A:H2' | 1:A:2299:G:O4' | 2.09 | 0.52 |
| 20:Y:43:ASN:OD1 | 20:Y:65:ALA:HB3 | 2.09 | 0.52 |
| 9:N:99:LEU:O | 9:N:103:VAL:HG23 | 2.10 | 0.52 |
| 1:A:2273:A:H2' | 1:A:2274:A:C8 | 2.45 | 0.52 |
| 1:A:934:G:H2' | 1:A:935:C:C6 | 2.45 | 0.52 |
| 1:A:2820:A:C5 | 13:R:4:LEU:HD11 | 2.45 | 0.52 |
| 14:S:58:LEU:HD12 | 14:S:65:VAL:HG13 | 1.91 | 0.52 |
| 3:D:172:TYR:CD1 | 3:D:186:HIS:HA | 2.45 | 0.52 |
| 1:A:234:C:H2' | 1:A:235:U:O4' | 2.10 | 0.52 |
| 1:A:1474:C:N4 | 34:A:3951:HOH:O | 2.42 | 0.52 |
| 23:1:23:LYS:HG2 | 23:1:29:GLY:HA3 | 1.92 | 0.52 |
| 1:A:1309:G:P | 29:7:9:ARG:HD3 | 2.50 | 0.52 |
| 7:H:139:GLN:HG3 | 7:H:140:LYS:N | 2.25 | 0.52 |
| 1:A:1833:U:H2' | 1:A:1834:U:H6 | 1.75 | 0.52 |
| 5:F:53:THR:HG22 | 5:F:56:GLU:HG3 | 1.92 | 0.51 |
| 1:A:323:G:C8 | 5:F:171:PRO:HG3 | 2.45 | 0.51 |
| 1:A:1165:U:H2' | 1:A:1166:C:C6 | 2.45 | 0.51 |
| 28:6:34:LEU:HD22 | 28:6:36:LEU:HD11 | 1.91 | 0.51 |
| 10:O:25:LEU:HD12 | 10:O:38:VAL:HG12 | 1.92 | 0.51 |
| 7:H:43:VAL:HG22 | 7:H:52:VAL:HG22 | 1.92 | 0.51 |
| 1:A:493:G:H2' | 1:A:494:G:O4' | 2.10 | 0.51 |
| 1:A:9:U:O2' | 1:A:10:G:OP1 | 2.28 | 0.51 |
| 1:A:1466:G:HO2' | 1:A:1546:C:HO2' | 1.49 | 0.51 |
| 1:A:2582:G:C2 | 1:A:2583:G:C8 | 2.98 | 0.51 |
| 27:5:41:PRO:O | 27:5:44:THR:OG1 | 2.28 | 0.51 |
| 1:A:2079:U:OP1 | 23:1:21:ARG:NH2 | 2.42 | 0.51 |
| 1:A:2107:C:H41 | 1:A:2108:C:H42 | 1.58 | 0.51 |
| 14:S:58:LEU:HB2 | 14:S:59:LYS:HB2 | 1.92 | 0.51 |
| 1:A:2734:A:H2' | 1:A:2735:G:O4' | 2.11 | 0.51 |
| 1:A:1547:C:H2' | 1:A:1548:C:H6 | 1.75 | 0.51 |
| 11:P:26:GLY:O | 11:P:28:GLY:N | 2.44 | 0.51 |
| 3:D:175:LEU:HD12 | 3:D:185:VAL:HG21 | 1.91 | 0.51 |
| 1:A:2126:A:H1' | 1:A:2127:G:OP2 | 2.10 | 0.51 |
| 1:A:903:C:H2' | 1:A:904:C:C6 | 2.44 | 0.51 |
| 21:Z:101:PRO:O | 21:Z:102:LEU:HD12 | 2.10 | 0.51 |
| 1:A:2815:C:H5' | 27:5:29:THR:HG21 | 1.92 | 0.51 |
| 12:Q:42:ILE:HD13 | 12:Q:97:VAL:HG21 | 1.91 | 0.51 |
| 1:A:57:C:H2' | 1:A:58:G:O4' | 2.11 | 0.51 |
| 1:A:2286:A:OP1 | 28:6:29:ASN:ND2 | 2.44 | 0.51 |
| 1:A:2292:C:OP1 | 14:S:17:ARG:NH2 | 2.43 | 0.51 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:1140:C:O3' | 9:N:25:ARG:NH1 | 2.43 | 0.51 |
| 1:A:2163:C:OP2 | 1:A:2164:C:N4 | 2.41 | 0.51 |
| 8:I:70:GLU:O | 8:I:74:ASN:ND2 | 2.43 | 0.51 |
| 17:V:16:PRO:HA | 17:V:96:ILE:HG22 | 1.93 | 0.51 |
| 1:A:1779:U:H6 | 1:A:1784:A:H62 | 1.57 | 0.51 |
| 1:A:287:C:N3 | 1:A:354:G:N1 | 2.46 | 0.51 |
| 1:A:2114:A:H2' | 1:A:2115:G:O4' | 2.11 | 0.51 |
| 1:A:2102:U:O2 | 1:A:2187:G:O6 | 2.29 | 0.51 |
| 1:A:2572:A:N7 | 4:E:145:LYS:HB2 | 2.25 | 0.51 |
| 14:S:83:LYS:O | 14:S:111:GLU:HG3 | 2.11 | 0.51 |
| 24:2:29:LYS:HD3 | 24:2:57:ILE:HD13 | 1.92 | 0.51 |
| 1:A:443:A:H1' | 1:A:1201:C:O4' | 2.10 | 0.51 |
| 23:1:51:VAL:HG11 | 23:1:74:VAL:HG21 | 1.92 | 0.51 |
| 1:A:1358:G:H2' | 1:A:1359:A:H2 | 1.76 | 0.51 |
| 19:X:11:PRO:HD3 | 24:2:37:PHE:CE2 | 2.46 | 0.51 |
| 24:2:48:HIS:O | 24:2:52:ASP:HB2 | 2.11 | 0.51 |
| 3:D:71:ASP:OD1 | 3:D:103:ARG:NH2 | 2.35 | 0.51 |
| 1:A:995:C:OP2 | 16:U:54:LYS:HE3 | 2.11 | 0.51 |
| 12:Q:5:ARG:O | 21:Z:194:PRO:HD2 | 2.11 | 0.51 |
| 6:G:60:LEU:O | 6:G:64:THR:N | 2.40 | 0.51 |
| 1:A:2420:C:OP2 | 30:8:33:ASN:HB2 | 2.11 | 0.51 |
| 23:1:82:LEU:HA | 23:1:85:LEU:HD23 | 1.92 | 0.51 |
| 3:D:12:SER:HB3 | 3:D:208:LYS:HB3 | 1.91 | 0.51 |
| 2:B:43:C:H4' | 6:G:66:GLN:OE1 | 2.11 | 0.51 |
| 1:A:2131:G:H8 | 1:A:2131:G:OP2 | 1.93 | 0.50 |
| 14:S:7:TYR:CE1 | 14:S:91:PRO:HG3 | 2.46 | 0.50 |
| 18:W:19:LEU:HB3 | 27:5:25:LEU:HD11 | 1.93 | 0.50 |
| 25:3:6:VAL:HG12 | 25:3:54:VAL:HG11 | 1.93 | 0.50 |
| 21:Z:110:GLY:HA3 | 21:Z:174:VAL:HG11 | 1.93 | 0.50 |
| 19:X:41:ASN:O | 19:X:45:THR:HG23 | 2.12 | 0.50 |
| 1:A:2305:A:H2' | 1:A:2306:C:O4' | 2.11 | 0.50 |
| 1:A:1047:G:H2' | 1:A:1110:G:N2 | 2.26 | 0.50 |
| 21:Z:128:VAL:HG22 | 21:Z:161:VAL:H | 1.75 | 0.50 |
| 1:A:1593:G:H2' | 1:A:1594:G:H8 | 1.76 | 0.50 |
| 1:A:1043:C:H2' | 1:A:1044:G:O4' | 2.11 | 0.50 |
| 24:2:69:ARG:O | 24:2:70:GLN:HB2 | 2.11 | 0.50 |
| 1:A:2199:A:OP2 | 1:A:2200:C:H5 | 1.94 | 0.50 |
| 1:A:2439:A:H5' | 1:A:2439:A:C8 | 2.46 | 0.50 |
| 1:A:1141:U:H4' | 1:A:1142(A):A:O4' | 2.11 | 0.50 |
| 1:A:639:U:H2' | 1:A:640:C:H6 | 1.77 | 0.50 |
| 9:N:33:LEU:HD12 | 9:N:38:HIS:CE1 | 2.47 | 0.50 |
| 8:I:87:LYS:HA | 8:I:121:LYS:O | 2.11 | 0.50 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:1816:G:H1 | 3:D:35:LYS:HD3 | 1.76 | 0.50 |
| 1:A:1377:G:O6 | 34:A:3680:HOH:O | 2.19 | 0.50 |
| 21:Z:24:LEU:HB2 | 21:Z:41:LEU:HD23 | 1.94 | 0.50 |
| 1:A:795:C:H2' | 1:A:796:C:H6 | 1.77 | 0.50 |
| 1:A:1638:C:H4' | 1:A:2710:C:O2 | 2.11 | 0.50 |
| 20:Y:23:ARG:HH11 | 20:Y:23:ARG:HB2 | 1.77 | 0.50 |
| 14:S:11:LYS:HG3 | 14:S:91:PRO:HD3 | 1.92 | 0.50 |
| 1:A:1602:U:O4 | 34:A:3687:HOH:O | 2.20 | 0.50 |
| 13:R:21:TYR:OH | 13:R:43:GLU:HG2 | 2.12 | 0.50 |
| 1:A:863:A:H2' | 1:A:864:G:C8 | 2.47 | 0.50 |
| 1:A:1379:A:H4' | 1:A:1380:G:OP2 | 2.11 | 0.50 |
| 1:A:271(N):U:O2' | 1:A:271(O):C:H5' | 2.12 | 0.50 |
| 7:H:69:ARG:HG3 | 7:H:70:THR:N | 2.26 | 0.50 |
| 1:A:1720:U:H2' | 1:A:1721:G:O4' | 2.11 | 0.50 |
| 19:X:11:PRO:HD3 | 24:2:37:PHE:CZ | 2.45 | 0.50 |
| 19:X:27:THR:HG23 | 19:X:80:ILE:HG13 | 1.94 | 0.50 |
| 1:A:1497:U:H5'' | 1:A:1498:C:H5 | 1.77 | 0.50 |
| 8:I:77:LEU:HB3 | 8:I:142:VAL:HG12 | 1.94 | 0.50 |
| 1:A:1810:A:H2' | 1:A:1811:G:O4' | 2.11 | 0.50 |
| 9:N:34:LEU:O | 9:N:49:GLY:HA3 | 2.11 | 0.50 |
| 1:A:251:A:OP1 | 30:8:7:HIS:HE1 | 1.95 | 0.50 |
| 1:A:252:G:OP2 | 11:P:50:ARG:NH1 | 2.40 | 0.50 |
| 28:6:8:LYS:HD3 | 30:8:34:TRP:CD2 | 2.46 | 0.50 |
| 30:8:32:LEU:O | 30:8:36:LYS:HE3 | 2.12 | 0.50 |
| 1:A:873:G:N2 | 1:A:905:U:C2 | 2.80 | 0.50 |
| 10:O:64:ARG:NH1 | 10:O:81:ASP:OD1 | 2.45 | 0.50 |
| 6:G:125:PHE:HB3 | 6:G:166:ASP:CG | 2.32 | 0.50 |
| 14:S:29:PHE:CD2 | 14:S:30:ARG:N | 2.79 | 0.50 |
| 1:A:910:A:C5 | 12:Q:13:GLN:HG3 | 2.47 | 0.50 |
| 1:A:479:A:N3 | 1:A:481:G:H5'' | 2.25 | 0.50 |
| 11:P:38:GLN:HA | 11:P:41:ARG:HG2 | 1.93 | 0.50 |
| 1:A:1547:C:H2' | 1:A:1548:C:C6 | 2.47 | 0.50 |
| 2:B:38:C:O4' | 14:S:95:HIS:NE2 | 2.44 | 0.50 |
| 1:A:1945:G:H2' | 1:A:1946:U:H6 | 1.77 | 0.49 |
| 1:A:910:A:H62 | 12:Q:12:GLN:HA | 1.77 | 0.49 |
| 1:A:1794:U:H2' | 1:A:1795:C:C6 | 2.47 | 0.49 |
| 1:A:1669:A:H5'' | 1:A:2550:G:OP1 | 2.12 | 0.49 |
| 1:A:524:U:H2' | 1:A:525:U:C6 | 2.47 | 0.49 |
| 1:A:1575:C:H2' | 1:A:1576:U:C6 | 2.47 | 0.49 |
| 9:N:96:GLU:H | 9:N:96:GLU:CD | 2.15 | 0.49 |
| 5:F:22:ALA:HB1 | 5:F:24:LEU:HD22 | 1.93 | 0.49 |
| 12:Q:6:ARG:HG2 | 21:Z:194:PRO:HG2 | 1.93 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 18:W:46:PHE:O | 18:W:50:VAL:HG23 | 2.13 | 0.49 |
| 1:A:946:G:P | 34:A:3959:HOH:O | 2.71 | 0.49 |
| 1:A:863:A:H2' | 1:A:864:G:H8 | 1.76 | 0.49 |
| 1:A:236:C:H2' | 1:A:237:C:C6 | 2.47 | 0.49 |
| 1:A:253:C:OP2 | 30:8:5:LYS:NZ | 2.37 | 0.49 |
| 5:F:149:ASP:OD2 | 5:F:149:ASP:N | 2.42 | 0.49 |
| 1:A:2131:G:N3 | 1:A:2133:G:N2 | 2.54 | 0.49 |
| 1:A:856:C:O4' | 22:0:27:GLU:HB3 | 2.12 | 0.49 |
| 1:A:902:C:H2' | 1:A:903:C:H6 | 1.77 | 0.49 |
| 1:A:1780:A:N6 | 34:A:3750:HOH:O | 2.44 | 0.49 |
| 10:O:71:ARG:HB3 | 10:O:73:ASP:OD2 | 2.13 | 0.49 |
| 10:O:77:ILE:HG12 | 15:T:74:ARG:HD3 | 1.95 | 0.49 |
| 2:B:94:C:H2' | 2:B:95:C:H6 | 1.76 | 0.49 |
| 1:A:307:G:H21 | 1:A:330:A:H62 | 1.60 | 0.49 |
| 7:H:70:THR:HA | 7:H:73:ALA:HB3 | 1.95 | 0.49 |
| 14:S:10:ARG:NH2 | 14:S:91:PRO:HB2 | 2.25 | 0.49 |
| 1:A:1935:G:H1' | 1:A:1964:G:N2 | 2.27 | 0.49 |
| 6:G:41:GLN:O | 6:G:89:GLY:HA2 | 2.12 | 0.49 |
| 5:F:158:THR:O | 5:F:164:ARG:NH1 | 2.45 | 0.49 |
| 1:A:851:U:OP1 | 25:3:49:LYS:HE2 | 2.13 | 0.49 |
| 12:Q:110:THR:HG23 | 12:Q:113:GLN:OE1 | 2.12 | 0.49 |
| 2:B:111:G:H2' | 2:B:112:U:H6 | 1.78 | 0.49 |
| 1:A:2311:A:O2' | 1:A:2312:U:O4' | 2.22 | 0.49 |
| 1:A:1514:U:H2' | 1:A:1515:G:C8 | 2.47 | 0.49 |
| 1:A:2611:U:C4 | 27:5:3:LYS:HG2 | 2.47 | 0.49 |
| 1:A:628:G:H2' | 1:A:629:G:C8 | 2.46 | 0.49 |
| 1:A:1501:C:O4' | 3:D:100:GLY:HA2 | 2.12 | 0.49 |
| 21:Z:152:ALA:HA | 21:Z:155:LEU:HD13 | 1.94 | 0.49 |
| 1:A:1769:G:O2' | 1:A:1958:C:OP1 | 2.18 | 0.49 |
| 24:2:23:LYS:O | 24:2:27:GLU:HG2 | 2.12 | 0.49 |
| 1:A:774:A:N3 | 1:A:774:A:H2' | 2.27 | 0.49 |
| 1:A:903:C:H2' | 1:A:904:C:H6 | 1.77 | 0.49 |
| 5:F:187:VAL:HG13 | 11:P:1:MET:O | 2.13 | 0.49 |
| 1:A:857:C:H4' | 22:0:23:VAL:HG21 | 1.94 | 0.49 |
| 1:A:2712:U:H1' | 1:A:2712(A):A:C8 | 2.48 | 0.49 |
| 1:A:934:G:H2' | 1:A:935:C:H6 | 1.78 | 0.49 |
| 1:A:792:G:H5'' | 1:A:793:A:H5' | 1.93 | 0.49 |
| 21:Z:144:LEU:CD2 | 21:Z:150:LEU:HG | 2.43 | 0.49 |
| 1:A:1908:C:H1' | 34:A:4163:HOH:O | 2.13 | 0.49 |
| 1:A:644:A:H4' | 1:A:645:C:C5 | 2.47 | 0.49 |
| 1:A:2820:A:O2' | 1:A:2821:A:OP1 | 2.30 | 0.49 |
| 8:I:40:THR:O | 8:I:44:LEU:HB2 | 2.13 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:1479:G:O2' | 1:A:1558:A:H5' | 2.13 | 0.49 |
| 1:A:1558:A:H8 | 34:A:3530:HOH:O | 1.96 | 0.49 |
| 1:A:2281:C:O2' | 1:A:2282:G:H5' | 2.13 | 0.49 |
| 3:D:2:ALA:N | 3:D:200:ASP:OD2 | 2.46 | 0.49 |
| 8:I:130:TYR:HB3 | 8:I:138:ILE:HB | 1.93 | 0.49 |
| 2:B:66:A:H61 | 2:B:109:C:H5'' | 1.76 | 0.49 |
| 1:A:2124:G:H1 | 1:A:2174:C:N4 | 2.10 | 0.49 |
| 1:A:2123:G:H1 | 1:A:2175:C:N4 | 2.11 | 0.49 |
| 1:A:274:G:H2' | 1:A:275:G:C8 | 2.47 | 0.49 |
| 1:A:1657:C:H2' | 1:A:1658:C:C6 | 2.47 | 0.49 |
| 1:A:2313:C:H2' | 1:A:2314:C:C6 | 2.48 | 0.49 |
| 1:A:2312:U:H5' | 6:G:88:ILE:HD12 | 1.95 | 0.49 |
| 1:A:1800:C:OP1 | 3:D:266:SER:OG | 2.16 | 0.49 |
| 1:A:821:A:H2' | 1:A:946:G:H5'' | 1.94 | 0.49 |
| 5:F:32:LEU:HD12 | 5:F:32:LEU:HA | 1.60 | 0.49 |
| 1:A:125:G:H5'' | 29:7:19:ARG:HD3 | 1.94 | 0.49 |
| 1:A:857:C:OP2 | 22:0:77:ARG:NH2 | 2.46 | 0.49 |
| 1:A:1794:U:H2' | 1:A:1795:C:H6 | 1.78 | 0.49 |
| 28:6:11:LEU:HB3 | 28:6:49:HIS:HB3 | 1.95 | 0.49 |
| 1:A:2687:U:H2' | 1:A:2688:U:O4' | 2.13 | 0.49 |
| 1:A:2699:C:H2' | 1:A:2700:C:O4' | 2.11 | 0.49 |
| 1:A:848:G:H2' | 1:A:849:A:C8 | 2.47 | 0.49 |
| 30:8:7:HIS:HD2 | 30:8:10:ALA:N | 2.01 | 0.48 |
| 1:A:1108:U:O2 | 1:A:1108:U:H2' | 2.13 | 0.48 |
| 1:A:855:G:H2' | 1:A:856:C:C6 | 2.48 | 0.48 |
| 24:2:64:LEU:HD21 | 24:2:68:ARG:HE | 1.78 | 0.48 |
| 21:Z:104:PHE:HB3 | 21:Z:141:VAL:HG21 | 1.94 | 0.48 |
| 11:P:101:VAL:HA | 11:P:106:LEU:O | 2.13 | 0.48 |
| 1:A:517:C:OP1 | 27:5:16:ARG:NH2 | 2.42 | 0.48 |
| 1:A:2208:A:H1' | 1:A:2219:G:C4 | 2.48 | 0.48 |
| 1:A:1292:U:H2' | 1:A:1293:C:C6 | 2.48 | 0.48 |
| 2:B:33:G:C2 | 2:B:50:G:C2 | 3.01 | 0.48 |
| 1:A:7:G:H2' | 1:A:8:A:O4' | 2.12 | 0.48 |
| 2:B:5:C:O2' | 2:B:27:C:O2 | 2.30 | 0.48 |
| 18:W:60:ASN:N | 18:W:60:ASN:ND2 | 2.60 | 0.48 |
| 1:A:2646:C:H2' | 1:A:2647:U:O4' | 2.12 | 0.48 |
| 1:A:2854:G:H2' | 1:A:2855:C:C6 | 2.47 | 0.48 |
| 16:U:74:LEU:HD11 | 16:U:110:VAL:HG13 | 1.95 | 0.48 |
| 12:Q:109:VAL:HG22 | 12:Q:113:GLN:OE1 | 2.13 | 0.48 |
| 24:2:44:LEU:HG | 24:2:45:SER:O | 2.12 | 0.48 |
| 11:P:82:GLY:HA2 | 11:P:113:LYS:O | 2.12 | 0.48 |
| 11:P:27:HIS:O | 11:P:31:ALA:HA | 2.13 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 1:A:1745(A):C:H5' | 1:A:1746:G:OP2 | 2.13 | 0.48 |
| 1:A:2287:A:N6 | 1:A:2344:U:N3 | 2.50 | 0.48 |
| 1:A:1239:G:H2' | 1:A:1240:U:O4' | 2.14 | 0.48 |
| 21:Z:72:ARG:NH2 | 21:Z:97:GLU:O | 2.46 | 0.48 |
| 18:W:14:PRO:HG2 | 18:W:78:GLU:HG2 | 1.94 | 0.48 |
| 1:A:511:U:C5 | 1:A:512:G:C5 | 3.01 | 0.48 |
| 1:A:1985:G:O2' | 1:A:1986:A:H5' | 2.12 | 0.48 |
| 9:N:23:LEU:HG | 9:N:24:GLY:H | 1.78 | 0.48 |
| 1:A:2723:C:OP2 | 4:E:109:LYS:NZ | 2.46 | 0.48 |
| 2:B:55:U:H1' | 6:G:29:TRP:HE1 | 1.78 | 0.48 |
| 2:B:32:C:N3 | 2:B:51:G:C2 | 2.82 | 0.48 |
| 1:A:1434:A:H61 | 1:A:1558:A:H62 | 1.61 | 0.48 |
| 21:Z:144:LEU:HD21 | 21:Z:150:LEU:HG | 1.96 | 0.48 |
| 1:A:848:G:N9 | 1:A:933:A:H8 | 2.12 | 0.48 |
| 1:A:911:A:H2' | 12:Q:9:TYR:OH | 2.13 | 0.48 |
| 1:A:1441:G:H2' | 1:A:1442:G:H8 | 1.77 | 0.48 |
| 20:Y:38:ILE:HD11 | 20:Y:66:PRO:HG3 | 1.94 | 0.48 |
| 11:P:84:ASN:HB3 | 11:P:117:GLU:O | 2.13 | 0.48 |
| 1:A:2098:U:H2' | 1:A:2099:U:O4' | 2.14 | 0.48 |
| 7:H:24:VAL:HG22 | 7:H:35:VAL:HB | 1.94 | 0.48 |
| 22:O:11:ARG:O | 22:O:14:ARG:NH2 | 2.46 | 0.48 |
| 1:A:2698:U:O4 | 34:A:4097:HOH:O | 2.19 | 0.48 |
| 1:A:251:A:C5 | 1:A:252:G:H1' | 2.49 | 0.48 |
| 3:D:17:THR:O | 3:D:211:ARG:NH2 | 2.40 | 0.48 |
| 22:O:26:TYR:O | 22:O:29:GLN:HB2 | 2.14 | 0.48 |
| 20:Y:28:LYS:HG2 | 20:Y:40:GLU:HG2 | 1.96 | 0.48 |
| 1:A:258:G:N7 | 34:A:4026:HOH:O | 2.35 | 0.48 |
| 6:G:73:ALA:HB2 | 6:G:88:ILE:HD11 | 1.95 | 0.48 |
| 1:A:1253:A:N6 | 34:A:3584:HOH:O | 2.45 | 0.48 |
| 16:U:76:TYR:OH | 16:U:92:ARG:NH1 | 2.47 | 0.48 |
| 21:Z:111:VAL:O | 21:Z:113:ALA:N | 2.46 | 0.48 |
| 1:A:2690:C:N4 | 1:A:2713:A:H1' | 2.28 | 0.48 |
| 1:A:1790:C:H5'' | 1:A:1791:A:OP1 | 2.13 | 0.48 |
| 4:E:35:GLN:OE1 | 4:E:66:HIS:HE1 | 1.95 | 0.48 |
| 2:B:90:A:C5 | 2:B:91:C:H1' | 2.49 | 0.48 |
| 23:1:94:LEU:O | 23:1:97:LEU:HB2 | 2.13 | 0.48 |
| 4:E:112:GLY:O | 4:E:159:HIS:HA | 2.13 | 0.48 |
| 1:A:1914:C:OP2 | 1:A:1914:C:H6 | 1.96 | 0.48 |
| 13:R:103:ARG:HH12 | 13:R:110:PRO:HD3 | 1.78 | 0.48 |
| 1:A:495:G:N7 | 34:A:4055:HOH:O | 2.35 | 0.48 |
| 31:9:32:HIS:O | 31:9:34:GLN:HG3 | 2.13 | 0.48 |
| 1:A:2162:G:H4' | 1:A:2172:U:O2' | 2.14 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:2331:G:H4' | 22:0:43:THR:H | 1.79 | 0.48 |
| 1:A:154:G:H8 | 1:A:154:G:H5'' | 1.79 | 0.48 |
| 1:A:958:U:H5'' | 12:Q:14:ARG:HD3 | 1.95 | 0.48 |
| 1:A:2134:A:C2 | 1:A:2159:G:H1' | 2.49 | 0.48 |
| 25:3:8:LEU:HD13 | 25:3:31:LEU:HA | 1.96 | 0.48 |
| 14:S:96:GLY:N | 14:S:99:LYS:H | 2.12 | 0.48 |
| 1:A:2834:G:C8 | 1:A:2834:G:H5'' | 2.49 | 0.48 |
| 1:A:1506:C:C2' | 1:A:1507:A:H5' | 2.44 | 0.48 |
| 1:A:1575:C:H2' | 1:A:1576:U:H6 | 1.78 | 0.48 |
| 1:A:2378:A:H4' | 14:S:23:ARG:NH1 | 2.29 | 0.48 |
| 26:4:16:CYS:SG | 26:4:20:ASN:N | 2.87 | 0.48 |
| 11:P:100:LEU:HD12 | 11:P:112:LEU:HD11 | 1.95 | 0.48 |
| 1:A:30:G:H2' | 1:A:31:C:C6 | 2.48 | 0.48 |
| 1:A:7:G:H1 | 1:A:2896:C:H42 | 1.62 | 0.47 |
| 30:8:34:TRP:CE2 | 30:8:35:GLN:HG3 | 2.49 | 0.47 |
| 2:B:29:A:H5'' | 2:B:30:C:OP2 | 2.14 | 0.47 |
| 1:A:795:C:H2' | 1:A:796:C:C6 | 2.49 | 0.47 |
| 1:A:2610:C:H4' | 1:A:2611:U:OP2 | 2.14 | 0.47 |
| 8:I:14:ASP:N | 8:I:17:GLN:OE1 | 2.34 | 0.47 |
| 1:A:1025:G:C4 | 1:A:1135:C:H1' | 2.49 | 0.47 |
| 17:V:62:LEU:HD21 | 17:V:95:LEU:HB2 | 1.95 | 0.47 |
| 29:7:8:ASN:OD1 | 29:7:8:ASN:C | 2.52 | 0.47 |
| 1:A:271(P):C:H2' | 1:A:271(Q):G:H5' | 1.95 | 0.47 |
| 30:8:62:LEU:HB3 | 30:8:65:GLU:HG2 | 1.96 | 0.47 |
| 1:A:957:A:H5' | 12:Q:76:LYS:HG3 | 1.96 | 0.47 |
| 15:T:23:ARG:HG3 | 15:T:120:ARG:NH1 | 2.29 | 0.47 |
| 18:W:83:LYS:O | 18:W:84:ARG:HD3 | 2.15 | 0.47 |
| 1:A:649:G:H2' | 1:A:650:C:O4' | 2.14 | 0.47 |
| 1:A:271(L):U:C4' | 1:A:271(M):G:OP1 | 2.61 | 0.47 |
| 1:A:1405:U:H2' | 1:A:1406:U:H6 | 1.78 | 0.47 |
| 17:V:58:VAL:HG12 | 17:V:97:LYS:HB2 | 1.96 | 0.47 |
| 1:A:359:A:H2' | 1:A:360:G:O4' | 2.14 | 0.47 |
| 1:A:1106:G:H4' | 1:A:1107:G:OP2 | 2.14 | 0.47 |
| 1:A:1364:G:P | 23:1:3:LYS:HG2 | 2.54 | 0.47 |
| 1:A:1486:A:H2' | 1:A:1487:G:C8 | 2.46 | 0.47 |
| 12:Q:84:GLY:O | 12:Q:85:LYS:HB2 | 2.14 | 0.47 |
| 5:F:32:LEU:HD11 | 5:F:105:VAL:HG13 | 1.96 | 0.47 |
| 4:E:105:THR:OG1 | 4:E:199:ARG:NH2 | 2.46 | 0.47 |
| 1:A:1041:C:H5' | 1:A:1042:G:OP2 | 2.15 | 0.47 |
| 1:A:2836:U:H2' | 1:A:2837:G:C8 | 2.49 | 0.47 |
| 1:A:1839:G:C8 | 1:A:1927:A:H1' | 2.49 | 0.47 |
| 21:Z:5:LEU:HD22 | 21:Z:6:LYS:H | 1.80 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:92:A:C2' | 1:A:93:G:H5' | 2.45 | 0.47 |
| 2:B:111:G:H2' | 2:B:112:U:C6 | 2.49 | 0.47 |
| 1:A:1223:G:N2 | 1:A:1226:A:OP2 | 2.40 | 0.47 |
| 1:A:2478:A:H5' | 31:9:31:LYS:HE2 | 1.96 | 0.47 |
| 10:O:2:ILE:HD12 | 10:O:6:THR:HG21 | 1.96 | 0.47 |
| 1:A:857:C:H1' | 22:O:26:TYR:CE2 | 2.49 | 0.47 |
| 1:A:542:C:H2' | 1:A:543:C:H6 | 1.79 | 0.47 |
| 1:A:864:G:C6 | 1:A:865:C:N4 | 2.83 | 0.47 |
| 1:A:362:U:O2' | 1:A:363:G:H5'' | 2.15 | 0.47 |
| 7:H:33:LEU:HD21 | 7:H:136:ILE:HG13 | 1.96 | 0.47 |
| 1:A:1652:A:OP1 | 13:R:8:ARG:HD3 | 2.14 | 0.47 |
| 19:X:53:LYS:HB3 | 19:X:82:GLN:HB3 | 1.96 | 0.47 |
| 1:A:2693:A:H2' | 1:A:2694:G:H8 | 1.78 | 0.47 |
| 23:1:82:LEU:HD22 | 23:1:90:ILE:HG23 | 1.97 | 0.47 |
| 1:A:2497:A:H5'' | 34:A:3634:HOH:O | 2.13 | 0.47 |
| 1:A:819:A:C2' | 1:A:820:A:H5' | 2.45 | 0.47 |
| 9:N:34:LEU:HD12 | 9:N:34:LEU:HA | 1.73 | 0.47 |
| 1:A:29:U:H2' | 1:A:30:G:C8 | 2.50 | 0.47 |
| 30:8:62:LEU:HB3 | 30:8:65:GLU:CG | 2.45 | 0.47 |
| 1:A:458:G:O2' | 29:7:39:ARG:HD3 | 2.14 | 0.47 |
| 1:A:2016:U:H1' | 27:5:6:VAL:HG13 | 1.96 | 0.47 |
| 1:A:2884:U:O2 | 27:5:53:ALA:HB2 | 2.15 | 0.47 |
| 29:7:16:HIS:HB2 | 29:7:44:PRO:HG2 | 1.97 | 0.47 |
| 1:A:975(A):G:H1' | 1:A:990:A:C2 | 2.49 | 0.47 |
| 1:A:2659:G:P | 7:H:158:HIS:HE2 | 2.36 | 0.47 |
| 1:A:824:A:H1' | 1:A:2358:G:N7 | 2.29 | 0.47 |
| 1:A:2317:C:H2' | 1:A:2318:G:H5' | 1.96 | 0.47 |
| 3:D:267:SER:C | 3:D:269:PHE:H | 2.18 | 0.47 |
| 1:A:1533:G:O5' | 1:A:1533:G:H8 | 1.98 | 0.47 |
| 1:A:1557:C:OP2 | 1:A:1558:A:O2' | 2.25 | 0.47 |
| 1:A:1329:U:H5'' | 1:A:1330:C:H5 | 1.80 | 0.47 |
| 7:H:144:VAL:O | 7:H:148:ILE:HG12 | 2.14 | 0.47 |
| 1:A:2894:G:N3 | 1:A:2894:G:H2' | 2.30 | 0.47 |
| 1:A:2337:G:C2 | 1:A:2338:G:C8 | 3.03 | 0.47 |
| 31:9:8:LYS:O | 31:9:34:GLN:NE2 | 2.45 | 0.47 |
| 14:S:3:ARG:HG3 | 14:S:4:LEU:N | 2.24 | 0.47 |
| 16:U:65:ILE:HD11 | 16:U:95:LEU:HB3 | 1.97 | 0.47 |
| 1:A:2315:G:C6 | 1:A:2316:C:N4 | 2.83 | 0.47 |
| 18:W:40:ASN:O | 18:W:41:LYS:HG3 | 2.14 | 0.47 |
| 1:A:720:C:H2' | 1:A:721:C:C6 | 2.48 | 0.47 |
| 21:Z:141:VAL:O | 21:Z:144:LEU:HB2 | 2.14 | 0.47 |
| 1:A:143:G:H2' | 1:A:143(A):C:C6 | 2.50 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 3:D:26:LYS:HE2 | 3:D:28:GLU:O | 2.14 | 0.47 |
| 7:H:40:GLU:OE2 | 7:H:60:ARG:NH1 | 2.48 | 0.47 |
| 1:A:2287:A:O2' | 1:A:2288:A:H3' | 2.15 | 0.47 |
| 27:5:35:GLU:HG3 | 27:5:51:TYR:CB | 2.45 | 0.47 |
| 1:A:811:U:H2' | 11:P:21:ARG:HA | 1.96 | 0.47 |
| 2:B:49:C:OP1 | 14:S:97:ARG:HB2 | 2.15 | 0.47 |
| 5:F:89:VAL:O | 5:F:91:GLY:N | 2.48 | 0.47 |
| 1:A:860:U:C2 | 1:A:2268:A:C8 | 3.03 | 0.47 |
| 5:F:64:ILE:HD12 | 5:F:65:TRP:CZ3 | 2.50 | 0.47 |
| 1:A:760:G:H2' | 1:A:761:A:O4' | 2.14 | 0.47 |
| 1:A:307:G:N7 | 34:A:3949:HOH:O | 2.35 | 0.46 |
| 21:Z:30:ASN:HD22 | 21:Z:90:VAL:HB | 1.79 | 0.46 |
| 1:A:657:U:H2' | 1:A:658:C:C6 | 2.50 | 0.46 |
| 1:A:1970:A:H4' | 1:A:1971:A:OP1 | 2.15 | 0.46 |
| 15:T:84:GLN:NE2 | 15:T:85:LYS:HG2 | 2.30 | 0.46 |
| 4:E:97:LYS:O | 4:E:100:GLU:HG3 | 2.15 | 0.46 |
| 1:A:1889:A:H2' | 1:A:1890:A:C8 | 2.50 | 0.46 |
| 15:T:23:ARG:HG3 | 15:T:120:ARG:CZ | 2.45 | 0.46 |
| 19:X:26:TYR:CE1 | 19:X:89:ILE:HG13 | 2.50 | 0.46 |
| 5:F:103:LYS:HA | 5:F:106:ARG:HG3 | 1.97 | 0.46 |
| 3:D:142:VAL:HG23 | 3:D:193:VAL:HA | 1.97 | 0.46 |
| 3:D:147:LEU:HD13 | 3:D:155:LEU:HD21 | 1.97 | 0.46 |
| 1:A:64:A:O3' | 19:X:71:GLY:HA3 | 2.15 | 0.46 |
| 4:E:36:ARG:HG2 | 4:E:47:VAL:HG22 | 1.96 | 0.46 |
| 1:A:1180:C:H2' | 1:A:1181:C:H6 | 1.79 | 0.46 |
| 1:A:278:A:H4' | 1:A:279:C:OP1 | 2.15 | 0.46 |
| 26:4:14:ILE:HA | 26:4:31:ILE:O | 2.16 | 0.46 |
| 28:6:11:LEU:HB2 | 28:6:21:TYR:HB2 | 1.97 | 0.46 |
| 14:S:49:VAL:HG12 | 14:S:73:LEU:HD12 | 1.96 | 0.46 |
| 1:A:1582:C:O2' | 1:A:1586:A:N3 | 2.47 | 0.46 |
| 1:A:2106:G:N1 | 1:A:2107:C:O2 | 2.48 | 0.46 |
| 1:A:1494:A:C6 | 1:A:1495:A:C6 | 3.04 | 0.46 |
| 9:N:111:PRO:HA | 9:N:114:ARG:NH1 | 2.30 | 0.46 |
| 18:W:86:LEU:HD22 | 18:W:96:ILE:HD11 | 1.96 | 0.46 |
| 3:D:101:GLU:OE1 | 3:D:103:ARG:HD3 | 2.15 | 0.46 |
| 28:6:21:TYR:CE2 | 28:6:38:LYS:HG2 | 2.51 | 0.46 |
| 6:G:145:THR:HG23 | 6:G:148:MET:SD | 2.55 | 0.46 |
| 22:0:72:ARG:HB2 | 22:0:75:LEU:HB2 | 1.98 | 0.46 |
| 17:V:99:ILE:HG22 | 17:V:101:GLY:H | 1.80 | 0.46 |
| 1:A:955:C:OP1 | 12:Q:87:LYS:HE2 | 2.14 | 0.46 |
| 1:A:1568:G:H5'' | 3:D:61:LEU:HD22 | 1.96 | 0.46 |
| 1:A:1021:A:N6 | 1:A:1142(A):A:H61 | 2.13 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 2:B:8:U:OP1 | 14:S:11:LYS:NZ | 2.41 | 0.46 |
| 1:A:2238:G:H2' | 1:A:2238:G:N3 | 2.30 | 0.46 |
| 1:A:492:A:H2' | 1:A:493:G:O4' | 2.15 | 0.46 |
| 1:A:415:A:H2' | 1:A:416:C:C6 | 2.50 | 0.46 |
| 3:D:68:LYS:O | 3:D:70:TRP:CD1 | 2.69 | 0.46 |
| 10:O:47:ILE:HB | 10:O:48:PRO:HD2 | 1.97 | 0.46 |
| 1:A:2275:C:H5' | 1:A:2275:C:H6 | 1.80 | 0.46 |
| 1:A:2286:A:H4' | 1:A:2287:A:O4' | 2.15 | 0.46 |
| 23:1:3:LYS:HE3 | 23:1:3:LYS:HB3 | 1.52 | 0.46 |
| 4:E:111:ARG:HB3 | 13:R:1:MET:HE2 | 1.97 | 0.46 |
| 21:Z:111:VAL:C | 21:Z:113:ALA:N | 2.68 | 0.46 |
| 1:A:919:G:N2 | 1:A:2269:A:OP2 | 2.45 | 0.46 |
| 14:S:96:GLY:H | 14:S:99:LYS:H | 1.63 | 0.46 |
| 14:S:83:LYS:C | 14:S:111:GLU:HG3 | 2.36 | 0.46 |
| 2:B:65:C:N4 | 2:B:109:C:C2 | 2.83 | 0.46 |
| 1:A:272(J):C:H2' | 1:A:274:G:O4' | 2.15 | 0.46 |
| 1:A:322:A:H5' | 1:A:340:A:H1' | 1.96 | 0.46 |
| 1:A:1171:G:H1 | 1:A:1178:C:H42 | 1.63 | 0.46 |
| 4:E:115:GLY:O | 4:E:119:ARG:HB2 | 2.15 | 0.46 |
| 8:I:61:ARG:HH11 | 8:I:61:ARG:HA | 1.81 | 0.46 |
| 6:G:16:ARG:NH2 | 6:G:28:VAL:O | 2.48 | 0.46 |
| 1:A:2080:G:P | 23:1:35:THR:HG1 | 2.38 | 0.46 |
| 4:E:52:LEU:O | 4:E:75:VAL:HG22 | 2.16 | 0.46 |
| 5:F:127:GLU:HA | 5:F:196:LEU:HD12 | 1.97 | 0.46 |
| 19:X:57:LEU:HD21 | 19:X:78:LYS:HE2 | 1.97 | 0.46 |
| 22:O:24:LYS:O | 22:O:25:ARG:HD3 | 2.16 | 0.46 |
| 1:A:469:G:H2' | 1:A:470:A:H5'' | 1.96 | 0.46 |
| 1:A:1202:C:N4 | 1:A:1203:G:C6 | 2.83 | 0.46 |
| 1:A:2615:U:C2 | 27:5:7:PRO:HA | 2.51 | 0.46 |
| 15:T:118:ARG:HG3 | 15:T:118:ARG:HH11 | 1.80 | 0.46 |
| 10:O:68:GLU:HB3 | 10:O:78:ARG:HD3 | 1.98 | 0.46 |
| 1:A:2636:U:H4' | 4:E:80:GLU:OE2 | 2.16 | 0.46 |
| 5:F:178:PRO:HG2 | 5:F:179:GLU:OE1 | 2.15 | 0.46 |
| 3:D:69:ARG:NH2 | 3:D:128:GLY:O | 2.38 | 0.46 |
| 1:A:1418:G:H8 | 1:A:1418:G:O5' | 1.99 | 0.46 |
| 1:A:2748:A:OP1 | 7:H:70:THR:HG21 | 2.16 | 0.46 |
| 12:Q:16:ARG:O | 12:Q:17:LEU:HD23 | 2.15 | 0.46 |
| 1:A:234:C:H2' | 1:A:235:U:H6 | 1.81 | 0.46 |
| 3:D:38:LYS:HD2 | 3:D:39:LYS:N | 2.30 | 0.46 |
| 5:F:133:ASN:HA | 5:F:162:LEU:HD23 | 1.98 | 0.46 |
| 1:A:2818:G:O2' | 1:A:2819:G:H5' | 2.16 | 0.46 |
| 1:A:2285:C:OP2 | 28:6:6:ARG:NH1 | 2.47 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:2850:A:OP2 | 1:A:2866:U:H5 | 1.98 | 0.46 |
| 8:I:97:ILE:O | 8:I:100:ALA:HB3 | 2.16 | 0.46 |
| 1:A:708:C:H5' | 1:A:709:U:OP2 | 2.16 | 0.46 |
| 1:A:271(R):G:H2' | 1:A:271(S):G:C8 | 2.49 | 0.46 |
| 1:A:901:A:H2' | 1:A:902:C:C6 | 2.51 | 0.46 |
| 1:A:1721:G:N1 | 1:A:1739:U:OP2 | 2.49 | 0.46 |
| 1:A:923:C:C4' | 22:0:29:GLN:HE21 | 2.28 | 0.46 |
| 25:3:4:LEU:N | 25:3:37:LEU:O | 2.45 | 0.46 |
| 8:I:124:GLY:N | 8:I:144:VAL:HG13 | 2.31 | 0.46 |
| 1:A:2747:G:O6 | 1:A:2755:C:H5'' | 2.16 | 0.46 |
| 15:T:11:GLU:O | 15:T:15:VAL:HG23 | 2.16 | 0.46 |
| 1:A:128:C:H2' | 1:A:129:C:H6 | 1.80 | 0.46 |
| 1:A:2867:G:OP2 | 15:T:119:LYS:NZ | 2.41 | 0.46 |
| 1:A:2142:C:N3 | 1:A:2149:G:O6 | 2.49 | 0.46 |
| 1:A:1108:U:O2' | 1:A:1109:C:O4' | 2.34 | 0.46 |
| 7:H:5:GLY:HA2 | 7:H:69:ARG:HB3 | 1.97 | 0.46 |
| 1:A:1815:A:C5 | 1:A:1817:G:C6 | 3.04 | 0.46 |
| 4:E:60:ASN:OD1 | 4:E:62:PRO:HD2 | 2.15 | 0.46 |
| 1:A:655:A:H8 | 1:A:656:G:O4' | 1.98 | 0.46 |
| 1:A:646:A:N3 | 1:A:646:A:H5' | 2.31 | 0.46 |
| 1:A:2784:C:H1' | 4:E:37:ARG:NH1 | 2.30 | 0.46 |
| 12:Q:35:VAL:HG13 | 12:Q:130:LYS:HB3 | 1.98 | 0.46 |
| 1:A:2345:G:N3 | 1:A:2381:C:H2' | 2.31 | 0.46 |
| 1:A:1204:A:H61 | 1:A:1240:U:H2' | 1.81 | 0.45 |
| 1:A:1364:G:OP2 | 23:1:3:LYS:HG2 | 2.16 | 0.45 |
| 1:A:2406:U:C4 | 11:P:72:PRO:HD2 | 2.51 | 0.45 |
| 1:A:1026:U:O2' | 1:A:1027:A:H8 | 2.00 | 0.45 |
| 1:A:1027:A:N6 | 1:A:1126:A:C4 | 2.84 | 0.45 |
| 1:A:2760:C:C2' | 1:A:2761:G:H5'' | 2.44 | 0.45 |
| 30:8:61:LEU:C | 30:8:63:PRO:HD3 | 2.36 | 0.45 |
| 1:A:2250:G:N2 | 12:Q:84:GLY:HA3 | 2.31 | 0.45 |
| 2:B:50:G:H5'' | 14:S:61:ASN:HD21 | 1.81 | 0.45 |
| 1:A:2716:U:O2' | 1:A:2717:G:H5' | 2.16 | 0.45 |
| 1:A:2626:C:H2' | 1:A:2627:G:O4' | 2.15 | 0.45 |
| 6:G:102:PHE:CE2 | 6:G:141:PHE:HE1 | 2.33 | 0.45 |
| 17:V:52:VAL:HG22 | 17:V:55:ALA:HB3 | 1.97 | 0.45 |
| 6:G:63:ILE:HD13 | 6:G:155:MET:HE1 | 1.98 | 0.45 |
| 30:8:9:GLY:O | 30:8:13:ARG:HG3 | 2.16 | 0.45 |
| 1:A:2512:C:H4' | 4:E:122:PHE:CE2 | 2.51 | 0.45 |
| 1:A:1922:G:H2' | 1:A:1923:U:O4' | 2.16 | 0.45 |
| 23:1:60:PHE:N | 23:1:60:PHE:CD2 | 2.84 | 0.45 |
| 1:A:195:A:H4' | 1:A:251:A:O2' | 2.17 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 1:A:241:A:O4' | 1:A:243:U:C6 | 2.70 | 0.45 |
| 1:A:1536:C:O2' | 1:A:1537:G:O5' | 2.28 | 0.45 |
| 14:S:65:VAL:O | 14:S:69:VAL:HG12 | 2.16 | 0.45 |
| 1:A:861:A:N3 | 2:B:79:C:O2' | 2.47 | 0.45 |
| 12:Q:12:GLN:HG2 | 12:Q:73:PRO:HD2 | 1.97 | 0.45 |
| 1:A:1364:G:N7 | 23:1:3:LYS:HD3 | 2.30 | 0.45 |
| 1:A:330:A:H2 | 1:A:1210:A:HO2' | 1.62 | 0.45 |
| 1:A:916:G:O2' | 1:A:917:A:O4' | 2.31 | 0.45 |
| 22:O:53:MET:HA | 22:O:58:THR:O | 2.16 | 0.45 |
| 23:1:64:ALA:HA | 23:1:67:ILE:HG13 | 1.97 | 0.45 |
| 1:A:2191:G:H3' | 1:A:2192:G:H8 | 1.81 | 0.45 |
| 6:G:174:GLU:O | 6:G:177:GLY:N | 2.45 | 0.45 |
| 1:A:2390:U:O2' | 1:A:2391:G:H5' | 2.16 | 0.45 |
| 17:V:21:ARG:HG3 | 17:V:93:GLU:HG3 | 1.98 | 0.45 |
| 12:Q:119:ARG:HE | 12:Q:119:ARG:HB3 | 1.62 | 0.45 |
| 1:A:26:G:C6 | 1:A:27:G:N1 | 2.85 | 0.45 |
| 1:A:2115:G:C2 | 1:A:2117:A:N7 | 2.84 | 0.45 |
| 24:2:51:ARG:O | 24:2:51:ARG:HG2 | 2.16 | 0.45 |
| 1:A:2107:C:N4 | 1:A:2108:C:N4 | 2.64 | 0.45 |
| 1:A:2109:U:O2 | 1:A:2181:G:N1 | 2.49 | 0.45 |
| 1:A:2302:G:C6 | 1:A:2315:G:C6 | 3.04 | 0.45 |
| 1:A:2146:C:H4' | 1:A:2147:G:C8 | 2.51 | 0.45 |
| 1:A:1510:G:H2' | 1:A:1511:C:C6 | 2.51 | 0.45 |
| 1:A:1478:G:H2' | 1:A:1479:G:H8 | 1.82 | 0.45 |
| 1:A:1592:C:H2' | 1:A:1593:G:H8 | 1.82 | 0.45 |
| 21:Z:144:LEU:HD12 | 21:Z:144:LEU:HA | 1.78 | 0.45 |
| 19:X:18:TYR:O | 19:X:20:GLY:N | 2.50 | 0.45 |
| 1:A:196:A:H2' | 1:A:196:A:N3 | 2.31 | 0.45 |
| 1:A:2793:G:N2 | 1:A:2804:C:H1' | 2.32 | 0.45 |
| 5:F:197:ASP:OD2 | 5:F:197:ASP:N | 2.49 | 0.45 |
| 1:A:2304:G:O6 | 1:A:2312:U:O4 | 2.34 | 0.45 |
| 1:A:2126:A:N1 | 1:A:2162:G:O2' | 2.40 | 0.45 |
| 1:A:2591:C:OP1 | 3:D:239:ARG:HG2 | 2.17 | 0.45 |
| 21:Z:53:ILE:HG22 | 21:Z:71:VAL:O | 2.17 | 0.45 |
| 1:A:643:A:C2 | 1:A:644:A:C4 | 3.04 | 0.45 |
| 1:A:645:C:H2' | 1:A:645:C:O2 | 2.15 | 0.45 |
| 1:A:1651:G:H2' | 1:A:1652:A:O4' | 2.17 | 0.45 |
| 1:A:1319:G:C6 | 1:A:1320:C:N4 | 2.85 | 0.45 |
| 3:D:213:ARG:HA | 3:D:213:ARG:HD2 | 1.61 | 0.45 |
| 1:A:1106:G:N3 | 1:A:1106:G:H2' | 2.31 | 0.45 |
| 1:A:1235:G:C6 | 1:A:1236:G:N1 | 2.84 | 0.45 |
| 1:A:997:G:OP1 | 16:U:92:ARG:HG2 | 2.16 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:902:C:H2' | 1:A:903:C:C6 | 2.51 | 0.45 |
| 25:3:43:ILE:O | 25:3:47:VAL:HG23 | 2.16 | 0.45 |
| 1:A:2483:C:N3 | 12:Q:124:LYS:NZ | 2.63 | 0.45 |
| 2:B:46:A:C5 | 2:B:47:C:C4 | 3.04 | 0.45 |
| 17:V:20:LEU:HA | 17:V:20:LEU:HD12 | 1.79 | 0.45 |
| 9:N:22:THR:O | 9:N:23:LEU:O | 2.34 | 0.45 |
| 26:4:40:HIS:HB3 | 26:4:43:TYR:HB3 | 1.98 | 0.45 |
| 1:A:583:G:OP2 | 16:U:10:ARG:HD2 | 2.17 | 0.45 |
| 21:Z:5:LEU:O | 21:Z:59:LEU:HA | 2.16 | 0.45 |
| 1:A:2427:C:H5'' | 1:A:2428:G:OP1 | 2.16 | 0.45 |
| 12:Q:7:MET:HE1 | 21:Z:193:GLU:CB | 2.47 | 0.45 |
| 1:A:815:C:H2' | 1:A:816:C:H6 | 1.81 | 0.45 |
| 1:A:1634:A:OP2 | 34:A:3693:HOH:O | 2.21 | 0.45 |
| 5:F:68:LYS:HB2 | 5:F:69:HIS:CD2 | 2.52 | 0.45 |
| 1:A:2785:C:OP1 | 4:E:41:LYS:NZ | 2.40 | 0.45 |
| 31:9:25:VAL:HB | 31:9:34:GLN:HB2 | 1.98 | 0.45 |
| 1:A:2131:G:OP2 | 1:A:2131:G:H3' | 2.16 | 0.45 |
| 1:A:2173:A:C6 | 1:A:2174:C:C2 | 3.05 | 0.45 |
| 2:B:29:A:OP2 | 14:S:32:LEU:HD12 | 2.17 | 0.45 |
| 7:H:75:ALA:O | 7:H:79:VAL:HG22 | 2.17 | 0.45 |
| 26:4:15:ILE:HG13 | 26:4:21:VAL:HG22 | 1.97 | 0.45 |
| 1:A:2360:A:H2' | 1:A:2361:A:O4' | 2.17 | 0.45 |
| 3:D:17:THR:HG23 | 3:D:205:VAL:HB | 1.98 | 0.45 |
| 1:A:1545:A:H2' | 1:A:1546:C:O4' | 2.17 | 0.45 |
| 1:A:1316:U:H2' | 1:A:1317:A:C8 | 2.51 | 0.45 |
| 3:D:221:VAL:HG22 | 3:D:226:MET:CE | 2.47 | 0.45 |
| 1:A:271(K):U:O2' | 1:A:271(L):U:OP1 | 2.29 | 0.45 |
| 1:A:271(M):G:O2' | 1:A:271(N):U:H3' | 2.17 | 0.45 |
| 3:D:71:ASP:HB3 | 3:D:103:ARG:NH2 | 2.31 | 0.45 |
| 12:Q:26:TYR:CD1 | 12:Q:28:ALA:HB2 | 2.51 | 0.45 |
| 1:A:2387:U:O2' | 22:0:41:ARG:NH2 | 2.42 | 0.45 |
| 1:A:725:G:C6 | 1:A:726:G:N1 | 2.85 | 0.45 |
| 1:A:1332:G:N3 | 1:A:1332:G:H5' | 2.32 | 0.45 |
| 1:A:2322:A:H2' | 1:A:2323:G:O4' | 2.17 | 0.45 |
| 22:0:51:VAL:HG23 | 22:0:81:VAL:HG23 | 1.97 | 0.45 |
| 1:A:1538:G:O2' | 1:A:1539:G:OP1 | 2.27 | 0.45 |
| 1:A:1341:U:O2 | 19:X:80:ILE:HD13 | 2.17 | 0.45 |
| 1:A:637:A:H8 | 11:P:117:GLU:HG3 | 1.82 | 0.45 |
| 19:X:5:TYR:HD1 | 24:2:33:MET:CE | 2.30 | 0.45 |
| 6:G:47:LYS:HD3 | 6:G:81:LYS:CB | 2.47 | 0.45 |
| 12:Q:75:THR:HA | 12:Q:89:ASN:O | 2.17 | 0.45 |
| 1:A:1009:A:O4' | 16:U:59:ARG:HG2 | 2.16 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:510:C:H2' | 1:A:511:U:O4' | 2.17 | 0.44 |
| 1:A:90:U:O2' | 1:A:92:A:P | 2.74 | 0.44 |
| 8:I:77:LEU:HD22 | 8:I:104:GLN:OE1 | 2.17 | 0.44 |
| 1:A:1027:A:C6 | 1:A:1126:A:C4 | 3.04 | 0.44 |
| 1:A:2420:C:O5' | 1:A:2420:C:H6 | 2.01 | 0.44 |
| 5:F:29:ASN:H | 5:F:112:MET:CE | 2.30 | 0.44 |
| 10:O:2:ILE:HB | 10:O:33:ALA:HB3 | 1.99 | 0.44 |
| 1:A:2018:G:H2' | 1:A:2019:A:O4' | 2.17 | 0.44 |
| 6:G:5:VAL:HG23 | 6:G:104:GLU:OE1 | 2.17 | 0.44 |
| 3:D:274:ARG:H | 3:D:274:ARG:HG3 | 1.47 | 0.44 |
| 1:A:1359:A:C6 | 1:A:1372:U:O4 | 2.68 | 0.44 |
| 1:A:2133:G:O2' | 1:A:2158:A:N1 | 2.43 | 0.44 |
| 1:A:723:G:H2' | 1:A:724:U:O4' | 2.17 | 0.44 |
| 23:1:86:SER:OG | 23:1:89:GLU:HG2 | 2.16 | 0.44 |
| 1:A:247:G:H4' | 1:A:386:G:C6 | 2.52 | 0.44 |
| 1:A:2574:G:N3 | 4:E:143:ASN:ND2 | 2.66 | 0.44 |
| 1:A:2236:C:C2' | 1:A:2237:G:H5' | 2.47 | 0.44 |
| 1:A:500:G:N2 | 1:A:502:A:H3' | 2.33 | 0.44 |
| 1:A:947:G:N2 | 1:A:971:C:C2 | 2.85 | 0.44 |
| 1:A:2461:C:H2' | 1:A:2462:U:C6 | 2.52 | 0.44 |
| 1:A:2371:G:HO2' | 28:6:46:HIS:CE1 | 2.26 | 0.44 |
| 1:A:2320:A:N3 | 1:A:2320:A:H2' | 2.31 | 0.44 |
| 30:8:4:MET:HE3 | 30:8:63:PRO:CG | 2.47 | 0.44 |
| 1:A:1036:G:H1 | 1:A:1119:C:N4 | 2.13 | 0.44 |
| 1:A:1537:G:H2' | 1:A:1538:G:H8 | 1.82 | 0.44 |
| 1:A:2009:G:OP1 | 18:W:41:LYS:HE2 | 2.17 | 0.44 |
| 3:D:76:PRO:HB2 | 3:D:116:GLN:NE2 | 2.32 | 0.44 |
| 1:A:1575:C:O2' | 1:A:1576:U:H5' | 2.16 | 0.44 |
| 21:Z:151:HIS:C | 21:Z:153:SER:H | 2.20 | 0.44 |
| 1:A:1526:G:C6 | 1:A:1527:G:C2 | 3.06 | 0.44 |
| 1:A:2028:U:H2' | 1:A:2029:G:O4' | 2.17 | 0.44 |
| 1:A:2586:C:H1' | 34:A:3975:HOH:O | 2.16 | 0.44 |
| 1:A:652(A):A:H4' | 1:A:652(B):A:OP1 | 2.17 | 0.44 |
| 1:A:2319:G:C2 | 14:S:3:ARG:HA | 2.53 | 0.44 |
| 1:A:2186:G:N1 | 1:A:2187:G:C5 | 2.85 | 0.44 |
| 12:Q:21:THR:HA | 12:Q:98:LYS:HB2 | 1.98 | 0.44 |
| 1:A:1533:G:H2' | 1:A:1534:U:O4' | 2.17 | 0.44 |
| 3:D:97:TYR:HB2 | 3:D:101:GLU:O | 2.17 | 0.44 |
| 21:Z:5:LEU:HD22 | 21:Z:6:LYS:N | 2.32 | 0.44 |
| 1:A:192:C:O2' | 1:A:802:A:N3 | 2.40 | 0.44 |
| 20:Y:68:HIS:ND1 | 20:Y:70:SER:HB3 | 2.32 | 0.44 |
| 1:A:1930:G:O2' | 1:A:1931:U:P | 2.76 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 6:G:74:LYS:O | 6:G:84:LYS:HG2 | 2.17 | 0.44 |
| 3:D:184:LYS:HG3 | 3:D:271:ILE:HD11 | 1.99 | 0.44 |
| 24:2:53:LEU:O | 24:2:57:ILE:HG13 | 2.17 | 0.44 |
| 1:A:1141:U:OP1 | 9:N:25:ARG:NH1 | 2.51 | 0.44 |
| 9:N:23:LEU:O | 9:N:25:ARG:N | 2.50 | 0.44 |
| 26:4:15:ILE:HB | 26:4:32:TYR:CE2 | 2.53 | 0.44 |
| 1:A:125:G:C6 | 29:7:10:ARG:HG3 | 2.52 | 0.44 |
| 8:I:75:LEU:HD12 | 8:I:105:HIS:ND1 | 2.33 | 0.44 |
| 5:F:88:VAL:HG23 | 5:F:89:VAL:O | 2.18 | 0.44 |
| 25:3:4:LEU:HD23 | 25:3:4:LEU:HA | 1.81 | 0.44 |
| 13:R:103:ARG:NH1 | 13:R:108:GLY:O | 2.51 | 0.44 |
| 4:E:116:VAL:HG13 | 4:E:122:PHE:CG | 2.52 | 0.44 |
| 1:A:249:C:O2 | 30:8:12:LYS:NZ | 2.40 | 0.44 |
| 28:6:13:CYS:HB2 | 28:6:20:ASN:HD21 | 1.82 | 0.44 |
| 3:D:245:PRO:HA | 3:D:246:PRO:HD3 | 1.84 | 0.44 |
| 20:Y:77:PRO:HD3 | 20:Y:106:LEU:HD23 | 1.98 | 0.44 |
| 1:A:2820:A:C6 | 13:R:4:LEU:HD11 | 2.53 | 0.44 |
| 8:I:78:THR:N | 8:I:104:GLN:OE1 | 2.43 | 0.44 |
| 1:A:2723:C:O3' | 13:R:1:MET:HE3 | 2.18 | 0.44 |
| 12:Q:72:LYS:HA | 12:Q:73:PRO:HD3 | 1.88 | 0.44 |
| 1:A:2313:C:H5'' | 6:G:91:ARG:HG3 | 1.98 | 0.44 |
| 21:Z:19:ARG:NH1 | 21:Z:84:GLU:O | 2.51 | 0.44 |
| 28:6:14:THR:HG21 | 28:6:48:VAL:HG13 | 2.00 | 0.44 |
| 1:A:2110:G:O2' | 1:A:2120:G:H5' | 2.17 | 0.44 |
| 14:S:110:LEU:HD12 | 14:S:110:LEU:HA | 1.81 | 0.44 |
| 15:T:50:ILE:HG22 | 15:T:102:ILE:HD11 | 2.00 | 0.44 |
| 21:Z:63:ASP:OD1 | 21:Z:65:GLN:HB3 | 2.17 | 0.44 |
| 8:I:123:LEU:H | 8:I:123:LEU:HG | 1.58 | 0.44 |
| 5:F:116:ASP:CG | 11:P:1:MET:HB2 | 2.38 | 0.44 |
| 1:A:71:A:H5'' | 1:A:73:A:C8 | 2.52 | 0.44 |
| 1:A:271(Y):U:O3' | 1:A:271(Z):C:H6 | 2.00 | 0.44 |
| 1:A:829:A:N7 | 1:A:2248:C:H5' | 2.33 | 0.44 |
| 1:A:2038:G:O6 | 34:A:3653:HOH:O | 2.20 | 0.44 |
| 13:R:44:LEU:HD23 | 13:R:44:LEU:HA | 1.86 | 0.44 |
| 16:U:27:LEU:HA | 16:U:30:LYS:HB2 | 2.00 | 0.44 |
| 1:A:2615:U:H2' | 1:A:2616:C:H6 | 1.82 | 0.44 |
| 1:A:1015:G:C2' | 1:A:1016:G:H5' | 2.48 | 0.44 |
| 1:A:1615:C:C5 | 1:A:1617:C:C4 | 3.06 | 0.44 |
| 14:S:63:THR:O | 14:S:66:ALA:HB3 | 2.18 | 0.44 |
| 1:A:2418:A:H2' | 1:A:2419:U:C6 | 2.53 | 0.44 |
| 5:F:46:ARG:CG | 5:F:46:ARG:HH11 | 2.21 | 0.44 |
| 1:A:2562:U:C1' | 10:O:23:ARG:HH11 | 2.25 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:A:2186:G:N2 | 1:A:2187:G:C4 | 2.86 | 0.44 |
| 1:A:2316:C:H1' | 6:G:128:ARG:NH2 | 2.32 | 0.44 |
| 1:A:1792:G:H2' | 1:A:1793:C:H6 | 1.81 | 0.44 |
| 20:Y:102:CYS:O | 20:Y:104:GLY:N | 2.51 | 0.44 |
| 9:N:42:TRP:CE3 | 16:U:63:VAL:HG11 | 2.52 | 0.44 |
| 2:B:32:C:N3 | 2:B:51:G:N2 | 2.65 | 0.44 |
| 16:U:106:PHE:O | 16:U:110:VAL:HG23 | 2.18 | 0.44 |
| 5:F:150:GLY:HA2 | 5:F:172:TRP:CE3 | 2.53 | 0.44 |
| 1:A:1592:C:H2' | 1:A:1593:G:C8 | 2.53 | 0.44 |
| 2:B:31:C:O2' | 2:B:53:A:N6 | 2.51 | 0.44 |
| 1:A:1833:U:H2' | 1:A:1834:U:C6 | 2.51 | 0.44 |
| 1:A:1436:G:H1' | 1:A:1477:A:O2' | 2.18 | 0.44 |
| 1:A:1310:G:H1' | 1:A:1611:C:H5' | 2.00 | 0.43 |
| 1:A:2356:C:O3' | 22:O:20:ARG:HD3 | 2.18 | 0.43 |
| 1:A:1187:G:H5'' | 17:V:81:TYR:CE2 | 2.53 | 0.43 |
| 1:A:271(Q):G:O2' | 1:A:271(R):G:OP2 | 2.36 | 0.43 |
| 1:A:2833:G:H3' | 1:A:2834:G:H5'' | 2.00 | 0.43 |
| 1:A:2772:C:H2' | 1:A:2773:C:C6 | 2.53 | 0.43 |
| 1:A:1049:C:O2' | 1:A:1050:A:P | 2.76 | 0.43 |
| 21:Z:48:PHE:CE2 | 21:Z:52:SER:HA | 2.53 | 0.43 |
| 14:S:110:LEU:HB3 | 14:S:112:PHE:HE2 | 1.83 | 0.43 |
| 12:Q:66:ILE:HG12 | 12:Q:104:PHE:CE2 | 2.53 | 0.43 |
| 22:O:17:GLN:OE1 | 22:O:17:GLN:HA | 2.18 | 0.43 |
| 8:I:97:ILE:O | 8:I:101:LEU:N | 2.51 | 0.43 |
| 1:A:2141:G:C6 | 1:A:2151:G:C6 | 3.06 | 0.43 |
| 1:A:2146:C:H4' | 1:A:2147:G:O4' | 2.19 | 0.43 |
| 9:N:128:HIS:HA | 9:N:129:PRO:HD2 | 1.64 | 0.43 |
| 26:4:30:GLU:O | 26:4:31:ILE:HG13 | 2.18 | 0.43 |
| 1:A:1914:C:H2' | 1:A:1915:U:C6 | 2.53 | 0.43 |
| 1:A:2093:G:H1 | 1:A:2196:C:H42 | 1.66 | 0.43 |
| 1:A:2404:C:O3' | 11:P:77:ARG:NH2 | 2.51 | 0.43 |
| 5:F:123:LEU:HD12 | 5:F:124:LEU:N | 2.33 | 0.43 |
| 1:A:1047:G:H21 | 1:A:1111:A:N6 | 2.17 | 0.43 |
| 1:A:2562:U:O2' | 10:O:23:ARG:HD3 | 2.18 | 0.43 |
| 1:A:1142(A):A:C4 | 1:A:1144:G:C8 | 3.06 | 0.43 |
| 1:A:271(F):C:C2 | 1:A:271(G):C:C6 | 3.06 | 0.43 |
| 3:D:108:PRO:HG2 | 3:D:111:LEU:HG | 1.99 | 0.43 |
| 14:S:11:LYS:O | 14:S:15:ARG:HB2 | 2.18 | 0.43 |
| 15:T:127:ALA:HA | 15:T:129:ARG:N | 2.33 | 0.43 |
| 1:A:1049:C:H2' | 1:A:1050:A:C8 | 2.53 | 0.43 |
| 9:N:38:HIS:O | 16:U:67:ALA:HB1 | 2.18 | 0.43 |
| 6:G:125:PHE:HB3 | 6:G:166:ASP:OD2 | 2.18 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 19:X:57:LEU:HD13 | 19:X:78:LYS:HG2 | 1.99 | 0.43 |
| 1:A:191:A:H2' | 1:A:192:C:C6 | 2.53 | 0.43 |
| 1:A:868:U:C4 | 1:A:869:G:N7 | 2.86 | 0.43 |
| 11:P:138:LEU:HD23 | 11:P:145:PRO:HG3 | 1.99 | 0.43 |
| 22:0:31:VAL:HB | 22:0:35:ASN:ND2 | 2.33 | 0.43 |
| 5:F:32:LEU:HB3 | 5:F:112:MET:HE1 | 2.00 | 0.43 |
| 1:A:2273:A:O2' | 1:A:2274:A:H5' | 2.19 | 0.43 |
| 1:A:1639:U:O2' | 1:A:1640:C:H5'' | 2.18 | 0.43 |
| 6:G:64:THR:OG1 | 6:G:65:GLY:N | 2.51 | 0.43 |
| 6:G:166:ASP:O | 6:G:170:ARG:N | 2.37 | 0.43 |
| 16:U:17:ILE:HA | 16:U:17:ILE:HD13 | 1.86 | 0.43 |
| 1:A:836:G:H5'' | 1:A:837:C:OP2 | 2.17 | 0.43 |
| 1:A:1676:A:N7 | 34:A:4077:HOH:O | 2.36 | 0.43 |
| 14:S:24:LEU:HD23 | 14:S:24:LEU:HA | 1.84 | 0.43 |
| 1:A:1210:A:H4' | 1:A:1211:U:O5' | 2.18 | 0.43 |
| 1:A:2572:A:C8 | 4:E:144:ARG:HD2 | 2.54 | 0.43 |
| 9:N:112:LEU:O | 9:N:115:ARG:N | 2.48 | 0.43 |
| 1:A:1537:G:H2' | 1:A:1538:G:C8 | 2.53 | 0.43 |
| 2:B:113:G:H2' | 2:B:114:C:H6 | 1.82 | 0.43 |
| 1:A:2262:U:H4' | 1:A:2328:A:C2 | 2.54 | 0.43 |
| 22:0:72:ARG:CB | 22:0:75:LEU:HB2 | 2.48 | 0.43 |
| 1:A:375:C:H2' | 1:A:376:C:C6 | 2.54 | 0.43 |
| 1:A:1396:U:H5'' | 34:A:4128:HOH:O | 2.17 | 0.43 |
| 16:U:104:GLN:CD | 16:U:104:GLN:H | 2.22 | 0.43 |
| 1:A:2109:U:C6 | 1:A:2109:U:C3' | 3.01 | 0.43 |
| 22:0:65:GLY:CA | 22:0:81:VAL:HG12 | 2.46 | 0.43 |
| 3:D:33:LEU:HA | 3:D:33:LEU:HD23 | 1.39 | 0.43 |
| 1:A:2564:A:C2 | 1:A:2647:U:H4' | 2.54 | 0.43 |
| 1:A:904:C:H2' | 1:A:905:U:C6 | 2.54 | 0.43 |
| 1:A:1885:A:H2' | 1:A:1886:C:O4' | 2.18 | 0.43 |
| 16:U:43:GLY:HA3 | 17:V:73:SER:OG | 2.19 | 0.43 |
| 1:A:265:A:H1' | 1:A:266:G:O4' | 2.19 | 0.43 |
| 1:A:459:U:H5'' | 29:7:40:TRP:CD2 | 2.53 | 0.43 |
| 1:A:839:U:H2' | 1:A:840:C:C6 | 2.53 | 0.43 |
| 5:F:101:LEU:HA | 5:F:101:LEU:HD12 | 1.79 | 0.43 |
| 21:Z:128:VAL:HG12 | 21:Z:129:SER:N | 2.33 | 0.43 |
| 5:F:181:LEU:HB3 | 5:F:205:ARG:NH2 | 2.33 | 0.43 |
| 1:A:2350:C:H2' | 1:A:2351:G:O4' | 2.18 | 0.43 |
| 1:A:2815:C:H2' | 1:A:2816:C:C6 | 2.53 | 0.43 |
| 1:A:1668:A:C8 | 1:A:1674:G:C6 | 3.07 | 0.43 |
| 4:E:116:VAL:HG13 | 4:E:122:PHE:HB2 | 2.01 | 0.43 |
| 12:Q:1:MET:HG2 | 12:Q:2:LEU:H | 1.83 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:A:24:G:H2' | 1:A:25:U:O4' | 2.19 | 0.43 |
| 1:A:1754:C:OP1 | 15:T:96:ARG:NH1 | 2.45 | 0.43 |
| 15:T:35:LYS:HE2 | 15:T:35:LYS:HB3 | 1.76 | 0.43 |
| 1:A:2186:G:C2 | 1:A:2187:G:C5 | 3.07 | 0.43 |
| 1:A:953:A:OP2 | 12:Q:16:ARG:NE | 2.47 | 0.43 |
| 1:A:1681:G:H1' | 1:A:1762:A:H2' | 2.00 | 0.43 |
| 6:G:107:LEU:HD23 | 6:G:111:LEU:HD12 | 2.01 | 0.43 |
| 8:I:134:PRO:O | 8:I:136:VAL:N | 2.51 | 0.43 |
| 3:D:71:ASP:HB3 | 3:D:103:ARG:HH22 | 1.83 | 0.43 |
| 25:3:11:SER:OG | 25:3:13:ILE:HG13 | 2.19 | 0.43 |
| 21:Z:98:MET:SD | 21:Z:133:ILE:HD13 | 2.59 | 0.43 |
| 29:7:27:GLY:O | 29:7:30:VAL:HB | 2.17 | 0.43 |
| 15:T:27:THR:HB | 15:T:90:GLN:HB3 | 2.00 | 0.43 |
| 1:A:1500:G:N2 | 3:D:99:ASP:O | 2.48 | 0.43 |
| 1:A:1383:C:O5' | 1:A:1383:C:H6 | 2.01 | 0.43 |
| 1:A:662:G:H5' | 11:P:14:LYS:O | 2.19 | 0.43 |
| 15:T:2:ASN:O | 15:T:6:LEU:HD22 | 2.19 | 0.43 |
| 1:A:2880:C:O3' | 13:R:90:ARG:NH1 | 2.51 | 0.43 |
| 1:A:2056:G:C2 | 1:A:2057:A:C8 | 3.06 | 0.43 |
| 1:A:1535:A:OP1 | 1:A:1535:A:H3' | 2.19 | 0.43 |
| 1:A:1029:A:H8 | 1:A:1029:A:O5' | 2.01 | 0.43 |
| 1:A:1211:U:H4' | 1:A:1212:G:OP2 | 2.18 | 0.43 |
| 12:Q:38:GLU:O | 12:Q:127:ILE:HG21 | 2.19 | 0.43 |
| 1:A:601:C:O2 | 1:A:605:C:H4' | 2.19 | 0.43 |
| 1:A:1486:A:C4 | 1:A:1487:G:C8 | 3.06 | 0.43 |
| 5:F:110:LEU:HD21 | 5:F:181:LEU:HG | 2.00 | 0.43 |
| 21:Z:79:ARG:HD2 | 21:Z:80:ARG:HH21 | 1.83 | 0.43 |
| 2:B:38:C:H2' | 2:B:39:A:O4' | 2.19 | 0.43 |
| 29:7:34:ARG:NH1 | 29:7:39:ARG:HG3 | 2.34 | 0.43 |
| 4:E:51:PHE:CE2 | 4:E:52:LEU:HD13 | 2.54 | 0.43 |
| 1:A:2483:C:H2' | 1:A:2484:G:O4' | 2.19 | 0.43 |
| 1:A:1324:G:C5 | 1:A:1328:G:O6 | 2.72 | 0.43 |
| 14:S:80:LEU:HD12 | 14:S:80:LEU:HA | 1.76 | 0.43 |
| 1:A:89:G:OP2 | 1:A:90:U:H3' | 2.19 | 0.43 |
| 1:A:2169:A:O2' | 1:A:2170:A:H5' | 2.18 | 0.43 |
| 24:2:50:ILE:O | 24:2:51:ARG:CB | 2.63 | 0.43 |
| 1:A:1858:G:H2' | 1:A:1883:G:N2 | 2.34 | 0.43 |
| 5:F:74:ARG:H | 5:F:74:ARG:HG3 | 1.27 | 0.43 |
| 5:F:32:LEU:O | 5:F:35:GLU:N | 2.52 | 0.43 |
| 6:G:137:GLU:HG3 | 6:G:152:LEU:HD21 | 1.99 | 0.43 |
| 1:A:107:C:C2 | 1:A:108:U:C5 | 3.07 | 0.43 |
| 1:A:1638:C:H5'' | 1:A:2710:C:O2' | 2.19 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 4:E:174:ASP:OD2 | 4:E:175:VAL:N | 2.52 | 0.43 |
| 1:A:1300:U:H4' | 1:A:1301:A:H5'' | 2.01 | 0.43 |
| 1:A:10:G:H1' | 1:A:2801(A):A:C2 | 2.54 | 0.42 |
| 1:A:639:U:O2' | 1:A:640:C:H5' | 2.19 | 0.42 |
| 3:D:242:ARG:N | 3:D:242:ARG:HD3 | 2.33 | 0.42 |
| 1:A:1721:G:C2 | 1:A:1739:U:OP2 | 2.72 | 0.42 |
| 1:A:952:G:C6 | 1:A:953:A:N7 | 2.87 | 0.42 |
| 10:O:106:LEU:HD23 | 10:O:106:LEU:HA | 1.78 | 0.42 |
| 1:A:1711:C:H2' | 1:A:1712:C:C6 | 2.54 | 0.42 |
| 1:A:1268:A:C2 | 1:A:2013:A:C4 | 3.07 | 0.42 |
| 1:A:805:G:H4' | 11:P:38:GLN:HB3 | 2.00 | 0.42 |
| 1:A:2108:C:C3' | 1:A:2108:C:C6 | 3.02 | 0.42 |
| 21:Z:30:ASN:OD1 | 21:Z:32:HIS:N | 2.46 | 0.42 |
| 1:A:1796:U:H4' | 3:D:256:GLY:N | 2.33 | 0.42 |
| 1:A:1529:G:H8 | 1:A:1529:G:O5' | 2.02 | 0.42 |
| 1:A:1900:A:N1 | 1:A:1970:A:C6 | 2.88 | 0.42 |
| 2:B:57:A:H1' | 6:G:29:TRP:HB2 | 2.01 | 0.42 |
| 6:G:89:GLY:O | 6:G:90:LEU:HD23 | 2.19 | 0.42 |
| 1:A:2557:G:H2' | 1:A:2558:C:H6 | 1.84 | 0.42 |
| 1:A:642:G:H21 | 1:A:646:A:H2 | 1.66 | 0.42 |
| 1:A:1833:U:O2' | 1:A:1969:A:N1 | 2.41 | 0.42 |
| 1:A:236:C:H2' | 1:A:237:C:H6 | 1.84 | 0.42 |
| 1:A:415:A:H2' | 1:A:416:C:H6 | 1.83 | 0.42 |
| 6:G:43:LEU:HB3 | 6:G:44:GLY:H | 1.58 | 0.42 |
| 4:E:21:VAL:HA | 4:E:22:PRO:HD2 | 1.74 | 0.42 |
| 1:A:1419:A:C8 | 1:A:1421:G:C6 | 3.08 | 0.42 |
| 1:A:1805:U:O2 | 3:D:50:THR:HB | 2.19 | 0.42 |
| 1:A:2294:C:OP1 | 14:S:89:ARG:NH1 | 2.43 | 0.42 |
| 6:G:24:GLY:O | 6:G:26:GLN:NE2 | 2.53 | 0.42 |
| 10:O:3:GLN:HB2 | 10:O:4:PRO:HD2 | 2.00 | 0.42 |
| 4:E:93:VAL:H | 4:E:93:VAL:HG22 | 1.55 | 0.42 |
| 23:1:15:ALA:O | 23:1:40:ARG:HG3 | 2.19 | 0.42 |
| 1:A:2140:C:H2' | 1:A:2141:G:C8 | 2.54 | 0.42 |
| 1:A:1827:C:H5' | 1:A:1971:A:H4' | 2.01 | 0.42 |
| 28:6:10:LEU:HD23 | 28:6:22:ALA:HB2 | 2.01 | 0.42 |
| 1:A:2065:C:H2' | 1:A:2066:C:H6 | 1.84 | 0.42 |
| 1:A:1161:C:H1' | 17:V:8:GLY:O | 2.19 | 0.42 |
| 5:F:130:ALA:HB2 | 5:F:142:TRP:HD1 | 1.84 | 0.42 |
| 10:O:10:VAL:HG21 | 10:O:16:ALA:HB3 | 1.99 | 0.42 |
| 1:A:2287:A:N3 | 1:A:2289:G:C8 | 2.88 | 0.42 |
| 14:S:34:HIS:CG | 14:S:53:SER:HG | 2.31 | 0.42 |
| 12:Q:21:THR:O | 21:Z:78:LYS:HD3 | 2.19 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:A:2111:C:C4 | 1:A:2145:C:C2 | 3.08 | 0.42 |
| 1:A:387:U:H5'' | 34:A:3739:HOH:O | 2.19 | 0.42 |
| 1:A:2575:C:H2' | 1:A:2578:G:O6 | 2.19 | 0.42 |
| 1:A:1639:U:H2' | 1:A:1640:C:H5'' | 2.00 | 0.42 |
| 21:Z:67:LEU:HA | 21:Z:68:PRO:HD3 | 1.74 | 0.42 |
| 2:B:7:G:H4' | 14:S:29:PHE:CD1 | 2.54 | 0.42 |
| 24:2:27:GLU:H | 24:2:27:GLU:HG2 | 1.68 | 0.42 |
| 1:A:30:G:O2' | 1:A:1214:A:N3 | 2.46 | 0.42 |
| 1:A:1138:G:H5'' | 1:A:1139:G:OP2 | 2.18 | 0.42 |
| 1:A:1425:G:H2' | 1:A:1426:G:O4' | 2.19 | 0.42 |
| 6:G:33:ARG:O | 6:G:161:THR:HG22 | 2.19 | 0.42 |
| 1:A:1311:G:O6 | 29:7:9:ARG:NH2 | 2.53 | 0.42 |
| 1:A:354:G:H2' | 1:A:355:G:C8 | 2.55 | 0.42 |
| 26:4:15:ILE:O | 26:4:33:VAL:N | 2.49 | 0.42 |
| 13:R:67:LEU:HD13 | 13:R:67:LEU:HA | 1.75 | 0.42 |
| 6:G:126:ASP:CG | 6:G:130:ASN:HD22 | 2.23 | 0.42 |
| 1:A:2772:C:H2' | 1:A:2773:C:H6 | 1.84 | 0.42 |
| 6:G:7:LEU:HD11 | 6:G:107:LEU:HD12 | 2.01 | 0.42 |
| 3:D:13:ARG:HA | 3:D:13:ARG:HD2 | 1.83 | 0.42 |
| 1:A:542:C:C6 | 1:A:542:C:H3' | 2.53 | 0.42 |
| 1:A:1816:G:N1 | 3:D:35:LYS:HD3 | 2.33 | 0.42 |
| 12:Q:50:ALA:HB2 | 12:Q:125:LEU:HD21 | 2.02 | 0.42 |
| 15:T:106:SER:O | 15:T:110:ILE:HG13 | 2.20 | 0.42 |
| 1:A:937:U:H2' | 1:A:938:G:O4' | 2.19 | 0.42 |
| 6:G:86:MET:HA | 6:G:87:PRO:HD3 | 1.84 | 0.42 |
| 26:4:25:TYR:N | 26:4:25:TYR:CD1 | 2.88 | 0.42 |
| 27:5:19:ARG:HD2 | 27:5:19:ARG:HH11 | 1.65 | 0.42 |
| 8:I:5:LEU:HD12 | 8:I:5:LEU:N | 2.35 | 0.42 |
| 1:A:2773:C:OP1 | 4:E:166:THR:OG1 | 2.34 | 0.42 |
| 1:A:990:A:OP2 | 1:A:991:C:OP2 | 2.38 | 0.42 |
| 2:B:77:U:OP1 | 21:Z:19:ARG:NH2 | 2.52 | 0.42 |
| 4:E:176:ILE:HG22 | 4:E:179:GLU:HB2 | 2.01 | 0.42 |
| 9:N:73:THR:HA | 9:N:83:LYS:O | 2.19 | 0.42 |
| 1:A:2095:C:H2' | 1:A:2096:U:O4' | 2.20 | 0.42 |
| 7:H:91:GLY:HA3 | 7:H:160:LYS:HG3 | 2.02 | 0.42 |
| 1:A:2600:A:C6 | 1:A:2601:C:N4 | 2.88 | 0.42 |
| 1:A:1001:A:H2' | 1:A:1002:G:O4' | 2.19 | 0.42 |
| 1:A:67:U:C2' | 1:A:68:G:H5' | 2.50 | 0.42 |
| 1:A:252:G:P | 11:P:50:ARG:HH11 | 2.43 | 0.42 |
| 7:H:3:ARG:HG2 | 7:H:6:ARG:NE | 2.31 | 0.42 |
| 7:H:121:ILE:HD11 | 7:H:140:LYS:HG2 | 2.01 | 0.42 |
| 5:F:160:ASN:ND2 | 5:F:163:VAL:HG23 | 2.35 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:479:A:H4' | 1:A:480:A:OP1 | 2.19 | 0.42 |
| 1:A:475:U:C4 | 1:A:481:G:O6 | 2.73 | 0.42 |
| 12:Q:35:VAL:CG1 | 12:Q:130:LYS:HB3 | 2.49 | 0.42 |
| 1:A:2070:G:C2 | 1:A:2442:C:C2 | 3.07 | 0.42 |
| 1:A:1130:U:O2 | 4:E:149:ARG:NH2 | 2.50 | 0.42 |
| 1:A:1637:A:H4' | 1:A:2711:A:O2' | 2.20 | 0.42 |
| 10:O:66:LYS:HA | 10:O:79:PHE:O | 2.20 | 0.42 |
| 4:E:201:THR:OG1 | 4:E:202:LYS:N | 2.53 | 0.42 |
| 1:A:1685:C:H2' | 1:A:1686:C:C6 | 2.55 | 0.42 |
| 4:E:181:LEU:HA | 4:E:181:LEU:HD12 | 1.71 | 0.42 |
| 1:A:545:G:OP1 | 1:A:545:G:H4' | 2.19 | 0.42 |
| 21:Z:125:LEU:HB3 | 21:Z:165:VAL:CG1 | 2.49 | 0.42 |
| 1:A:580:C:H2' | 1:A:581:C:C6 | 2.55 | 0.42 |
| 24:2:64:LEU:O | 24:2:68:ARG:HG2 | 2.19 | 0.42 |
| 1:A:2805:G:H2' | 1:A:2807:G:C8 | 2.52 | 0.42 |
| 1:A:819:A:C4 | 1:A:1189:A:C2 | 3.08 | 0.42 |
| 5:F:106:ARG:HG2 | 5:F:106:ARG:H | 1.51 | 0.42 |
| 1:A:1015:G:O2' | 1:A:1016:G:H5' | 2.20 | 0.42 |
| 1:A:2232:U:P | 23:1:40:ARG:HH12 | 2.43 | 0.42 |
| 4:E:38:THR:O | 4:E:42:ASP:N | 2.47 | 0.42 |
| 16:U:28:ARG:NH1 | 16:U:38:THR:OG1 | 2.48 | 0.42 |
| 1:A:2287:A:C4 | 1:A:2289:G:C8 | 3.07 | 0.42 |
| 1:A:2133:G:H2' | 1:A:2157:G:N2 | 2.35 | 0.42 |
| 1:A:1828:G:H5'' | 34:A:3601:HOH:O | 2.20 | 0.42 |
| 15:T:3:ARG:HH21 | 15:T:3:ARG:CB | 2.32 | 0.42 |
| 1:A:848:G:N3 | 1:A:933:A:H1' | 2.35 | 0.42 |
| 1:A:2391:G:O6 | 1:A:2425:A:H8 | 2.03 | 0.42 |
| 16:U:17:ILE:HG23 | 16:U:39:LEU:HD12 | 2.01 | 0.42 |
| 1:A:1711:C:H2' | 1:A:1712:C:H6 | 1.85 | 0.42 |
| 17:V:87:HIS:NE2 | 17:V:89:GLN:HG2 | 2.35 | 0.42 |
| 1:A:1911:U:C2 | 1:A:1918:A:C2 | 3.08 | 0.42 |
| 1:A:1777:U:O2' | 1:A:1778:U:H5' | 2.19 | 0.42 |
| 5:F:46:ARG:HG2 | 5:F:46:ARG:NH1 | 2.22 | 0.42 |
| 1:A:656:G:H2' | 1:A:657:U:O4' | 2.19 | 0.42 |
| 1:A:2521:C:O2' | 1:A:2564:A:N3 | 2.46 | 0.42 |
| 4:E:73:GLU:HA | 4:E:74:PRO:HD3 | 1.78 | 0.42 |
| 1:A:128:C:H2' | 1:A:129:C:C6 | 2.55 | 0.42 |
| 17:V:42:GLY:O | 17:V:43:GLU:HG2 | 2.20 | 0.42 |
| 10:O:104:ARG:NH1 | 15:T:34:VAL:HG21 | 2.35 | 0.42 |
| 3:D:228:PRO:HD3 | 3:D:235:GLY:HA3 | 2.02 | 0.42 |
| 2:B:59:A:H2' | 2:B:60:C:C6 | 2.55 | 0.42 |
| 1:A:1936:A:H5' | 34:A:3540:HOH:O | 2.19 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-----------------|-------------|----------|
| 4:E:12:THR:HG22 | 15:T:58:ASN:OD1 | 2.20 | 0.42 |
| 25:3:30:ARG:HG3 | 25:3:30:ARG:H | 1.66 | 0.42 |
| 21:Z:183:LEU:HD23 | 21:Z:183:LEU:HA | 1.81 | 0.42 |
| 1:A:225:A:H2' | 1:A:226:G:H5' | 2.03 | 0.41 |
| 5:F:22:ALA:HB1 | 5:F:24:LEU:CD2 | 2.50 | 0.41 |
| 24:2:45:SER:O | 24:2:46:GLN:HB2 | 2.20 | 0.41 |
| 1:A:2317:C:H2' | 1:A:2318:G:C5' | 2.50 | 0.41 |
| 1:A:1568:G:H5' | 3:D:60:ARG:HA | 2.02 | 0.41 |
| 10:O:4:PRO:O | 10:O:5:GLN:HB2 | 2.19 | 0.41 |
| 6:G:96:ARG:O | 6:G:99:MET:HB3 | 2.19 | 0.41 |
| 1:A:2517:C:C6 | 1:A:2542:A:N7 | 2.88 | 0.41 |
| 23:1:4:VAL:HG11 | 23:1:11:ARG:NH1 | 2.35 | 0.41 |
| 3:D:29:PRO:HA | 3:D:83:GLU:OE1 | 2.20 | 0.41 |
| 20:Y:67:LEU:HD23 | 20:Y:67:LEU:HA | 1.69 | 0.41 |
| 1:A:546:C:H2' | 1:A:546:C:H6 | 1.63 | 0.41 |
| 30:8:33:ASN:O | 30:8:34:TRP:O | 2.38 | 0.41 |
| 14:S:34:HIS:ND1 | 14:S:53:SER:OG | 2.31 | 0.41 |
| 31:9:4:ARG:O | 31:9:36:GLN:HA | 2.19 | 0.41 |
| 1:A:861:A:H2' | 1:A:862:G:O4' | 2.20 | 0.41 |
| 1:A:2065:C:H2' | 1:A:2066:C:C6 | 2.54 | 0.41 |
| 20:Y:2:ARG:HA | 20:Y:2:ARG:HD3 | 1.78 | 0.41 |
| 22:0:70:GLN:HG2 | 22:0:72:ARG:HG2 | 2.02 | 0.41 |
| 6:G:44:GLY:O | 6:G:47:LYS:NZ | 2.35 | 0.41 |
| 1:A:1930:G:O2' | 1:A:1931:U:OP2 | 2.38 | 0.41 |
| 1:A:1224:C:O2' | 17:V:85:LYS:HA | 2.20 | 0.41 |
| 31:9:12:ASP:OD1 | 31:9:13:LYS:HG3 | 2.19 | 0.41 |
| 1:A:1693:U:H4' | 1:A:1694:C:OP2 | 2.19 | 0.41 |
| 22:0:21:LEU:HD23 | 22:0:21:LEU:HA | 1.82 | 0.41 |
| 1:A:2157:G:H2' | 1:A:2158:A:C8 | 2.55 | 0.41 |
| 5:F:52:LYS:HA | 5:F:56:GLU:OE2 | 2.21 | 0.41 |
| 1:A:528:A:C2 | 1:A:2043:C:H4' | 2.56 | 0.41 |
| 1:A:708:C:N4 | 1:A:723:G:H1 | 2.16 | 0.41 |
| 21:Z:111:VAL:HG12 | 21:Z:112:ARG:H | 1.86 | 0.41 |
| 2:B:49:C:OP1 | 14:S:96:GLY:HA2 | 2.21 | 0.41 |
| 1:A:271(Q):G:O2' | 1:A:271(R):G:P | 2.78 | 0.41 |
| 1:A:1529:G:C6 | 1:A:1530:C:C4 | 3.07 | 0.41 |
| 1:A:1792:G:H2' | 1:A:1793:C:C6 | 2.55 | 0.41 |
| 9:N:18:ALA:O | 9:N:21:LYS:HB2 | 2.20 | 0.41 |
| 1:A:1668:A:H4' | 1:A:1669:A:O5' | 2.20 | 0.41 |
| 28:6:6:ARG:NH1 | 28:6:26:ASN:HB2 | 2.36 | 0.41 |
| 1:A:1759:A:H1' | 1:A:2711:A:C2 | 2.55 | 0.41 |
| 1:A:2519:U:C6 | 1:A:2542:A:N6 | 2.88 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:A:1783:A:C2 | 1:A:2587:A:C5 | 3.09 | 0.41 |
| 24:2:4:SER:HA | 24:2:7:ARG:NH1 | 2.35 | 0.41 |
| 4:E:50:GLY:HA2 | 4:E:77:ILE:O | 2.21 | 0.41 |
| 12:Q:63:LYS:HD2 | 21:Z:175:VAL:HG21 | 2.01 | 0.41 |
| 1:A:634:C:H2' | 1:A:635:C:C6 | 2.55 | 0.41 |
| 1:A:2205:C:O2 | 1:A:2220:G:C2 | 2.73 | 0.41 |
| 1:A:529:A:OP2 | 9:N:114:ARG:NH2 | 2.54 | 0.41 |
| 11:P:96:THR:OG1 | 11:P:99:LEU:HG | 2.20 | 0.41 |
| 16:U:47:TYR:HA | 16:U:50:ARG:NH2 | 2.35 | 0.41 |
| 2:B:11:C:H3' | 2:B:12:C:H6 | 1.82 | 0.41 |
| 1:A:196:A:O4' | 11:P:46:LYS:HE2 | 2.20 | 0.41 |
| 19:X:5:TYR:HD1 | 24:2:33:MET:HE2 | 1.85 | 0.41 |
| 5:F:95:ARG:HG3 | 5:F:97:TYR:CE2 | 2.55 | 0.41 |
| 1:A:807:U:OP2 | 11:P:36:LYS:HD3 | 2.20 | 0.41 |
| 1:A:2845:G:O2' | 1:A:2846:G:H5' | 2.20 | 0.41 |
| 1:A:289:A:H2' | 1:A:290:G:O4' | 2.20 | 0.41 |
| 1:A:250:G:H2' | 1:A:251:A:C8 | 2.56 | 0.41 |
| 1:A:271(H):G:O2' | 1:A:271(I):G:P | 2.79 | 0.41 |
| 1:A:271(P):C:C2' | 1:A:271(Q):G:H5' | 2.51 | 0.41 |
| 2:B:20:C:H2' | 2:B:21:G:O4' | 2.19 | 0.41 |
| 2:B:79:C:H2' | 2:B:80:U:O4' | 2.20 | 0.41 |
| 21:Z:138:GLU:HB3 | 21:Z:156:LYS:NZ | 2.35 | 0.41 |
| 1:A:2811:G:N2 | 1:A:2891:G:H1' | 2.35 | 0.41 |
| 30:8:54:GLU:OE1 | 30:8:57:ARG:NH1 | 2.50 | 0.41 |
| 1:A:216:A:C4 | 1:A:432:A:C2 | 3.08 | 0.41 |
| 3:D:137:PRO:HB2 | 3:D:140:THR:HG23 | 2.03 | 0.41 |
| 4:E:128:SER:OG | 4:E:129:HIS:N | 2.53 | 0.41 |
| 5:F:117:ARG:HD3 | 5:F:117:ARG:HA | 1.87 | 0.41 |
| 1:A:92:A:O2' | 1:A:93:G:H5' | 2.20 | 0.41 |
| 1:A:2170:A:H8 | 1:A:2170:A:OP2 | 2.04 | 0.41 |
| 2:B:117:G:H2' | 2:B:118:G:O4' | 2.21 | 0.41 |
| 1:A:2104:G:O6 | 1:A:2186:G:C4 | 2.74 | 0.41 |
| 1:A:900:A:O2' | 1:A:901:A:OP1 | 2.36 | 0.41 |
| 5:F:13:SER:HA | 5:F:14:PRO:HD2 | 1.82 | 0.41 |
| 8:I:133:HIS:CE1 | 8:I:134:PRO:O | 2.73 | 0.41 |
| 2:B:37:C:C5 | 2:B:38:C:C5 | 3.09 | 0.41 |
| 10:O:120:GLU:HG2 | 10:O:122:LEU:HG | 2.03 | 0.41 |
| 1:A:1469:A:C2 | 1:A:1524:G:C2 | 3.09 | 0.41 |
| 5:F:7:TYR:N | 5:F:22:ALA:HB3 | 2.31 | 0.41 |
| 1:A:2572:A:N7 | 4:E:144:ARG:HD2 | 2.35 | 0.41 |
| 1:A:2352:A:N6 | 1:A:2365:G:O2' | 2.54 | 0.41 |
| 6:G:126:ASP:HB2 | 6:G:130:ASN:O | 2.20 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 1:A:2147:G:H2' | 1:A:2148:G:O4' | 2.21 | 0.41 |
| 1:A:582:G:H2' | 1:A:583:G:C8 | 2.56 | 0.41 |
| 3:D:3:VAL:HG12 | 3:D:17:THR:HB | 2.03 | 0.41 |
| 4:E:105:THR:HG23 | 4:E:166:THR:OG1 | 2.20 | 0.41 |
| 2:B:2:C:H2' | 2:B:3:C:H6 | 1.84 | 0.41 |
| 1:A:1999:C:H2' | 1:A:2000:G:O4' | 2.19 | 0.41 |
| 9:N:54:VAL:HG11 | 9:N:99:LEU:HD12 | 2.01 | 0.41 |
| 1:A:468:G:N7 | 29:7:39:ARG:NH2 | 2.61 | 0.41 |
| 1:A:2441:C:OP2 | 1:A:2586:C:O2' | 2.36 | 0.41 |
| 1:A:1161:C:O2' | 17:V:8:GLY:HA2 | 2.21 | 0.41 |
| 1:A:1425:G:H2' | 1:A:1426:G:C8 | 2.55 | 0.41 |
| 25:3:22:ALA:O | 25:3:25:ALA:HB3 | 2.21 | 0.41 |
| 17:V:77:ALA:C | 17:V:79:VAL:H | 2.24 | 0.41 |
| 16:U:61:TRP:CD2 | 16:U:93:LYS:HA | 2.55 | 0.41 |
| 15:T:24:PRO:HA | 15:T:49:VAL:HG22 | 2.02 | 0.41 |
| 6:G:57:ALA:HB1 | 6:G:68:PRO:HD2 | 2.03 | 0.41 |
| 1:A:1028:A:N6 | 1:A:1125:G:H2' | 2.35 | 0.41 |
| 1:A:7:G:H4' | 9:N:13:TRP:CZ2 | 2.56 | 0.41 |
| 24:2:35:LEU:HA | 24:2:35:LEU:HD23 | 1.92 | 0.41 |
| 8:I:5:LEU:HD11 | 8:I:19:VAL:CG2 | 2.48 | 0.41 |
| 1:A:580:C:H2' | 1:A:581:C:H6 | 1.85 | 0.41 |
| 1:A:1048:A:O2' | 1:A:1049:C:P | 2.78 | 0.41 |
| 1:A:1504:C:O2' | 1:A:1505:C:H5' | 2.20 | 0.41 |
| 1:A:2577:A:O4' | 27:5:3:LYS:HB2 | 2.21 | 0.41 |
| 1:A:2484:G:C2 | 1:A:2485:G:C8 | 3.08 | 0.41 |
| 1:A:1695:G:H2' | 1:A:1696:G:O4' | 2.21 | 0.41 |
| 18:W:1:MET:HE2 | 18:W:2:GLU:O | 2.20 | 0.41 |
| 16:U:105:VAL:HG11 | 17:V:39:LEU:HD21 | 2.02 | 0.41 |
| 1:A:483:A:O4' | 20:Y:48:ALA:HB1 | 2.20 | 0.41 |
| 1:A:2679:A:H2' | 1:A:2680:C:O4' | 2.20 | 0.41 |
| 1:A:1840:G:C6 | 1:A:1841:U:C4 | 3.09 | 0.41 |
| 1:A:2340:G:O2' | 1:A:2341:G:H5' | 2.20 | 0.41 |
| 1:A:2335:A:C8 | 1:A:2337:G:N7 | 2.89 | 0.41 |
| 1:A:2304:G:H21 | 6:G:156:ASP:CG | 2.25 | 0.41 |
| 2:B:28:C:C2 | 2:B:29:A:C8 | 3.09 | 0.41 |
| 27:5:49:CYS:SG | 27:5:51:TYR:HD1 | 2.44 | 0.41 |
| 1:A:2833:G:O2' | 1:A:2834:G:P | 2.78 | 0.41 |
| 1:A:922:U:H2' | 1:A:923:C:C6 | 2.55 | 0.41 |
| 1:A:1049:C:H1' | 1:A:1113:U:H4' | 2.02 | 0.41 |
| 1:A:118:A:C8 | 1:A:119:A:C8 | 3.09 | 0.41 |
| 1:A:117:G:C6 | 1:A:119:A:C6 | 3.09 | 0.41 |
| 15:T:99:LEU:O | 15:T:100:TYR:C | 2.59 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 7:H:33:LEU:HD11 | 7:H:136:ILE:O | 2.21 | 0.41 |
| 1:A:1651:G:N2 | 1:A:2007:C:C2 | 2.89 | 0.41 |
| 7:H:32:GLU:O | 7:H:33:LEU:HD23 | 2.21 | 0.41 |
| 1:A:1587:A:H2' | 1:A:1588:C:C6 | 2.55 | 0.41 |
| 22:0:41:ARG:HD2 | 22:0:41:ARG:HA | 1.80 | 0.41 |
| 1:A:1382:G:H2' | 1:A:1383:C:C6 | 2.56 | 0.41 |
| 23:1:40:ARG:HE | 23:1:40:ARG:HB2 | 1.67 | 0.41 |
| 8:I:59:ALA:O | 8:I:63:ALA:N | 2.54 | 0.41 |
| 2:B:78:A:C2 | 2:B:100:A:C4 | 3.09 | 0.41 |
| 1:A:773:U:H5' | 3:D:47:GLY:HA3 | 2.02 | 0.41 |
| 13:R:26:LYS:HE2 | 13:R:70:LEU:O | 2.21 | 0.41 |
| 5:F:167:ALA:HB1 | 5:F:173:VAL:HG11 | 2.01 | 0.41 |
| 18:W:68:ARG:O | 18:W:109:GLU:HA | 2.21 | 0.41 |
| 1:A:1433:U:O2 | 1:A:1561:G:C2 | 2.74 | 0.41 |
| 1:A:2115:G:H5'' | 1:A:2116:G:OP2 | 2.21 | 0.41 |
| 8:I:78:THR:HA | 8:I:143:SER:O | 2.21 | 0.41 |
| 1:A:107:C:H2' | 1:A:108:U:C6 | 2.54 | 0.41 |
| 28:6:14:THR:O | 28:6:17:LYS:NZ | 2.30 | 0.41 |
| 2:B:59:A:H2' | 2:B:60:C:H6 | 1.85 | 0.41 |
| 1:A:729:G:H2' | 1:A:1775:U:H1' | 2.04 | 0.41 |
| 4:E:137:HIS:HB3 | 4:E:138:PRO:HD2 | 2.02 | 0.41 |
| 1:A:2400:G:C5 | 1:A:2401:U:C5 | 3.09 | 0.41 |
| 1:A:2702:U:H4' | 1:A:2703:C:OP1 | 2.20 | 0.41 |
| 19:X:94:GLY:HA3 | 19:X:95:LEU:HA | 1.66 | 0.41 |
| 30:8:26:LYS:HZ2 | 30:8:26:LYS:HG2 | 1.72 | 0.41 |
| 1:A:2752:C:O5' | 1:A:2752:C:H6 | 2.04 | 0.41 |
| 1:A:2127:G:HO2' | 1:A:2173:A:H2 | 1.63 | 0.40 |
| 1:A:271(H):G:O2' | 1:A:271(I):G:OP2 | 2.28 | 0.40 |
| 30:8:34:TRP:CD2 | 30:8:35:GLN:HB2 | 2.56 | 0.40 |
| 1:A:271(S):G:C6 | 1:A:271(T):C:C4 | 3.08 | 0.40 |
| 1:A:188:G:H1 | 1:A:208:C:N4 | 2.18 | 0.40 |
| 1:A:2834:G:N2 | 1:A:2882:A:N6 | 2.69 | 0.40 |
| 5:F:126:VAL:HG21 | 5:F:129:PHE:CE1 | 2.55 | 0.40 |
| 10:O:35:VAL:HG21 | 10:O:103:ALA:HB3 | 2.03 | 0.40 |
| 15:T:3:ARG:HB2 | 15:T:3:ARG:NH2 | 2.36 | 0.40 |
| 3:D:9:TYR:CZ | 3:D:13:ARG:HG2 | 2.56 | 0.40 |
| 1:A:858:U:O2 | 1:A:2268:A:H2' | 2.20 | 0.40 |
| 1:A:1138:G:C4 | 1:A:1139:G:H1' | 2.56 | 0.40 |
| 13:R:38:VAL:HB | 13:R:39:PRO:HD3 | 2.02 | 0.40 |
| 1:A:626:U:O4 | 11:P:107:LYS:HE2 | 2.21 | 0.40 |
| 30:8:29:LYS:HD3 | 30:8:44:LYS:C | 2.41 | 0.40 |
| 1:A:1420:U:H2' | 1:A:1420:U:H6 | 1.61 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:226:G:N2 | 1:A:228:A:N6 | 2.68 | 0.40 |
| 2:B:117:G:C4' | 14:S:54:LEU:HD23 | 2.47 | 0.40 |
| 1:A:243:U:O2' | 1:A:244:A:H5' | 2.22 | 0.40 |
| 18:W:79:GLY:CA | 18:W:100:THR:HG22 | 2.49 | 0.40 |
| 12:Q:18:LYS:O | 12:Q:98:LYS:HD3 | 2.21 | 0.40 |
| 1:A:2583:G:H2' | 1:A:2584:U:H6 | 1.86 | 0.40 |
| 1:A:1586:A:H2' | 1:A:1587:A:H5' | 2.03 | 0.40 |
| 19:X:18:TYR:C | 19:X:20:GLY:N | 2.75 | 0.40 |
| 1:A:1421:G:C2 | 1:A:1422:G:N7 | 2.89 | 0.40 |
| 1:A:2648:C:H2' | 1:A:2649:U:C6 | 2.56 | 0.40 |
| 1:A:706:A:H2' | 1:A:707:G:O4' | 2.21 | 0.40 |
| 1:A:950:G:C6 | 1:A:951:C:C4 | 3.10 | 0.40 |
| 1:A:2788:C:OP1 | 4:E:61:ARG:NH2 | 2.53 | 0.40 |
| 23:1:58:ILE:HG21 | 23:1:58:ILE:HD13 | 1.76 | 0.40 |
| 1:A:2119:A:C6 | 1:A:2171:A:C5 | 3.10 | 0.40 |
| 28:6:23:THR:HG1 | 28:6:24:GLU:N | 2.17 | 0.40 |
| 1:A:330:A:C2 | 1:A:1210:A:H2' | 2.52 | 0.40 |
| 1:A:1753:G:OP1 | 15:T:95:ARG:HD3 | 2.21 | 0.40 |
| 7:H:56:SER:OG | 7:H:57:ASP:N | 2.55 | 0.40 |
| 15:T:118:ARG:NH1 | 15:T:118:ARG:HG3 | 2.37 | 0.40 |
| 8:I:75:LEU:CD2 | 8:I:140:LEU:HD21 | 2.52 | 0.40 |
| 9:N:18:ALA:HB3 | 9:N:56:ASN:O | 2.21 | 0.40 |
| 14:S:58:LEU:HB2 | 14:S:59:LYS:CB | 2.50 | 0.40 |
| 10:O:68:GLU:HG2 | 10:O:68:GLU:O | 2.21 | 0.40 |
| 1:A:1799:G:C8 | 3:D:181:GLU:OE2 | 2.74 | 0.40 |
| 10:O:59:LYS:NZ | 10:O:89:ASN:HD21 | 2.19 | 0.40 |
| 22:O:10:THR:HG22 | 22:O:12:ASN:H | 1.86 | 0.40 |
| 1:A:827:U:O2 | 1:A:2246:G:H4' | 2.22 | 0.40 |
| 16:U:109:LEU:HD23 | 16:U:109:LEU:HA | 1.83 | 0.40 |
| 26:4:6:HIS:HA | 26:4:7:PRO:HD2 | 1.83 | 0.40 |
| 1:A:631:A:H2' | 1:A:632:A:O4' | 2.21 | 0.40 |
| 8:I:44:LEU:HA | 8:I:44:LEU:HD12 | 1.39 | 0.40 |
| 4:E:24:THR:HG23 | 4:E:184:VAL:HG12 | 2.04 | 0.40 |
| 1:A:1529:G:O2' | 1:A:1530:C:H5' | 2.21 | 0.40 |
| 18:W:41:LYS:HE3 | 27:5:25:LEU:HD21 | 2.04 | 0.40 |
| 1:A:1504:C:H2' | 1:A:1505:C:H6 | 1.86 | 0.40 |
| 1:A:2192:G:C2 | 1:A:2193:G:C8 | 3.09 | 0.40 |
| 1:A:826:U:OP1 | 1:A:2428:G:H3' | 2.21 | 0.40 |
| 13:R:70:LEU:HD23 | 13:R:70:LEU:HA | 1.84 | 0.40 |
| 1:A:979:G:C6 | 1:A:982:C:C5 | 3.09 | 0.40 |
| 1:A:1266:G:O5' | 18:W:15:ARG:NH2 | 2.54 | 0.40 |
| 1:A:754:C:H2' | 1:A:755:C:H6 | 1.86 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-----------------|-------------|----------|
| 6:G:105:LYS:HE2 | 6:G:105:LYS:HB2 | 1.91 | 0.40 |
| 1:A:2416:C:O5' | 1:A:2416:C:H6 | 2.04 | 0.40 |
| 1:A:2109:U:H3' | 1:A:2109:U:C6 | 2.53 | 0.40 |
| 14:S:102:ALA:HA | 14:S:105:ALA:H | 1.85 | 0.40 |
| 26:4:16:CYS:HB2 | 26:4:36:CYS:SG | 2.62 | 0.40 |
| 1:A:811:U:O2' | 11:P:21:ARG:HG3 | 2.22 | 0.40 |
| 1:A:2732:G:H3' | 1:A:2733:A:O4' | 2.20 | 0.40 |
| 1:A:271(T):C:H2' | 1:A:271(U):G:H8 | 1.86 | 0.40 |
| 9:N:134:ARG:HA | 9:N:135:PRO:HD3 | 1.61 | 0.40 |
| 1:A:1721:G:N3 | 1:A:1721:G:H5'' | 2.37 | 0.40 |
| 28:6:10:LEU:CD1 | 28:6:54:ILE:HA | 2.51 | 0.40 |
| 1:A:916:G:C2' | 1:A:917:A:H5'' | 2.52 | 0.40 |
| 1:A:469:G:C2' | 1:A:470:A:H5'' | 2.51 | 0.40 |
| 1:A:754:C:H2' | 1:A:755:C:C6 | 2.57 | 0.40 |
| 7:H:13:LYS:HA | 7:H:14:GLY:HA2 | 1.54 | 0.40 |
| 6:G:153:ARG:HB2 | 6:G:153:ARG:HE | 1.55 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 3 | D | 273/276 (99%) | 258 (94%) | 14 (5%) | 1 (0%) | 43 | 87 |
| 4 | E | 202/206 (98%) | 189 (94%) | 11 (5%) | 2 (1%) | 22 | 70 |
| 5 | F | 201/210 (96%) | 188 (94%) | 12 (6%) | 1 (0%) | 38 | 84 |
| 6 | G | 179/182 (98%) | 151 (84%) | 27 (15%) | 1 (1%) | 33 | 81 |
| 7 | H | 172/180 (96%) | 158 (92%) | 12 (7%) | 2 (1%) | 19 | 64 |
| 8 | I | 144/148 (97%) | 113 (78%) | 29 (20%) | 2 (1%) | 16 | 60 |
| 9 | N | 138/140 (99%) | 126 (91%) | 7 (5%) | 5 (4%) | 5 | 29 |
| 10 | O | 120/122 (98%) | 112 (93%) | 8 (7%) | 0 | 100 | 100 |
| 11 | P | 147/150 (98%) | 134 (91%) | 13 (9%) | 0 | 100 | 100 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 12 | Q | 139/141 (99%) | 125 (90%) | 14 (10%) | 0 | 100 | 100 |
| 13 | R | 116/118 (98%) | 112 (97%) | 4 (3%) | 0 | 100 | 100 |
| 14 | S | 108/112 (96%) | 97 (90%) | 10 (9%) | 1 (1%) | 25 | 73 |
| 15 | T | 129/146 (88%) | 126 (98%) | 3 (2%) | 0 | 100 | 100 |
| 16 | U | 114/118 (97%) | 113 (99%) | 1 (1%) | 0 | 100 | 100 |
| 17 | V | 99/101 (98%) | 94 (95%) | 5 (5%) | 0 | 100 | 100 |
| 18 | W | 110/113 (97%) | 106 (96%) | 4 (4%) | 0 | 100 | 100 |
| 19 | X | 93/96 (97%) | 88 (95%) | 5 (5%) | 0 | 100 | 100 |
| 20 | Y | 105/110 (96%) | 95 (90%) | 8 (8%) | 2 (2%) | 12 | 51 |
| 21 | Z | 196/206 (95%) | 177 (90%) | 16 (8%) | 3 (2%) | 15 | 58 |
| 22 | 0 | 74/85 (87%) | 71 (96%) | 3 (4%) | 0 | 100 | 100 |
| 23 | 1 | 95/98 (97%) | 93 (98%) | 1 (1%) | 1 (1%) | 21 | 67 |
| 24 | 2 | 68/72 (94%) | 65 (96%) | 3 (4%) | 0 | 100 | 100 |
| 25 | 3 | 57/60 (95%) | 53 (93%) | 4 (7%) | 0 | 100 | 100 |
| 26 | 4 | 44/71 (62%) | 38 (86%) | 6 (14%) | 0 | 100 | 100 |
| 27 | 5 | 57/60 (95%) | 52 (91%) | 5 (9%) | 0 | 100 | 100 |
| 28 | 6 | 51/54 (94%) | 49 (96%) | 2 (4%) | 0 | 100 | 100 |
| 29 | 7 | 46/49 (94%) | 45 (98%) | 0 | 1 (2%) | 10 | 45 |
| 30 | 8 | 62/65 (95%) | 59 (95%) | 1 (2%) | 2 (3%) | 6 | 33 |
| 31 | 9 | 34/37 (92%) | 34 (100%) | 0 | 0 | 100 | 100 |
| All | All | 3373/3526 (96%) | 3121 (92%) | 228 (7%) | 24 (1%) | 30 | 78 |

All (24) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9 | N | 23 | LEU |
| 9 | N | 24 | GLY |
| 30 | 8 | 34 | TRP |
| 30 | 8 | 35 | GLN |
| 5 | F | 89 | VAL |
| 8 | I | 117 | GLU |
| 20 | Y | 103 | GLY |
| 7 | H | 65 | HIS |
| 7 | H | 92 | ILE |
| 9 | N | 4 | TYR |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9 | N | 5 | VAL |
| 9 | N | 19 | GLU |
| 23 | 1 | 3 | LYS |
| 29 | 7 | 46 | VAL |
| 4 | E | 52 | LEU |
| 6 | G | 171 | ALA |
| 3 | D | 3 | VAL |
| 4 | E | 72 | VAL |
| 8 | I | 107 | VAL |
| 21 | Z | 161 | VAL |
| 21 | Z | 193 | GLU |
| 14 | S | 85 | VAL |
| 20 | Y | 3 | VAL |
| 21 | Z | 39 | VAL |

5.3.2 Protein sidechains ⓘ

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 3 | D | 215/218 (99%) | 180 (84%) | 35 (16%) | 3 | 17 |
| 4 | E | 163/166 (98%) | 135 (83%) | 28 (17%) | 3 | 14 |
| 5 | F | 159/166 (96%) | 133 (84%) | 26 (16%) | 3 | 16 |
| 6 | G | 128/156 (82%) | 106 (83%) | 22 (17%) | 3 | 14 |
| 7 | H | 141/148 (95%) | 127 (90%) | 14 (10%) | 11 | 40 |
| 8 | I | 98/124 (79%) | 67 (68%) | 31 (32%) | 0 | 2 |
| 9 | N | 117/119 (98%) | 93 (80%) | 24 (20%) | 2 | 9 |
| 10 | O | 98/100 (98%) | 90 (92%) | 8 (8%) | 17 | 52 |
| 11 | P | 114/116 (98%) | 100 (88%) | 14 (12%) | 7 | 28 |
| 12 | Q | 111/111 (100%) | 96 (86%) | 15 (14%) | 6 | 24 |
| 13 | R | 101/101 (100%) | 83 (82%) | 18 (18%) | 2 | 14 |
| 14 | S | 84/88 (96%) | 72 (86%) | 12 (14%) | 5 | 22 |
| 15 | T | 110/127 (87%) | 92 (84%) | 18 (16%) | 3 | 16 |
| 16 | U | 93/94 (99%) | 84 (90%) | 9 (10%) | 12 | 42 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 17 | V | 80/82 (98%) | 64 (80%) | 16 (20%) | 2 | 10 |
| 18 | W | 89/92 (97%) | 76 (85%) | 13 (15%) | 5 | 21 |
| 19 | X | 75/78 (96%) | 70 (93%) | 5 (7%) | 23 | 64 |
| 20 | Y | 80/91 (88%) | 63 (79%) | 17 (21%) | 1 | 8 |
| 21 | Z | 159/179 (89%) | 141 (89%) | 18 (11%) | 9 | 33 |
| 22 | 0 | 59/67 (88%) | 54 (92%) | 5 (8%) | 15 | 51 |
| 23 | 1 | 78/83 (94%) | 67 (86%) | 11 (14%) | 5 | 23 |
| 24 | 2 | 65/67 (97%) | 58 (89%) | 7 (11%) | 9 | 35 |
| 25 | 3 | 49/52 (94%) | 42 (86%) | 7 (14%) | 5 | 22 |
| 26 | 4 | 39/63 (62%) | 29 (74%) | 10 (26%) | 1 | 4 |
| 27 | 5 | 50/52 (96%) | 45 (90%) | 5 (10%) | 11 | 39 |
| 28 | 6 | 50/52 (96%) | 37 (74%) | 13 (26%) | 1 | 4 |
| 29 | 7 | 41/42 (98%) | 34 (83%) | 7 (17%) | 3 | 15 |
| 30 | 8 | 52/55 (94%) | 43 (83%) | 9 (17%) | 3 | 14 |
| 31 | 9 | 32/34 (94%) | 29 (91%) | 3 (9%) | 13 | 44 |
| All | All | 2730/2923 (93%) | 2310 (85%) | 420 (15%) | 4 | 19 |

All (420) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | D | 12 | SER |
| 3 | D | 13 | ARG |
| 3 | D | 25 | THR |
| 3 | D | 32 | SER |
| 3 | D | 35 | LYS |
| 3 | D | 37 | LEU |
| 3 | D | 39 | LYS |
| 3 | D | 54 | ARG |
| 3 | D | 61 | LEU |
| 3 | D | 88 | ARG |
| 3 | D | 89 | SER |
| 3 | D | 94 | LEU |
| 3 | D | 99 | ASP |
| 3 | D | 101 | GLU |
| 3 | D | 103 | ARG |
| 3 | D | 126 | GLN |
| 3 | D | 138 | VAL |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | D | 141 | VAL |
| 3 | D | 147 | LEU |
| 3 | D | 150 | LYS |
| 3 | D | 155 | LEU |
| 3 | D | 173 | VAL |
| 3 | D | 192 | THR |
| 3 | D | 193 | VAL |
| 3 | D | 211 | ARG |
| 3 | D | 212 | SER |
| 3 | D | 217 | ARG |
| 3 | D | 221 | VAL |
| 3 | D | 229 | VAL |
| 3 | D | 242 | ARG |
| 3 | D | 257 | LEU |
| 3 | D | 259 | THR |
| 3 | D | 260 | ARG |
| 3 | D | 270 | ILE |
| 3 | D | 274 | ARG |
| 4 | E | 9 | VAL |
| 4 | E | 12 | THR |
| 4 | E | 21 | VAL |
| 4 | E | 24 | THR |
| 4 | E | 34 | VAL |
| 4 | E | 38 | THR |
| 4 | E | 49 | LEU |
| 4 | E | 52 | LEU |
| 4 | E | 54 | GLN |
| 4 | E | 75 | VAL |
| 4 | E | 78 | LEU |
| 4 | E | 82 | ARG |
| 4 | E | 89 | ASP |
| 4 | E | 93 | VAL |
| 4 | E | 105 | THR |
| 4 | E | 113 | PHE |
| 4 | E | 116 | VAL |
| 4 | E | 119 | ARG |
| 4 | E | 144 | ARG |
| 4 | E | 152 | LYS |
| 4 | E | 154 | LYS |
| 4 | E | 163 | GLU |
| 4 | E | 170 | LEU |
| 4 | E | 175 | VAL |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | E | 179 | GLU |
| 4 | E | 181 | LEU |
| 4 | E | 182 | LEU |
| 4 | E | 184 | VAL |
| 5 | F | 15 | SER |
| 5 | F | 18 | ARG |
| 5 | F | 20 | LEU |
| 5 | F | 24 | LEU |
| 5 | F | 33 | LEU |
| 5 | F | 46 | ARG |
| 5 | F | 50 | SER |
| 5 | F | 53 | THR |
| 5 | F | 57 | VAL |
| 5 | F | 60 | SER |
| 5 | F | 74 | ARG |
| 5 | F | 77 | ASP |
| 5 | F | 82 | ILE |
| 5 | F | 88 | VAL |
| 5 | F | 96 | ASP |
| 5 | F | 106 | ARG |
| 5 | F | 110 | LEU |
| 5 | F | 117 | ARG |
| 5 | F | 133 | ASN |
| 5 | F | 135 | LYS |
| 5 | F | 140 | LEU |
| 5 | F | 152 | GLU |
| 5 | F | 158 | THR |
| 5 | F | 183 | VAL |
| 5 | F | 192 | LEU |
| 5 | F | 197 | ASP |
| 6 | G | 3 | LEU |
| 6 | G | 13 | GLU |
| 6 | G | 20 | ILE |
| 6 | G | 21 | ARG |
| 6 | G | 31 | VAL |
| 6 | G | 33 | ARG |
| 6 | G | 43 | LEU |
| 6 | G | 88 | ILE |
| 6 | G | 96 | ARG |
| 6 | G | 117 | PHE |
| 6 | G | 135 | LEU |
| 6 | G | 138 | GLN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6 | G | 143 | GLU |
| 6 | G | 145 | THR |
| 6 | G | 146 | TYR |
| 6 | G | 148 | MET |
| 6 | G | 149 | VAL |
| 6 | G | 150 | ASP |
| 6 | G | 153 | ARG |
| 6 | G | 159 | VAL |
| 6 | G | 161 | THR |
| 6 | G | 170 | ARG |
| 7 | H | 7 | LEU |
| 7 | H | 15 | VAL |
| 7 | H | 16 | SER |
| 7 | H | 41 | MET |
| 7 | H | 51 | ARG |
| 7 | H | 69 | ARG |
| 7 | H | 70 | THR |
| 7 | H | 88 | LEU |
| 7 | H | 98 | LEU |
| 7 | H | 106 | THR |
| 7 | H | 129 | THR |
| 7 | H | 132 | ARG |
| 7 | H | 139 | GLN |
| 7 | H | 171 | LEU |
| 8 | I | 1 | MET |
| 8 | I | 7 | GLU |
| 8 | I | 9 | LEU |
| 8 | I | 12 | LEU |
| 8 | I | 15 | VAL |
| 8 | I | 41 | GLU |
| 8 | I | 43 | ASN |
| 8 | I | 44 | LEU |
| 8 | I | 47 | LEU |
| 8 | I | 61 | ARG |
| 8 | I | 66 | GLU |
| 8 | I | 72 | LEU |
| 8 | I | 75 | LEU |
| 8 | I | 76 | THR |
| 8 | I | 77 | LEU |
| 8 | I | 78 | THR |
| 8 | I | 79 | ILE |
| 8 | I | 88 | ILE |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8 | I | 92 | VAL |
| 8 | I | 93 | THR |
| 8 | I | 97 | ILE |
| 8 | I | 105 | HIS |
| 8 | I | 116 | LEU |
| 8 | I | 117 | GLU |
| 8 | I | 120 | ILE |
| 8 | I | 123 | LEU |
| 8 | I | 133 | HIS |
| 8 | I | 140 | LEU |
| 8 | I | 142 | VAL |
| 8 | I | 144 | VAL |
| 8 | I | 145 | VAL |
| 9 | N | 2 | LYS |
| 9 | N | 9 | VAL |
| 9 | N | 12 | ARG |
| 9 | N | 15 | LEU |
| 9 | N | 22 | THR |
| 9 | N | 28 | THR |
| 9 | N | 33 | LEU |
| 9 | N | 34 | LEU |
| 9 | N | 43 | THR |
| 9 | N | 46 | VAL |
| 9 | N | 48 | MET |
| 9 | N | 55 | VAL |
| 9 | N | 62 | VAL |
| 9 | N | 63 | THR |
| 9 | N | 73 | THR |
| 9 | N | 87 | LEU |
| 9 | N | 93 | THR |
| 9 | N | 97 | ARG |
| 9 | N | 99 | LEU |
| 9 | N | 120 | LEU |
| 9 | N | 131 | GLN |
| 9 | N | 133 | GLN |
| 9 | N | 137 | LYS |
| 9 | N | 138 | LEU |
| 10 | O | 8 | LEU |
| 10 | O | 21 | CYS |
| 10 | O | 26 | LYS |
| 10 | O | 28 | SER |
| 10 | O | 42 | SER |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10 | O | 77 | ILE |
| 10 | O | 94 | ARG |
| 10 | O | 113 | LYS |
| 11 | P | 21 | ARG |
| 11 | P | 33 | ARG |
| 11 | P | 42 | SER |
| 11 | P | 55 | ARG |
| 11 | P | 59 | LEU |
| 11 | P | 64 | LYS |
| 11 | P | 86 | LYS |
| 11 | P | 98 | GLU |
| 11 | P | 106 | LEU |
| 11 | P | 112 | LEU |
| 11 | P | 117 | GLU |
| 11 | P | 125 | VAL |
| 11 | P | 133 | SER |
| 11 | P | 147 | LEU |
| 12 | Q | 1 | MET |
| 12 | Q | 5 | ARG |
| 12 | Q | 7 | MET |
| 12 | Q | 16 | ARG |
| 12 | Q | 21 | THR |
| 12 | Q | 25 | ASP |
| 12 | Q | 45 | GLN |
| 12 | Q | 55 | VAL |
| 12 | Q | 56 | ARG |
| 12 | Q | 75 | THR |
| 12 | Q | 79 | LEU |
| 12 | Q | 109 | VAL |
| 12 | Q | 119 | ARG |
| 12 | Q | 127 | ILE |
| 12 | Q | 138 | ASP |
| 13 | R | 6 | SER |
| 13 | R | 8 | ARG |
| 13 | R | 18 | LEU |
| 13 | R | 28 | LEU |
| 13 | R | 29 | LEU |
| 13 | R | 33 | ARG |
| 13 | R | 36 | THR |
| 13 | R | 44 | LEU |
| 13 | R | 48 | VAL |
| 13 | R | 54 | LEU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13 | R | 60 | LEU |
| 13 | R | 65 | LEU |
| 13 | R | 67 | LEU |
| 13 | R | 75 | LEU |
| 13 | R | 79 | LEU |
| 13 | R | 91 | GLN |
| 13 | R | 95 | THR |
| 13 | R | 100 | LEU |
| 14 | S | 3 | ARG |
| 14 | S | 11 | LYS |
| 14 | S | 19 | LYS |
| 14 | S | 20 | ARG |
| 14 | S | 25 | ARG |
| 14 | S | 42 | ASP |
| 14 | S | 50 | SER |
| 14 | S | 54 | LEU |
| 14 | S | 67 | ARG |
| 14 | S | 98 | VAL |
| 14 | S | 110 | LEU |
| 14 | S | 111 | GLU |
| 15 | T | 1 | MET |
| 15 | T | 6 | LEU |
| 15 | T | 13 | ARG |
| 15 | T | 16 | ARG |
| 15 | T | 23 | ARG |
| 15 | T | 28 | VAL |
| 15 | T | 34 | VAL |
| 15 | T | 39 | ARG |
| 15 | T | 49 | VAL |
| 15 | T | 53 | ARG |
| 15 | T | 59 | THR |
| 15 | T | 64 | ARG |
| 15 | T | 74 | ARG |
| 15 | T | 82 | LEU |
| 15 | T | 93 | ARG |
| 15 | T | 96 | ARG |
| 15 | T | 107 | ASP |
| 15 | T | 118 | ARG |
| 16 | U | 8 | VAL |
| 16 | U | 31 | SER |
| 16 | U | 36 | ARG |
| 16 | U | 58 | ARG |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 16 | U | 60 | LEU |
| 16 | U | 74 | LEU |
| 16 | U | 83 | LEU |
| 16 | U | 104 | GLN |
| 16 | U | 108 | GLU |
| 17 | V | 5 | VAL |
| 17 | V | 7 | THR |
| 17 | V | 18 | LEU |
| 17 | V | 28 | GLU |
| 17 | V | 33 | VAL |
| 17 | V | 35 | LEU |
| 17 | V | 38 | LEU |
| 17 | V | 46 | VAL |
| 17 | V | 51 | VAL |
| 17 | V | 57 | VAL |
| 17 | V | 61 | VAL |
| 17 | V | 62 | LEU |
| 17 | V | 72 | VAL |
| 17 | V | 89 | GLN |
| 17 | V | 95 | LEU |
| 17 | V | 100 | ARG |
| 18 | W | 11 | ARG |
| 18 | W | 15 | ARG |
| 18 | W | 17 | VAL |
| 18 | W | 23 | LEU |
| 18 | W | 27 | LYS |
| 18 | W | 28 | SER |
| 18 | W | 51 | LEU |
| 18 | W | 60 | ASN |
| 18 | W | 67 | ASP |
| 18 | W | 98 | LYS |
| 18 | W | 100 | THR |
| 18 | W | 103 | ILE |
| 18 | W | 107 | LEU |
| 19 | X | 23 | GLU |
| 19 | X | 35 | THR |
| 19 | X | 45 | THR |
| 19 | X | 52 | VAL |
| 19 | X | 57 | LEU |
| 20 | Y | 2 | ARG |
| 20 | Y | 5 | MET |
| 20 | Y | 6 | HIS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20 | Y | 7 | VAL |
| 20 | Y | 23 | ARG |
| 20 | Y | 29 | GLU |
| 20 | Y | 31 | LEU |
| 20 | Y | 44 | ILE |
| 20 | Y | 55 | TYR |
| 20 | Y | 72 | VAL |
| 20 | Y | 79 | CYS |
| 20 | Y | 85 | VAL |
| 20 | Y | 90 | LEU |
| 20 | Y | 92 | ASN |
| 20 | Y | 97 | ARG |
| 20 | Y | 99 | CYS |
| 20 | Y | 102 | CYS |
| 21 | Z | 3 | TYR |
| 21 | Z | 11 | GLU |
| 21 | Z | 19 | ARG |
| 21 | Z | 20 | ARG |
| 21 | Z | 41 | LEU |
| 21 | Z | 42 | VAL |
| 21 | Z | 72 | ARG |
| 21 | Z | 76 | LEU |
| 21 | Z | 80 | ARG |
| 21 | Z | 86 | VAL |
| 21 | Z | 89 | PHE |
| 21 | Z | 112 | ARG |
| 21 | Z | 126 | VAL |
| 21 | Z | 132 | ASN |
| 21 | Z | 133 | ILE |
| 21 | Z | 155 | LEU |
| 21 | Z | 156 | LYS |
| 21 | Z | 170 | THR |
| 22 | 0 | 20 | ARG |
| 22 | 0 | 43 | THR |
| 22 | 0 | 46 | LYS |
| 22 | 0 | 55 | ARG |
| 22 | 0 | 63 | VAL |
| 23 | 1 | 4 | VAL |
| 23 | 1 | 20 | ARG |
| 23 | 1 | 21 | ARG |
| 23 | 1 | 30 | VAL |
| 23 | 1 | 35 | THR |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23 | 1 | 40 | ARG |
| 23 | 1 | 58 | ILE |
| 23 | 1 | 59 | THR |
| 23 | 1 | 60 | PHE |
| 23 | 1 | 62 | VAL |
| 23 | 1 | 95 | LEU |
| 24 | 2 | 16 | LEU |
| 24 | 2 | 27 | GLU |
| 24 | 2 | 30 | ARG |
| 24 | 2 | 32 | LEU |
| 24 | 2 | 40 | SER |
| 24 | 2 | 53 | LEU |
| 24 | 2 | 55 | ARG |
| 25 | 3 | 6 | VAL |
| 25 | 3 | 8 | LEU |
| 25 | 3 | 23 | LEU |
| 25 | 3 | 24 | LYS |
| 25 | 3 | 30 | ARG |
| 25 | 3 | 31 | LEU |
| 25 | 3 | 40 | THR |
| 26 | 4 | 14 | ILE |
| 26 | 4 | 16 | CYS |
| 26 | 4 | 18 | CYS |
| 26 | 4 | 20 | ASN |
| 26 | 4 | 34 | GLU |
| 26 | 4 | 35 | VAL |
| 26 | 4 | 37 | SER |
| 26 | 4 | 39 | CYS |
| 26 | 4 | 43 | TYR |
| 26 | 4 | 44 | THR |
| 27 | 5 | 16 | ARG |
| 27 | 5 | 29 | THR |
| 27 | 5 | 37 | LYS |
| 27 | 5 | 40 | LYS |
| 27 | 5 | 55 | ARG |
| 28 | 6 | 6 | ARG |
| 28 | 6 | 14 | THR |
| 28 | 6 | 18 | ARG |
| 28 | 6 | 20 | ASN |
| 28 | 6 | 23 | THR |
| 28 | 6 | 28 | ARG |
| 28 | 6 | 33 | LYS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28 | 6 | 35 | GLU |
| 28 | 6 | 38 | LYS |
| 28 | 6 | 40 | CYS |
| 28 | 6 | 44 | ARG |
| 28 | 6 | 48 | VAL |
| 28 | 6 | 49 | HIS |
| 29 | 7 | 1 | MET |
| 29 | 7 | 4 | THR |
| 29 | 7 | 8 | ASN |
| 29 | 7 | 10 | ARG |
| 29 | 7 | 24 | THR |
| 29 | 7 | 32 | LYS |
| 29 | 7 | 47 | ARG |
| 30 | 8 | 26 | LYS |
| 30 | 8 | 29 | LYS |
| 30 | 8 | 30 | ARG |
| 30 | 8 | 31 | HIS |
| 30 | 8 | 32 | LEU |
| 30 | 8 | 34 | TRP |
| 30 | 8 | 37 | SER |
| 30 | 8 | 58 | ILE |
| 30 | 8 | 59 | LYS |
| 31 | 9 | 17 | ILE |
| 31 | 9 | 25 | VAL |
| 31 | 9 | 26 | ILE |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | D | 87 | ASN |
| 3 | D | 96 | HIS |
| 3 | D | 143 | HIS |
| 5 | F | 8 | GLN |
| 5 | F | 69 | HIS |
| 6 | G | 123 | ASN |
| 6 | G | 130 | ASN |
| 6 | G | 138 | GLN |
| 8 | I | 105 | HIS |
| 9 | N | 38 | HIS |
| 9 | N | 133 | GLN |
| 10 | O | 88 | ASN |
| 10 | O | 89 | ASN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12 | Q | 89 | ASN |
| 15 | T | 58 | ASN |
| 15 | T | 84 | GLN |
| 16 | U | 72 | HIS |
| 18 | W | 60 | ASN |
| 19 | X | 31 | HIS |
| 19 | X | 55 | ASN |
| 20 | Y | 6 | HIS |
| 21 | Z | 151 | HIS |
| 28 | 6 | 20 | ASN |
| 29 | 7 | 6 | GLN |
| 30 | 8 | 7 | HIS |
| 31 | 9 | 36 | GLN |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | A | 2808/2915 (96%) | 552 (19%) | 63 (2%) |
| 2 | B | 119/122 (97%) | 21 (17%) | 0 |
| All | All | 2927/3037 (96%) | 573 (19%) | 63 (2%) |

All (573) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 10 | G |
| 1 | A | 15 | G |
| 1 | A | 34 | C |
| 1 | A | 36 | G |
| 1 | A | 45 | C |
| 1 | A | 61 | G |
| 1 | A | 68 | G |
| 1 | A | 69 | C |
| 1 | A | 71 | A |
| 1 | A | 74 | A |
| 1 | A | 75 | G |
| 1 | A | 84 | A |
| 1 | A | 90 | U |
| 1 | A | 92 | A |
| 1 | A | 94 | C |
| 1 | A | 95 | G |
| 1 | A | 102 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | A | 118 | A |
| 1 | A | 119 | A |
| 1 | A | 120 | U |
| 1 | A | 121 | G |
| 1 | A | 125 | G |
| 1 | A | 131 | G |
| 1 | A | 139(A) | G |
| 1 | A | 141 | A |
| 1 | A | 154 | G |
| 1 | A | 154(A) | C |
| 1 | A | 157 | U |
| 1 | A | 172 | C |
| 1 | A | 181 | A |
| 1 | A | 182 | A |
| 1 | A | 196 | A |
| 1 | A | 199 | A |
| 1 | A | 204 | A |
| 1 | A | 205 | G |
| 1 | A | 215 | G |
| 1 | A | 216 | A |
| 1 | A | 221 | A |
| 1 | A | 222 | A |
| 1 | A | 225 | A |
| 1 | A | 229 | A |
| 1 | A | 232 | G |
| 1 | A | 233 | A |
| 1 | A | 248 | G |
| 1 | A | 250 | G |
| 1 | A | 271(I) | G |
| 1 | A | 271(K) | U |
| 1 | A | 271(L) | U |
| 1 | A | 271(M) | G |
| 1 | A | 271(N) | U |
| 1 | A | 271(O) | C |
| 1 | A | 271(P) | C |
| 1 | A | 271(R) | G |
| 1 | A | 272(B) | G |
| 1 | A | 272(H) | C |
| 1 | A | 272(I) | U |
| 1 | A | 272(J) | C |
| 1 | A | 277 | C |
| 1 | A | 278 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | A | 279 | C |
| 1 | A | 283 | A |
| 1 | A | 286 | C |
| 1 | A | 311 | A |
| 1 | A | 324 | A |
| 1 | A | 329 | G |
| 1 | A | 330 | A |
| 1 | A | 332 | A |
| 1 | A | 333 | G |
| 1 | A | 352 | G |
| 1 | A | 363 | G |
| 1 | A | 363(F) | A |
| 1 | A | 382 | G |
| 1 | A | 386 | G |
| 1 | A | 399 | G |
| 1 | A | 411 | G |
| 1 | A | 412 | A |
| 1 | A | 414 | C |
| 1 | A | 426 | C |
| 1 | A | 427 | U |
| 1 | A | 428 | A |
| 1 | A | 444 | C |
| 1 | A | 448 | U |
| 1 | A | 454 | A |
| 1 | A | 456 | C |
| 1 | A | 457 | A |
| 1 | A | 470 | A |
| 1 | A | 471 | A |
| 1 | A | 481 | G |
| 1 | A | 492 | A |
| 1 | A | 504 | U |
| 1 | A | 505 | A |
| 1 | A | 509 | C |
| 1 | A | 510 | C |
| 1 | A | 512 | G |
| 1 | A | 530 | G |
| 1 | A | 531 | C |
| 1 | A | 532 | A |
| 1 | A | 533 | G |
| 1 | A | 543 | C |
| 1 | A | 545 | G |
| 1 | A | 546 | C |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | A | 547 | A |
| 1 | A | 548 | A |
| 1 | A | 563 | G |
| 1 | A | 571 | A |
| 1 | A | 573 | G |
| 1 | A | 575 | A |
| 1 | A | 586 | A |
| 1 | A | 588 | U |
| 1 | A | 603 | A |
| 1 | A | 604 | G |
| 1 | A | 606 | U |
| 1 | A | 607 | U |
| 1 | A | 614 | U |
| 1 | A | 614(A) | U |
| 1 | A | 614(B) | G |
| 1 | A | 615 | G |
| 1 | A | 619 | G |
| 1 | A | 627 | A |
| 1 | A | 637 | A |
| 1 | A | 644 | A |
| 1 | A | 645 | C |
| 1 | A | 646 | A |
| 1 | A | 652(B) | A |
| 1 | A | 652(C) | G |
| 1 | A | 652(D) | C |
| 1 | A | 652(U) | G |
| 1 | A | 669 | G |
| 1 | A | 686 | G |
| 1 | A | 708 | C |
| 1 | A | 709 | U |
| 1 | A | 717 | G |
| 1 | A | 730 | C |
| 1 | A | 752 | A |
| 1 | A | 753 | C |
| 1 | A | 762 | U |
| 1 | A | 765 | G |
| 1 | A | 775 | G |
| 1 | A | 776 | G |
| 1 | A | 782 | A |
| 1 | A | 784 | A |
| 1 | A | 785 | G |
| 1 | A | 792 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | A | 802 | A |
| 1 | A | 805 | G |
| 1 | A | 810 | U |
| 1 | A | 812 | C |
| 1 | A | 819 | A |
| 1 | A | 827 | U |
| 1 | A | 828 | U |
| 1 | A | 830 | G |
| 1 | A | 836 | G |
| 1 | A | 857 | C |
| 1 | A | 859 | G |
| 1 | A | 869 | G |
| 1 | A | 879 | G |
| 1 | A | 880 | G |
| 1 | A | 896 | A |
| 1 | A | 897 | C |
| 1 | A | 899 | A |
| 1 | A | 900 | A |
| 1 | A | 901 | A |
| 1 | A | 910 | A |
| 1 | A | 917 | A |
| 1 | A | 922 | U |
| 1 | A | 923 | C |
| 1 | A | 932 | G |
| 1 | A | 934 | G |
| 1 | A | 938 | G |
| 1 | A | 941 | A |
| 1 | A | 945 | A |
| 1 | A | 946 | G |
| 1 | A | 958 | U |
| 1 | A | 959 | A |
| 1 | A | 961 | C |
| 1 | A | 968 | G |
| 1 | A | 974 | G |
| 1 | A | 975 | C |
| 1 | A | 975(A) | G |
| 1 | A | 983 | A |
| 1 | A | 990 | A |
| 1 | A | 996 | A |
| 1 | A | 1012 | U |
| 1 | A | 1013 | C |
| 1 | A | 1016 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | A | 1020 | A |
| 1 | A | 1022 | G |
| 1 | A | 1024 | G |
| 1 | A | 1025 | G |
| 1 | A | 1026 | U |
| 1 | A | 1027 | A |
| 1 | A | 1033 | U |
| 1 | A | 1034 | G |
| 1 | A | 1038 | C |
| 1 | A | 1041 | C |
| 1 | A | 1042 | G |
| 1 | A | 1044 | G |
| 1 | A | 1045 | A |
| 1 | A | 1046 | A |
| 1 | A | 1047 | G |
| 1 | A | 1048 | A |
| 1 | A | 1049 | C |
| 1 | A | 1050 | A |
| 1 | A | 1052 | C |
| 1 | A | 1107 | G |
| 1 | A | 1108 | U |
| 1 | A | 1109 | C |
| 1 | A | 1110 | G |
| 1 | A | 1111 | A |
| 1 | A | 1112 | G |
| 1 | A | 1115 | G |
| 1 | A | 1129 | A |
| 1 | A | 1135 | C |
| 1 | A | 1136 | G |
| 1 | A | 1139 | G |
| 1 | A | 1141 | U |
| 1 | A | 1142 | U |
| 1 | A | 1142(A) | A |
| 1 | A | 1149 | G |
| 1 | A | 1155 | A |
| 1 | A | 1164 | G |
| 1 | A | 1211 | U |
| 1 | A | 1218 | C |
| 1 | A | 1253 | A |
| 1 | A | 1256 | G |
| 1 | A | 1268 | A |
| 1 | A | 1271 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1272 | A |
| 1 | A | 1273 | U |
| 1 | A | 1298 | C |
| 1 | A | 1300 | U |
| 1 | A | 1301 | A |
| 1 | A | 1314 | C |
| 1 | A | 1321 | A |
| 1 | A | 1329 | U |
| 1 | A | 1338 | G |
| 1 | A | 1358 | G |
| 1 | A | 1365 | A |
| 1 | A | 1367 | A |
| 1 | A | 1368 | G |
| 1 | A | 1370 | C |
| 1 | A | 1374 | G |
| 1 | A | 1380 | G |
| 1 | A | 1384 | A |
| 1 | A | 1385 | G |
| 1 | A | 1391 | U |
| 1 | A | 1416 | G |
| 1 | A | 1417 | C |
| 1 | A | 1419 | A |
| 1 | A | 1420 | U |
| 1 | A | 1421 | G |
| 1 | A | 1427 | A |
| 1 | A | 1428 | C |
| 1 | A | 1429 | G |
| 1 | A | 1445 | A |
| 1 | A | 1449 | A |
| 1 | A | 1450 | G |
| 1 | A | 1459 | G |
| 1 | A | 1461 | G |
| 1 | A | 1467 | C |
| 1 | A | 1471 | A |
| 1 | A | 1481 | U |
| 1 | A | 1482 | G |
| 1 | A | 1488 | G |
| 1 | A | 1490 | A |
| 1 | A | 1493 | C |
| 1 | A | 1497 | U |
| 1 | A | 1507 | A |
| 1 | A | 1508 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | A | 1509 | C |
| 1 | A | 1509(A) | A |
| 1 | A | 1518 | U |
| 1 | A | 1520 | G |
| 1 | A | 1531 | C |
| 1 | A | 1533 | G |
| 1 | A | 1534 | U |
| 1 | A | 1535 | A |
| 1 | A | 1536 | C |
| 1 | A | 1537 | G |
| 1 | A | 1539 | G |
| 1 | A | 1542 | A |
| 1 | A | 1543 | C |
| 1 | A | 1554 | A |
| 1 | A | 1558 | A |
| 1 | A | 1559 | G |
| 1 | A | 1566 | A |
| 1 | A | 1569 | A |
| 1 | A | 1578 | U |
| 1 | A | 1580 | A |
| 1 | A | 1582 | C |
| 1 | A | 1584 | C |
| 1 | A | 1586 | A |
| 1 | A | 1598 | C |
| 1 | A | 1608 | A |
| 1 | A | 1609 | A |
| 1 | A | 1610 | A |
| 1 | A | 1617 | C |
| 1 | A | 1625 | C |
| 1 | A | 1639 | U |
| 1 | A | 1640 | C |
| 1 | A | 1641 | A |
| 1 | A | 1648 | C |
| 1 | A | 1654 | A |
| 1 | A | 1674 | G |
| 1 | A | 1675 | C |
| 1 | A | 1696 | G |
| 1 | A | 1700 | A |
| 1 | A | 1701 | A |
| 1 | A | 1703 | G |
| 1 | A | 1721 | G |
| 1 | A | 1722 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1746 | G |
| 1 | A | 1750 | G |
| 1 | A | 1756 | G |
| 1 | A | 1762 | A |
| 1 | A | 1763 | G |
| 1 | A | 1764 | G |
| 1 | A | 1773 | A |
| 1 | A | 1780 | A |
| 1 | A | 1781 | C |
| 1 | A | 1782 | C |
| 1 | A | 1791 | A |
| 1 | A | 1799 | G |
| 1 | A | 1800 | C |
| 1 | A | 1801 | G |
| 1 | A | 1816 | G |
| 1 | A | 1819 | A |
| 1 | A | 1820 | U |
| 1 | A | 1829 | A |
| 1 | A | 1835 | G |
| 1 | A | 1836 | C |
| 1 | A | 1847 | A |
| 1 | A | 1848 | A |
| 1 | A | 1858 | G |
| 1 | A | 1877 | A |
| 1 | A | 1878 | G |
| 1 | A | 1889 | A |
| 1 | A | 1900 | A |
| 1 | A | 1906 | G |
| 1 | A | 1913 | A |
| 1 | A | 1914 | C |
| 1 | A | 1929 | G |
| 1 | A | 1930 | G |
| 1 | A | 1934 | C |
| 1 | A | 1936 | A |
| 1 | A | 1938 | A |
| 1 | A | 1955 | U |
| 1 | A | 1962 | C |
| 1 | A | 1963 | U |
| 1 | A | 1967 | C |
| 1 | A | 1969 | A |
| 1 | A | 1970 | A |
| 1 | A | 1971 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1972 | A |
| 1 | A | 1982 | C |
| 1 | A | 1991 | U |
| 1 | A | 1992 | G |
| 1 | A | 1993 | U |
| 1 | A | 1997 | G |
| 1 | A | 2020 | A |
| 1 | A | 2023 | G |
| 1 | A | 2031 | A |
| 1 | A | 2032 | G |
| 1 | A | 2033 | A |
| 1 | A | 2036 | C |
| 1 | A | 2039 | C |
| 1 | A | 2043 | C |
| 1 | A | 2049 | G |
| 1 | A | 2055 | C |
| 1 | A | 2056 | G |
| 1 | A | 2060 | A |
| 1 | A | 2061 | G |
| 1 | A | 2062 | A |
| 1 | A | 2063 | C |
| 1 | A | 2069 | G |
| 1 | A | 2093 | G |
| 1 | A | 2099 | U |
| 1 | A | 2103 | C |
| 1 | A | 2104 | G |
| 1 | A | 2105 | C |
| 1 | A | 2106 | G |
| 1 | A | 2108 | C |
| 1 | A | 2109 | U |
| 1 | A | 2110 | G |
| 1 | A | 2111 | C |
| 1 | A | 2116 | G |
| 1 | A | 2117 | A |
| 1 | A | 2118 | U |
| 1 | A | 2119 | A |
| 1 | A | 2126 | A |
| 1 | A | 2127 | G |
| 1 | A | 2131 | G |
| 1 | A | 2133 | G |
| 1 | A | 2134 | A |
| 1 | A | 2135 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 2143 | C |
| 1 | A | 2146 | C |
| 1 | A | 2147 | G |
| 1 | A | 2148 | G |
| 1 | A | 2161 | C |
| 1 | A | 2162 | G |
| 1 | A | 2170 | A |
| 1 | A | 2172 | U |
| 1 | A | 2173 | A |
| 1 | A | 2175 | C |
| 1 | A | 2176 | A |
| 1 | A | 2181 | G |
| 1 | A | 2185 | C |
| 1 | A | 2187 | G |
| 1 | A | 2188 | C |
| 1 | A | 2190 | G |
| 1 | A | 2191 | G |
| 1 | A | 2192 | G |
| 1 | A | 2196 | C |
| 1 | A | 2198 | A |
| 1 | A | 2199 | A |
| 1 | A | 2200 | C |
| 1 | A | 2206 | G |
| 1 | A | 2207 | G |
| 1 | A | 2208 | A |
| 1 | A | 2218 | U |
| 1 | A | 2225 | A |
| 1 | A | 2235 | G |
| 1 | A | 2238 | G |
| 1 | A | 2239 | G |
| 1 | A | 2240 | C |
| 1 | A | 2259 | G |
| 1 | A | 2267 | A |
| 1 | A | 2268 | A |
| 1 | A | 2269 | A |
| 1 | A | 2273 | A |
| 1 | A | 2275 | C |
| 1 | A | 2280 | G |
| 1 | A | 2283 | C |
| 1 | A | 2287 | A |
| 1 | A | 2289 | G |
| 1 | A | 2304 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 2305 | A |
| 1 | A | 2306 | C |
| 1 | A | 2308 | G |
| 1 | A | 2309 | A |
| 1 | A | 2311 | A |
| 1 | A | 2316 | C |
| 1 | A | 2318 | G |
| 1 | A | 2319 | G |
| 1 | A | 2320 | A |
| 1 | A | 2325 | G |
| 1 | A | 2327 | A |
| 1 | A | 2334 | G |
| 1 | A | 2336 | A |
| 1 | A | 2347 | C |
| 1 | A | 2348 | U |
| 1 | A | 2350 | C |
| 1 | A | 2354 | G |
| 1 | A | 2355 | C |
| 1 | A | 2371 | G |
| 1 | A | 2372 | G |
| 1 | A | 2383 | G |
| 1 | A | 2385 | C |
| 1 | A | 2388 | A |
| 1 | A | 2396 | G |
| 1 | A | 2405 | G |
| 1 | A | 2406 | U |
| 1 | A | 2410 | G |
| 1 | A | 2413 | G |
| 1 | A | 2414 | G |
| 1 | A | 2422 | A |
| 1 | A | 2423 | U |
| 1 | A | 2425 | A |
| 1 | A | 2429 | G |
| 1 | A | 2430 | A |
| 1 | A | 2435 | A |
| 1 | A | 2439 | A |
| 1 | A | 2440 | C |
| 1 | A | 2441 | C |
| 1 | A | 2448 | A |
| 1 | A | 2460 | U |
| 1 | A | 2461 | C |
| 1 | A | 2468 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | A | 2469 | A |
| 1 | A | 2476 | A |
| 1 | A | 2478 | A |
| 1 | A | 2487 | G |
| 1 | A | 2494 | G |
| 1 | A | 2502 | G |
| 1 | A | 2505 | G |
| 1 | A | 2506 | U |
| 1 | A | 2518 | A |
| 1 | A | 2520 | C |
| 1 | A | 2525 | G |
| 1 | A | 2529 | G |
| 1 | A | 2535 | G |
| 1 | A | 2554 | U |
| 1 | A | 2566 | A |
| 1 | A | 2567 | G |
| 1 | A | 2569 | G |
| 1 | A | 2573 | C |
| 1 | A | 2584 | U |
| 1 | A | 2585 | U |
| 1 | A | 2586 | C |
| 1 | A | 2602 | A |
| 1 | A | 2603 | G |
| 1 | A | 2608 | G |
| 1 | A | 2611 | U |
| 1 | A | 2612 | C |
| 1 | A | 2615 | U |
| 1 | A | 2629 | A |
| 1 | A | 2630 | G |
| 1 | A | 2632 | A |
| 1 | A | 2643 | G |
| 1 | A | 2663 | G |
| 1 | A | 2673 | G |
| 1 | A | 2689 | U |
| 1 | A | 2690 | C |
| 1 | A | 2700 | C |
| 1 | A | 2702 | U |
| 1 | A | 2703 | C |
| 1 | A | 2707 | G |
| 1 | A | 2712 | U |
| 1 | A | 2712(A) | A |
| 1 | A | 2713 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 2714 | G |
| 1 | A | 2726 | U |
| 1 | A | 2733 | A |
| 1 | A | 2757 | A |
| 1 | A | 2758 | A |
| 1 | A | 2761 | G |
| 1 | A | 2762 | G |
| 1 | A | 2764 | A |
| 1 | A | 2765 | A |
| 1 | A | 2766 | G |
| 1 | A | 2769 | C |
| 1 | A | 2778 | A |
| 1 | A | 2791 | C |
| 1 | A | 2802 | G |
| 1 | A | 2803 | C |
| 1 | A | 2805 | G |
| 1 | A | 2808 | U |
| 1 | A | 2820 | A |
| 1 | A | 2821 | A |
| 1 | A | 2834 | G |
| 1 | A | 2835 | A |
| 1 | A | 2846 | G |
| 1 | A | 2850 | A |
| 1 | A | 2851 | A |
| 1 | A | 2872 | G |
| 1 | A | 2875 | C |
| 1 | A | 2880 | C |
| 1 | A | 2892 | A |
| 1 | A | 2893 | G |
| 1 | A | 2894 | G |
| 1 | A | 2895 | U |
| 2 | B | 2 | C |
| 2 | B | 8 | U |
| 2 | B | 9 | G |
| 2 | B | 12 | C |
| 2 | B | 13 | A |
| 2 | B | 22 | U |
| 2 | B | 24 | G |
| 2 | B | 29 | A |
| 2 | B | 32 | C |
| 2 | B | 34 | U |
| 2 | B | 39 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 45 | A |
| 2 | B | 52 | A |
| 2 | B | 53 | A |
| 2 | B | 56 | G |
| 2 | B | 59 | A |
| 2 | B | 64 | C |
| 2 | B | 73 | A |
| 2 | B | 106 | G |
| 2 | B | 110 | G |
| 2 | B | 116 | G |

All (63) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | A | 9 | U |
| 1 | A | 90 | U |
| 1 | A | 196 | A |
| 1 | A | 221 | A |
| 1 | A | 249 | C |
| 1 | A | 271(K) | U |
| 1 | A | 271(L) | U |
| 1 | A | 271(M) | G |
| 1 | A | 277 | C |
| 1 | A | 278 | A |
| 1 | A | 310 | A |
| 1 | A | 363(E) | U |
| 1 | A | 512 | G |
| 1 | A | 542 | C |
| 1 | A | 547 | A |
| 1 | A | 652(A) | A |
| 1 | A | 752 | A |
| 1 | A | 764 | A |
| 1 | A | 774 | A |
| 1 | A | 776 | G |
| 1 | A | 827 | U |
| 1 | A | 856 | C |
| 1 | A | 859 | G |
| 1 | A | 896 | A |
| 1 | A | 900 | A |
| 1 | A | 974 | G |
| 1 | A | 1026 | U |
| 1 | A | 1033 | U |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1047 | G |
| 1 | A | 1048 | A |
| 1 | A | 1049 | C |
| 1 | A | 1106 | G |
| 1 | A | 1108 | U |
| 1 | A | 1210 | A |
| 1 | A | 1378 | A |
| 1 | A | 1379 | A |
| 1 | A | 1427 | A |
| 1 | A | 1507 | A |
| 1 | A | 1530 | C |
| 1 | A | 1536 | C |
| 1 | A | 1538 | G |
| 1 | A | 1558 | A |
| 1 | A | 1608 | A |
| 1 | A | 1617 | C |
| 1 | A | 1653 | G |
| 1 | A | 1799 | G |
| 1 | A | 1819 | A |
| 1 | A | 1992 | G |
| 1 | A | 2126 | A |
| 1 | A | 2171 | A |
| 1 | A | 2172 | U |
| 1 | A | 2308 | G |
| 1 | A | 2318 | G |
| 1 | A | 2405 | G |
| 1 | A | 2439 | A |
| 1 | A | 2602 | A |
| 1 | A | 2610 | C |
| 1 | A | 2689 | U |
| 1 | A | 2712 | U |
| 1 | A | 2756 | U |
| 1 | A | 2778 | A |
| 1 | A | 2802 | G |
| 1 | A | 2873 | 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 446 ligands modelled in this entry, 446 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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 | A | 2814/2915 (96%) | -0.05 | 57 (2%) 62 12 | 34, 56, 138, 189 | 0 |
| 2 | B | 120/122 (98%) | 0.22 | 3 (2%) 54 11 | 63, 90, 111, 129 | 0 |
| 3 | D | 275/276 (99%) | 0.04 | 4 (1%) 70 16 | 36, 55, 72, 119 | 0 |
| 4 | E | 204/206 (99%) | 0.02 | 2 (0%) 79 22 | 35, 61, 84, 101 | 0 |
| 5 | F | 203/210 (96%) | 0.00 | 1 (0%) 88 36 | 34, 67, 96, 136 | 0 |
| 6 | G | 181/182 (99%) | 0.66 | 22 (12%) 5 1 | 92, 126, 146, 156 | 0 |
| 7 | H | 174/180 (96%) | 0.32 | 10 (5%) 23 5 | 70, 92, 107, 122 | 0 |
| 8 | I | 146/148 (98%) | 0.17 | 3 (2%) 60 12 | 60, 108, 127, 131 | 0 |
| 9 | N | 140/140 (100%) | -0.05 | 0 100 100 | 45, 63, 89, 101 | 0 |
| 10 | O | 122/122 (100%) | -0.05 | 0 100 100 | 46, 62, 82, 86 | 0 |
| 11 | P | 149/150 (99%) | 0.28 | 8 (5%) 25 5 | 38, 70, 102, 111 | 0 |
| 12 | Q | 141/141 (100%) | 0.10 | 2 (1%) 72 18 | 47, 67, 85, 94 | 0 |
| 13 | R | 118/118 (100%) | 0.12 | 5 (4%) 35 7 | 42, 55, 73, 82 | 0 |
| 14 | S | 110/112 (98%) | 0.32 | 6 (5%) 24 5 | 64, 82, 99, 110 | 0 |
| 15 | T | 131/146 (89%) | 0.05 | 1 (0%) 83 26 | 55, 67, 101, 118 | 0 |
| 16 | U | 116/118 (98%) | 0.06 | 2 (1%) 67 15 | 40, 56, 76, 86 | 0 |
| 17 | V | 101/101 (100%) | 0.05 | 1 (0%) 79 22 | 40, 72, 90, 98 | 0 |
| 18 | W | 112/113 (99%) | -0.22 | 0 100 100 | 40, 48, 69, 95 | 0 |
| 19 | X | 95/96 (98%) | -0.07 | 0 100 100 | 47, 56, 80, 102 | 0 |
| 20 | Y | 107/110 (97%) | 0.55 | 13 (12%) 5 1 | 59, 72, 96, 116 | 0 |
| 21 | Z | 198/206 (96%) | 0.28 | 6 (3%) 48 9 | 73, 92, 115, 132 | 0 |
| 22 | 0 | 76/85 (89%) | 0.14 | 0 100 100 | 53, 61, 76, 90 | 0 |
| 23 | 1 | 97/98 (98%) | 0.15 | 2 (2%) 60 12 | 41, 61, 91, 108 | 0 |
| 24 | 2 | 70/72 (97%) | 0.21 | 5 (7%) 16 4 | 55, 71, 88, 112 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 25 | 3 | 59/60 (98%) | 0.14 | 2 (3%) 43 8 | 49, 64, 92, 112 | 0 |
| 26 | 4 | 46/71 (64%) | -0.12 | 0 100 100 | 113, 141, 152, 163 | 0 |
| 27 | 5 | 59/60 (98%) | -0.03 | 3 (5%) 27 6 | 37, 55, 73, 95 | 0 |
| 28 | 6 | 53/54 (98%) | 0.05 | 1 (1%) 64 13 | 56, 65, 79, 82 | 0 |
| 29 | 7 | 48/49 (97%) | 0.41 | 4 (8%) 11 3 | 36, 40, 64, 83 | 0 |
| 30 | 8 | 64/65 (98%) | 0.03 | 0 100 100 | 46, 53, 62, 72 | 0 |
| 31 | 9 | 36/37 (97%) | 0.83 | 3 (8%) 11 3 | 58, 68, 81, 91 | 0 |
| All | All | 6365/6563 (96%) | 0.06 | 166 (2%) 54 10 | 34, 62, 126, 189 | 0 |

All (166) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 1 | A | 2117 | A | 7.5 |
| 7 | H | 171 | LEU | 7.3 |
| 5 | F | 208 | GLY | 7.0 |
| 1 | A | 2116 | G | 6.2 |
| 1 | A | 652(B) | A | 5.9 |
| 1 | A | 2124 | G | 5.7 |
| 1 | A | 2174 | C | 5.6 |
| 1 | A | 271(K) | U | 5.1 |
| 20 | Y | 1 | MET | 5.0 |
| 3 | D | 276 | LYS | 4.9 |
| 1 | A | 2790 | A | 4.8 |
| 24 | 2 | 8 | LYS | 4.7 |
| 1 | A | 2129 | C | 4.7 |
| 1 | A | 2150 | U | 4.7 |
| 1 | A | 1535 | A | 4.6 |
| 1 | A | 2173 | A | 4.5 |
| 6 | G | 35 | GLU | 4.5 |
| 6 | G | 136 | ARG | 4.5 |
| 1 | A | 2789 | C | 4.4 |
| 7 | H | 172 | LYS | 4.3 |
| 6 | G | 82 | LEU | 4.2 |
| 29 | 7 | 47 | ARG | 4.1 |
| 6 | G | 152 | LEU | 4.1 |
| 11 | P | 74 | GLU | 4.0 |
| 1 | A | 652(A) | A | 4.0 |
| 1 | A | 2175 | C | 4.0 |
| 31 | 9 | 37 | GLY | 4.0 |
| 1 | A | 655 | A | 3.8 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 1 | A | 2140 | C | 3.7 |
| 1 | A | 2118 | U | 3.7 |
| 1 | A | 362 | U | 3.6 |
| 20 | Y | 94 | LYS | 3.6 |
| 14 | S | 8 | GLU | 3.6 |
| 6 | G | 93 | THR | 3.6 |
| 20 | Y | 93 | GLY | 3.6 |
| 6 | G | 137 | GLU | 3.6 |
| 1 | A | 2132 | U | 3.5 |
| 23 | 1 | 37 | ILE | 3.4 |
| 1 | A | 271(L) | U | 3.4 |
| 1 | A | 2176 | A | 3.4 |
| 31 | 9 | 22 | ARG | 3.3 |
| 21 | Z | 140 | ASP | 3.3 |
| 3 | D | 5 | LYS | 3.2 |
| 1 | A | 2136 | C | 3.2 |
| 16 | U | 89 | GLU | 3.2 |
| 1 | A | 2122 | U | 3.2 |
| 27 | 5 | 59 | GLU | 3.1 |
| 11 | P | 108 | LYS | 3.1 |
| 20 | Y | 73 | ARG | 3.1 |
| 1 | A | 2149 | G | 3.1 |
| 20 | Y | 2 | ARG | 3.0 |
| 1 | A | 2128 | C | 3.0 |
| 1 | A | 1906 | G | 3.0 |
| 1 | A | 1331 | A | 3.0 |
| 7 | H | 109 | PHE | 3.0 |
| 1 | A | 2148 | G | 3.0 |
| 13 | R | 77 | ARG | 2.9 |
| 6 | G | 162 | THR | 2.9 |
| 1 | A | 361 | G | 2.8 |
| 7 | H | 108 | GLY | 2.8 |
| 1 | A | 2111 | C | 2.8 |
| 25 | 3 | 19 | GLN | 2.8 |
| 1 | A | 2125 | G | 2.8 |
| 11 | P | 73 | GLY | 2.8 |
| 11 | P | 109 | GLY | 2.8 |
| 1 | A | 2791 | C | 2.7 |
| 6 | G | 164 | GLU | 2.7 |
| 14 | S | 7 | TYR | 2.7 |
| 16 | U | 5 | LYS | 2.7 |
| 2 | B | 56 | G | 2.7 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 1 | A | 272(A) | U | 2.7 |
| 7 | H | 155 | SER | 2.7 |
| 1 | A | 2164 | C | 2.6 |
| 20 | Y | 92 | ASN | 2.6 |
| 7 | H | 159 | GLU | 2.6 |
| 14 | S | 43 | GLU | 2.6 |
| 1 | A | 2191 | G | 2.6 |
| 20 | Y | 22 | GLY | 2.6 |
| 1 | A | 896 | A | 2.6 |
| 6 | G | 33 | ARG | 2.6 |
| 20 | Y | 3 | VAL | 2.6 |
| 6 | G | 84 | LYS | 2.6 |
| 13 | R | 100 | LEU | 2.5 |
| 24 | 2 | 7 | ARG | 2.5 |
| 1 | A | 1905 | C | 2.5 |
| 15 | T | 113 | LYS | 2.5 |
| 1 | A | 2165 | G | 2.5 |
| 7 | H | 60 | ARG | 2.5 |
| 2 | B | 27 | C | 2.5 |
| 27 | 5 | 60 | VAL | 2.5 |
| 14 | S | 84 | GLN | 2.5 |
| 6 | G | 81 | LYS | 2.5 |
| 7 | H | 81 | GLU | 2.4 |
| 23 | 1 | 22 | GLY | 2.4 |
| 1 | A | 2121 | G | 2.4 |
| 1 | A | 2666 | C | 2.4 |
| 20 | Y | 55 | TYR | 2.4 |
| 20 | Y | 54 | LYS | 2.4 |
| 1 | A | 2120 | G | 2.4 |
| 2 | B | 24 | G | 2.4 |
| 21 | Z | 99 | TYR | 2.4 |
| 21 | Z | 141 | VAL | 2.4 |
| 1 | A | 2151 | G | 2.4 |
| 24 | 2 | 9 | GLN | 2.4 |
| 21 | Z | 78 | LYS | 2.3 |
| 12 | Q | 22 | LYS | 2.3 |
| 7 | H | 156 | ALA | 2.3 |
| 1 | A | 2068 | U | 2.3 |
| 1 | A | 2110 | G | 2.3 |
| 1 | A | 2123 | G | 2.3 |
| 6 | G | 36 | LYS | 2.3 |
| 24 | 2 | 49 | LYS | 2.3 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 11 | P | 79 | ARG | 2.3 |
| 1 | A | 1907 | G | 2.2 |
| 1 | A | 1609 | A | 2.2 |
| 1 | A | 1052 | C | 2.2 |
| 6 | G | 34 | LEU | 2.2 |
| 31 | 9 | 18 | ARG | 2.2 |
| 13 | R | 91 | GLN | 2.2 |
| 14 | S | 20 | ARG | 2.2 |
| 29 | 7 | 23 | ARG | 2.2 |
| 1 | A | 2172 | U | 2.2 |
| 21 | Z | 56 | VAL | 2.2 |
| 3 | D | 57 | GLY | 2.2 |
| 20 | Y | 87 | LYS | 2.2 |
| 8 | I | 57 | ARG | 2.2 |
| 6 | G | 50 | ALA | 2.2 |
| 6 | G | 97 | ASP | 2.2 |
| 29 | 7 | 46 | VAL | 2.2 |
| 8 | I | 35 | LEU | 2.2 |
| 28 | 6 | 54 | ILE | 2.2 |
| 11 | P | 92 | GLU | 2.2 |
| 11 | P | 76 | LYS | 2.1 |
| 8 | I | 36 | ALA | 2.1 |
| 6 | G | 145 | THR | 2.1 |
| 4 | E | 27 | LEU | 2.1 |
| 1 | A | 658 | C | 2.1 |
| 1 | A | 2109 | U | 2.1 |
| 4 | E | 8 | LYS | 2.1 |
| 6 | G | 134 | GLY | 2.1 |
| 6 | G | 182 | LYS | 2.1 |
| 27 | 5 | 58 | LEU | 2.1 |
| 1 | A | 1051 | G | 2.1 |
| 1 | A | 2792 | G | 2.1 |
| 3 | D | 275 | LYS | 2.1 |
| 14 | S | 44 | LYS | 2.1 |
| 21 | Z | 103 | ARG | 2.1 |
| 1 | A | 2169 | A | 2.1 |
| 25 | 3 | 24 | LYS | 2.1 |
| 1 | A | 2190 | G | 2.1 |
| 13 | R | 102 | GLU | 2.1 |
| 24 | 2 | 12 | GLU | 2.1 |
| 20 | Y | 29 | GLU | 2.1 |
| 6 | G | 138 | GLN | 2.1 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 20 | Y | 91 | GLU | 2.1 |
| 6 | G | 26 | GLN | 2.1 |
| 29 | 7 | 36 | GLN | 2.1 |
| 11 | P | 110 | TYR | 2.1 |
| 6 | G | 150 | ASP | 2.1 |
| 13 | R | 56 | LYS | 2.0 |
| 7 | H | 19 | VAL | 2.0 |
| 1 | A | 654 | A | 2.0 |
| 6 | G | 95 | ARG | 2.0 |
| 1 | A | 504 | U | 2.0 |
| 12 | Q | 1 | MET | 2.0 |
| 17 | V | 68 | LYS | 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 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 32 | MG | A | 3123 | 1/1 | 0.27 | - | 66,66,66,66 | 0 |
| 32 | MG | A | 3348 | 1/1 | 0.24 | - | 50,50,50,50 | 0 |
| 32 | MG | A | 3010 | 1/1 | 0.55 | - | 60,60,60,60 | 0 |
| 32 | MG | A | 3150 | 1/1 | 0.53 | - | 58,58,58,58 | 0 |
| 32 | MG | A | 3017 | 1/1 | 0.23 | - | 41,41,41,41 | 0 |
| 32 | MG | A | 3070 | 1/1 | 0.44 | - | 50,50,50,50 | 0 |
| 32 | MG | A | 3042 | 1/1 | 0.30 | - | 51,51,51,51 | 0 |
| 32 | MG | A | 3119 | 1/1 | 0.26 | - | 53,53,53,53 | 0 |
| 32 | MG | A | 3294 | 1/1 | 0.23 | - | 50,50,50,50 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 32 | MG | A | 3363 | 1/1 | 0.23 | - | 50,50,50,50 | 0 |
| 32 | MG | A | 3030 | 1/1 | 0.22 | - | 43,43,43,43 | 0 |
| 32 | MG | A | 3263 | 1/1 | 0.16 | - | 39,39,39,39 | 0 |
| 32 | MG | A | 3272 | 1/1 | 0.13 | - | 35,35,35,35 | 0 |
| 32 | MG | A | 3388 | 1/1 | 0.44 | - | 69,69,69,69 | 0 |
| 32 | MG | A | 3002 | 1/1 | 0.16 | - | 59,59,59,59 | 0 |
| 32 | MG | A | 3032 | 1/1 | 0.11 | - | 74,74,74,74 | 0 |
| 32 | MG | A | 3340 | 1/1 | 0.17 | - | 41,41,41,41 | 0 |
| 32 | MG | A | 3410 | 1/1 | 0.15 | - | 45,45,45,45 | 0 |
| 32 | MG | A | 3039 | 1/1 | 0.63 | - | 49,49,49,49 | 0 |
| 32 | MG | A | 3399 | 1/1 | 0.10 | - | 85,85,85,85 | 0 |
| 32 | MG | A | 3051 | 1/1 | 0.25 | - | 54,54,54,54 | 0 |
| 32 | MG | A | 3101 | 1/1 | 0.51 | - | 71,71,71,71 | 0 |
| 32 | MG | A | 3049 | 1/1 | 0.86 | - | 43,43,43,43 | 0 |
| 33 | ZN | 5 | 101 | 1/1 | 0.06 | - | 65,65,65,65 | 0 |
| 32 | MG | A | 3360 | 1/1 | 0.05 | - | 63,63,63,63 | 0 |
| 32 | MG | A | 3132 | 1/1 | 0.52 | - | 64,64,64,64 | 0 |
| 32 | MG | A | 3122 | 1/1 | 0.27 | - | 35,35,35,35 | 0 |
| 32 | MG | B | 205 | 1/1 | 0.11 | - | 70,70,70,70 | 0 |
| 32 | MG | A | 3131 | 1/1 | 0.49 | - | 78,78,78,78 | 0 |
| 32 | MG | A | 3343 | 1/1 | 0.50 | - | 100,100,100,100 | 0 |
| 32 | MG | A | 3216 | 1/1 | 0.31 | - | 53,53,53,53 | 0 |
| 32 | MG | A | 3256 | 1/1 | 0.43 | - | 56,56,56,56 | 0 |
| 32 | MG | A | 3108 | 1/1 | 0.34 | - | 46,46,46,46 | 0 |
| 32 | MG | A | 3267 | 1/1 | 0.09 | - | 54,54,54,54 | 0 |
| 32 | MG | A | 3330 | 1/1 | 0.12 | - | 62,62,62,62 | 0 |
| 32 | MG | A | 3087 | 1/1 | 0.96 | - | 82,82,82,82 | 0 |
| 32 | MG | A | 3261 | 1/1 | 0.15 | - | 70,70,70,70 | 0 |
| 32 | MG | A | 3068 | 1/1 | 0.37 | - | 53,53,53,53 | 0 |
| 32 | MG | A | 3283 | 1/1 | 0.12 | - | 52,52,52,52 | 0 |
| 32 | MG | A | 3231 | 1/1 | 0.24 | - | 43,43,43,43 | 0 |
| 32 | MG | A | 3240 | 1/1 | 0.46 | - | 38,38,38,38 | 0 |
| 32 | MG | A | 3331 | 1/1 | 0.11 | - | 53,53,53,53 | 0 |
| 32 | MG | A | 3194 | 1/1 | 0.16 | - | 63,63,63,63 | 0 |
| 32 | MG | A | 3242 | 1/1 | 0.28 | - | 35,35,35,35 | 0 |
| 32 | MG | A | 3018 | 1/1 | 0.45 | - | 39,39,39,39 | 0 |
| 32 | MG | A | 3223 | 1/1 | 0.28 | - | 64,64,64,64 | 0 |
| 32 | MG | A | 3179 | 1/1 | 0.24 | - | 51,51,51,51 | 0 |
| 32 | MG | A | 3065 | 1/1 | 0.31 | - | 32,32,32,32 | 0 |
| 32 | MG | D | 301 | 1/1 | 0.07 | - | 40,40,40,40 | 0 |
| 32 | MG | A | 3006 | 1/1 | 0.32 | - | 48,48,48,48 | 0 |
| 32 | MG | A | 3180 | 1/1 | 0.49 | - | 59,59,59,59 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 32 | MG | A | 3098 | 1/1 | 0.35 | - | 61,61,61,61 | 0 |
| 32 | MG | A | 3361 | 1/1 | 0.21 | - | 72,72,72,72 | 0 |
| 32 | MG | A | 3063 | 1/1 | 0.32 | - | 58,58,58,58 | 0 |
| 32 | MG | A | 3359 | 1/1 | 0.12 | - | 67,67,67,67 | 0 |
| 32 | MG | A | 3207 | 1/1 | 1.70 | - | 79,79,79,79 | 0 |
| 32 | MG | A | 3023 | 1/1 | 0.32 | - | 57,57,57,57 | 0 |
| 32 | MG | A | 3059 | 1/1 | 0.69 | - | 52,52,52,52 | 0 |
| 32 | MG | A | 3342 | 1/1 | 0.17 | - | 51,51,51,51 | 0 |
| 32 | MG | A | 3050 | 1/1 | 0.73 | - | 71,71,71,71 | 0 |
| 32 | MG | B | 203 | 1/1 | 0.33 | - | 61,61,61,61 | 0 |
| 32 | MG | A | 3184 | 1/1 | 0.44 | - | 42,42,42,42 | 0 |
| 32 | MG | A | 3384 | 1/1 | 0.12 | - | 63,63,63,63 | 0 |
| 32 | MG | A | 3102 | 1/1 | 0.39 | - | 57,57,57,57 | 0 |
| 32 | MG | A | 3210 | 1/1 | 0.35 | - | 38,38,38,38 | 0 |
| 32 | MG | A | 3115 | 1/1 | 0.24 | - | 34,34,34,34 | 0 |
| 32 | MG | A | 3407 | 1/1 | 0.20 | - | 79,79,79,79 | 0 |
| 32 | MG | A | 3095 | 1/1 | 0.61 | - | 64,64,64,64 | 0 |
| 32 | MG | A | 3220 | 1/1 | 0.22 | - | 47,47,47,47 | 0 |
| 32 | MG | A | 3135 | 1/1 | 0.75 | - | 64,64,64,64 | 0 |
| 32 | MG | A | 3165 | 1/1 | 1.22 | - | 59,59,59,59 | 0 |
| 32 | MG | A | 3217 | 1/1 | 0.21 | - | 38,38,38,38 | 0 |
| 32 | MG | A | 3125 | 1/1 | 0.97 | - | 63,63,63,63 | 0 |
| 32 | MG | F | 302 | 1/1 | 1.13 | - | 64,64,64,64 | 0 |
| 32 | MG | A | 3080 | 1/1 | 0.43 | - | 51,51,51,51 | 0 |
| 32 | MG | A | 3420 | 1/1 | 0.17 | - | 75,75,75,75 | 0 |
| 32 | MG | A | 3147 | 1/1 | 0.24 | - | 36,36,36,36 | 0 |
| 32 | MG | A | 3034 | 1/1 | 0.24 | - | 65,65,65,65 | 0 |
| 32 | MG | A | 3249 | 1/1 | 0.45 | - | 39,39,39,39 | 0 |
| 32 | MG | A | 3145 | 1/1 | 0.43 | - | 78,78,78,78 | 0 |
| 32 | MG | A | 3209 | 1/1 | 0.13 | - | 53,53,53,53 | 0 |
| 32 | MG | A | 3332 | 1/1 | 0.11 | - | 56,56,56,56 | 0 |
| 32 | MG | A | 3282 | 1/1 | 0.17 | - | 61,61,61,61 | 0 |
| 32 | MG | A | 3003 | 1/1 | 0.62 | - | 64,64,64,64 | 0 |
| 32 | MG | A | 3202 | 1/1 | 0.29 | - | 37,37,37,37 | 0 |
| 32 | MG | A | 3398 | 1/1 | 0.56 | - | 95,95,95,95 | 0 |
| 32 | MG | A | 3110 | 1/1 | 0.42 | - | 60,60,60,60 | 0 |
| 32 | MG | A | 3107 | 1/1 | 0.75 | - | 70,70,70,70 | 0 |
| 32 | MG | A | 3254 | 1/1 | 0.35 | - | 59,59,59,59 | 0 |
| 32 | MG | A | 3061 | 1/1 | 0.20 | - | 54,54,54,54 | 0 |
| 32 | MG | A | 3028 | 1/1 | 0.26 | - | 52,52,52,52 | 0 |
| 32 | MG | A | 3375 | 1/1 | 0.12 | - | 61,61,61,61 | 0 |
| 32 | MG | A | 3044 | 1/1 | 0.65 | - | 43,43,43,43 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 32 | MG | A | 3215 | 1/1 | 0.67 | - | 69,69,69,69 | 0 |
| 32 | MG | A | 3345 | 1/1 | 0.24 | - | 76,76,76,76 | 0 |
| 32 | MG | A | 3386 | 1/1 | 0.29 | - | 72,72,72,72 | 0 |
| 32 | MG | A | 3016 | 1/1 | 0.22 | - | 42,42,42,42 | 0 |
| 32 | MG | A | 3327 | 1/1 | 0.13 | - | 47,47,47,47 | 0 |
| 32 | MG | A | 3072 | 1/1 | 0.31 | - | 38,38,38,38 | 0 |
| 32 | MG | A | 3159 | 1/1 | 0.41 | - | 55,55,55,55 | 0 |
| 32 | MG | A | 3086 | 1/1 | 0.29 | - | 65,65,65,65 | 0 |
| 32 | MG | A | 3413 | 1/1 | 0.09 | - | 89,89,89,89 | 0 |
| 32 | MG | A | 3252 | 1/1 | 0.25 | - | 43,43,43,43 | 0 |
| 32 | MG | A | 3146 | 1/1 | 0.21 | - | 70,70,70,70 | 0 |
| 32 | MG | A | 3255 | 1/1 | 0.26 | - | 59,59,59,59 | 0 |
| 32 | MG | A | 3276 | 1/1 | 0.16 | - | 46,46,46,46 | 0 |
| 32 | MG | A | 3204 | 1/1 | 0.60 | - | 75,75,75,75 | 0 |
| 32 | MG | A | 3367 | 1/1 | 0.20 | - | 57,57,57,57 | 0 |
| 32 | MG | A | 3310 | 1/1 | 0.19 | - | 67,67,67,67 | 0 |
| 32 | MG | A | 3100 | 1/1 | 0.53 | - | 79,79,79,79 | 0 |
| 32 | MG | A | 3266 | 1/1 | 0.16 | - | 43,43,43,43 | 0 |
| 32 | MG | A | 3027 | 1/1 | 0.69 | - | 72,72,72,72 | 0 |
| 32 | MG | A | 3157 | 1/1 | 0.33 | - | 59,59,59,59 | 0 |
| 32 | MG | A | 3198 | 1/1 | 0.31 | - | 67,67,67,67 | 0 |
| 32 | MG | A | 3230 | 1/1 | 0.20 | - | 46,46,46,46 | 0 |
| 32 | MG | A | 3289 | 1/1 | 0.41 | - | 43,43,43,43 | 0 |
| 32 | MG | A | 3109 | 1/1 | 0.48 | - | 60,60,60,60 | 0 |
| 32 | MG | A | 3387 | 1/1 | 0.15 | - | 58,58,58,58 | 0 |
| 33 | ZN | 6 | 101 | 1/1 | 0.09 | - | 86,86,86,86 | 0 |
| 32 | MG | A | 3419 | 1/1 | 0.10 | - | 69,69,69,69 | 0 |
| 32 | MG | E | 301 | 1/1 | 0.27 | - | 37,37,37,37 | 0 |
| 32 | MG | A | 3192 | 1/1 | 0.56 | - | 77,77,77,77 | 0 |
| 32 | MG | A | 3011 | 1/1 | 0.24 | - | 41,41,41,41 | 0 |
| 32 | MG | A | 3040 | 1/1 | 0.36 | - | 46,46,46,46 | 0 |
| 32 | MG | A | 3339 | 1/1 | 0.09 | - | 39,39,39,39 | 0 |
| 32 | MG | A | 3013 | 1/1 | 0.50 | - | 71,71,71,71 | 0 |
| 32 | MG | A | 3071 | 1/1 | 0.25 | - | 54,54,54,54 | 0 |
| 32 | MG | A | 3238 | 1/1 | 0.32 | - | 67,67,67,67 | 0 |
| 32 | MG | A | 3138 | 1/1 | 0.88 | - | 70,70,70,70 | 0 |
| 32 | MG | A | 3060 | 1/1 | 0.34 | - | 65,65,65,65 | 0 |
| 32 | MG | A | 3347 | 1/1 | 0.29 | - | 54,54,54,54 | 0 |
| 32 | MG | A | 3302 | 1/1 | 0.12 | - | 38,38,38,38 | 0 |
| 32 | MG | A | 3311 | 1/1 | 0.16 | - | 64,64,64,64 | 0 |
| 32 | MG | A | 3093 | 1/1 | 0.30 | - | 71,71,71,71 | 0 |
| 32 | MG | A | 3408 | 1/1 | 0.29 | - | 72,72,72,72 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 32 | MG | A | 3218 | 1/1 | 0.22 | - | 48,48,48,48 | 0 |
| 32 | MG | A | 3334 | 1/1 | 0.39 | - | 87,87,87,87 | 0 |
| 32 | MG | A | 3274 | 1/1 | 0.15 | - | 51,51,51,51 | 0 |
| 32 | MG | A | 3389 | 1/1 | 0.27 | - | 67,67,67,67 | 0 |
| 32 | MG | A | 3337 | 1/1 | 0.12 | - | 48,48,48,48 | 0 |
| 32 | MG | A | 3164 | 1/1 | 0.36 | - | 55,55,55,55 | 0 |
| 32 | MG | A | 3036 | 1/1 | 0.23 | - | 39,39,39,39 | 0 |
| 32 | MG | A | 3008 | 1/1 | 0.39 | - | 43,43,43,43 | 0 |
| 32 | MG | B | 201 | 1/1 | 0.40 | - | 75,75,75,75 | 0 |
| 32 | MG | A | 3193 | 1/1 | 0.30 | - | 75,75,75,75 | 0 |
| 32 | MG | A | 3246 | 1/1 | 0.37 | - | 44,44,44,44 | 0 |
| 32 | MG | A | 3379 | 1/1 | 0.15 | - | 79,79,79,79 | 0 |
| 32 | MG | A | 3148 | 1/1 | 0.20 | - | 41,41,41,41 | 0 |
| 32 | MG | A | 3189 | 1/1 | 0.56 | - | 50,50,50,50 | 0 |
| 32 | MG | A | 3094 | 1/1 | 0.20 | - | 46,46,46,46 | 0 |
| 32 | MG | A | 3167 | 1/1 | 0.21 | - | 39,39,39,39 | 0 |
| 32 | MG | A | 3221 | 1/1 | 0.77 | - | 104,104,104,104 | 0 |
| 32 | MG | A | 3047 | 1/1 | 0.40 | - | 58,58,58,58 | 0 |
| 32 | MG | B | 202 | 1/1 | 0.31 | - | 86,86,86,86 | 0 |
| 32 | MG | A | 3412 | 1/1 | 0.30 | - | 68,68,68,68 | 0 |
| 32 | MG | A | 3082 | 1/1 | 0.40 | - | 62,62,62,62 | 0 |
| 32 | MG | A | 3299 | 1/1 | 0.16 | - | 55,55,55,55 | 0 |
| 32 | MG | A | 3425 | 1/1 | 0.16 | - | 40,40,40,40 | 0 |
| 32 | MG | A | 3318 | 1/1 | 0.16 | - | 57,57,57,57 | 0 |
| 32 | MG | A | 3203 | 1/1 | 0.19 | - | 82,82,82,82 | 0 |
| 32 | MG | A | 3090 | 1/1 | 0.42 | - | 63,63,63,63 | 0 |
| 32 | MG | A | 3280 | 1/1 | 0.13 | - | 42,42,42,42 | 0 |
| 32 | MG | A | 3219 | 1/1 | 0.32 | - | 69,69,69,69 | 0 |
| 32 | MG | A | 3045 | 1/1 | 0.49 | - | 65,65,65,65 | 0 |
| 32 | MG | A | 3033 | 1/1 | 0.64 | - | 68,68,68,68 | 0 |
| 32 | MG | A | 3121 | 1/1 | 0.32 | - | 56,56,56,56 | 0 |
| 32 | MG | P | 201 | 1/1 | 0.48 | - | 58,58,58,58 | 0 |
| 32 | MG | A | 3414 | 1/1 | 0.07 | - | 32,32,32,32 | 0 |
| 32 | MG | A | 3041 | 1/1 | 0.26 | - | 63,63,63,63 | 0 |
| 32 | MG | A | 3365 | 1/1 | 0.19 | - | 68,68,68,68 | 0 |
| 32 | MG | A | 3213 | 1/1 | 0.24 | - | 58,58,58,58 | 0 |
| 32 | MG | A | 3264 | 1/1 | 0.06 | - | 58,58,58,58 | 0 |
| 32 | MG | A | 3344 | 1/1 | 0.13 | - | 89,89,89,89 | 0 |
| 32 | MG | A | 3141 | 1/1 | 0.46 | - | 62,62,62,62 | 0 |
| 32 | MG | A | 3303 | 1/1 | 0.14 | - | 55,55,55,55 | 0 |
| 32 | MG | A | 3133 | 1/1 | 0.20 | - | 44,44,44,44 | 0 |
| 32 | MG | A | 3356 | 1/1 | 0.61 | - | 68,68,68,68 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 32 | MG | A | 3161 | 1/1 | 0.35 | - | 56,56,56,56 | 0 |
| 32 | MG | A | 3426 | 1/1 | 0.14 | - | 81,81,81,81 | 0 |
| 32 | MG | A | 3333 | 1/1 | 0.41 | - | 72,72,72,72 | 0 |
| 32 | MG | A | 3397 | 1/1 | 0.48 | - | 60,60,60,60 | 0 |
| 32 | MG | B | 204 | 1/1 | 0.23 | - | 74,74,74,74 | 0 |
| 32 | MG | A | 3114 | 1/1 | 0.39 | - | 46,46,46,46 | 0 |
| 32 | MG | A | 3373 | 1/1 | 0.10 | - | 50,50,50,50 | 0 |
| 32 | MG | A | 3309 | 1/1 | 0.21 | - | 65,65,65,65 | 0 |
| 32 | MG | A | 3067 | 1/1 | 0.20 | - | 61,61,61,61 | 0 |
| 32 | MG | A | 3285 | 1/1 | 0.15 | - | 46,46,46,46 | 0 |
| 32 | MG | A | 3224 | 1/1 | 0.28 | - | 53,53,53,53 | 0 |
| 32 | MG | A | 3118 | 1/1 | 0.45 | - | 52,52,52,52 | 0 |
| 32 | MG | A | 3143 | 1/1 | 0.22 | - | 47,47,47,47 | 0 |
| 32 | MG | A | 3316 | 1/1 | 0.13 | - | 66,66,66,66 | 0 |
| 32 | MG | A | 3022 | 1/1 | 0.51 | - | 49,49,49,49 | 0 |
| 32 | MG | A | 3055 | 1/1 | 0.33 | - | 67,67,67,67 | 0 |
| 32 | MG | A | 3196 | 1/1 | 0.21 | - | 55,55,55,55 | 0 |
| 32 | MG | A | 3341 | 1/1 | 0.13 | - | 35,35,35,35 | 0 |
| 32 | MG | A | 3286 | 1/1 | 0.07 | - | 37,37,37,37 | 0 |
| 32 | MG | A | 3077 | 1/1 | 0.29 | - | 60,60,60,60 | 0 |
| 32 | MG | A | 3177 | 1/1 | 0.56 | - | 62,62,62,62 | 0 |
| 32 | MG | A | 3074 | 1/1 | 0.09 | - | 70,70,70,70 | 0 |
| 32 | MG | A | 3188 | 1/1 | 0.16 | - | 57,57,57,57 | 0 |
| 32 | MG | A | 3128 | 1/1 | 0.52 | - | 59,59,59,59 | 0 |
| 32 | MG | A | 3404 | 1/1 | 0.11 | - | 35,35,35,35 | 0 |
| 32 | MG | A | 3417 | 1/1 | 0.25 | - | 50,50,50,50 | 0 |
| 32 | MG | 8 | 101 | 1/1 | 0.31 | - | 49,49,49,49 | 0 |
| 32 | MG | A | 3305 | 1/1 | 0.14 | - | 39,39,39,39 | 0 |
| 32 | MG | A | 3385 | 1/1 | 0.20 | - | 71,71,71,71 | 0 |
| 32 | MG | A | 3225 | 1/1 | 0.26 | - | 65,65,65,65 | 0 |
| 32 | MG | A | 3091 | 1/1 | 0.62 | - | 66,66,66,66 | 0 |
| 32 | MG | A | 3160 | 1/1 | 0.60 | - | 55,55,55,55 | 0 |
| 32 | MG | A | 3298 | 1/1 | 0.16 | - | 62,62,62,62 | 0 |
| 32 | MG | A | 3313 | 1/1 | 0.24 | - | 59,59,59,59 | 0 |
| 32 | MG | A | 3092 | 1/1 | 0.26 | - | 39,39,39,39 | 0 |
| 32 | MG | A | 3378 | 1/1 | 0.15 | - | 91,91,91,91 | 0 |
| 32 | MG | A | 3314 | 1/1 | 0.28 | - | 75,75,75,75 | 0 |
| 32 | MG | A | 3308 | 1/1 | 0.18 | - | 56,56,56,56 | 0 |
| 32 | MG | A | 3195 | 1/1 | 0.88 | - | 66,66,66,66 | 0 |
| 32 | MG | A | 3323 | 1/1 | 0.32 | - | 36,36,36,36 | 0 |
| 32 | MG | A | 3172 | 1/1 | 0.33 | - | 60,60,60,60 | 0 |
| 32 | MG | A | 3162 | 1/1 | 0.16 | - | 46,46,46,46 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 32 | MG | A | 3287 | 1/1 | 0.18 | - | 52,52,52,52 | 0 |
| 32 | MG | A | 3268 | 1/1 | 0.07 | - | 34,34,34,34 | 0 |
| 32 | MG | A | 3346 | 1/1 | 0.18 | - | 85,85,85,85 | 0 |
| 32 | MG | A | 3007 | 1/1 | 0.38 | - | 54,54,54,54 | 0 |
| 32 | MG | A | 3099 | 1/1 | 0.29 | - | 62,62,62,62 | 0 |
| 32 | MG | A | 3251 | 1/1 | 0.20 | - | 42,42,42,42 | 0 |
| 32 | MG | A | 3081 | 1/1 | 0.37 | - | 55,55,55,55 | 0 |
| 32 | MG | A | 3021 | 1/1 | 0.47 | - | 61,61,61,61 | 0 |
| 32 | MG | A | 3262 | 1/1 | 0.28 | - | 46,46,46,46 | 0 |
| 32 | MG | A | 3052 | 1/1 | 0.51 | - | 75,75,75,75 | 0 |
| 32 | MG | A | 3166 | 1/1 | 0.16 | - | 42,42,42,42 | 0 |
| 32 | MG | A | 3129 | 1/1 | 0.22 | - | 39,39,39,39 | 0 |
| 32 | MG | A | 3247 | 1/1 | 0.27 | - | 67,67,67,67 | 0 |
| 32 | MG | A | 3064 | 1/1 | 0.21 | - | 56,56,56,56 | 0 |
| 32 | MG | A | 3151 | 1/1 | 0.58 | - | 38,38,38,38 | 0 |
| 32 | MG | A | 3377 | 1/1 | 0.31 | - | 94,94,94,94 | 0 |
| 32 | MG | A | 3300 | 1/1 | 0.16 | - | 36,36,36,36 | 0 |
| 32 | MG | A | 3144 | 1/1 | 0.31 | - | 35,35,35,35 | 0 |
| 32 | MG | A | 3066 | 1/1 | 0.19 | - | 48,48,48,48 | 0 |
| 33 | ZN | 9 | 101 | 1/1 | 0.04 | - | 87,87,87,87 | 0 |
| 32 | MG | A | 3245 | 1/1 | 0.17 | - | 52,52,52,52 | 0 |
| 32 | MG | A | 3326 | 1/1 | 0.06 | - | 34,34,34,34 | 0 |
| 32 | MG | A | 3183 | 1/1 | 0.55 | - | 47,47,47,47 | 0 |
| 32 | MG | A | 3416 | 1/1 | 0.13 | - | 39,39,39,39 | 0 |
| 32 | MG | A | 3158 | 1/1 | 0.36 | - | 48,48,48,48 | 0 |
| 32 | MG | A | 3269 | 1/1 | 0.13 | - | 57,57,57,57 | 0 |
| 32 | MG | A | 3015 | 1/1 | 0.24 | - | 61,61,61,61 | 0 |
| 32 | MG | A | 3024 | 1/1 | 0.93 | - | 49,49,49,49 | 0 |
| 32 | MG | A | 3250 | 1/1 | 0.21 | - | 41,41,41,41 | 0 |
| 32 | MG | A | 3075 | 1/1 | 0.34 | - | 66,66,66,66 | 0 |
| 33 | ZN | Y | 201 | 1/1 | 0.03 | - | 128,128,128,128 | 0 |
| 32 | MG | A | 3124 | 1/1 | 0.22 | - | 80,80,80,80 | 0 |
| 32 | MG | A | 3004 | 1/1 | 0.78 | - | 44,44,44,44 | 0 |
| 32 | MG | A | 3236 | 1/1 | 0.61 | - | 52,52,52,52 | 0 |
| 32 | MG | A | 3155 | 1/1 | 0.33 | - | 69,69,69,69 | 0 |
| 32 | MG | A | 3369 | 1/1 | 0.28 | - | 50,50,50,50 | 0 |
| 32 | MG | A | 3402 | 1/1 | 0.25 | - | 53,53,53,53 | 0 |
| 32 | MG | A | 3259 | 1/1 | 0.43 | - | 56,56,56,56 | 0 |
| 32 | MG | A | 3153 | 1/1 | 0.26 | - | 57,57,57,57 | 0 |
| 32 | MG | A | 3201 | 1/1 | 0.15 | - | 48,48,48,48 | 0 |
| 32 | MG | A | 3175 | 1/1 | 0.68 | - | 59,59,59,59 | 0 |
| 32 | MG | A | 3306 | 1/1 | 0.24 | - | 49,49,49,49 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 32 | MG | A | 3393 | 1/1 | 0.21 | - | 37,37,37,37 | 0 |
| 32 | MG | A | 3037 | 1/1 | 0.17 | - | 41,41,41,41 | 0 |
| 32 | MG | A | 3427 | 1/1 | 0.13 | - | 44,44,44,44 | 0 |
| 32 | MG | A | 3403 | 1/1 | 0.19 | - | 70,70,70,70 | 0 |
| 32 | MG | A | 3170 | 1/1 | 0.28 | - | 50,50,50,50 | 0 |
| 32 | MG | A | 3054 | 1/1 | 0.77 | - | 61,61,61,61 | 0 |
| 32 | MG | A | 3197 | 1/1 | 0.14 | - | 74,74,74,74 | 0 |
| 32 | MG | A | 3035 | 1/1 | 1.05 | - | 49,49,49,49 | 0 |
| 32 | MG | A | 3111 | 1/1 | 0.26 | - | 42,42,42,42 | 0 |
| 32 | MG | A | 3260 | 1/1 | 0.22 | - | 46,46,46,46 | 0 |
| 32 | MG | A | 3152 | 1/1 | 0.31 | - | 62,62,62,62 | 0 |
| 32 | MG | A | 3366 | 1/1 | 0.27 | - | 78,78,78,78 | 0 |
| 32 | MG | A | 3053 | 1/1 | 0.35 | - | 43,43,43,43 | 0 |
| 32 | MG | A | 3228 | 1/1 | 0.52 | - | 67,67,67,67 | 0 |
| 32 | MG | A | 3358 | 1/1 | 0.33 | - | 63,63,63,63 | 0 |
| 32 | MG | A | 3248 | 1/1 | 0.21 | - | 41,41,41,41 | 0 |
| 32 | MG | A | 3182 | 1/1 | 0.30 | - | 39,39,39,39 | 0 |
| 32 | MG | A | 3351 | 1/1 | 0.11 | - | 40,40,40,40 | 0 |
| 32 | MG | A | 3304 | 1/1 | 0.10 | - | 88,88,88,88 | 0 |
| 32 | MG | A | 3227 | 1/1 | 0.46 | - | 55,55,55,55 | 0 |
| 32 | MG | A | 3335 | 1/1 | 0.20 | - | 42,42,42,42 | 0 |
| 32 | MG | A | 3383 | 1/1 | 0.30 | - | 49,49,49,49 | 0 |
| 32 | MG | A | 3112 | 1/1 | 0.15 | - | 51,51,51,51 | 0 |
| 32 | MG | A | 3297 | 1/1 | 0.14 | - | 54,54,54,54 | 0 |
| 32 | MG | A | 3097 | 1/1 | 0.27 | - | 40,40,40,40 | 0 |
| 32 | MG | A | 3257 | 1/1 | 0.30 | - | 64,64,64,64 | 0 |
| 32 | MG | A | 3149 | 1/1 | 0.42 | - | 58,58,58,58 | 0 |
| 32 | MG | A | 3271 | 1/1 | 0.23 | - | 37,37,37,37 | 0 |
| 32 | MG | A | 3243 | 1/1 | 0.39 | - | 47,47,47,47 | 0 |
| 32 | MG | A | 3422 | 1/1 | 0.08 | - | 130,130,130,130 | 0 |
| 32 | MG | A | 3273 | 1/1 | 0.21 | - | 48,48,48,48 | 0 |
| 32 | MG | A | 3400 | 1/1 | 0.28 | - | 59,59,59,59 | 0 |
| 32 | MG | A | 3395 | 1/1 | 0.22 | - | 65,65,65,65 | 0 |
| 32 | MG | A | 3048 | 1/1 | 0.26 | - | 90,90,90,90 | 0 |
| 32 | MG | A | 3025 | 1/1 | 0.23 | - | 51,51,51,51 | 0 |
| 32 | MG | A | 3174 | 1/1 | 0.52 | - | 61,61,61,61 | 0 |
| 32 | MG | A | 3005 | 1/1 | 0.17 | - | 36,36,36,36 | 0 |
| 32 | MG | A | 3181 | 1/1 | 0.16 | - | 50,50,50,50 | 0 |
| 32 | MG | A | 3428 | 1/1 | 0.07 | - | 72,72,72,72 | 0 |
| 32 | MG | A | 3222 | 1/1 | 0.38 | - | 80,80,80,80 | 0 |
| 32 | MG | A | 3239 | 1/1 | 0.24 | - | 63,63,63,63 | 0 |
| 32 | MG | A | 3126 | 1/1 | 0.48 | - | 72,72,72,72 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 32 | MG | A | 3353 | 1/1 | 0.24 | - | 37,37,37,37 | 0 |
| 32 | MG | A | 3043 | 1/1 | 0.58 | - | 72,72,72,72 | 0 |
| 32 | MG | A | 3026 | 1/1 | 0.20 | - | 53,53,53,53 | 0 |
| 32 | MG | A | 3130 | 1/1 | 0.33 | - | 49,49,49,49 | 0 |
| 32 | MG | A | 3073 | 1/1 | 0.69 | - | 71,71,71,71 | 0 |
| 32 | MG | A | 3096 | 1/1 | 0.36 | - | 62,62,62,62 | 0 |
| 32 | MG | A | 3301 | 1/1 | 0.10 | - | 37,37,37,37 | 0 |
| 32 | MG | A | 3372 | 1/1 | 0.21 | - | 44,44,44,44 | 0 |
| 32 | MG | A | 3139 | 1/1 | 0.87 | - | 74,74,74,74 | 0 |
| 32 | MG | A | 3185 | 1/1 | 0.47 | - | 47,47,47,47 | 0 |
| 32 | MG | A | 3329 | 1/1 | 0.17 | - | 69,69,69,69 | 0 |
| 32 | MG | A | 3411 | 1/1 | 0.13 | - | 37,37,37,37 | 0 |
| 32 | MG | A | 3423 | 1/1 | 0.07 | - | 60,60,60,60 | 0 |
| 32 | MG | A | 3200 | 1/1 | 0.30 | - | 37,37,37,37 | 0 |
| 32 | MG | A | 3325 | 1/1 | 0.60 | - | 94,94,94,94 | 0 |
| 32 | MG | A | 3085 | 1/1 | 0.39 | - | 58,58,58,58 | 0 |
| 32 | MG | A | 3352 | 1/1 | 0.18 | - | 41,41,41,41 | 0 |
| 32 | MG | A | 3038 | 1/1 | 0.58 | - | 50,50,50,50 | 0 |
| 32 | MG | A | 3178 | 1/1 | 0.51 | - | 78,78,78,78 | 0 |
| 32 | MG | A | 3120 | 1/1 | 0.28 | - | 47,47,47,47 | 0 |
| 32 | MG | A | 3270 | 1/1 | 0.18 | - | 47,47,47,47 | 0 |
| 32 | MG | A | 3083 | 1/1 | 0.22 | - | 51,51,51,51 | 0 |
| 32 | MG | A | 3390 | 1/1 | 0.12 | - | 56,56,56,56 | 0 |
| 32 | MG | A | 3127 | 1/1 | 1.72 | - | 78,78,78,78 | 0 |
| 32 | MG | A | 3140 | 1/1 | 0.34 | - | 46,46,46,46 | 0 |
| 32 | MG | A | 3088 | 1/1 | 0.27 | - | 53,53,53,53 | 0 |
| 32 | MG | A | 3370 | 1/1 | 0.23 | - | 40,40,40,40 | 0 |
| 32 | MG | A | 3154 | 1/1 | 0.75 | - | 52,52,52,52 | 0 |
| 32 | MG | A | 3187 | 1/1 | 0.71 | - | 66,66,66,66 | 0 |
| 32 | MG | A | 3265 | 1/1 | 0.21 | - | 59,59,59,59 | 0 |
| 32 | MG | A | 3069 | 1/1 | 0.28 | - | 60,60,60,60 | 0 |
| 32 | MG | A | 3350 | 1/1 | 0.23 | - | 61,61,61,61 | 0 |
| 32 | MG | A | 3062 | 1/1 | 0.34 | - | 53,53,53,53 | 0 |
| 32 | MG | A | 3076 | 1/1 | 0.51 | - | 53,53,53,53 | 0 |
| 32 | MG | A | 3190 | 1/1 | 0.21 | - | 66,66,66,66 | 0 |
| 32 | MG | A | 3237 | 1/1 | 0.18 | - | 39,39,39,39 | 0 |
| 32 | MG | A | 3046 | 1/1 | 0.54 | - | 53,53,53,53 | 0 |
| 32 | MG | A | 3258 | 1/1 | 0.20 | - | 44,44,44,44 | 0 |
| 32 | MG | A | 3278 | 1/1 | 0.23 | - | 40,40,40,40 | 0 |
| 32 | MG | A | 3396 | 1/1 | 0.19 | - | 52,52,52,52 | 0 |
| 32 | MG | A | 3205 | 1/1 | 0.38 | - | 53,53,53,53 | 0 |
| 32 | MG | A | 3229 | 1/1 | 0.32 | - | 54,54,54,54 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 32 | MG | A | 3106 | 1/1 | 0.35 | - | 80,80,80,80 | 0 |
| 32 | MG | A | 3380 | 1/1 | 0.22 | - | 53,53,53,53 | 0 |
| 32 | MG | A | 3312 | 1/1 | 0.31 | - | 54,54,54,54 | 0 |
| 32 | MG | A | 3029 | 1/1 | 0.33 | - | 43,43,43,43 | 0 |
| 32 | MG | A | 3019 | 1/1 | 0.43 | - | 53,53,53,53 | 0 |
| 32 | MG | A | 3406 | 1/1 | 0.21 | - | 65,65,65,65 | 0 |
| 32 | MG | A | 3142 | 1/1 | 0.19 | - | 42,42,42,42 | 0 |
| 32 | MG | F | 301 | 1/1 | 0.49 | - | 58,58,58,58 | 0 |
| 32 | MG | A | 3405 | 1/1 | 0.19 | - | 59,59,59,59 | 0 |
| 32 | MG | A | 3296 | 1/1 | 0.16 | - | 71,71,71,71 | 0 |
| 32 | MG | A | 3392 | 1/1 | 0.28 | - | 56,56,56,56 | 0 |
| 32 | MG | A | 3105 | 1/1 | 0.36 | - | 47,47,47,47 | 0 |
| 32 | MG | A | 3235 | 1/1 | 0.30 | - | 39,39,39,39 | 0 |
| 32 | MG | A | 3241 | 1/1 | 0.13 | - | 53,53,53,53 | 0 |
| 32 | MG | A | 3291 | 1/1 | 0.24 | - | 50,50,50,50 | 0 |
| 32 | MG | A | 3211 | 1/1 | 0.13 | - | 64,64,64,64 | 0 |
| 32 | MG | A | 3136 | 1/1 | 0.69 | - | 60,60,60,60 | 0 |
| 32 | MG | A | 3031 | 1/1 | 0.28 | - | 68,68,68,68 | 0 |
| 32 | MG | A | 3319 | 1/1 | 0.19 | - | 53,53,53,53 | 0 |
| 32 | MG | A | 3349 | 1/1 | 0.17 | - | 78,78,78,78 | 0 |
| 32 | MG | A | 3020 | 1/1 | 0.20 | - | 52,52,52,52 | 0 |
| 32 | MG | A | 3232 | 1/1 | 0.46 | - | 56,56,56,56 | 0 |
| 32 | MG | A | 3295 | 1/1 | 0.16 | - | 66,66,66,66 | 0 |
| 32 | MG | A | 3113 | 1/1 | 0.52 | - | 39,39,39,39 | 0 |
| 32 | MG | A | 3169 | 1/1 | 0.17 | - | 53,53,53,53 | 0 |
| 32 | MG | A | 3137 | 1/1 | 0.30 | - | 65,65,65,65 | 0 |
| 32 | MG | A | 3012 | 1/1 | 0.12 | - | 52,52,52,52 | 0 |
| 32 | MG | A | 3418 | 1/1 | 0.07 | - | 97,97,97,97 | 0 |
| 32 | MG | A | 3324 | 1/1 | 0.20 | - | 95,95,95,95 | 0 |
| 32 | MG | A | 3084 | 1/1 | 0.54 | - | 54,54,54,54 | 0 |
| 32 | MG | A | 3176 | 1/1 | 0.45 | - | 58,58,58,58 | 0 |
| 32 | MG | A | 3338 | 1/1 | 0.13 | - | 44,44,44,44 | 0 |
| 32 | MG | A | 3381 | 1/1 | 0.34 | - | 63,63,63,63 | 0 |
| 32 | MG | A | 3409 | 1/1 | 0.12 | - | 90,90,90,90 | 0 |
| 32 | MG | A | 3244 | 1/1 | 0.30 | - | 41,41,41,41 | 0 |
| 32 | MG | A | 3253 | 1/1 | 0.34 | - | 63,63,63,63 | 0 |
| 32 | MG | A | 3057 | 1/1 | 0.31 | - | 55,55,55,55 | 0 |
| 32 | MG | A | 3322 | 1/1 | 0.14 | - | 64,64,64,64 | 0 |
| 32 | MG | A | 3104 | 1/1 | 0.86 | - | 56,56,56,56 | 0 |
| 32 | MG | A | 3320 | 1/1 | 0.18 | - | 35,35,35,35 | 0 |
| 32 | MG | A | 3156 | 1/1 | 0.30 | - | 72,72,72,72 | 0 |
| 32 | MG | A | 3277 | 1/1 | 0.14 | - | 40,40,40,40 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 32 | MG | A | 3368 | 1/1 | 0.30 | - | 51,51,51,51 | 0 |
| 32 | MG | A | 3421 | 1/1 | 0.18 | - | 79,79,79,79 | 0 |
| 32 | MG | A | 3186 | 1/1 | 0.23 | - | 54,54,54,54 | 0 |
| 32 | MG | A | 3199 | 1/1 | 0.21 | - | 69,69,69,69 | 0 |
| 32 | MG | A | 3233 | 1/1 | 0.16 | - | 36,36,36,36 | 0 |
| 32 | MG | A | 3293 | 1/1 | 0.17 | - | 42,42,42,42 | 0 |
| 32 | MG | A | 3401 | 1/1 | 0.16 | - | 49,49,49,49 | 0 |
| 32 | MG | A | 3315 | 1/1 | 0.12 | - | 94,94,94,94 | 0 |
| 32 | MG | A | 3328 | 1/1 | 0.10 | - | 44,44,44,44 | 0 |
| 32 | MG | A | 3214 | 1/1 | 0.19 | - | 53,53,53,53 | 0 |
| 32 | MG | A | 3226 | 1/1 | 0.20 | - | 51,51,51,51 | 0 |
| 32 | MG | A | 3307 | 1/1 | 0.25 | - | 48,48,48,48 | 0 |
| 32 | MG | A | 3357 | 1/1 | 0.20 | - | 49,49,49,49 | 0 |
| 32 | MG | A | 3173 | 1/1 | 0.35 | - | 69,69,69,69 | 0 |
| 32 | MG | A | 3116 | 1/1 | 0.26 | - | 44,44,44,44 | 0 |
| 32 | MG | 6 | 102 | 1/1 | 0.41 | - | 64,64,64,64 | 0 |
| 32 | MG | A | 3371 | 1/1 | 0.12 | - | 38,38,38,38 | 0 |
| 32 | MG | A | 3134 | 1/1 | 0.23 | - | 42,42,42,42 | 0 |
| 33 | ZN | 4 | 101 | 1/1 | 0.05 | - | 176,176,176,176 | 0 |
| 32 | MG | A | 3275 | 1/1 | 0.18 | - | 42,42,42,42 | 0 |
| 32 | MG | A | 3206 | 1/1 | 0.25 | - | 52,52,52,52 | 0 |
| 32 | MG | A | 3089 | 1/1 | 0.17 | - | 70,70,70,70 | 0 |
| 32 | MG | A | 3234 | 1/1 | 0.29 | - | 44,44,44,44 | 0 |
| 32 | MG | A | 3009 | 1/1 | 0.30 | - | 46,46,46,46 | 0 |
| 32 | MG | A | 3163 | 1/1 | 0.27 | - | 58,58,58,58 | 0 |
| 32 | MG | A | 3056 | 1/1 | 0.26 | - | 51,51,51,51 | 0 |
| 32 | MG | A | 3424 | 1/1 | 0.28 | - | 94,94,94,94 | 0 |
| 32 | MG | A | 3391 | 1/1 | 0.20 | - | 81,81,81,81 | 0 |
| 32 | MG | A | 3079 | 1/1 | 0.32 | - | 52,52,52,52 | 0 |
| 32 | MG | A | 3288 | 1/1 | 0.12 | - | 42,42,42,42 | 0 |
| 32 | MG | A | 3364 | 1/1 | 0.11 | - | 35,35,35,35 | 0 |
| 32 | MG | A | 3281 | 1/1 | 0.11 | - | 48,48,48,48 | 0 |
| 32 | MG | A | 3078 | 1/1 | 0.59 | - | 73,73,73,73 | 0 |
| 32 | MG | A | 3336 | 1/1 | 0.31 | - | 50,50,50,50 | 0 |
| 32 | MG | A | 3362 | 1/1 | 0.23 | - | 67,67,67,67 | 0 |
| 32 | MG | A | 3321 | 1/1 | 0.11 | - | 36,36,36,36 | 0 |
| 32 | MG | A | 3382 | 1/1 | 0.25 | - | 57,57,57,57 | 0 |
| 32 | MG | 7 | 101 | 1/1 | 0.33 | - | 52,52,52,52 | 0 |
| 32 | MG | A | 3058 | 1/1 | 0.86 | - | 60,60,60,60 | 0 |
| 32 | MG | A | 3279 | 1/1 | 0.07 | - | 36,36,36,36 | 0 |
| 32 | MG | A | 3355 | 1/1 | 0.19 | - | 53,53,53,53 | 0 |
| 32 | MG | A | 3103 | 1/1 | 0.56 | - | 33,33,33,33 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 32 | MG | A | 3374 | 1/1 | 0.09 | - | 43,43,43,43 | 0 |
| 32 | MG | A | 3191 | 1/1 | 0.78 | - | 63,63,63,63 | 0 |
| 32 | MG | A | 3117 | 1/1 | 0.45 | - | 57,57,57,57 | 0 |
| 32 | MG | A | 3292 | 1/1 | 0.42 | - | 52,52,52,52 | 0 |
| 32 | MG | A | 3001 | 1/1 | 0.34 | - | 35,35,35,35 | 0 |
| 32 | MG | A | 3376 | 1/1 | 0.19 | - | 98,98,98,98 | 0 |
| 32 | MG | A | 3014 | 1/1 | 0.58 | - | 41,41,41,41 | 0 |
| 32 | MG | A | 3354 | 1/1 | 0.09 | - | 42,42,42,42 | 0 |
| 32 | MG | A | 3394 | 1/1 | 0.13 | - | 37,37,37,37 | 0 |
| 32 | MG | A | 3415 | 1/1 | 0.18 | - | 81,81,81,81 | 0 |
| 32 | MG | A | 3284 | 1/1 | 0.20 | - | 50,50,50,50 | 0 |
| 32 | MG | A | 3212 | 1/1 | 0.89 | - | 74,74,74,74 | 0 |
| 32 | MG | A | 3290 | 1/1 | 0.16 | - | 39,39,39,39 | 0 |
| 32 | MG | A | 3171 | 1/1 | 0.30 | - | 49,49,49,49 | 0 |
| 32 | MG | A | 3208 | 1/1 | 0.32 | - | 60,60,60,60 | 0 |
| 32 | MG | A | 3168 | 1/1 | 0.42 | - | 52,52,52,52 | 0 |
| 32 | MG | A | 3317 | 1/1 | 0.06 | - | 59,59,59,59 | 0 |

6.5 Other polymers ⓘ

There are no such residues in this entry.