



# Full wwPDB EM Validation Report (i)

Nov 19, 2022 – 12:07 PM EST

PDB ID : 4V6Z  
EMDB ID : EMD-2472  
Title : E. coli 70S-fMetVal-tRNAVal-tRNAAfMet complex in classic pre-translocation state (pre1b)  
Authors : Blau, C.; Bock, L.V.; Schroder, G.F.; Davydov, I.; Fischer, N.; Stark, H.; Rodnina, M.V.; Vaiana, A.C.; Grubmuller, H.  
Deposited on : 2013-10-14  
Resolution : 12.00 Å (reported)  
Based on initial models : 2WRI, 2HGP, 3I1O, 2K4C

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at  
<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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

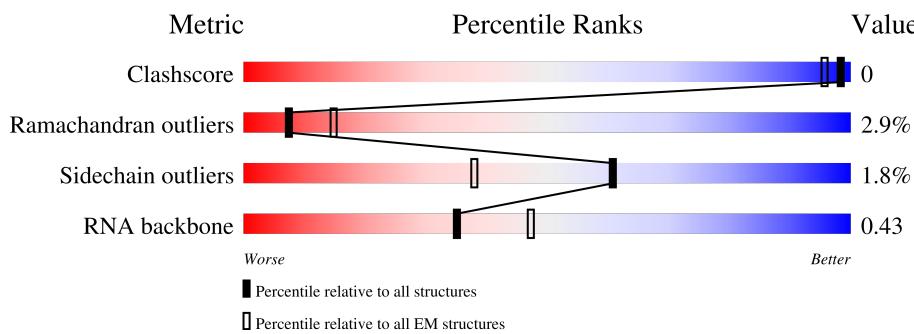
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:  
**ELECTRON MICROSCOPY**

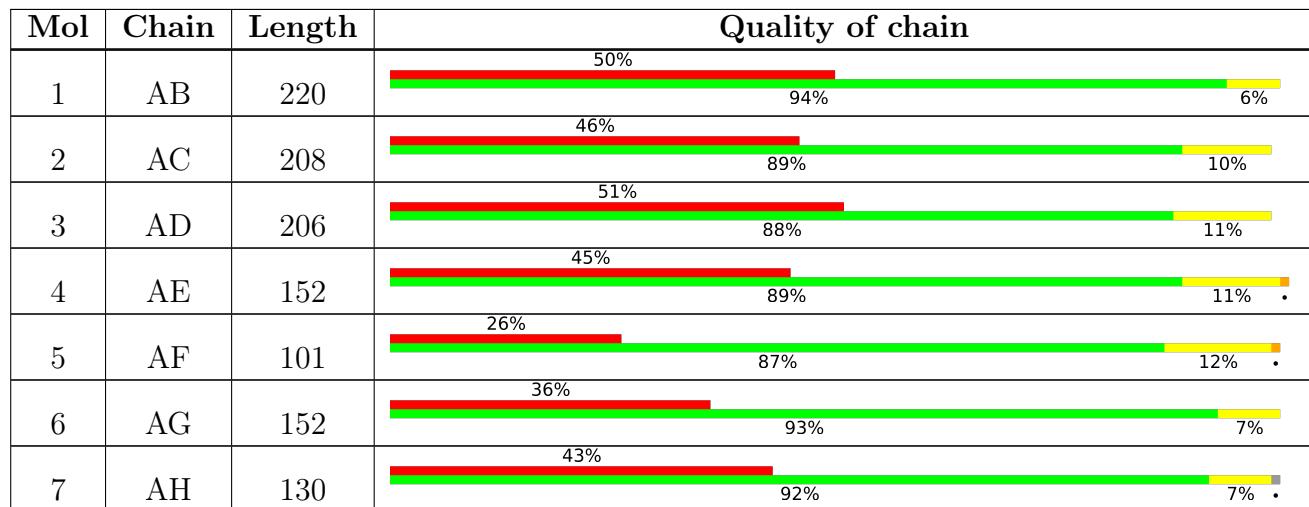
The reported resolution of this entry is 12.00 Å.

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.



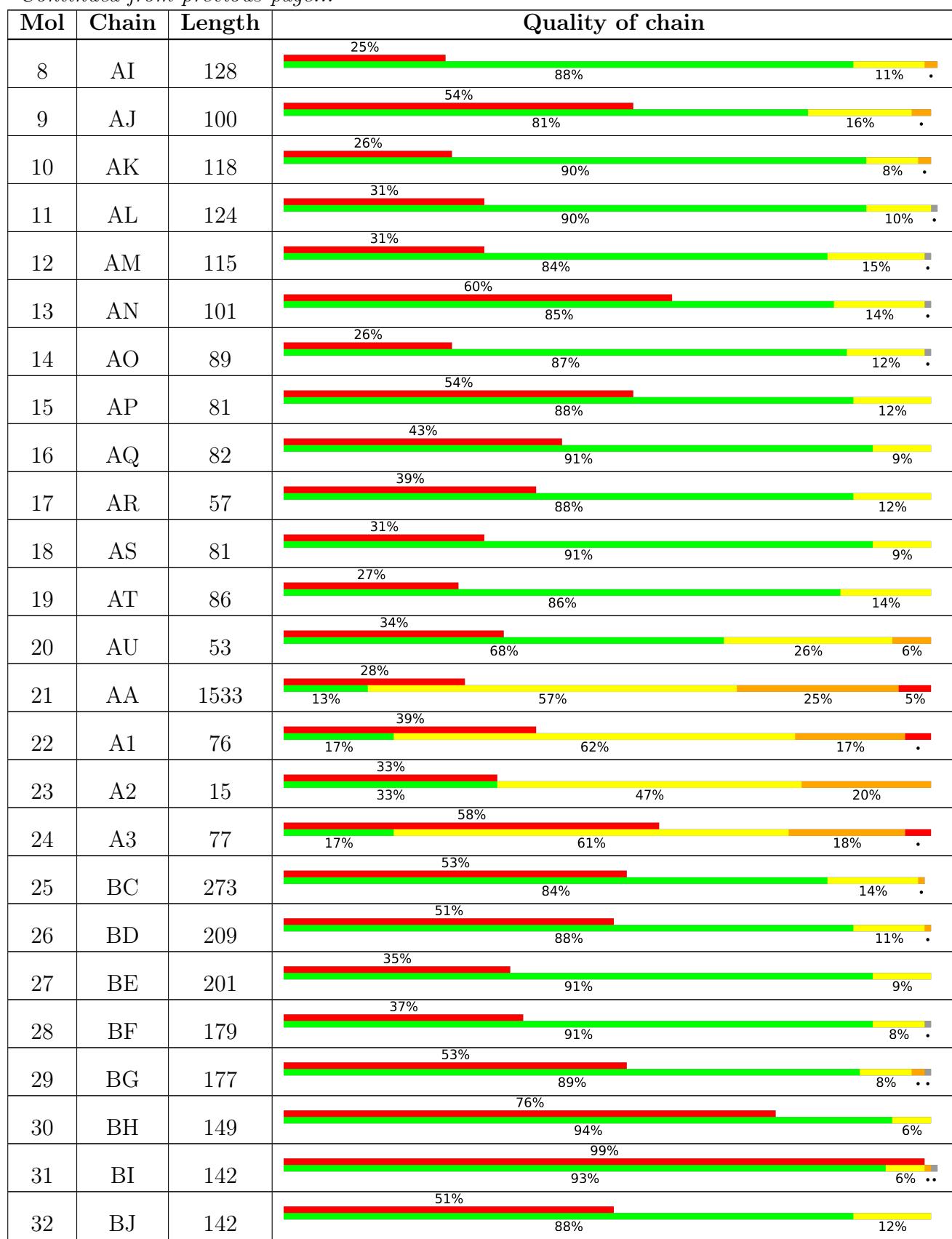
| Metric                | Whole archive (#Entries) | EM structures (#Entries) |
|-----------------------|--------------------------|--------------------------|
| Clashscore            | 158937                   | 4297                     |
| Ramachandran outliers | 154571                   | 4023                     |
| Sidechain outliers    | 154315                   | 3826                     |
| RNA backbone          | 4643                     | 859                      |

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



Continued on next page...

*Continued from previous page...*



*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain |     |       |    |
|-----|-------|--------|------------------|-----|-------|----|
| 33  | BK    | 123    | 51%              | 87% | 11%   | .. |
| 34  | BL    | 144    | 33%              | 81% | 17%   | .. |
| 35  | BM    | 136    | 54%              | 89% | 11%   |    |
| 36  | BN    | 121    | 42%              | 85% | 14%   | .  |
| 37  | BO    | 117    | 11%              | 88% | 11%   | .  |
| 38  | BP    | 115    | 53%              | 84% | 13%   | .. |
| 39  | BQ    | 118    | 43%              | 88% | 10%   | .. |
| 40  | BR    | 103    | 31%              | 89% | 11%   |    |
| 41  | BS    | 110    | 46%              | 90% | 10%   |    |
| 42  | BT    | 94     | 36%              | 89% | 11%   |    |
| 43  | BU    | 104    | 39%              | 91% | 7%    | .. |
| 44  | BV    | 94     | 34%              | 93% | 7%    |    |
| 45  | BW    | 80     | 39%              | 84% | 12%   | .  |
| 46  | BX    | 79     | 49%              | 84% | 13%   | .. |
| 47  | BY    | 63     | 40%              | 92% | 8%    |    |
| 48  | BZ    | 59     | 51%              | 86% | 12%   | .  |
| 49  | B0    | 57     | 23%              | 84% | 12%   | .. |
| 50  | B1    | 52     | 48%              | 83% | 17%   |    |
| 51  | B2    | 46     | 57%              | 74% | 26%   |    |
| 52  | B3    | 65     | 51%              | 91% | 6%    | .. |
| 53  | B4    | 38     | 45%              | 87% | 13%   |    |
| 54  | BA    | 2903   | 35%              | 57% | 26%   | 5% |
| 55  | BB    | 118    | 23%              | 57% | 31%   | .. |
| 56  | B5    | 234    | 60%              | 90% | 5% 5% |    |

## 2 Entry composition (i)

There are 58 unique types of molecules in this entry. The entry contains 147653 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
|     |       |          | Total | C    | N   | O   | S |         |       |
| 1   | AB    | 220      | 1708  | 1083 | 306 | 312 | 7 | 0       | 1     |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment     | Reference  |
|-------|---------|----------|--------|-------------|------------|
| AB    | 7       | ACE      | -      | acetylation | UNP P0A7V0 |
| AB    | 226     | NH2      | -      | amidation   | UNP P0A7V0 |

- Molecule 2 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
|     |       |          | Total | C    | N   | O   | S |         |       |
| 2   | AC    | 207      | 1625  | 1028 | 306 | 288 | 3 | 0       | 1     |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment   | Reference  |
|-------|---------|----------|--------|-----------|------------|
| AC    | 207     | NH2      | -      | amidation | UNP P0A7V3 |

- Molecule 3 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
|     |       |          | Total | C    | N   | O   | S |         |       |
| 3   | AD    | 205      | 1643  | 1026 | 315 | 298 | 4 | 0       | 0     |

- Molecule 4 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 4   | AE    | 152      | 1109  | 689 | 212 | 202 | 6 | 0       | 1     |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment     | Reference  |
|-------|---------|----------|--------|-------------|------------|
| AE    | 8       | ACE      | -      | acetylation | UNP P0A7W1 |
| AE    | 159     | NH2      | -      | amidation   | UNP P0A7W1 |

- Molecule 5 is a protein called 30S ribosomal protein S6.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 5   | AF    | 101      | Total | C   | N   | O   | S       |       |
|     |       |          | 818   | 515 | 149 | 148 | 6       | 0 1   |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment   | Reference  |
|-------|---------|----------|--------|-----------|------------|
| AF    | 101     | NH2      | -      | amidation | UNP P02358 |

- Molecule 6 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 6   | AG    | 152      | Total | C   | N   | O   | S       |       |
|     |       |          | 1178  | 732 | 227 | 215 | 4       | 0 1   |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment     | Reference  |
|-------|---------|----------|--------|-------------|------------|
| AG    | 1       | ACE      | -      | acetylation | UNP P02359 |
| AG    | 152     | NH2      | -      | amidation   | UNP P02359 |

- Molecule 7 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 7   | AH    | 129      | Total | C   | N   | O   | S       |       |
|     |       |          | 979   | 616 | 173 | 184 | 6       | 0 0   |

- Molecule 8 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 8   | AI    | 128      | Total | C   | N   | O   | S       |       |
|     |       |          | 1025  | 636 | 206 | 180 | 3       | 0 0   |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment     | Reference  |
|-------|---------|----------|--------|-------------|------------|
| AI    | 2       | ACE      | -      | acetylation | UNP P0A7X3 |

- Molecule 9 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 9   | AJ    | 100      | 790   | 495 | 151 | 143 | 1 | 0       | 1     |
|     |       |          |       |     |     |     |   |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment     | Reference  |
|-------|---------|----------|--------|-------------|------------|
| AJ    | 4       | ACE      | -      | acetylation | UNP P0A7R5 |
| AJ    | 103     | NH2      | -      | amidation   | UNP P0A7R5 |

- Molecule 10 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 10  | AK    | 118      | 880   | 542 | 174 | 161 | 3 | 0       | 0     |
|     |       |          |       |     |     |     |   |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment     | Reference  |
|-------|---------|----------|--------|-------------|------------|
| AK    | 11      | ACE      | -      | acetylation | UNP P0A7R9 |

- Molecule 11 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 11  | AL    | 123      | 955   | 590 | 196 | 165 | 4 | 0       | 0     |
|     |       |          |       |     |     |     |   |         |       |

- Molecule 12 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 12  | AM    | 114      | 877   | 541 | 178 | 155 | 3 | 0       | 1     |
|     |       |          |       |     |     |     |   |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment   | Reference  |
|-------|---------|----------|--------|-----------|------------|
| AM    | 114     | NH2      | -      | amidation | UNP P0A7S9 |

- Molecule 13 is a protein called 30S ribosomal protein S14.

| Mol | Chain | Residues | Atoms |   |   |   |   | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|-------|
| 13  | AN    | 100      | Total | C | N | O | S | 0       | 0     |

- Molecule 14 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms |   |   |   |   | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|-------|
| 14  | AO    | 88       | Total | C | N | O | S | 0       | 0     |

- Molecule 15 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms |   |   |   |   | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|-------|
| 15  | AP    | 81       | Total | C | N | O | S | 0       | 1     |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment   | Reference  |
|-------|---------|----------|--------|-----------|------------|
| AP    | 81      | NH2      | -      | amidation | UNP P0A7T3 |

- Molecule 16 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms |   |   |   |   | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|-------|
| 16  | AQ    | 82       | Total | C | N | O | S | 0       | 1     |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment     | Reference  |
|-------|---------|----------|--------|-------------|------------|
| AQ    | 2       | ACE      | -      | acetylation | UNP P0AG63 |
| AQ    | 83      | NH2      | -      | amidation   | UNP P0AG63 |

- Molecule 17 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms |   |   |   |  | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|--|---------|-------|
| 17  | AR    | 57       | Total | C | N | O |  | 0       | 1     |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment     | Reference  |
|-------|---------|----------|--------|-------------|------------|
| AR    | 18      | ACE      | -      | acetylation | UNP P0A7T7 |

*Continued on next page...*

*Continued from previous page...*

| Chain | Residue | Modelled | Actual | Comment   | Reference  |
|-------|---------|----------|--------|-----------|------------|
| AR    | 74      | NH2      | -      | amidation | UNP P0A7T7 |

- Molecule 18 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | AS    | 81       | Total | C   | N   | O   | S | 0       | 1     |
|     |       |          | 641   | 410 | 121 | 108 | 2 |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment     | Reference  |
|-------|---------|----------|--------|-------------|------------|
| AS    | 1       | ACE      | -      | acetylation | UNP P0A7U3 |
| AS    | 81      | NH2      | -      | amidation   | UNP P0A7U3 |

- Molecule 19 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | AT    | 86       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 668   | 413 | 137 | 115 | 3 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment     | Reference  |
|-------|---------|----------|--------|-------------|------------|
| AT    | 1       | ACE      | -      | acetylation | UNP P0A7U7 |

- Molecule 20 is a protein called 30S ribosomal protein S21.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 20  | AU    | 53       | Total | C   | N  | O  | S | 0       | 1     |
|     |       |          | 429   | 267 | 87 | 74 | 1 |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment     | Reference  |
|-------|---------|----------|--------|-------------|------------|
| AU    | 2       | ACE      | -      | acetylation | UNP P68679 |
| AU    | 54      | NH2      | -      | amidation   | UNP P68679 |

- Molecule 21 is a RNA chain called 16S ribosomal RNA.

| Mol | Chain | Residues | Atoms |   |   |   |   | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|-------|
| 21  | AA    | 1530     | Total | C | N | O | P | 0       | 0     |

- Molecule 22 is a RNA chain called fMet-Val-tRNA-Val.

| Mol | Chain | Residues | Atoms |   |   |   |   | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|-------|
| 22  | A1    | 76       | Total | C | N | O | P | S       | 0     |

- Molecule 23 is a RNA chain called 5'-R(\*AP\*CP\*UP\*AP\*UP\*GP\*GP\*UP\*UP\*UP\*UP\*U P\*AP\*UP\*U)-3'.

| Mol | Chain | Residues | Atoms |   |   |   |   | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|-------|
| 23  | A2    | 15       | Total | C | N | O | P |         | 0     |

- Molecule 24 is a RNA chain called tRNA-fMet.

| Mol | Chain | Residues | Atoms |   |   |   |   | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|-------|
| 24  | A3    | 77       | Total | C | N | O | P | S       | 0     |

- Molecule 25 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms |   |   |   |   | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|-------|
| 25  | BC    | 272      | Total | C | N | O | P | S       | 0     |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment   | Reference  |
|-------|---------|----------|--------|-----------|------------|
| BC    | 272     | NH2      | -      | amidation | UNP P60422 |

- Molecule 26 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |   |   |   |   | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|-------|
| 26  | BD    | 209      | Total | C | N | O | S |         | 0     |

- Molecule 27 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms   |     |     |     | AltConf | Trace |
|-----|-------|----------|---------|-----|-----|-----|---------|-------|
| 27  | BE    | 201      | Total C | N   | O   | S   | 0       | 0     |
|     |       |          | 1552    | 974 | 283 | 290 | 5       |       |

- Molecule 28 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms   |     |     |     | AltConf | Trace |
|-----|-------|----------|---------|-----|-----|-----|---------|-------|
| 28  | BF    | 178      | Total C | N   | O   | S   | 0       | 0     |
|     |       |          | 1420    | 905 | 251 | 258 | 6       |       |

- Molecule 29 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms   |     |     |     | AltConf | Trace |
|-----|-------|----------|---------|-----|-----|-----|---------|-------|
| 29  | BG    | 176      | Total C | N   | O   | S   | 0       | 0     |
|     |       |          | 1323    | 832 | 243 | 246 | 2       |       |

- Molecule 30 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms   |     |     |     | AltConf | Trace |
|-----|-------|----------|---------|-----|-----|-----|---------|-------|
| 30  | BH    | 149      | Total C | N   | O   | S   | 0       | 0     |
|     |       |          | 1111    | 699 | 197 | 214 | 1       |       |

- Molecule 31 is a protein called 50S ribosomal protein L11.

| Mol | Chain | Residues | Atoms   |     |     |     | AltConf | Trace |
|-----|-------|----------|---------|-----|-----|-----|---------|-------|
| 31  | BI    | 141      | Total C | N   | O   | S   | 0       | 0     |
|     |       |          | 1032    | 651 | 179 | 196 | 6       |       |

- Molecule 32 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms   |     |     |     | AltConf | Trace |
|-----|-------|----------|---------|-----|-----|-----|---------|-------|
| 32  | BJ    | 142      | Total C | N   | O   | S   | 0       | 0     |
|     |       |          | 1129    | 714 | 212 | 199 | 4       |       |

- Molecule 33 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms   |     |     |     | AltConf | Trace |
|-----|-------|----------|---------|-----|-----|-----|---------|-------|
| 33  | BK    | 123      | Total C | N   | O   | S   | 0       | 1     |
|     |       |          | 939     | 587 | 181 | 165 | 6       |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment   | Reference  |
|-------|---------|----------|--------|-----------|------------|
| BK    | 123     | NH2      | -      | amidation | UNP P0ADY3 |

- Molecule 34 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms |   |   |   |   | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|-------|
| 34  | BL    | 143      | Total | C | N | O | S | 0       | 0     |

1045    649    206    189    1

- Molecule 35 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms |   |   |   |   | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|-------|
| 35  | BM    | 136      | Total | C | N | O | S | 0       | 0     |

1074    686    205    177    6

- Molecule 36 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms |   |   |   |   | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|-------|
| 36  | BN    | 121      | Total | C | N | O | S | 0       | 1     |

961    593    197    166    5

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment   | Reference  |
|-------|---------|----------|--------|-----------|------------|
| BN    | 121     | NH2      | -      | amidation | UNP P0AG44 |

- Molecule 37 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms |   |   |   |  | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|--|---------|-------|
| 37  | BO    | 116      | Total | C | N | O |  | 0       | 0     |

892    552    178    162

- Molecule 38 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms |   |   |   |   | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|-------|
| 38  | BP    | 114      | Total | C | N | O | S | 0       | 0     |

917    574    179    163    1

- Molecule 39 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms |   |   |   |  | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|--|---------|-------|
| 39  | BQ    | 117      | Total | C | N | O |  | 0       | 0     |

947    604    192    151

- Molecule 40 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40  | BR    | 103      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 816   | 516 | 153 | 145 | 2 |         |       |

- Molecule 41 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 41  | BS    | 110      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 857   | 532 | 166 | 156 | 3 |         |       |

- Molecule 42 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 42  | BT    | 94       | Total | C   | N   | O   | S | 0       | 1     |
|     |       |          | 739   | 466 | 140 | 131 | 2 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment   | Reference  |
|-------|---------|----------|--------|-----------|------------|
| BT    | 94      | NH2      | -      | amidation | UNP P0ADZ0 |

- Molecule 43 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 43  | BU    | 103      | Total | C   | N   | O   | 0 | 1       |       |
|     |       |          | 780   | 492 | 147 | 141 |   |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment   | Reference  |
|-------|---------|----------|--------|-----------|------------|
| BU    | 103     | NH2      | -      | amidation | UNP P60624 |

- Molecule 44 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 44  | BV    | 94       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 753   | 479 | 137 | 134 | 3 |         |       |

- Molecule 45 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |   |   |   |   | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|-------|
| 45  | BW    | 80       | Total | C | N | O | S | 0       | 0     |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment     | Reference  |
|-------|---------|----------|--------|-------------|------------|
| BW    | 5       | ACE      | -      | acetylation | UNP P0A7L8 |

- Molecule 46 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms |   |   |   |   | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|-------|
| 46  | BX    | 77       | Total | C | N | O | S | 0       | 0     |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment     | Reference  |
|-------|---------|----------|--------|-------------|------------|
| BX    | -1      | ACE      | -      | acetylation | UNP P0A7M2 |

- Molecule 47 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms |   |   |   |   | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|-------|
| 47  | BY    | 63       | Total | C | N | O | S | 0       | 0     |

- Molecule 48 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms |   |   |   |   | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|-------|
| 48  | BZ    | 58       | Total | C | N | O | S | 0       | 0     |

- Molecule 49 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |   |   |   |   | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|-------|
| 49  | B0    | 56       | Total | C | N | O | S | 0       | 0     |

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

| Mol | Chain | Residues | Atoms |   |   |   |  | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|--|---------|-------|
| 50  | B1    | 52       | Total | C | N | O |  | 0       | 1     |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment     | Reference  |
|-------|---------|----------|--------|-------------|------------|
| B1    | 2       | ACE      | -      | acetylation | UNP P0A7N9 |
| B1    | 53      | NH2      | -      | amidation   | UNP P0A7N9 |

- Molecule 51 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 51  | B2    | 46       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 377   | 228 | 90 | 57 | 2 |         |       |

- Molecule 52 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 52  | B3    | 64       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 504   | 323 | 105 | 74 | 2 |         |       |

- Molecule 53 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 53  | B4    | 38       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 302   | 185 | 65 | 48 | 4 |         |       |

- Molecule 54 is a RNA chain called 23S ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 54  | BA    | 2903     | Total | C     | N     | O     | P    | 0       | 0     |
|     |       |          | 62317 | 27801 | 11467 | 20147 | 2902 |         |       |

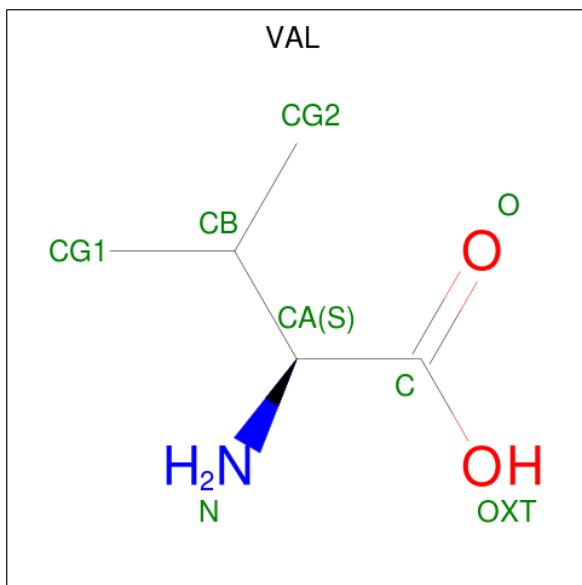
- Molecule 55 is a RNA chain called 5S ribosomal RNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 55  | BB    | 117      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 2504  | 1116 | 459 | 813 | 116 |         |       |

- Molecule 56 is a protein called 50S ribosomal protein L1.

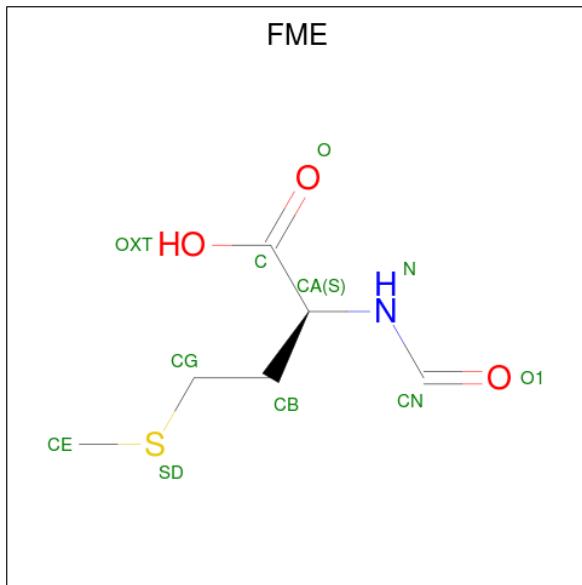
| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 56  | B5    | 223      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1658  | 1038 | 302 | 312 | 6 |         |       |

- Molecule 57 is VALINE (three-letter code: VAL) (formula: C<sub>5</sub>H<sub>11</sub>NO<sub>2</sub>).



| Mol | Chain | Residues | Atoms |   |   |   | AltConf |
|-----|-------|----------|-------|---|---|---|---------|
|     |       |          | Total | C | N | O |         |
| 57  | A1    | 1        | 7     | 5 | 1 | 1 | 0       |

- Molecule 58 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: C<sub>6</sub>H<sub>11</sub>NO<sub>3</sub>S).



| Mol | Chain | Residues | Atoms |   |   |   | AltConf |
|-----|-------|----------|-------|---|---|---|---------|
|     |       |          | Total | C | N | O | S       |
| 58  | BA    | 1        | 10    | 6 | 1 | 2 | 1       |

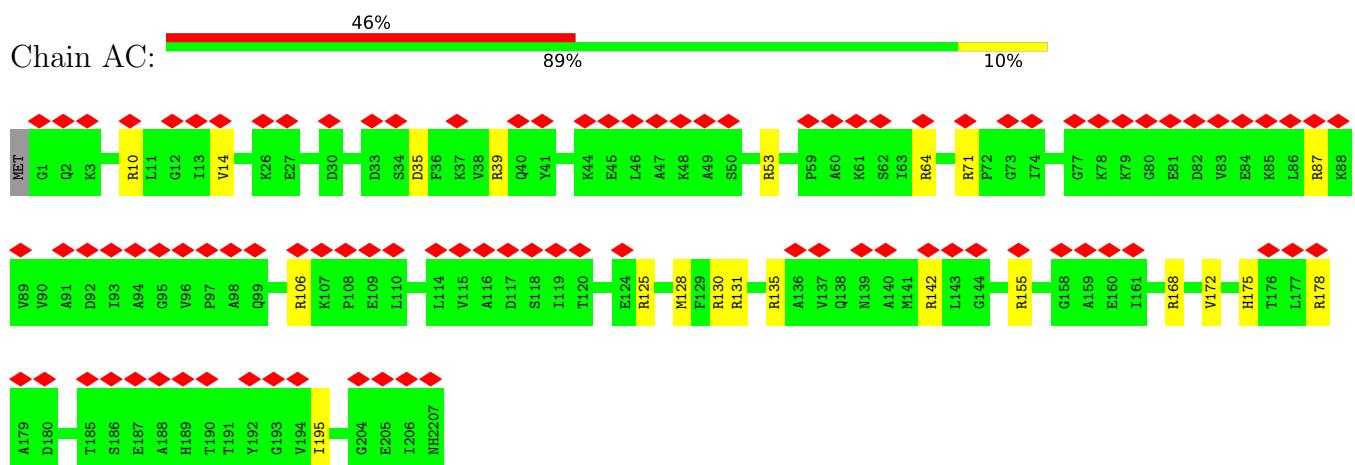
### 3 Residue-property plots [\(i\)](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

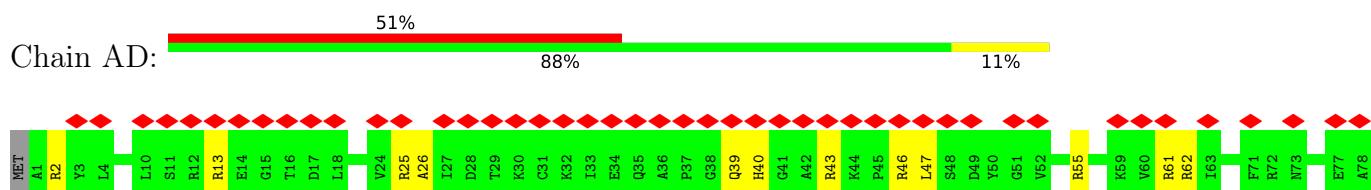
- Molecule 1: 30S ribosomal protein S2

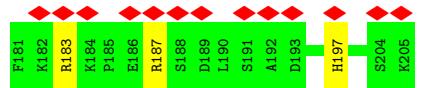


- Molecule 2: 30S ribosomal protein S3

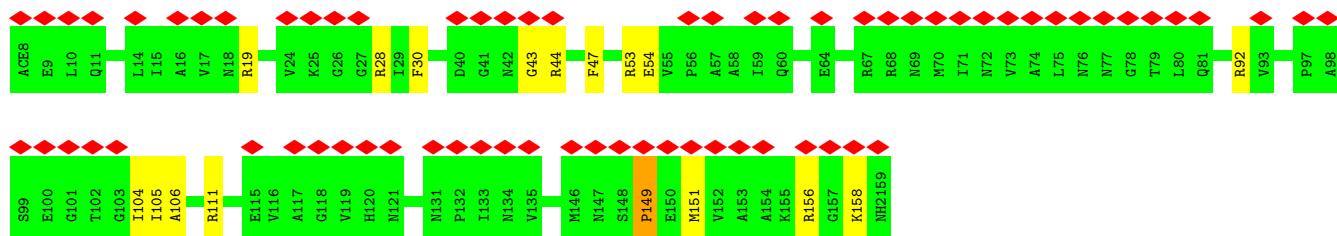
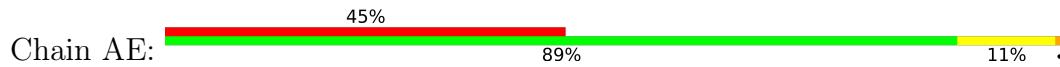


- Molecule 3: 30S ribosomal protein S4

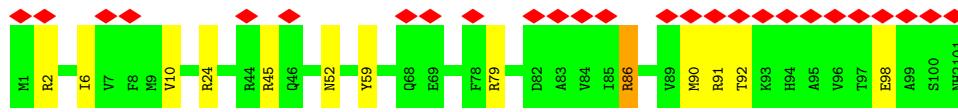




- Molecule 4: 30S ribosomal protein S5



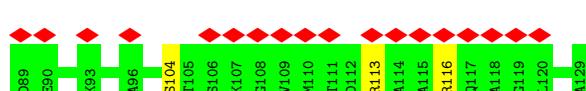
- Molecule 5: 30S ribosomal protein S6



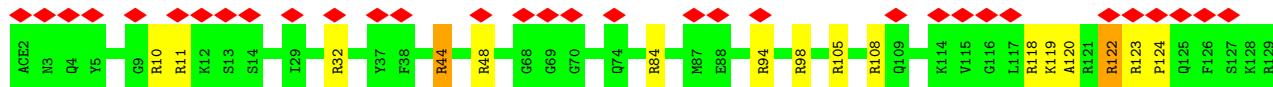
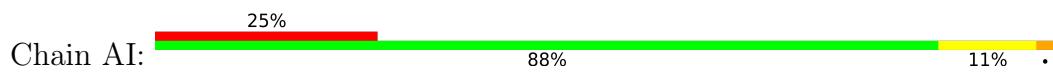
- Molecule 6: 30S ribosomal protein S7



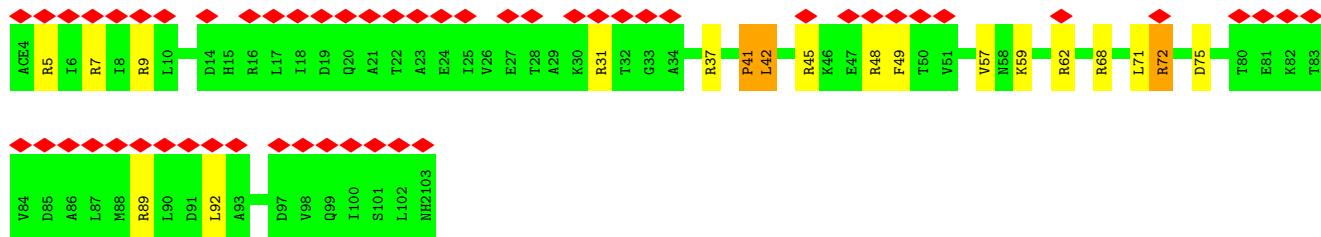
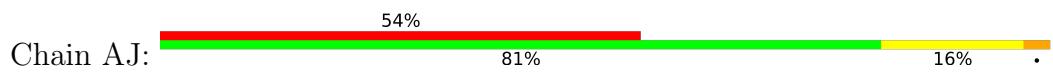
- Molecule 7: 30S ribosomal protein S8



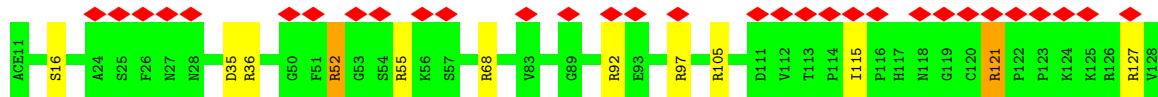
- Molecule 8: 30S ribosomal protein S9



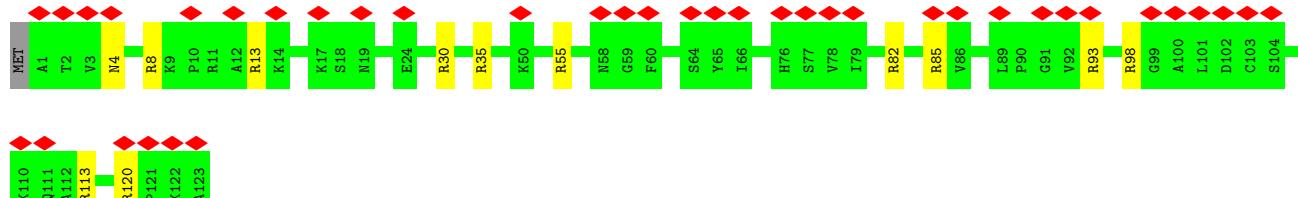
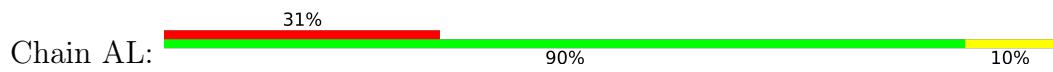
- Molecule 9: 30S ribosomal protein S10



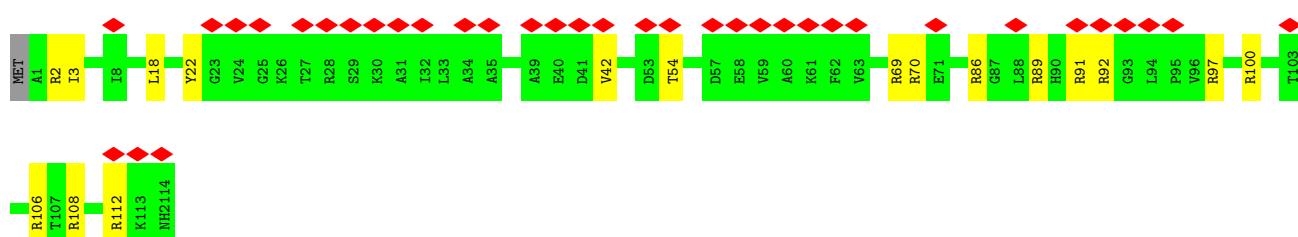
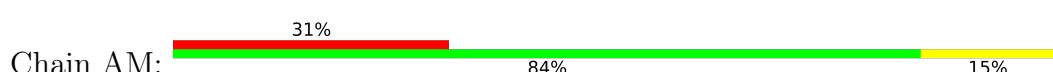
- Molecule 10: 30S ribosomal protein S11



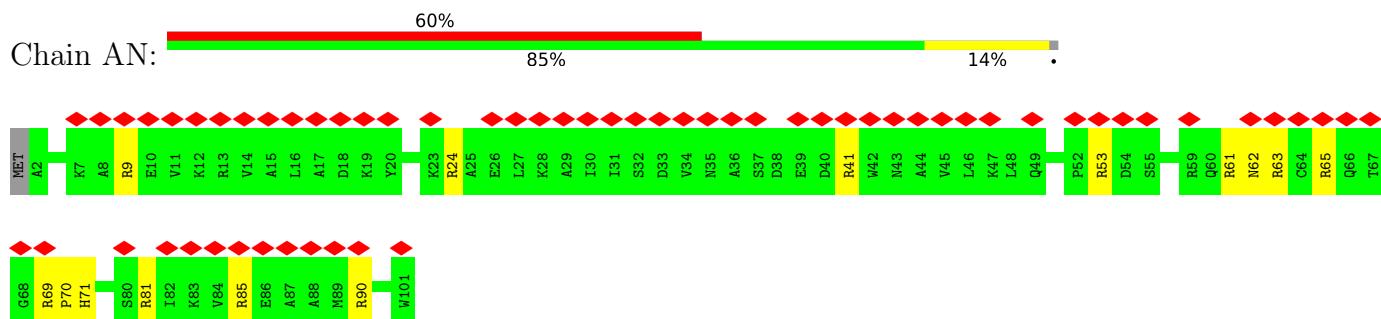
- Molecule 11: 30S ribosomal protein S12



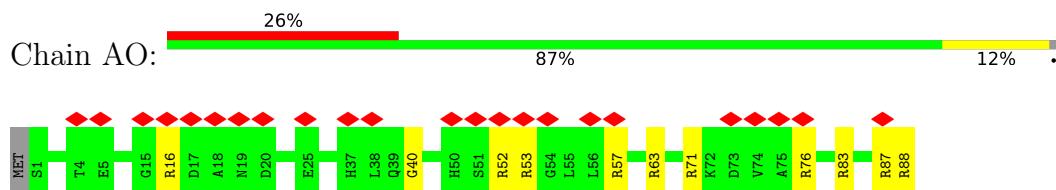
- Molecule 12: 30S ribosomal protein S13



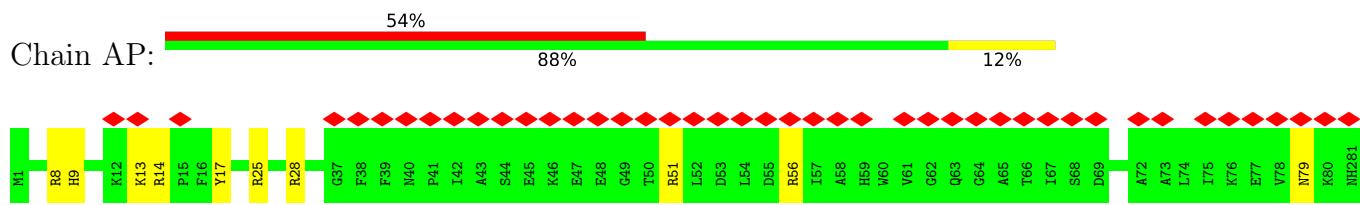
- Molecule 13: 30S ribosomal protein S14



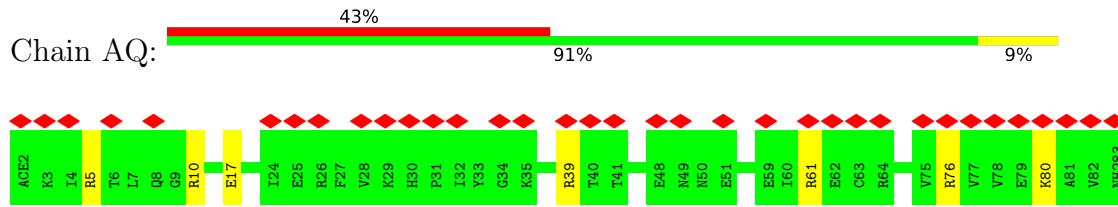
- Molecule 14: 30S ribosomal protein S15



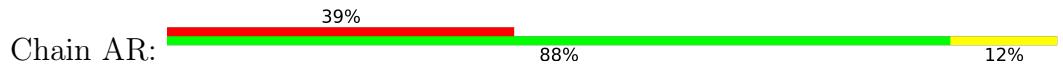
- Molecule 15: 30S ribosomal protein S16



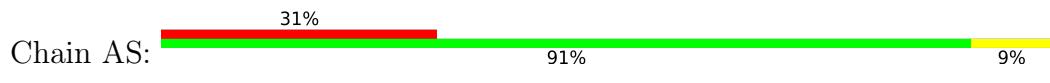
- Molecule 16: 30S ribosomal protein S17



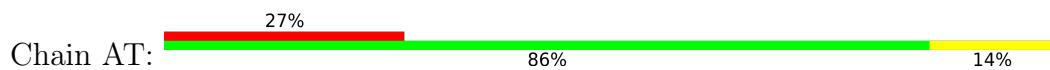
- Molecule 17: 30S ribosomal protein S18



- Molecule 18: 30S ribosomal protein S19



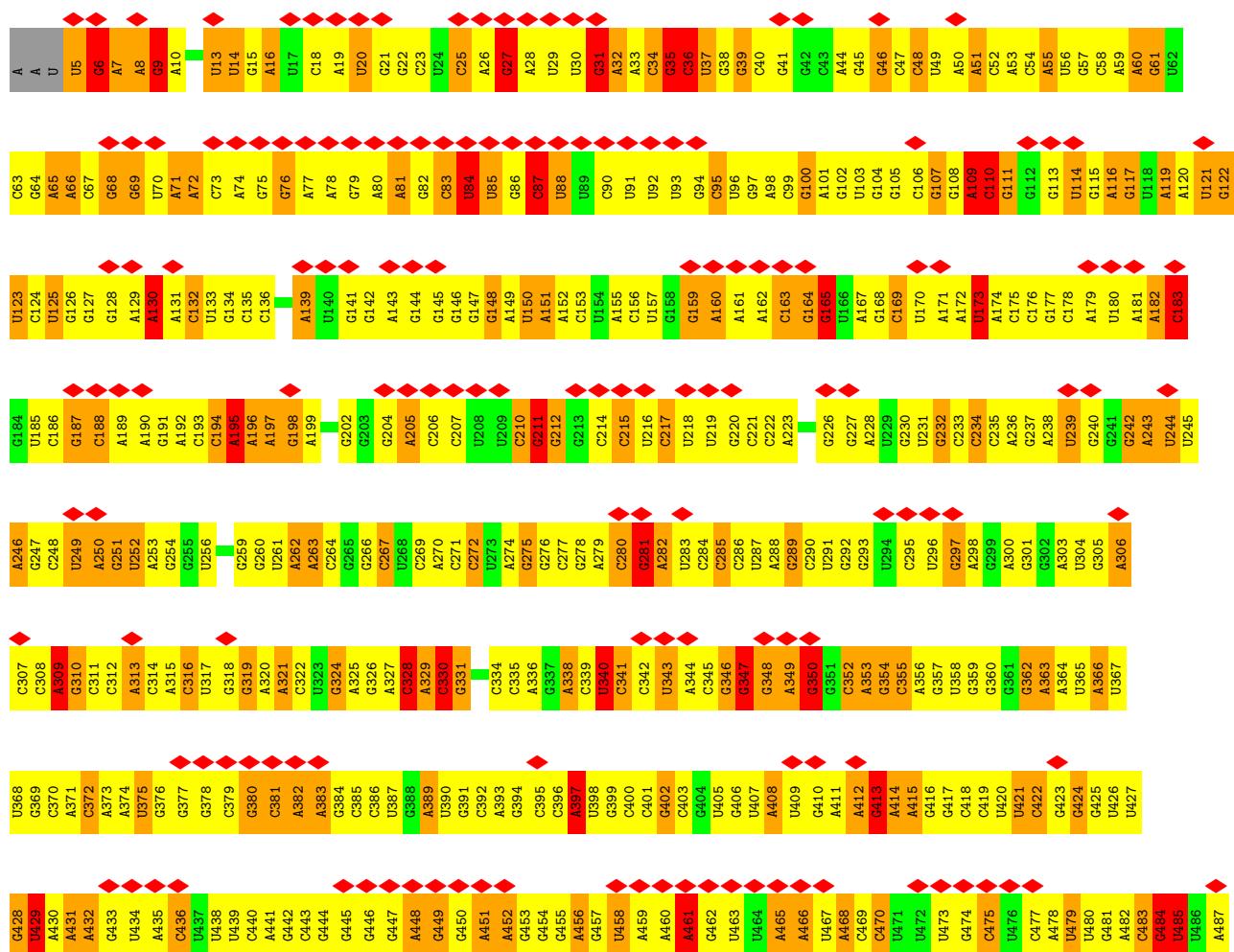
- Molecule 19: 30S ribosomal protein S20



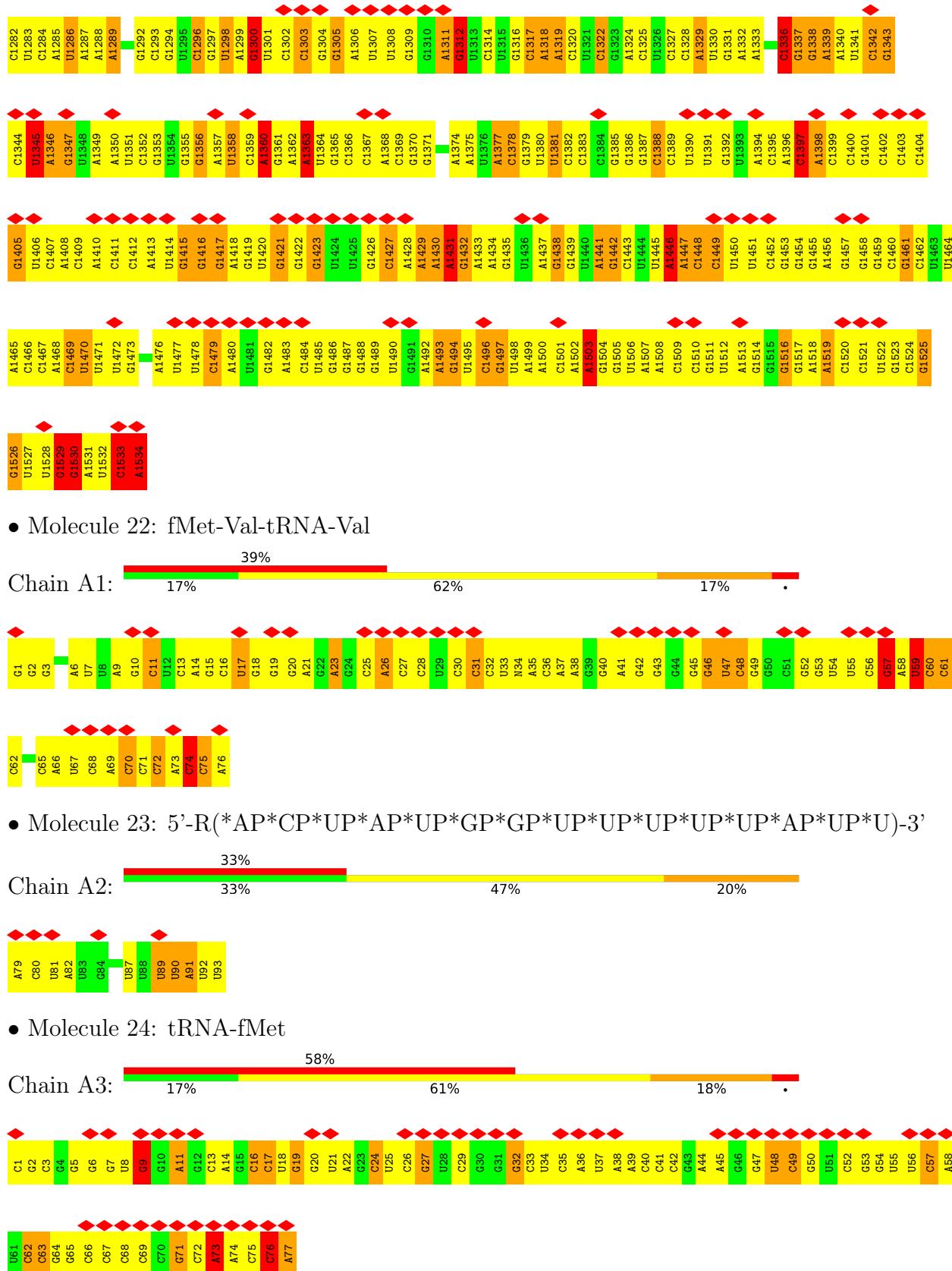
- Molecule 20: 30S ribosomal protein S21

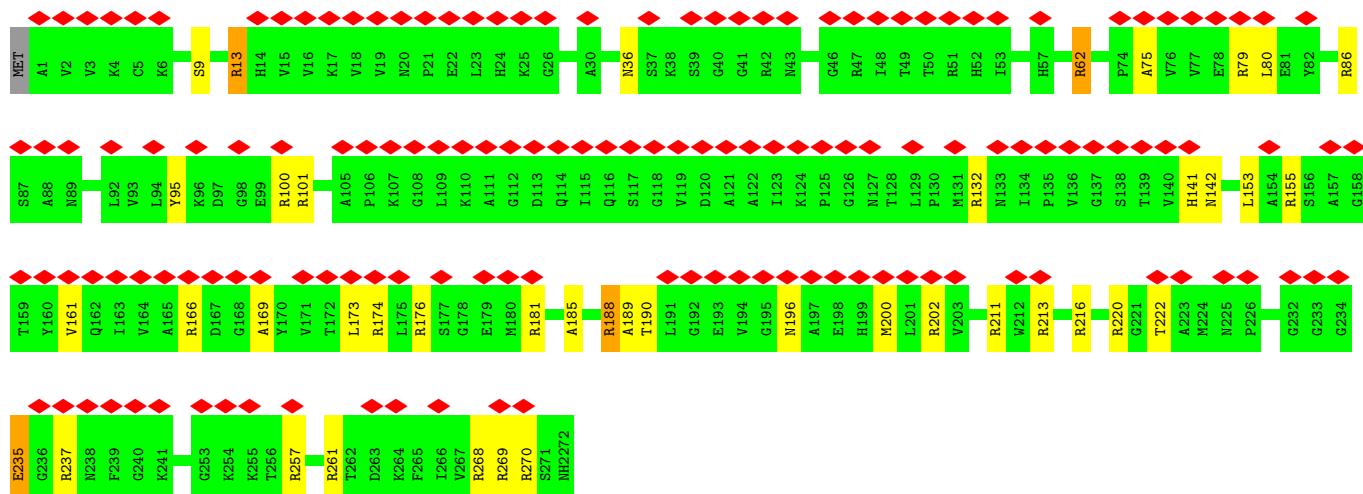
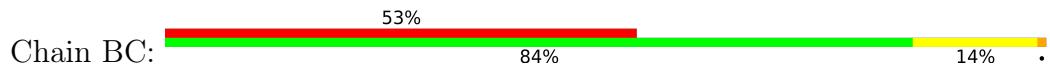


- Molecule 21: 16S ribosomal RNA

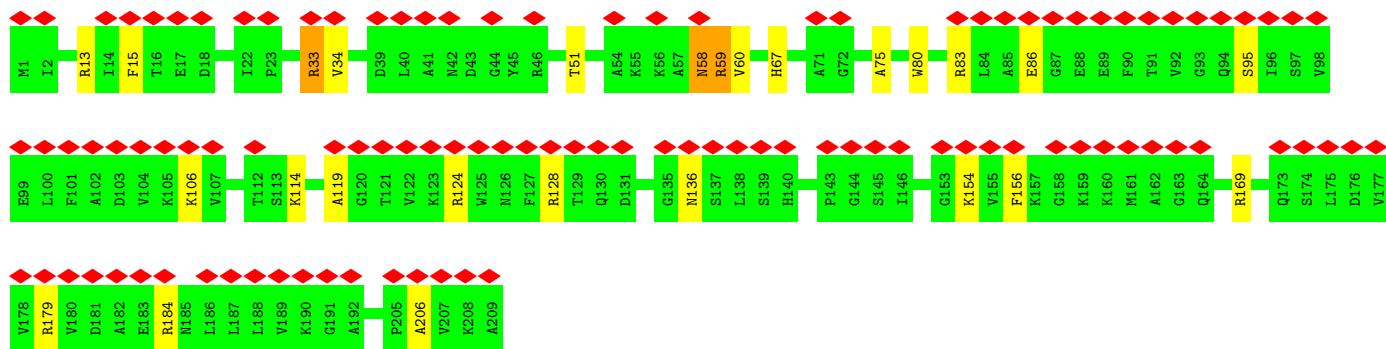
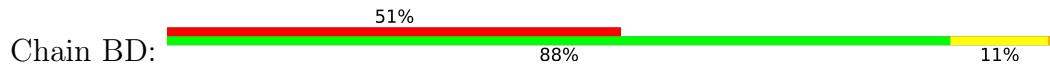




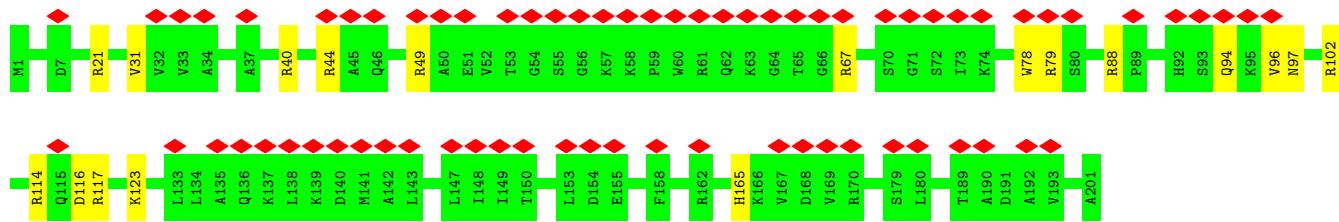




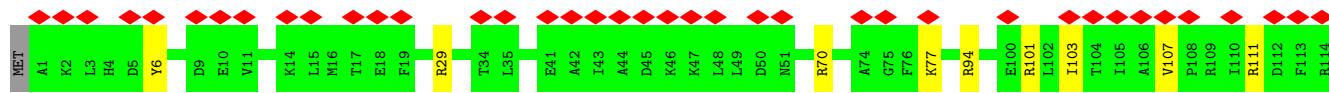
- Molecule 26: 50S ribosomal protein L3



- Molecule 27: 50S ribosomal protein L4

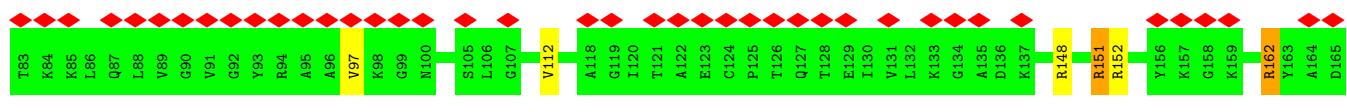


- Molecule 28: 50S ribosomal protein L5

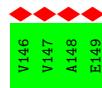
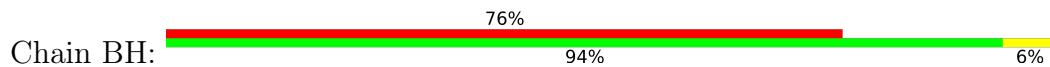




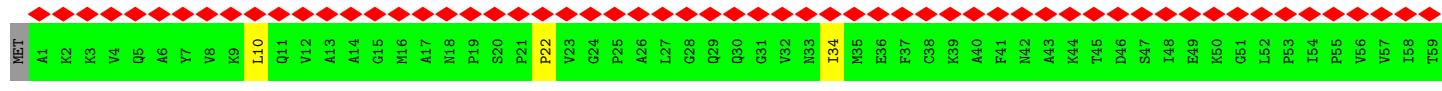
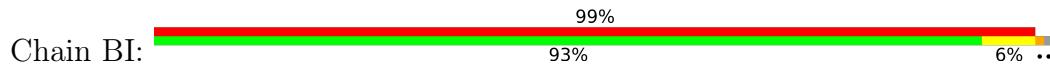
- Molecule 29: 50S ribosomal protein L6



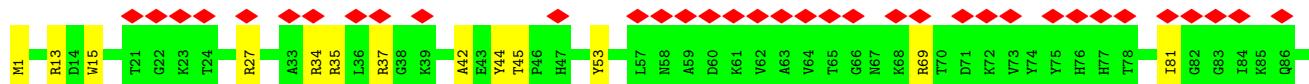
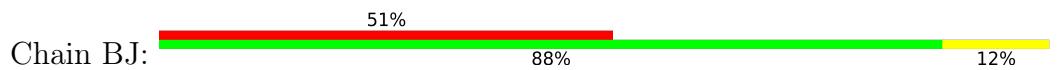
- Molecule 30: 50S ribosomal protein L9



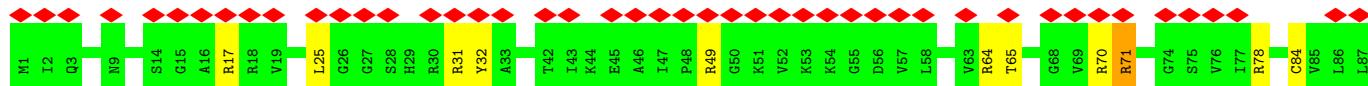
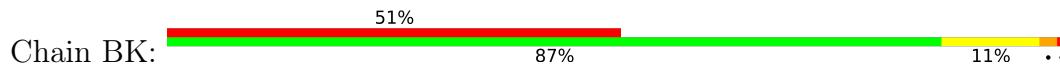
- Molecule 31: 50S ribosomal protein L11



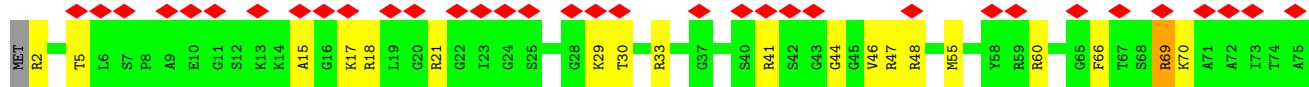
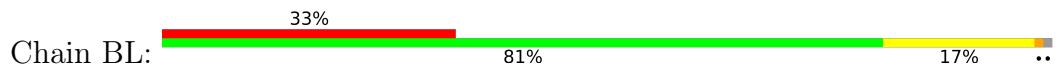
- Molecule 32: 50S ribosomal protein L13



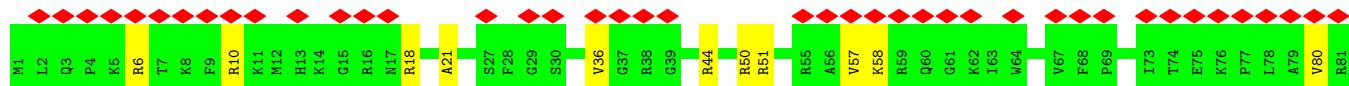
- Molecule 33: 50S ribosomal protein L14



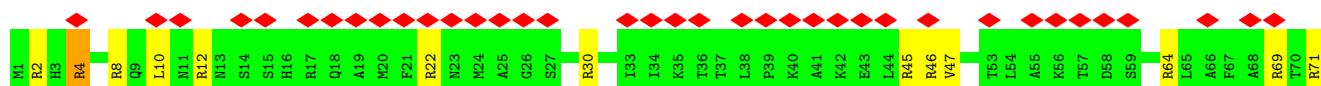
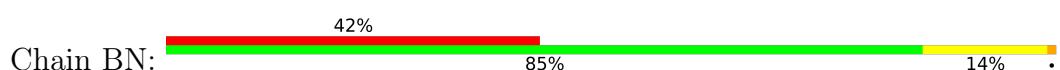
- Molecule 34: 50S ribosomal protein L15



- Molecule 35: 50S ribosomal protein L16

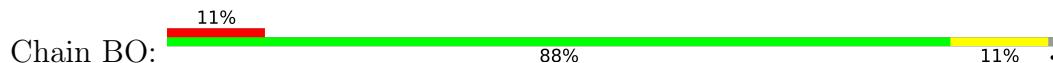


- Molecule 36: 50S ribosomal protein L17

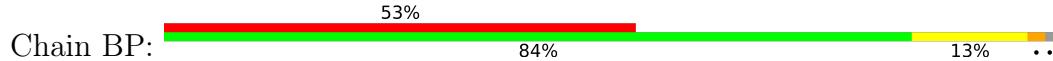




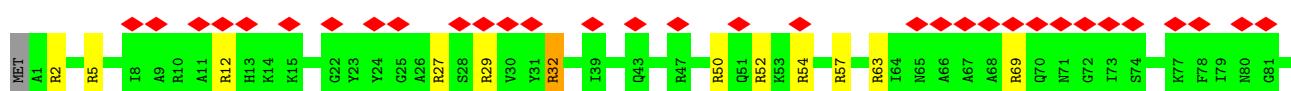
- Molecule 37: 50S ribosomal protein L18



- Molecule 38: 50S ribosomal protein L19



- Molecule 39: 50S ribosomal protein L20



- Molecule 40: 50S ribosomal protein L21

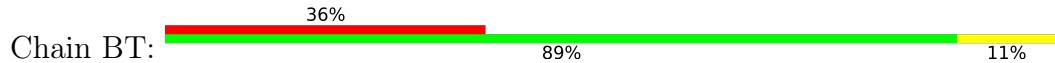


- Molecule 41: 50S ribosomal protein L22

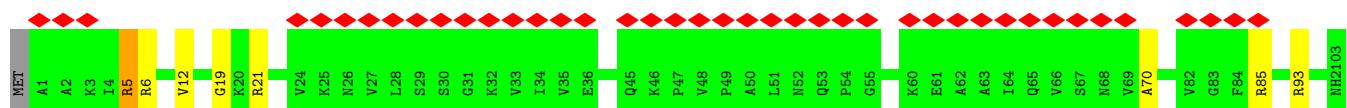
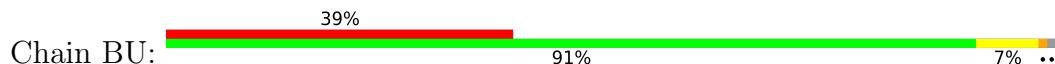




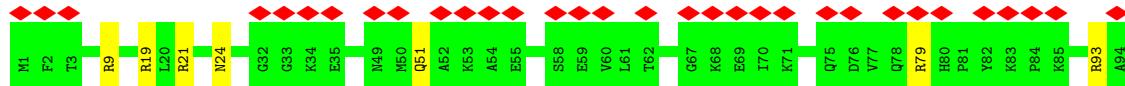
- Molecule 42: 50S ribosomal protein L23



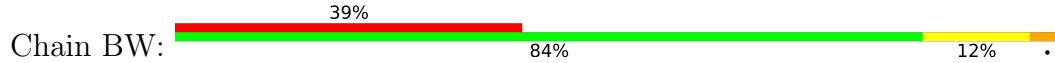
- Molecule 43: 50S ribosomal protein L24



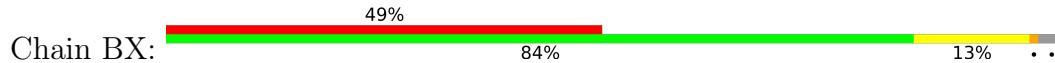
- Molecule 44: 50S ribosomal protein L25



- Molecule 45: 50S ribosomal protein L27



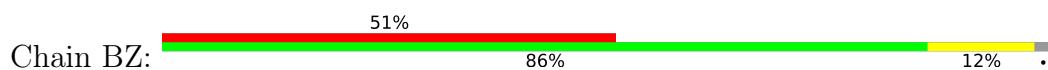
- Molecule 46: 50S ribosomal protein L28



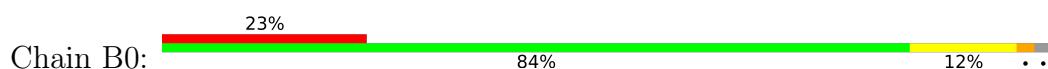
- Molecule 47: 50S ribosomal protein L29



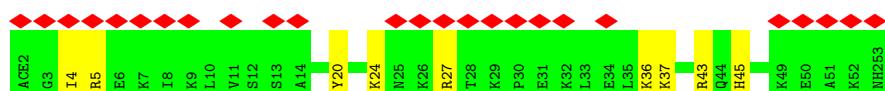
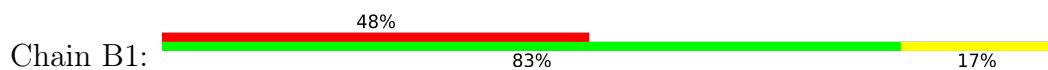
- Molecule 48: 50S ribosomal protein L30



- Molecule 49: 50S ribosomal protein L32



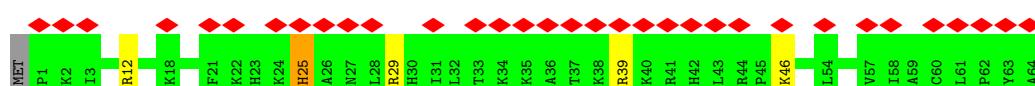
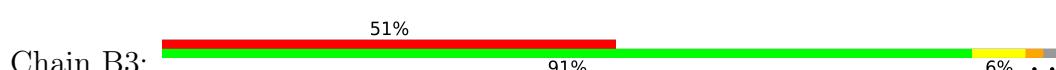
- Molecule 50: 50S ribosomal protein L33



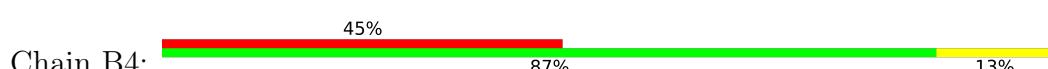
- Molecule 51: 50S ribosomal protein L34



- Molecule 52: 50S ribosomal protein L35



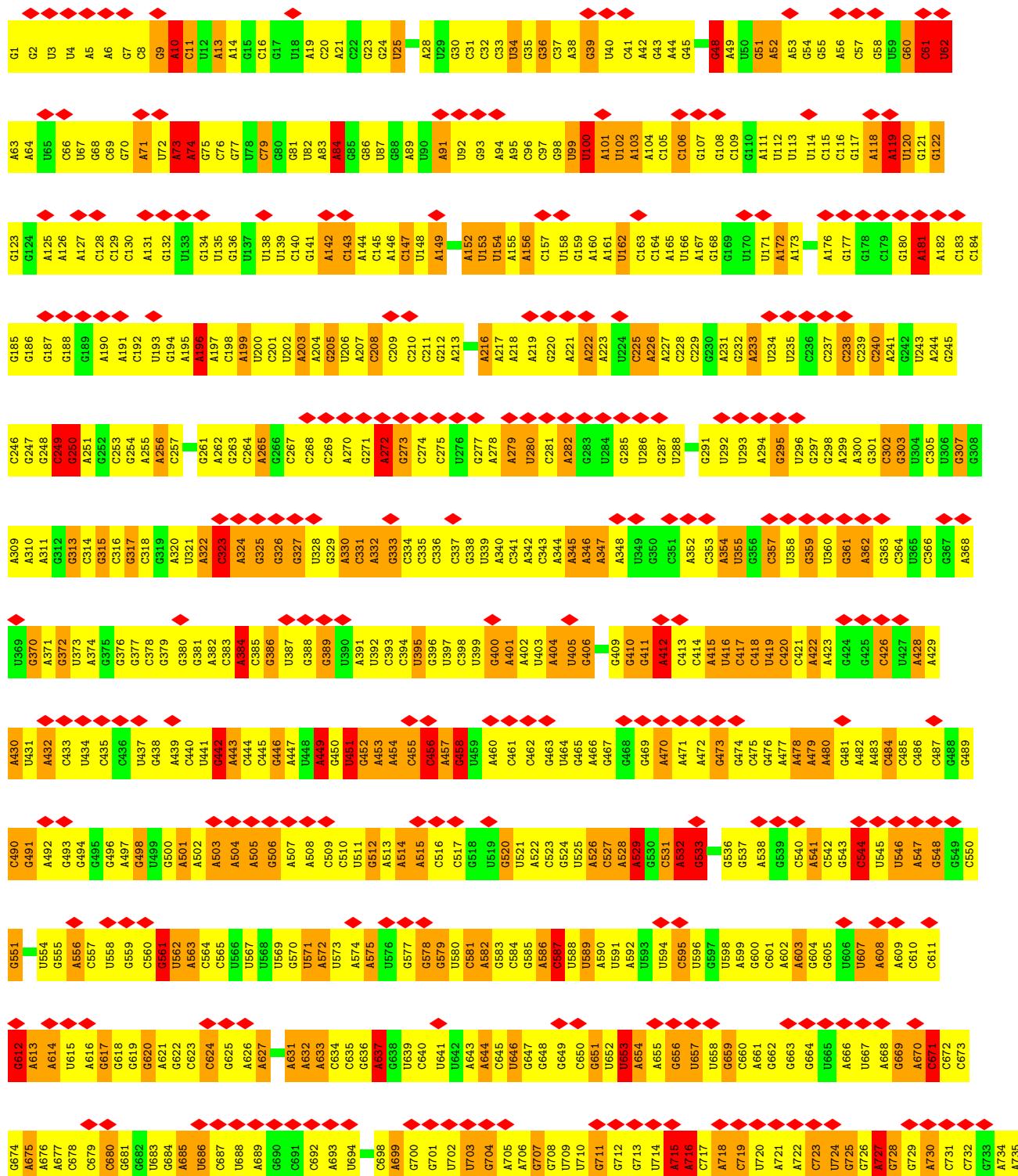
- Molecule 53: 50S ribosomal protein L36

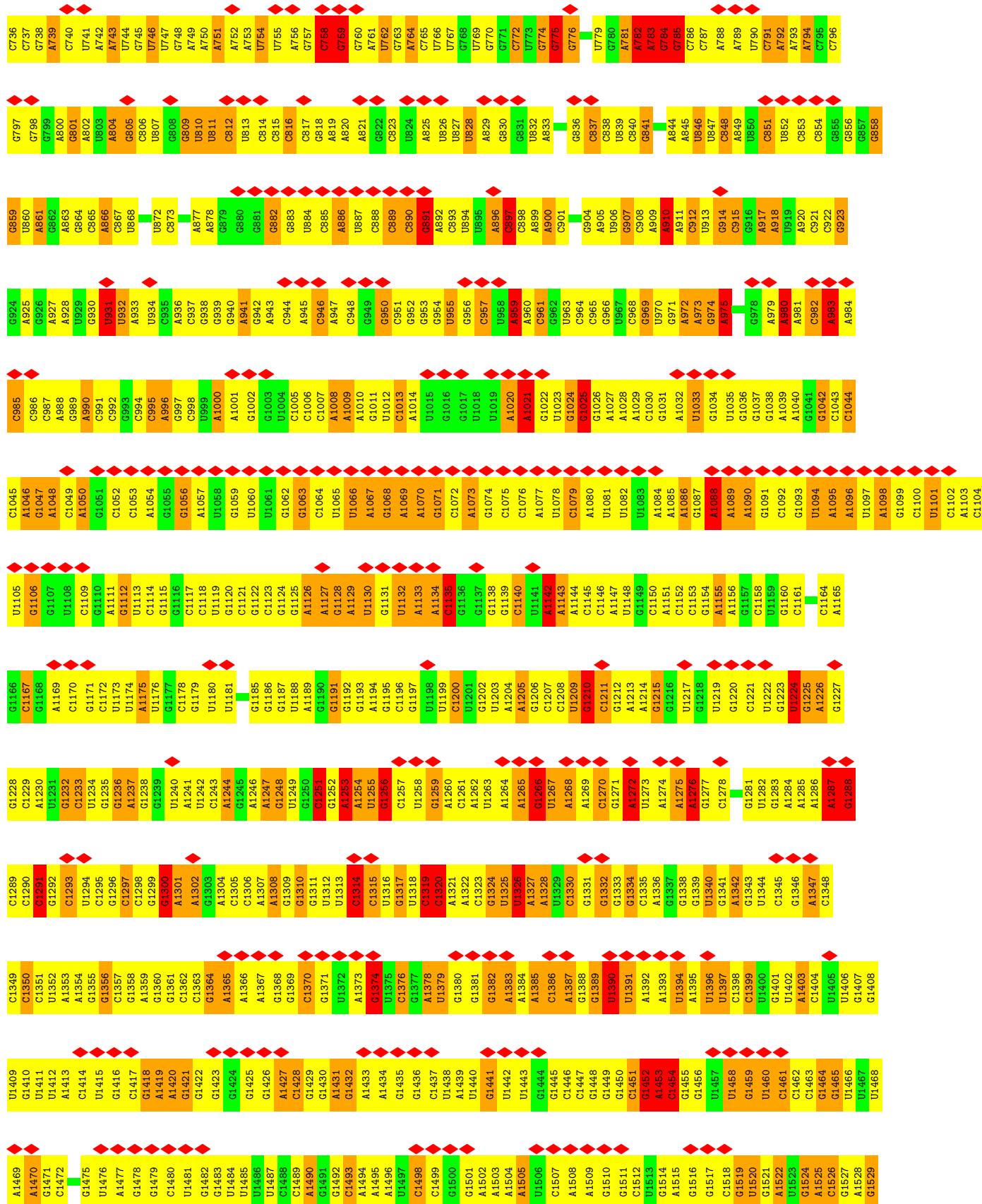


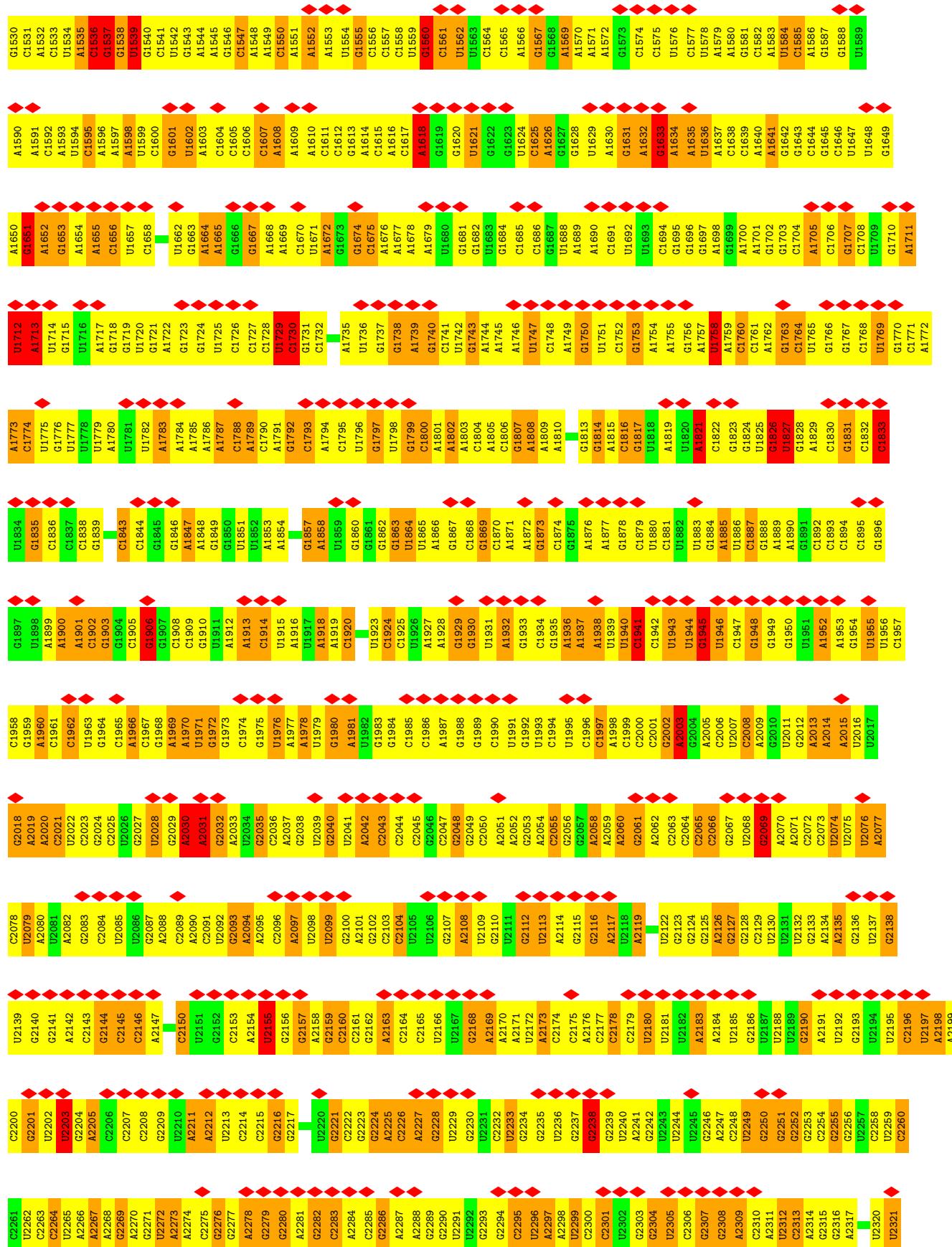


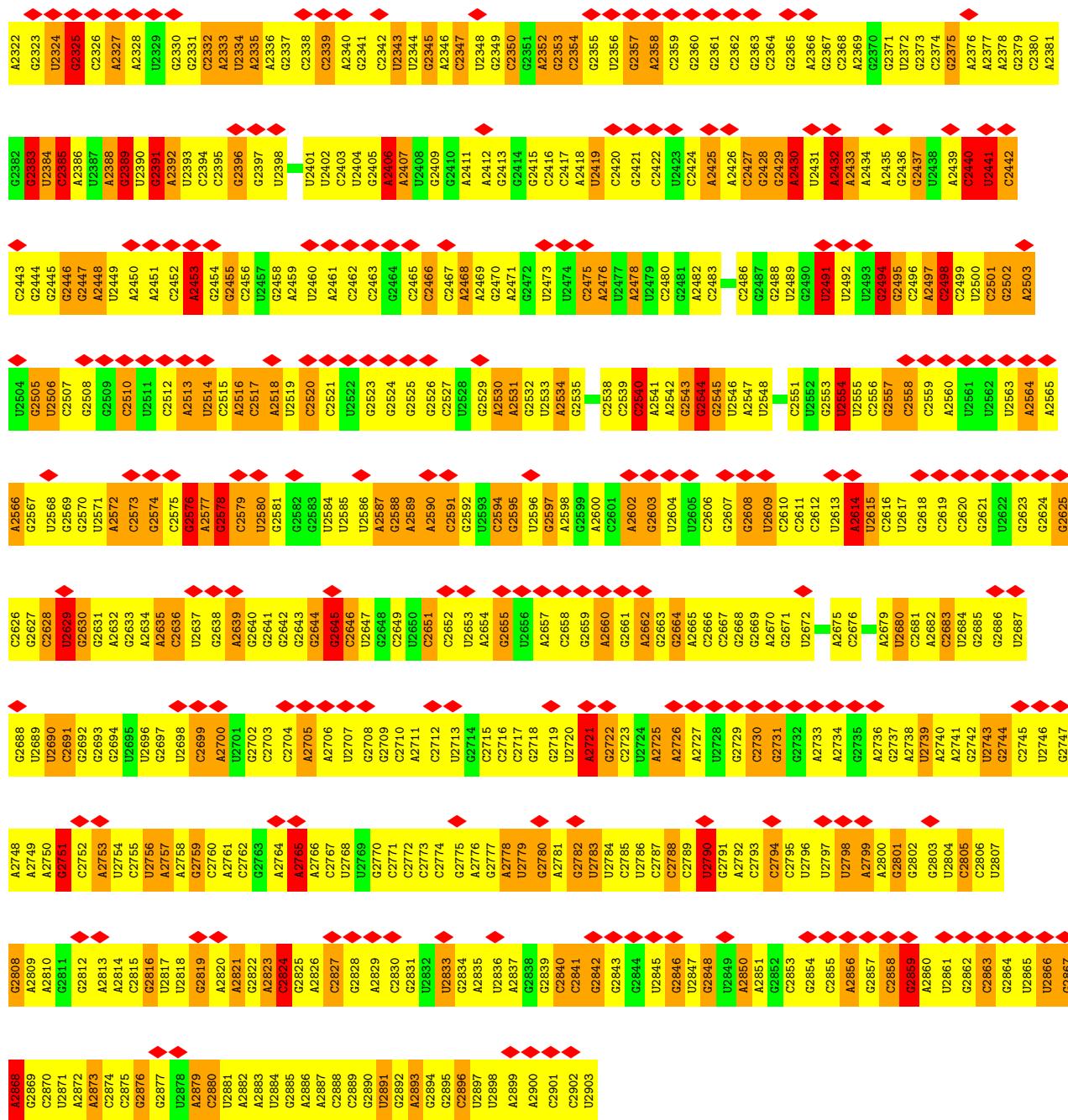
- Molecule 54: 23S ribosomal RNA

Chain BA: 13% 35% 57% 26% 5%



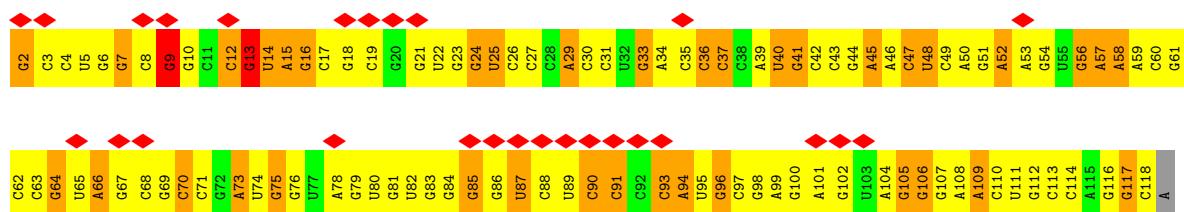






- Molecule 55: 5S ribosomal RNA

Chain BB: 9% 23% 57% 31% :.



- Molecule 56: 50S ribosomal protein L1



## 4 Experimental information i

| Property                             | Value                   | Source    |
|--------------------------------------|-------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE         | Depositor |
| Imposed symmetry                     | POINT, C1               | Depositor |
| Number of particles used             | 13091                   | Depositor |
| Resolution determination method      | FSC 0.5 CUT-OFF         | Depositor |
| CTF correction method                | Not provided            |           |
| Microscope                           | FEI/PHILIPS CM200FEG    | Depositor |
| Voltage (kV)                         | 160                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 20                      | Depositor |
| Minimum defocus (nm)                 | 500                     | Depositor |
| Maximum defocus (nm)                 | 2000                    | Depositor |
| Magnification                        | 161000                  | Depositor |
| Image detector                       | GENERIC TVIPS (4k x 4k) | Depositor |
| Maximum map value                    | 191.487                 | Depositor |
| Minimum map value                    | -133.057                | Depositor |
| Average map value                    | -0.914                  | Depositor |
| Map value standard deviation         | 20.362                  | Depositor |
| Recommended contour level            | 25.0                    | Depositor |
| Map size ( $\text{\AA}$ )            | 358.4, 358.4, 358.4     | wwPDB     |
| Map dimensions                       | 128, 128, 128           | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0        | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 2.8, 2.8, 2.8           | Depositor |

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 6MZ, ACE, FME, NH2, OMC, PSU, 5MU, 4SU, 7MG, CM0, H2U

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   | AB    | 0.76         | 0/1736           | 1.10        | 10/2340 (0.4%)    |
| 2   | AC    | 0.81         | 0/1651           | 1.19        | 17/2225 (0.8%)    |
| 3   | AD    | 0.83         | 0/1665           | 1.27        | 20/2227 (0.9%)    |
| 4   | AE    | 0.79         | 0/1119           | 1.16        | 9/1506 (0.6%)     |
| 5   | AF    | 0.79         | 0/835            | 1.15        | 7/1128 (0.6%)     |
| 6   | AG    | 0.81         | 0/1188           | 1.19        | 11/1593 (0.7%)    |
| 7   | AH    | 0.80         | 0/989            | 1.09        | 8/1326 (0.6%)     |
| 8   | AI    | 0.88         | 0/1035           | 1.34        | 14/1377 (1.0%)    |
| 9   | AJ    | 0.81         | 0/797            | 1.22        | 11/1079 (1.0%)    |
| 10  | AK    | 0.85         | 0/894            | 1.20        | 10/1207 (0.8%)    |
| 11  | AL    | 0.85         | 0/969            | 1.25        | 13/1300 (1.0%)    |
| 12  | AM    | 0.84         | 0/884            | 1.30        | 14/1181 (1.2%)    |
| 13  | AN    | 0.88         | 1/817 (0.1%)     | 1.43        | 16/1088 (1.5%)    |
| 14  | AO    | 0.86         | 0/722            | 1.26        | 12/964 (1.2%)     |
| 15  | AP    | 0.88         | 0/648            | 1.25        | 6/870 (0.7%)      |
| 16  | AQ    | 0.78         | 0/658            | 1.13        | 5/883 (0.6%)      |
| 17  | AR    | 0.85         | 0/463            | 1.25        | 8/623 (1.3%)      |
| 18  | AS    | 0.84         | 0/653            | 1.26        | 8/879 (0.9%)      |
| 19  | AT    | 0.79         | 0/672            | 1.24        | 8/890 (0.9%)      |
| 20  | AU    | 0.96         | 0/431            | 1.57        | 12/572 (2.1%)     |
| 21  | AA    | 2.03         | 752/36759 (2.0%) | 2.33        | 2571/57346 (4.5%) |
| 22  | A1    | 2.04         | 28/1668 (1.7%)   | 2.30        | 106/2595 (4.1%)   |
| 23  | A2    | 1.81         | 3/343 (0.9%)     | 2.39        | 25/531 (4.7%)     |
| 24  | A3    | 2.06         | 38/1722 (2.2%)   | 2.29        | 111/2685 (4.1%)   |
| 25  | BC    | 0.85         | 0/2121           | 1.31        | 31/2852 (1.1%)    |
| 26  | BD    | 0.77         | 0/1586           | 1.22        | 10/2134 (0.5%)    |
| 27  | BE    | 0.75         | 0/1571           | 1.20        | 13/2113 (0.6%)    |
| 28  | BF    | 0.79         | 0/1444           | 1.21        | 11/1937 (0.6%)    |
| 29  | BG    | 0.76         | 0/1343           | 1.18        | 10/1816 (0.6%)    |
| 30  | BH    | 0.72         | 0/1122           | 1.10        | 7/1515 (0.5%)     |
| 31  | BI    | 0.71         | 0/1046           | 1.07        | 3/1410 (0.2%)     |
| 32  | BJ    | 0.77         | 0/1152           | 1.24        | 12/1551 (0.8%)    |

| Mol | Chain | Bond lengths |                    | Bond angles |                    |
|-----|-------|--------------|--------------------|-------------|--------------------|
|     |       | RMSZ         | # Z  >5            | RMSZ        | # Z  >5            |
| 33  | BK    | 0.79         | 0/947              | 1.30        | 11/1268 (0.9%)     |
| 34  | BL    | 0.82         | 0/1054             | 1.36        | 14/1403 (1.0%)     |
| 35  | BM    | 0.84         | 0/1093             | 1.24        | 9/1460 (0.6%)      |
| 36  | BN    | 0.89         | 0/973              | 1.43        | 19/1301 (1.5%)     |
| 37  | BO    | 0.85         | 0/902              | 1.32        | 11/1209 (0.9%)     |
| 38  | BP    | 0.85         | 0/929              | 1.42        | 13/1242 (1.0%)     |
| 39  | BQ    | 0.86         | 0/960              | 1.33        | 14/1278 (1.1%)     |
| 40  | BR    | 0.79         | 0/829              | 1.18        | 6/1107 (0.5%)      |
| 41  | BS    | 0.76         | 0/864              | 1.20        | 8/1156 (0.7%)      |
| 42  | BT    | 0.77         | 0/744              | 1.27        | 8/994 (0.8%)       |
| 43  | BU    | 0.78         | 0/787              | 1.20        | 5/1051 (0.5%)      |
| 44  | BV    | 0.75         | 0/766              | 1.17        | 6/1025 (0.6%)      |
| 45  | BW    | 0.84         | 0/604              | 1.29        | 5/799 (0.6%)       |
| 46  | BX    | 0.87         | 0/635              | 1.39        | 11/848 (1.3%)      |
| 47  | BY    | 0.77         | 0/510              | 1.26        | 4/677 (0.6%)       |
| 48  | BZ    | 0.84         | 0/453              | 1.29        | 5/605 (0.8%)       |
| 49  | B0    | 0.85         | 0/450              | 1.33        | 7/599 (1.2%)       |
| 50  | B1    | 0.77         | 0/417              | 1.21        | 4/556 (0.7%)       |
| 51  | B2    | 0.98         | 0/380              | 1.49        | 10/498 (2.0%)      |
| 52  | B3    | 0.76         | 0/513              | 1.16        | 4/676 (0.6%)       |
| 53  | B4    | 0.86         | 0/303              | 1.39        | 5/397 (1.3%)       |
| 54  | BA    | 1.91         | 1309/69796 (1.9%)  | 2.32        | 5106/108888 (4.7%) |
| 55  | BB    | 2.03         | 85/2800 (3.0%)     | 2.33        | 222/4367 (5.1%)    |
| 56  | B5    | 0.71         | 0/1673             | 1.10        | 10/2255 (0.4%)     |
| All | All   | 1.71         | 2216/160085 (1.4%) | 2.09        | 8646/239402 (3.6%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 2   | AC    | 0                   | 2                   |
| 8   | AI    | 0                   | 1                   |
| 10  | AK    | 0                   | 1                   |
| 21  | AA    | 0                   | 365                 |
| 22  | A1    | 0                   | 10                  |
| 23  | A2    | 0                   | 1                   |
| 24  | A3    | 0                   | 14                  |
| 25  | BC    | 0                   | 2                   |
| 33  | BK    | 0                   | 1                   |
| 34  | BL    | 0                   | 1                   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 54  | BA    | 0                   | 666                 |
| 55  | BB    | 0                   | 30                  |
| All | All   | 0                   | 1094                |

All (2216) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 54  | BA    | 1044 | C    | C4-N4 | -7.34 | 1.27        | 1.33     |
| 54  | BA    | 2752 | C    | C4-N4 | -7.31 | 1.27        | 1.33     |
| 24  | A3    | 3    | C    | C4-N4 | -7.23 | 1.27        | 1.33     |
| 21  | AA    | 6    | G    | C6-N1 | -7.22 | 1.34        | 1.39     |
| 21  | AA    | 1479 | C    | C4-N4 | -7.20 | 1.27        | 1.33     |
| 21  | AA    | 330  | C    | C4-N4 | -7.18 | 1.27        | 1.33     |
| 55  | BB    | 113  | C    | C4-N4 | -7.17 | 1.27        | 1.33     |
| 21  | AA    | 176  | C    | C4-N4 | -7.17 | 1.27        | 1.33     |
| 54  | BA    | 565  | C    | C4-N4 | -7.17 | 1.27        | 1.33     |
| 54  | BA    | 2723 | C    | C4-N4 | -7.14 | 1.27        | 1.33     |
| 21  | AA    | 1509 | C    | C4-N4 | -7.10 | 1.27        | 1.33     |
| 21  | AA    | 824  | G    | C2-N2 | -7.09 | 1.27        | 1.34     |
| 54  | BA    | 2104 | C    | C4-N4 | -7.09 | 1.27        | 1.33     |
| 54  | BA    | 624  | C    | C4-N4 | -7.07 | 1.27        | 1.33     |
| 54  | BA    | 1595 | C    | C4-N4 | -7.05 | 1.27        | 1.33     |
| 54  | BA    | 1558 | C    | C4-N4 | -7.05 | 1.27        | 1.33     |
| 21  | AA    | 341  | C    | C4-N4 | -7.04 | 1.27        | 1.33     |
| 54  | BA    | 1550 | C    | C4-N4 | -7.02 | 1.27        | 1.33     |
| 54  | BA    | 616  | A    | C6-N1 | -7.01 | 1.30        | 1.35     |
| 54  | BA    | 2777 | G    | C2-N2 | -7.00 | 1.27        | 1.34     |
| 54  | BA    | 2620 | C    | C4-N4 | -6.99 | 1.27        | 1.33     |
| 22  | A1    | 62   | C    | C4-N4 | -6.98 | 1.27        | 1.33     |
| 54  | BA    | 1793 | C    | C4-N4 | -6.97 | 1.27        | 1.33     |
| 54  | BA    | 527  | C    | C4-N4 | -6.96 | 1.27        | 1.33     |
| 54  | BA    | 1832 | C    | C4-N4 | -6.96 | 1.27        | 1.33     |
| 21  | AA    | 547  | A    | C6-N1 | -6.95 | 1.30        | 1.35     |
| 54  | BA    | 2062 | A    | C6-N1 | -6.94 | 1.30        | 1.35     |
| 54  | BA    | 2359 | C    | C4-N4 | -6.92 | 1.27        | 1.33     |
| 55  | BB    | 71   | C    | C4-N4 | -6.88 | 1.27        | 1.33     |
| 54  | BA    | 2045 | C    | C4-N4 | -6.88 | 1.27        | 1.33     |
| 54  | BA    | 2717 | C    | C4-N4 | -6.87 | 1.27        | 1.33     |
| 54  | BA    | 1821 | A    | C6-N1 | -6.86 | 1.30        | 1.35     |
| 55  | BB    | 37   | C    | C4-N4 | -6.86 | 1.27        | 1.33     |
| 55  | BB    | 75   | G    | C6-N1 | -6.85 | 1.34        | 1.39     |
| 21  | AA    | 1063 | C    | C4-N4 | -6.84 | 1.27        | 1.33     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 21  | AA    | 675  | A    | C6-N1 | -6.84 | 1.30        | 1.35     |
| 54  | BA    | 433  | C    | C4-N4 | -6.83 | 1.27        | 1.33     |
| 54  | BA    | 1398 | C    | C4-N4 | -6.83 | 1.27        | 1.33     |
| 22  | A1    | 65   | C    | N3-C4 | -6.82 | 1.29        | 1.33     |
| 21  | AA    | 499  | A    | C6-N1 | -6.82 | 1.30        | 1.35     |
| 54  | BA    | 704  | G    | C6-N1 | -6.82 | 1.34        | 1.39     |
| 54  | BA    | 2025 | C    | C4-N4 | -6.82 | 1.27        | 1.33     |
| 54  | BA    | 2428 | G    | C6-N1 | -6.81 | 1.34        | 1.39     |
| 21  | AA    | 403  | C    | C4-N4 | -6.80 | 1.27        | 1.33     |
| 54  | BA    | 2863 | C    | C4-N4 | -6.80 | 1.27        | 1.33     |
| 21  | AA    | 58   | C    | C4-N4 | -6.80 | 1.27        | 1.33     |
| 21  | AA    | 1496 | C    | C4-N4 | -6.80 | 1.27        | 1.33     |
| 54  | BA    | 2385 | C    | C4-N4 | -6.80 | 1.27        | 1.33     |
| 54  | BA    | 2031 | A    | C6-N1 | -6.80 | 1.30        | 1.35     |
| 54  | BA    | 2795 | C    | C4-N4 | -6.79 | 1.27        | 1.33     |
| 54  | BA    | 2636 | C    | C4-N4 | -6.78 | 1.27        | 1.33     |
| 21  | AA    | 1193 | G    | C2-N2 | -6.78 | 1.27        | 1.34     |
| 21  | AA    | 1108 | G    | C2-N2 | -6.77 | 1.27        | 1.34     |
| 54  | BA    | 2452 | C    | C4-N4 | -6.77 | 1.27        | 1.33     |
| 55  | BB    | 19   | C    | C4-N4 | -6.77 | 1.27        | 1.33     |
| 21  | AA    | 392  | C    | C4-N4 | -6.76 | 1.27        | 1.33     |
| 21  | AA    | 277  | C    | C4-N4 | -6.76 | 1.27        | 1.33     |
| 54  | BA    | 2196 | C    | N3-C4 | -6.76 | 1.29        | 1.33     |
| 21  | AA    | 1141 | C    | C4-N4 | -6.75 | 1.27        | 1.33     |
| 21  | AA    | 470  | C    | C4-N4 | -6.75 | 1.27        | 1.33     |
| 21  | AA    | 1412 | C    | C4-N4 | -6.75 | 1.27        | 1.33     |
| 54  | BA    | 1704 | C    | C4-N4 | -6.75 | 1.27        | 1.33     |
| 21  | AA    | 188  | C    | C4-N4 | -6.75 | 1.27        | 1.33     |
| 54  | BA    | 2282 | G    | C2-N2 | -6.74 | 1.27        | 1.34     |
| 21  | AA    | 186  | C    | C4-N4 | -6.74 | 1.27        | 1.33     |
| 54  | BA    | 167  | A    | C6-N1 | -6.74 | 1.30        | 1.35     |
| 55  | BB    | 24   | G    | C6-N1 | -6.73 | 1.34        | 1.39     |
| 24  | A3    | 69   | C    | C4-N4 | -6.73 | 1.27        | 1.33     |
| 54  | BA    | 2103 | C    | C4-N4 | -6.73 | 1.27        | 1.33     |
| 54  | BA    | 2326 | C    | C4-N4 | -6.73 | 1.27        | 1.33     |
| 21  | AA    | 1094 | G    | C2-N2 | -6.72 | 1.27        | 1.34     |
| 54  | BA    | 645  | C    | C4-N4 | -6.71 | 1.27        | 1.33     |
| 54  | BA    | 2283 | C    | N3-C4 | -6.71 | 1.29        | 1.33     |
| 54  | BA    | 1413 | A    | C6-N1 | -6.71 | 1.30        | 1.35     |
| 21  | AA    | 363  | A    | C6-N1 | -6.71 | 1.30        | 1.35     |
| 54  | BA    | 2442 | C    | N3-C4 | -6.70 | 1.29        | 1.33     |
| 54  | BA    | 2901 | C    | C4-N4 | -6.70 | 1.27        | 1.33     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 24  | A3    | 68   | C    | C4-N4 | -6.69 | 1.27        | 1.33     |
| 54  | BA    | 378  | C    | C4-N4 | -6.69 | 1.27        | 1.33     |
| 54  | BA    | 717  | C    | C4-N4 | -6.69 | 1.27        | 1.33     |
| 54  | BA    | 371  | A    | C6-N1 | -6.68 | 1.30        | 1.35     |
| 55  | BB    | 116  | G    | C2-N2 | -6.68 | 1.27        | 1.34     |
| 54  | BA    | 31   | C    | C4-N4 | -6.67 | 1.27        | 1.33     |
| 54  | BA    | 1768 | C    | C4-N4 | -6.67 | 1.27        | 1.33     |
| 54  | BA    | 2112 | G    | C2-N2 | -6.67 | 1.27        | 1.34     |
| 54  | BA    | 2175 | C    | C4-N4 | -6.66 | 1.27        | 1.33     |
| 24  | A3    | 62   | C    | C4-N4 | -6.66 | 1.27        | 1.33     |
| 22  | A1    | 1    | G    | C2-N2 | -6.66 | 1.27        | 1.34     |
| 54  | BA    | 781  | A    | C6-N1 | -6.66 | 1.30        | 1.35     |
| 54  | BA    | 2374 | C    | C4-N4 | -6.66 | 1.27        | 1.33     |
| 54  | BA    | 2823 | A    | C6-N1 | -6.66 | 1.30        | 1.35     |
| 21  | AA    | 685  | G    | C2-N2 | -6.65 | 1.27        | 1.34     |
| 54  | BA    | 411  | G    | C2-N2 | -6.65 | 1.27        | 1.34     |
| 54  | BA    | 1386 | C    | C4-N4 | -6.64 | 1.27        | 1.33     |
| 54  | BA    | 2428 | G    | C2-N2 | -6.64 | 1.27        | 1.34     |
| 21  | AA    | 1188 | A    | C6-N1 | -6.64 | 1.30        | 1.35     |
| 54  | BA    | 1514 | G    | C2-N2 | -6.64 | 1.27        | 1.34     |
| 54  | BA    | 2091 | C    | C4-N4 | -6.64 | 1.27        | 1.33     |
| 54  | BA    | 1556 | C    | C4-N4 | -6.63 | 1.27        | 1.33     |
| 54  | BA    | 2644 | G    | C2-N2 | -6.63 | 1.27        | 1.34     |
| 21  | AA    | 776  | G    | C2-N2 | -6.63 | 1.27        | 1.34     |
| 54  | BA    | 1753 | G    | C6-N1 | -6.63 | 1.34        | 1.39     |
| 54  | BA    | 2038 | G    | C6-N1 | -6.63 | 1.34        | 1.39     |
| 21  | AA    | 841  | C    | C4-N4 | -6.62 | 1.27        | 1.33     |
| 54  | BA    | 2623 | G    | C2-N2 | -6.62 | 1.27        | 1.34     |
| 54  | BA    | 1426 | G    | C2-N2 | -6.62 | 1.27        | 1.34     |
| 54  | BA    | 1788 | C    | C4-N4 | -6.61 | 1.27        | 1.33     |
| 21  | AA    | 1231 | G    | C2-N2 | -6.61 | 1.27        | 1.34     |
| 21  | AA    | 1482 | G    | C2-N2 | -6.61 | 1.27        | 1.34     |
| 21  | AA    | 292  | G    | C6-N1 | -6.61 | 1.34        | 1.39     |
| 24  | A3    | 73   | A    | C5-C4 | -6.61 | 1.34        | 1.38     |
| 21  | AA    | 359  | G    | C2-N2 | -6.60 | 1.27        | 1.34     |
| 22  | A1    | 72   | C    | C4-N4 | -6.60 | 1.28        | 1.33     |
| 54  | BA    | 2544 | G    | C6-N1 | -6.59 | 1.34        | 1.39     |
| 54  | BA    | 2683 | C    | C4-N4 | -6.58 | 1.28        | 1.33     |
| 21  | AA    | 1182 | G    | C2-N2 | -6.58 | 1.27        | 1.34     |
| 54  | BA    | 2043 | C    | N3-C4 | -6.57 | 1.29        | 1.33     |
| 21  | AA    | 930  | C    | N3-C4 | -6.57 | 1.29        | 1.33     |
| 54  | BA    | 54   | G    | C6-N1 | -6.57 | 1.34        | 1.39     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 21  | AA    | 379  | C    | C4-N4 | -6.57 | 1.28        | 1.33     |
| 21  | AA    | 1193 | G    | C6-N1 | -6.57 | 1.34        | 1.39     |
| 54  | BA    | 51   | G    | C2-N2 | -6.56 | 1.27        | 1.34     |
| 21  | AA    | 156  | C    | N3-C4 | -6.56 | 1.29        | 1.33     |
| 54  | BA    | 2222 | C    | C4-N4 | -6.56 | 1.28        | 1.33     |
| 21  | AA    | 1066 | C    | C4-N4 | -6.56 | 1.28        | 1.33     |
| 54  | BA    | 2048 | G    | C6-N1 | -6.56 | 1.34        | 1.39     |
| 54  | BA    | 440  | C    | C4-N4 | -6.55 | 1.28        | 1.33     |
| 21  | AA    | 412  | A    | C6-N1 | -6.55 | 1.30        | 1.35     |
| 24  | A3    | 6    | G    | C2-N2 | -6.55 | 1.28        | 1.34     |
| 54  | BA    | 45   | G    | C6-N1 | -6.55 | 1.34        | 1.39     |
| 54  | BA    | 1601 | G    | C2-N2 | -6.55 | 1.28        | 1.34     |
| 21  | AA    | 1280 | A    | C6-N1 | -6.54 | 1.30        | 1.35     |
| 54  | BA    | 2638 | G    | C2-N2 | -6.54 | 1.28        | 1.34     |
| 21  | AA    | 926  | G    | C6-N1 | -6.54 | 1.34        | 1.39     |
| 54  | BA    | 623  | C    | C4-N4 | -6.54 | 1.28        | 1.33     |
| 54  | BA    | 1102 | C    | C4-N4 | -6.54 | 1.28        | 1.33     |
| 54  | BA    | 2443 | C    | C4-N4 | -6.54 | 1.28        | 1.33     |
| 54  | BA    | 2281 | A    | C6-N1 | -6.53 | 1.30        | 1.35     |
| 21  | AA    | 450  | G    | C6-N1 | -6.53 | 1.34        | 1.39     |
| 54  | BA    | 385  | C    | C4-N4 | -6.53 | 1.28        | 1.33     |
| 54  | BA    | 1614 | A    | C6-N1 | -6.53 | 1.30        | 1.35     |
| 54  | BA    | 2044 | C    | C4-N4 | -6.53 | 1.28        | 1.33     |
| 54  | BA    | 449  | A    | C6-N1 | -6.53 | 1.30        | 1.35     |
| 54  | BA    | 1803 | A    | C6-N1 | -6.53 | 1.30        | 1.35     |
| 54  | BA    | 679  | C    | N3-C4 | -6.53 | 1.29        | 1.33     |
| 21  | AA    | 396  | C    | N3-C4 | -6.53 | 1.29        | 1.33     |
| 54  | BA    | 1370 | C    | C4-N4 | -6.51 | 1.28        | 1.33     |
| 54  | BA    | 1759 | A    | C6-N1 | -6.51 | 1.30        | 1.35     |
| 21  | AA    | 1431 | A    | C6-N1 | -6.51 | 1.30        | 1.35     |
| 55  | BB    | 4    | C    | C4-N4 | -6.51 | 1.28        | 1.33     |
| 21  | AA    | 342  | C    | C4-N4 | -6.51 | 1.28        | 1.33     |
| 21  | AA    | 520  | A    | C6-N1 | -6.51 | 1.30        | 1.35     |
| 54  | BA    | 2362 | C    | C4-N4 | -6.51 | 1.28        | 1.33     |
| 21  | AA    | 1129 | C    | C4-N4 | -6.50 | 1.28        | 1.33     |
| 54  | BA    | 1414 | C    | N3-C4 | -6.50 | 1.29        | 1.33     |
| 54  | BA    | 32   | C    | C4-N4 | -6.50 | 1.28        | 1.33     |
| 54  | BA    | 275  | C    | C4-N4 | -6.50 | 1.28        | 1.33     |
| 54  | BA    | 1430 | G    | C2-N2 | -6.49 | 1.28        | 1.34     |
| 21  | AA    | 1476 | A    | C6-N1 | -6.49 | 1.31        | 1.35     |
| 21  | AA    | 931  | C    | N3-C4 | -6.49 | 1.29        | 1.33     |
| 54  | BA    | 1365 | A    | C6-N1 | -6.49 | 1.31        | 1.35     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 21  | AA    | 207  | C    | N3-C4   | -6.49 | 1.29        | 1.33     |
| 54  | BA    | 456  | C    | C4-N4   | -6.49 | 1.28        | 1.33     |
| 54  | BA    | 1667 | G    | C2-N2   | -6.49 | 1.28        | 1.34     |
| 54  | BA    | 1678 | A    | C6-N1   | -6.49 | 1.31        | 1.35     |
| 54  | BA    | 2161 | C    | C4-N4   | -6.49 | 1.28        | 1.33     |
| 55  | BB    | 98   | G    | C2-N2   | -6.48 | 1.28        | 1.34     |
| 21  | AA    | 1084 | G    | C2-N2   | -6.48 | 1.28        | 1.34     |
| 54  | BA    | 2767 | C    | C4-N4   | -6.48 | 1.28        | 1.33     |
| 21  | AA    | 1109 | C    | C4-N4   | -6.47 | 1.28        | 1.33     |
| 54  | BA    | 2589 | A    | C6-N1   | -6.47 | 1.31        | 1.35     |
| 21  | AA    | 494  | G    | C2-N2   | -6.47 | 1.28        | 1.34     |
| 54  | BA    | 1395 | A    | C6-N1   | -6.47 | 1.31        | 1.35     |
| 21  | AA    | 347  | G    | C2-N2   | -6.46 | 1.28        | 1.34     |
| 21  | AA    | 113  | G    | C2-N2   | -6.46 | 1.28        | 1.34     |
| 22  | A1    | 1    | G    | C6-N1   | -6.46 | 1.35        | 1.39     |
| 22  | A1    | 52   | G    | C2-N2   | -6.46 | 1.28        | 1.34     |
| 21  | AA    | 778  | G    | C2-N2   | -6.46 | 1.28        | 1.34     |
| 24  | A3    | 73   | A    | C6-N6   | -6.45 | 1.28        | 1.33     |
| 54  | BA    | 295  | G    | C2-N2   | -6.45 | 1.28        | 1.34     |
| 54  | BA    | 704  | G    | C2-N2   | -6.45 | 1.28        | 1.34     |
| 54  | BA    | 2269 | G    | C2-N2   | -6.45 | 1.28        | 1.34     |
| 54  | BA    | 2721 | A    | C6-N1   | -6.45 | 1.31        | 1.35     |
| 21  | AA    | 354  | G    | C2-N2   | -6.44 | 1.28        | 1.34     |
| 21  | AA    | 308  | C    | C4-N4   | -6.44 | 1.28        | 1.33     |
| 21  | AA    | 663  | A    | C6-N1   | -6.44 | 1.31        | 1.35     |
| 54  | BA    | 574  | A    | C6-N1   | -6.44 | 1.31        | 1.35     |
| 21  | AA    | 275  | G    | C2-N2   | -6.44 | 1.28        | 1.34     |
| 21  | AA    | 1494 | G    | C2-N2   | -6.44 | 1.28        | 1.34     |
| 21  | AA    | 36   | C    | C4'-C3' | -6.44 | 1.46        | 1.53     |
| 22  | A1    | 60   | C    | C4-N4   | -6.44 | 1.28        | 1.33     |
| 54  | BA    | 1345 | C    | C4-N4   | -6.44 | 1.28        | 1.33     |
| 24  | A3    | 5    | G    | C6-N1   | -6.43 | 1.35        | 1.39     |
| 54  | BA    | 2854 | G    | C2-N2   | -6.43 | 1.28        | 1.34     |
| 54  | BA    | 60   | G    | C6-N1   | -6.43 | 1.35        | 1.39     |
| 21  | AA    | 369  | G    | C2-N2   | -6.43 | 1.28        | 1.34     |
| 54  | BA    | 2201 | G    | C2-N2   | -6.42 | 1.28        | 1.34     |
| 54  | BA    | 1436 | G    | C2-N2   | -6.42 | 1.28        | 1.34     |
| 54  | BA    | 2503 | A    | C6-N1   | -6.42 | 1.31        | 1.35     |
| 21  | AA    | 453  | G    | C2-N2   | -6.41 | 1.28        | 1.34     |
| 21  | AA    | 1405 | G    | C2-N2   | -6.41 | 1.28        | 1.34     |
| 55  | BB    | 52   | A    | C6-N1   | -6.41 | 1.31        | 1.35     |
| 54  | BA    | 192  | C    | C4-N4   | -6.41 | 1.28        | 1.33     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 54  | BA    | 2595 | G    | C2-N2 | -6.41 | 1.28        | 1.34     |
| 54  | BA    | 1031 | G    | N1-C2 | -6.41 | 1.32        | 1.37     |
| 21  | AA    | 848  | C    | C4-N4 | -6.41 | 1.28        | 1.33     |
| 21  | AA    | 1469 | C    | C4-N4 | -6.41 | 1.28        | 1.33     |
| 24  | A3    | 71   | G    | C2-N2 | -6.41 | 1.28        | 1.34     |
| 54  | BA    | 2851 | A    | C5-C4 | -6.41 | 1.34        | 1.38     |
| 54  | BA    | 1950 | G    | C2-N2 | -6.40 | 1.28        | 1.34     |
| 54  | BA    | 37   | C    | C4-N4 | -6.40 | 1.28        | 1.33     |
| 54  | BA    | 1537 | G    | C6-N1 | -6.40 | 1.35        | 1.39     |
| 54  | BA    | 1570 | A    | C6-N1 | -6.39 | 1.31        | 1.35     |
| 54  | BA    | 2544 | G    | C2-N2 | -6.39 | 1.28        | 1.34     |
| 21  | AA    | 146  | G    | C2-N2 | -6.39 | 1.28        | 1.34     |
| 21  | AA    | 1281 | C    | N3-C4 | -6.39 | 1.29        | 1.33     |
| 54  | BA    | 422  | A    | C6-N1 | -6.38 | 1.31        | 1.35     |
| 21  | AA    | 1427 | C    | N3-C4 | -6.38 | 1.29        | 1.33     |
| 21  | AA    | 1147 | C    | N3-C4 | -6.38 | 1.29        | 1.33     |
| 54  | BA    | 2050 | C    | C4-N4 | -6.38 | 1.28        | 1.33     |
| 54  | BA    | 2083 | G    | C2-N2 | -6.38 | 1.28        | 1.34     |
| 54  | BA    | 2350 | C    | C4-N4 | -6.38 | 1.28        | 1.33     |
| 21  | AA    | 247  | G    | C2-N2 | -6.38 | 1.28        | 1.34     |
| 55  | BB    | 91   | C    | C4-N4 | -6.37 | 1.28        | 1.33     |
| 21  | AA    | 484  | G    | C2-N2 | -6.37 | 1.28        | 1.34     |
| 21  | AA    | 869  | G    | C2-N2 | -6.37 | 1.28        | 1.34     |
| 54  | BA    | 176  | A    | C6-N1 | -6.37 | 1.31        | 1.35     |
| 54  | BA    | 1826 | G    | C2-N2 | -6.37 | 1.28        | 1.34     |
| 54  | BA    | 2306 | C    | C4-N4 | -6.37 | 1.28        | 1.33     |
| 54  | BA    | 577  | G    | C6-N1 | -6.37 | 1.35        | 1.39     |
| 54  | BA    | 982  | C    | N3-C4 | -6.36 | 1.29        | 1.33     |
| 21  | AA    | 440  | C    | N3-C4 | -6.36 | 1.29        | 1.33     |
| 54  | BA    | 39   | G    | C2-N2 | -6.36 | 1.28        | 1.34     |
| 54  | BA    | 1349 | C    | C4-N4 | -6.36 | 1.28        | 1.33     |
| 55  | BB    | 34   | A    | C6-N1 | -6.36 | 1.31        | 1.35     |
| 55  | BB    | 61   | G    | N1-C2 | -6.36 | 1.32        | 1.37     |
| 54  | BA    | 2338 | C    | C4-N4 | -6.36 | 1.28        | 1.33     |
| 54  | BA    | 885  | C    | C4-N4 | -6.35 | 1.28        | 1.33     |
| 21  | AA    | 210  | C    | C4-N4 | -6.35 | 1.28        | 1.33     |
| 21  | AA    | 1346 | A    | C6-N6 | -6.35 | 1.28        | 1.33     |
| 54  | BA    | 611  | C    | N3-C4 | -6.35 | 1.29        | 1.33     |
| 21  | AA    | 776  | G    | C6-N1 | -6.35 | 1.35        | 1.39     |
| 54  | BA    | 2770 | G    | C2-N2 | -6.35 | 1.28        | 1.34     |
| 21  | AA    | 1531 | A    | C6-N1 | -6.35 | 1.31        | 1.35     |
| 21  | AA    | 941  | G    | C6-N1 | -6.34 | 1.35        | 1.39     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 54  | BA    | 2355 | G    | C2-N2 | -6.34 | 1.28        | 1.34     |
| 24  | A3    | 72   | C    | N3-C4 | -6.34 | 1.29        | 1.33     |
| 54  | BA    | 564  | C    | C4-N4 | -6.34 | 1.28        | 1.33     |
| 54  | BA    | 2289 | G    | C2-N2 | -6.33 | 1.28        | 1.34     |
| 21  | AA    | 164  | G    | C2-N2 | -6.33 | 1.28        | 1.34     |
| 21  | AA    | 292  | G    | C2-N2 | -6.33 | 1.28        | 1.34     |
| 54  | BA    | 1437 | C    | N3-C4 | -6.33 | 1.29        | 1.33     |
| 54  | BA    | 1965 | C    | C4-N4 | -6.33 | 1.28        | 1.33     |
| 21  | AA    | 779  | C    | N3-C4 | -6.33 | 1.29        | 1.33     |
| 21  | AA    | 1488 | G    | C2-N2 | -6.33 | 1.28        | 1.34     |
| 54  | BA    | 605  | G    | C6-N1 | -6.33 | 1.35        | 1.39     |
| 54  | BA    | 892  | A    | C6-N1 | -6.33 | 1.31        | 1.35     |
| 21  | AA    | 52   | C    | C4-N4 | -6.33 | 1.28        | 1.33     |
| 21  | AA    | 880  | C    | N3-C4 | -6.33 | 1.29        | 1.33     |
| 54  | BA    | 2380 | C    | C4-N4 | -6.33 | 1.28        | 1.33     |
| 54  | BA    | 2422 | C    | C4-N4 | -6.32 | 1.28        | 1.33     |
| 21  | AA    | 153  | C    | C4-N4 | -6.32 | 1.28        | 1.33     |
| 55  | BB    | 8    | C    | N3-C4 | -6.32 | 1.29        | 1.33     |
| 54  | BA    | 2759 | G    | C2-N2 | -6.32 | 1.28        | 1.34     |
| 54  | BA    | 2760 | C    | N3-C4 | -6.32 | 1.29        | 1.33     |
| 21  | AA    | 146  | G    | C6-N1 | -6.31 | 1.35        | 1.39     |
| 54  | BA    | 128  | C    | N3-C4 | -6.31 | 1.29        | 1.33     |
| 54  | BA    | 2271 | G    | C2-N2 | -6.31 | 1.28        | 1.34     |
| 54  | BA    | 2048 | G    | C2-N2 | -6.31 | 1.28        | 1.34     |
| 54  | BA    | 2224 | G    | C2-N2 | -6.31 | 1.28        | 1.34     |
| 54  | BA    | 291  | G    | C2-N2 | -6.30 | 1.28        | 1.34     |
| 54  | BA    | 2021 | C    | C4-N4 | -6.30 | 1.28        | 1.33     |
| 54  | BA    | 2253 | G    | C2-N2 | -6.30 | 1.28        | 1.34     |
| 54  | BA    | 116  | C    | C4-N4 | -6.30 | 1.28        | 1.33     |
| 54  | BA    | 2623 | G    | C6-N1 | -6.30 | 1.35        | 1.39     |
| 54  | BA    | 1470 | A    | C6-N1 | -6.30 | 1.31        | 1.35     |
| 54  | BA    | 2162 | G    | C2-N2 | -6.30 | 1.28        | 1.34     |
| 54  | BA    | 2389 | G    | C2-N2 | -6.30 | 1.28        | 1.34     |
| 21  | AA    | 526  | C    | C4-N4 | -6.30 | 1.28        | 1.33     |
| 54  | BA    | 692  | C    | N3-C4 | -6.30 | 1.29        | 1.33     |
| 55  | BB    | 7    | G    | C2-N2 | -6.30 | 1.28        | 1.34     |
| 55  | BB    | 30   | C    | N3-C4 | -6.30 | 1.29        | 1.33     |
| 21  | AA    | 1404 | C    | N3-C4 | -6.29 | 1.29        | 1.33     |
| 21  | AA    | 335  | C    | N3-C4 | -6.29 | 1.29        | 1.33     |
| 21  | AA    | 1320 | C    | C4-N4 | -6.29 | 1.28        | 1.33     |
| 54  | BA    | 1748 | C    | C4-N4 | -6.29 | 1.28        | 1.33     |
| 54  | BA    | 830  | G    | N1-C2 | -6.29 | 1.32        | 1.37     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 21  | AA    | 1171 | A    | C6-N1 | -6.29 | 1.31        | 1.35     |
| 21  | AA    | 1208 | C    | N3-C4 | -6.29 | 1.29        | 1.33     |
| 21  | AA    | 866  | C    | N3-C4 | -6.29 | 1.29        | 1.33     |
| 21  | AA    | 1501 | C    | N3-C4 | -6.29 | 1.29        | 1.33     |
| 21  | AA    | 449  | G    | C2-N2 | -6.28 | 1.28        | 1.34     |
| 21  | AA    | 443  | C    | N3-C4 | -6.28 | 1.29        | 1.33     |
| 21  | AA    | 865  | A    | C6-N1 | -6.28 | 1.31        | 1.35     |
| 54  | BA    | 2123 | G    | C2-N2 | -6.28 | 1.28        | 1.34     |
| 21  | AA    | 840  | C    | C4-N4 | -6.28 | 1.28        | 1.33     |
| 21  | AA    | 882  | C    | C4-N4 | -6.28 | 1.28        | 1.33     |
| 21  | AA    | 462  | G    | C2-N2 | -6.28 | 1.28        | 1.34     |
| 21  | AA    | 704  | A    | C6-N1 | -6.28 | 1.31        | 1.35     |
| 54  | BA    | 2745 | C    | C4-N4 | -6.28 | 1.28        | 1.33     |
| 54  | BA    | 2886 | A    | C6-N1 | -6.28 | 1.31        | 1.35     |
| 54  | BA    | 353  | C    | N3-C4 | -6.27 | 1.29        | 1.33     |
| 54  | BA    | 2800 | A    | C6-N1 | -6.27 | 1.31        | 1.35     |
| 21  | AA    | 778  | G    | C6-N1 | -6.27 | 1.35        | 1.39     |
| 24  | A3    | 63   | C    | C4-N4 | -6.27 | 1.28        | 1.33     |
| 54  | BA    | 2822 | G    | C2-N2 | -6.27 | 1.28        | 1.34     |
| 54  | BA    | 1401 | G    | C2-N2 | -6.26 | 1.28        | 1.34     |
| 54  | BA    | 2186 | G    | N1-C2 | -6.26 | 1.32        | 1.37     |
| 21  | AA    | 366  | A    | C6-N1 | -6.26 | 1.31        | 1.35     |
| 21  | AA    | 422  | C    | C4-N4 | -6.26 | 1.28        | 1.33     |
| 21  | AA    | 674  | G    | C2-N2 | -6.26 | 1.28        | 1.34     |
| 21  | AA    | 1366 | C    | N3-C4 | -6.26 | 1.29        | 1.33     |
| 54  | BA    | 2391 | G    | N1-C2 | -6.26 | 1.32        | 1.37     |
| 54  | BA    | 2228 | G    | C2-N2 | -6.26 | 1.28        | 1.34     |
| 54  | BA    | 2073 | C    | N3-C4 | -6.26 | 1.29        | 1.33     |
| 21  | AA    | 1421 | G    | C2-N2 | -6.25 | 1.28        | 1.34     |
| 54  | BA    | 1493 | C    | N3-C4 | -6.25 | 1.29        | 1.33     |
| 21  | AA    | 1410 | A    | C6-N1 | -6.25 | 1.31        | 1.35     |
| 54  | BA    | 1080 | A    | C6-N1 | -6.25 | 1.31        | 1.35     |
| 54  | BA    | 1695 | G    | C2-N2 | -6.25 | 1.28        | 1.34     |
| 21  | AA    | 314  | C    | C4-N4 | -6.25 | 1.28        | 1.33     |
| 22  | A1    | 61   | C    | C4-N4 | -6.25 | 1.28        | 1.33     |
| 21  | AA    | 1177 | G    | C2-N2 | -6.25 | 1.28        | 1.34     |
| 54  | BA    | 2626 | C    | C4-N4 | -6.25 | 1.28        | 1.33     |
| 55  | BB    | 41   | G    | C2-N2 | -6.25 | 1.28        | 1.34     |
| 21  | AA    | 528  | C    | N3-C4 | -6.24 | 1.29        | 1.33     |
| 54  | BA    | 364  | C    | C4-N4 | -6.24 | 1.28        | 1.33     |
| 54  | BA    | 2785 | C    | C4-N4 | -6.24 | 1.28        | 1.33     |
| 54  | BA    | 937  | C    | N3-C4 | -6.24 | 1.29        | 1.33     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 55  | BB    | 64   | G    | C6-N1 | -6.24 | 1.35        | 1.39     |
| 21  | AA    | 802  | A    | C6-N1 | -6.24 | 1.31        | 1.35     |
| 24  | A3    | 19   | G    | C2-N2 | -6.24 | 1.28        | 1.34     |
| 54  | BA    | 2699 | C    | C4-N4 | -6.24 | 1.28        | 1.33     |
| 54  | BA    | 1537 | G    | C2-N2 | -6.23 | 1.28        | 1.34     |
| 54  | BA    | 1564 | C    | C4-N4 | -6.23 | 1.28        | 1.33     |
| 21  | AA    | 1517 | G    | C2-N2 | -6.23 | 1.28        | 1.34     |
| 21  | AA    | 495  | A    | C6-N1 | -6.23 | 1.31        | 1.35     |
| 21  | AA    | 1347 | G    | C2-N2 | -6.23 | 1.28        | 1.34     |
| 21  | AA    | 251  | G    | C2-N2 | -6.23 | 1.28        | 1.34     |
| 54  | BA    | 1446 | C    | N3-C4 | -6.23 | 1.29        | 1.33     |
| 55  | BB    | 31   | C    | C4-N4 | -6.23 | 1.28        | 1.33     |
| 21  | AA    | 1447 | A    | C6-N1 | -6.23 | 1.31        | 1.35     |
| 54  | BA    | 2427 | C    | C4-N4 | -6.22 | 1.28        | 1.33     |
| 54  | BA    | 2    | G    | C2-N2 | -6.22 | 1.28        | 1.34     |
| 54  | BA    | 774  | G    | C2-N2 | -6.22 | 1.28        | 1.34     |
| 54  | BA    | 1472 | C    | C4-N4 | -6.22 | 1.28        | 1.33     |
| 54  | BA    | 1990 | C    | N3-C4 | -6.22 | 1.29        | 1.33     |
| 54  | BA    | 343  | C    | C4-N4 | -6.22 | 1.28        | 1.33     |
| 54  | BA    | 1973 | G    | C2-N2 | -6.22 | 1.28        | 1.34     |
| 55  | BB    | 64   | G    | C2-N2 | -6.21 | 1.28        | 1.34     |
| 21  | AA    | 879  | C    | N3-C4 | -6.21 | 1.29        | 1.33     |
| 21  | AA    | 1342 | C    | C4-N4 | -6.21 | 1.28        | 1.33     |
| 54  | BA    | 1870 | C    | C4-N4 | -6.21 | 1.28        | 1.33     |
| 55  | BB    | 97   | C    | C4-N4 | -6.21 | 1.28        | 1.33     |
| 55  | BB    | 114  | C    | C4-N4 | -6.20 | 1.28        | 1.33     |
| 54  | BA    | 1609 | A    | C6-N1 | -6.20 | 1.31        | 1.35     |
| 54  | BA    | 2737 | G    | C6-N1 | -6.20 | 1.35        | 1.39     |
| 54  | BA    | 2747 | G    | C2-N2 | -6.20 | 1.28        | 1.34     |
| 21  | AA    | 348  | G    | C6-N1 | -6.20 | 1.35        | 1.39     |
| 54  | BA    | 454  | A    | C6-N1 | -6.20 | 1.31        | 1.35     |
| 54  | BA    | 2443 | C    | N3-C4 | -6.20 | 1.29        | 1.33     |
| 54  | BA    | 2885 | G    | C2-N2 | -6.20 | 1.28        | 1.34     |
| 21  | AA    | 637  | C    | N3-C4 | -6.19 | 1.29        | 1.33     |
| 54  | BA    | 2038 | G    | C2-N2 | -6.19 | 1.28        | 1.34     |
| 55  | BB    | 41   | G    | C6-N1 | -6.19 | 1.35        | 1.39     |
| 21  | AA    | 1151 | A    | C6-N1 | -6.19 | 1.31        | 1.35     |
| 55  | BB    | 62   | C    | C4-N4 | -6.19 | 1.28        | 1.33     |
| 21  | AA    | 1139 | G    | C2-N2 | -6.19 | 1.28        | 1.34     |
| 21  | AA    | 1484 | C    | C4-N4 | -6.18 | 1.28        | 1.33     |
| 21  | AA    | 494  | G    | C6-N1 | -6.18 | 1.35        | 1.39     |
| 54  | BA    | 412  | A    | C6-N1 | -6.18 | 1.31        | 1.35     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 21  | AA    | 444  | G    | C2-N2 | -6.18 | 1.28        | 1.34     |
| 54  | BA    | 2770 | G    | C6-N1 | -6.18 | 1.35        | 1.39     |
| 55  | BB    | 79   | G    | C2-N2 | -6.18 | 1.28        | 1.34     |
| 21  | AA    | 483  | C    | C4-N4 | -6.17 | 1.28        | 1.33     |
| 54  | BA    | 161  | A    | C5-C4 | -6.17 | 1.34        | 1.38     |
| 54  | BA    | 1229 | C    | C4-N4 | -6.17 | 1.28        | 1.33     |
| 54  | BA    | 1774 | C    | C4-N4 | -6.17 | 1.28        | 1.33     |
| 55  | BB    | 29   | A    | C6-N1 | -6.17 | 1.31        | 1.35     |
| 54  | BA    | 2890 | G    | C2-N2 | -6.17 | 1.28        | 1.34     |
| 54  | BA    | 2160 | C    | C4-N4 | -6.17 | 1.28        | 1.33     |
| 21  | AA    | 197  | A    | C6-N1 | -6.17 | 1.31        | 1.35     |
| 54  | BA    | 1761 | C    | C4-N4 | -6.17 | 1.28        | 1.33     |
| 21  | AA    | 297  | G    | C2-N2 | -6.17 | 1.28        | 1.34     |
| 54  | BA    | 140  | C    | C4-N4 | -6.16 | 1.28        | 1.33     |
| 21  | AA    | 926  | G    | C2-N2 | -6.16 | 1.28        | 1.34     |
| 54  | BA    | 806  | C    | C4-N4 | -6.16 | 1.28        | 1.33     |
| 54  | BA    | 901  | C    | C4-N4 | -6.16 | 1.28        | 1.33     |
| 21  | AA    | 369  | G    | C6-N1 | -6.16 | 1.35        | 1.39     |
| 21  | AA    | 527  | G    | C6-N1 | -6.16 | 1.35        | 1.39     |
| 54  | BA    | 36   | G    | N1-C2 | -6.16 | 1.32        | 1.37     |
| 21  | AA    | 457  | G    | C2-N2 | -6.16 | 1.28        | 1.34     |
| 24  | A3    | 66   | C    | N3-C4 | -6.16 | 1.29        | 1.33     |
| 21  | AA    | 187  | G    | N1-C2 | -6.15 | 1.32        | 1.37     |
| 54  | BA    | 383  | C    | N3-C4 | -6.15 | 1.29        | 1.33     |
| 54  | BA    | 601  | C    | C4-N4 | -6.15 | 1.28        | 1.33     |
| 21  | AA    | 1534 | A    | C6-N1 | -6.15 | 1.31        | 1.35     |
| 54  | BA    | 1514 | G    | C6-N1 | -6.15 | 1.35        | 1.39     |
| 54  | BA    | 473  | G    | C2-N2 | -6.15 | 1.28        | 1.34     |
| 21  | AA    | 347  | G    | C6-N1 | -6.15 | 1.35        | 1.39     |
| 21  | AA    | 1102 | A    | C6-N1 | -6.15 | 1.31        | 1.35     |
| 54  | BA    | 961  | C    | N3-C4 | -6.15 | 1.29        | 1.33     |
| 54  | BA    | 474  | G    | C6-N1 | -6.14 | 1.35        | 1.39     |
| 54  | BA    | 2215 | C    | N3-C4 | -6.14 | 1.29        | 1.33     |
| 55  | BB    | 85   | G    | C2-N2 | -6.14 | 1.28        | 1.34     |
| 21  | AA    | 1526 | G    | C2-N2 | -6.14 | 1.28        | 1.34     |
| 54  | BA    | 1129 | A    | C6-N1 | -6.14 | 1.31        | 1.35     |
| 54  | BA    | 347  | A    | C6-N1 | -6.14 | 1.31        | 1.35     |
| 54  | BA    | 626  | A    | C6-N1 | -6.14 | 1.31        | 1.35     |
| 54  | BA    | 332  | A    | C6-N1 | -6.14 | 1.31        | 1.35     |
| 54  | BA    | 936  | A    | C6-N1 | -6.14 | 1.31        | 1.35     |
| 54  | BA    | 671  | C    | C4-N4 | -6.14 | 1.28        | 1.33     |
| 54  | BA    | 69   | C    | C4-N4 | -6.14 | 1.28        | 1.33     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 54  | BA    | 587  | C    | C4-N4 | -6.13 | 1.28        | 1.33     |
| 54  | BA    | 1800 | C    | C4-N4 | -6.13 | 1.28        | 1.33     |
| 54  | BA    | 2628 | C    | C4-N4 | -6.13 | 1.28        | 1.33     |
| 21  | AA    | 481  | G    | C2-N2 | -6.13 | 1.28        | 1.34     |
| 21  | AA    | 1097 | C    | N3-C4 | -6.13 | 1.29        | 1.33     |
| 21  | AA    | 1415 | G    | C6-N1 | -6.13 | 1.35        | 1.39     |
| 21  | AA    | 1432 | G    | C2-N2 | -6.13 | 1.28        | 1.34     |
| 21  | AA    | 1521 | C    | N3-C4 | -6.13 | 1.29        | 1.33     |
| 21  | AA    | 376  | G    | C2-N2 | -6.13 | 1.28        | 1.34     |
| 21  | AA    | 1388 | C    | C4-N4 | -6.13 | 1.28        | 1.33     |
| 55  | BB    | 116  | G    | C6-N1 | -6.13 | 1.35        | 1.39     |
| 21  | AA    | 1428 | A    | C5-C4 | -6.12 | 1.34        | 1.38     |
| 54  | BA    | 2234 | G    | C2-N2 | -6.12 | 1.28        | 1.34     |
| 54  | BA    | 1036 | G    | C6-N1 | -6.12 | 1.35        | 1.39     |
| 54  | BA    | 2710 | C    | C4-N4 | -6.12 | 1.28        | 1.33     |
| 54  | BA    | 2827 | C    | N3-C4 | -6.12 | 1.29        | 1.33     |
| 21  | AA    | 475  | C    | C4-N4 | -6.12 | 1.28        | 1.33     |
| 21  | AA    | 1178 | G    | N1-C2 | -6.12 | 1.32        | 1.37     |
| 54  | BA    | 391  | A    | C6-N1 | -6.12 | 1.31        | 1.35     |
| 54  | BA    | 570  | G    | C2-N2 | -6.12 | 1.28        | 1.34     |
| 54  | BA    | 1077 | A    | C6-N1 | -6.12 | 1.31        | 1.35     |
| 55  | BB    | 23   | G    | C6-N1 | -6.12 | 1.35        | 1.39     |
| 54  | BA    | 2614 | A    | C5-C4 | -6.12 | 1.34        | 1.38     |
| 54  | BA    | 1114 | C    | C4-N4 | -6.12 | 1.28        | 1.33     |
| 54  | BA    | 2507 | C    | N3-C4 | -6.12 | 1.29        | 1.33     |
| 21  | AA    | 728  | A    | C5-C4 | -6.12 | 1.34        | 1.38     |
| 54  | BA    | 719  | C    | N3-C4 | -6.12 | 1.29        | 1.33     |
| 54  | BA    | 1075 | C    | C4-N4 | -6.12 | 1.28        | 1.33     |
| 55  | BB    | 102  | G    | N1-C2 | -6.12 | 1.32        | 1.37     |
| 54  | BA    | 223  | A    | C5-C4 | -6.11 | 1.34        | 1.38     |
| 54  | BA    | 423  | A    | C5-C4 | -6.11 | 1.34        | 1.38     |
| 54  | BA    | 1787 | A    | C6-N1 | -6.11 | 1.31        | 1.35     |
| 54  | BA    | 2587 | A    | C5-C4 | -6.11 | 1.34        | 1.38     |
| 22  | A1    | 28   | C    | C4-N4 | -6.11 | 1.28        | 1.33     |
| 54  | BA    | 550  | C    | N3-C4 | -6.11 | 1.29        | 1.33     |
| 55  | BB    | 94   | A    | C6-N1 | -6.11 | 1.31        | 1.35     |
| 21  | AA    | 1077 | G    | N1-C2 | -6.11 | 1.32        | 1.37     |
| 21  | AA    | 1344 | C    | C4-N4 | -6.11 | 1.28        | 1.33     |
| 54  | BA    | 226  | A    | C6-N1 | -6.11 | 1.31        | 1.35     |
| 55  | BB    | 7    | G    | C6-N1 | -6.11 | 1.35        | 1.39     |
| 54  | BA    | 585  | G    | C2-N2 | -6.10 | 1.28        | 1.34     |
| 54  | BA    | 1441 | G    | C2-N2 | -6.10 | 1.28        | 1.34     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 54  | BA    | 1208 | C    | N3-C4 | -6.10 | 1.29        | 1.33     |
| 21  | AA    | 355  | C    | N3-C4 | -6.10 | 1.29        | 1.33     |
| 21  | AA    | 360  | G    | N1-C2 | -6.10 | 1.32        | 1.37     |
| 21  | AA    | 878  | A    | C6-N1 | -6.10 | 1.31        | 1.35     |
| 21  | AA    | 1061 | G    | C6-N1 | -6.10 | 1.35        | 1.39     |
| 21  | AA    | 1369 | C    | C4-N4 | -6.10 | 1.28        | 1.33     |
| 54  | BA    | 2850 | A    | C6-N1 | -6.10 | 1.31        | 1.35     |
| 21  | AA    | 1433 | A    | C6-N1 | -6.10 | 1.31        | 1.35     |
| 54  | BA    | 570  | G    | C6-N1 | -6.10 | 1.35        | 1.39     |
| 55  | BB    | 60   | C    | C4-N4 | -6.10 | 1.28        | 1.33     |
| 54  | BA    | 398  | C    | C4-N4 | -6.09 | 1.28        | 1.33     |
| 54  | BA    | 1741 | C    | C4-N4 | -6.09 | 1.28        | 1.33     |
| 54  | BA    | 2870 | C    | C4-N4 | -6.09 | 1.28        | 1.33     |
| 24  | A3    | 6    | G    | C6-N1 | -6.09 | 1.35        | 1.39     |
| 54  | BA    | 121  | G    | C2-N2 | -6.09 | 1.28        | 1.34     |
| 54  | BA    | 1686 | C    | C4-N4 | -6.09 | 1.28        | 1.33     |
| 54  | BA    | 160  | A    | C6-N1 | -6.09 | 1.31        | 1.35     |
| 54  | BA    | 945  | A    | C6-N1 | -6.09 | 1.31        | 1.35     |
| 54  | BA    | 2078 | C    | N3-C4 | -6.09 | 1.29        | 1.33     |
| 21  | AA    | 1207 | G    | C2-N2 | -6.08 | 1.28        | 1.34     |
| 21  | AA    | 1038 | C    | C4-N4 | -6.08 | 1.28        | 1.33     |
| 54  | BA    | 54   | G    | C2-N2 | -6.08 | 1.28        | 1.34     |
| 54  | BA    | 393  | C    | C4-N4 | -6.08 | 1.28        | 1.33     |
| 54  | BA    | 2234 | G    | C6-N1 | -6.08 | 1.35        | 1.39     |
| 21  | AA    | 1438 | G    | C6-N1 | -6.08 | 1.35        | 1.39     |
| 21  | AA    | 155  | A    | C6-N1 | -6.08 | 1.31        | 1.35     |
| 21  | AA    | 983  | A    | C6-N1 | -6.07 | 1.31        | 1.35     |
| 54  | BA    | 386  | G    | C2-N2 | -6.07 | 1.28        | 1.34     |
| 21  | AA    | 703  | G    | N1-C2 | -6.07 | 1.32        | 1.37     |
| 54  | BA    | 2734 | A    | C6-N6 | -6.07 | 1.29        | 1.33     |
| 54  | BA    | 2828 | G    | N1-C2 | -6.06 | 1.32        | 1.37     |
| 54  | BA    | 1454 | C    | C4-N4 | -6.06 | 1.28        | 1.33     |
| 21  | AA    | 233  | C    | C4-N4 | -6.06 | 1.28        | 1.33     |
| 21  | AA    | 1061 | G    | C2-N2 | -6.06 | 1.28        | 1.34     |
| 54  | BA    | 1401 | G    | C6-N1 | -6.06 | 1.35        | 1.39     |
| 21  | AA    | 1407 | C    | C4-N4 | -6.06 | 1.28        | 1.33     |
| 54  | BA    | 1043 | C    | C4-N4 | -6.06 | 1.28        | 1.33     |
| 55  | BB    | 75   | G    | C2-N2 | -6.06 | 1.28        | 1.34     |
| 21  | AA    | 1397 | C    | C4-N4 | -6.05 | 1.28        | 1.33     |
| 21  | AA    | 775  | G    | C2-N2 | -6.05 | 1.28        | 1.34     |
| 54  | BA    | 706  | A    | C6-N1 | -6.05 | 1.31        | 1.35     |
| 54  | BA    | 893  | C    | N3-C4 | -6.05 | 1.29        | 1.33     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 21  | AA    | 806  | C    | N3-C4 | -6.05 | 1.29        | 1.33     |
| 54  | BA    | 285  | G    | C2-N2 | -6.05 | 1.28        | 1.34     |
| 54  | BA    | 1646 | C    | C4-N4 | -6.05 | 1.28        | 1.33     |
| 54  | BA    | 2332 | C    | C4-N4 | -6.05 | 1.28        | 1.33     |
| 21  | AA    | 222  | C    | C4-N4 | -6.05 | 1.28        | 1.33     |
| 54  | BA    | 1361 | G    | C2-N2 | -6.05 | 1.28        | 1.34     |
| 54  | BA    | 1927 | A    | C6-N1 | -6.05 | 1.31        | 1.35     |
| 54  | BA    | 2618 | G    | C2-N2 | -6.05 | 1.28        | 1.34     |
| 21  | AA    | 489  | C    | N3-C4 | -6.05 | 1.29        | 1.33     |
| 54  | BA    | 738  | G    | C2-N2 | -6.05 | 1.28        | 1.34     |
| 54  | BA    | 1700 | A    | C6-N6 | -6.05 | 1.29        | 1.33     |
| 21  | AA    | 1210 | C    | C4-N4 | -6.04 | 1.28        | 1.33     |
| 54  | BA    | 1593 | A    | C6-N1 | -6.04 | 1.31        | 1.35     |
| 54  | BA    | 2367 | G    | C2-N2 | -6.04 | 1.28        | 1.34     |
| 21  | AA    | 32   | A    | C6-N1 | -6.03 | 1.31        | 1.35     |
| 54  | BA    | 1220 | G    | C2-N2 | -6.03 | 1.28        | 1.34     |
| 21  | AA    | 39   | G    | C2-N2 | -6.03 | 1.28        | 1.34     |
| 54  | BA    | 1613 | G    | C2-N2 | -6.03 | 1.28        | 1.34     |
| 21  | AA    | 490  | C    | C4-N4 | -6.03 | 1.28        | 1.33     |
| 54  | BA    | 44   | A    | C6-N1 | -6.03 | 1.31        | 1.35     |
| 54  | BA    | 45   | G    | C2-N2 | -6.03 | 1.28        | 1.34     |
| 54  | BA    | 2323 | G    | C2-N2 | -6.03 | 1.28        | 1.34     |
| 54  | BA    | 1046 | A    | C6-N1 | -6.02 | 1.31        | 1.35     |
| 54  | BA    | 33   | C    | C4-N4 | -6.02 | 1.28        | 1.33     |
| 54  | BA    | 443  | A    | C6-N1 | -6.02 | 1.31        | 1.35     |
| 21  | AA    | 1487 | G    | C2-N2 | -6.02 | 1.28        | 1.34     |
| 54  | BA    | 1221 | C    | N3-C4 | -6.02 | 1.29        | 1.33     |
| 54  | BA    | 444  | C    | N3-C4 | -6.02 | 1.29        | 1.33     |
| 54  | BA    | 2207 | C    | N3-C4 | -6.02 | 1.29        | 1.33     |
| 54  | BA    | 180  | G    | C2-N2 | -6.02 | 1.28        | 1.34     |
| 54  | BA    | 1121 | C    | C4-N4 | -6.02 | 1.28        | 1.33     |
| 54  | BA    | 1830 | C    | N3-C4 | -6.02 | 1.29        | 1.33     |
| 54  | BA    | 1753 | G    | C2-N2 | -6.01 | 1.28        | 1.34     |
| 54  | BA    | 2624 | G    | C6-N1 | -6.01 | 1.35        | 1.39     |
| 21  | AA    | 1507 | A    | C6-N1 | -6.01 | 1.31        | 1.35     |
| 54  | BA    | 60   | G    | C2-N2 | -6.01 | 1.28        | 1.34     |
| 21  | AA    | 370  | C    | N3-C4 | -6.01 | 1.29        | 1.33     |
| 21  | AA    | 519  | C    | C4-N4 | -6.01 | 1.28        | 1.33     |
| 21  | AA    | 1103 | C    | N3-C4 | -6.01 | 1.29        | 1.33     |
| 54  | BA    | 208  | C    | N3-C4 | -6.01 | 1.29        | 1.33     |
| 54  | BA    | 758  | C    | C4-N4 | -6.01 | 1.28        | 1.33     |
| 54  | BA    | 1090 | A    | C5-C4 | -6.01 | 1.34        | 1.38     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 54  | BA    | 1426 | G    | C6-N1 | -6.01 | 1.35        | 1.39     |
| 54  | BA    | 84   | A    | C6-N1 | -6.00 | 1.31        | 1.35     |
| 21  | AA    | 730  | G    | C2-N2 | -6.00 | 1.28        | 1.34     |
| 54  | BA    | 1512 | C    | C4-N4 | -6.00 | 1.28        | 1.33     |
| 54  | BA    | 2    | G    | C6-N1 | -6.00 | 1.35        | 1.39     |
| 21  | AA    | 1169 | A    | C5-C4 | -6.00 | 1.34        | 1.38     |
| 54  | BA    | 2821 | A    | C6-N1 | -6.00 | 1.31        | 1.35     |
| 21  | AA    | 453  | G    | C6-N1 | -6.00 | 1.35        | 1.39     |
| 54  | BA    | 382  | A    | C6-N1 | -6.00 | 1.31        | 1.35     |
| 54  | BA    | 2801 | G    | C2-N2 | -6.00 | 1.28        | 1.34     |
| 21  | AA    | 192  | A    | C5-C4 | -6.00 | 1.34        | 1.38     |
| 54  | BA    | 2342 | C    | N3-C4 | -5.99 | 1.29        | 1.33     |
| 21  | AA    | 614  | C    | C4-N4 | -5.99 | 1.28        | 1.33     |
| 54  | BA    | 729  | G    | C2-N2 | -5.99 | 1.28        | 1.34     |
| 54  | BA    | 1561 | C    | N3-C4 | -5.99 | 1.29        | 1.33     |
| 54  | BA    | 2704 | C    | N3-C4 | -5.99 | 1.29        | 1.33     |
| 54  | BA    | 2712 | C    | C4-N4 | -5.99 | 1.28        | 1.33     |
| 54  | BA    | 2323 | G    | C6-N1 | -5.99 | 1.35        | 1.39     |
| 54  | BA    | 2692 | G    | C6-N1 | -5.99 | 1.35        | 1.39     |
| 55  | BB    | 117  | G    | C2-N2 | -5.99 | 1.28        | 1.34     |
| 54  | BA    | 2369 | A    | C6-N6 | -5.99 | 1.29        | 1.33     |
| 54  | BA    | 2597 | G    | C2-N2 | -5.99 | 1.28        | 1.34     |
| 55  | BB    | 105  | G    | C6-N1 | -5.99 | 1.35        | 1.39     |
| 21  | AA    | 451  | A    | C6-N1 | -5.98 | 1.31        | 1.35     |
| 21  | AA    | 747  | A    | C6-N1 | -5.98 | 1.31        | 1.35     |
| 54  | BA    | 1987 | A    | C6-N6 | -5.98 | 1.29        | 1.33     |
| 22  | A1    | 52   | G    | C6-N1 | -5.98 | 1.35        | 1.39     |
| 21  | AA    | 348  | G    | C2-N2 | -5.98 | 1.28        | 1.34     |
| 21  | AA    | 825  | A    | C6-N1 | -5.98 | 1.31        | 1.35     |
| 21  | AA    | 1409 | C    | N3-C4 | -5.98 | 1.29        | 1.33     |
| 22  | A1    | 41   | A    | C6-N1 | -5.98 | 1.31        | 1.35     |
| 55  | BB    | 105  | G    | C2-N2 | -5.98 | 1.28        | 1.34     |
| 21  | AA    | 1226 | C    | C4-N4 | -5.97 | 1.28        | 1.33     |
| 54  | BA    | 1037 | G    | N1-C2 | -5.97 | 1.32        | 1.37     |
| 21  | AA    | 1416 | G    | C2-N2 | -5.97 | 1.28        | 1.34     |
| 21  | AA    | 940  | C    | N3-C4 | -5.97 | 1.29        | 1.33     |
| 54  | BA    | 2090 | A    | C5-C4 | -5.97 | 1.34        | 1.38     |
| 54  | BA    | 2855 | C    | N3-C4 | -5.97 | 1.29        | 1.33     |
| 54  | BA    | 145  | C    | C4-N4 | -5.96 | 1.28        | 1.33     |
| 54  | BA    | 620  | G    | C2-N2 | -5.96 | 1.28        | 1.34     |
| 54  | BA    | 2285 | C    | C4-N4 | -5.96 | 1.28        | 1.33     |
| 54  | BA    | 2301 | C    | C4-N4 | -5.96 | 1.28        | 1.33     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 54  | BA    | 2379 | G    | C2-N2   | -5.96 | 1.28        | 1.34     |
| 21  | AA    | 868  | C    | C4-N4   | -5.96 | 1.28        | 1.33     |
| 54  | BA    | 845  | A    | C6-N1   | -5.96 | 1.31        | 1.35     |
| 54  | BA    | 58   | G    | C2-N2   | -5.96 | 1.28        | 1.34     |
| 54  | BA    | 1703 | G    | N1-C2   | -5.96 | 1.32        | 1.37     |
| 21  | AA    | 1113 | C    | C4-N4   | -5.96 | 1.28        | 1.33     |
| 21  | AA    | 1133 | G    | C6-N1   | -5.96 | 1.35        | 1.39     |
| 54  | BA    | 730  | A    | C6-N1   | -5.96 | 1.31        | 1.35     |
| 54  | BA    | 1347 | A    | C6-N1   | -5.96 | 1.31        | 1.35     |
| 54  | BA    | 1452 | G    | C2-N2   | -5.96 | 1.28        | 1.34     |
| 21  | AA    | 712  | A    | C4'-C3' | -5.95 | 1.46        | 1.52     |
| 54  | BA    | 1740 | G    | C6-N1   | -5.95 | 1.35        | 1.39     |
| 54  | BA    | 2737 | G    | C2-N2   | -5.95 | 1.28        | 1.34     |
| 54  | BA    | 2824 | C    | N3-C4   | -5.95 | 1.29        | 1.33     |
| 21  | AA    | 1133 | G    | C2-N2   | -5.95 | 1.28        | 1.34     |
| 21  | AA    | 783  | C    | N3-C4   | -5.95 | 1.29        | 1.33     |
| 54  | BA    | 1592 | C    | N3-C4   | -5.95 | 1.29        | 1.33     |
| 54  | BA    | 2023 | C    | N3-C4   | -5.95 | 1.29        | 1.33     |
| 54  | BA    | 2136 | G    | C2-N2   | -5.95 | 1.28        | 1.34     |
| 54  | BA    | 2358 | A    | C6-N6   | -5.95 | 1.29        | 1.33     |
| 21  | AA    | 1084 | G    | C6-N1   | -5.95 | 1.35        | 1.39     |
| 54  | BA    | 2330 | G    | C6-N1   | -5.95 | 1.35        | 1.39     |
| 21  | AA    | 319  | G    | N1-C2   | -5.95 | 1.32        | 1.37     |
| 54  | BA    | 341  | C    | C4-N4   | -5.95 | 1.28        | 1.33     |
| 54  | BA    | 2341 | G    | C2-N2   | -5.94 | 1.28        | 1.34     |
| 54  | BA    | 1276 | A    | C6-N1   | -5.94 | 1.31        | 1.35     |
| 54  | BA    | 1362 | C    | N3-C4   | -5.94 | 1.29        | 1.33     |
| 21  | AA    | 838  | G    | C2-N2   | -5.94 | 1.28        | 1.34     |
| 54  | BA    | 647  | G    | C2-N2   | -5.94 | 1.28        | 1.34     |
| 54  | BA    | 217  | A    | C6-N1   | -5.93 | 1.31        | 1.35     |
| 54  | BA    | 1674 | G    | N1-C2   | -5.93 | 1.33        | 1.37     |
| 21  | AA    | 509  | A    | C5-C4   | -5.93 | 1.34        | 1.38     |
| 54  | BA    | 2896 | C    | C4-N4   | -5.93 | 1.28        | 1.33     |
| 21  | AA    | 394  | G    | C2-N2   | -5.93 | 1.28        | 1.34     |
| 21  | AA    | 1041 | G    | C2-N2   | -5.93 | 1.28        | 1.34     |
| 54  | BA    | 1822 | C    | C4-N4   | -5.93 | 1.28        | 1.33     |
| 54  | BA    | 2208 | C    | N3-C4   | -5.93 | 1.29        | 1.33     |
| 54  | BA    | 2339 | C    | C4-N4   | -5.93 | 1.28        | 1.33     |
| 21  | AA    | 999  | C    | C4-N4   | -5.92 | 1.28        | 1.33     |
| 54  | BA    | 1833 | C    | C4-N4   | -5.92 | 1.28        | 1.33     |
| 54  | BA    | 516  | C    | C4-N4   | -5.92 | 1.28        | 1.33     |
| 54  | BA    | 557  | C    | C4-N4   | -5.92 | 1.28        | 1.33     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 54  | BA    | 1773 | A    | C6-N1 | -5.92 | 1.31        | 1.35     |
| 21  | AA    | 1150 | A    | C6-N1 | -5.92 | 1.31        | 1.35     |
| 21  | AA    | 1422 | G    | C2-N2 | -5.92 | 1.28        | 1.34     |
| 21  | AA    | 449  | G    | C6-N1 | -5.92 | 1.35        | 1.39     |
| 54  | BA    | 316  | C    | C4-N4 | -5.92 | 1.28        | 1.33     |
| 54  | BA    | 1408 | G    | C2-N2 | -5.92 | 1.28        | 1.34     |
| 54  | BA    | 2597 | G    | C6-N1 | -5.92 | 1.35        | 1.39     |
| 21  | AA    | 372  | C    | C4-N4 | -5.91 | 1.28        | 1.33     |
| 21  | AA    | 469  | C    | N3-C4 | -5.91 | 1.29        | 1.33     |
| 54  | BA    | 1134 | A    | C6-N1 | -5.91 | 1.31        | 1.35     |
| 54  | BA    | 1587 | G    | C2-N2 | -5.91 | 1.28        | 1.34     |
| 55  | BB    | 118  | C    | C4-N4 | -5.91 | 1.28        | 1.33     |
| 21  | AA    | 929  | G    | C2-N2 | -5.91 | 1.28        | 1.34     |
| 21  | AA    | 939  | G    | C2-N2 | -5.91 | 1.28        | 1.34     |
| 54  | BA    | 882  | G    | C2-N2 | -5.91 | 1.28        | 1.34     |
| 21  | AA    | 63   | C    | C4-N4 | -5.91 | 1.28        | 1.33     |
| 24  | A3    | 53   | G    | C2-N2 | -5.91 | 1.28        | 1.34     |
| 54  | BA    | 757  | G    | N1-C2 | -5.91 | 1.33        | 1.37     |
| 21  | AA    | 1228 | C    | C4-N4 | -5.91 | 1.28        | 1.33     |
| 21  | AA    | 528  | C    | C4-N4 | -5.91 | 1.28        | 1.33     |
| 21  | AA    | 1164 | G    | N1-C2 | -5.91 | 1.33        | 1.37     |
| 54  | BA    | 1980 | G    | N1-C2 | -5.91 | 1.33        | 1.37     |
| 54  | BA    | 2736 | A    | C6-N1 | -5.90 | 1.31        | 1.35     |
| 54  | BA    | 2851 | A    | C6-N6 | -5.90 | 1.29        | 1.33     |
| 55  | BB    | 86   | G    | C2-N2 | -5.90 | 1.28        | 1.34     |
| 21  | AA    | 349  | A    | C5-C4 | -5.90 | 1.34        | 1.38     |
| 54  | BA    | 1036 | G    | C2-N2 | -5.90 | 1.28        | 1.34     |
| 21  | AA    | 145  | G    | C2-N2 | -5.90 | 1.28        | 1.34     |
| 54  | BA    | 1679 | A    | C5-C4 | -5.90 | 1.34        | 1.38     |
| 21  | AA    | 179  | A    | C6-N1 | -5.90 | 1.31        | 1.35     |
| 54  | BA    | 2890 | G    | C6-N1 | -5.89 | 1.35        | 1.39     |
| 21  | AA    | 40   | C    | C4-N4 | -5.89 | 1.28        | 1.33     |
| 21  | AA    | 1524 | C    | C4-N4 | -5.89 | 1.28        | 1.33     |
| 54  | BA    | 1373 | A    | C6-N1 | -5.89 | 1.31        | 1.35     |
| 54  | BA    | 2201 | G    | C6-N1 | -5.89 | 1.35        | 1.39     |
| 21  | AA    | 1375 | A    | C5-C4 | -5.89 | 1.34        | 1.38     |
| 21  | AA    | 1132 | C    | N3-C4 | -5.89 | 1.29        | 1.33     |
| 22  | A1    | 42   | G    | C6-N1 | -5.89 | 1.35        | 1.39     |
| 21  | AA    | 1411 | C    | N3-C4 | -5.89 | 1.29        | 1.33     |
| 54  | BA    | 585  | G    | C6-N1 | -5.89 | 1.35        | 1.39     |
| 54  | BA    | 2762 | C    | N3-C4 | -5.89 | 1.29        | 1.33     |
| 55  | BB    | 53   | A    | C6-N1 | -5.89 | 1.31        | 1.35     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 21  | AA    | 1482 | G    | C6-N1 | -5.88 | 1.35        | 1.39     |
| 54  | BA    | 536  | G    | C2-N2 | -5.88 | 1.28        | 1.34     |
| 54  | BA    | 1799 | G    | N1-C2 | -5.88 | 1.33        | 1.37     |
| 54  | BA    | 2638 | G    | C6-N1 | -5.88 | 1.35        | 1.39     |
| 54  | BA    | 2854 | G    | C6-N1 | -5.88 | 1.35        | 1.39     |
| 21  | AA    | 1473 | G    | N1-C2 | -5.88 | 1.33        | 1.37     |
| 54  | BA    | 474  | G    | C2-N2 | -5.88 | 1.28        | 1.34     |
| 54  | BA    | 891  | G    | C2-N2 | -5.88 | 1.28        | 1.34     |
| 54  | BA    | 1874 | C    | C4-N4 | -5.88 | 1.28        | 1.33     |
| 54  | BA    | 2633 | G    | C2-N2 | -5.88 | 1.28        | 1.34     |
| 21  | AA    | 1156 | G    | C6-N1 | -5.88 | 1.35        | 1.39     |
| 54  | BA    | 1954 | G    | C6-N1 | -5.88 | 1.35        | 1.39     |
| 21  | AA    | 1031 | C    | N3-C4 | -5.88 | 1.29        | 1.33     |
| 21  | AA    | 478  | A    | C6-N1 | -5.87 | 1.31        | 1.35     |
| 54  | BA    | 450  | G    | N1-C2 | -5.87 | 1.33        | 1.37     |
| 54  | BA    | 2358 | A    | C5-C4 | -5.87 | 1.34        | 1.38     |
| 54  | BA    | 2794 | C    | C4-N4 | -5.87 | 1.28        | 1.33     |
| 21  | AA    | 1340 | A    | C6-N1 | -5.87 | 1.31        | 1.35     |
| 21  | AA    | 1367 | C    | C4-N4 | -5.87 | 1.28        | 1.33     |
| 54  | BA    | 1519 | G    | C2-N2 | -5.87 | 1.28        | 1.34     |
| 54  | BA    | 1527 | G    | C6-N1 | -5.87 | 1.35        | 1.39     |
| 54  | BA    | 2174 | C    | C4-N4 | -5.87 | 1.28        | 1.33     |
| 54  | BA    | 2676 | C    | C4-N4 | -5.87 | 1.28        | 1.33     |
| 54  | BA    | 2813 | A    | C6-N1 | -5.87 | 1.31        | 1.35     |
| 55  | BB    | 16   | G    | C2-N2 | -5.87 | 1.28        | 1.34     |
| 21  | AA    | 658  | C    | C4-N4 | -5.87 | 1.28        | 1.33     |
| 54  | BA    | 1156 | A    | C6-N1 | -5.87 | 1.31        | 1.35     |
| 54  | BA    | 1361 | G    | C6-N1 | -5.87 | 1.35        | 1.39     |
| 54  | BA    | 1587 | G    | C6-N1 | -5.87 | 1.35        | 1.39     |
| 21  | AA    | 127  | G    | C2-N2 | -5.86 | 1.28        | 1.34     |
| 54  | BA    | 1084 | A    | C5-C4 | -5.86 | 1.34        | 1.38     |
| 21  | AA    | 498  | A    | C5-C4 | -5.86 | 1.34        | 1.38     |
| 21  | AA    | 1177 | G    | C6-N1 | -5.86 | 1.35        | 1.39     |
| 54  | BA    | 2602 | A    | C5-C4 | -5.86 | 1.34        | 1.38     |
| 55  | BB    | 70   | C    | C4-N4 | -5.86 | 1.28        | 1.33     |
| 54  | BA    | 2140 | G    | C2-N2 | -5.86 | 1.28        | 1.34     |
| 54  | BA    | 2619 | C    | C4-N4 | -5.86 | 1.28        | 1.33     |
| 55  | BB    | 27   | C    | C4-N4 | -5.86 | 1.28        | 1.33     |
| 21  | AA    | 1418 | A    | C5-C4 | -5.86 | 1.34        | 1.38     |
| 54  | BA    | 1548 | A    | C6-N1 | -5.86 | 1.31        | 1.35     |
| 54  | BA    | 2708 | G    | C2-N2 | -5.86 | 1.28        | 1.34     |
| 54  | BA    | 2618 | G    | C6-N1 | -5.86 | 1.35        | 1.39     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 54  | BA    | 2667 | C    | C4-N4 | -5.86 | 1.28        | 1.33     |
| 54  | BA    | 2887 | A    | C6-N6 | -5.86 | 1.29        | 1.33     |
| 21  | AA    | 506  | G    | C2-N2 | -5.85 | 1.28        | 1.34     |
| 55  | BB    | 49   | C    | C4-N4 | -5.85 | 1.28        | 1.33     |
| 21  | AA    | 664  | G    | C2-N2 | -5.85 | 1.28        | 1.34     |
| 24  | A3    | 17   | C    | C4-N4 | -5.85 | 1.28        | 1.33     |
| 54  | BA    | 651  | G    | C2-N2 | -5.85 | 1.28        | 1.34     |
| 54  | BA    | 420  | C    | N3-C4 | -5.85 | 1.29        | 1.33     |
| 54  | BA    | 1434 | A    | C6-N6 | -5.85 | 1.29        | 1.33     |
| 21  | AA    | 1192 | C    | C4-N4 | -5.85 | 1.28        | 1.33     |
| 54  | BA    | 1389 | G    | C2-N2 | -5.85 | 1.28        | 1.34     |
| 54  | BA    | 1545 | A    | C5-C4 | -5.85 | 1.34        | 1.38     |
| 21  | AA    | 527  | G    | C2-N2 | -5.84 | 1.28        | 1.34     |
| 21  | AA    | 623  | C    | C4-N4 | -5.84 | 1.28        | 1.33     |
| 21  | AA    | 419  | C    | C4-N4 | -5.84 | 1.28        | 1.33     |
| 21  | AA    | 846  | G    | C2-N2 | -5.84 | 1.28        | 1.34     |
| 21  | AA    | 1152 | A    | C5-C4 | -5.84 | 1.34        | 1.38     |
| 21  | AA    | 708  | C    | N3-C4 | -5.84 | 1.29        | 1.33     |
| 54  | BA    | 1677 | A    | C6-N1 | -5.84 | 1.31        | 1.35     |
| 21  | AA    | 290  | C    | C4-N4 | -5.84 | 1.28        | 1.33     |
| 54  | BA    | 1407 | G    | C2-N2 | -5.84 | 1.28        | 1.34     |
| 54  | BA    | 1947 | C    | C4-N4 | -5.84 | 1.28        | 1.33     |
| 54  | BA    | 2330 | G    | C2-N2 | -5.84 | 1.28        | 1.34     |
| 54  | BA    | 1090 | A    | C6-N6 | -5.83 | 1.29        | 1.33     |
| 54  | BA    | 1691 | C    | N3-C4 | -5.83 | 1.29        | 1.33     |
| 21  | AA    | 1483 | A    | C6-N1 | -5.83 | 1.31        | 1.35     |
| 54  | BA    | 439  | A    | C5-C4 | -5.83 | 1.34        | 1.38     |
| 54  | BA    | 544  | C    | C4-N4 | -5.83 | 1.28        | 1.33     |
| 54  | BA    | 1374 | G    | N1-C2 | -5.83 | 1.33        | 1.37     |
| 54  | BA    | 1339 | G    | C2-N2 | -5.83 | 1.28        | 1.34     |
| 54  | BA    | 1382 | G    | C2-N2 | -5.83 | 1.28        | 1.34     |
| 54  | BA    | 2405 | G    | C2-N2 | -5.83 | 1.28        | 1.34     |
| 54  | BA    | 1569 | A    | C6-N1 | -5.83 | 1.31        | 1.35     |
| 54  | BA    | 1598 | A    | C5-C4 | -5.83 | 1.34        | 1.38     |
| 21  | AA    | 175  | C    | C4-N4 | -5.83 | 1.28        | 1.33     |
| 54  | BA    | 1738 | G    | C2-N2 | -5.83 | 1.28        | 1.34     |
| 54  | BA    | 2254 | C    | N3-C4 | -5.83 | 1.29        | 1.33     |
| 54  | BA    | 2815 | C    | C4-N4 | -5.83 | 1.28        | 1.33     |
| 21  | AA    | 359  | G    | C6-N1 | -5.82 | 1.35        | 1.39     |
| 54  | BA    | 2655 | G    | C2-N2 | -5.82 | 1.28        | 1.34     |
| 21  | AA    | 6    | G    | C2-N2 | -5.82 | 1.28        | 1.34     |
| 21  | AA    | 124  | C    | C4-N4 | -5.82 | 1.28        | 1.33     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 54  | BA    | 363  | G    | N1-C2 | -5.82 | 1.33        | 1.37     |
| 54  | BA    | 2040 | G    | N1-C2 | -5.82 | 1.33        | 1.37     |
| 54  | BA    | 2063 | C    | N3-C4 | -5.82 | 1.29        | 1.33     |
| 55  | BB    | 3    | C    | C4-N4 | -5.82 | 1.28        | 1.33     |
| 55  | BB    | 24   | G    | C2-N2 | -5.82 | 1.28        | 1.34     |
| 21  | AA    | 1349 | A    | C6-N1 | -5.82 | 1.31        | 1.35     |
| 54  | BA    | 1901 | A    | C6-N1 | -5.82 | 1.31        | 1.35     |
| 54  | BA    | 2097 | A    | C6-N1 | -5.82 | 1.31        | 1.35     |
| 54  | BA    | 42   | A    | C6-N6 | -5.82 | 1.29        | 1.33     |
| 21  | AA    | 356  | A    | C5-C4 | -5.81 | 1.34        | 1.38     |
| 54  | BA    | 2682 | A    | C6-N1 | -5.81 | 1.31        | 1.35     |
| 54  | BA    | 2872 | A    | C6-N6 | -5.81 | 1.29        | 1.33     |
| 21  | AA    | 1510 | C    | C4-N4 | -5.81 | 1.28        | 1.33     |
| 21  | AA    | 1184 | G    | N1-C2 | -5.81 | 1.33        | 1.37     |
| 54  | BA    | 187  | G    | C2-N2 | -5.81 | 1.28        | 1.34     |
| 54  | BA    | 445  | C    | C4-N4 | -5.81 | 1.28        | 1.33     |
| 54  | BA    | 651  | G    | C6-N1 | -5.81 | 1.35        | 1.39     |
| 54  | BA    | 2239 | G    | C2-N2 | -5.81 | 1.28        | 1.34     |
| 21  | AA    | 1438 | G    | C2-N2 | -5.81 | 1.28        | 1.34     |
| 54  | BA    | 1120 | G    | N1-C2 | -5.81 | 1.33        | 1.37     |
| 54  | BA    | 2032 | G    | C2-N2 | -5.81 | 1.28        | 1.34     |
| 21  | AA    | 385  | C    | N3-C4 | -5.81 | 1.29        | 1.33     |
| 21  | AA    | 395  | C    | N3-C4 | -5.80 | 1.29        | 1.33     |
| 54  | BA    | 7    | G    | C2-N2 | -5.80 | 1.28        | 1.34     |
| 54  | BA    | 2270 | A    | C6-N1 | -5.80 | 1.31        | 1.35     |
| 54  | BA    | 439  | A    | C6-N6 | -5.80 | 1.29        | 1.33     |
| 21  | AA    | 484  | G    | C6-N1 | -5.80 | 1.35        | 1.39     |
| 21  | AA    | 1181 | G    | C2-N2 | -5.80 | 1.28        | 1.34     |
| 21  | AA    | 1331 | G    | C2-N2 | -5.80 | 1.28        | 1.34     |
| 54  | BA    | 209  | C    | C4-N4 | -5.80 | 1.28        | 1.33     |
| 55  | BB    | 33   | G    | C2-N2 | -5.80 | 1.28        | 1.34     |
| 21  | AA    | 305  | G    | C2-N2 | -5.80 | 1.28        | 1.34     |
| 54  | BA    | 2499 | C    | C4-N4 | -5.80 | 1.28        | 1.33     |
| 21  | AA    | 215  | C    | N3-C4 | -5.79 | 1.29        | 1.33     |
| 24  | A3    | 67   | C    | C4-N4 | -5.79 | 1.28        | 1.33     |
| 54  | BA    | 1317 | G    | C2-N2 | -5.79 | 1.28        | 1.34     |
| 54  | BA    | 2282 | G    | C6-N1 | -5.79 | 1.35        | 1.39     |
| 54  | BA    | 2900 | A    | C5-C4 | -5.79 | 1.34        | 1.38     |
| 54  | BA    | 2364 | C    | C4-N4 | -5.79 | 1.28        | 1.33     |
| 21  | AA    | 1365 | G    | C2-N2 | -5.79 | 1.28        | 1.34     |
| 54  | BA    | 1447 | C    | N3-C4 | -5.79 | 1.29        | 1.33     |
| 21  | AA    | 141  | G    | C2-N2 | -5.79 | 1.28        | 1.34     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 21  | AA    | 1182 | G    | C6-N1 | -5.79 | 1.35        | 1.39     |
| 54  | BA    | 2738 | A    | C5-C4 | -5.79 | 1.34        | 1.38     |
| 54  | BA    | 1348 | C    | N3-C4 | -5.78 | 1.29        | 1.33     |
| 54  | BA    | 2080 | A    | C5-C4 | -5.78 | 1.34        | 1.38     |
| 54  | BA    | 1069 | A    | C6-N1 | -5.78 | 1.31        | 1.35     |
| 54  | BA    | 1339 | G    | C6-N1 | -5.78 | 1.35        | 1.39     |
| 54  | BA    | 1684 | G    | C2-N2 | -5.78 | 1.28        | 1.34     |
| 21  | AA    | 852  | G    | C2-N2 | -5.78 | 1.28        | 1.34     |
| 21  | AA    | 1051 | C    | C4-N4 | -5.78 | 1.28        | 1.33     |
| 24  | A3    | 5    | G    | C2-N2 | -5.78 | 1.28        | 1.34     |
| 54  | BA    | 2208 | C    | C4-N4 | -5.78 | 1.28        | 1.33     |
| 54  | BA    | 2263 | C    | N3-C4 | -5.78 | 1.29        | 1.33     |
| 54  | BA    | 122  | G    | C2-N2 | -5.78 | 1.28        | 1.34     |
| 54  | BA    | 2899 | A    | C6-N1 | -5.78 | 1.31        | 1.35     |
| 21  | AA    | 522  | C    | C4-N4 | -5.78 | 1.28        | 1.33     |
| 54  | BA    | 1770 | G    | C2-N2 | -5.78 | 1.28        | 1.34     |
| 54  | BA    | 1961 | C    | C4-N4 | -5.78 | 1.28        | 1.33     |
| 54  | BA    | 2226 | C    | C4-N4 | -5.78 | 1.28        | 1.33     |
| 54  | BA    | 2591 | C    | C4-N4 | -5.78 | 1.28        | 1.33     |
| 55  | BB    | 6    | G    | C2-N2 | -5.78 | 1.28        | 1.34     |
| 54  | BA    | 605  | G    | C2-N2 | -5.77 | 1.28        | 1.34     |
| 54  | BA    | 1073 | A    | C5-C4 | -5.77 | 1.34        | 1.38     |
| 54  | BA    | 2856 | A    | C5-C4 | -5.77 | 1.34        | 1.38     |
| 21  | AA    | 1517 | G    | C6-N1 | -5.77 | 1.35        | 1.39     |
| 54  | BA    | 2369 | A    | C5-C4 | -5.77 | 1.34        | 1.38     |
| 54  | BA    | 417  | C    | C4-N4 | -5.77 | 1.28        | 1.33     |
| 54  | BA    | 2846 | G    | C2-N2 | -5.77 | 1.28        | 1.34     |
| 54  | BA    | 1441 | G    | C6-N1 | -5.77 | 1.35        | 1.39     |
| 54  | BA    | 1975 | G    | N1-C2 | -5.76 | 1.33        | 1.37     |
| 54  | BA    | 837  | C    | N3-C4 | -5.76 | 1.29        | 1.33     |
| 55  | BB    | 101  | A    | C6-N1 | -5.76 | 1.31        | 1.35     |
| 21  | AA    | 34   | C    | C4-N4 | -5.76 | 1.28        | 1.33     |
| 21  | AA    | 1437 | A    | C6-N1 | -5.76 | 1.31        | 1.35     |
| 54  | BA    | 410  | G    | C2-N2 | -5.76 | 1.28        | 1.34     |
| 54  | BA    | 1334 | G    | C2-N2 | -5.76 | 1.28        | 1.34     |
| 21  | AA    | 376  | G    | C6-N1 | -5.76 | 1.35        | 1.39     |
| 21  | AA    | 703  | G    | C2-N2 | -5.76 | 1.28        | 1.34     |
| 21  | AA    | 1415 | G    | C2-N2 | -5.76 | 1.28        | 1.34     |
| 54  | BA    | 2357 | G    | N1-C2 | -5.76 | 1.33        | 1.37     |
| 54  | BA    | 1760 | C    | N3-C4 | -5.76 | 1.29        | 1.33     |
| 21  | AA    | 976  | G    | C2-N2 | -5.76 | 1.28        | 1.34     |
| 21  | AA    | 1467 | C    | C4-N4 | -5.76 | 1.28        | 1.33     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 54  | BA    | 1427 | A    | C5-C4 | -5.76 | 1.34        | 1.38     |
| 54  | BA    | 2607 | G    | C2-N2 | -5.75 | 1.28        | 1.34     |
| 21  | AA    | 839  | C    | C4-N4 | -5.75 | 1.28        | 1.33     |
| 21  | AA    | 1117 | A    | C5-C4 | -5.75 | 1.34        | 1.38     |
| 21  | AA    | 1128 | C    | C4-N4 | -5.75 | 1.28        | 1.33     |
| 54  | BA    | 129  | C    | C4-N4 | -5.75 | 1.28        | 1.33     |
| 54  | BA    | 1123 | C    | N3-C4 | -5.75 | 1.29        | 1.33     |
| 54  | BA    | 2077 | A    | C6-N1 | -5.75 | 1.31        | 1.35     |
| 21  | AA    | 1502 | A    | C6-N1 | -5.75 | 1.31        | 1.35     |
| 21  | AA    | 1504 | G    | N1-C2 | -5.75 | 1.33        | 1.37     |
| 54  | BA    | 1243 | C    | N3-C4 | -5.75 | 1.29        | 1.33     |
| 54  | BA    | 1359 | A    | C5-C4 | -5.75 | 1.34        | 1.38     |
| 54  | BA    | 1771 | C    | N3-C4 | -5.75 | 1.29        | 1.33     |
| 21  | AA    | 313  | A    | C6-N6 | -5.75 | 1.29        | 1.33     |
| 21  | AA    | 383  | A    | C5-C4 | -5.75 | 1.34        | 1.38     |
| 54  | BA    | 2590 | A    | C6-N1 | -5.75 | 1.31        | 1.35     |
| 21  | AA    | 1174 | G    | N1-C2 | -5.75 | 1.33        | 1.37     |
| 54  | BA    | 2241 | A    | C5-C4 | -5.75 | 1.34        | 1.38     |
| 54  | BA    | 2349 | G    | N1-C2 | -5.75 | 1.33        | 1.37     |
| 21  | AA    | 826  | C    | N3-C4 | -5.74 | 1.29        | 1.33     |
| 54  | BA    | 104  | A    | C6-N6 | -5.74 | 1.29        | 1.33     |
| 21  | AA    | 1047 | G    | C2-N2 | -5.74 | 1.28        | 1.34     |
| 54  | BA    | 2297 | A    | C6-N1 | -5.74 | 1.31        | 1.35     |
| 54  | BA    | 612  | G    | N1-C2 | -5.74 | 1.33        | 1.37     |
| 54  | BA    | 1985 | C    | N3-C4 | -5.74 | 1.29        | 1.33     |
| 21  | AA    | 1209 | C    | C4-N4 | -5.74 | 1.28        | 1.33     |
| 54  | BA    | 57   | C    | C4-N4 | -5.74 | 1.28        | 1.33     |
| 54  | BA    | 1989 | G    | C2-N2 | -5.74 | 1.28        | 1.34     |
| 54  | BA    | 2521 | C    | C4-N4 | -5.74 | 1.28        | 1.33     |
| 21  | AA    | 1449 | C    | N3-C4 | -5.73 | 1.29        | 1.33     |
| 54  | BA    | 2030 | A    | C5-C4 | -5.73 | 1.34        | 1.38     |
| 21  | AA    | 354  | G    | C6-N1 | -5.73 | 1.35        | 1.39     |
| 21  | AA    | 496  | A    | C6-N1 | -5.73 | 1.31        | 1.35     |
| 21  | AA    | 447  | G    | C2-N2 | -5.73 | 1.28        | 1.34     |
| 55  | BB    | 79   | G    | C6-N1 | -5.73 | 1.35        | 1.39     |
| 54  | BA    | 1968 | G    | C2-N2 | -5.73 | 1.28        | 1.34     |
| 21  | AA    | 521  | G    | C2-N2 | -5.73 | 1.28        | 1.34     |
| 22  | A1    | 66   | A    | C5-C4 | -5.73 | 1.34        | 1.38     |
| 54  | BA    | 64   | A    | C6-N6 | -5.73 | 1.29        | 1.33     |
| 54  | BA    | 2088 | A    | C6-N1 | -5.73 | 1.31        | 1.35     |
| 54  | BA    | 2217 | G    | N1-C2 | -5.73 | 1.33        | 1.37     |
| 54  | BA    | 2602 | A    | C6-N6 | -5.73 | 1.29        | 1.33     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 21  | AA    | 1094 | G    | C6-N1 | -5.73 | 1.35        | 1.39     |
| 24  | A3    | 77   | A    | C6-N1 | -5.73 | 1.31        | 1.35     |
| 55  | BB    | 96   | G    | N1-C2 | -5.72 | 1.33        | 1.37     |
| 21  | AA    | 1093 | A    | C6-N1 | -5.72 | 1.31        | 1.35     |
| 21  | AA    | 1421 | G    | C6-N1 | -5.72 | 1.35        | 1.39     |
| 54  | BA    | 1630 | A    | C5-C4 | -5.72 | 1.34        | 1.38     |
| 21  | AA    | 468  | A    | C6-N6 | -5.72 | 1.29        | 1.33     |
| 54  | BA    | 352  | A    | C6-N1 | -5.72 | 1.31        | 1.35     |
| 21  | AA    | 450  | G    | C2-N2 | -5.72 | 1.28        | 1.34     |
| 21  | AA    | 799  | G    | N1-C2 | -5.72 | 1.33        | 1.37     |
| 21  | AA    | 803  | G    | N1-C2 | -5.72 | 1.33        | 1.37     |
| 54  | BA    | 14   | A    | C6-N1 | -5.72 | 1.31        | 1.35     |
| 54  | BA    | 1477 | A    | C5-C4 | -5.72 | 1.34        | 1.38     |
| 54  | BA    | 2361 | G    | C2-N2 | -5.72 | 1.28        | 1.34     |
| 54  | BA    | 2425 | A    | C6-N1 | -5.72 | 1.31        | 1.35     |
| 21  | AA    | 371  | A    | C6-N6 | -5.71 | 1.29        | 1.33     |
| 24  | A3    | 54   | G    | C6-N1 | -5.71 | 1.35        | 1.39     |
| 54  | BA    | 55   | G    | N1-C2 | -5.71 | 1.33        | 1.37     |
| 54  | BA    | 1112 | G    | C2-N2 | -5.71 | 1.28        | 1.34     |
| 54  | BA    | 2368 | C    | C4-N4 | -5.71 | 1.28        | 1.33     |
| 54  | BA    | 2862 | G    | N1-C2 | -5.71 | 1.33        | 1.37     |
| 55  | BB    | 2    | G    | C2-N2 | -5.71 | 1.28        | 1.34     |
| 54  | BA    | 2354 | C    | N3-C4 | -5.71 | 1.29        | 1.33     |
| 21  | AA    | 313  | A    | C5-C4 | -5.71 | 1.34        | 1.38     |
| 21  | AA    | 328  | C    | C4-N4 | -5.71 | 1.28        | 1.33     |
| 21  | AA    | 784  | A    | C6-N1 | -5.71 | 1.31        | 1.35     |
| 24  | A3    | 50   | G    | N1-C2 | -5.71 | 1.33        | 1.37     |
| 54  | BA    | 2072 | C    | N3-C4 | -5.71 | 1.29        | 1.33     |
| 54  | BA    | 2304 | G    | C2-N2 | -5.71 | 1.28        | 1.34     |
| 54  | BA    | 1996 | C    | N3-C4 | -5.71 | 1.29        | 1.33     |
| 54  | BA    | 2260 | C    | C4-N4 | -5.71 | 1.28        | 1.33     |
| 54  | BA    | 668  | A    | C6-N1 | -5.71 | 1.31        | 1.35     |
| 54  | BA    | 1645 | G    | C2-N2 | -5.71 | 1.28        | 1.34     |
| 54  | BA    | 173  | A    | C5-C4 | -5.71 | 1.34        | 1.38     |
| 21  | AA    | 445  | G    | N1-C2 | -5.71 | 1.33        | 1.37     |
| 21  | AA    | 568  | G    | C2-N2 | -5.71 | 1.28        | 1.34     |
| 54  | BA    | 63   | A    | C5-C4 | -5.71 | 1.34        | 1.38     |
| 21  | AA    | 237  | G    | C2-N2 | -5.70 | 1.28        | 1.34     |
| 21  | AA    | 353  | A    | C6-N6 | -5.70 | 1.29        | 1.33     |
| 55  | BB    | 117  | G    | C6-N1 | -5.70 | 1.35        | 1.39     |
| 54  | BA    | 2697 | G    | C2-N2 | -5.70 | 1.28        | 1.34     |
| 54  | BA    | 164  | C    | C4-N4 | -5.70 | 1.28        | 1.33     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 21  | AA    | 959  | A    | C5-C4 | -5.70 | 1.34        | 1.38     |
| 21  | AA    | 1466 | C    | N3-C4 | -5.70 | 1.29        | 1.33     |
| 21  | AA    | 1519 | A    | C5-C4 | -5.70 | 1.34        | 1.38     |
| 54  | BA    | 1987 | A    | C5-C4 | -5.70 | 1.34        | 1.38     |
| 21  | AA    | 521  | G    | N1-C2 | -5.69 | 1.33        | 1.37     |
| 54  | BA    | 789  | A    | C6-N1 | -5.69 | 1.31        | 1.35     |
| 21  | AA    | 498  | A    | C6-N6 | -5.69 | 1.29        | 1.33     |
| 54  | BA    | 529  | A    | C5-C4 | -5.69 | 1.34        | 1.38     |
| 54  | BA    | 1087 | G    | C2-N2 | -5.69 | 1.28        | 1.34     |
| 21  | AA    | 553  | A    | C6-N6 | -5.69 | 1.29        | 1.33     |
| 21  | AA    | 1111 | A    | C6-N1 | -5.69 | 1.31        | 1.35     |
| 54  | BA    | 1549 | A    | C5-C4 | -5.69 | 1.34        | 1.38     |
| 54  | BA    | 2190 | G    | C2-N2 | -5.69 | 1.28        | 1.34     |
| 21  | AA    | 226  | G    | C2-N2 | -5.69 | 1.28        | 1.34     |
| 54  | BA    | 377  | G    | C2-N2 | -5.69 | 1.28        | 1.34     |
| 54  | BA    | 1819 | A    | C5-C4 | -5.69 | 1.34        | 1.38     |
| 54  | BA    | 1404 | C    | N3-C4 | -5.69 | 1.29        | 1.33     |
| 54  | BA    | 2639 | A    | C6-N1 | -5.69 | 1.31        | 1.35     |
| 54  | BA    | 2706 | A    | C6-N1 | -5.69 | 1.31        | 1.35     |
| 21  | AA    | 941  | G    | C2-N2 | -5.68 | 1.28        | 1.34     |
| 54  | BA    | 161  | A    | C6-N6 | -5.68 | 1.29        | 1.33     |
| 54  | BA    | 1204 | A    | C6-N6 | -5.68 | 1.29        | 1.33     |
| 21  | AA    | 364  | A    | C5-C4 | -5.68 | 1.34        | 1.38     |
| 54  | BA    | 228  | C    | N3-C4 | -5.68 | 1.29        | 1.33     |
| 54  | BA    | 2498 | C    | C4-N4 | -5.68 | 1.28        | 1.33     |
| 21  | AA    | 844  | G    | C2-N2 | -5.68 | 1.28        | 1.34     |
| 54  | BA    | 1124 | G    | N1-C2 | -5.68 | 1.33        | 1.37     |
| 21  | AA    | 33   | A    | C5-C4 | -5.68 | 1.34        | 1.38     |
| 54  | BA    | 1822 | C    | N3-C4 | -5.68 | 1.29        | 1.33     |
| 54  | BA    | 2090 | A    | C6-N6 | -5.68 | 1.29        | 1.33     |
| 54  | BA    | 2315 | G    | C2-N2 | -5.68 | 1.28        | 1.34     |
| 54  | BA    | 2888 | C    | C4-N4 | -5.68 | 1.28        | 1.33     |
| 54  | BA    | 134  | G    | C2-N2 | -5.67 | 1.28        | 1.34     |
| 54  | BA    | 2748 | A    | C6-N1 | -5.67 | 1.31        | 1.35     |
| 21  | AA    | 1516 | G    | C2-N2 | -5.67 | 1.28        | 1.34     |
| 54  | BA    | 9    | G    | N1-C2 | -5.67 | 1.33        | 1.37     |
| 54  | BA    | 2083 | G    | C6-N1 | -5.67 | 1.35        | 1.39     |
| 21  | AA    | 248  | C    | N3-C4 | -5.67 | 1.29        | 1.33     |
| 24  | A3    | 54   | G    | C2-N2 | -5.67 | 1.28        | 1.34     |
| 54  | BA    | 1210 | G    | C2-N2 | -5.67 | 1.28        | 1.34     |
| 21  | AA    | 111  | G    | N1-C2 | -5.67 | 1.33        | 1.37     |
| 21  | AA    | 569  | C    | N3-C4 | -5.67 | 1.29        | 1.33     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 21  | AA    | 1371 | G    | C2-N2 | -5.67 | 1.28        | 1.34     |
| 54  | BA    | 48   | G    | C6-N1 | -5.67 | 1.35        | 1.39     |
| 54  | BA    | 291  | G    | C6-N1 | -5.67 | 1.35        | 1.39     |
| 54  | BA    | 617  | G    | N1-C2 | -5.67 | 1.33        | 1.37     |
| 54  | BA    | 1382 | G    | C6-N1 | -5.67 | 1.35        | 1.39     |
| 54  | BA    | 1959 | G    | C2-N2 | -5.67 | 1.28        | 1.34     |
| 54  | BA    | 2608 | G    | C2-N2 | -5.67 | 1.28        | 1.34     |
| 21  | AA    | 1169 | A    | C6-N6 | -5.67 | 1.29        | 1.33     |
| 54  | BA    | 1355 | G    | C2-N2 | -5.67 | 1.28        | 1.34     |
| 54  | BA    | 1404 | C    | C4-N4 | -5.67 | 1.28        | 1.33     |
| 54  | BA    | 2726 | A    | C6-N1 | -5.67 | 1.31        | 1.35     |
| 21  | AA    | 554  | A    | N9-C4 | -5.67 | 1.34        | 1.37     |
| 54  | BA    | 42   | A    | C5-C4 | -5.67 | 1.34        | 1.38     |
| 21  | AA    | 68   | G    | C2-N2 | -5.66 | 1.28        | 1.34     |
| 54  | BA    | 1389 | G    | C6-N1 | -5.66 | 1.35        | 1.39     |
| 21  | AA    | 748  | G    | C2-N2 | -5.66 | 1.28        | 1.34     |
| 54  | BA    | 198  | C    | C4-N4 | -5.66 | 1.28        | 1.33     |
| 54  | BA    | 1630 | A    | C6-N6 | -5.66 | 1.29        | 1.33     |
| 54  | BA    | 2371 | G    | C2-N2 | -5.66 | 1.28        | 1.34     |
| 22  | A1    | 2    | G    | C6-N1 | -5.66 | 1.35        | 1.39     |
| 21  | AA    | 77   | A    | C6-N1 | -5.66 | 1.31        | 1.35     |
| 21  | AA    | 442  | G    | C2-N2 | -5.66 | 1.28        | 1.34     |
| 22  | A1    | 66   | A    | C6-N6 | -5.66 | 1.29        | 1.33     |
| 54  | BA    | 362  | A    | C6-N1 | -5.66 | 1.31        | 1.35     |
| 54  | BA    | 1335 | C    | C4-N4 | -5.66 | 1.28        | 1.33     |
| 54  | BA    | 1538 | G    | N1-C2 | -5.66 | 1.33        | 1.37     |
| 54  | BA    | 2228 | G    | C6-N1 | -5.66 | 1.35        | 1.39     |
| 54  | BA    | 2426 | A    | C6-N1 | -5.66 | 1.31        | 1.35     |
| 54  | BA    | 2872 | A    | C5-C4 | -5.66 | 1.34        | 1.38     |
| 21  | AA    | 191  | G    | C6-N1 | -5.65 | 1.35        | 1.39     |
| 54  | BA    | 1314 | C    | C4-N4 | -5.65 | 1.28        | 1.33     |
| 54  | BA    | 1428 | C    | C4-N4 | -5.65 | 1.28        | 1.33     |
| 54  | BA    | 2855 | C    | C4-N4 | -5.65 | 1.28        | 1.33     |
| 21  | AA    | 621  | A    | C6-N1 | -5.65 | 1.31        | 1.35     |
| 21  | AA    | 1500 | A    | C6-N1 | -5.65 | 1.31        | 1.35     |
| 54  | BA    | 2293 | G    | C2-N2 | -5.65 | 1.28        | 1.34     |
| 54  | BA    | 2614 | A    | C6-N6 | -5.65 | 1.29        | 1.33     |
| 54  | BA    | 1295 | C    | C4-N4 | -5.65 | 1.28        | 1.33     |
| 54  | BA    | 2315 | G    | C6-N1 | -5.65 | 1.35        | 1.39     |
| 54  | BA    | 2643 | G    | C2-N2 | -5.65 | 1.28        | 1.34     |
| 54  | BA    | 729  | G    | C6-N1 | -5.65 | 1.35        | 1.39     |
| 54  | BA    | 2651 | C    | C4-N4 | -5.65 | 1.28        | 1.33     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 54  | BA    | 2708 | G    | C6-N1 | -5.65 | 1.35        | 1.39     |
| 24  | A3    | 19   | G    | C6-N1 | -5.65 | 1.35        | 1.39     |
| 54  | BA    | 1204 | A    | C5-C4 | -5.65 | 1.34        | 1.38     |
| 21  | AA    | 481  | G    | C6-N1 | -5.65 | 1.35        | 1.39     |
| 21  | AA    | 1140 | C    | C4-N4 | -5.64 | 1.28        | 1.33     |
| 54  | BA    | 1252 | G    | C2-N2 | -5.64 | 1.28        | 1.34     |
| 54  | BA    | 2127 | G    | C2-N2 | -5.64 | 1.28        | 1.34     |
| 55  | BB    | 39   | A    | C6-N1 | -5.64 | 1.31        | 1.35     |
| 21  | AA    | 1037 | C    | C4-N4 | -5.64 | 1.28        | 1.33     |
| 54  | BA    | 432  | A    | C5-C4 | -5.64 | 1.34        | 1.38     |
| 54  | BA    | 674  | G    | C2-N2 | -5.64 | 1.28        | 1.34     |
| 54  | BA    | 1471 | G    | N1-C2 | -5.64 | 1.33        | 1.37     |
| 21  | AA    | 1338 | G    | N1-C2 | -5.64 | 1.33        | 1.37     |
| 54  | BA    | 809  | G    | C2-N2 | -5.64 | 1.28        | 1.34     |
| 54  | BA    | 1376 | C    | C4-N4 | -5.64 | 1.28        | 1.33     |
| 21  | AA    | 518  | C    | N3-C4 | -5.64 | 1.30        | 1.33     |
| 21  | AA    | 893  | C    | N3-C4 | -5.64 | 1.30        | 1.33     |
| 21  | AA    | 1375 | A    | C6-N6 | -5.64 | 1.29        | 1.33     |
| 54  | BA    | 1351 | C    | N3-C4 | -5.64 | 1.30        | 1.33     |
| 54  | BA    | 1436 | G    | C6-N1 | -5.64 | 1.35        | 1.39     |
| 54  | BA    | 1669 | A    | C6-N1 | -5.64 | 1.31        | 1.35     |
| 54  | BA    | 1681 | G    | C2-N2 | -5.64 | 1.28        | 1.34     |
| 54  | BA    | 2084 | C    | C4-N4 | -5.64 | 1.28        | 1.33     |
| 54  | BA    | 731  | C    | C4-N4 | -5.64 | 1.28        | 1.33     |
| 54  | BA    | 927  | A    | C6-N1 | -5.64 | 1.31        | 1.35     |
| 54  | BA    | 2757 | A    | C5-C4 | -5.64 | 1.34        | 1.38     |
| 21  | AA    | 136  | C    | C4-N4 | -5.64 | 1.28        | 1.33     |
| 21  | AA    | 560  | A    | C5-C4 | -5.64 | 1.34        | 1.38     |
| 54  | BA    | 2693 | G    | N1-C2 | -5.64 | 1.33        | 1.37     |
| 54  | BA    | 1122 | G    | C2-N2 | -5.63 | 1.28        | 1.34     |
| 21  | AA    | 192  | A    | C6-N6 | -5.63 | 1.29        | 1.33     |
| 21  | AA    | 563  | A    | C6-N1 | -5.63 | 1.31        | 1.35     |
| 54  | BA    | 2061 | G    | C2-N2 | -5.63 | 1.28        | 1.34     |
| 21  | AA    | 1042 | A    | C6-N1 | -5.63 | 1.31        | 1.35     |
| 54  | BA    | 104  | A    | C5-C4 | -5.63 | 1.34        | 1.38     |
| 54  | BA    | 109  | C    | C4-N4 | -5.63 | 1.28        | 1.33     |
| 54  | BA    | 281  | C    | N3-C4 | -5.63 | 1.30        | 1.33     |
| 54  | BA    | 1772 | A    | C5-C4 | -5.63 | 1.34        | 1.38     |
| 54  | BA    | 2237 | G    | C2-N2 | -5.63 | 1.28        | 1.34     |
| 54  | BA    | 2824 | C    | C4-N4 | -5.63 | 1.28        | 1.33     |
| 24  | A3    | 65   | G    | C2-N2 | -5.62 | 1.28        | 1.34     |
| 54  | BA    | 1448 | G    | N1-C2 | -5.62 | 1.33        | 1.37     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 22  | A1    | 53   | G    | C6-N1 | -5.62 | 1.35        | 1.39     |
| 21  | AA    | 168  | G    | C2-N2 | -5.62 | 1.28        | 1.34     |
| 54  | BA    | 1802 | A    | C6-N1 | -5.62 | 1.31        | 1.35     |
| 55  | BB    | 26   | C    | C4-N4 | -5.62 | 1.28        | 1.33     |
| 21  | AA    | 984  | C    | N3-C4 | -5.62 | 1.30        | 1.33     |
| 21  | AA    | 371  | A    | C5-C4 | -5.62 | 1.34        | 1.38     |
| 21  | AA    | 1402 | C    | C4-N4 | -5.62 | 1.28        | 1.33     |
| 22  | A1    | 2    | G    | N1-C2 | -5.62 | 1.33        | 1.37     |
| 54  | BA    | 2224 | G    | C6-N1 | -5.62 | 1.35        | 1.39     |
| 54  | BA    | 105  | C    | C4-N4 | -5.62 | 1.28        | 1.33     |
| 54  | BA    | 338  | G    | N1-C2 | -5.62 | 1.33        | 1.37     |
| 54  | BA    | 604  | G    | C2-N2 | -5.62 | 1.28        | 1.34     |
| 54  | BA    | 2084 | C    | N3-C4 | -5.62 | 1.30        | 1.33     |
| 54  | BA    | 1582 | C    | C4-N4 | -5.61 | 1.28        | 1.33     |
| 54  | BA    | 1675 | C    | N3-C4 | -5.61 | 1.30        | 1.33     |
| 54  | BA    | 1008 | A    | C6-N1 | -5.61 | 1.31        | 1.35     |
| 21  | AA    | 915  | A    | C6-N6 | -5.61 | 1.29        | 1.33     |
| 54  | BA    | 144  | A    | C6-N1 | -5.61 | 1.31        | 1.35     |
| 54  | BA    | 282  | A    | C6-N6 | -5.61 | 1.29        | 1.33     |
| 54  | BA    | 1089 | A    | C5-C4 | -5.61 | 1.34        | 1.38     |
| 54  | BA    | 1723 | G    | C2-N2 | -5.61 | 1.28        | 1.34     |
| 54  | BA    | 2789 | C    | N3-C4 | -5.61 | 1.30        | 1.33     |
| 54  | BA    | 172  | A    | C6-N1 | -5.61 | 1.31        | 1.35     |
| 54  | BA    | 285  | G    | C6-N1 | -5.61 | 1.35        | 1.39     |
| 54  | BA    | 2730 | C    | N3-C4 | -5.61 | 1.30        | 1.33     |
| 55  | BB    | 90   | C    | C4-N4 | -5.61 | 1.28        | 1.33     |
| 21  | AA    | 106  | C    | N3-C4 | -5.61 | 1.30        | 1.33     |
| 21  | AA    | 110  | C    | N3-C4 | -5.61 | 1.30        | 1.33     |
| 21  | AA    | 874  | G    | C2-N2 | -5.61 | 1.28        | 1.34     |
| 21  | AA    | 962  | C    | N3-C4 | -5.61 | 1.30        | 1.33     |
| 21  | AA    | 248  | C    | C4-N4 | -5.60 | 1.28        | 1.33     |
| 21  | AA    | 553  | A    | C5-C4 | -5.60 | 1.34        | 1.38     |
| 21  | AA    | 281  | G    | C2-N2 | -5.60 | 1.28        | 1.34     |
| 54  | BA    | 155  | A    | C5-C4 | -5.60 | 1.34        | 1.38     |
| 54  | BA    | 619  | G    | C2-N2 | -5.60 | 1.28        | 1.34     |
| 21  | AA    | 346  | G    | N1-C2 | -5.60 | 1.33        | 1.37     |
| 54  | BA    | 1371 | G    | C2-N2 | -5.60 | 1.28        | 1.34     |
| 54  | BA    | 203  | A    | C6-N1 | -5.60 | 1.31        | 1.35     |
| 54  | BA    | 1084 | A    | C6-N6 | -5.60 | 1.29        | 1.33     |
| 54  | BA    | 1475 | G    | N1-C2 | -5.60 | 1.33        | 1.37     |
| 54  | BA    | 2128 | G    | C6-N1 | -5.60 | 1.35        | 1.39     |
| 54  | BA    | 2761 | A    | C6-N1 | -5.60 | 1.31        | 1.35     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 21  | AA    | 728  | A    | C6-N6   | -5.60 | 1.29        | 1.33     |
| 21  | AA    | 1350 | A    | C5-C4   | -5.60 | 1.34        | 1.38     |
| 54  | BA    | 1601 | G    | C6-N1   | -5.60 | 1.35        | 1.39     |
| 54  | BA    | 2355 | G    | C6-N1   | -5.60 | 1.35        | 1.39     |
| 54  | BA    | 2640 | G    | N1-C2   | -5.60 | 1.33        | 1.37     |
| 22  | A1    | 71   | C    | C4-N4   | -5.59 | 1.28        | 1.33     |
| 54  | BA    | 2365 | G    | C2-N2   | -5.59 | 1.28        | 1.34     |
| 54  | BA    | 2808 | G    | N1-C2   | -5.59 | 1.33        | 1.37     |
| 54  | BA    | 563  | A    | C6-N1   | -5.59 | 1.31        | 1.35     |
| 54  | BA    | 2209 | G    | N1-C2   | -5.59 | 1.33        | 1.37     |
| 54  | BA    | 216  | A    | C6-N1   | -5.59 | 1.31        | 1.35     |
| 54  | BA    | 784  | G    | C2-N2   | -5.59 | 1.28        | 1.34     |
| 54  | BA    | 1878 | G    | C6-N1   | -5.59 | 1.35        | 1.39     |
| 54  | BA    | 2668 | G    | C2-N2   | -5.59 | 1.28        | 1.34     |
| 21  | AA    | 339  | C    | N3-C4   | -5.59 | 1.30        | 1.33     |
| 21  | AA    | 1108 | G    | C6-N1   | -5.59 | 1.35        | 1.39     |
| 54  | BA    | 173  | A    | C6-N6   | -5.59 | 1.29        | 1.33     |
| 54  | BA    | 2232 | C    | C4-N4   | -5.59 | 1.28        | 1.33     |
| 54  | BA    | 2069 | G    | N1-C2   | -5.58 | 1.33        | 1.37     |
| 21  | AA    | 744  | C    | C4-N4   | -5.58 | 1.28        | 1.33     |
| 54  | BA    | 107  | G    | C2-N2   | -5.58 | 1.28        | 1.34     |
| 21  | AA    | 39   | G    | C6-N1   | -5.58 | 1.35        | 1.39     |
| 55  | BB    | 100  | G    | C2-N2   | -5.58 | 1.28        | 1.34     |
| 21  | AA    | 441  | A    | C5-C4   | -5.58 | 1.34        | 1.38     |
| 54  | BA    | 97   | C    | O3'-P   | -5.58 | 1.54        | 1.61     |
| 21  | AA    | 954  | G    | C2-N2   | -5.58 | 1.28        | 1.34     |
| 54  | BA    | 281  | C    | C4-N4   | -5.57 | 1.28        | 1.33     |
| 54  | BA    | 1710 | G    | C6-N1   | -5.57 | 1.35        | 1.39     |
| 55  | BB    | 51   | G    | C2-N2   | -5.57 | 1.28        | 1.34     |
| 54  | BA    | 207  | A    | C6-N1   | -5.57 | 1.31        | 1.35     |
| 54  | BA    | 2140 | G    | C6-N1   | -5.57 | 1.35        | 1.39     |
| 21  | AA    | 1446 | A    | C6-N1   | -5.57 | 1.31        | 1.35     |
| 54  | BA    | 410  | G    | C6-N1   | -5.57 | 1.35        | 1.39     |
| 54  | BA    | 2289 | G    | C6-N1   | -5.57 | 1.35        | 1.39     |
| 21  | AA    | 601  | G    | C4'-O4' | -5.57 | 1.38        | 1.45     |
| 21  | AA    | 1346 | A    | C5-C4   | -5.57 | 1.34        | 1.38     |
| 21  | AA    | 1355 | G    | C2-N2   | -5.57 | 1.28        | 1.34     |
| 54  | BA    | 1718 | G    | C2-N2   | -5.57 | 1.28        | 1.34     |
| 54  | BA    | 299  | A    | C5-C4   | -5.57 | 1.34        | 1.38     |
| 21  | AA    | 1071 | C    | N3-C4   | -5.56 | 1.30        | 1.33     |
| 21  | AA    | 1429 | A    | C5-C4   | -5.56 | 1.34        | 1.38     |
| 22  | A1    | 53   | G    | C2-N2   | -5.56 | 1.28        | 1.34     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 54  | BA    | 2108 | A    | C6-N1 | -5.56 | 1.31        | 1.35     |
| 21  | AA    | 833  | G    | N1-C2 | -5.56 | 1.33        | 1.37     |
| 21  | AA    | 1336 | C    | C4-N4 | -5.56 | 1.28        | 1.33     |
| 54  | BA    | 517  | C    | C4-N4 | -5.56 | 1.28        | 1.33     |
| 54  | BA    | 1378 | A    | C6-N1 | -5.56 | 1.31        | 1.35     |
| 54  | BA    | 1756 | G    | N1-C2 | -5.56 | 1.33        | 1.37     |
| 21  | AA    | 1462 | C    | C4-N4 | -5.56 | 1.28        | 1.33     |
| 54  | BA    | 2227 | A    | C6-N6 | -5.56 | 1.29        | 1.33     |
| 54  | BA    | 2368 | C    | N3-C4 | -5.56 | 1.30        | 1.33     |
| 54  | BA    | 2565 | A    | C6-N1 | -5.56 | 1.31        | 1.35     |
| 54  | BA    | 2782 | G    | C2-N2 | -5.56 | 1.28        | 1.34     |
| 54  | BA    | 210  | C    | C4-N4 | -5.55 | 1.28        | 1.33     |
| 54  | BA    | 883  | G    | N1-C2 | -5.55 | 1.33        | 1.37     |
| 54  | BA    | 1800 | C    | N3-C4 | -5.55 | 1.30        | 1.33     |
| 54  | BA    | 1973 | G    | C6-N1 | -5.55 | 1.35        | 1.39     |
| 21  | AA    | 329  | A    | C6-N1 | -5.55 | 1.31        | 1.35     |
| 54  | BA    | 184  | C    | C4-N4 | -5.55 | 1.28        | 1.33     |
| 54  | BA    | 680  | C    | N3-C4 | -5.55 | 1.30        | 1.33     |
| 21  | AA    | 165  | G    | N1-C2 | -5.55 | 1.33        | 1.37     |
| 54  | BA    | 1986 | C    | C4-N4 | -5.55 | 1.28        | 1.33     |
| 54  | BA    | 2089 | C    | N3-C4 | -5.55 | 1.30        | 1.33     |
| 54  | BA    | 2112 | G    | C6-N1 | -5.55 | 1.35        | 1.39     |
| 54  | BA    | 2616 | C    | C4-N4 | -5.55 | 1.28        | 1.33     |
| 21  | AA    | 105  | G    | C2-N2 | -5.55 | 1.29        | 1.34     |
| 21  | AA    | 1489 | G    | N1-C2 | -5.55 | 1.33        | 1.37     |
| 22  | A1    | 42   | G    | C2-N2 | -5.55 | 1.29        | 1.34     |
| 54  | BA    | 1056 | G    | C2-N2 | -5.55 | 1.29        | 1.34     |
| 54  | BA    | 1752 | C    | N3-C4 | -5.55 | 1.30        | 1.33     |
| 54  | BA    | 1950 | G    | C6-N1 | -5.55 | 1.35        | 1.39     |
| 54  | BA    | 2692 | G    | C2-N2 | -5.55 | 1.29        | 1.34     |
| 21  | AA    | 174  | A    | C6-N1 | -5.54 | 1.31        | 1.35     |
| 54  | BA    | 282  | A    | C5-C4 | -5.54 | 1.34        | 1.38     |
| 54  | BA    | 732  | C    | C4-N4 | -5.54 | 1.28        | 1.33     |
| 54  | BA    | 2660 | A    | C6-N1 | -5.54 | 1.31        | 1.35     |
| 55  | BB    | 23   | G    | C2-N2 | -5.54 | 1.29        | 1.34     |
| 54  | BA    | 1071 | G    | C2-N2 | -5.54 | 1.29        | 1.34     |
| 54  | BA    | 1700 | A    | C5-C4 | -5.54 | 1.34        | 1.38     |
| 54  | BA    | 2606 | C    | C4-N4 | -5.54 | 1.28        | 1.33     |
| 54  | BA    | 2731 | G    | C2-N2 | -5.54 | 1.29        | 1.34     |
| 55  | BB    | 30   | C    | C4-N4 | -5.54 | 1.28        | 1.33     |
| 21  | AA    | 386  | C    | N3-C4 | -5.54 | 1.30        | 1.33     |
| 22  | A1    | 30   | C    | C4-N4 | -5.54 | 1.28        | 1.33     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 54  | BA    | 228  | C    | C4-N4   | -5.54 | 1.28        | 1.33     |
| 54  | BA    | 473  | G    | C6-N1   | -5.54 | 1.35        | 1.39     |
| 54  | BA    | 532  | A    | C5-C4   | -5.54 | 1.34        | 1.38     |
| 54  | BA    | 1958 | C    | N3-C4   | -5.54 | 1.30        | 1.33     |
| 54  | BA    | 2814 | A    | C5-C4   | -5.54 | 1.34        | 1.38     |
| 21  | AA    | 193  | C    | C4-N4   | -5.54 | 1.28        | 1.33     |
| 54  | BA    | 2080 | A    | C6-N6   | -5.54 | 1.29        | 1.33     |
| 54  | BA    | 1986 | C    | N3-C4   | -5.54 | 1.30        | 1.33     |
| 21  | AA    | 732  | C    | C4-N4   | -5.53 | 1.28        | 1.33     |
| 21  | AA    | 1374 | A    | C6-N1   | -5.53 | 1.31        | 1.35     |
| 21  | AA    | 1399 | C    | N3-C4   | -5.53 | 1.30        | 1.33     |
| 54  | BA    | 145  | C    | N3-C4   | -5.53 | 1.30        | 1.33     |
| 54  | BA    | 201  | C    | C4-N4   | -5.53 | 1.28        | 1.33     |
| 54  | BA    | 1431 | A    | C6-N1   | -5.53 | 1.31        | 1.35     |
| 54  | BA    | 1732 | C    | C4-N4   | -5.53 | 1.28        | 1.33     |
| 54  | BA    | 2454 | G    | C2-N2   | -5.53 | 1.29        | 1.34     |
| 21  | AA    | 713  | G    | C4'-C3' | -5.53 | 1.47        | 1.52     |
| 54  | BA    | 1465 | G    | N1-C2   | -5.53 | 1.33        | 1.37     |
| 54  | BA    | 1996 | C    | C4-N4   | -5.53 | 1.28        | 1.33     |
| 54  | BA    | 2624 | G    | C2-N2   | -5.53 | 1.29        | 1.34     |
| 54  | BA    | 1878 | G    | C2-N2   | -5.53 | 1.29        | 1.34     |
| 21  | AA    | 41   | G    | N1-C2   | -5.53 | 1.33        | 1.37     |
| 21  | AA    | 234  | C    | C4-N4   | -5.53 | 1.28        | 1.33     |
| 54  | BA    | 71   | A    | C6-N6   | -5.53 | 1.29        | 1.33     |
| 54  | BA    | 1098 | A    | C5-C4   | -5.53 | 1.34        | 1.38     |
| 21  | AA    | 1170 | A    | C6-N6   | -5.53 | 1.29        | 1.33     |
| 54  | BA    | 295  | G    | C6-N1   | -5.53 | 1.35        | 1.39     |
| 54  | BA    | 467  | G    | C2-N2   | -5.53 | 1.29        | 1.34     |
| 54  | BA    | 728  | G    | C2-N2   | -5.53 | 1.29        | 1.34     |
| 21  | AA    | 1104 | G    | C2-N2   | -5.52 | 1.29        | 1.34     |
| 21  | AA    | 382  | A    | C5-C4   | -5.52 | 1.34        | 1.38     |
| 54  | BA    | 149  | A    | C5-C4   | -5.52 | 1.34        | 1.38     |
| 54  | BA    | 608  | A    | C5-C4   | -5.52 | 1.34        | 1.38     |
| 54  | BA    | 1797 | G    | C2-N2   | -5.52 | 1.29        | 1.34     |
| 54  | BA    | 2777 | G    | C6-N1   | -5.52 | 1.35        | 1.39     |
| 54  | BA    | 63   | A    | C6-N6   | -5.52 | 1.29        | 1.33     |
| 54  | BA    | 386  | G    | C6-N1   | -5.52 | 1.35        | 1.39     |
| 54  | BA    | 445  | C    | N3-C4   | -5.52 | 1.30        | 1.33     |
| 54  | BA    | 684  | G    | C2-N2   | -5.52 | 1.29        | 1.34     |
| 54  | BA    | 1925 | C    | C4-N4   | -5.52 | 1.28        | 1.33     |
| 54  | BA    | 2110 | G    | N1-C2   | -5.52 | 1.33        | 1.37     |
| 21  | AA    | 336  | A    | C5-C4   | -5.52 | 1.34        | 1.38     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 54  | BA    | 49   | A    | C5-C4   | -5.52 | 1.34        | 1.38     |
| 54  | BA    | 1447 | C    | C4-N4   | -5.52 | 1.28        | 1.33     |
| 54  | BA    | 1527 | G    | C2-N2   | -5.52 | 1.29        | 1.34     |
| 21  | AA    | 1081 | A    | C5-C4   | -5.52 | 1.34        | 1.38     |
| 54  | BA    | 447  | A    | C5-C4   | -5.52 | 1.34        | 1.38     |
| 21  | AA    | 44   | A    | C6-N1   | -5.51 | 1.31        | 1.35     |
| 21  | AA    | 312  | C    | C4-N4   | -5.51 | 1.28        | 1.33     |
| 21  | AA    | 1343 | G    | N1-C2   | -5.51 | 1.33        | 1.37     |
| 54  | BA    | 1359 | A    | C6-N1   | -5.51 | 1.31        | 1.35     |
| 54  | BA    | 2543 | G    | C2-N2   | -5.51 | 1.29        | 1.34     |
| 21  | AA    | 1057 | G    | N1-C2   | -5.51 | 1.33        | 1.37     |
| 24  | A3    | 57   | C    | N3-C4   | -5.51 | 1.30        | 1.33     |
| 54  | BA    | 1071 | G    | C6-N1   | -5.51 | 1.35        | 1.39     |
| 21  | AA    | 242  | G    | C2-N2   | -5.51 | 1.29        | 1.34     |
| 54  | BA    | 68   | G    | N1-C2   | -5.51 | 1.33        | 1.37     |
| 21  | AA    | 1147 | C    | C4-N4   | -5.51 | 1.28        | 1.33     |
| 24  | A3    | 2    | G    | N1-C2   | -5.51 | 1.33        | 1.37     |
| 54  | BA    | 426  | C    | N3-C4   | -5.51 | 1.30        | 1.33     |
| 54  | BA    | 1269 | A    | C6-N1   | -5.51 | 1.31        | 1.35     |
| 54  | BA    | 1560 | G    | C2-N2   | -5.51 | 1.29        | 1.34     |
| 54  | BA    | 2379 | G    | C6-N1   | -5.51 | 1.35        | 1.39     |
| 54  | BA    | 2657 | A    | C6-N1   | -5.51 | 1.31        | 1.35     |
| 54  | BA    | 1817 | G    | C2-N2   | -5.50 | 1.29        | 1.34     |
| 21  | AA    | 1343 | G    | C4'-O4' | -5.50 | 1.38        | 1.45     |
| 54  | BA    | 41   | C    | N3-C4   | -5.50 | 1.30        | 1.33     |
| 54  | BA    | 377  | G    | C6-N1   | -5.50 | 1.35        | 1.39     |
| 54  | BA    | 1432 | G    | N1-C2   | -5.50 | 1.33        | 1.37     |
| 54  | BA    | 2221 | G    | C2-N2   | -5.50 | 1.29        | 1.34     |
| 54  | BA    | 2733 | A    | C6-N1   | -5.50 | 1.31        | 1.35     |
| 54  | BA    | 2771 | C    | C4-N4   | -5.50 | 1.28        | 1.33     |
| 54  | BA    | 2822 | G    | C6-N1   | -5.50 | 1.35        | 1.39     |
| 21  | AA    | 164  | G    | C6-N1   | -5.50 | 1.35        | 1.39     |
| 21  | AA    | 1418 | A    | C6-N6   | -5.50 | 1.29        | 1.33     |
| 54  | BA    | 41   | C    | C4-N4   | -5.50 | 1.29        | 1.33     |
| 24  | A3    | 53   | G    | C6-N1   | -5.50 | 1.35        | 1.39     |
| 54  | BA    | 938  | G    | N1-C2   | -5.50 | 1.33        | 1.37     |
| 54  | BA    | 1767 | G    | N1-C2   | -5.50 | 1.33        | 1.37     |
| 21  | AA    | 468  | A    | C5-C4   | -5.49 | 1.34        | 1.38     |
| 54  | BA    | 1710 | G    | C2-N2   | -5.49 | 1.29        | 1.34     |
| 54  | BA    | 2856 | A    | C6-N6   | -5.49 | 1.29        | 1.33     |
| 21  | AA    | 377  | G    | N1-C2   | -5.49 | 1.33        | 1.37     |
| 54  | BA    | 2154 | A    | C6-N1   | -5.49 | 1.31        | 1.35     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 54  | BA    | 322  | A    | C5-C4   | -5.49 | 1.34        | 1.38     |
| 54  | BA    | 647  | G    | C6-N1   | -5.49 | 1.35        | 1.39     |
| 54  | BA    | 1740 | G    | C2-N2   | -5.49 | 1.29        | 1.34     |
| 54  | BA    | 2591 | C    | N3-C4   | -5.49 | 1.30        | 1.33     |
| 21  | AA    | 335  | C    | C4-N4   | -5.49 | 1.29        | 1.33     |
| 21  | AA    | 546  | A    | C4'-C3' | -5.49 | 1.47        | 1.52     |
| 21  | AA    | 998  | C    | C4-N4   | -5.49 | 1.29        | 1.33     |
| 21  | AA    | 1191 | A    | C6-N6   | -5.49 | 1.29        | 1.33     |
| 54  | BA    | 79   | C    | C4-N4   | -5.49 | 1.29        | 1.33     |
| 54  | BA    | 801  | G    | N1-C2   | -5.49 | 1.33        | 1.37     |
| 54  | BA    | 1836 | C    | C4-N4   | -5.49 | 1.29        | 1.33     |
| 54  | BA    | 2179 | C    | N3-C4   | -5.49 | 1.30        | 1.33     |
| 21  | AA    | 873  | A    | C5-C4   | -5.49 | 1.34        | 1.38     |
| 54  | BA    | 1451 | C    | N3-C4   | -5.49 | 1.30        | 1.33     |
| 54  | BA    | 1552 | A    | C6-N1   | -5.49 | 1.31        | 1.35     |
| 54  | BA    | 1696 | G    | N1-C2   | -5.49 | 1.33        | 1.37     |
| 54  | BA    | 115  | C    | N3-C4   | -5.48 | 1.30        | 1.33     |
| 54  | BA    | 2264 | C    | N3-C4   | -5.48 | 1.30        | 1.33     |
| 54  | BA    | 301  | G    | C2-N2   | -5.48 | 1.29        | 1.34     |
| 54  | BA    | 1954 | G    | C2-N2   | -5.48 | 1.29        | 1.34     |
| 54  | BA    | 2060 | A    | C5-C4   | -5.48 | 1.34        | 1.38     |
| 54  | BA    | 71   | A    | C5-C4   | -5.48 | 1.34        | 1.38     |
| 21  | AA    | 1163 | A    | C6-N1   | -5.48 | 1.31        | 1.35     |
| 21  | AA    | 1428 | A    | C6-N6   | -5.48 | 1.29        | 1.33     |
| 21  | AA    | 800  | G    | C2-N2   | -5.48 | 1.29        | 1.34     |
| 54  | BA    | 1867 | G    | C2-N2   | -5.48 | 1.29        | 1.34     |
| 54  | BA    | 2349 | G    | C2-N2   | -5.48 | 1.29        | 1.34     |
| 54  | BA    | 2633 | G    | C6-N1   | -5.48 | 1.35        | 1.39     |
| 54  | BA    | 1665 | A    | C6-N6   | -5.48 | 1.29        | 1.33     |
| 54  | BA    | 2176 | A    | C6-N6   | -5.48 | 1.29        | 1.33     |
| 54  | BA    | 2496 | C    | C4-N4   | -5.47 | 1.29        | 1.33     |
| 54  | BA    | 2755 | C    | N3-C4   | -5.47 | 1.30        | 1.33     |
| 21  | AA    | 418  | C    | C4-N4   | -5.47 | 1.29        | 1.33     |
| 21  | AA    | 474  | G    | N1-C2   | -5.47 | 1.33        | 1.37     |
| 21  | AA    | 1071 | C    | C4-N4   | -5.47 | 1.29        | 1.33     |
| 54  | BA    | 2012 | G    | C2-N2   | -5.47 | 1.29        | 1.34     |
| 21  | AA    | 970  | C    | C4-N4   | -5.47 | 1.29        | 1.33     |
| 54  | BA    | 2608 | G    | C6-N1   | -5.47 | 1.35        | 1.39     |
| 21  | AA    | 386  | C    | C4-N4   | -5.47 | 1.29        | 1.33     |
| 21  | AA    | 1426 | G    | C2-N2   | -5.47 | 1.29        | 1.34     |
| 54  | BA    | 2691 | C    | N3-C4   | -5.47 | 1.30        | 1.33     |
| 55  | BB    | 24   | G    | N1-C2   | -5.47 | 1.33        | 1.37     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 21  | AA    | 1155 | A    | C6-N1 | -5.46 | 1.31        | 1.35     |
| 54  | BA    | 2258 | C    | N3-C4 | -5.46 | 1.30        | 1.33     |
| 54  | BA    | 2688 | G    | N1-C2 | -5.46 | 1.33        | 1.37     |
| 54  | BA    | 442  | G    | C2-N2 | -5.46 | 1.29        | 1.34     |
| 21  | AA    | 1072 | G    | N1-C2 | -5.46 | 1.33        | 1.37     |
| 54  | BA    | 2373 | G    | C2-N2 | -5.46 | 1.29        | 1.34     |
| 54  | BA    | 2719 | G    | C2-N2 | -5.46 | 1.29        | 1.34     |
| 54  | BA    | 2353 | G    | C2-N2 | -5.46 | 1.29        | 1.34     |
| 21  | AA    | 336  | A    | C6-N6 | -5.46 | 1.29        | 1.33     |
| 21  | AA    | 604  | G    | C2-N2 | -5.46 | 1.29        | 1.34     |
| 54  | BA    | 1555 | G    | N1-C2 | -5.46 | 1.33        | 1.37     |
| 54  | BA    | 625  | G    | C2-N2 | -5.46 | 1.29        | 1.34     |
| 54  | BA    | 2136 | G    | C6-N1 | -5.46 | 1.35        | 1.39     |
| 54  | BA    | 1788 | C    | N3-C4 | -5.46 | 1.30        | 1.33     |
| 21  | AA    | 914  | A    | C6-N1 | -5.45 | 1.31        | 1.35     |
| 21  | AA    | 735  | C    | N3-C4 | -5.45 | 1.30        | 1.33     |
| 54  | BA    | 299  | A    | C6-N6 | -5.45 | 1.29        | 1.33     |
| 54  | BA    | 5    | A    | C6-N6 | -5.45 | 1.29        | 1.33     |
| 54  | BA    | 1857 | G    | C2-N2 | -5.45 | 1.29        | 1.34     |
| 54  | BA    | 2123 | G    | C6-N1 | -5.45 | 1.35        | 1.39     |
| 21  | AA    | 1322 | C    | C4-N4 | -5.45 | 1.29        | 1.33     |
| 54  | BA    | 1407 | G    | C6-N1 | -5.45 | 1.35        | 1.39     |
| 54  | BA    | 2253 | G    | C6-N1 | -5.45 | 1.35        | 1.39     |
| 54  | BA    | 208  | C    | C4-N4 | -5.45 | 1.29        | 1.33     |
| 54  | BA    | 1320 | C    | C4-N4 | -5.45 | 1.29        | 1.33     |
| 21  | AA    | 311  | C    | N3-C4 | -5.44 | 1.30        | 1.33     |
| 54  | BA    | 1238 | G    | N1-C2 | -5.44 | 1.33        | 1.37     |
| 54  | BA    | 2226 | C    | N3-C4 | -5.44 | 1.30        | 1.33     |
| 21  | AA    | 620  | C    | C4-N4 | -5.44 | 1.29        | 1.33     |
| 21  | AA    | 1190 | G    | C2-N2 | -5.44 | 1.29        | 1.34     |
| 54  | BA    | 531  | C    | N3-C4 | -5.44 | 1.30        | 1.33     |
| 54  | BA    | 2587 | A    | C6-N6 | -5.44 | 1.29        | 1.33     |
| 54  | BA    | 2782 | G    | C6-N1 | -5.44 | 1.35        | 1.39     |
| 54  | BA    | 2808 | G    | C2-N2 | -5.44 | 1.29        | 1.34     |
| 54  | BA    | 2902 | C    | C4-N4 | -5.44 | 1.29        | 1.33     |
| 55  | BB    | 106  | G    | N1-C2 | -5.44 | 1.33        | 1.37     |
| 54  | BA    | 608  | A    | C6-N6 | -5.44 | 1.29        | 1.33     |
| 54  | BA    | 1063 | G    | C2-N2 | -5.44 | 1.29        | 1.34     |
| 21  | AA    | 212  | G    | N1-C2 | -5.44 | 1.33        | 1.37     |
| 54  | BA    | 48   | G    | C2-N2 | -5.44 | 1.29        | 1.34     |
| 54  | BA    | 2663 | G    | C2-N2 | -5.44 | 1.29        | 1.34     |
| 54  | BA    | 2762 | C    | C4-N4 | -5.44 | 1.29        | 1.33     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 54  | BA    | 56   | A    | C6-N6   | -5.44 | 1.29        | 1.33     |
| 54  | BA    | 1632 | A    | C6-N1   | -5.44 | 1.31        | 1.35     |
| 54  | BA    | 1902 | C    | N3-C4   | -5.43 | 1.30        | 1.33     |
| 21  | AA    | 353  | A    | C5-C4   | -5.43 | 1.34        | 1.38     |
| 21  | AA    | 383  | A    | C6-N6   | -5.43 | 1.29        | 1.33     |
| 21  | AA    | 1112 | C    | N3-C4   | -5.43 | 1.30        | 1.33     |
| 22  | A1    | 68   | C    | C4-N4   | -5.43 | 1.29        | 1.33     |
| 54  | BA    | 804  | A    | C6-N1   | -5.43 | 1.31        | 1.35     |
| 21  | AA    | 92   | U    | C4'-O4' | -5.43 | 1.38        | 1.45     |
| 21  | AA    | 839  | C    | N3-C4   | -5.43 | 1.30        | 1.33     |
| 54  | BA    | 1357 | C    | C4-N4   | -5.43 | 1.29        | 1.33     |
| 54  | BA    | 2053 | G    | C2-N2   | -5.43 | 1.29        | 1.34     |
| 21  | AA    | 664  | G    | N1-C2   | -5.43 | 1.33        | 1.37     |
| 54  | BA    | 301  | G    | C6-N1   | -5.43 | 1.35        | 1.39     |
| 54  | BA    | 372  | G    | C2-N2   | -5.43 | 1.29        | 1.34     |
| 21  | AA    | 1143 | G    | C2-N2   | -5.43 | 1.29        | 1.34     |
| 54  | BA    | 147  | C    | C4-N4   | -5.43 | 1.29        | 1.33     |
| 54  | BA    | 164  | C    | N3-C4   | -5.43 | 1.30        | 1.33     |
| 54  | BA    | 2102 | G    | C2-N2   | -5.43 | 1.29        | 1.34     |
| 54  | BA    | 2444 | G    | N1-C2   | -5.43 | 1.33        | 1.37     |
| 54  | BA    | 2894 | G    | N1-C2   | -5.43 | 1.33        | 1.37     |
| 54  | BA    | 1929 | G    | C2-N2   | -5.42 | 1.29        | 1.34     |
| 21  | AA    | 441  | A    | C6-N6   | -5.42 | 1.29        | 1.33     |
| 54  | BA    | 2014 | A    | C6-N1   | -5.42 | 1.31        | 1.35     |
| 21  | AA    | 566  | G    | C2-N2   | -5.42 | 1.29        | 1.34     |
| 21  | AA    | 1082 | A    | C6-N6   | -5.42 | 1.29        | 1.33     |
| 54  | BA    | 1654 | A    | C6-N6   | -5.42 | 1.29        | 1.33     |
| 21  | AA    | 355  | C    | C4-N4   | -5.42 | 1.29        | 1.33     |
| 21  | AA    | 674  | G    | C6-N1   | -5.42 | 1.35        | 1.39     |
| 21  | AA    | 784  | A    | C5-C4   | -5.42 | 1.34        | 1.38     |
| 54  | BA    | 396  | G    | C2-N2   | -5.42 | 1.29        | 1.34     |
| 21  | AA    | 171  | A    | C5-C4   | -5.42 | 1.34        | 1.38     |
| 21  | AA    | 980  | C    | C4-N4   | -5.42 | 1.29        | 1.33     |
| 21  | AA    | 1365 | G    | C6-N1   | -5.42 | 1.35        | 1.39     |
| 54  | BA    | 277  | G    | N1-C2   | -5.42 | 1.33        | 1.37     |
| 54  | BA    | 1319 | C    | C4-N4   | -5.42 | 1.29        | 1.33     |
| 54  | BA    | 1356 | G    | C2-N2   | -5.42 | 1.29        | 1.34     |
| 55  | BB    | 8    | C    | C4-N4   | -5.42 | 1.29        | 1.33     |
| 21  | AA    | 275  | G    | C6-N1   | -5.42 | 1.35        | 1.39     |
| 21  | AA    | 152  | A    | C6-N1   | -5.41 | 1.31        | 1.35     |
| 21  | AA    | 821  | G    | N1-C2   | -5.41 | 1.33        | 1.37     |
| 21  | AA    | 127  | G    | C6-N1   | -5.41 | 1.35        | 1.39     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 54  | BA    | 155  | A    | C6-N6 | -5.41 | 1.29        | 1.33     |
| 54  | BA    | 637  | A    | C6-N1 | -5.41 | 1.31        | 1.35     |
| 21  | AA    | 1156 | G    | C2-N2 | -5.41 | 1.29        | 1.34     |
| 24  | A3    | 20   | G    | N1-C2 | -5.41 | 1.33        | 1.37     |
| 54  | BA    | 2625 | G    | N1-C2 | -5.41 | 1.33        | 1.37     |
| 21  | AA    | 57   | G    | C2-N2 | -5.41 | 1.29        | 1.34     |
| 21  | AA    | 550  | G    | C2-N2 | -5.41 | 1.29        | 1.34     |
| 21  | AA    | 838  | G    | C6-N1 | -5.41 | 1.35        | 1.39     |
| 21  | AA    | 1136 | C    | C4-N4 | -5.41 | 1.29        | 1.33     |
| 21  | AA    | 1187 | G    | C2-N2 | -5.41 | 1.29        | 1.34     |
| 21  | AA    | 1511 | G    | C2-N2 | -5.41 | 1.29        | 1.34     |
| 54  | BA    | 334  | C    | N3-C4 | -5.41 | 1.30        | 1.33     |
| 54  | BA    | 614  | A    | C6-N1 | -5.41 | 1.31        | 1.35     |
| 54  | BA    | 716  | A    | C5-C4 | -5.41 | 1.34        | 1.38     |
| 54  | BA    | 2191 | A    | C6-N1 | -5.41 | 1.31        | 1.35     |
| 54  | BA    | 2435 | A    | C6-N1 | -5.41 | 1.31        | 1.35     |
| 54  | BA    | 2644 | G    | C6-N1 | -5.41 | 1.35        | 1.39     |
| 54  | BA    | 2705 | A    | C6-N6 | -5.41 | 1.29        | 1.33     |
| 21  | AA    | 145  | G    | C6-N1 | -5.41 | 1.35        | 1.39     |
| 21  | AA    | 570  | G    | N1-C2 | -5.41 | 1.33        | 1.37     |
| 22  | A1    | 32   | C    | N3-C4 | -5.41 | 1.30        | 1.33     |
| 54  | BA    | 396  | G    | C6-N1 | -5.41 | 1.35        | 1.39     |
| 54  | BA    | 103  | A    | C6-N1 | -5.41 | 1.31        | 1.35     |
| 54  | BA    | 2284 | A    | C5-C4 | -5.41 | 1.34        | 1.38     |
| 54  | BA    | 2303 | G    | C2-N2 | -5.41 | 1.29        | 1.34     |
| 54  | BA    | 1430 | G    | C6-N1 | -5.40 | 1.35        | 1.39     |
| 21  | AA    | 661  | G    | C2-N2 | -5.40 | 1.29        | 1.34     |
| 54  | BA    | 1574 | C    | N3-C4 | -5.40 | 1.30        | 1.33     |
| 54  | BA    | 2267 | A    | C5-C4 | -5.40 | 1.34        | 1.38     |
| 21  | AA    | 408  | A    | C6-N1 | -5.40 | 1.31        | 1.35     |
| 21  | AA    | 687  | A    | C6-N1 | -5.40 | 1.31        | 1.35     |
| 54  | BA    | 130  | C    | C4-N4 | -5.40 | 1.29        | 1.33     |
| 54  | BA    | 1265 | A    | C6-N1 | -5.40 | 1.31        | 1.35     |
| 54  | BA    | 1343 | G    | C2-N2 | -5.40 | 1.29        | 1.34     |
| 21  | AA    | 1513 | A    | C5-C4 | -5.40 | 1.34        | 1.38     |
| 54  | BA    | 418  | C    | C4-N4 | -5.40 | 1.29        | 1.33     |
| 21  | AA    | 509  | A    | C6-N6 | -5.40 | 1.29        | 1.33     |
| 54  | BA    | 254  | G    | O3'-P | -5.40 | 1.54        | 1.61     |
| 21  | AA    | 141  | G    | C6-N1 | -5.40 | 1.35        | 1.39     |
| 54  | BA    | 1336 | A    | C6-N6 | -5.40 | 1.29        | 1.33     |
| 21  | AA    | 26   | A    | C5-C4 | -5.39 | 1.34        | 1.38     |
| 54  | BA    | 218  | A    | C5-C4 | -5.39 | 1.34        | 1.38     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 54  | BA    | 1368 | G    | C6-N1   | -5.39 | 1.35        | 1.39     |
| 54  | BA    | 2027 | G    | C2-N2   | -5.39 | 1.29        | 1.34     |
| 21  | AA    | 217  | C    | C4-N4   | -5.39 | 1.29        | 1.33     |
| 21  | AA    | 1401 | G    | N1-C2   | -5.39 | 1.33        | 1.37     |
| 54  | BA    | 796  | C    | N3-C4   | -5.39 | 1.30        | 1.33     |
| 55  | BB    | 26   | C    | N3-C4   | -5.39 | 1.30        | 1.33     |
| 21  | AA    | 227  | G    | C2-N2   | -5.39 | 1.29        | 1.34     |
| 21  | AA    | 425  | G    | C2-N2   | -5.39 | 1.29        | 1.34     |
| 54  | BA    | 225  | C    | C4-N4   | -5.39 | 1.29        | 1.33     |
| 54  | BA    | 2341 | G    | C6-N1   | -5.39 | 1.35        | 1.39     |
| 54  | BA    | 2380 | C    | N3-C4   | -5.39 | 1.30        | 1.33     |
| 21  | AA    | 791  | G    | C4'-O4' | -5.39 | 1.38        | 1.45     |
| 24  | A3    | 76   | C    | C4-N4   | -5.39 | 1.29        | 1.33     |
| 23  | A2    | 91   | A    | C6-N6   | -5.39 | 1.29        | 1.33     |
| 54  | BA    | 2174 | C    | N3-C4   | -5.39 | 1.30        | 1.33     |
| 54  | BA    | 8    | C    | N3-C4   | -5.38 | 1.30        | 1.33     |
| 54  | BA    | 1809 | A    | C6-N1   | -5.38 | 1.31        | 1.35     |
| 54  | BA    | 2829 | A    | C5-C4   | -5.38 | 1.34        | 1.38     |
| 54  | BA    | 267  | C    | C4-N4   | -5.38 | 1.29        | 1.33     |
| 54  | BA    | 1088 | A    | C6-N1   | -5.38 | 1.31        | 1.35     |
| 54  | BA    | 1757 | A    | C6-N1   | -5.38 | 1.31        | 1.35     |
| 54  | BA    | 2734 | A    | C5-C4   | -5.38 | 1.34        | 1.38     |
| 21  | AA    | 1172 | C    | N3-C4   | -5.38 | 1.30        | 1.33     |
| 54  | BA    | 933  | A    | C6-N6   | -5.38 | 1.29        | 1.33     |
| 54  | BA    | 1241 | A    | C6-N6   | -5.38 | 1.29        | 1.33     |
| 54  | BA    | 409  | G    | C2-N2   | -5.38 | 1.29        | 1.34     |
| 54  | BA    | 2658 | C    | C4-N4   | -5.38 | 1.29        | 1.33     |
| 21  | AA    | 402  | G    | N1-C2   | -5.38 | 1.33        | 1.37     |
| 54  | BA    | 544  | C    | N3-C4   | -5.38 | 1.30        | 1.33     |
| 54  | BA    | 2230 | G    | C2-N2   | -5.38 | 1.29        | 1.34     |
| 21  | AA    | 1069 | C    | N3-C4   | -5.38 | 1.30        | 1.33     |
| 54  | BA    | 2367 | G    | C6-N1   | -5.38 | 1.35        | 1.39     |
| 21  | AA    | 1434 | A    | C5-C4   | -5.38 | 1.34        | 1.38     |
| 54  | BA    | 274  | C    | C4-N4   | -5.38 | 1.29        | 1.33     |
| 54  | BA    | 1776 | G    | C2-N2   | -5.38 | 1.29        | 1.34     |
| 54  | BA    | 2389 | G    | C6-N1   | -5.38 | 1.35        | 1.39     |
| 54  | BA    | 2611 | C    | N3-C4   | -5.38 | 1.30        | 1.33     |
| 54  | BA    | 2670 | A    | C5-C4   | -5.38 | 1.34        | 1.38     |
| 54  | BA    | 2679 | A    | C6-N1   | -5.38 | 1.31        | 1.35     |
| 55  | BB    | 17   | C    | N3-C4   | -5.38 | 1.30        | 1.33     |
| 21  | AA    | 1488 | G    | C6-N1   | -5.37 | 1.35        | 1.39     |
| 54  | BA    | 354  | A    | C5-C4   | -5.37 | 1.34        | 1.38     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 54  | BA    | 995  | C    | C4-N4   | -5.37 | 1.29        | 1.33     |
| 54  | BA    | 2128 | G    | C2-N2   | -5.37 | 1.29        | 1.34     |
| 54  | BA    | 2227 | A    | C5-C4   | -5.37 | 1.34        | 1.38     |
| 21  | AA    | 1374 | A    | C5-C4   | -5.37 | 1.34        | 1.38     |
| 54  | BA    | 273  | G    | C2-N2   | -5.37 | 1.29        | 1.34     |
| 54  | BA    | 400  | G    | C2-N2   | -5.37 | 1.29        | 1.34     |
| 54  | BA    | 1064 | C    | N3-C4   | -5.37 | 1.30        | 1.33     |
| 54  | BA    | 1697 | G    | C2-N2   | -5.37 | 1.29        | 1.34     |
| 54  | BA    | 2391 | G    | C2-N2   | -5.37 | 1.29        | 1.34     |
| 21  | AA    | 380  | G    | C2-N2   | -5.37 | 1.29        | 1.34     |
| 54  | BA    | 1792 | G    | N1-C2   | -5.37 | 1.33        | 1.37     |
| 54  | BA    | 2294 | G    | C2-N2   | -5.37 | 1.29        | 1.34     |
| 54  | BA    | 2515 | C    | C4-N4   | -5.37 | 1.29        | 1.33     |
| 24  | A3    | 7    | G    | N1-C2   | -5.37 | 1.33        | 1.37     |
| 21  | AA    | 1508 | A    | C5-C4   | -5.36 | 1.34        | 1.38     |
| 55  | BB    | 36   | C    | C4-N4   | -5.36 | 1.29        | 1.33     |
| 21  | AA    | 573  | A    | C4'-O4' | -5.36 | 1.38        | 1.45     |
| 21  | AA    | 874  | G    | N1-C2   | -5.36 | 1.33        | 1.37     |
| 21  | AA    | 276  | G    | C2-N2   | -5.36 | 1.29        | 1.34     |
| 21  | AA    | 931  | C    | C4-N4   | -5.36 | 1.29        | 1.33     |
| 54  | BA    | 2311 | A    | C6-N1   | -5.36 | 1.31        | 1.35     |
| 21  | AA    | 1254 | A    | O3'-P   | -5.36 | 1.54        | 1.61     |
| 21  | AA    | 1336 | C    | N3-C4   | -5.36 | 1.30        | 1.33     |
| 54  | BA    | 342  | A    | C6-N6   | -5.36 | 1.29        | 1.33     |
| 54  | BA    | 136  | G    | N1-C2   | -5.36 | 1.33        | 1.37     |
| 54  | BA    | 1620 | G    | C2-N2   | -5.36 | 1.29        | 1.34     |
| 54  | BA    | 1984 | G    | C2-N2   | -5.36 | 1.29        | 1.34     |
| 54  | BA    | 2342 | C    | C4-N4   | -5.36 | 1.29        | 1.33     |
| 21  | AA    | 228  | A    | C6-N6   | -5.35 | 1.29        | 1.33     |
| 54  | BA    | 487  | C    | C4-N4   | -5.35 | 1.29        | 1.33     |
| 54  | BA    | 1608 | A    | C6-N1   | -5.35 | 1.31        | 1.35     |
| 54  | BA    | 2781 | A    | C6-N6   | -5.35 | 1.29        | 1.33     |
| 54  | BA    | 223  | A    | C6-N6   | -5.35 | 1.29        | 1.33     |
| 21  | AA    | 462  | G    | C6-N1   | -5.35 | 1.35        | 1.39     |
| 54  | BA    | 1014 | A    | O3'-P   | -5.35 | 1.54        | 1.61     |
| 54  | BA    | 2280 | G    | C2-N2   | -5.35 | 1.29        | 1.34     |
| 54  | BA    | 2801 | G    | C6-N1   | -5.35 | 1.35        | 1.39     |
| 21  | AA    | 247  | G    | C6-N1   | -5.35 | 1.35        | 1.39     |
| 21  | AA    | 324  | G    | N1-C2   | -5.35 | 1.33        | 1.37     |
| 21  | AA    | 352  | C    | N3-C4   | -5.35 | 1.30        | 1.33     |
| 54  | BA    | 914  | G    | N1-C2   | -5.35 | 1.33        | 1.37     |
| 54  | BA    | 1034 | G    | C2-N2   | -5.35 | 1.29        | 1.34     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 54  | BA    | 2199 | A    | C6-N6   | -5.35 | 1.29        | 1.33     |
| 54  | BA    | 2686 | G    | C2-N2   | -5.35 | 1.29        | 1.34     |
| 54  | BA    | 1092 | C    | C4-N4   | -5.35 | 1.29        | 1.33     |
| 54  | BA    | 1353 | A    | C6-N1   | -5.35 | 1.31        | 1.35     |
| 21  | AA    | 872  | A    | C5-C4   | -5.34 | 1.35        | 1.38     |
| 21  | AA    | 1191 | A    | C5-C4   | -5.34 | 1.35        | 1.38     |
| 54  | BA    | 2024 | G    | N1-C2   | -5.34 | 1.33        | 1.37     |
| 24  | A3    | 29   | C    | C4-N4   | -5.34 | 1.29        | 1.33     |
| 54  | BA    | 910  | A    | C6-N1   | -5.34 | 1.31        | 1.35     |
| 54  | BA    | 1676 | A    | C8-N7   | -5.34 | 1.27        | 1.31     |
| 21  | AA    | 664  | G    | C6-N1   | -5.34 | 1.35        | 1.39     |
| 54  | BA    | 297  | G    | N1-C2   | -5.34 | 1.33        | 1.37     |
| 54  | BA    | 1557 | C    | C4-N4   | -5.34 | 1.29        | 1.33     |
| 54  | BA    | 2061 | G    | C6-N1   | -5.34 | 1.35        | 1.39     |
| 54  | BA    | 2846 | G    | C6-N1   | -5.34 | 1.35        | 1.39     |
| 54  | BA    | 2170 | A    | C5-C4   | -5.34 | 1.35        | 1.38     |
| 54  | BA    | 2862 | G    | C2-N2   | -5.34 | 1.29        | 1.34     |
| 24  | A3    | 1    | C    | N3-C4   | -5.33 | 1.30        | 1.33     |
| 54  | BA    | 1241 | A    | C5-C4   | -5.33 | 1.35        | 1.38     |
| 55  | BB    | 81   | G    | C2-N2   | -5.33 | 1.29        | 1.34     |
| 21  | AA    | 1158 | C    | C4-N4   | -5.33 | 1.29        | 1.33     |
| 21  | AA    | 1422 | G    | C6-N1   | -5.33 | 1.35        | 1.39     |
| 54  | BA    | 1567 | G    | O3'-P   | -5.33 | 1.54        | 1.61     |
| 54  | BA    | 1785 | A    | C6-N6   | -5.33 | 1.29        | 1.33     |
| 54  | BA    | 2230 | G    | N1-C2   | -5.33 | 1.33        | 1.37     |
| 21  | AA    | 93   | U    | C4'-O4' | -5.33 | 1.38        | 1.45     |
| 54  | BA    | 2089 | C    | C4-N4   | -5.33 | 1.29        | 1.33     |
| 21  | AA    | 1225 | A    | C6-N1   | -5.33 | 1.31        | 1.35     |
| 21  | AA    | 191  | G    | C2-N2   | -5.33 | 1.29        | 1.34     |
| 54  | BA    | 1572 | A    | C5-C4   | -5.33 | 1.35        | 1.38     |
| 54  | BA    | 2420 | C    | C4-N4   | -5.33 | 1.29        | 1.33     |
| 54  | BA    | 297  | G    | C2-N2   | -5.32 | 1.29        | 1.34     |
| 54  | BA    | 1124 | G    | C2-N2   | -5.32 | 1.29        | 1.34     |
| 54  | BA    | 1364 | G    | N1-C2   | -5.32 | 1.33        | 1.37     |
| 54  | BA    | 1726 | C    | C4-N4   | -5.32 | 1.29        | 1.33     |
| 54  | BA    | 2831 | G    | C2-N2   | -5.32 | 1.29        | 1.34     |
| 21  | AA    | 331  | G    | C2-N2   | -5.32 | 1.29        | 1.34     |
| 21  | AA    | 576  | C    | O3'-P   | -5.32 | 1.54        | 1.61     |
| 54  | BA    | 604  | G    | C6-N1   | -5.32 | 1.35        | 1.39     |
| 21  | AA    | 780  | A    | C6-N6   | -5.32 | 1.29        | 1.33     |
| 54  | BA    | 446  | G    | N1-C2   | -5.32 | 1.33        | 1.37     |
| 54  | BA    | 873  | C    | C4-N4   | -5.32 | 1.29        | 1.33     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 54  | BA    | 676  | A    | C5-C4 | -5.32 | 1.35        | 1.38     |
| 54  | BA    | 2545 | G    | C2-N2 | -5.32 | 1.29        | 1.34     |
| 21  | AA    | 162  | A    | C6-N6 | -5.32 | 1.29        | 1.33     |
| 24  | A3    | 77   | A    | C5-C4 | -5.32 | 1.35        | 1.38     |
| 54  | BA    | 2812 | G    | C2-N2 | -5.32 | 1.29        | 1.34     |
| 54  | BA    | 2722 | G    | N1-C2 | -5.32 | 1.33        | 1.37     |
| 21  | AA    | 1105 | A    | C5-C4 | -5.31 | 1.35        | 1.38     |
| 54  | BA    | 294  | A    | C5-C4 | -5.31 | 1.35        | 1.38     |
| 21  | AA    | 305  | G    | N1-C2 | -5.31 | 1.33        | 1.37     |
| 54  | BA    | 1920 | C    | C4-N4 | -5.31 | 1.29        | 1.33     |
| 54  | BA    | 1099 | G    | C2-N2 | -5.31 | 1.29        | 1.34     |
| 54  | BA    | 1633 | G    | N1-C2 | -5.31 | 1.33        | 1.37     |
| 54  | BA    | 232  | G    | C2-N2 | -5.31 | 1.29        | 1.34     |
| 54  | BA    | 279  | A    | C6-N1 | -5.31 | 1.31        | 1.35     |
| 54  | BA    | 294  | A    | C6-N6 | -5.31 | 1.29        | 1.33     |
| 54  | BA    | 1093 | G    | C2-N2 | -5.31 | 1.29        | 1.34     |
| 55  | BB    | 21   | G    | C2-N2 | -5.31 | 1.29        | 1.34     |
| 21  | AA    | 858  | G    | C2-N2 | -5.31 | 1.29        | 1.34     |
| 21  | AA    | 1105 | A    | C6-N6 | -5.31 | 1.29        | 1.33     |
| 54  | BA    | 1363 | C    | C4-N4 | -5.31 | 1.29        | 1.33     |
| 21  | AA    | 425  | G    | C6-N1 | -5.30 | 1.35        | 1.39     |
| 54  | BA    | 188  | G    | N1-C2 | -5.30 | 1.33        | 1.37     |
| 54  | BA    | 2887 | A    | C5-C4 | -5.30 | 1.35        | 1.38     |
| 21  | AA    | 860  | A    | C6-N6 | -5.30 | 1.29        | 1.33     |
| 21  | AA    | 1523 | G    | N1-C2 | -5.30 | 1.33        | 1.37     |
| 54  | BA    | 1232 | G    | C2-N2 | -5.30 | 1.29        | 1.34     |
| 21  | AA    | 522  | C    | N3-C4 | -5.30 | 1.30        | 1.33     |
| 21  | AA    | 826  | C    | C4-N4 | -5.30 | 1.29        | 1.33     |
| 21  | AA    | 1003 | G    | C2-N2 | -5.30 | 1.29        | 1.34     |
| 54  | BA    | 1278 | C    | C4-N4 | -5.30 | 1.29        | 1.33     |
| 54  | BA    | 2212 | A    | C6-N6 | -5.30 | 1.29        | 1.33     |
| 54  | BA    | 2592 | G    | C8-N7 | -5.30 | 1.27        | 1.30     |
| 21  | AA    | 175  | C    | N3-C4 | -5.30 | 1.30        | 1.33     |
| 21  | AA    | 1187 | G    | C6-N1 | -5.30 | 1.35        | 1.39     |
| 54  | BA    | 2440 | C    | C4-N4 | -5.30 | 1.29        | 1.33     |
| 54  | BA    | 341  | C    | N3-C4 | -5.29 | 1.30        | 1.33     |
| 54  | BA    | 2114 | A    | C5-C4 | -5.29 | 1.35        | 1.38     |
| 21  | AA    | 356  | A    | C6-N6 | -5.29 | 1.29        | 1.33     |
| 21  | AA    | 860  | A    | C5-C4 | -5.29 | 1.35        | 1.38     |
| 21  | AA    | 861  | G    | C2-N2 | -5.29 | 1.29        | 1.34     |
| 54  | BA    | 640  | C    | N3-C4 | -5.29 | 1.30        | 1.33     |
| 54  | BA    | 1479 | G    | C2-N2 | -5.29 | 1.29        | 1.34     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 54  | BA    | 1493 | C    | C4-N4   | -5.29 | 1.29        | 1.33     |
| 54  | BA    | 2749 | A    | C5-C4   | -5.29 | 1.35        | 1.38     |
| 21  | AA    | 370  | C    | C4-N4   | -5.29 | 1.29        | 1.33     |
| 21  | AA    | 525  | C    | C4-N4   | -5.29 | 1.29        | 1.33     |
| 54  | BA    | 429  | A    | C6-N1   | -5.29 | 1.31        | 1.35     |
| 54  | BA    | 1654 | A    | C5-C4   | -5.29 | 1.35        | 1.38     |
| 54  | BA    | 2055 | C    | N3-C4   | -5.29 | 1.30        | 1.33     |
| 21  | AA    | 1429 | A    | C5'-C4' | 5.29  | 1.57        | 1.51     |
| 54  | BA    | 101  | A    | C6-N1   | -5.29 | 1.31        | 1.35     |
| 54  | BA    | 2738 | A    | C6-N6   | -5.29 | 1.29        | 1.33     |
| 21  | AA    | 510  | A    | C5-C4   | -5.29 | 1.35        | 1.38     |
| 24  | A3    | 71   | G    | C6-N1   | -5.29 | 1.35        | 1.39     |
| 54  | BA    | 333  | G    | C2-N2   | -5.29 | 1.29        | 1.34     |
| 54  | BA    | 2652 | C    | C4-N4   | -5.29 | 1.29        | 1.33     |
| 21  | AA    | 1217 | C    | C4-N4   | -5.29 | 1.29        | 1.33     |
| 54  | BA    | 269  | C    | N3-C4   | -5.29 | 1.30        | 1.33     |
| 54  | BA    | 712  | G    | N1-C2   | -5.29 | 1.33        | 1.37     |
| 54  | BA    | 1429 | G    | C2-N2   | -5.29 | 1.29        | 1.34     |
| 54  | BA    | 1435 | G    | C2-N2   | -5.29 | 1.29        | 1.34     |
| 54  | BA    | 2598 | A    | C6-N1   | -5.29 | 1.31        | 1.35     |
| 54  | BA    | 2819 | G    | N1-C2   | -5.29 | 1.33        | 1.37     |
| 21  | AA    | 530  | G    | N1-C2   | -5.28 | 1.33        | 1.37     |
| 21  | AA    | 797  | C    | C4-N4   | -5.28 | 1.29        | 1.33     |
| 54  | BA    | 579  | G    | O3'-P   | -5.28 | 1.54        | 1.61     |
| 54  | BA    | 681  | G    | N1-C2   | -5.28 | 1.33        | 1.37     |
| 54  | BA    | 1256 | G    | C2-N2   | -5.28 | 1.29        | 1.34     |
| 54  | BA    | 1810 | A    | C6-N1   | -5.28 | 1.31        | 1.35     |
| 54  | BA    | 2829 | A    | C6-N6   | -5.28 | 1.29        | 1.33     |
| 55  | BB    | 73   | A    | C6-N6   | -5.28 | 1.29        | 1.33     |
| 22  | A1    | 15   | G    | C2-N2   | -5.28 | 1.29        | 1.34     |
| 54  | BA    | 520  | G    | C2-N2   | -5.28 | 1.29        | 1.34     |
| 54  | BA    | 2501 | C    | O3'-P   | -5.28 | 1.54        | 1.61     |
| 22  | A1    | 75   | C    | C4-N4   | -5.28 | 1.29        | 1.33     |
| 54  | BA    | 354  | A    | C6-N6   | -5.28 | 1.29        | 1.33     |
| 54  | BA    | 1766 | G    | N1-C2   | -5.28 | 1.33        | 1.37     |
| 21  | AA    | 881  | G    | N1-C2   | -5.27 | 1.33        | 1.37     |
| 21  | AA    | 1385 | G    | C2-N2   | -5.27 | 1.29        | 1.34     |
| 54  | BA    | 1724 | G    | C6-N1   | -5.27 | 1.35        | 1.39     |
| 54  | BA    | 2049 | G    | C6-N1   | -5.27 | 1.35        | 1.39     |
| 54  | BA    | 2124 | G    | C2-N2   | -5.27 | 1.29        | 1.34     |
| 21  | AA    | 807  | A    | C4'-C3' | -5.27 | 1.47        | 1.52     |
| 21  | AA    | 1423 | G    | N1-C2   | -5.27 | 1.33        | 1.37     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 54  | BA    | 937  | C    | C4-N4   | -5.27 | 1.29        | 1.33     |
| 54  | BA    | 1981 | A    | C5-C4   | -5.27 | 1.35        | 1.38     |
| 55  | BB    | 35   | C    | C4-N4   | -5.27 | 1.29        | 1.33     |
| 21  | AA    | 57   | G    | N1-C2   | -5.27 | 1.33        | 1.37     |
| 54  | BA    | 805  | G    | C2-N2   | -5.27 | 1.29        | 1.34     |
| 54  | BA    | 1236 | G    | C2-N2   | -5.27 | 1.29        | 1.34     |
| 54  | BA    | 381  | G    | C2-N2   | -5.27 | 1.29        | 1.34     |
| 54  | BA    | 1118 | C    | C4-N4   | -5.27 | 1.29        | 1.33     |
| 54  | BA    | 2716 | C    | N3-C4   | -5.27 | 1.30        | 1.33     |
| 21  | AA    | 230  | G    | C2-N2   | -5.27 | 1.29        | 1.34     |
| 21  | AA    | 1080 | A    | C6-N1   | -5.27 | 1.31        | 1.35     |
| 54  | BA    | 1135 | C    | O3'-P   | -5.27 | 1.54        | 1.61     |
| 54  | BA    | 1420 | A    | C6-N6   | -5.27 | 1.29        | 1.33     |
| 21  | AA    | 1358 | U    | C4'-O4' | -5.26 | 1.38        | 1.45     |
| 21  | AA    | 1405 | G    | C6-N1   | -5.26 | 1.35        | 1.39     |
| 54  | BA    | 1571 | A    | C5-C4   | -5.26 | 1.35        | 1.38     |
| 21  | AA    | 115  | G    | N1-C2   | -5.26 | 1.33        | 1.37     |
| 21  | AA    | 149  | A    | C6-N6   | -5.26 | 1.29        | 1.33     |
| 21  | AA    | 888  | G    | C4'-O4' | -5.26 | 1.38        | 1.45     |
| 54  | BA    | 577  | G    | C2-N2   | -5.26 | 1.29        | 1.34     |
| 54  | BA    | 2036 | C    | C4-N4   | -5.26 | 1.29        | 1.33     |
| 21  | AA    | 958  | A    | C6-N6   | -5.26 | 1.29        | 1.33     |
| 54  | BA    | 529  | A    | C6-N6   | -5.26 | 1.29        | 1.33     |
| 54  | BA    | 740  | C    | N3-C4   | -5.26 | 1.30        | 1.33     |
| 54  | BA    | 1785 | A    | C5-C4   | -5.26 | 1.35        | 1.38     |
| 54  | BA    | 2383 | G    | C2-N2   | -5.26 | 1.29        | 1.34     |
| 21  | AA    | 413  | G    | C2-N2   | -5.26 | 1.29        | 1.34     |
| 21  | AA    | 604  | G    | C6-N1   | -5.26 | 1.35        | 1.39     |
| 54  | BA    | 177  | G    | C2-N2   | -5.26 | 1.29        | 1.34     |
| 54  | BA    | 2124 | G    | N1-C2   | -5.26 | 1.33        | 1.37     |
| 54  | BA    | 2744 | G    | N1-C2   | -5.26 | 1.33        | 1.37     |
| 21  | AA    | 128  | G    | C2-N2   | -5.25 | 1.29        | 1.34     |
| 21  | AA    | 444  | G    | C6-N1   | -5.25 | 1.35        | 1.39     |
| 54  | BA    | 2825 | G    | N1-C2   | -5.25 | 1.33        | 1.37     |
| 21  | AA    | 362  | G    | C2-N2   | -5.25 | 1.29        | 1.34     |
| 21  | AA    | 1362 | A    | C6-N1   | -5.25 | 1.31        | 1.35     |
| 54  | BA    | 1631 | G    | C2-N2   | -5.25 | 1.29        | 1.34     |
| 54  | BA    | 1819 | A    | C6-N6   | -5.25 | 1.29        | 1.33     |
| 54  | BA    | 2032 | G    | C6-N1   | -5.25 | 1.35        | 1.39     |
| 55  | BB    | 98   | G    | C6-N1   | -5.25 | 1.35        | 1.39     |
| 21  | AA    | 1204 | A    | C5-C4   | -5.25 | 1.35        | 1.38     |
| 21  | AA    | 1467 | C    | N3-C4   | -5.25 | 1.30        | 1.33     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 21  | AA    | 1519 | A    | C6-N6   | -5.25 | 1.29        | 1.33     |
| 54  | BA    | 739  | A    | C6-N1   | -5.25 | 1.31        | 1.35     |
| 21  | AA    | 925  | G    | C2-N2   | -5.25 | 1.29        | 1.34     |
| 54  | BA    | 143  | C    | N3-C4   | -5.25 | 1.30        | 1.33     |
| 54  | BA    | 250  | G    | C2-N2   | -5.25 | 1.29        | 1.34     |
| 54  | BA    | 1045 | C    | C4-N4   | -5.25 | 1.29        | 1.33     |
| 54  | BA    | 1248 | G    | C2-N2   | -5.25 | 1.29        | 1.34     |
| 54  | BA    | 1611 | C    | C4-N4   | -5.25 | 1.29        | 1.33     |
| 21  | AA    | 446  | G    | N1-C2   | -5.25 | 1.33        | 1.37     |
| 21  | AA    | 502  | A    | C4'-O4' | -5.25 | 1.38        | 1.45     |
| 54  | BA    | 376  | G    | C2-N2   | -5.25 | 1.29        | 1.34     |
| 54  | BA    | 1399 | C    | C4-N4   | -5.25 | 1.29        | 1.33     |
| 54  | BA    | 2097 | A    | C5-C4   | -5.25 | 1.35        | 1.38     |
| 54  | BA    | 35   | G    | C2-N2   | -5.25 | 1.29        | 1.34     |
| 54  | BA    | 528  | A    | C6-N6   | -5.25 | 1.29        | 1.33     |
| 54  | BA    | 2037 | A    | C6-N1   | -5.25 | 1.31        | 1.35     |
| 21  | AA    | 310  | G    | C2-N2   | -5.24 | 1.29        | 1.34     |
| 21  | AA    | 903  | G    | O3'-P   | -5.24 | 1.54        | 1.61     |
| 54  | BA    | 1607 | C    | N3-C4   | -5.24 | 1.30        | 1.33     |
| 54  | BA    | 2830 | C    | C4-N4   | -5.24 | 1.29        | 1.33     |
| 55  | BB    | 76   | G    | N1-C2   | -5.24 | 1.33        | 1.37     |
| 21  | AA    | 918  | A    | C6-N1   | -5.24 | 1.31        | 1.35     |
| 24  | A3    | 7    | G    | C2-N2   | -5.24 | 1.29        | 1.34     |
| 54  | BA    | 656  | G    | C2-N2   | -5.24 | 1.29        | 1.34     |
| 54  | BA    | 930  | G    | C2-N2   | -5.24 | 1.29        | 1.34     |
| 54  | BA    | 1615 | C    | C4-N4   | -5.24 | 1.29        | 1.33     |
| 54  | BA    | 2314 | A    | C6-N1   | -5.24 | 1.31        | 1.35     |
| 21  | AA    | 1200 | C    | N3-C4   | -5.24 | 1.30        | 1.33     |
| 54  | BA    | 442  | G    | C6-N1   | -5.24 | 1.35        | 1.39     |
| 54  | BA    | 2156 | G    | C2-N2   | -5.24 | 1.29        | 1.34     |
| 21  | AA    | 746  | A    | C6-N1   | -5.24 | 1.31        | 1.35     |
| 54  | BA    | 1380 | G    | N1-C2   | -5.24 | 1.33        | 1.37     |
| 54  | BA    | 1616 | A    | C6-N1   | -5.24 | 1.31        | 1.35     |
| 54  | BA    | 1974 | C    | C4-N4   | -5.24 | 1.29        | 1.33     |
| 21  | AA    | 1092 | A    | N9-C4   | -5.23 | 1.34        | 1.37     |
| 21  | AA    | 147  | G    | C2-N2   | -5.23 | 1.29        | 1.34     |
| 54  | BA    | 64   | A    | C5-C4   | -5.23 | 1.35        | 1.38     |
| 55  | BB    | 2    | G    | N1-C2   | -5.23 | 1.33        | 1.37     |
| 21  | AA    | 318  | G    | N1-C2   | -5.23 | 1.33        | 1.37     |
| 54  | BA    | 711  | G    | C2-N2   | -5.23 | 1.29        | 1.34     |
| 54  | BA    | 1464 | G    | C2-N2   | -5.23 | 1.29        | 1.34     |
| 54  | BA    | 1068 | G    | N1-C2   | -5.23 | 1.33        | 1.37     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 54  | BA    | 1533 | C    | C4-N4   | -5.23 | 1.29        | 1.33     |
| 21  | AA    | 1204 | A    | C6-N6   | -5.22 | 1.29        | 1.33     |
| 54  | BA    | 1369 | G    | N1-C2   | -5.22 | 1.33        | 1.37     |
| 54  | BA    | 1489 | C    | C4-N4   | -5.22 | 1.29        | 1.33     |
| 54  | BA    | 1772 | A    | C6-N6   | -5.22 | 1.29        | 1.33     |
| 54  | BA    | 2803 | G    | N1-C2   | -5.22 | 1.33        | 1.37     |
| 21  | AA    | 1095 | U    | C4'-O4' | -5.22 | 1.38        | 1.45     |
| 54  | BA    | 1702 | G    | C6-N1   | -5.22 | 1.35        | 1.39     |
| 54  | BA    | 2757 | A    | C6-N6   | -5.22 | 1.29        | 1.33     |
| 54  | BA    | 1220 | G    | C6-N1   | -5.22 | 1.35        | 1.39     |
| 54  | BA    | 1257 | C    | N3-C4   | -5.22 | 1.30        | 1.33     |
| 21  | AA    | 542  | G    | C2-N2   | -5.22 | 1.29        | 1.34     |
| 21  | AA    | 974  | A    | C6-N1   | -5.22 | 1.31        | 1.35     |
| 54  | BA    | 1207 | C    | N3-C4   | -5.22 | 1.30        | 1.33     |
| 54  | BA    | 1549 | A    | C6-N6   | -5.22 | 1.29        | 1.33     |
| 54  | BA    | 1724 | G    | C2-N2   | -5.22 | 1.29        | 1.34     |
| 54  | BA    | 1823 | G    | N1-C2   | -5.22 | 1.33        | 1.37     |
| 54  | BA    | 680  | C    | C4-N4   | -5.22 | 1.29        | 1.33     |
| 54  | BA    | 1073 | A    | C6-N6   | -5.22 | 1.29        | 1.33     |
| 21  | AA    | 260  | G    | O3'-P   | -5.22 | 1.54        | 1.61     |
| 21  | AA    | 880  | C    | C4-N4   | -5.22 | 1.29        | 1.33     |
| 21  | AA    | 906  | A    | C4'-O4' | -5.22 | 1.38        | 1.45     |
| 21  | AA    | 953  | G    | C2-N2   | -5.22 | 1.29        | 1.34     |
| 21  | AA    | 969  | A    | C5-C4   | -5.22 | 1.35        | 1.38     |
| 21  | AA    | 1392 | G    | N1-C2   | -5.22 | 1.33        | 1.37     |
| 54  | BA    | 220  | G    | C6-N1   | -5.22 | 1.35        | 1.39     |
| 54  | BA    | 1665 | A    | C5-C4   | -5.22 | 1.35        | 1.38     |
| 21  | AA    | 204  | G    | N1-C2   | -5.21 | 1.33        | 1.37     |
| 54  | BA    | 346  | A    | C5-C4   | -5.21 | 1.35        | 1.38     |
| 54  | BA    | 673  | C    | N3-C4   | -5.21 | 1.30        | 1.33     |
| 54  | BA    | 2239 | G    | C6-N1   | -5.21 | 1.35        | 1.39     |
| 54  | BA    | 2663 | G    | C6-N1   | -5.21 | 1.35        | 1.39     |
| 21  | AA    | 474  | G    | C2-N2   | -5.21 | 1.29        | 1.34     |
| 54  | BA    | 2619 | C    | N3-C4   | -5.21 | 1.30        | 1.33     |
| 21  | AA    | 1209 | C    | N3-C4   | -5.21 | 1.30        | 1.33     |
| 54  | BA    | 1059 | G    | C2-N2   | -5.21 | 1.29        | 1.34     |
| 21  | AA    | 220  | G    | C2-N2   | -5.21 | 1.29        | 1.34     |
| 21  | AA    | 1448 | C    | C4-C5   | -5.21 | 1.38        | 1.43     |
| 54  | BA    | 229  | C    | C4-N4   | -5.21 | 1.29        | 1.33     |
| 55  | BB    | 15   | A    | C6-N6   | -5.21 | 1.29        | 1.33     |
| 21  | AA    | 845  | A    | C5-C4   | -5.21 | 1.35        | 1.38     |
| 54  | BA    | 1333 | G    | C2-N2   | -5.21 | 1.29        | 1.34     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 54  | BA    | 1572 | A    | C6-N6   | -5.21 | 1.29        | 1.33     |
| 54  | BA    | 2096 | C    | N3-C4   | -5.21 | 1.30        | 1.33     |
| 21  | AA    | 1514 | G    | N1-C2   | -5.21 | 1.33        | 1.37     |
| 54  | BA    | 627  | A    | C5-C4   | -5.21 | 1.35        | 1.38     |
| 54  | BA    | 760  | G    | C2-N2   | -5.21 | 1.29        | 1.34     |
| 54  | BA    | 1649 | G    | O3'-P   | -5.21 | 1.54        | 1.61     |
| 54  | BA    | 2610 | C    | C4-N4   | -5.21 | 1.29        | 1.33     |
| 21  | AA    | 252  | U    | C4'-O4' | -5.20 | 1.38        | 1.45     |
| 21  | AA    | 312  | C    | N3-C4   | -5.20 | 1.30        | 1.33     |
| 21  | AA    | 506  | G    | C6-N1   | -5.20 | 1.35        | 1.39     |
| 21  | AA    | 624  | C    | N3-C4   | -5.20 | 1.30        | 1.33     |
| 21  | AA    | 1134 | G    | N1-C2   | -5.20 | 1.33        | 1.37     |
| 54  | BA    | 1538 | G    | C2-N2   | -5.20 | 1.29        | 1.34     |
| 21  | AA    | 958  | A    | C5-C4   | -5.20 | 1.35        | 1.38     |
| 54  | BA    | 739  | A    | C5-C4   | -5.20 | 1.35        | 1.38     |
| 21  | AA    | 580  | C    | C4-N4   | -5.20 | 1.29        | 1.33     |
| 54  | BA    | 1783 | A    | C5-C4   | -5.20 | 1.35        | 1.38     |
| 54  | BA    | 1826 | G    | C6-N1   | -5.20 | 1.35        | 1.39     |
| 54  | BA    | 2030 | A    | C6-N6   | -5.20 | 1.29        | 1.33     |
| 54  | BA    | 2575 | C    | C4-N4   | -5.20 | 1.29        | 1.33     |
| 21  | AA    | 971  | G    | C2-N2   | -5.20 | 1.29        | 1.34     |
| 21  | AA    | 991  | U    | C4'-O4' | -5.20 | 1.38        | 1.45     |
| 54  | BA    | 1049 | C    | C4-N4   | -5.20 | 1.29        | 1.33     |
| 54  | BA    | 2279 | G    | C2-N2   | -5.20 | 1.29        | 1.34     |
| 54  | BA    | 1477 | A    | C6-N6   | -5.20 | 1.29        | 1.33     |
| 54  | BA    | 2295 | C    | C4-N4   | -5.20 | 1.29        | 1.33     |
| 21  | AA    | 378  | G    | N1-C2   | -5.20 | 1.33        | 1.37     |
| 21  | AA    | 755  | G    | C2-N2   | -5.20 | 1.29        | 1.34     |
| 54  | BA    | 183  | C    | N3-C4   | -5.20 | 1.30        | 1.33     |
| 54  | BA    | 348  | A    | C5-C4   | -5.20 | 1.35        | 1.38     |
| 54  | BA    | 620  | G    | C6-N1   | -5.20 | 1.35        | 1.39     |
| 54  | BA    | 2287 | A    | C6-N6   | -5.20 | 1.29        | 1.33     |
| 54  | BA    | 1667 | G    | C6-N1   | -5.19 | 1.35        | 1.39     |
| 21  | AA    | 823  | C    | C4-N4   | -5.19 | 1.29        | 1.33     |
| 54  | BA    | 186  | G    | C2-N2   | -5.19 | 1.29        | 1.34     |
| 54  | BA    | 1544 | A    | C6-N1   | -5.19 | 1.31        | 1.35     |
| 54  | BA    | 2200 | C    | N3-C4   | -5.19 | 1.30        | 1.33     |
| 21  | AA    | 488  | C    | N3-C4   | -5.19 | 1.30        | 1.33     |
| 21  | AA    | 869  | G    | C6-N1   | -5.19 | 1.35        | 1.39     |
| 54  | BA    | 792  | A    | C5-C4   | -5.19 | 1.35        | 1.38     |
| 21  | AA    | 377  | G    | C2-N2   | -5.19 | 1.29        | 1.34     |
| 21  | AA    | 1064 | G    | C2-N2   | -5.19 | 1.29        | 1.34     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 21  | AA    | 687  | A    | C5-C4   | -5.19 | 1.35        | 1.38     |
| 54  | BA    | 81   | G    | C2-N2   | -5.19 | 1.29        | 1.34     |
| 54  | BA    | 1009 | A    | C6-N1   | -5.19 | 1.31        | 1.35     |
| 54  | BA    | 2731 | G    | C6-N1   | -5.19 | 1.35        | 1.39     |
| 55  | BB    | 54   | G    | N1-C2   | -5.19 | 1.33        | 1.37     |
| 21  | AA    | 853  | C    | N3-C4   | -5.18 | 1.30        | 1.33     |
| 21  | AA    | 890  | G    | C2-N2   | -5.18 | 1.29        | 1.34     |
| 21  | AA    | 993  | G    | C2-N2   | -5.18 | 1.29        | 1.34     |
| 21  | AA    | 1055 | A    | C6-N1   | -5.18 | 1.31        | 1.35     |
| 54  | BA    | 1658 | C    | C4-N4   | -5.18 | 1.29        | 1.33     |
| 21  | AA    | 406  | G    | C2-N2   | -5.18 | 1.29        | 1.34     |
| 21  | AA    | 925  | G    | N1-C2   | -5.18 | 1.33        | 1.37     |
| 21  | AA    | 1241 | G    | C4'-O4' | -5.18 | 1.38        | 1.45     |
| 54  | BA    | 302  | C    | N3-C4   | -5.18 | 1.30        | 1.33     |
| 54  | BA    | 1368 | G    | C2-N2   | -5.18 | 1.29        | 1.34     |
| 54  | BA    | 159  | G    | N1-C2   | -5.18 | 1.33        | 1.37     |
| 54  | BA    | 1252 | G    | C6-N1   | -5.18 | 1.35        | 1.39     |
| 54  | BA    | 1675 | C    | C4-N4   | -5.18 | 1.29        | 1.33     |
| 55  | BB    | 85   | G    | C6-N1   | -5.18 | 1.35        | 1.39     |
| 54  | BA    | 277  | G    | C2-N2   | -5.18 | 1.29        | 1.34     |
| 54  | BA    | 1519 | G    | C6-N1   | -5.18 | 1.35        | 1.39     |
| 54  | BA    | 2776 | A    | C5-C4   | -5.18 | 1.35        | 1.38     |
| 54  | BA    | 1    | G    | C2-N2   | -5.18 | 1.29        | 1.34     |
| 54  | BA    | 2216 | G    | N1-C2   | -5.18 | 1.33        | 1.37     |
| 21  | AA    | 21   | G    | N1-C2   | -5.18 | 1.33        | 1.37     |
| 21  | AA    | 780  | A    | C5-C4   | -5.18 | 1.35        | 1.38     |
| 21  | AA    | 1152 | A    | C6-N6   | -5.18 | 1.29        | 1.33     |
| 54  | BA    | 584  | C    | C4-N4   | -5.18 | 1.29        | 1.33     |
| 54  | BA    | 1042 | G    | C2-N2   | -5.18 | 1.29        | 1.34     |
| 54  | BA    | 2294 | G    | C6-N1   | -5.18 | 1.35        | 1.39     |
| 54  | BA    | 2750 | A    | C6-N1   | -5.18 | 1.31        | 1.35     |
| 54  | BA    | 2834 | G    | C2-N2   | -5.18 | 1.29        | 1.34     |
| 21  | AA    | 295  | C    | N3-C4   | -5.17 | 1.30        | 1.33     |
| 54  | BA    | 2588 | G    | C2-N2   | -5.17 | 1.29        | 1.34     |
| 54  | BA    | 152  | A    | C6-N1   | -5.17 | 1.31        | 1.35     |
| 54  | BA    | 648  | G    | N1-C2   | -5.17 | 1.33        | 1.37     |
| 54  | BA    | 1480 | C    | N3-C4   | -5.17 | 1.30        | 1.33     |
| 54  | BA    | 2895 | G    | N1-C2   | -5.17 | 1.33        | 1.37     |
| 21  | AA    | 1214 | C    | C2'-C1' | -5.17 | 1.47        | 1.53     |
| 54  | BA    | 1616 | A    | C5-C4   | -5.17 | 1.35        | 1.38     |
| 54  | BA    | 2788 | C    | N3-C4   | -5.17 | 1.30        | 1.33     |
| 54  | BA    | 2716 | C    | C4-N4   | -5.17 | 1.29        | 1.33     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 21  | AA    | 668  | G    | C4'-C3' | -5.17 | 1.47        | 1.52     |
| 21  | AA    | 1416 | G    | C6-N1   | -5.17 | 1.35        | 1.39     |
| 22  | A1    | 40   | G    | C2-N2   | -5.17 | 1.29        | 1.34     |
| 54  | BA    | 340  | A    | C6-N1   | -5.17 | 1.31        | 1.35     |
| 54  | BA    | 492  | A    | C6-N1   | -5.17 | 1.31        | 1.35     |
| 54  | BA    | 736  | C    | C4-N4   | -5.17 | 1.29        | 1.33     |
| 54  | BA    | 1072 | C    | N3-C4   | -5.17 | 1.30        | 1.33     |
| 54  | BA    | 1385 | A    | C5-C4   | -5.17 | 1.35        | 1.38     |
| 54  | BA    | 1566 | A    | C5-C4   | -5.17 | 1.35        | 1.38     |
| 54  | BA    | 1585 | C    | C4-N4   | -5.17 | 1.29        | 1.33     |
| 21  | AA    | 518  | C    | C4-N4   | -5.17 | 1.29        | 1.33     |
| 54  | BA    | 447  | A    | C6-N6   | -5.17 | 1.29        | 1.33     |
| 54  | BA    | 1516 | G    | C2-N2   | -5.17 | 1.29        | 1.34     |
| 54  | BA    | 1524 | G    | N1-C2   | -5.17 | 1.33        | 1.37     |
| 54  | BA    | 2361 | G    | C6-N1   | -5.17 | 1.35        | 1.39     |
| 21  | AA    | 104  | G    | C2-N2   | -5.17 | 1.29        | 1.34     |
| 21  | AA    | 382  | A    | C6-N6   | -5.17 | 1.29        | 1.33     |
| 21  | AA    | 658  | C    | C4'-O4' | -5.17 | 1.38        | 1.45     |
| 54  | BA    | 323  | C    | C4-N4   | -5.16 | 1.29        | 1.33     |
| 54  | BA    | 654  | A    | C6-N6   | -5.16 | 1.29        | 1.33     |
| 21  | AA    | 774  | G    | C4'-O4' | -5.16 | 1.38        | 1.45     |
| 21  | AA    | 1163 | A    | C5-C4   | -5.16 | 1.35        | 1.38     |
| 21  | AA    | 125  | U    | C4'-O4' | -5.16 | 1.38        | 1.45     |
| 21  | AA    | 244  | U    | C2'-C1' | -5.16 | 1.47        | 1.53     |
| 54  | BA    | 1702 | G    | C2-N2   | -5.16 | 1.29        | 1.34     |
| 54  | BA    | 2049 | G    | C2-N2   | -5.16 | 1.29        | 1.34     |
| 21  | AA    | 507  | C    | N3-C4   | -5.16 | 1.30        | 1.33     |
| 21  | AA    | 1098 | C    | N3-C4   | -5.16 | 1.30        | 1.33     |
| 21  | AA    | 1336 | C    | C2'-C1' | -5.16 | 1.47        | 1.53     |
| 54  | BA    | 1450 | G    | C2-N2   | -5.16 | 1.29        | 1.34     |
| 54  | BA    | 2802 | G    | C6-N1   | -5.16 | 1.35        | 1.39     |
| 54  | BA    | 1025 | G    | O3'-P   | -5.16 | 1.54        | 1.61     |
| 54  | BA    | 1112 | G    | C6-N1   | -5.16 | 1.35        | 1.39     |
| 54  | BA    | 2709 | G    | N1-C2   | -5.16 | 1.33        | 1.37     |
| 21  | AA    | 40   | C    | N3-C4   | -5.15 | 1.30        | 1.33     |
| 54  | BA    | 526  | A    | C6-N1   | -5.15 | 1.31        | 1.35     |
| 54  | BA    | 2705 | A    | C5-C4   | -5.15 | 1.35        | 1.38     |
| 21  | AA    | 171  | A    | C6-N1   | -5.15 | 1.31        | 1.35     |
| 21  | AA    | 477  | C    | C4-N4   | -5.15 | 1.29        | 1.33     |
| 21  | AA    | 1274 | A    | C6-N1   | -5.15 | 1.31        | 1.35     |
| 24  | A3    | 52   | C    | C4-N4   | -5.15 | 1.29        | 1.33     |
| 21  | AA    | 186  | C    | N3-C4   | -5.15 | 1.30        | 1.33     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 21  | AA    | 575  | G    | N1-C2   | -5.15 | 1.33        | 1.37     |
| 54  | BA    | 220  | G    | C2-N2   | -5.15 | 1.29        | 1.34     |
| 54  | BA    | 853  | C    | N3-C4   | -5.15 | 1.30        | 1.33     |
| 21  | AA    | 444  | G    | N1-C2   | -5.15 | 1.33        | 1.37     |
| 21  | AA    | 779  | C    | C4-N4   | -5.15 | 1.29        | 1.33     |
| 21  | AA    | 808  | C    | C4'-C3' | -5.15 | 1.47        | 1.52     |
| 21  | AA    | 1429 | A    | C6-N6   | -5.15 | 1.29        | 1.33     |
| 21  | AA    | 1497 | G    | N1-C2   | -5.15 | 1.33        | 1.37     |
| 54  | BA    | 342  | A    | C5-C4   | -5.14 | 1.35        | 1.38     |
| 54  | BA    | 800  | A    | N9-C4   | -5.14 | 1.34        | 1.37     |
| 54  | BA    | 2107 | G    | C2-N2   | -5.14 | 1.29        | 1.34     |
| 54  | BA    | 2446 | G    | C2-N2   | -5.14 | 1.29        | 1.34     |
| 21  | AA    | 205  | A    | C6-N6   | -5.14 | 1.29        | 1.33     |
| 21  | AA    | 350  | G    | N1-C2   | -5.14 | 1.33        | 1.37     |
| 54  | BA    | 2255 | G    | N1-C2   | -5.14 | 1.33        | 1.37     |
| 54  | BA    | 2598 | A    | C5-C4   | -5.14 | 1.35        | 1.38     |
| 54  | BA    | 792  | A    | C6-N6   | -5.14 | 1.29        | 1.33     |
| 13  | AN    | 69   | ARG  | CZ-NH2  | -5.14 | 1.26        | 1.33     |
| 21  | AA    | 785  | G    | N1-C2   | -5.14 | 1.33        | 1.37     |
| 21  | AA    | 1525 | G    | C2-N2   | -5.14 | 1.29        | 1.34     |
| 54  | BA    | 359  | G    | C2-N2   | -5.14 | 1.29        | 1.34     |
| 54  | BA    | 2290 | G    | N1-C2   | -5.14 | 1.33        | 1.37     |
| 54  | BA    | 2328 | A    | C6-N1   | -5.14 | 1.31        | 1.35     |
| 54  | BA    | 2376 | A    | C5-C4   | -5.14 | 1.35        | 1.38     |
| 54  | BA    | 231  | A    | C6-N1   | -5.14 | 1.31        | 1.35     |
| 54  | BA    | 2165 | C    | C4-N4   | -5.14 | 1.29        | 1.33     |
| 21  | AA    | 1104 | G    | N1-C2   | -5.14 | 1.33        | 1.37     |
| 54  | BA    | 749  | A    | C5-C4   | -5.14 | 1.35        | 1.38     |
| 54  | BA    | 1455 | G    | N1-C2   | -5.13 | 1.33        | 1.37     |
| 54  | BA    | 2664 | G    | N1-C2   | -5.13 | 1.33        | 1.37     |
| 21  | AA    | 852  | G    | C6-N1   | -5.13 | 1.35        | 1.39     |
| 21  | AA    | 1153 | G    | N1-C2   | -5.13 | 1.33        | 1.37     |
| 55  | BB    | 76   | G    | C2-N2   | -5.13 | 1.29        | 1.34     |
| 21  | AA    | 284  | C    | C4-N4   | -5.13 | 1.29        | 1.33     |
| 21  | AA    | 418  | C    | C4'-O4' | -5.13 | 1.38        | 1.45     |
| 21  | AA    | 1439 | G    | C2-N2   | -5.13 | 1.29        | 1.34     |
| 24  | A3    | 29   | C    | C4'-O4' | -5.13 | 1.38        | 1.45     |
| 54  | BA    | 1050 | A    | O3'-P   | -5.13 | 1.54        | 1.61     |
| 54  | BA    | 1246 | A    | O3'-P   | -5.13 | 1.54        | 1.61     |
| 21  | AA    | 156  | C    | C4-N4   | -5.13 | 1.29        | 1.33     |
| 54  | BA    | 685  | A    | C6-N1   | -5.13 | 1.31        | 1.35     |
| 54  | BA    | 2168 | G    | C2-N2   | -5.13 | 1.29        | 1.34     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 55  | BB    | 112  | G    | N1-C2 | -5.13 | 1.33        | 1.37     |
| 21  | AA    | 149  | A    | C5-C4 | -5.13 | 1.35        | 1.38     |
| 21  | AA    | 236  | A    | C6-N1 | -5.13 | 1.31        | 1.35     |
| 54  | BA    | 1567 | G    | N1-C2 | -5.13 | 1.33        | 1.37     |
| 54  | BA    | 1598 | A    | C6-N6 | -5.13 | 1.29        | 1.33     |
| 21  | AA    | 1074 | G    | C2-N2 | -5.13 | 1.29        | 1.34     |
| 22  | A1    | 27   | C    | C4-N4 | -5.13 | 1.29        | 1.33     |
| 54  | BA    | 809  | G    | C6-N1 | -5.13 | 1.35        | 1.39     |
| 54  | BA    | 844  | A    | C6-N1 | -5.13 | 1.31        | 1.35     |
| 21  | AA    | 50   | A    | C6-N1 | -5.12 | 1.31        | 1.35     |
| 21  | AA    | 178  | C    | C4-N4 | -5.12 | 1.29        | 1.33     |
| 21  | AA    | 1184 | G    | C2-N2 | -5.12 | 1.29        | 1.34     |
| 54  | BA    | 1128 | G    | C2-N2 | -5.12 | 1.29        | 1.34     |
| 54  | BA    | 1338 | G    | C2-N2 | -5.12 | 1.29        | 1.34     |
| 54  | BA    | 1490 | A    | C6-N1 | -5.12 | 1.31        | 1.35     |
| 54  | BA    | 1972 | G    | C2-N2 | -5.12 | 1.29        | 1.34     |
| 21  | AA    | 113  | G    | C6-N1 | -5.12 | 1.35        | 1.39     |
| 54  | BA    | 413  | C    | C4-N4 | -5.12 | 1.29        | 1.33     |
| 54  | BA    | 2284 | A    | C6-N6 | -5.12 | 1.29        | 1.33     |
| 54  | BA    | 2669 | G    | C2-N2 | -5.12 | 1.29        | 1.34     |
| 21  | AA    | 457  | G    | C6-N1 | -5.12 | 1.35        | 1.39     |
| 54  | BA    | 1632 | A    | C5-C4 | -5.12 | 1.35        | 1.38     |
| 22  | A1    | 38   | A    | C5-C4 | -5.12 | 1.35        | 1.38     |
| 54  | BA    | 1732 | C    | N3-C4 | -5.12 | 1.30        | 1.33     |
| 54  | BA    | 2513 | A    | C6-N1 | -5.12 | 1.31        | 1.35     |
| 21  | AA    | 159  | G    | N1-C2 | -5.12 | 1.33        | 1.37     |
| 54  | BA    | 2300 | C    | C4-N4 | -5.12 | 1.29        | 1.33     |
| 21  | AA    | 161  | A    | C6-N6 | -5.12 | 1.29        | 1.33     |
| 21  | AA    | 521  | G    | C6-N1 | -5.12 | 1.35        | 1.39     |
| 21  | AA    | 876  | C    | C4-N4 | -5.12 | 1.29        | 1.33     |
| 21  | AA    | 1162 | C    | N3-C4 | -5.12 | 1.30        | 1.33     |
| 21  | AA    | 1468 | A    | C5-C4 | -5.12 | 1.35        | 1.38     |
| 54  | BA    | 537  | G    | C6-N1 | -5.12 | 1.35        | 1.39     |
| 54  | BA    | 1933 | G    | C2-N2 | -5.12 | 1.29        | 1.34     |
| 54  | BA    | 2044 | C    | N3-C4 | -5.12 | 1.30        | 1.33     |
| 21  | AA    | 741  | G    | C2-N2 | -5.11 | 1.29        | 1.34     |
| 21  | AA    | 1382 | C    | C4-N4 | -5.11 | 1.29        | 1.33     |
| 54  | BA    | 1766 | G    | C2-N2 | -5.11 | 1.29        | 1.34     |
| 54  | BA    | 2114 | A    | C6-N6 | -5.11 | 1.29        | 1.33     |
| 21  | AA    | 919  | A    | C5-C4 | -5.11 | 1.35        | 1.38     |
| 54  | BA    | 51   | G    | C6-N1 | -5.11 | 1.35        | 1.39     |
| 54  | BA    | 1684 | G    | C6-N1 | -5.11 | 1.35        | 1.39     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 54  | BA    | 1545 | A    | C6-N6   | -5.11 | 1.29        | 1.33     |
| 54  | BA    | 2436 | G    | N1-C2   | -5.11 | 1.33        | 1.37     |
| 21  | AA    | 877  | G    | C2-N2   | -5.11 | 1.29        | 1.34     |
| 54  | BA    | 1211 | C    | C4-N4   | -5.11 | 1.29        | 1.33     |
| 54  | BA    | 144  | A    | C5-C4   | -5.11 | 1.35        | 1.38     |
| 54  | BA    | 1900 | A    | C5-C4   | -5.11 | 1.35        | 1.38     |
| 54  | BA    | 1974 | C    | N3-C4   | -5.11 | 1.30        | 1.33     |
| 54  | BA    | 2774 | C    | N3-C4   | -5.11 | 1.30        | 1.33     |
| 54  | BA    | 24   | G    | C6-N1   | -5.11 | 1.35        | 1.39     |
| 54  | BA    | 797  | G    | N1-C2   | -5.11 | 1.33        | 1.37     |
| 54  | BA    | 1783 | A    | C6-N6   | -5.11 | 1.29        | 1.33     |
| 54  | BA    | 2012 | G    | C6-N1   | -5.11 | 1.35        | 1.39     |
| 54  | BA    | 1085 | A    | C5-C4   | -5.10 | 1.35        | 1.38     |
| 21  | AA    | 602  | A    | C4'-O4' | -5.10 | 1.39        | 1.45     |
| 21  | AA    | 859  | G    | C2-N2   | -5.10 | 1.29        | 1.34     |
| 21  | AA    | 1039 | G    | C2-N2   | -5.10 | 1.29        | 1.34     |
| 21  | AA    | 382  | A    | C6-N1   | -5.10 | 1.31        | 1.35     |
| 21  | AA    | 685  | G    | C6-N1   | -5.10 | 1.35        | 1.39     |
| 21  | AA    | 1457 | G    | C2-N2   | -5.10 | 1.29        | 1.34     |
| 21  | AA    | 589  | U    | C4'-O4' | -5.10 | 1.39        | 1.45     |
| 21  | AA    | 1417 | G    | N1-C2   | -5.10 | 1.33        | 1.37     |
| 21  | AA    | 1518 | A    | C6-N1   | -5.10 | 1.31        | 1.35     |
| 24  | A3    | 57   | C    | C4-N4   | -5.10 | 1.29        | 1.33     |
| 54  | BA    | 23   | G    | C2-N2   | -5.10 | 1.29        | 1.34     |
| 54  | BA    | 2325 | G    | N1-C2   | -5.10 | 1.33        | 1.37     |
| 54  | BA    | 2681 | C    | N3-C4   | -5.10 | 1.30        | 1.33     |
| 21  | AA    | 1179 | A    | C4'-O4' | -5.10 | 1.39        | 1.45     |
| 54  | BA    | 1702 | G    | N1-C2   | -5.10 | 1.33        | 1.37     |
| 54  | BA    | 1776 | G    | C6-N1   | -5.10 | 1.35        | 1.39     |
| 54  | BA    | 2429 | G    | C2-N2   | -5.10 | 1.29        | 1.34     |
| 55  | BB    | 59   | A    | C6-N1   | -5.10 | 1.31        | 1.35     |
| 54  | BA    | 24   | G    | C2-N2   | -5.10 | 1.29        | 1.34     |
| 54  | BA    | 2024 | G    | C2-N2   | -5.10 | 1.29        | 1.34     |
| 21  | AA    | 705  | G    | C2-N2   | -5.09 | 1.29        | 1.34     |
| 21  | AA    | 1352 | C    | C4-N4   | -5.09 | 1.29        | 1.33     |
| 54  | BA    | 346  | A    | C6-N1   | -5.09 | 1.31        | 1.35     |
| 54  | BA    | 2805 | C    | C4-N4   | -5.09 | 1.29        | 1.33     |
| 21  | AA    | 461  | A    | C6-N1   | -5.09 | 1.31        | 1.35     |
| 21  | AA    | 862  | C    | N3-C4   | -5.09 | 1.30        | 1.33     |
| 54  | BA    | 2002 | G    | C2-N2   | -5.09 | 1.29        | 1.34     |
| 21  | AA    | 745  | G    | C2-N2   | -5.09 | 1.29        | 1.34     |
| 21  | AA    | 1002 | G    | C2-N2   | -5.09 | 1.29        | 1.34     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 54  | BA    | 1591 | A    | C6-N1 | -5.09 | 1.31        | 1.35     |
| 54  | BA    | 2307 | G    | N1-C2 | -5.09 | 1.33        | 1.37     |
| 21  | AA    | 384  | G    | C2-N2 | -5.09 | 1.29        | 1.34     |
| 21  | AA    | 1114 | C    | N3-C4 | -5.09 | 1.30        | 1.33     |
| 54  | BA    | 1118 | C    | N3-C4 | -5.09 | 1.30        | 1.33     |
| 54  | BA    | 1750 | G    | C2-N2 | -5.09 | 1.29        | 1.34     |
| 54  | BA    | 2216 | G    | C6-N1 | -5.09 | 1.35        | 1.39     |
| 55  | BB    | 12   | C    | N3-C4 | -5.09 | 1.30        | 1.33     |
| 54  | BA    | 1804 | C    | C4-N4 | -5.09 | 1.29        | 1.33     |
| 54  | BA    | 2373 | G    | C6-N1 | -5.09 | 1.35        | 1.39     |
| 21  | AA    | 917  | G    | C2-N2 | -5.09 | 1.29        | 1.34     |
| 54  | BA    | 1679 | A    | C6-N6 | -5.09 | 1.29        | 1.33     |
| 21  | AA    | 932  | C    | C4-N4 | -5.08 | 1.29        | 1.33     |
| 21  | AA    | 47   | C    | N3-C4 | -5.08 | 1.30        | 1.33     |
| 21  | AA    | 873  | A    | C6-N6 | -5.08 | 1.29        | 1.33     |
| 21  | AA    | 1170 | A    | C5-C4 | -5.08 | 1.35        | 1.38     |
| 54  | BA    | 2071 | A    | C6-N1 | -5.08 | 1.31        | 1.35     |
| 21  | AA    | 132  | C    | C4-N4 | -5.08 | 1.29        | 1.33     |
| 54  | BA    | 1053 | C    | C4-N4 | -5.08 | 1.29        | 1.33     |
| 54  | BA    | 2718 | G    | C8-N7 | -5.08 | 1.27        | 1.30     |
| 54  | BA    | 2437 | G    | N1-C2 | -5.08 | 1.33        | 1.37     |
| 21  | AA    | 364  | A    | C6-N6 | -5.08 | 1.29        | 1.33     |
| 21  | AA    | 497  | G    | N1-C2 | -5.08 | 1.33        | 1.37     |
| 21  | AA    | 1234 | C    | C4-N4 | -5.08 | 1.29        | 1.33     |
| 54  | BA    | 1988 | G    | N1-C2 | -5.08 | 1.33        | 1.37     |
| 54  | BA    | 2634 | A    | C6-N1 | -5.08 | 1.31        | 1.35     |
| 54  | BA    | 2900 | A    | C6-N6 | -5.08 | 1.29        | 1.33     |
| 21  | AA    | 1027 | C    | O3'-P | -5.08 | 1.55        | 1.61     |
| 54  | BA    | 1522 | A    | C6-N1 | -5.08 | 1.31        | 1.35     |
| 54  | BA    | 1708 | C    | C4-N4 | -5.08 | 1.29        | 1.33     |
| 21  | AA    | 177  | G    | N1-C2 | -5.08 | 1.33        | 1.37     |
| 21  | AA    | 178  | C    | C4-C5 | -5.08 | 1.38        | 1.43     |
| 21  | AA    | 557  | G    | C2-N2 | -5.08 | 1.29        | 1.34     |
| 54  | BA    | 249  | C    | C4-N4 | -5.08 | 1.29        | 1.33     |
| 54  | BA    | 389  | G    | C2-N2 | -5.08 | 1.29        | 1.34     |
| 54  | BA    | 1233 | C    | N3-C4 | -5.08 | 1.30        | 1.33     |
| 54  | BA    | 1566 | A    | C6-N1 | -5.08 | 1.31        | 1.35     |
| 54  | BA    | 1638 | C    | C4-N4 | -5.08 | 1.29        | 1.33     |
| 55  | BB    | 73   | A    | C5-C4 | -5.08 | 1.35        | 1.38     |
| 21  | AA    | 491  | G    | N1-C2 | -5.07 | 1.33        | 1.37     |
| 54  | BA    | 1403 | A    | C5-C4 | -5.07 | 1.35        | 1.38     |
| 54  | BA    | 1461 | C    | C4-N4 | -5.07 | 1.29        | 1.33     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 54  | BA    | 1902 | C    | C4-N4 | -5.07 | 1.29        | 1.33     |
| 54  | BA    | 1948 | G    | C8-N7 | -5.07 | 1.27        | 1.30     |
| 54  | BA    | 2890 | G    | N1-C2 | -5.07 | 1.33        | 1.37     |
| 21  | AA    | 396  | C    | C4-N4 | -5.07 | 1.29        | 1.33     |
| 21  | AA    | 1493 | A    | C6-N6 | -5.07 | 1.29        | 1.33     |
| 54  | BA    | 1999 | C    | C4-N4 | -5.07 | 1.29        | 1.33     |
| 54  | BA    | 2749 | A    | C6-N1 | -5.07 | 1.31        | 1.35     |
| 54  | BA    | 287  | G    | N1-C2 | -5.07 | 1.33        | 1.37     |
| 54  | BA    | 1427 | A    | C6-N6 | -5.07 | 1.29        | 1.33     |
| 54  | BA    | 2738 | A    | C6-N1 | -5.07 | 1.32        | 1.35     |
| 21  | AA    | 1047 | G    | C6-N1 | -5.07 | 1.36        | 1.39     |
| 54  | BA    | 245  | G    | O3'-P | -5.07 | 1.55        | 1.61     |
| 54  | BA    | 432  | A    | C6-N6 | -5.07 | 1.29        | 1.33     |
| 21  | AA    | 243  | A    | C6-N1 | -5.07 | 1.32        | 1.35     |
| 21  | AA    | 513  | C    | C4-N4 | -5.07 | 1.29        | 1.33     |
| 21  | AA    | 584  | G    | C2-N2 | -5.07 | 1.29        | 1.34     |
| 54  | BA    | 35   | G    | C6-N1 | -5.07 | 1.36        | 1.39     |
| 54  | BA    | 528  | A    | C5-C4 | -5.07 | 1.35        | 1.38     |
| 54  | BA    | 1264 | A    | C6-N6 | -5.07 | 1.29        | 1.33     |
| 54  | BA    | 1828 | G    | N1-C2 | -5.07 | 1.33        | 1.37     |
| 55  | BB    | 118  | C    | N3-C4 | -5.07 | 1.30        | 1.33     |
| 21  | AA    | 18   | C    | C4-N4 | -5.07 | 1.29        | 1.33     |
| 21  | AA    | 97   | G    | N1-C2 | -5.07 | 1.33        | 1.37     |
| 21  | AA    | 134  | G    | C2-N2 | -5.07 | 1.29        | 1.34     |
| 21  | AA    | 349  | A    | C6-N6 | -5.07 | 1.29        | 1.33     |
| 54  | BA    | 705  | A    | C6-N1 | -5.07 | 1.32        | 1.35     |
| 54  | BA    | 1547 | C    | N3-C4 | -5.07 | 1.30        | 1.33     |
| 54  | BA    | 1797 | G    | C6-N1 | -5.07 | 1.36        | 1.39     |
| 54  | BA    | 2235 | G    | C2-N2 | -5.07 | 1.29        | 1.34     |
| 21  | AA    | 436  | C    | C4-N4 | -5.06 | 1.29        | 1.33     |
| 54  | BA    | 740  | C    | C4-N4 | -5.06 | 1.29        | 1.33     |
| 21  | AA    | 1281 | C    | C4-N4 | -5.06 | 1.29        | 1.33     |
| 21  | AA    | 1389 | C    | C4-N4 | -5.06 | 1.29        | 1.33     |
| 54  | BA    | 784  | G    | C6-N1 | -5.06 | 1.36        | 1.39     |
| 21  | AA    | 172  | A    | C5-C4 | -5.06 | 1.35        | 1.38     |
| 54  | BA    | 1831 | G    | C2-N2 | -5.06 | 1.29        | 1.34     |
| 21  | AA    | 424  | G    | C2-N2 | -5.06 | 1.29        | 1.34     |
| 54  | BA    | 944  | C    | N3-C4 | -5.06 | 1.30        | 1.33     |
| 54  | BA    | 1575 | C    | N3-C4 | -5.06 | 1.30        | 1.33     |
| 54  | BA    | 2033 | A    | C6-N1 | -5.06 | 1.32        | 1.35     |
| 54  | BA    | 2280 | G    | C6-N1 | -5.06 | 1.36        | 1.39     |
| 21  | AA    | 109  | A    | C6-N1 | -5.05 | 1.32        | 1.35     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 54  | BA    | 818  | G    | O3'-P   | -5.05 | 1.55        | 1.61     |
| 54  | BA    | 1664 | A    | C6-N6   | -5.05 | 1.29        | 1.33     |
| 54  | BA    | 2872 | A    | N1-C2   | -5.05 | 1.29        | 1.34     |
| 21  | AA    | 126  | G    | C2-N2   | -5.05 | 1.29        | 1.34     |
| 23  | A2    | 80   | C    | C4-N4   | -5.05 | 1.29        | 1.33     |
| 54  | BA    | 532  | A    | C6-N6   | -5.05 | 1.29        | 1.33     |
| 54  | BA    | 1879 | C    | N3-C4   | -5.05 | 1.30        | 1.33     |
| 54  | BA    | 2171 | A    | C6-N6   | -5.05 | 1.29        | 1.33     |
| 54  | BA    | 190  | A    | C6-N1   | -5.05 | 1.32        | 1.35     |
| 54  | BA    | 2173 | A    | C6-N1   | -5.05 | 1.32        | 1.35     |
| 21  | AA    | 1350 | A    | C6-N6   | -5.05 | 1.29        | 1.33     |
| 54  | BA    | 268  | C    | N3-C4   | -5.05 | 1.30        | 1.33     |
| 54  | BA    | 836  | G    | C2-N2   | -5.05 | 1.29        | 1.34     |
| 54  | BA    | 1167 | C    | N3-C4   | -5.05 | 1.30        | 1.33     |
| 54  | BA    | 2579 | C    | N3-C4   | -5.05 | 1.30        | 1.33     |
| 54  | BA    | 2802 | G    | N1-C2   | -5.05 | 1.33        | 1.37     |
| 21  | AA    | 1353 | G    | C2-N2   | -5.05 | 1.29        | 1.34     |
| 54  | BA    | 1718 | G    | C6-N1   | -5.05 | 1.36        | 1.39     |
| 54  | BA    | 2386 | A    | C6-N6   | -5.05 | 1.29        | 1.33     |
| 54  | BA    | 2545 | G    | C6-N1   | -5.05 | 1.36        | 1.39     |
| 21  | AA    | 128  | G    | C6-N1   | -5.05 | 1.36        | 1.39     |
| 54  | BA    | 132  | G    | C2-N2   | -5.05 | 1.29        | 1.34     |
| 54  | BA    | 751  | A    | C5-C4   | -5.05 | 1.35        | 1.38     |
| 54  | BA    | 2157 | G    | C2-N2   | -5.05 | 1.29        | 1.34     |
| 54  | BA    | 2462 | C    | C4-N4   | -5.05 | 1.29        | 1.33     |
| 54  | BA    | 2064 | C    | C4-N4   | -5.04 | 1.29        | 1.33     |
| 54  | BA    | 2816 | G    | C2-N2   | -5.04 | 1.29        | 1.34     |
| 21  | AA    | 634  | C    | C4-N4   | -5.04 | 1.29        | 1.33     |
| 21  | AA    | 764  | C    | C4-N4   | -5.04 | 1.29        | 1.33     |
| 21  | AA    | 373  | A    | C6-N6   | -5.04 | 1.29        | 1.33     |
| 21  | AA    | 995  | C    | C4'-C3' | -5.04 | 1.47        | 1.52     |
| 21  | AA    | 1181 | G    | C6-N1   | -5.04 | 1.36        | 1.39     |
| 54  | BA    | 477  | A    | C6-N1   | -5.04 | 1.32        | 1.35     |
| 54  | BA    | 610  | C    | N3-C4   | -5.04 | 1.30        | 1.33     |
| 21  | AA    | 1526 | G    | C6-N1   | -5.04 | 1.36        | 1.39     |
| 54  | BA    | 1518 | C    | C4-N4   | -5.04 | 1.29        | 1.33     |
| 54  | BA    | 1577 | C    | C4-N4   | -5.04 | 1.29        | 1.33     |
| 21  | AA    | 172  | A    | C6-N6   | -5.04 | 1.29        | 1.33     |
| 23  | A2    | 91   | A    | C5-C4   | -5.04 | 1.35        | 1.38     |
| 54  | BA    | 2316 | G    | C2-N2   | -5.04 | 1.29        | 1.34     |
| 55  | BB    | 86   | G    | C6-N1   | -5.04 | 1.36        | 1.39     |
| 21  | AA    | 142  | G    | N1-C2   | -5.04 | 1.33        | 1.37     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 21  | AA    | 942  | G    | C2-N2   | -5.04 | 1.29        | 1.34     |
| 21  | AA    | 95   | C    | N3-C4   | -5.04 | 1.30        | 1.33     |
| 21  | AA    | 1366 | C    | C4-N4   | -5.04 | 1.29        | 1.33     |
| 21  | AA    | 433  | G    | C2-N2   | -5.03 | 1.29        | 1.34     |
| 21  | AA    | 1082 | A    | C5-C4   | -5.03 | 1.35        | 1.38     |
| 54  | BA    | 1048 | A    | C6-N1   | -5.03 | 1.32        | 1.35     |
| 54  | BA    | 2242 | G    | N1-C2   | -5.03 | 1.33        | 1.37     |
| 54  | BA    | 5    | A    | C5-C4   | -5.03 | 1.35        | 1.38     |
| 54  | BA    | 35   | G    | N1-C2   | -5.03 | 1.33        | 1.37     |
| 54  | BA    | 1420 | A    | C5-C4   | -5.03 | 1.35        | 1.38     |
| 54  | BA    | 2136 | G    | O3'-P   | -5.03 | 1.55        | 1.61     |
| 21  | AA    | 566  | G    | C6-N1   | -5.03 | 1.36        | 1.39     |
| 21  | AA    | 1368 | A    | C6-N6   | -5.03 | 1.29        | 1.33     |
| 54  | BA    | 438  | G    | N1-C2   | -5.03 | 1.33        | 1.37     |
| 54  | BA    | 911  | A    | C5-C4   | -5.03 | 1.35        | 1.38     |
| 54  | BA    | 2694 | G    | N1-C2   | -5.03 | 1.33        | 1.37     |
| 21  | AA    | 1002 | G    | C6-N1   | -5.03 | 1.36        | 1.39     |
| 21  | AA    | 1330 | U    | C4'-O4' | -5.03 | 1.39        | 1.45     |
| 54  | BA    | 2433 | A    | C5-C4   | -5.03 | 1.35        | 1.38     |
| 21  | AA    | 1038 | C    | C4'-O4' | -5.03 | 1.39        | 1.45     |
| 21  | AA    | 1503 | A    | C6-N1   | -5.03 | 1.32        | 1.35     |
| 54  | BA    | 89   | A    | C6-N1   | -5.03 | 1.32        | 1.35     |
| 54  | BA    | 1098 | A    | C6-N6   | -5.03 | 1.29        | 1.33     |
| 54  | BA    | 1831 | G    | N1-C2   | -5.03 | 1.33        | 1.37     |
| 54  | BA    | 2212 | A    | C5-C4   | -5.03 | 1.35        | 1.38     |
| 21  | AA    | 48   | C    | N3-C4   | -5.02 | 1.30        | 1.33     |
| 21  | AA    | 626  | G    | C2-N2   | -5.02 | 1.29        | 1.34     |
| 54  | BA    | 911  | A    | C6-N6   | -5.02 | 1.29        | 1.33     |
| 21  | AA    | 26   | A    | C6-N6   | -5.02 | 1.29        | 1.33     |
| 21  | AA    | 129  | A    | C5-C4   | -5.02 | 1.35        | 1.38     |
| 54  | BA    | 655  | A    | C6-N6   | -5.02 | 1.29        | 1.33     |
| 54  | BA    | 2567 | G    | O3'-P   | -5.02 | 1.55        | 1.61     |
| 54  | BA    | 2686 | G    | C6-N1   | -5.02 | 1.36        | 1.39     |
| 54  | BA    | 2753 | A    | N9-C4   | -5.02 | 1.34        | 1.37     |
| 21  | AA    | 270  | A    | C4'-O4' | -5.02 | 1.39        | 1.45     |
| 21  | AA    | 391  | G    | N1-C2   | -5.02 | 1.33        | 1.37     |
| 21  | AA    | 572  | A    | C4'-O4' | -5.02 | 1.39        | 1.45     |
| 21  | AA    | 824  | G    | C6-N1   | -5.02 | 1.36        | 1.39     |
| 21  | AA    | 1112 | C    | C4-N4   | -5.02 | 1.29        | 1.33     |
| 54  | BA    | 986  | C    | C4-N4   | -5.02 | 1.29        | 1.33     |
| 54  | BA    | 2733 | A    | C5-C4   | -5.02 | 1.35        | 1.38     |
| 21  | AA    | 1059 | C    | C4-N4   | -5.02 | 1.29        | 1.33     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 21  | AA    | 1317 | C    | N3-C4   | -5.02 | 1.30        | 1.33     |
| 54  | BA    | 764  | A    | C6-N1   | -5.02 | 1.32        | 1.35     |
| 54  | BA    | 1469 | A    | C6-N1   | -5.02 | 1.32        | 1.35     |
| 54  | BA    | 411  | G    | C6-N1   | -5.02 | 1.36        | 1.39     |
| 54  | BA    | 2024 | G    | C6-N1   | -5.02 | 1.36        | 1.39     |
| 54  | BA    | 9    | G    | C2-N2   | -5.01 | 1.29        | 1.34     |
| 54  | BA    | 336  | C    | N3-C4   | -5.01 | 1.30        | 1.33     |
| 54  | BA    | 490  | C    | N3-C4   | -5.01 | 1.30        | 1.33     |
| 54  | BA    | 1317 | G    | C6-N1   | -5.01 | 1.36        | 1.39     |
| 21  | AA    | 833  | G    | C2-N2   | -5.01 | 1.29        | 1.34     |
| 54  | BA    | 1037 | G    | C2-N2   | -5.01 | 1.29        | 1.34     |
| 54  | BA    | 2406 | A    | C6-N1   | -5.01 | 1.32        | 1.35     |
| 21  | AA    | 288  | A    | C5-C4   | -5.01 | 1.35        | 1.38     |
| 21  | AA    | 492  | C    | C4-N4   | -5.01 | 1.29        | 1.33     |
| 21  | AA    | 1454 | G    | C4'-O4' | -5.01 | 1.39        | 1.45     |
| 54  | BA    | 2432 | A    | C6-N1   | -5.01 | 1.32        | 1.35     |
| 21  | AA    | 1499 | A    | C6-N1   | -5.01 | 1.32        | 1.35     |
| 21  | AA    | 1533 | C    | C4-N4   | -5.01 | 1.29        | 1.33     |
| 54  | BA    | 270  | A    | C5-C4   | -5.01 | 1.35        | 1.38     |
| 54  | BA    | 318  | C    | C4-N4   | -5.01 | 1.29        | 1.33     |
| 54  | BA    | 1089 | A    | C6-N6   | -5.01 | 1.29        | 1.33     |
| 54  | BA    | 2750 | A    | C5-C4   | -5.01 | 1.35        | 1.38     |
| 55  | BB    | 68   | C    | C4-N4   | -5.01 | 1.29        | 1.33     |
| 21  | AA    | 962  | C    | C4-N4   | -5.01 | 1.29        | 1.33     |
| 54  | BA    | 2862 | G    | C6-N1   | -5.01 | 1.36        | 1.39     |
| 21  | AA    | 1048 | G    | C2-N2   | -5.01 | 1.29        | 1.34     |
| 21  | AA    | 1403 | C    | N3-C4   | -5.01 | 1.30        | 1.33     |
| 54  | BA    | 1698 | A    | C6-N6   | -5.01 | 1.29        | 1.33     |
| 54  | BA    | 1893 | C    | O3'-P   | -5.01 | 1.55        | 1.61     |
| 54  | BA    | 2087 | G    | C2-N2   | -5.01 | 1.29        | 1.34     |
| 55  | BB    | 16   | G    | C6-N1   | -5.01 | 1.36        | 1.39     |
| 54  | BA    | 1434 | A    | C5-C4   | -5.00 | 1.35        | 1.38     |
| 54  | BA    | 1721 | G    | C2-N2   | -5.00 | 1.29        | 1.34     |
| 54  | BA    | 716  | A    | C6-N6   | -5.00 | 1.29        | 1.33     |
| 54  | BA    | 1746 | A    | C6-N1   | -5.00 | 1.32        | 1.35     |
| 54  | BA    | 2381 | A    | C6-N6   | -5.00 | 1.29        | 1.33     |
| 21  | AA    | 745  | G    | C4'-O4' | -5.00 | 1.39        | 1.45     |
| 54  | BA    | 2335 | A    | C4'-O4' | -5.00 | 1.39        | 1.45     |
| 54  | BA    | 2569 | G    | C2-N2   | -5.00 | 1.29        | 1.34     |

All (8646) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 54  | BA    | 2510 | C    | N3-C2-O2   | -15.56 | 111.01      | 121.90   |
| 54  | BA    | 975  | A    | N1-C6-N6   | -13.84 | 110.30      | 118.60   |
| 54  | BA    | 479  | A    | N1-C6-N6   | -13.45 | 110.53      | 118.60   |
| 21  | AA    | 412  | A    | N1-C6-N6   | -12.78 | 110.93      | 118.60   |
| 54  | BA    | 900  | A    | N1-C6-N6   | -12.71 | 110.97      | 118.60   |
| 54  | BA    | 2062 | A    | N1-C6-N6   | -12.44 | 111.14      | 118.60   |
| 21  | AA    | 172  | A    | N1-C6-N6   | -12.39 | 111.17      | 118.60   |
| 23  | A2    | 91   | A    | N1-C6-N6   | -12.35 | 111.19      | 118.60   |
| 54  | BA    | 2433 | A    | N1-C6-N6   | -12.34 | 111.19      | 118.60   |
| 54  | BA    | 2198 | A    | N1-C6-N6   | -12.33 | 111.20      | 118.60   |
| 21  | AA    | 845  | A    | N1-C6-N6   | -12.29 | 111.23      | 118.60   |
| 21  | AA    | 665  | A    | N1-C6-N6   | -12.21 | 111.28      | 118.60   |
| 21  | AA    | 1117 | A    | N1-C6-N6   | -12.15 | 111.31      | 118.60   |
| 21  | AA    | 676  | A    | N1-C6-N6   | -12.11 | 111.33      | 118.60   |
| 55  | BB    | 94   | A    | N1-C6-N6   | -12.04 | 111.37      | 118.60   |
| 54  | BA    | 1073 | A    | N1-C6-N6   | -12.01 | 111.39      | 118.60   |
| 25  | BC    | 176  | ARG  | NE-CZ-NH1  | 11.98  | 126.29      | 120.30   |
| 21  | AA    | 364  | A    | N1-C6-N6   | -11.94 | 111.44      | 118.60   |
| 21  | AA    | 1188 | A    | N1-C6-N6   | -11.92 | 111.45      | 118.60   |
| 21  | AA    | 792  | A    | N1-C6-N6   | -11.85 | 111.49      | 118.60   |
| 21  | AA    | 1150 | A    | N1-C6-N6   | -11.84 | 111.49      | 118.60   |
| 54  | BA    | 910  | A    | N1-C6-N6   | -11.82 | 111.50      | 118.60   |
| 54  | BA    | 1359 | A    | N1-C6-N6   | -11.82 | 111.51      | 118.60   |
| 54  | BA    | 761  | A    | N1-C6-N6   | -11.80 | 111.52      | 118.60   |
| 22  | A1    | 66   | A    | N1-C6-N6   | -11.78 | 111.53      | 118.60   |
| 21  | AA    | 547  | A    | N1-C6-N6   | -11.78 | 111.53      | 118.60   |
| 54  | BA    | 1821 | A    | N1-C6-N6   | -11.77 | 111.54      | 118.60   |
| 54  | BA    | 371  | A    | N1-C6-N6   | -11.77 | 111.54      | 118.60   |
| 54  | BA    | 932  | U    | O4'-C1'-N1 | 11.77  | 117.62      | 108.20   |
| 54  | BA    | 1970 | A    | N1-C6-N6   | -11.77 | 111.54      | 118.60   |
| 54  | BA    | 1404 | C    | N3-C2-O2   | -11.75 | 113.68      | 121.90   |
| 54  | BA    | 323  | C    | O4'-C1'-N1 | 11.74  | 117.59      | 108.20   |
| 21  | AA    | 825  | A    | N1-C6-N6   | -11.74 | 111.56      | 118.60   |
| 54  | BA    | 931  | U    | O4'-C1'-N1 | 11.73  | 117.58      | 108.20   |
| 21  | AA    | 493  | A    | N1-C6-N6   | -11.67 | 111.60      | 118.60   |
| 54  | BA    | 1021 | A    | N1-C6-N6   | -11.67 | 111.60      | 118.60   |
| 54  | BA    | 643  | A    | O4'-C1'-N9 | 11.65  | 117.52      | 108.20   |
| 54  | BA    | 1552 | A    | N1-C6-N6   | -11.62 | 111.63      | 118.60   |
| 21  | AA    | 1042 | A    | N1-C6-N6   | -11.58 | 111.65      | 118.60   |
| 54  | BA    | 1641 | A    | N1-C6-N6   | -11.58 | 111.65      | 118.60   |
| 54  | BA    | 19   | A    | N1-C6-N6   | -11.55 | 111.67      | 118.60   |
| 54  | BA    | 2288 | A    | N1-C6-N6   | -11.54 | 111.68      | 118.60   |
| 55  | BB    | 34   | A    | N1-C6-N6   | -11.51 | 111.70      | 118.60   |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms     | Z      | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|-----------|--------|------------------------|---------------------|
| 54  | BA    | 2872 | A    | N1-C6-N6  | -11.48 | 111.71                 | 118.60              |
| 54  | BA    | 1142 | A    | N1-C6-N6  | -11.46 | 111.73                 | 118.60              |
| 13  | AN    | 63   | ARG  | NE-CZ-NH1 | 11.43  | 126.02                 | 120.30              |
| 54  | BA    | 2090 | A    | N1-C6-N6  | -11.43 | 111.74                 | 118.60              |
| 54  | BA    | 982  | C    | N3-C2-O2  | -11.41 | 113.91                 | 121.90              |
| 21  | AA    | 510  | A    | N1-C6-N6  | -11.41 | 111.75                 | 118.60              |
| 54  | BA    | 631  | A    | N1-C6-N6  | -11.39 | 111.77                 | 118.60              |
| 54  | BA    | 2311 | A    | N1-C6-N6  | -11.39 | 111.77                 | 118.60              |
| 54  | BA    | 1008 | A    | N1-C6-N6  | -11.38 | 111.77                 | 118.60              |
| 21  | AA    | 914  | A    | N1-C6-N6  | -11.38 | 111.77                 | 118.60              |
| 54  | BA    | 2426 | A    | N1-C6-N6  | -11.37 | 111.78                 | 118.60              |
| 13  | AN    | 69   | ARG  | NE-CZ-NH1 | 11.36  | 125.98                 | 120.30              |
| 54  | BA    | 706  | A    | N1-C6-N6  | -11.28 | 111.83                 | 118.60              |
| 21  | AA    | 382  | A    | N1-C6-N6  | -11.28 | 111.83                 | 118.60              |
| 54  | BA    | 1545 | A    | N1-C6-N6  | -11.27 | 111.84                 | 118.60              |
| 21  | AA    | 1285 | A    | N1-C6-N6  | -11.24 | 111.86                 | 118.60              |
| 21  | AA    | 560  | A    | N1-C6-N6  | -11.21 | 111.88                 | 118.60              |
| 54  | BA    | 825  | A    | N1-C6-N6  | -11.20 | 111.88                 | 118.60              |
| 54  | BA    | 582  | A    | N1-C6-N6  | -11.18 | 111.89                 | 118.60              |
| 21  | AA    | 152  | A    | N1-C6-N6  | -11.16 | 111.90                 | 118.60              |
| 54  | BA    | 1404 | C    | N1-C2-O2  | 11.14  | 125.58                 | 118.90              |
| 54  | BA    | 2060 | A    | N1-C6-N6  | -11.13 | 111.92                 | 118.60              |
| 54  | BA    | 497  | A    | N1-C6-N6  | -11.13 | 111.92                 | 118.60              |
| 54  | BA    | 1133 | A    | N1-C6-N6  | -11.13 | 111.92                 | 118.60              |
| 54  | BA    | 2823 | A    | N1-C6-N6  | -11.13 | 111.92                 | 118.60              |
| 21  | AA    | 520  | A    | N1-C6-N6  | -11.12 | 111.93                 | 118.60              |
| 54  | BA    | 1746 | A    | N1-C6-N6  | -11.11 | 111.93                 | 118.60              |
| 21  | AA    | 1251 | A    | N1-C6-N6  | -11.09 | 111.95                 | 118.60              |
| 54  | BA    | 1328 | A    | N1-C6-N6  | -11.08 | 111.95                 | 118.60              |
| 54  | BA    | 750  | A    | N1-C6-N6  | -11.08 | 111.95                 | 118.60              |
| 21  | AA    | 1197 | A    | N1-C6-N6  | -11.07 | 111.96                 | 118.60              |
| 54  | BA    | 1505 | A    | N1-C6-N6  | -11.06 | 111.96                 | 118.60              |
| 21  | AA    | 622  | A    | N1-C6-N6  | -11.06 | 111.96                 | 118.60              |
| 54  | BA    | 347  | A    | N1-C6-N6  | -11.03 | 111.98                 | 118.60              |
| 24  | A3    | 77   | A    | N1-C6-N6  | -11.03 | 111.98                 | 118.60              |
| 21  | AA    | 1502 | A    | N1-C6-N6  | -11.02 | 111.99                 | 118.60              |
| 54  | BA    | 2810 | A    | N1-C6-N6  | -11.02 | 111.99                 | 118.60              |
| 21  | AA    | 1429 | A    | N1-C6-N6  | -10.99 | 112.01                 | 118.60              |
| 54  | BA    | 2411 | A    | N1-C6-N6  | -10.99 | 112.00                 | 118.60              |
| 54  | BA    | 2406 | A    | N1-C6-N6  | -10.98 | 112.01                 | 118.60              |
| 54  | BA    | 161  | A    | N1-C6-N6  | -10.97 | 112.02                 | 118.60              |
| 46  | BX    | 44   | ARG  | NE-CZ-NH1 | 10.96  | 125.78                 | 120.30              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z      | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|------------|--------|------------------------|---------------------|
| 54  | BA    | 821  | A    | N1-C6-N6   | -10.95 | 112.03                 | 118.60              |
| 21  | AA    | 468  | A    | N1-C6-N6   | -10.93 | 112.05                 | 118.60              |
| 21  | AA    | 181  | A    | N1-C6-N6   | -10.92 | 112.05                 | 118.60              |
| 21  | AA    | 363  | A    | N1-C6-N6   | -10.90 | 112.06                 | 118.60              |
| 54  | BA    | 529  | A    | N1-C6-N6   | -10.89 | 112.07                 | 118.60              |
| 21  | AA    | 179  | A    | N1-C6-N6   | -10.88 | 112.07                 | 118.60              |
| 54  | BA    | 1490 | A    | N1-C6-N6   | -10.88 | 112.07                 | 118.60              |
| 54  | BA    | 384  | A    | N1-C6-N6   | -10.88 | 112.07                 | 118.60              |
| 54  | BA    | 1759 | A    | N1-C6-N6   | -10.88 | 112.07                 | 118.60              |
| 54  | BA    | 10   | A    | N1-C6-N6   | -10.87 | 112.08                 | 118.60              |
| 54  | BA    | 2147 | A    | N1-C6-N6   | -10.86 | 112.08                 | 118.60              |
| 21  | AA    | 1105 | A    | N1-C6-N6   | -10.86 | 112.09                 | 118.60              |
| 54  | BA    | 217  | A    | N1-C6-N6   | -10.84 | 112.09                 | 118.60              |
| 54  | BA    | 346  | A    | N1-C6-N6   | -10.83 | 112.10                 | 118.60              |
| 54  | BA    | 1385 | A    | N1-C6-N6   | -10.83 | 112.10                 | 118.60              |
| 21  | AA    | 523  | A    | N1-C6-N6   | -10.82 | 112.11                 | 118.60              |
| 54  | BA    | 752  | A    | O4'-C1'-N9 | 10.82  | 116.86                 | 108.20              |
| 54  | BA    | 2598 | A    | N1-C6-N6   | -10.82 | 112.11                 | 118.60              |
| 54  | BA    | 2267 | A    | N1-C6-N6   | -10.81 | 112.11                 | 118.60              |
| 17  | AR    | 56   | ARG  | NE-CZ-NH1  | 10.80  | 125.70                 | 120.30              |
| 21  | AA    | 1288 | A    | N1-C6-N6   | -10.80 | 112.12                 | 118.60              |
| 54  | BA    | 279  | A    | N1-C6-N6   | -10.80 | 112.12                 | 118.60              |
| 54  | BA    | 1260 | A    | N1-C6-N6   | -10.80 | 112.12                 | 118.60              |
| 54  | BA    | 1420 | A    | N1-C6-N6   | -10.80 | 112.12                 | 118.60              |
| 21  | AA    | 546  | A    | N1-C6-N6   | -10.79 | 112.12                 | 118.60              |
| 54  | BA    | 2850 | A    | N1-C6-N6   | -10.79 | 112.12                 | 118.60              |
| 15  | AP    | 25   | ARG  | NE-CZ-NH1  | 10.78  | 125.69                 | 120.30              |
| 21  | AA    | 356  | A    | N1-C6-N6   | -10.78 | 112.13                 | 118.60              |
| 54  | BA    | 1098 | A    | N1-C6-N6   | -10.78 | 112.13                 | 118.60              |
| 54  | BA    | 2439 | A    | N1-C6-N6   | -10.77 | 112.14                 | 118.60              |
| 54  | BA    | 2381 | A    | N1-C6-N6   | -10.77 | 112.14                 | 118.60              |
| 21  | AA    | 171  | A    | N1-C6-N6   | -10.76 | 112.15                 | 118.60              |
| 21  | AA    | 1238 | A    | N1-C6-N6   | -10.75 | 112.15                 | 118.60              |
| 54  | BA    | 2900 | A    | N1-C6-N6   | -10.75 | 112.15                 | 118.60              |
| 21  | AA    | 366  | A    | N1-C6-N6   | -10.74 | 112.15                 | 118.60              |
| 21  | AA    | 563  | A    | N1-C6-N6   | -10.74 | 112.16                 | 118.60              |
| 54  | BA    | 2142 | A    | N1-C6-N6   | -10.74 | 112.16                 | 118.60              |
| 21  | AA    | 109  | A    | N1-C6-N6   | -10.73 | 112.16                 | 118.60              |
| 21  | AA    | 681  | A    | N1-C6-N6   | -10.73 | 112.16                 | 118.60              |
| 54  | BA    | 504  | A    | N1-C6-N6   | -10.73 | 112.16                 | 118.60              |
| 21  | AA    | 1374 | A    | N1-C6-N6   | -10.72 | 112.17                 | 118.60              |
| 54  | BA    | 676  | A    | N1-C6-N6   | -10.71 | 112.17                 | 118.60              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z      | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|------------|--------|------------------------|---------------------|
| 54  | BA    | 861  | A    | N1-C6-N6   | -10.71 | 112.17                 | 118.60              |
| 54  | BA    | 528  | A    | N1-C6-N6   | -10.70 | 112.18                 | 118.60              |
| 54  | BA    | 983  | A    | N1-C6-N6   | -10.69 | 112.19                 | 118.60              |
| 21  | AA    | 1225 | A    | N1-C6-N6   | -10.68 | 112.19                 | 118.60              |
| 38  | BP    | 100  | ARG  | NE-CZ-NH1  | 10.68  | 125.64                 | 120.30              |
| 54  | BA    | 1566 | A    | N1-C6-N6   | -10.65 | 112.21                 | 118.60              |
| 24  | A3    | 60   | A    | N1-C6-N6   | -10.65 | 112.21                 | 118.60              |
| 21  | AA    | 1151 | A    | N1-C6-N6   | -10.65 | 112.21                 | 118.60              |
| 21  | AA    | 1441 | A    | N1-C6-N6   | -10.65 | 112.21                 | 118.60              |
| 54  | BA    | 2734 | A    | N1-C6-N6   | -10.65 | 112.21                 | 118.60              |
| 36  | BN    | 64   | ARG  | NE-CZ-NH1  | 10.62  | 125.61                 | 120.30              |
| 54  | BA    | 223  | A    | N1-C6-N6   | -10.61 | 112.23                 | 118.60              |
| 54  | BA    | 1808 | A    | N1-C6-N6   | -10.61 | 112.23                 | 118.60              |
| 54  | BA    | 1652 | A    | N1-C6-N6   | -10.61 | 112.24                 | 118.60              |
| 21  | AA    | 1518 | A    | N1-C6-N6   | -10.60 | 112.24                 | 118.60              |
| 21  | AA    | 509  | A    | N1-C6-N6   | -10.59 | 112.25                 | 118.60              |
| 54  | BA    | 614  | A    | N1-C6-N6   | -10.59 | 112.25                 | 118.60              |
| 54  | BA    | 1916 | A    | N1-C6-N6   | -10.59 | 112.25                 | 118.60              |
| 21  | AA    | 1468 | A    | N1-C6-N6   | -10.59 | 112.25                 | 118.60              |
| 21  | AA    | 766  | A    | N1-C6-N6   | -10.57 | 112.26                 | 118.60              |
| 54  | BA    | 2031 | A    | N1-C6-N6   | -10.57 | 112.26                 | 118.60              |
| 54  | BA    | 715  | A    | N1-C6-N6   | -10.57 | 112.26                 | 118.60              |
| 54  | BA    | 1327 | A    | N1-C6-N6   | -10.55 | 112.27                 | 118.60              |
| 55  | BB    | 15   | A    | N1-C6-N6   | -10.55 | 112.27                 | 118.60              |
| 21  | AA    | 383  | A    | N1-C6-N6   | -10.54 | 112.27                 | 118.60              |
| 54  | BA    | 2751 | G    | O4'-C1'-N9 | 10.54  | 116.63                 | 108.20              |
| 3   | AD    | 110  | ARG  | NE-CZ-NH1  | 10.53  | 125.56                 | 120.30              |
| 11  | AL    | 30   | ARG  | NE-CZ-NH1  | 10.51  | 125.56                 | 120.30              |
| 21  | AA    | 1434 | A    | N1-C6-N6   | -10.48 | 112.31                 | 118.60              |
| 54  | BA    | 1129 | A    | N1-C6-N6   | -10.48 | 112.31                 | 118.60              |
| 54  | BA    | 172  | A    | N1-C6-N6   | -10.47 | 112.32                 | 118.60              |
| 21  | AA    | 696  | A    | N1-C6-N6   | -10.47 | 112.32                 | 118.60              |
| 54  | BA    | 94   | A    | N1-C6-N6   | -10.46 | 112.32                 | 118.60              |
| 21  | AA    | 162  | A    | N1-C6-N6   | -10.44 | 112.34                 | 118.60              |
| 24  | A3    | 73   | A    | C5-C6-N1   | 10.44  | 122.92                 | 117.70              |
| 54  | BA    | 1773 | A    | N1-C6-N6   | -10.44 | 112.34                 | 118.60              |
| 54  | BA    | 1535 | A    | N1-C6-N6   | -10.44 | 112.34                 | 118.60              |
| 54  | BA    | 1966 | A    | N1-C6-N6   | -10.44 | 112.34                 | 118.60              |
| 54  | BA    | 2080 | A    | N1-C6-N6   | -10.44 | 112.34                 | 118.60              |
| 54  | BA    | 1614 | A    | N1-C6-N6   | -10.43 | 112.34                 | 118.60              |
| 21  | AA    | 807  | A    | N1-C6-N6   | -10.42 | 112.35                 | 118.60              |
| 54  | BA    | 1365 | A    | N1-C6-N6   | -10.41 | 112.35                 | 118.60              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z      | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|------------|--------|------------------------|---------------------|
| 54  | BA    | 91   | A    | O4'-C1'-N9 | 10.41  | 116.53                 | 108.20              |
| 54  | BA    | 144  | A    | N1-C6-N6   | -10.41 | 112.35                 | 118.60              |
| 54  | BA    | 2274 | A    | N1-C6-N6   | -10.41 | 112.35                 | 118.60              |
| 54  | BA    | 2307 | G    | O4'-C1'-N9 | 10.41  | 116.53                 | 108.20              |
| 21  | AA    | 1022 | A    | N1-C6-N6   | -10.40 | 112.36                 | 118.60              |
| 54  | BA    | 1711 | A    | N1-C6-N6   | -10.39 | 112.36                 | 118.60              |
| 54  | BA    | 1134 | A    | N1-C6-N6   | -10.39 | 112.37                 | 118.60              |
| 54  | BA    | 2358 | A    | N1-C6-N6   | -10.39 | 112.37                 | 118.60              |
| 54  | BA    | 1276 | A    | N1-C6-N6   | -10.39 | 112.37                 | 118.60              |
| 54  | BA    | 127  | A    | N1-C6-N6   | -10.38 | 112.37                 | 118.60              |
| 4   | AE    | 28   | ARG  | NE-CZ-NH1  | 10.38  | 125.49                 | 120.30              |
| 54  | BA    | 2451 | A    | N1-C6-N6   | -10.37 | 112.38                 | 118.60              |
| 54  | BA    | 1847 | A    | O4'-C1'-N9 | 10.37  | 116.50                 | 108.20              |
| 54  | BA    | 352  | A    | N1-C6-N6   | -10.37 | 112.38                 | 118.60              |
| 54  | BA    | 2721 | A    | N1-C6-N6   | -10.37 | 112.38                 | 118.60              |
| 21  | AA    | 873  | A    | N1-C6-N6   | -10.36 | 112.38                 | 118.60              |
| 3   | AD    | 62   | ARG  | NE-CZ-NH1  | 10.34  | 125.47                 | 120.30              |
| 6   | AG    | 69   | ARG  | NE-CZ-NH1  | 10.33  | 125.47                 | 120.30              |
| 21  | AA    | 1191 | A    | N1-C6-N6   | -10.33 | 112.40                 | 118.60              |
| 54  | BA    | 1981 | A    | N1-C6-N6   | -10.32 | 112.41                 | 118.60              |
| 54  | BA    | 2158 | A    | N1-C6-N6   | -10.32 | 112.41                 | 118.60              |
| 54  | BA    | 1654 | A    | N1-C6-N6   | -10.32 | 112.41                 | 118.60              |
| 21  | AA    | 243  | A    | N1-C6-N6   | -10.31 | 112.41                 | 118.60              |
| 54  | BA    | 1088 | A    | N1-C6-N6   | -10.31 | 112.41                 | 118.60              |
| 19  | AT    | 73   | ARG  | NE-CZ-NH1  | 10.31  | 125.45                 | 120.30              |
| 54  | BA    | 556  | A    | N1-C6-N6   | -10.30 | 112.42                 | 118.60              |
| 54  | BA    | 2639 | A    | N1-C6-N6   | -10.30 | 112.42                 | 118.60              |
| 21  | AA    | 1318 | A    | N1-C6-N6   | -10.30 | 112.42                 | 118.60              |
| 54  | BA    | 1679 | A    | N1-C6-N6   | -10.29 | 112.42                 | 118.60              |
| 21  | AA    | 845  | A    | C5-C6-N1   | 10.28  | 122.84                 | 117.70              |
| 21  | AA    | 704  | A    | N1-C6-N6   | -10.27 | 112.44                 | 118.60              |
| 54  | BA    | 996  | A    | N1-C6-N6   | -10.26 | 112.44                 | 118.60              |
| 21  | AA    | 329  | A    | N1-C6-N6   | -10.25 | 112.45                 | 118.60              |
| 54  | BA    | 661  | A    | N1-C6-N6   | -10.25 | 112.45                 | 118.60              |
| 54  | BA    | 2381 | A    | C4-C5-C6   | -10.25 | 111.88                 | 117.00              |
| 21  | AA    | 937  | A    | N1-C6-N6   | -10.24 | 112.45                 | 118.60              |
| 54  | BA    | 2726 | A    | N1-C6-N6   | -10.23 | 112.46                 | 118.60              |
| 21  | AA    | 1036 | A    | N1-C6-N6   | -10.23 | 112.46                 | 118.60              |
| 21  | AA    | 1167 | A    | N1-C6-N6   | -10.23 | 112.46                 | 118.60              |
| 54  | BA    | 653  | U    | O4'-C1'-N1 | 10.23  | 116.38                 | 108.20              |
| 54  | BA    | 526  | A    | N1-C6-N6   | -10.22 | 112.47                 | 118.60              |
| 54  | BA    | 270  | A    | N1-C6-N6   | -10.22 | 112.47                 | 118.60              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z      | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|------------|--------|------------------------|---------------------|
| 21  | AA    | 130  | A    | N1-C6-N6   | -10.22 | 112.47                 | 118.60              |
| 54  | BA    | 739  | A    | N1-C6-N6   | -10.21 | 112.47                 | 118.60              |
| 54  | BA    | 2654 | A    | N1-C6-N6   | -10.21 | 112.47                 | 118.60              |
| 21  | AA    | 1362 | A    | N1-C6-N6   | -10.21 | 112.47                 | 118.60              |
| 21  | AA    | 1152 | A    | N1-C6-N6   | -10.21 | 112.48                 | 118.60              |
| 21  | AA    | 495  | A    | N1-C6-N6   | -10.20 | 112.48                 | 118.60              |
| 54  | BA    | 480  | A    | N1-C6-N6   | -10.20 | 112.48                 | 118.60              |
| 54  | BA    | 2666 | C    | O4'-C1'-N1 | 10.19  | 116.35                 | 108.20              |
| 54  | BA    | 1969 | A    | N1-C6-N6   | -10.19 | 112.49                 | 118.60              |
| 26  | BD    | 83   | ARG  | NE-CZ-NH1  | 10.19  | 125.39                 | 120.30              |
| 54  | BA    | 2873 | A    | N1-C6-N6   | -10.18 | 112.49                 | 118.60              |
| 54  | BA    | 515  | A    | N1-C6-N6   | -10.18 | 112.49                 | 118.60              |
| 21  | AA    | 576  | C    | N3-C2-O2   | -10.18 | 114.78                 | 121.90              |
| 54  | BA    | 877  | A    | N1-C6-N6   | -10.18 | 112.49                 | 118.60              |
| 54  | BA    | 1854 | A    | N1-C6-N6   | -10.17 | 112.50                 | 118.60              |
| 21  | AA    | 162  | A    | C4-C5-C6   | -10.17 | 111.92                 | 117.00              |
| 54  | BA    | 1241 | A    | N1-C6-N6   | -10.16 | 112.50                 | 118.60              |
| 21  | AA    | 573  | A    | N1-C6-N6   | -10.14 | 112.52                 | 118.60              |
| 54  | BA    | 280  | U    | O4'-C1'-N1 | 10.14  | 116.31                 | 108.20              |
| 55  | BB    | 29   | A    | N1-C6-N6   | -10.13 | 112.52                 | 118.60              |
| 54  | BA    | 265  | A    | N1-C6-N6   | -10.13 | 112.52                 | 118.60              |
| 21  | AA    | 251  | G    | O4'-C1'-N9 | 10.11  | 116.28                 | 108.20              |
| 54  | BA    | 1900 | A    | N1-C6-N6   | -10.10 | 112.54                 | 118.60              |
| 21  | AA    | 949  | A    | N1-C6-N6   | -10.09 | 112.55                 | 118.60              |
| 54  | BA    | 735  | A    | N1-C6-N6   | -10.09 | 112.55                 | 118.60              |
| 21  | AA    | 353  | A    | C5-C6-N1   | 10.08  | 122.74                 | 117.70              |
| 47  | BY    | 23   | ARG  | NE-CZ-NH1  | 10.07  | 125.34                 | 120.30              |
| 54  | BA    | 945  | A    | N1-C6-N6   | -10.07 | 112.56                 | 118.60              |
| 21  | AA    | 1508 | A    | N1-C6-N6   | -10.06 | 112.56                 | 118.60              |
| 54  | BA    | 2386 | A    | N1-C6-N6   | -10.06 | 112.56                 | 118.60              |
| 21  | AA    | 1324 | A    | N1-C6-N6   | -10.06 | 112.57                 | 118.60              |
| 21  | AA    | 1346 | A    | C5-C6-N1   | 10.05  | 122.72                 | 117.70              |
| 54  | BA    | 1678 | A    | N1-C6-N6   | -10.04 | 112.58                 | 118.60              |
| 22  | A1    | 41   | A    | N1-C6-N6   | -10.04 | 112.58                 | 118.60              |
| 54  | BA    | 439  | A    | N1-C6-N6   | -10.04 | 112.58                 | 118.60              |
| 54  | BA    | 1810 | A    | N1-C6-N6   | -10.04 | 112.58                 | 118.60              |
| 54  | BA    | 160  | A    | N1-C6-N6   | -10.03 | 112.58                 | 118.60              |
| 54  | BA    | 227  | A    | N1-C6-N6   | -10.03 | 112.58                 | 118.60              |
| 54  | BA    | 447  | A    | N1-C6-N6   | -10.03 | 112.58                 | 118.60              |
| 54  | BA    | 2227 | A    | N1-C6-N6   | -10.03 | 112.58                 | 118.60              |
| 27  | BE    | 114  | ARG  | NE-CZ-NH1  | 10.02  | 125.31                 | 120.30              |
| 54  | BA    | 1927 | A    | N1-C6-N6   | -9.99  | 112.60                 | 118.60              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|------------|-------|------------------------|---------------------|
| 21  | AA    | 131  | A    | N1-C6-N6   | -9.99 | 112.61                 | 118.60              |
| 54  | BA    | 1809 | A    | N1-C6-N6   | -9.99 | 112.61                 | 118.60              |
| 54  | BA    | 1204 | A    | C5-C6-N1   | 9.98  | 122.69                 | 117.70              |
| 54  | BA    | 1819 | A    | C5-C6-N1   | 9.98  | 122.69                 | 117.70              |
| 54  | BA    | 42   | A    | N1-C6-N6   | -9.98 | 112.61                 | 118.60              |
| 54  | BA    | 71   | A    | N1-C6-N6   | -9.97 | 112.62                 | 118.60              |
| 54  | BA    | 1758 | U    | O4'-C1'-N1 | 9.97  | 116.18                 | 108.20              |
| 54  | BA    | 1819 | A    | N1-C6-N6   | -9.97 | 112.62                 | 118.60              |
| 21  | AA    | 959  | A    | N1-C6-N6   | -9.97 | 112.62                 | 118.60              |
| 21  | AA    | 781  | A    | N1-C6-N6   | -9.97 | 112.62                 | 118.60              |
| 54  | BA    | 507  | A    | N1-C6-N6   | -9.96 | 112.62                 | 118.60              |
| 54  | BA    | 2761 | A    | N1-C6-N6   | -9.96 | 112.62                 | 118.60              |
| 21  | AA    | 161  | A    | N1-C6-N6   | -9.95 | 112.63                 | 118.60              |
| 54  | BA    | 2503 | A    | N1-C6-N6   | -9.95 | 112.63                 | 118.60              |
| 21  | AA    | 468  | A    | C5-C6-N1   | 9.95  | 122.67                 | 117.70              |
| 21  | AA    | 382  | A    | C5-C6-N1   | 9.93  | 122.67                 | 117.70              |
| 34  | BL    | 41   | ARG  | NE-CZ-NH1  | 9.93  | 125.27                 | 120.30              |
| 21  | AA    | 892  | A    | N1-C6-N6   | -9.93 | 112.64                 | 118.60              |
| 54  | BA    | 1147 | A    | N1-C6-N6   | -9.92 | 112.64                 | 118.60              |
| 54  | BA    | 2590 | A    | N1-C6-N6   | -9.92 | 112.65                 | 118.60              |
| 21  | AA    | 51   | A    | N1-C6-N6   | -9.92 | 112.65                 | 118.60              |
| 21  | AA    | 1428 | A    | N1-C6-N6   | -9.92 | 112.65                 | 118.60              |
| 21  | AA    | 892  | A    | C4-C5-C6   | -9.91 | 112.04                 | 117.00              |
| 21  | AA    | 1269 | A    | N1-C6-N6   | -9.91 | 112.65                 | 118.60              |
| 21  | AA    | 935  | A    | N1-C6-N6   | -9.91 | 112.66                 | 118.60              |
| 35  | BM    | 6    | ARG  | NE-CZ-NH1  | 9.91  | 125.25                 | 120.30              |
| 54  | BA    | 1987 | A    | N1-C6-N6   | -9.91 | 112.66                 | 118.60              |
| 21  | AA    | 958  | A    | N1-C6-N6   | -9.89 | 112.66                 | 118.60              |
| 23  | A2    | 91   | A    | C5-C6-N1   | 9.89  | 122.64                 | 117.70              |
| 21  | AA    | 32   | A    | N1-C6-N6   | -9.88 | 112.67                 | 118.60              |
| 55  | BB    | 46   | A    | N1-C6-N6   | -9.88 | 112.67                 | 118.60              |
| 3   | AD    | 164  | ARG  | NE-CZ-NH1  | 9.87  | 125.24                 | 120.30              |
| 54  | BA    | 374  | A    | N1-C6-N6   | -9.87 | 112.68                 | 118.60              |
| 54  | BA    | 1772 | A    | C5-C6-N1   | 9.87  | 122.64                 | 117.70              |
| 54  | BA    | 2030 | A    | N1-C6-N6   | -9.87 | 112.68                 | 118.60              |
| 21  | AA    | 1252 | A    | N1-C6-N6   | -9.87 | 112.68                 | 118.60              |
| 54  | BA    | 1847 | A    | N1-C6-N6   | -9.87 | 112.68                 | 118.60              |
| 54  | BA    | 2850 | A    | O4'-C1'-N9 | 9.86  | 116.09                 | 108.20              |
| 54  | BA    | 2670 | A    | N1-C6-N6   | -9.86 | 112.68                 | 118.60              |
| 21  | AA    | 665  | A    | C5-C6-N1   | 9.86  | 122.63                 | 117.70              |
| 54  | BA    | 412  | A    | N1-C6-N6   | -9.85 | 112.69                 | 118.60              |
| 54  | BA    | 2482 | A    | N1-C6-N6   | -9.85 | 112.69                 | 118.60              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 21  | AA    | 872  | A    | N1-C6-N6    | -9.85 | 112.69      | 118.60   |
| 36  | BN    | 30   | ARG  | NE-CZ-NH1   | 9.85  | 125.22      | 120.30   |
| 54  | BA    | 527  | C    | N3-C2-O2    | -9.85 | 115.01      | 121.90   |
| 21  | AA    | 1534 | A    | C1'-O4'-C4' | -9.85 | 102.02      | 109.90   |
| 21  | AA    | 1534 | A    | N1-C6-N6    | -9.84 | 112.70      | 118.60   |
| 54  | BA    | 83   | A    | N1-C6-N6    | -9.84 | 112.70      | 118.60   |
| 54  | BA    | 101  | A    | N1-C6-N6    | -9.84 | 112.70      | 118.60   |
| 54  | BA    | 2634 | A    | N1-C6-N6    | -9.84 | 112.70      | 118.60   |
| 21  | AA    | 607  | A    | N1-C6-N6    | -9.84 | 112.70      | 118.60   |
| 54  | BA    | 2419 | U    | O4'-C1'-N1  | 9.84  | 116.07      | 108.20   |
| 54  | BA    | 49   | A    | N1-C6-N6    | -9.83 | 112.70      | 118.60   |
| 21  | AA    | 196  | A    | N1-C6-N6    | -9.83 | 112.70      | 118.60   |
| 54  | BA    | 2530 | A    | N1-C6-N6    | -9.83 | 112.70      | 118.60   |
| 54  | BA    | 368  | A    | N1-C6-N6    | -9.82 | 112.71      | 118.60   |
| 21  | AA    | 1340 | A    | N1-C6-N6    | -9.81 | 112.71      | 118.60   |
| 54  | BA    | 2872 | A    | C5-C6-N1    | 9.81  | 122.61      | 117.70   |
| 54  | BA    | 2781 | A    | C4-C5-C6    | -9.81 | 112.10      | 117.00   |
| 13  | AN    | 85   | ARG  | NE-CZ-NH1   | 9.80  | 125.20      | 120.30   |
| 21  | AA    | 608  | A    | N1-C6-N6    | -9.80 | 112.72      | 118.60   |
| 54  | BA    | 161  | A    | C5-C6-N1    | 9.80  | 122.60      | 117.70   |
| 21  | AA    | 687  | A    | N1-C6-N6    | -9.80 | 112.72      | 118.60   |
| 54  | BA    | 608  | A    | C5-C6-N1    | 9.80  | 122.60      | 117.70   |
| 54  | BA    | 793  | A    | N1-C6-N6    | -9.79 | 112.72      | 118.60   |
| 54  | BA    | 1757 | A    | N1-C6-N6    | -9.79 | 112.73      | 118.60   |
| 54  | BA    | 2281 | A    | N1-C6-N6    | -9.78 | 112.73      | 118.60   |
| 54  | BA    | 2176 | A    | N1-C6-N6    | -9.78 | 112.73      | 118.60   |
| 54  | BA    | 2469 | A    | N1-C6-N6    | -9.77 | 112.74      | 118.60   |
| 21  | AA    | 478  | A    | N1-C6-N6    | -9.77 | 112.74      | 118.60   |
| 54  | BA    | 1528 | A    | N1-C6-N6    | -9.77 | 112.74      | 118.60   |
| 54  | BA    | 1772 | A    | N1-C6-N6    | -9.77 | 112.74      | 118.60   |
| 54  | BA    | 478  | A    | N1-C6-N6    | -9.76 | 112.74      | 118.60   |
| 21  | AA    | 907  | A    | N1-C6-N6    | -9.76 | 112.74      | 118.60   |
| 12  | AM    | 106  | ARG  | NE-CZ-NH1   | 9.76  | 125.18      | 120.30   |
| 54  | BA    | 1353 | A    | N1-C6-N6    | -9.75 | 112.75      | 118.60   |
| 54  | BA    | 1073 | A    | C5-C6-N1    | 9.74  | 122.57      | 117.70   |
| 55  | BB    | 101  | A    | N1-C6-N6    | -9.74 | 112.75      | 118.60   |
| 54  | BA    | 529  | A    | C5-C6-N1    | 9.74  | 122.57      | 117.70   |
| 54  | BA    | 1009 | A    | N1-C6-N6    | -9.74 | 112.76      | 118.60   |
| 54  | BA    | 1603 | A    | N1-C6-N6    | -9.73 | 112.76      | 118.60   |
| 54  | BA    | 574  | A    | N1-C6-N6    | -9.73 | 112.76      | 118.60   |
| 21  | AA    | 728  | A    | C5-C6-N1    | 9.72  | 122.56      | 117.70   |
| 21  | AA    | 1289 | A    | N1-C6-N6    | -9.71 | 112.77      | 118.60   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|------------|-------|------------------------|---------------------|
| 54  | BA    | 627  | A    | N1-C6-N6   | -9.70 | 112.78                 | 118.60              |
| 54  | BA    | 2792 | A    | N1-C6-N6   | -9.70 | 112.78                 | 118.60              |
| 21  | AA    | 313  | A    | N1-C6-N6   | -9.70 | 112.78                 | 118.60              |
| 54  | BA    | 1143 | A    | N1-C6-N6   | -9.70 | 112.78                 | 118.60              |
| 54  | BA    | 878  | A    | N1-C6-N6   | -9.69 | 112.78                 | 118.60              |
| 21  | AA    | 460  | A    | N1-C6-N6   | -9.68 | 112.79                 | 118.60              |
| 54  | BA    | 241  | A    | N1-C6-N6   | -9.68 | 112.79                 | 118.60              |
| 54  | BA    | 670  | A    | N1-C6-N6   | -9.68 | 112.79                 | 118.60              |
| 54  | BA    | 1559 | U    | O4'-C1'-N1 | 9.68  | 115.94                 | 108.20              |
| 54  | BA    | 633  | A    | N1-C6-N6   | -9.68 | 112.79                 | 118.60              |
| 21  | AA    | 498  | A    | N1-C6-N6   | -9.67 | 112.80                 | 118.60              |
| 54  | BA    | 1211 | C    | O4'-C1'-N1 | 9.66  | 115.93                 | 108.20              |
| 54  | BA    | 1057 | A    | N1-C6-N6   | -9.66 | 112.80                 | 118.60              |
| 21  | AA    | 919  | A    | N1-C6-N6   | -9.65 | 112.81                 | 118.60              |
| 24  | A3    | 44   | A    | N1-C6-N6   | -9.65 | 112.81                 | 118.60              |
| 54  | BA    | 428  | A    | N1-C6-N6   | -9.64 | 112.82                 | 118.60              |
| 21  | AA    | 964  | A    | N1-C6-N6   | -9.63 | 112.82                 | 118.60              |
| 54  | BA    | 2170 | A    | N1-C6-N6   | -9.63 | 112.82                 | 118.60              |
| 54  | BA    | 1987 | A    | C5-C6-N1   | 9.63  | 122.51                 | 117.70              |
| 21  | AA    | 784  | A    | N1-C6-N6   | -9.62 | 112.83                 | 118.60              |
| 54  | BA    | 982  | C    | N1-C2-O2   | 9.62  | 124.67                 | 118.90              |
| 54  | BA    | 1593 | A    | N1-C6-N6   | -9.62 | 112.83                 | 118.60              |
| 54  | BA    | 1084 | A    | C5-C6-N1   | 9.60  | 122.50                 | 117.70              |
| 54  | BA    | 207  | A    | N1-C6-N6   | -9.60 | 112.84                 | 118.60              |
| 21  | AA    | 1336 | C    | N3-C2-O2   | -9.59 | 115.19                 | 121.90              |
| 21  | AA    | 1180 | A    | N1-C6-N6   | -9.59 | 112.85                 | 118.60              |
| 21  | AA    | 1410 | A    | N1-C6-N6   | -9.59 | 112.85                 | 118.60              |
| 54  | BA    | 300  | A    | N1-C6-N6   | -9.59 | 112.85                 | 118.60              |
| 54  | BA    | 2126 | A    | O4'-C1'-N9 | 9.59  | 115.87                 | 108.20              |
| 54  | BA    | 196  | A    | N1-C6-N6   | -9.58 | 112.85                 | 118.60              |
| 21  | AA    | 498  | A    | C5-C6-N1   | 9.58  | 122.49                 | 117.70              |
| 54  | BA    | 430  | A    | N1-C6-N6   | -9.58 | 112.85                 | 118.60              |
| 21  | AA    | 1428 | A    | C5-C6-N1   | 9.57  | 122.49                 | 117.70              |
| 6   | AG    | 95   | ARG  | NE-CZ-NH1  | 9.57  | 125.09                 | 120.30              |
| 54  | BA    | 233  | A    | N1-C6-N6   | -9.57 | 112.86                 | 118.60              |
| 21  | AA    | 364  | A    | C5-C6-N1   | 9.57  | 122.48                 | 117.70              |
| 21  | AA    | 1357 | A    | C4-C5-C6   | -9.56 | 112.22                 | 117.00              |
| 54  | BA    | 2358 | A    | C5-C6-N1   | 9.56  | 122.48                 | 117.70              |
| 54  | BA    | 457  | A    | N1-C6-N6   | -9.56 | 112.86                 | 118.60              |
| 54  | BA    | 1404 | C    | O4'-C1'-N1 | 9.56  | 115.85                 | 108.20              |
| 21  | AA    | 353  | A    | N1-C6-N6   | -9.55 | 112.87                 | 118.60              |
| 55  | BB    | 52   | A    | N1-C6-N6   | -9.55 | 112.87                 | 118.60              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 54  | BA    | 299  | A    | C5-C6-N1   | 9.55  | 122.47      | 117.70   |
| 54  | BA    | 2882 | A    | N1-C6-N6   | -9.55 | 112.87      | 118.60   |
| 54  | BA    | 2108 | A    | N1-C6-N6   | -9.54 | 112.87      | 118.60   |
| 54  | BA    | 2453 | A    | N1-C6-N6   | -9.54 | 112.87      | 118.60   |
| 54  | BA    | 1413 | A    | N1-C6-N6   | -9.54 | 112.88      | 118.60   |
| 54  | BA    | 1630 | A    | N1-C6-N6   | -9.54 | 112.88      | 118.60   |
| 8   | AI    | 105  | ARG  | NE-CZ-NH1  | 9.53  | 125.06      | 120.30   |
| 21  | AA    | 749  | A    | N1-C6-N6   | -9.52 | 112.89      | 118.60   |
| 22  | A1    | 38   | A    | N1-C6-N6   | -9.51 | 112.89      | 118.60   |
| 54  | BA    | 1532 | A    | N1-C6-N6   | -9.51 | 112.89      | 118.60   |
| 54  | BA    | 896  | A    | N1-C6-N6   | -9.51 | 112.90      | 118.60   |
| 54  | BA    | 792  | A    | N1-C6-N6   | -9.50 | 112.90      | 118.60   |
| 54  | BA    | 1772 | A    | C4-C5-C6   | -9.50 | 112.25      | 117.00   |
| 54  | BA    | 1713 | A    | N1-C6-N6   | -9.50 | 112.90      | 118.60   |
| 54  | BA    | 1616 | A    | N1-C6-N6   | -9.49 | 112.90      | 118.60   |
| 54  | BA    | 2733 | A    | N1-C6-N6   | -9.49 | 112.91      | 118.60   |
| 40  | BR    | 79   | ARG  | NE-CZ-NH1  | 9.49  | 125.04      | 120.30   |
| 54  | BA    | 792  | A    | C5-C6-N1   | 9.49  | 122.44      | 117.70   |
| 21  | AA    | 451  | A    | N1-C6-N6   | -9.49 | 112.91      | 118.60   |
| 54  | BA    | 563  | A    | N1-C6-N6   | -9.49 | 112.91      | 118.60   |
| 54  | BA    | 1274 | A    | C5-C6-N1   | 9.48  | 122.44      | 117.70   |
| 21  | AA    | 675  | A    | N1-C6-N6   | -9.47 | 112.92      | 118.60   |
| 54  | BA    | 423  | A    | C5-C6-N1   | 9.47  | 122.44      | 117.70   |
| 54  | BA    | 2309 | A    | N1-C6-N6   | -9.47 | 112.92      | 118.60   |
| 21  | AA    | 767  | A    | N1-C6-N6   | -9.47 | 112.92      | 118.60   |
| 20  | AU    | 17   | ARG  | NE-CZ-NH1  | 9.47  | 125.03      | 120.30   |
| 54  | BA    | 103  | A    | N1-C6-N6   | -9.47 | 112.92      | 118.60   |
| 21  | AA    | 499  | A    | N1-C6-N6   | -9.47 | 112.92      | 118.60   |
| 38  | BP    | 88   | ARG  | NE-CZ-NH1  | 9.46  | 125.03      | 120.30   |
| 54  | BA    | 846  | U    | O4'-C1'-N1 | 9.46  | 115.77      | 108.20   |
| 54  | BA    | 432  | A    | N1-C6-N6   | -9.45 | 112.93      | 118.60   |
| 4   | AE    | 53   | ARG  | NE-CZ-NH1  | 9.45  | 125.03      | 120.30   |
| 54  | BA    | 1427 | A    | C5-C6-N1   | 9.45  | 122.43      | 117.70   |
| 53  | B4    | 36   | ARG  | NE-CZ-NH1  | 9.45  | 125.03      | 120.30   |
| 21  | AA    | 349  | A    | N1-C6-N6   | -9.45 | 112.93      | 118.60   |
| 21  | AA    | 923  | A    | N1-C6-N6   | -9.45 | 112.93      | 118.60   |
| 54  | BA    | 599  | A    | N1-C6-N6   | -9.45 | 112.93      | 118.60   |
| 54  | BA    | 1609 | A    | N1-C6-N6   | -9.45 | 112.93      | 118.60   |
| 21  | AA    | 246  | A    | N1-C6-N6   | -9.44 | 112.93      | 118.60   |
| 54  | BA    | 2587 | A    | N1-C6-N6   | -9.45 | 112.93      | 118.60   |
| 54  | BA    | 1340 | U    | O4'-C1'-N1 | 9.44  | 115.75      | 108.20   |
| 54  | BA    | 2174 | C    | N3-C2-O2   | -9.44 | 115.29      | 121.90   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 54  | BA    | 415  | A    | N1-C6-N6  | -9.44 | 112.94      | 118.60   |
| 21  | AA    | 915  | A    | C5-C6-N1  | 9.44  | 122.42      | 117.70   |
| 21  | AA    | 1519 | A    | N1-C6-N6  | -9.43 | 112.94      | 118.60   |
| 54  | BA    | 2734 | A    | C5-C6-N1  | 9.43  | 122.42      | 117.70   |
| 54  | BA    | 1084 | A    | N1-C6-N6  | -9.43 | 112.94      | 118.60   |
| 54  | BA    | 1477 | A    | C5-C6-N1  | 9.43  | 122.41      | 117.70   |
| 54  | BA    | 1626 | A    | N1-C6-N6  | -9.43 | 112.94      | 118.60   |
| 54  | BA    | 190  | A    | N1-C6-N6  | -9.43 | 112.94      | 118.60   |
| 21  | AA    | 872  | A    | C5-C6-N1  | 9.42  | 122.41      | 117.70   |
| 54  | BA    | 668  | A    | N1-C6-N6  | -9.42 | 112.95      | 118.60   |
| 54  | BA    | 2851 | A    | C5-C6-N1  | 9.42  | 122.41      | 117.70   |
| 54  | BA    | 2886 | A    | N1-C6-N6  | -9.42 | 112.95      | 118.60   |
| 54  | BA    | 2176 | A    | C4-C5-C6  | -9.41 | 112.29      | 117.00   |
| 54  | BA    | 176  | A    | N1-C6-N6  | -9.41 | 112.95      | 118.60   |
| 21  | AA    | 356  | A    | C5-C6-N1  | 9.41  | 122.40      | 117.70   |
| 54  | BA    | 592  | A    | N1-C6-N6  | -9.40 | 112.96      | 118.60   |
| 21  | AA    | 1476 | A    | N1-C6-N6  | -9.40 | 112.96      | 118.60   |
| 54  | BA    | 2267 | A    | C5-C6-N1  | 9.39  | 122.40      | 117.70   |
| 54  | BA    | 470  | A    | N1-C6-N6  | -9.39 | 112.97      | 118.60   |
| 21  | AA    | 250  | A    | N1-C6-N6  | -9.38 | 112.97      | 118.60   |
| 54  | BA    | 2369 | A    | C5-C6-N1  | 9.38  | 122.39      | 117.70   |
| 21  | AA    | 1145 | A    | N1-C6-N6  | -9.38 | 112.97      | 118.60   |
| 54  | BA    | 2273 | A    | N1-C6-N6  | -9.38 | 112.97      | 118.60   |
| 21  | AA    | 371  | A    | N1-C6-N6  | -9.37 | 112.98      | 118.60   |
| 21  | AA    | 1171 | A    | N1-C6-N6  | -9.37 | 112.98      | 118.60   |
| 54  | BA    | 2009 | A    | N1-C6-N6  | -9.37 | 112.98      | 118.60   |
| 54  | BA    | 716  | A    | N1-C6-N6  | -9.37 | 112.98      | 118.60   |
| 54  | BA    | 1347 | A    | N1-C6-N6  | -9.37 | 112.98      | 118.60   |
| 21  | AA    | 26   | A    | C5-C6-N1  | 9.37  | 122.38      | 117.70   |
| 54  | BA    | 44   | A    | N1-C6-N6  | -9.37 | 112.98      | 118.60   |
| 54  | BA    | 2750 | A    | N1-C6-N6  | -9.37 | 112.98      | 118.60   |
| 54  | BA    | 1434 | A    | N1-C6-N6  | -9.36 | 112.98      | 118.60   |
| 54  | BA    | 322  | A    | C5-C6-N1  | 9.36  | 122.38      | 117.70   |
| 21  | AA    | 1219 | A    | N1-C6-N6  | -9.36 | 112.99      | 118.60   |
| 22  | A1    | 66   | A    | C5-C6-N1  | 9.35  | 122.38      | 117.70   |
| 13  | AN    | 24   | ARG  | NE-CZ-NH1 | 9.35  | 124.97      | 120.30   |
| 54  | BA    | 1046 | A    | N1-C6-N6  | -9.35 | 112.99      | 118.60   |
| 54  | BA    | 218  | A    | N1-C6-N6  | -9.34 | 112.99      | 118.60   |
| 54  | BA    | 167  | A    | N1-C6-N6  | -9.33 | 113.00      | 118.60   |
| 54  | BA    | 941  | A    | N1-C6-N6  | -9.33 | 113.00      | 118.60   |
| 21  | AA    | 397  | A    | N1-C6-N6  | -9.33 | 113.00      | 118.60   |
| 54  | BA    | 1264 | A    | N1-C6-N6  | -9.33 | 113.00      | 118.60   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 54  | BA    | 2749 | A    | N1-C6-N6   | -9.32 | 113.00      | 118.60   |
| 21  | AA    | 819  | A    | N1-C6-N6   | -9.32 | 113.01      | 118.60   |
| 21  | AA    | 1357 | A    | N1-C6-N6   | -9.32 | 113.01      | 118.60   |
| 54  | BA    | 1901 | A    | N1-C6-N6   | -9.32 | 113.01      | 118.60   |
| 21  | AA    | 1044 | A    | N1-C6-N6   | -9.32 | 113.01      | 118.60   |
| 54  | BA    | 927  | A    | N1-C6-N6   | -9.32 | 113.01      | 118.60   |
| 21  | AA    | 1513 | A    | C5-C6-N1   | 9.31  | 122.36      | 117.70   |
| 21  | AA    | 143  | A    | N1-C6-N6   | -9.31 | 113.01      | 118.60   |
| 54  | BA    | 655  | A    | C5-C6-N1   | 9.31  | 122.36      | 117.70   |
| 21  | AA    | 510  | A    | C5-C6-N1   | 9.31  | 122.35      | 117.70   |
| 54  | BA    | 2800 | A    | N1-C6-N6   | -9.31 | 113.02      | 118.60   |
| 55  | BB    | 39   | A    | N1-C6-N6   | -9.31 | 113.02      | 118.60   |
| 8   | AI    | 122  | ARG  | NE-CZ-NH2  | 9.31  | 124.95      | 120.30   |
| 21  | AA    | 300  | A    | N1-C6-N6   | -9.30 | 113.02      | 118.60   |
| 54  | BA    | 1598 | A    | C5-C6-N1   | 9.30  | 122.35      | 117.70   |
| 42  | BT    | 77   | ARG  | NE-CZ-NH1  | 9.30  | 124.95      | 120.30   |
| 54  | BA    | 613  | A    | N1-C6-N6   | -9.30 | 113.02      | 118.60   |
| 21  | AA    | 383  | A    | C5-C6-N1   | 9.30  | 122.35      | 117.70   |
| 54  | BA    | 1204 | A    | N1-C6-N6   | -9.30 | 113.02      | 118.60   |
| 54  | BA    | 2886 | A    | O4'-C1'-N9 | 9.30  | 115.64      | 108.20   |
| 54  | BA    | 456  | C    | N3-C2-O2   | -9.30 | 115.39      | 121.90   |
| 21  | AA    | 579  | A    | N1-C6-N6   | -9.29 | 113.03      | 118.60   |
| 21  | AA    | 873  | A    | C5-C6-N1   | 9.29  | 122.34      | 117.70   |
| 54  | BA    | 1434 | A    | C5-C6-N1   | 9.29  | 122.34      | 117.70   |
| 38  | BP    | 20   | ARG  | NE-CZ-NH1  | 9.28  | 124.94      | 120.30   |
| 54  | BA    | 125  | A    | C5-C6-N1   | 9.28  | 122.34      | 117.70   |
| 54  | BA    | 693  | A    | N1-C6-N6   | -9.28 | 113.03      | 118.60   |
| 21  | AA    | 205  | A    | C5-C6-N1   | 9.28  | 122.34      | 117.70   |
| 39  | BQ    | 91   | ARG  | NE-CZ-NH1  | 9.27  | 124.94      | 120.30   |
| 54  | BA    | 2602 | A    | C5-C6-N1   | 9.27  | 122.33      | 117.70   |
| 54  | BA    | 2227 | A    | C5-C6-N1   | 9.27  | 122.33      | 117.70   |
| 54  | BA    | 354  | A    | N1-C6-N6   | -9.26 | 113.04      | 118.60   |
| 54  | BA    | 1610 | A    | N1-C6-N6   | -9.26 | 113.04      | 118.60   |
| 54  | BA    | 2614 | A    | C5-C6-N1   | 9.26  | 122.33      | 117.70   |
| 54  | BA    | 477  | A    | N1-C6-N6   | -9.26 | 113.04      | 118.60   |
| 54  | BA    | 2322 | A    | C4-C5-C6   | -9.26 | 112.37      | 117.00   |
| 21  | AA    | 414  | A    | N1-C6-N6   | -9.25 | 113.05      | 118.60   |
| 34  | BL    | 18   | ARG  | NE-CZ-NH1  | 9.25  | 124.92      | 120.30   |
| 54  | BA    | 346  | A    | C5-C6-N1   | 9.24  | 122.32      | 117.70   |
| 21  | AA    | 493  | A    | C5-C6-N1   | 9.24  | 122.32      | 117.70   |
| 18  | AS    | 77   | ARG  | NE-CZ-NH1  | 9.23  | 124.92      | 120.30   |
| 54  | BA    | 1549 | A    | N1-C6-N6   | -9.23 | 113.06      | 118.60   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|------------|-------|------------------------|---------------------|
| 54  | BA    | 1937 | A    | N1-C6-N6   | -9.23 | 113.06                 | 118.60              |
| 23  | A2    | 79   | A    | N1-C6-N6   | -9.23 | 113.06                 | 118.60              |
| 54  | BA    | 2705 | A    | C5-C6-N1   | 9.23  | 122.31                 | 117.70              |
| 55  | BB    | 15   | A    | C5-C6-N1   | 9.23  | 122.31                 | 117.70              |
| 40  | BR    | 21   | ARG  | NE-CZ-NH1  | 9.22  | 124.91                 | 120.30              |
| 48  | BZ    | 37   | ARG  | NE-CZ-NH1  | 9.22  | 124.91                 | 120.30              |
| 54  | BA    | 721  | A    | N1-C6-N6   | -9.22 | 113.07                 | 118.60              |
| 54  | BA    | 1803 | A    | N1-C6-N6   | -9.22 | 113.07                 | 118.60              |
| 21  | AA    | 1375 | A    | C5-C6-N1   | 9.21  | 122.31                 | 117.70              |
| 54  | BA    | 2119 | A    | N1-C6-N6   | -9.21 | 113.07                 | 118.60              |
| 54  | BA    | 973  | A    | N1-C6-N6   | -9.21 | 113.07                 | 118.60              |
| 54  | BA    | 382  | A    | N1-C6-N6   | -9.21 | 113.08                 | 118.60              |
| 54  | BA    | 979  | A    | N1-C6-N6   | -9.21 | 113.08                 | 118.60              |
| 54  | BA    | 2675 | A    | N1-C6-N6   | -9.20 | 113.08                 | 118.60              |
| 21  | AA    | 1513 | A    | N1-C6-N6   | -9.20 | 113.08                 | 118.60              |
| 54  | BA    | 2450 | A    | N1-C6-N6   | -9.20 | 113.08                 | 118.60              |
| 54  | BA    | 63   | A    | C5-C6-N1   | 9.19  | 122.29                 | 117.70              |
| 54  | BA    | 1630 | A    | C5-C6-N1   | 9.19  | 122.30                 | 117.70              |
| 21  | AA    | 553  | A    | C5-C6-N1   | 9.19  | 122.29                 | 117.70              |
| 21  | AA    | 1285 | A    | C5-C6-N1   | 9.19  | 122.29                 | 117.70              |
| 54  | BA    | 2308 | G    | O4'-C1'-N9 | 9.19  | 115.55                 | 108.20              |
| 21  | AA    | 1299 | A    | C5-C6-N1   | 9.18  | 122.29                 | 117.70              |
| 54  | BA    | 1236 | G    | O4'-C1'-N9 | 9.18  | 115.55                 | 108.20              |
| 54  | BA    | 2090 | A    | C4-C5-C6   | -9.18 | 112.41                 | 117.00              |
| 21  | AA    | 1170 | A    | N1-C6-N6   | -9.18 | 113.09                 | 118.60              |
| 54  | BA    | 911  | A    | C5-C6-N1   | 9.18  | 122.29                 | 117.70              |
| 54  | BA    | 1262 | A    | N1-C6-N6   | -9.18 | 113.09                 | 118.60              |
| 54  | BA    | 513  | A    | N1-C6-N6   | -9.18 | 113.09                 | 118.60              |
| 54  | BA    | 1247 | A    | N1-C6-N6   | -9.17 | 113.10                 | 118.60              |
| 21  | AA    | 509  | A    | C5-C6-N1   | 9.17  | 122.28                 | 117.70              |
| 54  | BA    | 2060 | A    | C5-C6-N1   | 9.17  | 122.28                 | 117.70              |
| 54  | BA    | 490  | C    | N3-C2-O2   | -9.17 | 115.48                 | 121.90              |
| 54  | BA    | 1853 | A    | N1-C6-N6   | -9.17 | 113.10                 | 118.60              |
| 54  | BA    | 2030 | A    | C5-C6-N1   | 9.16  | 122.28                 | 117.70              |
| 21  | AA    | 1360 | A    | N1-C6-N6   | -9.16 | 113.10                 | 118.60              |
| 54  | BA    | 244  | A    | N1-C6-N6   | -9.16 | 113.11                 | 118.60              |
| 54  | BA    | 1090 | A    | N1-C6-N6   | -9.15 | 113.11                 | 118.60              |
| 54  | BA    | 330  | A    | O4'-C1'-N9 | 9.15  | 115.52                 | 108.20              |
| 54  | BA    | 743  | A    | N1-C6-N6   | -9.15 | 113.11                 | 118.60              |
| 54  | BA    | 2173 | A    | N1-C6-N6   | -9.15 | 113.11                 | 118.60              |
| 54  | BA    | 2211 | A    | N1-C6-N6   | -9.15 | 113.11                 | 118.60              |
| 54  | BA    | 2825 | G    | O4'-C1'-N9 | 9.15  | 115.52                 | 108.20              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 54  | BA    | 1655 | A    | N1-C6-N6   | -9.14 | 113.11      | 118.60   |
| 21  | AA    | 1170 | A    | C5-C6-N1   | 9.14  | 122.27      | 117.70   |
| 33  | BK    | 78   | ARG  | NE-CZ-NH1  | 9.14  | 124.87      | 120.30   |
| 21  | AA    | 1346 | A    | N1-C6-N6   | -9.14 | 113.12      | 118.60   |
| 54  | BA    | 502  | A    | N1-C6-N6   | -9.14 | 113.12      | 118.60   |
| 54  | BA    | 626  | A    | N1-C6-N6   | -9.14 | 113.11      | 118.60   |
| 21  | AA    | 1280 | A    | N1-C6-N6   | -9.14 | 113.12      | 118.60   |
| 54  | BA    | 1858 | A    | N1-C6-N6   | -9.13 | 113.12      | 118.60   |
| 54  | BA    | 2090 | A    | C5-C6-N1   | 9.13  | 122.27      | 117.70   |
| 21  | AA    | 931  | C    | N3-C2-O2   | -9.13 | 115.51      | 121.90   |
| 42  | BT    | 69   | ARG  | NE-CZ-NH1  | 9.13  | 124.86      | 120.30   |
| 54  | BA    | 91   | A    | N1-C6-N6   | -9.13 | 113.12      | 118.60   |
| 18  | AS    | 80   | ARG  | NE-CZ-NH1  | 9.12  | 124.86      | 120.30   |
| 21  | AA    | 371  | A    | C5-C6-N1   | 9.12  | 122.26      | 117.70   |
| 54  | BA    | 990  | A    | N1-C6-N6   | -9.12 | 113.13      | 118.60   |
| 54  | BA    | 928  | A    | N1-C6-N6   | -9.12 | 113.13      | 118.60   |
| 54  | BA    | 483  | A    | N1-C6-N6   | -9.12 | 113.13      | 118.60   |
| 21  | AA    | 441  | A    | C5-C6-N1   | 9.11  | 122.26      | 117.70   |
| 54  | BA    | 1014 | A    | N1-C6-N6   | -9.11 | 113.13      | 118.60   |
| 14  | AO    | 76   | ARG  | NE-CZ-NH1  | 9.11  | 124.86      | 120.30   |
| 54  | BA    | 654  | A    | C5-C6-N1   | 9.11  | 122.25      | 117.70   |
| 54  | BA    | 920  | A    | N1-C6-N6   | -9.11 | 113.14      | 118.60   |
| 54  | BA    | 943  | A    | N1-C6-N6   | -9.11 | 113.14      | 118.60   |
| 54  | BA    | 1027 | A    | N1-C6-N6   | -9.11 | 113.14      | 118.60   |
| 54  | BA    | 1637 | A    | N1-C6-N6   | -9.11 | 113.14      | 118.60   |
| 54  | BA    | 2766 | A    | N1-C6-N6   | -9.11 | 113.14      | 118.60   |
| 21  | AA    | 958  | A    | C5-C6-N1   | 9.10  | 122.25      | 117.70   |
| 21  | AA    | 1031 | C    | N3-C2-O2   | -9.10 | 115.53      | 121.90   |
| 24  | A3    | 73   | A    | N1-C6-N6   | -9.10 | 113.14      | 118.60   |
| 54  | BA    | 905  | A    | N1-C6-N6   | -9.10 | 113.14      | 118.60   |
| 54  | BA    | 1780 | A    | N1-C6-N6   | -9.10 | 113.14      | 118.60   |
| 54  | BA    | 104  | A    | C5-C6-N1   | 9.10  | 122.25      | 117.70   |
| 54  | BA    | 42   | A    | C4-C5-C6   | -9.10 | 112.45      | 117.00   |
| 21  | AA    | 155  | A    | N1-C6-N6   | -9.09 | 113.14      | 118.60   |
| 21  | AA    | 199  | A    | N1-C6-N6   | -9.09 | 113.14      | 118.60   |
| 37  | BO    | 33   | ARG  | NE-CZ-NH2  | 9.09  | 124.84      | 120.30   |
| 21  | AA    | 298  | A    | C4-C5-C6   | -9.08 | 112.46      | 117.00   |
| 21  | AA    | 1216 | A    | N1-C6-N6   | -9.08 | 113.15      | 118.60   |
| 54  | BA    | 1385 | A    | C5-C6-N1   | 9.08  | 122.24      | 117.70   |
| 21  | AA    | 1418 | A    | C5-C6-N1   | 9.08  | 122.24      | 117.70   |
| 54  | BA    | 546  | U    | O4'-C1'-N1 | 9.08  | 115.47      | 108.20   |
| 54  | BA    | 2386 | A    | C4-C5-C6   | -9.08 | 112.46      | 117.00   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|------------|-------|------------------------|---------------------|
| 21  | AA    | 1287 | A    | N1-C6-N6   | -9.08 | 113.15                 | 118.60              |
| 54  | BA    | 432  | A    | C5-C6-N1   | 9.08  | 122.24                 | 117.70              |
| 21  | AA    | 1169 | A    | N1-C6-N6   | -9.07 | 113.16                 | 118.60              |
| 21  | AA    | 192  | A    | N1-C6-N6   | -9.07 | 113.16                 | 118.60              |
| 38  | BP    | 38   | ARG  | NE-CZ-NH1  | 9.07  | 124.84                 | 120.30              |
| 54  | BA    | 205  | G    | O4'-C1'-N9 | 9.07  | 115.46                 | 108.20              |
| 54  | BA    | 1932 | A    | C5-C6-N1   | 9.07  | 122.24                 | 117.70              |
| 54  | BA    | 2199 | A    | N1-C6-N6   | -9.07 | 113.16                 | 118.60              |
| 21  | AA    | 313  | A    | C4-C5-C6   | -9.07 | 112.47                 | 117.00              |
| 54  | BA    | 1395 | A    | N1-C6-N6   | -9.07 | 113.16                 | 118.60              |
| 54  | BA    | 2284 | A    | C5-C6-N1   | 9.07  | 122.23                 | 117.70              |
| 54  | BA    | 1890 | A    | N1-C6-N6   | -9.06 | 113.16                 | 118.60              |
| 54  | BA    | 959  | A    | N1-C6-N6   | -9.06 | 113.16                 | 118.60              |
| 54  | BA    | 270  | A    | C5-C6-N1   | 9.06  | 122.23                 | 117.70              |
| 54  | BA    | 1085 | A    | C5-C6-N1   | 9.06  | 122.23                 | 117.70              |
| 21  | AA    | 408  | A    | N1-C6-N6   | -9.06 | 113.17                 | 118.60              |
| 54  | BA    | 718  | A    | N1-C6-N6   | -9.06 | 113.17                 | 118.60              |
| 54  | BA    | 1378 | A    | N1-C6-N6   | -9.06 | 113.17                 | 118.60              |
| 21  | AA    | 913  | A    | N1-C6-N6   | -9.05 | 113.17                 | 118.60              |
| 54  | BA    | 2560 | A    | N1-C6-N6   | -9.05 | 113.17                 | 118.60              |
| 54  | BA    | 1900 | A    | C5-C6-N1   | 9.05  | 122.23                 | 117.70              |
| 54  | BA    | 2665 | A    | N1-C6-N6   | -9.05 | 113.17                 | 118.60              |
| 21  | AA    | 712  | A    | N1-C6-N6   | -9.05 | 113.17                 | 118.60              |
| 54  | BA    | 2154 | A    | N1-C6-N6   | -9.04 | 113.17                 | 118.60              |
| 54  | BA    | 28   | A    | N1-C6-N6   | -9.04 | 113.17                 | 118.60              |
| 54  | BA    | 104  | A    | N1-C6-N6   | -9.04 | 113.18                 | 118.60              |
| 54  | BA    | 804  | A    | N1-C6-N6   | -9.04 | 113.17                 | 118.60              |
| 54  | BA    | 1427 | A    | N1-C6-N6   | -9.04 | 113.18                 | 118.60              |
| 54  | BA    | 1509 | A    | N1-C6-N6   | -9.04 | 113.18                 | 118.60              |
| 54  | BA    | 1580 | A    | N1-C6-N6   | -9.04 | 113.18                 | 118.60              |
| 21  | AA    | 279  | A    | N1-C6-N6   | -9.04 | 113.18                 | 118.60              |
| 54  | BA    | 1089 | A    | C5-C6-N1   | 9.04  | 122.22                 | 117.70              |
| 37  | BO    | 102  | ARG  | NE-CZ-NH1  | 9.03  | 124.82                 | 120.30              |
| 54  | BA    | 2887 | A    | C5-C6-N1   | 9.03  | 122.22                 | 117.70              |
| 21  | AA    | 228  | A    | C5-C6-N1   | 9.03  | 122.21                 | 117.70              |
| 54  | BA    | 2899 | A    | N1-C6-N6   | -9.03 | 113.19                 | 118.60              |
| 54  | BA    | 1960 | A    | N1-C6-N6   | -9.02 | 113.19                 | 118.60              |
| 21  | AA    | 44   | A    | N1-C6-N6   | -9.01 | 113.19                 | 118.60              |
| 54  | BA    | 896  | A    | C5-C6-N1   | 9.01  | 122.21                 | 117.70              |
| 54  | BA    | 2283 | C    | O4'-C1'-N1 | 9.01  | 115.41                 | 108.20              |
| 21  | AA    | 1021 | A    | N1-C6-N6   | -9.01 | 113.19                 | 118.60              |
| 54  | BA    | 56   | A    | C4-C5-C6   | -9.01 | 112.49                 | 117.00              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|-------------|-------|------------------------|---------------------|
| 54  | BA    | 423  | A    | N1-C6-N6    | -9.01 | 113.19                 | 118.60              |
| 54  | BA    | 2534 | A    | N1-C6-N6    | -9.01 | 113.20                 | 118.60              |
| 21  | AA    | 695  | A    | N1-C6-N6    | -9.00 | 113.20                 | 118.60              |
| 21  | AA    | 915  | A    | C4-C5-C6    | -9.00 | 112.50                 | 117.00              |
| 21  | AA    | 1337 | G    | C1'-O4'-C4' | -9.00 | 102.70                 | 109.90              |
| 54  | BA    | 218  | A    | C5-C6-N1    | 9.00  | 122.20                 | 117.70              |
| 21  | AA    | 181  | A    | C5-C6-N1    | 9.00  | 122.20                 | 117.70              |
| 21  | AA    | 906  | A    | N1-C6-N6    | -9.00 | 113.20                 | 118.60              |
| 54  | BA    | 1142 | A    | C5-C6-N1    | 9.00  | 122.20                 | 117.70              |
| 21  | AA    | 900  | A    | N1-C6-N6    | -8.99 | 113.20                 | 118.60              |
| 21  | AA    | 949  | A    | C5-C6-N1    | 8.99  | 122.20                 | 117.70              |
| 21  | AA    | 1152 | A    | C5-C6-N1    | 8.99  | 122.20                 | 117.70              |
| 54  | BA    | 348  | A    | N1-C6-N6    | -8.99 | 113.20                 | 118.60              |
| 54  | BA    | 1918 | A    | N1-C6-N6    | -8.99 | 113.20                 | 118.60              |
| 54  | BA    | 1808 | A    | C5-C6-N1    | 8.99  | 122.19                 | 117.70              |
| 54  | BA    | 2241 | A    | N1-C6-N6    | -8.99 | 113.21                 | 118.60              |
| 55  | BB    | 59   | A    | N1-C6-N6    | -8.99 | 113.21                 | 118.60              |
| 21  | AA    | 1275 | A    | N1-C6-N6    | -8.98 | 113.21                 | 118.60              |
| 54  | BA    | 1700 | A    | C5-C6-N1    | 8.98  | 122.19                 | 117.70              |
| 54  | BA    | 2542 | A    | N1-C6-N6    | -8.98 | 113.21                 | 118.60              |
| 54  | BA    | 2739 | U    | O4'-C1'-N1  | 8.98  | 115.38                 | 108.20              |
| 54  | BA    | 2781 | A    | C5-C6-N1    | 8.98  | 122.19                 | 117.70              |
| 21  | AA    | 1109 | C    | N3-C2-O2    | -8.97 | 115.62                 | 121.90              |
| 54  | BA    | 2392 | A    | N1-C6-N6    | -8.97 | 113.22                 | 118.60              |
| 21  | AA    | 1163 | A    | N1-C6-N6    | -8.96 | 113.22                 | 118.60              |
| 21  | AA    | 1346 | A    | C4-C5-C6    | -8.96 | 112.52                 | 117.00              |
| 54  | BA    | 1570 | A    | N1-C6-N6    | -8.96 | 113.22                 | 118.60              |
| 54  | BA    | 1275 | A    | C5-C6-N1    | 8.96  | 122.18                 | 117.70              |
| 54  | BA    | 2706 | A    | N1-C6-N6    | -8.96 | 113.22                 | 118.60              |
| 21  | AA    | 635  | A    | N1-C6-N6    | -8.96 | 113.23                 | 118.60              |
| 21  | AA    | 715  | A    | N1-C6-N6    | -8.96 | 113.23                 | 118.60              |
| 21  | AA    | 101  | A    | N1-C6-N6    | -8.96 | 113.23                 | 118.60              |
| 21  | AA    | 889  | A    | N1-C6-N6    | -8.96 | 113.23                 | 118.60              |
| 54  | BA    | 2346 | A    | N1-C6-N6    | -8.96 | 113.23                 | 118.60              |
| 21  | AA    | 938  | A    | N1-C6-N6    | -8.95 | 113.23                 | 118.60              |
| 21  | AA    | 649  | A    | N1-C6-N6    | -8.95 | 113.23                 | 118.60              |
| 54  | BA    | 2740 | A    | N1-C6-N6    | -8.95 | 113.23                 | 118.60              |
| 21  | AA    | 72   | A    | N1-C6-N6    | -8.94 | 113.23                 | 118.60              |
| 21  | AA    | 238  | A    | N1-C6-N6    | -8.95 | 113.23                 | 118.60              |
| 21  | AA    | 546  | A    | C5-C6-N1    | 8.94  | 122.17                 | 117.70              |
| 30  | BH    | 27   | ARG  | NE-CZ-NH1   | 8.94  | 124.77                 | 120.30              |
| 21  | AA    | 129  | A    | N1-C6-N6    | -8.94 | 113.24                 | 118.60              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|-------------|-------|------------------------|---------------------|
| 54  | BA    | 2868 | A    | N1-C6-N6    | -8.94 | 113.24                 | 118.60              |
| 21  | AA    | 1508 | A    | C5-C6-N1    | 8.93  | 122.17                 | 117.70              |
| 21  | AA    | 1519 | A    | C5-C6-N1    | 8.93  | 122.17                 | 117.70              |
| 25  | BC    | 237  | ARG  | NE-CZ-NH1   | 8.93  | 124.77                 | 120.30              |
| 54  | BA    | 14   | A    | N1-C6-N6    | -8.93 | 113.24                 | 118.60              |
| 54  | BA    | 433  | C    | N3-C2-O2    | -8.93 | 115.65                 | 121.90              |
| 54  | BA    | 1494 | A    | N1-C6-N6    | -8.93 | 113.24                 | 118.60              |
| 54  | BA    | 479  | A    | C5-C6-N1    | 8.93  | 122.16                 | 117.70              |
| 21  | AA    | 1117 | A    | C5-C6-N1    | 8.93  | 122.16                 | 117.70              |
| 54  | BA    | 2114 | A    | C5-C6-N1    | 8.92  | 122.16                 | 117.70              |
| 54  | BA    | 2510 | C    | N1-C2-O2    | 8.92  | 124.25                 | 118.90              |
| 21  | AA    | 129  | A    | C5-C6-N1    | 8.92  | 122.16                 | 117.70              |
| 21  | AA    | 192  | A    | C5-C6-N1    | 8.92  | 122.16                 | 117.70              |
| 21  | AA    | 1231 | G    | C1'-O4'-C4' | -8.92 | 102.77                 | 109.90              |
| 54  | BA    | 1302 | A    | N1-C6-N6    | -8.92 | 113.25                 | 118.60              |
| 54  | BA    | 1783 | A    | N1-C6-N6    | -8.92 | 113.25                 | 118.60              |
| 25  | BC    | 216  | ARG  | NE-CZ-NH1   | 8.91  | 124.76                 | 120.30              |
| 54  | BA    | 2171 | A    | C5-C6-N1    | 8.91  | 122.16                 | 117.70              |
| 54  | BA    | 155  | A    | C5-C6-N1    | 8.91  | 122.16                 | 117.70              |
| 54  | BA    | 2814 | A    | C5-C6-N1    | 8.91  | 122.15                 | 117.70              |
| 21  | AA    | 1429 | A    | C4-C5-C6    | -8.91 | 112.55                 | 117.00              |
| 54  | BA    | 675  | A    | N1-C6-N6    | -8.91 | 113.26                 | 118.60              |
| 21  | AA    | 415  | A    | N1-C6-N6    | -8.90 | 113.26                 | 118.60              |
| 33  | BK    | 31   | ARG  | NE-CZ-NH1   | 8.90  | 124.75                 | 120.30              |
| 54  | BA    | 1783 | A    | C5-C6-N1    | 8.90  | 122.15                 | 117.70              |
| 22  | A1    | 38   | A    | C5-C6-N1    | 8.90  | 122.15                 | 117.70              |
| 54  | BA    | 111  | A    | N1-C6-N6    | -8.90 | 113.26                 | 118.60              |
| 54  | BA    | 204  | A    | N1-C6-N6    | -8.90 | 113.26                 | 118.60              |
| 54  | BA    | 1287 | A    | N1-C6-N6    | -8.89 | 113.26                 | 118.60              |
| 34  | BL    | 78   | ARG  | NE-CZ-NH1   | 8.89  | 124.75                 | 120.30              |
| 54  | BA    | 63   | A    | N1-C6-N6    | -8.89 | 113.26                 | 118.60              |
| 24  | A3    | 22   | A    | N1-C6-N6    | -8.89 | 113.27                 | 118.60              |
| 21  | AA    | 65   | A    | C5-C6-N1    | 8.89  | 122.14                 | 117.70              |
| 21  | AA    | 969  | A    | C5-C6-N1    | 8.89  | 122.14                 | 117.70              |
| 54  | BA    | 752  | A    | C5-C6-N1    | 8.89  | 122.14                 | 117.70              |
| 54  | BA    | 2058 | A    | N1-C6-N6    | -8.89 | 113.27                 | 118.60              |
| 21  | AA    | 994  | A    | N1-C6-N6    | -8.88 | 113.27                 | 118.60              |
| 54  | BA    | 1784 | A    | N1-C6-N6    | -8.88 | 113.27                 | 118.60              |
| 54  | BA    | 56   | A    | N1-C6-N6    | -8.88 | 113.27                 | 118.60              |
| 54  | BA    | 1552 | A    | O4'-C1'-N9  | 8.88  | 115.30                 | 108.20              |
| 54  | BA    | 1654 | A    | C5-C6-N1    | 8.87  | 122.14                 | 117.70              |
| 21  | AA    | 74   | A    | C5-C6-N1    | 8.87  | 122.13                 | 117.70              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms     | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|-----------|-------|------------------------|---------------------|
| 54  | BA    | 223  | A    | C5-C6-N1  | 8.87  | 122.13                 | 117.70              |
| 54  | BA    | 1322 | A    | C5-C6-N1  | 8.86  | 122.13                 | 117.70              |
| 21  | AA    | 959  | A    | C5-C6-N1  | 8.86  | 122.13                 | 117.70              |
| 36  | BN    | 45   | ARG  | NE-CZ-NH1 | 8.86  | 124.73                 | 120.30              |
| 21  | AA    | 1110 | A    | N1-C6-N6  | -8.86 | 113.28                 | 118.60              |
| 54  | BA    | 2322 | A    | N1-C6-N6  | -8.86 | 113.28                 | 118.60              |
| 54  | BA    | 1264 | A    | C4-C5-C6  | -8.86 | 112.57                 | 117.00              |
| 54  | BA    | 1701 | A    | N1-C6-N6  | -8.86 | 113.28                 | 118.60              |
| 54  | BA    | 2227 | A    | C4-C5-C6  | -8.86 | 112.57                 | 117.00              |
| 54  | BA    | 645  | C    | N3-C2-O2  | -8.86 | 115.70                 | 121.90              |
| 54  | BA    | 2799 | A    | N1-C6-N6  | -8.86 | 113.29                 | 118.60              |
| 21  | AA    | 1111 | A    | N1-C6-N6  | -8.85 | 113.29                 | 118.60              |
| 54  | BA    | 1020 | A    | N1-C6-N6  | -8.85 | 113.29                 | 118.60              |
| 54  | BA    | 1431 | A    | N1-C6-N6  | -8.85 | 113.29                 | 118.60              |
| 42  | BT    | 3    | ARG  | NE-CZ-NH1 | 8.85  | 124.72                 | 120.30              |
| 54  | BA    | 1336 | A    | C5-C6-N1  | 8.85  | 122.13                 | 117.70              |
| 54  | BA    | 2734 | A    | C4-C5-C6  | -8.85 | 112.58                 | 117.00              |
| 54  | BA    | 5    | A    | C5-C6-N1  | 8.85  | 122.12                 | 117.70              |
| 11  | AL    | 98   | ARG  | NE-CZ-NH1 | 8.85  | 124.72                 | 120.30              |
| 21  | AA    | 915  | A    | N1-C6-N6  | -8.85 | 113.29                 | 118.60              |
| 54  | BA    | 1264 | A    | C5-C6-N1  | 8.85  | 122.12                 | 117.70              |
| 54  | BA    | 2829 | A    | N1-C6-N6  | -8.85 | 113.29                 | 118.60              |
| 54  | BA    | 1885 | A    | N1-C6-N6  | -8.85 | 113.29                 | 118.60              |
| 54  | BA    | 2434 | A    | C5-C6-N1  | 8.85  | 122.12                 | 117.70              |
| 21  | AA    | 1368 | A    | C5-C6-N1  | 8.85  | 122.12                 | 117.70              |
| 54  | BA    | 1566 | A    | C5-C6-N1  | 8.85  | 122.12                 | 117.70              |
| 21  | AA    | 1377 | A    | N1-C6-N6  | -8.84 | 113.30                 | 118.60              |
| 24  | A3    | 38   | A    | N1-C6-N6  | -8.84 | 113.30                 | 118.60              |
| 54  | BA    | 829  | A    | N1-C6-N6  | -8.84 | 113.30                 | 118.60              |
| 54  | BA    | 988  | A    | C5-C6-N1  | 8.84  | 122.12                 | 117.70              |
| 54  | BA    | 2781 | A    | N1-C6-N6  | -8.84 | 113.30                 | 118.60              |
| 21  | AA    | 1500 | A    | N1-C6-N6  | -8.83 | 113.30                 | 118.60              |
| 54  | BA    | 984  | A    | N1-C6-N6  | -8.83 | 113.30                 | 118.60              |
| 21  | AA    | 841  | C    | N1-C2-O2  | 8.83  | 124.20                 | 118.90              |
| 54  | BA    | 439  | A    | C5-C6-N1  | 8.83  | 122.11                 | 117.70              |
| 54  | BA    | 1111 | A    | N1-C6-N6  | -8.83 | 113.30                 | 118.60              |
| 54  | BA    | 2900 | A    | C5-C6-N1  | 8.83  | 122.11                 | 117.70              |
| 54  | BA    | 637  | A    | N1-C6-N6  | -8.81 | 113.31                 | 118.60              |
| 21  | AA    | 611  | C    | N3-C2-O2  | -8.81 | 115.73                 | 121.90              |
| 21  | AA    | 482  | A    | N1-C6-N6  | -8.81 | 113.31                 | 118.60              |
| 54  | BA    | 1098 | A    | C5-C6-N1  | 8.81  | 122.10                 | 117.70              |
| 21  | AA    | 860  | A    | C5-C6-N1  | 8.80  | 122.10                 | 117.70              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 54  | BA    | 911  | A    | N1-C6-N6   | -8.81 | 113.32      | 118.60   |
| 54  | BA    | 1969 | A    | C5-C6-N1   | 8.81  | 122.10      | 117.70   |
| 54  | BA    | 2654 | A    | C4-C5-C6   | -8.81 | 112.60      | 117.00   |
| 54  | BA    | 195  | A    | C5-C6-N1   | 8.80  | 122.10      | 117.70   |
| 54  | BA    | 1760 | C    | N3-C2-O2   | -8.80 | 115.74      | 121.90   |
| 10  | AK    | 52   | ARG  | NE-CZ-NH1  | 8.80  | 124.70      | 120.30   |
| 1   | AB    | 62   | ARG  | NE-CZ-NH1  | 8.80  | 124.70      | 120.30   |
| 21  | AA    | 572  | A    | C4-C5-C6   | -8.79 | 112.60      | 117.00   |
| 54  | BA    | 616  | A    | N1-C6-N6   | -8.79 | 113.32      | 118.60   |
| 54  | BA    | 2376 | A    | C5-C6-N1   | 8.79  | 122.10      | 117.70   |
| 21  | AA    | 313  | A    | C5-C6-N1   | 8.79  | 122.10      | 117.70   |
| 21  | AA    | 345  | C    | O4'-C1'-N1 | 8.79  | 115.23      | 108.20   |
| 54  | BA    | 532  | A    | N1-C6-N6   | -8.79 | 113.33      | 118.60   |
| 54  | BA    | 1086 | A    | C5-C6-N1   | 8.79  | 122.10      | 117.70   |
| 54  | BA    | 2635 | A    | N1-C6-N6   | -8.79 | 113.33      | 118.60   |
| 54  | BA    | 1930 | G    | O4'-C1'-N9 | 8.79  | 115.23      | 108.20   |
| 54  | BA    | 1783 | A    | C4-C5-C6   | -8.79 | 112.61      | 117.00   |
| 54  | BA    | 789  | A    | N1-C6-N6   | -8.78 | 113.33      | 118.60   |
| 54  | BA    | 74   | A    | C5-C6-N1   | 8.78  | 122.09      | 117.70   |
| 54  | BA    | 909  | A    | N1-C6-N6   | -8.77 | 113.34      | 118.60   |
| 21  | AA    | 1203 | C    | N3-C2-O2   | -8.77 | 115.76      | 121.90   |
| 21  | AA    | 681  | A    | C5-C6-N1   | 8.77  | 122.08      | 117.70   |
| 21  | AA    | 729  | A    | N1-C6-N6   | -8.77 | 113.34      | 118.60   |
| 21  | AA    | 518  | C    | N3-C2-O2   | -8.76 | 115.77      | 121.90   |
| 54  | BA    | 1241 | A    | C5-C6-N1   | 8.76  | 122.08      | 117.70   |
| 54  | BA    | 1754 | A    | N1-C6-N6   | -8.76 | 113.34      | 118.60   |
| 43  | BU    | 6    | ARG  | NE-CZ-NH1  | 8.76  | 124.68      | 120.30   |
| 54  | BA    | 2058 | A    | C4-C5-C6   | -8.76 | 112.62      | 117.00   |
| 17  | AR    | 52   | ARG  | NE-CZ-NH2  | -8.75 | 115.92      | 120.30   |
| 21  | AA    | 162  | A    | C5-C6-N1   | 8.75  | 122.08      | 117.70   |
| 54  | BA    | 2856 | A    | C5-C6-N1   | 8.75  | 122.08      | 117.70   |
| 2   | AC    | 130  | ARG  | NE-CZ-NH1  | 8.75  | 124.67      | 120.30   |
| 21  | AA    | 794  | A    | N1-C6-N6   | -8.75 | 113.35      | 118.60   |
| 21  | AA    | 864  | A    | N1-C6-N6   | -8.75 | 113.35      | 118.60   |
| 54  | BA    | 1889 | A    | N1-C6-N6   | -8.75 | 113.35      | 118.60   |
| 54  | BA    | 2711 | A    | N1-C6-N6   | -8.75 | 113.35      | 118.60   |
| 55  | BB    | 109  | A    | N1-C6-N6   | -8.75 | 113.35      | 118.60   |
| 21  | AA    | 1311 | A    | N1-C6-N6   | -8.74 | 113.35      | 118.60   |
| 54  | BA    | 1095 | A    | N1-C6-N6   | -8.74 | 113.36      | 118.60   |
| 54  | BA    | 1126 | A    | N1-C6-N6   | -8.74 | 113.36      | 118.60   |
| 21  | AA    | 78   | A    | N1-C6-N6   | -8.74 | 113.36      | 118.60   |
| 21  | AA    | 373  | A    | C5-C6-N1   | 8.74  | 122.07      | 117.70   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|------------|-------|------------------------|---------------------|
| 54  | BA    | 125  | A    | N1-C6-N6   | -8.74 | 113.36                 | 118.60              |
| 21  | AA    | 1248 | A    | N1-C6-N6   | -8.73 | 113.36                 | 118.60              |
| 54  | BA    | 2813 | A    | N1-C6-N6   | -8.73 | 113.36                 | 118.60              |
| 54  | BA    | 64   | A    | N1-C6-N6   | -8.73 | 113.36                 | 118.60              |
| 54  | BA    | 1551 | A    | C4-C5-C6   | -8.73 | 112.64                 | 117.00              |
| 54  | BA    | 2829 | A    | C5-C6-N1   | 8.73  | 122.06                 | 117.70              |
| 54  | BA    | 1987 | A    | C4-C5-C6   | -8.73 | 112.64                 | 117.00              |
| 54  | BA    | 527  | C    | N1-C2-O2   | 8.73  | 124.14                 | 118.90              |
| 54  | BA    | 2762 | C    | N3-C2-O2   | -8.72 | 115.79                 | 121.90              |
| 18  | AS    | 54   | ARG  | NE-CZ-NH1  | 8.72  | 124.66                 | 120.30              |
| 54  | BA    | 294  | A    | C5-C6-N1   | 8.72  | 122.06                 | 117.70              |
| 54  | BA    | 2540 | C    | O4'-C1'-N1 | 8.72  | 115.18                 | 108.20              |
| 21  | AA    | 74   | A    | N1-C6-N6   | -8.72 | 113.37                 | 118.60              |
| 54  | BA    | 1876 | A    | C5-C6-N1   | 8.72  | 122.06                 | 117.70              |
| 54  | BA    | 718  | A    | C5-C6-N1   | 8.72  | 122.06                 | 117.70              |
| 54  | BA    | 1700 | A    | N1-C6-N6   | -8.72 | 113.37                 | 118.60              |
| 54  | BA    | 2439 | A    | C5-C6-N1   | 8.72  | 122.06                 | 117.70              |
| 54  | BA    | 788  | A    | N1-C6-N6   | -8.71 | 113.37                 | 118.60              |
| 21  | AA    | 780  | A    | C5-C6-N1   | 8.71  | 122.06                 | 117.70              |
| 22  | A1    | 6    | A    | N1-C6-N6   | -8.71 | 113.37                 | 118.60              |
| 54  | BA    | 119  | A    | N1-C6-N6   | -8.71 | 113.37                 | 118.60              |
| 54  | BA    | 676  | A    | C5-C6-N1   | 8.71  | 122.06                 | 117.70              |
| 21  | AA    | 205  | A    | N1-C6-N6   | -8.71 | 113.38                 | 118.60              |
| 54  | BA    | 833  | A    | N1-C6-N6   | -8.71 | 113.38                 | 118.60              |
| 33  | BK    | 108  | ARG  | NE-CZ-NH1  | 8.71  | 124.65                 | 120.30              |
| 21  | AA    | 1016 | A    | N1-C6-N6   | -8.70 | 113.38                 | 118.60              |
| 25  | BC    | 220  | ARG  | NE-CZ-NH1  | 8.70  | 124.65                 | 120.30              |
| 54  | BA    | 1665 | A    | C4-C5-C6   | -8.70 | 112.65                 | 117.00              |
| 54  | BA    | 1761 | C    | N3-C2-O2   | -8.70 | 115.81                 | 121.90              |
| 54  | BA    | 2080 | A    | C5-C6-N1   | 8.70  | 122.05                 | 117.70              |
| 21  | AA    | 1170 | A    | C4-C5-C6   | -8.70 | 112.65                 | 117.00              |
| 54  | BA    | 222  | A    | N1-C6-N6   | -8.70 | 113.38                 | 118.60              |
| 54  | BA    | 1156 | A    | N1-C6-N6   | -8.70 | 113.38                 | 118.60              |
| 21  | AA    | 1082 | A    | C4-C5-C6   | -8.70 | 112.65                 | 117.00              |
| 21  | AA    | 792  | A    | C4-C5-C6   | -8.69 | 112.66                 | 117.00              |
| 24  | A3    | 16   | C    | N3-C2-O2   | -8.69 | 115.82                 | 121.90              |
| 36  | BN    | 12   | ARG  | NE-CZ-NH2  | -8.69 | 115.96                 | 120.30              |
| 54  | BA    | 587  | C    | N3-C2-O2   | -8.69 | 115.82                 | 121.90              |
| 54  | BA    | 2654 | A    | C5-C6-N1   | 8.69  | 122.04                 | 117.70              |
| 54  | BA    | 2097 | A    | N1-C6-N6   | -8.69 | 113.39                 | 118.60              |
| 21  | AA    | 533  | A    | N1-C6-N6   | -8.69 | 113.39                 | 118.60              |
| 54  | BA    | 1302 | A    | C5-C6-N1   | 8.69  | 122.04                 | 117.70              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|------------|-------|------------------------|---------------------|
| 54  | BA    | 2829 | A    | C4-C5-C6   | -8.68 | 112.66                 | 117.00              |
| 21  | AA    | 1480 | A    | C4-C5-C6   | -8.68 | 112.66                 | 117.00              |
| 54  | BA    | 2565 | A    | N1-C6-N6   | -8.68 | 113.39                 | 118.60              |
| 54  | BA    | 1419 | A    | N1-C6-N6   | -8.68 | 113.39                 | 118.60              |
| 54  | BA    | 2433 | A    | C5-C6-N1   | 8.68  | 122.04                 | 117.70              |
| 21  | AA    | 1046 | A    | N1-C6-N6   | -8.67 | 113.40                 | 118.60              |
| 54  | BA    | 1785 | A    | C5-C6-N1   | 8.67  | 122.04                 | 117.70              |
| 21  | AA    | 1204 | A    | C5-C6-N1   | 8.67  | 122.03                 | 117.70              |
| 54  | BA    | 1032 | A    | C4-C5-C6   | -8.67 | 112.67                 | 117.00              |
| 21  | AA    | 1012 | A    | N1-C6-N6   | -8.67 | 113.40                 | 118.60              |
| 54  | BA    | 2425 | A    | O4'-C1'-N9 | 8.67  | 115.13                 | 108.20              |
| 54  | BA    | 1451 | C    | O4'-C1'-N1 | 8.66  | 115.13                 | 108.20              |
| 54  | BA    | 2856 | A    | N1-C6-N6   | -8.66 | 113.40                 | 118.60              |
| 54  | BA    | 1211 | C    | N1-C2-O2   | 8.66  | 124.10                 | 118.90              |
| 44  | BV    | 9    | ARG  | NE-CZ-NH1  | 8.66  | 124.63                 | 120.30              |
| 54  | BA    | 2478 | A    | N1-C6-N6   | -8.66 | 113.41                 | 118.60              |
| 54  | BA    | 1936 | A    | N1-C6-N6   | -8.66 | 113.41                 | 118.60              |
| 2   | AC    | 142  | ARG  | NE-CZ-NH1  | 8.65  | 124.63                 | 120.30              |
| 54  | BA    | 1366 | A    | N1-C6-N6   | -8.65 | 113.41                 | 118.60              |
| 54  | BA    | 1664 | A    | C5-C6-N1   | 8.65  | 122.03                 | 117.70              |
| 54  | BA    | 439  | A    | C4-C5-C6   | -8.65 | 112.68                 | 117.00              |
| 54  | BA    | 2879 | A    | N1-C6-N6   | -8.64 | 113.41                 | 118.60              |
| 54  | BA    | 2468 | A    | C5-C6-N1   | 8.64  | 122.02                 | 117.70              |
| 54  | BA    | 1260 | A    | C4-C5-C6   | -8.64 | 112.68                 | 117.00              |
| 21  | AA    | 1493 | A    | C5-C6-N1   | 8.63  | 122.02                 | 117.70              |
| 54  | BA    | 2054 | A    | N1-C6-N6   | -8.63 | 113.42                 | 118.60              |
| 21  | AA    | 288  | A    | C5-C6-N1   | 8.63  | 122.02                 | 117.70              |
| 21  | AA    | 743  | A    | N1-C6-N6   | -8.63 | 113.42                 | 118.60              |
| 21  | AA    | 1281 | C    | N3-C2-O2   | -8.63 | 115.86                 | 121.90              |
| 54  | BA    | 429  | A    | N1-C6-N6   | -8.63 | 113.42                 | 118.60              |
| 54  | BA    | 532  | A    | C5-C6-N1   | 8.63  | 122.02                 | 117.70              |
| 54  | BA    | 1272 | A    | O4'-C1'-N9 | 8.63  | 115.11                 | 108.20              |
| 21  | AA    | 1337 | G    | O4'-C1'-N9 | 8.63  | 115.10                 | 108.20              |
| 54  | BA    | 1213 | A    | N1-C6-N6   | -8.63 | 113.42                 | 118.60              |
| 54  | BA    | 1628 | G    | O4'-C1'-N9 | 8.63  | 115.10                 | 108.20              |
| 21  | AA    | 172  | A    | C4-C5-C6   | -8.63 | 112.69                 | 117.00              |
| 8   | AI    | 98   | ARG  | NE-CZ-NH1  | 8.62  | 124.61                 | 120.30              |
| 21  | AA    | 573  | A    | C4-C5-C6   | -8.62 | 112.69                 | 117.00              |
| 12  | AM    | 106  | ARG  | NE-CZ-NH2  | -8.62 | 115.99                 | 120.30              |
| 21  | AA    | 889  | A    | C4-C5-C6   | -8.61 | 112.69                 | 117.00              |
| 21  | AA    | 1429 | A    | C5-C6-N1   | 8.61  | 122.01                 | 117.70              |
| 54  | BA    | 140  | C    | N3-C2-O2   | -8.61 | 115.87                 | 121.90              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|------------|-------|------------------------|---------------------|
| 54  | BA    | 282  | A    | C5-C6-N1   | 8.61  | 122.01                 | 117.70              |
| 54  | BA    | 2518 | A    | C4-C5-C6   | -8.61 | 112.69                 | 117.00              |
| 21  | AA    | 1533 | C    | N3-C2-O2   | -8.61 | 115.87                 | 121.90              |
| 54  | BA    | 1913 | A    | N1-C6-N6   | -8.61 | 113.43                 | 118.60              |
| 54  | BA    | 2346 | A    | C5-C6-N1   | 8.61  | 122.00                 | 117.70              |
| 54  | BA    | 742  | A    | N1-C6-N6   | -8.61 | 113.44                 | 118.60              |
| 21  | AA    | 1105 | A    | C4-C5-C6   | -8.60 | 112.70                 | 117.00              |
| 54  | BA    | 2076 | U    | O4'-C1'-N1 | 8.60  | 115.08                 | 108.20              |
| 54  | BA    | 2602 | A    | N1-C6-N6   | -8.60 | 113.44                 | 118.60              |
| 24  | A3    | 74   | A    | N1-C6-N6   | -8.60 | 113.44                 | 118.60              |
| 22  | A1    | 73   | A    | N1-C6-N6   | -8.60 | 113.44                 | 118.60              |
| 21  | AA    | 676  | A    | C5-C6-N1   | 8.59  | 122.00                 | 117.70              |
| 21  | AA    | 560  | A    | C5-C6-N1   | 8.59  | 122.00                 | 117.70              |
| 54  | BA    | 1090 | A    | C5-C6-N1   | 8.59  | 122.00                 | 117.70              |
| 54  | BA    | 1420 | A    | C5-C6-N1   | 8.59  | 122.00                 | 117.70              |
| 54  | BA    | 2101 | A    | N1-C6-N6   | -8.59 | 113.45                 | 118.60              |
| 16  | AQ    | 5    | ARG  | NE-CZ-NH1  | 8.59  | 124.59                 | 120.30              |
| 21  | AA    | 373  | A    | N1-C6-N6   | -8.59 | 113.45                 | 118.60              |
| 21  | AA    | 1105 | A    | C5-C6-N1   | 8.59  | 121.99                 | 117.70              |
| 21  | AA    | 236  | A    | N1-C6-N6   | -8.58 | 113.45                 | 118.60              |
| 21  | AA    | 371  | A    | C4-C5-C6   | -8.58 | 112.71                 | 117.00              |
| 54  | BA    | 2587 | A    | C5-C6-N1   | 8.58  | 121.99                 | 117.70              |
| 54  | BA    | 71   | A    | C5-C6-N1   | 8.57  | 121.99                 | 117.70              |
| 54  | BA    | 980  | A    | C5-C6-N1   | 8.57  | 121.99                 | 117.70              |
| 54  | BA    | 2750 | A    | C5-C6-N1   | 8.57  | 121.99                 | 117.70              |
| 21  | AA    | 1434 | A    | C5-C6-N1   | 8.57  | 121.98                 | 117.70              |
| 54  | BA    | 1047 | G    | O4'-C1'-N9 | 8.57  | 115.06                 | 108.20              |
| 54  | BA    | 1050 | A    | N1-C6-N6   | -8.57 | 113.46                 | 118.60              |
| 54  | BA    | 1549 | A    | C5-C6-N1   | 8.57  | 121.99                 | 117.70              |
| 23  | A2    | 80   | C    | N3-C2-O2   | -8.57 | 115.90                 | 121.90              |
| 54  | BA    | 152  | A    | N1-C6-N6   | -8.57 | 113.46                 | 118.60              |
| 54  | BA    | 2238 | G    | O4'-C1'-N9 | 8.57  | 115.05                 | 108.20              |
| 11  | AL    | 120  | ARG  | NE-CZ-NH1  | 8.56  | 124.58                 | 120.30              |
| 21  | AA    | 729  | A    | C4-C5-C6   | -8.56 | 112.72                 | 117.00              |
| 54  | BA    | 792  | A    | C4-C5-C6   | -8.56 | 112.72                 | 117.00              |
| 21  | AA    | 160  | A    | N1-C6-N6   | -8.56 | 113.46                 | 118.60              |
| 54  | BA    | 750  | A    | C4-C5-C6   | -8.56 | 112.72                 | 117.00              |
| 54  | BA    | 936  | A    | N1-C6-N6   | -8.56 | 113.46                 | 118.60              |
| 21  | AA    | 53   | A    | N1-C6-N6   | -8.56 | 113.47                 | 118.60              |
| 21  | AA    | 977  | A    | N1-C6-N6   | -8.56 | 113.47                 | 118.60              |
| 21  | AA    | 1329 | A    | C5-C6-N1   | 8.55  | 121.98                 | 117.70              |
| 54  | BA    | 1244 | A    | N1-C6-N6   | -8.56 | 113.47                 | 118.60              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms     | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|-----------|-------|------------------------|---------------------|
| 54  | BA    | 354  | A    | C5-C6-N1  | 8.55  | 121.98                 | 117.70              |
| 54  | BA    | 2776 | A    | C5-C6-N1  | 8.55  | 121.98                 | 117.70              |
| 21  | AA    | 223  | A    | N1-C6-N6  | -8.55 | 113.47                 | 118.60              |
| 21  | AA    | 308  | C    | N3-C2-O2  | -8.55 | 115.91                 | 121.90              |
| 27  | BE    | 21   | ARG  | NE-CZ-NH1 | 8.55  | 124.58                 | 120.30              |
| 54  | BA    | 454  | A    | N1-C6-N6  | -8.55 | 113.47                 | 118.60              |
| 21  | AA    | 328  | C    | N1-C2-O2  | 8.55  | 124.03                 | 118.90              |
| 21  | AA    | 901  | A    | N1-C6-N6  | -8.55 | 113.47                 | 118.60              |
| 21  | AA    | 172  | A    | C5-C6-N1  | 8.55  | 121.97                 | 117.70              |
| 21  | AA    | 937  | A    | C5-C6-N1  | 8.54  | 121.97                 | 117.70              |
| 21  | AA    | 1468 | A    | C5-C6-N1  | 8.54  | 121.97                 | 117.70              |
| 54  | BA    | 1981 | A    | C5-C6-N1  | 8.54  | 121.97                 | 117.70              |
| 54  | BA    | 2740 | A    | C5-C6-N1  | 8.54  | 121.97                 | 117.70              |
| 54  | BA    | 42   | A    | C5-C6-N1  | 8.54  | 121.97                 | 117.70              |
| 54  | BA    | 1054 | A    | N1-C6-N6  | -8.54 | 113.48                 | 118.60              |
| 20  | AU    | 6    | ARG  | NE-CZ-NH1 | 8.53  | 124.57                 | 120.30              |
| 21  | AA    | 694  | A    | N1-C6-N6  | -8.53 | 113.48                 | 118.60              |
| 54  | BA    | 119  | A    | C4-C5-C6  | -8.53 | 112.73                 | 117.00              |
| 51  | B2    | 33   | ARG  | NE-CZ-NH1 | 8.53  | 124.56                 | 120.30              |
| 14  | AO    | 16   | ARG  | NE-CZ-NH1 | 8.53  | 124.56                 | 120.30              |
| 54  | BA    | 627  | A    | C5-C6-N1  | 8.53  | 121.96                 | 117.70              |
| 2   | AC    | 10   | ARG  | NE-CZ-NH1 | 8.52  | 124.56                 | 120.30              |
| 54  | BA    | 1872 | A    | N1-C6-N6  | -8.52 | 113.49                 | 118.60              |
| 54  | BA    | 221  | A    | N1-C6-N6  | -8.52 | 113.49                 | 118.60              |
| 54  | BA    | 582  | A    | C4-C5-C6  | -8.52 | 112.74                 | 117.00              |
| 21  | AA    | 663  | A    | N1-C6-N6  | -8.52 | 113.49                 | 118.60              |
| 21  | AA    | 702  | A    | N1-C6-N6  | -8.52 | 113.49                 | 118.60              |
| 21  | AA    | 1411 | C    | N3-C2-O2  | -8.52 | 115.94                 | 121.90              |
| 54  | BA    | 1359 | A    | C5-C6-N1  | 8.52  | 121.96                 | 117.70              |
| 54  | BA    | 1515 | A    | N1-C6-N6  | -8.52 | 113.49                 | 118.60              |
| 54  | BA    | 309  | A    | N1-C6-N6  | -8.52 | 113.49                 | 118.60              |
| 22  | A1    | 58   | A    | N1-C6-N6  | -8.51 | 113.49                 | 118.60              |
| 44  | BV    | 93   | ARG  | NE-CZ-NH1 | 8.51  | 124.56                 | 120.30              |
| 54  | BA    | 2088 | A    | N1-C6-N6  | -8.51 | 113.49                 | 118.60              |
| 54  | BA    | 2814 | A    | N1-C6-N6  | -8.51 | 113.49                 | 118.60              |
| 21  | AA    | 349  | A    | C5-C6-N1  | 8.51  | 121.95                 | 117.70              |
| 21  | AA    | 546  | A    | C4-C5-C6  | -8.51 | 112.75                 | 117.00              |
| 54  | BA    | 608  | A    | N1-C6-N6  | -8.51 | 113.50                 | 118.60              |
| 54  | BA    | 1788 | C    | N3-C2-O2  | -8.51 | 115.94                 | 121.90              |
| 55  | BB    | 73   | A    | N1-C6-N6  | -8.51 | 113.49                 | 118.60              |
| 21  | AA    | 780  | A    | N1-C6-N6  | -8.51 | 113.50                 | 118.60              |
| 46  | BX    | 49   | ARG  | NE-CZ-NH1 | 8.51  | 124.55                 | 120.30              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|------------|-------|------------------------|---------------------|
| 21  | AA    | 510  | A    | C4-C5-C6   | -8.51 | 112.75                 | 117.00              |
| 54  | BA    | 1634 | A    | N1-C6-N6   | -8.51 | 113.50                 | 118.60              |
| 21  | AA    | 841  | C    | N3-C2-O2   | -8.50 | 115.95                 | 121.90              |
| 54  | BA    | 482  | A    | N1-C6-N6   | -8.50 | 113.50                 | 118.60              |
| 54  | BA    | 2381 | A    | C5-C6-N1   | 8.50  | 121.95                 | 117.70              |
| 54  | BA    | 2328 | A    | N1-C6-N6   | -8.50 | 113.50                 | 118.60              |
| 13  | AN    | 90   | ARG  | NE-CZ-NH1  | 8.50  | 124.55                 | 120.30              |
| 21  | AA    | 673  | A    | N1-C6-N6   | -8.50 | 113.50                 | 118.60              |
| 21  | AA    | 1342 | C    | N3-C2-O2   | -8.50 | 115.95                 | 121.90              |
| 54  | BA    | 1969 | A    | C4-C5-C6   | -8.50 | 112.75                 | 117.00              |
| 54  | BA    | 2432 | A    | N1-C6-N6   | -8.50 | 113.50                 | 118.60              |
| 21  | AA    | 33   | A    | N1-C6-N6   | -8.49 | 113.50                 | 118.60              |
| 21  | AA    | 65   | A    | N1-C6-N6   | -8.49 | 113.50                 | 118.60              |
| 21  | AA    | 1169 | A    | C5-C6-N1   | 8.49  | 121.95                 | 117.70              |
| 54  | BA    | 889  | C    | N3-C2-O2   | -8.49 | 115.96                 | 121.90              |
| 54  | BA    | 1403 | A    | C5-C6-N1   | 8.49  | 121.95                 | 117.70              |
| 54  | BA    | 1876 | A    | N1-C6-N6   | -8.49 | 113.50                 | 118.60              |
| 55  | BB    | 78   | A    | N1-C6-N6   | -8.49 | 113.50                 | 118.60              |
| 21  | AA    | 151  | A    | N1-C6-N6   | -8.49 | 113.51                 | 118.60              |
| 54  | BA    | 716  | A    | O4'-C1'-N9 | 8.48  | 114.99                 | 108.20              |
| 54  | BA    | 1420 | A    | C4-C5-C6   | -8.48 | 112.76                 | 117.00              |
| 54  | BA    | 2657 | A    | N1-C6-N6   | -8.48 | 113.51                 | 118.60              |
| 54  | BA    | 1008 | A    | C5-C6-N1   | 8.48  | 121.94                 | 117.70              |
| 54  | BA    | 2288 | A    | C5-C6-N1   | 8.48  | 121.94                 | 117.70              |
| 54  | BA    | 2448 | A    | C4-C5-C6   | -8.48 | 112.76                 | 117.00              |
| 55  | BB    | 109  | A    | C4-C5-C6   | -8.48 | 112.76                 | 117.00              |
| 54  | BA    | 1490 | A    | C5-C6-N1   | 8.47  | 121.94                 | 117.70              |
| 54  | BA    | 2139 | U    | O4'-C1'-N1 | 8.47  | 114.98                 | 108.20              |
| 21  | AA    | 80   | A    | N1-C6-N6   | -8.47 | 113.52                 | 118.60              |
| 21  | AA    | 968  | A    | N1-C6-N6   | -8.47 | 113.52                 | 118.60              |
| 54  | BA    | 149  | A    | N1-C6-N6   | -8.47 | 113.52                 | 118.60              |
| 54  | BA    | 2757 | A    | C5-C6-N1   | 8.47  | 121.94                 | 117.70              |
| 54  | BA    | 2451 | A    | C5-C6-N1   | 8.47  | 121.94                 | 117.70              |
| 21  | AA    | 65   | A    | C4-C5-C6   | -8.47 | 112.77                 | 117.00              |
| 21  | AA    | 1054 | C    | O4'-C1'-N1 | 8.46  | 114.97                 | 108.20              |
| 19  | AT    | 24   | ARG  | NE-CZ-NH1  | 8.46  | 124.53                 | 120.30              |
| 21  | AA    | 60   | A    | N1-C6-N6   | -8.46 | 113.52                 | 118.60              |
| 54  | BA    | 528  | A    | C5-C6-N1   | 8.46  | 121.93                 | 117.70              |
| 54  | BA    | 526  | A    | C5-C6-N1   | 8.46  | 121.93                 | 117.70              |
| 21  | AA    | 8    | A    | N1-C6-N6   | -8.46 | 113.53                 | 118.60              |
| 21  | AA    | 1501 | C    | N3-C2-O2   | -8.46 | 115.98                 | 121.90              |
| 54  | BA    | 1321 | A    | N1-C6-N6   | -8.46 | 113.53                 | 118.60              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms     | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|-----------|-------|------------------------|---------------------|
| 21  | AA    | 131  | A    | C4-C5-C6  | -8.45 | 112.78                 | 117.00              |
| 32  | BJ    | 37   | ARG  | NE-CZ-NH1 | 8.45  | 124.53                 | 120.30              |
| 21  | AA    | 303  | A    | N1-C6-N6  | -8.45 | 113.53                 | 118.60              |
| 54  | BA    | 2176 | A    | C5-C6-N1  | 8.45  | 121.92                 | 117.70              |
| 21  | AA    | 576  | C    | N1-C2-O2  | 8.45  | 123.97                 | 118.90              |
| 54  | BA    | 2809 | A    | N1-C6-N6  | -8.45 | 113.53                 | 118.60              |
| 21  | AA    | 161  | A    | C4-C5-C6  | -8.44 | 112.78                 | 117.00              |
| 54  | BA    | 2376 | A    | N1-C6-N6  | -8.44 | 113.53                 | 118.60              |
| 21  | AA    | 466  | A    | N1-C6-N6  | -8.44 | 113.53                 | 118.60              |
| 54  | BA    | 2899 | A    | C5-C6-N1  | 8.44  | 121.92                 | 117.70              |
| 4   | AE    | 149  | PRO  | CA-N-CD   | -8.44 | 99.68                  | 111.50              |
| 54  | BA    | 94   | A    | C5-C6-N1  | 8.44  | 121.92                 | 117.70              |
| 54  | BA    | 1550 | C    | N3-C2-O2  | -8.44 | 115.99                 | 121.90              |
| 54  | BA    | 433  | C    | N1-C2-O2  | 8.44  | 123.96                 | 118.90              |
| 54  | BA    | 866  | A    | N1-C6-N6  | -8.44 | 113.54                 | 118.60              |
| 21  | AA    | 795  | C    | N3-C2-O2  | -8.44 | 116.00                 | 121.90              |
| 54  | BA    | 2435 | A    | N1-C6-N6  | -8.44 | 113.54                 | 118.60              |
| 21  | AA    | 1082 | A    | C5-C6-N1  | 8.43  | 121.92                 | 117.70              |
| 26  | BD    | 128  | ARG  | NE-CZ-NH1 | 8.43  | 124.52                 | 120.30              |
| 21  | AA    | 1531 | A    | N1-C6-N6  | -8.43 | 113.54                 | 118.60              |
| 21  | AA    | 1447 | A    | N1-C6-N6  | -8.43 | 113.54                 | 118.60              |
| 32  | BJ    | 116  | ARG  | NE-CZ-NH1 | 8.43  | 124.51                 | 120.30              |
| 54  | BA    | 764  | A    | N1-C6-N6  | -8.43 | 113.55                 | 118.60              |
| 54  | BA    | 2518 | A    | C5-C6-N1  | 8.43  | 121.91                 | 117.70              |
| 21  | AA    | 747  | A    | N1-C6-N6  | -8.42 | 113.55                 | 118.60              |
| 54  | BA    | 2434 | A    | N1-C6-N6  | -8.42 | 113.55                 | 118.60              |
| 43  | BU    | 85   | ARG  | NE-CZ-NH1 | 8.42  | 124.51                 | 120.30              |
| 54  | BA    | 644  | A    | C5-C6-N1  | 8.42  | 121.91                 | 117.70              |
| 21  | AA    | 53   | A    | C4-C5-C6  | -8.42 | 112.79                 | 117.00              |
| 21  | AA    | 7    | A    | C4-C5-C6  | -8.41 | 112.79                 | 117.00              |
| 21  | AA    | 174  | A    | N1-C6-N6  | -8.41 | 113.55                 | 118.60              |
| 54  | BA    | 2851 | A    | N1-C6-N6  | -8.41 | 113.55                 | 118.60              |
| 21  | AA    | 498  | A    | C4-C5-C6  | -8.41 | 112.80                 | 117.00              |
| 54  | BA    | 2199 | A    | C5-C6-N1  | 8.41  | 121.90                 | 117.70              |
| 54  | BA    | 1336 | A    | C4-C5-C6  | -8.41 | 112.80                 | 117.00              |
| 54  | BA    | 2547 | A    | N1-C6-N6  | -8.41 | 113.56                 | 118.60              |
| 21  | AA    | 816  | A    | N1-C6-N6  | -8.40 | 113.56                 | 118.60              |
| 54  | BA    | 654  | A    | N1-C6-N6  | -8.40 | 113.56                 | 118.60              |
| 54  | BA    | 819  | A    | N1-C6-N6  | -8.40 | 113.56                 | 118.60              |
| 21  | AA    | 1503 | A    | N1-C6-N6  | -8.40 | 113.56                 | 118.60              |
| 26  | BD    | 13   | ARG  | NE-CZ-NH1 | 8.40  | 124.50                 | 120.30              |
| 54  | BA    | 756  | A    | N1-C6-N6  | -8.40 | 113.56                 | 118.60              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 54  | BA    | 1366 | A    | C4-C5-C6   | -8.40 | 112.80      | 117.00   |
| 54  | BA    | 2191 | A    | N1-C6-N6   | -8.40 | 113.56      | 118.60   |
| 53  | B4    | 24   | ARG  | NE-CZ-NH1  | 8.40  | 124.50      | 120.30   |
| 54  | BA    | 1655 | A    | C4-C5-C6   | -8.40 | 112.80      | 117.00   |
| 54  | BA    | 1057 | A    | C5-C6-N1   | 8.39  | 121.90      | 117.70   |
| 54  | BA    | 1786 | A    | N1-C6-N6   | -8.39 | 113.56      | 118.60   |
| 21  | AA    | 743  | A    | C5-C6-N1   | 8.39  | 121.89      | 117.70   |
| 54  | BA    | 31   | C    | N3-C2-O2   | -8.39 | 116.03      | 121.90   |
| 54  | BA    | 2411 | A    | C5-C6-N1   | 8.39  | 121.89      | 117.70   |
| 54  | BA    | 716  | A    | C5-C6-N1   | 8.39  | 121.89      | 117.70   |
| 54  | BA    | 1647 | U    | O4'-C1'-N1 | 8.39  | 114.91      | 108.20   |
| 54  | BA    | 721  | A    | C4-C5-C6   | -8.39 | 112.81      | 117.00   |
| 54  | BA    | 2738 | A    | C5-C6-N1   | 8.39  | 121.89      | 117.70   |
| 21  | AA    | 1213 | A    | N1-C6-N6   | -8.38 | 113.57      | 118.60   |
| 54  | BA    | 1871 | A    | N1-C6-N6   | -8.38 | 113.57      | 118.60   |
| 21  | AA    | 1191 | A    | C5-C6-N1   | 8.38  | 121.89      | 117.70   |
| 54  | BA    | 2776 | A    | N1-C6-N6   | -8.38 | 113.57      | 118.60   |
| 54  | BA    | 149  | A    | C5-C6-N1   | 8.38  | 121.89      | 117.70   |
| 54  | BA    | 1732 | C    | N3-C2-O2   | -8.38 | 116.04      | 121.90   |
| 54  | BA    | 1789 | A    | C4-C5-C6   | -8.38 | 112.81      | 117.00   |
| 21  | AA    | 279  | A    | C5-C6-N1   | 8.37  | 121.89      | 117.70   |
| 21  | AA    | 441  | A    | C4-C5-C6   | -8.37 | 112.81      | 117.00   |
| 54  | BA    | 2212 | A    | C5-C6-N1   | 8.37  | 121.89      | 117.70   |
| 54  | BA    | 2287 | A    | C5-C6-N1   | 8.37  | 121.89      | 117.70   |
| 21  | AA    | 1480 | A    | N1-C6-N6   | -8.37 | 113.58      | 118.60   |
| 21  | AA    | 77   | A    | N1-C6-N6   | -8.37 | 113.58      | 118.60   |
| 54  | BA    | 1522 | A    | N1-C6-N6   | -8.37 | 113.58      | 118.60   |
| 25  | BC    | 211  | ARG  | NE-CZ-NH1  | 8.36  | 124.48      | 120.30   |
| 21  | AA    | 389  | A    | N1-C6-N6   | -8.36 | 113.58      | 118.60   |
| 21  | AA    | 932  | C    | N3-C2-O2   | -8.36 | 116.05      | 121.90   |
| 54  | BA    | 2700 | A    | N1-C6-N6   | -8.36 | 113.58      | 118.60   |
| 54  | BA    | 1784 | A    | C4-C5-C6   | -8.36 | 112.82      | 117.00   |
| 54  | BA    | 1952 | A    | N1-C6-N6   | -8.36 | 113.58      | 118.60   |
| 21  | AA    | 1046 | A    | C4-C5-C6   | -8.35 | 112.82      | 117.00   |
| 21  | AA    | 1014 | A    | N1-C6-N6   | -8.35 | 113.59      | 118.60   |
| 54  | BA    | 219  | A    | N1-C6-N6   | -8.35 | 113.59      | 118.60   |
| 54  | BA    | 1960 | A    | C5-C6-N1   | 8.35  | 121.88      | 117.70   |
| 56  | B5    | 71   | ARG  | NE-CZ-NH1  | 8.35  | 124.48      | 120.30   |
| 56  | B5    | 164  | ARG  | NE-CZ-NH1  | 8.35  | 124.48      | 120.30   |
| 1   | AB    | 138  | ARG  | NE-CZ-NH1  | 8.35  | 124.47      | 120.30   |
| 24  | A3    | 77   | A    | C5-C6-N1   | 8.35  | 121.87      | 117.70   |
| 54  | BA    | 2682 | A    | N1-C6-N6   | -8.35 | 113.59      | 118.60   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|------------|-------|------------------------|---------------------|
| 21  | AA    | 1299 | A    | N1-C6-N6   | -8.35 | 113.59                 | 118.60              |
| 24  | A3    | 74   | A    | C5-C6-N1   | 8.35  | 121.87                 | 117.70              |
| 54  | BA    | 1548 | A    | N1-C6-N6   | -8.35 | 113.59                 | 118.60              |
| 21  | AA    | 629  | A    | N1-C6-N6   | -8.34 | 113.59                 | 118.60              |
| 20  | AU    | 33   | ARG  | NE-CZ-NH1  | 8.34  | 124.47                 | 120.30              |
| 21  | AA    | 1274 | A    | N1-C6-N6   | -8.34 | 113.59                 | 118.60              |
| 54  | BA    | 1301 | A    | C5-C6-N1   | 8.34  | 121.87                 | 117.70              |
| 55  | BB    | 70   | C    | N3-C2-O2   | -8.34 | 116.06                 | 121.90              |
| 54  | BA    | 2032 | G    | C8-N9-C4   | -8.34 | 103.06                 | 106.40              |
| 22  | A1    | 9    | A    | N1-C6-N6   | -8.34 | 113.60                 | 118.60              |
| 54  | BA    | 332  | A    | N1-C6-N6   | -8.33 | 113.60                 | 118.60              |
| 54  | BA    | 1545 | A    | C5-C6-N1   | 8.33  | 121.86                 | 117.70              |
| 21  | AA    | 1081 | A    | N1-C6-N6   | -8.33 | 113.60                 | 118.60              |
| 21  | AA    | 495  | A    | C5-C6-N1   | 8.33  | 121.86                 | 117.70              |
| 54  | BA    | 1080 | A    | N1-C6-N6   | -8.33 | 113.61                 | 118.60              |
| 54  | BA    | 1535 | A    | C5-C6-N1   | 8.33  | 121.86                 | 117.70              |
| 54  | BA    | 1650 | A    | N1-C6-N6   | -8.33 | 113.60                 | 118.60              |
| 54  | BA    | 528  | A    | C4-C5-C6   | -8.32 | 112.84                 | 117.00              |
| 54  | BA    | 2165 | C    | N3-C2-O2   | -8.32 | 116.07                 | 121.90              |
| 21  | AA    | 50   | A    | C5-C6-N1   | 8.32  | 121.86                 | 117.70              |
| 54  | BA    | 56   | A    | C5-C6-N1   | 8.32  | 121.86                 | 117.70              |
| 54  | BA    | 177  | G    | O4'-C1'-N9 | 8.32  | 114.86                 | 108.20              |
| 21  | AA    | 26   | A    | N1-C6-N6   | -8.32 | 113.61                 | 118.60              |
| 21  | AA    | 325  | A    | N1-C6-N6   | -8.32 | 113.61                 | 118.60              |
| 54  | BA    | 699  | A    | N1-C6-N6   | -8.32 | 113.61                 | 118.60              |
| 54  | BA    | 218  | A    | C4-C5-C6   | -8.32 | 112.84                 | 117.00              |
| 29  | BG    | 34   | ARG  | NE-CZ-NH1  | 8.31  | 124.46                 | 120.30              |
| 24  | A3    | 75   | C    | N3-C2-O2   | -8.31 | 116.08                 | 121.90              |
| 54  | BA    | 449  | A    | N1-C6-N6   | -8.31 | 113.61                 | 118.60              |
| 21  | AA    | 728  | A    | N1-C6-N6   | -8.31 | 113.61                 | 118.60              |
| 54  | BA    | 2476 | A    | N1-C6-N6   | -8.31 | 113.61                 | 118.60              |
| 54  | BA    | 2766 | A    | C5-C6-N1   | 8.31  | 121.86                 | 117.70              |
| 54  | BA    | 2541 | A    | N1-C6-N6   | -8.31 | 113.61                 | 118.60              |
| 21  | AA    | 328  | C    | N3-C2-O2   | -8.31 | 116.08                 | 121.90              |
| 21  | AA    | 1101 | A    | C4-C5-C6   | -8.31 | 112.85                 | 117.00              |
| 54  | BA    | 213  | A    | N1-C6-N6   | -8.30 | 113.62                 | 118.60              |
| 54  | BA    | 2741 | A    | N1-C6-N6   | -8.30 | 113.62                 | 118.60              |
| 55  | BB    | 15   | A    | O4'-C1'-N9 | 8.30  | 114.84                 | 108.20              |
| 21  | AA    | 431  | A    | N1-C6-N6   | -8.30 | 113.62                 | 118.60              |
| 54  | BA    | 2589 | A    | N1-C6-N6   | -8.30 | 113.62                 | 118.60              |
| 54  | BA    | 2882 | A    | C4-C5-C6   | -8.30 | 112.85                 | 117.00              |
| 54  | BA    | 1090 | A    | C4-C5-C6   | -8.30 | 112.85                 | 117.00              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 54  | BA    | 2575 | C    | N3-C2-O2   | -8.30 | 116.09      | 121.90   |
| 21  | AA    | 50   | A    | N1-C6-N6   | -8.29 | 113.62      | 118.60   |
| 54  | BA    | 1175 | A    | N1-C6-N6   | -8.29 | 113.62      | 118.60   |
| 54  | BA    | 1913 | A    | C5-C6-N1   | 8.29  | 121.85      | 117.70   |
| 48  | BZ    | 30   | ARG  | NE-CZ-NH1  | 8.29  | 124.44      | 120.30   |
| 54  | BA    | 727  | A    | C5-C6-N1   | 8.29  | 121.85      | 117.70   |
| 55  | BB    | 57   | A    | C5-C6-N1   | 8.29  | 121.85      | 117.70   |
| 21  | AA    | 559  | A    | N1-C6-N6   | -8.29 | 113.63      | 118.60   |
| 54  | BA    | 910  | A    | C5-C6-N1   | 8.29  | 121.84      | 117.70   |
| 54  | BA    | 1698 | A    | C5-C6-N1   | 8.29  | 121.84      | 117.70   |
| 54  | BA    | 655  | A    | C4-C5-C6   | -8.28 | 112.86      | 117.00   |
| 54  | BA    | 1810 | A    | C5-C6-N1   | 8.28  | 121.84      | 117.70   |
| 54  | BA    | 2407 | A    | N1-C6-N6   | -8.28 | 113.63      | 118.60   |
| 21  | AA    | 10   | A    | C4-C5-C6   | -8.28 | 112.86      | 117.00   |
| 22  | A1    | 35   | A    | C4-C5-C6   | -8.28 | 112.86      | 117.00   |
| 54  | BA    | 1237 | A    | N1-C6-N6   | -8.28 | 113.63      | 118.60   |
| 54  | BA    | 1801 | A    | N1-C6-N6   | -8.28 | 113.63      | 118.60   |
| 54  | BA    | 1938 | A    | C5-C6-N1   | 8.28  | 121.84      | 117.70   |
| 1   | AB    | 112  | ARG  | NE-CZ-NH1  | 8.28  | 124.44      | 120.30   |
| 21  | AA    | 1441 | A    | C5-C6-N1   | 8.28  | 121.84      | 117.70   |
| 54  | BA    | 497  | A    | C5-C6-N1   | 8.28  | 121.84      | 117.70   |
| 54  | BA    | 63   | A    | C4-C5-C6   | -8.28 | 112.86      | 117.00   |
| 54  | BA    | 196  | A    | O4'-C1'-N9 | 8.28  | 114.82      | 108.20   |
| 54  | BA    | 1050 | A    | C5-C6-N1   | 8.28  | 121.84      | 117.70   |
| 54  | BA    | 1876 | A    | C4-C5-C6   | -8.28 | 112.86      | 117.00   |
| 54  | BA    | 979  | A    | C5-C6-N1   | 8.27  | 121.84      | 117.70   |
| 54  | BA    | 1165 | A    | N1-C6-N6   | -8.27 | 113.64      | 118.60   |
| 21  | AA    | 865  | A    | N1-C6-N6   | -8.27 | 113.64      | 118.60   |
| 45  | BW    | 76   | ARG  | NE-CZ-NH1  | 8.27  | 124.44      | 120.30   |
| 54  | BA    | 2660 | A    | N1-C6-N6   | -8.27 | 113.64      | 118.60   |
| 21  | AA    | 336  | A    | N1-C6-N6   | -8.27 | 113.64      | 118.60   |
| 54  | BA    | 2199 | A    | C4-C5-C6   | -8.27 | 112.86      | 117.00   |
| 28  | BF    | 177  | ARG  | NE-CZ-NH2  | 8.27  | 124.43      | 120.30   |
| 54  | BA    | 2184 | A    | N1-C6-N6   | -8.27 | 113.64      | 118.60   |
| 34  | BL    | 47   | ARG  | NE-CZ-NH1  | 8.26  | 124.43      | 120.30   |
| 54  | BA    | 2598 | A    | C5-C6-N1   | 8.26  | 121.83      | 117.70   |
| 54  | BA    | 1569 | A    | N1-C6-N6   | -8.26 | 113.64      | 118.60   |
| 19  | AT    | 9    | ARG  | NE-CZ-NH1  | 8.26  | 124.43      | 120.30   |
| 22  | A1    | 21   | A    | N1-C6-N6   | -8.26 | 113.64      | 118.60   |
| 21  | AA    | 356  | A    | C4-C5-C6   | -8.26 | 112.87      | 117.00   |
| 54  | BA    | 342  | A    | C5-C6-N1   | 8.26  | 121.83      | 117.70   |
| 54  | BA    | 582  | A    | C5-C6-N1   | 8.26  | 121.83      | 117.70   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|------------|-------|------------------------|---------------------|
| 54  | BA    | 1571 | A    | C5-C6-N1   | 8.26  | 121.83                 | 117.70              |
| 21  | AA    | 1398 | A    | C5-C6-N1   | 8.26  | 121.83                 | 117.70              |
| 21  | AA    | 149  | A    | C5-C6-N1   | 8.26  | 121.83                 | 117.70              |
| 54  | BA    | 1800 | C    | N3-C2-O2   | -8.26 | 116.12                 | 121.90              |
| 54  | BA    | 2254 | C    | N3-C2-O2   | -8.26 | 116.12                 | 121.90              |
| 21  | AA    | 262  | A    | N1-C6-N6   | -8.25 | 113.65                 | 118.60              |
| 54  | BA    | 374  | A    | C5-C6-N1   | 8.25  | 121.83                 | 117.70              |
| 54  | BA    | 1762 | A    | C5-C6-N1   | 8.25  | 121.83                 | 117.70              |
| 21  | AA    | 522  | C    | N3-C2-O2   | -8.25 | 116.13                 | 121.90              |
| 54  | BA    | 689  | A    | C4-C5-C6   | -8.25 | 112.88                 | 117.00              |
| 54  | BA    | 1020 | A    | C5-C6-N1   | 8.25  | 121.82                 | 117.70              |
| 54  | BA    | 2635 | A    | C5-C6-N1   | 8.25  | 121.82                 | 117.70              |
| 21  | AA    | 448  | A    | C5-C6-N1   | 8.24  | 121.82                 | 117.70              |
| 49  | B0    | 15   | ARG  | NE-CZ-NH1  | 8.24  | 124.42                 | 120.30              |
| 54  | BA    | 2644 | G    | O4'-C1'-N9 | 8.24  | 114.80                 | 108.20              |
| 21  | AA    | 1204 | A    | N1-C6-N6   | -8.24 | 113.66                 | 118.60              |
| 21  | AA    | 1285 | A    | C4-C5-C6   | -8.24 | 112.88                 | 117.00              |
| 54  | BA    | 2810 | A    | C5-C6-N1   | 8.24  | 121.82                 | 117.70              |
| 54  | BA    | 1655 | A    | C5-C6-N1   | 8.23  | 121.82                 | 117.70              |
| 21  | AA    | 1196 | A    | N1-C6-N6   | -8.23 | 113.66                 | 118.60              |
| 54  | BA    | 2391 | G    | O4'-C1'-N9 | 8.23  | 114.79                 | 108.20              |
| 54  | BA    | 1493 | C    | N3-C2-O2   | -8.23 | 116.14                 | 121.90              |
| 21  | AA    | 640  | A    | N1-C6-N6   | -8.23 | 113.66                 | 118.60              |
| 21  | AA    | 1368 | A    | N1-C6-N6   | -8.23 | 113.66                 | 118.60              |
| 54  | BA    | 1936 | A    | C5-C6-N1   | 8.23  | 121.82                 | 117.70              |
| 54  | BA    | 1847 | A    | C5-C6-N1   | 8.23  | 121.81                 | 117.70              |
| 54  | BA    | 2434 | A    | C4-C5-C6   | -8.23 | 112.89                 | 117.00              |
| 54  | BA    | 204  | A    | C4-C5-C6   | -8.23 | 112.89                 | 117.00              |
| 54  | BA    | 2764 | A    | N1-C6-N6   | -8.23 | 113.66                 | 118.60              |
| 1   | AB    | 224  | ARG  | NE-CZ-NH1  | 8.22  | 124.41                 | 120.30              |
| 21  | AA    | 466  | A    | C5-C6-N1   | 8.22  | 121.81                 | 117.70              |
| 54  | BA    | 1111 | A    | C5-C6-N1   | 8.22  | 121.81                 | 117.70              |
| 54  | BA    | 2566 | A    | C5-C6-N1   | 8.22  | 121.81                 | 117.70              |
| 24  | A3    | 45   | A    | N1-C6-N6   | -8.22 | 113.67                 | 118.60              |
| 54  | BA    | 64   | A    | C5-C6-N1   | 8.22  | 121.81                 | 117.70              |
| 54  | BA    | 2513 | A    | N1-C6-N6   | -8.22 | 113.67                 | 118.60              |
| 54  | BA    | 1528 | A    | C5-C6-N1   | 8.22  | 121.81                 | 117.70              |
| 54  | BA    | 2418 | A    | N1-C6-N6   | -8.22 | 113.67                 | 118.60              |
| 54  | BA    | 1088 | A    | C5-C6-N1   | 8.21  | 121.81                 | 117.70              |
| 55  | BB    | 8    | C    | N3-C2-O2   | -8.21 | 116.15                 | 121.90              |
| 21  | AA    | 274  | A    | N1-C6-N6   | -8.21 | 113.67                 | 118.60              |
| 41  | BS    | 18   | ARG  | NE-CZ-NH1  | 8.21  | 124.41                 | 120.30              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 8   | AI    | 118  | ARG  | NE-CZ-NH1  | 8.21  | 124.40      | 120.30   |
| 36  | BN    | 12   | ARG  | NE-CZ-NH1  | 8.21  | 124.40      | 120.30   |
| 21  | AA    | 815  | A    | N1-C6-N6   | -8.21 | 113.68      | 118.60   |
| 54  | BA    | 715  | A    | C5-C6-N1   | 8.21  | 121.80      | 117.70   |
| 54  | BA    | 2335 | A    | C5-C6-N1   | 8.21  | 121.80      | 117.70   |
| 21  | AA    | 1418 | A    | N1-C6-N6   | -8.20 | 113.68      | 118.60   |
| 54  | BA    | 443  | A    | N1-C6-N6   | -8.20 | 113.68      | 118.60   |
| 54  | BA    | 1354 | A    | C5-C6-N1   | 8.20  | 121.80      | 117.70   |
| 54  | BA    | 2170 | A    | C5-C6-N1   | 8.20  | 121.80      | 117.70   |
| 21  | AA    | 19   | A    | N1-C6-N6   | -8.20 | 113.68      | 118.60   |
| 21  | AA    | 1238 | A    | C5-C6-N1   | 8.20  | 121.80      | 117.70   |
| 54  | BA    | 2021 | C    | N3-C2-O2   | -8.20 | 116.16      | 121.90   |
| 54  | BA    | 49   | A    | C5-C6-N1   | 8.20  | 121.80      | 117.70   |
| 21  | AA    | 149  | A    | N1-C6-N6   | -8.19 | 113.68      | 118.60   |
| 54  | BA    | 575  | A    | N1-C6-N6   | -8.19 | 113.69      | 118.60   |
| 54  | BA    | 1308 | A    | N1-C6-N6   | -8.19 | 113.69      | 118.60   |
| 54  | BA    | 64   | A    | C4-C5-C6   | -8.19 | 112.91      | 117.00   |
| 54  | BA    | 1077 | A    | N1-C6-N6   | -8.19 | 113.69      | 118.60   |
| 54  | BA    | 1533 | C    | N3-C2-O2   | -8.19 | 116.17      | 121.90   |
| 54  | BA    | 1953 | A    | N1-C6-N6   | -8.18 | 113.69      | 118.60   |
| 54  | BA    | 1000 | A    | C5-C6-N1   | 8.18  | 121.79      | 117.70   |
| 47  | BY    | 48   | ARG  | NE-CZ-NH1  | 8.18  | 124.39      | 120.30   |
| 54  | BA    | 2060 | A    | C4-C5-C6   | -8.18 | 112.91      | 117.00   |
| 54  | BA    | 735  | A    | C5-C6-N1   | 8.17  | 121.79      | 117.70   |
| 54  | BA    | 2407 | A    | C5-C6-N1   | 8.17  | 121.79      | 117.70   |
| 56  | B5    | 122  | ARG  | NE-CZ-NH1  | 8.17  | 124.39      | 120.30   |
| 27  | BE    | 49   | ARG  | NE-CZ-NH1  | 8.17  | 124.39      | 120.30   |
| 54  | BA    | 320  | A    | N1-C6-N6   | -8.17 | 113.70      | 118.60   |
| 13  | AN    | 53   | ARG  | NE-CZ-NH1  | 8.17  | 124.38      | 120.30   |
| 54  | BA    | 6    | A    | N1-C6-N6   | -8.17 | 113.70      | 118.60   |
| 54  | BA    | 458  | G    | O4'-C1'-N9 | 8.17  | 114.73      | 108.20   |
| 54  | BA    | 1899 | A    | N1-C6-N6   | -8.17 | 113.70      | 118.60   |
| 13  | AN    | 63   | ARG  | NE-CZ-NH2  | -8.16 | 116.22      | 120.30   |
| 21  | AA    | 243  | A    | C5-C6-N1   | 8.16  | 121.78      | 117.70   |
| 54  | BA    | 1679 | A    | C5-C6-N1   | 8.16  | 121.78      | 117.70   |
| 21  | AA    | 1030 | U    | O4'-C1'-N1 | 8.16  | 114.73      | 108.20   |
| 21  | AA    | 228  | A    | N1-C6-N6   | -8.16 | 113.70      | 118.60   |
| 54  | BA    | 1606 | C    | N3-C2-O2   | -8.16 | 116.19      | 121.90   |
| 54  | BA    | 2384 | U    | O4'-C1'-N1 | 8.16  | 114.73      | 108.20   |
| 12  | AM    | 100  | ARG  | NE-CZ-NH1  | 8.16  | 124.38      | 120.30   |
| 21  | AA    | 435  | A    | C5-C6-N1   | 8.16  | 121.78      | 117.70   |
| 21  | AA    | 1214 | C    | N3-C2-O2   | -8.16 | 116.19      | 121.90   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|------------|-------|------------------------|---------------------|
| 36  | BN    | 4    | ARG  | NE-CZ-NH1  | 8.16  | 124.38                 | 120.30              |
| 22  | A1    | 60   | C    | N3-C2-O2   | -8.15 | 116.19                 | 121.90              |
| 54  | BA    | 1451 | C    | N3-C2-O2   | -8.15 | 116.19                 | 121.90              |
| 54  | BA    | 1367 | A    | N1-C6-N6   | -8.15 | 113.71                 | 118.60              |
| 54  | BA    | 1762 | A    | N1-C6-N6   | -8.15 | 113.71                 | 118.60              |
| 21  | AA    | 1368 | A    | C4-C5-C6   | -8.15 | 112.92                 | 117.00              |
| 54  | BA    | 1383 | A    | C5-C6-N1   | 8.15  | 121.78                 | 117.70              |
| 17  | AR    | 52   | ARG  | NE-CZ-NH1  | 8.15  | 124.37                 | 120.30              |
| 54  | BA    | 1454 | C    | N3-C2-O2   | -8.15 | 116.20                 | 121.90              |
| 54  | BA    | 1785 | A    | N1-C6-N6   | -8.15 | 113.71                 | 118.60              |
| 21  | AA    | 389  | A    | C4-C5-C6   | -8.14 | 112.93                 | 117.00              |
| 54  | BA    | 739  | A    | C5-C6-N1   | 8.14  | 121.77                 | 117.70              |
| 54  | BA    | 1941 | C    | N3-C2-O2   | -8.14 | 116.20                 | 121.90              |
| 21  | AA    | 784  | A    | C5-C6-N1   | 8.14  | 121.77                 | 117.70              |
| 54  | BA    | 1617 | C    | N3-C2-O2   | -8.14 | 116.20                 | 121.90              |
| 54  | BA    | 41   | C    | N3-C2-O2   | -8.14 | 116.20                 | 121.90              |
| 54  | BA    | 1085 | A    | N1-C6-N6   | -8.14 | 113.72                 | 118.60              |
| 54  | BA    | 2077 | A    | N1-C6-N6   | -8.14 | 113.72                 | 118.60              |
| 54  | BA    | 1552 | A    | C5-C6-N1   | 8.14  | 121.77                 | 117.70              |
| 37  | BO    | 94   | ARG  | NE-CZ-NH1  | 8.14  | 124.37                 | 120.30              |
| 54  | BA    | 5    | A    | C4-C5-C6   | -8.13 | 112.93                 | 117.00              |
| 54  | BA    | 182  | A    | N1-C6-N6   | -8.14 | 113.72                 | 118.60              |
| 54  | BA    | 563  | A    | C5-C6-N1   | 8.14  | 121.77                 | 117.70              |
| 54  | BA    | 1593 | A    | C5-C6-N1   | 8.13  | 121.77                 | 117.70              |
| 54  | BA    | 2317 | A    | N1-C6-N6   | -8.13 | 113.72                 | 118.60              |
| 21  | AA    | 33   | A    | C5-C6-N1   | 8.13  | 121.77                 | 117.70              |
| 21  | AA    | 59   | A    | N1-C6-N6   | -8.13 | 113.72                 | 118.60              |
| 21  | AA    | 1483 | A    | N1-C6-N6   | -8.13 | 113.72                 | 118.60              |
| 54  | BA    | 2070 | A    | C4-C5-C6   | -8.13 | 112.94                 | 117.00              |
| 46  | BX    | 73   | ARG  | NE-CZ-NH1  | 8.13  | 124.36                 | 120.30              |
| 54  | BA    | 975  | A    | C5-C6-N1   | 8.13  | 121.76                 | 117.70              |
| 54  | BA    | 1289 | C    | N3-C2-O2   | -8.12 | 116.21                 | 121.90              |
| 54  | BA    | 2670 | A    | C5-C6-N1   | 8.12  | 121.76                 | 117.70              |
| 21  | AA    | 1433 | A    | N1-C6-N6   | -8.12 | 113.73                 | 118.60              |
| 54  | BA    | 1067 | A    | N1-C6-N6   | -8.12 | 113.73                 | 118.60              |
| 54  | BA    | 1630 | A    | C4-C5-C6   | -8.12 | 112.94                 | 117.00              |
| 21  | AA    | 396  | C    | N3-C2-O2   | -8.12 | 116.22                 | 121.90              |
| 54  | BA    | 1544 | A    | N1-C6-N6   | -8.12 | 113.73                 | 118.60              |
| 54  | BA    | 2063 | C    | N3-C2-O2   | -8.12 | 116.22                 | 121.90              |
| 55  | BB    | 40   | U    | O4'-C1'-N1 | 8.12  | 114.70                 | 108.20              |
| 21  | AA    | 1110 | A    | C4-C5-C6   | -8.12 | 112.94                 | 117.00              |
| 54  | BA    | 802  | A    | C5-C6-N1   | 8.12  | 121.76                 | 117.70              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|------------|-------|------------------------|---------------------|
| 21  | AA    | 106  | C    | N3-C2-O2   | -8.11 | 116.22                 | 121.90              |
| 21  | AA    | 386  | C    | N3-C2-O2   | -8.11 | 116.22                 | 121.90              |
| 54  | BA    | 877  | A    | C5-C6-N1   | 8.11  | 121.76                 | 117.70              |
| 54  | BA    | 1787 | A    | N1-C6-N6   | -8.11 | 113.73                 | 118.60              |
| 2   | AC    | 53   | ARG  | NE-CZ-NH1  | 8.11  | 124.36                 | 120.30              |
| 54  | BA    | 1001 | A    | N1-C6-N6   | -8.11 | 113.73                 | 118.60              |
| 54  | BA    | 2736 | A    | N1-C6-N6   | -8.11 | 113.73                 | 118.60              |
| 21  | AA    | 572  | A    | C5-C6-N1   | 8.11  | 121.75                 | 117.70              |
| 23  | A2    | 91   | A    | C4-C5-C6   | -8.11 | 112.95                 | 117.00              |
| 54  | BA    | 2368 | C    | N3-C2-O2   | -8.11 | 116.22                 | 121.90              |
| 54  | BA    | 833  | A    | C4-C5-C6   | -8.10 | 112.95                 | 117.00              |
| 54  | BA    | 323  | C    | N1-C2-O2   | 8.10  | 123.76                 | 118.90              |
| 54  | BA    | 1962 | C    | N3-C2-O2   | -8.10 | 116.23                 | 121.90              |
| 55  | BB    | 26   | C    | N3-C2-O2   | -8.10 | 116.23                 | 121.90              |
| 10  | AK    | 92   | ARG  | NE-CZ-NH1  | 8.10  | 124.35                 | 120.30              |
| 21  | AA    | 972  | C    | N3-C2-O2   | -8.10 | 116.23                 | 121.90              |
| 21  | AA    | 1339 | A    | C4-C5-C6   | -8.10 | 112.95                 | 117.00              |
| 54  | BA    | 199  | A    | O4'-C1'-N9 | 8.10  | 114.68                 | 108.20              |
| 54  | BA    | 2700 | A    | C4-C5-C6   | -8.10 | 112.95                 | 117.00              |
| 54  | BA    | 2679 | A    | N1-C6-N6   | -8.10 | 113.74                 | 118.60              |
| 21  | AA    | 1257 | A    | N1-C6-N6   | -8.10 | 113.74                 | 118.60              |
| 37  | BO    | 30   | ARG  | NE-CZ-NH1  | 8.10  | 124.35                 | 120.30              |
| 54  | BA    | 900  | A    | C5-C6-N1   | 8.10  | 121.75                 | 117.70              |
| 54  | BA    | 2297 | A    | N1-C6-N6   | -8.10 | 113.74                 | 118.60              |
| 19  | AT    | 28   | ARG  | NE-CZ-NH1  | 8.09  | 124.35                 | 120.30              |
| 54  | BA    | 1616 | A    | C5-C6-N1   | 8.09  | 121.75                 | 117.70              |
| 54  | BA    | 142  | A    | N1-C6-N6   | -8.09 | 113.75                 | 118.60              |
| 54  | BA    | 197  | A    | N1-C6-N6   | -8.09 | 113.75                 | 118.60              |
| 54  | BA    | 1744 | A    | N1-C6-N6   | -8.09 | 113.75                 | 118.60              |
| 54  | BA    | 2425 | A    | N1-C6-N6   | -8.09 | 113.75                 | 118.60              |
| 54  | BA    | 1765 | U    | O4'-C1'-N1 | 8.09  | 114.67                 | 108.20              |
| 21  | AA    | 355  | C    | N3-C2-O2   | -8.09 | 116.24                 | 121.90              |
| 22  | A1    | 76   | A    | C5-C6-N1   | 8.09  | 121.74                 | 117.70              |
| 54  | BA    | 2560 | A    | C5-C6-N1   | 8.09  | 121.74                 | 117.70              |
| 54  | BA    | 2835 | A    | N1-C6-N6   | -8.09 | 113.75                 | 118.60              |
| 21  | AA    | 320  | A    | C4-C5-C6   | -8.09 | 112.96                 | 117.00              |
| 54  | BA    | 160  | A    | C5-C6-N1   | 8.09  | 121.74                 | 117.70              |
| 54  | BA    | 422  | A    | N1-C6-N6   | -8.09 | 113.75                 | 118.60              |
| 54  | BA    | 1044 | C    | N3-C2-O2   | -8.09 | 116.24                 | 121.90              |
| 21  | AA    | 195  | A    | N1-C6-N6   | -8.08 | 113.75                 | 118.60              |
| 54  | BA    | 821  | A    | C5-C6-N1   | 8.08  | 121.74                 | 117.70              |
| 54  | BA    | 2471 | A    | N1-C6-N6   | -8.08 | 113.75                 | 118.60              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|------------|-------|------------------------|---------------------|
| 38  | BP    | 92   | ARG  | NE-CZ-NH1  | 8.08  | 124.34                 | 120.30              |
| 54  | BA    | 119  | A    | C5-C6-N1   | 8.08  | 121.74                 | 117.70              |
| 54  | BA    | 222  | A    | C5-C6-N1   | 8.08  | 121.74                 | 117.70              |
| 54  | BA    | 1010 | A    | C5-C6-N1   | 8.08  | 121.74                 | 117.70              |
| 54  | BA    | 1607 | C    | N3-C2-O2   | -8.08 | 116.24                 | 121.90              |
| 54  | BA    | 1672 | A    | C5-C6-N1   | 8.08  | 121.74                 | 117.70              |
| 54  | BA    | 1919 | A    | N1-C6-N6   | -8.08 | 113.75                 | 118.60              |
| 21  | AA    | 250  | A    | C5-C6-N1   | 8.08  | 121.74                 | 117.70              |
| 54  | BA    | 2690 | U    | O4'-C1'-N1 | 8.08  | 114.66                 | 108.20              |
| 54  | BA    | 1433 | A    | C4-C5-C6   | -8.07 | 112.96                 | 117.00              |
| 54  | BA    | 2453 | A    | C5-C6-N1   | 8.07  | 121.74                 | 117.70              |
| 54  | BA    | 2448 | A    | C5-C6-N1   | 8.07  | 121.74                 | 117.70              |
| 21  | AA    | 40   | C    | N3-C2-O2   | -8.07 | 116.25                 | 121.90              |
| 21  | AA    | 1213 | A    | C5-C6-N1   | 8.07  | 121.74                 | 117.70              |
| 54  | BA    | 2287 | A    | O4'-C1'-N9 | 8.07  | 114.66                 | 108.20              |
| 54  | BA    | 447  | A    | C5-C6-N1   | 8.07  | 121.73                 | 117.70              |
| 54  | BA    | 1253 | A    | N1-C6-N6   | -8.07 | 113.76                 | 118.60              |
| 21  | AA    | 7    | A    | N1-C6-N6   | -8.07 | 113.76                 | 118.60              |
| 54  | BA    | 1322 | A    | N1-C6-N6   | -8.07 | 113.76                 | 118.60              |
| 55  | BB    | 73   | A    | C5-C6-N1   | 8.07  | 121.73                 | 117.70              |
| 54  | BA    | 2761 | A    | C5-C6-N1   | 8.07  | 121.73                 | 117.70              |
| 21  | AA    | 919  | A    | C5-C6-N1   | 8.06  | 121.73                 | 117.70              |
| 29  | BG    | 148  | ARG  | NE-CZ-NH1  | 8.06  | 124.33                 | 120.30              |
| 46  | BX    | 2    | ARG  | NE-CZ-NH1  | 8.06  | 124.33                 | 120.30              |
| 54  | BA    | 2507 | C    | N3-C2-O2   | -8.06 | 116.25                 | 121.90              |
| 54  | BA    | 2893 | A    | N1-C6-N6   | -8.06 | 113.76                 | 118.60              |
| 21  | AA    | 182  | A    | N1-C6-N6   | -8.06 | 113.77                 | 118.60              |
| 21  | AA    | 1339 | A    | C5-C6-N1   | 8.06  | 121.73                 | 117.70              |
| 21  | AA    | 1431 | A    | N1-C6-N6   | -8.05 | 113.77                 | 118.60              |
| 54  | BA    | 1717 | A    | N1-C6-N6   | -8.06 | 113.77                 | 118.60              |
| 54  | BA    | 2084 | C    | N3-C2-O2   | -8.05 | 116.26                 | 121.90              |
| 49  | B0    | 9    | ARG  | NE-CZ-NH2  | 8.05  | 124.33                 | 120.30              |
| 21  | AA    | 860  | A    | C4-C5-C6   | -8.05 | 112.97                 | 117.00              |
| 54  | BA    | 82   | U    | O4'-C1'-N1 | 8.05  | 114.64                 | 108.20              |
| 54  | BA    | 925  | A    | N1-C6-N6   | -8.05 | 113.77                 | 118.60              |
| 54  | BA    | 547  | A    | N1-C6-N6   | -8.05 | 113.77                 | 118.60              |
| 54  | BA    | 689  | A    | C5-C6-N1   | 8.05  | 121.72                 | 117.70              |
| 54  | BA    | 1637 | A    | C5-C6-N1   | 8.05  | 121.72                 | 117.70              |
| 54  | BA    | 1089 | A    | N1-C6-N6   | -8.05 | 113.77                 | 118.60              |
| 54  | BA    | 742  | A    | C5-C6-N1   | 8.05  | 121.72                 | 117.70              |
| 54  | BA    | 1664 | A    | N1-C6-N6   | -8.05 | 113.77                 | 118.60              |
| 54  | BA    | 819  | A    | C5-C6-N1   | 8.04  | 121.72                 | 117.70              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 54  | BA    | 984  | A    | C5-C6-N1   | 8.04  | 121.72      | 117.70   |
| 54  | BA    | 1741 | C    | N3-C2-O2   | -8.04 | 116.27      | 121.90   |
| 23  | A2    | 82   | A    | N1-C6-N6   | -8.04 | 113.77      | 118.60   |
| 21  | AA    | 1016 | A    | C5-C6-N1   | 8.04  | 121.72      | 117.70   |
| 54  | BA    | 282  | A    | C4-C5-C6   | -8.04 | 112.98      | 117.00   |
| 54  | BA    | 821  | A    | C4-C5-C6   | -8.04 | 112.98      | 117.00   |
| 54  | BA    | 2386 | A    | C5-C6-N1   | 8.04  | 121.72      | 117.70   |
| 21  | AA    | 607  | A    | C5-C6-N1   | 8.04  | 121.72      | 117.70   |
| 55  | BB    | 45   | A    | C5-C6-N1   | 8.04  | 121.72      | 117.70   |
| 21  | AA    | 964  | A    | C5-C6-N1   | 8.03  | 121.72      | 117.70   |
| 54  | BA    | 1572 | A    | C5-C6-N1   | 8.03  | 121.72      | 117.70   |
| 54  | BA    | 1961 | C    | N3-C2-O2   | -8.03 | 116.28      | 121.90   |
| 54  | BA    | 2241 | A    | C5-C6-N1   | 8.03  | 121.72      | 117.70   |
| 54  | BA    | 2726 | A    | O4'-C1'-N9 | 8.03  | 114.62      | 108.20   |
| 21  | AA    | 665  | A    | C4-C5-C6   | -8.03 | 112.99      | 117.00   |
| 41  | BS    | 11   | ARG  | NE-CZ-NH1  | 8.03  | 124.31      | 120.30   |
| 49  | B0    | 39   | ARG  | NE-CZ-NH1  | 8.02  | 124.31      | 120.30   |
| 54  | BA    | 731  | C    | N3-C2-O2   | -8.02 | 116.28      | 121.90   |
| 54  | BA    | 829  | A    | C5-C6-N1   | 8.02  | 121.71      | 117.70   |
| 54  | BA    | 1632 | A    | C5-C6-N1   | 8.02  | 121.71      | 117.70   |
| 1   | AB    | 207  | ARG  | NE-CZ-NH2  | -8.02 | 116.29      | 120.30   |
| 15  | AP    | 8    | ARG  | NE-CZ-NH1  | 8.02  | 124.31      | 120.30   |
| 54  | BA    | 1970 | A    | C5-C6-N1   | 8.02  | 121.71      | 117.70   |
| 54  | BA    | 2198 | A    | C5-C6-N1   | 8.02  | 121.71      | 117.70   |
| 54  | BA    | 204  | A    | C5-C6-N1   | 8.02  | 121.71      | 117.70   |
| 21  | AA    | 523  | A    | C5-C6-N1   | 8.01  | 121.71      | 117.70   |
| 21  | AA    | 790  | A    | N1-C6-N6   | -8.01 | 113.79      | 118.60   |
| 21  | AA    | 1112 | C    | N3-C2-O2   | -8.01 | 116.29      | 121.90   |
| 54  | BA    | 1084 | A    | C4-C5-C6   | -8.01 | 112.99      | 117.00   |
| 21  | AA    | 681  | A    | C4-C5-C6   | -8.01 | 113.00      | 117.00   |
| 54  | BA    | 1525 | A    | C4-C5-C6   | -8.01 | 113.00      | 117.00   |
| 21  | AA    | 860  | A    | N1-C6-N6   | -8.01 | 113.80      | 118.60   |
| 54  | BA    | 1067 | A    | C5-C6-N1   | 8.01  | 121.70      | 117.70   |
| 54  | BA    | 2119 | A    | C5-C6-N1   | 8.01  | 121.70      | 117.70   |
| 21  | AA    | 792  | A    | C5-C6-N1   | 8.00  | 121.70      | 117.70   |
| 33  | BK    | 49   | ARG  | NE-CZ-NH1  | 8.00  | 124.30      | 120.30   |
| 38  | BP    | 108  | ARG  | NE-CZ-NH2  | 8.00  | 124.30      | 120.30   |
| 54  | BA    | 2468 | A    | N1-C6-N6   | -8.00 | 113.80      | 118.60   |
| 55  | BB    | 60   | C    | N3-C2-O2   | -8.00 | 116.30      | 121.90   |
| 54  | BA    | 1618 | A    | N1-C6-N6   | -8.00 | 113.80      | 118.60   |
| 21  | AA    | 1229 | A    | N1-C6-N6   | -8.00 | 113.80      | 118.60   |
| 54  | BA    | 1254 | A    | C5-C6-N1   | 8.00  | 121.70      | 117.70   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 54  | BA    | 2352 | A    | N1-C6-N6  | -8.00 | 113.80      | 118.60   |
| 54  | BA    | 2311 | A    | C5-C6-N1  | 8.00  | 121.70      | 117.70   |
| 54  | BA    | 2451 | A    | C4-C5-C6  | -8.00 | 113.00      | 117.00   |
| 21  | AA    | 374  | A    | C4-C5-C6  | -7.99 | 113.00      | 117.00   |
| 22  | A1    | 58   | A    | C4-C5-C6  | -7.99 | 113.00      | 117.00   |
| 54  | BA    | 330  | A    | N1-C6-N6  | -7.99 | 113.80      | 118.60   |
| 54  | BA    | 761  | A    | C5-C6-N1  | 7.99  | 121.70      | 117.70   |
| 54  | BA    | 1010 | A    | N1-C6-N6  | -7.99 | 113.80      | 118.60   |
| 21  | AA    | 1333 | A    | N1-C6-N6  | -7.99 | 113.81      | 118.60   |
| 40  | BR    | 68   | ARG  | NE-CZ-NH1 | 7.99  | 124.30      | 120.30   |
| 54  | BA    | 146  | A    | C5-C6-N1  | 7.99  | 121.69      | 117.70   |
| 54  | BA    | 1307 | A    | N1-C6-N6  | -7.99 | 113.81      | 118.60   |
| 21  | AA    | 802  | A    | N1-C6-N6  | -7.99 | 113.81      | 118.60   |
| 54  | BA    | 341  | C    | N3-C2-O2  | -7.99 | 116.31      | 121.90   |
| 54  | BA    | 1665 | A    | C5-C6-N1  | 7.99  | 121.69      | 117.70   |
| 54  | BA    | 2856 | A    | C4-C5-C6  | -7.99 | 113.00      | 117.00   |
| 36  | BN    | 71   | ARG  | NE-CZ-NH1 | 7.99  | 124.29      | 120.30   |
| 21  | AA    | 729  | A    | C5-C6-N1  | 7.99  | 121.69      | 117.70   |
| 21  | AA    | 1413 | A    | C4-C5-C6  | -7.99 | 113.01      | 117.00   |
| 21  | AA    | 448  | A    | C4-C5-C6  | -7.98 | 113.01      | 117.00   |
| 54  | BA    | 1675 | C    | N3-C2-O2  | -7.98 | 116.31      | 121.90   |
| 21  | AA    | 288  | A    | N1-C6-N6  | -7.97 | 113.81      | 118.60   |
| 54  | BA    | 556  | A    | C5-C6-N1  | 7.97  | 121.69      | 117.70   |
| 21  | AA    | 780  | A    | C4-C5-C6  | -7.97 | 113.02      | 117.00   |
| 54  | BA    | 391  | A    | N1-C6-N6  | -7.97 | 113.82      | 118.60   |
| 54  | BA    | 1916 | A    | C5-C6-N1  | 7.97  | 121.69      | 117.70   |
| 21  | AA    | 253  | A    | N1-C6-N6  | -7.97 | 113.82      | 118.60   |
| 21  | AA    | 554  | A    | N1-C6-N6  | -7.97 | 113.82      | 118.60   |
| 54  | BA    | 1877 | A    | N1-C6-N6  | -7.97 | 113.82      | 118.60   |
| 21  | AA    | 1167 | A    | C5-C6-N1  | 7.96  | 121.68      | 117.70   |
| 54  | BA    | 173  | A    | C5-C6-N1  | 7.96  | 121.68      | 117.70   |
| 54  | BA    | 281  | C    | N3-C2-O2  | -7.96 | 116.32      | 121.90   |
| 21  | AA    | 280  | C    | N3-C2-O2  | -7.96 | 116.33      | 121.90   |
| 54  | BA    | 1189 | A    | N1-C6-N6  | -7.96 | 113.82      | 118.60   |
| 21  | AA    | 1374 | A    | C5-C6-N1  | 7.96  | 121.68      | 117.70   |
| 54  | BA    | 750  | A    | C5-C6-N1  | 7.96  | 121.68      | 117.70   |
| 54  | BA    | 155  | A    | C4-C5-C6  | -7.96 | 113.02      | 117.00   |
| 45  | BW    | 38   | ARG  | NE-CZ-NH1 | 7.96  | 124.28      | 120.30   |
| 54  | BA    | 564  | C    | N3-C2-O2  | -7.96 | 116.33      | 121.90   |
| 54  | BA    | 2665 | A    | C5-C6-N1  | 7.96  | 121.68      | 117.70   |
| 54  | BA    | 2352 | A    | C4-C5-C6  | -7.96 | 113.02      | 117.00   |
| 12  | AM    | 89   | ARG  | NE-CZ-NH1 | 7.95  | 124.28      | 120.30   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 21  | AA    | 248  | C    | N3-C2-O2   | -7.95 | 116.33      | 121.90   |
| 54  | BA    | 550  | C    | N3-C2-O2   | -7.95 | 116.33      | 121.90   |
| 54  | BA    | 2700 | A    | C5-C6-N1   | 7.95  | 121.68      | 117.70   |
| 55  | BB    | 35   | C    | N3-C2-O2   | -7.95 | 116.33      | 121.90   |
| 54  | BA    | 384  | A    | C5-C6-N1   | 7.95  | 121.68      | 117.70   |
| 54  | BA    | 2247 | A    | C4-C5-C6   | -7.95 | 113.02      | 117.00   |
| 54  | BA    | 94   | A    | C4-C5-C6   | -7.95 | 113.03      | 117.00   |
| 21  | AA    | 164  | G    | O4'-C1'-N9 | 7.95  | 114.56      | 108.20   |
| 21  | AA    | 321  | A    | N1-C6-N6   | -7.95 | 113.83      | 118.60   |
| 54  | BA    | 614  | A    | C5-C6-N1   | 7.95  | 121.67      | 117.70   |
| 54  | BA    | 825  | A    | C5-C6-N1   | 7.95  | 121.67      | 117.70   |
| 54  | BA    | 1268 | A    | C4-C5-C6   | -7.95 | 113.03      | 117.00   |
| 54  | BA    | 2824 | C    | N3-C2-O2   | -7.95 | 116.34      | 121.90   |
| 21  | AA    | 1339 | A    | N1-C6-N6   | -7.95 | 113.83      | 118.60   |
| 54  | BA    | 718  | A    | C4-C5-C6   | -7.95 | 113.03      | 117.00   |
| 21  | AA    | 284  | C    | N3-C2-O2   | -7.94 | 116.34      | 121.90   |
| 25  | BC    | 86   | ARG  | NE-CZ-NH2  | -7.94 | 116.33      | 120.30   |
| 53  | B4    | 4    | ARG  | NE-CZ-NH1  | 7.94  | 124.27      | 120.30   |
| 21  | AA    | 1349 | A    | N1-C6-N6   | -7.94 | 113.83      | 118.60   |
| 54  | BA    | 262  | A    | N1-C6-N6   | -7.94 | 113.83      | 118.60   |
| 54  | BA    | 402  | A    | N1-C6-N6   | -7.94 | 113.83      | 118.60   |
| 54  | BA    | 1258 | U    | O4'-C1'-N1 | 7.94  | 114.56      | 108.20   |
| 55  | BB    | 118  | C    | N3-C2-O2   | -7.94 | 116.34      | 121.90   |
| 54  | BA    | 721  | A    | C5-C6-N1   | 7.94  | 121.67      | 117.70   |
| 54  | BA    | 294  | A    | N1-C6-N6   | -7.94 | 113.84      | 118.60   |
| 54  | BA    | 749  | A    | N1-C6-N6   | -7.94 | 113.84      | 118.60   |
| 21  | AA    | 205  | A    | C4-C5-C6   | -7.93 | 113.03      | 117.00   |
| 21  | AA    | 345  | C    | N3-C2-O2   | -7.93 | 116.34      | 121.90   |
| 54  | BA    | 2374 | C    | N3-C2-O2   | -7.93 | 116.35      | 121.90   |
| 21  | AA    | 305  | G    | N1-C6-O6   | -7.93 | 115.14      | 119.90   |
| 54  | BA    | 84   | A    | N1-C6-N6   | -7.93 | 113.84      | 118.60   |
| 54  | BA    | 1439 | A    | N1-C6-N6   | -7.93 | 113.84      | 118.60   |
| 54  | BA    | 2025 | C    | N3-C2-O2   | -7.93 | 116.35      | 121.90   |
| 21  | AA    | 1261 | A    | N1-C6-N6   | -7.93 | 113.84      | 118.60   |
| 21  | AA    | 1467 | C    | N3-C2-O2   | -7.93 | 116.35      | 121.90   |
| 54  | BA    | 994  | C    | N3-C2-O2   | -7.93 | 116.35      | 121.90   |
| 54  | BA    | 1584 | U    | O4'-C1'-N1 | 7.93  | 114.54      | 108.20   |
| 21  | AA    | 1004 | A    | N1-C6-N6   | -7.92 | 113.85      | 118.60   |
| 54  | BA    | 190  | A    | C5-C6-N1   | 7.92  | 121.66      | 117.70   |
| 21  | AA    | 539  | A    | N1-C6-N6   | -7.92 | 113.85      | 118.60   |
| 54  | BA    | 1791 | A    | C5-C6-N1   | 7.92  | 121.66      | 117.70   |
| 24  | A3    | 36   | A    | N1-C6-N6   | -7.91 | 113.85      | 118.60   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|------------|-------|------------------------|---------------------|
| 54  | BA    | 2298 | A    | N1-C6-N6   | -7.91 | 113.85                 | 118.60              |
| 7   | AH    | 113  | ARG  | NE-CZ-NH1  | 7.91  | 124.25                 | 120.30              |
| 47  | BY    | 7    | ARG  | NE-CZ-NH1  | 7.91  | 124.25                 | 120.30              |
| 54  | BA    | 2003 | A    | N1-C6-N6   | -7.91 | 113.86                 | 118.60              |
| 21  | AA    | 131  | A    | C5-C6-N1   | 7.91  | 121.65                 | 117.70              |
| 21  | AA    | 728  | A    | C4-C5-C6   | -7.91 | 113.05                 | 117.00              |
| 54  | BA    | 2350 | C    | N3-C2-O2   | -7.91 | 116.37                 | 121.90              |
| 54  | BA    | 2412 | A    | C5-C6-N1   | 7.91  | 121.65                 | 117.70              |
| 54  | BA    | 2564 | A    | N1-C6-N6   | -7.91 | 113.86                 | 118.60              |
| 54  | BA    | 1118 | C    | N3-C2-O2   | -7.90 | 116.37                 | 121.90              |
| 21  | AA    | 978  | A    | N1-C6-N6   | -7.90 | 113.86                 | 118.60              |
| 21  | AA    | 1191 | A    | C4-C5-C6   | -7.90 | 113.05                 | 117.00              |
| 21  | AA    | 1319 | A    | N1-C6-N6   | -7.90 | 113.86                 | 118.60              |
| 54  | BA    | 2126 | A    | N1-C6-N6   | -7.90 | 113.86                 | 118.60              |
| 21  | AA    | 1098 | C    | N3-C2-O2   | -7.90 | 116.37                 | 121.90              |
| 54  | BA    | 1635 | A    | N1-C6-N6   | -7.90 | 113.86                 | 118.60              |
| 54  | BA    | 1686 | C    | N3-C2-O2   | -7.90 | 116.37                 | 121.90              |
| 54  | BA    | 2342 | C    | N3-C2-O2   | -7.90 | 116.37                 | 121.90              |
| 21  | AA    | 414  | A    | C5-C6-N1   | 7.90  | 121.65                 | 117.70              |
| 54  | BA    | 1774 | C    | N3-C2-O2   | -7.90 | 116.37                 | 121.90              |
| 54  | BA    | 2520 | C    | N3-C2-O2   | -7.89 | 116.38                 | 121.90              |
| 55  | BB    | 57   | A    | N1-C6-N6   | -7.89 | 113.86                 | 118.60              |
| 54  | BA    | 1780 | A    | C5-C6-N1   | 7.89  | 121.65                 | 117.70              |
| 21  | AA    | 309  | A    | N1-C6-N6   | -7.89 | 113.87                 | 118.60              |
| 54  | BA    | 1996 | C    | N3-C2-O2   | -7.89 | 116.38                 | 121.90              |
| 54  | BA    | 2740 | A    | C4-C5-C6   | -7.89 | 113.06                 | 117.00              |
| 54  | BA    | 2780 | G    | O4'-C1'-N9 | 7.89  | 114.51                 | 108.20              |
| 54  | BA    | 145  | C    | N3-C2-O2   | -7.89 | 116.38                 | 121.90              |
| 54  | BA    | 572  | A    | C5-C6-N1   | 7.89  | 121.64                 | 117.70              |
| 21  | AA    | 431  | A    | C5-C6-N1   | 7.89  | 121.64                 | 117.70              |
| 54  | BA    | 1211 | C    | N3-C2-O2   | -7.89 | 116.38                 | 121.90              |
| 54  | BA    | 1353 | A    | C5-C6-N1   | 7.89  | 121.64                 | 117.70              |
| 54  | BA    | 917  | A    | N1-C6-N6   | -7.88 | 113.87                 | 118.60              |
| 21  | AA    | 161  | A    | C5-C6-N1   | 7.88  | 121.64                 | 117.70              |
| 54  | BA    | 323  | C    | N3-C2-O2   | -7.88 | 116.38                 | 121.90              |
| 54  | BA    | 983  | A    | C5-C6-N1   | 7.88  | 121.64                 | 117.70              |
| 54  | BA    | 1321 | A    | C5-C6-N1   | 7.88  | 121.64                 | 117.70              |
| 18  | AS    | 36   | ARG  | NE-CZ-NH1  | 7.88  | 124.24                 | 120.30              |
| 21  | AA    | 51   | A    | C5-C6-N1   | 7.88  | 121.64                 | 117.70              |
| 54  | BA    | 1048 | A    | N1-C6-N6   | -7.88 | 113.87                 | 118.60              |
| 19  | AT    | 9    | ARG  | NE-CZ-NH2  | -7.88 | 116.36                 | 120.30              |
| 54  | BA    | 751  | A    | C5-C6-N1   | 7.88  | 121.64                 | 117.70              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 54  | BA    | 2247 | A    | N1-C6-N6   | -7.88 | 113.87      | 118.60   |
| 21  | AA    | 448  | A    | N1-C6-N6   | -7.88 | 113.87      | 118.60   |
| 54  | BA    | 2058 | A    | C5-C6-N1   | 7.88  | 121.64      | 117.70   |
| 21  | AA    | 59   | A    | C4-C5-C6   | -7.88 | 113.06      | 117.00   |
| 54  | BA    | 1151 | A    | N1-C6-N6   | -7.88 | 113.88      | 118.60   |
| 54  | BA    | 2560 | A    | C4-C5-C6   | -7.88 | 113.06      | 117.00   |
| 54  | BA    | 1387 | A    | C5-C6-N1   | 7.87  | 121.64      | 117.70   |
| 21  | AA    | 1227 | A    | N1-C6-N6   | -7.87 | 113.88      | 118.60   |
| 21  | AA    | 1237 | C    | N3-C2-O2   | -7.87 | 116.39      | 121.90   |
| 21  | AA    | 1479 | C    | N3-C2-O2   | -7.87 | 116.39      | 121.90   |
| 21  | AA    | 1155 | A    | N1-C6-N6   | -7.87 | 113.88      | 118.60   |
| 38  | BP    | 52   | ARG  | NE-CZ-NH1  | 7.87  | 124.23      | 120.30   |
| 38  | BP    | 52   | ARG  | NE-CZ-NH2  | -7.87 | 116.37      | 120.30   |
| 54  | BA    | 2452 | C    | N3-C2-O2   | -7.87 | 116.39      | 121.90   |
| 21  | AA    | 441  | A    | N1-C6-N6   | -7.86 | 113.88      | 118.60   |
| 54  | BA    | 1508 | A    | N1-C6-N6   | -7.86 | 113.88      | 118.60   |
| 54  | BA    | 1809 | A    | C5-C6-N1   | 7.86  | 121.63      | 117.70   |
| 54  | BA    | 2435 | A    | C5-C6-N1   | 7.86  | 121.63      | 117.70   |
| 54  | BA    | 1009 | A    | C5-C6-N1   | 7.86  | 121.63      | 117.70   |
| 54  | BA    | 1254 | A    | C4-C5-C6   | -7.86 | 113.07      | 117.00   |
| 54  | BA    | 503  | A    | C5-C6-N1   | 7.86  | 121.63      | 117.70   |
| 54  | BA    | 1085 | A    | C4-C5-C6   | -7.86 | 113.07      | 117.00   |
| 21  | AA    | 1507 | A    | N1-C6-N6   | -7.86 | 113.89      | 118.60   |
| 34  | BL    | 69   | ARG  | NE-CZ-NH1  | 7.86  | 124.23      | 120.30   |
| 54  | BA    | 1269 | A    | N1-C6-N6   | -7.86 | 113.89      | 118.60   |
| 54  | BA    | 2044 | C    | N3-C2-O2   | -7.86 | 116.40      | 121.90   |
| 54  | BA    | 2774 | C    | N3-C2-O2   | -7.86 | 116.40      | 121.90   |
| 11  | AL    | 55   | ARG  | NE-CZ-NH1  | 7.85  | 124.23      | 120.30   |
| 21  | AA    | 782  | A    | N1-C6-N6   | -7.85 | 113.89      | 118.60   |
| 54  | BA    | 282  | A    | N1-C6-N6   | -7.85 | 113.89      | 118.60   |
| 21  | AA    | 156  | C    | N3-C2-O2   | -7.85 | 116.41      | 121.90   |
| 27  | BE    | 117  | ARG  | NE-CZ-NH1  | 7.85  | 124.22      | 120.30   |
| 54  | BA    | 531  | C    | N3-C2-O2   | -7.85 | 116.41      | 121.90   |
| 54  | BA    | 972  | A    | N1-C6-N6   | -7.85 | 113.89      | 118.60   |
| 54  | BA    | 1913 | A    | O4'-C1'-N9 | 7.85  | 114.48      | 108.20   |
| 4   | AE    | 111  | ARG  | NE-CZ-NH1  | 7.85  | 124.22      | 120.30   |
| 54  | BA    | 947  | A    | N1-C6-N6   | -7.84 | 113.89      | 118.60   |
| 54  | BA    | 2534 | A    | C5-C6-N1   | 7.84  | 121.62      | 117.70   |
| 54  | BA    | 2717 | C    | N3-C2-O2   | -7.84 | 116.41      | 121.90   |
| 24  | A3    | 35   | C    | N3-C2-O2   | -7.84 | 116.41      | 121.90   |
| 54  | BA    | 1789 | A    | N1-C6-N6   | -7.84 | 113.89      | 118.60   |
| 21  | AA    | 98   | A    | C5-C6-N1   | 7.84  | 121.62      | 117.70   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 54  | BA    | 482  | A    | C5-C6-N1   | 7.84  | 121.62      | 117.70   |
| 54  | BA    | 644  | A    | N1-C6-N6   | -7.84 | 113.90      | 118.60   |
| 54  | BA    | 671  | C    | N1-C2-O2   | 7.84  | 123.60      | 118.90   |
| 54  | BA    | 1952 | A    | C5-C6-N1   | 7.84  | 121.62      | 117.70   |
| 54  | BA    | 2369 | A    | C4-C5-C6   | -7.84 | 113.08      | 117.00   |
| 54  | BA    | 2726 | A    | C5-C6-N1   | 7.84  | 121.62      | 117.70   |
| 54  | BA    | 191  | A    | C5-C6-N1   | 7.84  | 121.62      | 117.70   |
| 54  | BA    | 429  | A    | C5-C6-N1   | 7.84  | 121.62      | 117.70   |
| 54  | BA    | 1366 | A    | C5-C6-N1   | 7.84  | 121.62      | 117.70   |
| 54  | BA    | 2666 | C    | N3-C2-O2   | -7.83 | 116.42      | 121.90   |
| 21  | AA    | 298  | A    | N1-C6-N6   | -7.83 | 113.90      | 118.60   |
| 54  | BA    | 1453 | A    | C5-C6-N1   | 7.83  | 121.62      | 117.70   |
| 54  | BA    | 1966 | A    | C5-C6-N1   | 7.83  | 121.62      | 117.70   |
| 21  | AA    | 1375 | A    | C4-C5-C6   | -7.83 | 113.08      | 117.00   |
| 54  | BA    | 2266 | A    | N1-C6-N6   | -7.83 | 113.90      | 118.60   |
| 21  | AA    | 1519 | A    | C4-C5-C6   | -7.83 | 113.09      | 117.00   |
| 54  | BA    | 208  | C    | N3-C2-O2   | -7.83 | 116.42      | 121.90   |
| 54  | BA    | 457  | A    | C5-C6-N1   | 7.83  | 121.61      | 117.70   |
| 54  | BA    | 1284 | A    | C5-C6-N1   | 7.83  | 121.61      | 117.70   |
| 21  | AA    | 160  | A    | C5-C6-N1   | 7.82  | 121.61      | 117.70   |
| 21  | AA    | 573  | A    | C5-C6-N1   | 7.82  | 121.61      | 117.70   |
| 54  | BA    | 353  | C    | N3-C2-O2   | -7.82 | 116.43      | 121.90   |
| 54  | BA    | 1226 | A    | C5-C6-N1   | 7.82  | 121.61      | 117.70   |
| 21  | AA    | 907  | A    | C5-C6-N1   | 7.82  | 121.61      | 117.70   |
| 21  | AA    | 171  | A    | C5-C6-N1   | 7.82  | 121.61      | 117.70   |
| 21  | AA    | 1256 | A    | C5-C6-N1   | 7.82  | 121.61      | 117.70   |
| 54  | BA    | 1784 | A    | C5-C6-N1   | 7.82  | 121.61      | 117.70   |
| 21  | AA    | 98   | A    | C4-C5-C6   | -7.82 | 113.09      | 117.00   |
| 21  | AA    | 983  | A    | N1-C6-N6   | -7.82 | 113.91      | 118.60   |
| 54  | BA    | 1866 | A    | N1-C6-N6   | -7.82 | 113.91      | 118.60   |
| 54  | BA    | 988  | A    | N1-C6-N6   | -7.81 | 113.91      | 118.60   |
| 54  | BA    | 1244 | A    | C5-C6-N1   | 7.81  | 121.61      | 117.70   |
| 21  | AA    | 985  | C    | N3-C2-O2   | -7.81 | 116.43      | 121.90   |
| 54  | BA    | 1942 | C    | N3-C2-O2   | -7.81 | 116.43      | 121.90   |
| 54  | BA    | 1870 | C    | N3-C2-O2   | -7.81 | 116.43      | 121.90   |
| 54  | BA    | 2503 | A    | O4'-C1'-N9 | 7.81  | 114.45      | 108.20   |
| 21  | AA    | 48   | C    | N3-C2-O2   | -7.81 | 116.44      | 121.90   |
| 21  | AA    | 1250 | A    | C5-C6-N1   | 7.81  | 121.60      | 117.70   |
| 54  | BA    | 1749 | A    | C4-C5-C6   | -7.81 | 113.10      | 117.00   |
| 21  | AA    | 1163 | A    | C5-C6-N1   | 7.80  | 121.60      | 117.70   |
| 21  | AA    | 279  | A    | C4-C5-C6   | -7.80 | 113.10      | 117.00   |
| 21  | AA    | 188  | C    | N3-C2-O2   | -7.80 | 116.44      | 121.90   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 21  | AA    | 502  | A    | C4-C5-C6   | -7.80 | 113.10      | 117.00   |
| 21  | AA    | 1129 | C    | N3-C2-O2   | -7.80 | 116.44      | 121.90   |
| 21  | AA    | 655  | A    | N1-C6-N6   | -7.80 | 113.92      | 118.60   |
| 21  | AA    | 781  | A    | C5-C6-N1   | 7.80  | 121.60      | 117.70   |
| 54  | BA    | 146  | A    | N1-C6-N6   | -7.80 | 113.92      | 118.60   |
| 54  | BA    | 1503 | A    | N1-C6-N6   | -7.80 | 113.92      | 118.60   |
| 54  | BA    | 2556 | C    | N3-C2-O2   | -7.80 | 116.44      | 121.90   |
| 3   | AD    | 61   | ARG  | NE-CZ-NH1  | 7.79  | 124.20      | 120.30   |
| 54  | BA    | 1067 | A    | C4-C5-C6   | -7.79 | 113.10      | 117.00   |
| 22  | A1    | 35   | A    | C5-C6-N1   | 7.79  | 121.60      | 117.70   |
| 54  | BA    | 1128 | G    | O4'-C1'-N9 | 7.79  | 114.43      | 108.20   |
| 54  | BA    | 155  | A    | N1-C6-N6   | -7.79 | 113.93      | 118.60   |
| 54  | BA    | 899  | A    | N1-C6-N6   | -7.79 | 113.93      | 118.60   |
| 54  | BA    | 1877 | A    | C4-C5-C6   | -7.79 | 113.11      | 117.00   |
| 21  | AA    | 194  | C    | N3-C2-O2   | -7.79 | 116.45      | 121.90   |
| 21  | AA    | 1364 | U    | O4'-C1'-N1 | 7.79  | 114.43      | 108.20   |
| 54  | BA    | 794  | A    | C4-C5-C6   | -7.79 | 113.11      | 117.00   |
| 54  | BA    | 358  | U    | O4'-C1'-N1 | 7.79  | 114.43      | 108.20   |
| 21  | AA    | 60   | A    | C5-C6-N1   | 7.79  | 121.59      | 117.70   |
| 54  | BA    | 1827 | U    | O4'-C1'-N1 | 7.79  | 114.43      | 108.20   |
| 54  | BA    | 2711 | A    | C4-C5-C6   | -7.79 | 113.11      | 117.00   |
| 21  | AA    | 1398 | A    | N1-C6-N6   | -7.78 | 113.93      | 118.60   |
| 54  | BA    | 322  | A    | N1-C6-N6   | -7.78 | 113.93      | 118.60   |
| 54  | BA    | 899  | A    | C5-C6-N1   | 7.78  | 121.59      | 117.70   |
| 54  | BA    | 928  | A    | C5-C6-N1   | 7.78  | 121.59      | 117.70   |
| 54  | BA    | 2887 | A    | N1-C6-N6   | -7.78 | 113.93      | 118.60   |
| 21  | AA    | 889  | A    | C5-C6-N1   | 7.78  | 121.59      | 117.70   |
| 54  | BA    | 173  | A    | N1-C6-N6   | -7.78 | 113.93      | 118.60   |
| 54  | BA    | 2749 | A    | C5-C6-N1   | 7.78  | 121.59      | 117.70   |
| 54  | BA    | 1351 | C    | O4'-C1'-N1 | 7.78  | 114.42      | 108.20   |
| 54  | BA    | 456  | C    | N1-C2-O2   | 7.78  | 123.56      | 118.90   |
| 54  | BA    | 2778 | A    | C5-C6-N1   | 7.78  | 121.59      | 117.70   |
| 28  | BF    | 70   | ARG  | NE-CZ-NH1  | 7.77  | 124.19      | 120.30   |
| 54  | BA    | 1899 | A    | C5-C6-N1   | 7.77  | 121.59      | 117.70   |
| 54  | BA    | 2572 | A    | C4-C5-C6   | -7.77 | 113.11      | 117.00   |
| 54  | BA    | 1274 | A    | N1-C6-N6   | -7.77 | 113.94      | 118.60   |
| 54  | BA    | 1265 | A    | N1-C6-N6   | -7.77 | 113.94      | 118.60   |
| 54  | BA    | 1284 | A    | N1-C6-N6   | -7.77 | 113.94      | 118.60   |
| 21  | AA    | 66   | A    | N1-C6-N6   | -7.77 | 113.94      | 118.60   |
| 54  | BA    | 2699 | C    | N3-C2-O2   | -7.77 | 116.46      | 121.90   |
| 54  | BA    | 294  | A    | C4-C5-C6   | -7.76 | 113.12      | 117.00   |
| 54  | BA    | 538  | A    | N1-C6-N6   | -7.76 | 113.94      | 118.60   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 54  | BA    | 2080 | A    | C4-C5-C6   | -7.76 | 113.12      | 117.00   |
| 54  | BA    | 541  | A    | N1-C6-N6   | -7.76 | 113.94      | 118.60   |
| 54  | BA    | 794  | A    | C5-C6-N1   | 7.76  | 121.58      | 117.70   |
| 24  | A3    | 73   | A    | C4-C5-C6   | -7.76 | 113.12      | 117.00   |
| 54  | BA    | 479  | A    | C4-C5-C6   | -7.76 | 113.12      | 117.00   |
| 54  | BA    | 671  | C    | N3-C2-O2   | -7.76 | 116.47      | 121.90   |
| 54  | BA    | 787  | C    | N3-C2-O2   | -7.76 | 116.47      | 121.90   |
| 54  | BA    | 943  | A    | C5-C6-N1   | 7.76  | 121.58      | 117.70   |
| 54  | BA    | 1470 | A    | N1-C6-N6   | -7.76 | 113.94      | 118.60   |
| 21  | AA    | 1287 | A    | C5-C6-N1   | 7.76  | 121.58      | 117.70   |
| 21  | AA    | 539  | A    | C5-C6-N1   | 7.76  | 121.58      | 117.70   |
| 54  | BA    | 947  | A    | C5-C6-N1   | 7.76  | 121.58      | 117.70   |
| 54  | BA    | 1711 | A    | C5-C6-N1   | 7.76  | 121.58      | 117.70   |
| 54  | BA    | 603  | A    | C5-C6-N1   | 7.75  | 121.58      | 117.70   |
| 54  | BA    | 794  | A    | N1-C6-N6   | -7.75 | 113.95      | 118.60   |
| 21  | AA    | 475  | C    | N3-C2-O2   | -7.75 | 116.47      | 121.90   |
| 21  | AA    | 482  | A    | C5-C6-N1   | 7.75  | 121.58      | 117.70   |
| 33  | BK    | 64   | ARG  | NE-CZ-NH1  | 7.75  | 124.17      | 120.30   |
| 54  | BA    | 265  | A    | C5-C6-N1   | 7.75  | 121.58      | 117.70   |
| 21  | AA    | 10   | A    | N1-C6-N6   | -7.75 | 113.95      | 118.60   |
| 21  | AA    | 143  | A    | C5-C6-N1   | 7.75  | 121.57      | 117.70   |
| 21  | AA    | 1396 | A    | N1-C6-N6   | -7.75 | 113.95      | 118.60   |
| 54  | BA    | 861  | A    | C5-C6-N1   | 7.75  | 121.58      | 117.70   |
| 55  | BB    | 89   | U    | O4'-C1'-N1 | 7.75  | 114.40      | 108.20   |
| 21  | AA    | 435  | A    | C4-C5-C6   | -7.75 | 113.13      | 117.00   |
| 54  | BA    | 165  | A    | C4-C5-C6   | -7.75 | 113.13      | 117.00   |
| 54  | BA    | 2126 | A    | C5-C6-N1   | 7.75  | 121.57      | 117.70   |
| 54  | BA    | 2208 | C    | N3-C2-O2   | -7.75 | 116.48      | 121.90   |
| 54  | BA    | 2655 | G    | O4'-C1'-N9 | 7.75  | 114.40      | 108.20   |
| 54  | BA    | 2777 | G    | C8-N9-C4   | -7.75 | 103.30      | 106.40   |
| 21  | AA    | 909  | A    | N1-C6-N6   | -7.75 | 113.95      | 118.60   |
| 50  | B1    | 27   | ARG  | NE-CZ-NH1  | 7.75  | 124.17      | 120.30   |
| 18  | AS    | 54   | ARG  | NE-CZ-NH2  | -7.74 | 116.43      | 120.30   |
| 39  | BQ    | 27   | ARG  | NE-CZ-NH1  | 7.74  | 124.17      | 120.30   |
| 54  | BA    | 764  | A    | C5-C6-N1   | 7.74  | 121.57      | 117.70   |
| 21  | AA    | 1367 | C    | N3-C2-O2   | -7.74 | 116.48      | 121.90   |
| 54  | BA    | 2591 | C    | N3-C2-O2   | -7.74 | 116.48      | 121.90   |
| 54  | BA    | 272  | A    | N1-C6-N6   | -7.74 | 113.95      | 118.60   |
| 54  | BA    | 368  | A    | C5-C6-N1   | 7.73  | 121.57      | 117.70   |
| 54  | BA    | 2268 | A    | C5-C6-N1   | 7.73  | 121.57      | 117.70   |
| 21  | AA    | 223  | A    | C4-C5-C6   | -7.73 | 113.13      | 117.00   |
| 21  | AA    | 451  | A    | C5-C6-N1   | 7.73  | 121.56      | 117.70   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 54  | BA    | 2453 | A    | C4-C5-C6   | -7.73 | 113.14      | 117.00   |
| 54  | BA    | 544  | C    | N3-C2-O2   | -7.73 | 116.49      | 121.90   |
| 21  | AA    | 880  | C    | N3-C2-O2   | -7.73 | 116.49      | 121.90   |
| 21  | AA    | 1518 | A    | C5-C6-N1   | 7.73  | 121.56      | 117.70   |
| 27  | BE    | 44   | ARG  | NE-CZ-NH1  | 7.73  | 124.16      | 120.30   |
| 36  | BN    | 46   | ARG  | NE-CZ-NH1  | 7.73  | 124.16      | 120.30   |
| 54  | BA    | 2705 | A    | N1-C6-N6   | -7.73 | 113.96      | 118.60   |
| 54  | BA    | 2738 | A    | N1-C6-N6   | -7.73 | 113.96      | 118.60   |
| 14  | AO    | 57   | ARG  | NE-CZ-NH1  | 7.72  | 124.16      | 120.30   |
| 54  | BA    | 226  | A    | N1-C6-N6   | -7.72 | 113.97      | 118.60   |
| 54  | BA    | 1213 | A    | C5-C6-N1   | 7.72  | 121.56      | 117.70   |
| 5   | AF    | 24   | ARG  | NE-CZ-NH1  | 7.72  | 124.16      | 120.30   |
| 6   | AG    | 4    | ARG  | NE-CZ-NH1  | 7.72  | 124.16      | 120.30   |
| 15  | AP    | 14   | ARG  | NE-CZ-NH1  | 7.72  | 124.16      | 120.30   |
| 54  | BA    | 1785 | A    | C4-C5-C6   | -7.72 | 113.14      | 117.00   |
| 55  | BB    | 78   | A    | C4-C5-C6   | -7.72 | 113.14      | 117.00   |
| 54  | BA    | 655  | A    | N1-C6-N6   | -7.72 | 113.97      | 118.60   |
| 21  | AA    | 768  | A    | N1-C6-N6   | -7.72 | 113.97      | 118.60   |
| 21  | AA    | 1375 | A    | N1-C6-N6   | -7.72 | 113.97      | 118.60   |
| 54  | BA    | 1754 | A    | C5-C6-N1   | 7.72  | 121.56      | 117.70   |
| 54  | BA    | 1103 | A    | C5-C6-N1   | 7.71  | 121.56      | 117.70   |
| 21  | AA    | 609  | A    | N1-C6-N6   | -7.71 | 113.97      | 118.60   |
| 54  | BA    | 1046 | A    | C5-C6-N1   | 7.71  | 121.56      | 117.70   |
| 9   | AJ    | 37   | ARG  | NE-CZ-NH1  | 7.71  | 124.15      | 120.30   |
| 54  | BA    | 1274 | A    | C4-C5-C6   | -7.71 | 113.15      | 117.00   |
| 54  | BA    | 2723 | C    | N3-C2-O2   | -7.71 | 116.50      | 121.90   |
| 6   | AG    | 77   | ARG  | NE-CZ-NH1  | 7.71  | 124.15      | 120.30   |
| 21  | AA    | 186  | C    | N3-C2-O2   | -7.71 | 116.51      | 121.90   |
| 54  | BA    | 457  | A    | C4-C5-C6   | -7.71 | 113.15      | 117.00   |
| 54  | BA    | 477  | A    | C5-C6-N1   | 7.71  | 121.55      | 117.70   |
| 54  | BA    | 960  | A    | N1-C6-N6   | -7.71 | 113.98      | 118.60   |
| 54  | BA    | 1885 | A    | C5-C6-N1   | 7.71  | 121.55      | 117.70   |
| 21  | AA    | 336  | A    | C5-C6-N1   | 7.70  | 121.55      | 117.70   |
| 21  | AA    | 622  | A    | C5-C6-N1   | 7.70  | 121.55      | 117.70   |
| 21  | AA    | 1254 | A    | N1-C6-N6   | -7.70 | 113.98      | 118.60   |
| 54  | BA    | 1414 | C    | N3-C2-O2   | -7.70 | 116.51      | 121.90   |
| 54  | BA    | 2448 | A    | N1-C6-N6   | -7.70 | 113.98      | 118.60   |
| 54  | BA    | 933  | A    | C5-C6-N1   | 7.70  | 121.55      | 117.70   |
| 54  | BA    | 800  | A    | C4-C5-C6   | -7.70 | 113.15      | 117.00   |
| 21  | AA    | 1049 | U    | O4'-C1'-N1 | 7.70  | 114.36      | 108.20   |
| 54  | BA    | 383  | C    | O4'-C1'-N1 | 7.70  | 114.36      | 108.20   |
| 54  | BA    | 982  | C    | C2-N1-C1'  | 7.70  | 127.27      | 118.80   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 54  | BA    | 1912 | A    | C5-C6-N1   | 7.70  | 121.55      | 117.70   |
| 54  | BA    | 2900 | A    | C4-C5-C6   | -7.70 | 113.15      | 117.00   |
| 24  | A3    | 62   | C    | N3-C2-O2   | -7.70 | 116.51      | 121.90   |
| 19  | AT    | 23   | ARG  | NE-CZ-NH1  | 7.69  | 124.15      | 120.30   |
| 21  | AA    | 918  | A    | N1-C6-N6   | -7.69 | 113.98      | 118.60   |
| 21  | AA    | 1252 | A    | C5-C6-N1   | 7.69  | 121.55      | 117.70   |
| 45  | BW    | 40   | ARG  | NE-CZ-NH1  | 7.69  | 124.14      | 120.30   |
| 54  | BA    | 453  | A    | N1-C6-N6   | -7.69 | 113.99      | 118.60   |
| 54  | BA    | 2169 | A    | N1-C6-N6   | -7.69 | 113.99      | 118.60   |
| 21  | AA    | 55   | A    | N1-C6-N6   | -7.69 | 113.99      | 118.60   |
| 54  | BA    | 1054 | A    | C5-C6-N1   | 7.69  | 121.54      | 117.70   |
| 54  | BA    | 337  | C    | N3-C2-O2   | -7.68 | 116.52      | 121.90   |
| 54  | BA    | 286  | U    | O4'-C1'-N1 | 7.68  | 114.35      | 108.20   |
| 54  | BA    | 1230 | A    | N1-C6-N6   | -7.68 | 113.99      | 118.60   |
| 54  | BA    | 2314 | A    | N1-C6-N6   | -7.68 | 113.99      | 118.60   |
| 54  | BA    | 2461 | A    | C5-C6-N1   | 7.68  | 121.54      | 117.70   |
| 21  | AA    | 210  | C    | N3-C2-O2   | -7.68 | 116.52      | 121.90   |
| 21  | AA    | 1288 | A    | C5-C6-N1   | 7.68  | 121.54      | 117.70   |
| 21  | AA    | 1394 | A    | N1-C6-N6   | -7.68 | 113.99      | 118.60   |
| 54  | BA    | 704  | G    | C8-N9-C4   | -7.68 | 103.33      | 106.40   |
| 54  | BA    | 1102 | C    | N3-C2-O2   | -7.68 | 116.53      | 121.90   |
| 21  | AA    | 977  | A    | C4-C5-C6   | -7.68 | 113.16      | 117.00   |
| 54  | BA    | 2733 | A    | C5-C6-N1   | 7.68  | 121.54      | 117.70   |
| 3   | AD    | 43   | ARG  | NE-CZ-NH1  | 7.67  | 124.14      | 120.30   |
| 21  | AA    | 143  | A    | C4-C5-C6   | -7.67 | 113.16      | 117.00   |
| 54  | BA    | 2134 | A    | N1-C6-N6   | -7.67 | 114.00      | 118.60   |
| 54  | BA    | 2882 | A    | C5-C6-N1   | 7.67  | 121.54      | 117.70   |
| 21  | AA    | 1231 | G    | O4'-C1'-N9 | 7.67  | 114.34      | 108.20   |
| 21  | AA    | 1136 | C    | N3-C2-O2   | -7.67 | 116.53      | 121.90   |
| 54  | BA    | 2450 | A    | C5-C6-N1   | 7.67  | 121.53      | 117.70   |
| 54  | BA    | 1127 | A    | N1-C6-N6   | -7.67 | 114.00      | 118.60   |
| 54  | BA    | 1508 | A    | C5-C6-N1   | 7.67  | 121.53      | 117.70   |
| 54  | BA    | 1736 | U    | O4'-C1'-N1 | 7.67  | 114.33      | 108.20   |
| 54  | BA    | 1848 | A    | N1-C6-N6   | -7.67 | 114.00      | 118.60   |
| 50  | B1    | 5    | ARG  | NE-CZ-NH1  | 7.67  | 124.13      | 120.30   |
| 54  | BA    | 693  | A    | C5-C6-N1   | 7.67  | 121.53      | 117.70   |
| 54  | BA    | 918  | A    | C5-C6-N1   | 7.67  | 121.53      | 117.70   |
| 54  | BA    | 631  | A    | C5-C6-N1   | 7.66  | 121.53      | 117.70   |
| 21  | AA    | 737  | C    | N3-C2-O2   | -7.66 | 116.54      | 121.90   |
| 24  | A3    | 1    | C    | N3-C2-O2   | -7.66 | 116.54      | 121.90   |
| 54  | BA    | 2377 | A    | C5-C6-N1   | 7.66  | 121.53      | 117.70   |
| 21  | AA    | 1329 | A    | N1-C6-N6   | -7.66 | 114.00      | 118.60   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 55  | BB    | 101  | A    | C5-C6-N1    | 7.66  | 121.53      | 117.70   |
| 24  | A3    | 67   | C    | N3-C2-O2    | -7.66 | 116.54      | 121.90   |
| 54  | BA    | 1632 | A    | N1-C6-N6    | -7.66 | 114.01      | 118.60   |
| 25  | BC    | 86   | ARG  | NE-CZ-NH1   | 7.66  | 124.13      | 120.30   |
| 54  | BA    | 1363 | C    | N3-C2-O2    | -7.66 | 116.54      | 121.90   |
| 54  | BA    | 2284 | A    | C4-C5-C6    | -7.66 | 113.17      | 117.00   |
| 14  | AO    | 53   | ARG  | NE-CZ-NH1   | 7.65  | 124.13      | 120.30   |
| 21  | AA    | 182  | A    | C4-C5-C6    | -7.65 | 113.17      | 117.00   |
| 54  | BA    | 1352 | U    | O4'-C1'-N1  | 7.65  | 114.32      | 108.20   |
| 54  | BA    | 1805 | A    | N1-C6-N6    | -7.64 | 114.02      | 118.60   |
| 54  | BA    | 6    | A    | C4-C5-C6    | -7.64 | 113.18      | 117.00   |
| 54  | BA    | 2540 | C    | C1'-O4'-C4' | -7.64 | 103.79      | 109.90   |
| 21  | AA    | 1213 | A    | C4-C5-C6    | -7.64 | 113.18      | 117.00   |
| 54  | BA    | 83   | A    | C5-C6-N1    | 7.64  | 121.52      | 117.70   |
| 54  | BA    | 471  | A    | C5-C6-N1    | 7.63  | 121.52      | 117.70   |
| 54  | BA    | 492  | A    | N1-C6-N6    | -7.63 | 114.02      | 118.60   |
| 54  | BA    | 752  | A    | N1-C6-N6    | -7.63 | 114.02      | 118.60   |
| 21  | AA    | 345  | C    | N1-C2-O2    | 7.63  | 123.48      | 118.90   |
| 54  | BA    | 144  | A    | C5-C6-N1    | 7.63  | 121.51      | 117.70   |
| 21  | AA    | 892  | A    | C5-C6-N1    | 7.63  | 121.51      | 117.70   |
| 54  | BA    | 1362 | C    | N3-C2-O2    | -7.63 | 116.56      | 121.90   |
| 54  | BA    | 1854 | A    | C4-C5-C6    | -7.63 | 113.19      | 117.00   |
| 54  | BA    | 984  | A    | C4-C5-C6    | -7.62 | 113.19      | 117.00   |
| 54  | BA    | 1403 | A    | C4-C5-C6    | -7.62 | 113.19      | 117.00   |
| 54  | BA    | 2270 | A    | N1-C6-N6    | -7.62 | 114.03      | 118.60   |
| 21  | AA    | 596  | A    | N1-C6-N6    | -7.62 | 114.03      | 118.60   |
| 54  | BA    | 2610 | C    | N3-C2-O2    | -7.62 | 116.57      | 121.90   |
| 55  | BB    | 30   | C    | N3-C2-O2    | -7.62 | 116.57      | 121.90   |
| 54  | BA    | 1537 | G    | N3-C4-C5    | -7.62 | 124.79      | 128.60   |
| 21  | AA    | 116  | A    | C5-C6-N1    | 7.62  | 121.51      | 117.70   |
| 22  | A1    | 26   | A    | C5-C6-N1    | 7.62  | 121.51      | 117.70   |
| 32  | BJ    | 27   | ARG  | NE-CZ-NH1   | 7.62  | 124.11      | 120.30   |
| 36  | BN    | 86   | ARG  | NE-CZ-NH1   | 7.62  | 124.11      | 120.30   |
| 54  | BA    | 172  | A    | C5-C6-N1    | 7.62  | 121.51      | 117.70   |
| 54  | BA    | 802  | A    | C4-C5-C6    | -7.62 | 113.19      | 117.00   |
| 54  | BA    | 1387 | A    | C4-C5-C6    | -7.62 | 113.19      | 117.00   |
| 21  | AA    | 924  | C    | N3-C2-O2    | -7.61 | 116.57      | 121.90   |
| 21  | AA    | 1509 | C    | N3-C2-O2    | -7.61 | 116.57      | 121.90   |
| 54  | BA    | 1548 | A    | C5-C6-N1    | 7.61  | 121.51      | 117.70   |
| 21  | AA    | 602  | A    | N1-C6-N6    | -7.61 | 114.03      | 118.60   |
| 21  | AA    | 554  | A    | C4-C5-C6    | -7.61 | 113.19      | 117.00   |
| 54  | BA    | 129  | C    | N3-C2-O2    | -7.61 | 116.57      | 121.90   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 54  | BA    | 231  | A    | N1-C6-N6   | -7.61 | 114.03      | 118.60   |
| 54  | BA    | 571  | U    | O4'-C1'-N1 | 7.61  | 114.29      | 108.20   |
| 54  | BA    | 2025 | C    | N1-C2-O2   | 7.61  | 123.47      | 118.90   |
| 21  | AA    | 1197 | A    | C5-C6-N1   | 7.61  | 121.50      | 117.70   |
| 55  | BB    | 58   | A    | C4-C5-C6   | -7.61 | 113.20      | 117.00   |
| 21  | AA    | 1071 | C    | N3-C2-O2   | -7.60 | 116.58      | 121.90   |
| 54  | BA    | 2432 | A    | O4'-C1'-N9 | 7.60  | 114.28      | 108.20   |
| 21  | AA    | 766  | A    | C5-C6-N1   | 7.60  | 121.50      | 117.70   |
| 21  | AA    | 535  | A    | N1-C6-N6   | -7.60 | 114.04      | 118.60   |
| 54  | BA    | 2541 | A    | C5-C6-N1   | 7.60  | 121.50      | 117.70   |
| 23  | A2    | 82   | A    | C5-C6-N1   | 7.60  | 121.50      | 117.70   |
| 54  | BA    | 1434 | A    | C4-C5-C6   | -7.60 | 113.20      | 117.00   |
| 15  | AP    | 28   | ARG  | NE-CZ-NH1  | 7.60  | 124.10      | 120.30   |
| 21  | AA    | 974  | A    | N1-C6-N6   | -7.59 | 114.04      | 118.60   |
| 21  | AA    | 1081 | A    | C5-C6-N1   | 7.59  | 121.50      | 117.70   |
| 54  | BA    | 127  | A    | C5-C6-N1   | 7.59  | 121.50      | 117.70   |
| 21  | AA    | 10   | A    | C5-C6-N1   | 7.59  | 121.50      | 117.70   |
| 54  | BA    | 213  | A    | C5-C6-N1   | 7.59  | 121.50      | 117.70   |
| 54  | BA    | 217  | A    | C5-C6-N1   | 7.59  | 121.50      | 117.70   |
| 54  | BA    | 1000 | A    | N1-C6-N6   | -7.59 | 114.05      | 118.60   |
| 21  | AA    | 1250 | A    | N1-C6-N6   | -7.59 | 114.05      | 118.60   |
| 37  | BO    | 16   | ARG  | NE-CZ-NH1  | 7.59  | 124.09      | 120.30   |
| 54  | BA    | 316  | C    | N3-C2-O2   | -7.59 | 116.59      | 121.90   |
| 54  | BA    | 2860 | A    | N1-C6-N6   | -7.59 | 114.05      | 118.60   |
| 21  | AA    | 600  | A    | N1-C6-N6   | -7.59 | 114.05      | 118.60   |
| 21  | AA    | 148  | G    | C5-C6-N1   | 7.59  | 115.29      | 111.50   |
| 54  | BA    | 730  | A    | N1-C6-N6   | -7.59 | 114.05      | 118.60   |
| 54  | BA    | 2278 | A    | C4-C5-C6   | -7.59 | 113.21      | 117.00   |
| 54  | BA    | 2332 | C    | N3-C2-O2   | -7.59 | 116.59      | 121.90   |
| 21  | AA    | 1082 | A    | N1-C6-N6   | -7.58 | 114.05      | 118.60   |
| 54  | BA    | 2073 | C    | N3-C2-O2   | -7.58 | 116.59      | 121.90   |
| 54  | BA    | 2145 | C    | O4'-C1'-N1 | 7.58  | 114.27      | 108.20   |
| 21  | AA    | 440  | C    | N3-C2-O2   | -7.58 | 116.59      | 121.90   |
| 21  | AA    | 1350 | A    | C5-C6-N1   | 7.58  | 121.49      | 117.70   |
| 40  | BR    | 78   | ARG  | NE-CZ-NH2  | 7.58  | 124.09      | 120.30   |
| 54  | BA    | 2070 | A    | N1-C6-N6   | -7.58 | 114.05      | 118.60   |
| 54  | BA    | 1822 | C    | N3-C2-O2   | -7.58 | 116.59      | 121.90   |
| 54  | BA    | 2377 | A    | C4-C5-C6   | -7.58 | 113.21      | 117.00   |
| 43  | BU    | 5    | ARG  | NE-CZ-NH1  | 7.58  | 124.09      | 120.30   |
| 54  | BA    | 911  | A    | C4-C5-C6   | -7.58 | 113.21      | 117.00   |
| 21  | AA    | 109  | A    | C5-C6-N1   | 7.57  | 121.49      | 117.70   |
| 21  | AA    | 648  | A    | N1-C6-N6   | -7.57 | 114.06      | 118.60   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 54  | BA    | 2687 | U    | O4'-C1'-N1  | 7.57  | 114.26      | 108.20   |
| 21  | AA    | 16   | A    | C5-C6-N1    | 7.57  | 121.49      | 117.70   |
| 21  | AA    | 233  | C    | N3-C2-O2    | -7.57 | 116.60      | 121.90   |
| 54  | BA    | 1302 | A    | C4-C5-C6    | -7.57 | 113.21      | 117.00   |
| 21  | AA    | 430  | A    | N1-C6-N6    | -7.57 | 114.06      | 118.60   |
| 21  | AA    | 487  | A    | C4-C5-C6    | -7.57 | 113.22      | 117.00   |
| 21  | AA    | 196  | A    | C5-C6-N1    | 7.57  | 121.48      | 117.70   |
| 21  | AA    | 819  | A    | C5-C6-N1    | 7.57  | 121.48      | 117.70   |
| 8   | AI    | 11   | ARG  | NE-CZ-NH1   | 7.56  | 124.08      | 120.30   |
| 54  | BA    | 806  | C    | N3-C2-O2    | -7.56 | 116.61      | 121.90   |
| 54  | BA    | 1070 | A    | N1-C6-N6    | -7.56 | 114.06      | 118.60   |
| 54  | BA    | 793  | A    | C5-C6-N1    | 7.56  | 121.48      | 117.70   |
| 54  | BA    | 1808 | A    | C4-C5-C6    | -7.56 | 113.22      | 117.00   |
| 21  | AA    | 47   | C    | N3-C2-O2    | -7.56 | 116.61      | 121.90   |
| 21  | AA    | 1317 | C    | N3-C2-O2    | -7.56 | 116.61      | 121.90   |
| 54  | BA    | 300  | A    | C5-C6-N1    | 7.56  | 121.48      | 117.70   |
| 54  | BA    | 2346 | A    | C4-C5-C6    | -7.56 | 113.22      | 117.00   |
| 2   | AC    | 155  | ARG  | NE-CZ-NH1   | 7.56  | 124.08      | 120.30   |
| 7   | AH    | 12   | ARG  | NE-CZ-NH1   | 7.56  | 124.08      | 120.30   |
| 54  | BA    | 10   | A    | C5-C6-N1    | 7.56  | 121.48      | 117.70   |
| 54  | BA    | 241  | A    | C5-C6-N1    | 7.56  | 121.48      | 117.70   |
| 3   | AD    | 13   | ARG  | NE-CZ-NH1   | 7.55  | 124.08      | 120.30   |
| 55  | BB    | 57   | A    | C4-C5-C6    | -7.55 | 113.22      | 117.00   |
| 8   | AI    | 84   | ARG  | NE-CZ-NH1   | 7.55  | 124.08      | 120.30   |
| 54  | BA    | 109  | C    | N3-C2-O2    | -7.55 | 116.61      | 121.90   |
| 54  | BA    | 960  | A    | C5-C6-N1    | 7.55  | 121.48      | 117.70   |
| 55  | BB    | 24   | G    | N3-C4-C5    | -7.55 | 124.82      | 128.60   |
| 55  | BB    | 3    | C    | N3-C2-O2    | -7.55 | 116.61      | 121.90   |
| 21  | AA    | 938  | A    | C4-C5-C6    | -7.55 | 113.23      | 117.00   |
| 54  | BA    | 1072 | C    | N3-C2-O2    | -7.55 | 116.62      | 121.90   |
| 54  | BA    | 2112 | G    | C8-N9-C4    | -7.55 | 103.38      | 106.40   |
| 54  | BA    | 2727 | A    | C5-C6-N1    | 7.55  | 121.47      | 117.70   |
| 21  | AA    | 1030 | U    | C1'-O4'-C4' | -7.54 | 103.86      | 109.90   |
| 54  | BA    | 886  | A    | C4-C5-C6    | -7.54 | 113.23      | 117.00   |
| 54  | BA    | 2586 | U    | O4'-C1'-N1  | 7.54  | 114.23      | 108.20   |
| 54  | BA    | 300  | A    | C4-C5-C6    | -7.54 | 113.23      | 117.00   |
| 54  | BA    | 2809 | A    | C5-C6-N1    | 7.54  | 121.47      | 117.70   |
| 54  | BA    | 1562 | U    | O4'-C1'-N1  | 7.54  | 114.23      | 108.20   |
| 54  | BA    | 131  | A    | C5-C6-N1    | 7.54  | 121.47      | 117.70   |
| 54  | BA    | 443  | A    | C5-C6-N1    | 7.54  | 121.47      | 117.70   |
| 54  | BA    | 644  | A    | C4-C5-C6    | -7.54 | 113.23      | 117.00   |
| 54  | BA    | 1596 | A    | C5-C6-N1    | 7.54  | 121.47      | 117.70   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 54  | BA    | 1749 | A    | N1-C6-N6    | -7.54 | 114.08      | 118.60   |
| 54  | BA    | 2134 | A    | C4-C5-C6    | -7.54 | 113.23      | 117.00   |
| 54  | BA    | 722  | A    | C5-C6-N1    | 7.53  | 121.47      | 117.70   |
| 54  | BA    | 1996 | C    | N1-C2-O2    | 7.53  | 123.42      | 118.90   |
| 55  | BB    | 53   | A    | C5-C6-N1    | 7.53  | 121.47      | 117.70   |
| 54  | BA    | 227  | A    | C5-C6-N1    | 7.53  | 121.47      | 117.70   |
| 16  | AQ    | 39   | ARG  | NE-CZ-NH1   | 7.53  | 124.06      | 120.30   |
| 21  | AA    | 859  | G    | N1-C6-O6    | -7.53 | 115.38      | 119.90   |
| 54  | BA    | 348  | A    | C5-C6-N1    | 7.53  | 121.46      | 117.70   |
| 54  | BA    | 783  | A    | N1-C6-N6    | -7.53 | 114.08      | 118.60   |
| 21  | AA    | 28   | A    | C4-C5-C6    | -7.53 | 113.24      | 117.00   |
| 21  | AA    | 490  | C    | N3-C2-O2    | -7.53 | 116.63      | 121.90   |
| 54  | BA    | 325  | G    | O4'-C1'-N9  | 7.53  | 114.22      | 108.20   |
| 54  | BA    | 2872 | A    | C4-C5-C6    | -7.52 | 113.24      | 117.00   |
| 3   | AD    | 153  | ARG  | NE-CZ-NH1   | 7.52  | 124.06      | 120.30   |
| 54  | BA    | 945  | A    | C5-C6-N1    | 7.52  | 121.46      | 117.70   |
| 22  | A1    | 75   | C    | C1'-O4'-C4' | -7.52 | 103.89      | 109.90   |
| 24  | A3    | 58   | A    | C5-C6-N1    | 7.52  | 121.46      | 117.70   |
| 54  | BA    | 609  | A    | C4-C5-C6    | -7.52 | 113.24      | 117.00   |
| 54  | BA    | 749  | A    | C5-C6-N1    | 7.52  | 121.46      | 117.70   |
| 54  | BA    | 1597 | A    | N1-C6-N6    | -7.52 | 114.09      | 118.60   |
| 21  | AA    | 98   | A    | N1-C6-N6    | -7.52 | 114.09      | 118.60   |
| 23  | A2    | 79   | A    | C5-C6-N1    | 7.52  | 121.46      | 117.70   |
| 54  | BA    | 275  | C    | N3-C2-O2    | -7.52 | 116.64      | 121.90   |
| 54  | BA    | 2013 | A    | C5-C6-N1    | 7.52  | 121.46      | 117.70   |
| 2   | AC    | 135  | ARG  | NE-CZ-NH1   | 7.52  | 124.06      | 120.30   |
| 21  | AA    | 1337 | G    | N3-C4-C5    | -7.52 | 124.84      | 128.60   |
| 21  | AA    | 1210 | C    | N3-C2-O2    | -7.51 | 116.64      | 121.90   |
| 54  | BA    | 1248 | G    | O4'-C1'-N9  | 7.51  | 114.21      | 108.20   |
| 21  | AA    | 1480 | A    | C5-C6-N1    | 7.51  | 121.45      | 117.70   |
| 54  | BA    | 2742 | G    | O4'-C1'-N9  | 7.51  | 114.21      | 108.20   |
| 54  | BA    | 277  | G    | N3-C4-C5    | -7.51 | 124.85      | 128.60   |
| 55  | BB    | 17   | C    | O4'-C1'-N1  | 7.51  | 114.21      | 108.20   |
| 54  | BA    | 2764 | A    | C4-C5-C6    | -7.51 | 113.25      | 117.00   |
| 21  | AA    | 994  | A    | C5-C6-N1    | 7.50  | 121.45      | 117.70   |
| 39  | BQ    | 69   | ARG  | NE-CZ-NH1   | 7.50  | 124.05      | 120.30   |
| 54  | BA    | 1504 | A    | N1-C6-N6    | -7.50 | 114.10      | 118.60   |
| 54  | BA    | 2459 | A    | N1-C6-N6    | -7.50 | 114.10      | 118.60   |
| 55  | BB    | 37   | C    | N3-C2-O2    | -7.50 | 116.65      | 121.90   |
| 26  | BD    | 59   | ARG  | NE-CZ-NH1   | 7.50  | 124.05      | 120.30   |
| 55  | BB    | 109  | A    | C5-C6-N1    | 7.50  | 121.45      | 117.70   |
| 24  | A3    | 45   | A    | C5-C6-N1    | 7.50  | 121.45      | 117.70   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 22  | A1    | 23   | A    | C5-C6-N1   | 7.50  | 121.45      | 117.70   |
| 27  | BE    | 79   | ARG  | NE-CZ-NH1  | 7.50  | 124.05      | 120.30   |
| 54  | BA    | 632  | A    | N1-C6-N6   | -7.50 | 114.10      | 118.60   |
| 54  | BA    | 1610 | A    | O4'-C1'-N9 | 7.50  | 114.20      | 108.20   |
| 54  | BA    | 2335 | A    | C4-C5-C6   | -7.50 | 113.25      | 117.00   |
| 54  | BA    | 946  | C    | N3-C2-O2   | -7.50 | 116.65      | 121.90   |
| 54  | BA    | 1575 | C    | N3-C2-O2   | -7.50 | 116.65      | 121.90   |
| 54  | BA    | 1744 | A    | C5-C6-N1   | 7.50  | 121.45      | 117.70   |
| 54  | BA    | 2380 | C    | N3-C2-O2   | -7.50 | 116.65      | 121.90   |
| 21  | AA    | 906  | A    | C4-C5-C6   | -7.50 | 113.25      | 117.00   |
| 54  | BA    | 2003 | A    | C5-C6-N1   | 7.50  | 121.45      | 117.70   |
| 21  | AA    | 167  | A    | C4-C5-C6   | -7.49 | 113.25      | 117.00   |
| 21  | AA    | 1493 | A    | C4-C5-C6   | -7.49 | 113.25      | 117.00   |
| 22  | A1    | 9    | A    | C5-C6-N1   | 7.49  | 121.44      | 117.70   |
| 54  | BA    | 502  | A    | C5-C6-N1   | 7.49  | 121.44      | 117.70   |
| 54  | BA    | 515  | A    | C5-C6-N1   | 7.49  | 121.44      | 117.70   |
| 54  | BA    | 1731 | G    | O4'-C1'-N9 | 7.49  | 114.19      | 108.20   |
| 54  | BA    | 2666 | C    | N1-C2-O2   | 7.49  | 123.39      | 118.90   |
| 55  | BB    | 45   | A    | N1-C6-N6   | -7.49 | 114.11      | 118.60   |
| 24  | A3    | 17   | C    | N3-C2-O2   | -7.49 | 116.66      | 121.90   |
| 54  | BA    | 654  | A    | C4-C5-C6   | -7.49 | 113.26      | 117.00   |
| 54  | BA    | 961  | C    | N3-C2-O2   | -7.49 | 116.66      | 121.90   |
| 54  | BA    | 1871 | A    | C5-C6-N1   | 7.49  | 121.44      | 117.70   |
| 54  | BA    | 2160 | C    | N3-C2-O2   | -7.49 | 116.66      | 121.90   |
| 21  | AA    | 6    | G    | N3-C4-C5   | -7.48 | 124.86      | 128.60   |
| 21  | AA    | 152  | A    | C5-C6-N1   | 7.48  | 121.44      | 117.70   |
| 24  | A3    | 59   | A    | C5-C6-N1   | 7.48  | 121.44      | 117.70   |
| 54  | BA    | 996  | A    | C4-C5-C6   | -7.48 | 113.26      | 117.00   |
| 14  | AO    | 63   | ARG  | NE-CZ-NH1  | 7.48  | 124.04      | 120.30   |
| 21  | AA    | 189  | A    | C4-C5-C6   | -7.48 | 113.26      | 117.00   |
| 54  | BA    | 460  | A    | N1-C6-N6   | -7.48 | 114.11      | 118.60   |
| 54  | BA    | 1144 | A    | C5-C6-N1   | 7.48  | 121.44      | 117.70   |
| 54  | BA    | 2212 | A    | C4-C5-C6   | -7.48 | 113.26      | 117.00   |
| 21  | AA    | 149  | A    | C4-C5-C6   | -7.48 | 113.26      | 117.00   |
| 21  | AA    | 1176 | A    | N1-C6-N6   | -7.48 | 114.11      | 118.60   |
| 54  | BA    | 457  | A    | O4'-C1'-N9 | 7.48  | 114.18      | 108.20   |
| 54  | BA    | 2211 | A    | C5-C6-N1   | 7.48  | 121.44      | 117.70   |
| 21  | AA    | 366  | A    | P-O3'-C3'  | 7.48  | 128.67      | 119.70   |
| 51  | B2    | 28   | ARG  | NE-CZ-NH1  | 7.47  | 124.04      | 120.30   |
| 54  | BA    | 1001 | A    | C5-C6-N1   | 7.47  | 121.44      | 117.70   |
| 54  | BA    | 1143 | A    | C5-C6-N1   | 7.47  | 121.44      | 117.70   |
| 54  | BA    | 378  | C    | N3-C2-O2   | -7.47 | 116.67      | 121.90   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|------------|-------|------------------------|---------------------|
| 21  | AA    | 501  | C    | N3-C2-O2   | -7.47 | 116.67                 | 121.90              |
| 21  | AA    | 432  | A    | N1-C6-N6   | -7.47 | 114.12                 | 118.60              |
| 54  | BA    | 1805 | A    | C5-C6-N1   | 7.47  | 121.44                 | 117.70              |
| 54  | BA    | 1382 | G    | N3-C4-C5   | -7.47 | 124.87                 | 128.60              |
| 54  | BA    | 1590 | A    | C4-C5-C6   | -7.46 | 113.27                 | 117.00              |
| 21  | AA    | 340  | U    | O4'-C1'-N1 | 7.46  | 114.17                 | 108.20              |
| 54  | BA    | 1991 | U    | O4'-C1'-N1 | 7.46  | 114.17                 | 108.20              |
| 54  | BA    | 1874 | C    | O4'-C1'-N1 | 7.46  | 114.17                 | 108.20              |
| 54  | BA    | 2727 | A    | N1-C6-N6   | -7.46 | 114.12                 | 118.60              |
| 54  | BA    | 941  | A    | C5-C6-N1   | 7.46  | 121.43                 | 117.70              |
| 54  | BA    | 2496 | C    | N3-C2-O2   | -7.46 | 116.68                 | 121.90              |
| 21  | AA    | 840  | C    | N3-C2-O2   | -7.46 | 116.68                 | 121.90              |
| 21  | AA    | 461  | A    | N1-C6-N6   | -7.46 | 114.13                 | 118.60              |
| 24  | A3    | 57   | C    | N3-C2-O2   | -7.46 | 116.68                 | 121.90              |
| 54  | BA    | 849  | A    | C5-C6-N1   | 7.46  | 121.43                 | 117.70              |
| 21  | AA    | 811  | C    | N3-C2-O2   | -7.46 | 116.68                 | 121.90              |
| 21  | AA    | 967  | C    | N3-C2-O2   | -7.46 | 116.68                 | 121.90              |
| 54  | BA    | 2406 | A    | C5-C6-N1   | 7.46  | 121.43                 | 117.70              |
| 21  | AA    | 465  | A    | O4'-C1'-N9 | 7.45  | 114.16                 | 108.20              |
| 54  | BA    | 959  | A    | C5-C6-N1   | 7.45  | 121.43                 | 117.70              |
| 54  | BA    | 1178 | C    | N3-C2-O2   | -7.45 | 116.68                 | 121.90              |
| 54  | BA    | 1268 | A    | C5-C6-N1   | 7.45  | 121.42                 | 117.70              |
| 54  | BA    | 1494 | A    | C5-C6-N1   | 7.45  | 121.42                 | 117.70              |
| 54  | BA    | 2362 | C    | N3-C2-O2   | -7.45 | 116.69                 | 121.90              |
| 54  | BA    | 2818 | U    | O4'-C1'-N1 | 7.45  | 114.16                 | 108.20              |
| 25  | BC    | 181  | ARG  | NE-CZ-NH1  | 7.45  | 124.02                 | 120.30              |
| 54  | BA    | 2284 | A    | N1-C6-N6   | -7.45 | 114.13                 | 118.60              |
| 21  | AA    | 1180 | A    | C4-C5-C6   | -7.45 | 113.28                 | 117.00              |
| 54  | BA    | 789  | A    | C5-C6-N1   | 7.45  | 121.42                 | 117.70              |
| 54  | BA    | 1571 | A    | N1-C6-N6   | -7.45 | 114.13                 | 118.60              |
| 54  | BA    | 1826 | G    | O4'-C1'-N9 | 7.45  | 114.16                 | 108.20              |
| 21  | AA    | 572  | A    | N1-C6-N6   | -7.45 | 114.13                 | 118.60              |
| 54  | BA    | 1447 | C    | N3-C2-O2   | -7.45 | 116.69                 | 121.90              |
| 54  | BA    | 2619 | C    | N3-C2-O2   | -7.45 | 116.69                 | 121.90              |
| 54  | BA    | 1698 | A    | C4-C5-C6   | -7.44 | 113.28                 | 117.00              |
| 21  | AA    | 528  | C    | N3-C2-O2   | -7.44 | 116.69                 | 121.90              |
| 54  | BA    | 383  | C    | N3-C2-O2   | -7.44 | 116.69                 | 121.90              |
| 54  | BA    | 1054 | A    | C4-C5-C6   | -7.44 | 113.28                 | 117.00              |
| 54  | BA    | 2268 | A    | N1-C6-N6   | -7.44 | 114.14                 | 118.60              |
| 21  | AA    | 864  | A    | C4-C5-C6   | -7.44 | 113.28                 | 117.00              |
| 54  | BA    | 362  | A    | N1-C6-N6   | -7.44 | 114.14                 | 118.60              |
| 54  | BA    | 2317 | A    | C5-C6-N1   | 7.44  | 121.42                 | 117.70              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 54  | BA    | 1288 | G    | O4'-C1'-N9 | 7.44  | 114.15      | 108.20   |
| 54  | BA    | 2753 | A    | C4-C5-C6   | -7.44 | 113.28      | 117.00   |
| 21  | AA    | 415  | A    | C5-C6-N1   | 7.44  | 121.42      | 117.70   |
| 54  | BA    | 126  | A    | N1-C6-N6   | -7.44 | 114.14      | 118.60   |
| 54  | BA    | 1328 | A    | C5-C6-N1   | 7.44  | 121.42      | 117.70   |
| 21  | AA    | 465  | A    | N1-C6-N6   | -7.43 | 114.14      | 118.60   |
| 32  | BJ    | 13   | ARG  | NE-CZ-NH1  | 7.43  | 124.02      | 120.30   |
| 54  | BA    | 740  | C    | N3-C2-O2   | -7.43 | 116.70      | 121.90   |
| 54  | BA    | 2827 | C    | O4'-C1'-N1 | 7.43  | 114.15      | 108.20   |
| 21  | AA    | 393  | A    | C4-C5-C6   | -7.43 | 113.28      | 117.00   |
| 21  | AA    | 1246 | A    | N1-C6-N6   | -7.43 | 114.14      | 118.60   |
| 54  | BA    | 893  | C    | N3-C2-O2   | -7.43 | 116.70      | 121.90   |
| 54  | BA    | 1069 | A    | N1-C6-N6   | -7.43 | 114.14      | 118.60   |
| 54  | BA    | 1872 | A    | C5-C6-N1   | 7.43  | 121.42      | 117.70   |
| 21  | AA    | 221  | C    | N3-C2-O2   | -7.43 | 116.70      | 121.90   |
| 21  | AA    | 1320 | C    | N3-C2-O2   | -7.43 | 116.70      | 121.90   |
| 54  | BA    | 1427 | A    | C4-C5-C6   | -7.43 | 113.29      | 117.00   |
| 54  | BA    | 2600 | A    | N1-C6-N6   | -7.43 | 114.14      | 118.60   |
| 54  | BA    | 2692 | G    | N3-C4-C5   | -7.43 | 124.89      | 128.60   |
| 5   | AF    | 2    | ARG  | NE-CZ-NH1  | 7.43  | 124.01      | 120.30   |
| 11  | AL    | 82   | ARG  | NE-CZ-NH1  | 7.43  | 124.01      | 120.30   |
| 21  | AA    | 1446 | A    | N1-C6-N6   | -7.43 | 114.14      | 118.60   |
| 54  | BA    | 470  | A    | C5-C6-N1   | 7.43  | 121.41      | 117.70   |
| 54  | BA    | 1646 | C    | N3-C2-O2   | -7.43 | 116.70      | 121.90   |
| 54  | BA    | 103  | A    | C5-C6-N1   | 7.42  | 121.41      | 117.70   |
| 54  | BA    | 1144 | A    | N1-C6-N6   | -7.42 | 114.14      | 118.60   |
| 54  | BA    | 2014 | A    | N1-C6-N6   | -7.42 | 114.14      | 118.60   |
| 54  | BA    | 2510 | C    | C2-N3-C4   | -7.42 | 116.19      | 119.90   |
| 21  | AA    | 130  | A    | C5-C6-N1   | 7.42  | 121.41      | 117.70   |
| 21  | AA    | 938  | A    | C5-C6-N1   | 7.42  | 121.41      | 117.70   |
| 21  | AA    | 329  | A    | C5-C6-N1   | 7.42  | 121.41      | 117.70   |
| 54  | BA    | 1021 | A    | C4-C5-C6   | -7.42 | 113.29      | 117.00   |
| 54  | BA    | 2015 | A    | N1-C6-N6   | -7.42 | 114.15      | 118.60   |
| 21  | AA    | 489  | C    | N3-C2-O2   | -7.42 | 116.71      | 121.90   |
| 54  | BA    | 1320 | C    | N3-C2-O2   | -7.42 | 116.71      | 121.90   |
| 54  | BA    | 1532 | A    | C5-C6-N1   | 7.42  | 121.41      | 117.70   |
| 54  | BA    | 861  | A    | C4-C5-C6   | -7.42 | 113.29      | 117.00   |
| 10  | AK    | 36   | ARG  | NE-CZ-NH1  | 7.42  | 124.01      | 120.30   |
| 21  | AA    | 456  | A    | N1-C6-N6   | -7.42 | 114.15      | 118.60   |
| 21  | AA    | 74   | A    | C4-C5-C6   | -7.41 | 113.30      | 117.00   |
| 21  | AA    | 485  | U    | O4'-C1'-N1 | 7.41  | 114.13      | 108.20   |
| 21  | AA    | 1216 | A    | C5-C6-N1   | 7.41  | 121.40      | 117.70   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 54  | BA    | 2443 | C    | N3-C2-O2   | -7.41 | 116.72      | 121.90   |
| 21  | AA    | 1169 | A    | C4-C5-C6   | -7.40 | 113.30      | 117.00   |
| 21  | AA    | 59   | A    | C5-C6-N1   | 7.40  | 121.40      | 117.70   |
| 54  | BA    | 513  | A    | C5-C6-N1   | 7.40  | 121.40      | 117.70   |
| 54  | BA    | 1027 | A    | C4-C5-C6   | -7.40 | 113.30      | 117.00   |
| 54  | BA    | 1285 | A    | C5-C6-N1   | 7.40  | 121.40      | 117.70   |
| 54  | BA    | 1700 | A    | C4-C5-C6   | -7.40 | 113.30      | 117.00   |
| 54  | BA    | 1780 | A    | C4-C5-C6   | -7.40 | 113.30      | 117.00   |
| 54  | BA    | 2273 | A    | C4-C5-C6   | -7.40 | 113.30      | 117.00   |
| 3   | AD    | 153  | ARG  | NE-CZ-NH2  | -7.40 | 116.60      | 120.30   |
| 21  | AA    | 977  | A    | C5-C6-N1   | 7.40  | 121.40      | 117.70   |
| 54  | BA    | 2274 | A    | C5-C6-N1   | 7.40  | 121.40      | 117.70   |
| 54  | BA    | 2378 | A    | N1-C6-N6   | -7.40 | 114.16      | 118.60   |
| 21  | AA    | 1214 | C    | N1-C2-O2   | 7.40  | 123.34      | 118.90   |
| 54  | BA    | 1365 | A    | C5-C6-N1   | 7.40  | 121.40      | 117.70   |
| 54  | BA    | 1480 | C    | N3-C2-O2   | -7.40 | 116.72      | 121.90   |
| 21  | AA    | 58   | C    | N3-C2-O2   | -7.39 | 116.72      | 121.90   |
| 54  | BA    | 2164 | C    | N3-C2-O2   | -7.39 | 116.72      | 121.90   |
| 6   | AG    | 94   | ARG  | NE-CZ-NH1  | 7.39  | 124.00      | 120.30   |
| 21  | AA    | 962  | C    | N3-C2-O2   | -7.39 | 116.73      | 121.90   |
| 43  | BU    | 93   | ARG  | NE-CZ-NH1  | 7.39  | 124.00      | 120.30   |
| 21  | AA    | 246  | A    | C5-C6-N1   | 7.39  | 121.39      | 117.70   |
| 22  | A1    | 71   | C    | N3-C2-O2   | -7.39 | 116.73      | 121.90   |
| 54  | BA    | 1640 | A    | N1-C6-N6   | -7.39 | 114.17      | 118.60   |
| 54  | BA    | 2006 | C    | N3-C2-O2   | -7.39 | 116.73      | 121.90   |
| 54  | BA    | 2789 | C    | O4'-C1'-N1 | 7.39  | 114.11      | 108.20   |
| 54  | BA    | 710  | U    | O4'-C1'-N1 | 7.39  | 114.11      | 108.20   |
| 21  | AA    | 1462 | C    | N3-C2-O2   | -7.39 | 116.73      | 121.90   |
| 54  | BA    | 302  | C    | N3-C2-O2   | -7.39 | 116.73      | 121.90   |
| 54  | BA    | 487  | C    | N3-C2-O2   | -7.39 | 116.73      | 121.90   |
| 54  | BA    | 1384 | A    | N1-C6-N6   | -7.39 | 114.17      | 118.60   |
| 54  | BA    | 1932 | A    | C4-C5-C6   | -7.39 | 113.31      | 117.00   |
| 21  | AA    | 1158 | C    | N3-C2-O2   | -7.38 | 116.73      | 121.90   |
| 21  | AA    | 1322 | C    | N3-C2-O2   | -7.38 | 116.73      | 121.90   |
| 54  | BA    | 1735 | A    | N1-C6-N6   | -7.38 | 114.17      | 118.60   |
| 54  | BA    | 611  | C    | N3-C2-O2   | -7.38 | 116.74      | 121.90   |
| 54  | BA    | 2426 | A    | C5-C6-N1   | 7.38  | 121.39      | 117.70   |
| 54  | BA    | 933  | A    | C4-C5-C6   | -7.38 | 113.31      | 117.00   |
| 21  | AA    | 1102 | A    | N1-C6-N6   | -7.37 | 114.17      | 118.60   |
| 54  | BA    | 719  | C    | N3-C2-O2   | -7.37 | 116.74      | 121.90   |
| 54  | BA    | 1431 | A    | C5-C6-N1   | 7.37  | 121.39      | 117.70   |
| 54  | BA    | 2614 | A    | N1-C6-N6   | -7.37 | 114.18      | 118.60   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 21  | AA    | 705  | G    | N1-C6-O6    | -7.37 | 115.48      | 119.90   |
| 22  | A1    | 27   | C    | N3-C2-O2    | -7.37 | 116.74      | 121.90   |
| 21  | AA    | 139  | A    | N1-C6-N6    | -7.37 | 114.18      | 118.60   |
| 21  | AA    | 167  | A    | N1-C6-N6    | -7.37 | 114.18      | 118.60   |
| 21  | AA    | 1100 | C    | N3-C2-O2    | -7.37 | 116.74      | 121.90   |
| 54  | BA    | 401  | A    | N1-C6-N6    | -7.37 | 114.18      | 118.60   |
| 54  | BA    | 2823 | A    | C5-C6-N1    | 7.37  | 121.38      | 117.70   |
| 54  | BA    | 980  | A    | C4-C5-C6    | -7.37 | 113.32      | 117.00   |
| 21  | AA    | 1363 | A    | C4-C5-C6    | -7.37 | 113.32      | 117.00   |
| 54  | BA    | 342  | A    | C4-C5-C6    | -7.37 | 113.32      | 117.00   |
| 21  | AA    | 130  | A    | C4-C5-C6    | -7.36 | 113.32      | 117.00   |
| 21  | AA    | 1012 | A    | C5-C6-N1    | 7.36  | 121.38      | 117.70   |
| 55  | BB    | 45   | A    | C4-C5-C6    | -7.36 | 113.32      | 117.00   |
| 54  | BA    | 279  | A    | C5-C6-N1    | 7.36  | 121.38      | 117.70   |
| 21  | AA    | 1433 | A    | C5-C6-N1    | 7.36  | 121.38      | 117.70   |
| 54  | BA    | 76   | C    | N3-C2-O2    | -7.36 | 116.75      | 121.90   |
| 21  | AA    | 306  | A    | N1-C6-N6    | -7.36 | 114.19      | 118.60   |
| 21  | AA    | 932  | C    | C1'-O4'-C4' | -7.36 | 104.01      | 109.90   |
| 21  | AA    | 1046 | A    | C5-C6-N1    | 7.36  | 121.38      | 117.70   |
| 37  | BO    | 25   | ARG  | NE-CZ-NH1   | 7.36  | 123.98      | 120.30   |
| 54  | BA    | 431  | U    | O4'-C1'-N1  | 7.36  | 114.09      | 108.20   |
| 54  | BA    | 599  | A    | C4-C5-C6    | -7.36 | 113.32      | 117.00   |
| 54  | BA    | 1550 | C    | N1-C2-O2    | 7.36  | 123.31      | 118.90   |
| 54  | BA    | 1771 | C    | O4'-C1'-N1  | 7.36  | 114.09      | 108.20   |
| 54  | BA    | 2094 | A    | C4-C5-C6    | -7.36 | 113.32      | 117.00   |
| 55  | BB    | 36   | C    | N3-C2-O2    | -7.36 | 116.75      | 121.90   |
| 21  | AA    | 6    | G    | N1-C6-O6    | -7.36 | 115.49      | 119.90   |
| 21  | AA    | 1350 | A    | N1-C6-N6    | -7.36 | 114.19      | 118.60   |
| 54  | BA    | 717  | C    | N3-C2-O2    | -7.36 | 116.75      | 121.90   |
| 54  | BA    | 419  | U    | O4'-C1'-N1  | 7.35  | 114.08      | 108.20   |
| 54  | BA    | 751  | A    | C4-C5-C6    | -7.35 | 113.32      | 117.00   |
| 21  | AA    | 642  | A    | N1-C6-N6    | -7.35 | 114.19      | 118.60   |
| 21  | AA    | 900  | A    | C5-C6-N1    | 7.35  | 121.37      | 117.70   |
| 54  | BA    | 572  | A    | C4-C5-C6    | -7.35 | 113.33      | 117.00   |
| 54  | BA    | 2517 | C    | O4'-C1'-N1  | 7.35  | 114.08      | 108.20   |
| 39  | BQ    | 12   | ARG  | NE-CZ-NH2   | 7.35  | 123.97      | 120.30   |
| 54  | BA    | 2051 | A    | N1-C6-N6    | -7.35 | 114.19      | 118.60   |
| 54  | BA    | 156  | A    | C4-C5-C6    | -7.34 | 113.33      | 117.00   |
| 54  | BA    | 2531 | A    | N1-C6-N6    | -7.34 | 114.19      | 118.60   |
| 54  | BA    | 2516 | A    | N1-C6-N6    | -7.34 | 114.19      | 118.60   |
| 21  | AA    | 487  | A    | N1-C6-N6    | -7.34 | 114.20      | 118.60   |
| 21  | AA    | 794  | A    | C5-C6-N1    | 7.34  | 121.37      | 117.70   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 54  | BA    | 833  | A    | C5-C6-N1    | 7.34  | 121.37      | 117.70   |
| 54  | BA    | 1786 | A    | C5-C6-N1    | 7.34  | 121.37      | 117.70   |
| 54  | BA    | 756  | A    | C5-C6-N1    | 7.34  | 121.37      | 117.70   |
| 54  | BA    | 2556 | C    | O4'-C1'-N1  | 7.34  | 114.07      | 108.20   |
| 21  | AA    | 753  | A    | C5-C6-N1    | 7.34  | 121.37      | 117.70   |
| 21  | AA    | 779  | C    | N3-C2-O2    | -7.34 | 116.77      | 121.90   |
| 21  | AA    | 839  | C    | N3-C2-O2    | -7.34 | 116.76      | 121.90   |
| 54  | BA    | 670  | A    | C5-C6-N1    | 7.34  | 121.37      | 117.70   |
| 54  | BA    | 1804 | C    | N3-C2-O2    | -7.34 | 116.76      | 121.90   |
| 54  | BA    | 2054 | A    | C5-C6-N1    | 7.34  | 121.37      | 117.70   |
| 21  | AA    | 949  | A    | C4-C5-C6    | -7.33 | 113.33      | 117.00   |
| 54  | BA    | 146  | A    | C4-C5-C6    | -7.33 | 113.33      | 117.00   |
| 54  | BA    | 514  | A    | C5-C6-N1    | 7.33  | 121.37      | 117.70   |
| 54  | BA    | 2226 | C    | N3-C2-O2    | -7.33 | 116.77      | 121.90   |
| 54  | BA    | 2510 | C    | N1-C2-N3    | 7.33  | 124.33      | 119.20   |
| 54  | BA    | 2860 | A    | C4-C5-C6    | -7.33 | 113.33      | 117.00   |
| 21  | AA    | 608  | A    | C4-C5-C6    | -7.33 | 113.33      | 117.00   |
| 21  | AA    | 914  | A    | C5-C6-N1    | 7.33  | 121.37      | 117.70   |
| 54  | BA    | 1801 | A    | C5-C6-N1    | 7.33  | 121.36      | 117.70   |
| 54  | BA    | 2222 | C    | N3-C2-O2    | -7.33 | 116.77      | 121.90   |
| 54  | BA    | 621  | A    | N1-C6-N6    | -7.33 | 114.20      | 118.60   |
| 54  | BA    | 173  | A    | C4-C5-C6    | -7.33 | 113.34      | 117.00   |
| 25  | BC    | 132  | ARG  | NE-CZ-NH1   | 7.32  | 123.96      | 120.30   |
| 54  | BA    | 1454 | C    | N1-C2-O2    | 7.32  | 123.29      | 118.90   |
| 54  | BA    | 1998 | A    | N1-C6-N6    | -7.32 | 114.21      | 118.60   |
| 21  | AA    | 1137 | C    | N3-C2-O2    | -7.32 | 116.78      | 121.90   |
| 54  | BA    | 324  | A    | C5-C6-N1    | 7.32  | 121.36      | 117.70   |
| 54  | BA    | 1977 | A    | C4-C5-C6    | -7.32 | 113.34      | 117.00   |
| 21  | AA    | 640  | A    | C5-C6-N1    | 7.32  | 121.36      | 117.70   |
| 21  | AA    | 913  | A    | C5-C6-N1    | 7.32  | 121.36      | 117.70   |
| 54  | BA    | 2062 | A    | C5-C6-N1    | 7.32  | 121.36      | 117.70   |
| 21  | AA    | 1377 | A    | C4-C5-C6    | -7.31 | 113.34      | 117.00   |
| 54  | BA    | 295  | G    | C8-N9-C4    | -7.31 | 103.47      | 106.40   |
| 54  | BA    | 1534 | U    | O4'-C1'-N1  | 7.31  | 114.05      | 108.20   |
| 54  | BA    | 2704 | C    | N3-C2-O2    | -7.31 | 116.78      | 121.90   |
| 21  | AA    | 344  | A    | C5-C6-N1    | 7.31  | 121.35      | 117.70   |
| 21  | AA    | 1158 | C    | N1-C2-O2    | 7.31  | 123.28      | 118.90   |
| 21  | AA    | 1403 | C    | N3-C2-O2    | -7.31 | 116.78      | 121.90   |
| 54  | BA    | 1938 | A    | C1'-O4'-C4' | -7.31 | 104.05      | 109.90   |
| 54  | BA    | 2564 | A    | C4-C5-C6    | -7.31 | 113.35      | 117.00   |
| 54  | BA    | 675  | A    | C5-C6-N1    | 7.30  | 121.35      | 117.70   |
| 54  | BA    | 229  | C    | O4'-C1'-N1  | 7.30  | 114.04      | 108.20   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|-------------|-------|------------------------|---------------------|
| 54  | BA    | 1226 | A    | C4-C5-C6    | -7.30 | 113.35                 | 117.00              |
| 54  | BA    | 2135 | A    | C4-C5-C6    | -7.30 | 113.35                 | 117.00              |
| 54  | BA    | 74   | A    | C4-C5-C6    | -7.30 | 113.35                 | 117.00              |
| 22  | A1    | 66   | A    | C4-C5-C6    | -7.30 | 113.35                 | 117.00              |
| 54  | BA    | 240  | C    | N3-C2-O2    | -7.30 | 116.79                 | 121.90              |
| 54  | BA    | 1354 | A    | C4-C5-C6    | -7.30 | 113.35                 | 117.00              |
| 21  | AA    | 156  | C    | O4'-C1'-N1  | 7.29  | 114.03                 | 108.20              |
| 54  | BA    | 165  | A    | N1-C6-N6    | -7.29 | 114.22                 | 118.60              |
| 54  | BA    | 595  | C    | N3-C2-O2    | -7.29 | 116.80                 | 121.90              |
| 54  | BA    | 2748 | A    | N1-C6-N6    | -7.29 | 114.22                 | 118.60              |
| 21  | AA    | 1201 | A    | C4-C5-C6    | -7.29 | 113.35                 | 117.00              |
| 54  | BA    | 9    | G    | N1-C6-O6    | -7.29 | 115.53                 | 119.90              |
| 54  | BA    | 430  | A    | C5-C6-N1    | 7.29  | 121.35                 | 117.70              |
| 54  | BA    | 1999 | C    | N3-C2-O2    | -7.29 | 116.80                 | 121.90              |
| 54  | BA    | 2590 | A    | C5-C6-N1    | 7.29  | 121.34                 | 117.70              |
| 5   | AF    | 79   | ARG  | NE-CZ-NH1   | 7.29  | 123.94                 | 120.30              |
| 21  | AA    | 848  | C    | N3-C2-O2    | -7.29 | 116.80                 | 121.90              |
| 54  | BA    | 1336 | A    | N1-C6-N6    | -7.29 | 114.23                 | 118.60              |
| 21  | AA    | 1520 | C    | N3-C2-O2    | -7.29 | 116.80                 | 121.90              |
| 54  | BA    | 896  | A    | O4'-C1'-N9  | 7.29  | 114.03                 | 108.20              |
| 54  | BA    | 13   | A    | N1-C6-N6    | -7.29 | 114.23                 | 118.60              |
| 54  | BA    | 508  | A    | C4-C5-C6    | -7.29 | 113.36                 | 117.00              |
| 54  | BA    | 973  | A    | C5-C6-N1    | 7.29  | 121.34                 | 117.70              |
| 54  | BA    | 2635 | A    | C4-C5-C6    | -7.29 | 113.36                 | 117.00              |
| 54  | BA    | 2660 | A    | O4'-C1'-N9  | 7.29  | 114.03                 | 108.20              |
| 54  | BA    | 2755 | C    | N3-C2-O2    | -7.29 | 116.80                 | 121.90              |
| 21  | AA    | 262  | A    | C5-C6-N1    | 7.28  | 121.34                 | 117.70              |
| 21  | AA    | 370  | C    | N3-C2-O2    | -7.28 | 116.80                 | 121.90              |
| 22  | A1    | 69   | A    | N1-C6-N6    | -7.28 | 114.23                 | 118.60              |
| 54  | BA    | 1103 | A    | C4-C5-C6    | -7.28 | 113.36                 | 117.00              |
| 54  | BA    | 1606 | C    | N1-C2-O2    | 7.28  | 123.27                 | 118.90              |
| 21  | AA    | 197  | A    | N1-C6-N6    | -7.28 | 114.23                 | 118.60              |
| 54  | BA    | 2287 | A    | C4-C5-C6    | -7.28 | 113.36                 | 117.00              |
| 24  | A3    | 39   | A    | C5-C6-N1    | 7.28  | 121.34                 | 117.70              |
| 54  | BA    | 1769 | U    | C4'-C3'-C2' | -7.28 | 95.32                  | 102.60              |
| 21  | AA    | 853  | C    | N3-C2-O2    | -7.28 | 116.81                 | 121.90              |
| 21  | AA    | 1245 | C    | N3-C2-O2    | -7.28 | 116.80                 | 121.90              |
| 21  | AA    | 1318 | A    | C5-C6-N1    | 7.28  | 121.34                 | 117.70              |
| 54  | BA    | 1221 | C    | N3-C2-O2    | -7.28 | 116.80                 | 121.90              |
| 54  | BA    | 2459 | A    | C5-C6-N1    | 7.28  | 121.34                 | 117.70              |
| 43  | BU    | 21   | ARG  | NE-CZ-NH1   | 7.28  | 123.94                 | 120.30              |
| 54  | BA    | 1459 | G    | O4'-C1'-N9  | 7.28  | 114.02                 | 108.20              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 54  | BA    | 19   | A    | C5-C6-N1   | 7.28  | 121.34      | 117.70   |
| 54  | BA    | 1952 | A    | C4-C5-C6   | -7.28 | 113.36      | 117.00   |
| 21  | AA    | 1469 | C    | N3-C2-O2   | -7.27 | 116.81      | 121.90   |
| 21  | AA    | 1226 | C    | N3-C2-O2   | -7.27 | 116.81      | 121.90   |
| 54  | BA    | 116  | C    | N3-C2-O2   | -7.27 | 116.81      | 121.90   |
| 54  | BA    | 920  | A    | C4-C5-C6   | -7.27 | 113.36      | 117.00   |
| 21  | AA    | 907  | A    | C4-C5-C6   | -7.27 | 113.36      | 117.00   |
| 54  | BA    | 753  | A    | C4-C5-C6   | -7.27 | 113.36      | 117.00   |
| 54  | BA    | 1986 | C    | N3-C2-O2   | -7.27 | 116.81      | 121.90   |
| 54  | BA    | 2452 | C    | N1-C2-O2   | 7.27  | 123.26      | 118.90   |
| 21  | AA    | 1225 | A    | C5-C6-N1   | 7.27  | 121.33      | 117.70   |
| 34  | BL    | 33   | ARG  | NE-CZ-NH1  | 7.27  | 123.93      | 120.30   |
| 54  | BA    | 783  | A    | C5-C6-N1   | 7.27  | 121.33      | 117.70   |
| 21  | AA    | 1267 | C    | N3-C2-O2   | -7.26 | 116.81      | 121.90   |
| 54  | BA    | 1641 | A    | C5-C6-N1   | 7.26  | 121.33      | 117.70   |
| 56  | B5    | 134  | ARG  | NE-CZ-NH1  | 7.26  | 123.93      | 120.30   |
| 54  | BA    | 192  | C    | N1-C2-O2   | 7.26  | 123.25      | 118.90   |
| 54  | BA    | 1070 | A    | C4-C5-C6   | -7.26 | 113.37      | 117.00   |
| 54  | BA    | 71   | A    | C4-C5-C6   | -7.26 | 113.37      | 117.00   |
| 21  | AA    | 1408 | A    | C4-C5-C6   | -7.26 | 113.37      | 117.00   |
| 54  | BA    | 480  | A    | C5-C6-N1   | 7.26  | 121.33      | 117.70   |
| 22  | A1    | 56   | C    | N3-C2-O2   | -7.25 | 116.82      | 121.90   |
| 54  | BA    | 2760 | C    | N3-C2-O2   | -7.25 | 116.82      | 121.90   |
| 11  | AL    | 85   | ARG  | NE-CZ-NH1  | 7.25  | 123.93      | 120.30   |
| 21  | AA    | 1319 | A    | C5-C6-N1   | 7.25  | 121.33      | 117.70   |
| 54  | BA    | 1746 | A    | C5-C6-N1   | 7.25  | 121.33      | 117.70   |
| 54  | BA    | 1796 | U    | O4'-C1'-N1 | 7.25  | 114.00      | 108.20   |
| 54  | BA    | 1900 | A    | C4-C5-C6   | -7.25 | 113.37      | 117.00   |
| 25  | BC    | 213  | ARG  | NE-CZ-NH1  | 7.25  | 123.92      | 120.30   |
| 54  | BA    | 1134 | A    | C5-C6-N1   | 7.25  | 121.33      | 117.70   |
| 21  | AA    | 1398 | A    | C4-C5-C6   | -7.25 | 113.38      | 117.00   |
| 54  | BA    | 108  | G    | N1-C6-O6   | -7.25 | 115.55      | 119.90   |
| 54  | BA    | 478  | A    | C5-C6-N1   | 7.25  | 121.32      | 117.70   |
| 54  | BA    | 722  | A    | C4-C5-C6   | -7.25 | 113.38      | 117.00   |
| 54  | BA    | 2050 | C    | N3-C2-O2   | -7.25 | 116.83      | 121.90   |
| 21  | AA    | 1254 | A    | C5-C6-N1   | 7.25  | 121.32      | 117.70   |
| 24  | A3    | 60   | A    | C5-C6-N1   | 7.25  | 121.32      | 117.70   |
| 54  | BA    | 1879 | C    | N3-C2-O2   | -7.25 | 116.83      | 121.90   |
| 21  | AA    | 1031 | C    | N1-C2-O2   | 7.24  | 123.25      | 118.90   |
| 27  | BE    | 49   | ARG  | NE-CZ-NH2  | -7.24 | 116.68      | 120.30   |
| 39  | BQ    | 50   | ARG  | NE-CZ-NH2  | 7.24  | 123.92      | 120.30   |
| 54  | BA    | 2794 | C    | N3-C2-O2   | -7.24 | 116.83      | 121.90   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 21  | AA    | 983  | A    | C5-C6-N1   | 7.24  | 121.32      | 117.70   |
| 21  | AA    | 1101 | A    | C5-C6-N1   | 7.24  | 121.32      | 117.70   |
| 54  | BA    | 742  | A    | C4-C5-C6   | -7.24 | 113.38      | 117.00   |
| 54  | BA    | 2310 | C    | N3-C2-O2   | -7.24 | 116.83      | 121.90   |
| 54  | BA    | 2266 | A    | C5-C6-N1   | 7.24  | 121.32      | 117.70   |
| 54  | BA    | 2708 | G    | O4'-C1'-N9 | 7.24  | 113.99      | 108.20   |
| 42  | BT    | 76   | ARG  | NE-CZ-NH1  | 7.24  | 123.92      | 120.30   |
| 54  | BA    | 340  | A    | N1-C6-N6   | -7.24 | 114.26      | 118.60   |
| 54  | BA    | 1142 | A    | C4-C5-C6   | -7.24 | 113.38      | 117.00   |
| 54  | BA    | 1561 | C    | N3-C2-O2   | -7.23 | 116.84      | 121.90   |
| 21  | AA    | 298  | A    | C5-C6-N1   | 7.23  | 121.32      | 117.70   |
| 21  | AA    | 478  | A    | C5-C6-N1   | 7.23  | 121.32      | 117.70   |
| 21  | AA    | 583  | A    | N1-C6-N6   | -7.23 | 114.26      | 118.60   |
| 36  | BN    | 118  | ARG  | NE-CZ-NH1  | 7.23  | 123.92      | 120.30   |
| 54  | BA    | 1496 | A    | N1-C6-N6   | -7.23 | 114.26      | 118.60   |
| 54  | BA    | 1650 | A    | C5-C6-N1   | 7.23  | 121.32      | 117.70   |
| 21  | AA    | 1413 | A    | C5-C6-N1   | 7.23  | 121.31      | 117.70   |
| 54  | BA    | 1419 | A    | C5-C6-N1   | 7.23  | 121.31      | 117.70   |
| 54  | BA    | 1757 | A    | C5-C6-N1   | 7.23  | 121.32      | 117.70   |
| 54  | BA    | 1789 | A    | C5-C6-N1   | 7.23  | 121.31      | 117.70   |
| 20  | AU    | 20   | ARG  | NE-CZ-NH1  | 7.23  | 123.91      | 120.30   |
| 21  | AA    | 583  | A    | C5-C6-N1   | 7.23  | 121.31      | 117.70   |
| 54  | BA    | 475  | C    | N3-C2-O2   | -7.23 | 116.84      | 121.90   |
| 54  | BA    | 2880 | C    | N3-C2-O2   | -7.23 | 116.84      | 121.90   |
| 6   | AG    | 110  | ARG  | NE-CZ-NH1  | 7.23  | 123.91      | 120.30   |
| 21  | AA    | 28   | A    | N1-C6-N6   | -7.23 | 114.27      | 118.60   |
| 35  | BM    | 50   | ARG  | NE-CZ-NH1  | 7.23  | 123.91      | 120.30   |
| 54  | BA    | 590  | A    | C5-C6-N1   | 7.22  | 121.31      | 117.70   |
| 54  | BA    | 915  | C    | N3-C2-O2   | -7.22 | 116.84      | 121.90   |
| 54  | BA    | 990  | A    | C5-C6-N1   | 7.22  | 121.31      | 117.70   |
| 54  | BA    | 2089 | C    | N3-C2-O2   | -7.22 | 116.84      | 121.90   |
| 54  | BA    | 1230 | A    | C4-C5-C6   | -7.22 | 113.39      | 117.00   |
| 54  | BA    | 52   | A    | C5-C6-N1   | 7.22  | 121.31      | 117.70   |
| 54  | BA    | 581  | C    | O4'-C1'-N1 | 7.22  | 113.97      | 108.20   |
| 54  | BA    | 2283 | C    | N3-C2-O2   | -7.22 | 116.85      | 121.90   |
| 54  | BA    | 849  | A    | N1-C6-N6   | -7.22 | 114.27      | 118.60   |
| 54  | BA    | 2264 | C    | N3-C2-O2   | -7.22 | 116.85      | 121.90   |
| 21  | AA    | 435  | A    | N1-C6-N6   | -7.21 | 114.27      | 118.60   |
| 29  | BG    | 169  | ARG  | NE-CZ-NH1  | 7.21  | 123.91      | 120.30   |
| 54  | BA    | 1260 | A    | C5-C6-N1   | 7.21  | 121.31      | 117.70   |
| 54  | BA    | 2851 | A    | C4-C5-C6   | -7.21 | 113.39      | 117.00   |
| 21  | AA    | 263  | A    | N1-C6-N6   | -7.21 | 114.27      | 118.60   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 21  | AA    | 1357 | A    | C5-C6-N1   | 7.21  | 121.31      | 117.70   |
| 54  | BA    | 184  | C    | N3-C2-O2   | -7.21 | 116.85      | 121.90   |
| 21  | AA    | 767  | A    | C5-C6-N1   | 7.21  | 121.31      | 117.70   |
| 22  | A1    | 14   | A    | N1-C6-N6   | -7.21 | 114.27      | 118.60   |
| 22  | A1    | 16   | C    | N3-C2-O2   | -7.21 | 116.85      | 121.90   |
| 51  | B2    | 3    | ARG  | NE-CZ-NH2  | 7.21  | 123.91      | 120.30   |
| 21  | AA    | 946  | A    | C5-C6-N1   | 7.21  | 121.31      | 117.70   |
| 54  | BA    | 1947 | C    | N3-C2-O2   | -7.21 | 116.85      | 121.90   |
| 21  | AA    | 716  | A    | C4-C5-C6   | -7.21 | 113.39      | 117.00   |
| 54  | BA    | 391  | A    | C5-C6-N1   | 7.21  | 121.30      | 117.70   |
| 54  | BA    | 1773 | A    | C5-C6-N1   | 7.21  | 121.31      | 117.70   |
| 54  | BA    | 2287 | A    | N1-C6-N6   | -7.21 | 114.28      | 118.60   |
| 54  | BA    | 2717 | C    | N3-C4-C5   | 7.21  | 124.78      | 121.90   |
| 54  | BA    | 1238 | G    | C5-C6-N1   | 7.21  | 115.10      | 111.50   |
| 54  | BA    | 1626 | A    | C5-C6-N1   | 7.21  | 121.30      | 117.70   |
| 54  | BA    | 1732 | C    | N1-C2-O2   | 7.21  | 123.22      | 118.90   |
| 21  | AA    | 1289 | A    | C5-C6-N1   | 7.21  | 121.30      | 117.70   |
| 21  | AA    | 640  | A    | C4-C5-C6   | -7.20 | 113.40      | 117.00   |
| 45  | BW    | 76   | ARG  | NE-CZ-NH2  | -7.20 | 116.70      | 120.30   |
| 54  | BA    | 661  | A    | C5-C6-N1   | 7.20  | 121.30      | 117.70   |
| 54  | BA    | 2103 | C    | N3-C2-O2   | -7.20 | 116.86      | 121.90   |
| 54  | BA    | 2544 | G    | C8-N9-C4   | -7.20 | 103.52      | 106.40   |
| 55  | BB    | 66   | A    | C4-C5-C6   | -7.20 | 113.40      | 117.00   |
| 54  | BA    | 161  | A    | C4-C5-C6   | -7.20 | 113.40      | 117.00   |
| 2   | AC    | 71   | ARG  | NE-CZ-NH1  | 7.20  | 123.90      | 120.30   |
| 21  | AA    | 696  | A    | C5-C6-N1   | 7.20  | 121.30      | 117.70   |
| 54  | BA    | 2071 | A    | N1-C6-N6   | -7.20 | 114.28      | 118.60   |
| 37  | BO    | 7    | ARG  | NE-CZ-NH1  | 7.19  | 123.90      | 120.30   |
| 21  | AA    | 913  | A    | C4-C5-C6   | -7.19 | 113.40      | 117.00   |
| 54  | BA    | 192  | C    | N3-C2-O2   | -7.19 | 116.87      | 121.90   |
| 54  | BA    | 1829 | A    | C5-C6-N1   | 7.19  | 121.30      | 117.70   |
| 9   | AJ    | 31   | ARG  | NE-CZ-NH1  | 7.19  | 123.90      | 120.30   |
| 21  | AA    | 1201 | A    | N1-C6-N6   | -7.19 | 114.29      | 118.60   |
| 54  | BA    | 503  | A    | N1-C6-N6   | -7.19 | 114.28      | 118.60   |
| 54  | BA    | 1653 | G    | O4'-C1'-N9 | 7.19  | 113.95      | 108.20   |
| 54  | BA    | 2134 | A    | C5-C6-N1   | 7.19  | 121.30      | 117.70   |
| 6   | AG    | 78   | ARG  | NE-CZ-NH1  | 7.19  | 123.89      | 120.30   |
| 21  | AA    | 1394 | A    | C5-C6-N1   | 7.19  | 121.29      | 117.70   |
| 21  | AA    | 238  | A    | C5-C6-N1   | 7.19  | 121.29      | 117.70   |
| 21  | AA    | 547  | A    | C5-C6-N1   | 7.19  | 121.29      | 117.70   |
| 54  | BA    | 251  | A    | C5-C6-N1   | 7.19  | 121.29      | 117.70   |
| 54  | BA    | 1096 | A    | N1-C6-N6   | -7.19 | 114.29      | 118.60   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 21  | AA    | 422  | C    | N3-C2-O2   | -7.18 | 116.87      | 121.90   |
| 54  | BA    | 633  | A    | C5-C6-N1   | 7.18  | 121.29      | 117.70   |
| 54  | BA    | 782  | A    | N1-C6-N6   | -7.18 | 114.29      | 118.60   |
| 54  | BA    | 933  | A    | N1-C6-N6   | -7.18 | 114.29      | 118.60   |
| 54  | BA    | 2855 | C    | N3-C2-O2   | -7.18 | 116.87      | 121.90   |
| 54  | BA    | 2510 | C    | C6-N1-C2   | -7.18 | 117.43      | 120.30   |
| 54  | BA    | 445  | C    | N3-C2-O2   | -7.18 | 116.87      | 121.90   |
| 54  | BA    | 1933 | G    | O4'-C1'-N9 | 7.18  | 113.94      | 108.20   |
| 21  | AA    | 84   | U    | N3-C2-O2   | -7.18 | 117.18      | 122.20   |
| 24  | A3    | 45   | A    | C4-C5-C6   | -7.18 | 113.41      | 117.00   |
| 54  | BA    | 99   | U    | O4'-C1'-N1 | 7.18  | 113.94      | 108.20   |
| 54  | BA    | 324  | A    | N1-C6-N6   | -7.18 | 114.29      | 118.60   |
| 54  | BA    | 514  | A    | N1-C6-N6   | -7.18 | 114.29      | 118.60   |
| 54  | BA    | 1829 | A    | C4-C5-C6   | -7.18 | 113.41      | 117.00   |
| 54  | BA    | 1782 | U    | O4'-C1'-N1 | 7.17  | 113.94      | 108.20   |
| 21  | AA    | 101  | A    | C5-C6-N1   | 7.17  | 121.29      | 117.70   |
| 21  | AA    | 1306 | A    | C5-C6-N1   | 7.17  | 121.29      | 117.70   |
| 54  | BA    | 244  | A    | C5-C6-N1   | 7.17  | 121.29      | 117.70   |
| 54  | BA    | 603  | A    | C4-C5-C6   | -7.17 | 113.42      | 117.00   |
| 54  | BA    | 1676 | A    | C5-C6-N1   | 7.17  | 121.29      | 117.70   |
| 5   | AF    | 24   | ARG  | NE-CZ-NH2  | -7.17 | 116.72      | 120.30   |
| 13  | AN    | 69   | ARG  | NH1-CZ-NH2 | -7.17 | 111.52      | 119.40   |
| 21  | AA    | 642  | A    | C5-C6-N1   | 7.17  | 121.28      | 117.70   |
| 21  | AA    | 1397 | C    | N3-C2-O2   | -7.17 | 116.88      | 121.90   |
| 54  | BA    | 1392 | A    | C5-C6-N1   | 7.17  | 121.28      | 117.70   |
| 54  | BA    | 164  | C    | N3-C2-O2   | -7.17 | 116.88      | 121.90   |
| 21  | AA    | 612  | C    | N3-C2-O2   | -7.17 | 116.88      | 121.90   |
| 39  | BQ    | 57   | ARG  | NE-CZ-NH1  | 7.16  | 123.88      | 120.30   |
| 54  | BA    | 504  | A    | C5-C6-N1   | 7.16  | 121.28      | 117.70   |
| 54  | BA    | 677  | A    | C4-C5-C6   | -7.16 | 113.42      | 117.00   |
| 21  | AA    | 403  | C    | N3-C2-O2   | -7.16 | 116.89      | 121.90   |
| 54  | BA    | 104  | A    | C4-C5-C6   | -7.16 | 113.42      | 117.00   |
| 54  | BA    | 2145 | C    | N3-C2-O2   | -7.16 | 116.89      | 121.90   |
| 21  | AA    | 78   | A    | C5-C6-N1   | 7.16  | 121.28      | 117.70   |
| 21  | AA    | 1430 | A    | C4-C5-C6   | -7.16 | 113.42      | 117.00   |
| 29  | BG    | 54   | ARG  | NE-CZ-NH1  | 7.16  | 123.88      | 120.30   |
| 54  | BA    | 1266 | G    | O4'-C1'-N9 | 7.16  | 113.93      | 108.20   |
| 21  | AA    | 34   | C    | N3-C2-O2   | -7.16 | 116.89      | 121.90   |
| 21  | AA    | 412  | A    | C5-C6-N1   | 7.16  | 121.28      | 117.70   |
| 21  | AA    | 706  | A    | C4-C5-C6   | -7.16 | 113.42      | 117.00   |
| 54  | BA    | 1433 | A    | C5-C6-N1   | 7.16  | 121.28      | 117.70   |
| 54  | BA    | 2392 | A    | C5-C6-N1   | 7.16  | 121.28      | 117.70   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|------------|-------|------------------------|---------------------|
| 21  | AA    | 969  | A    | N1-C6-N6   | -7.16 | 114.31                 | 118.60              |
| 21  | AA    | 496  | A    | N1-C6-N6   | -7.16 | 114.31                 | 118.60              |
| 21  | AA    | 937  | A    | C4-C5-C6   | -7.16 | 113.42                 | 117.00              |
| 24  | A3    | 60   | A    | C4-C5-C6   | -7.16 | 113.42                 | 117.00              |
| 54  | BA    | 404  | A    | N1-C6-N6   | -7.16 | 114.31                 | 118.60              |
| 54  | BA    | 1558 | C    | N1-C2-O2   | 7.16  | 123.19                 | 118.90              |
| 54  | BA    | 2009 | A    | C5-C6-N1   | 7.16  | 121.28                 | 117.70              |
| 21  | AA    | 502  | A    | C5-C6-N1   | 7.15  | 121.28                 | 117.70              |
| 21  | AA    | 312  | C    | N3-C2-O2   | -7.15 | 116.89                 | 121.90              |
| 21  | AA    | 393  | A    | N1-C6-N6   | -7.15 | 114.31                 | 118.60              |
| 21  | AA    | 687  | A    | C5-C6-N1   | 7.15  | 121.28                 | 117.70              |
| 21  | AA    | 1139 | G    | N3-C2-N2   | -7.15 | 114.89                 | 119.90              |
| 34  | BL    | 2    | ARG  | NE-CZ-NH2  | -7.15 | 116.72                 | 120.30              |
| 54  | BA    | 1039 | A    | C5-C6-N1   | 7.15  | 121.28                 | 117.70              |
| 54  | BA    | 1086 | A    | N1-C6-N6   | -7.15 | 114.31                 | 118.60              |
| 54  | BA    | 2033 | A    | N1-C6-N6   | -7.15 | 114.31                 | 118.60              |
| 13  | AN    | 61   | ARG  | NE-CZ-NH1  | 7.15  | 123.88                 | 120.30              |
| 21  | AA    | 996  | A    | N1-C6-N6   | -7.15 | 114.31                 | 118.60              |
| 54  | BA    | 191  | A    | C4-C5-C6   | -7.15 | 113.42                 | 117.00              |
| 54  | BA    | 371  | A    | C5-C6-N1   | 7.15  | 121.28                 | 117.70              |
| 54  | BA    | 2579 | C    | C6-N1-C2   | -7.15 | 117.44                 | 120.30              |
| 54  | BA    | 788  | A    | C5-C6-N1   | 7.15  | 121.28                 | 117.70              |
| 21  | AA    | 1179 | A    | C4-C5-C6   | -7.15 | 113.43                 | 117.00              |
| 39  | BQ    | 29   | ARG  | NE-CZ-NH1  | 7.15  | 123.87                 | 120.30              |
| 54  | BA    | 2658 | C    | N3-C2-O2   | -7.15 | 116.90                 | 121.90              |
| 21  | AA    | 176  | C    | N3-C4-C5   | 7.15  | 124.76                 | 121.90              |
| 21  | AA    | 635  | A    | C4-C5-C6   | -7.15 | 113.43                 | 117.00              |
| 54  | BA    | 1043 | C    | N3-C2-O2   | -7.15 | 116.90                 | 121.90              |
| 12  | AM    | 91   | ARG  | NE-CZ-NH1  | 7.14  | 123.87                 | 120.30              |
| 54  | BA    | 1354 | A    | N1-C6-N6   | -7.14 | 114.31                 | 118.60              |
| 21  | AA    | 460  | A    | C4-C5-C6   | -7.14 | 113.43                 | 117.00              |
| 39  | BQ    | 54   | ARG  | NE-CZ-NH1  | 7.14  | 123.87                 | 120.30              |
| 21  | AA    | 49   | U    | O4'-C1'-N1 | 7.14  | 113.91                 | 108.20              |
| 54  | BA    | 1689 | A    | C5-C6-N1   | 7.14  | 121.27                 | 117.70              |
| 54  | BA    | 2716 | C    | N3-C2-O2   | -7.14 | 116.90                 | 121.90              |
| 21  | AA    | 246  | A    | C4-C5-C6   | -7.14 | 113.43                 | 117.00              |
| 54  | BA    | 753  | A    | C5-C6-N1   | 7.14  | 121.27                 | 117.70              |
| 54  | BA    | 2322 | A    | C5-C6-N1   | 7.14  | 121.27                 | 117.70              |
| 54  | BA    | 2572 | A    | N1-C6-N6   | -7.14 | 114.32                 | 118.60              |
| 54  | BA    | 1754 | A    | C4-C5-C6   | -7.13 | 113.43                 | 117.00              |
| 54  | BA    | 1894 | C    | N3-C2-O2   | -7.13 | 116.91                 | 121.90              |
| 54  | BA    | 2430 | A    | C5-C6-N1   | 7.13  | 121.27                 | 117.70              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|------------|-------|------------------------|---------------------|
| 31  | BI    | 64   | ARG  | NE-CZ-NH1  | 7.13  | 123.87                 | 120.30              |
| 54  | BA    | 1276 | A    | C5-C6-N1   | 7.13  | 121.27                 | 117.70              |
| 54  | BA    | 2278 | A    | N1-C6-N6   | -7.13 | 114.32                 | 118.60              |
| 54  | BA    | 223  | A    | C4-C5-C6   | -7.13 | 113.43                 | 117.00              |
| 54  | BA    | 2124 | G    | N1-C6-O6   | -7.13 | 115.62                 | 119.90              |
| 54  | BA    | 2875 | C    | O4'-C1'-N1 | 7.13  | 113.91                 | 108.20              |
| 21  | AA    | 1492 | A    | N1-C6-N6   | -7.13 | 114.32                 | 118.60              |
| 54  | BA    | 2542 | A    | C5-C6-N1   | 7.13  | 121.27                 | 117.70              |
| 21  | AA    | 1408 | A    | C5-C6-N1   | 7.13  | 121.27                 | 117.70              |
| 54  | BA    | 1705 | A    | C4-C5-C6   | -7.13 | 113.44                 | 117.00              |
| 54  | BA    | 2795 | C    | N3-C2-O2   | -7.13 | 116.91                 | 121.90              |
| 54  | BA    | 497  | A    | C4-C5-C6   | -7.13 | 113.44                 | 117.00              |
| 54  | BA    | 1382 | G    | O4'-C1'-N9 | 7.13  | 113.90                 | 108.20              |
| 54  | BA    | 2327 | A    | C4-C5-C6   | -7.13 | 113.44                 | 117.00              |
| 21  | AA    | 1509 | C    | N1-C2-O2   | 7.12  | 123.17                 | 118.90              |
| 38  | BP    | 92   | ARG  | NE-CZ-NH2  | -7.12 | 116.74                 | 120.30              |
| 54  | BA    | 229  | C    | N3-C2-O2   | -7.12 | 116.91                 | 121.90              |
| 21  | AA    | 483  | C    | N1-C2-O2   | 7.12  | 123.17                 | 118.90              |
| 21  | AA    | 1044 | A    | C5-C6-N1   | 7.12  | 121.26                 | 117.70              |
| 21  | AA    | 1195 | C    | N3-C2-O2   | -7.12 | 116.91                 | 121.90              |
| 24  | A3    | 66   | C    | N3-C2-O2   | -7.12 | 116.91                 | 121.90              |
| 54  | BA    | 590  | A    | N1-C6-N6   | -7.12 | 114.33                 | 118.60              |
| 54  | BA    | 1644 | C    | O4'-C1'-N1 | 7.12  | 113.90                 | 108.20              |
| 54  | BA    | 2518 | A    | N1-C6-N6   | -7.12 | 114.33                 | 118.60              |
| 21  | AA    | 336  | A    | C4-C5-C6   | -7.12 | 113.44                 | 117.00              |
| 21  | AA    | 1502 | A    | C5-C6-N1   | 7.12  | 121.26                 | 117.70              |
| 54  | BA    | 975  | A    | C4-C5-C6   | -7.12 | 113.44                 | 117.00              |
| 54  | BA    | 1240 | U    | O4'-C1'-N1 | 7.12  | 113.90                 | 108.20              |
| 54  | BA    | 1998 | A    | C5-C6-N1   | 7.12  | 121.26                 | 117.70              |
| 21  | AA    | 600  | A    | C4-C5-C6   | -7.12 | 113.44                 | 117.00              |
| 10  | AK    | 97   | ARG  | NE-CZ-NH1  | 7.12  | 123.86                 | 120.30              |
| 21  | AA    | 132  | C    | N3-C2-O2   | -7.12 | 116.92                 | 121.90              |
| 21  | AA    | 309  | A    | C4-C5-C6   | -7.12 | 113.44                 | 117.00              |
| 33  | BK    | 98   | ARG  | NE-CZ-NH1  | 7.12  | 123.86                 | 120.30              |
| 54  | BA    | 156  | A    | C5-C6-N1   | 7.12  | 121.26                 | 117.70              |
| 54  | BA    | 1014 | A    | C5-C6-N1   | 7.12  | 121.26                 | 117.70              |
| 24  | A3    | 22   | A    | C5-C6-N1   | 7.12  | 121.26                 | 117.70              |
| 54  | BA    | 2711 | A    | C5-C6-N1   | 7.12  | 121.26                 | 117.70              |
| 21  | AA    | 210  | C    | N1-C2-O2   | 7.11  | 123.17                 | 118.90              |
| 54  | BA    | 164  | C    | O4'-C1'-N1 | 7.11  | 113.89                 | 108.20              |
| 54  | BA    | 1290 | C    | N3-C2-O2   | -7.11 | 116.92                 | 121.90              |
| 54  | BA    | 1572 | A    | C4-C5-C6   | -7.11 | 113.44                 | 117.00              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 21  | AA    | 189  | A    | C5-C6-N1    | 7.11  | 121.26      | 117.70   |
| 54  | BA    | 209  | C    | N3-C2-O2    | -7.11 | 116.92      | 121.90   |
| 21  | AA    | 85   | U    | N3-C2-O2    | -7.11 | 117.22      | 122.20   |
| 54  | BA    | 398  | C    | N3-C2-O2    | -7.11 | 116.92      | 121.90   |
| 21  | AA    | 335  | C    | N3-C2-O2    | -7.11 | 116.92      | 121.90   |
| 21  | AA    | 532  | A    | C1'-O4'-C4' | -7.11 | 104.22      | 109.90   |
| 21  | AA    | 1479 | C    | N1-C2-O2    | 7.11  | 123.17      | 118.90   |
| 54  | BA    | 699  | A    | C5-C6-N1    | 7.11  | 121.25      | 117.70   |
| 54  | BA    | 1689 | A    | C4-C5-C6    | -7.11 | 113.45      | 117.00   |
| 4   | AE    | 92   | ARG  | NE-CZ-NH1   | 7.11  | 123.85      | 120.30   |
| 21  | AA    | 521  | G    | N1-C6-O6    | -7.11 | 115.64      | 119.90   |
| 54  | BA    | 909  | A    | C5-C6-N1    | 7.11  | 121.25      | 117.70   |
| 54  | BA    | 1853 | A    | C4-C5-C6    | -7.11 | 113.45      | 117.00   |
| 54  | BA    | 1918 | A    | O4'-C1'-N9  | 7.11  | 113.89      | 108.20   |
| 54  | BA    | 2758 | A    | C4-C5-C6    | -7.11 | 113.45      | 117.00   |
| 21  | AA    | 946  | A    | C4-C5-C6    | -7.10 | 113.45      | 117.00   |
| 54  | BA    | 1730 | C    | N3-C2-O2    | -7.10 | 116.93      | 121.90   |
| 12  | AM    | 112  | ARG  | NE-CZ-NH1   | 7.10  | 123.85      | 120.30   |
| 21  | AA    | 16   | A    | N1-C6-N6    | -7.10 | 114.34      | 118.60   |
| 21  | AA    | 1101 | A    | P-O3'-C3'   | 7.10  | 128.22      | 119.70   |
| 54  | BA    | 331  | C    | N3-C2-O2    | -7.10 | 116.93      | 121.90   |
| 21  | AA    | 759  | A    | N1-C6-N6    | -7.10 | 114.34      | 118.60   |
| 21  | AA    | 694  | A    | C4-C5-C6    | -7.10 | 113.45      | 117.00   |
| 37  | BO    | 13   | ARG  | NE-CZ-NH1   | 7.10  | 123.85      | 120.30   |
| 54  | BA    | 1618 | A    | C5-C6-N1    | 7.10  | 121.25      | 117.70   |
| 54  | BA    | 2743 | U    | O4'-C1'-N1  | 7.10  | 113.88      | 108.20   |
| 21  | AA    | 1318 | A    | C4-C5-C6    | -7.10 | 113.45      | 117.00   |
| 22  | A1    | 19   | G    | O4'-C1'-N9  | 7.10  | 113.88      | 108.20   |
| 54  | BA    | 1268 | A    | N1-C6-N6    | -7.10 | 114.34      | 118.60   |
| 54  | BA    | 2870 | C    | N3-C2-O2    | -7.10 | 116.93      | 121.90   |
| 21  | AA    | 718  | A    | C5-C6-N1    | 7.10  | 121.25      | 117.70   |
| 21  | AA    | 270  | A    | N1-C6-N6    | -7.09 | 114.34      | 118.60   |
| 21  | AA    | 655  | A    | C5-C6-N1    | 7.09  | 121.25      | 117.70   |
| 21  | AA    | 1054 | C    | N3-C2-O2    | -7.09 | 116.93      | 121.90   |
| 24  | A3    | 59   | A    | C4-C5-C6    | -7.09 | 113.45      | 117.00   |
| 54  | BA    | 1226 | A    | N1-C6-N6    | -7.09 | 114.34      | 118.60   |
| 54  | BA    | 2321 | U    | O4'-C1'-N1  | 7.09  | 113.88      | 108.20   |
| 21  | AA    | 81   | A    | N1-C6-N6    | -7.09 | 114.34      | 118.60   |
| 21  | AA    | 1000 | A    | C4-C5-C6    | -7.09 | 113.45      | 117.00   |
| 54  | BA    | 2822 | G    | N1-C6-O6    | -7.09 | 115.64      | 119.90   |
| 21  | AA    | 579  | A    | C5-C6-N1    | 7.09  | 121.25      | 117.70   |
| 54  | BA    | 905  | A    | C5-C6-N1    | 7.09  | 121.25      | 117.70   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 54  | BA    | 1974 | C    | N3-C2-O2   | -7.09 | 116.94      | 121.90   |
| 54  | BA    | 522  | A    | C5-C6-N1   | 7.09  | 121.24      | 117.70   |
| 21  | AA    | 175  | C    | N3-C2-O2   | -7.09 | 116.94      | 121.90   |
| 21  | AA    | 702  | A    | C5-C6-N1   | 7.09  | 121.24      | 117.70   |
| 22  | A1    | 38   | A    | C4-C5-C6   | -7.09 | 113.46      | 117.00   |
| 54  | BA    | 1304 | A    | C5-C6-N1   | 7.09  | 121.24      | 117.70   |
| 54  | BA    | 1544 | A    | C5-C6-N1   | 7.09  | 121.24      | 117.70   |
| 54  | BA    | 2708 | G    | N1-C6-O6   | -7.09 | 115.65      | 119.90   |
| 21  | AA    | 600  | A    | C5-C6-N1   | 7.08  | 121.24      | 117.70   |
| 21  | AA    | 1288 | A    | C4-C5-C6   | -7.08 | 113.46      | 117.00   |
| 54  | BA    | 1977 | A    | C5-C6-N1   | 7.08  | 121.24      | 117.70   |
| 54  | BA    | 2482 | A    | C5-C6-N1   | 7.08  | 121.24      | 117.70   |
| 21  | AA    | 1281 | C    | N3-C4-N4   | -7.08 | 113.04      | 118.00   |
| 21  | AA    | 470  | C    | N3-C2-O2   | -7.08 | 116.94      | 121.90   |
| 21  | AA    | 980  | C    | N3-C2-O2   | -7.08 | 116.94      | 121.90   |
| 21  | AA    | 1378 | C    | N3-C2-O2   | -7.08 | 116.94      | 121.90   |
| 21  | AA    | 1019 | A    | N1-C6-N6   | -7.08 | 114.35      | 118.60   |
| 54  | BA    | 1762 | A    | C4-C5-C6   | -7.08 | 113.46      | 117.00   |
| 21  | AA    | 411  | A    | C5-C6-N1   | 7.07  | 121.24      | 117.70   |
| 21  | AA    | 621  | A    | N1-C6-N6   | -7.07 | 114.36      | 118.60   |
| 21  | AA    | 1261 | A    | C5-C6-N1   | 7.07  | 121.24      | 117.70   |
| 54  | BA    | 378  | C    | O4'-C1'-N1 | 7.07  | 113.86      | 108.20   |
| 54  | BA    | 2150 | C    | O4'-C1'-N1 | 7.07  | 113.86      | 108.20   |
| 54  | BA    | 2826 | A    | N1-C6-N6   | -7.07 | 114.36      | 118.60   |
| 54  | BA    | 139  | U    | O4'-C1'-N1 | 7.07  | 113.86      | 108.20   |
| 54  | BA    | 1955 | U    | O4'-C1'-N1 | 7.07  | 113.86      | 108.20   |
| 21  | AA    | 831  | A    | N1-C6-N6   | -7.07 | 114.36      | 118.60   |
| 21  | AA    | 1496 | C    | N3-C2-O2   | -7.07 | 116.95      | 121.90   |
| 54  | BA    | 2427 | C    | N3-C2-O2   | -7.07 | 116.95      | 121.90   |
| 10  | AK    | 105  | ARG  | NE-CZ-NH1  | 7.07  | 123.83      | 120.30   |
| 54  | BA    | 1243 | C    | N3-C2-O2   | -7.07 | 116.95      | 121.90   |
| 54  | BA    | 1585 | C    | N3-C2-O2   | -7.07 | 116.95      | 121.90   |
| 54  | BA    | 1665 | A    | N1-C6-N6   | -7.07 | 114.36      | 118.60   |
| 21  | AA    | 66   | A    | C5-C6-N1   | 7.06  | 121.23      | 117.70   |
| 21  | AA    | 575  | G    | N1-C6-O6   | -7.06 | 115.66      | 119.90   |
| 54  | BA    | 1702 | G    | N1-C6-O6   | -7.06 | 115.66      | 119.90   |
| 54  | BA    | 1348 | C    | O4'-C1'-N1 | 7.06  | 113.85      | 108.20   |
| 54  | BA    | 28   | A    | C5-C6-N1   | 7.06  | 121.23      | 117.70   |
| 54  | BA    | 892  | A    | N1-C6-N6   | -7.06 | 114.37      | 118.60   |
| 54  | BA    | 1549 | A    | C4-C5-C6   | -7.06 | 113.47      | 117.00   |
| 54  | BA    | 1578 | U    | O4'-C1'-N1 | 7.06  | 113.85      | 108.20   |
| 54  | BA    | 1916 | A    | C4-C5-C6   | -7.06 | 113.47      | 117.00   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 54  | BA    | 1691 | C    | O4'-C1'-N1 | 7.06  | 113.84      | 108.20   |
| 54  | BA    | 2091 | C    | N3-C2-O2   | -7.06 | 116.96      | 121.90   |
| 21  | AA    | 325  | A    | C4-C5-C6   | -7.05 | 113.47      | 117.00   |
| 21  | AA    | 1239 | A    | N1-C6-N6   | -7.05 | 114.37      | 118.60   |
| 54  | BA    | 199  | A    | C5-C6-N1   | 7.05  | 121.23      | 117.70   |
| 54  | BA    | 689  | A    | N1-C6-N6   | -7.05 | 114.37      | 118.60   |
| 54  | BA    | 1553 | A    | C4-C5-C6   | -7.05 | 113.47      | 117.00   |
| 21  | AA    | 629  | A    | C5-C6-N1   | 7.05  | 121.22      | 117.70   |
| 21  | AA    | 1248 | A    | C5-C6-N1   | 7.05  | 121.22      | 117.70   |
| 54  | BA    | 274  | C    | N3-C2-O2   | -7.05 | 116.97      | 121.90   |
| 54  | BA    | 2031 | A    | C5-C6-N1   | 7.05  | 121.22      | 117.70   |
| 54  | BA    | 680  | C    | N3-C2-O2   | -7.05 | 116.97      | 121.90   |
| 25  | BC    | 269  | ARG  | NE-CZ-NH1  | 7.05  | 123.82      | 120.30   |
| 54  | BA    | 1985 | C    | O4'-C1'-N1 | 7.05  | 113.84      | 108.20   |
| 55  | BB    | 113  | C    | N3-C2-O2   | -7.05 | 116.97      | 121.90   |
| 54  | BA    | 1509 | A    | C5-C6-N1   | 7.04  | 121.22      | 117.70   |
| 21  | AA    | 7    | A    | C5-C6-N1   | 7.04  | 121.22      | 117.70   |
| 54  | BA    | 1373 | A    | N1-C6-N6   | -7.04 | 114.37      | 118.60   |
| 54  | BA    | 609  | A    | C5-C6-N1   | 7.04  | 121.22      | 117.70   |
| 54  | BA    | 1877 | A    | C5-C6-N1   | 7.04  | 121.22      | 117.70   |
| 21  | AA    | 73   | C    | N3-C2-O2   | -7.04 | 116.97      | 121.90   |
| 21  | AA    | 533  | A    | C5-C6-N1   | 7.04  | 121.22      | 117.70   |
| 54  | BA    | 2163 | A    | N1-C6-N6   | -7.04 | 114.38      | 118.60   |
| 21  | AA    | 275  | G    | C8-N9-C4   | -7.04 | 103.58      | 106.40   |
| 54  | BA    | 2676 | C    | N3-C2-O2   | -7.04 | 116.97      | 121.90   |
| 54  | BA    | 1030 | C    | N3-C2-O2   | -7.04 | 116.97      | 121.90   |
| 54  | BA    | 1815 | A    | N1-C6-N6   | -7.04 | 114.38      | 118.60   |
| 54  | BA    | 2103 | C    | N3-C4-C5   | 7.04  | 124.71      | 121.90   |
| 21  | AA    | 483  | C    | N3-C2-O2   | -7.03 | 116.98      | 121.90   |
| 21  | AA    | 1412 | C    | N3-C2-O2   | -7.03 | 116.98      | 121.90   |
| 54  | BA    | 2169 | A    | C5-C6-N1   | 7.03  | 121.22      | 117.70   |
| 54  | BA    | 2332 | C    | N1-C2-O2   | 7.03  | 123.12      | 118.90   |
| 27  | BE    | 40   | ARG  | NE-CZ-NH2  | -7.03 | 116.78      | 120.30   |
| 54  | BA    | 920  | A    | C5-C6-N1   | 7.03  | 121.22      | 117.70   |
| 12  | AM    | 70   | ARG  | NE-CZ-NH1  | 7.03  | 123.81      | 120.30   |
| 21  | AA    | 1209 | C    | N3-C2-O2   | -7.03 | 116.98      | 121.90   |
| 54  | BA    | 1895 | C    | N3-C2-O2   | -7.03 | 116.98      | 121.90   |
| 21  | AA    | 228  | A    | C4-C5-C6   | -7.03 | 113.48      | 117.00   |
| 28  | BF    | 124  | ARG  | NE-CZ-NH1  | 7.03  | 123.81      | 120.30   |
| 21  | AA    | 630  | A    | N1-C6-N6   | -7.03 | 114.38      | 118.60   |
| 54  | BA    | 270  | A    | C4-C5-C6   | -7.03 | 113.49      | 117.00   |
| 54  | BA    | 2814 | A    | C4-C5-C6   | -7.03 | 113.49      | 117.00   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | AD    | 55   | ARG  | NE-CZ-NH1   | 7.03  | 123.81      | 120.30   |
| 54  | BA    | 1027 | A    | C5-C6-N1    | 7.03  | 121.21      | 117.70   |
| 54  | BA    | 734  | A    | N1-C6-N6    | -7.02 | 114.39      | 118.60   |
| 54  | BA    | 2275 | C    | N3-C2-O2    | -7.02 | 116.98      | 121.90   |
| 21  | AA    | 264  | C    | N3-C2-O2    | -7.02 | 116.98      | 121.90   |
| 54  | BA    | 21   | A    | C5-C6-N1    | 7.02  | 121.21      | 117.70   |
| 54  | BA    | 837  | C    | N3-C2-O2    | -7.02 | 116.98      | 121.90   |
| 54  | BA    | 2827 | C    | N3-C2-O2    | -7.02 | 116.98      | 121.90   |
| 54  | BA    | 2117 | A    | O4'-C1'-N9  | 7.02  | 113.82      | 108.20   |
| 54  | BA    | 2097 | A    | C5-C6-N1    | 7.02  | 121.21      | 117.70   |
| 18  | AS    | 35   | ARG  | NE-CZ-NH1   | 7.02  | 123.81      | 120.30   |
| 54  | BA    | 1020 | A    | C4-C5-C6    | -7.02 | 113.49      | 117.00   |
| 54  | BA    | 1194 | A    | C5-C6-N1    | 7.02  | 121.21      | 117.70   |
| 54  | BA    | 1254 | A    | N1-C6-N6    | -7.02 | 114.39      | 118.60   |
| 21  | AA    | 1246 | A    | C5-C6-N1    | 7.02  | 121.21      | 117.70   |
| 54  | BA    | 1205 | A    | N1-C6-N6    | -7.02 | 114.39      | 118.60   |
| 21  | AA    | 596  | A    | C5-C6-N1    | 7.01  | 121.21      | 117.70   |
| 21  | AA    | 249  | U    | N3-C2-O2    | -7.01 | 117.29      | 122.20   |
| 21  | AA    | 176  | C    | N3-C2-O2    | -7.01 | 116.99      | 121.90   |
| 21  | AA    | 723  | U    | N3-C2-O2    | -7.01 | 117.29      | 122.20   |
| 21  | AA    | 1489 | G    | N1-C6-O6    | -7.01 | 115.69      | 119.90   |
| 54  | BA    | 244  | A    | C4-C5-C6    | -7.01 | 113.49      | 117.00   |
| 54  | BA    | 1755 | A    | N1-C6-N6    | -7.01 | 114.39      | 118.60   |
| 54  | BA    | 2614 | A    | C4-C5-C6    | -7.01 | 113.49      | 117.00   |
| 54  | BA    | 2755 | C    | O4'-C1'-N1  | 7.01  | 113.81      | 108.20   |
| 21  | AA    | 790  | A    | C4-C5-C6    | -7.01 | 113.50      | 117.00   |
| 21  | AA    | 807  | A    | C5-C6-N1    | 7.01  | 121.20      | 117.70   |
| 46  | BX    | 17   | ARG  | NE-CZ-NH1   | 7.01  | 123.81      | 120.30   |
| 54  | BA    | 840  | C    | N3-C2-O2    | -7.01 | 116.99      | 121.90   |
| 54  | BA    | 2777 | G    | N9-C4-C5    | 7.01  | 108.20      | 105.40   |
| 21  | AA    | 1035 | A    | C5-C6-N1    | 7.01  | 121.20      | 117.70   |
| 21  | AA    | 1521 | C    | N3-C2-O2    | -7.01 | 116.99      | 121.90   |
| 54  | BA    | 1109 | C    | C3'-C2'-C1' | 7.01  | 107.11      | 101.50   |
| 54  | BA    | 1964 | G    | C3'-C2'-C1' | 7.01  | 107.11      | 101.50   |
| 21  | AA    | 676  | A    | C4-C5-C6    | -7.01 | 113.50      | 117.00   |
| 21  | AA    | 814  | A    | N1-C6-N6    | -7.01 | 114.40      | 118.60   |
| 21  | AA    | 978  | A    | C5-C6-N1    | 7.01  | 121.20      | 117.70   |
| 54  | BA    | 2003 | A    | C4-C5-C6    | -7.01 | 113.50      | 117.00   |
| 55  | BB    | 99   | A    | N1-C6-N6    | -7.01 | 114.40      | 118.60   |
| 54  | BA    | 793  | A    | C4-C5-C6    | -7.00 | 113.50      | 117.00   |
| 21  | AA    | 1179 | A    | N1-C6-N6    | -7.00 | 114.40      | 118.60   |
| 21  | AA    | 971  | G    | N1-C6-O6    | -7.00 | 115.70      | 119.90   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 54  | BA    | 1387 | A    | N1-C6-N6    | -7.00 | 114.40      | 118.60   |
| 54  | BA    | 1603 | A    | C4-C5-C6    | -7.00 | 113.50      | 117.00   |
| 54  | BA    | 19   | A    | C4-C5-C6    | -7.00 | 113.50      | 117.00   |
| 54  | BA    | 1854 | A    | C5-C6-N1    | 7.00  | 121.20      | 117.70   |
| 21  | AA    | 559  | A    | C5-C6-N1    | 7.00  | 121.20      | 117.70   |
| 54  | BA    | 1032 | A    | C5-C6-N1    | 7.00  | 121.20      | 117.70   |
| 54  | BA    | 1794 | A    | C4-C5-C6    | -7.00 | 113.50      | 117.00   |
| 21  | AA    | 702  | A    | C4-C5-C6    | -7.00 | 113.50      | 117.00   |
| 54  | BA    | 1953 | A    | C4-C5-C6    | -7.00 | 113.50      | 117.00   |
| 54  | BA    | 1537 | G    | O4'-C1'-N9  | 6.99  | 113.80      | 108.20   |
| 54  | BA    | 2682 | A    | C5-C6-N1    | 6.99  | 121.20      | 117.70   |
| 21  | AA    | 1055 | A    | N1-C6-N6    | -6.99 | 114.41      | 118.60   |
| 54  | BA    | 95   | A    | N1-C6-N6    | -6.99 | 114.41      | 118.60   |
| 54  | BA    | 613  | A    | C4-C5-C6    | -6.99 | 113.50      | 117.00   |
| 54  | BA    | 705  | A    | N1-C6-N6    | -6.99 | 114.41      | 118.60   |
| 54  | BA    | 1434 | A    | O4'-C1'-N9  | 6.99  | 113.79      | 108.20   |
| 28  | BF    | 111  | ARG  | NE-CZ-NH1   | 6.99  | 123.79      | 120.30   |
| 54  | BA    | 272  | A    | O4'-C1'-N9  | 6.99  | 113.79      | 108.20   |
| 54  | BA    | 2158 | A    | C5-C6-N1    | 6.99  | 121.19      | 117.70   |
| 21  | AA    | 325  | A    | C5-C6-N1    | 6.99  | 121.19      | 117.70   |
| 54  | BA    | 2761 | A    | O4'-C1'-N9  | 6.99  | 113.79      | 108.20   |
| 21  | AA    | 768  | A    | C5-C6-N1    | 6.98  | 121.19      | 117.70   |
| 54  | BA    | 788  | A    | C4-C5-C6    | -6.98 | 113.51      | 117.00   |
| 21  | AA    | 1130 | A    | C4-C5-C6    | -6.98 | 113.51      | 117.00   |
| 54  | BA    | 1551 | A    | C5-C6-N1    | 6.98  | 121.19      | 117.70   |
| 54  | BA    | 2385 | C    | N3-C2-O2    | -6.98 | 117.01      | 121.90   |
| 54  | BA    | 2823 | A    | C3'-C2'-C1' | 6.98  | 107.09      | 101.50   |
| 21  | AA    | 824  | G    | N9-C4-C5    | 6.98  | 108.19      | 105.40   |
| 54  | BA    | 1551 | A    | N1-C6-N6    | -6.98 | 114.41      | 118.60   |
| 54  | BA    | 2620 | C    | N3-C4-C5    | 6.98  | 124.69      | 121.90   |
| 21  | AA    | 364  | A    | C4-C5-C6    | -6.98 | 113.51      | 117.00   |
| 54  | BA    | 31   | C    | N1-C2-O2    | 6.98  | 123.09      | 118.90   |
| 54  | BA    | 1040 | A    | N1-C6-N6    | -6.98 | 114.41      | 118.60   |
| 21  | AA    | 116  | A    | N1-C6-N6    | -6.98 | 114.41      | 118.60   |
| 21  | AA    | 411  | A    | C4-C5-C6    | -6.98 | 113.51      | 117.00   |
| 54  | BA    | 845  | A    | N1-C6-N6    | -6.98 | 114.41      | 118.60   |
| 54  | BA    | 2572 | A    | C5-C6-N1    | 6.98  | 121.19      | 117.70   |
| 21  | AA    | 1061 | G    | N3-C4-C5    | -6.98 | 125.11      | 128.60   |
| 54  | BA    | 2691 | C    | N3-C2-O2    | -6.98 | 117.02      | 121.90   |
| 21  | AA    | 553  | A    | C4-C5-C6    | -6.97 | 113.51      | 117.00   |
| 54  | BA    | 948  | C    | N3-C2-O2    | -6.97 | 117.02      | 121.90   |
| 54  | BA    | 1885 | A    | C4-C5-C6    | -6.97 | 113.51      | 117.00   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|------------|-------|------------------------|---------------------|
| 54  | BA    | 2753 | A    | N1-C6-N6   | -6.97 | 114.42                 | 118.60              |
| 21  | AA    | 1004 | A    | C5-C6-N1   | 6.97  | 121.19                 | 117.70              |
| 54  | BA    | 1095 | A    | C5-C6-N1   | 6.97  | 121.19                 | 117.70              |
| 54  | BA    | 1990 | C    | O4'-C1'-N1 | 6.97  | 113.78                 | 108.20              |
| 54  | BA    | 2612 | C    | N3-C2-O2   | -6.97 | 117.02                 | 121.90              |
| 21  | AA    | 499  | A    | C5-C6-N1   | 6.97  | 121.19                 | 117.70              |
| 22  | A1    | 21   | A    | C5-C6-N1   | 6.97  | 121.19                 | 117.70              |
| 54  | BA    | 1753 | G    | N3-C4-C5   | -6.97 | 125.11                 | 128.60              |
| 54  | BA    | 2461 | A    | N1-C6-N6   | -6.97 | 114.42                 | 118.60              |
| 54  | BA    | 2705 | A    | C4-C5-C6   | -6.97 | 113.51                 | 117.00              |
| 21  | AA    | 263  | A    | C5-C6-N1   | 6.97  | 121.18                 | 117.70              |
| 21  | AA    | 1179 | A    | C5-C6-N1   | 6.97  | 121.19                 | 117.70              |
| 21  | AA    | 1217 | C    | N3-C2-O2   | -6.97 | 117.02                 | 121.90              |
| 21  | AA    | 1314 | C    | N3-C2-O2   | -6.97 | 117.02                 | 121.90              |
| 54  | BA    | 251  | A    | N1-C6-N6   | -6.97 | 114.42                 | 118.60              |
| 54  | BA    | 547  | A    | C5-C6-N1   | 6.97  | 121.19                 | 117.70              |
| 54  | BA    | 2090 | A    | C6-C5-N7   | 6.97  | 137.18                 | 132.30              |
| 54  | BA    | 2723 | C    | N1-C2-O2   | 6.97  | 123.08                 | 118.90              |
| 21  | AA    | 1147 | C    | N3-C2-O2   | -6.97 | 117.02                 | 121.90              |
| 22  | A1    | 58   | A    | C5-C6-N1   | 6.97  | 121.18                 | 117.70              |
| 54  | BA    | 61   | C    | N3-C2-O2   | -6.97 | 117.02                 | 121.90              |
| 54  | BA    | 332  | A    | C5-C6-N1   | 6.96  | 121.18                 | 117.70              |
| 54  | BA    | 641  | U    | O4'-C1'-N1 | 6.96  | 113.77                 | 108.20              |
| 54  | BA    | 1039 | A    | C4-C5-C6   | -6.96 | 113.52                 | 117.00              |
| 54  | BA    | 1800 | C    | N1-C2-O2   | 6.96  | 123.08                 | 118.90              |
| 21  | AA    | 460  | A    | C5-C6-N1   | 6.96  | 121.18                 | 117.70              |
| 21  | AA    | 1045 | C    | N3-C2-O2   | -6.96 | 117.03                 | 121.90              |
| 8   | AI    | 94   | ARG  | NE-CZ-NH1  | 6.96  | 123.78                 | 120.30              |
| 21  | AA    | 1204 | A    | C4-C5-C6   | -6.96 | 113.52                 | 117.00              |
| 54  | BA    | 1621 | U    | O4'-C1'-N1 | 6.96  | 113.77                 | 108.20              |
| 21  | AA    | 811  | C    | O4'-C1'-N1 | 6.96  | 113.77                 | 108.20              |
| 21  | AA    | 825  | A    | C5-C6-N1   | 6.96  | 121.18                 | 117.70              |
| 21  | AA    | 1151 | A    | C5-C6-N1   | 6.96  | 121.18                 | 117.70              |
| 54  | BA    | 829  | A    | C4-C5-C6   | -6.96 | 113.52                 | 117.00              |
| 54  | BA    | 1050 | A    | C4-C5-C6   | -6.96 | 113.52                 | 117.00              |
| 54  | BA    | 1310 | G    | O4'-C1'-N9 | 6.96  | 113.77                 | 108.20              |
| 54  | BA    | 2207 | C    | N3-C2-O2   | -6.96 | 117.03                 | 121.90              |
| 21  | AA    | 119  | A    | N1-C6-N6   | -6.95 | 114.43                 | 118.60              |
| 21  | AA    | 706  | A    | N1-C6-N6   | -6.95 | 114.43                 | 118.60              |
| 21  | AA    | 998  | C    | N3-C2-O2   | -6.95 | 117.03                 | 121.90              |
| 54  | BA    | 1475 | G    | C5-C6-N1   | 6.95  | 114.98                 | 111.50              |
| 55  | BB    | 34   | A    | C5-C6-N1   | 6.95  | 121.18                 | 117.70              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 54  | BA    | 337  | C    | O4'-C1'-N1  | 6.95  | 113.76      | 108.20   |
| 54  | BA    | 1558 | C    | N3-C2-O2    | -6.95 | 117.03      | 121.90   |
| 21  | AA    | 819  | A    | C4-C5-C6    | -6.95 | 113.53      | 117.00   |
| 54  | BA    | 623  | C    | N3-C2-O2    | -6.95 | 117.03      | 121.90   |
| 54  | BA    | 717  | C    | N1-C2-O2    | 6.95  | 123.07      | 118.90   |
| 54  | BA    | 2019 | A    | C5-C6-N1    | 6.95  | 121.17      | 117.70   |
| 54  | BA    | 2471 | A    | C5-C6-N1    | 6.95  | 121.17      | 117.70   |
| 21  | AA    | 564  | C    | N3-C2-O2    | -6.95 | 117.04      | 121.90   |
| 29  | BG    | 2    | ARG  | NE-CZ-NH1   | 6.95  | 123.77      | 120.30   |
| 54  | BA    | 1146 | C    | N3-C2-O2    | -6.95 | 117.04      | 121.90   |
| 54  | BA    | 1328 | A    | C4-C5-C6    | -6.95 | 113.53      | 117.00   |
| 54  | BA    | 1598 | A    | N1-C6-N6    | -6.95 | 114.43      | 118.60   |
| 54  | BA    | 2681 | C    | N3-C2-O2    | -6.94 | 117.04      | 121.90   |
| 21  | AA    | 1401 | G    | C5-C6-N1    | 6.94  | 114.97      | 111.50   |
| 54  | BA    | 587  | C    | N1-C2-O2    | 6.94  | 123.07      | 118.90   |
| 54  | BA    | 1135 | C    | N3-C2-O2    | -6.94 | 117.04      | 121.90   |
| 54  | BA    | 2841 | C    | N3-C2-O2    | -6.94 | 117.04      | 121.90   |
| 21  | AA    | 346  | G    | C5-C6-N1    | 6.94  | 114.97      | 111.50   |
| 24  | A3    | 11   | A    | N1-C6-N6    | -6.94 | 114.44      | 118.60   |
| 31  | BI    | 102  | ARG  | NE-CZ-NH1   | 6.94  | 123.77      | 120.30   |
| 54  | BA    | 2198 | A    | C4-C5-C6    | -6.94 | 113.53      | 117.00   |
| 54  | BA    | 2217 | G    | C5-C6-N1    | 6.94  | 114.97      | 111.50   |
| 32  | BJ    | 69   | ARG  | NE-CZ-NH1   | 6.94  | 123.77      | 120.30   |
| 21  | AA    | 397  | A    | C5-C6-N1    | 6.94  | 121.17      | 117.70   |
| 21  | AA    | 1157 | A    | N1-C6-N6    | -6.94 | 114.44      | 118.60   |
| 54  | BA    | 1323 | C    | N3-C2-O2    | -6.94 | 117.04      | 121.90   |
| 39  | BQ    | 32   | ARG  | NE-CZ-NH2   | 6.94  | 123.77      | 120.30   |
| 54  | BA    | 1596 | A    | C4-C5-C6    | -6.94 | 113.53      | 117.00   |
| 54  | BA    | 2515 | C    | N3-C2-O2    | -6.94 | 117.05      | 121.90   |
| 21  | AA    | 712  | A    | C4-C5-C6    | -6.93 | 113.53      | 117.00   |
| 54  | BA    | 1476 | U    | O4'-C1'-N1  | 6.93  | 113.75      | 108.20   |
| 54  | BA    | 2516 | A    | C4-C5-C6    | -6.93 | 113.53      | 117.00   |
| 5   | AF    | 45   | ARG  | NE-CZ-NH1   | 6.93  | 123.77      | 120.30   |
| 21  | AA    | 71   | A    | C5-C6-N1    | 6.93  | 121.17      | 117.70   |
| 21  | AA    | 1365 | G    | N3-C2-N2    | -6.93 | 115.05      | 119.90   |
| 54  | BA    | 2114 | A    | C4-C5-C6    | -6.93 | 113.53      | 117.00   |
| 21  | AA    | 1329 | A    | C4-C5-C6    | -6.93 | 113.53      | 117.00   |
| 54  | BA    | 21   | A    | C4-C5-C6    | -6.93 | 113.53      | 117.00   |
| 54  | BA    | 2068 | U    | C1'-O4'-C4' | -6.93 | 104.36      | 109.90   |
| 54  | BA    | 634  | C    | N3-C2-O2    | -6.93 | 117.05      | 121.90   |
| 54  | BA    | 1652 | A    | C5-C6-N1    | 6.93  | 121.16      | 117.70   |
| 54  | BA    | 2683 | C    | N3-C2-O2    | -6.93 | 117.05      | 121.90   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|------------|-------|------------------------|---------------------|
| 4   | AE    | 44   | ARG  | NE-CZ-NH1  | 6.93  | 123.76                 | 120.30              |
| 21  | AA    | 383  | A    | C4-C5-C6   | -6.93 | 113.54                 | 117.00              |
| 21  | AA    | 806  | C    | N3-C2-O2   | -6.93 | 117.05                 | 121.90              |
| 54  | BA    | 2029 | G    | C5-C6-N1   | 6.93  | 114.96                 | 111.50              |
| 54  | BA    | 2045 | C    | N3-C2-O2   | -6.93 | 117.05                 | 121.90              |
| 54  | BA    | 2758 | A    | C5-C6-N1   | 6.93  | 121.16                 | 117.70              |
| 54  | BA    | 1669 | A    | N1-C6-N6   | -6.93 | 114.44                 | 118.60              |
| 54  | BA    | 1821 | A    | C5-C6-N1   | 6.93  | 121.16                 | 117.70              |
| 54  | BA    | 2104 | C    | N3-C4-C5   | 6.93  | 124.67                 | 121.90              |
| 55  | BB    | 53   | A    | N1-C6-N6   | -6.93 | 114.44                 | 118.60              |
| 54  | BA    | 233  | A    | C5-C6-N1   | 6.92  | 121.16                 | 117.70              |
| 54  | BA    | 1021 | A    | C5-C6-N1   | 6.92  | 121.16                 | 117.70              |
| 54  | BA    | 1367 | A    | C4-C5-C6   | -6.92 | 113.54                 | 117.00              |
| 54  | BA    | 2403 | C    | N3-C2-O2   | -6.92 | 117.05                 | 121.90              |
| 21  | AA    | 267  | C    | N3-C2-O2   | -6.92 | 117.06                 | 121.90              |
| 21  | AA    | 1484 | C    | N3-C2-O2   | -6.92 | 117.06                 | 121.90              |
| 54  | BA    | 854  | C    | N3-C2-O2   | -6.92 | 117.06                 | 121.90              |
| 21  | AA    | 1042 | A    | C5-C6-N1   | 6.92  | 121.16                 | 117.70              |
| 54  | BA    | 2297 | A    | C5-C6-N1   | 6.92  | 121.16                 | 117.70              |
| 54  | BA    | 2819 | G    | C5-C6-N1   | 6.92  | 114.96                 | 111.50              |
| 55  | BB    | 52   | A    | C5-C6-N1   | 6.92  | 121.16                 | 117.70              |
| 54  | BA    | 781  | A    | N1-C6-N6   | -6.92 | 114.45                 | 118.60              |
| 54  | BA    | 1933 | G    | C8-N9-C4   | -6.92 | 103.63                 | 106.40              |
| 54  | BA    | 2808 | G    | N1-C6-O6   | -6.92 | 115.75                 | 119.90              |
| 54  | BA    | 2858 | C    | O4'-C1'-N1 | 6.92  | 113.73                 | 108.20              |
| 54  | BA    | 1386 | C    | N3-C2-O2   | -6.92 | 117.06                 | 121.90              |
| 54  | BA    | 95   | A    | C5-C6-N1   | 6.91  | 121.16                 | 117.70              |
| 54  | BA    | 1954 | G    | N3-C4-C5   | -6.91 | 125.14                 | 128.60              |
| 54  | BA    | 1029 | A    | N1-C6-N6   | -6.91 | 114.45                 | 118.60              |
| 54  | BA    | 1208 | C    | N3-C2-O2   | -6.91 | 117.06                 | 121.90              |
| 54  | BA    | 2469 | A    | C5-C6-N1   | 6.91  | 121.16                 | 117.70              |
| 21  | AA    | 797  | C    | N3-C2-O2   | -6.91 | 117.06                 | 121.90              |
| 21  | AA    | 599  | C    | N3-C2-O2   | -6.91 | 117.06                 | 121.90              |
| 54  | BA    | 2043 | C    | N3-C2-O2   | -6.91 | 117.06                 | 121.90              |
| 54  | BA    | 2483 | C    | N3-C2-O2   | -6.91 | 117.06                 | 121.90              |
| 21  | AA    | 932  | C    | O4'-C1'-N1 | 6.91  | 113.72                 | 108.20              |
| 55  | BB    | 99   | A    | C4-C5-C6   | -6.91 | 113.55                 | 117.00              |
| 54  | BA    | 1057 | A    | C4-C5-C6   | -6.90 | 113.55                 | 117.00              |
| 54  | BA    | 2183 | A    | N1-C6-N6   | -6.90 | 114.46                 | 118.60              |
| 7   | AH    | 14   | ARG  | NE-CZ-NH1  | 6.90  | 123.75                 | 120.30              |
| 21  | AA    | 382  | A    | C4-C5-C6   | -6.90 | 113.55                 | 117.00              |
| 54  | BA    | 158  | U    | O4'-C1'-N1 | 6.90  | 113.72                 | 108.20              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|------------|-------|------------------------|---------------------|
| 54  | BA    | 2338 | C    | N3-C4-C5   | 6.90  | 124.66                 | 121.90              |
| 21  | AA    | 972  | C    | N1-C2-O2   | 6.90  | 123.04                 | 118.90              |
| 21  | AA    | 1340 | A    | C5-C6-N1   | 6.90  | 121.15                 | 117.70              |
| 54  | BA    | 1717 | A    | C5-C6-N1   | 6.90  | 121.15                 | 117.70              |
| 54  | BA    | 2333 | A    | N1-C6-N6   | -6.90 | 114.46                 | 118.60              |
| 54  | BA    | 2512 | C    | O4'-C1'-N1 | 6.90  | 113.72                 | 108.20              |
| 21  | AA    | 1231 | G    | N9-C4-C5   | 6.90  | 108.16                 | 105.40              |
| 54  | BA    | 1040 | A    | C5-C6-N1   | 6.90  | 121.15                 | 117.70              |
| 54  | BA    | 1654 | A    | C4-C5-C6   | -6.90 | 113.55                 | 117.00              |
| 21  | AA    | 358  | U    | O4'-C1'-N1 | 6.89  | 113.72                 | 108.20              |
| 11  | AL    | 93   | ARG  | NE-CZ-NH1  | 6.89  | 123.75                 | 120.30              |
| 54  | BA    | 1204 | A    | O4'-C1'-N9 | 6.89  | 113.71                 | 108.20              |
| 21  | AA    | 545  | C    | N3-C2-O2   | -6.89 | 117.08                 | 121.90              |
| 21  | AA    | 212  | G    | O4'-C1'-N9 | 6.89  | 113.71                 | 108.20              |
| 21  | AA    | 756  | C    | N3-C2-O2   | -6.89 | 117.08                 | 121.90              |
| 54  | BA    | 2675 | A    | C5-C6-N1   | 6.89  | 121.14                 | 117.70              |
| 21  | AA    | 1269 | A    | C5-C6-N1   | 6.89  | 121.14                 | 117.70              |
| 22  | A1    | 61   | C    | N3-C2-O2   | -6.89 | 117.08                 | 121.90              |
| 24  | A3    | 11   | A    | C5-C6-N1   | 6.89  | 121.14                 | 117.70              |
| 54  | BA    | 226  | A    | C5-C6-N1   | 6.89  | 121.14                 | 117.70              |
| 54  | BA    | 1053 | C    | N3-C2-O2   | -6.89 | 117.08                 | 121.90              |
| 54  | BA    | 1382 | G    | C8-N9-C4   | -6.89 | 103.64                 | 106.40              |
| 21  | AA    | 866  | C    | N3-C2-O2   | -6.88 | 117.08                 | 121.90              |
| 54  | BA    | 2378 | A    | C4-C5-C6   | -6.88 | 113.56                 | 117.00              |
| 54  | BA    | 2887 | A    | C4-C5-C6   | -6.88 | 113.56                 | 117.00              |
| 54  | BA    | 1214 | A    | N1-C6-N6   | -6.88 | 114.47                 | 118.60              |
| 54  | BA    | 1233 | C    | N3-C2-O2   | -6.88 | 117.08                 | 121.90              |
| 54  | BA    | 1558 | C    | N3-C4-C5   | 6.88  | 124.65                 | 121.90              |
| 54  | BA    | 2042 | A    | N1-C6-N6   | -6.88 | 114.47                 | 118.60              |
| 54  | BA    | 2091 | C    | N1-C2-O2   | 6.88  | 123.03                 | 118.90              |
| 54  | BA    | 1096 | A    | C5-C6-N1   | 6.88  | 121.14                 | 117.70              |
| 54  | BA    | 1293 | C    | N3-C2-O2   | -6.88 | 117.08                 | 121.90              |
| 54  | BA    | 2288 | A    | C4-C5-C6   | -6.88 | 113.56                 | 117.00              |
| 54  | BA    | 482  | A    | C4-C5-C6   | -6.88 | 113.56                 | 117.00              |
| 21  | AA    | 1140 | C    | N3-C2-O2   | -6.88 | 117.09                 | 121.90              |
| 21  | AA    | 1286 | U    | N3-C2-O2   | -6.88 | 117.39                 | 122.20              |
| 54  | BA    | 128  | C    | N3-C2-O2   | -6.88 | 117.09                 | 121.90              |
| 54  | BA    | 1213 | A    | C4-C5-C6   | -6.88 | 113.56                 | 117.00              |
| 54  | BA    | 1953 | A    | C5-C6-N1   | 6.88  | 121.14                 | 117.70              |
| 54  | BA    | 2793 | C    | N3-C2-O2   | -6.88 | 117.09                 | 121.90              |
| 21  | AA    | 1130 | A    | C5-C6-N1   | 6.88  | 121.14                 | 117.70              |
| 21  | AA    | 1092 | A    | C4-C5-C6   | -6.87 | 113.56                 | 117.00              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|------------|-------|------------------------|---------------------|
| 21  | AA    | 1145 | A    | C5-C6-N1   | 6.87  | 121.14                 | 117.70              |
| 54  | BA    | 2005 | A    | N1-C6-N6   | -6.87 | 114.48                 | 118.60              |
| 44  | BV    | 21   | ARG  | NE-CZ-NH1  | 6.87  | 123.74                 | 120.30              |
| 54  | BA    | 1207 | C    | C6-N1-C2   | -6.87 | 117.55                 | 120.30              |
| 54  | BA    | 2070 | A    | C5-C6-N1   | 6.87  | 121.14                 | 117.70              |
| 54  | BA    | 2398 | U    | O4'-C1'-N1 | 6.87  | 113.70                 | 108.20              |
| 21  | AA    | 695  | A    | C5-C6-N1   | 6.87  | 121.14                 | 117.70              |
| 36  | BN    | 69   | ARG  | NE-CZ-NH1  | 6.87  | 123.73                 | 120.30              |
| 54  | BA    | 1685 | C    | N3-C2-O2   | -6.87 | 117.09                 | 121.90              |
| 35  | BM    | 114  | ARG  | NE-CZ-NH1  | 6.87  | 123.73                 | 120.30              |
| 54  | BA    | 666  | A    | N1-C6-N6   | -6.87 | 114.48                 | 118.60              |
| 54  | BA    | 1247 | A    | C5-C6-N1   | 6.87  | 121.13                 | 117.70              |
| 54  | BA    | 1477 | A    | N1-C6-N6   | -6.87 | 114.48                 | 118.60              |
| 54  | BA    | 1525 | A    | N1-C6-N6   | -6.87 | 114.48                 | 118.60              |
| 55  | BB    | 108  | A    | C5-C6-N1   | 6.87  | 121.13                 | 117.70              |
| 21  | AA    | 247  | G    | N9-C4-C5   | 6.87  | 108.15                 | 105.40              |
| 21  | AA    | 1101 | A    | N1-C6-N6   | -6.87 | 114.48                 | 118.60              |
| 54  | BA    | 14   | A    | C5-C6-N1   | 6.87  | 121.13                 | 117.70              |
| 54  | BA    | 139  | U    | N3-C2-O2   | -6.87 | 117.39                 | 122.20              |
| 54  | BA    | 1073 | A    | C4-C5-C6   | -6.87 | 113.57                 | 117.00              |
| 54  | BA    | 1114 | C    | N3-C2-O2   | -6.87 | 117.09                 | 121.90              |
| 55  | BB    | 116  | G    | C8-N9-C4   | -6.87 | 103.65                 | 106.40              |
| 21  | AA    | 55   | A    | C4-C5-C6   | -6.86 | 113.57                 | 117.00              |
| 54  | BA    | 2020 | A    | C5-C6-N1   | 6.86  | 121.13                 | 117.70              |
| 54  | BA    | 2727 | A    | C4-C5-C6   | -6.86 | 113.57                 | 117.00              |
| 21  | AA    | 1126 | U    | N3-C2-O2   | -6.86 | 117.40                 | 122.20              |
| 21  | AA    | 716  | A    | N1-C6-N6   | -6.86 | 114.48                 | 118.60              |
| 54  | BA    | 820  | A    | C5-C6-N1   | 6.86  | 121.13                 | 117.70              |
| 54  | BA    | 1392 | A    | C4-C5-C6   | -6.86 | 113.57                 | 117.00              |
| 54  | BA    | 2644 | G    | N1-C6-O6   | -6.86 | 115.78                 | 119.90              |
| 54  | BA    | 2883 | A    | C5-C6-N1   | 6.86  | 121.13                 | 117.70              |
| 21  | AA    | 25   | C    | N3-C2-O2   | -6.86 | 117.10                 | 121.90              |
| 21  | AA    | 826  | C    | N3-C2-O2   | -6.86 | 117.10                 | 121.90              |
| 21  | AA    | 1508 | A    | C4-C5-C6   | -6.86 | 113.57                 | 117.00              |
| 54  | BA    | 426  | C    | O4'-C1'-N1 | 6.86  | 113.69                 | 108.20              |
| 54  | BA    | 937  | C    | N3-C2-O2   | -6.86 | 117.10                 | 121.90              |
| 54  | BA    | 2469 | A    | O4'-C1'-N9 | 6.86  | 113.69                 | 108.20              |
| 21  | AA    | 1111 | A    | C5-C6-N1   | 6.86  | 121.13                 | 117.70              |
| 54  | BA    | 1912 | A    | N1-C6-N6   | -6.86 | 114.49                 | 118.60              |
| 54  | BA    | 698  | C    | N3-C2-O2   | -6.85 | 117.10                 | 121.90              |
| 54  | BA    | 2795 | C    | N1-C2-O2   | 6.85  | 123.01                 | 118.90              |
| 55  | BB    | 73   | A    | C4-C5-C6   | -6.85 | 113.57                 | 117.00              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 21  | AA    | 413  | G    | C5'-C4'-C3' | -6.85 | 105.04      | 116.00   |
| 54  | BA    | 1437 | C    | N3-C2-O2    | -6.85 | 117.11      | 121.90   |
| 21  | AA    | 445  | G    | C5-C6-N1    | 6.85  | 114.92      | 111.50   |
| 54  | BA    | 1288 | G    | N1-C6-O6    | -6.85 | 115.79      | 119.90   |
| 21  | AA    | 919  | A    | C4-C5-C6    | -6.85 | 113.58      | 117.00   |
| 6   | AG    | 3    | ARG  | NE-CZ-NH1   | 6.85  | 123.72      | 120.30   |
| 21  | AA    | 114  | U    | O4'-C1'-N1  | 6.84  | 113.67      | 108.20   |
| 22  | A1    | 72   | C    | N1-C2-O2    | 6.84  | 123.01      | 118.90   |
| 54  | BA    | 2778 | A    | C4-C5-C6    | -6.84 | 113.58      | 117.00   |
| 21  | AA    | 679  | C    | N3-C2-O2    | -6.84 | 117.11      | 121.90   |
| 21  | AA    | 878  | A    | N1-C6-N6    | -6.84 | 114.49      | 118.60   |
| 21  | AA    | 1196 | A    | C5-C6-N1    | 6.84  | 121.12      | 117.70   |
| 21  | AA    | 1338 | G    | C1'-O4'-C4' | -6.84 | 104.43      | 109.90   |
| 54  | BA    | 1122 | G    | N3-C2-N2    | -6.84 | 115.11      | 119.90   |
| 54  | BA    | 1595 | C    | N1-C2-O2    | 6.84  | 123.01      | 118.90   |
| 54  | BA    | 631  | A    | C4-C5-C6    | -6.84 | 113.58      | 117.00   |
| 54  | BA    | 1610 | A    | C5-C6-N1    | 6.84  | 121.12      | 117.70   |
| 21  | AA    | 766  | A    | C4-C5-C6    | -6.84 | 113.58      | 117.00   |
| 21  | AA    | 1103 | C    | N3-C2-O2    | -6.84 | 117.11      | 121.90   |
| 54  | BA    | 1801 | A    | C4-C5-C6    | -6.84 | 113.58      | 117.00   |
| 54  | BA    | 2530 | A    | C4-C5-C6    | -6.84 | 113.58      | 117.00   |
| 54  | BA    | 800  | A    | N1-C6-N6    | -6.84 | 114.50      | 118.60   |
| 54  | BA    | 985  | C    | N3-C2-O2    | -6.84 | 117.11      | 121.90   |
| 54  | BA    | 1495 | A    | C5-C6-N1    | 6.84  | 121.12      | 117.70   |
| 21  | AA    | 1188 | A    | C5-C6-N1    | 6.83  | 121.12      | 117.70   |
| 54  | BA    | 2771 | C    | N3-C2-O2    | -6.83 | 117.12      | 121.90   |
| 54  | BA    | 643  | A    | N1-C6-N6    | -6.83 | 114.50      | 118.60   |
| 21  | AA    | 177  | G    | C5-C6-N1    | 6.83  | 114.92      | 111.50   |
| 44  | BV    | 79   | ARG  | NE-CZ-NH1   | 6.83  | 123.72      | 120.30   |
| 54  | BA    | 2466 | C    | O4'-C1'-N1  | 6.83  | 113.66      | 108.20   |
| 27  | BE    | 67   | ARG  | NE-CZ-NH1   | 6.83  | 123.72      | 120.30   |
| 21  | AA    | 893  | C    | N3-C2-O2    | -6.83 | 117.12      | 121.90   |
| 54  | BA    | 2785 | C    | N3-C2-O2    | -6.83 | 117.12      | 121.90   |
| 21  | AA    | 1429 | A    | O4'-C1'-N9  | 6.83  | 113.66      | 108.20   |
| 34  | BL    | 2    | ARG  | NE-CZ-NH1   | 6.83  | 123.71      | 120.30   |
| 54  | BA    | 975  | A    | C6-C5-N7    | 6.83  | 137.08      | 132.30   |
| 54  | BA    | 1625 | C    | N3-C2-O2    | -6.83 | 117.12      | 121.90   |
| 21  | AA    | 341  | C    | N3-C2-O2    | -6.83 | 117.12      | 121.90   |
| 21  | AA    | 1251 | A    | C5-C6-N1    | 6.83  | 121.11      | 117.70   |
| 54  | BA    | 68   | G    | C5-C6-N1    | 6.83  | 114.91      | 111.50   |
| 21  | AA    | 906  | A    | C5-C6-N1    | 6.82  | 121.11      | 117.70   |
| 54  | BA    | 1172 | C    | N3-C2-O2    | -6.82 | 117.12      | 121.90   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|-------------|-------|------------------------|---------------------|
| 54  | BA    | 1463 | C    | O4'-C1'-N1  | 6.82  | 113.66                 | 108.20              |
| 54  | BA    | 1495 | A    | N1-C6-N6    | -6.82 | 114.51                 | 118.60              |
| 21  | AA    | 195  | A    | C5-C6-N1    | 6.82  | 121.11                 | 117.70              |
| 54  | BA    | 1101 | U    | O4'-C1'-N1  | 6.82  | 113.66                 | 108.20              |
| 54  | BA    | 2335 | A    | N1-C6-N6    | -6.82 | 114.51                 | 118.60              |
| 21  | AA    | 765  | G    | O4'-C1'-N9  | 6.82  | 113.65                 | 108.20              |
| 54  | BA    | 203  | A    | N1-C6-N6    | -6.82 | 114.51                 | 118.60              |
| 54  | BA    | 2338 | C    | N1-C2-O2    | 6.82  | 122.99                 | 118.90              |
| 54  | BA    | 2527 | C    | N3-C2-O2    | -6.82 | 117.13                 | 121.90              |
| 55  | BB    | 58   | A    | C5-C6-N1    | 6.82  | 121.11                 | 117.70              |
| 21  | AA    | 1523 | G    | C5-C6-N1    | 6.81  | 114.91                 | 111.50              |
| 54  | BA    | 1287 | A    | C5-C6-N1    | 6.81  | 121.11                 | 117.70              |
| 55  | BB    | 110  | C    | N3-C2-O2    | -6.81 | 117.13                 | 121.90              |
| 3   | AD    | 183  | ARG  | NE-CZ-NH1   | 6.81  | 123.71                 | 120.30              |
| 54  | BA    | 142  | A    | C4-C5-C6    | -6.81 | 113.59                 | 117.00              |
| 54  | BA    | 2174 | C    | N1-C2-O2    | 6.81  | 122.99                 | 118.90              |
| 54  | BA    | 2717 | C    | N1-C2-O2    | 6.81  | 122.99                 | 118.90              |
| 54  | BA    | 254  | G    | C5'-C4'-O4' | 6.81  | 117.27                 | 109.10              |
| 54  | BA    | 1348 | C    | N3-C2-O2    | -6.81 | 117.13                 | 121.90              |
| 21  | AA    | 938  | A    | O4'-C1'-N9  | 6.81  | 113.65                 | 108.20              |
| 21  | AA    | 1183 | U    | O4'-C1'-N1  | 6.81  | 113.65                 | 108.20              |
| 22  | A1    | 72   | C    | N3-C2-O2    | -6.81 | 117.13                 | 121.90              |
| 21  | AA    | 67   | C    | N3-C2-O2    | -6.81 | 117.13                 | 121.90              |
| 21  | AA    | 561  | U    | C3'-C2'-C1' | 6.81  | 106.95                 | 101.50              |
| 54  | BA    | 2354 | C    | O4'-C1'-N1  | 6.81  | 113.65                 | 108.20              |
| 54  | BA    | 219  | A    | C4-C5-C6    | -6.81 | 113.60                 | 117.00              |
| 54  | BA    | 2767 | C    | N3-C2-O2    | -6.81 | 117.14                 | 121.90              |
| 54  | BA    | 995  | C    | N3-C2-O2    | -6.80 | 117.14                 | 121.90              |
| 55  | BB    | 99   | A    | C5-C6-N1    | 6.80  | 121.10                 | 117.70              |
| 21  | AA    | 1037 | C    | N3-C2-O2    | -6.80 | 117.14                 | 121.90              |
| 21  | AA    | 1229 | A    | C4-C5-C6    | -6.80 | 113.60                 | 117.00              |
| 21  | AA    | 1336 | C    | N1-C2-O2    | 6.80  | 122.98                 | 118.90              |
| 21  | AA    | 1366 | C    | N3-C2-O2    | -6.80 | 117.14                 | 121.90              |
| 21  | AA    | 1410 | A    | C5-C6-N1    | 6.80  | 121.10                 | 117.70              |
| 54  | BA    | 979  | A    | C4-C5-C6    | -6.80 | 113.60                 | 117.00              |
| 21  | AA    | 372  | C    | N3-C2-O2    | -6.80 | 117.14                 | 121.90              |
| 21  | AA    | 415  | A    | C4-C5-C6    | -6.80 | 113.60                 | 117.00              |
| 21  | AA    | 658  | C    | N3-C2-O2    | -6.80 | 117.14                 | 121.90              |
| 21  | AA    | 715  | A    | C5-C6-N1    | 6.80  | 121.10                 | 117.70              |
| 21  | AA    | 770  | C    | N3-C2-O2    | -6.80 | 117.14                 | 121.90              |
| 54  | BA    | 2079 | U    | O4'-C1'-N1  | 6.80  | 113.64                 | 108.20              |
| 21  | AA    | 608  | A    | C5-C6-N1    | 6.80  | 121.10                 | 117.70              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 54  | BA    | 111  | A    | C4-C5-C6   | -6.80 | 113.60      | 117.00   |
| 54  | BA    | 2790 | U    | O4'-C1'-N1 | 6.80  | 113.64      | 108.20   |
| 21  | AA    | 1265 | C    | N3-C2-O2   | -6.79 | 117.14      | 121.90   |
| 54  | BA    | 507  | A    | C5-C6-N1   | 6.79  | 121.10      | 117.70   |
| 54  | BA    | 886  | A    | N1-C6-N6   | -6.79 | 114.52      | 118.60   |
| 31  | BI    | 133  | ARG  | NE-CZ-NH1  | 6.79  | 123.70      | 120.30   |
| 54  | BA    | 125  | A    | C4-C5-C6   | -6.79 | 113.60      | 117.00   |
| 54  | BA    | 131  | A    | C4-C5-C6   | -6.79 | 113.60      | 117.00   |
| 54  | BA    | 1595 | C    | N3-C2-O2   | -6.79 | 117.14      | 121.90   |
| 54  | BA    | 1668 | A    | N1-C6-N6   | -6.79 | 114.52      | 118.60   |
| 54  | BA    | 2879 | A    | C5-C6-N1   | 6.79  | 121.10      | 117.70   |
| 54  | BA    | 311  | A    | C4-C5-C6   | -6.79 | 113.61      | 117.00   |
| 54  | BA    | 2559 | C    | N3-C2-O2   | -6.79 | 117.15      | 121.90   |
| 54  | BA    | 2707 | U    | O4'-C1'-N1 | 6.79  | 113.63      | 108.20   |
| 54  | BA    | 1858 | A    | C5-C6-N1   | 6.79  | 121.09      | 117.70   |
| 27  | BE    | 88   | ARG  | NE-CZ-NH2  | -6.79 | 116.91      | 120.30   |
| 54  | BA    | 2463 | C    | O4'-C1'-N1 | 6.79  | 113.63      | 108.20   |
| 54  | BA    | 2901 | C    | N3-C4-C5   | 6.79  | 124.61      | 121.90   |
| 21  | AA    | 703  | G    | N3-C4-C5   | -6.79 | 125.21      | 128.60   |
| 54  | BA    | 264  | C    | N3-C2-O2   | -6.79 | 117.15      | 121.90   |
| 54  | BA    | 299  | A    | C4-C5-C6   | -6.79 | 113.61      | 117.00   |
| 54  | BA    | 374  | A    | C4-C5-C6   | -6.79 | 113.61      | 117.00   |
| 54  | BA    | 1044 | C    | N1-C2-O2   | 6.79  | 122.97      | 118.90   |
| 54  | BA    | 1349 | C    | N3-C2-O2   | -6.79 | 117.15      | 121.90   |
| 54  | BA    | 1414 | C    | O4'-C1'-N1 | 6.79  | 113.63      | 108.20   |
| 54  | BA    | 1658 | C    | N3-C2-O2   | -6.79 | 117.15      | 121.90   |
| 54  | BA    | 2295 | C    | N3-C2-O2   | -6.79 | 117.15      | 121.90   |
| 21  | AA    | 1362 | A    | C5-C6-N1   | 6.78  | 121.09      | 117.70   |
| 54  | BA    | 1246 | A    | C5-C6-N1   | 6.78  | 121.09      | 117.70   |
| 54  | BA    | 1317 | G    | O4'-C1'-N9 | 6.78  | 113.63      | 108.20   |
| 54  | BA    | 2171 | A    | N1-C6-N6   | -6.78 | 114.53      | 118.60   |
| 54  | BA    | 2215 | C    | N3-C2-O2   | -6.78 | 117.15      | 121.90   |
| 54  | BA    | 2009 | A    | C4-C5-C6   | -6.78 | 113.61      | 117.00   |
| 33  | BK    | 17   | ARG  | NE-CZ-NH1  | 6.78  | 123.69      | 120.30   |
| 54  | BA    | 483  | A    | C5-C6-N1   | 6.78  | 121.09      | 117.70   |
| 54  | BA    | 538  | A    | C5-C6-N1   | 6.78  | 121.09      | 117.70   |
| 21  | AA    | 215  | C    | N3-C2-O2   | -6.78 | 117.16      | 121.90   |
| 54  | BA    | 1638 | C    | N3-C2-O2   | -6.78 | 117.16      | 121.90   |
| 54  | BA    | 2099 | U    | O4'-C1'-N1 | 6.78  | 113.62      | 108.20   |
| 54  | BA    | 2171 | A    | C4-C5-C6   | -6.78 | 113.61      | 117.00   |
| 55  | BB    | 54   | G    | N1-C6-O6   | -6.78 | 115.83      | 119.90   |
| 21  | AA    | 1405 | G    | N9-C4-C5   | 6.78  | 108.11      | 105.40   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 54  | BA    | 345  | A    | N1-C6-N6   | -6.78 | 114.53      | 118.60   |
| 55  | BB    | 12   | C    | N3-C2-O2   | -6.78 | 117.16      | 121.90   |
| 21  | AA    | 706  | A    | C5-C6-N1   | 6.78  | 121.09      | 117.70   |
| 54  | BA    | 2253 | G    | C8-N9-C4   | -6.78 | 103.69      | 106.40   |
| 54  | BA    | 589  | U    | O4'-C1'-N1 | 6.77  | 113.62      | 108.20   |
| 54  | BA    | 1241 | A    | C4-C5-C6   | -6.77 | 113.61      | 117.00   |
| 22  | A1    | 35   | A    | N1-C6-N6   | -6.77 | 114.54      | 118.60   |
| 54  | BA    | 1362 | C    | O4'-C1'-N1 | 6.77  | 113.62      | 108.20   |
| 54  | BA    | 1398 | C    | N1-C2-O2   | 6.77  | 122.96      | 118.90   |
| 54  | BA    | 163  | C    | N3-C2-O2   | -6.77 | 117.16      | 121.90   |
| 54  | BA    | 354  | A    | C4-C5-C6   | -6.77 | 113.61      | 117.00   |
| 54  | BA    | 1322 | A    | C4-C5-C6   | -6.77 | 113.61      | 117.00   |
| 21  | AA    | 1360 | A    | C4-C5-C6   | -6.77 | 113.61      | 117.00   |
| 54  | BA    | 330  | A    | C5-C6-N1   | 6.77  | 121.08      | 117.70   |
| 54  | BA    | 522  | A    | N1-C6-N6   | -6.77 | 114.54      | 118.60   |
| 54  | BA    | 575  | A    | C4-C5-C6   | -6.77 | 113.62      | 117.00   |
| 54  | BA    | 1853 | A    | C5-C6-N1   | 6.77  | 121.08      | 117.70   |
| 21  | AA    | 1250 | A    | C4-C5-C6   | -6.77 | 113.62      | 117.00   |
| 54  | BA    | 2196 | C    | O4'-C1'-N1 | 6.77  | 113.61      | 108.20   |
| 21  | AA    | 320  | A    | C5-C6-N1   | 6.77  | 121.08      | 117.70   |
| 21  | AA    | 1044 | A    | C4-C5-C6   | -6.77 | 113.62      | 117.00   |
| 21  | AA    | 1129 | C    | N1-C2-O2   | 6.77  | 122.96      | 118.90   |
| 21  | AA    | 996  | A    | C5-C6-N1   | 6.76  | 121.08      | 117.70   |
| 21  | AA    | 1427 | C    | N3-C2-O2   | -6.76 | 117.16      | 121.90   |
| 25  | BC    | 101  | ARG  | NE-CZ-NH1  | 6.76  | 123.68      | 120.30   |
| 54  | BA    | 2883 | A    | C4-C5-C6   | -6.76 | 113.62      | 117.00   |
| 21  | AA    | 147  | G    | N1-C6-O6   | -6.76 | 115.84      | 119.90   |
| 21  | AA    | 523  | A    | C4-C5-C6   | -6.76 | 113.62      | 117.00   |
| 54  | BA    | 1109 | C    | O4'-C1'-N1 | 6.76  | 113.61      | 108.20   |
| 21  | AA    | 782  | A    | C4-C5-C6   | -6.76 | 113.62      | 117.00   |
| 22  | A1    | 72   | C    | N3-C4-C5   | 6.76  | 124.60      | 121.90   |
| 25  | BC    | 155  | ARG  | NE-CZ-NH1  | 6.76  | 123.68      | 120.30   |
| 54  | BA    | 1802 | A    | N1-C6-N6   | -6.76 | 114.55      | 118.60   |
| 54  | BA    | 2821 | A    | N1-C6-N6   | -6.76 | 114.55      | 118.60   |
| 55  | BB    | 46   | A    | C5-C6-N1   | 6.76  | 121.08      | 117.70   |
| 54  | BA    | 509  | C    | N3-C2-O2   | -6.76 | 117.17      | 121.90   |
| 21  | AA    | 172  | A    | C6-C5-N7   | 6.76  | 137.03      | 132.30   |
| 54  | BA    | 115  | C    | N3-C2-O2   | -6.76 | 117.17      | 121.90   |
| 54  | BA    | 1614 | A    | C5-C6-N1   | 6.76  | 121.08      | 117.70   |
| 54  | BA    | 1676 | A    | C4-C5-C6   | -6.76 | 113.62      | 117.00   |
| 54  | BA    | 275  | C    | N1-C2-O2   | 6.75  | 122.95      | 118.90   |
| 21  | AA    | 767  | A    | C4-C5-C6   | -6.75 | 113.62      | 117.00   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|-------------|-------|------------------------|---------------------|
| 21  | AA    | 1479 | C    | N3-C4-C5    | 6.75  | 124.60                 | 121.90              |
| 54  | BA    | 873  | C    | N3-C2-O2    | -6.75 | 117.17                 | 121.90              |
| 54  | BA    | 925  | A    | C4-C5-C6    | -6.75 | 113.62                 | 117.00              |
| 54  | BA    | 1367 | A    | C5-C6-N1    | 6.75  | 121.08                 | 117.70              |
| 21  | AA    | 80   | A    | C5-C6-N1    | 6.75  | 121.08                 | 117.70              |
| 21  | AA    | 1342 | C    | N1-C2-O2    | 6.75  | 122.95                 | 118.90              |
| 54  | BA    | 980  | A    | N1-C6-N6    | -6.75 | 114.55                 | 118.60              |
| 54  | BA    | 344  | A    | N1-C6-N6    | -6.75 | 114.55                 | 118.60              |
| 54  | BA    | 2270 | A    | C5-C6-N1    | 6.75  | 121.07                 | 117.70              |
| 54  | BA    | 2634 | A    | C5-C6-N1    | 6.75  | 121.07                 | 117.70              |
| 54  | BA    | 1289 | C    | O4'-C1'-N1  | 6.75  | 113.60                 | 108.20              |
| 54  | BA    | 1902 | C    | N3-C2-O2    | -6.75 | 117.18                 | 121.90              |
| 55  | BB    | 18   | G    | N1-C6-O6    | -6.75 | 115.85                 | 119.90              |
| 54  | BA    | 2273 | A    | C5-C6-N1    | 6.75  | 121.07                 | 117.70              |
| 21  | AA    | 1167 | A    | C4-C5-C6    | -6.74 | 113.63                 | 117.00              |
| 24  | A3    | 14   | A    | C5-C6-N1    | 6.74  | 121.07                 | 117.70              |
| 54  | BA    | 599  | A    | C5-C6-N1    | 6.74  | 121.07                 | 117.70              |
| 54  | BA    | 1932 | A    | N1-C6-N6    | -6.74 | 114.55                 | 118.60              |
| 55  | BB    | 108  | A    | C4-C5-C6    | -6.74 | 113.63                 | 117.00              |
| 21  | AA    | 899  | C    | N3-C2-O2    | -6.74 | 117.18                 | 121.90              |
| 21  | AA    | 366  | A    | C5-C6-N1    | 6.74  | 121.07                 | 117.70              |
| 21  | AA    | 1236 | A    | N1-C6-N6    | -6.74 | 114.56                 | 118.60              |
| 54  | BA    | 462  | C    | N3-C2-O2    | -6.74 | 117.18                 | 121.90              |
| 54  | BA    | 1145 | C    | N3-C2-O2    | -6.74 | 117.18                 | 121.90              |
| 54  | BA    | 2725 | A    | N1-C6-N6    | -6.74 | 114.56                 | 118.60              |
| 22  | A1    | 76   | A    | C4-C5-C6    | -6.74 | 113.63                 | 117.00              |
| 54  | BA    | 126  | A    | C5-C6-N1    | 6.74  | 121.07                 | 117.70              |
| 54  | BA    | 2870 | C    | N1-C2-O2    | 6.74  | 122.94                 | 118.90              |
| 21  | AA    | 1116 | U    | C5-C6-N1    | -6.74 | 119.33                 | 122.70              |
| 21  | AA    | 1410 | A    | O4'-C1'-N9  | 6.74  | 113.59                 | 108.20              |
| 21  | AA    | 1534 | A    | C5-C6-N1    | 6.74  | 121.07                 | 117.70              |
| 54  | BA    | 256  | A    | N1-C6-N6    | -6.74 | 114.56                 | 118.60              |
| 54  | BA    | 613  | A    | C5-C6-N1    | 6.74  | 121.07                 | 117.70              |
| 54  | BA    | 1594 | U    | C5-C6-N1    | -6.74 | 119.33                 | 122.70              |
| 21  | AA    | 680  | C    | N3-C2-O2    | -6.73 | 117.19                 | 121.90              |
| 21  | AA    | 694  | A    | C5-C6-N1    | 6.73  | 121.07                 | 117.70              |
| 21  | AA    | 750  | C    | N3-C2-O2    | -6.73 | 117.19                 | 121.90              |
| 54  | BA    | 751  | A    | N1-C6-N6    | -6.73 | 114.56                 | 118.60              |
| 54  | BA    | 2620 | C    | N3-C2-O2    | -6.73 | 117.19                 | 121.90              |
| 21  | AA    | 270  | A    | C4-C5-C6    | -6.73 | 113.64                 | 117.00              |
| 21  | AA    | 483  | C    | C3'-C2'-C1' | 6.73  | 106.89                 | 101.50              |
| 21  | AA    | 1236 | A    | C5-C6-N1    | 6.73  | 121.07                 | 117.70              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 54  | BA    | 1832 | C    | N3-C2-O2    | -6.73 | 117.19      | 121.90   |
| 21  | AA    | 1337 | G    | N3-C4-N9    | 6.73  | 130.04      | 126.00   |
| 22  | A1    | 2    | G    | N3-C4-C5    | -6.73 | 125.24      | 128.60   |
| 54  | BA    | 1056 | G    | O4'-C1'-N9  | 6.73  | 113.58      | 108.20   |
| 54  | BA    | 1446 | C    | N3-C2-O2    | -6.73 | 117.19      | 121.90   |
| 54  | BA    | 2008 | C    | N3-C2-O2    | -6.73 | 117.19      | 121.90   |
| 54  | BA    | 2135 | A    | N1-C6-N6    | -6.73 | 114.56      | 118.60   |
| 54  | BA    | 863  | A    | N1-C6-N6    | -6.73 | 114.56      | 118.60   |
| 21  | AA    | 840  | C    | N1-C2-O2    | 6.73  | 122.94      | 118.90   |
| 54  | BA    | 1579 | A    | C5-C6-N1    | 6.73  | 121.06      | 117.70   |
| 21  | AA    | 285  | C    | N3-C2-O2    | -6.72 | 117.19      | 121.90   |
| 54  | BA    | 2204 | G    | C5-C6-N1    | 6.72  | 114.86      | 111.50   |
| 21  | AA    | 414  | A    | C4-C5-C6    | -6.72 | 113.64      | 117.00   |
| 54  | BA    | 196  | A    | C5-C6-N1    | 6.72  | 121.06      | 117.70   |
| 54  | BA    | 900  | A    | C4-C5-C6    | -6.72 | 113.64      | 117.00   |
| 54  | BA    | 1504 | A    | C5-C6-N1    | 6.72  | 121.06      | 117.70   |
| 21  | AA    | 1136 | C    | N1-C2-O2    | 6.72  | 122.93      | 118.90   |
| 54  | BA    | 96   | C    | N3-C2-O2    | -6.72 | 117.19      | 121.90   |
| 21  | AA    | 408  | A    | C5-C6-N1    | 6.72  | 121.06      | 117.70   |
| 21  | AA    | 833  | G    | N1-C6-O6    | -6.72 | 115.87      | 119.90   |
| 54  | BA    | 471  | A    | N1-C6-N6    | -6.72 | 114.57      | 118.60   |
| 54  | BA    | 1114 | C    | N1-C2-O2    | 6.72  | 122.93      | 118.90   |
| 55  | BB    | 3    | C    | O4'-C1'-N1  | 6.72  | 113.57      | 108.20   |
| 54  | BA    | 1278 | C    | N3-C2-O2    | -6.72 | 117.20      | 121.90   |
| 54  | BA    | 1829 | A    | N1-C6-N6    | -6.72 | 114.57      | 118.60   |
| 54  | BA    | 2104 | C    | N3-C2-O2    | -6.72 | 117.20      | 121.90   |
| 54  | BA    | 2575 | C    | N1-C2-O2    | 6.72  | 122.93      | 118.90   |
| 54  | BA    | 2620 | C    | N1-C2-O2    | 6.72  | 122.93      | 118.90   |
| 21  | AA    | 758  | C    | N3-C2-O2    | -6.71 | 117.20      | 121.90   |
| 54  | BA    | 201  | C    | N3-C2-O2    | -6.71 | 117.20      | 121.90   |
| 54  | BA    | 398  | C    | N1-C2-O2    | 6.71  | 122.93      | 118.90   |
| 54  | BA    | 505  | A    | N1-C6-N6    | -6.71 | 114.57      | 118.60   |
| 21  | AA    | 968  | A    | C5-C6-N1    | 6.71  | 121.06      | 117.70   |
| 21  | AA    | 1431 | A    | C3'-C2'-C1' | 6.71  | 106.87      | 101.50   |
| 54  | BA    | 1672 | A    | C4-C5-C6    | -6.71 | 113.64      | 117.00   |
| 54  | BA    | 2636 | C    | N1-C2-O2    | 6.71  | 122.93      | 118.90   |
| 54  | BA    | 1640 | A    | C5-C6-N1    | 6.71  | 121.05      | 117.70   |
| 54  | BA    | 2275 | C    | C3'-C2'-C1' | 6.71  | 106.87      | 101.50   |
| 21  | AA    | 129  | A    | C4-C5-C6    | -6.71 | 113.65      | 117.00   |
| 21  | AA    | 519  | C    | C1'-O4'-C4' | -6.71 | 104.53      | 109.90   |
| 21  | AA    | 1452 | C    | N3-C2-O2    | -6.71 | 117.20      | 121.90   |
| 54  | BA    | 505  | A    | C5-C6-N1    | 6.71  | 121.05      | 117.70   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|-------------|-------|------------------------|---------------------|
| 54  | BA    | 1724 | G    | N3-C4-C5    | -6.71 | 125.25                 | 128.60              |
| 25  | BC    | 174  | ARG  | NE-CZ-NH1   | 6.71  | 123.65                 | 120.30              |
| 54  | BA    | 336  | C    | O4'-C1'-N1  | 6.71  | 113.56                 | 108.20              |
| 54  | BA    | 453  | A    | C5-C6-N1    | 6.71  | 121.05                 | 117.70              |
| 54  | BA    | 849  | A    | C4-C5-C6    | -6.71 | 113.65                 | 117.00              |
| 54  | BA    | 859  | G    | O4'-C1'-N9  | 6.71  | 113.56                 | 108.20              |
| 54  | BA    | 2739 | U    | C5-C6-N1    | -6.71 | 119.35                 | 122.70              |
| 21  | AA    | 83   | C    | N3-C2-O2    | -6.70 | 117.21                 | 121.90              |
| 54  | BA    | 706  | A    | C5-C6-N1    | 6.70  | 121.05                 | 117.70              |
| 54  | BA    | 1253 | A    | C5-C6-N1    | 6.70  | 121.05                 | 117.70              |
| 54  | BA    | 1626 | A    | C4-C5-C6    | -6.70 | 113.65                 | 117.00              |
| 54  | BA    | 2471 | A    | C4-C5-C6    | -6.70 | 113.65                 | 117.00              |
| 54  | BA    | 2739 | U    | N3-C2-O2    | -6.70 | 117.51                 | 122.20              |
| 54  | BA    | 957  | C    | N3-C2-O2    | -6.70 | 117.21                 | 121.90              |
| 54  | BA    | 364  | C    | N3-C2-O2    | -6.70 | 117.21                 | 121.90              |
| 54  | BA    | 743  | A    | C4-C5-C6    | -6.70 | 113.65                 | 117.00              |
| 24  | A3    | 39   | A    | N1-C6-N6    | -6.70 | 114.58                 | 118.60              |
| 54  | BA    | 1133 | A    | C5-C6-N1    | 6.70  | 121.05                 | 117.70              |
| 54  | BA    | 1871 | A    | C4-C5-C6    | -6.70 | 113.65                 | 117.00              |
| 24  | A3    | 11   | A    | C4-C5-C6    | -6.70 | 113.65                 | 117.00              |
| 54  | BA    | 899  | A    | C4-C5-C6    | -6.70 | 113.65                 | 117.00              |
| 54  | BA    | 2534 | A    | C4-C5-C6    | -6.70 | 113.65                 | 117.00              |
| 21  | AA    | 145  | G    | N3-C2-N2    | -6.69 | 115.21                 | 119.90              |
| 54  | BA    | 1695 | G    | C8-N9-C4    | -6.69 | 103.72                 | 106.40              |
| 54  | BA    | 1776 | G    | N3-C4-C5    | -6.69 | 125.25                 | 128.60              |
| 21  | AA    | 575  | G    | C5-C6-N1    | 6.69  | 114.85                 | 111.50              |
| 54  | BA    | 1155 | A    | N1-C6-N6    | -6.69 | 114.58                 | 118.60              |
| 54  | BA    | 1906 | G    | N1-C6-O6    | -6.69 | 115.89                 | 119.90              |
| 54  | BA    | 515  | A    | C4-C5-C6    | -6.69 | 113.66                 | 117.00              |
| 54  | BA    | 918  | A    | N1-C6-N6    | -6.69 | 114.59                 | 118.60              |
| 54  | BA    | 1805 | A    | C4-C5-C6    | -6.69 | 113.66                 | 117.00              |
| 54  | BA    | 2282 | G    | N1-C6-O6    | -6.69 | 115.89                 | 119.90              |
| 54  | BA    | 2418 | A    | C5-C6-N1    | 6.69  | 121.05                 | 117.70              |
| 21  | AA    | 1035 | A    | N1-C6-N6    | -6.69 | 114.59                 | 118.60              |
| 21  | AA    | 270  | A    | C5-C6-N1    | 6.69  | 121.04                 | 117.70              |
| 21  | AA    | 463  | U    | C5-C6-N1    | -6.69 | 119.36                 | 122.70              |
| 21  | AA    | 1345 | U    | C1'-O4'-C4' | -6.69 | 104.55                 | 109.90              |
| 54  | BA    | 239  | C    | N3-C2-O2    | -6.69 | 117.22                 | 121.90              |
| 54  | BA    | 1889 | A    | C5-C6-N1    | 6.69  | 121.04                 | 117.70              |
| 54  | BA    | 2782 | G    | C8-N9-C4    | -6.69 | 103.72                 | 106.40              |
| 21  | AA    | 204  | G    | C5-C6-N1    | 6.69  | 114.84                 | 111.50              |
| 54  | BA    | 886  | A    | C5-C6-N1    | 6.69  | 121.04                 | 117.70              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 21  | AA    | 349  | A    | C4-C5-C6    | -6.68 | 113.66      | 117.00   |
| 33  | BK    | 71   | ARG  | NE-CZ-NH1   | 6.68  | 123.64      | 120.30   |
| 54  | BA    | 228  | C    | N3-C2-O2    | -6.68 | 117.22      | 121.90   |
| 7   | AH    | 116  | ARG  | NE-CZ-NH1   | 6.68  | 123.64      | 120.30   |
| 21  | AA    | 754  | C    | N3-C2-O2    | -6.68 | 117.22      | 121.90   |
| 54  | BA    | 404  | A    | C5-C6-N1    | 6.68  | 121.04      | 117.70   |
| 54  | BA    | 1275 | A    | C4-C5-C6    | -6.68 | 113.66      | 117.00   |
| 54  | BA    | 1689 | A    | N1-C6-N6    | -6.68 | 114.59      | 118.60   |
| 54  | BA    | 1794 | A    | N1-C6-N6    | -6.68 | 114.59      | 118.60   |
| 54  | BA    | 2150 | C    | N3-C2-O2    | -6.68 | 117.22      | 121.90   |
| 54  | BA    | 2433 | A    | C4-C5-C6    | -6.68 | 113.66      | 117.00   |
| 55  | BB    | 51   | G    | O4'-C1'-N9  | 6.68  | 113.54      | 108.20   |
| 21  | AA    | 462  | G    | N1-C6-O6    | -6.68 | 115.89      | 119.90   |
| 54  | BA    | 118  | A    | C5-C6-N1    | 6.68  | 121.04      | 117.70   |
| 54  | BA    | 281  | C    | O4'-C1'-N1  | 6.68  | 113.54      | 108.20   |
| 54  | BA    | 2234 | G    | C8-N9-C4    | -6.68 | 103.73      | 106.40   |
| 54  | BA    | 345  | A    | C5-C6-N1    | 6.68  | 121.04      | 117.70   |
| 54  | BA    | 508  | A    | C5-C6-N1    | 6.68  | 121.04      | 117.70   |
| 21  | AA    | 413  | G    | O4'-C1'-N9  | 6.67  | 113.54      | 108.20   |
| 21  | AA    | 1021 | A    | C5-C6-N1    | 6.67  | 121.04      | 117.70   |
| 24  | A3    | 13   | C    | N3-C2-O2    | -6.67 | 117.23      | 121.90   |
| 54  | BA    | 83   | A    | C4-C5-C6    | -6.67 | 113.66      | 117.00   |
| 54  | BA    | 2092 | U    | N3-C2-O2    | -6.67 | 117.53      | 122.20   |
| 54  | BA    | 2632 | A    | N1-C6-N6    | -6.67 | 114.60      | 118.60   |
| 21  | AA    | 1016 | A    | C4-C5-C6    | -6.67 | 113.66      | 117.00   |
| 54  | BA    | 1369 | G    | C5-C6-N1    | 6.67  | 114.84      | 111.50   |
| 54  | BA    | 2305 | U    | O4'-C1'-N1  | 6.67  | 113.54      | 108.20   |
| 21  | AA    | 1197 | A    | C4-C5-C6    | -6.67 | 113.67      | 117.00   |
| 54  | BA    | 1959 | G    | N1-C6-O6    | -6.67 | 115.90      | 119.90   |
| 21  | AA    | 716  | A    | C5-C6-N1    | 6.67  | 121.03      | 117.70   |
| 21  | AA    | 1152 | A    | C4-C5-C6    | -6.67 | 113.67      | 117.00   |
| 21  | AA    | 1503 | A    | C1'-O4'-C4' | -6.67 | 104.57      | 109.90   |
| 54  | BA    | 453  | A    | O4'-C1'-N9  | 6.67  | 113.53      | 108.20   |
| 54  | BA    | 819  | A    | C4-C5-C6    | -6.67 | 113.67      | 117.00   |
| 54  | BA    | 1384 | A    | C4-C5-C6    | -6.67 | 113.67      | 117.00   |
| 54  | BA    | 1439 | A    | O4'-C1'-N9  | 6.67  | 113.53      | 108.20   |
| 54  | BA    | 2411 | A    | C4-C5-C6    | -6.67 | 113.67      | 117.00   |
| 54  | BA    | 32   | C    | N1-C2-O2    | 6.67  | 122.90      | 118.90   |
| 54  | BA    | 1678 | A    | C5-C6-N1    | 6.67  | 121.03      | 117.70   |
| 54  | BA    | 1803 | A    | C5-C6-N1    | 6.67  | 121.03      | 117.70   |
| 54  | BA    | 2756 | U    | N3-C2-O2    | -6.67 | 117.53      | 122.20   |
| 21  | AA    | 752  | G    | O4'-C1'-N9  | 6.66  | 113.53      | 108.20   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|------------|-------|------------------------|---------------------|
| 24  | A3    | 17   | C    | N1-C2-O2   | 6.66  | 122.90                 | 118.90              |
| 54  | BA    | 758  | C    | N3-C2-O2   | -6.66 | 117.24                 | 121.90              |
| 54  | BA    | 1204 | A    | C4-C5-C6   | -6.66 | 113.67                 | 117.00              |
| 54  | BA    | 1327 | A    | C5-C6-N1   | 6.66  | 121.03                 | 117.70              |
| 21  | AA    | 790  | A    | C5-C6-N1   | 6.66  | 121.03                 | 117.70              |
| 54  | BA    | 472  | A    | C4-C5-C6   | -6.66 | 113.67                 | 117.00              |
| 54  | BA    | 981  | A    | N1-C6-N6   | -6.66 | 114.60                 | 118.60              |
| 21  | AA    | 60   | A    | C4-C5-C6   | -6.66 | 113.67                 | 117.00              |
| 24  | A3    | 58   | A    | C4-C5-C6   | -6.66 | 113.67                 | 117.00              |
| 54  | BA    | 2039 | U    | O4'-C1'-N1 | 6.66  | 113.53                 | 108.20              |
| 54  | BA    | 2810 | A    | C4-C5-C6   | -6.66 | 113.67                 | 117.00              |
| 54  | BA    | 800  | A    | C5-C6-N1   | 6.66  | 121.03                 | 117.70              |
| 54  | BA    | 2019 | A    | C4-C5-C6   | -6.66 | 113.67                 | 117.00              |
| 54  | BA    | 2655 | G    | C8-N9-C4   | -6.66 | 103.74                 | 106.40              |
| 54  | BA    | 2752 | C    | N3-C2-O2   | -6.66 | 117.24                 | 121.90              |
| 54  | BA    | 2129 | C    | N3-C2-O2   | -6.66 | 117.24                 | 121.90              |
| 54  | BA    | 2385 | C    | N1-C2-O2   | 6.66  | 122.89                 | 118.90              |
| 54  | BA    | 2863 | C    | N3-C2-O2   | -6.66 | 117.24                 | 121.90              |
| 54  | BA    | 529  | A    | C4-C5-C6   | -6.66 | 113.67                 | 117.00              |
| 54  | BA    | 635  | C    | N3-C2-O2   | -6.65 | 117.24                 | 121.90              |
| 54  | BA    | 901  | C    | N3-C2-O2   | -6.65 | 117.24                 | 121.90              |
| 54  | BA    | 2862 | G    | N1-C6-O6   | -6.65 | 115.91                 | 119.90              |
| 21  | AA    | 879  | C    | N3-C2-O2   | -6.65 | 117.25                 | 121.90              |
| 21  | AA    | 1005 | A    | N1-C6-N6   | -6.65 | 114.61                 | 118.60              |
| 22  | A1    | 6    | A    | C5-C6-N1   | 6.65  | 121.03                 | 117.70              |
| 39  | BQ    | 63   | ARG  | NE-CZ-NH1  | 6.65  | 123.62                 | 120.30              |
| 54  | BA    | 1189 | A    | C5-C6-N1   | 6.65  | 121.03                 | 117.70              |
| 54  | BA    | 2013 | A    | N1-C6-N6   | -6.65 | 114.61                 | 118.60              |
| 21  | AA    | 222  | C    | N3-C2-O2   | -6.65 | 117.25                 | 121.90              |
| 54  | BA    | 2158 | A    | C4-C5-C6   | -6.65 | 113.68                 | 117.00              |
| 52  | B3    | 12   | ARG  | NE-CZ-NH1  | 6.65  | 123.62                 | 120.30              |
| 54  | BA    | 316  | C    | N1-C2-O2   | 6.65  | 122.89                 | 118.90              |
| 54  | BA    | 1285 | A    | N1-C6-N6   | -6.65 | 114.61                 | 118.60              |
| 54  | BA    | 1294 | U    | O4'-C1'-N1 | 6.65  | 113.52                 | 108.20              |
| 54  | BA    | 1786 | A    | C4-C5-C6   | -6.65 | 113.68                 | 117.00              |
| 21  | AA    | 1437 | A    | N1-C6-N6   | -6.65 | 114.61                 | 118.60              |
| 22  | A1    | 68   | C    | N3-C2-O2   | -6.65 | 117.25                 | 121.90              |
| 54  | BA    | 1919 | A    | C5-C6-N1   | 6.65  | 121.02                 | 117.70              |
| 21  | AA    | 177  | G    | C2-N3-C4   | 6.64  | 115.22                 | 111.90              |
| 21  | AA    | 338  | A    | N1-C6-N6   | -6.64 | 114.61                 | 118.60              |
| 21  | AA    | 1325 | C    | N3-C2-O2   | -6.64 | 117.25                 | 121.90              |
| 54  | BA    | 1031 | G    | N1-C6-O6   | -6.64 | 115.92                 | 119.90              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|-------------|-------|------------------------|---------------------|
| 54  | BA    | 1920 | C    | N3-C2-O2    | -6.64 | 117.25                 | 121.90              |
| 26  | BD    | 184  | ARG  | NE-CZ-NH1   | 6.64  | 123.62                 | 120.30              |
| 54  | BA    | 651  | G    | C5'-C4'-O4' | 6.64  | 117.07                 | 109.10              |
| 54  | BA    | 1978 | A    | C4-C5-C6    | -6.64 | 113.68                 | 117.00              |
| 10  | AK    | 55   | ARG  | NE-CZ-NH1   | 6.64  | 123.62                 | 120.30              |
| 35  | BM    | 44   | ARG  | NE-CZ-NH1   | 6.64  | 123.62                 | 120.30              |
| 54  | BA    | 1794 | A    | C5-C6-N1    | 6.64  | 121.02                 | 117.70              |
| 21  | AA    | 210  | C    | N3-C4-C5    | 6.64  | 124.56                 | 121.90              |
| 21  | AA    | 431  | A    | C4-C5-C6    | -6.64 | 113.68                 | 117.00              |
| 54  | BA    | 346  | A    | C2-N3-C4    | 6.64  | 113.92                 | 110.60              |
| 54  | BA    | 513  | A    | C4-C5-C6    | -6.64 | 113.68                 | 117.00              |
| 54  | BA    | 998  | C    | N3-C2-O2    | -6.63 | 117.26                 | 121.90              |
| 21  | AA    | 494  | G    | C8-N9-C4    | -6.63 | 103.75                 | 106.40              |
| 21  | AA    | 1022 | A    | C5-C6-N1    | 6.63  | 121.02                 | 117.70              |
| 21  | AA    | 1428 | A    | C4-C5-C6    | -6.63 | 113.69                 | 117.00              |
| 21  | AA    | 1399 | C    | N3-C2-O2    | -6.63 | 117.26                 | 121.90              |
| 54  | BA    | 181  | A    | C4-C5-C6    | -6.63 | 113.69                 | 117.00              |
| 54  | BA    | 182  | A    | C5-C6-N1    | 6.63  | 121.02                 | 117.70              |
| 54  | BA    | 1307 | A    | C5-C6-N1    | 6.63  | 121.02                 | 117.70              |
| 54  | BA    | 1977 | A    | N1-C6-N6    | -6.63 | 114.62                 | 118.60              |
| 21  | AA    | 188  | C    | N1-C2-O2    | 6.63  | 122.88                 | 118.90              |
| 21  | AA    | 338  | A    | C4-C5-C6    | -6.63 | 113.69                 | 117.00              |
| 21  | AA    | 602  | A    | C4-C5-C6    | -6.63 | 113.69                 | 117.00              |
| 54  | BA    | 1565 | C    | O4'-C1'-N1  | 6.63  | 113.50                 | 108.20              |
| 54  | BA    | 2051 | A    | C4-C5-C6    | -6.63 | 113.69                 | 117.00              |
| 54  | BA    | 2251 | G    | C5-C6-N1    | 6.63  | 114.81                 | 111.50              |
| 54  | BA    | 2393 | U    | O4'-C1'-N1  | 6.63  | 113.50                 | 108.20              |
| 21  | AA    | 1395 | C    | N3-C2-O2    | -6.62 | 117.26                 | 121.90              |
| 21  | AA    | 1418 | A    | C4-C5-C6    | -6.62 | 113.69                 | 117.00              |
| 54  | BA    | 2013 | A    | C4-C5-C6    | -6.62 | 113.69                 | 117.00              |
| 54  | BA    | 2503 | A    | C5-C6-N1    | 6.62  | 121.01                 | 117.70              |
| 54  | BA    | 1663 | G    | C5-C6-N1    | 6.62  | 114.81                 | 111.50              |
| 54  | BA    | 2055 | C    | N3-C2-O2    | -6.62 | 117.27                 | 121.90              |
| 21  | AA    | 432  | A    | C5-C6-N1    | 6.62  | 121.01                 | 117.70              |
| 21  | AA    | 489  | C    | O4'-C1'-N1  | 6.62  | 113.50                 | 108.20              |
| 21  | AA    | 526  | C    | N3-C2-O2    | -6.62 | 117.27                 | 121.90              |
| 21  | AA    | 1189 | U    | C5-C6-N1    | -6.62 | 119.39                 | 122.70              |
| 54  | BA    | 1595 | C    | N3-C4-C5    | 6.62  | 124.55                 | 121.90              |
| 55  | BB    | 30   | C    | O4'-C1'-N1  | 6.62  | 113.49                 | 108.20              |
| 46  | BX    | 26   | ARG  | NE-CZ-NH1   | 6.62  | 123.61                 | 120.30              |
| 54  | BA    | 341  | C    | O4'-C1'-N1  | 6.62  | 113.49                 | 108.20              |
| 54  | BA    | 832  | U    | O4'-C1'-N1  | 6.62  | 113.49                 | 108.20              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 54  | BA    | 1863 | G    | N1-C6-O6   | -6.62 | 115.93      | 119.90   |
| 2   | AC    | 142  | ARG  | NE-CZ-NH2  | -6.62 | 116.99      | 120.30   |
| 21  | AA    | 6    | G    | C8-N9-C4   | -6.62 | 103.75      | 106.40   |
| 54  | BA    | 838  | C    | N3-C2-O2   | -6.62 | 117.27      | 121.90   |
| 54  | BA    | 1634 | A    | C4-C5-C6   | -6.62 | 113.69      | 117.00   |
| 54  | BA    | 1771 | C    | N3-C2-O2   | -6.62 | 117.27      | 121.90   |
| 54  | BA    | 2265 | U    | O4'-C1'-N1 | 6.62  | 113.49      | 108.20   |
| 54  | BA    | 2300 | C    | N3-C2-O2   | -6.62 | 117.27      | 121.90   |
| 54  | BA    | 981  | A    | C4-C5-C6   | -6.61 | 113.69      | 117.00   |
| 54  | BA    | 1368 | G    | N3-C4-C5   | -6.61 | 125.29      | 128.60   |
| 54  | BA    | 462  | C    | O4'-C1'-N1 | 6.61  | 113.49      | 108.20   |
| 21  | AA    | 315  | A    | C5-C6-N1   | 6.61  | 121.00      | 117.70   |
| 54  | BA    | 758  | C    | N1-C2-O2   | 6.61  | 122.86      | 118.90   |
| 54  | BA    | 1848 | A    | C5-C6-N1   | 6.61  | 121.00      | 117.70   |
| 54  | BA    | 2162 | G    | C8-N9-C4   | -6.61 | 103.76      | 106.40   |
| 54  | BA    | 2420 | C    | N3-C2-O2   | -6.61 | 117.27      | 121.90   |
| 54  | BA    | 278  | A    | N1-C6-N6   | -6.61 | 114.64      | 118.60   |
| 54  | BA    | 988  | A    | C4-C5-C6   | -6.61 | 113.70      | 117.00   |
| 54  | BA    | 1248 | G    | N3-C4-C5   | -6.61 | 125.30      | 128.60   |
| 54  | BA    | 2874 | C    | N3-C2-O2   | -6.61 | 117.28      | 121.90   |
| 24  | A3    | 68   | C    | N3-C2-O2   | -6.60 | 117.28      | 121.90   |
| 12  | AM    | 2    | ARG  | NE-CZ-NH2  | 6.60  | 123.60      | 120.30   |
| 54  | BA    | 560  | C    | N3-C2-O2   | -6.60 | 117.28      | 121.90   |
| 54  | BA    | 1049 | C    | N3-C2-O2   | -6.60 | 117.28      | 121.90   |
| 21  | AA    | 715  | A    | C4-C5-C6   | -6.60 | 113.70      | 117.00   |
| 54  | BA    | 2000 | C    | N3-C2-O2   | -6.60 | 117.28      | 121.90   |
| 54  | BA    | 577  | G    | N1-C6-O6   | -6.60 | 115.94      | 119.90   |
| 54  | BA    | 699  | A    | C4-C5-C6   | -6.60 | 113.70      | 117.00   |
| 54  | BA    | 912  | C    | N3-C2-O2   | -6.60 | 117.28      | 121.90   |
| 54  | BA    | 1937 | A    | C5-C6-N1   | 6.60  | 121.00      | 117.70   |
| 54  | BA    | 2037 | A    | N1-C6-N6   | -6.60 | 114.64      | 118.60   |
| 55  | BB    | 15   | A    | C4-C5-C6   | -6.60 | 113.70      | 117.00   |
| 54  | BA    | 1352 | U    | C5-C6-N1   | -6.60 | 119.40      | 122.70   |
| 21  | AA    | 630  | A    | C5-C6-N1   | 6.59  | 121.00      | 117.70   |
| 21  | AA    | 1341 | U    | O4'-C1'-N1 | 6.59  | 113.48      | 108.20   |
| 54  | BA    | 1169 | A    | C5-C6-N1   | 6.59  | 121.00      | 117.70   |
| 21  | AA    | 1487 | G    | C8-N9-C4   | -6.59 | 103.76      | 106.40   |
| 21  | AA    | 277  | C    | N3-C2-O2   | -6.59 | 117.29      | 121.90   |
| 21  | AA    | 1381 | U    | N3-C2-O2   | -6.59 | 117.59      | 122.20   |
| 54  | BA    | 378  | C    | N3-C4-C5   | 6.59  | 124.54      | 121.90   |
| 54  | BA    | 617  | G    | C5-C6-N1   | 6.59  | 114.80      | 111.50   |
| 54  | BA    | 2723 | C    | N3-C4-C5   | 6.59  | 124.54      | 121.90   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|-------------|-------|------------------------|---------------------|
| 54  | BA    | 2860 | A    | C5-C6-N1    | 6.59  | 121.00                 | 117.70              |
| 54  | BA    | 609  | A    | N1-C6-N6    | -6.59 | 114.65                 | 118.60              |
| 54  | BA    | 2030 | A    | C4-C5-C6    | -6.59 | 113.70                 | 117.00              |
| 54  | BA    | 2875 | C    | N3-C2-O2    | -6.59 | 117.29                 | 121.90              |
| 15  | AP    | 56   | ARG  | NE-CZ-NH1   | 6.59  | 123.59                 | 120.30              |
| 21  | AA    | 101  | A    | C4-C5-C6    | -6.59 | 113.71                 | 117.00              |
| 54  | BA    | 1451 | C    | N1-C2-O2    | 6.59  | 122.85                 | 118.90              |
| 21  | AA    | 207  | C    | N3-C2-O2    | -6.59 | 117.29                 | 121.90              |
| 21  | AA    | 560  | A    | C4-C5-C6    | -6.59 | 113.71                 | 117.00              |
| 54  | BA    | 219  | A    | C5-C6-N1    | 6.59  | 120.99                 | 117.70              |
| 54  | BA    | 1870 | C    | N1-C2-O2    | 6.59  | 122.85                 | 118.90              |
| 54  | BA    | 2312 | U    | O4'-C1'-N1  | 6.59  | 113.47                 | 108.20              |
| 54  | BA    | 2432 | A    | C5-C6-N1    | 6.59  | 120.99                 | 117.70              |
| 21  | AA    | 327  | A    | N1-C6-N6    | -6.58 | 114.65                 | 118.60              |
| 21  | AA    | 1172 | C    | N3-C2-O2    | -6.58 | 117.29                 | 121.90              |
| 21  | AA    | 1201 | A    | C5-C6-N1    | 6.58  | 120.99                 | 117.70              |
| 50  | B1    | 43   | ARG  | NE-CZ-NH1   | 6.58  | 123.59                 | 120.30              |
| 54  | BA    | 1774 | C    | N1-C2-O2    | 6.58  | 122.85                 | 118.90              |
| 54  | BA    | 2175 | C    | N3-C2-O2    | -6.58 | 117.29                 | 121.90              |
| 54  | BA    | 2340 | A    | N1-C6-N6    | -6.58 | 114.65                 | 118.60              |
| 54  | BA    | 255  | A    | C5-C6-N1    | 6.58  | 120.99                 | 117.70              |
| 54  | BA    | 941  | A    | C4-C5-C6    | -6.58 | 113.71                 | 117.00              |
| 54  | BA    | 2169 | A    | O4'-C1'-N9  | 6.58  | 113.47                 | 108.20              |
| 54  | BA    | 183  | C    | O4'-C1'-N1  | 6.58  | 113.47                 | 108.20              |
| 54  | BA    | 1352 | U    | N1-C2-N3    | 6.58  | 118.85                 | 114.90              |
| 54  | BA    | 1991 | U    | C5-C6-N1    | -6.58 | 119.41                 | 122.70              |
| 54  | BA    | 1713 | A    | C5-C6-N1    | 6.58  | 120.99                 | 117.70              |
| 24  | A3    | 63   | C    | N3-C2-O2    | -6.58 | 117.30                 | 121.90              |
| 54  | BA    | 1301 | A    | N1-C6-N6    | -6.58 | 114.65                 | 118.60              |
| 54  | BA    | 1978 | A    | N1-C6-N6    | -6.58 | 114.65                 | 118.60              |
| 54  | BA    | 2374 | C    | N1-C2-O2    | 6.58  | 122.85                 | 118.90              |
| 24  | A3    | 38   | A    | C5-C6-N1    | 6.58  | 120.99                 | 117.70              |
| 54  | BA    | 687  | C    | O4'-C1'-N1  | 6.58  | 113.46                 | 108.20              |
| 54  | BA    | 1691 | C    | N3-C2-O2    | -6.58 | 117.30                 | 121.90              |
| 3   | AD    | 103  | ARG  | NE-CZ-NH1   | 6.58  | 123.59                 | 120.30              |
| 21  | AA    | 300  | A    | C5-C6-N1    | 6.58  | 120.99                 | 117.70              |
| 21  | AA    | 308  | C    | N1-C2-O2    | 6.58  | 122.84                 | 118.90              |
| 21  | AA    | 566  | G    | N3-C4-C5    | -6.58 | 125.31                 | 128.60              |
| 21  | AA    | 1128 | C    | N3-C2-O2    | -6.58 | 117.30                 | 121.90              |
| 54  | BA    | 2494 | G    | N1-C6-O6    | -6.58 | 115.95                 | 119.90              |
| 21  | AA    | 36   | C    | C5'-C4'-C3' | -6.57 | 105.48                 | 116.00              |
| 54  | BA    | 420  | C    | N3-C2-O2    | -6.57 | 117.30                 | 121.90              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 54  | BA    | 1453 | A    | C4-C5-C6    | -6.57 | 113.71      | 117.00   |
| 54  | BA    | 2835 | A    | C5-C6-N1    | 6.57  | 120.99      | 117.70   |
| 21  | AA    | 165  | G    | N1-C6-O6    | -6.57 | 115.96      | 119.90   |
| 21  | AA    | 274  | A    | C5-C6-N1    | 6.57  | 120.99      | 117.70   |
| 54  | BA    | 421  | C    | N3-C2-O2    | -6.57 | 117.30      | 121.90   |
| 54  | BA    | 2478 | A    | C5-C6-N1    | 6.57  | 120.99      | 117.70   |
| 21  | AA    | 321  | A    | C4-C5-C6    | -6.57 | 113.71      | 117.00   |
| 21  | AA    | 1029 | U    | N3-C2-O2    | -6.57 | 117.60      | 122.20   |
| 54  | BA    | 1971 | U    | O4'-C1'-N1  | 6.57  | 113.46      | 108.20   |
| 21  | AA    | 1408 | A    | N1-C6-N6    | -6.57 | 114.66      | 118.60   |
| 21  | AA    | 511  | C    | N3-C2-O2    | -6.57 | 117.30      | 121.90   |
| 21  | AA    | 595  | A    | N1-C6-N6    | -6.57 | 114.66      | 118.60   |
| 22  | A1    | 60   | C    | N1-C2-O2    | 6.57  | 122.84      | 118.90   |
| 42  | BT    | 73   | ARG  | NE-CZ-NH1   | 6.57  | 123.58      | 120.30   |
| 54  | BA    | 820  | A    | N1-C6-N6    | -6.57 | 114.66      | 118.60   |
| 54  | BA    | 2338 | C    | N3-C2-O2    | -6.57 | 117.30      | 121.90   |
| 54  | BA    | 2354 | C    | N3-C2-O2    | -6.57 | 117.30      | 121.90   |
| 21  | AA    | 610  | U    | C1'-O4'-C4' | -6.57 | 104.65      | 109.90   |
| 54  | BA    | 255  | A    | N1-C6-N6    | -6.57 | 114.66      | 118.60   |
| 54  | BA    | 269  | C    | O4'-C1'-N1  | 6.57  | 113.45      | 108.20   |
| 54  | BA    | 1028 | A    | C4-C5-C6    | -6.57 | 113.72      | 117.00   |
| 54  | BA    | 2096 | C    | N3-C2-O2    | -6.57 | 117.30      | 121.90   |
| 21  | AA    | 251  | G    | C8-N9-C4    | -6.56 | 103.77      | 106.40   |
| 54  | BA    | 415  | A    | C5-C6-N1    | 6.56  | 120.98      | 117.70   |
| 54  | BA    | 1562 | U    | C5-C6-N1    | -6.56 | 119.42      | 122.70   |
| 21  | AA    | 381  | C    | N3-C2-O2    | -6.56 | 117.31      | 121.90   |
| 21  | AA    | 580  | C    | N3-C2-O2    | -6.56 | 117.31      | 121.90   |
| 54  | BA    | 1788 | C    | N1-C2-O2    | 6.56  | 122.84      | 118.90   |
| 17  | AR    | 72   | ARG  | NE-CZ-NH1   | 6.56  | 123.58      | 120.30   |
| 54  | BA    | 474  | G    | O4'-C1'-N9  | 6.56  | 113.45      | 108.20   |
| 54  | BA    | 2060 | A    | C6-C5-N7    | 6.56  | 136.89      | 132.30   |
| 54  | BA    | 2539 | C    | N3-C2-O2    | -6.56 | 117.31      | 121.90   |
| 21  | AA    | 379  | C    | N1-C2-O2    | 6.56  | 122.83      | 118.90   |
| 36  | BN    | 22   | ARG  | NE-CZ-NH1   | 6.56  | 123.58      | 120.30   |
| 54  | BA    | 501  | A    | N1-C6-N6    | -6.56 | 114.67      | 118.60   |
| 54  | BA    | 575  | A    | C1'-O4'-C4' | -6.56 | 104.65      | 109.90   |
| 54  | BA    | 586  | A    | N1-C6-N6    | -6.56 | 114.67      | 118.60   |
| 54  | BA    | 2873 | A    | C5-C6-N1    | 6.56  | 120.98      | 117.70   |
| 54  | BA    | 1173 | U    | O4'-C1'-N1  | 6.55  | 113.44      | 108.20   |
| 54  | BA    | 2053 | G    | N3-C2-N2    | -6.55 | 115.31      | 119.90   |
| 54  | BA    | 2343 | U    | O4'-C1'-N1  | 6.55  | 113.44      | 108.20   |
| 54  | BA    | 2173 | A    | C5-C6-N1    | 6.55  | 120.98      | 117.70   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 21  | AA    | 111  | G    | C5-C6-N1   | 6.55  | 114.78      | 111.50   |
| 21  | AA    | 1093 | A    | N1-C6-N6   | -6.55 | 114.67      | 118.60   |
| 29  | BG    | 151  | ARG  | NE-CZ-NH1  | 6.55  | 123.58      | 120.30   |
| 54  | BA    | 2327 | A    | C5-C6-N1   | 6.55  | 120.98      | 117.70   |
| 54  | BA    | 2345 | G    | C5-C6-N1   | 6.55  | 114.78      | 111.50   |
| 54  | BA    | 2820 | A    | C4-C5-C6   | -6.55 | 113.72      | 117.00   |
| 21  | AA    | 5    | U    | O4'-C1'-N1 | 6.55  | 113.44      | 108.20   |
| 21  | AA    | 969  | A    | C4-C5-C6   | -6.55 | 113.72      | 117.00   |
| 54  | BA    | 197  | A    | C5-C6-N1   | 6.55  | 120.97      | 117.70   |
| 54  | BA    | 670  | A    | P-O3'-C3'  | 6.55  | 127.56      | 119.70   |
| 54  | BA    | 996  | A    | C5-C6-N1   | 6.55  | 120.97      | 117.70   |
| 54  | BA    | 1309 | G    | O4'-C1'-N9 | 6.55  | 113.44      | 108.20   |
| 54  | BA    | 1872 | A    | C4-C5-C6   | -6.55 | 113.73      | 117.00   |
| 54  | BA    | 2789 | C    | N3-C2-O2   | -6.55 | 117.31      | 121.90   |
| 21  | AA    | 1004 | A    | C4-C5-C6   | -6.55 | 113.73      | 117.00   |
| 54  | BA    | 554  | U    | O4'-C1'-N1 | 6.55  | 113.44      | 108.20   |
| 21  | AA    | 445  | G    | N1-C6-O6   | -6.55 | 115.97      | 119.90   |
| 54  | BA    | 221  | A    | C5-C6-N1   | 6.55  | 120.97      | 117.70   |
| 54  | BA    | 532  | A    | C2-N3-C4   | 6.55  | 113.87      | 110.60   |
| 54  | BA    | 1639 | C    | N3-C2-O2   | -6.55 | 117.32      | 121.90   |
| 54  | BA    | 2820 | A    | C5-C6-N1   | 6.55  | 120.97      | 117.70   |
| 54  | BA    | 660  | C    | N3-C2-O2   | -6.54 | 117.32      | 121.90   |
| 54  | BA    | 2076 | U    | N3-C2-O2   | -6.54 | 117.62      | 122.20   |
| 21  | AA    | 1121 | U    | O4'-C1'-N1 | 6.54  | 113.44      | 108.20   |
| 54  | BA    | 1230 | A    | C5-C6-N1   | 6.54  | 120.97      | 117.70   |
| 54  | BA    | 2078 | C    | N3-C2-O2   | -6.54 | 117.32      | 121.90   |
| 21  | AA    | 1259 | C    | N3-C2-O2   | -6.54 | 117.32      | 121.90   |
| 54  | BA    | 364  | C    | O4'-C1'-N1 | 6.54  | 113.43      | 108.20   |
| 54  | BA    | 727  | A    | C4-C5-C6   | -6.54 | 113.73      | 117.00   |
| 54  | BA    | 2258 | C    | N3-C2-O2   | -6.54 | 117.32      | 121.90   |
| 17  | AR    | 47   | ARG  | NE-CZ-NH1  | 6.54  | 123.57      | 120.30   |
| 51  | B2    | 41   | ARG  | NE-CZ-NH1  | 6.54  | 123.57      | 120.30   |
| 54  | BA    | 1996 | C    | O4'-C1'-N1 | 6.54  | 113.43      | 108.20   |
| 54  | BA    | 2147 | A    | C5-C6-N1   | 6.54  | 120.97      | 117.70   |
| 54  | BA    | 2225 | A    | N1-C6-N6   | -6.54 | 114.68      | 118.60   |
| 54  | BA    | 2646 | C    | N3-C2-O2   | -6.54 | 117.32      | 121.90   |
| 54  | BA    | 608  | A    | C4-C5-C6   | -6.54 | 113.73      | 117.00   |
| 54  | BA    | 2278 | A    | C5-C6-N1   | 6.54  | 120.97      | 117.70   |
| 24  | A3    | 24   | C    | N3-C2-O2   | -6.53 | 117.33      | 121.90   |
| 54  | BA    | 1402 | U    | C5-C6-N1   | -6.53 | 119.43      | 122.70   |
| 21  | AA    | 816  | A    | C5-C6-N1   | 6.53  | 120.97      | 117.70   |
| 21  | AA    | 81   | A    | C5-C6-N1   | 6.53  | 120.96      | 117.70   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 21  | AA    | 430  | A    | C5-C6-N1   | 6.53  | 120.96      | 117.70   |
| 54  | BA    | 1936 | A    | C4-C5-C6   | -6.53 | 113.74      | 117.00   |
| 54  | BA    | 2117 | A    | C5-C6-N1   | 6.53  | 120.96      | 117.70   |
| 54  | BA    | 2458 | G    | N3-C4-C5   | -6.53 | 125.34      | 128.60   |
| 22  | A1    | 73   | A    | C4-C5-C6   | -6.53 | 113.74      | 117.00   |
| 54  | BA    | 1304 | A    | C4-C5-C6   | -6.53 | 113.74      | 117.00   |
| 54  | BA    | 1502 | A    | C5-C6-N1   | 6.53  | 120.96      | 117.70   |
| 54  | BA    | 2032 | G    | N7-C8-N9   | 6.53  | 116.36      | 113.10   |
| 21  | AA    | 453  | G    | C8-N9-C4   | -6.52 | 103.79      | 106.40   |
| 54  | BA    | 423  | A    | C4-C5-C6   | -6.52 | 113.74      | 117.00   |
| 21  | AA    | 215  | C    | O4'-C1'-N1 | 6.52  | 113.42      | 108.20   |
| 21  | AA    | 373  | A    | C4-C5-C6   | -6.52 | 113.74      | 117.00   |
| 21  | AA    | 1279 | G    | N1-C6-O6   | -6.52 | 115.99      | 119.90   |
| 54  | BA    | 791  | C    | N3-C2-O2   | -6.52 | 117.33      | 121.90   |
| 54  | BA    | 1480 | C    | O4'-C1'-N1 | 6.52  | 113.42      | 108.20   |
| 54  | BA    | 1505 | A    | C4-C5-C6   | -6.52 | 113.74      | 117.00   |
| 54  | BA    | 2644 | G    | N3-C2-N2   | -6.52 | 115.33      | 119.90   |
| 21  | AA    | 115  | G    | C5-C6-N1   | 6.52  | 114.76      | 111.50   |
| 21  | AA    | 996  | A    | C4-C5-C6   | -6.52 | 113.74      | 117.00   |
| 22  | A1    | 43   | G    | N1-C6-O6   | -6.52 | 115.99      | 119.90   |
| 54  | BA    | 1793 | C    | N3-C4-C5   | 6.52  | 124.51      | 121.90   |
| 21  | AA    | 609  | A    | C4-C5-C6   | -6.52 | 113.74      | 117.00   |
| 54  | BA    | 310  | A    | C5-C6-N1   | 6.52  | 120.96      | 117.70   |
| 54  | BA    | 1103 | A    | N1-C6-N6   | -6.52 | 114.69      | 118.60   |
| 54  | BA    | 1344 | U    | O4'-C1'-N1 | 6.52  | 113.41      | 108.20   |
| 21  | AA    | 52   | C    | N3-C2-O2   | -6.51 | 117.34      | 121.90   |
| 21  | AA    | 502  | A    | N1-C6-N6   | -6.51 | 114.69      | 118.60   |
| 54  | BA    | 1502 | A    | N1-C6-N6   | -6.51 | 114.69      | 118.60   |
| 54  | BA    | 2764 | A    | C5-C6-N1   | 6.51  | 120.96      | 117.70   |
| 12  | AM    | 92   | ARG  | NE-CZ-NH1  | 6.51  | 123.56      | 120.30   |
| 21  | AA    | 810  | C    | N3-C2-O2   | -6.51 | 117.34      | 121.90   |
| 54  | BA    | 812  | C    | N3-C2-O2   | -6.51 | 117.34      | 121.90   |
| 54  | BA    | 934  | U    | O4'-C1'-N1 | 6.51  | 113.41      | 108.20   |
| 54  | BA    | 1300 | G    | P-O3'-C3'  | 6.51  | 127.51      | 119.70   |
| 23  | A2    | 82   | A    | C4-C5-C6   | -6.51 | 113.75      | 117.00   |
| 21  | AA    | 703  | G    | N1-C6-O6   | -6.51 | 116.00      | 119.90   |
| 21  | AA    | 1507 | A    | C5-C6-N1   | 6.51  | 120.95      | 117.70   |
| 25  | BC    | 166  | ARG  | NE-CZ-NH1  | 6.51  | 123.55      | 120.30   |
| 21  | AA    | 274  | A    | C4-C5-C6   | -6.51 | 113.75      | 117.00   |
| 54  | BA    | 1304 | A    | N1-C6-N6   | -6.51 | 114.70      | 118.60   |
| 54  | BA    | 1833 | C    | N3-C2-O2   | -6.51 | 117.35      | 121.90   |
| 54  | BA    | 154  | U    | C5-C6-N1   | -6.50 | 119.45      | 122.70   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|-------------|-------|------------------------|---------------------|
| 54  | BA    | 1650 | A    | C4-C5-C6    | -6.50 | 113.75                 | 117.00              |
| 21  | AA    | 620  | C    | N3-C2-O2    | -6.50 | 117.35                 | 121.90              |
| 21  | AA    | 787  | A    | N1-C6-N6    | -6.50 | 114.70                 | 118.60              |
| 21  | AA    | 1493 | A    | N1-C6-N6    | -6.50 | 114.70                 | 118.60              |
| 54  | BA    | 256  | A    | C5-C6-N1    | 6.50  | 120.95                 | 117.70              |
| 54  | BA    | 1398 | C    | N3-C2-O2    | -6.50 | 117.35                 | 121.90              |
| 54  | BA    | 1938 | A    | O4'-C1'-N9  | 6.50  | 113.40                 | 108.20              |
| 21  | AA    | 874  | G    | N1-C6-O6    | -6.50 | 116.00                 | 119.90              |
| 54  | BA    | 180  | G    | O4'-C1'-N9  | 6.50  | 113.40                 | 108.20              |
| 54  | BA    | 1126 | A    | C5-C6-N1    | 6.50  | 120.95                 | 117.70              |
| 54  | BA    | 811  | U    | O4'-C1'-N1  | 6.50  | 113.40                 | 108.20              |
| 21  | AA    | 484  | G    | C8-N9-C4    | -6.50 | 103.80                 | 106.40              |
| 21  | AA    | 530  | G    | N3-C4-C5    | -6.50 | 125.35                 | 128.60              |
| 54  | BA    | 730  | A    | C5-C6-N1    | 6.50  | 120.95                 | 117.70              |
| 54  | BA    | 1436 | G    | C8-N9-C4    | -6.50 | 103.80                 | 106.40              |
| 21  | AA    | 481  | G    | N1-C6-O6    | -6.50 | 116.00                 | 119.90              |
| 21  | AA    | 1238 | A    | C4-C5-C6    | -6.50 | 113.75                 | 117.00              |
| 20  | AU    | 32   | ARG  | NE-CZ-NH1   | 6.49  | 123.55                 | 120.30              |
| 54  | BA    | 2573 | C    | N3-C2-O2    | -6.49 | 117.36                 | 121.90              |
| 21  | AA    | 32   | A    | C5-C6-N1    | 6.49  | 120.94                 | 117.70              |
| 21  | AA    | 578  | C    | N3-C2-O2    | -6.49 | 117.36                 | 121.90              |
| 29  | BG    | 162  | ARG  | NE-CZ-NH1   | 6.49  | 123.55                 | 120.30              |
| 54  | BA    | 1286 | A    | C5-C6-N1    | 6.49  | 120.94                 | 117.70              |
| 54  | BA    | 1662 | U    | O4'-C1'-N1  | 6.49  | 113.39                 | 108.20              |
| 21  | AA    | 374  | A    | C5-C6-N1    | 6.49  | 120.94                 | 117.70              |
| 38  | BP    | 102  | ARG  | NE-CZ-NH1   | 6.49  | 123.54                 | 120.30              |
| 54  | BA    | 1417 | C    | O4'-C1'-N1  | 6.49  | 113.39                 | 108.20              |
| 54  | BA    | 2031 | A    | C3'-C2'-C1' | 6.49  | 106.69                 | 101.50              |
| 54  | BA    | 1930 | G    | C3'-C2'-C1' | -6.49 | 96.31                  | 101.50              |
| 21  | AA    | 181  | A    | C4-C5-C6    | -6.49 | 113.76                 | 117.00              |
| 21  | AA    | 401  | C    | N3-C2-O2    | -6.49 | 117.36                 | 121.90              |
| 21  | AA    | 1251 | A    | C4-C5-C6    | -6.49 | 113.76                 | 117.00              |
| 35  | BM    | 18   | ARG  | NE-CZ-NH1   | 6.49  | 123.54                 | 120.30              |
| 54  | BA    | 2166 | U    | C5-C6-N1    | -6.49 | 119.46                 | 122.70              |
| 54  | BA    | 2340 | A    | C4-C5-C6    | -6.49 | 113.76                 | 117.00              |
| 21  | AA    | 5    | U    | N3-C2-O2    | -6.48 | 117.66                 | 122.20              |
| 21  | AA    | 320  | A    | N1-C6-N6    | -6.48 | 114.71                 | 118.60              |
| 44  | BV    | 19   | ARG  | NE-CZ-NH1   | 6.48  | 123.54                 | 120.30              |
| 21  | AA    | 330  | C    | N3-C2-O2    | -6.48 | 117.36                 | 121.90              |
| 54  | BA    | 138  | U    | N3-C2-O2    | -6.48 | 117.67                 | 122.20              |
| 54  | BA    | 2693 | G    | C5-C6-N1    | 6.48  | 114.74                 | 111.50              |
| 21  | AA    | 462  | G    | N9-C4-C5    | 6.48  | 107.99                 | 105.40              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|-------------|-------|------------------------|---------------------|
| 21  | AA    | 487  | A    | C5-C6-N1    | 6.48  | 120.94                 | 117.70              |
| 54  | BA    | 2097 | A    | O4'-C1'-N9  | 6.48  | 113.38                 | 108.20              |
| 54  | BA    | 2590 | A    | O4'-C1'-N9  | 6.48  | 113.38                 | 108.20              |
| 54  | BA    | 2837 | A    | C5-C6-N1    | 6.48  | 120.94                 | 117.70              |
| 55  | BB    | 80   | U    | O4'-C1'-N1  | 6.48  | 113.38                 | 108.20              |
| 21  | AA    | 330  | C    | N3-C4-C5    | 6.47  | 124.49                 | 121.90              |
| 21  | AA    | 458  | U    | C5-C6-N1    | -6.47 | 119.46                 | 122.70              |
| 21  | AA    | 1117 | A    | C4-C5-C6    | -6.47 | 113.76                 | 117.00              |
| 21  | AA    | 1364 | U    | N3-C2-O2    | -6.47 | 117.67                 | 122.20              |
| 37  | BO    | 10   | ARG  | NE-CZ-NH1   | 6.47  | 123.54                 | 120.30              |
| 54  | BA    | 1472 | C    | N3-C2-O2    | -6.47 | 117.37                 | 121.90              |
| 21  | AA    | 182  | A    | C5-C6-N1    | 6.47  | 120.94                 | 117.70              |
| 21  | AA    | 282  | A    | C5-C6-N1    | 6.47  | 120.94                 | 117.70              |
| 54  | BA    | 816  | C    | N3-C2-O2    | -6.47 | 117.37                 | 121.90              |
| 54  | BA    | 1155 | A    | C5-C6-N1    | 6.47  | 120.94                 | 117.70              |
| 54  | BA    | 1606 | C    | O4'-C1'-N1  | 6.47  | 113.38                 | 108.20              |
| 54  | BA    | 1476 | U    | C5-C6-N1    | -6.47 | 119.47                 | 122.70              |
| 54  | BA    | 2020 | A    | C4-C5-C6    | -6.47 | 113.76                 | 117.00              |
| 21  | AA    | 1218 | C    | N3-C2-O2    | -6.47 | 117.37                 | 121.90              |
| 54  | BA    | 639  | U    | O4'-C1'-N1  | 6.47  | 113.38                 | 108.20              |
| 54  | BA    | 719  | C    | O4'-C1'-N1  | 6.47  | 113.38                 | 108.20              |
| 21  | AA    | 696  | A    | C4-C5-C6    | -6.47 | 113.77                 | 117.00              |
| 21  | AA    | 719  | C    | N3-C2-O2    | -6.47 | 117.37                 | 121.90              |
| 54  | BA    | 1158 | C    | N3-C2-O2    | -6.47 | 117.37                 | 121.90              |
| 54  | BA    | 1293 | C    | O4'-C1'-N1  | 6.47  | 113.37                 | 108.20              |
| 54  | BA    | 1745 | A    | C5-C6-N1    | 6.47  | 120.93                 | 117.70              |
| 54  | BA    | 2861 | U    | O4'-C1'-N1  | 6.47  | 113.37                 | 108.20              |
| 21  | AA    | 80   | A    | C4-C5-C6    | -6.46 | 113.77                 | 117.00              |
| 21  | AA    | 607  | A    | C4-C5-C6    | -6.46 | 113.77                 | 117.00              |
| 21  | AA    | 641  | U    | C3'-C2'-C1' | 6.46  | 106.67                 | 101.50              |
| 21  | AA    | 1141 | C    | N3-C2-O2    | -6.46 | 117.38                 | 121.90              |
| 54  | BA    | 685  | A    | N1-C6-N6    | -6.46 | 114.72                 | 118.60              |
| 54  | BA    | 2649 | C    | N3-C2-O2    | -6.46 | 117.38                 | 121.90              |
| 54  | BA    | 2717 | C    | O4'-C1'-N1  | 6.46  | 113.37                 | 108.20              |
| 54  | BA    | 1869 | G    | N1-C6-O6    | -6.46 | 116.02                 | 119.90              |
| 3   | AD    | 46   | ARG  | NE-CZ-NH1   | 6.46  | 123.53                 | 120.30              |
| 21  | AA    | 1110 | A    | C5-C6-N1    | 6.46  | 120.93                 | 117.70              |
| 56  | B5    | 7    | ARG  | NE-CZ-NH1   | 6.46  | 123.53                 | 120.30              |
| 21  | AA    | 177  | G    | N3-C4-C5    | -6.46 | 125.37                 | 128.60              |
| 21  | AA    | 271  | C    | N3-C2-O2    | -6.46 | 117.38                 | 121.90              |
| 54  | BA    | 1912 | A    | C4-C5-C6    | -6.46 | 113.77                 | 117.00              |
| 21  | AA    | 156  | C    | N3-C4-N4    | -6.46 | 113.48                 | 118.00              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|-------------|-------|------------------------|---------------------|
| 21  | AA    | 174  | A    | C5-C6-N1    | 6.46  | 120.93                 | 117.70              |
| 21  | AA    | 549  | C    | N3-C2-O2    | -6.46 | 117.38                 | 121.90              |
| 21  | AA    | 1252 | A    | C4-C5-C6    | -6.46 | 113.77                 | 117.00              |
| 21  | AA    | 1303 | C    | N3-C2-O2    | -6.46 | 117.38                 | 121.90              |
| 41  | BS    | 25   | ARG  | NE-CZ-NH1   | 6.46  | 123.53                 | 120.30              |
| 54  | BA    | 314  | C    | N3-C2-O2    | -6.46 | 117.38                 | 121.90              |
| 54  | BA    | 590  | A    | C4-C5-C6    | -6.46 | 113.77                 | 117.00              |
| 21  | AA    | 55   | A    | C5-C6-N1    | 6.46  | 120.93                 | 117.70              |
| 54  | BA    | 180  | G    | N1-C6-O6    | -6.46 | 116.03                 | 119.90              |
| 54  | BA    | 632  | A    | C5-C6-N1    | 6.46  | 120.93                 | 117.70              |
| 54  | BA    | 1545 | A    | C4-C5-C6    | -6.46 | 113.77                 | 117.00              |
| 54  | BA    | 2094 | A    | N1-C6-N6    | -6.46 | 114.73                 | 118.60              |
| 54  | BA    | 1761 | C    | N1-C2-O2    | 6.46  | 122.77                 | 118.90              |
| 24  | A3    | 49   | C    | N3-C2-O2    | -6.45 | 117.38                 | 121.90              |
| 54  | BA    | 678  | C    | N3-C2-O2    | -6.45 | 117.38                 | 121.90              |
| 54  | BA    | 1032 | A    | N1-C6-N6    | -6.45 | 114.73                 | 118.60              |
| 54  | BA    | 2712 | C    | N3-C2-O2    | -6.45 | 117.38                 | 121.90              |
| 21  | AA    | 379  | C    | N3-C4-C5    | 6.45  | 124.48                 | 121.90              |
| 54  | BA    | 1439 | A    | C5-C6-N1    | 6.45  | 120.93                 | 117.70              |
| 54  | BA    | 1974 | C    | O4'-C1'-N1  | 6.45  | 113.36                 | 108.20              |
| 21  | AA    | 1478 | U    | N3-C2-O2    | -6.45 | 117.69                 | 122.20              |
| 54  | BA    | 565  | C    | N1-C2-O2    | 6.45  | 122.77                 | 118.90              |
| 54  | BA    | 1098 | A    | C4-C5-C6    | -6.45 | 113.78                 | 117.00              |
| 54  | BA    | 2355 | G    | N1-C6-O6    | -6.45 | 116.03                 | 119.90              |
| 21  | AA    | 432  | A    | C4-C5-C6    | -6.45 | 113.78                 | 117.00              |
| 21  | AA    | 452  | A    | N1-C6-N6    | -6.45 | 114.73                 | 118.60              |
| 28  | BF    | 94   | ARG  | NE-CZ-NH1   | 6.45  | 123.53                 | 120.30              |
| 54  | BA    | 1113 | U    | C5-C6-N1    | -6.45 | 119.47                 | 122.70              |
| 54  | BA    | 2381 | A    | C6-C5-N7    | 6.45  | 136.81                 | 132.30              |
| 54  | BA    | 692  | C    | N3-C2-O2    | -6.45 | 117.39                 | 121.90              |
| 54  | BA    | 1938 | A    | C4-C5-C6    | -6.45 | 113.78                 | 117.00              |
| 21  | AA    | 8    | A    | C5-C6-N1    | 6.45  | 120.92                 | 117.70              |
| 24  | A3    | 44   | A    | C5-C6-N1    | 6.45  | 120.92                 | 117.70              |
| 54  | BA    | 1735 | A    | C5-C6-N1    | 6.45  | 120.92                 | 117.70              |
| 54  | BA    | 1741 | C    | N1-C2-O2    | 6.45  | 122.77                 | 118.90              |
| 54  | BA    | 1985 | C    | N3-C2-O2    | -6.45 | 117.39                 | 121.90              |
| 54  | BA    | 2110 | G    | C3'-C2'-C1' | -6.45 | 96.34                  | 101.50              |
| 55  | BB    | 78   | A    | C5-C6-N1    | 6.45  | 120.92                 | 117.70              |
| 54  | BA    | 28   | A    | C4-C5-C6    | -6.44 | 113.78                 | 117.00              |
| 54  | BA    | 2358 | A    | C4-C5-C6    | -6.44 | 113.78                 | 117.00              |
| 55  | BB    | 46   | A    | C4-C5-C6    | -6.44 | 113.78                 | 117.00              |
| 23  | A2    | 79   | A    | C4-C5-C6    | -6.44 | 113.78                 | 117.00              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|------------|-------|------------------------|---------------------|
| 30  | BH    | 116  | ARG  | NE-CZ-NH2  | -6.44 | 117.08                 | 120.30              |
| 54  | BA    | 299  | A    | N1-C6-N6   | -6.44 | 114.73                 | 118.60              |
| 54  | BA    | 890  | C    | N3-C2-O2   | -6.44 | 117.39                 | 121.90              |
| 24  | A3    | 26   | C    | N3-C2-O2   | -6.44 | 117.39                 | 121.90              |
| 54  | BA    | 16   | C    | N3-C2-O2   | -6.44 | 117.39                 | 121.90              |
| 54  | BA    | 70   | G    | O4'-C1'-N9 | 6.44  | 113.35                 | 108.20              |
| 54  | BA    | 582  | A    | C6-C5-N7   | 6.44  | 136.81                 | 132.30              |
| 54  | BA    | 970  | U    | O4'-C1'-N1 | 6.44  | 113.35                 | 108.20              |
| 54  | BA    | 1028 | A    | C5-C6-N1   | 6.44  | 120.92                 | 117.70              |
| 54  | BA    | 1210 | G    | O4'-C1'-N9 | 6.44  | 113.35                 | 108.20              |
| 54  | BA    | 1580 | A    | C5-C6-N1   | 6.44  | 120.92                 | 117.70              |
| 21  | AA    | 896  | C    | N3-C2-O2   | -6.44 | 117.39                 | 121.90              |
| 54  | BA    | 188  | G    | N1-C6-O6   | -6.44 | 116.04                 | 119.90              |
| 54  | BA    | 2236 | U    | O4'-C1'-N1 | 6.44  | 113.35                 | 108.20              |
| 23  | A2    | 80   | C    | N1-C2-O2   | 6.44  | 122.76                 | 118.90              |
| 54  | BA    | 2191 | A    | C5-C6-N1   | 6.44  | 120.92                 | 117.70              |
| 54  | BA    | 2486 | C    | N3-C2-O2   | -6.44 | 117.39                 | 121.90              |
| 54  | BA    | 1175 | A    | C5-C6-N1   | 6.43  | 120.92                 | 117.70              |
| 55  | BB    | 22   | U    | O4'-C1'-N1 | 6.43  | 113.35                 | 108.20              |
| 54  | BA    | 411  | G    | N3-C2-N2   | -6.43 | 115.40                 | 119.90              |
| 54  | BA    | 1889 | A    | C4-C5-C6   | -6.43 | 113.78                 | 117.00              |
| 54  | BA    | 2858 | C    | N3-C2-O2   | -6.43 | 117.40                 | 121.90              |
| 54  | BA    | 1335 | C    | N3-C2-O2   | -6.43 | 117.40                 | 121.90              |
| 54  | BA    | 1868 | C    | N3-C2-O2   | -6.43 | 117.40                 | 121.90              |
| 24  | A3    | 62   | C    | N1-C2-O2   | 6.43  | 122.76                 | 118.90              |
| 21  | AA    | 418  | C    | N3-C2-O2   | -6.43 | 117.40                 | 121.90              |
| 21  | AA    | 610  | U    | O4'-C1'-N1 | 6.43  | 113.34                 | 108.20              |
| 21  | AA    | 1022 | A    | C4-C5-C6   | -6.43 | 113.79                 | 117.00              |
| 22  | A1    | 26   | A    | C4-C5-C6   | -6.43 | 113.79                 | 117.00              |
| 54  | BA    | 1583 | A    | N1-C6-N6   | -6.43 | 114.74                 | 118.60              |
| 54  | BA    | 2024 | G    | N1-C6-O6   | -6.43 | 116.04                 | 119.90              |
| 54  | BA    | 297  | G    | N1-C6-O6   | -6.42 | 116.05                 | 119.90              |
| 21  | AA    | 726  | C    | N3-C2-O2   | -6.42 | 117.40                 | 121.90              |
| 21  | AA    | 853  | C    | O4'-C1'-N1 | 6.42  | 113.34                 | 108.20              |
| 54  | BA    | 1553 | A    | N1-C6-N6   | -6.42 | 114.75                 | 118.60              |
| 54  | BA    | 2901 | C    | N3-C2-O2   | -6.42 | 117.40                 | 121.90              |
| 21  | AA    | 1363 | A    | C5-C6-N1   | 6.42  | 120.91                 | 117.70              |
| 3   | AD    | 127  | ARG  | NE-CZ-NH1  | 6.42  | 123.51                 | 120.30              |
| 21  | AA    | 231  | U    | O4'-C1'-N1 | 6.42  | 113.34                 | 108.20              |
| 21  | AA    | 459  | A    | C4-C5-C6   | -6.42 | 113.79                 | 117.00              |
| 21  | AA    | 779  | C    | O4'-C1'-N1 | 6.42  | 113.33                 | 108.20              |
| 54  | BA    | 13   | A    | C5-C6-N1   | 6.42  | 120.91                 | 117.70              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|-------------|-------|------------------------|---------------------|
| 54  | BA    | 227  | A    | C4-C5-C6    | -6.42 | 113.79                 | 117.00              |
| 54  | BA    | 564  | C    | N1-C2-O2    | 6.42  | 122.75                 | 118.90              |
| 54  | BA    | 1189 | A    | C4-C5-C6    | -6.42 | 113.79                 | 117.00              |
| 54  | BA    | 1590 | A    | N1-C6-N6    | -6.42 | 114.75                 | 118.60              |
| 54  | BA    | 2790 | U    | N3-C2-O2    | -6.42 | 117.71                 | 122.20              |
| 21  | AA    | 536  | C    | N3-C2-O2    | -6.42 | 117.41                 | 121.90              |
| 54  | BA    | 654  | A    | O4'-C1'-N9  | 6.42  | 113.33                 | 108.20              |
| 54  | BA    | 2205 | A    | N1-C6-N6    | -6.42 | 114.75                 | 118.60              |
| 21  | AA    | 167  | A    | C5-C6-N1    | 6.42  | 120.91                 | 117.70              |
| 54  | BA    | 1370 | C    | N3-C2-O2    | -6.42 | 117.41                 | 121.90              |
| 54  | BA    | 1586 | A    | N1-C6-N6    | -6.41 | 114.75                 | 118.60              |
| 21  | AA    | 344  | A    | C4-C5-C6    | -6.41 | 113.79                 | 117.00              |
| 21  | AA    | 926  | G    | N1-C6-O6    | -6.41 | 116.05                 | 119.90              |
| 21  | AA    | 990  | C    | N3-C2-O2    | -6.41 | 117.41                 | 121.90              |
| 21  | AA    | 1280 | A    | C5-C6-N1    | 6.41  | 120.91                 | 117.70              |
| 54  | BA    | 52   | A    | C4-C5-C6    | -6.41 | 113.80                 | 117.00              |
| 54  | BA    | 241  | A    | C4-C5-C6    | -6.41 | 113.80                 | 117.00              |
| 54  | BA    | 1056 | G    | N3-C4-C5    | -6.41 | 125.39                 | 128.60              |
| 54  | BA    | 1934 | C    | O4'-C1'-N1  | 6.41  | 113.33                 | 108.20              |
| 55  | BB    | 118  | C    | N1-C2-O2    | 6.41  | 122.75                 | 118.90              |
| 21  | AA    | 251  | G    | N7-C8-N9    | 6.41  | 116.30                 | 113.10              |
| 21  | AA    | 304  | U    | O4'-C1'-N1  | 6.41  | 113.33                 | 108.20              |
| 21  | AA    | 736  | C    | N3-C2-O2    | -6.41 | 117.41                 | 121.90              |
| 21  | AA    | 999  | C    | N3-C4-C5    | 6.41  | 124.46                 | 121.90              |
| 54  | BA    | 1143 | A    | C4-C5-C6    | -6.41 | 113.80                 | 117.00              |
| 54  | BA    | 1679 | A    | C4-C5-C6    | -6.41 | 113.80                 | 117.00              |
| 54  | BA    | 1744 | A    | C4-C5-C6    | -6.41 | 113.80                 | 117.00              |
| 54  | BA    | 1927 | A    | C5-C6-N1    | 6.41  | 120.91                 | 117.70              |
| 54  | BA    | 2578 | G    | C1'-O4'-C4' | -6.41 | 104.77                 | 109.90              |
| 54  | BA    | 757  | G    | C5-C6-N1    | 6.41  | 114.70                 | 111.50              |
| 54  | BA    | 1151 | A    | C4-C5-C6    | -6.41 | 113.80                 | 117.00              |
| 21  | AA    | 1324 | A    | C5-C6-N1    | 6.40  | 120.90                 | 117.70              |
| 21  | AA    | 664  | G    | N3-C4-C5    | -6.40 | 125.40                 | 128.60              |
| 54  | BA    | 581  | C    | N3-C2-O2    | -6.40 | 117.42                 | 121.90              |
| 54  | BA    | 2359 | C    | N3-C2-O2    | -6.40 | 117.42                 | 121.90              |
| 21  | AA    | 53   | A    | C5-C6-N1    | 6.40  | 120.90                 | 117.70              |
| 21  | AA    | 739  | C    | N3-C2-O2    | -6.40 | 117.42                 | 121.90              |
| 21  | AA    | 1130 | A    | N1-C6-N6    | -6.40 | 114.76                 | 118.60              |
| 32  | BJ    | 37   | ARG  | NE-CZ-NH2   | -6.40 | 117.10                 | 120.30              |
| 21  | AA    | 1134 | G    | N1-C6-O6    | -6.40 | 116.06                 | 119.90              |
| 54  | BA    | 450  | G    | N3-C4-C5    | -6.40 | 125.40                 | 128.60              |
| 54  | BA    | 572  | A    | N1-C6-N6    | -6.40 | 114.76                 | 118.60              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|-------------|-------|------------------------|---------------------|
| 54  | BA    | 661  | A    | C4-C5-C6    | -6.40 | 113.80                 | 117.00              |
| 54  | BA    | 921  | C    | N3-C2-O2    | -6.40 | 117.42                 | 121.90              |
| 54  | BA    | 2752 | C    | N3-C4-C5    | 6.40  | 124.46                 | 121.90              |
| 21  | AA    | 1299 | A    | C4-C5-C6    | -6.40 | 113.80                 | 117.00              |
| 38  | BP    | 100  | ARG  | NE-CZ-NH2   | -6.40 | 117.10                 | 120.30              |
| 54  | BA    | 540  | C    | N3-C2-O2    | -6.40 | 117.42                 | 121.90              |
| 54  | BA    | 908  | C    | N3-C2-O2    | -6.40 | 117.42                 | 121.90              |
| 54  | BA    | 1383 | A    | C4-C5-C6    | -6.40 | 113.80                 | 117.00              |
| 54  | BA    | 1609 | A    | C5-C6-N1    | 6.40  | 120.90                 | 117.70              |
| 54  | BA    | 2001 | C    | O4'-C1'-N1  | 6.39  | 113.32                 | 108.20              |
| 54  | BA    | 1823 | G    | C5-C6-N1    | 6.39  | 114.70                 | 111.50              |
| 54  | BA    | 2442 | C    | N3-C2-O2    | -6.39 | 117.42                 | 121.90              |
| 54  | BA    | 2757 | A    | N1-C6-N6    | -6.39 | 114.77                 | 118.60              |
| 21  | AA    | 569  | C    | N3-C2-O2    | -6.39 | 117.43                 | 121.90              |
| 21  | AA    | 709  | U    | O4'-C1'-N1  | 6.39  | 113.31                 | 108.20              |
| 21  | AA    | 941  | G    | N1-C6-O6    | -6.39 | 116.06                 | 119.90              |
| 21  | AA    | 1494 | G    | C8-N9-C4    | -6.39 | 103.84                 | 106.40              |
| 54  | BA    | 195  | A    | C4-C5-C6    | -6.39 | 113.81                 | 117.00              |
| 54  | BA    | 1498 | C    | N3-C2-O2    | -6.39 | 117.43                 | 121.90              |
| 54  | BA    | 2765 | A    | N1-C6-N6    | -6.39 | 114.77                 | 118.60              |
| 21  | AA    | 509  | A    | C4-C5-C6    | -6.39 | 113.81                 | 117.00              |
| 21  | AA    | 1108 | G    | N9-C4-C5    | 6.39  | 107.95                 | 105.40              |
| 54  | BA    | 32   | C    | N3-C2-O2    | -6.39 | 117.43                 | 121.90              |
| 54  | BA    | 2755 | C    | C3'-C2'-C1' | 6.39  | 106.61                 | 101.50              |
| 7   | AH    | 83   | ARG  | NE-CZ-NH1   | 6.39  | 123.49                 | 120.30              |
| 21  | AA    | 1070 | U    | O4'-C1'-N1  | 6.39  | 113.31                 | 108.20              |
| 54  | BA    | 473  | G    | C8-N9-C4    | -6.39 | 103.85                 | 106.40              |
| 54  | BA    | 1045 | C    | N3-C2-O2    | -6.39 | 117.43                 | 121.90              |
| 54  | BA    | 2758 | A    | N1-C6-N6    | -6.39 | 114.77                 | 118.60              |
| 21  | AA    | 288  | A    | C4-C5-C6    | -6.38 | 113.81                 | 117.00              |
| 21  | AA    | 1496 | C    | N3-C4-C5    | 6.38  | 124.45                 | 121.90              |
| 54  | BA    | 732  | C    | N3-C2-O2    | -6.38 | 117.43                 | 121.90              |
| 54  | BA    | 753  | A    | N1-C6-N6    | -6.38 | 114.77                 | 118.60              |
| 54  | BA    | 1807 | G    | O4'-C1'-N9  | 6.38  | 113.31                 | 108.20              |
| 54  | BA    | 2336 | A    | N1-C6-N6    | -6.38 | 114.77                 | 118.60              |
| 54  | BA    | 2619 | C    | O4'-C1'-N1  | 6.38  | 113.31                 | 108.20              |
| 21  | AA    | 127  | G    | C8-N9-C4    | -6.38 | 103.85                 | 106.40              |
| 21  | AA    | 353  | A    | C4-C5-C6    | -6.38 | 113.81                 | 117.00              |
| 21  | AA    | 374  | A    | N1-C6-N6    | -6.38 | 114.77                 | 118.60              |
| 21  | AA    | 897  | C    | N3-C2-O2    | -6.38 | 117.43                 | 121.90              |
| 54  | BA    | 1830 | C    | N3-C2-O2    | -6.38 | 117.43                 | 121.90              |
| 54  | BA    | 2788 | C    | N3-C2-O2    | -6.38 | 117.43                 | 121.90              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|------------|-------|------------------------|---------------------|
| 13  | AN    | 9    | ARG  | NE-CZ-NH1  | 6.38  | 123.49                 | 120.30              |
| 54  | BA    | 4    | U    | C5-C6-N1   | -6.38 | 119.51                 | 122.70              |
| 54  | BA    | 320  | A    | C5-C6-N1   | 6.38  | 120.89                 | 117.70              |
| 54  | BA    | 1368 | G    | C5-C6-N1   | 6.38  | 114.69                 | 111.50              |
| 21  | AA    | 34   | C    | N1-C2-O2   | 6.38  | 122.73                 | 118.90              |
| 21  | AA    | 189  | A    | N1-C6-N6   | -6.38 | 114.77                 | 118.60              |
| 21  | AA    | 1000 | A    | C5-C6-N1   | 6.38  | 120.89                 | 117.70              |
| 21  | AA    | 1287 | A    | C4-C5-C6   | -6.38 | 113.81                 | 117.00              |
| 54  | BA    | 95   | A    | C4-C5-C6   | -6.38 | 113.81                 | 117.00              |
| 54  | BA    | 2639 | A    | C5-C6-N1   | 6.38  | 120.89                 | 117.70              |
| 54  | BA    | 2668 | G    | N9-C4-C5   | 6.38  | 107.95                 | 105.40              |
| 21  | AA    | 807  | A    | C4-C5-C6   | -6.38 | 113.81                 | 117.00              |
| 21  | AA    | 815  | A    | C5-C6-N1   | 6.38  | 120.89                 | 117.70              |
| 21  | AA    | 930  | C    | N3-C2-O2   | -6.38 | 117.44                 | 121.90              |
| 54  | BA    | 416  | U    | O4'-C1'-N1 | 6.38  | 113.30                 | 108.20              |
| 54  | BA    | 1535 | A    | C4-C5-C6   | -6.38 | 113.81                 | 117.00              |
| 9   | AJ    | 89   | ARG  | NE-CZ-NH1  | 6.37  | 123.49                 | 120.30              |
| 11  | AL    | 35   | ARG  | NE-CZ-NH1  | 6.37  | 123.49                 | 120.30              |
| 21  | AA    | 1413 | A    | N1-C6-N6   | -6.37 | 114.78                 | 118.60              |
| 21  | AA    | 1504 | G    | C5-C6-N1   | 6.37  | 114.69                 | 111.50              |
| 22  | A1    | 32   | C    | N3-C2-O2   | -6.37 | 117.44                 | 121.90              |
| 22  | A1    | 52   | G    | C8-N9-C4   | -6.37 | 103.85                 | 106.40              |
| 54  | BA    | 641  | U    | C5-C6-N1   | -6.37 | 119.51                 | 122.70              |
| 54  | BA    | 1844 | C    | N3-C2-O2   | -6.37 | 117.44                 | 121.90              |
| 54  | BA    | 2362 | C    | N3-C4-C5   | 6.37  | 124.45                 | 121.90              |
| 55  | BB    | 29   | A    | C5-C6-N1   | 6.37  | 120.89                 | 117.70              |
| 54  | BA    | 181  | A    | N1-C6-N6   | -6.37 | 114.78                 | 118.60              |
| 54  | BA    | 1330 | C    | N3-C2-O2   | -6.37 | 117.44                 | 121.90              |
| 54  | BA    | 1205 | A    | C5-C6-N1   | 6.37  | 120.88                 | 117.70              |
| 21  | AA    | 389  | A    | C5-C6-N1   | 6.37  | 120.88                 | 117.70              |
| 54  | BA    | 79   | C    | N3-C2-O2   | -6.37 | 117.44                 | 121.90              |
| 54  | BA    | 1477 | A    | C4-C5-C6   | -6.37 | 113.82                 | 117.00              |
| 21  | AA    | 759  | A    | C5-C6-N1   | 6.37  | 120.88                 | 117.70              |
| 21  | AA    | 984  | C    | N3-C2-O2   | -6.37 | 117.44                 | 121.90              |
| 40  | BR    | 80   | ARG  | NE-CZ-NH2  | 6.37  | 123.48                 | 120.30              |
| 54  | BA    | 896  | A    | C4-C5-C6   | -6.37 | 113.82                 | 117.00              |
| 54  | BA    | 930  | G    | N1-C6-O6   | -6.37 | 116.08                 | 119.90              |
| 54  | BA    | 2813 | A    | C5-C6-N1   | 6.37  | 120.88                 | 117.70              |
| 21  | AA    | 120  | A    | N1-C6-N6   | -6.36 | 114.78                 | 118.60              |
| 21  | AA    | 651  | C    | N3-C2-O2   | -6.36 | 117.44                 | 121.90              |
| 21  | AA    | 1201 | A    | P-O3'-C3'  | 6.36  | 127.34                 | 119.70              |
| 21  | AA    | 1363 | A    | N1-C6-N6   | -6.36 | 114.78                 | 118.60              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 27  | BE    | 40   | ARG  | NE-CZ-NH1   | 6.36  | 123.48      | 120.30   |
| 54  | BA    | 292  | U    | C5-C6-N1    | -6.36 | 119.52      | 122.70   |
| 54  | BA    | 438  | G    | O4'-C1'-N9  | 6.36  | 113.29      | 108.20   |
| 21  | AA    | 1469 | C    | C3'-C2'-C1' | 6.36  | 106.59      | 101.50   |
| 54  | BA    | 1345 | C    | N3-C2-O2    | -6.36 | 117.45      | 121.90   |
| 54  | BA    | 1636 | U    | O4'-C1'-N1  | 6.36  | 113.29      | 108.20   |
| 54  | BA    | 2079 | U    | C5-C6-N1    | -6.36 | 119.52      | 122.70   |
| 54  | BA    | 2183 | A    | C4-C5-C6    | -6.36 | 113.82      | 117.00   |
| 54  | BA    | 2646 | C    | N1-C2-O2    | 6.36  | 122.72      | 118.90   |
| 54  | BA    | 140  | C    | C2-N3-C4    | -6.36 | 116.72      | 119.90   |
| 54  | BA    | 314  | C    | O4'-C1'-N1  | 6.36  | 113.28      | 108.20   |
| 54  | BA    | 2146 | C    | N3-C2-O2    | -6.36 | 117.45      | 121.90   |
| 54  | BA    | 2587 | A    | C4-C5-C6    | -6.36 | 113.82      | 117.00   |
| 21  | AA    | 609  | A    | C5-C6-N1    | 6.36  | 120.88      | 117.70   |
| 54  | BA    | 171  | U    | O4'-C1'-N1  | 6.36  | 113.28      | 108.20   |
| 54  | BA    | 1151 | A    | C5-C6-N1    | 6.36  | 120.88      | 117.70   |
| 54  | BA    | 1975 | G    | C5-C6-N1    | 6.36  | 114.68      | 111.50   |
| 21  | AA    | 1234 | C    | N3-C2-O2    | -6.35 | 117.45      | 121.90   |
| 54  | BA    | 1272 | A    | N1-C6-N6    | -6.35 | 114.79      | 118.60   |
| 21  | AA    | 303  | A    | C5-C6-N1    | 6.35  | 120.88      | 117.70   |
| 21  | AA    | 1036 | A    | C5-C6-N1    | 6.35  | 120.88      | 117.70   |
| 21  | AA    | 1429 | A    | C6-C5-N7    | 6.35  | 136.75      | 132.30   |
| 54  | BA    | 767  | U    | O4'-C1'-N1  | 6.35  | 113.28      | 108.20   |
| 54  | BA    | 1426 | G    | C8-N9-C4    | -6.35 | 103.86      | 106.40   |
| 54  | BA    | 1603 | A    | C5-C6-N1    | 6.35  | 120.88      | 117.70   |
| 54  | BA    | 1686 | C    | O4'-C1'-N1  | 6.35  | 113.28      | 108.20   |
| 22  | A1    | 28   | C    | N3-C2-O2    | -6.35 | 117.45      | 121.90   |
| 41  | BS    | 92   | ARG  | NE-CZ-NH1   | 6.35  | 123.47      | 120.30   |
| 54  | BA    | 402  | A    | C5-C6-N1    | 6.35  | 120.88      | 117.70   |
| 54  | BA    | 1053 | C    | O4'-C1'-N1  | 6.35  | 113.28      | 108.20   |
| 54  | BA    | 1070 | A    | C5-C6-N1    | 6.35  | 120.88      | 117.70   |
| 54  | BA    | 2355 | G    | N3-C4-C5    | -6.35 | 125.43      | 128.60   |
| 55  | BB    | 37   | C    | N3-C4-C5    | 6.35  | 124.44      | 121.90   |
| 21  | AA    | 16   | A    | C4-C5-C6    | -6.35 | 113.83      | 117.00   |
| 21  | AA    | 136  | C    | N3-C2-O2    | -6.35 | 117.46      | 121.90   |
| 54  | BA    | 743  | A    | C5-C6-N1    | 6.35  | 120.87      | 117.70   |
| 54  | BA    | 1204 | A    | C2-N3-C4    | 6.35  | 113.77      | 110.60   |
| 54  | BA    | 1325 | U    | C4-C5-C6    | 6.35  | 123.51      | 119.70   |
| 54  | BA    | 1594 | U    | O4'-C1'-N1  | 6.35  | 113.28      | 108.20   |
| 54  | BA    | 2837 | A    | N1-C6-N6    | -6.35 | 114.79      | 118.60   |
| 21  | AA    | 1412 | C    | N3-C4-C5    | 6.35  | 124.44      | 121.90   |
| 54  | BA    | 1637 | A    | C4-C5-C6    | -6.35 | 113.83      | 117.00   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|------------|-------|------------------------|---------------------|
| 54  | BA    | 2547 | A    | C5-C6-N1   | 6.35  | 120.87                 | 117.70              |
| 21  | AA    | 465  | A    | C5-C6-N1   | 6.34  | 120.87                 | 117.70              |
| 22  | A1    | 27   | C    | N1-C2-O2   | 6.34  | 122.71                 | 118.90              |
| 54  | BA    | 275  | C    | N3-C4-C5   | 6.34  | 124.44                 | 121.90              |
| 54  | BA    | 607  | U    | O4'-C1'-N1 | 6.34  | 113.28                 | 108.20              |
| 54  | BA    | 2201 | G    | N1-C6-O6   | -6.34 | 116.09                 | 119.90              |
| 54  | BA    | 2212 | A    | N1-C6-N6   | -6.34 | 114.79                 | 118.60              |
| 21  | AA    | 1469 | C    | N1-C2-O2   | 6.34  | 122.71                 | 118.90              |
| 54  | BA    | 461  | C    | N3-C2-O2   | -6.34 | 117.46                 | 121.90              |
| 3   | AD    | 2    | ARG  | NE-CZ-NH1  | 6.34  | 123.47                 | 120.30              |
| 21  | AA    | 359  | G    | N9-C4-C5   | 6.34  | 107.94                 | 105.40              |
| 21  | AA    | 912  | C    | N3-C2-O2   | -6.34 | 117.46                 | 121.90              |
| 21  | AA    | 1328 | C    | N3-C2-O2   | -6.34 | 117.46                 | 121.90              |
| 25  | BC    | 268  | ARG  | NE-CZ-NH1  | 6.34  | 123.47                 | 120.30              |
| 54  | BA    | 817  | C    | N3-C2-O2   | -6.34 | 117.46                 | 121.90              |
| 54  | BA    | 1402 | U    | O4'-C1'-N1 | 6.34  | 113.27                 | 108.20              |
| 54  | BA    | 1704 | C    | N3-C2-O2   | -6.34 | 117.46                 | 121.90              |
| 54  | BA    | 1997 | C    | N3-C2-O2   | -6.34 | 117.46                 | 121.90              |
| 54  | BA    | 2144 | G    | N1-C6-O6   | -6.34 | 116.10                 | 119.90              |
| 21  | AA    | 1311 | A    | C5-C6-N1   | 6.34  | 120.87                 | 117.70              |
| 22  | A1    | 62   | C    | N3-C4-C5   | 6.34  | 124.43                 | 121.90              |
| 54  | BA    | 1990 | C    | N3-C2-O2   | -6.34 | 117.47                 | 121.90              |
| 54  | BA    | 2541 | A    | C4-C5-C6   | -6.34 | 113.83                 | 117.00              |
| 55  | BB    | 90   | C    | N3-C2-O2   | -6.34 | 117.46                 | 121.90              |
| 21  | AA    | 1267 | C    | N1-C2-O2   | 6.33  | 122.70                 | 118.90              |
| 24  | A3    | 3    | C    | N3-C4-C5   | 6.33  | 124.43                 | 121.90              |
| 54  | BA    | 992  | C    | N3-C2-O2   | -6.33 | 117.47                 | 121.90              |
| 54  | BA    | 1385 | A    | C4-C5-C6   | -6.33 | 113.83                 | 117.00              |
| 21  | AA    | 120  | A    | C5-C6-N1   | 6.33  | 120.87                 | 117.70              |
| 21  | AA    | 226  | G    | N3-C2-N2   | -6.33 | 115.47                 | 119.90              |
| 21  | AA    | 510  | A    | C6-C5-N7   | 6.33  | 136.73                 | 132.30              |
| 54  | BA    | 740  | C    | O4'-C1'-N1 | 6.33  | 113.27                 | 108.20              |
| 54  | BA    | 2668 | G    | C8-N9-C4   | -6.33 | 103.87                 | 106.40              |
| 55  | BB    | 97   | C    | N3-C2-O2   | -6.33 | 117.47                 | 121.90              |
| 41  | BS    | 8    | ARG  | NE-CZ-NH1  | 6.33  | 123.47                 | 120.30              |
| 54  | BA    | 1214 | A    | C5-C6-N1   | 6.33  | 120.86                 | 117.70              |
| 54  | BA    | 1965 | C    | N3-C4-C5   | 6.33  | 124.43                 | 121.90              |
| 55  | BB    | 105  | G    | O4'-C1'-N9 | 6.33  | 113.27                 | 108.20              |
| 21  | AA    | 148  | G    | N3-C4-C5   | -6.33 | 125.44                 | 128.60              |
| 21  | AA    | 699  | C    | N3-C2-O2   | -6.33 | 117.47                 | 121.90              |
| 54  | BA    | 1133 | A    | C4-C5-C6   | -6.33 | 113.84                 | 117.00              |
| 54  | BA    | 2062 | A    | O4'-C1'-N9 | 6.33  | 113.26                 | 108.20              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|-------------|-------|------------------------|---------------------|
| 21  | AA    | 23   | C    | N3-C2-O2    | -6.33 | 117.47                 | 121.90              |
| 54  | BA    | 508  | A    | N1-C6-N6    | -6.33 | 114.80                 | 118.60              |
| 54  | BA    | 1000 | A    | C4-C5-C6    | -6.33 | 113.84                 | 117.00              |
| 21  | AA    | 718  | A    | N1-C6-N6    | -6.32 | 114.81                 | 118.60              |
| 21  | AA    | 728  | A    | C2-N3-C4    | 6.32  | 113.76                 | 110.60              |
| 21  | AA    | 1036 | A    | C4-C5-C6    | -6.32 | 113.84                 | 117.00              |
| 54  | BA    | 447  | A    | C4-C5-C6    | -6.32 | 113.84                 | 117.00              |
| 54  | BA    | 1570 | A    | O4'-C1'-N9  | 6.32  | 113.26                 | 108.20              |
| 54  | BA    | 2564 | A    | C5-C6-N1    | 6.32  | 120.86                 | 117.70              |
| 21  | AA    | 1011 | C    | N3-C2-O2    | -6.32 | 117.47                 | 121.90              |
| 51  | B2    | 35   | ARG  | NE-CZ-NH1   | 6.32  | 123.46                 | 120.30              |
| 54  | BA    | 246  | C    | N3-C2-O2    | -6.32 | 117.47                 | 121.90              |
| 8   | AI    | 10   | ARG  | NE-CZ-NH1   | 6.32  | 123.46                 | 120.30              |
| 24  | A3    | 72   | C    | N3-C2-O2    | -6.32 | 117.48                 | 121.90              |
| 54  | BA    | 89   | A    | N1-C6-N6    | -6.32 | 114.81                 | 118.60              |
| 54  | BA    | 948  | C    | O4'-C1'-N1  | 6.32  | 113.26                 | 108.20              |
| 54  | BA    | 1114 | C    | N3-C4-C5    | 6.32  | 124.43                 | 121.90              |
| 54  | BA    | 1286 | A    | N1-C6-N6    | -6.32 | 114.81                 | 118.60              |
| 21  | AA    | 195  | A    | C4-C5-C6    | -6.32 | 113.84                 | 117.00              |
| 21  | AA    | 1005 | A    | C5-C6-N1    | 6.32  | 120.86                 | 117.70              |
| 14  | AO    | 87   | ARG  | NE-CZ-NH1   | 6.32  | 123.46                 | 120.30              |
| 18  | AS    | 2    | ARG  | NE-CZ-NH1   | 6.32  | 123.46                 | 120.30              |
| 21  | AA    | 217  | C    | N3-C2-O2    | -6.32 | 117.48                 | 121.90              |
| 21  | AA    | 572  | A    | C1'-O4'-C4' | -6.32 | 104.85                 | 109.90              |
| 21  | AA    | 1085 | U    | C5-C6-N1    | -6.32 | 119.54                 | 122.70              |
| 24  | A3    | 22   | A    | C4-C5-C6    | -6.32 | 113.84                 | 117.00              |
| 45  | BW    | 24   | ARG  | NE-CZ-NH1   | 6.32  | 123.46                 | 120.30              |
| 54  | BA    | 1140 | C    | N3-C2-O2    | -6.32 | 117.48                 | 121.90              |
| 54  | BA    | 1755 | A    | C4-C5-C6    | -6.32 | 113.84                 | 117.00              |
| 19  | AT    | 73   | ARG  | NH1-CZ-NH2  | -6.32 | 112.45                 | 119.40              |
| 21  | AA    | 534  | U    | N3-C2-O2    | -6.32 | 117.78                 | 122.20              |
| 21  | AA    | 740  | U    | O4'-C1'-N1  | 6.32  | 113.25                 | 108.20              |
| 24  | A3    | 14   | A    | N1-C6-N6    | -6.32 | 114.81                 | 118.60              |
| 29  | BG    | 152  | ARG  | NE-CZ-NH1   | 6.32  | 123.46                 | 120.30              |
| 54  | BA    | 501  | A    | C5-C6-N1    | 6.32  | 120.86                 | 117.70              |
| 54  | BA    | 729  | G    | C8-N9-C4    | -6.32 | 103.87                 | 106.40              |
| 54  | BA    | 2640 | G    | C5-C6-N1    | 6.32  | 114.66                 | 111.50              |
| 55  | BB    | 43   | C    | N3-C2-O2    | -6.32 | 117.48                 | 121.90              |
| 21  | AA    | 514  | C    | N3-C2-O2    | -6.31 | 117.48                 | 121.90              |
| 21  | AA    | 190  | A    | C5-C6-N1    | 6.31  | 120.86                 | 117.70              |
| 21  | AA    | 1239 | A    | C5-C6-N1    | 6.31  | 120.86                 | 117.70              |
| 55  | BB    | 16   | G    | C8-N9-C4    | -6.31 | 103.88                 | 106.40              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 21  | AA    | 308  | C    | N3-C4-N4   | -6.31 | 113.58      | 118.00   |
| 21  | AA    | 379  | C    | N3-C2-O2   | -6.31 | 117.48      | 121.90   |
| 54  | BA    | 2068 | U    | C5-C6-N1   | -6.31 | 119.55      | 122.70   |
| 21  | AA    | 689  | C    | N3-C2-O2   | -6.31 | 117.48      | 121.90   |
| 54  | BA    | 166  | U    | O4'-C1'-N1 | 6.31  | 113.25      | 108.20   |
| 54  | BA    | 965  | C    | N3-C2-O2   | -6.31 | 117.48      | 121.90   |
| 54  | BA    | 640  | C    | N3-C2-O2   | -6.31 | 117.48      | 121.90   |
| 54  | BA    | 1318 | U    | N3-C2-O2   | -6.31 | 117.79      | 122.20   |
| 54  | BA    | 435  | C    | N3-C2-O2   | -6.30 | 117.49      | 121.90   |
| 54  | BA    | 486  | C    | N3-C2-O2   | -6.30 | 117.49      | 121.90   |
| 54  | BA    | 1257 | C    | N3-C2-O2   | -6.30 | 117.49      | 121.90   |
| 54  | BA    | 1755 | A    | C5-C6-N1   | 6.30  | 120.85      | 117.70   |
| 54  | BA    | 257  | C    | N3-C2-O2   | -6.30 | 117.49      | 121.90   |
| 22  | A1    | 65   | C    | N3-C2-O2   | -6.30 | 117.49      | 121.90   |
| 24  | A3    | 16   | C    | N1-C2-O2   | 6.30  | 122.68      | 118.90   |
| 54  | BA    | 516  | C    | N1-C2-O2   | 6.30  | 122.68      | 118.90   |
| 54  | BA    | 814  | C    | O4'-C1'-N1 | 6.30  | 113.24      | 108.20   |
| 54  | BA    | 2815 | C    | N3-C2-O2   | -6.30 | 117.49      | 121.90   |
| 55  | BB    | 113  | C    | N1-C2-O2   | 6.30  | 122.68      | 118.90   |
| 17  | AR    | 72   | ARG  | NE-CZ-NH2  | -6.30 | 117.15      | 120.30   |
| 54  | BA    | 1014 | A    | C4-C5-C6   | -6.30 | 113.85      | 117.00   |
| 54  | BA    | 2521 | C    | N3-C2-O2   | -6.30 | 117.49      | 121.90   |
| 54  | BA    | 2530 | A    | C5-C6-N1   | 6.30  | 120.85      | 117.70   |
| 54  | BA    | 2232 | C    | N3-C2-O2   | -6.30 | 117.49      | 121.90   |
| 55  | BB    | 14   | U    | O4'-C1'-N1 | 6.30  | 113.24      | 108.20   |
| 10  | AK    | 68   | ARG  | NE-CZ-NH1  | 6.30  | 123.45      | 120.30   |
| 21  | AA    | 15   | G    | C5-C6-N1   | 6.30  | 114.65      | 111.50   |
| 21  | AA    | 1320 | C    | N1-C2-O2   | 6.30  | 122.68      | 118.90   |
| 54  | BA    | 765  | C    | N3-C2-O2   | -6.30 | 117.49      | 121.90   |
| 54  | BA    | 972  | A    | C5-C6-N1   | 6.30  | 120.85      | 117.70   |
| 54  | BA    | 1442 | U    | C5-C6-N1   | -6.30 | 119.55      | 122.70   |
| 54  | BA    | 2305 | U    | C5-C6-N1   | -6.30 | 119.55      | 122.70   |
| 54  | BA    | 2636 | C    | N3-C2-O2   | -6.30 | 117.49      | 121.90   |
| 21  | AA    | 931  | C    | N1-C2-O2   | 6.29  | 122.68      | 118.90   |
| 22  | A1    | 26   | A    | N1-C6-N6   | -6.29 | 114.82      | 118.60   |
| 54  | BA    | 2863 | C    | N3-C4-C5   | 6.29  | 124.42      | 121.90   |
| 41  | BS    | 110  | ARG  | NE-CZ-NH1  | 6.29  | 123.45      | 120.30   |
| 54  | BA    | 1042 | G    | N1-C6-O6   | -6.29 | 116.12      | 119.90   |
| 54  | BA    | 1527 | G    | N1-C6-O6   | -6.29 | 116.12      | 119.90   |
| 21  | AA    | 743  | A    | C4-C5-C6   | -6.29 | 113.86      | 117.00   |
| 51  | B2    | 34   | ARG  | NE-CZ-NH1  | 6.29  | 123.45      | 120.30   |
| 54  | BA    | 334  | C    | N3-C2-O2   | -6.29 | 117.50      | 121.90   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|------------|-------|------------------------|---------------------|
| 8   | AI    | 108  | ARG  | NE-CZ-NH1  | 6.29  | 123.44                 | 120.30              |
| 21  | AA    | 304  | U    | N1-C2-N3   | 6.29  | 118.67                 | 114.90              |
| 21  | AA    | 352  | C    | N3-C2-O2   | -6.29 | 117.50                 | 121.90              |
| 54  | BA    | 645  | C    | N1-C2-O2   | 6.29  | 122.67                 | 118.90              |
| 54  | BA    | 2546 | U    | C5-C6-N1   | -6.29 | 119.56                 | 122.70              |
| 54  | BA    | 2800 | A    | C5-C6-N1   | 6.29  | 120.84                 | 117.70              |
| 24  | A3    | 27   | G    | N3-C2-N2   | -6.29 | 115.50                 | 119.90              |
| 55  | BB    | 65   | U    | C5-C6-N1   | -6.29 | 119.56                 | 122.70              |
| 21  | AA    | 311  | C    | C6-N1-C2   | -6.29 | 117.79                 | 120.30              |
| 21  | AA    | 872  | A    | C2-N3-C4   | 6.29  | 113.74                 | 110.60              |
| 21  | AA    | 1456 | A    | N1-C6-N6   | -6.29 | 114.83                 | 118.60              |
| 54  | BA    | 1705 | A    | N1-C6-N6   | -6.29 | 114.83                 | 118.60              |
| 54  | BA    | 191  | A    | N1-C6-N6   | -6.28 | 114.83                 | 118.60              |
| 54  | BA    | 2468 | A    | C4-C5-C6   | -6.28 | 113.86                 | 117.00              |
| 21  | AA    | 223  | A    | C5-C6-N1   | 6.28  | 120.84                 | 117.70              |
| 21  | AA    | 833  | G    | O4'-C1'-N9 | 6.28  | 113.23                 | 108.20              |
| 54  | BA    | 1558 | C    | O4'-C1'-N1 | 6.28  | 113.22                 | 108.20              |
| 21  | AA    | 519  | C    | N3-C2-O2   | -6.28 | 117.50                 | 121.90              |
| 21  | AA    | 1100 | C    | N1-C2-O2   | 6.28  | 122.67                 | 118.90              |
| 54  | BA    | 1512 | C    | N3-C2-O2   | -6.28 | 117.50                 | 121.90              |
| 54  | BA    | 2135 | A    | C5-C6-N1   | 6.28  | 120.84                 | 117.70              |
| 54  | BA    | 2386 | A    | C6-C5-N7   | 6.28  | 136.70                 | 132.30              |
| 21  | AA    | 469  | C    | N3-C2-O2   | -6.28 | 117.51                 | 121.90              |
| 21  | AA    | 595  | A    | C5-C6-N1   | 6.28  | 120.84                 | 117.70              |
| 54  | BA    | 796  | C    | N3-C2-O2   | -6.28 | 117.50                 | 121.90              |
| 54  | BA    | 1836 | C    | O4'-C1'-N1 | 6.28  | 113.22                 | 108.20              |
| 20  | AU    | 46   | ARG  | NE-CZ-NH1  | 6.28  | 123.44                 | 120.30              |
| 54  | BA    | 1539 | U    | N3-C2-O2   | -6.28 | 117.81                 | 122.20              |
| 54  | BA    | 2388 | A    | C4-C5-C6   | -6.28 | 113.86                 | 117.00              |
| 54  | BA    | 2458 | G    | O4'-C1'-N9 | 6.28  | 113.22                 | 108.20              |
| 54  | BA    | 2741 | A    | C4-C5-C6   | -6.28 | 113.86                 | 117.00              |
| 54  | BA    | 2886 | A    | C5-C6-N1   | 6.28  | 120.84                 | 117.70              |
| 21  | AA    | 1109 | C    | N1-C2-O2   | 6.27  | 122.66                 | 118.90              |
| 21  | AA    | 1256 | A    | N1-C6-N6   | -6.27 | 114.84                 | 118.60              |
| 21  | AA    | 1404 | C    | N3-C2-O2   | -6.27 | 117.51                 | 121.90              |
| 54  | BA    | 1833 | C    | N1-C2-O2   | 6.27  | 122.66                 | 118.90              |
| 54  | BA    | 2051 | A    | C5-C6-N1   | 6.27  | 120.84                 | 117.70              |
| 21  | AA    | 142  | G    | C5-C6-N1   | 6.27  | 114.64                 | 111.50              |
| 21  | AA    | 926  | G    | C8-N9-C4   | -6.27 | 103.89                 | 106.40              |
| 54  | BA    | 950  | G    | N3-C2-N2   | -6.27 | 115.51                 | 119.90              |
| 54  | BA    | 2224 | G    | C8-N9-C4   | -6.27 | 103.89                 | 106.40              |
| 54  | BA    | 2531 | A    | C5-C6-N1   | 6.27  | 120.84                 | 117.70              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|-------------|-------|------------------------|---------------------|
| 11  | AL    | 13   | ARG  | NE-CZ-NH1   | 6.27  | 123.44                 | 120.30              |
| 54  | BA    | 1759 | A    | C5-C6-N1    | 6.27  | 120.83                 | 117.70              |
| 54  | BA    | 1806 | C    | N3-C2-O2    | -6.27 | 117.51                 | 121.90              |
| 54  | BA    | 2456 | C    | N3-C2-O2    | -6.27 | 117.51                 | 121.90              |
| 21  | AA    | 182  | A    | O4'-C1'-N9  | 6.27  | 113.21                 | 108.20              |
| 21  | AA    | 494  | G    | O4'-C1'-N9  | 6.27  | 113.22                 | 108.20              |
| 21  | AA    | 793  | U    | C1'-O4'-C4' | -6.27 | 104.89                 | 109.90              |
| 54  | BA    | 6    | A    | C5-C6-N1    | 6.27  | 120.83                 | 117.70              |
| 54  | BA    | 1690 | A    | N1-C6-N6    | -6.27 | 114.84                 | 118.60              |
| 54  | BA    | 2247 | A    | C5-C6-N1    | 6.27  | 120.83                 | 117.70              |
| 55  | BB    | 12   | C    | O4'-C1'-N1  | 6.27  | 113.21                 | 108.20              |
| 21  | AA    | 526  | C    | N1-C2-O2    | 6.27  | 122.66                 | 118.90              |
| 21  | AA    | 872  | A    | C4-C5-C6    | -6.27 | 113.87                 | 117.00              |
| 21  | AA    | 919  | A    | C6-C5-N7    | 6.27  | 136.69                 | 132.30              |
| 54  | BA    | 1701 | A    | C4-C5-C6    | -6.27 | 113.87                 | 117.00              |
| 54  | BA    | 1515 | A    | C4-C5-C6    | -6.26 | 113.87                 | 117.00              |
| 54  | BA    | 1722 | A    | C5-C6-N1    | 6.26  | 120.83                 | 117.70              |
| 54  | BA    | 2040 | G    | C5-C6-N1    | 6.26  | 114.63                 | 111.50              |
| 54  | BA    | 2498 | C    | N3-C2-O2    | -6.26 | 117.52                 | 121.90              |
| 55  | BB    | 113  | C    | N3-C4-C5    | 6.26  | 124.41                 | 121.90              |
| 24  | A3    | 58   | A    | N1-C6-N6    | -6.26 | 114.84                 | 118.60              |
| 21  | AA    | 1139 | G    | N9-C4-C5    | 6.26  | 107.91                 | 105.40              |
| 54  | BA    | 990  | A    | C4-C5-C6    | -6.26 | 113.87                 | 117.00              |
| 54  | BA    | 2788 | C    | O4'-C1'-N1  | 6.26  | 113.21                 | 108.20              |
| 14  | AO    | 52   | ARG  | NE-CZ-NH1   | 6.26  | 123.43                 | 120.30              |
| 21  | AA    | 164  | G    | C8-N9-C4    | -6.26 | 103.90                 | 106.40              |
| 54  | BA    | 430  | A    | C4-C5-C6    | -6.26 | 113.87                 | 117.00              |
| 54  | BA    | 195  | A    | N1-C6-N6    | -6.26 | 114.84                 | 118.60              |
| 54  | BA    | 2439 | A    | C4-C5-C6    | -6.26 | 113.87                 | 117.00              |
| 21  | AA    | 970  | C    | N1-C2-O2    | 6.26  | 122.65                 | 118.90              |
| 21  | AA    | 1430 | A    | N1-C6-N6    | -6.26 | 114.85                 | 118.60              |
| 54  | BA    | 385  | C    | N3-C2-O2    | -6.26 | 117.52                 | 121.90              |
| 54  | BA    | 2045 | C    | N1-C2-O2    | 6.26  | 122.65                 | 118.90              |
| 54  | BA    | 2336 | A    | C5-C6-N1    | 6.26  | 120.83                 | 117.70              |
| 55  | BB    | 80   | U    | N1-C2-N3    | 6.26  | 118.65                 | 114.90              |
| 54  | BA    | 592  | A    | C4-C5-C6    | -6.25 | 113.87                 | 117.00              |
| 21  | AA    | 1108 | G    | N3-C2-N2    | -6.25 | 115.52                 | 119.90              |
| 21  | AA    | 1449 | C    | N3-C2-O2    | -6.25 | 117.52                 | 121.90              |
| 54  | BA    | 2028 | U    | O4'-C1'-N1  | 6.25  | 113.20                 | 108.20              |
| 21  | AA    | 493  | A    | C2-N3-C4    | 6.25  | 113.73                 | 110.60              |
| 54  | BA    | 130  | C    | N3-C2-O2    | -6.25 | 117.52                 | 121.90              |
| 54  | BA    | 1587 | G    | N3-C4-C5    | -6.25 | 125.47                 | 128.60              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 20  | AU    | 44   | ARG  | NE-CZ-NH1  | 6.25  | 123.42      | 120.30   |
| 21  | AA    | 970  | C    | N3-C2-O2   | -6.25 | 117.53      | 121.90   |
| 21  | AA    | 1263 | C    | N3-C2-O2   | -6.25 | 117.53      | 121.90   |
| 54  | BA    | 2108 | A    | C5-C6-N1   | 6.25  | 120.83      | 117.70   |
| 54  | BA    | 2443 | C    | N3-C4-C5   | 6.25  | 124.40      | 121.90   |
| 54  | BA    | 2469 | A    | C4-C5-C6   | -6.25 | 113.88      | 117.00   |
| 21  | AA    | 19   | A    | C4-C5-C6   | -6.25 | 113.88      | 117.00   |
| 21  | AA    | 269  | C    | N3-C2-O2   | -6.25 | 117.53      | 121.90   |
| 54  | BA    | 2052 | A    | N1-C6-N6   | -6.25 | 114.85      | 118.60   |
| 54  | BA    | 2693 | G    | N1-C6-O6   | -6.25 | 116.15      | 119.90   |
| 54  | BA    | 2715 | C    | N3-C2-O2   | -6.25 | 117.53      | 121.90   |
| 54  | BA    | 2808 | G    | C5-C6-N1   | 6.25  | 114.62      | 111.50   |
| 21  | AA    | 67   | C    | O4'-C1'-N1 | 6.25  | 113.20      | 108.20   |
| 54  | BA    | 1759 | A    | C8-N9-C4   | -6.25 | 103.30      | 105.80   |
| 54  | BA    | 1890 | A    | C5-C6-N1   | 6.25  | 120.82      | 117.70   |
| 54  | BA    | 746  | U    | C5-C6-N1   | -6.25 | 119.58      | 122.70   |
| 54  | BA    | 1980 | G    | C5-C6-N1   | 6.25  | 114.62      | 111.50   |
| 54  | BA    | 2269 | G    | N9-C4-C5   | 6.25  | 107.90      | 105.40   |
| 21  | AA    | 614  | C    | N3-C2-O2   | -6.24 | 117.53      | 121.90   |
| 21  | AA    | 1526 | G    | C8-N9-C4   | -6.24 | 103.90      | 106.40   |
| 22  | A1    | 47   | U    | N3-C2-O2   | -6.24 | 117.83      | 122.20   |
| 54  | BA    | 1100 | C    | N3-C2-O2   | -6.24 | 117.53      | 121.90   |
| 54  | BA    | 1340 | U    | P-O3'-C3'  | 6.24  | 127.19      | 119.70   |
| 21  | AA    | 176  | C    | N1-C2-O2   | 6.24  | 122.64      | 118.90   |
| 21  | AA    | 892  | A    | C5-N7-C8   | -6.24 | 100.78      | 103.90   |
| 54  | BA    | 311  | A    | C5-C6-N1   | 6.24  | 120.82      | 117.70   |
| 54  | BA    | 749  | A    | C4-C5-C6   | -6.24 | 113.88      | 117.00   |
| 54  | BA    | 1095 | A    | C4-C5-C6   | -6.24 | 113.88      | 117.00   |
| 54  | BA    | 1357 | C    | N3-C2-O2   | -6.24 | 117.53      | 121.90   |
| 21  | AA    | 13   | U    | O4'-C1'-N1 | 6.24  | 113.19      | 108.20   |
| 21  | AA    | 110  | C    | O4'-C1'-N1 | 6.24  | 113.19      | 108.20   |
| 21  | AA    | 1157 | A    | C4-C5-C6   | -6.24 | 113.88      | 117.00   |
| 54  | BA    | 36   | G    | C5-C6-N1   | 6.24  | 114.62      | 111.50   |
| 54  | BA    | 1315 | C    | C6-N1-C2   | -6.24 | 117.81      | 120.30   |
| 54  | BA    | 1641 | A    | C4-C5-C6   | -6.24 | 113.88      | 117.00   |
| 54  | BA    | 2160 | C    | N1-C2-O2   | 6.24  | 122.64      | 118.90   |
| 21  | AA    | 110  | C    | N3-C2-O2   | -6.24 | 117.53      | 121.90   |
| 54  | BA    | 1030 | C    | O4'-C1'-N1 | 6.24  | 113.19      | 108.20   |
| 54  | BA    | 2095 | A    | N1-C6-N6   | -6.24 | 114.86      | 118.60   |
| 24  | A3    | 36   | A    | C4-C5-C6   | -6.24 | 113.88      | 117.00   |
| 54  | BA    | 2704 | C    | O4'-C1'-N1 | 6.24  | 113.19      | 108.20   |
| 55  | BB    | 19   | C    | N3-C2-O2   | -6.24 | 117.53      | 121.90   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|-------------|-------|------------------------|---------------------|
| 22  | A1    | 17   | U    | N3-C2-O2    | -6.23 | 117.84                 | 122.20              |
| 54  | BA    | 1928 | A    | C5-C6-N1    | 6.23  | 120.82                 | 117.70              |
| 54  | BA    | 2230 | G    | O4'-C1'-N9  | 6.23  | 113.19                 | 108.20              |
| 21  | AA    | 427  | U    | N3-C2-O2    | -6.23 | 117.84                 | 122.20              |
| 21  | AA    | 1324 | A    | C4-C5-C6    | -6.23 | 113.89                 | 117.00              |
| 21  | AA    | 1478 | U    | C5-C6-N1    | -6.23 | 119.58                 | 122.70              |
| 54  | BA    | 177  | G    | N3-C2-N2    | -6.23 | 115.54                 | 119.90              |
| 54  | BA    | 1798 | U    | C5-C6-N1    | -6.23 | 119.58                 | 122.70              |
| 54  | BA    | 1393 | A    | C4-C5-C6    | -6.23 | 113.89                 | 117.00              |
| 54  | BA    | 1443 | U    | C5-C6-N1    | -6.23 | 119.58                 | 122.70              |
| 54  | BA    | 2902 | C    | N3-C2-O2    | -6.23 | 117.54                 | 121.90              |
| 21  | AA    | 648  | A    | C5-C6-N1    | 6.23  | 120.81                 | 117.70              |
| 21  | AA    | 1522 | U    | N3-C2-O2    | -6.23 | 117.84                 | 122.20              |
| 22  | A1    | 62   | C    | N3-C2-O2    | -6.23 | 117.54                 | 121.90              |
| 54  | BA    | 565  | C    | N3-C4-C5    | 6.23  | 124.39                 | 121.90              |
| 54  | BA    | 1924 | C    | N3-C2-O2    | -6.23 | 117.54                 | 121.90              |
| 21  | AA    | 1274 | A    | C5-C6-N1    | 6.23  | 120.81                 | 117.70              |
| 54  | BA    | 643  | A    | C5-C6-N1    | 6.23  | 120.81                 | 117.70              |
| 54  | BA    | 897  | C    | C6-N1-C2    | -6.23 | 117.81                 | 120.30              |
| 54  | BA    | 1535 | A    | O4'-C1'-N9  | 6.23  | 113.18                 | 108.20              |
| 21  | AA    | 1256 | A    | O4'-C1'-N9  | 6.22  | 113.18                 | 108.20              |
| 54  | BA    | 1117 | C    | N3-C2-O2    | -6.22 | 117.54                 | 121.90              |
| 54  | BA    | 1543 | G    | C5-C6-N1    | 6.22  | 114.61                 | 111.50              |
| 54  | BA    | 1847 | A    | C1'-O4'-C4' | -6.22 | 104.92                 | 109.90              |
| 21  | AA    | 369  | G    | N9-C4-C5    | 6.22  | 107.89                 | 105.40              |
| 54  | BA    | 532  | A    | C4-C5-C6    | -6.22 | 113.89                 | 117.00              |
| 21  | AA    | 814  | A    | C5-C6-N1    | 6.22  | 120.81                 | 117.70              |
| 54  | BA    | 2555 | U    | O4'-C1'-N1  | 6.22  | 113.18                 | 108.20              |
| 21  | AA    | 459  | A    | N1-C6-N6    | -6.22 | 114.87                 | 118.60              |
| 54  | BA    | 1161 | C    | N3-C2-O2    | -6.22 | 117.55                 | 121.90              |
| 54  | BA    | 1384 | A    | C5-C6-N1    | 6.22  | 120.81                 | 117.70              |
| 54  | BA    | 1550 | C    | N3-C4-C5    | 6.22  | 124.39                 | 121.90              |
| 54  | BA    | 2825 | G    | C5-C6-N1    | 6.22  | 114.61                 | 111.50              |
| 13  | AN    | 24   | ARG  | NE-CZ-NH2   | -6.22 | 117.19                 | 120.30              |
| 21  | AA    | 36   | C    | C5'-C4'-O4' | 6.22  | 116.56                 | 109.10              |
| 21  | AA    | 233  | C    | N1-C2-O2    | 6.22  | 122.63                 | 118.90              |
| 54  | BA    | 927  | A    | C5-C6-N1    | 6.22  | 120.81                 | 117.70              |
| 54  | BA    | 1266 | G    | C5-C6-N1    | 6.22  | 114.61                 | 111.50              |
| 54  | BA    | 198  | C    | N3-C2-O2    | -6.21 | 117.55                 | 121.90              |
| 54  | BA    | 1495 | A    | C4-C5-C6    | -6.21 | 113.89                 | 117.00              |
| 54  | BA    | 1516 | G    | O4'-C1'-N9  | 6.21  | 113.17                 | 108.20              |
| 54  | BA    | 310  | A    | N1-C6-N6    | -6.21 | 114.87                 | 118.60              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|------------|-------|------------------------|---------------------|
| 54  | BA    | 2088 | A    | C5-C6-N1   | 6.21  | 120.81                 | 117.70              |
| 54  | BA    | 2144 | G    | O4'-C1'-N9 | 6.21  | 113.17                 | 108.20              |
| 21  | AA    | 95   | C    | N3-C2-O2   | -6.21 | 117.55                 | 121.90              |
| 21  | AA    | 1509 | C    | N3-C4-C5   | 6.21  | 124.38                 | 121.90              |
| 54  | BA    | 269  | C    | N3-C2-O2   | -6.21 | 117.55                 | 121.90              |
| 54  | BA    | 2624 | G    | N3-C4-C5   | -6.21 | 125.49                 | 128.60              |
| 54  | BA    | 1428 | C    | N3-C2-O2   | -6.21 | 117.55                 | 121.90              |
| 55  | BB    | 81   | G    | N3-C4-C5   | -6.21 | 125.50                 | 128.60              |
| 21  | AA    | 363  | A    | C5-C6-N1   | 6.21  | 120.80                 | 117.70              |
| 54  | BA    | 34   | U    | O4'-C1'-N1 | 6.21  | 113.17                 | 108.20              |
| 54  | BA    | 1601 | G    | N9-C4-C5   | 6.21  | 107.88                 | 105.40              |
| 54  | BA    | 1604 | C    | N3-C2-O2   | -6.21 | 117.55                 | 121.90              |
| 54  | BA    | 1692 | U    | C5-C6-N1   | -6.21 | 119.60                 | 122.70              |
| 21  | AA    | 402  | G    | N1-C6-O6   | -6.21 | 116.18                 | 119.90              |
| 21  | AA    | 1275 | A    | C5-C6-N1   | 6.21  | 120.80                 | 117.70              |
| 21  | AA    | 1468 | A    | C4-C5-C6   | -6.21 | 113.90                 | 117.00              |
| 26  | BD    | 58   | ASN  | C-N-CA     | 6.21  | 137.21                 | 121.70              |
| 54  | BA    | 439  | A    | C6-C5-N7   | 6.21  | 136.65                 | 132.30              |
| 54  | BA    | 889  | C    | N1-C2-O2   | 6.21  | 122.62                 | 118.90              |
| 54  | BA    | 1052 | C    | N3-C2-O2   | -6.21 | 117.56                 | 121.90              |
| 54  | BA    | 1325 | U    | N1-C2-N3   | 6.21  | 118.62                 | 114.90              |
| 54  | BA    | 2795 | C    | N3-C4-C5   | 6.21  | 124.38                 | 121.90              |
| 54  | BA    | 1357 | C    | O4'-C1'-N1 | 6.21  | 113.16                 | 108.20              |
| 54  | BA    | 474  | G    | N1-C6-O6   | -6.20 | 116.18                 | 119.90              |
| 54  | BA    | 2274 | A    | C4-C5-C6   | -6.20 | 113.90                 | 117.00              |
| 54  | BA    | 2142 | A    | C5-C6-N1   | 6.20  | 120.80                 | 117.70              |
| 21  | AA    | 1141 | C    | N1-C2-O2   | 6.20  | 122.62                 | 118.90              |
| 21  | AA    | 1360 | A    | C5-C6-N1   | 6.20  | 120.80                 | 117.70              |
| 21  | AA    | 1443 | C    | N3-C2-O2   | -6.20 | 117.56                 | 121.90              |
| 54  | BA    | 485  | C    | N3-C2-O2   | -6.20 | 117.56                 | 121.90              |
| 54  | BA    | 1577 | C    | N3-C2-O2   | -6.20 | 117.56                 | 121.90              |
| 54  | BA    | 2807 | U    | O4'-C1'-N1 | 6.20  | 113.16                 | 108.20              |
| 54  | BA    | 1437 | C    | O4'-C1'-N1 | 6.20  | 113.16                 | 108.20              |
| 55  | BB    | 13   | G    | O4'-C1'-N9 | 6.20  | 113.16                 | 108.20              |
| 55  | BB    | 42   | C    | N3-C2-O2   | -6.20 | 117.56                 | 121.90              |
| 21  | AA    | 1438 | G    | O4'-C1'-N9 | 6.20  | 113.16                 | 108.20              |
| 54  | BA    | 1422 | G    | N1-C6-O6   | -6.20 | 116.18                 | 119.90              |
| 21  | AA    | 1067 | A    | C5-C6-N1   | 6.20  | 120.80                 | 117.70              |
| 54  | BA    | 353  | C    | O4'-C1'-N1 | 6.20  | 113.16                 | 108.20              |
| 54  | BA    | 368  | A    | C4-C5-C6   | -6.20 | 113.90                 | 117.00              |
| 54  | BA    | 1298 | C    | N3-C2-O2   | -6.20 | 117.56                 | 121.90              |
| 54  | BA    | 1817 | G    | C5-C6-N1   | 6.20  | 114.60                 | 111.50              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|-------------|-------|------------------------|---------------------|
| 54  | BA    | 2123 | G    | N1-C6-O6    | -6.20 | 116.18                 | 119.90              |
| 54  | BA    | 2799 | A    | C5-C6-N1    | 6.20  | 120.80                 | 117.70              |
| 54  | BA    | 2197 | U    | C5-C6-N1    | -6.19 | 119.60                 | 122.70              |
| 54  | BA    | 2021 | C    | N1-C2-O2    | 6.19  | 122.62                 | 118.90              |
| 24  | A3    | 63   | C    | N1-C2-O2    | 6.19  | 122.61                 | 118.90              |
| 54  | BA    | 578  | G    | N1-C6-O6    | -6.19 | 116.19                 | 119.90              |
| 54  | BA    | 2072 | C    | N3-C2-O2    | -6.19 | 117.57                 | 121.90              |
| 54  | BA    | 2638 | G    | C8-N9-C4    | -6.19 | 103.92                 | 106.40              |
| 55  | BB    | 39   | A    | C5-C6-N1    | 6.19  | 120.80                 | 117.70              |
| 21  | AA    | 188  | C    | N3-C4-C5    | 6.19  | 124.38                 | 121.90              |
| 54  | BA    | 585  | G    | C8-N9-C4    | -6.19 | 103.92                 | 106.40              |
| 21  | AA    | 1226 | C    | N1-C2-O2    | 6.19  | 122.61                 | 118.90              |
| 21  | AA    | 1405 | G    | N1-C6-O6    | -6.19 | 116.19                 | 119.90              |
| 54  | BA    | 909  | A    | C4-C5-C6    | -6.19 | 113.91                 | 117.00              |
| 54  | BA    | 2222 | C    | N1-C2-O2    | 6.18  | 122.61                 | 118.90              |
| 21  | AA    | 72   | A    | C5-C6-N1    | 6.18  | 120.79                 | 117.70              |
| 21  | AA    | 1322 | C    | N1-C2-O2    | 6.18  | 122.61                 | 118.90              |
| 54  | BA    | 1978 | A    | C5-C6-N1    | 6.18  | 120.79                 | 117.70              |
| 54  | BA    | 428  | A    | C5-C6-N1    | 6.18  | 120.79                 | 117.70              |
| 54  | BA    | 605  | G    | N1-C6-O6    | -6.18 | 116.19                 | 119.90              |
| 54  | BA    | 692  | C    | O4'-C1'-N1  | 6.18  | 113.14                 | 108.20              |
| 54  | BA    | 782  | A    | C4-C5-C6    | -6.18 | 113.91                 | 117.00              |
| 54  | BA    | 898  | C    | N3-C2-O2    | -6.18 | 117.57                 | 121.90              |
| 54  | BA    | 1936 | A    | P-O3'-C3'   | 6.18  | 127.12                 | 119.70              |
| 54  | BA    | 1955 | U    | C1'-O4'-C4' | -6.18 | 104.96                 | 109.90              |
| 54  | BA    | 1970 | A    | C4-C5-C6    | -6.18 | 113.91                 | 117.00              |
| 54  | BA    | 2173 | A    | C4-C5-C6    | -6.18 | 113.91                 | 117.00              |
| 54  | BA    | 2476 | A    | C5-C6-N1    | 6.18  | 120.79                 | 117.70              |
| 21  | AA    | 1237 | C    | N1-C2-O2    | 6.18  | 122.61                 | 118.90              |
| 54  | BA    | 878  | A    | C5-C6-N1    | 6.18  | 120.79                 | 117.70              |
| 54  | BA    | 1251 | C    | N3-C2-O2    | -6.18 | 117.58                 | 121.90              |
| 21  | AA    | 340  | U    | N1-C2-N3    | 6.18  | 118.61                 | 114.90              |
| 54  | BA    | 344  | A    | C4-C5-C6    | -6.18 | 113.91                 | 117.00              |
| 54  | BA    | 1967 | C    | N3-C2-O2    | -6.18 | 117.58                 | 121.90              |
| 54  | BA    | 2052 | A    | C5-C6-N1    | 6.18  | 120.79                 | 117.70              |
| 54  | BA    | 2404 | U    | O4'-C1'-N1  | 6.18  | 113.14                 | 108.20              |
| 54  | BA    | 2517 | C    | N3-C2-O2    | -6.18 | 117.58                 | 121.90              |
| 54  | BA    | 2855 | C    | O4'-C1'-N1  | 6.18  | 113.14                 | 108.20              |
| 12  | AM    | 97   | ARG  | NE-CZ-NH1   | 6.17  | 123.39                 | 120.30              |
| 21  | AA    | 36   | C    | N3-C2-O2    | -6.17 | 117.58                 | 121.90              |
| 54  | BA    | 1113 | U    | O4'-C1'-N1  | 6.17  | 113.14                 | 108.20              |
| 21  | AA    | 449  | G    | C8-N9-C4    | -6.17 | 103.93                 | 106.40              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|------------|-------|------------------------|---------------------|
| 21  | AA    | 890  | G    | O4'-C1'-N9 | 6.17  | 113.14                 | 108.20              |
| 54  | BA    | 9    | G    | C5-C6-N1   | 6.17  | 114.59                 | 111.50              |
| 54  | BA    | 734  | A    | C5-C6-N1   | 6.17  | 120.79                 | 117.70              |
| 54  | BA    | 66   | C    | O4'-C1'-N1 | 6.17  | 113.14                 | 108.20              |
| 54  | BA    | 460  | A    | C5-C6-N1   | 6.17  | 120.79                 | 117.70              |
| 54  | BA    | 1010 | A    | C4-C5-C6   | -6.17 | 113.91                 | 117.00              |
| 3   | AD    | 62   | ARG  | NH1-CZ-NH2 | -6.17 | 112.61                 | 119.40              |
| 21  | AA    | 845  | A    | C2-N3-C4   | 6.17  | 113.69                 | 110.60              |
| 21  | AA    | 1112 | C    | N1-C2-O2   | 6.17  | 122.60                 | 118.90              |
| 54  | BA    | 1285 | A    | C4-C5-C6   | -6.17 | 113.92                 | 117.00              |
| 21  | AA    | 99   | C    | N3-C2-O2   | -6.17 | 117.58                 | 121.90              |
| 21  | AA    | 193  | C    | N3-C4-C5   | 6.17  | 124.37                 | 121.90              |
| 21  | AA    | 712  | A    | C5-C6-N1   | 6.17  | 120.78                 | 117.70              |
| 54  | BA    | 1320 | C    | N1-C2-O2   | 6.17  | 122.60                 | 118.90              |
| 21  | AA    | 1173 | U    | C5-C6-N1   | -6.17 | 119.62                 | 122.70              |
| 54  | BA    | 1209 | U    | C5-C6-N1   | -6.17 | 119.62                 | 122.70              |
| 54  | BA    | 2333 | A    | C5-C6-N1   | 6.17  | 120.78                 | 117.70              |
| 54  | BA    | 84   | A    | C5-C6-N1   | 6.17  | 120.78                 | 117.70              |
| 54  | BA    | 2465 | C    | N3-C2-O2   | -6.17 | 117.58                 | 121.90              |
| 21  | AA    | 732  | C    | N3-C2-O2   | -6.16 | 117.58                 | 121.90              |
| 54  | BA    | 515  | A    | O4'-C1'-N9 | 6.16  | 113.13                 | 108.20              |
| 54  | BA    | 928  | A    | C4-C5-C6   | -6.16 | 113.92                 | 117.00              |
| 54  | BA    | 2876 | G    | C5-C6-N1   | 6.16  | 114.58                 | 111.50              |
| 21  | AA    | 777  | A    | C5-C6-N1   | 6.16  | 120.78                 | 117.70              |
| 21  | AA    | 995  | C    | N3-C2-O2   | -6.16 | 117.59                 | 121.90              |
| 21  | AA    | 493  | A    | C4-C5-C6   | -6.16 | 113.92                 | 117.00              |
| 21  | AA    | 663  | A    | C5-C6-N1   | 6.16  | 120.78                 | 117.70              |
| 54  | BA    | 1674 | G    | C5-C6-N1   | 6.16  | 114.58                 | 111.50              |
| 54  | BA    | 2636 | C    | N3-C4-C5   | 6.16  | 124.36                 | 121.90              |
| 21  | AA    | 81   | A    | C4-C5-C6   | -6.16 | 113.92                 | 117.00              |
| 21  | AA    | 226  | G    | C8-N9-C4   | -6.16 | 103.94                 | 106.40              |
| 21  | AA    | 1275 | A    | C4-C5-C6   | -6.16 | 113.92                 | 117.00              |
| 24  | A3    | 36   | A    | C5-C6-N1   | 6.16  | 120.78                 | 117.70              |
| 54  | BA    | 677  | A    | N1-C6-N6   | -6.16 | 114.91                 | 118.60              |
| 54  | BA    | 947  | A    | C4-C5-C6   | -6.16 | 113.92                 | 117.00              |
| 54  | BA    | 1914 | C    | N3-C2-O2   | -6.16 | 117.59                 | 121.90              |
| 21  | AA    | 971  | G    | O4'-C1'-N9 | 6.16  | 113.12                 | 108.20              |
| 21  | AA    | 1174 | G    | C5-C6-N1   | 6.16  | 114.58                 | 111.50              |
| 32  | BJ    | 27   | ARG  | NE-CZ-NH2  | -6.16 | 117.22                 | 120.30              |
| 54  | BA    | 1112 | G    | N1-C6-O6   | -6.16 | 116.21                 | 119.90              |
| 54  | BA    | 2074 | U    | C5-C6-N1   | -6.16 | 119.62                 | 122.70              |
| 21  | AA    | 535  | A    | C5-C6-N1   | 6.15  | 120.78                 | 117.70              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 30  | BH    | 116  | ARG  | NE-CZ-NH1   | 6.15  | 123.38      | 120.30   |
| 21  | AA    | 31   | G    | O4'-C1'-N9  | 6.15  | 113.12      | 108.20   |
| 21  | AA    | 286  | C    | N3-C2-O2    | -6.15 | 117.59      | 121.90   |
| 54  | BA    | 2545 | G    | N1-C6-O6    | -6.15 | 116.21      | 119.90   |
| 21  | AA    | 26   | A    | C4-C5-C6    | -6.15 | 113.92      | 117.00   |
| 54  | BA    | 112  | U    | O4'-C1'-N1  | 6.15  | 113.12      | 108.20   |
| 54  | BA    | 645  | C    | N3-C4-C5    | 6.15  | 124.36      | 121.90   |
| 54  | BA    | 671  | C    | N3-C4-C5    | 6.15  | 124.36      | 121.90   |
| 21  | AA    | 753  | A    | N1-C6-N6    | -6.15 | 114.91      | 118.60   |
| 21  | AA    | 1394 | A    | C4-C5-C6    | -6.15 | 113.92      | 117.00   |
| 54  | BA    | 1553 | A    | C5-C6-N1    | 6.15  | 120.78      | 117.70   |
| 54  | BA    | 2352 | A    | C5-C6-N1    | 6.15  | 120.77      | 117.70   |
| 21  | AA    | 135  | C    | N3-C2-O2    | -6.15 | 117.60      | 121.90   |
| 54  | BA    | 722  | A    | N1-C6-N6    | -6.15 | 114.91      | 118.60   |
| 54  | BA    | 2691 | C    | O4'-C1'-N1  | 6.15  | 113.12      | 108.20   |
| 54  | BA    | 32   | C    | N3-C4-C5    | 6.15  | 124.36      | 121.90   |
| 54  | BA    | 347  | A    | C5-C6-N1    | 6.15  | 120.77      | 117.70   |
| 54  | BA    | 1438 | U    | C5-C6-N1    | -6.15 | 119.63      | 122.70   |
| 54  | BA    | 2142 | A    | C4-C5-C6    | -6.15 | 113.93      | 117.00   |
| 16  | AQ    | 10   | ARG  | NE-CZ-NH1   | 6.14  | 123.37      | 120.30   |
| 21  | AA    | 346  | G    | N3-C4-C5    | -6.14 | 125.53      | 128.60   |
| 21  | AA    | 1377 | A    | C5-C6-N1    | 6.14  | 120.77      | 117.70   |
| 54  | BA    | 2280 | G    | C4'-C3'-C2' | -6.14 | 96.45       | 102.60   |
| 54  | BA    | 2540 | C    | N3-C2-O2    | -6.14 | 117.60      | 121.90   |
| 54  | BA    | 2632 | A    | C4-C5-C6    | -6.14 | 113.93      | 117.00   |
| 54  | BA    | 663  | G    | O4'-C1'-N9  | 6.14  | 113.11      | 108.20   |
| 55  | BB    | 2    | G    | N1-C6-O6    | -6.14 | 116.22      | 119.90   |
| 21  | AA    | 474  | G    | N1-C6-O6    | -6.14 | 116.22      | 119.90   |
| 24  | A3    | 20   | G    | C5-C6-N1    | 6.14  | 114.57      | 111.50   |
| 54  | BA    | 1282 | U    | O4'-C1'-N1  | 6.14  | 113.11      | 108.20   |
| 54  | BA    | 2655 | G    | N7-C8-N9    | 6.14  | 116.17      | 113.10   |
| 54  | BA    | 600  | G    | C5-C6-N1    | 6.14  | 114.57      | 111.50   |
| 54  | BA    | 1468 | U    | O4'-C1'-N1  | 6.14  | 113.11      | 108.20   |
| 21  | AA    | 908  | A    | C5-C6-N1    | 6.14  | 120.77      | 117.70   |
| 21  | AA    | 1190 | G    | P-O3'-C3'   | 6.14  | 127.06      | 119.70   |
| 21  | AA    | 1400 | C    | N3-C2-O2    | -6.14 | 117.61      | 121.90   |
| 54  | BA    | 2016 | U    | N3-C2-O2    | -6.14 | 117.90      | 122.20   |
| 54  | BA    | 2309 | A    | C5-C6-N1    | 6.14  | 120.77      | 117.70   |
| 21  | AA    | 20   | U    | N1-C2-N3    | 6.13  | 118.58      | 114.90   |
| 21  | AA    | 1488 | G    | N9-C4-C5    | 6.13  | 107.85      | 105.40   |
| 22  | A1    | 14   | A    | C5-C6-N1    | 6.13  | 120.77      | 117.70   |
| 54  | BA    | 301  | G    | N3-C4-C5    | -6.13 | 125.53      | 128.60   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|-------------|-------|------------------------|---------------------|
| 54  | BA    | 693  | A    | C4-C5-C6    | -6.13 | 113.93                 | 117.00              |
| 54  | BA    | 995  | C    | N1-C2-O2    | 6.13  | 122.58                 | 118.90              |
| 54  | BA    | 1722 | A    | C4-C5-C6    | -6.13 | 113.93                 | 117.00              |
| 55  | BB    | 24   | G    | N1-C6-O6    | -6.13 | 116.22                 | 119.90              |
| 54  | BA    | 352  | A    | C5-C6-N1    | 6.13  | 120.77                 | 117.70              |
| 21  | AA    | 1099 | G    | N1-C6-O6    | -6.13 | 116.22                 | 119.90              |
| 51  | B2    | 21   | ARG  | NE-CZ-NH1   | 6.13  | 123.37                 | 120.30              |
| 54  | BA    | 717  | C    | N3-C4-C5    | 6.13  | 124.35                 | 121.90              |
| 54  | BA    | 2240 | U    | O4'-C1'-N1  | 6.13  | 113.11                 | 108.20              |
| 54  | BA    | 1222 | U    | C5-C6-N1    | -6.13 | 119.64                 | 122.70              |
| 21  | AA    | 339  | C    | O4'-C1'-N1  | 6.13  | 113.10                 | 108.20              |
| 32  | BJ    | 35   | ARG  | NE-CZ-NH1   | 6.13  | 123.36                 | 120.30              |
| 54  | BA    | 2496 | C    | C3'-C2'-C1' | 6.13  | 106.40                 | 101.50              |
| 1   | AB    | 207  | ARG  | NE-CZ-NH1   | 6.13  | 123.36                 | 120.30              |
| 21  | AA    | 619  | U    | N3-C2-O2    | -6.13 | 117.91                 | 122.20              |
| 21  | AA    | 946  | A    | N1-C6-N6    | -6.13 | 114.92                 | 118.60              |
| 21  | AA    | 1406 | U    | N1-C2-N3    | 6.13  | 118.58                 | 114.90              |
| 21  | AA    | 1516 | G    | C8-N9-C4    | -6.13 | 103.95                 | 106.40              |
| 22  | A1    | 76   | A    | O4'-C1'-N9  | 6.13  | 113.10                 | 108.20              |
| 24  | A3    | 39   | A    | C4-C5-C6    | -6.13 | 113.94                 | 117.00              |
| 54  | BA    | 482  | A    | C3'-C2'-C1' | 6.13  | 106.40                 | 101.50              |
| 54  | BA    | 2066 | C    | O4'-C1'-N1  | 6.13  | 113.10                 | 108.20              |
| 54  | BA    | 2449 | U    | C5-C6-N1    | -6.13 | 119.64                 | 122.70              |
| 21  | AA    | 1012 | A    | C4-C5-C6    | -6.12 | 113.94                 | 117.00              |
| 21  | AA    | 1120 | C    | N3-C2-O2    | -6.12 | 117.61                 | 121.90              |
| 54  | BA    | 38   | A    | C5-C6-N1    | 6.12  | 120.76                 | 117.70              |
| 54  | BA    | 1124 | G    | N1-C6-O6    | -6.12 | 116.22                 | 119.90              |
| 54  | BA    | 1937 | A    | C4-C5-C6    | -6.12 | 113.94                 | 117.00              |
| 54  | BA    | 2799 | A    | C4-C5-C6    | -6.12 | 113.94                 | 117.00              |
| 21  | AA    | 339  | C    | N3-C2-O2    | -6.12 | 117.61                 | 121.90              |
| 21  | AA    | 457  | G    | N1-C6-O6    | -6.12 | 116.23                 | 119.90              |
| 21  | AA    | 1249 | C    | N3-C2-O2    | -6.12 | 117.61                 | 121.90              |
| 55  | BB    | 65   | U    | N3-C2-O2    | -6.12 | 117.91                 | 122.20              |
| 21  | AA    | 637  | C    | N3-C2-O2    | -6.12 | 117.61                 | 121.90              |
| 54  | BA    | 249  | C    | P-O3'-C3'   | 6.12  | 127.05                 | 119.70              |
| 54  | BA    | 2514 | U    | C5-C6-N1    | -6.12 | 119.64                 | 122.70              |
| 54  | BA    | 1908 | C    | N3-C2-O2    | -6.12 | 117.62                 | 121.90              |
| 54  | BA    | 2082 | A    | C5-C6-N1    | 6.12  | 120.76                 | 117.70              |
| 21  | AA    | 605  | U    | C5-C6-N1    | -6.12 | 119.64                 | 122.70              |
| 54  | BA    | 165  | A    | C5-C6-N1    | 6.12  | 120.76                 | 117.70              |
| 54  | BA    | 415  | A    | C4-C5-C6    | -6.12 | 113.94                 | 117.00              |
| 54  | BA    | 1308 | A    | C5-C6-N1    | 6.12  | 120.76                 | 117.70              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 54  | BA    | 1712 | U    | C5-C6-N1    | -6.12 | 119.64      | 122.70   |
| 54  | BA    | 1866 | A    | C5-C6-N1    | 6.12  | 120.76      | 117.70   |
| 54  | BA    | 2132 | U    | C5-C6-N1    | -6.12 | 119.64      | 122.70   |
| 54  | BA    | 670  | A    | C4-C5-C6    | -6.12 | 113.94      | 117.00   |
| 54  | BA    | 55   | G    | N1-C6-O6    | -6.12 | 116.23      | 119.90   |
| 54  | BA    | 1233 | C    | O4'-C1'-N1  | 6.12  | 113.09      | 108.20   |
| 54  | BA    | 1393 | A    | C5-C6-N1    | 6.12  | 120.76      | 117.70   |
| 54  | BA    | 1592 | C    | N3-C2-O2    | -6.12 | 117.62      | 121.90   |
| 54  | BA    | 2350 | C    | N1-C2-O2    | 6.12  | 122.57      | 118.90   |
| 55  | BB    | 71   | C    | N3-C2-O2    | -6.12 | 117.62      | 121.90   |
| 54  | BA    | 373  | U    | N3-C2-O2    | -6.11 | 117.92      | 122.20   |
| 54  | BA    | 1965 | C    | N3-C2-O2    | -6.11 | 117.62      | 121.90   |
| 54  | BA    | 2068 | U    | N3-C2-O2    | -6.11 | 117.92      | 122.20   |
| 2   | AC    | 10   | ARG  | NE-CZ-NH2   | -6.11 | 117.25      | 120.30   |
| 21  | AA    | 615  | G    | C5-C6-N1    | 6.11  | 114.56      | 111.50   |
| 21  | AA    | 697  | U    | O4'-C1'-N1  | 6.11  | 113.09      | 108.20   |
| 21  | AA    | 869  | G    | N3-C2-N2    | -6.11 | 115.62      | 119.90   |
| 21  | AA    | 119  | A    | O4'-C1'-N9  | 6.11  | 113.09      | 108.20   |
| 21  | AA    | 355  | C    | N3-C4-N4    | -6.11 | 113.72      | 118.00   |
| 21  | AA    | 411  | A    | N1-C6-N6    | -6.11 | 114.93      | 118.60   |
| 54  | BA    | 340  | A    | C5-C6-N1    | 6.11  | 120.75      | 117.70   |
| 54  | BA    | 839  | U    | O4'-C1'-N1  | 6.11  | 113.09      | 108.20   |
| 54  | BA    | 2754 | U    | O4'-C1'-N1  | 6.11  | 113.09      | 108.20   |
| 24  | A3    | 74   | A    | C4-C5-C6    | -6.11 | 113.95      | 117.00   |
| 36  | BN    | 64   | ARG  | NE-CZ-NH2   | -6.11 | 117.25      | 120.30   |
| 54  | BA    | 523  | C    | N3-C2-O2    | -6.11 | 117.62      | 121.90   |
| 54  | BA    | 533  | G    | C5-C6-N1    | 6.11  | 114.55      | 111.50   |
| 54  | BA    | 1455 | G    | C5-C6-N1    | 6.11  | 114.55      | 111.50   |
| 54  | BA    | 2576 | G    | N3-C4-C5    | -6.11 | 125.55      | 128.60   |
| 21  | AA    | 452  | A    | C5-C6-N1    | 6.11  | 120.75      | 117.70   |
| 21  | AA    | 1409 | C    | N3-C2-O2    | -6.11 | 117.63      | 121.90   |
| 54  | BA    | 782  | A    | C5-C6-N1    | 6.11  | 120.75      | 117.70   |
| 54  | BA    | 1646 | C    | N3-C4-C5    | 6.11  | 124.34      | 121.90   |
| 54  | BA    | 2427 | C    | N3-C4-C5    | 6.11  | 124.34      | 121.90   |
| 21  | AA    | 1332 | A    | N1-C6-N6    | -6.10 | 114.94      | 118.60   |
| 54  | BA    | 1194 | A    | C4-C5-C6    | -6.10 | 113.95      | 117.00   |
| 54  | BA    | 2788 | C    | C5'-C4'-O4' | 6.10  | 116.42      | 109.10   |
| 54  | BA    | 311  | A    | N1-C6-N6    | -6.10 | 114.94      | 118.60   |
| 54  | BA    | 1033 | U    | C5-C6-N1    | -6.10 | 119.65      | 122.70   |
| 54  | BA    | 2467 | C    | N3-C2-O2    | -6.10 | 117.63      | 121.90   |
| 55  | BB    | 106  | G    | C5-C6-N1    | 6.10  | 114.55      | 111.50   |
| 21  | AA    | 619  | U    | C5-C6-N1    | -6.10 | 119.65      | 122.70   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 21  | AA    | 873  | A    | C4-C5-C6    | -6.10 | 113.95      | 117.00   |
| 54  | BA    | 2336 | A    | C4-C5-C6    | -6.10 | 113.95      | 117.00   |
| 21  | AA    | 496  | A    | C5-C6-N1    | 6.10  | 120.75      | 117.70   |
| 21  | AA    | 658  | C    | N1-C2-O2    | 6.10  | 122.56      | 118.90   |
| 54  | BA    | 91   | A    | C5-C6-N1    | 6.10  | 120.75      | 117.70   |
| 54  | BA    | 679  | C    | N3-C2-O2    | -6.10 | 117.63      | 121.90   |
| 54  | BA    | 2430 | A    | N1-C6-N6    | -6.10 | 114.94      | 118.60   |
| 21  | AA    | 354  | G    | C8-N9-C4    | -6.10 | 103.96      | 106.40   |
| 21  | AA    | 535  | A    | C3'-C2'-C1' | 6.10  | 106.38      | 101.50   |
| 54  | BA    | 917  | A    | C5-C6-N1    | 6.10  | 120.75      | 117.70   |
| 54  | BA    | 1380 | G    | C5-C6-N1    | 6.10  | 114.55      | 111.50   |
| 54  | BA    | 1442 | U    | N3-C2-O2    | -6.10 | 117.93      | 122.20   |
| 54  | BA    | 2441 | U    | O4'-C1'-N1  | 6.10  | 113.08      | 108.20   |
| 21  | AA    | 1230 | C    | O4'-C1'-N1  | 6.10  | 113.08      | 108.20   |
| 21  | AA    | 1256 | A    | C4-C5-C6    | -6.10 | 113.95      | 117.00   |
| 54  | BA    | 490  | C    | O4'-C1'-N1  | 6.10  | 113.08      | 108.20   |
| 54  | BA    | 1938 | A    | N1-C6-N6    | -6.10 | 114.94      | 118.60   |
| 21  | AA    | 901  | A    | C5-C6-N1    | 6.09  | 120.75      | 117.70   |
| 21  | AA    | 1063 | C    | N3-C2-O2    | -6.09 | 117.63      | 121.90   |
| 21  | AA    | 1510 | C    | N3-C2-O2    | -6.09 | 117.63      | 121.90   |
| 54  | BA    | 487  | C    | N1-C2-O2    | 6.09  | 122.56      | 118.90   |
| 54  | BA    | 1862 | G    | N1-C6-O6    | -6.09 | 116.24      | 119.90   |
| 21  | AA    | 151  | A    | C4-C5-C6    | -6.09 | 113.95      | 117.00   |
| 21  | AA    | 974  | A    | C5-C6-N1    | 6.09  | 120.75      | 117.70   |
| 54  | BA    | 91   | A    | C4-C5-C6    | -6.09 | 113.95      | 117.00   |
| 54  | BA    | 944  | C    | N3-C2-O2    | -6.09 | 117.64      | 121.90   |
| 54  | BA    | 2126 | A    | C4-C5-C6    | -6.09 | 113.95      | 117.00   |
| 21  | AA    | 1513 | A    | C4-C5-C6    | -6.09 | 113.96      | 117.00   |
| 54  | BA    | 807  | U    | N3-C2-O2    | -6.09 | 117.94      | 122.20   |
| 54  | BA    | 2496 | C    | N1-C2-O2    | 6.09  | 122.55      | 118.90   |
| 54  | BA    | 2628 | C    | O4'-C1'-N1  | 6.09  | 113.07      | 108.20   |
| 21  | AA    | 28   | A    | C5-C6-N1    | 6.09  | 120.74      | 117.70   |
| 21  | AA    | 49   | U    | C5-C6-N1    | -6.09 | 119.66      | 122.70   |
| 54  | BA    | 2513 | A    | C5-C6-N1    | 6.09  | 120.74      | 117.70   |
| 21  | AA    | 27   | G    | C5-C6-N1    | 6.09  | 114.54      | 111.50   |
| 21  | AA    | 532  | A    | C4-C5-C6    | -6.09 | 113.96      | 117.00   |
| 21  | AA    | 948  | C    | N3-C2-O2    | -6.09 | 117.64      | 121.90   |
| 23  | A2    | 89   | U    | O4'-C1'-N1  | 6.08  | 113.07      | 108.20   |
| 39  | BQ    | 52   | ARG  | NE-CZ-NH1   | 6.08  | 123.34      | 120.30   |
| 54  | BA    | 413  | C    | N3-C2-O2    | -6.08 | 117.64      | 121.90   |
| 54  | BA    | 761  | A    | C4-C5-C6    | -6.08 | 113.96      | 117.00   |
| 54  | BA    | 974  | G    | O4'-C1'-N9  | 6.08  | 113.07      | 108.20   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|-------------|-------|------------------------|---------------------|
| 21  | AA    | 527  | G    | N1-C6-O6    | -6.08 | 116.25                 | 119.90              |
| 21  | AA    | 1248 | A    | C4-C5-C6    | -6.08 | 113.96                 | 117.00              |
| 54  | BA    | 565  | C    | N3-C2-O2    | -6.08 | 117.64                 | 121.90              |
| 54  | BA    | 892  | A    | C5-C6-N1    | 6.08  | 120.74                 | 117.70              |
| 54  | BA    | 1123 | C    | O4'-C1'-N1  | 6.08  | 113.07                 | 108.20              |
| 54  | BA    | 1999 | C    | N1-C2-O2    | 6.08  | 122.55                 | 118.90              |
| 55  | BB    | 71   | C    | N3-C4-C5    | 6.08  | 124.33                 | 121.90              |
| 21  | AA    | 63   | C    | N3-C2-O2    | -6.08 | 117.64                 | 121.90              |
| 21  | AA    | 313  | A    | C6-C5-N7    | 6.08  | 136.56                 | 132.30              |
| 21  | AA    | 455  | G    | N7-C8-N9    | 6.08  | 116.14                 | 113.10              |
| 21  | AA    | 1430 | A    | C5-C6-N1    | 6.08  | 120.74                 | 117.70              |
| 54  | BA    | 546  | U    | N3-C2-O2    | -6.08 | 117.94                 | 122.20              |
| 54  | BA    | 809  | G    | C8-N9-C4    | -6.08 | 103.97                 | 106.40              |
| 54  | BA    | 866  | A    | C4-C5-C6    | -6.08 | 113.96                 | 117.00              |
| 54  | BA    | 1499 | C    | N3-C2-O2    | -6.08 | 117.64                 | 121.90              |
| 54  | BA    | 1826 | G    | C4'-C3'-C2' | -6.08 | 96.52                  | 102.60              |
| 21  | AA    | 480  | U    | C5-C6-N1    | -6.08 | 119.66                 | 122.70              |
| 54  | BA    | 38   | A    | C4-C5-C6    | -6.08 | 113.96                 | 117.00              |
| 54  | BA    | 401  | A    | C5-C6-N1    | 6.08  | 120.74                 | 117.70              |
| 54  | BA    | 1102 | C    | N3-C4-C5    | 6.08  | 124.33                 | 121.90              |
| 54  | BA    | 2166 | U    | O4'-C1'-N1  | 6.08  | 113.06                 | 108.20              |
| 54  | BA    | 2521 | C    | N1-C2-O2    | 6.08  | 122.55                 | 118.90              |
| 54  | BA    | 527  | C    | N3-C4-C5    | 6.08  | 124.33                 | 121.90              |
| 54  | BA    | 1206 | G    | N7-C8-N9    | 6.08  | 116.14                 | 113.10              |
| 54  | BA    | 2317 | A    | C4-C5-C6    | -6.08 | 113.96                 | 117.00              |
| 54  | BA    | 2416 | C    | N3-C2-O2    | -6.08 | 117.65                 | 121.90              |
| 54  | BA    | 69   | C    | N1-C2-O2    | 6.08  | 122.55                 | 118.90              |
| 54  | BA    | 1819 | A    | C4-C5-C6    | -6.08 | 113.96                 | 117.00              |
| 54  | BA    | 2216 | G    | C5-C6-N1    | 6.08  | 114.54                 | 111.50              |
| 54  | BA    | 2333 | A    | C4-C5-C6    | -6.08 | 113.96                 | 117.00              |
| 55  | BB    | 4    | C    | N3-C2-O2    | -6.08 | 117.65                 | 121.90              |
| 21  | AA    | 57   | G    | N1-C6-O6    | -6.07 | 116.26                 | 119.90              |
| 54  | BA    | 233  | A    | C4-C5-C6    | -6.07 | 113.96                 | 117.00              |
| 54  | BA    | 716  | A    | C4-C5-C6    | -6.07 | 113.96                 | 117.00              |
| 54  | BA    | 1753 | G    | C8-N9-C4    | -6.07 | 103.97                 | 106.40              |
| 54  | BA    | 2080 | A    | C6-C5-N7    | 6.07  | 136.55                 | 132.30              |
| 21  | AA    | 507  | C    | N3-C2-O2    | -6.07 | 117.65                 | 121.90              |
| 54  | BA    | 222  | A    | C4-C5-C6    | -6.07 | 113.96                 | 117.00              |
| 54  | BA    | 1406 | U    | O4'-C1'-N1  | 6.07  | 113.06                 | 108.20              |
| 54  | BA    | 1742 | U    | O4'-C1'-N1  | 6.07  | 113.06                 | 108.20              |
| 21  | AA    | 56   | U    | O4'-C1'-N1  | 6.07  | 113.06                 | 108.20              |
| 21  | AA    | 171  | A    | C4-C5-C6    | -6.07 | 113.97                 | 117.00              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|------------|-------|------------------------|---------------------|
| 54  | BA    | 433  | C    | N3-C4-C5   | 6.07  | 124.33                 | 121.90              |
| 54  | BA    | 676  | A    | C4-C5-C6   | -6.07 | 113.96                 | 117.00              |
| 54  | BA    | 873  | C    | N1-C2-O2   | 6.07  | 122.54                 | 118.90              |
| 54  | BA    | 1175 | A    | C4-C5-C6   | -6.07 | 113.97                 | 117.00              |
| 54  | BA    | 1576 | U    | C5-C6-N1   | -6.07 | 119.67                 | 122.70              |
| 54  | BA    | 1634 | A    | C5-C6-N1   | 6.07  | 120.73                 | 117.70              |
| 54  | BA    | 2094 | A    | C5-C6-N1   | 6.07  | 120.73                 | 117.70              |
| 54  | BA    | 2216 | G    | N3-C4-C5   | -6.07 | 125.56                 | 128.60              |
| 54  | BA    | 2449 | U    | N3-C2-O2   | -6.07 | 117.95                 | 122.20              |
| 21  | AA    | 451  | A    | O4'-C1'-N9 | 6.07  | 113.05                 | 108.20              |
| 54  | BA    | 484  | C    | N3-C2-O2   | -6.07 | 117.65                 | 121.90              |
| 54  | BA    | 2312 | U    | C5-C6-N1   | -6.07 | 119.67                 | 122.70              |
| 21  | AA    | 553  | A    | N1-C6-N6   | -6.07 | 114.96                 | 118.60              |
| 21  | AA    | 1097 | C    | N3-C2-O2   | -6.07 | 117.66                 | 121.90              |
| 21  | AA    | 1505 | G    | O4'-C1'-N9 | 6.07  | 113.05                 | 108.20              |
| 54  | BA    | 168  | G    | C5-C6-N1   | 6.07  | 114.53                 | 111.50              |
| 54  | BA    | 2778 | A    | N1-C6-N6   | -6.07 | 114.96                 | 118.60              |
| 21  | AA    | 929  | G    | C8-N9-C4   | -6.06 | 103.97                 | 106.40              |
| 54  | BA    | 1611 | C    | N3-C2-O2   | -6.06 | 117.66                 | 121.90              |
| 54  | BA    | 1772 | A    | C6-C5-N7   | 6.06  | 136.54                 | 132.30              |
| 21  | AA    | 347  | G    | C8-N9-C4   | -6.06 | 103.97                 | 106.40              |
| 21  | AA    | 789  | U    | N3-C2-O2   | -6.06 | 117.96                 | 122.20              |
| 54  | BA    | 754  | U    | O4'-C1'-N1 | 6.06  | 113.05                 | 108.20              |
| 54  | BA    | 951  | C    | N3-C2-O2   | -6.06 | 117.66                 | 121.90              |
| 54  | BA    | 1104 | C    | N3-C2-O2   | -6.06 | 117.66                 | 121.90              |
| 54  | BA    | 1752 | C    | O4'-C1'-N1 | 6.06  | 113.05                 | 108.20              |
| 54  | BA    | 2044 | C    | N1-C2-O2   | 6.06  | 122.54                 | 118.90              |
| 54  | BA    | 2356 | U    | C5-C6-N1   | -6.06 | 119.67                 | 122.70              |
| 54  | BA    | 2417 | C    | N3-C2-O2   | -6.06 | 117.66                 | 121.90              |
| 22  | A1    | 74   | C    | N3-C2-O2   | -6.06 | 117.66                 | 121.90              |
| 54  | BA    | 466  | A    | C5-C6-N1   | 6.06  | 120.73                 | 117.70              |
| 54  | BA    | 541  | A    | C5-C6-N1   | 6.06  | 120.73                 | 117.70              |
| 28  | BF    | 6    | TYR  | CB-CG-CD2  | -6.06 | 117.36                 | 121.00              |
| 54  | BA    | 1640 | A    | C4-C5-C6   | -6.06 | 113.97                 | 117.00              |
| 21  | AA    | 1533 | C    | N1-C2-O2   | 6.06  | 122.53                 | 118.90              |
| 54  | BA    | 142  | A    | C5-C6-N1   | 6.06  | 120.73                 | 117.70              |
| 54  | BA    | 1698 | A    | N1-C6-N6   | -6.06 | 114.97                 | 118.60              |
| 21  | AA    | 160  | A    | C4-C5-C6   | -6.06 | 113.97                 | 117.00              |
| 21  | AA    | 41   | G    | C5-C6-N1   | 6.05  | 114.53                 | 111.50              |
| 22  | A1    | 20   | G    | O4'-C1'-N9 | 6.05  | 113.04                 | 108.20              |
| 54  | BA    | 159  | G    | C5-C6-N1   | 6.05  | 114.53                 | 111.50              |
| 55  | BB    | 14   | U    | C5-C6-N1   | -6.05 | 119.67                 | 122.70              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 27  | BE    | 88   | ARG  | NE-CZ-NH1   | 6.05  | 123.33      | 120.30   |
| 54  | BA    | 181  | A    | C5-C6-N1    | 6.05  | 120.73      | 117.70   |
| 55  | BB    | 91   | C    | N3-C2-O2    | -6.05 | 117.66      | 121.90   |
| 55  | BB    | 112  | G    | C5-C6-N1    | 6.05  | 114.53      | 111.50   |
| 21  | AA    | 378  | G    | C5-C6-N1    | 6.05  | 114.53      | 111.50   |
| 21  | AA    | 1341 | U    | C5-C6-N1    | -6.05 | 119.67      | 122.70   |
| 21  | AA    | 1510 | C    | N1-C2-O2    | 6.05  | 122.53      | 118.90   |
| 54  | BA    | 20   | C    | N3-C2-O2    | -6.05 | 117.66      | 121.90   |
| 54  | BA    | 309  | A    | C5-C6-N1    | 6.05  | 120.73      | 117.70   |
| 54  | BA    | 1918 | A    | C4-C5-C6    | -6.05 | 113.97      | 117.00   |
| 54  | BA    | 2113 | U    | C5-C6-N1    | -6.05 | 119.67      | 122.70   |
| 54  | BA    | 2377 | A    | N1-C6-N6    | -6.05 | 114.97      | 118.60   |
| 54  | BA    | 522  | A    | C4-C5-C6    | -6.05 | 113.97      | 117.00   |
| 54  | BA    | 1625 | C    | O4'-C1'-N1  | 6.05  | 113.04      | 108.20   |
| 54  | BA    | 2050 | C    | N1-C2-O2    | 6.05  | 122.53      | 118.90   |
| 54  | BA    | 2281 | A    | C5-C6-N1    | 6.05  | 120.72      | 117.70   |
| 54  | BA    | 2710 | C    | N3-C2-O2    | -6.05 | 117.67      | 121.90   |
| 54  | BA    | 1119 | U    | O4'-C1'-N1  | 6.05  | 113.04      | 108.20   |
| 54  | BA    | 1130 | U    | O4'-C1'-N1  | 6.05  | 113.04      | 108.20   |
| 54  | BA    | 1503 | A    | C5-C6-N1    | 6.05  | 120.72      | 117.70   |
| 54  | BA    | 1617 | C    | N1-C2-O2    | 6.05  | 122.53      | 118.90   |
| 54  | BA    | 1828 | G    | C3'-C2'-C1' | -6.05 | 96.66       | 101.50   |
| 21  | AA    | 352  | C    | C6-N1-C2    | -6.05 | 117.88      | 120.30   |
| 21  | AA    | 525  | C    | N3-C2-O2    | -6.05 | 117.67      | 121.90   |
| 23  | A2    | 92   | U    | N3-C2-O2    | -6.05 | 117.97      | 122.20   |
| 54  | BA    | 246  | C    | O4'-C1'-N1  | 6.05  | 113.04      | 108.20   |
| 54  | BA    | 405  | U    | O4'-C1'-N1  | 6.05  | 113.04      | 108.20   |
| 54  | BA    | 444  | C    | N3-C2-O2    | -6.05 | 117.67      | 121.90   |
| 54  | BA    | 681  | G    | C5-C6-N1    | 6.05  | 114.52      | 111.50   |
| 54  | BA    | 2289 | G    | C8-N9-C4    | -6.05 | 103.98      | 106.40   |
| 21  | AA    | 108  | G    | N3-C4-C5    | -6.04 | 125.58      | 128.60   |
| 21  | AA    | 468  | A    | C2-N3-C4    | 6.04  | 113.62      | 110.60   |
| 21  | AA    | 1401 | G    | N3-C4-C5    | -6.04 | 125.58      | 128.60   |
| 54  | BA    | 1379 | U    | O4'-C1'-N1  | 6.04  | 113.04      | 108.20   |
| 54  | BA    | 1395 | A    | C5-C6-N1    | 6.04  | 120.72      | 117.70   |
| 54  | BA    | 1667 | G    | C8-N9-C4    | -6.04 | 103.98      | 106.40   |
| 54  | BA    | 2024 | G    | N3-C4-C5    | -6.04 | 125.58      | 128.60   |
| 54  | BA    | 2183 | A    | C5-C6-N1    | 6.04  | 120.72      | 117.70   |
| 54  | BA    | 2246 | G    | N3-C4-C5    | -6.04 | 125.58      | 128.60   |
| 6   | AG    | 108  | ARG  | NE-CZ-NH1   | 6.04  | 123.32      | 120.30   |
| 21  | AA    | 193  | C    | N3-C2-O2    | -6.04 | 117.67      | 121.90   |
| 21  | AA    | 272  | C    | N3-C2-O2    | -6.04 | 117.67      | 121.90   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|-------------|-------|------------------------|---------------------|
| 21  | AA    | 744  | C    | N3-C2-O2    | -6.04 | 117.67                 | 121.90              |
| 21  | AA    | 1091 | U    | N1-C2-N3    | 6.04  | 118.53                 | 114.90              |
| 21  | AA    | 1369 | C    | N3-C2-O2    | -6.04 | 117.67                 | 121.90              |
| 28  | BF    | 147  | ARG  | NE-CZ-NH1   | 6.04  | 123.32                 | 120.30              |
| 54  | BA    | 42   | A    | C6-C5-N7    | 6.04  | 136.53                 | 132.30              |
| 54  | BA    | 60   | G    | O4'-C1'-N9  | 6.04  | 113.03                 | 108.20              |
| 54  | BA    | 474  | G    | N9-C4-C5    | 6.04  | 107.82                 | 105.40              |
| 54  | BA    | 633  | A    | C4-C5-C6    | -6.04 | 113.98                 | 117.00              |
| 54  | BA    | 2331 | G    | N3-C4-C5    | -6.04 | 125.58                 | 128.60              |
| 21  | AA    | 900  | A    | C4-C5-C6    | -6.04 | 113.98                 | 117.00              |
| 54  | BA    | 517  | C    | N3-C2-O2    | -6.04 | 117.67                 | 121.90              |
| 54  | BA    | 960  | A    | C4-C5-C6    | -6.04 | 113.98                 | 117.00              |
| 54  | BA    | 2340 | A    | C5-C6-N1    | 6.04  | 120.72                 | 117.70              |
| 54  | BA    | 2390 | U    | O4'-C1'-N1  | 6.04  | 113.03                 | 108.20              |
| 54  | BA    | 2394 | C    | O4'-C1'-N1  | 6.04  | 113.03                 | 108.20              |
| 21  | AA    | 1093 | A    | C5-C6-N1    | 6.04  | 120.72                 | 117.70              |
| 54  | BA    | 715  | A    | C3'-C2'-C1' | 6.04  | 106.33                 | 101.50              |
| 54  | BA    | 1918 | A    | C5-C6-N1    | 6.04  | 120.72                 | 117.70              |
| 54  | BA    | 2712 | C    | N3-C4-C5    | 6.04  | 124.32                 | 121.90              |
| 21  | AA    | 360  | G    | C5-C6-N1    | 6.04  | 114.52                 | 111.50              |
| 54  | BA    | 184  | C    | N1-C2-O2    | 6.04  | 122.52                 | 118.90              |
| 54  | BA    | 1317 | G    | N1-C6-O6    | -6.04 | 116.28                 | 119.90              |
| 54  | BA    | 272  | A    | C4-C5-C6    | -6.04 | 113.98                 | 117.00              |
| 54  | BA    | 685  | A    | C5-C6-N1    | 6.04  | 120.72                 | 117.70              |
| 54  | BA    | 2276 | G    | C5-C6-N1    | 6.04  | 114.52                 | 111.50              |
| 54  | BA    | 2349 | G    | N1-C6-O6    | -6.04 | 116.28                 | 119.90              |
| 21  | AA    | 342  | C    | N3-C2-O2    | -6.04 | 117.67                 | 121.90              |
| 21  | AA    | 611  | C    | N1-C2-O2    | 6.03  | 122.52                 | 118.90              |
| 21  | AA    | 1423 | G    | C5-C6-N1    | 6.03  | 114.52                 | 111.50              |
| 54  | BA    | 1768 | C    | N1-C2-O2    | 6.03  | 122.52                 | 118.90              |
| 54  | BA    | 2805 | C    | N3-C2-O2    | -6.03 | 117.68                 | 121.90              |
| 21  | AA    | 1076 | U    | C5-C6-N1    | -6.03 | 119.68                 | 122.70              |
| 54  | BA    | 548  | G    | C3'-C2'-C1' | 6.03  | 106.33                 | 101.50              |
| 54  | BA    | 1321 | A    | C4-C5-C6    | -6.03 | 113.98                 | 117.00              |
| 21  | AA    | 1000 | A    | N1-C6-N6    | -6.03 | 114.98                 | 118.60              |
| 54  | BA    | 39   | G    | N3-C2-N2    | -6.03 | 115.68                 | 119.90              |
| 54  | BA    | 411  | G    | N9-C4-C5    | 6.03  | 107.81                 | 105.40              |
| 54  | BA    | 478  | A    | C4-C5-C6    | -6.03 | 113.98                 | 117.00              |
| 54  | BA    | 2311 | A    | C4-C5-C6    | -6.03 | 113.98                 | 117.00              |
| 54  | BA    | 2371 | G    | C4'-C3'-C2' | -6.03 | 96.57                  | 102.60              |
| 21  | AA    | 1447 | A    | C5-C6-N1    | 6.03  | 120.71                 | 117.70              |
| 54  | BA    | 1082 | U    | C5-C6-N1    | -6.03 | 119.69                 | 122.70              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 54  | BA    | 1668 | A    | C4-C5-C6    | -6.03 | 113.99      | 117.00   |
| 54  | BA    | 1946 | U    | O4'-C1'-N1  | 6.03  | 113.02      | 108.20   |
| 21  | AA    | 1117 | A    | C6-C5-N7    | 6.03  | 136.52      | 132.30   |
| 54  | BA    | 544  | C    | N1-C2-O2    | 6.03  | 122.52      | 118.90   |
| 54  | BA    | 1049 | C    | O4'-C1'-N1  | 6.03  | 113.02      | 108.20   |
| 54  | BA    | 1670 | C    | N3-C2-O2    | -6.03 | 117.68      | 121.90   |
| 54  | BA    | 1764 | C    | O4'-C1'-N1  | 6.03  | 113.02      | 108.20   |
| 54  | BA    | 2591 | C    | O4'-C1'-N1  | 6.03  | 113.02      | 108.20   |
| 54  | BA    | 622  | G    | C5-C6-N1    | 6.02  | 114.51      | 111.50   |
| 54  | BA    | 1040 | A    | C4-C5-C6    | -6.02 | 113.99      | 117.00   |
| 54  | BA    | 2049 | G    | N3-C4-C5    | -6.02 | 125.59      | 128.60   |
| 54  | BA    | 1867 | G    | O4'-C1'-N9  | 6.02  | 113.02      | 108.20   |
| 54  | BA    | 2228 | G    | C8-N9-C4    | -6.02 | 103.99      | 106.40   |
| 54  | BA    | 2478 | A    | C4-C5-C6    | -6.02 | 113.99      | 117.00   |
| 54  | BA    | 2506 | U    | O4'-C1'-N1  | 6.02  | 113.02      | 108.20   |
| 54  | BA    | 2580 | U    | N3-C2-O2    | -6.02 | 117.98      | 122.20   |
| 21  | AA    | 1499 | A    | N1-C6-N6    | -6.02 | 114.99      | 118.60   |
| 54  | BA    | 382  | A    | C5-C6-N1    | 6.02  | 120.71      | 117.70   |
| 54  | BA    | 502  | A    | C4-C5-C6    | -6.02 | 113.99      | 117.00   |
| 54  | BA    | 712  | G    | C5-C6-N1    | 6.02  | 114.51      | 111.50   |
| 54  | BA    | 2085 | U    | O4'-C1'-N1  | 6.02  | 113.02      | 108.20   |
| 54  | BA    | 2743 | U    | C5-C6-N1    | -6.02 | 119.69      | 122.70   |
| 55  | BB    | 19   | C    | N1-C2-O2    | 6.02  | 122.51      | 118.90   |
| 21  | AA    | 1522 | U    | N1-C2-N3    | 6.02  | 118.51      | 114.90   |
| 54  | BA    | 1096 | A    | C4-C5-C6    | -6.02 | 113.99      | 117.00   |
| 54  | BA    | 2170 | A    | C4-C5-C6    | -6.02 | 113.99      | 117.00   |
| 22  | A1    | 69   | A    | C3'-C2'-C1' | 6.02  | 106.31      | 101.50   |
| 21  | AA    | 459  | A    | C5-C6-N1    | 6.01  | 120.71      | 117.70   |
| 54  | BA    | 972  | A    | C4-C5-C6    | -6.01 | 113.99      | 117.00   |
| 54  | BA    | 2130 | U    | N1-C2-N3    | 6.01  | 118.51      | 114.90   |
| 54  | BA    | 2345 | G    | N1-C6-O6    | -6.01 | 116.29      | 119.90   |
| 21  | AA    | 551  | U    | C5-C6-N1    | -6.01 | 119.69      | 122.70   |
| 54  | BA    | 378  | C    | N1-C2-O2    | 6.01  | 122.51      | 118.90   |
| 54  | BA    | 2045 | C    | N3-C4-C5    | 6.01  | 124.31      | 121.90   |
| 55  | BB    | 27   | C    | N1-C2-O2    | 6.01  | 122.51      | 118.90   |
| 21  | AA    | 975  | A    | C5-C6-N1    | 6.01  | 120.70      | 117.70   |
| 21  | AA    | 1115 | U    | C5-C6-N1    | -6.01 | 119.69      | 122.70   |
| 21  | AA    | 1237 | C    | O4'-C1'-N1  | 6.01  | 113.01      | 108.20   |
| 54  | BA    | 610  | C    | N3-C2-O2    | -6.01 | 117.69      | 121.90   |
| 54  | BA    | 1031 | G    | C5-C6-N1    | 6.01  | 114.51      | 111.50   |
| 54  | BA    | 1874 | C    | N3-C2-O2    | -6.01 | 117.69      | 121.90   |
| 54  | BA    | 2443 | C    | N1-C2-O2    | 6.01  | 122.51      | 118.90   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|-------------|-------|------------------------|---------------------|
| 21  | AA    | 935  | A    | C5-C6-N1    | 6.01  | 120.70                 | 117.70              |
| 21  | AA    | 1239 | A    | C4-C5-C6    | -6.01 | 114.00                 | 117.00              |
| 21  | AA    | 1282 | C    | N3-C2-O2    | -6.01 | 117.69                 | 121.90              |
| 54  | BA    | 1260 | A    | C6-C5-N7    | 6.01  | 136.51                 | 132.30              |
| 54  | BA    | 1870 | C    | N3-C4-C5    | 6.01  | 124.30                 | 121.90              |
| 54  | BA    | 2110 | G    | C1'-O4'-C4' | -6.01 | 105.09                 | 109.90              |
| 54  | BA    | 2321 | U    | N3-C2-O2    | -6.01 | 117.99                 | 122.20              |
| 54  | BA    | 2608 | G    | N3-C4-C5    | -6.01 | 125.59                 | 128.60              |
| 21  | AA    | 789  | U    | C5-C6-N1    | -6.01 | 119.70                 | 122.70              |
| 21  | AA    | 832  | G    | N1-C6-O6    | -6.01 | 116.30                 | 119.90              |
| 54  | BA    | 1044 | C    | N3-C4-C5    | 6.01  | 124.30                 | 121.90              |
| 21  | AA    | 841  | C    | N3-C4-C5    | 6.01  | 124.30                 | 121.90              |
| 21  | AA    | 1227 | A    | C4-C5-C6    | -6.01 | 114.00                 | 117.00              |
| 54  | BA    | 1327 | A    | C4-C5-C6    | -6.01 | 114.00                 | 117.00              |
| 54  | BA    | 2379 | G    | N1-C6-O6    | -6.01 | 116.30                 | 119.90              |
| 54  | BA    | 2557 | G    | O4'-C1'-N9  | 6.01  | 113.00                 | 108.20              |
| 54  | BA    | 981  | A    | C5-C6-N1    | 6.00  | 120.70                 | 117.70              |
| 54  | BA    | 2395 | C    | O4'-C1'-N1  | 6.00  | 113.00                 | 108.20              |
| 21  | AA    | 319  | G    | C5-C6-N1    | 6.00  | 114.50                 | 111.50              |
| 21  | AA    | 782  | A    | C5-C6-N1    | 6.00  | 120.70                 | 117.70              |
| 21  | AA    | 926  | G    | N9-C4-C5    | 6.00  | 107.80                 | 105.40              |
| 21  | AA    | 1146 | A    | N1-C6-N6    | -6.00 | 115.00                 | 118.60              |
| 21  | AA    | 1434 | A    | C4-C5-C6    | -6.00 | 114.00                 | 117.00              |
| 54  | BA    | 673  | C    | O4'-C1'-N1  | 6.00  | 113.00                 | 108.20              |
| 54  | BA    | 1505 | A    | C5-C6-N1    | 6.00  | 120.70                 | 117.70              |
| 21  | AA    | 417  | G    | N1-C6-O6    | -6.00 | 116.30                 | 119.90              |
| 21  | AA    | 920  | U    | N3-C2-O2    | -6.00 | 118.00                 | 122.20              |
| 21  | AA    | 940  | C    | N3-C2-O2    | -6.00 | 117.70                 | 121.90              |
| 21  | AA    | 1148 | U    | C5-C6-N1    | -6.00 | 119.70                 | 122.70              |
| 21  | AA    | 1522 | U    | C5-C6-N1    | -6.00 | 119.70                 | 122.70              |
| 54  | BA    | 952  | G    | N1-C6-O6    | -6.00 | 116.30                 | 119.90              |
| 54  | BA    | 2437 | G    | C5-C6-N1    | 6.00  | 114.50                 | 111.50              |
| 21  | AA    | 1019 | A    | C4-C5-C6    | -6.00 | 114.00                 | 117.00              |
| 54  | BA    | 1768 | C    | N3-C4-C5    | 6.00  | 124.30                 | 121.90              |
| 54  | BA    | 2606 | C    | N3-C4-C5    | 6.00  | 124.30                 | 121.90              |
| 54  | BA    | 1766 | G    | C5-C6-N1    | 6.00  | 114.50                 | 111.50              |
| 55  | BB    | 86   | G    | N1-C6-O6    | -6.00 | 116.30                 | 119.90              |
| 21  | AA    | 532  | A    | N1-C6-N6    | -6.00 | 115.00                 | 118.60              |
| 21  | AA    | 277  | C    | N3-C4-C5    | 6.00  | 124.30                 | 121.90              |
| 54  | BA    | 602  | A    | N1-C6-N6    | -5.99 | 115.00                 | 118.60              |
| 54  | BA    | 1251 | C    | C3'-C2'-C1' | 5.99  | 106.30                 | 101.50              |
| 54  | BA    | 1316 | U    | O4'-C1'-N1  | 5.99  | 113.00                 | 108.20              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|-------------|-------|------------------------|---------------------|
| 54  | BA    | 1417 | C    | N3-C2-O2    | -5.99 | 117.70                 | 121.90              |
| 54  | BA    | 1793 | C    | N3-C2-O2    | -5.99 | 117.70                 | 121.90              |
| 54  | BA    | 2347 | C    | C3'-C2'-C1' | 5.99  | 106.30                 | 101.50              |
| 54  | BA    | 2873 | A    | O4'-C1'-N9  | 5.99  | 112.99                 | 108.20              |
| 55  | BB    | 80   | U    | C5-C6-N1    | -5.99 | 119.70                 | 122.70              |
| 21  | AA    | 631  | C    | N3-C2-O2    | -5.99 | 117.71                 | 121.90              |
| 54  | BA    | 905  | A    | C4-C5-C6    | -5.99 | 114.00                 | 117.00              |
| 54  | BA    | 2765 | A    | O4'-C1'-N9  | 5.99  | 112.99                 | 108.20              |
| 21  | AA    | 1297 | G    | N3-C2-N2    | -5.99 | 115.71                 | 119.90              |
| 54  | BA    | 1154 | G    | O4'-C1'-N9  | 5.99  | 112.99                 | 108.20              |
| 54  | BA    | 2497 | A    | C5-C6-N1    | 5.99  | 120.69                 | 117.70              |
| 21  | AA    | 197  | A    | C5-C6-N1    | 5.99  | 120.69                 | 117.70              |
| 21  | AA    | 328  | C    | C1'-O4'-C4' | -5.99 | 105.11                 | 109.90              |
| 54  | BA    | 938  | G    | N1-C6-O6    | -5.99 | 116.31                 | 119.90              |
| 54  | BA    | 1106 | G    | N1-C6-O6    | -5.99 | 116.31                 | 119.90              |
| 54  | BA    | 1187 | G    | N1-C6-O6    | -5.99 | 116.31                 | 119.90              |
| 54  | BA    | 1420 | A    | C6-C5-N7    | 5.99  | 136.49                 | 132.30              |
| 54  | BA    | 2883 | A    | N1-C6-N6    | -5.99 | 115.01                 | 118.60              |
| 21  | AA    | 613  | C    | N3-C2-O2    | -5.99 | 117.71                 | 121.90              |
| 54  | BA    | 542  | C    | O4'-C1'-N1  | 5.99  | 112.99                 | 108.20              |
| 21  | AA    | 214  | C    | N3-C2-O2    | -5.99 | 117.71                 | 121.90              |
| 21  | AA    | 385  | C    | N3-C2-O2    | -5.99 | 117.71                 | 121.90              |
| 22  | A1    | 73   | A    | C5-C6-N1    | 5.99  | 120.69                 | 117.70              |
| 54  | BA    | 2113 | U    | N3-C2-O2    | -5.99 | 118.01                 | 122.20              |
| 54  | BA    | 2196 | C    | N3-C2-O2    | -5.99 | 117.71                 | 121.90              |
| 21  | AA    | 111  | G    | N1-C6-O6    | -5.98 | 116.31                 | 119.90              |
| 21  | AA    | 1281 | C    | N1-C2-O2    | 5.98  | 122.49                 | 118.90              |
| 54  | BA    | 118  | A    | C4-C5-C6    | -5.98 | 114.01                 | 117.00              |
| 54  | BA    | 757  | G    | N1-C6-O6    | -5.98 | 116.31                 | 119.90              |
| 54  | BA    | 1502 | A    | C4-C5-C6    | -5.98 | 114.01                 | 117.00              |
| 54  | BA    | 1704 | C    | N1-C2-O2    | 5.98  | 122.49                 | 118.90              |
| 54  | BA    | 2568 | U    | O4'-C1'-N1  | 5.98  | 112.99                 | 108.20              |
| 21  | AA    | 422  | C    | N1-C2-O2    | 5.98  | 122.49                 | 118.90              |
| 21  | AA    | 533  | A    | C4-C5-C6    | -5.98 | 114.01                 | 117.00              |
| 21  | AA    | 1072 | G    | C5-C6-N1    | 5.98  | 114.49                 | 111.50              |
| 21  | AA    | 1332 | A    | C5-C6-N1    | 5.98  | 120.69                 | 117.70              |
| 21  | AA    | 1477 | U    | N1-C2-N3    | 5.98  | 118.49                 | 114.90              |
| 47  | BY    | 29   | ARG  | NE-CZ-NH1   | 5.98  | 123.29                 | 120.30              |
| 54  | BA    | 1359 | A    | C4-C5-C6    | -5.98 | 114.01                 | 117.00              |
| 54  | BA    | 1392 | A    | N1-C6-N6    | -5.98 | 115.01                 | 118.60              |
| 54  | BA    | 1515 | A    | C5-C6-N1    | 5.98  | 120.69                 | 117.70              |
| 54  | BA    | 1602 | U    | O4'-C1'-N1  | 5.98  | 112.98                 | 108.20              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|------------|-------|------------------------|---------------------|
| 21  | AA    | 527  | G    | O4'-C1'-N9 | 5.98  | 112.98                 | 108.20              |
| 54  | BA    | 3    | U    | C5-C6-N1   | -5.98 | 119.71                 | 122.70              |
| 55  | BB    | 25   | U    | C5-C6-N1   | -5.98 | 119.71                 | 122.70              |
| 21  | AA    | 171  | A    | C6-C5-N7   | 5.98  | 136.48                 | 132.30              |
| 21  | AA    | 423  | G    | O4'-C1'-N9 | 5.98  | 112.98                 | 108.20              |
| 21  | AA    | 1151 | A    | P-O3'-C3'  | 5.98  | 126.87                 | 119.70              |
| 24  | A3    | 3    | C    | N3-C2-O2   | -5.98 | 117.72                 | 121.90              |
| 24  | A3    | 63   | C    | N3-C4-C5   | 5.98  | 124.29                 | 121.90              |
| 54  | BA    | 1924 | C    | O4'-C1'-N1 | 5.98  | 112.98                 | 108.20              |
| 54  | BA    | 2044 | C    | N3-C4-C5   | 5.98  | 124.29                 | 121.90              |
| 54  | BA    | 2624 | G    | C5-C6-N1   | 5.98  | 114.49                 | 111.50              |
| 21  | AA    | 186  | C    | N1-C2-O2   | 5.98  | 122.48                 | 118.90              |
| 54  | BA    | 678  | C    | C6-N1-C2   | -5.98 | 117.91                 | 120.30              |
| 54  | BA    | 2683 | C    | N3-C4-C5   | 5.98  | 124.29                 | 121.90              |
| 21  | AA    | 635  | A    | C5-C6-N1   | 5.97  | 120.69                 | 117.70              |
| 54  | BA    | 1601 | G    | C8-N9-C4   | -5.97 | 104.01                 | 106.40              |
| 54  | BA    | 1752 | C    | N3-C2-O2   | -5.97 | 117.72                 | 121.90              |
| 21  | AA    | 1037 | C    | N1-C2-O2   | 5.97  | 122.48                 | 118.90              |
| 21  | AA    | 1056 | U    | C5-C6-N1   | -5.97 | 119.71                 | 122.70              |
| 54  | BA    | 143  | C    | N3-C2-O2   | -5.97 | 117.72                 | 121.90              |
| 54  | BA    | 844  | A    | N1-C6-N6   | -5.97 | 115.02                 | 118.60              |
| 54  | BA    | 1496 | A    | C5-C6-N1   | 5.97  | 120.69                 | 117.70              |
| 54  | BA    | 2135 | A    | O4'-C1'-N9 | 5.97  | 112.98                 | 108.20              |
| 21  | AA    | 311  | C    | N3-C2-O2   | -5.97 | 117.72                 | 121.90              |
| 21  | AA    | 674  | G    | C8-N9-C4   | -5.97 | 104.01                 | 106.40              |
| 21  | AA    | 1182 | G    | N1-C6-O6   | -5.97 | 116.32                 | 119.90              |
| 24  | A3    | 68   | C    | N1-C2-O2   | 5.97  | 122.48                 | 118.90              |
| 54  | BA    | 2512 | C    | N3-C2-O2   | -5.97 | 117.72                 | 121.90              |
| 21  | AA    | 183  | C    | N3-C2-O2   | -5.97 | 117.72                 | 121.90              |
| 54  | BA    | 297  | G    | C5-C6-N1   | 5.97  | 114.48                 | 111.50              |
| 54  | BA    | 411  | G    | C8-N9-C4   | -5.97 | 104.01                 | 106.40              |
| 54  | BA    | 1165 | A    | C5-C6-N1   | 5.97  | 120.68                 | 117.70              |
| 54  | BA    | 1705 | A    | C5-C6-N1   | 5.97  | 120.68                 | 117.70              |
| 54  | BA    | 2847 | U    | O4'-C1'-N1 | 5.97  | 112.97                 | 108.20              |
| 54  | BA    | 712  | G    | N1-C6-O6   | -5.97 | 116.32                 | 119.90              |
| 54  | BA    | 1013 | C    | N3-C2-O2   | -5.97 | 117.72                 | 121.90              |
| 54  | BA    | 1332 | G    | C5-C6-N1   | 5.97  | 114.48                 | 111.50              |
| 54  | BA    | 2033 | A    | C5-C6-N1   | 5.97  | 120.68                 | 117.70              |
| 54  | BA    | 2175 | C    | N3-C4-C5   | 5.97  | 124.29                 | 121.90              |
| 21  | AA    | 356  | A    | C6-C5-N7   | 5.96  | 136.47                 | 132.30              |
| 21  | AA    | 409  | U    | C5-C6-N1   | -5.96 | 119.72                 | 122.70              |
| 21  | AA    | 768  | A    | C4-C5-C6   | -5.96 | 114.02                 | 117.00              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 21  | AA    | 1087 | G    | C5-C6-N1    | 5.96  | 114.48      | 111.50   |
| 54  | BA    | 907  | G    | O4'-C1'-N9  | 5.96  | 112.97      | 108.20   |
| 54  | BA    | 1241 | A    | O4'-C1'-N9  | 5.96  | 112.97      | 108.20   |
| 54  | BA    | 1514 | G    | C8-N9-C4    | -5.96 | 104.01      | 106.40   |
| 54  | BA    | 1873 | G    | O4'-C1'-N9  | 5.96  | 112.97      | 108.20   |
| 21  | AA    | 931  | C    | O4'-C1'-N1  | 5.96  | 112.97      | 108.20   |
| 54  | BA    | 2290 | G    | C5-C6-N1    | 5.96  | 114.48      | 111.50   |
| 54  | BA    | 2426 | A    | O4'-C1'-N9  | 5.96  | 112.97      | 108.20   |
| 21  | AA    | 749  | A    | C5-C6-N1    | 5.96  | 120.68      | 117.70   |
| 21  | AA    | 803  | G    | N1-C6-O6    | -5.96 | 116.32      | 119.90   |
| 21  | AA    | 877  | G    | N7-C8-N9    | 5.96  | 116.08      | 113.10   |
| 21  | AA    | 934  | C    | N3-C2-O2    | -5.96 | 117.73      | 121.90   |
| 21  | AA    | 1054 | C    | N1-C2-O2    | 5.96  | 122.48      | 118.90   |
| 27  | BE    | 102  | ARG  | NE-CZ-NH1   | 5.96  | 123.28      | 120.30   |
| 54  | BA    | 301  | G    | O4'-C1'-N9  | 5.96  | 112.97      | 108.20   |
| 54  | BA    | 1229 | C    | N1-C2-O2    | 5.96  | 122.48      | 118.90   |
| 55  | BB    | 95   | U    | N3-C2-O2    | -5.96 | 118.03      | 122.20   |
| 54  | BA    | 1730 | C    | N1-C2-O2    | 5.96  | 122.48      | 118.90   |
| 54  | BA    | 1814 | G    | C5-C6-N1    | 5.96  | 114.48      | 111.50   |
| 21  | AA    | 817  | C    | N3-C2-O2    | -5.96 | 117.73      | 121.90   |
| 21  | AA    | 881  | G    | C5-C6-N1    | 5.96  | 114.48      | 111.50   |
| 54  | BA    | 69   | C    | N3-C2-O2    | -5.96 | 117.73      | 121.90   |
| 54  | BA    | 121  | G    | O4'-C1'-N9  | 5.96  | 112.97      | 108.20   |
| 54  | BA    | 265  | A    | O4'-C1'-N9  | 5.96  | 112.97      | 108.20   |
| 54  | BA    | 579  | G    | C5'-C4'-O4' | 5.96  | 116.25      | 109.10   |
| 54  | BA    | 1140 | C    | O4'-C1'-N1  | 5.96  | 112.97      | 108.20   |
| 54  | BA    | 1156 | A    | C5-C6-N1    | 5.96  | 120.68      | 117.70   |
| 54  | BA    | 1973 | G    | C8-N9-C4    | -5.96 | 104.02      | 106.40   |
| 54  | BA    | 2775 | G    | C5-C6-N1    | 5.96  | 114.48      | 111.50   |
| 21  | AA    | 1021 | A    | C4-C5-C6    | -5.96 | 114.02      | 117.00   |
| 54  | BA    | 736  | C    | N3-C2-O2    | -5.96 | 117.73      | 121.90   |
| 54  | BA    | 922  | C    | N3-C2-O2    | -5.96 | 117.73      | 121.90   |
| 54  | BA    | 2174 | C    | N3-C4-N4    | -5.96 | 113.83      | 118.00   |
| 22  | A1    | 76   | A    | N1-C6-N6    | -5.96 | 115.03      | 118.60   |
| 54  | BA    | 4    | U    | O4'-C1'-N1  | 5.96  | 112.96      | 108.20   |
| 54  | BA    | 2579 | C    | N3-C2-O2    | -5.96 | 117.73      | 121.90   |
| 54  | BA    | 35   | G    | N1-C6-O6    | -5.95 | 116.33      | 119.90   |
| 54  | BA    | 624  | C    | N1-C2-O2    | 5.95  | 122.47      | 118.90   |
| 54  | BA    | 1170 | C    | N3-C2-O2    | -5.95 | 117.73      | 121.90   |
| 21  | AA    | 196  | A    | C4-C5-C6    | -5.95 | 114.02      | 117.00   |
| 21  | AA    | 816  | A    | C4-C5-C6    | -5.95 | 114.02      | 117.00   |
| 54  | BA    | 995  | C    | N3-C4-C5    | 5.95  | 124.28      | 121.90   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|-------------|-------|------------------------|---------------------|
| 54  | BA    | 1284 | A    | C4-C5-C6    | -5.95 | 114.02                 | 117.00              |
| 21  | AA    | 35   | G    | C1'-O4'-C4' | -5.95 | 105.14                 | 109.90              |
| 21  | AA    | 718  | A    | C4-C5-C6    | -5.95 | 114.03                 | 117.00              |
| 21  | AA    | 793  | U    | C5-C6-N1    | -5.95 | 119.72                 | 122.70              |
| 46  | BX    | 10   | ARG  | NE-CZ-NH1   | 5.95  | 123.28                 | 120.30              |
| 54  | BA    | 471  | A    | C4-C5-C6    | -5.95 | 114.03                 | 117.00              |
| 54  | BA    | 804  | A    | C5-C6-N1    | 5.95  | 120.68                 | 117.70              |
| 54  | BA    | 1727 | C    | N3-C2-O2    | -5.95 | 117.73                 | 121.90              |
| 54  | BA    | 2165 | C    | N1-C2-O2    | 5.95  | 122.47                 | 118.90              |
| 54  | BA    | 2326 | C    | N1-C2-O2    | 5.95  | 122.47                 | 118.90              |
| 21  | AA    | 1494 | G    | N9-C4-C5    | 5.95  | 107.78                 | 105.40              |
| 54  | BA    | 100  | U    | N1-C2-N3    | 5.95  | 118.47                 | 114.90              |
| 54  | BA    | 109  | C    | N1-C2-O2    | 5.95  | 122.47                 | 118.90              |
| 54  | BA    | 1363 | C    | N1-C2-O2    | 5.95  | 122.47                 | 118.90              |
| 54  | BA    | 1652 | A    | C4-C5-C6    | -5.95 | 114.03                 | 117.00              |
| 54  | BA    | 1696 | G    | C5-C6-N1    | 5.95  | 114.47                 | 111.50              |
| 54  | BA    | 1768 | C    | N3-C2-O2    | -5.95 | 117.74                 | 121.90              |
| 54  | BA    | 1892 | C    | N3-C2-O2    | -5.95 | 117.74                 | 121.90              |
| 54  | BA    | 2326 | C    | N3-C4-C5    | 5.95  | 124.28                 | 121.90              |
| 54  | BA    | 680  | C    | O4'-C1'-N1  | 5.95  | 112.96                 | 108.20              |
| 54  | BA    | 883  | G    | N1-C6-O6    | -5.95 | 116.33                 | 119.90              |
| 21  | AA    | 194  | C    | N1-C2-O2    | 5.95  | 122.47                 | 118.90              |
| 21  | AA    | 779  | C    | N3-C4-N4    | -5.95 | 113.84                 | 118.00              |
| 21  | AA    | 1496 | C    | N1-C2-O2    | 5.95  | 122.47                 | 118.90              |
| 54  | BA    | 759  | G    | N7-C8-N9    | 5.95  | 116.07                 | 113.10              |
| 54  | BA    | 828  | U    | N3-C2-O2    | -5.95 | 118.04                 | 122.20              |
| 54  | BA    | 1223 | G    | C5-C6-N1    | 5.95  | 114.47                 | 111.50              |
| 54  | BA    | 1816 | C    | N3-C2-O2    | -5.95 | 117.74                 | 121.90              |
| 54  | BA    | 2102 | G    | N3-C4-C5    | -5.95 | 125.63                 | 128.60              |
| 21  | AA    | 612  | C    | N1-C2-O2    | 5.94  | 122.47                 | 118.90              |
| 54  | BA    | 750  | A    | P-O3'-C3'   | 5.94  | 126.83                 | 119.70              |
| 54  | BA    | 2331 | G    | C5-C6-N1    | 5.94  | 114.47                 | 111.50              |
| 10  | AK    | 127  | ARG  | NE-CZ-NH1   | 5.94  | 123.27                 | 120.30              |
| 21  | AA    | 443  | C    | N3-C2-O2    | -5.94 | 117.74                 | 121.90              |
| 21  | AA    | 1228 | C    | N1-C2-O2    | 5.94  | 122.47                 | 118.90              |
| 54  | BA    | 7    | G    | N3-C2-N2    | -5.94 | 115.74                 | 119.90              |
| 54  | BA    | 503  | A    | O4'-C1'-N9  | 5.94  | 112.95                 | 108.20              |
| 54  | BA    | 516  | C    | N3-C2-O2    | -5.94 | 117.74                 | 121.90              |
| 54  | BA    | 1967 | C    | O4'-C1'-N1  | 5.94  | 112.95                 | 108.20              |
| 54  | BA    | 2645 | G    | C5-C6-N1    | 5.94  | 114.47                 | 111.50              |
| 8   | AI    | 44   | ARG  | NE-CZ-NH1   | 5.94  | 123.27                 | 120.30              |
| 54  | BA    | 720  | U    | C5-C6-N1    | -5.94 | 119.73                 | 122.70              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 54  | BA    | 1229 | C    | N3-C2-O2    | -5.94 | 117.74      | 121.90   |
| 54  | BA    | 1267 | U    | C5-C6-N1    | -5.94 | 119.73      | 122.70   |
| 54  | BA    | 2098 | U    | C5-C6-N1    | -5.94 | 119.73      | 122.70   |
| 21  | AA    | 1207 | G    | N3-C2-N2    | -5.94 | 115.74      | 119.90   |
| 22  | A1    | 23   | A    | N1-C6-N6    | -5.94 | 115.04      | 118.60   |
| 25  | BC    | 13   | ARG  | NE-CZ-NH1   | 5.94  | 123.27      | 120.30   |
| 54  | BA    | 450  | G    | N1-C6-O6    | -5.94 | 116.34      | 119.90   |
| 54  | BA    | 1165 | A    | C4-C5-C6    | -5.94 | 114.03      | 117.00   |
| 54  | BA    | 2258 | C    | O4'-C1'-N1  | 5.94  | 112.95      | 108.20   |
| 54  | BA    | 2660 | A    | C5-C6-N1    | 5.94  | 120.67      | 117.70   |
| 21  | AA    | 461  | A    | C5-C6-N1    | 5.94  | 120.67      | 117.70   |
| 54  | BA    | 888  | C    | N3-C2-O2    | -5.94 | 117.75      | 121.90   |
| 54  | BA    | 2840 | C    | N3-C2-O2    | -5.94 | 117.75      | 121.90   |
| 21  | AA    | 1289 | A    | C4-C5-C6    | -5.93 | 114.03      | 117.00   |
| 21  | AA    | 1320 | C    | N3-C4-C5    | 5.93  | 124.27      | 121.90   |
| 54  | BA    | 1    | G    | C4'-C3'-C2' | -5.93 | 96.67       | 102.60   |
| 54  | BA    | 1119 | U    | C5-C6-N1    | -5.93 | 119.73      | 122.70   |
| 54  | BA    | 1205 | A    | C4-C5-C6    | -5.93 | 114.03      | 117.00   |
| 54  | BA    | 1878 | G    | C8-N9-C4    | -5.93 | 104.03      | 106.40   |
| 54  | BA    | 2516 | A    | C5-C6-N1    | 5.93  | 120.67      | 117.70   |
| 13  | AN    | 41   | ARG  | NE-CZ-NH1   | 5.93  | 123.27      | 120.30   |
| 21  | AA    | 132  | C    | N1-C2-O2    | 5.93  | 122.46      | 118.90   |
| 21  | AA    | 1065 | U    | C3'-C2'-C1' | 5.93  | 106.25      | 101.50   |
| 54  | BA    | 5    | A    | N1-C6-N6    | -5.93 | 115.04      | 118.60   |
| 54  | BA    | 77   | G    | N1-C6-O6    | -5.93 | 116.34      | 119.90   |
| 54  | BA    | 490  | C    | N1-C2-O2    | 5.93  | 122.46      | 118.90   |
| 54  | BA    | 1827 | U    | N3-C2-O2    | -5.93 | 118.05      | 122.20   |
| 54  | BA    | 2577 | A    | N1-C6-N6    | -5.93 | 115.04      | 118.60   |
| 21  | AA    | 1014 | A    | C4-C5-C6    | -5.93 | 114.03      | 117.00   |
| 54  | BA    | 2186 | G    | N1-C6-O6    | -5.93 | 116.34      | 119.90   |
| 21  | AA    | 840  | C    | N3-C4-C5    | 5.93  | 124.27      | 121.90   |
| 21  | AA    | 1296 | C    | N3-C2-O2    | -5.93 | 117.75      | 121.90   |
| 54  | BA    | 1066 | U    | O4'-C1'-N1  | 5.93  | 112.94      | 108.20   |
| 54  | BA    | 1472 | C    | N1-C2-O2    | 5.93  | 122.46      | 118.90   |
| 54  | BA    | 1940 | U    | N3-C2-O2    | -5.93 | 118.05      | 122.20   |
| 54  | BA    | 1989 | G    | C8-N9-C4    | -5.93 | 104.03      | 106.40   |
| 54  | BA    | 2420 | C    | N1-C2-O2    | 5.93  | 122.46      | 118.90   |
| 55  | BB    | 76   | G    | N3-C4-C5    | -5.93 | 125.64      | 128.60   |
| 54  | BA    | 2372 | U    | O4'-C1'-N1  | 5.93  | 112.94      | 108.20   |
| 54  | BA    | 1485 | U    | O4'-C1'-N1  | 5.93  | 112.94      | 108.20   |
| 54  | BA    | 2616 | C    | N3-C2-O2    | -5.93 | 117.75      | 121.90   |
| 21  | AA    | 869  | G    | N9-C4-C5    | 5.92  | 107.77      | 105.40   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 21  | AA    | 964  | A    | C4-C5-C6    | -5.92 | 114.04      | 117.00   |
| 29  | BG    | 68   | ARG  | NE-CZ-NH1   | 5.92  | 123.26      | 120.30   |
| 54  | BA    | 3    | U    | O4'-C1'-N1  | 5.92  | 112.94      | 108.20   |
| 54  | BA    | 1126 | A    | C4-C5-C6    | -5.92 | 114.04      | 117.00   |
| 54  | BA    | 1289 | C    | C3'-C2'-C1' | 5.92  | 106.24      | 101.50   |
| 54  | BA    | 1331 | G    | N1-C6-O6    | -5.92 | 116.35      | 119.90   |
| 54  | BA    | 1635 | A    | C4-C5-C6    | -5.92 | 114.04      | 117.00   |
| 54  | BA    | 2110 | G    | C5-C6-N1    | 5.92  | 114.46      | 111.50   |
| 21  | AA    | 882  | C    | N3-C2-O2    | -5.92 | 117.75      | 121.90   |
| 21  | AA    | 972  | C    | C3'-C2'-C1' | 5.92  | 106.24      | 101.50   |
| 21  | AA    | 1117 | A    | C2-N3-C4    | 5.92  | 113.56      | 110.60   |
| 21  | AA    | 1472 | U    | C5-C6-N1    | -5.92 | 119.74      | 122.70   |
| 54  | BA    | 723  | C    | N3-C2-O2    | -5.92 | 117.75      | 121.90   |
| 54  | BA    | 2349 | G    | N3-C4-C5    | -5.92 | 125.64      | 128.60   |
| 54  | BA    | 2600 | A    | C4-C5-C6    | -5.92 | 114.04      | 117.00   |
| 56  | B5    | 53   | ARG  | NE-CZ-NH1   | 5.92  | 123.26      | 120.30   |
| 21  | AA    | 1123 | U    | C1'-O4'-C4' | -5.92 | 105.16      | 109.90   |
| 54  | BA    | 2452 | C    | N3-C4-C5    | 5.92  | 124.27      | 121.90   |
| 54  | BA    | 2611 | C    | N3-C2-O2    | -5.92 | 117.76      | 121.90   |
| 21  | AA    | 468  | A    | C4-C5-C6    | -5.92 | 114.04      | 117.00   |
| 21  | AA    | 926  | G    | N3-C4-C5    | -5.92 | 125.64      | 128.60   |
| 24  | A3    | 44   | A    | C4-C5-C6    | -5.92 | 114.04      | 117.00   |
| 54  | BA    | 1383 | A    | N1-C6-N6    | -5.92 | 115.05      | 118.60   |
| 15  | AP    | 51   | ARG  | NE-CZ-NH1   | 5.92  | 123.26      | 120.30   |
| 21  | AA    | 1338 | G    | C5-C6-N1    | 5.92  | 114.46      | 111.50   |
| 55  | BB    | 100  | G    | C8-N9-C4    | -5.92 | 104.03      | 106.40   |
| 21  | AA    | 87   | C    | N3-C2-O2    | -5.92 | 117.76      | 121.90   |
| 54  | BA    | 2433 | A    | C6-C5-N7    | 5.92  | 136.44      | 132.30   |
| 21  | AA    | 186  | C    | N3-C4-C5    | 5.91  | 124.27      | 121.90   |
| 22  | A1    | 66   | A    | C6-C5-N7    | 5.91  | 136.44      | 132.30   |
| 54  | BA    | 108  | G    | O4'-C1'-N9  | 5.91  | 112.93      | 108.20   |
| 54  | BA    | 395  | U    | O4'-C1'-N1  | 5.91  | 112.93      | 108.20   |
| 54  | BA    | 1379 | U    | N3-C2-O2    | -5.91 | 118.06      | 122.20   |
| 54  | BA    | 2023 | C    | N3-C2-O2    | -5.91 | 117.76      | 121.90   |
| 21  | AA    | 1298 | U    | N3-C2-O2    | -5.91 | 118.06      | 122.20   |
| 21  | AA    | 1356 | G    | C5-C6-N1    | 5.91  | 114.46      | 111.50   |
| 54  | BA    | 702  | U    | O4'-C1'-N1  | 5.91  | 112.93      | 108.20   |
| 54  | BA    | 853  | C    | N3-C2-O2    | -5.91 | 117.76      | 121.90   |
| 21  | AA    | 973  | G    | N1-C6-O6    | -5.91 | 116.35      | 119.90   |
| 21  | AA    | 1389 | C    | C1'-O4'-C4' | -5.91 | 105.17      | 109.90   |
| 22  | A1    | 68   | C    | N1-C2-O2    | 5.91  | 122.45      | 118.90   |
| 54  | BA    | 1308 | A    | C4-C5-C6    | -5.91 | 114.04      | 117.00   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 54  | BA    | 1830 | C    | C6-N1-C2    | -5.91 | 117.94      | 120.30   |
| 54  | BA    | 1923 | U    | O4'-C1'-N1  | 5.91  | 112.93      | 108.20   |
| 54  | BA    | 2900 | A    | C6-C5-N7    | 5.91  | 136.44      | 132.30   |
| 21  | AA    | 685  | G    | N9-C4-C5    | 5.91  | 107.76      | 105.40   |
| 51  | B2    | 19   | ARG  | NE-CZ-NH1   | 5.91  | 123.25      | 120.30   |
| 54  | BA    | 1386 | C    | N1-C2-O2    | 5.91  | 122.45      | 118.90   |
| 54  | BA    | 2138 | G    | O4'-C1'-N9  | 5.91  | 112.93      | 108.20   |
| 21  | AA    | 306  | A    | C4-C5-C6    | -5.91 | 114.05      | 117.00   |
| 21  | AA    | 930  | C    | O4'-C1'-N1  | 5.91  | 112.92      | 108.20   |
| 21  | AA    | 1514 | G    | C5-C6-N1    | 5.91  | 114.45      | 111.50   |
| 22  | A1    | 59   | U    | O4'-C1'-N1  | 5.91  | 112.92      | 108.20   |
| 54  | BA    | 61   | C    | N1-C2-O2    | 5.91  | 122.44      | 118.90   |
| 54  | BA    | 363  | G    | C5-C6-N1    | 5.91  | 114.45      | 111.50   |
| 54  | BA    | 587  | C    | N3-C4-C5    | 5.91  | 124.26      | 121.90   |
| 54  | BA    | 1081 | U    | O4'-C1'-N1  | 5.91  | 112.92      | 108.20   |
| 21  | AA    | 1490 | U    | C5-C6-N1    | -5.90 | 119.75      | 122.70   |
| 36  | BN    | 96   | ARG  | NE-CZ-NH1   | 5.90  | 123.25      | 120.30   |
| 37  | BO    | 111  | ARG  | NE-CZ-NH1   | 5.90  | 123.25      | 120.30   |
| 54  | BA    | 145  | C    | N3-C4-N4    | -5.90 | 113.87      | 118.00   |
| 54  | BA    | 641  | U    | N3-C2-O2    | -5.90 | 118.07      | 122.20   |
| 54  | BA    | 1675 | C    | O4'-C1'-N1  | 5.90  | 112.92      | 108.20   |
| 54  | BA    | 1777 | U    | C5'-C4'-O4' | 5.90  | 116.18      | 109.10   |
| 9   | AJ    | 7    | ARG  | NE-CZ-NH1   | 5.90  | 123.25      | 120.30   |
| 21  | AA    | 971  | G    | C5-C6-N1    | 5.90  | 114.45      | 111.50   |
| 21  | AA    | 1527 | U    | N3-C2-O2    | -5.90 | 118.07      | 122.20   |
| 24  | A3    | 20   | G    | N1-C6-O6    | -5.90 | 116.36      | 119.90   |
| 35  | BM    | 51   | ARG  | NE-CZ-NH1   | 5.90  | 123.25      | 120.30   |
| 54  | BA    | 21   | A    | N1-C6-N6    | -5.90 | 115.06      | 118.60   |
| 54  | BA    | 121  | G    | N9-C4-C5    | 5.90  | 107.76      | 105.40   |
| 54  | BA    | 982  | C    | N1-C1'-C2'  | 5.90  | 121.67      | 114.00   |
| 54  | BA    | 1089 | A    | C2-N3-C4    | 5.90  | 113.55      | 110.60   |
| 54  | BA    | 1306 | C    | N3-C2-O2    | -5.90 | 117.77      | 121.90   |
| 54  | BA    | 1586 | A    | C5-C6-N1    | 5.90  | 120.65      | 117.70   |
| 54  | BA    | 1819 | A    | C2-N3-C4    | 5.90  | 113.55      | 110.60   |
| 54  | BA    | 2359 | C    | N1-C2-O2    | 5.90  | 122.44      | 118.90   |
| 54  | BA    | 2463 | C    | N3-C2-O2    | -5.90 | 117.77      | 121.90   |
| 54  | BA    | 438  | G    | C5-C6-N1    | 5.90  | 114.45      | 111.50   |
| 54  | BA    | 1398 | C    | N3-C4-C5    | 5.90  | 124.26      | 121.90   |
| 21  | AA    | 498  | A    | C6-C5-N7    | 5.90  | 136.43      | 132.30   |
| 21  | AA    | 570  | G    | C5-C6-N1    | 5.90  | 114.45      | 111.50   |
| 21  | AA    | 1019 | A    | C5-C6-N1    | 5.90  | 120.65      | 117.70   |
| 54  | BA    | 1378 | A    | C5-C6-N1    | 5.90  | 120.65      | 117.70   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 54  | BA    | 1646 | C    | O4'-C1'-N1 | 5.90  | 112.92      | 108.20   |
| 54  | BA    | 2005 | A    | C5-C6-N1   | 5.90  | 120.65      | 117.70   |
| 55  | BB    | 85   | G    | C8-N9-C4   | -5.90 | 104.04      | 106.40   |
| 21  | AA    | 532  | A    | C5-C6-N1   | 5.90  | 120.65      | 117.70   |
| 54  | BA    | 787  | C    | N1-C2-O2   | 5.90  | 122.44      | 118.90   |
| 54  | BA    | 2466 | C    | N3-C2-O2   | -5.90 | 117.77      | 121.90   |
| 54  | BA    | 2505 | G    | N1-C6-O6   | -5.90 | 116.36      | 119.90   |
| 55  | BB    | 104  | A    | C4-C5-C6   | -5.90 | 114.05      | 117.00   |
| 21  | AA    | 506  | G    | N1-C6-O6   | -5.89 | 116.36      | 119.90   |
| 54  | BA    | 648  | G    | C5-C6-N1   | 5.89  | 114.45      | 111.50   |
| 54  | BA    | 1025 | G    | N1-C6-O6   | -5.89 | 116.36      | 119.90   |
| 54  | BA    | 2497 | A    | P-O3'-C3'  | 5.89  | 126.77      | 119.70   |
| 21  | AA    | 162  | A    | C6-C5-N7   | 5.89  | 136.42      | 132.30   |
| 21  | AA    | 1350 | A    | C4-C5-C6   | -5.89 | 114.05      | 117.00   |
| 54  | BA    | 1402 | U    | N3-C2-O2   | -5.89 | 118.08      | 122.20   |
| 54  | BA    | 2202 | U    | O4'-C1'-N1 | 5.89  | 112.92      | 108.20   |
| 54  | BA    | 2551 | C    | N3-C2-O2   | -5.89 | 117.78      | 121.90   |
| 54  | BA    | 2868 | A    | C5-C6-N1   | 5.89  | 120.65      | 117.70   |
| 6   | AG    | 137  | ARG  | NE-CZ-NH1  | 5.89  | 123.25      | 120.30   |
| 21  | AA    | 58   | C    | N1-C2-O2   | 5.89  | 122.44      | 118.90   |
| 21  | AA    | 649  | A    | C5-C6-N1   | 5.89  | 120.64      | 117.70   |
| 21  | AA    | 705  | G    | C5-C6-N1   | 5.89  | 114.45      | 111.50   |
| 21  | AA    | 848  | C    | N3-C4-C5   | 5.89  | 124.26      | 121.90   |
| 54  | BA    | 457  | A    | C6-C5-N7   | 5.89  | 136.42      | 132.30   |
| 54  | BA    | 1686 | C    | N1-C2-O2   | 5.89  | 122.43      | 118.90   |
| 54  | BA    | 1788 | C    | N3-C4-C5   | 5.89  | 124.26      | 121.90   |
| 54  | BA    | 2316 | G    | N1-C6-O6   | -5.89 | 116.37      | 119.90   |
| 54  | BA    | 220  | G    | N3-C4-C5   | -5.89 | 125.66      | 128.60   |
| 54  | BA    | 396  | G    | N1-C6-O6   | -5.89 | 116.37      | 119.90   |
| 54  | BA    | 738  | G    | N9-C4-C5   | 5.89  | 107.75      | 105.40   |
| 54  | BA    | 2114 | A    | N1-C6-N6   | -5.89 | 115.07      | 118.60   |
| 21  | AA    | 621  | A    | C5-C6-N1   | 5.88  | 120.64      | 117.70   |
| 21  | AA    | 798  | U    | O4'-C1'-N1 | 5.88  | 112.91      | 108.20   |
| 54  | BA    | 406  | G    | N1-C6-O6   | -5.88 | 116.37      | 119.90   |
| 54  | BA    | 1979 | U    | O4'-C1'-N1 | 5.88  | 112.91      | 108.20   |
| 23  | A2    | 87   | U    | O4'-C1'-N1 | 5.88  | 112.91      | 108.20   |
| 54  | BA    | 1415 | U    | O4'-C1'-N1 | 5.88  | 112.91      | 108.20   |
| 55  | BB    | 118  | C    | N3-C4-C5   | 5.88  | 124.25      | 121.90   |
| 21  | AA    | 1421 | G    | C8-N9-C4   | -5.88 | 104.05      | 106.40   |
| 54  | BA    | 1048 | A    | C5-C6-N1   | 5.88  | 120.64      | 117.70   |
| 21  | AA    | 39   | G    | N1-C6-O6   | -5.88 | 116.37      | 119.90   |
| 54  | BA    | 48   | G    | C8-N9-C4   | -5.88 | 104.05      | 106.40   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|------------|-------|------------------------|---------------------|
| 25  | BC    | 261  | ARG  | NE-CZ-NH1  | 5.88  | 123.24                 | 120.30              |
| 42  | BT    | 12   | ARG  | NE-CZ-NH1  | 5.88  | 123.24                 | 120.30              |
| 54  | BA    | 1827 | U    | C5-C6-N1   | -5.88 | 119.76                 | 122.70              |
| 54  | BA    | 2640 | G    | N1-C6-O6   | -5.88 | 116.37                 | 119.90              |
| 55  | BB    | 94   | A    | C5-C6-N1   | 5.88  | 120.64                 | 117.70              |
| 21  | AA    | 1257 | A    | C4-C5-C6   | -5.88 | 114.06                 | 117.00              |
| 24  | A3    | 54   | G    | N3-C4-C5   | -5.88 | 125.66                 | 128.60              |
| 54  | BA    | 537  | G    | N1-C6-O6   | -5.88 | 116.37                 | 119.90              |
| 54  | BA    | 784  | G    | C8-N9-C4   | -5.88 | 104.05                 | 106.40              |
| 54  | BA    | 1071 | G    | C8-N9-C4   | -5.88 | 104.05                 | 106.40              |
| 54  | BA    | 53   | A    | N1-C6-N6   | -5.88 | 115.08                 | 118.60              |
| 54  | BA    | 2429 | G    | N1-C6-O6   | -5.88 | 116.38                 | 119.90              |
| 54  | BA    | 2698 | U    | O4'-C1'-N1 | 5.88  | 112.90                 | 108.20              |
| 21  | AA    | 56   | U    | N1-C2-N3   | 5.87  | 118.42                 | 114.90              |
| 21  | AA    | 395  | C    | N3-C2-O2   | -5.87 | 117.79                 | 121.90              |
| 21  | AA    | 999  | C    | N3-C2-O2   | -5.87 | 117.79                 | 121.90              |
| 21  | AA    | 1035 | A    | C4-C5-C6   | -5.87 | 114.06                 | 117.00              |
| 21  | AA    | 1428 | A    | C2-N3-C4   | 5.87  | 113.54                 | 110.60              |
| 22  | A1    | 25   | C    | N3-C2-O2   | -5.87 | 117.79                 | 121.90              |
| 54  | BA    | 422  | A    | C5-C6-N1   | 5.87  | 120.64                 | 117.70              |
| 54  | BA    | 1296 | G    | N3-C2-N2   | -5.87 | 115.79                 | 119.90              |
| 54  | BA    | 2784 | U    | C5-C6-N1   | -5.87 | 119.76                 | 122.70              |
| 21  | AA    | 563  | A    | C4-C5-C6   | -5.87 | 114.06                 | 117.00              |
| 21  | AA    | 1129 | C    | N3-C4-C5   | 5.87  | 124.25                 | 121.90              |
| 54  | BA    | 156  | A    | N1-C6-N6   | -5.87 | 115.08                 | 118.60              |
| 54  | BA    | 1147 | A    | C5-C6-N1   | 5.87  | 120.64                 | 117.70              |
| 54  | BA    | 1278 | C    | N1-C2-O2   | 5.87  | 122.42                 | 118.90              |
| 54  | BA    | 1567 | G    | C5-C6-N1   | 5.87  | 114.44                 | 111.50              |
| 54  | BA    | 1747 | U    | O4'-C1'-N1 | 5.87  | 112.90                 | 108.20              |
| 54  | BA    | 1987 | A    | C6-C5-N7   | 5.87  | 136.41                 | 132.30              |
| 54  | BA    | 2205 | A    | C4-C5-C6   | -5.87 | 114.06                 | 117.00              |
| 54  | BA    | 2443 | C    | N3-C4-N4   | -5.87 | 113.89                 | 118.00              |
| 54  | BA    | 2476 | A    | C4-C5-C6   | -5.87 | 114.06                 | 117.00              |
| 55  | BB    | 37   | C    | N1-C2-O2   | 5.87  | 122.42                 | 118.90              |
| 21  | AA    | 1530 | G    | N3-C2-N2   | -5.87 | 115.79                 | 119.90              |
| 54  | BA    | 2815 | C    | N1-C2-O2   | 5.87  | 122.42                 | 118.90              |
| 54  | BA    | 2901 | C    | N1-C2-O2   | 5.87  | 122.42                 | 118.90              |
| 21  | AA    | 308  | C    | N3-C4-C5   | 5.87  | 124.25                 | 121.90              |
| 21  | AA    | 324  | G    | C5-C6-N1   | 5.87  | 114.44                 | 111.50              |
| 21  | AA    | 1521 | C    | O4'-C1'-N1 | 5.87  | 112.89                 | 108.20              |
| 21  | AA    | 1254 | A    | C4-C5-C6   | -5.87 | 114.07                 | 117.00              |
| 54  | BA    | 1305 | C    | N3-C2-O2   | -5.87 | 117.79                 | 121.90              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 21  | AA    | 522  | C    | N3-C4-C5    | 5.87  | 124.25      | 121.90   |
| 21  | AA    | 821  | G    | C5-C6-N1    | 5.87  | 114.43      | 111.50   |
| 21  | AA    | 1365 | G    | C8-N9-C4    | -5.87 | 104.05      | 106.40   |
| 54  | BA    | 121  | G    | C3'-C2'-C1' | 5.87  | 106.19      | 101.50   |
| 54  | BA    | 205  | G    | N7-C8-N9    | 5.87  | 116.03      | 113.10   |
| 54  | BA    | 860  | U    | O4'-C1'-N1  | 5.87  | 112.89      | 108.20   |
| 54  | BA    | 2767 | C    | N3-C4-C5    | 5.87  | 124.25      | 121.90   |
| 21  | AA    | 276  | G    | N1-C6-O6    | -5.86 | 116.38      | 119.90   |
| 21  | AA    | 306  | A    | C5-C6-N1    | 5.86  | 120.63      | 117.70   |
| 21  | AA    | 402  | G    | C5-C6-N1    | 5.86  | 114.43      | 111.50   |
| 25  | BC    | 270  | ARG  | NE-CZ-NH1   | 5.86  | 123.23      | 120.30   |
| 54  | BA    | 210  | C    | N3-C2-O2    | -5.86 | 117.80      | 121.90   |
| 54  | BA    | 467  | G    | N1-C6-O6    | -5.86 | 116.38      | 119.90   |
| 54  | BA    | 901  | C    | N1-C2-O2    | 5.86  | 122.42      | 118.90   |
| 54  | BA    | 2535 | G    | C5-C6-N1    | 5.86  | 114.43      | 111.50   |
| 21  | AA    | 109  | A    | C1'-O4'-C4' | -5.86 | 105.21      | 109.90   |
| 21  | AA    | 783  | C    | N3-C2-O2    | -5.86 | 117.80      | 121.90   |
| 21  | AA    | 1122 | U    | C5-C6-N1    | -5.86 | 119.77      | 122.70   |
| 21  | AA    | 1452 | C    | N1-C2-O2    | 5.86  | 122.42      | 118.90   |
| 21  | AA    | 1477 | U    | C5-C6-N1    | -5.86 | 119.77      | 122.70   |
| 54  | BA    | 2073 | C    | O4'-C1'-N1  | 5.86  | 112.89      | 108.20   |
| 53  | B4    | 12   | ARG  | NE-CZ-NH1   | 5.86  | 123.23      | 120.30   |
| 54  | BA    | 208  | C    | O4'-C1'-N1  | 5.86  | 112.89      | 108.20   |
| 54  | BA    | 1001 | A    | C4-C5-C6    | -5.86 | 114.07      | 117.00   |
| 54  | BA    | 1175 | A    | O4'-C1'-N9  | 5.86  | 112.89      | 108.20   |
| 54  | BA    | 1537 | G    | N1-C6-O6    | -5.86 | 116.38      | 119.90   |
| 54  | BA    | 2269 | G    | N3-C2-N2    | -5.86 | 115.80      | 119.90   |
| 54  | BA    | 2602 | A    | C4-C5-C6    | -5.86 | 114.07      | 117.00   |
| 21  | AA    | 648  | A    | C4-C5-C6    | -5.86 | 114.07      | 117.00   |
| 54  | BA    | 293  | U    | C5-C6-N1    | -5.86 | 119.77      | 122.70   |
| 54  | BA    | 637  | A    | C4-C5-C6    | -5.86 | 114.07      | 117.00   |
| 54  | BA    | 766  | U    | O4'-C1'-N1  | 5.86  | 112.89      | 108.20   |
| 11  | AL    | 8    | ARG  | NE-CZ-NH1   | 5.86  | 123.23      | 120.30   |
| 54  | BA    | 1436 | G    | N9-C4-C5    | 5.86  | 107.74      | 105.40   |
| 54  | BA    | 2299 | U    | O4'-C1'-N1  | 5.86  | 112.89      | 108.20   |
| 55  | BB    | 50   | A    | N1-C6-N6    | -5.86 | 115.08      | 118.60   |
| 21  | AA    | 105  | G    | C8-N9-C4    | -5.86 | 104.06      | 106.40   |
| 21  | AA    | 284  | C    | N1-C2-O2    | 5.86  | 122.41      | 118.90   |
| 21  | AA    | 307  | C    | N3-C2-O2    | -5.86 | 117.80      | 121.90   |
| 21  | AA    | 556  | C    | N3-C2-O2    | -5.86 | 117.80      | 121.90   |
| 54  | BA    | 102  | U    | O4'-C1'-N1  | 5.86  | 112.88      | 108.20   |
| 54  | BA    | 249  | C    | N3-C2-O2    | -5.86 | 117.80      | 121.90   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|------------|-------|------------------------|---------------------|
| 54  | BA    | 490  | C    | C6-N1-C2   | -5.86 | 117.96                 | 120.30              |
| 54  | BA    | 2298 | A    | C5-C6-N1   | 5.86  | 120.63                 | 117.70              |
| 54  | BA    | 2324 | U    | O4'-C1'-N1 | 5.86  | 112.89                 | 108.20              |
| 54  | BA    | 2644 | G    | N9-C4-C5   | 5.86  | 107.74                 | 105.40              |
| 54  | BA    | 815  | C    | O4'-C1'-N1 | 5.85  | 112.88                 | 108.20              |
| 54  | BA    | 1077 | A    | C5-C6-N1   | 5.85  | 120.63                 | 117.70              |
| 54  | BA    | 2136 | G    | C8-N9-C4   | -5.85 | 104.06                 | 106.40              |
| 54  | BA    | 2667 | C    | N3-C4-C5   | 5.85  | 124.24                 | 121.90              |
| 21  | AA    | 681  | A    | C6-C5-N7   | 5.85  | 136.40                 | 132.30              |
| 21  | AA    | 1219 | A    | C5-C6-N1   | 5.85  | 120.63                 | 117.70              |
| 22  | A1    | 21   | A    | C4-C5-C6   | -5.85 | 114.07                 | 117.00              |
| 54  | BA    | 1695 | G    | N3-C2-N2   | -5.85 | 115.80                 | 119.90              |
| 54  | BA    | 2265 | U    | C5-C6-N1   | -5.85 | 119.77                 | 122.70              |
| 21  | AA    | 173  | U    | N3-C2-O2   | -5.85 | 118.10                 | 122.20              |
| 54  | BA    | 826  | U    | N3-C2-O2   | -5.85 | 118.10                 | 122.20              |
| 54  | BA    | 1826 | G    | N9-C4-C5   | 5.85  | 107.74                 | 105.40              |
| 55  | BB    | 50   | A    | C4-C5-C6   | -5.85 | 114.08                 | 117.00              |
| 21  | AA    | 276  | G    | C5-C6-N1   | 5.85  | 114.42                 | 111.50              |
| 21  | AA    | 925  | G    | C5-C6-N1   | 5.85  | 114.42                 | 111.50              |
| 54  | BA    | 612  | G    | C5-C6-N1   | 5.85  | 114.42                 | 111.50              |
| 54  | BA    | 1075 | C    | N3-C2-O2   | -5.85 | 117.81                 | 121.90              |
| 54  | BA    | 1217 | U    | O4'-C1'-N1 | 5.85  | 112.88                 | 108.20              |
| 54  | BA    | 1905 | C    | N3-C2-O2   | -5.85 | 117.81                 | 121.90              |
| 54  | BA    | 2039 | U    | C5-C6-N1   | -5.85 | 119.78                 | 122.70              |
| 54  | BA    | 2531 | A    | C4-C5-C6   | -5.85 | 114.08                 | 117.00              |
| 55  | BB    | 61   | G    | N1-C6-O6   | -5.85 | 116.39                 | 119.90              |
| 54  | BA    | 272  | A    | C5-C6-N1   | 5.85  | 120.62                 | 117.70              |
| 54  | BA    | 2064 | C    | N3-C2-O2   | -5.85 | 117.81                 | 121.90              |
| 54  | BA    | 2202 | U    | C5-C6-N1   | -5.85 | 119.78                 | 122.70              |
| 21  | AA    | 1137 | C    | N3-C4-C5   | 5.85  | 124.24                 | 121.90              |
| 54  | BA    | 472  | A    | C5-C6-N1   | 5.85  | 120.62                 | 117.70              |
| 54  | BA    | 2863 | C    | N1-C2-O2   | 5.85  | 122.41                 | 118.90              |
| 21  | AA    | 1416 | G    | N3-C4-C5   | -5.84 | 125.68                 | 128.60              |
| 54  | BA    | 2343 | U    | N3-C2-O2   | -5.84 | 118.11                 | 122.20              |
| 54  | BA    | 2731 | G    | N1-C6-O6   | -5.84 | 116.39                 | 119.90              |
| 54  | BA    | 1093 | G    | O4'-C1'-N9 | 5.84  | 112.88                 | 108.20              |
| 21  | AA    | 1214 | C    | O4'-C1'-N1 | 5.84  | 112.87                 | 108.20              |
| 54  | BA    | 115  | C    | O4'-C1'-N1 | 5.84  | 112.87                 | 108.20              |
| 54  | BA    | 1142 | A    | C6-C5-N7   | 5.84  | 136.39                 | 132.30              |
| 54  | BA    | 1224 | U    | C5-C6-N1   | -5.84 | 119.78                 | 122.70              |
| 54  | BA    | 1391 | U    | O4'-C1'-N1 | 5.84  | 112.87                 | 108.20              |
| 54  | BA    | 2143 | C    | N3-C2-O2   | -5.84 | 117.81                 | 121.90              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|-------------|-------|------------------------|---------------------|
| 54  | BA    | 2822 | G    | N3-C4-C5    | -5.84 | 125.68                 | 128.60              |
| 55  | BB    | 70   | C    | N1-C2-O2    | 5.84  | 122.41                 | 118.90              |
| 21  | AA    | 359  | G    | C8-N9-C4    | -5.84 | 104.06                 | 106.40              |
| 54  | BA    | 624  | C    | N3-C4-C5    | 5.84  | 124.24                 | 121.90              |
| 54  | BA    | 1122 | G    | C8-N9-C4    | -5.84 | 104.06                 | 106.40              |
| 5   | AF    | 86   | ARG  | NE-CZ-NH1   | 5.84  | 123.22                 | 120.30              |
| 21  | AA    | 315  | A    | N1-C6-N6    | -5.84 | 115.10                 | 118.60              |
| 21  | AA    | 392  | C    | N3-C2-O2    | -5.84 | 117.81                 | 121.90              |
| 21  | AA    | 513  | C    | N3-C2-O2    | -5.84 | 117.81                 | 121.90              |
| 54  | BA    | 1596 | A    | N1-C6-N6    | -5.84 | 115.10                 | 118.60              |
| 54  | BA    | 2690 | U    | N3-C2-O2    | -5.84 | 118.11                 | 122.20              |
| 21  | AA    | 479  | U    | N3-C2-O2    | -5.84 | 118.11                 | 122.20              |
| 21  | AA    | 1336 | C    | C1'-O4'-C4' | -5.84 | 105.23                 | 109.90              |
| 24  | A3    | 75   | C    | N1-C2-O2    | 5.84  | 122.40                 | 118.90              |
| 54  | BA    | 1349 | C    | N3-C4-C5    | 5.84  | 124.23                 | 121.90              |
| 54  | BA    | 2067 | G    | C5-C6-N1    | 5.84  | 114.42                 | 111.50              |
| 54  | BA    | 2306 | C    | N1-C2-O2    | 5.84  | 122.40                 | 118.90              |
| 21  | AA    | 199  | A    | C5-C6-N1    | 5.83  | 120.62                 | 117.70              |
| 54  | BA    | 182  | A    | C4-C5-C6    | -5.83 | 114.08                 | 117.00              |
| 54  | BA    | 1391 | U    | C5-C6-N1    | -5.83 | 119.78                 | 122.70              |
| 54  | BA    | 1427 | A    | P-O3'-C3'   | 5.83  | 126.70                 | 119.70              |
| 16  | AQ    | 61   | ARG  | NE-CZ-NH1   | 5.83  | 123.22                 | 120.30              |
| 21  | AA    | 238  | A    | C4-C5-C6    | -5.83 | 114.08                 | 117.00              |
| 21  | AA    | 421  | U    | C5-C6-N1    | -5.83 | 119.78                 | 122.70              |
| 54  | BA    | 602  | A    | C4-C5-C6    | -5.83 | 114.08                 | 117.00              |
| 54  | BA    | 2020 | A    | N1-C6-N6    | -5.83 | 115.10                 | 118.60              |
| 54  | BA    | 2418 | A    | C4-C5-C6    | -5.83 | 114.08                 | 117.00              |
| 21  | AA    | 14   | U    | N3-C2-O2    | -5.83 | 118.12                 | 122.20              |
| 21  | AA    | 428  | G    | N1-C6-O6    | -5.83 | 116.40                 | 119.90              |
| 21  | AA    | 1407 | C    | N3-C2-O2    | -5.83 | 117.82                 | 121.90              |
| 21  | AA    | 1456 | A    | C5-C6-N1    | 5.83  | 120.62                 | 117.70              |
| 54  | BA    | 776  | G    | N3-C2-N2    | -5.83 | 115.82                 | 119.90              |
| 54  | BA    | 898  | C    | O4'-C1'-N1  | 5.83  | 112.87                 | 108.20              |
| 54  | BA    | 2033 | A    | O4'-C1'-N9  | 5.83  | 112.86                 | 108.20              |
| 54  | BA    | 2059 | A    | C4-C5-C6    | -5.83 | 114.08                 | 117.00              |
| 55  | BB    | 26   | C    | N1-C2-O2    | 5.83  | 122.40                 | 118.90              |
| 21  | AA    | 153  | C    | N3-C4-C5    | 5.83  | 124.23                 | 121.90              |
| 21  | AA    | 262  | A    | C4-C5-C6    | -5.83 | 114.08                 | 117.00              |
| 54  | BA    | 292  | U    | O4'-C1'-N1  | 5.83  | 112.86                 | 108.20              |
| 54  | BA    | 1866 | A    | C4-C5-C6    | -5.83 | 114.08                 | 117.00              |
| 55  | BB    | 58   | A    | N1-C6-N6    | -5.83 | 115.10                 | 118.60              |
| 21  | AA    | 1396 | A    | C5-C6-N1    | 5.83  | 120.61                 | 117.70              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 21  | AA    | 1492 | A    | C4-C5-C6   | -5.83 | 114.09      | 117.00   |
| 54  | BA    | 362  | A    | C5-C6-N1   | 5.83  | 120.61      | 117.70   |
| 54  | BA    | 1187 | G    | N3-C4-C5   | -5.83 | 125.69      | 128.60   |
| 54  | BA    | 1961 | C    | N1-C2-O2   | 5.83  | 122.40      | 118.90   |
| 21  | AA    | 243  | A    | P-O3'-C3'  | 5.83  | 126.69      | 119.70   |
| 21  | AA    | 322  | C    | N3-C2-O2   | -5.83 | 117.82      | 121.90   |
| 21  | AA    | 1343 | G    | C5-C6-N1   | 5.83  | 114.41      | 111.50   |
| 32  | BJ    | 13   | ARG  | NE-CZ-NH2  | -5.83 | 117.39      | 120.30   |
| 54  | BA    | 1387 | A    | O4'-C1'-N9 | 5.83  | 112.86      | 108.20   |
| 21  | AA    | 1084 | G    | N1-C6-O6   | -5.82 | 116.41      | 119.90   |
| 22  | A1    | 75   | C    | N3-C2-O2   | -5.82 | 117.82      | 121.90   |
| 54  | BA    | 547  | A    | C4-C5-C6   | -5.82 | 114.09      | 117.00   |
| 54  | BA    | 1906 | G    | C5-C6-N1   | 5.82  | 114.41      | 111.50   |
| 54  | BA    | 2253 | G    | N9-C4-C5   | 5.82  | 107.73      | 105.40   |
| 54  | BA    | 2298 | A    | C4-C5-C6   | -5.82 | 114.09      | 117.00   |
| 54  | BA    | 2368 | C    | N1-C2-O2   | 5.82  | 122.39      | 118.90   |
| 54  | BA    | 2412 | A    | C4-C5-C6   | -5.82 | 114.09      | 117.00   |
| 54  | BA    | 2498 | C    | N1-C2-O2   | 5.82  | 122.39      | 118.90   |
| 21  | AA    | 784  | A    | C4-C5-C6   | -5.82 | 114.09      | 117.00   |
| 22  | A1    | 67   | U    | C5-C6-N1   | -5.82 | 119.79      | 122.70   |
| 54  | BA    | 663  | G    | C5-C6-N1   | 5.82  | 114.41      | 111.50   |
| 54  | BA    | 801  | G    | C5-C6-N1   | 5.82  | 114.41      | 111.50   |
| 54  | BA    | 2461 | A    | C4-C5-C6   | -5.82 | 114.09      | 117.00   |
| 54  | BA    | 2741 | A    | C5-C6-N1   | 5.82  | 120.61      | 117.70   |
| 54  | BA    | 2744 | G    | C5-C6-N1   | 5.82  | 114.41      | 111.50   |
| 54  | BA    | 1129 | A    | C5-C6-N1   | 5.82  | 120.61      | 117.70   |
| 54  | BA    | 1164 | C    | N3-C2-O2   | -5.82 | 117.83      | 121.90   |
| 54  | BA    | 1512 | C    | N1-C2-O2   | 5.82  | 122.39      | 118.90   |
| 54  | BA    | 1909 | C    | N3-C2-O2   | -5.82 | 117.83      | 121.90   |
| 54  | BA    | 2234 | G    | N7-C8-N9   | 5.82  | 116.01      | 113.10   |
| 54  | BA    | 2548 | U    | O4'-C1'-N1 | 5.82  | 112.86      | 108.20   |
| 54  | BA    | 2744 | G    | O4'-C1'-N9 | 5.82  | 112.86      | 108.20   |
| 21  | AA    | 634  | C    | N3-C2-O2   | -5.82 | 117.83      | 121.90   |
| 54  | BA    | 866  | A    | C5-C6-N1   | 5.82  | 120.61      | 117.70   |
| 54  | BA    | 1728 | C    | N3-C2-O2   | -5.82 | 117.83      | 121.90   |
| 54  | BA    | 1893 | C    | N3-C2-O2   | -5.82 | 117.83      | 121.90   |
| 21  | AA    | 647  | C    | N3-C2-O2   | -5.82 | 117.83      | 121.90   |
| 21  | AA    | 1074 | G    | N3-C2-N2   | -5.82 | 115.83      | 119.90   |
| 21  | AA    | 1352 | C    | N3-C2-O2   | -5.82 | 117.83      | 121.90   |
| 54  | BA    | 971  | G    | N3-C4-C5   | -5.82 | 125.69      | 128.60   |
| 54  | BA    | 1270 | C    | N3-C2-O2   | -5.82 | 117.83      | 121.90   |
| 54  | BA    | 1507 | C    | N3-C2-O2   | -5.82 | 117.83      | 121.90   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 54  | BA    | 1613 | G    | N9-C4-C5    | 5.82  | 107.73      | 105.40   |
| 54  | BA    | 2059 | A    | N1-C6-N6    | -5.82 | 115.11      | 118.60   |
| 54  | BA    | 2193 | G    | C5-C6-N1    | 5.82  | 114.41      | 111.50   |
| 54  | BA    | 2519 | U    | O4'-C1'-N1  | 5.82  | 112.85      | 108.20   |
| 54  | BA    | 2676 | C    | N1-C2-O2    | 5.82  | 122.39      | 118.90   |
| 54  | BA    | 1703 | G    | C5-C6-N1    | 5.81  | 114.41      | 111.50   |
| 54  | BA    | 2818 | U    | C5-C6-N1    | -5.81 | 119.79      | 122.70   |
| 3   | AD    | 25   | ARG  | NE-CZ-NH1   | 5.81  | 123.21      | 120.30   |
| 21  | AA    | 192  | A    | C4-C5-C6    | -5.81 | 114.09      | 117.00   |
| 21  | AA    | 1155 | A    | C4-C5-C6    | -5.81 | 114.09      | 117.00   |
| 54  | BA    | 176  | A    | C5-C6-N1    | 5.81  | 120.61      | 117.70   |
| 54  | BA    | 964  | C    | N3-C2-O2    | -5.81 | 117.83      | 121.90   |
| 54  | BA    | 1541 | C    | C4'-C3'-C2' | -5.81 | 96.79       | 102.60   |
| 54  | BA    | 1559 | U    | N3-C2-O2    | -5.81 | 118.13      | 122.20   |
| 54  | BA    | 1847 | A    | C4-C5-C6    | -5.81 | 114.09      | 117.00   |
| 54  | BA    | 38   | A    | N1-C6-N6    | -5.81 | 115.11      | 118.60   |
| 54  | BA    | 681  | G    | N1-C6-O6    | -5.81 | 116.41      | 119.90   |
| 54  | BA    | 1323 | C    | C5'-C4'-O4' | 5.81  | 116.07      | 109.10   |
| 54  | BA    | 2214 | C    | N3-C2-O2    | -5.81 | 117.83      | 121.90   |
| 54  | BA    | 2497 | A    | C4-C5-C6    | -5.81 | 114.09      | 117.00   |
| 21  | AA    | 170  | U    | C5-C6-N1    | -5.81 | 119.80      | 122.70   |
| 21  | AA    | 1228 | C    | N3-C4-C5    | 5.81  | 124.22      | 121.90   |
| 54  | BA    | 2803 | G    | C5-C6-N1    | 5.81  | 114.40      | 111.50   |
| 54  | BA    | 887  | U    | O4'-C1'-N1  | 5.81  | 112.85      | 108.20   |
| 54  | BA    | 1359 | A    | C6-C5-N7    | 5.81  | 136.37      | 132.30   |
| 21  | AA    | 732  | C    | N3-C4-C5    | 5.81  | 124.22      | 121.90   |
| 34  | BL    | 123  | ARG  | NE-CZ-NH1   | 5.81  | 123.20      | 120.30   |
| 54  | BA    | 8    | C    | N3-C2-O2    | -5.81 | 117.84      | 121.90   |
| 54  | BA    | 119  | A    | O4'-C1'-N9  | 5.81  | 112.84      | 108.20   |
| 54  | BA    | 1646 | C    | C2-N3-C4    | -5.81 | 117.00      | 119.90   |
| 21  | AA    | 1347 | G    | C8-N9-C4    | -5.80 | 104.08      | 106.40   |
| 54  | BA    | 2429 | G    | N3-C4-C5    | -5.80 | 125.70      | 128.60   |
| 54  | BA    | 2533 | U    | O4'-C1'-N1  | 5.80  | 112.84      | 108.20   |
| 54  | BA    | 234  | U    | C5-C6-N1    | -5.80 | 119.80      | 122.70   |
| 54  | BA    | 506  | G    | O4'-C1'-N9  | 5.80  | 112.84      | 108.20   |
| 54  | BA    | 1272 | A    | C5-C6-N1    | 5.80  | 120.60      | 117.70   |
| 21  | AA    | 303  | A    | C4-C5-C6    | -5.80 | 114.10      | 117.00   |
| 21  | AA    | 505  | G    | N3-C2-N2    | -5.80 | 115.84      | 119.90   |
| 54  | BA    | 805  | G    | N1-C6-O6    | -5.80 | 116.42      | 119.90   |
| 54  | BA    | 2015 | A    | C4-C5-C6    | -5.80 | 114.10      | 117.00   |
| 21  | AA    | 44   | A    | C5-C6-N1    | 5.80  | 120.60      | 117.70   |
| 21  | AA    | 994  | A    | C4-C5-C6    | -5.80 | 114.10      | 117.00   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 54  | BA    | 526  | A    | C4-C5-C6    | -5.80 | 114.10      | 117.00   |
| 54  | BA    | 673  | C    | N3-C2-O2    | -5.80 | 117.84      | 121.90   |
| 54  | BA    | 838  | C    | N1-C2-O2    | 5.80  | 122.38      | 118.90   |
| 54  | BA    | 1075 | C    | N1-C2-O2    | 5.80  | 122.38      | 118.90   |
| 54  | BA    | 1342 | A    | C5-C6-N1    | 5.80  | 120.60      | 117.70   |
| 54  | BA    | 1409 | U    | N3-C2-O2    | -5.80 | 118.14      | 122.20   |
| 54  | BA    | 1796 | U    | N1-C2-N3    | 5.80  | 118.38      | 114.90   |
| 54  | BA    | 1909 | C    | O4'-C1'-N1  | 5.80  | 112.84      | 108.20   |
| 54  | BA    | 2378 | A    | C5-C6-N1    | 5.80  | 120.60      | 117.70   |
| 12  | AM    | 86   | ARG  | NE-CZ-NH1   | 5.80  | 123.20      | 120.30   |
| 21  | AA    | 518  | C    | C3'-C2'-C1' | 5.80  | 106.14      | 101.50   |
| 21  | AA    | 1271 | A    | C5-C6-N1    | 5.80  | 120.60      | 117.70   |
| 21  | AA    | 45   | G    | O4'-C1'-N9  | 5.80  | 112.84      | 108.20   |
| 21  | AA    | 1109 | C    | C2-N3-C4    | -5.80 | 117.00      | 119.90   |
| 54  | BA    | 1339 | G    | N3-C4-C5    | -5.80 | 125.70      | 128.60   |
| 54  | BA    | 2048 | G    | C8-N9-C4    | -5.80 | 104.08      | 106.40   |
| 54  | BA    | 2230 | G    | N1-C6-O6    | -5.80 | 116.42      | 119.90   |
| 21  | AA    | 1327 | C    | N3-C2-O2    | -5.79 | 117.84      | 121.90   |
| 21  | AA    | 1421 | G    | N9-C4-C5    | 5.79  | 107.72      | 105.40   |
| 54  | BA    | 1767 | G    | C5-C6-N1    | 5.79  | 114.40      | 111.50   |
| 21  | AA    | 283  | U    | C5-C6-N1    | -5.79 | 119.80      | 122.70   |
| 21  | AA    | 421  | U    | O4'-C1'-N1  | 5.79  | 112.83      | 108.20   |
| 54  | BA    | 543  | G    | C5-C6-N1    | 5.79  | 114.40      | 111.50   |
| 54  | BA    | 1986 | C    | O4'-C1'-N1  | 5.79  | 112.83      | 108.20   |
| 21  | AA    | 331  | G    | O4'-C4'-C3' | 5.79  | 110.73      | 106.10   |
| 21  | AA    | 355  | C    | N1-C2-O2    | 5.79  | 122.38      | 118.90   |
| 21  | AA    | 387  | U    | N3-C2-O2    | -5.79 | 118.15      | 122.20   |
| 21  | AA    | 488  | C    | N3-C2-O2    | -5.79 | 117.85      | 121.90   |
| 21  | AA    | 633  | G    | N1-C6-O6    | -5.79 | 116.42      | 119.90   |
| 21  | AA    | 1208 | C    | N3-C2-O2    | -5.79 | 117.85      | 121.90   |
| 54  | BA    | 1711 | A    | P-O3'-C3'   | 5.79  | 126.65      | 119.70   |
| 54  | BA    | 2670 | A    | C4-C5-C6    | -5.79 | 114.10      | 117.00   |
| 11  | AL    | 113  | ARG  | NE-CZ-NH1   | 5.79  | 123.19      | 120.30   |
| 21  | AA    | 250  | A    | C4-C5-C6    | -5.79 | 114.11      | 117.00   |
| 21  | AA    | 422  | C    | N3-C4-C5    | 5.79  | 124.22      | 121.90   |
| 54  | BA    | 716  | A    | C1'-O4'-C4' | -5.79 | 105.27      | 109.90   |
| 54  | BA    | 1934 | C    | N3-C2-O2    | -5.79 | 117.85      | 121.90   |
| 54  | BA    | 1956 | U    | N3-C2-O2    | -5.79 | 118.15      | 122.20   |
| 54  | BA    | 2184 | A    | C4-C5-C6    | -5.79 | 114.11      | 117.00   |
| 54  | BA    | 2571 | U    | C5-C6-N1    | -5.79 | 119.81      | 122.70   |
| 1   | AB    | 224  | ARG  | NE-CZ-NH2   | -5.79 | 117.41      | 120.30   |
| 54  | BA    | 140  | C    | N3-C4-C5    | 5.79  | 124.22      | 121.90   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 54  | BA    | 1787 | A    | C5-C6-N1    | 5.79  | 120.59      | 117.70   |
| 54  | BA    | 2468 | A    | O4'-C1'-N9  | 5.79  | 112.83      | 108.20   |
| 21  | AA    | 701  | U    | C5-C6-N1    | -5.79 | 119.81      | 122.70   |
| 21  | AA    | 1412 | C    | N1-C2-O2    | 5.79  | 122.37      | 118.90   |
| 21  | AA    | 1529 | G    | O4'-C1'-N9  | 5.79  | 112.83      | 108.20   |
| 54  | BA    | 561  | G    | N1-C6-O6    | -5.79 | 116.43      | 119.90   |
| 54  | BA    | 845  | A    | C5-C6-N1    | 5.79  | 120.59      | 117.70   |
| 54  | BA    | 1029 | A    | C5-C6-N1    | 5.79  | 120.59      | 117.70   |
| 54  | BA    | 1717 | A    | C4-C5-C6    | -5.79 | 114.11      | 117.00   |
| 54  | BA    | 2280 | G    | C8-N9-C4    | -5.79 | 104.09      | 106.40   |
| 54  | BA    | 2792 | A    | C5-C6-N1    | 5.79  | 120.59      | 117.70   |
| 21  | AA    | 620  | C    | N1-C2-O2    | 5.78  | 122.37      | 118.90   |
| 21  | AA    | 1489 | G    | C5-C6-N1    | 5.78  | 114.39      | 111.50   |
| 54  | BA    | 41   | C    | N1-C2-O2    | 5.78  | 122.37      | 118.90   |
| 54  | BA    | 656  | G    | C8-N9-C4    | -5.78 | 104.09      | 106.40   |
| 54  | BA    | 821  | A    | C6-C5-N7    | 5.78  | 136.35      | 132.30   |
| 54  | BA    | 2350 | C    | N3-C4-C5    | 5.78  | 124.21      | 121.90   |
| 54  | BA    | 2854 | G    | N9-C4-C5    | 5.78  | 107.71      | 105.40   |
| 54  | BA    | 291  | G    | N3-C2-N2    | -5.78 | 115.85      | 119.90   |
| 54  | BA    | 1094 | U    | C5'-C4'-O4' | 5.78  | 116.04      | 109.10   |
| 21  | AA    | 49   | U    | N3-C2-O2    | -5.78 | 118.15      | 122.20   |
| 21  | AA    | 452  | A    | C4-C5-C6    | -5.78 | 114.11      | 117.00   |
| 21  | AA    | 1069 | C    | N3-C2-O2    | -5.78 | 117.85      | 121.90   |
| 22  | A1    | 18   | G    | C5-C6-N1    | 5.78  | 114.39      | 111.50   |
| 54  | BA    | 101  | A    | C4-C5-C6    | -5.78 | 114.11      | 117.00   |
| 54  | BA    | 216  | A    | N1-C6-N6    | -5.78 | 115.13      | 118.60   |
| 54  | BA    | 524  | G    | N1-C6-O6    | -5.78 | 116.43      | 119.90   |
| 54  | BA    | 1319 | C    | N3-C2-O2    | -5.78 | 117.85      | 121.90   |
| 21  | AA    | 354  | G    | N3-C4-C5    | -5.78 | 125.71      | 128.60   |
| 54  | BA    | 1389 | G    | C8-N9-C4    | -5.78 | 104.09      | 106.40   |
| 54  | BA    | 1592 | C    | O4'-C1'-N1  | 5.78  | 112.82      | 108.20   |
| 54  | BA    | 1677 | A    | N1-C6-N6    | -5.78 | 115.13      | 118.60   |
| 20  | AU    | 34   | ARG  | NE-CZ-NH1   | 5.78  | 123.19      | 120.30   |
| 22  | A1    | 70   | C    | N3-C2-O2    | -5.78 | 117.86      | 121.90   |
| 54  | BA    | 622  | G    | N1-C6-O6    | -5.78 | 116.43      | 119.90   |
| 54  | BA    | 1439 | A    | C4-C5-C6    | -5.78 | 114.11      | 117.00   |
| 54  | BA    | 1725 | U    | C5-C6-N1    | -5.78 | 119.81      | 122.70   |
| 54  | BA    | 2264 | C    | O4'-C1'-N1  | 5.78  | 112.82      | 108.20   |
| 54  | BA    | 2363 | G    | C5-C6-N1    | 5.78  | 114.39      | 111.50   |
| 21  | AA    | 799  | G    | C5-C6-N1    | 5.78  | 114.39      | 111.50   |
| 21  | AA    | 839  | C    | O4'-C1'-N1  | 5.78  | 112.82      | 108.20   |
| 54  | BA    | 225  | C    | N3-C2-O2    | -5.78 | 117.86      | 121.90   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 54  | BA    | 982  | C    | C6-N1-C2    | -5.78 | 117.99      | 120.30   |
| 54  | BA    | 1200 | C    | N3-C2-O2    | -5.78 | 117.86      | 121.90   |
| 54  | BA    | 1290 | C    | N1-C2-O2    | 5.78  | 122.36      | 118.90   |
| 54  | BA    | 2498 | C    | O4'-C1'-N1  | 5.78  | 112.82      | 108.20   |
| 21  | AA    | 394  | G    | N3-C2-N2    | -5.77 | 115.86      | 119.90   |
| 21  | AA    | 481  | G    | N3-C4-C5    | -5.77 | 125.71      | 128.60   |
| 25  | BC    | 213  | ARG  | NE-CZ-NH2   | -5.77 | 117.41      | 120.30   |
| 54  | BA    | 1374 | G    | N1-C6-O6    | -5.77 | 116.44      | 119.90   |
| 54  | BA    | 2422 | C    | N3-C2-O2    | -5.77 | 117.86      | 121.90   |
| 2   | AC    | 131  | ARG  | NE-CZ-NH1   | 5.77  | 123.19      | 120.30   |
| 21  | AA    | 857  | C    | N3-C2-O2    | -5.77 | 117.86      | 121.90   |
| 21  | AA    | 1438 | G    | N9-C4-C5    | 5.77  | 107.71      | 105.40   |
| 54  | BA    | 1383 | A    | O4'-C1'-N9  | 5.77  | 112.82      | 108.20   |
| 54  | BA    | 1545 | A    | C6-C5-N7    | 5.77  | 136.34      | 132.30   |
| 54  | BA    | 1692 | U    | N3-C2-O2    | -5.77 | 118.16      | 122.20   |
| 54  | BA    | 2362 | C    | O4'-C1'-N1  | 5.77  | 112.82      | 108.20   |
| 21  | AA    | 1508 | A    | C6-C5-N7    | 5.77  | 136.34      | 132.30   |
| 54  | BA    | 936  | A    | C5-C6-N1    | 5.77  | 120.58      | 117.70   |
| 54  | BA    | 2633 | G    | O4'-C1'-N9  | 5.77  | 112.82      | 108.20   |
| 55  | BB    | 35   | C    | C2-N3-C4    | -5.77 | 117.02      | 119.90   |
| 21  | AA    | 414  | A    | C3'-C2'-C1' | 5.77  | 106.12      | 101.50   |
| 21  | AA    | 1188 | A    | C6-C5-N7    | 5.77  | 136.34      | 132.30   |
| 21  | AA    | 1200 | C    | N3-C2-O2    | -5.77 | 117.86      | 121.90   |
| 21  | AA    | 1238 | A    | C6-C5-N7    | 5.77  | 136.34      | 132.30   |
| 21  | AA    | 1246 | A    | C4-C5-C6    | -5.77 | 114.11      | 117.00   |
| 54  | BA    | 487  | C    | C5'-C4'-O4' | 5.77  | 116.02      | 109.10   |
| 54  | BA    | 1633 | G    | C5-C6-N1    | 5.77  | 114.39      | 111.50   |
| 54  | BA    | 1947 | C    | O4'-C1'-N1  | 5.77  | 112.81      | 108.20   |
| 54  | BA    | 2087 | G    | C8-N9-C4    | -5.77 | 104.09      | 106.40   |
| 21  | AA    | 21   | G    | N3-C4-C5    | -5.77 | 125.72      | 128.60   |
| 21  | AA    | 217  | C    | N1-C2-O2    | 5.77  | 122.36      | 118.90   |
| 21  | AA    | 1063 | C    | N3-C4-C5    | 5.77  | 124.21      | 121.90   |
| 54  | BA    | 2433 | A    | O4'-C1'-N9  | 5.77  | 112.81      | 108.20   |
| 21  | AA    | 354  | G    | N9-C4-C5    | 5.77  | 107.71      | 105.40   |
| 21  | AA    | 738  | C    | N3-C2-O2    | -5.77 | 117.86      | 121.90   |
| 21  | AA    | 837  | U    | O4'-C1'-N1  | 5.77  | 112.81      | 108.20   |
| 21  | AA    | 1121 | U    | C5-C6-N1    | -5.77 | 119.82      | 122.70   |
| 21  | AA    | 1499 | A    | C4-C5-C6    | -5.77 | 114.12      | 117.00   |
| 24  | A3    | 6    | G    | C8-N9-C4    | -5.77 | 104.09      | 106.40   |
| 54  | BA    | 466  | A    | C4-C5-C6    | -5.77 | 114.12      | 117.00   |
| 54  | BA    | 1229 | C    | N3-C4-C5    | 5.77  | 124.21      | 121.90   |
| 54  | BA    | 1475 | G    | N1-C6-O6    | -5.77 | 116.44      | 119.90   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|------------|-------|------------------------|---------------------|
| 54  | BA    | 2163 | A    | C5-C6-N1   | 5.77  | 120.58                 | 117.70              |
| 54  | BA    | 2359 | C    | N3-C4-C5   | 5.77  | 124.21                 | 121.90              |
| 54  | BA    | 2604 | U    | C5-C6-N1   | -5.77 | 119.82                 | 122.70              |
| 21  | AA    | 100  | G    | N1-C6-O6   | -5.76 | 116.44                 | 119.90              |
| 21  | AA    | 357  | G    | N7-C8-N9   | 5.76  | 115.98                 | 113.10              |
| 54  | BA    | 223  | A    | C6-C5-N7   | 5.76  | 136.33                 | 132.30              |
| 14  | AO    | 71   | ARG  | NE-CZ-NH1  | 5.76  | 123.18                 | 120.30              |
| 21  | AA    | 463  | U    | O4'-C1'-N1 | 5.76  | 112.81                 | 108.20              |
| 21  | AA    | 723  | U    | N1-C2-N3   | 5.76  | 118.36                 | 114.90              |
| 29  | BG    | 162  | ARG  | NE-CZ-NH2  | -5.76 | 117.42                 | 120.30              |
| 54  | BA    | 1105 | U    | O4'-C1'-N1 | 5.76  | 112.81                 | 108.20              |
| 54  | BA    | 1150 | C    | N3-C2-O2   | -5.76 | 117.87                 | 121.90              |
| 54  | BA    | 2109 | U    | C5-C6-N1   | -5.76 | 119.82                 | 122.70              |
| 54  | BA    | 2543 | G    | N3-C2-N2   | -5.76 | 115.87                 | 119.90              |
| 54  | BA    | 2866 | U    | C5-C6-N1   | -5.76 | 119.82                 | 122.70              |
| 21  | AA    | 1148 | U    | N3-C2-O2   | -5.76 | 118.17                 | 122.20              |
| 21  | AA    | 1162 | C    | N3-C2-O2   | -5.76 | 117.87                 | 121.90              |
| 23  | A2    | 87   | U    | C5-C6-N1   | -5.76 | 119.82                 | 122.70              |
| 54  | BA    | 1281 | G    | N1-C6-O6   | -5.76 | 116.44                 | 119.90              |
| 54  | BA    | 1423 | G    | O4'-C1'-N9 | 5.76  | 112.81                 | 108.20              |
| 54  | BA    | 1434 | A    | C2-N3-C4   | 5.76  | 113.48                 | 110.60              |
| 54  | BA    | 1635 | A    | C5-C6-N1   | 5.76  | 120.58                 | 117.70              |
| 54  | BA    | 2178 | C    | C6-N1-C2   | -5.76 | 118.00                 | 120.30              |
| 54  | BA    | 2428 | G    | O4'-C1'-N9 | 5.76  | 112.81                 | 108.20              |
| 54  | BA    | 2762 | C    | O4'-C1'-N1 | 5.76  | 112.81                 | 108.20              |
| 54  | BA    | 2824 | C    | C2-N3-C4   | -5.76 | 117.02                 | 119.90              |
| 21  | AA    | 475  | C    | N1-C2-O2   | 5.76  | 122.36                 | 118.90              |
| 21  | AA    | 1181 | G    | C8-N9-C4   | -5.76 | 104.10                 | 106.40              |
| 54  | BA    | 738  | G    | N1-C6-O6   | -5.76 | 116.44                 | 119.90              |
| 55  | BB    | 23   | G    | N3-C4-C5   | -5.76 | 125.72                 | 128.60              |
| 21  | AA    | 211  | G    | O4'-C1'-N9 | 5.76  | 112.81                 | 108.20              |
| 21  | AA    | 1477 | U    | N3-C2-O2   | -5.76 | 118.17                 | 122.20              |
| 54  | BA    | 525  | U    | O4'-C1'-N1 | 5.76  | 112.81                 | 108.20              |
| 54  | BA    | 1764 | C    | N3-C2-O2   | -5.76 | 117.87                 | 121.90              |
| 54  | BA    | 2015 | A    | O4'-C1'-N9 | 5.76  | 112.81                 | 108.20              |
| 54  | BA    | 2289 | G    | N9-C4-C5   | 5.76  | 107.70                 | 105.40              |
| 54  | BA    | 2558 | C    | N3-C2-O2   | -5.76 | 117.87                 | 121.90              |
| 9   | AJ    | 68   | ARG  | NE-CZ-NH1  | 5.75  | 123.18                 | 120.30              |
| 21  | AA    | 280  | C    | N1-C2-O2   | 5.75  | 122.35                 | 118.90              |
| 54  | BA    | 2022 | U    | O4'-C1'-N1 | 5.75  | 112.80                 | 108.20              |
| 21  | AA    | 142  | G    | N1-C6-O6   | -5.75 | 116.45                 | 119.90              |
| 21  | AA    | 447  | G    | N7-C8-N9   | 5.75  | 115.98                 | 113.10              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|-------------|-------|------------------------|---------------------|
| 21  | AA    | 708  | C    | N3-C2-O2    | -5.75 | 117.87                 | 121.90              |
| 21  | AA    | 1096 | C    | C6-N1-C2    | -5.75 | 118.00                 | 120.30              |
| 21  | AA    | 1472 | U    | N3-C2-O2    | -5.75 | 118.17                 | 122.20              |
| 54  | BA    | 106  | C    | C6-N1-C2    | -5.75 | 118.00                 | 120.30              |
| 54  | BA    | 143  | C    | O4'-C1'-N1  | 5.75  | 112.80                 | 108.20              |
| 54  | BA    | 432  | A    | C4-C5-C6    | -5.75 | 114.12                 | 117.00              |
| 54  | BA    | 564  | C    | N3-C4-C5    | 5.75  | 124.20                 | 121.90              |
| 54  | BA    | 1123 | C    | N3-C2-O2    | -5.75 | 117.87                 | 121.90              |
| 54  | BA    | 1453 | A    | N1-C6-N6    | -5.75 | 115.15                 | 118.60              |
| 21  | AA    | 632  | U    | C5-C6-N1    | -5.75 | 119.82                 | 122.70              |
| 21  | AA    | 695  | A    | C4-C5-C6    | -5.75 | 114.12                 | 117.00              |
| 21  | AA    | 1180 | A    | C5-C6-N1    | 5.75  | 120.58                 | 117.70              |
| 54  | BA    | 1511 | G    | C5-C6-N1    | 5.75  | 114.38                 | 111.50              |
| 54  | BA    | 2833 | U    | C5-C6-N1    | -5.75 | 119.82                 | 122.70              |
| 55  | BB    | 30   | C    | N3-C4-N4    | -5.75 | 113.97                 | 118.00              |
| 21  | AA    | 371  | A    | C6-C5-N7    | 5.75  | 136.32                 | 132.30              |
| 24  | A3    | 42   | C    | N3-C2-O2    | -5.75 | 117.88                 | 121.90              |
| 25  | BC    | 202  | ARG  | NE-CZ-NH1   | 5.75  | 123.17                 | 120.30              |
| 54  | BA    | 986  | C    | N3-C2-O2    | -5.75 | 117.88                 | 121.90              |
| 54  | BA    | 2208 | C    | O4'-C1'-N1  | 5.75  | 112.80                 | 108.20              |
| 21  | AA    | 885  | G    | N3-C4-C5    | -5.75 | 125.72                 | 128.60              |
| 21  | AA    | 1132 | C    | N3-C2-O2    | -5.75 | 117.88                 | 121.90              |
| 21  | AA    | 1137 | C    | C2-N3-C4    | -5.75 | 117.03                 | 119.90              |
| 21  | AA    | 1267 | C    | O4'-C1'-N1  | 5.75  | 112.80                 | 108.20              |
| 22  | A1    | 11   | C    | N3-C2-O2    | -5.75 | 117.88                 | 121.90              |
| 54  | BA    | 97   | C    | N3-C2-O2    | -5.75 | 117.88                 | 121.90              |
| 54  | BA    | 854  | C    | O4'-C1'-N1  | 5.75  | 112.80                 | 108.20              |
| 54  | BA    | 1085 | A    | C1'-O4'-C4' | -5.75 | 105.30                 | 109.90              |
| 54  | BA    | 1167 | C    | N3-C2-O2    | -5.75 | 117.88                 | 121.90              |
| 21  | AA    | 1462 | C    | N1-C2-O2    | 5.75  | 122.35                 | 118.90              |
| 54  | BA    | 301  | G    | C8-N9-C4    | -5.75 | 104.10                 | 106.40              |
| 54  | BA    | 1391 | U    | N1-C2-N3    | 5.75  | 118.35                 | 114.90              |
| 54  | BA    | 1538 | G    | N1-C6-O6    | -5.75 | 116.45                 | 119.90              |
| 54  | BA    | 1749 | A    | C5-C6-N1    | 5.75  | 120.57                 | 117.70              |
| 21  | AA    | 90   | C    | N3-C2-O2    | -5.75 | 117.88                 | 121.90              |
| 21  | AA    | 159  | G    | C1'-O4'-C4' | -5.75 | 105.30                 | 109.90              |
| 21  | AA    | 232  | G    | N1-C6-O6    | -5.75 | 116.45                 | 119.90              |
| 21  | AA    | 334  | C    | N3-C2-O2    | -5.75 | 117.88                 | 121.90              |
| 21  | AA    | 1041 | G    | O4'-C1'-N9  | 5.75  | 112.80                 | 108.20              |
| 21  | AA    | 1395 | C    | N1-C2-O2    | 5.75  | 122.35                 | 118.90              |
| 54  | BA    | 58   | G    | N3-C2-N2    | -5.75 | 115.88                 | 119.90              |
| 54  | BA    | 512  | G    | O4'-C1'-N9  | 5.75  | 112.80                 | 108.20              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|-------------|-------|------------------------|---------------------|
| 54  | BA    | 1374 | G    | C5-C6-N1    | 5.75  | 114.37                 | 111.50              |
| 21  | AA    | 1472 | U    | O4'-C1'-N1  | 5.74  | 112.80                 | 108.20              |
| 54  | BA    | 194  | G    | N1-C6-O6    | -5.74 | 116.45                 | 119.90              |
| 54  | BA    | 1152 | C    | N3-C2-O2    | -5.74 | 117.88                 | 121.90              |
| 54  | BA    | 2205 | A    | C5-C6-N1    | 5.74  | 120.57                 | 117.70              |
| 54  | BA    | 2364 | C    | N3-C2-O2    | -5.74 | 117.88                 | 121.90              |
| 54  | BA    | 520  | G    | N1-C6-O6    | -5.74 | 116.45                 | 119.90              |
| 54  | BA    | 1690 | A    | C4-C5-C6    | -5.74 | 114.13                 | 117.00              |
| 18  | AS    | 36   | ARG  | NE-CZ-NH2   | -5.74 | 117.43                 | 120.30              |
| 21  | AA    | 522  | C    | N1-C2-O2    | 5.74  | 122.34                 | 118.90              |
| 25  | BC    | 62   | ARG  | NE-CZ-NH1   | 5.74  | 123.17                 | 120.30              |
| 54  | BA    | 73   | A    | N1-C6-N6    | -5.74 | 115.16                 | 118.60              |
| 54  | BA    | 1222 | U    | N3-C2-O2    | -5.74 | 118.18                 | 122.20              |
| 54  | BA    | 1702 | G    | N3-C4-C5    | -5.74 | 125.73                 | 128.60              |
| 55  | BB    | 106  | G    | N1-C6-O6    | -5.74 | 116.46                 | 119.90              |
| 21  | AA    | 963  | G    | C5-C6-N1    | 5.74  | 114.37                 | 111.50              |
| 21  | AA    | 1138 | G    | N3-C4-C5    | -5.74 | 125.73                 | 128.60              |
| 54  | BA    | 220  | G    | C8-N9-C4    | -5.74 | 104.10                 | 106.40              |
| 54  | BA    | 1145 | C    | O4'-C1'-N1  | 5.74  | 112.79                 | 108.20              |
| 54  | BA    | 1832 | C    | N3-C4-C5    | 5.74  | 124.20                 | 121.90              |
| 54  | BA    | 183  | C    | N3-C2-O2    | -5.74 | 117.88                 | 121.90              |
| 54  | BA    | 286  | U    | N1-C2-N3    | 5.74  | 118.34                 | 114.90              |
| 54  | BA    | 2792 | A    | C4-C5-C6    | -5.74 | 114.13                 | 117.00              |
| 21  | AA    | 403  | C    | N1-C2-O2    | 5.74  | 122.34                 | 118.90              |
| 21  | AA    | 583  | A    | C4-C5-C6    | -5.74 | 114.13                 | 117.00              |
| 21  | AA    | 1473 | G    | C5-C6-N1    | 5.74  | 114.37                 | 111.50              |
| 54  | BA    | 49   | A    | O4'-C1'-N9  | 5.74  | 112.79                 | 108.20              |
| 54  | BA    | 645  | C    | C2-N3-C4    | -5.74 | 117.03                 | 119.90              |
| 54  | BA    | 784  | G    | N1-C6-O6    | -5.74 | 116.46                 | 119.90              |
| 54  | BA    | 1356 | G    | O4'-C1'-N9  | 5.74  | 112.79                 | 108.20              |
| 54  | BA    | 1588 | G    | C5-C6-N1    | 5.74  | 114.37                 | 111.50              |
| 54  | BA    | 2667 | C    | N3-C2-O2    | -5.74 | 117.89                 | 121.90              |
| 54  | BA    | 2891 | U    | C5-C6-N1    | -5.74 | 119.83                 | 122.70              |
| 21  | AA    | 45   | G    | C5-C6-N1    | 5.73  | 114.37                 | 111.50              |
| 32  | BJ    | 95   | ARG  | NE-CZ-NH1   | 5.73  | 123.17                 | 120.30              |
| 54  | BA    | 469  | G    | N1-C6-O6    | -5.73 | 116.46                 | 119.90              |
| 54  | BA    | 669  | G    | C3'-C2'-C1' | 5.73  | 106.09                 | 101.50              |
| 21  | AA    | 722  | G    | C5-C6-N1    | 5.73  | 114.37                 | 111.50              |
| 21  | AA    | 966  | G    | N1-C6-O6    | -5.73 | 116.46                 | 119.90              |
| 54  | BA    | 45   | G    | N1-C6-O6    | -5.73 | 116.46                 | 119.90              |
| 54  | BA    | 802  | A    | N1-C6-N6    | -5.73 | 115.16                 | 118.60              |
| 54  | BA    | 1386 | C    | N3-C4-C5    | 5.73  | 124.19                 | 121.90              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|-------------|-------|------------------------|---------------------|
| 54  | BA    | 1463 | C    | N3-C2-O2    | -5.73 | 117.89                 | 121.90              |
| 54  | BA    | 2301 | C    | O4'-C1'-N1  | 5.73  | 112.79                 | 108.20              |
| 54  | BA    | 2321 | U    | N1-C2-N3    | 5.73  | 118.34                 | 114.90              |
| 21  | AA    | 221  | C    | C5'-C4'-O4' | 5.73  | 115.98                 | 109.10              |
| 21  | AA    | 316  | C    | C3'-C2'-C1' | 5.73  | 106.08                 | 101.50              |
| 21  | AA    | 501  | C    | N1-C2-O2    | 5.73  | 122.34                 | 118.90              |
| 23  | A2    | 89   | U    | C5-C6-N1    | -5.73 | 119.83                 | 122.70              |
| 54  | BA    | 140  | C    | N1-C2-O2    | 5.73  | 122.34                 | 118.90              |
| 54  | BA    | 441  | U    | C4'-C3'-C2' | -5.73 | 96.87                  | 102.60              |
| 54  | BA    | 474  | G    | N3-C4-C5    | -5.73 | 125.73                 | 128.60              |
| 54  | BA    | 1082 | U    | O4'-C1'-N1  | 5.73  | 112.78                 | 108.20              |
| 54  | BA    | 1460 | U    | O4'-C1'-N1  | 5.73  | 112.78                 | 108.20              |
| 21  | AA    | 1492 | A    | C5-C6-N1    | 5.73  | 120.56                 | 117.70              |
| 54  | BA    | 238  | C    | N3-C2-O2    | -5.73 | 117.89                 | 121.90              |
| 54  | BA    | 2112 | G    | N7-C8-N9    | 5.73  | 115.97                 | 113.10              |
| 54  | BA    | 2765 | A    | C5-C6-N1    | 5.73  | 120.56                 | 117.70              |
| 4   | AE    | 156  | ARG  | NE-CZ-NH1   | 5.73  | 123.16                 | 120.30              |
| 21  | AA    | 838  | G    | N1-C6-O6    | -5.73 | 116.46                 | 119.90              |
| 21  | AA    | 1285 | A    | C6-C5-N7    | 5.73  | 136.31                 | 132.30              |
| 54  | BA    | 316  | C    | N3-C4-C5    | 5.73  | 124.19                 | 121.90              |
| 54  | BA    | 624  | C    | N3-C2-O2    | -5.73 | 117.89                 | 121.90              |
| 54  | BA    | 735  | A    | C4-C5-C6    | -5.73 | 114.14                 | 117.00              |
| 54  | BA    | 1063 | G    | C1'-O4'-C4' | -5.73 | 105.32                 | 109.90              |
| 21  | AA    | 130  | A    | C6-C5-N7    | 5.73  | 136.31                 | 132.30              |
| 21  | AA    | 936  | C    | N3-C2-O2    | -5.73 | 117.89                 | 121.90              |
| 21  | AA    | 1150 | A    | C4-C5-C6    | -5.73 | 114.14                 | 117.00              |
| 54  | BA    | 2348 | U    | O4'-C1'-N1  | 5.73  | 112.78                 | 108.20              |
| 21  | AA    | 665  | A    | C6-C5-N7    | 5.72  | 136.31                 | 132.30              |
| 21  | AA    | 1369 | C    | N1-C2-O2    | 5.72  | 122.33                 | 118.90              |
| 21  | AA    | 1499 | A    | C5-C6-N1    | 5.72  | 120.56                 | 117.70              |
| 54  | BA    | 1583 | A    | C5-C6-N1    | 5.72  | 120.56                 | 117.70              |
| 54  | BA    | 1748 | C    | N3-C2-O2    | -5.72 | 117.89                 | 121.90              |
| 54  | BA    | 1964 | G    | O4'-C1'-N9  | 5.72  | 112.78                 | 108.20              |
| 54  | BA    | 2362 | C    | N3-C4-N4    | -5.72 | 113.99                 | 118.00              |
| 54  | BA    | 2782 | G    | N7-C8-N9    | 5.72  | 115.96                 | 113.10              |
| 2   | AC    | 39   | ARG  | NE-CZ-NH1   | 5.72  | 123.16                 | 120.30              |
| 2   | AC    | 64   | ARG  | NE-CZ-NH1   | 5.72  | 123.16                 | 120.30              |
| 21  | AA    | 263  | A    | C4-C5-C6    | -5.72 | 114.14                 | 117.00              |
| 21  | AA    | 495  | A    | C5'-C4'-C3' | -5.72 | 106.84                 | 116.00              |
| 21  | AA    | 582  | C    | N3-C4-C5    | 5.72  | 124.19                 | 121.90              |
| 21  | AA    | 808  | C    | N3-C2-O2    | -5.72 | 117.89                 | 121.90              |
| 54  | BA    | 865  | C    | N3-C2-O2    | -5.72 | 117.89                 | 121.90              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|-------------|-------|------------------------|---------------------|
| 54  | BA    | 1089 | A    | C4-C5-C6    | -5.72 | 114.14                 | 117.00              |
| 54  | BA    | 1102 | C    | N1-C2-O2    | 5.72  | 122.33                 | 118.90              |
| 54  | BA    | 1435 | G    | N7-C8-N9    | 5.72  | 115.96                 | 113.10              |
| 54  | BA    | 2018 | G    | N3-C4-C5    | -5.72 | 125.74                 | 128.60              |
| 54  | BA    | 2082 | A    | C4-C5-C6    | -5.72 | 114.14                 | 117.00              |
| 54  | BA    | 2854 | G    | N1-C6-O6    | -5.72 | 116.47                 | 119.90              |
| 12  | AM    | 108  | ARG  | NE-CZ-NH1   | 5.72  | 123.16                 | 120.30              |
| 21  | AA    | 121  | U    | O4'-C1'-N1  | 5.72  | 112.78                 | 108.20              |
| 24  | A3    | 5    | G    | N7-C8-N9    | 5.72  | 115.96                 | 113.10              |
| 54  | BA    | 73   | A    | C4-C5-C6    | -5.72 | 114.14                 | 117.00              |
| 54  | BA    | 473  | G    | N7-C8-N9    | 5.72  | 115.96                 | 113.10              |
| 21  | AA    | 61   | G    | N3-C4-C5    | -5.72 | 125.74                 | 128.60              |
| 21  | AA    | 72   | A    | C4-C5-C6    | -5.72 | 114.14                 | 117.00              |
| 21  | AA    | 128  | G    | O4'-C1'-N9  | 5.72  | 112.78                 | 108.20              |
| 34  | BL    | 41   | ARG  | NE-CZ-NH2   | -5.72 | 117.44                 | 120.30              |
| 54  | BA    | 621  | A    | C5'-C4'-C3' | -5.72 | 106.85                 | 116.00              |
| 54  | BA    | 732  | C    | N1-C2-O2    | 5.72  | 122.33                 | 118.90              |
| 54  | BA    | 1544 | A    | C5'-C4'-O4' | 5.72  | 115.96                 | 109.10              |
| 54  | BA    | 1901 | A    | C5-C6-N1    | 5.72  | 120.56                 | 117.70              |
| 54  | BA    | 2007 | U    | O4'-C1'-N1  | 5.72  | 112.78                 | 108.20              |
| 54  | BA    | 322  | A    | C4-C5-C6    | -5.72 | 114.14                 | 117.00              |
| 54  | BA    | 1397 | U    | N1-C2-N3    | 5.72  | 118.33                 | 114.90              |
| 21  | AA    | 340  | U    | N3-C2-O2    | -5.72 | 118.20                 | 122.20              |
| 21  | AA    | 350  | G    | C5-C6-N1    | 5.72  | 114.36                 | 111.50              |
| 21  | AA    | 814  | A    | C4-C5-C6    | -5.72 | 114.14                 | 117.00              |
| 54  | BA    | 744  | U    | O4'-C1'-N1  | 5.72  | 112.77                 | 108.20              |
| 54  | BA    | 1668 | A    | C5-C6-N1    | 5.72  | 120.56                 | 117.70              |
| 54  | BA    | 2375 | G    | C5-C6-N1    | 5.72  | 114.36                 | 111.50              |
| 54  | BA    | 2611 | C    | O4'-C1'-N1  | 5.72  | 112.77                 | 108.20              |
| 14  | AO    | 83   | ARG  | NE-CZ-NH1   | 5.71  | 123.16                 | 120.30              |
| 21  | AA    | 703  | G    | C5-C6-N1    | 5.71  | 114.36                 | 111.50              |
| 21  | AA    | 1080 | A    | C5-N7-C8    | -5.71 | 101.04                 | 103.90              |
| 21  | AA    | 1109 | C    | N3-C4-C5    | 5.71  | 124.19                 | 121.90              |
| 23  | A2    | 87   | U    | N3-C2-O2    | -5.71 | 118.20                 | 122.20              |
| 54  | BA    | 68   | G    | N1-C6-O6    | -5.71 | 116.47                 | 119.90              |
| 54  | BA    | 131  | A    | N1-C6-N6    | -5.71 | 115.17                 | 118.60              |
| 54  | BA    | 959  | A    | C4-C5-C6    | -5.71 | 114.14                 | 117.00              |
| 54  | BA    | 1527 | G    | N3-C4-C5    | -5.71 | 125.74                 | 128.60              |
| 26  | BD    | 169  | ARG  | NE-CZ-NH1   | 5.71  | 123.16                 | 120.30              |
| 21  | AA    | 1101 | A    | O4'-C1'-N9  | 5.71  | 112.77                 | 108.20              |
| 54  | BA    | 472  | A    | N1-C6-N6    | -5.71 | 115.17                 | 118.60              |
| 54  | BA    | 647  | G    | N3-C4-C5    | -5.71 | 125.74                 | 128.60              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|-------------|-------|------------------------|---------------------|
| 54  | BA    | 1100 | C    | O4'-C1'-N1  | 5.71  | 112.77                 | 108.20              |
| 21  | AA    | 676  | A    | C6-C5-N7    | 5.71  | 136.30                 | 132.30              |
| 21  | AA    | 1344 | C    | N3-C2-O2    | -5.71 | 117.90                 | 121.90              |
| 54  | BA    | 651  | G    | C8-N9-C4    | -5.71 | 104.12                 | 106.40              |
| 54  | BA    | 886  | A    | C4'-C3'-C2' | -5.71 | 96.89                  | 102.60              |
| 54  | BA    | 2880 | C    | N1-C2-O2    | 5.71  | 122.33                 | 118.90              |
| 21  | AA    | 842  | U    | O4'-C4'-C3' | 5.71  | 110.67                 | 106.10              |
| 22  | A1    | 1    | G    | N3-C4-C5    | -5.71 | 125.75                 | 128.60              |
| 54  | BA    | 457  | A    | C3'-C2'-C1' | -5.71 | 96.93                  | 101.50              |
| 54  | BA    | 479  | A    | C6-C5-N7    | 5.71  | 136.30                 | 132.30              |
| 54  | BA    | 1181 | U    | O4'-C1'-N1  | 5.71  | 112.77                 | 108.20              |
| 54  | BA    | 1851 | U    | O4'-C1'-N1  | 5.71  | 112.77                 | 108.20              |
| 54  | BA    | 2180 | U    | O4'-C1'-N1  | 5.71  | 112.77                 | 108.20              |
| 54  | BA    | 2355 | G    | N9-C4-C5    | 5.71  | 107.68                 | 105.40              |
| 54  | BA    | 2626 | C    | N3-C2-O2    | -5.71 | 117.91                 | 121.90              |
| 21  | AA    | 8    | A    | C4-C5-C6    | -5.71 | 114.15                 | 117.00              |
| 21  | AA    | 1432 | G    | C8-N9-C4    | -5.71 | 104.12                 | 106.40              |
| 54  | BA    | 343  | C    | N3-C2-O2    | -5.71 | 117.91                 | 121.90              |
| 54  | BA    | 343  | C    | N3-C4-C5    | 5.71  | 124.18                 | 121.90              |
| 54  | BA    | 1519 | G    | C8-N9-C4    | -5.71 | 104.12                 | 106.40              |
| 54  | BA    | 1738 | G    | N7-C8-N9    | 5.71  | 115.95                 | 113.10              |
| 55  | BB    | 88   | C    | N3-C2-O2    | -5.71 | 117.91                 | 121.90              |
| 21  | AA    | 275  | G    | N9-C4-C5    | 5.71  | 107.68                 | 105.40              |
| 21  | AA    | 1465 | A    | N1-C6-N6    | -5.71 | 115.18                 | 118.60              |
| 54  | BA    | 111  | A    | C5-C6-N1    | 5.71  | 120.55                 | 117.70              |
| 54  | BA    | 1073 | A    | C6-C5-N7    | 5.71  | 136.29                 | 132.30              |
| 54  | BA    | 1775 | U    | O4'-C1'-N1  | 5.71  | 112.76                 | 108.20              |
| 21  | AA    | 108  | G    | O4'-C1'-N9  | 5.70  | 112.76                 | 108.20              |
| 21  | AA    | 847  | G    | C5-C6-N1    | 5.70  | 114.35                 | 111.50              |
| 21  | AA    | 1061 | G    | C8-N9-C4    | -5.70 | 104.12                 | 106.40              |
| 21  | AA    | 1472 | U    | N1-C2-N3    | 5.70  | 118.32                 | 114.90              |
| 54  | BA    | 93   | G    | N3-C4-C5    | -5.70 | 125.75                 | 128.60              |
| 54  | BA    | 418  | C    | N3-C2-O2    | -5.70 | 117.91                 | 121.90              |
| 54  | BA    | 635  | C    | N1-C2-O2    | 5.70  | 122.32                 | 118.90              |
| 54  | BA    | 1320 | C    | N3-C4-C5    | 5.70  | 124.18                 | 121.90              |
| 54  | BA    | 2443 | C    | C5'-C4'-O4' | 5.70  | 115.94                 | 109.10              |
| 54  | BA    | 2544 | G    | N3-C4-C5    | -5.70 | 125.75                 | 128.60              |
| 55  | BB    | 81   | G    | C5-C6-N1    | 5.70  | 114.35                 | 111.50              |
| 54  | BA    | 1125 | G    | C5-C6-N1    | 5.70  | 114.35                 | 111.50              |
| 21  | AA    | 1141 | C    | N3-C4-C5    | 5.70  | 124.18                 | 121.90              |
| 54  | BA    | 83   | A    | C6-C5-N7    | 5.70  | 136.29                 | 132.30              |
| 54  | BA    | 601  | C    | N1-C2-O2    | 5.70  | 122.32                 | 118.90              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 54  | BA    | 2368 | C    | O4'-C1'-N1 | 5.70  | 112.76      | 108.20   |
| 54  | BA    | 2428 | G    | C8-N9-C4   | -5.70 | 104.12      | 106.40   |
| 21  | AA    | 466  | A    | C4-C5-C6   | -5.70 | 114.15      | 117.00   |
| 21  | AA    | 732  | C    | N1-C2-O2   | 5.70  | 122.32      | 118.90   |
| 22  | A1    | 53   | G    | N1-C6-O6   | -5.70 | 116.48      | 119.90   |
| 54  | BA    | 359  | G    | N3-C4-C5   | -5.70 | 125.75      | 128.60   |
| 54  | BA    | 1430 | G    | C8-N9-C4   | -5.70 | 104.12      | 106.40   |
| 26  | BD    | 59   | ARG  | NE-CZ-NH2  | -5.70 | 117.45      | 120.30   |
| 54  | BA    | 1830 | C    | O4'-C1'-N1 | 5.70  | 112.76      | 108.20   |
| 54  | BA    | 2611 | C    | C6-N1-C2   | -5.70 | 118.02      | 120.30   |
| 55  | BB    | 97   | C    | N1-C2-O2   | 5.70  | 122.32      | 118.90   |
| 21  | AA    | 202  | G    | C5-C6-N1   | 5.70  | 114.35      | 111.50   |
| 21  | AA    | 327  | A    | C5-C6-N1   | 5.70  | 120.55      | 117.70   |
| 54  | BA    | 707  | G    | C5-C6-N1   | 5.70  | 114.35      | 111.50   |
| 54  | BA    | 715  | A    | C4-C5-C6   | -5.70 | 114.15      | 117.00   |
| 54  | BA    | 2230 | G    | C5-C6-N1   | 5.70  | 114.35      | 111.50   |
| 21  | AA    | 573  | A    | C6-C5-N7   | 5.69  | 136.29      | 132.30   |
| 21  | AA    | 882  | C    | N1-C2-O2   | 5.69  | 122.32      | 118.90   |
| 38  | BP    | 87   | ARG  | NE-CZ-NH1  | 5.69  | 123.15      | 120.30   |
| 54  | BA    | 270  | A    | C6-C5-N7   | 5.69  | 136.29      | 132.30   |
| 54  | BA    | 1633 | G    | N1-C6-O6   | -5.69 | 116.48      | 119.90   |
| 21  | AA    | 1500 | A    | C4-C5-C6   | -5.69 | 114.15      | 117.00   |
| 54  | BA    | 1408 | G    | N1-C6-O6   | -5.69 | 116.48      | 119.90   |
| 54  | BA    | 2694 | G    | C5-C6-N1   | 5.69  | 114.35      | 111.50   |
| 2   | AC    | 87   | ARG  | NE-CZ-NH1  | 5.69  | 123.14      | 120.30   |
| 21  | AA    | 164  | G    | N1-C6-O6   | -5.69 | 116.49      | 119.90   |
| 21  | AA    | 391  | G    | N3-C4-C5   | -5.69 | 125.75      | 128.60   |
| 21  | AA    | 531  | U    | C5-C6-N1   | -5.69 | 119.86      | 122.70   |
| 21  | AA    | 1115 | U    | N1-C2-N3   | 5.69  | 118.31      | 114.90   |
| 21  | AA    | 1156 | G    | N3-C4-C5   | -5.69 | 125.75      | 128.60   |
| 32  | BJ    | 34   | ARG  | NE-CZ-NH1  | 5.69  | 123.14      | 120.30   |
| 54  | BA    | 584  | C    | N3-C2-O2   | -5.69 | 117.92      | 121.90   |
| 54  | BA    | 652  | U    | N1-C2-N3   | 5.69  | 118.31      | 114.90   |
| 54  | BA    | 2824 | C    | O4'-C1'-N1 | 5.69  | 112.75      | 108.20   |
| 54  | BA    | 54   | G    | N3-C4-C5   | -5.69 | 125.75      | 128.60   |
| 54  | BA    | 1740 | G    | N1-C6-O6   | -5.69 | 116.49      | 119.90   |
| 54  | BA    | 2374 | C    | N3-C4-C5   | 5.69  | 124.18      | 121.90   |
| 54  | BA    | 2638 | G    | N1-C6-O6   | -5.69 | 116.49      | 119.90   |
| 21  | AA    | 708  | C    | O4'-C1'-N1 | 5.69  | 112.75      | 108.20   |
| 54  | BA    | 296  | U    | C5-C6-N1   | -5.69 | 119.86      | 122.70   |
| 54  | BA    | 1311 | G    | N1-C6-O6   | -5.69 | 116.49      | 119.90   |
| 54  | BA    | 2364 | C    | N1-C2-O2   | 5.69  | 122.31      | 118.90   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 21  | AA    | 416  | G    | C5-C6-N1   | 5.69  | 114.34      | 111.50   |
| 54  | BA    | 1928 | A    | N1-C6-N6   | -5.69 | 115.19      | 118.60   |
| 21  | AA    | 372  | C    | N1-C2-O2   | 5.68  | 122.31      | 118.90   |
| 21  | AA    | 815  | A    | C4-C5-C6   | -5.68 | 114.16      | 117.00   |
| 21  | AA    | 923  | A    | C4-C5-C6   | -5.68 | 114.16      | 117.00   |
| 21  | AA    | 1219 | A    | C4-C5-C6   | -5.68 | 114.16      | 117.00   |
| 46  | BX    | 56   | ARG  | NE-CZ-NH1  | 5.68  | 123.14      | 120.30   |
| 54  | BA    | 277  | G    | O4'-C1'-N9 | 5.68  | 112.75      | 108.20   |
| 54  | BA    | 1024 | G    | O4'-C1'-N9 | 5.68  | 112.75      | 108.20   |
| 54  | BA    | 1081 | U    | N1-C2-N3   | 5.68  | 118.31      | 114.90   |
| 54  | BA    | 2565 | A    | C5-C6-N1   | 5.68  | 120.54      | 117.70   |
| 54  | BA    | 2566 | A    | N1-C6-N6   | -5.68 | 115.19      | 118.60   |
| 55  | BB    | 25   | U    | N1-C2-N3   | 5.68  | 118.31      | 114.90   |
| 13  | AN    | 41   | ARG  | NE-CZ-NH2  | -5.68 | 117.46      | 120.30   |
| 22  | A1    | 57   | G    | C5-C6-N1   | 5.68  | 114.34      | 111.50   |
| 24  | A3    | 7    | G    | N1-C6-O6   | -5.68 | 116.49      | 119.90   |
| 30  | BH    | 97   | ARG  | NE-CZ-NH1  | 5.68  | 123.14      | 120.30   |
| 40  | BR    | 90   | ARG  | NE-CZ-NH1  | 5.68  | 123.14      | 120.30   |
| 54  | BA    | 503  | A    | C4-C5-C6   | -5.68 | 114.16      | 117.00   |
| 54  | BA    | 599  | A    | C6-C5-N7   | 5.68  | 136.28      | 132.30   |
| 54  | BA    | 797  | G    | N1-C6-O6   | -5.68 | 116.49      | 119.90   |
| 54  | BA    | 848  | C    | N3-C2-O2   | -5.68 | 117.92      | 121.90   |
| 54  | BA    | 1005 | C    | N3-C2-O2   | -5.68 | 117.92      | 121.90   |
| 54  | BA    | 1390 | U    | O4'-C1'-N1 | 5.68  | 112.75      | 108.20   |
| 54  | BA    | 1790 | C    | N3-C2-O2   | -5.68 | 117.92      | 121.90   |
| 8   | AI    | 98   | ARG  | NH1-CZ-NH2 | -5.68 | 113.15      | 119.40   |
| 21  | AA    | 1533 | C    | P-O3'-C3'  | 5.68  | 126.52      | 119.70   |
| 54  | BA    | 40   | U    | N1-C2-N3   | 5.68  | 118.31      | 114.90   |
| 54  | BA    | 1496 | A    | C4-C5-C6   | -5.68 | 114.16      | 117.00   |
| 21  | AA    | 660  | C    | N3-C2-O2   | -5.68 | 117.92      | 121.90   |
| 21  | AA    | 664  | G    | N1-C6-O6   | -5.68 | 116.49      | 119.90   |
| 21  | AA    | 754  | C    | N1-C2-O2   | 5.68  | 122.31      | 118.90   |
| 21  | AA    | 1397 | C    | N1-C2-O2   | 5.68  | 122.31      | 118.90   |
| 21  | AA    | 1428 | A    | C6-C5-N7   | 5.68  | 136.28      | 132.30   |
| 54  | BA    | 577  | G    | C5-C6-N1   | 5.68  | 114.34      | 111.50   |
| 54  | BA    | 1677 | A    | N7-C8-N9   | 5.68  | 116.64      | 113.80   |
| 54  | BA    | 2233 | U    | O4'-C1'-N1 | 5.68  | 112.74      | 108.20   |
| 54  | BA    | 2301 | C    | N3-C2-O2   | -5.68 | 117.92      | 121.90   |
| 54  | BA    | 2702 | G    | N3-C2-N2   | -5.68 | 115.92      | 119.90   |
| 54  | BA    | 2738 | A    | C4-C5-C6   | -5.68 | 114.16      | 117.00   |
| 21  | AA    | 735  | C    | N3-C2-O2   | -5.68 | 117.93      | 121.90   |
| 21  | AA    | 1014 | A    | C5-C6-N1   | 5.68  | 120.54      | 117.70   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|-------------|-------|------------------------|---------------------|
| 21  | AA    | 1071 | C    | O4'-C1'-N1  | 5.68  | 112.74                 | 108.20              |
| 21  | AA    | 1487 | G    | N9-C4-C5    | 5.68  | 107.67                 | 105.40              |
| 54  | BA    | 25   | U    | C5-C6-N1    | -5.68 | 119.86                 | 122.70              |
| 54  | BA    | 25   | U    | N3-C2-O2    | -5.68 | 118.23                 | 122.20              |
| 54  | BA    | 316  | C    | O4'-C1'-N1  | 5.68  | 112.74                 | 108.20              |
| 54  | BA    | 650  | C    | N3-C2-O2    | -5.68 | 117.93                 | 121.90              |
| 54  | BA    | 668  | A    | C5-C6-N1    | 5.68  | 120.54                 | 117.70              |
| 54  | BA    | 1147 | A    | C4-C5-C6    | -5.68 | 114.16                 | 117.00              |
| 54  | BA    | 1267 | U    | O4'-C1'-N1  | 5.68  | 112.74                 | 108.20              |
| 54  | BA    | 2117 | A    | N1-C6-N6    | -5.68 | 115.19                 | 118.60              |
| 21  | AA    | 1426 | G    | N7-C8-N9    | 5.67  | 115.94                 | 113.10              |
| 22  | A1    | 18   | G    | N3-C4-C5    | -5.67 | 125.76                 | 128.60              |
| 54  | BA    | 1881 | C    | N3-C2-O2    | -5.67 | 117.93                 | 121.90              |
| 21  | AA    | 236  | A    | C4-C5-C6    | -5.67 | 114.16                 | 117.00              |
| 54  | BA    | 542  | C    | N3-C2-O2    | -5.67 | 117.93                 | 121.90              |
| 54  | BA    | 556  | A    | C4-C5-C6    | -5.67 | 114.16                 | 117.00              |
| 54  | BA    | 2473 | U    | O4'-C1'-N1  | 5.67  | 112.74                 | 108.20              |
| 21  | AA    | 1277 | C    | N3-C2-O2    | -5.67 | 117.93                 | 121.90              |
| 54  | BA    | 100  | U    | C5-C6-N1    | -5.67 | 119.86                 | 122.70              |
| 54  | BA    | 409  | G    | N7-C8-N9    | 5.67  | 115.94                 | 113.10              |
| 54  | BA    | 915  | C    | N1-C2-O2    | 5.67  | 122.30                 | 118.90              |
| 54  | BA    | 2063 | C    | C2-N3-C4    | -5.67 | 117.06                 | 119.90              |
| 54  | BA    | 2401 | U    | O4'-C1'-N1  | 5.67  | 112.74                 | 108.20              |
| 54  | BA    | 2577 | A    | C5-C6-N1    | 5.67  | 120.54                 | 117.70              |
| 21  | AA    | 925  | G    | N3-C4-C5    | -5.67 | 125.77                 | 128.60              |
| 54  | BA    | 31   | C    | N3-C4-C5    | 5.67  | 124.17                 | 121.90              |
| 54  | BA    | 2743 | U    | C5'-C4'-O4' | 5.67  | 115.91                 | 109.10              |
| 55  | BB    | 117  | G    | N1-C6-O6    | -5.67 | 116.50                 | 119.90              |
| 21  | AA    | 1027 | C    | N3-C2-O2    | -5.67 | 117.93                 | 121.90              |
| 21  | AA    | 1046 | A    | C6-C5-N7    | 5.67  | 136.27                 | 132.30              |
| 21  | AA    | 1504 | G    | C1'-O4'-C4' | -5.67 | 105.36                 | 109.90              |
| 54  | BA    | 806  | C    | N1-C2-O2    | 5.67  | 122.30                 | 118.90              |
| 54  | BA    | 814  | C    | N3-C2-O2    | -5.67 | 117.93                 | 121.90              |
| 54  | BA    | 1817 | G    | N1-C6-O6    | -5.67 | 116.50                 | 119.90              |
| 54  | BA    | 2862 | G    | N3-C4-C5    | -5.67 | 125.77                 | 128.60              |
| 21  | AA    | 124  | C    | N3-C2-O2    | -5.67 | 117.93                 | 121.90              |
| 21  | AA    | 705  | G    | C6-C5-N7    | 5.67  | 133.80                 | 130.40              |
| 21  | AA    | 796  | C    | N3-C2-O2    | -5.67 | 117.93                 | 121.90              |
| 54  | BA    | 2525 | G    | N1-C6-O6    | -5.67 | 116.50                 | 119.90              |
| 21  | AA    | 239  | U    | N3-C2-O2    | -5.67 | 118.23                 | 122.20              |
| 54  | BA    | 2039 | U    | N3-C2-O2    | -5.67 | 118.23                 | 122.20              |
| 21  | AA    | 496  | A    | C8-N9-C4    | -5.66 | 103.53                 | 105.80              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|------------|-------|------------------------|---------------------|
| 54  | BA    | 1624 | U    | O4'-C1'-N1 | 5.66  | 112.73                 | 108.20              |
| 54  | BA    | 1681 | G    | O4'-C1'-N9 | 5.66  | 112.73                 | 108.20              |
| 54  | BA    | 1864 | U    | O4'-C1'-N1 | 5.66  | 112.73                 | 108.20              |
| 54  | BA    | 1895 | C    | N1-C2-O2   | 5.66  | 122.30                 | 118.90              |
| 24  | A3    | 71   | G    | C8-N9-C4   | -5.66 | 104.14                 | 106.40              |
| 54  | BA    | 2798 | U    | O4'-C1'-N1 | 5.66  | 112.73                 | 108.20              |
| 21  | AA    | 709  | U    | N1-C2-N3   | 5.66  | 118.30                 | 114.90              |
| 21  | AA    | 1041 | G    | N9-C4-C5   | 5.66  | 107.66                 | 105.40              |
| 21  | AA    | 1098 | C    | N1-C2-O2   | 5.66  | 122.30                 | 118.90              |
| 21  | AA    | 1434 | A    | C6-C5-N7   | 5.66  | 136.26                 | 132.30              |
| 21  | AA    | 1520 | C    | C6-N1-C2   | -5.66 | 118.03                 | 120.30              |
| 54  | BA    | 237  | C    | N3-C2-O2   | -5.66 | 117.94                 | 121.90              |
| 54  | BA    | 1946 | U    | C5-C6-N1   | -5.66 | 119.87                 | 122.70              |
| 54  | BA    | 2074 | U    | O4'-C1'-N1 | 5.66  | 112.73                 | 108.20              |
| 54  | BA    | 2222 | C    | N3-C4-C5   | 5.66  | 124.16                 | 121.90              |
| 54  | BA    | 2903 | U    | O4'-C1'-N1 | 5.66  | 112.73                 | 108.20              |
| 21  | AA    | 1210 | C    | N1-C2-O2   | 5.66  | 122.30                 | 118.90              |
| 46  | BX    | 36   | ARG  | NE-CZ-NH1  | 5.66  | 123.13                 | 120.30              |
| 54  | BA    | 40   | U    | O4'-C1'-N1 | 5.66  | 112.73                 | 108.20              |
| 54  | BA    | 1319 | C    | N1-C2-O2   | 5.66  | 122.30                 | 118.90              |
| 55  | BB    | 71   | C    | O4'-C1'-N1 | 5.66  | 112.73                 | 108.20              |
| 54  | BA    | 1127 | A    | C5-C6-N1   | 5.66  | 120.53                 | 117.70              |
| 55  | BB    | 19   | C    | N3-C4-C5   | 5.66  | 124.16                 | 121.90              |
| 21  | AA    | 719  | C    | N1-C2-O2   | 5.66  | 122.29                 | 118.90              |
| 21  | AA    | 1416 | G    | N1-C6-O6   | -5.66 | 116.51                 | 119.90              |
| 54  | BA    | 274  | C    | O4'-C1'-N1 | 5.66  | 112.72                 | 108.20              |
| 54  | BA    | 738  | G    | O4'-C1'-N9 | 5.66  | 112.72                 | 108.20              |
| 54  | BA    | 833  | A    | O4'-C1'-N9 | 5.66  | 112.72                 | 108.20              |
| 54  | BA    | 1237 | A    | C5-C6-N1   | 5.66  | 120.53                 | 117.70              |
| 54  | BA    | 1694 | C    | N3-C2-O2   | -5.66 | 117.94                 | 121.90              |
| 54  | BA    | 2802 | G    | C5-C6-N1   | 5.66  | 114.33                 | 111.50              |
| 21  | AA    | 559  | A    | O4'-C1'-N9 | 5.65  | 112.72                 | 108.20              |
| 21  | AA    | 586  | C    | N3-C2-O2   | -5.65 | 117.94                 | 121.90              |
| 21  | AA    | 760  | G    | N1-C6-O6   | -5.65 | 116.51                 | 119.90              |
| 21  | AA    | 1411 | C    | O4'-C1'-N1 | 5.65  | 112.72                 | 108.20              |
| 54  | BA    | 2362 | C    | N1-C2-O2   | 5.65  | 122.29                 | 118.90              |
| 21  | AA    | 393  | A    | C5-C6-N1   | 5.65  | 120.53                 | 117.70              |
| 21  | AA    | 741  | G    | C8-N9-C4   | -5.65 | 104.14                 | 106.40              |
| 21  | AA    | 901  | A    | C4-C5-C6   | -5.65 | 114.17                 | 117.00              |
| 34  | BL    | 60   | ARG  | NE-CZ-NH1  | 5.65  | 123.13                 | 120.30              |
| 51  | B2    | 12   | ARG  | NE-CZ-NH1  | 5.65  | 123.13                 | 120.30              |
| 54  | BA    | 507  | A    | C4-C5-C6   | -5.65 | 114.17                 | 117.00              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 54  | BA    | 731  | C    | N1-C2-O2    | 5.65  | 122.29      | 118.90   |
| 54  | BA    | 1647 | U    | N3-C2-O2    | -5.65 | 118.24      | 122.20   |
| 54  | BA    | 1747 | U    | C5-C6-N1    | -5.65 | 119.87      | 122.70   |
| 54  | BA    | 2291 | U    | O4'-C1'-N1  | 5.65  | 112.72      | 108.20   |
| 54  | BA    | 2742 | G    | N1-C6-O6    | -5.65 | 116.51      | 119.90   |
| 21  | AA    | 356  | A    | C2-N3-C4    | 5.65  | 113.43      | 110.60   |
| 24  | A3    | 41   | C    | N3-C2-O2    | -5.65 | 117.94      | 121.90   |
| 54  | BA    | 123  | G    | N1-C6-O6    | -5.65 | 116.51      | 119.90   |
| 54  | BA    | 301  | G    | N1-C6-O6    | -5.65 | 116.51      | 119.90   |
| 54  | BA    | 1715 | G    | C5-C6-N1    | 5.65  | 114.33      | 111.50   |
| 54  | BA    | 1836 | C    | C3'-C2'-C1' | 5.65  | 106.02      | 101.50   |
| 55  | BB    | 84   | G    | N3-C2-N2    | -5.65 | 115.94      | 119.90   |
| 21  | AA    | 582  | C    | N3-C2-O2    | -5.65 | 117.95      | 121.90   |
| 54  | BA    | 161  | A    | C6-C5-N7    | 5.65  | 136.25      | 132.30   |
| 54  | BA    | 1234 | U    | C5-C6-N1    | -5.65 | 119.88      | 122.70   |
| 54  | BA    | 1419 | A    | C4-C5-C6    | -5.65 | 114.17      | 117.00   |
| 54  | BA    | 2123 | G    | N9-C4-C5    | 5.65  | 107.66      | 105.40   |
| 54  | BA    | 2324 | U    | N3-C2-O2    | -5.65 | 118.25      | 122.20   |
| 21  | AA    | 433  | G    | N3-C2-N2    | -5.65 | 115.95      | 119.90   |
| 54  | BA    | 358  | U    | N1-C2-N3    | 5.65  | 118.29      | 114.90   |
| 54  | BA    | 718  | A    | C2-N3-C4    | 5.65  | 113.42      | 110.60   |
| 54  | BA    | 1429 | G    | N7-C8-N9    | 5.65  | 115.92      | 113.10   |
| 54  | BA    | 1667 | G    | N9-C4-C5    | 5.65  | 107.66      | 105.40   |
| 54  | BA    | 1751 | U    | O4'-C1'-N1  | 5.65  | 112.72      | 108.20   |
| 54  | BA    | 2056 | G    | C5-C6-N1    | 5.65  | 114.32      | 111.50   |
| 54  | BA    | 2380 | C    | N1-C2-O2    | 5.65  | 122.29      | 118.90   |
| 21  | AA    | 1066 | C    | N3-C4-C5    | 5.65  | 124.16      | 121.90   |
| 24  | A3    | 64   | G    | N7-C8-N9    | 5.65  | 115.92      | 113.10   |
| 54  | BA    | 1711 | A    | C4-C5-C6    | -5.65 | 114.18      | 117.00   |
| 54  | BA    | 2708 | G    | N9-C4-C5    | 5.65  | 107.66      | 105.40   |
| 21  | AA    | 429  | U    | C5-C6-N1    | -5.64 | 119.88      | 122.70   |
| 21  | AA    | 519  | C    | N1-C2-O2    | 5.64  | 122.29      | 118.90   |
| 21  | AA    | 1441 | A    | C4-C5-C6    | -5.64 | 114.18      | 117.00   |
| 54  | BA    | 8    | C    | O4'-C1'-N1  | 5.64  | 112.72      | 108.20   |
| 54  | BA    | 153  | U    | O4'-C1'-N1  | 5.64  | 112.72      | 108.20   |
| 54  | BA    | 1071 | G    | C5'-C4'-C3' | -5.64 | 106.97      | 116.00   |
| 54  | BA    | 1253 | A    | C5'-C4'-C3' | -5.64 | 106.97      | 116.00   |
| 54  | BA    | 1345 | C    | N3-C4-C5    | 5.64  | 124.16      | 121.90   |
| 54  | BA    | 1579 | A    | N1-C6-N6    | -5.64 | 115.21      | 118.60   |
| 54  | BA    | 1992 | G    | C5-C6-N1    | 5.64  | 114.32      | 111.50   |
| 54  | BA    | 2072 | C    | O4'-C1'-N1  | 5.64  | 112.72      | 108.20   |
| 21  | AA    | 290  | C    | N1-C2-O2    | 5.64  | 122.29      | 118.90   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|-------------|-------|------------------------|---------------------|
| 21  | AA    | 295  | C    | C1'-O4'-C4' | -5.64 | 105.39                 | 109.90              |
| 21  | AA    | 1166 | G    | C3'-C2'-C1' | 5.64  | 106.01                 | 101.50              |
| 21  | AA    | 1450 | U    | C5-C6-N1    | -5.64 | 119.88                 | 122.70              |
| 54  | BA    | 315  | G    | N1-C6-O6    | -5.64 | 116.51                 | 119.90              |
| 54  | BA    | 1490 | A    | C4-C5-C6    | -5.64 | 114.18                 | 117.00              |
| 54  | BA    | 1738 | G    | C8-N9-C4    | -5.64 | 104.14                 | 106.40              |
| 54  | BA    | 1767 | G    | N1-C6-O6    | -5.64 | 116.52                 | 119.90              |
| 54  | BA    | 66   | C    | N3-C2-O2    | -5.64 | 117.95                 | 121.90              |
| 54  | BA    | 1481 | U    | C5-C6-N1    | -5.64 | 119.88                 | 122.70              |
| 54  | BA    | 2073 | C    | C5'-C4'-O4' | 5.64  | 115.87                 | 109.10              |
| 54  | BA    | 2246 | G    | C5-C6-N1    | 5.64  | 114.32                 | 111.50              |
| 21  | AA    | 315  | A    | C4-C5-C6    | -5.64 | 114.18                 | 117.00              |
| 54  | BA    | 2731 | G    | N3-C4-C5    | -5.64 | 125.78                 | 128.60              |
| 54  | BA    | 2751 | G    | N3-C4-C5    | -5.64 | 125.78                 | 128.60              |
| 55  | BB    | 102  | G    | C5-C6-N1    | 5.64  | 114.32                 | 111.50              |
| 55  | BB    | 104  | A    | N1-C6-N6    | -5.64 | 115.22                 | 118.60              |
| 21  | AA    | 1527 | U    | C5-C6-N1    | -5.64 | 119.88                 | 122.70              |
| 54  | BA    | 382  | A    | O4'-C1'-N9  | 5.64  | 112.71                 | 108.20              |
| 54  | BA    | 1941 | C    | N1-C2-O2    | 5.64  | 122.28                 | 118.90              |
| 21  | AA    | 551  | U    | N3-C2-O2    | -5.64 | 118.25                 | 122.20              |
| 21  | AA    | 689  | C    | O4'-C1'-N1  | 5.64  | 112.71                 | 108.20              |
| 21  | AA    | 1461 | G    | O4'-C1'-N9  | 5.64  | 112.71                 | 108.20              |
| 22  | A1    | 62   | C    | N1-C2-O2    | 5.64  | 122.28                 | 118.90              |
| 54  | BA    | 963  | U    | O4'-C1'-N1  | 5.64  | 112.71                 | 108.20              |
| 54  | BA    | 1925 | C    | N3-C2-O2    | -5.64 | 117.95                 | 121.90              |
| 54  | BA    | 2095 | A    | C4'-C3'-C2' | -5.64 | 96.96                  | 102.60              |
| 54  | BA    | 2179 | C    | N3-C2-O2    | -5.64 | 117.95                 | 121.90              |
| 54  | BA    | 2859 | G    | C5-C6-N1    | 5.64  | 114.32                 | 111.50              |
| 55  | BB    | 93   | C    | O4'-C1'-N1  | 5.64  | 112.71                 | 108.20              |
| 54  | BA    | 1524 | G    | C5-C6-N1    | 5.63  | 114.32                 | 111.50              |
| 54  | BA    | 1598 | A    | C4-C5-C6    | -5.63 | 114.18                 | 117.00              |
| 55  | BB    | 71   | C    | N1-C2-O2    | 5.63  | 122.28                 | 118.90              |
| 55  | BB    | 111  | U    | C5-C6-N1    | -5.63 | 119.88                 | 122.70              |
| 21  | AA    | 253  | A    | C4-C5-C6    | -5.63 | 114.18                 | 117.00              |
| 21  | AA    | 385  | C    | C6-N1-C2    | -5.63 | 118.05                 | 120.30              |
| 21  | AA    | 523  | A    | C6-C5-N7    | 5.63  | 136.24                 | 132.30              |
| 24  | A3    | 59   | A    | N1-C6-N6    | -5.63 | 115.22                 | 118.60              |
| 54  | BA    | 218  | A    | C6-C5-N7    | 5.63  | 136.24                 | 132.30              |
| 54  | BA    | 2161 | C    | N3-C2-O2    | -5.63 | 117.96                 | 121.90              |
| 54  | BA    | 2263 | C    | N3-C2-O2    | -5.63 | 117.96                 | 121.90              |
| 54  | BA    | 2450 | A    | C4-C5-C6    | -5.63 | 114.18                 | 117.00              |
| 55  | BB    | 60   | C    | O4'-C1'-N1  | 5.63  | 112.71                 | 108.20              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|-------------|-------|------------------------|---------------------|
| 21  | AA    | 1150 | A    | C5-C6-N1    | 5.63  | 120.52                 | 117.70              |
| 21  | AA    | 1333 | A    | C5-C6-N1    | 5.63  | 120.52                 | 117.70              |
| 21  | AA    | 1516 | G    | N3-C2-N2    | -5.63 | 115.96                 | 119.90              |
| 39  | BQ    | 5    | ARG  | NE-CZ-NH1   | 5.63  | 123.12                 | 120.30              |
| 54  | BA    | 167  | A    | C5-C6-N1    | 5.63  | 120.52                 | 117.70              |
| 54  | BA    | 180  | G    | N9-C4-C5    | 5.63  | 107.65                 | 105.40              |
| 54  | BA    | 1694 | C    | N1-C2-O2    | 5.63  | 122.28                 | 118.90              |
| 54  | BA    | 2393 | U    | N3-C2-O2    | -5.63 | 118.26                 | 122.20              |
| 55  | BB    | 59   | A    | C5-C6-N1    | 5.63  | 120.52                 | 117.70              |
| 21  | AA    | 292  | G    | C8-N9-C4    | -5.63 | 104.15                 | 106.40              |
| 23  | A2    | 93   | U    | C5-C6-N1    | -5.63 | 119.89                 | 122.70              |
| 28  | BF    | 29   | ARG  | NE-CZ-NH1   | 5.63  | 123.11                 | 120.30              |
| 54  | BA    | 1038 | G    | C5-C6-N1    | 5.63  | 114.31                 | 111.50              |
| 54  | BA    | 1574 | C    | N3-C2-O2    | -5.63 | 117.96                 | 121.90              |
| 21  | AA    | 40   | C    | N1-C2-O2    | 5.63  | 122.28                 | 118.90              |
| 21  | AA    | 340  | U    | C3'-C2'-C1' | 5.63  | 106.00                 | 101.50              |
| 54  | BA    | 724  | U    | O4'-C1'-N1  | 5.63  | 112.70                 | 108.20              |
| 54  | BA    | 893  | C    | O4'-C1'-N1  | 5.63  | 112.70                 | 108.20              |
| 54  | BA    | 1350 | C    | N3-C2-O2    | -5.63 | 117.96                 | 121.90              |
| 54  | BA    | 1402 | U    | N1-C2-N3    | 5.63  | 118.28                 | 114.90              |
| 54  | BA    | 2268 | A    | C4-C5-C6    | -5.63 | 114.19                 | 117.00              |
| 54  | BA    | 2895 | G    | C5-C6-N1    | 5.63  | 114.31                 | 111.50              |
| 54  | BA    | 1172 | C    | N1-C2-O2    | 5.63  | 122.28                 | 118.90              |
| 54  | BA    | 1410 | G    | C5-C6-N1    | 5.63  | 114.31                 | 111.50              |
| 54  | BA    | 2180 | U    | N1-C2-N3    | 5.63  | 118.28                 | 114.90              |
| 54  | BA    | 2279 | G    | N3-C2-N2    | -5.63 | 115.96                 | 119.90              |
| 21  | AA    | 803  | G    | C5-C6-N1    | 5.62  | 114.31                 | 111.50              |
| 54  | BA    | 2508 | G    | C5-C6-N1    | 5.62  | 114.31                 | 111.50              |
| 54  | BA    | 2808 | G    | N3-C4-C5    | -5.62 | 125.79                 | 128.60              |
| 54  | BA    | 2850 | A    | C5-C6-N1    | 5.62  | 120.51                 | 117.70              |
| 21  | AA    | 271  | C    | N1-C2-O2    | 5.62  | 122.27                 | 118.90              |
| 21  | AA    | 364  | A    | C6-C5-N7    | 5.62  | 136.24                 | 132.30              |
| 21  | AA    | 629  | A    | C4-C5-C6    | -5.62 | 114.19                 | 117.00              |
| 21  | AA    | 942  | G    | C5-C6-N1    | 5.62  | 114.31                 | 111.50              |
| 54  | BA    | 770  | G    | C5-C6-N1    | 5.62  | 114.31                 | 111.50              |
| 54  | BA    | 1346 | G    | N3-C2-N2    | -5.62 | 115.96                 | 119.90              |
| 54  | BA    | 1766 | G    | O4'-C1'-N9  | 5.62  | 112.70                 | 108.20              |
| 54  | BA    | 2366 | A    | C4-C5-C6    | -5.62 | 114.19                 | 117.00              |
| 54  | BA    | 2569 | G    | N1-C6-O6    | -5.62 | 116.53                 | 119.90              |
| 21  | AA    | 490  | C    | N3-C4-C5    | 5.62  | 124.15                 | 121.90              |
| 21  | AA    | 1417 | G    | C5-C6-N1    | 5.62  | 114.31                 | 111.50              |
| 24  | A3    | 40   | C    | N3-C2-O2    | -5.62 | 117.97                 | 121.90              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 24  | A3    | 68   | C    | N3-C4-C5    | 5.62  | 124.15      | 121.90   |
| 54  | BA    | 613  | A    | O4'-C1'-N9  | 5.62  | 112.70      | 108.20   |
| 54  | BA    | 711  | G    | N1-C6-O6    | -5.62 | 116.53      | 119.90   |
| 54  | BA    | 1776 | G    | C5'-C4'-C3' | -5.62 | 107.01      | 116.00   |
| 21  | AA    | 622  | A    | C4-C5-C6    | -5.62 | 114.19      | 117.00   |
| 21  | AA    | 824  | G    | C8-N9-C4    | -5.62 | 104.15      | 106.40   |
| 21  | AA    | 1178 | G    | C5-C6-N1    | 5.62  | 114.31      | 111.50   |
| 34  | BL    | 21   | ARG  | NE-CZ-NH1   | 5.62  | 123.11      | 120.30   |
| 54  | BA    | 120  | U    | O4'-C1'-N1  | 5.62  | 112.70      | 108.20   |
| 21  | AA    | 490  | C    | O4'-C1'-N1  | 5.62  | 112.70      | 108.20   |
| 21  | AA    | 728  | A    | C6-C5-N7    | 5.62  | 136.23      | 132.30   |
| 21  | AA    | 1105 | A    | C6-C5-N7    | 5.62  | 136.23      | 132.30   |
| 21  | AA    | 1271 | A    | C4-C5-C6    | -5.62 | 114.19      | 117.00   |
| 48  | BZ    | 44   | ARG  | NE-CZ-NH1   | 5.62  | 123.11      | 120.30   |
| 54  | BA    | 55   | G    | C5-C6-N1    | 5.62  | 114.31      | 111.50   |
| 54  | BA    | 135  | U    | C5-C6-N1    | -5.62 | 119.89      | 122.70   |
| 54  | BA    | 1236 | G    | N3-C2-N2    | -5.62 | 115.97      | 119.90   |
| 54  | BA    | 1542 | U    | O4'-C1'-N1  | 5.62  | 112.69      | 108.20   |
| 54  | BA    | 2545 | G    | N3-C4-C5    | -5.62 | 125.79      | 128.60   |
| 54  | BA    | 2802 | G    | N3-C4-C5    | -5.62 | 125.79      | 128.60   |
| 21  | AA    | 451  | A    | P-O3'-C3'   | 5.62  | 126.44      | 119.70   |
| 54  | BA    | 1517 | G    | C5-C6-N1    | 5.62  | 114.31      | 111.50   |
| 21  | AA    | 704  | A    | C5-C6-N1    | 5.62  | 120.51      | 117.70   |
| 21  | AA    | 941  | G    | N3-C4-C5    | -5.62 | 125.79      | 128.60   |
| 54  | BA    | 820  | A    | C4-C5-C6    | -5.62 | 114.19      | 117.00   |
| 54  | BA    | 2140 | G    | N1-C6-O6    | -5.62 | 116.53      | 119.90   |
| 21  | AA    | 338  | A    | C5-C6-N1    | 5.61  | 120.51      | 117.70   |
| 21  | AA    | 1070 | U    | N1-C2-N3    | 5.61  | 118.27      | 114.90   |
| 54  | BA    | 1719 | G    | N3-C4-C5    | -5.61 | 125.79      | 128.60   |
| 54  | BA    | 1793 | C    | N1-C2-O2    | 5.61  | 122.27      | 118.90   |
| 54  | BA    | 2185 | U    | O4'-C1'-N1  | 5.61  | 112.69      | 108.20   |
| 54  | BA    | 2429 | G    | C5-C6-N1    | 5.61  | 114.31      | 111.50   |
| 54  | BA    | 2630 | G    | C5-C6-N1    | 5.61  | 114.31      | 111.50   |
| 55  | BB    | 17   | C    | N3-C2-O2    | -5.61 | 117.97      | 121.90   |
| 21  | AA    | 923  | A    | C5-C6-N1    | 5.61  | 120.51      | 117.70   |
| 21  | AA    | 975  | A    | N1-C6-N6    | -5.61 | 115.23      | 118.60   |
| 54  | BA    | 199  | A    | N1-C6-N6    | -5.61 | 115.23      | 118.60   |
| 54  | BA    | 2403 | C    | O4'-C1'-N1  | 5.61  | 112.69      | 108.20   |
| 24  | A3    | 32   | G    | N1-C6-O6    | -5.61 | 116.53      | 119.90   |
| 54  | BA    | 346  | A    | O4'-C1'-N9  | 5.61  | 112.69      | 108.20   |
| 54  | BA    | 394  | C    | O4'-C1'-N1  | 5.61  | 112.69      | 108.20   |
| 54  | BA    | 1960 | A    | C4-C5-C6    | -5.61 | 114.20      | 117.00   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|------------|-------|------------------------|---------------------|
| 54  | BA    | 2385 | C    | N3-C4-C5   | 5.61  | 124.14                 | 121.90              |
| 21  | AA    | 97   | G    | C5-C6-N1   | 5.61  | 114.30                 | 111.50              |
| 54  | BA    | 203  | A    | C8-N9-C4   | -5.61 | 103.56                 | 105.80              |
| 54  | BA    | 863  | A    | C5-C6-N1   | 5.61  | 120.50                 | 117.70              |
| 21  | AA    | 1306 | A    | N1-C6-N6   | -5.61 | 115.24                 | 118.60              |
| 22  | A1    | 17   | U    | N1-C2-N3   | 5.61  | 118.26                 | 114.90              |
| 53  | B4    | 36   | ARG  | NE-CZ-NH2  | -5.61 | 117.50                 | 120.30              |
| 54  | BA    | 159  | G    | N3-C4-C5   | -5.61 | 125.80                 | 128.60              |
| 54  | BA    | 1478 | G    | N7-C8-N9   | 5.61  | 115.90                 | 113.10              |
| 54  | BA    | 1997 | C    | O4'-C1'-N1 | 5.61  | 112.69                 | 108.20              |
| 54  | BA    | 2455 | G    | N3-C4-C5   | -5.61 | 125.80                 | 128.60              |
| 54  | BA    | 2547 | A    | C4-C5-C6   | -5.61 | 114.20                 | 117.00              |
| 21  | AA    | 787  | A    | C5-C6-N1   | 5.60  | 120.50                 | 117.70              |
| 54  | BA    | 792  | A    | C6-C5-N7   | 5.60  | 136.22                 | 132.30              |
| 54  | BA    | 2896 | C    | N3-C2-O2   | -5.60 | 117.98                 | 121.90              |
| 21  | AA    | 19   | A    | C5-C6-N1   | 5.60  | 120.50                 | 117.70              |
| 21  | AA    | 193  | C    | N1-C2-O2   | 5.60  | 122.26                 | 118.90              |
| 21  | AA    | 1509 | C    | N3-C4-N4   | -5.60 | 114.08                 | 118.00              |
| 54  | BA    | 240  | C    | N1-C2-O2   | 5.60  | 122.26                 | 118.90              |
| 54  | BA    | 1029 | A    | O4'-C1'-N9 | 5.60  | 112.68                 | 108.20              |
| 54  | BA    | 1036 | G    | N1-C6-O6   | -5.60 | 116.54                 | 119.90              |
| 54  | BA    | 1943 | U    | O4'-C1'-N1 | 5.60  | 112.68                 | 108.20              |
| 54  | BA    | 2759 | G    | N3-C2-N2   | -5.60 | 115.98                 | 119.90              |
| 54  | BA    | 2767 | C    | N1-C2-O2   | 5.60  | 122.26                 | 118.90              |
| 54  | BA    | 2829 | A    | C6-C5-N7   | 5.60  | 136.22                 | 132.30              |
| 54  | BA    | 786  | C    | N3-C2-O2   | -5.60 | 117.98                 | 121.90              |
| 54  | BA    | 2253 | G    | N3-C2-N2   | -5.60 | 115.98                 | 119.90              |
| 54  | BA    | 2612 | C    | N1-C2-O2   | 5.60  | 122.26                 | 118.90              |
| 54  | BA    | 2721 | A    | O4'-C1'-N9 | 5.60  | 112.68                 | 108.20              |
| 21  | AA    | 453  | G    | N9-C4-C5   | 5.60  | 107.64                 | 105.40              |
| 54  | BA    | 239  | C    | O4'-C1'-N1 | 5.60  | 112.68                 | 108.20              |
| 54  | BA    | 1265 | A    | C4-C5-C6   | -5.60 | 114.20                 | 117.00              |
| 21  | AA    | 97   | G    | N1-C6-O6   | -5.60 | 116.54                 | 119.90              |
| 21  | AA    | 490  | C    | C2-N3-C4   | -5.60 | 117.10                 | 119.90              |
| 21  | AA    | 1191 | A    | C6-C5-N7   | 5.60  | 136.22                 | 132.30              |
| 54  | BA    | 1760 | C    | C2-N3-C4   | -5.60 | 117.10                 | 119.90              |
| 55  | BB    | 54   | G    | C5-C6-N1   | 5.60  | 114.30                 | 111.50              |
| 21  | AA    | 1365 | G    | N7-C8-N9   | 5.60  | 115.90                 | 113.10              |
| 54  | BA    | 2092 | U    | C5-C6-N1   | -5.60 | 119.90                 | 122.70              |
| 54  | BA    | 2499 | C    | N3-C2-O2   | -5.60 | 117.98                 | 121.90              |
| 21  | AA    | 776  | G    | C8-N9-C4   | -5.59 | 104.16                 | 106.40              |
| 54  | BA    | 321  | U    | O4'-C1'-N1 | 5.59  | 112.68                 | 108.20              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|-------------|-------|------------------------|---------------------|
| 54  | BA    | 359  | G    | N1-C6-O6    | -5.59 | 116.54                 | 119.90              |
| 54  | BA    | 1418 | G    | C5-C6-N1    | 5.59  | 114.30                 | 111.50              |
| 54  | BA    | 1795 | C    | N3-C2-O2    | -5.59 | 117.98                 | 121.90              |
| 54  | BA    | 2482 | A    | C4-C5-C6    | -5.59 | 114.20                 | 117.00              |
| 3   | AD    | 80   | ARG  | NE-CZ-NH1   | 5.59  | 123.10                 | 120.30              |
| 54  | BA    | 67   | U    | O4'-C1'-N1  | 5.59  | 112.67                 | 108.20              |
| 54  | BA    | 74   | A    | N1-C6-N6    | -5.59 | 115.24                 | 118.60              |
| 54  | BA    | 1880 | U    | C5-C6-N1    | -5.59 | 119.90                 | 122.70              |
| 21  | AA    | 172  | A    | C2-N3-C4    | 5.59  | 113.40                 | 110.60              |
| 21  | AA    | 1439 | G    | N1-C6-O6    | -5.59 | 116.55                 | 119.90              |
| 21  | AA    | 1471 | U    | O4'-C1'-N1  | 5.59  | 112.67                 | 108.20              |
| 54  | BA    | 564  | C    | C5'-C4'-O4' | 5.59  | 115.81                 | 109.10              |
| 54  | BA    | 627  | A    | C4-C5-C6    | -5.59 | 114.20                 | 117.00              |
| 54  | BA    | 1597 | A    | C4-C5-C6    | -5.59 | 114.20                 | 117.00              |
| 21  | AA    | 426  | U    | N3-C2-O2    | -5.59 | 118.29                 | 122.20              |
| 21  | AA    | 624  | C    | N3-C2-O2    | -5.59 | 117.99                 | 121.90              |
| 21  | AA    | 910  | C    | N3-C2-O2    | -5.59 | 117.99                 | 121.90              |
| 54  | BA    | 1043 | C    | N1-C2-O2    | 5.59  | 122.25                 | 118.90              |
| 54  | BA    | 1254 | A    | C3'-C2'-C1' | 5.59  | 105.97                 | 101.50              |
| 54  | BA    | 1314 | C    | N3-C2-O2    | -5.59 | 117.99                 | 121.90              |
| 54  | BA    | 1442 | U    | O4'-C1'-N1  | 5.59  | 112.67                 | 108.20              |
| 54  | BA    | 1980 | G    | N1-C6-O6    | -5.59 | 116.55                 | 119.90              |
| 54  | BA    | 2232 | C    | C5'-C4'-O4' | 5.59  | 115.81                 | 109.10              |
| 54  | BA    | 2306 | C    | N3-C2-O2    | -5.59 | 117.99                 | 121.90              |
| 54  | BA    | 2597 | G    | C8-N9-C4    | -5.59 | 104.16                 | 106.40              |
| 54  | BA    | 2756 | U    | C5-C6-N1    | -5.59 | 119.91                 | 122.70              |
| 21  | AA    | 831  | A    | C4-C5-C6    | -5.59 | 114.21                 | 117.00              |
| 21  | AA    | 1121 | U    | N3-C2-O2    | -5.59 | 118.29                 | 122.20              |
| 30  | BH    | 123  | ARG  | NE-CZ-NH1   | 5.59  | 123.09                 | 120.30              |
| 54  | BA    | 393  | C    | N1-C2-O2    | 5.59  | 122.25                 | 118.90              |
| 54  | BA    | 1933 | G    | N9-C4-C5    | 5.59  | 107.64                 | 105.40              |
| 54  | BA    | 2706 | A    | C4-C5-C6    | -5.59 | 114.21                 | 117.00              |
| 21  | AA    | 106  | C    | O4'-C1'-N1  | 5.59  | 112.67                 | 108.20              |
| 21  | AA    | 198  | G    | C5-C6-N1    | 5.59  | 114.29                 | 111.50              |
| 21  | AA    | 568  | G    | C8-N9-C4    | -5.59 | 104.17                 | 106.40              |
| 54  | BA    | 1992 | G    | N3-C4-C5    | -5.59 | 125.81                 | 128.60              |
| 54  | BA    | 2014 | A    | C5-C6-N1    | 5.59  | 120.49                 | 117.70              |
| 54  | BA    | 2065 | C    | N3-C2-O2    | -5.59 | 117.99                 | 121.90              |
| 54  | BA    | 2263 | C    | C6-N1-C2    | -5.59 | 118.06                 | 120.30              |
| 54  | BA    | 2308 | G    | N3-C4-C5    | -5.59 | 125.81                 | 128.60              |
| 54  | BA    | 2651 | C    | N3-C2-O2    | -5.59 | 117.99                 | 121.90              |
| 21  | AA    | 1306 | A    | C4-C5-C6    | -5.58 | 114.21                 | 117.00              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|------------|-------|------------------------|---------------------|
| 54  | BA    | 537  | G    | N3-C4-C5   | -5.58 | 125.81                 | 128.60              |
| 21  | AA    | 94   | G    | O4'-C1'-N9 | 5.58  | 112.67                 | 108.20              |
| 21  | AA    | 1227 | A    | C5-C6-N1   | 5.58  | 120.49                 | 117.70              |
| 54  | BA    | 558  | U    | O4'-C1'-N1 | 5.58  | 112.67                 | 108.20              |
| 54  | BA    | 1215 | G    | N3-C2-N2   | -5.58 | 115.99                 | 119.90              |
| 54  | BA    | 1583 | A    | C4-C5-C6   | -5.58 | 114.21                 | 117.00              |
| 21  | AA    | 123  | U    | O4'-C1'-N1 | 5.58  | 112.67                 | 108.20              |
| 21  | AA    | 1406 | U    | C5-C6-N1   | -5.58 | 119.91                 | 122.70              |
| 54  | BA    | 274  | C    | N1-C2-O2   | 5.58  | 122.25                 | 118.90              |
| 21  | AA    | 535  | A    | C4-C5-C6   | -5.58 | 114.21                 | 117.00              |
| 21  | AA    | 1524 | C    | N3-C4-C5   | 5.58  | 124.13                 | 121.90              |
| 22  | A1    | 1    | G    | C8-N9-C4   | -5.58 | 104.17                 | 106.40              |
| 54  | BA    | 728  | G    | N7-C8-N9   | 5.58  | 115.89                 | 113.10              |
| 54  | BA    | 1171 | G    | N1-C6-O6   | -5.58 | 116.55                 | 119.90              |
| 54  | BA    | 1665 | A    | C6-C5-N7   | 5.58  | 136.20                 | 132.30              |
| 54  | BA    | 1692 | U    | N1-C2-N3   | 5.58  | 118.25                 | 114.90              |
| 54  | BA    | 2015 | A    | C5-C6-N1   | 5.58  | 120.49                 | 117.70              |
| 54  | BA    | 2462 | C    | N3-C2-O2   | -5.58 | 118.00                 | 121.90              |
| 54  | BA    | 2752 | C    | O4'-C1'-N1 | 5.58  | 112.66                 | 108.20              |
| 55  | BB    | 112  | G    | N1-C6-O6   | -5.58 | 116.55                 | 119.90              |
| 21  | AA    | 84   | U    | O4'-C1'-N1 | 5.58  | 112.66                 | 108.20              |
| 21  | AA    | 1029 | U    | N1-C2-N3   | 5.58  | 118.25                 | 114.90              |
| 21  | AA    | 1170 | A    | C6-C5-N7   | 5.58  | 136.20                 | 132.30              |
| 54  | BA    | 741  | U    | C5-C6-N1   | -5.58 | 119.91                 | 122.70              |
| 54  | BA    | 1989 | G    | N7-C8-N9   | 5.58  | 115.89                 | 113.10              |
| 21  | AA    | 455  | G    | C5-N7-C8   | -5.58 | 101.51                 | 104.30              |
| 54  | BA    | 545  | U    | C5-C6-N1   | -5.58 | 119.91                 | 122.70              |
| 54  | BA    | 585  | G    | N7-C8-N9   | 5.58  | 115.89                 | 113.10              |
| 54  | BA    | 1415 | U    | C5-C6-N1   | -5.58 | 119.91                 | 122.70              |
| 54  | BA    | 1465 | G    | C5-C6-N1   | 5.58  | 114.29                 | 111.50              |
| 54  | BA    | 1630 | A    | C6-C5-N7   | 5.58  | 136.20                 | 132.30              |
| 21  | AA    | 157  | U    | N3-C2-O2   | -5.57 | 118.30                 | 122.20              |
| 21  | AA    | 785  | G    | C5-C6-N1   | 5.57  | 114.29                 | 111.50              |
| 21  | AA    | 936  | C    | O4'-C1'-N1 | 5.57  | 112.66                 | 108.20              |
| 54  | BA    | 193  | U    | N1-C2-N3   | 5.57  | 118.24                 | 114.90              |
| 54  | BA    | 209  | C    | O4'-C1'-N1 | 5.57  | 112.66                 | 108.20              |
| 54  | BA    | 372  | G    | N1-C6-O6   | -5.57 | 116.56                 | 119.90              |
| 54  | BA    | 587  | C    | O4'-C1'-N1 | 5.57  | 112.66                 | 108.20              |
| 54  | BA    | 694  | U    | N3-C2-O2   | -5.57 | 118.30                 | 122.20              |
| 54  | BA    | 775  | G    | O4'-C1'-N9 | 5.57  | 112.66                 | 108.20              |
| 54  | BA    | 1370 | C    | N1-C2-O2   | 5.57  | 122.25                 | 118.90              |
| 54  | BA    | 2323 | G    | C8-N9-C4   | -5.57 | 104.17                 | 106.40              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 54  | BA    | 2538 | C    | N3-C2-O2    | -5.57 | 118.00      | 121.90   |
| 54  | BA    | 2770 | G    | N1-C6-O6    | -5.57 | 116.56      | 119.90   |
| 54  | BA    | 130  | C    | O4'-C1'-N1  | 5.57  | 112.66      | 108.20   |
| 54  | BA    | 983  | A    | C4-C5-C6    | -5.57 | 114.21      | 117.00   |
| 54  | BA    | 1792 | G    | C5-C6-N1    | 5.57  | 114.29      | 111.50   |
| 54  | BA    | 861  | A    | C6-C5-N7    | 5.57  | 136.20      | 132.30   |
| 54  | BA    | 1259 | G    | C5-C6-N1    | 5.57  | 114.29      | 111.50   |
| 54  | BA    | 1531 | C    | N3-C2-O2    | -5.57 | 118.00      | 121.90   |
| 21  | AA    | 998  | C    | N1-C2-O2    | 5.57  | 122.24      | 118.90   |
| 22  | A1    | 43   | G    | C5-C6-N1    | 5.57  | 114.28      | 111.50   |
| 54  | BA    | 894  | U    | N3-C2-O2    | -5.57 | 118.30      | 122.20   |
| 54  | BA    | 2663 | G    | N3-C4-C5    | -5.57 | 125.82      | 128.60   |
| 54  | BA    | 2902 | C    | N1-C2-O2    | 5.57  | 122.24      | 118.90   |
| 23  | A2    | 91   | A    | C6-C5-N7    | 5.57  | 136.20      | 132.30   |
| 54  | BA    | 177  | G    | N7-C8-N9    | 5.57  | 115.88      | 113.10   |
| 54  | BA    | 1208 | C    | O4'-C1'-N1  | 5.57  | 112.66      | 108.20   |
| 54  | BA    | 1240 | U    | C3'-C2'-C1' | 5.57  | 105.95      | 101.50   |
| 54  | BA    | 2520 | C    | N1-C2-O2    | 5.57  | 122.24      | 118.90   |
| 55  | BB    | 42   | C    | C6-N1-C2    | -5.57 | 118.07      | 120.30   |
| 21  | AA    | 1051 | C    | N3-C2-O2    | -5.57 | 118.00      | 121.90   |
| 21  | AA    | 1069 | C    | O4'-C1'-N1  | 5.57  | 112.65      | 108.20   |
| 21  | AA    | 1128 | C    | N1-C2-O2    | 5.57  | 122.24      | 118.90   |
| 54  | BA    | 1097 | U    | C4-C5-C6    | 5.57  | 123.04      | 119.70   |
| 54  | BA    | 2393 | U    | C5-C6-N1    | -5.57 | 119.92      | 122.70   |
| 54  | BA    | 2578 | G    | N3-C2-N2    | -5.57 | 116.00      | 119.90   |
| 54  | BA    | 2781 | A    | C6-C5-N7    | 5.57  | 136.20      | 132.30   |
| 54  | BA    | 2785 | C    | N1-C2-O2    | 5.57  | 122.24      | 118.90   |
| 56  | B5    | 9    | ARG  | NE-CZ-NH1   | 5.57  | 123.08      | 120.30   |
| 54  | BA    | 53   | A    | C4'-C3'-C2' | -5.56 | 97.04       | 102.60   |
| 54  | BA    | 1169 | A    | N1-C6-N6    | -5.56 | 115.26      | 118.60   |
| 21  | AA    | 312  | C    | O4'-C1'-N1  | 5.56  | 112.65      | 108.20   |
| 21  | AA    | 1176 | A    | C4-C5-C6    | -5.56 | 114.22      | 117.00   |
| 21  | AA    | 1311 | A    | C4-C5-C6    | -5.56 | 114.22      | 117.00   |
| 21  | AA    | 1445 | U    | O4'-C1'-N1  | 5.56  | 112.65      | 108.20   |
| 21  | AA    | 1458 | G    | C5-C6-N1    | 5.56  | 114.28      | 111.50   |
| 54  | BA    | 556  | A    | O4'-C1'-N9  | 5.56  | 112.65      | 108.20   |
| 54  | BA    | 873  | C    | N3-C4-C5    | 5.56  | 124.12      | 121.90   |
| 54  | BA    | 1919 | A    | C4-C5-C6    | -5.56 | 114.22      | 117.00   |
| 54  | BA    | 2802 | G    | C5'-C4'-O4' | 5.56  | 115.77      | 109.10   |
| 21  | AA    | 535  | A    | O4'-C4'-C3' | 5.56  | 110.55      | 106.10   |
| 21  | AA    | 605  | U    | N1-C2-N3    | 5.56  | 118.24      | 114.90   |
| 21  | AA    | 1072 | G    | N1-C6-O6    | -5.56 | 116.56      | 119.90   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|------------|-------|------------------------|---------------------|
| 28  | BF    | 101  | ARG  | NE-CZ-NH1  | 5.56  | 123.08                 | 120.30              |
| 21  | AA    | 40   | C    | N3-C4-C5   | 5.56  | 124.12                 | 121.90              |
| 21  | AA    | 148  | G    | C2-N3-C4   | 5.56  | 114.68                 | 111.90              |
| 21  | AA    | 319  | G    | N1-C6-O6   | -5.56 | 116.56                 | 119.90              |
| 21  | AA    | 975  | A    | C4-C5-C6   | -5.56 | 114.22                 | 117.00              |
| 21  | AA    | 1403 | C    | C6-N1-C2   | -5.56 | 118.08                 | 120.30              |
| 21  | AA    | 1432 | G    | N3-C4-C5   | -5.56 | 125.82                 | 128.60              |
| 54  | BA    | 96   | C    | O4'-C1'-N1 | 5.56  | 112.65                 | 108.20              |
| 54  | BA    | 551  | G    | N1-C6-O6   | -5.56 | 116.56                 | 119.90              |
| 54  | BA    | 867  | C    | O4'-C1'-N1 | 5.56  | 112.65                 | 108.20              |
| 21  | AA    | 360  | G    | N1-C6-O6   | -5.56 | 116.57                 | 119.90              |
| 21  | AA    | 463  | U    | N3-C2-O2   | -5.56 | 118.31                 | 122.20              |
| 54  | BA    | 1262 | A    | C4-C5-C6   | -5.56 | 114.22                 | 117.00              |
| 54  | BA    | 1701 | A    | C5-C6-N1   | 5.56  | 120.48                 | 117.70              |
| 21  | AA    | 1221 | G    | N1-C6-O6   | -5.56 | 116.57                 | 119.90              |
| 54  | BA    | 19   | A    | C6-C5-N7   | 5.56  | 136.19                 | 132.30              |
| 54  | BA    | 739  | A    | C4-C5-C6   | -5.56 | 114.22                 | 117.00              |
| 54  | BA    | 1832 | C    | N1-C2-O2   | 5.56  | 122.23                 | 118.90              |
| 11  | AL    | 82   | ARG  | NE-CZ-NH2  | -5.55 | 117.52                 | 120.30              |
| 21  | AA    | 236  | A    | C5-C6-N1   | 5.55  | 120.48                 | 117.70              |
| 21  | AA    | 1442 | G    | N3-C2-N2   | -5.55 | 116.01                 | 119.90              |
| 54  | BA    | 603  | A    | N1-C6-N6   | -5.55 | 115.27                 | 118.60              |
| 54  | BA    | 622  | G    | N3-C4-C5   | -5.55 | 125.82                 | 128.60              |
| 54  | BA    | 679  | C    | O4'-C1'-N1 | 5.55  | 112.64                 | 108.20              |
| 54  | BA    | 1590 | A    | C5-C6-N1   | 5.55  | 120.48                 | 117.70              |
| 54  | BA    | 2226 | C    | N3-C4-C5   | 5.55  | 124.12                 | 121.90              |
| 54  | BA    | 2480 | C    | N3-C2-O2   | -5.55 | 118.01                 | 121.90              |
| 21  | AA    | 301  | G    | C5-C6-N1   | 5.55  | 114.28                 | 111.50              |
| 21  | AA    | 1319 | A    | C4-C5-C6   | -5.55 | 114.22                 | 117.00              |
| 54  | BA    | 286  | U    | C5-C6-N1   | -5.55 | 119.92                 | 122.70              |
| 54  | BA    | 1591 | A    | N1-C6-N6   | -5.55 | 115.27                 | 118.60              |
| 54  | BA    | 2176 | A    | C6-C5-N7   | 5.55  | 136.19                 | 132.30              |
| 21  | AA    | 868  | C    | N1-C2-O2   | 5.55  | 122.23                 | 118.90              |
| 21  | AA    | 1232 | U    | O4'-C1'-N1 | 5.55  | 112.64                 | 108.20              |
| 54  | BA    | 725  | G    | C5-C6-N1   | 5.55  | 114.28                 | 111.50              |
| 54  | BA    | 1265 | A    | C5-C6-N1   | 5.55  | 120.48                 | 117.70              |
| 54  | BA    | 1522 | A    | C5-C6-N1   | 5.55  | 120.48                 | 117.70              |
| 54  | BA    | 2349 | G    | C5-C6-N1   | 5.55  | 114.28                 | 111.50              |
| 54  | BA    | 2658 | C    | N1-C2-O2   | 5.55  | 122.23                 | 118.90              |
| 21  | AA    | 40   | C    | C2-N3-C4   | -5.55 | 117.12                 | 119.90              |
| 21  | AA    | 250  | A    | C2-N3-C4   | 5.55  | 113.37                 | 110.60              |
| 21  | AA    | 419  | C    | N3-C2-O2   | -5.55 | 118.02                 | 121.90              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 21  | AA    | 1450 | U    | N3-C2-O2    | -5.55 | 118.31      | 122.20   |
| 22  | A1    | 67   | U    | N3-C2-O2    | -5.55 | 118.31      | 122.20   |
| 54  | BA    | 34   | U    | N1-C2-N3    | 5.55  | 118.23      | 114.90   |
| 54  | BA    | 126  | A    | C5'-C4'-C3' | -5.55 | 107.12      | 116.00   |
| 21  | AA    | 993  | G    | N3-C4-C5    | -5.55 | 125.83      | 128.60   |
| 25  | BC    | 257  | ARG  | NE-CZ-NH1   | 5.55  | 123.07      | 120.30   |
| 54  | BA    | 404  | A    | O4'-C1'-N9  | 5.55  | 112.64      | 108.20   |
| 54  | BA    | 656  | G    | N7-C8-N9    | 5.55  | 115.87      | 113.10   |
| 54  | BA    | 1153 | C    | N3-C2-O2    | -5.55 | 118.02      | 121.90   |
| 54  | BA    | 2232 | C    | N1-C2-O2    | 5.55  | 122.23      | 118.90   |
| 21  | AA    | 222  | C    | N3-C4-C5    | 5.55  | 124.12      | 121.90   |
| 21  | AA    | 342  | C    | N3-C4-C5    | 5.55  | 124.12      | 121.90   |
| 24  | A3    | 71   | G    | N9-C4-C5    | 5.55  | 107.62      | 105.40   |
| 54  | BA    | 177  | G    | C8-N9-C4    | -5.55 | 104.18      | 106.40   |
| 54  | BA    | 1764 | C    | C6-N1-C2    | -5.55 | 118.08      | 120.30   |
| 54  | BA    | 2625 | G    | C5-C6-N1    | 5.55  | 114.27      | 111.50   |
| 54  | BA    | 1088 | A    | C2-N3-C4    | 5.54  | 113.37      | 110.60   |
| 54  | BA    | 1562 | U    | N3-C2-O2    | -5.54 | 118.32      | 122.20   |
| 54  | BA    | 2112 | G    | N3-C2-N2    | -5.54 | 116.02      | 119.90   |
| 54  | BA    | 2395 | C    | N3-C2-O2    | -5.54 | 118.02      | 121.90   |
| 54  | BA    | 2879 | A    | O4'-C1'-N9  | 5.54  | 112.64      | 108.20   |
| 21  | AA    | 102  | G    | C5-C6-N1    | 5.54  | 114.27      | 111.50   |
| 21  | AA    | 918  | A    | C5-C6-N1    | 5.54  | 120.47      | 117.70   |
| 21  | AA    | 1169 | A    | C6-C5-N7    | 5.54  | 136.18      | 132.30   |
| 54  | BA    | 752  | A    | C1'-O4'-C4' | -5.54 | 105.47      | 109.90   |
| 54  | BA    | 2441 | U    | C5'-C4'-O4' | 5.54  | 115.75      | 109.10   |
| 21  | AA    | 418  | C    | N1-C2-O2    | 5.54  | 122.22      | 118.90   |
| 54  | BA    | 402  | A    | C4-C5-C6    | -5.54 | 114.23      | 117.00   |
| 54  | BA    | 1538 | G    | N3-C4-C5    | -5.54 | 125.83      | 128.60   |
| 54  | BA    | 1797 | G    | N1-C6-O6    | -5.54 | 116.58      | 119.90   |
| 54  | BA    | 2326 | C    | N3-C2-O2    | -5.54 | 118.02      | 121.90   |
| 54  | BA    | 2894 | G    | N1-C6-O6    | -5.54 | 116.58      | 119.90   |
| 55  | BB    | 39   | A    | C4-C5-C6    | -5.54 | 114.23      | 117.00   |
| 2   | AC    | 125  | ARG  | NE-CZ-NH1   | 5.54  | 123.07      | 120.30   |
| 21  | AA    | 296  | U    | N1-C2-N3    | 5.54  | 118.22      | 114.90   |
| 54  | BA    | 380  | G    | C4'-C3'-C2' | -5.54 | 97.06       | 102.60   |
| 54  | BA    | 925  | A    | C5-C6-N1    | 5.54  | 120.47      | 117.70   |
| 54  | BA    | 1326 | U    | O4'-C1'-N1  | 5.54  | 112.63      | 108.20   |
| 21  | AA    | 377  | G    | N1-C6-O6    | -5.54 | 116.58      | 119.90   |
| 21  | AA    | 1113 | C    | N3-C2-O2    | -5.54 | 118.02      | 121.90   |
| 54  | BA    | 443  | A    | O4'-C1'-N9  | 5.54  | 112.63      | 108.20   |
| 54  | BA    | 997  | G    | N1-C6-O6    | -5.54 | 116.58      | 119.90   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|-------------|-------|------------------------|---------------------|
| 54  | BA    | 1381 | G    | N3-C2-N2    | -5.54 | 116.02                 | 119.90              |
| 54  | BA    | 1512 | C    | N3-C4-C5    | 5.54  | 124.12                 | 121.90              |
| 54  | BA    | 1704 | C    | N3-C4-C5    | 5.54  | 124.11                 | 121.90              |
| 54  | BA    | 2286 | G    | C3'-C2'-C1' | 5.54  | 105.93                 | 101.50              |
| 55  | BB    | 116  | G    | N9-C4-C5    | 5.54  | 107.62                 | 105.40              |
| 21  | AA    | 1482 | G    | N3-C4-C5    | -5.54 | 125.83                 | 128.60              |
| 54  | BA    | 687  | C    | N3-C2-O2    | -5.54 | 118.02                 | 121.90              |
| 54  | BA    | 2587 | A    | O4'-C1'-N9  | 5.54  | 112.63                 | 108.20              |
| 54  | BA    | 2686 | G    | N3-C4-C5    | -5.54 | 125.83                 | 128.60              |
| 21  | AA    | 344  | A    | N1-C6-N6    | -5.54 | 115.28                 | 118.60              |
| 21  | AA    | 1056 | U    | N1-C2-N3    | 5.54  | 118.22                 | 114.90              |
| 23  | A2    | 92   | U    | O4'-C1'-N1  | 5.54  | 112.63                 | 108.20              |
| 54  | BA    | 657  | U    | O4'-C1'-N1  | 5.54  | 112.63                 | 108.20              |
| 54  | BA    | 1779 | U    | C5-C6-N1    | -5.54 | 119.93                 | 122.70              |
| 54  | BA    | 2030 | A    | O4'-C1'-N9  | 5.54  | 112.63                 | 108.20              |
| 54  | BA    | 2526 | G    | N1-C6-O6    | -5.54 | 116.58                 | 119.90              |
| 21  | AA    | 377  | G    | C5-C6-N1    | 5.53  | 114.27                 | 111.50              |
| 21  | AA    | 993  | G    | C5'-C4'-C3' | -5.53 | 107.15                 | 116.00              |
| 21  | AA    | 1067 | A    | N1-C6-N6    | -5.53 | 115.28                 | 118.60              |
| 21  | AA    | 1517 | G    | C8-N9-C4    | -5.53 | 104.19                 | 106.40              |
| 54  | BA    | 623  | C    | N3-C4-C5    | 5.53  | 124.11                 | 121.90              |
| 54  | BA    | 1064 | C    | C6-N1-C2    | -5.53 | 118.09                 | 120.30              |
| 54  | BA    | 1104 | C    | C6-N1-C2    | -5.53 | 118.09                 | 120.30              |
| 54  | BA    | 2162 | G    | N9-C4-C5    | 5.53  | 107.61                 | 105.40              |
| 54  | BA    | 2785 | C    | N3-C4-C5    | 5.53  | 124.11                 | 121.90              |
| 21  | AA    | 164  | G    | N9-C4-C5    | 5.53  | 107.61                 | 105.40              |
| 21  | AA    | 254  | G    | N1-C6-O6    | -5.53 | 116.58                 | 119.90              |
| 54  | BA    | 541  | A    | C4-C5-C6    | -5.53 | 114.23                 | 117.00              |
| 54  | BA    | 2089 | C    | C2-N3-C4    | -5.53 | 117.13                 | 119.90              |
| 55  | BB    | 49   | C    | N3-C2-O2    | -5.53 | 118.03                 | 121.90              |
| 8   | AI    | 48   | ARG  | NE-CZ-NH1   | 5.53  | 123.06                 | 120.30              |
| 21  | AA    | 773  | G    | N1-C6-O6    | -5.53 | 116.58                 | 119.90              |
| 24  | A3    | 35   | C    | N1-C2-O2    | 5.53  | 122.22                 | 118.90              |
| 44  | BV    | 19   | ARG  | NE-CZ-NH2   | -5.53 | 117.53                 | 120.30              |
| 54  | BA    | 296  | U    | O4'-C1'-N1  | 5.53  | 112.62                 | 108.20              |
| 54  | BA    | 651  | G    | N3-C4-C5    | -5.53 | 125.83                 | 128.60              |
| 54  | BA    | 1799 | G    | N1-C6-O6    | -5.53 | 116.58                 | 119.90              |
| 21  | AA    | 68   | G    | O4'-C1'-N9  | 5.53  | 112.62                 | 108.20              |
| 21  | AA    | 327  | A    | C4-C5-C6    | -5.53 | 114.24                 | 117.00              |
| 21  | AA    | 927  | G    | C5-C6-N1    | 5.53  | 114.27                 | 111.50              |
| 21  | AA    | 1078 | U    | N3-C2-O2    | -5.53 | 118.33                 | 122.20              |
| 54  | BA    | 348  | A    | C4-C5-C6    | -5.53 | 114.23                 | 117.00              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|-------------|-------|------------------------|---------------------|
| 54  | BA    | 1968 | G    | C8-N9-C4    | -5.53 | 104.19                 | 106.40              |
| 54  | BA    | 2503 | A    | C1'-O4'-C4' | -5.53 | 105.48                 | 109.90              |
| 54  | BA    | 2687 | U    | N1-C2-N3    | 5.53  | 118.22                 | 114.90              |
| 21  | AA    | 434  | U    | C5-C6-N1    | -5.53 | 119.94                 | 122.70              |
| 21  | AA    | 848  | C    | N1-C2-O2    | 5.53  | 122.22                 | 118.90              |
| 48  | BZ    | 29   | ARG  | NE-CZ-NH1   | 5.53  | 123.06                 | 120.30              |
| 54  | BA    | 654  | A    | C2-N3-C4    | 5.53  | 113.36                 | 110.60              |
| 54  | BA    | 662  | G    | N1-C6-O6    | -5.53 | 116.58                 | 119.90              |
| 54  | BA    | 830  | G    | C5-C6-N1    | 5.53  | 114.26                 | 111.50              |
| 54  | BA    | 1446 | C    | O4'-C1'-N1  | 5.53  | 112.62                 | 108.20              |
| 54  | BA    | 1539 | U    | C5-C6-N1    | -5.53 | 119.94                 | 122.70              |
| 54  | BA    | 1732 | C    | N3-C4-C5    | 5.53  | 124.11                 | 121.90              |
| 54  | BA    | 2716 | C    | O4'-C1'-N1  | 5.53  | 112.62                 | 108.20              |
| 54  | BA    | 2894 | G    | C5-C6-N1    | 5.53  | 114.26                 | 111.50              |
| 21  | AA    | 1203 | C    | O4'-C1'-N1  | 5.53  | 112.62                 | 108.20              |
| 21  | AA    | 1218 | C    | N1-C2-O2    | 5.53  | 122.22                 | 118.90              |
| 21  | AA    | 1382 | C    | N3-C4-C5    | 5.53  | 124.11                 | 121.90              |
| 54  | BA    | 1365 | A    | O4'-C1'-N9  | 5.53  | 112.62                 | 108.20              |
| 54  | BA    | 1579 | A    | C5'-C4'-O4' | 5.53  | 115.73                 | 109.10              |
| 54  | BA    | 1962 | C    | N3-C4-N4    | -5.53 | 114.13                 | 118.00              |
| 54  | BA    | 2061 | G    | C8-N9-C4    | -5.53 | 104.19                 | 106.40              |
| 54  | BA    | 411  | G    | P-O3'-C3'   | 5.52  | 126.33                 | 119.70              |
| 54  | BA    | 1608 | A    | C5-C6-N1    | 5.52  | 120.46                 | 117.70              |
| 54  | BA    | 2746 | U    | O4'-C1'-N1  | 5.52  | 112.62                 | 108.20              |
| 21  | AA    | 253  | A    | C5-C6-N1    | 5.52  | 120.46                 | 117.70              |
| 21  | AA    | 368  | U    | C1'-O4'-C4' | -5.52 | 105.48                 | 109.90              |
| 21  | AA    | 757  | U    | O4'-C1'-N1  | 5.52  | 112.62                 | 108.20              |
| 54  | BA    | 190  | A    | C4-C5-C6    | -5.52 | 114.24                 | 117.00              |
| 54  | BA    | 900  | A    | C6-C5-N7    | 5.52  | 136.17                 | 132.30              |
| 21  | AA    | 179  | A    | C5-C6-N1    | 5.52  | 120.46                 | 117.70              |
| 21  | AA    | 522  | C    | N3-C4-N4    | -5.52 | 114.14                 | 118.00              |
| 54  | BA    | 1037 | G    | C5-C6-N1    | 5.52  | 114.26                 | 111.50              |
| 54  | BA    | 1547 | C    | O4'-C1'-N1  | 5.52  | 112.62                 | 108.20              |
| 21  | AA    | 199  | A    | C4-C5-C6    | -5.52 | 114.24                 | 117.00              |
| 24  | A3    | 5    | G    | C8-N9-C4    | -5.52 | 104.19                 | 106.40              |
| 54  | BA    | 253  | C    | N3-C2-O2    | -5.52 | 118.04                 | 121.90              |
| 54  | BA    | 417  | C    | O4'-C1'-N1  | 5.52  | 112.61                 | 108.20              |
| 54  | BA    | 1525 | A    | C5-C6-N1    | 5.52  | 120.46                 | 117.70              |
| 54  | BA    | 2892 | G    | C5-C6-N1    | 5.52  | 114.26                 | 111.50              |
| 14  | AO    | 88   | ARG  | NE-CZ-NH1   | 5.52  | 123.06                 | 120.30              |
| 21  | AA    | 1050 | G    | C5-C6-N1    | 5.52  | 114.26                 | 111.50              |
| 54  | BA    | 872  | U    | O4'-C1'-N1  | 5.52  | 112.61                 | 108.20              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 54  | BA    | 1954 | G    | C8-N9-C4    | -5.52 | 104.19      | 106.40   |
| 54  | BA    | 2723 | C    | C5'-C4'-O4' | 5.52  | 115.72      | 109.10   |
| 54  | BA    | 2865 | U    | O4'-C1'-N1  | 5.52  | 112.61      | 108.20   |
| 54  | BA    | 24   | G    | O4'-C1'-N9  | 5.51  | 112.61      | 108.20   |
| 54  | BA    | 364  | C    | N1-C2-O2    | 5.51  | 122.21      | 118.90   |
| 54  | BA    | 1759 | A    | N7-C8-N9    | 5.51  | 116.56      | 113.80   |
| 54  | BA    | 2067 | G    | N1-C6-O6    | -5.51 | 116.59      | 119.90   |
| 54  | BA    | 2812 | G    | C8-N9-C4    | -5.51 | 104.19      | 106.40   |
| 21  | AA    | 556  | C    | C6-N1-C2    | -5.51 | 118.09      | 120.30   |
| 21  | AA    | 1145 | A    | C4-C5-C6    | -5.51 | 114.24      | 117.00   |
| 37  | BO    | 81   | ARG  | NE-CZ-NH1   | 5.51  | 123.06      | 120.30   |
| 54  | BA    | 1537 | G    | C8-N9-C4    | -5.51 | 104.19      | 106.40   |
| 54  | BA    | 2669 | G    | N1-C6-O6    | -5.51 | 116.59      | 119.90   |
| 54  | BA    | 2771 | C    | N1-C2-O2    | 5.51  | 122.21      | 118.90   |
| 21  | AA    | 321  | A    | C5-C6-N1    | 5.51  | 120.46      | 117.70   |
| 21  | AA    | 1429 | A    | C5'-C4'-O4' | 5.51  | 115.71      | 109.10   |
| 54  | BA    | 884  | U    | C5-C6-N1    | -5.51 | 119.94      | 122.70   |
| 54  | BA    | 1758 | U    | N3-C2-O2    | -5.51 | 118.34      | 122.20   |
| 21  | AA    | 403  | C    | N3-C4-C5    | 5.51  | 124.10      | 121.90   |
| 21  | AA    | 862  | C    | N3-C2-O2    | -5.51 | 118.04      | 121.90   |
| 21  | AA    | 973  | G    | C5-C6-N1    | 5.51  | 114.25      | 111.50   |
| 54  | BA    | 331  | C    | O4'-C1'-N1  | 5.51  | 112.61      | 108.20   |
| 54  | BA    | 1064 | C    | N3-C2-O2    | -5.51 | 118.04      | 121.90   |
| 54  | BA    | 1468 | U    | N1-C2-N3    | 5.51  | 118.21      | 114.90   |
| 54  | BA    | 2147 | A    | C4-C5-C6    | -5.51 | 114.25      | 117.00   |
| 54  | BA    | 2717 | C    | C2-N3-C4    | -5.51 | 117.14      | 119.90   |
| 54  | BA    | 2779 | U    | O4'-C1'-N1  | 5.51  | 112.61      | 108.20   |
| 54  | BA    | 2160 | C    | N3-C4-C5    | 5.51  | 124.10      | 121.90   |
| 54  | BA    | 2339 | C    | N1-C2-O2    | 5.51  | 122.20      | 118.90   |
| 9   | AJ    | 5    | ARG  | NE-CZ-NH1   | 5.51  | 123.05      | 120.30   |
| 21  | AA    | 63   | C    | N1-C2-O2    | 5.51  | 122.20      | 118.90   |
| 21  | AA    | 353  | A    | C2-N3-C4    | 5.51  | 113.35      | 110.60   |
| 21  | AA    | 484  | G    | N9-C4-C5    | 5.51  | 107.60      | 105.40   |
| 21  | AA    | 1385 | G    | O4'-C1'-N9  | 5.51  | 112.61      | 108.20   |
| 24  | A3    | 69   | C    | N1-C2-O2    | 5.51  | 122.20      | 118.90   |
| 54  | BA    | 812  | C    | N1-C2-O2    | 5.51  | 122.20      | 118.90   |
| 54  | BA    | 1146 | C    | O4'-C1'-N1  | 5.51  | 112.61      | 108.20   |
| 54  | BA    | 1206 | G    | C5-N7-C8    | -5.51 | 101.55      | 104.30   |
| 23  | A2    | 92   | U    | C5-C6-N1    | -5.50 | 119.95      | 122.70   |
| 24  | A3    | 38   | A    | C4-C5-C6    | -5.50 | 114.25      | 117.00   |
| 54  | BA    | 474  | G    | C8-N9-C4    | -5.50 | 104.20      | 106.40   |
| 54  | BA    | 1275 | A    | N1-C6-N6    | -5.50 | 115.30      | 118.60   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|-------------|-------|------------------------|---------------------|
| 21  | AA    | 375  | U    | O4'-C1'-N1  | 5.50  | 112.60                 | 108.20              |
| 21  | AA    | 949  | A    | C6-C5-N7    | 5.50  | 136.15                 | 132.30              |
| 21  | AA    | 1064 | G    | N3-C2-N2    | -5.50 | 116.05                 | 119.90              |
| 21  | AA    | 1243 | C    | N3-C2-O2    | -5.50 | 118.05                 | 121.90              |
| 54  | BA    | 205  | G    | C8-N9-C4    | -5.50 | 104.20                 | 106.40              |
| 54  | BA    | 1378 | A    | C4-C5-C6    | -5.50 | 114.25                 | 117.00              |
| 54  | BA    | 1452 | G    | C8-N9-C4    | -5.50 | 104.20                 | 106.40              |
| 54  | BA    | 1475 | G    | N3-C4-C5    | -5.50 | 125.85                 | 128.60              |
| 54  | BA    | 2454 | G    | C8-N9-C4    | -5.50 | 104.20                 | 106.40              |
| 21  | AA    | 686  | U    | N1-C2-N3    | 5.50  | 118.20                 | 114.90              |
| 54  | BA    | 2103 | C    | N1-C2-O2    | 5.50  | 122.20                 | 118.90              |
| 21  | AA    | 272  | C    | C1'-O4'-C4' | -5.50 | 105.50                 | 109.90              |
| 21  | AA    | 369  | G    | N1-C6-O6    | -5.50 | 116.60                 | 119.90              |
| 21  | AA    | 847  | G    | N1-C6-O6    | -5.50 | 116.60                 | 119.90              |
| 54  | BA    | 1146 | C    | N1-C2-O2    | 5.50  | 122.20                 | 118.90              |
| 54  | BA    | 2597 | G    | N1-C6-O6    | -5.50 | 116.60                 | 119.90              |
| 54  | BA    | 2610 | C    | N1-C2-O2    | 5.50  | 122.20                 | 118.90              |
| 54  | BA    | 2773 | C    | N3-C2-O2    | -5.50 | 118.05                 | 121.90              |
| 12  | AM    | 69   | ARG  | NE-CZ-NH1   | 5.50  | 123.05                 | 120.30              |
| 21  | AA    | 71   | A    | C4-C5-C6    | -5.50 | 114.25                 | 117.00              |
| 54  | BA    | 139  | U    | C5-C6-N1    | -5.50 | 119.95                 | 122.70              |
| 54  | BA    | 144  | A    | C4-C5-C6    | -5.50 | 114.25                 | 117.00              |
| 54  | BA    | 1539 | U    | C1'-O4'-C4' | -5.50 | 105.50                 | 109.90              |
| 1   | AB    | 94   | ARG  | NE-CZ-NH1   | 5.50  | 123.05                 | 120.30              |
| 21  | AA    | 447  | G    | C8-N9-C4    | -5.50 | 104.20                 | 106.40              |
| 21  | AA    | 833  | G    | C5-C6-N1    | 5.50  | 114.25                 | 111.50              |
| 21  | AA    | 974  | A    | O4'-C1'-N9  | 5.50  | 112.60                 | 108.20              |
| 54  | BA    | 1476 | U    | N1-C2-N3    | 5.50  | 118.20                 | 114.90              |
| 54  | BA    | 2084 | C    | N1-C2-O2    | 5.50  | 122.20                 | 118.90              |
| 54  | BA    | 2240 | U    | C5-C6-N1    | -5.50 | 119.95                 | 122.70              |
| 54  | BA    | 2241 | A    | C4-C5-C6    | -5.50 | 114.25                 | 117.00              |
| 54  | BA    | 2748 | A    | C5-C6-N1    | 5.50  | 120.45                 | 117.70              |
| 21  | AA    | 822  | U    | C1'-O4'-C4' | -5.49 | 105.50                 | 109.90              |
| 21  | AA    | 849  | G    | C5-C6-N1    | 5.49  | 114.25                 | 111.50              |
| 21  | AA    | 1157 | A    | C5-C6-N1    | 5.49  | 120.45                 | 117.70              |
| 24  | A3    | 50   | G    | C5-C6-N1    | 5.49  | 114.25                 | 111.50              |
| 54  | BA    | 723  | C    | C4'-C3'-C2' | -5.49 | 97.11                  | 102.60              |
| 55  | BB    | 7    | G    | N9-C4-C5    | 5.49  | 107.60                 | 105.40              |
| 21  | AA    | 205  | A    | O4'-C4'-C3' | 5.49  | 110.49                 | 106.10              |
| 21  | AA    | 1146 | A    | C5-C6-N1    | 5.49  | 120.45                 | 117.70              |
| 21  | AA    | 1197 | A    | C3'-C2'-C1' | 5.49  | 105.89                 | 101.50              |
| 21  | AA    | 1262 | C    | N3-C2-O2    | -5.49 | 118.06                 | 121.90              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 54  | BA    | 537  | G    | C5-C6-N1    | 5.49  | 114.25      | 111.50   |
| 54  | BA    | 2638 | G    | N9-C4-C5    | 5.49  | 107.60      | 105.40   |
| 21  | AA    | 107  | G    | N1-C6-O6    | -5.49 | 116.61      | 119.90   |
| 21  | AA    | 187  | G    | C5-C6-N1    | 5.49  | 114.25      | 111.50   |
| 54  | BA    | 1    | G    | N7-C8-N9    | 5.49  | 115.84      | 113.10   |
| 54  | BA    | 361  | G    | N3-C2-N2    | -5.49 | 116.06      | 119.90   |
| 54  | BA    | 1826 | G    | N1-C6-O6    | -5.49 | 116.61      | 119.90   |
| 54  | BA    | 2087 | G    | O4'-C1'-N9  | 5.49  | 112.59      | 108.20   |
| 54  | BA    | 2828 | G    | N1-C6-O6    | -5.49 | 116.61      | 119.90   |
| 21  | AA    | 314  | C    | N1-C2-O2    | 5.49  | 122.19      | 118.90   |
| 21  | AA    | 341  | C    | N1-C2-O2    | 5.49  | 122.19      | 118.90   |
| 54  | BA    | 250  | G    | N1-C6-O6    | -5.49 | 116.61      | 119.90   |
| 54  | BA    | 492  | A    | C5-C6-N1    | 5.49  | 120.44      | 117.70   |
| 54  | BA    | 1035 | U    | N1-C2-N3    | 5.49  | 118.19      | 114.90   |
| 54  | BA    | 1775 | U    | C4'-C3'-C2' | -5.49 | 97.11       | 102.60   |
| 54  | BA    | 2328 | A    | C4-C5-C6    | -5.49 | 114.26      | 117.00   |
| 54  | BA    | 295  | G    | N7-C8-N9    | 5.49  | 115.84      | 113.10   |
| 54  | BA    | 2376 | A    | C4-C5-C6    | -5.49 | 114.26      | 117.00   |
| 22  | A1    | 28   | C    | N1-C2-O2    | 5.49  | 122.19      | 118.90   |
| 54  | BA    | 496  | G    | O4'-C1'-N9  | 5.49  | 112.59      | 108.20   |
| 54  | BA    | 577  | G    | N3-C4-C5    | -5.49 | 125.86      | 128.60   |
| 54  | BA    | 1209 | U    | O4'-C1'-N1  | 5.49  | 112.59      | 108.20   |
| 54  | BA    | 1409 | U    | C5-C6-N1    | -5.49 | 119.96      | 122.70   |
| 21  | AA    | 1375 | A    | C2-N3-C4    | 5.48  | 113.34      | 110.60   |
| 21  | AA    | 1495 | U    | N3-C2-O2    | -5.48 | 118.36      | 122.20   |
| 28  | BF    | 149  | ARG  | NE-CZ-NH1   | 5.48  | 123.04      | 120.30   |
| 21  | AA    | 328  | C    | O4'-C1'-N1  | 5.48  | 112.59      | 108.20   |
| 21  | AA    | 546  | A    | C6-C5-N7    | 5.48  | 136.14      | 132.30   |
| 21  | AA    | 1498 | U    | O4'-C1'-N1  | 5.48  | 112.59      | 108.20   |
| 30  | BH    | 51   | ARG  | NE-CZ-NH1   | 5.48  | 123.04      | 120.30   |
| 54  | BA    | 1290 | C    | N3-C4-C5    | 5.48  | 124.09      | 121.90   |
| 54  | BA    | 1560 | G    | N3-C2-N2    | -5.48 | 116.06      | 119.90   |
| 21  | AA    | 1465 | A    | C4-C5-C6    | -5.48 | 114.26      | 117.00   |
| 54  | BA    | 1112 | G    | N3-C4-C5    | -5.48 | 125.86      | 128.60   |
| 54  | BA    | 1404 | C    | N3-C4-N4    | -5.48 | 114.16      | 118.00   |
| 55  | BB    | 66   | A    | C5-C6-N1    | 5.48  | 120.44      | 117.70   |
| 55  | BB    | 91   | C    | N1-C2-O2    | 5.48  | 122.19      | 118.90   |
| 54  | BA    | 620  | G    | N3-C4-C5    | -5.48 | 125.86      | 128.60   |
| 54  | BA    | 806  | C    | N3-C4-C5    | 5.48  | 124.09      | 121.90   |
| 54  | BA    | 1325 | U    | N1-C1'-C2'  | 5.48  | 121.12      | 114.00   |
| 54  | BA    | 2127 | G    | N9-C4-C5    | 5.48  | 107.59      | 105.40   |
| 21  | AA    | 71   | A    | N1-C6-N6    | -5.48 | 115.31      | 118.60   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 54  | BA    | 1833 | C    | N3-C4-C5    | 5.48  | 124.09      | 121.90   |
| 54  | BA    | 1981 | A    | C4-C5-C6    | -5.48 | 114.26      | 117.00   |
| 54  | BA    | 2289 | G    | N1-C6-O6    | -5.48 | 116.61      | 119.90   |
| 54  | BA    | 2628 | C    | N3-C4-C5    | 5.48  | 124.09      | 121.90   |
| 21  | AA    | 170  | U    | N3-C2-O2    | -5.48 | 118.37      | 122.20   |
| 21  | AA    | 958  | A    | C4-C5-C6    | -5.48 | 114.26      | 117.00   |
| 54  | BA    | 403  | U    | O4'-C1'-N1  | 5.48  | 112.58      | 108.20   |
| 21  | AA    | 391  | G    | N1-C6-O6    | -5.47 | 116.61      | 119.90   |
| 21  | AA    | 1300 | G    | N1-C6-O6    | -5.47 | 116.61      | 119.90   |
| 54  | BA    | 1403 | A    | N1-C6-N6    | -5.47 | 115.31      | 118.60   |
| 54  | BA    | 1461 | C    | N3-C2-O2    | -5.47 | 118.07      | 121.90   |
| 54  | BA    | 1508 | A    | C4-C5-C6    | -5.47 | 114.26      | 117.00   |
| 54  | BA    | 1533 | C    | N1-C2-O2    | 5.47  | 122.19      | 118.90   |
| 54  | BA    | 2042 | A    | C4-C5-C6    | -5.47 | 114.26      | 117.00   |
| 21  | AA    | 1314 | C    | N1-C2-O2    | 5.47  | 122.18      | 118.90   |
| 21  | AA    | 1388 | C    | N3-C4-C5    | 5.47  | 124.09      | 121.90   |
| 21  | AA    | 1438 | G    | C8-N9-C4    | -5.47 | 104.21      | 106.40   |
| 54  | BA    | 51   | G    | C8-N9-C4    | -5.47 | 104.21      | 106.40   |
| 54  | BA    | 296  | U    | N1-C2-N3    | 5.47  | 118.18      | 114.90   |
| 54  | BA    | 1297 | C    | C6-N1-C2    | -5.47 | 118.11      | 120.30   |
| 54  | BA    | 2757 | A    | C4-C5-C6    | -5.47 | 114.26      | 117.00   |
| 55  | BB    | 3    | C    | N1-C2-O2    | 5.47  | 122.18      | 118.90   |
| 21  | AA    | 566  | G    | N1-C6-O6    | -5.47 | 116.62      | 119.90   |
| 21  | AA    | 859  | G    | C5-C6-N1    | 5.47  | 114.23      | 111.50   |
| 21  | AA    | 1055 | A    | C5-C6-N1    | 5.47  | 120.44      | 117.70   |
| 24  | A3    | 62   | C    | N3-C4-C5    | 5.47  | 124.09      | 121.90   |
| 54  | BA    | 144  | A    | C6-C5-N7    | 5.47  | 136.13      | 132.30   |
| 54  | BA    | 517  | C    | N1-C2-O2    | 5.47  | 122.18      | 118.90   |
| 54  | BA    | 1560 | G    | N7-C8-N9    | 5.47  | 115.84      | 113.10   |
| 54  | BA    | 2293 | G    | C8-N9-C4    | -5.47 | 104.21      | 106.40   |
| 54  | BA    | 2384 | U    | N1-C2-N3    | 5.47  | 118.18      | 114.90   |
| 21  | AA    | 1138 | G    | C5-C6-N1    | 5.47  | 114.23      | 111.50   |
| 21  | AA    | 1416 | G    | N9-C4-C5    | 5.47  | 107.59      | 105.40   |
| 54  | BA    | 1634 | A    | P-O3'-C3'   | 5.47  | 126.26      | 119.70   |
| 54  | BA    | 1846 | G    | C3'-C2'-C1' | 5.47  | 105.88      | 101.50   |
| 54  | BA    | 2296 | U    | N3-C2-O2    | -5.47 | 118.37      | 122.20   |
| 54  | BA    | 2344 | U    | N3-C2-O2    | -5.47 | 118.37      | 122.20   |
| 24  | A3    | 2    | G    | C5-C6-N1    | 5.47  | 114.23      | 111.50   |
| 21  | AA    | 650  | G    | N1-C6-O6    | -5.47 | 116.62      | 119.90   |
| 21  | AA    | 851  | G    | N7-C8-N9    | 5.47  | 115.83      | 113.10   |
| 54  | BA    | 688  | U    | O4'-C1'-N1  | 5.47  | 112.57      | 108.20   |
| 54  | BA    | 2018 | G    | C5-C6-N1    | 5.47  | 114.23      | 111.50   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|-------------|-------|------------------------|---------------------|
| 54  | BA    | 2295 | C    | O4'-C1'-N1  | 5.47  | 112.57                 | 108.20              |
| 54  | BA    | 2342 | C    | O4'-C1'-N1  | 5.47  | 112.57                 | 108.20              |
| 21  | AA    | 117  | G    | C5-C6-N1    | 5.46  | 114.23                 | 111.50              |
| 21  | AA    | 152  | A    | O4'-C1'-N9  | 5.46  | 112.57                 | 108.20              |
| 21  | AA    | 819  | A    | C6-C5-N7    | 5.46  | 136.12                 | 132.30              |
| 54  | BA    | 1178 | C    | N1-C2-O2    | 5.46  | 122.18                 | 118.90              |
| 54  | BA    | 1616 | A    | C4-C5-C6    | -5.46 | 114.27                 | 117.00              |
| 54  | BA    | 1950 | G    | C8-N9-C4    | -5.46 | 104.21                 | 106.40              |
| 21  | AA    | 131  | A    | C6-C5-N7    | 5.46  | 136.12                 | 132.30              |
| 21  | AA    | 403  | C    | O4'-C1'-N1  | 5.46  | 112.57                 | 108.20              |
| 22  | A1    | 36   | C    | N3-C2-O2    | -5.46 | 118.08                 | 121.90              |
| 54  | BA    | 1719 | G    | C5-C6-N1    | 5.46  | 114.23                 | 111.50              |
| 54  | BA    | 1748 | C    | N1-C2-O2    | 5.46  | 122.18                 | 118.90              |
| 21  | AA    | 96   | U    | C5-C6-N1    | -5.46 | 119.97                 | 122.70              |
| 21  | AA    | 711  | G    | N1-C6-O6    | -5.46 | 116.62                 | 119.90              |
| 21  | AA    | 1211 | U    | O4'-C4'-C3' | 5.46  | 110.47                 | 106.10              |
| 21  | AA    | 1526 | G    | N9-C4-C5    | 5.46  | 107.58                 | 105.40              |
| 54  | BA    | 138  | U    | O4'-C1'-N1  | 5.46  | 112.57                 | 108.20              |
| 54  | BA    | 198  | C    | N1-C2-O2    | 5.46  | 122.18                 | 118.90              |
| 54  | BA    | 769  | U    | C5'-C4'-O4' | 5.46  | 115.65                 | 109.10              |
| 54  | BA    | 1037 | G    | N1-C6-O6    | -5.46 | 116.62                 | 119.90              |
| 54  | BA    | 1099 | G    | N3-C2-N2    | -5.46 | 116.08                 | 119.90              |
| 54  | BA    | 1556 | C    | N3-C4-C5    | 5.46  | 124.08                 | 121.90              |
| 54  | BA    | 2053 | G    | C8-N9-C4    | -5.46 | 104.22                 | 106.40              |
| 51  | B2    | 39   | ARG  | NE-CZ-NH1   | 5.46  | 123.03                 | 120.30              |
| 54  | BA    | 60   | G    | N3-C4-C5    | -5.46 | 125.87                 | 128.60              |
| 54  | BA    | 592  | A    | C5-C6-N1    | 5.46  | 120.43                 | 117.70              |
| 54  | BA    | 748  | G    | N1-C6-O6    | -5.46 | 116.62                 | 119.90              |
| 54  | BA    | 1135 | C    | O4'-C1'-N1  | 5.46  | 112.57                 | 108.20              |
| 54  | BA    | 2286 | G    | C1'-O4'-C4' | -5.46 | 105.53                 | 109.90              |
| 54  | BA    | 2397 | G    | N1-C6-O6    | -5.46 | 116.62                 | 119.90              |
| 21  | AA    | 110  | C    | C1'-O4'-C4' | -5.46 | 105.53                 | 109.90              |
| 21  | AA    | 290  | C    | N3-C2-O2    | -5.46 | 118.08                 | 121.90              |
| 21  | AA    | 482  | A    | C4-C5-C6    | -5.46 | 114.27                 | 117.00              |
| 21  | AA    | 1512 | U    | O4'-C1'-N1  | 5.46  | 112.57                 | 108.20              |
| 54  | BA    | 100  | U    | C4-C5-C6    | 5.46  | 122.97                 | 119.70              |
| 54  | BA    | 1448 | G    | C5-C6-N1    | 5.46  | 114.23                 | 111.50              |
| 54  | BA    | 1509 | A    | C4-C5-C6    | -5.46 | 114.27                 | 117.00              |
| 54  | BA    | 1607 | C    | N1-C2-O2    | 5.46  | 122.17                 | 118.90              |
| 54  | BA    | 2087 | G    | N3-C2-N2    | -5.46 | 116.08                 | 119.90              |
| 21  | AA    | 955  | U    | C5-C6-N1    | -5.46 | 119.97                 | 122.70              |
| 54  | BA    | 567  | U    | O4'-C1'-N1  | 5.46  | 112.56                 | 108.20              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|-------------|-------|------------------------|---------------------|
| 54  | BA    | 1343 | G    | C8-N9-C4    | -5.46 | 104.22                 | 106.40              |
| 54  | BA    | 2127 | G    | C8-N9-C4    | -5.46 | 104.22                 | 106.40              |
| 54  | BA    | 2311 | A    | C6-C5-N7    | 5.46  | 136.12                 | 132.30              |
| 54  | BA    | 2355 | G    | C8-N9-C4    | -5.46 | 104.22                 | 106.40              |
| 54  | BA    | 2715 | C    | O4'-C1'-N1  | 5.46  | 112.56                 | 108.20              |
| 23  | A2    | 90   | U    | C5-C6-N1    | -5.46 | 119.97                 | 122.70              |
| 54  | BA    | 752  | A    | C2-N3-C4    | 5.46  | 113.33                 | 110.60              |
| 54  | BA    | 1348 | C    | C2-N3-C4    | -5.46 | 117.17                 | 119.90              |
| 54  | BA    | 1672 | A    | N1-C6-N6    | -5.46 | 115.33                 | 118.60              |
| 55  | BB    | 15   | A    | C2-N3-C4    | 5.46  | 113.33                 | 110.60              |
| 21  | AA    | 453  | G    | N1-C6-O6    | -5.45 | 116.63                 | 119.90              |
| 21  | AA    | 469  | C    | C6-N1-C2    | -5.45 | 118.12                 | 120.30              |
| 21  | AA    | 1162 | C    | C6-N1-C2    | -5.45 | 118.12                 | 120.30              |
| 21  | AA    | 1390 | U    | O4'-C1'-N1  | 5.45  | 112.56                 | 108.20              |
| 54  | BA    | 287  | G    | N1-C6-O6    | -5.45 | 116.63                 | 119.90              |
| 54  | BA    | 417  | C    | N3-C2-O2    | -5.45 | 118.08                 | 121.90              |
| 54  | BA    | 1726 | C    | N3-C2-O2    | -5.45 | 118.08                 | 121.90              |
| 54  | BA    | 2095 | A    | C4-C5-C6    | -5.45 | 114.27                 | 117.00              |
| 54  | BA    | 2430 | A    | C4-C5-C6    | -5.45 | 114.27                 | 117.00              |
| 54  | BA    | 2722 | G    | C5-C6-N1    | 5.45  | 114.23                 | 111.50              |
| 54  | BA    | 2862 | G    | C5-C6-N1    | 5.45  | 114.23                 | 111.50              |
| 54  | BA    | 2870 | C    | N3-C4-C5    | 5.45  | 124.08                 | 121.90              |
| 21  | AA    | 233  | C    | N3-C4-C5    | 5.45  | 124.08                 | 121.90              |
| 54  | BA    | 11   | C    | N3-C2-O2    | -5.45 | 118.08                 | 121.90              |
| 54  | BA    | 1351 | C    | N3-C2-O2    | -5.45 | 118.08                 | 121.90              |
| 54  | BA    | 1396 | U    | N3-C2-O2    | -5.45 | 118.39                 | 122.20              |
| 21  | AA    | 139  | A    | C4-C5-C6    | -5.45 | 114.28                 | 117.00              |
| 21  | AA    | 194  | C    | C3'-C2'-C1' | 5.45  | 105.86                 | 101.50              |
| 21  | AA    | 553  | A    | C2-N3-C4    | 5.45  | 113.32                 | 110.60              |
| 21  | AA    | 1059 | C    | N3-C2-O2    | -5.45 | 118.08                 | 121.90              |
| 25  | BC    | 188  | ARG  | NE-CZ-NH1   | 5.45  | 123.02                 | 120.30              |
| 54  | BA    | 71   | A    | C6-C5-N7    | 5.45  | 136.11                 | 132.30              |
| 54  | BA    | 943  | A    | C5'-C4'-O4' | 5.45  | 115.64                 | 109.10              |
| 54  | BA    | 1314 | C    | N1-C2-O2    | 5.45  | 122.17                 | 118.90              |
| 54  | BA    | 1782 | U    | N1-C2-N3    | 5.45  | 118.17                 | 114.90              |
| 54  | BA    | 1928 | A    | C4-C5-C6    | -5.45 | 114.28                 | 117.00              |
| 21  | AA    | 1534 | A    | C5'-C4'-O4' | 5.45  | 115.64                 | 109.10              |
| 54  | BA    | 2597 | G    | N9-C4-C5    | 5.45  | 107.58                 | 105.40              |
| 54  | BA    | 1890 | A    | C4-C5-C6    | -5.45 | 114.28                 | 117.00              |
| 24  | A3    | 20   | G    | N3-C4-C5    | -5.44 | 125.88                 | 128.60              |
| 54  | BA    | 514  | A    | C4-C5-C6    | -5.44 | 114.28                 | 117.00              |
| 54  | BA    | 700  | G    | O4'-C1'-N9  | 5.44  | 112.56                 | 108.20              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|-------------|-------|------------------------|---------------------|
| 54  | BA    | 2300 | C    | O4'-C1'-N1  | 5.44  | 112.56                 | 108.20              |
| 21  | AA    | 890  | G    | C8-N9-C4    | -5.44 | 104.22                 | 106.40              |
| 54  | BA    | 262  | A    | C5-C6-N1    | 5.44  | 120.42                 | 117.70              |
| 54  | BA    | 1069 | A    | C5-C6-N1    | 5.44  | 120.42                 | 117.70              |
| 54  | BA    | 1291 | C    | N3-C2-O2    | -5.44 | 118.09                 | 121.90              |
| 54  | BA    | 2242 | G    | C5-C6-N1    | 5.44  | 114.22                 | 111.50              |
| 54  | BA    | 2628 | C    | N1-C2-O2    | 5.44  | 122.17                 | 118.90              |
| 54  | BA    | 2760 | C    | O4'-C1'-N1  | 5.44  | 112.55                 | 108.20              |
| 21  | AA    | 30   | U    | N3-C2-O2    | -5.44 | 118.39                 | 122.20              |
| 21  | AA    | 825  | A    | C6-C5-N7    | 5.44  | 136.11                 | 132.30              |
| 21  | AA    | 1527 | U    | O4'-C1'-N1  | 5.44  | 112.55                 | 108.20              |
| 54  | BA    | 295  | G    | N9-C4-C5    | 5.44  | 107.58                 | 105.40              |
| 54  | BA    | 1339 | G    | C8-N9-C4    | -5.44 | 104.22                 | 106.40              |
| 54  | BA    | 1965 | C    | C2-N3-C4    | -5.44 | 117.18                 | 119.90              |
| 54  | BA    | 2411 | A    | C6-C5-N7    | 5.44  | 136.11                 | 132.30              |
| 21  | AA    | 120  | A    | C4-C5-C6    | -5.44 | 114.28                 | 117.00              |
| 54  | BA    | 277  | G    | C5-C6-N1    | 5.44  | 114.22                 | 111.50              |
| 54  | BA    | 1900 | A    | C6-C5-N7    | 5.44  | 136.11                 | 132.30              |
| 54  | BA    | 2584 | U    | C4'-C3'-C2' | -5.44 | 97.16                  | 102.60              |
| 54  | BA    | 2902 | C    | C4'-C3'-C2' | -5.44 | 97.16                  | 102.60              |
| 21  | AA    | 129  | A    | C6-C5-N7    | 5.44  | 136.11                 | 132.30              |
| 54  | BA    | 1385 | A    | C1'-O4'-C4' | -5.44 | 105.55                 | 109.90              |
| 54  | BA    | 1594 | U    | N3-C2-O2    | -5.44 | 118.39                 | 122.20              |
| 54  | BA    | 2406 | A    | C4-C5-C6    | -5.44 | 114.28                 | 117.00              |
| 54  | BA    | 2756 | U    | N1-C2-N3    | 5.44  | 118.16                 | 114.90              |
| 55  | BB    | 14   | U    | N3-C2-O2    | -5.44 | 118.39                 | 122.20              |
| 21  | AA    | 159  | G    | C5-C6-N1    | 5.44  | 114.22                 | 111.50              |
| 21  | AA    | 384  | G    | N7-C8-N9    | 5.44  | 115.82                 | 113.10              |
| 21  | AA    | 444  | G    | N1-C6-O6    | -5.44 | 116.64                 | 119.90              |
| 54  | BA    | 366  | C    | N3-C2-O2    | -5.44 | 118.09                 | 121.90              |
| 54  | BA    | 623  | C    | N1-C2-O2    | 5.44  | 122.16                 | 118.90              |
| 54  | BA    | 1564 | C    | N3-C2-O2    | -5.44 | 118.09                 | 121.90              |
| 54  | BA    | 1836 | C    | N3-C2-O2    | -5.44 | 118.09                 | 121.90              |
| 54  | BA    | 1970 | A    | C6-C5-N7    | 5.44  | 136.10                 | 132.30              |
| 54  | BA    | 2080 | A    | O4'-C1'-N9  | 5.44  | 112.55                 | 108.20              |
| 54  | BA    | 2743 | U    | N3-C2-O2    | -5.44 | 118.39                 | 122.20              |
| 21  | AA    | 275  | G    | N3-C2-N2    | -5.43 | 116.10                 | 119.90              |
| 21  | AA    | 383  | A    | C2-N3-C4    | 5.43  | 113.32                 | 110.60              |
| 21  | AA    | 1359 | C    | N3-C2-O2    | -5.43 | 118.09                 | 121.90              |
| 54  | BA    | 286  | U    | C4-C5-C6    | 5.43  | 122.96                 | 119.70              |
| 54  | BA    | 466  | A    | N1-C6-N6    | -5.43 | 115.34                 | 118.60              |
| 54  | BA    | 1287 | A    | C4-C5-C6    | -5.43 | 114.28                 | 117.00              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|-------------|-------|------------------------|---------------------|
| 54  | BA    | 545  | U    | N3-C2-O2    | -5.43 | 118.40                 | 122.20              |
| 54  | BA    | 762  | U    | P-O3'-C3'   | 5.43  | 126.22                 | 119.70              |
| 54  | BA    | 1325 | U    | O4'-C1'-C2' | -5.43 | 100.37                 | 105.80              |
| 54  | BA    | 1471 | G    | C5-C6-N1    | 5.43  | 114.22                 | 111.50              |
| 21  | AA    | 1202 | U    | O4'-C1'-N1  | 5.43  | 112.55                 | 108.20              |
| 21  | AA    | 1210 | C    | N3-C4-C5    | 5.43  | 124.07                 | 121.90              |
| 54  | BA    | 234  | U    | N3-C2-O2    | -5.43 | 118.40                 | 122.20              |
| 54  | BA    | 523  | C    | N1-C2-O2    | 5.43  | 122.16                 | 118.90              |
| 54  | BA    | 2209 | G    | N1-C6-O6    | -5.43 | 116.64                 | 119.90              |
| 54  | BA    | 2255 | G    | C5-C6-N1    | 5.43  | 114.22                 | 111.50              |
| 21  | AA    | 369  | G    | C8-N9-C4    | -5.43 | 104.23                 | 106.40              |
| 21  | AA    | 1067 | A    | C4-C5-C6    | -5.43 | 114.29                 | 117.00              |
| 54  | BA    | 602  | A    | C5-C6-N1    | 5.43  | 120.42                 | 117.70              |
| 54  | BA    | 2229 | U    | C5-C6-N1    | -5.43 | 119.98                 | 122.70              |
| 54  | BA    | 2314 | A    | C4-C5-C6    | -5.43 | 114.28                 | 117.00              |
| 55  | BB    | 63   | C    | O4'-C1'-N1  | 5.43  | 112.54                 | 108.20              |
| 21  | AA    | 977  | A    | O4'-C1'-N9  | 5.43  | 112.54                 | 108.20              |
| 22  | A1    | 17   | U    | C5-C6-N1    | -5.43 | 119.99                 | 122.70              |
| 54  | BA    | 1426 | G    | N9-C4-C5    | 5.43  | 107.57                 | 105.40              |
| 21  | AA    | 185  | U    | N1-C2-N3    | 5.43  | 118.16                 | 114.90              |
| 21  | AA    | 331  | G    | C8-N9-C4    | -5.43 | 104.23                 | 106.40              |
| 21  | AA    | 1069 | C    | C6-N1-C2    | -5.43 | 118.13                 | 120.30              |
| 21  | AA    | 1497 | G    | C5-C6-N1    | 5.43  | 114.21                 | 111.50              |
| 54  | BA    | 704  | G    | N3-C4-C5    | -5.43 | 125.89                 | 128.60              |
| 54  | BA    | 961  | C    | C6-N1-C2    | -5.43 | 118.13                 | 120.30              |
| 54  | BA    | 1152 | C    | O4'-C1'-N1  | 5.43  | 112.54                 | 108.20              |
| 54  | BA    | 1429 | G    | C8-N9-C4    | -5.43 | 104.23                 | 106.40              |
| 54  | BA    | 1538 | G    | C5-C6-N1    | 5.43  | 114.21                 | 111.50              |
| 54  | BA    | 2161 | C    | N1-C2-O2    | 5.43  | 122.16                 | 118.90              |
| 54  | BA    | 2687 | U    | N3-C2-O2    | -5.43 | 118.40                 | 122.20              |
| 54  | BA    | 2867 | G    | C5-C6-N1    | 5.43  | 114.21                 | 111.50              |
| 21  | AA    | 206  | C    | N3-C2-O2    | -5.42 | 118.10                 | 121.90              |
| 21  | AA    | 655  | A    | C4-C5-C6    | -5.42 | 114.29                 | 117.00              |
| 21  | AA    | 1184 | G    | N1-C6-O6    | -5.42 | 116.64                 | 119.90              |
| 49  | B0    | 49   | ARG  | NE-CZ-NH1   | 5.42  | 123.01                 | 120.30              |
| 54  | BA    | 291  | G    | N9-C4-C5    | 5.42  | 107.57                 | 105.40              |
| 54  | BA    | 431  | U    | C4-C5-C6    | 5.42  | 122.95                 | 119.70              |
| 54  | BA    | 485  | C    | O4'-C1'-N1  | 5.42  | 112.54                 | 108.20              |
| 54  | BA    | 923  | G    | N1-C6-O6    | -5.42 | 116.64                 | 119.90              |
| 54  | BA    | 1703 | G    | N1-C6-O6    | -5.42 | 116.65                 | 119.90              |
| 54  | BA    | 1807 | G    | N1-C6-O6    | -5.42 | 116.64                 | 119.90              |
| 4   | AE    | 19   | ARG  | NE-CZ-NH1   | 5.42  | 123.01                 | 120.30              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 21  | AA    | 247  | G    | C4-C5-N7    | -5.42 | 108.63      | 110.80   |
| 21  | AA    | 473  | U    | C4-C5-C6    | 5.42  | 122.95      | 119.70   |
| 21  | AA    | 1201 | A    | C5'-C4'-C3' | -5.42 | 107.32      | 116.00   |
| 54  | BA    | 130  | C    | N3-C4-C5    | 5.42  | 124.07      | 121.90   |
| 54  | BA    | 2603 | G    | C5-C6-N1    | 5.42  | 114.21      | 111.50   |
| 21  | AA    | 1143 | G    | C8-N9-C4    | -5.42 | 104.23      | 106.40   |
| 21  | AA    | 1368 | A    | C6-C5-N7    | 5.42  | 136.09      | 132.30   |
| 54  | BA    | 1739 | A    | C5-C6-N1    | 5.42  | 120.41      | 117.70   |
| 54  | BA    | 2699 | C    | N1-C2-O2    | 5.42  | 122.15      | 118.90   |
| 54  | BA    | 2821 | A    | C5-C6-N1    | 5.42  | 120.41      | 117.70   |
| 55  | BB    | 27   | C    | N3-C2-O2    | -5.42 | 118.11      | 121.90   |
| 21  | AA    | 438  | U    | N1-C2-N3    | 5.42  | 118.15      | 114.90   |
| 21  | AA    | 477  | C    | N3-C2-O2    | -5.42 | 118.11      | 121.90   |
| 21  | AA    | 1431 | A    | C5-C6-N1    | 5.42  | 120.41      | 117.70   |
| 54  | BA    | 1376 | C    | N3-C2-O2    | -5.42 | 118.11      | 121.90   |
| 54  | BA    | 2104 | C    | N1-C2-O2    | 5.42  | 122.15      | 118.90   |
| 55  | BB    | 109  | A    | C1'-O4'-C4' | -5.42 | 105.56      | 109.90   |
| 21  | AA    | 917  | G    | N7-C8-N9    | 5.42  | 115.81      | 113.10   |
| 54  | BA    | 1503 | A    | C4-C5-C6    | -5.42 | 114.29      | 117.00   |
| 54  | BA    | 2269 | G    | C8-N9-C4    | -5.42 | 104.23      | 106.40   |
| 54  | BA    | 2652 | C    | N3-C2-O2    | -5.42 | 118.11      | 121.90   |
| 21  | AA    | 580  | C    | N3-C4-C5    | 5.42  | 124.07      | 121.90   |
| 21  | AA    | 1331 | G    | C8-N9-C4    | -5.42 | 104.23      | 106.40   |
| 24  | A3    | 1    | C    | N3-C4-N4    | -5.42 | 114.21      | 118.00   |
| 54  | BA    | 423  | A    | C2-N3-C4    | 5.42  | 113.31      | 110.60   |
| 54  | BA    | 1373 | A    | C5-C6-N1    | 5.42  | 120.41      | 117.70   |
| 54  | BA    | 1675 | C    | C2-N3-C4    | -5.42 | 117.19      | 119.90   |
| 54  | BA    | 2524 | G    | O4'-C1'-N9  | 5.42  | 112.53      | 108.20   |
| 24  | A3    | 67   | C    | O4'-C1'-N1  | 5.42  | 112.53      | 108.20   |
| 54  | BA    | 211  | C    | N3-C2-O2    | -5.42 | 118.11      | 121.90   |
| 54  | BA    | 405  | U    | N3-C2-O2    | -5.42 | 118.41      | 122.20   |
| 55  | BB    | 16   | G    | N7-C8-N9    | 5.42  | 115.81      | 113.10   |
| 21  | AA    | 115  | G    | N3-C4-C5    | -5.41 | 125.89      | 128.60   |
| 21  | AA    | 251  | G    | C3'-C2'-C1' | 5.41  | 105.83      | 101.50   |
| 21  | AA    | 497  | G    | C5-C6-N1    | 5.41  | 114.21      | 111.50   |
| 21  | AA    | 818  | G    | C5-C6-N1    | 5.41  | 114.21      | 111.50   |
| 21  | AA    | 1009 | U    | O4'-C1'-N1  | 5.41  | 112.53      | 108.20   |
| 21  | AA    | 1127 | G    | C5-C6-N1    | 5.41  | 114.21      | 111.50   |
| 21  | AA    | 1441 | A    | C6-C5-N7    | 5.41  | 136.09      | 132.30   |
| 24  | A3    | 69   | C    | C5'-C4'-C3' | -5.41 | 107.34      | 116.00   |
| 54  | BA    | 423  | A    | C6-C5-N7    | 5.41  | 136.09      | 132.30   |
| 54  | BA    | 720  | U    | O4'-C1'-N1  | 5.41  | 112.53      | 108.20   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 54  | BA    | 2772 | C    | N3-C2-O2    | -5.41 | 118.11      | 121.90   |
| 21  | AA    | 165  | G    | C5-C6-N1    | 5.41  | 114.21      | 111.50   |
| 54  | BA    | 305  | C    | N3-C2-O2    | -5.41 | 118.11      | 121.90   |
| 54  | BA    | 2368 | C    | N3-C4-C5    | 5.41  | 124.06      | 121.90   |
| 21  | AA    | 720  | C    | N3-C2-O2    | -5.41 | 118.11      | 121.90   |
| 21  | AA    | 1223 | C    | N3-C2-O2    | -5.41 | 118.11      | 121.90   |
| 22  | A1    | 69   | A    | C5-C6-N1    | 5.41  | 120.41      | 117.70   |
| 54  | BA    | 1618 | A    | C4-C5-C6    | -5.41 | 114.29      | 117.00   |
| 54  | BA    | 2847 | U    | C5-C6-N1    | -5.41 | 120.00      | 122.70   |
| 21  | AA    | 753  | A    | C4-C5-C6    | -5.41 | 114.30      | 117.00   |
| 21  | AA    | 925  | G    | N1-C6-O6    | -5.41 | 116.66      | 119.90   |
| 21  | AA    | 1028 | C    | N3-C2-O2    | -5.41 | 118.11      | 121.90   |
| 21  | AA    | 1078 | U    | C5-C6-N1    | -5.41 | 120.00      | 122.70   |
| 49  | B0    | 51   | ARG  | NE-CZ-NH1   | 5.41  | 123.00      | 120.30   |
| 54  | BA    | 601  | C    | N3-C2-O2    | -5.41 | 118.11      | 121.90   |
| 54  | BA    | 815  | C    | N3-C2-O2    | -5.41 | 118.11      | 121.90   |
| 54  | BA    | 1655 | A    | C6-C5-N7    | 5.41  | 136.09      | 132.30   |
| 54  | BA    | 2130 | U    | C4-C5-C6    | 5.41  | 122.94      | 119.70   |
| 54  | BA    | 2853 | C    | O4'-C1'-N1  | 5.41  | 112.53      | 108.20   |
| 54  | BA    | 338  | G    | C5-C6-N1    | 5.41  | 114.20      | 111.50   |
| 54  | BA    | 455  | C    | O4'-C4'-C3' | 5.41  | 110.43      | 106.10   |
| 54  | BA    | 825  | A    | C4-C5-C6    | -5.41 | 114.30      | 117.00   |
| 21  | AA    | 1236 | A    | C4-C5-C6    | -5.41 | 114.30      | 117.00   |
| 54  | BA    | 1281 | G    | O4'-C1'-N9  | 5.41  | 112.52      | 108.20   |
| 54  | BA    | 1571 | A    | C4-C5-C6    | -5.41 | 114.30      | 117.00   |
| 54  | BA    | 1758 | U    | C3'-C2'-C1' | -5.41 | 97.18       | 101.50   |
| 54  | BA    | 1958 | C    | N3-C2-O2    | -5.41 | 118.12      | 121.90   |
| 54  | BA    | 2098 | U    | N3-C2-O2    | -5.41 | 118.42      | 122.20   |
| 54  | BA    | 2211 | A    | C4-C5-C6    | -5.41 | 114.30      | 117.00   |
| 54  | BA    | 2699 | C    | N3-C4-C5    | 5.41  | 124.06      | 121.90   |
| 54  | BA    | 1241 | A    | C2-N3-C4    | 5.40  | 113.30      | 110.60   |
| 54  | BA    | 2178 | C    | O4'-C1'-N1  | 5.40  | 112.52      | 108.20   |
| 54  | BA    | 2227 | A    | C6-C5-N7    | 5.40  | 136.08      | 132.30   |
| 21  | AA    | 342  | C    | N1-C2-O2    | 5.40  | 122.14      | 118.90   |
| 21  | AA    | 1150 | A    | C6-C5-N7    | 5.40  | 136.08      | 132.30   |
| 21  | AA    | 1207 | G    | C8-N9-C4    | -5.40 | 104.24      | 106.40   |
| 21  | AA    | 1293 | C    | N3-C2-O2    | -5.40 | 118.12      | 121.90   |
| 54  | BA    | 44   | A    | C5-C6-N1    | 5.40  | 120.40      | 117.70   |
| 54  | BA    | 677  | A    | C5-N7-C8    | -5.40 | 101.20      | 103.90   |
| 54  | BA    | 832  | U    | C5-C6-N1    | -5.40 | 120.00      | 122.70   |
| 54  | BA    | 2025 | C    | N3-C4-C5    | 5.40  | 124.06      | 121.90   |
| 54  | BA    | 2881 | U    | N3-C2-O2    | -5.40 | 118.42      | 122.20   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 21  | AA    | 1207 | G    | N9-C4-C5    | 5.40  | 107.56      | 105.40   |
| 54  | BA    | 207  | A    | C5-C6-N1    | 5.40  | 120.40      | 117.70   |
| 54  | BA    | 646  | U    | O4'-C1'-N1  | 5.40  | 112.52      | 108.20   |
| 54  | BA    | 901  | C    | N3-C4-C5    | 5.40  | 124.06      | 121.90   |
| 54  | BA    | 1307 | A    | C4-C5-C6    | -5.40 | 114.30      | 117.00   |
| 54  | BA    | 1315 | C    | N3-C2-O2    | -5.40 | 118.12      | 121.90   |
| 54  | BA    | 1981 | A    | O4'-C4'-C3' | 5.40  | 110.42      | 106.10   |
| 54  | BA    | 2617 | U    | C5'-C4'-O4' | 5.40  | 115.58      | 109.10   |
| 4   | AE    | 28   | ARG  | CD-NE-CZ    | 5.40  | 131.16      | 123.60   |
| 21  | AA    | 114  | U    | N1-C2-N3    | 5.40  | 118.14      | 114.90   |
| 21  | AA    | 125  | U    | C1'-O4'-C4' | -5.40 | 105.58      | 109.90   |
| 21  | AA    | 765  | G    | N3-C4-C5    | -5.40 | 125.90      | 128.60   |
| 54  | BA    | 1098 | A    | C6-C5-N7    | 5.40  | 136.08      | 132.30   |
| 54  | BA    | 2050 | C    | N3-C4-C5    | 5.40  | 124.06      | 121.90   |
| 21  | AA    | 164  | G    | C1'-O4'-C4' | -5.40 | 105.58      | 109.90   |
| 21  | AA    | 837  | U    | N1-C2-N3    | 5.40  | 118.14      | 114.90   |
| 21  | AA    | 1328 | C    | N1-C2-O2    | 5.40  | 122.14      | 118.90   |
| 54  | BA    | 20   | C    | O4'-C1'-N1  | 5.40  | 112.52      | 108.20   |
| 54  | BA    | 39   | G    | C8-N9-C4    | -5.40 | 104.24      | 106.40   |
| 54  | BA    | 705  | A    | C5-C6-N1    | 5.40  | 120.40      | 117.70   |
| 54  | BA    | 1370 | C    | O4'-C1'-N1  | 5.40  | 112.52      | 108.20   |
| 54  | BA    | 2373 | G    | N1-C6-O6    | -5.40 | 116.66      | 119.90   |
| 54  | BA    | 2698 | U    | N3-C2-O2    | -5.40 | 118.42      | 122.20   |
| 7   | AH    | 79   | ARG  | NE-CZ-NH1   | 5.40  | 123.00      | 120.30   |
| 21  | AA    | 173  | U    | C1'-O4'-C4' | -5.40 | 105.58      | 109.90   |
| 21  | AA    | 539  | A    | C4-C5-C6    | -5.40 | 114.30      | 117.00   |
| 21  | AA    | 1056 | U    | O4'-C1'-N1  | 5.40  | 112.52      | 108.20   |
| 21  | AA    | 1092 | A    | C5-C6-N1    | 5.40  | 120.40      | 117.70   |
| 54  | BA    | 2162 | G    | N3-C2-N2    | -5.40 | 116.12      | 119.90   |
| 54  | BA    | 2861 | U    | N1-C2-N3    | 5.40  | 118.14      | 114.90   |
| 21  | AA    | 730  | G    | C8-N9-C4    | -5.39 | 104.24      | 106.40   |
| 21  | AA    | 831  | A    | C5-C6-N1    | 5.39  | 120.40      | 117.70   |
| 54  | BA    | 257  | C    | O4'-C1'-N1  | 5.39  | 112.52      | 108.20   |
| 54  | BA    | 1232 | G    | N3-C2-N2    | -5.39 | 116.12      | 119.90   |
| 54  | BA    | 1530 | G    | N7-C8-N9    | 5.39  | 115.80      | 113.10   |
| 54  | BA    | 1701 | A    | O4'-C1'-N9  | 5.39  | 112.52      | 108.20   |
| 54  | BA    | 1915 | U    | O4'-C1'-N1  | 5.39  | 112.52      | 108.20   |
| 54  | BA    | 2722 | G    | N1-C6-O6    | -5.39 | 116.66      | 119.90   |
| 54  | BA    | 2745 | C    | N3-C2-O2    | -5.39 | 118.12      | 121.90   |
| 54  | BA    | 557  | C    | N3-C2-O2    | -5.39 | 118.12      | 121.90   |
| 55  | BB    | 22   | U    | N1-C2-N3    | 5.39  | 118.14      | 114.90   |
| 21  | AA    | 967  | C    | N1-C2-O2    | 5.39  | 122.13      | 118.90   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|-------------|-------|------------------------|---------------------|
| 23  | A2    | 90   | U    | N3-C2-O2    | -5.39 | 118.43                 | 122.20              |
| 54  | BA    | 409  | G    | C8-N9-C4    | -5.39 | 104.24                 | 106.40              |
| 54  | BA    | 1197 | G    | N1-C6-O6    | -5.39 | 116.67                 | 119.90              |
| 54  | BA    | 1340 | U    | N3-C2-O2    | -5.39 | 118.43                 | 122.20              |
| 21  | AA    | 52   | C    | N3-C4-C5    | 5.39  | 124.06                 | 121.90              |
| 21  | AA    | 64   | G    | O4'-C1'-N9  | 5.39  | 112.51                 | 108.20              |
| 24  | A3    | 65   | G    | N3-C2-N2    | -5.39 | 116.13                 | 119.90              |
| 24  | A3    | 67   | C    | C2-N3-C4    | -5.39 | 117.20                 | 119.90              |
| 54  | BA    | 543  | G    | N1-C6-O6    | -5.39 | 116.67                 | 119.90              |
| 54  | BA    | 906  | U    | C5-C6-N1    | -5.39 | 120.01                 | 122.70              |
| 54  | BA    | 1091 | G    | C5-C6-N1    | 5.39  | 114.19                 | 111.50              |
| 54  | BA    | 1282 | U    | C5-C6-N1    | -5.39 | 120.00                 | 122.70              |
| 54  | BA    | 1432 | G    | C5-C6-N1    | 5.39  | 114.19                 | 111.50              |
| 54  | BA    | 2574 | G    | C5-C6-N1    | 5.39  | 114.19                 | 111.50              |
| 55  | BB    | 60   | C    | N1-C2-O2    | 5.39  | 122.13                 | 118.90              |
| 21  | AA    | 242  | G    | N1-C6-O6    | -5.39 | 116.67                 | 119.90              |
| 21  | AA    | 764  | C    | N3-C2-O2    | -5.39 | 118.13                 | 121.90              |
| 54  | BA    | 116  | C    | O4'-C1'-N1  | 5.39  | 112.51                 | 108.20              |
| 54  | BA    | 401  | A    | C4-C5-C6    | -5.39 | 114.31                 | 117.00              |
| 54  | BA    | 2614 | A    | C6-C5-N7    | 5.39  | 136.07                 | 132.30              |
| 54  | BA    | 2634 | A    | C4-C5-C6    | -5.39 | 114.31                 | 117.00              |
| 54  | BA    | 2745 | C    | N3-C4-C5    | 5.39  | 124.06                 | 121.90              |
| 55  | BB    | 18   | G    | O4'-C1'-N9  | 5.39  | 112.51                 | 108.20              |
| 21  | AA    | 358  | U    | C3'-C2'-C1' | 5.39  | 105.81                 | 101.50              |
| 21  | AA    | 512  | U    | C5-C6-N1    | -5.39 | 120.01                 | 122.70              |
| 22  | A1    | 40   | G    | N7-C8-N9    | 5.39  | 115.79                 | 113.10              |
| 46  | BX    | 27   | ARG  | NE-CZ-NH1   | 5.39  | 122.99                 | 120.30              |
| 54  | BA    | 420  | C    | C6-N1-C2    | -5.39 | 118.14                 | 120.30              |
| 54  | BA    | 455  | C    | C3'-C2'-C1' | 5.39  | 105.81                 | 101.50              |
| 54  | BA    | 1352 | U    | C4-C5-C6    | 5.39  | 122.93                 | 119.70              |
| 54  | BA    | 1476 | U    | N3-C2-O2    | -5.39 | 118.43                 | 122.20              |
| 54  | BA    | 2380 | C    | N3-C4-C5    | 5.39  | 124.06                 | 121.90              |
| 54  | BA    | 2783 | U    | O4'-C1'-N1  | 5.39  | 112.51                 | 108.20              |
| 21  | AA    | 716  | A    | O4'-C1'-N9  | 5.38  | 112.51                 | 108.20              |
| 21  | AA    | 1057 | G    | C5-C6-N1    | 5.38  | 114.19                 | 111.50              |
| 22  | A1    | 48   | C    | N3-C2-O2    | -5.38 | 118.13                 | 121.90              |
| 54  | BA    | 385  | C    | N1-C2-O2    | 5.38  | 122.13                 | 118.90              |
| 54  | BA    | 1319 | C    | C1'-O4'-C4' | -5.38 | 105.59                 | 109.90              |
| 54  | BA    | 1677 | A    | C8-N9-C4    | -5.38 | 103.65                 | 105.80              |
| 54  | BA    | 1826 | G    | C2'-C3'-O3' | 5.38  | 122.31                 | 113.70              |
| 54  | BA    | 2828 | G    | C5-C6-N1    | 5.38  | 114.19                 | 111.50              |
| 55  | BB    | 109  | A    | O4'-C1'-N9  | 5.38  | 112.51                 | 108.20              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|-------------|-------|------------------------|---------------------|
| 21  | AA    | 861  | G    | N7-C8-N9    | 5.38  | 115.79                 | 113.10              |
| 21  | AA    | 1184 | G    | C5-C6-N1    | 5.38  | 114.19                 | 111.50              |
| 54  | BA    | 805  | G    | C5-C6-N1    | 5.38  | 114.19                 | 111.50              |
| 54  | BA    | 2371 | G    | O4'-C1'-N9  | 5.38  | 112.51                 | 108.20              |
| 21  | AA    | 387  | U    | C5-C6-N1    | -5.38 | 120.01                 | 122.70              |
| 21  | AA    | 1153 | G    | C5-C6-N1    | 5.38  | 114.19                 | 111.50              |
| 54  | BA    | 33   | C    | N3-C2-O2    | -5.38 | 118.13                 | 121.90              |
| 54  | BA    | 385  | C    | N3-C4-C5    | 5.38  | 124.05                 | 121.90              |
| 54  | BA    | 1011 | G    | O4'-C1'-N9  | 5.38  | 112.51                 | 108.20              |
| 54  | BA    | 1090 | A    | C6-C5-N7    | 5.38  | 136.07                 | 132.30              |
| 54  | BA    | 1256 | G    | C8-N9-C4    | -5.38 | 104.25                 | 106.40              |
| 54  | BA    | 1973 | G    | N9-C4-C5    | 5.38  | 107.55                 | 105.40              |
| 54  | BA    | 2389 | G    | N3-C2-N2    | -5.38 | 116.13                 | 119.90              |
| 54  | BA    | 372  | G    | N3-C4-C5    | -5.38 | 125.91                 | 128.60              |
| 21  | AA    | 9    | G    | C5-C6-N1    | 5.38  | 114.19                 | 111.50              |
| 21  | AA    | 309  | A    | C5-C6-N1    | 5.38  | 120.39                 | 117.70              |
| 21  | AA    | 560  | A    | C6-C5-N7    | 5.38  | 136.06                 | 132.30              |
| 21  | AA    | 1234 | C    | N1-C2-O2    | 5.38  | 122.13                 | 118.90              |
| 54  | BA    | 76   | C    | N1-C2-O2    | 5.38  | 122.13                 | 118.90              |
| 54  | BA    | 278  | A    | C5-C6-N1    | 5.38  | 120.39                 | 117.70              |
| 54  | BA    | 841  | G    | N1-C6-O6    | -5.38 | 116.67                 | 119.90              |
| 54  | BA    | 1543 | G    | N3-C4-C5    | -5.38 | 125.91                 | 128.60              |
| 54  | BA    | 2683 | C    | O4'-C1'-N1  | 5.38  | 112.50                 | 108.20              |
| 21  | AA    | 70   | U    | O4'-C4'-C3' | 5.38  | 110.40                 | 106.10              |
| 21  | AA    | 77   | A    | C5-C6-N1    | 5.38  | 120.39                 | 117.70              |
| 21  | AA    | 625  | U    | N1-C2-N3    | 5.38  | 118.13                 | 114.90              |
| 21  | AA    | 995  | C    | C1'-O4'-C4' | -5.38 | 105.60                 | 109.90              |
| 22  | A1    | 31   | C    | N3-C2-O2    | -5.38 | 118.14                 | 121.90              |
| 54  | BA    | 1    | G    | C8-N9-C4    | -5.38 | 104.25                 | 106.40              |
| 54  | BA    | 774  | G    | C8-N9-C4    | -5.38 | 104.25                 | 106.40              |
| 54  | BA    | 2339 | C    | N3-C4-C5    | 5.38  | 124.05                 | 121.90              |
| 54  | BA    | 2389 | G    | C8-N9-C4    | -5.38 | 104.25                 | 106.40              |
| 55  | BB    | 18   | G    | C5-C6-N1    | 5.38  | 114.19                 | 111.50              |
| 21  | AA    | 1477 | U    | O4'-C1'-N1  | 5.38  | 112.50                 | 108.20              |
| 54  | BA    | 13   | A    | C4-C5-C6    | -5.38 | 114.31                 | 117.00              |
| 54  | BA    | 374  | A    | C6-C5-N7    | 5.38  | 136.06                 | 132.30              |
| 21  | AA    | 1526 | G    | N3-C4-C5    | -5.37 | 125.91                 | 128.60              |
| 54  | BA    | 134  | G    | N1-C6-O6    | -5.37 | 116.68                 | 119.90              |
| 54  | BA    | 386  | G    | N3-C4-C5    | -5.37 | 125.91                 | 128.60              |
| 54  | BA    | 540  | C    | N1-C2-O2    | 5.37  | 122.12                 | 118.90              |
| 54  | BA    | 736  | C    | N1-C2-O2    | 5.37  | 122.12                 | 118.90              |
| 54  | BA    | 863  | A    | C4-C5-C6    | -5.37 | 114.31                 | 117.00              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|-------------|-------|------------------------|---------------------|
| 54  | BA    | 946  | C    | N1-C2-O2    | 5.37  | 122.12                 | 118.90              |
| 1   | AB    | 62   | ARG  | NE-CZ-NH2   | -5.37 | 117.61                 | 120.30              |
| 21  | AA    | 525  | C    | N1-C2-O2    | 5.37  | 122.12                 | 118.90              |
| 21  | AA    | 1031 | C    | C1'-O4'-C4' | -5.37 | 105.60                 | 109.90              |
| 21  | AA    | 1355 | G    | N1-C6-O6    | -5.37 | 116.68                 | 119.90              |
| 36  | BN    | 103  | ARG  | NE-CZ-NH1   | 5.37  | 122.99                 | 120.30              |
| 54  | BA    | 548  | G    | N1-C6-O6    | -5.37 | 116.68                 | 119.90              |
| 54  | BA    | 974  | G    | N3-C4-C5    | -5.37 | 125.91                 | 128.60              |
| 54  | BA    | 1121 | C    | C4'-C3'-C2' | -5.37 | 97.23                  | 102.60              |
| 54  | BA    | 1465 | G    | P-O3'-C3'   | 5.37  | 126.15                 | 119.70              |
| 54  | BA    | 1945 | G    | C8-N9-C4    | -5.37 | 104.25                 | 106.40              |
| 54  | BA    | 2526 | G    | O4'-C1'-N9  | 5.37  | 112.50                 | 108.20              |
| 21  | AA    | 1486 | G    | C5-C6-N1    | 5.37  | 114.19                 | 111.50              |
| 54  | BA    | 1037 | G    | N3-C4-C5    | -5.37 | 125.92                 | 128.60              |
| 54  | BA    | 1489 | C    | N3-C2-O2    | -5.37 | 118.14                 | 121.90              |
| 54  | BA    | 2325 | G    | N1-C6-O6    | -5.37 | 116.68                 | 119.90              |
| 8   | AI    | 123  | ARG  | NE-CZ-NH1   | 5.37  | 122.98                 | 120.30              |
| 21  | AA    | 893  | C    | C6-N1-C2    | -5.37 | 118.15                 | 120.30              |
| 22  | A1    | 17   | U    | C4-C5-C6    | 5.37  | 122.92                 | 119.70              |
| 54  | BA    | 746  | U    | N3-C2-O2    | -5.37 | 118.44                 | 122.20              |
| 54  | BA    | 1261 | C    | N3-C2-O2    | -5.37 | 118.14                 | 121.90              |
| 54  | BA    | 1345 | C    | O4'-C1'-N1  | 5.37  | 112.50                 | 108.20              |
| 54  | BA    | 2030 | A    | C6-C5-N7    | 5.37  | 136.06                 | 132.30              |
| 54  | BA    | 2161 | C    | N3-C4-C5    | 5.37  | 124.05                 | 121.90              |
| 21  | AA    | 340  | U    | C5-C6-N1    | -5.37 | 120.02                 | 122.70              |
| 21  | AA    | 653  | U    | O4'-C1'-N1  | 5.37  | 112.49                 | 108.20              |
| 21  | AA    | 1495 | U    | N1-C2-N3    | 5.37  | 118.12                 | 114.90              |
| 54  | BA    | 70   | G    | C8-N9-C4    | -5.37 | 104.25                 | 106.40              |
| 54  | BA    | 199  | A    | C4-C5-C6    | -5.37 | 114.32                 | 117.00              |
| 54  | BA    | 501  | A    | C4-C5-C6    | -5.37 | 114.32                 | 117.00              |
| 54  | BA    | 2324 | U    | C3'-C2'-C1' | 5.37  | 105.79                 | 101.50              |
| 55  | BB    | 9    | G    | N3-C4-C5    | -5.37 | 125.92                 | 128.60              |
| 21  | AA    | 417  | G    | C5-C6-N1    | 5.37  | 114.18                 | 111.50              |
| 21  | AA    | 932  | C    | N1-C2-O2    | 5.37  | 122.12                 | 118.90              |
| 54  | BA    | 2    | G    | C8-N9-C4    | -5.37 | 104.25                 | 106.40              |
| 54  | BA    | 756  | A    | C4-C5-C6    | -5.37 | 114.32                 | 117.00              |
| 54  | BA    | 1101 | U    | C5-C6-N1    | -5.37 | 120.02                 | 122.70              |
| 54  | BA    | 1305 | C    | O4'-C1'-N1  | 5.37  | 112.49                 | 108.20              |
| 54  | BA    | 1799 | G    | C5-C6-N1    | 5.37  | 114.18                 | 111.50              |
| 54  | BA    | 1940 | U    | O4'-C1'-N1  | 5.37  | 112.49                 | 108.20              |
| 54  | BA    | 2136 | G    | N9-C4-C5    | 5.37  | 107.55                 | 105.40              |
| 54  | BA    | 2422 | C    | N3-C4-C5    | 5.37  | 124.05                 | 121.90              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | A1    | 57   | G    | N1-C6-O6    | -5.36 | 116.68      | 119.90   |
| 25  | BC    | 79   | ARG  | NE-CZ-NH1   | 5.36  | 122.98      | 120.30   |
| 54  | BA    | 121  | G    | N3-C2-N2    | -5.36 | 116.15      | 119.90   |
| 54  | BA    | 721  | A    | C6-C5-N7    | 5.36  | 136.06      | 132.30   |
| 54  | BA    | 1128 | G    | N1-C6-O6    | -5.36 | 116.68      | 119.90   |
| 54  | BA    | 1370 | C    | N3-C4-C5    | 5.36  | 124.05      | 121.90   |
| 54  | BA    | 1464 | G    | N3-C4-C5    | -5.36 | 125.92      | 128.60   |
| 54  | BA    | 1501 | G    | N3-C2-N2    | -5.36 | 116.15      | 119.90   |
| 54  | BA    | 1685 | C    | C4'-C3'-C2' | -5.36 | 97.24       | 102.60   |
| 54  | BA    | 1822 | C    | N3-C4-C5    | 5.36  | 124.05      | 121.90   |
| 54  | BA    | 1244 | A    | C4-C5-C6    | -5.36 | 114.32      | 117.00   |
| 54  | BA    | 1558 | C    | N3-C4-N4    | -5.36 | 114.25      | 118.00   |
| 54  | BA    | 1945 | G    | N3-C2-N2    | -5.36 | 116.15      | 119.90   |
| 54  | BA    | 2822 | G    | C5-C6-N1    | 5.36  | 114.18      | 111.50   |
| 21  | AA    | 264  | C    | O4'-C1'-N1  | 5.36  | 112.49      | 108.20   |
| 21  | AA    | 1332 | A    | C4-C5-C6    | -5.36 | 114.32      | 117.00   |
| 22  | A1    | 41   | A    | C4-C5-C6    | -5.36 | 114.32      | 117.00   |
| 54  | BA    | 830  | G    | N1-C6-O6    | -5.36 | 116.69      | 119.90   |
| 54  | BA    | 1569 | A    | C5-C6-N1    | 5.36  | 120.38      | 117.70   |
| 54  | BA    | 2271 | G    | N9-C4-C5    | 5.36  | 107.54      | 105.40   |
| 21  | AA    | 84   | U    | C5-C6-N1    | -5.36 | 120.02      | 122.70   |
| 21  | AA    | 976  | G    | C8-N9-C4    | -5.36 | 104.26      | 106.40   |
| 21  | AA    | 1002 | G    | C8-N9-C4    | -5.36 | 104.26      | 106.40   |
| 21  | AA    | 1217 | C    | N1-C2-O2    | 5.36  | 122.11      | 118.90   |
| 21  | AA    | 1517 | G    | N1-C6-O6    | -5.36 | 116.69      | 119.90   |
| 54  | BA    | 1277 | G    | C5-C6-N1    | 5.36  | 114.18      | 111.50   |
| 54  | BA    | 1541 | C    | N3-C2-O2    | -5.36 | 118.15      | 121.90   |
| 54  | BA    | 1588 | G    | N1-C6-O6    | -5.36 | 116.69      | 119.90   |
| 54  | BA    | 1607 | C    | O4'-C1'-N1  | 5.36  | 112.49      | 108.20   |
| 54  | BA    | 1643 | G    | O4'-C1'-N9  | 5.36  | 112.49      | 108.20   |
| 54  | BA    | 1931 | U    | N3-C2-O2    | -5.36 | 118.45      | 122.20   |
| 54  | BA    | 2356 | U    | N3-C2-O2    | -5.36 | 118.45      | 122.20   |
| 54  | BA    | 2687 | U    | C5-C6-N1    | -5.36 | 120.02      | 122.70   |
| 55  | BB    | 6    | G    | C4'-C3'-C2' | -5.36 | 97.24       | 102.60   |
| 21  | AA    | 71   | A    | C3'-C2'-C1' | 5.36  | 105.78      | 101.50   |
| 21  | AA    | 874  | G    | N3-C4-C5    | -5.36 | 125.92      | 128.60   |
| 54  | BA    | 233  | A    | C6-C5-N7    | 5.36  | 136.05      | 132.30   |
| 54  | BA    | 653  | U    | N3-C2-O2    | -5.36 | 118.45      | 122.20   |
| 54  | BA    | 996  | A    | C6-C5-N7    | 5.36  | 136.05      | 132.30   |
| 54  | BA    | 1185 | G    | N3-C2-N2    | -5.36 | 116.15      | 119.90   |
| 54  | BA    | 1470 | A    | C5-C6-N1    | 5.36  | 120.38      | 117.70   |
| 54  | BA    | 2153 | C    | N3-C2-O2    | -5.36 | 118.15      | 121.90   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 54  | BA    | 2494 | G    | O4'-C1'-N9  | 5.36  | 112.48      | 108.20   |
| 54  | BA    | 2890 | G    | N3-C4-C5    | -5.36 | 125.92      | 128.60   |
| 33  | BK    | 105  | ARG  | NE-CZ-NH1   | 5.35  | 122.98      | 120.30   |
| 54  | BA    | 58   | G    | C8-N9-C4    | -5.35 | 104.26      | 106.40   |
| 54  | BA    | 528  | A    | C6-C5-N7    | 5.35  | 136.05      | 132.30   |
| 54  | BA    | 1065 | U    | O4'-C1'-N1  | 5.35  | 112.48      | 108.20   |
| 21  | AA    | 1058 | G    | C3'-C2'-C1' | 5.35  | 105.78      | 101.50   |
| 54  | BA    | 684  | G    | N1-C6-O6    | -5.35 | 116.69      | 119.90   |
| 54  | BA    | 885  | C    | N3-C4-C5    | 5.35  | 124.04      | 121.90   |
| 54  | BA    | 2239 | G    | N7-C8-N9    | 5.35  | 115.78      | 113.10   |
| 54  | BA    | 2307 | G    | C5-C6-N1    | 5.35  | 114.18      | 111.50   |
| 54  | BA    | 2680 | U    | N1-C2-N3    | 5.35  | 118.11      | 114.90   |
| 21  | AA    | 248  | C    | O4'-C1'-N1  | 5.35  | 112.48      | 108.20   |
| 21  | AA    | 968  | A    | O4'-C1'-N9  | 5.35  | 112.48      | 108.20   |
| 54  | BA    | 341  | C    | C2-N3-C4    | -5.35 | 117.22      | 119.90   |
| 54  | BA    | 675  | A    | C4'-C3'-C2' | -5.35 | 97.25       | 102.60   |
| 54  | BA    | 984  | A    | O4'-C4'-C3' | 5.35  | 110.38      | 106.10   |
| 54  | BA    | 2002 | G    | N3-C4-C5    | -5.35 | 125.92      | 128.60   |
| 55  | BB    | 110  | C    | N1-C2-O2    | 5.35  | 122.11      | 118.90   |
| 21  | AA    | 575  | G    | P-O3'-C3'   | 5.35  | 126.12      | 119.70   |
| 21  | AA    | 929  | G    | N7-C8-N9    | 5.35  | 115.77      | 113.10   |
| 54  | BA    | 116  | C    | N3-C4-C5    | 5.35  | 124.04      | 121.90   |
| 54  | BA    | 143  | C    | C6-N1-C2    | -5.35 | 118.16      | 120.30   |
| 54  | BA    | 291  | G    | C8-N9-C4    | -5.35 | 104.26      | 106.40   |
| 54  | BA    | 360  | U    | C5-C6-N1    | -5.35 | 120.03      | 122.70   |
| 54  | BA    | 1097 | U    | N1-C2-N3    | 5.35  | 118.11      | 114.90   |
| 54  | BA    | 2669 | G    | O4'-C1'-N9  | 5.35  | 112.48      | 108.20   |
| 21  | AA    | 170  | U    | N1-C2-N3    | 5.35  | 118.11      | 114.90   |
| 21  | AA    | 392  | C    | N3-C4-C5    | 5.35  | 124.04      | 121.90   |
| 21  | AA    | 874  | G    | C5-C6-N1    | 5.35  | 114.17      | 111.50   |
| 54  | BA    | 1887 | C    | N3-C2-O2    | -5.35 | 118.16      | 121.90   |
| 54  | BA    | 2089 | C    | O4'-C1'-N1  | 5.35  | 112.48      | 108.20   |
| 54  | BA    | 2155 | U    | O4'-C1'-N1  | 5.35  | 112.48      | 108.20   |
| 54  | BA    | 2325 | G    | C5-C6-N1    | 5.35  | 114.17      | 111.50   |
| 21  | AA    | 1367 | C    | N1-C2-O2    | 5.35  | 122.11      | 118.90   |
| 54  | BA    | 2069 | G    | C5-C6-N1    | 5.35  | 114.17      | 111.50   |
| 54  | BA    | 2684 | U    | O4'-C1'-N1  | 5.35  | 112.48      | 108.20   |
| 55  | BB    | 94   | A    | C5-C6-N6    | 5.35  | 127.98      | 123.70   |
| 21  | AA    | 247  | G    | C8-N9-C4    | -5.34 | 104.26      | 106.40   |
| 21  | AA    | 1172 | C    | O4'-C1'-N1  | 5.34  | 112.47      | 108.20   |
| 23  | A2    | 92   | U    | N1-C2-N3    | 5.34  | 118.11      | 114.90   |
| 35  | BM    | 18   | ARG  | NE-CZ-NH2   | -5.34 | 117.63      | 120.30   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|------------|-------|------------------------|---------------------|
| 36  | BN    | 90   | ARG  | NE-CZ-NH1  | 5.34  | 122.97                 | 120.30              |
| 54  | BA    | 182  | A    | O4'-C1'-N9 | 5.34  | 112.48                 | 108.20              |
| 54  | BA    | 2174 | C    | N3-C4-C5   | 5.34  | 124.04                 | 121.90              |
| 54  | BA    | 2730 | C    | N3-C2-O2   | -5.34 | 118.16                 | 121.90              |
| 55  | BB    | 104  | A    | C5-C6-N1   | 5.34  | 120.37                 | 117.70              |
| 21  | AA    | 917  | G    | C8-N9-C4   | -5.34 | 104.26                 | 106.40              |
| 21  | AA    | 1038 | C    | N3-C4-C5   | 5.34  | 124.04                 | 121.90              |
| 21  | AA    | 1423 | G    | C2-N3-C4   | 5.34  | 114.57                 | 111.90              |
| 54  | BA    | 279  | A    | C4-C5-C6   | -5.34 | 114.33                 | 117.00              |
| 54  | BA    | 280  | U    | N3-C2-O2   | -5.34 | 118.46                 | 122.20              |
| 54  | BA    | 605  | G    | C8-N9-C4   | -5.34 | 104.26                 | 106.40              |
| 54  | BA    | 1612 | C    | O4'-C1'-N1 | 5.34  | 112.47                 | 108.20              |
| 54  | BA    | 1727 | C    | O4'-C1'-N1 | 5.34  | 112.47                 | 108.20              |
| 55  | BB    | 76   | G    | C5-C6-N1   | 5.34  | 114.17                 | 111.50              |
| 9   | AJ    | 62   | ARG  | NE-CZ-NH1  | 5.34  | 122.97                 | 120.30              |
| 21  | AA    | 864  | A    | C5-C6-N1   | 5.34  | 120.37                 | 117.70              |
| 54  | BA    | 79   | C    | N1-C2-O2   | 5.34  | 122.11                 | 118.90              |
| 54  | BA    | 938  | G    | C5-C6-N1   | 5.34  | 114.17                 | 111.50              |
| 54  | BA    | 94   | A    | C6-C5-N7   | 5.34  | 136.04                 | 132.30              |
| 54  | BA    | 605  | G    | N3-C4-C5   | -5.34 | 125.93                 | 128.60              |
| 54  | BA    | 1443 | U    | N3-C2-O2   | -5.34 | 118.46                 | 122.20              |
| 54  | BA    | 1995 | U    | N1-C2-N3   | 5.34  | 118.10                 | 114.90              |
| 54  | BA    | 2554 | U    | C4-C5-C6   | 5.34  | 122.90                 | 119.70              |
| 54  | BA    | 1121 | C    | N3-C2-O2   | -5.34 | 118.16                 | 121.90              |
| 54  | BA    | 1636 | U    | N1-C2-N3   | 5.34  | 118.10                 | 114.90              |
| 54  | BA    | 2035 | G    | N3-C2-N2   | -5.34 | 116.16                 | 119.90              |
| 54  | BA    | 2876 | G    | N1-C6-O6   | -5.34 | 116.70                 | 119.90              |
| 20  | AU    | 47   | ALA  | C-N-CA     | 5.34  | 135.04                 | 121.70              |
| 21  | AA    | 1257 | A    | C5-C6-N1   | 5.34  | 120.37                 | 117.70              |
| 21  | AA    | 1524 | C    | N3-C2-O2   | -5.34 | 118.16                 | 121.90              |
| 54  | BA    | 779  | U    | O4'-C1'-N1 | 5.34  | 112.47                 | 108.20              |
| 54  | BA    | 885  | C    | N1-C2-O2   | 5.34  | 122.10                 | 118.90              |
| 54  | BA    | 1770 | G    | N3-C2-N2   | -5.34 | 116.16                 | 119.90              |
| 54  | BA    | 2146 | C    | O4'-C1'-N1 | 5.34  | 112.47                 | 108.20              |
| 21  | AA    | 152  | A    | C6-C5-N7   | 5.33  | 136.03                 | 132.30              |
| 3   | AD    | 80   | ARG  | NE-CZ-NH2  | -5.33 | 117.63                 | 120.30              |
| 21  | AA    | 759  | A    | C4-C5-C6   | -5.33 | 114.33                 | 117.00              |
| 21  | AA    | 1138 | G    | N1-C6-O6   | -5.33 | 116.70                 | 119.90              |
| 41  | BS    | 92   | ARG  | NH1-CZ-NH2 | -5.33 | 113.53                 | 119.40              |
| 54  | BA    | 1299 | G    | O4'-C1'-N9 | 5.33  | 112.47                 | 108.20              |
| 54  | BA    | 1522 | A    | C4-C5-C6   | -5.33 | 114.33                 | 117.00              |
| 54  | BA    | 2574 | G    | N1-C6-O6   | -5.33 | 116.70                 | 119.90              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|------------|-------|------------------------|---------------------|
| 54  | BA    | 2848 | G    | N1-C6-O6   | -5.33 | 116.70                 | 119.90              |
| 21  | AA    | 1177 | G    | O4'-C1'-N9 | 5.33  | 112.47                 | 108.20              |
| 24  | A3    | 29   | C    | N3-C2-O2   | -5.33 | 118.17                 | 121.90              |
| 54  | BA    | 97   | C    | O4'-C1'-N1 | 5.33  | 112.47                 | 108.20              |
| 54  | BA    | 201  | C    | N3-C4-C5   | 5.33  | 124.03                 | 121.90              |
| 54  | BA    | 640  | C    | O4'-C1'-N1 | 5.33  | 112.47                 | 108.20              |
| 54  | BA    | 781  | A    | C5-C6-N1   | 5.33  | 120.37                 | 117.70              |
| 54  | BA    | 1155 | A    | C4-C5-C6   | -5.33 | 114.33                 | 117.00              |
| 54  | BA    | 2427 | C    | C2-N3-C4   | -5.33 | 117.23                 | 119.90              |
| 54  | BA    | 2497 | A    | N1-C6-N6   | -5.33 | 115.40                 | 118.60              |
| 54  | BA    | 2807 | U    | N3-C2-O2   | -5.33 | 118.47                 | 122.20              |
| 21  | AA    | 1357 | A    | C6-C5-N7   | 5.33  | 136.03                 | 132.30              |
| 54  | BA    | 574  | A    | C5-C6-N1   | 5.33  | 120.36                 | 117.70              |
| 54  | BA    | 1318 | U    | C5-C6-N1   | -5.33 | 120.03                 | 122.70              |
| 54  | BA    | 2342 | C    | N1-C2-O2   | 5.33  | 122.10                 | 118.90              |
| 55  | BB    | 105  | G    | N1-C6-O6   | -5.33 | 116.70                 | 119.90              |
| 55  | BB    | 108  | A    | N1-C6-N6   | -5.33 | 115.40                 | 118.60              |
| 1   | AB    | 20   | ARG  | NE-CZ-NH1  | 5.33  | 122.97                 | 120.30              |
| 21  | AA    | 748  | G    | C8-N9-C4   | -5.33 | 104.27                 | 106.40              |
| 21  | AA    | 777  | A    | N1-C6-N6   | -5.33 | 115.40                 | 118.60              |
| 41  | BS    | 92   | ARG  | NE-CZ-NH2  | 5.33  | 122.96                 | 120.30              |
| 54  | BA    | 30   | G    | N1-C6-O6   | -5.33 | 116.70                 | 119.90              |
| 54  | BA    | 213  | A    | O4'-C1'-N9 | 5.33  | 112.46                 | 108.20              |
| 54  | BA    | 1271 | G    | C5-C6-N1   | 5.33  | 114.16                 | 111.50              |
| 54  | BA    | 1647 | U    | N1-C2-N3   | 5.33  | 118.10                 | 114.90              |
| 54  | BA    | 2822 | G    | N9-C4-C5   | 5.33  | 107.53                 | 105.40              |
| 21  | AA    | 494  | G    | N3-C4-C5   | -5.33 | 125.94                 | 128.60              |
| 54  | BA    | 292  | U    | N3-C2-O2   | -5.33 | 118.47                 | 122.20              |
| 54  | BA    | 1391 | U    | N3-C2-O2   | -5.33 | 118.47                 | 122.20              |
| 21  | AA    | 407  | U    | N1-C2-N3   | 5.33  | 118.09                 | 114.90              |
| 22  | A1    | 13   | C    | N3-C2-O2   | -5.33 | 118.17                 | 121.90              |
| 48  | BZ    | 37   | ARG  | NH1-CZ-NH2 | -5.33 | 113.54                 | 119.40              |
| 54  | BA    | 598  | U    | O4'-C1'-N1 | 5.33  | 112.46                 | 108.20              |
| 54  | BA    | 720  | U    | N3-C2-O2   | -5.33 | 118.47                 | 122.20              |
| 54  | BA    | 1195 | G    | N3-C2-N2   | -5.33 | 116.17                 | 119.90              |
| 54  | BA    | 1228 | G    | C5-C6-N1   | 5.33  | 114.16                 | 111.50              |
| 54  | BA    | 1390 | U    | N1-C2-N3   | 5.33  | 118.10                 | 114.90              |
| 54  | BA    | 2095 | A    | C5-C6-N1   | 5.33  | 120.36                 | 117.70              |
| 54  | BA    | 2287 | A    | C2-N3-C4   | 5.33  | 113.26                 | 110.60              |
| 54  | BA    | 2465 | C    | O4'-C1'-N1 | 5.33  | 112.46                 | 108.20              |
| 54  | BA    | 2570 | G    | N1-C6-O6   | -5.33 | 116.70                 | 119.90              |
| 54  | BA    | 2626 | C    | N3-C4-C5   | 5.33  | 124.03                 | 121.90              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|-------------|-------|------------------------|---------------------|
| 21  | AA    | 234  | C    | N3-C4-C5    | 5.32  | 124.03                 | 121.90              |
| 21  | AA    | 658  | C    | O4'-C1'-N1  | 5.32  | 112.46                 | 108.20              |
| 21  | AA    | 1421 | G    | N1-C6-O6    | -5.32 | 116.70                 | 119.90              |
| 54  | BA    | 1942 | C    | N1-C2-O2    | 5.32  | 122.09                 | 118.90              |
| 54  | BA    | 2279 | G    | C4'-C3'-C2' | -5.32 | 97.28                  | 102.60              |
| 21  | AA    | 96   | U    | O4'-C1'-N1  | 5.32  | 112.46                 | 108.20              |
| 21  | AA    | 396  | C    | N1-C2-O2    | 5.32  | 122.09                 | 118.90              |
| 26  | BD    | 179  | ARG  | NE-CZ-NH1   | 5.32  | 122.96                 | 120.30              |
| 54  | BA    | 599  | A    | O4'-C1'-N9  | 5.32  | 112.46                 | 108.20              |
| 54  | BA    | 1561 | C    | O4'-C1'-N1  | 5.32  | 112.46                 | 108.20              |
| 54  | BA    | 2091 | C    | N3-C4-C5    | 5.32  | 124.03                 | 121.90              |
| 21  | AA    | 386  | C    | N1-C2-O2    | 5.32  | 122.09                 | 118.90              |
| 21  | AA    | 446  | G    | C5-C6-N1    | 5.32  | 114.16                 | 111.50              |
| 21  | AA    | 1150 | A    | C5-C6-N6    | 5.32  | 127.96                 | 123.70              |
| 21  | AA    | 1529 | G    | N3-C4-C5    | -5.32 | 125.94                 | 128.60              |
| 22  | A1    | 16   | C    | N1-C2-O2    | 5.32  | 122.09                 | 118.90              |
| 54  | BA    | 196  | A    | C4-C5-C6    | -5.32 | 114.34                 | 117.00              |
| 54  | BA    | 397  | U    | C5-C6-N1    | -5.32 | 120.04                 | 122.70              |
| 54  | BA    | 1776 | G    | N1-C6-O6    | -5.32 | 116.71                 | 119.90              |
| 54  | BA    | 2175 | C    | N1-C2-O2    | 5.32  | 122.09                 | 118.90              |
| 54  | BA    | 2762 | C    | N1-C2-O2    | 5.32  | 122.09                 | 118.90              |
| 55  | BB    | 76   | G    | N1-C6-O6    | -5.32 | 116.71                 | 119.90              |
| 55  | BB    | 95   | U    | C5-C6-N1    | -5.32 | 120.04                 | 122.70              |
| 21  | AA    | 1468 | A    | C6-C5-N7    | 5.32  | 136.02                 | 132.30              |
| 54  | BA    | 1671 | U    | N3-C2-O2    | -5.32 | 118.48                 | 122.20              |
| 54  | BA    | 1869 | G    | O4'-C1'-N9  | 5.32  | 112.46                 | 108.20              |
| 21  | AA    | 57   | G    | N3-C4-C5    | -5.32 | 125.94                 | 128.60              |
| 21  | AA    | 1286 | U    | C5-C6-N1    | -5.32 | 120.04                 | 122.70              |
| 54  | BA    | 1161 | C    | N1-C2-O2    | 5.32  | 122.09                 | 118.90              |
| 54  | BA    | 1564 | C    | N1-C2-O2    | 5.32  | 122.09                 | 118.90              |
| 54  | BA    | 1607 | C    | C6-N1-C2    | -5.32 | 118.17                 | 120.30              |
| 54  | BA    | 2201 | G    | O4'-C1'-N9  | 5.32  | 112.45                 | 108.20              |
| 54  | BA    | 2676 | C    | N3-C4-C5    | 5.32  | 124.03                 | 121.90              |
| 54  | BA    | 2843 | G    | C5-C6-N1    | 5.32  | 114.16                 | 111.50              |
| 20  | AU    | 44   | ARG  | NH1-CZ-NH2  | -5.32 | 113.55                 | 119.40              |
| 21  | AA    | 845  | A    | C4-C5-C6    | -5.32 | 114.34                 | 117.00              |
| 21  | AA    | 868  | C    | N3-C2-O2    | -5.32 | 118.18                 | 121.90              |
| 21  | AA    | 1076 | U    | N3-C2-O2    | -5.32 | 118.48                 | 122.20              |
| 22  | A1    | 38   | A    | C6-C5-N7    | 5.32  | 136.02                 | 132.30              |
| 24  | A3    | 9    | G    | N3-C4-C5    | -5.32 | 125.94                 | 128.60              |
| 54  | BA    | 111  | A    | C5'-C4'-O4' | 5.32  | 115.48                 | 109.10              |
| 54  | BA    | 114  | U    | O4'-C1'-N1  | 5.32  | 112.45                 | 108.20              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|-------------|-------|------------------------|---------------------|
| 54  | BA    | 2893 | A    | C5-C6-N1    | 5.32  | 120.36                 | 117.70              |
| 55  | BB    | 24   | G    | C3'-C2'-C1' | 5.32  | 105.75                 | 101.50              |
| 21  | AA    | 354  | G    | N1-C6-O6    | -5.31 | 116.71                 | 119.90              |
| 21  | AA    | 493  | A    | C6-C5-N7    | 5.31  | 136.02                 | 132.30              |
| 21  | AA    | 945  | G    | C5-C6-N1    | 5.31  | 114.16                 | 111.50              |
| 21  | AA    | 1251 | A    | C6-C5-N7    | 5.31  | 136.02                 | 132.30              |
| 24  | A3    | 6    | G    | N9-C4-C5    | 5.31  | 107.53                 | 105.40              |
| 28  | BF    | 124  | ARG  | NE-CZ-NH2   | -5.31 | 117.64                 | 120.30              |
| 54  | BA    | 2226 | C    | O4'-C1'-N1  | 5.31  | 112.45                 | 108.20              |
| 20  | AU    | 44   | ARG  | NE-CZ-NH2   | 5.31  | 122.96                 | 120.30              |
| 21  | AA    | 943  | U    | C5-C6-N1    | -5.31 | 120.04                 | 122.70              |
| 21  | AA    | 1160 | G    | N3-C2-N2    | -5.31 | 116.18                 | 119.90              |
| 21  | AA    | 1189 | U    | N3-C2-O2    | -5.31 | 118.48                 | 122.20              |
| 54  | BA    | 937  | C    | O4'-C1'-N1  | 5.31  | 112.45                 | 108.20              |
| 21  | AA    | 469  | C    | O4'-C1'-N1  | 5.31  | 112.45                 | 108.20              |
| 54  | BA    | 1514 | G    | N9-C4-C5    | 5.31  | 107.52                 | 105.40              |
| 54  | BA    | 2712 | C    | N1-C2-O2    | 5.31  | 122.09                 | 118.90              |
| 21  | AA    | 68   | G    | N3-C4-C5    | -5.31 | 125.94                 | 128.60              |
| 21  | AA    | 504  | C    | N3-C2-O2    | -5.31 | 118.18                 | 121.90              |
| 54  | BA    | 956  | G    | N3-C2-N2    | -5.31 | 116.18                 | 119.90              |
| 54  | BA    | 1795 | C    | C4'-C3'-C2' | -5.31 | 97.29                  | 102.60              |
| 54  | BA    | 2309 | A    | C4-C5-C6    | -5.31 | 114.34                 | 117.00              |
| 21  | AA    | 330  | C    | N1-C2-O2    | 5.31  | 122.08                 | 118.90              |
| 21  | AA    | 1467 | C    | C2-N3-C4    | -5.31 | 117.25                 | 119.90              |
| 25  | BC    | 211  | ARG  | NE-CZ-NH2   | -5.31 | 117.65                 | 120.30              |
| 54  | BA    | 399  | U    | O4'-C1'-N1  | 5.31  | 112.45                 | 108.20              |
| 54  | BA    | 797  | G    | C5-C6-N1    | 5.31  | 114.15                 | 111.50              |
| 54  | BA    | 1602 | U    | N3-C2-O2    | -5.31 | 118.48                 | 122.20              |
| 54  | BA    | 1813 | G    | N1-C6-O6    | -5.31 | 116.72                 | 119.90              |
| 54  | BA    | 2556 | C    | N1-C2-O2    | 5.31  | 122.08                 | 118.90              |
| 55  | BB    | 87   | U    | N3-C2-O2    | -5.31 | 118.48                 | 122.20              |
| 22  | A1    | 14   | A    | C4-C5-C6    | -5.31 | 114.35                 | 117.00              |
| 54  | BA    | 323  | C    | C3'-C2'-C1' | 5.31  | 105.75                 | 101.50              |
| 54  | BA    | 1739 | A    | C4-C5-C6    | -5.31 | 114.35                 | 117.00              |
| 54  | BA    | 2216 | G    | N1-C6-O6    | -5.31 | 116.72                 | 119.90              |
| 54  | BA    | 2848 | G    | O4'-C1'-N9  | 5.31  | 112.44                 | 108.20              |
| 21  | AA    | 1041 | G    | C8-N9-C4    | -5.30 | 104.28                 | 106.40              |
| 21  | AA    | 1407 | C    | N3-C4-C5    | 5.30  | 124.02                 | 121.90              |
| 54  | BA    | 40   | U    | C4-C5-C6    | 5.30  | 122.88                 | 119.70              |
| 54  | BA    | 56   | A    | C6-C5-N7    | 5.30  | 136.01                 | 132.30              |
| 54  | BA    | 414  | C    | N3-C2-O2    | -5.30 | 118.19                 | 121.90              |
| 54  | BA    | 1192 | G    | C5-C6-N1    | 5.30  | 114.15                 | 111.50              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 54  | BA    | 1782 | U    | N3-C2-O2    | -5.30 | 118.49      | 122.20   |
| 54  | BA    | 2021 | C    | N3-C4-C5    | 5.30  | 124.02      | 121.90   |
| 55  | BB    | 50   | A    | C5-C6-N1    | 5.30  | 120.35      | 117.70   |
| 21  | AA    | 349  | A    | C6-C5-N7    | 5.30  | 136.01      | 132.30   |
| 54  | BA    | 145  | C    | N1-C2-O2    | 5.30  | 122.08      | 118.90   |
| 54  | BA    | 353  | C    | N3-C4-N4    | -5.30 | 114.29      | 118.00   |
| 54  | BA    | 1154 | G    | N7-C8-N9    | 5.30  | 115.75      | 113.10   |
| 54  | BA    | 2391 | G    | N1-C6-O6    | -5.30 | 116.72      | 119.90   |
| 21  | AA    | 152  | A    | C4-C5-C6    | -5.30 | 114.35      | 117.00   |
| 21  | AA    | 1221 | G    | C5-C6-N1    | 5.30  | 114.15      | 111.50   |
| 24  | A3    | 7    | G    | C5-C6-N1    | 5.30  | 114.15      | 111.50   |
| 54  | BA    | 379  | G    | C5-C6-N1    | 5.30  | 114.15      | 111.50   |
| 54  | BA    | 775  | G    | N3-C2-N2    | -5.30 | 116.19      | 119.90   |
| 54  | BA    | 1317 | G    | N9-C4-C5    | 5.30  | 107.52      | 105.40   |
| 54  | BA    | 1369 | G    | N3-C4-C5    | -5.30 | 125.95      | 128.60   |
| 54  | BA    | 2872 | A    | C6-C5-N7    | 5.30  | 136.01      | 132.30   |
| 21  | AA    | 494  | G    | N9-C4-C5    | 5.30  | 107.52      | 105.40   |
| 21  | AA    | 657  | U    | O4'-C1'-N1  | 5.30  | 112.44      | 108.20   |
| 21  | AA    | 1031 | C    | O4'-C1'-N1  | 5.30  | 112.44      | 108.20   |
| 21  | AA    | 1284 | C    | N3-C2-O2    | -5.30 | 118.19      | 121.90   |
| 21  | AA    | 1379 | G    | C5-C6-N1    | 5.30  | 114.15      | 111.50   |
| 54  | BA    | 192  | C    | O4'-C1'-N1  | 5.30  | 112.44      | 108.20   |
| 54  | BA    | 737  | C    | N3-C2-O2    | -5.30 | 118.19      | 121.90   |
| 54  | BA    | 759  | G    | N3-C2-N2    | -5.30 | 116.19      | 119.90   |
| 54  | BA    | 809  | G    | C4'-C3'-C2' | -5.30 | 97.30       | 102.60   |
| 54  | BA    | 1894 | C    | N1-C2-O2    | 5.30  | 122.08      | 118.90   |
| 54  | BA    | 2444 | G    | C5-C6-N1    | 5.30  | 114.15      | 111.50   |
| 21  | AA    | 938  | A    | C1'-O4'-C4' | -5.30 | 105.66      | 109.90   |
| 21  | AA    | 673  | A    | C4-C5-C6    | -5.30 | 114.35      | 117.00   |
| 22  | A1    | 2    | G    | C5-C6-N1    | 5.30  | 114.15      | 111.50   |
| 54  | BA    | 498  | G    | N1-C6-O6    | -5.30 | 116.72      | 119.90   |
| 54  | BA    | 1332 | G    | C1'-O4'-C4' | -5.30 | 105.66      | 109.90   |
| 54  | BA    | 1526 | C    | O4'-C1'-N1  | 5.30  | 112.44      | 108.20   |
| 54  | BA    | 1678 | A    | O4'-C1'-N9  | 5.30  | 112.44      | 108.20   |
| 54  | BA    | 2101 | A    | C5-C6-N1    | 5.30  | 120.35      | 117.70   |
| 54  | BA    | 2280 | G    | O4'-C1'-N9  | 5.30  | 112.44      | 108.20   |
| 55  | BB    | 79   | G    | C8-N9-C4    | -5.30 | 104.28      | 106.40   |
| 21  | AA    | 526  | C    | N3-C4-C5    | 5.29  | 124.02      | 121.90   |
| 21  | AA    | 1182 | G    | C5-C6-N1    | 5.29  | 114.15      | 111.50   |
| 54  | BA    | 337  | C    | N3-C4-N4    | -5.29 | 114.29      | 118.00   |
| 54  | BA    | 704  | G    | N7-C8-N9    | 5.29  | 115.75      | 113.10   |
| 54  | BA    | 1702 | G    | C5-C6-N1    | 5.29  | 114.15      | 111.50   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|-------------|-------|------------------------|---------------------|
| 54  | BA    | 2000 | C    | N1-C2-O2    | 5.29  | 122.08                 | 118.90              |
| 21  | AA    | 545  | C    | O4'-C1'-N1  | 5.29  | 112.43                 | 108.20              |
| 54  | BA    | 184  | C    | N3-C4-C5    | 5.29  | 124.02                 | 121.90              |
| 54  | BA    | 442  | G    | N7-C8-N9    | 5.29  | 115.75                 | 113.10              |
| 54  | BA    | 1154 | G    | C8-N9-C4    | -5.29 | 104.28                 | 106.40              |
| 54  | BA    | 2794 | C    | N1-C2-O2    | 5.29  | 122.08                 | 118.90              |
| 21  | AA    | 13   | U    | N1-C2-N3    | 5.29  | 118.08                 | 114.90              |
| 21  | AA    | 426  | U    | C5-C6-N1    | -5.29 | 120.06                 | 122.70              |
| 21  | AA    | 478  | A    | C4-C5-C6    | -5.29 | 114.36                 | 117.00              |
| 21  | AA    | 744  | C    | N1-C2-O2    | 5.29  | 122.08                 | 118.90              |
| 21  | AA    | 1432 | G    | N9-C4-C5    | 5.29  | 107.52                 | 105.40              |
| 54  | BA    | 16   | C    | N1-C2-O2    | 5.29  | 122.08                 | 118.90              |
| 54  | BA    | 48   | G    | N1-C6-O6    | -5.29 | 116.73                 | 119.90              |
| 54  | BA    | 1092 | C    | N3-C2-O2    | -5.29 | 118.20                 | 121.90              |
| 54  | BA    | 1720 | U    | O4'-C1'-N1  | 5.29  | 112.43                 | 108.20              |
| 54  | BA    | 1874 | C    | N1-C2-O2    | 5.29  | 122.07                 | 118.90              |
| 54  | BA    | 1976 | U    | C5-C6-N1    | -5.29 | 120.05                 | 122.70              |
| 54  | BA    | 2788 | C    | C4'-C3'-C2' | -5.29 | 97.31                  | 102.60              |
| 21  | AA    | 51   | A    | C4-C5-C6    | -5.29 | 114.36                 | 117.00              |
| 54  | BA    | 621  | A    | C5-C6-N1    | 5.29  | 120.34                 | 117.70              |
| 21  | AA    | 383  | A    | C6-C5-N7    | 5.29  | 136.00                 | 132.30              |
| 21  | AA    | 1363 | A    | O4'-C1'-N9  | 5.29  | 112.43                 | 108.20              |
| 21  | AA    | 1504 | G    | N1-C6-O6    | -5.29 | 116.73                 | 119.90              |
| 24  | A3    | 54   | G    | N1-C6-O6    | -5.29 | 116.73                 | 119.90              |
| 54  | BA    | 713  | G    | N3-C2-N2    | -5.29 | 116.20                 | 119.90              |
| 54  | BA    | 975  | A    | C5-C6-N6    | 5.29  | 127.93                 | 123.70              |
| 54  | BA    | 2112 | G    | N9-C4-C5    | 5.29  | 107.52                 | 105.40              |
| 21  | AA    | 852  | G    | C8-N9-C4    | -5.29 | 104.28                 | 106.40              |
| 54  | BA    | 451  | U    | N3-C2-O2    | -5.29 | 118.50                 | 122.20              |
| 21  | AA    | 22   | G    | N3-C4-C5    | -5.29 | 125.96                 | 128.60              |
| 21  | AA    | 234  | C    | N3-C2-O2    | -5.29 | 118.20                 | 121.90              |
| 21  | AA    | 576  | C    | O4'-C1'-N1  | 5.29  | 112.43                 | 108.20              |
| 21  | AA    | 1516 | G    | O4'-C4'-C3' | 5.29  | 110.33                 | 106.10              |
| 24  | A3    | 7    | G    | N3-C4-C5    | -5.29 | 125.96                 | 128.60              |
| 54  | BA    | 160  | A    | C5'-C4'-O4' | 5.29  | 115.44                 | 109.10              |
| 54  | BA    | 984  | A    | C6-C5-N7    | 5.29  | 136.00                 | 132.30              |
| 54  | BA    | 1084 | A    | C6-C5-N7    | 5.29  | 136.00                 | 132.30              |
| 54  | BA    | 1115 | G    | C5-C6-N1    | 5.29  | 114.14                 | 111.50              |
| 54  | BA    | 2008 | C    | N1-C2-O2    | 5.29  | 122.07                 | 118.90              |
| 54  | BA    | 2019 | A    | N1-C6-N6    | -5.29 | 115.43                 | 118.60              |
| 54  | BA    | 2226 | C    | C2-N3-C4    | -5.29 | 117.26                 | 119.90              |
| 54  | BA    | 2356 | U    | O4'-C1'-N1  | 5.29  | 112.43                 | 108.20              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|-------------|-------|------------------------|---------------------|
| 21  | AA    | 5    | U    | C1'-O4'-C4' | -5.28 | 105.67                 | 109.90              |
| 21  | AA    | 524  | G    | C5-C6-N1    | 5.28  | 114.14                 | 111.50              |
| 22  | A1    | 2    | G    | N1-C6-O6    | -5.28 | 116.73                 | 119.90              |
| 22  | A1    | 47   | U    | C3'-C2'-C1' | 5.28  | 105.73                 | 101.50              |
| 54  | BA    | 1356 | G    | C8-N9-C4    | -5.28 | 104.29                 | 106.40              |
| 54  | BA    | 1549 | A    | C6-C5-N7    | 5.28  | 136.00                 | 132.30              |
| 54  | BA    | 1947 | C    | N1-C2-O2    | 5.28  | 122.07                 | 118.90              |
| 54  | BA    | 2310 | C    | N1-C2-O2    | 5.28  | 122.07                 | 118.90              |
| 21  | AA    | 1383 | C    | N3-C2-O2    | -5.28 | 118.20                 | 121.90              |
| 54  | BA    | 578  | G    | C5-C6-N1    | 5.28  | 114.14                 | 111.50              |
| 54  | BA    | 907  | G    | N1-C6-O6    | -5.28 | 116.73                 | 119.90              |
| 54  | BA    | 1585 | C    | N1-C2-O2    | 5.28  | 122.07                 | 118.90              |
| 54  | BA    | 1636 | U    | C4-C5-C6    | 5.28  | 122.87                 | 119.70              |
| 21  | AA    | 602  | A    | C5-C6-N1    | 5.28  | 120.34                 | 117.70              |
| 21  | AA    | 614  | C    | N3-C4-C5    | 5.28  | 124.01                 | 121.90              |
| 21  | AA    | 1173 | U    | N3-C2-O2    | -5.28 | 118.50                 | 122.20              |
| 21  | AA    | 1452 | C    | N3-C4-C5    | 5.28  | 124.01                 | 121.90              |
| 21  | AA    | 1487 | G    | N7-C8-N9    | 5.28  | 115.74                 | 113.10              |
| 54  | BA    | 1128 | G    | C1'-O4'-C4' | -5.28 | 105.68                 | 109.90              |
| 54  | BA    | 1290 | C    | C4'-C3'-C2' | -5.28 | 97.32                  | 102.60              |
| 54  | BA    | 1963 | U    | N3-C2-O2    | -5.28 | 118.50                 | 122.20              |
| 54  | BA    | 2267 | A    | C4-C5-C6    | -5.28 | 114.36                 | 117.00              |
| 21  | AA    | 1152 | A    | C6-C5-N7    | 5.28  | 136.00                 | 132.30              |
| 54  | BA    | 2427 | C    | N1-C2-O2    | 5.28  | 122.07                 | 118.90              |
| 54  | BA    | 2793 | C    | O4'-C1'-N1  | 5.28  | 112.42                 | 108.20              |
| 21  | AA    | 275  | G    | N3-C4-C5    | -5.28 | 125.96                 | 128.60              |
| 21  | AA    | 639  | G    | C5-C6-N1    | 5.28  | 114.14                 | 111.50              |
| 21  | AA    | 892  | A    | C6-C5-N7    | 5.28  | 136.00                 | 132.30              |
| 22  | A1    | 33   | U    | N3-C2-O2    | -5.28 | 118.50                 | 122.20              |
| 54  | BA    | 193  | U    | O4'-C1'-N1  | 5.28  | 112.42                 | 108.20              |
| 54  | BA    | 362  | A    | C5'-C4'-C3' | -5.28 | 107.55                 | 116.00              |
| 54  | BA    | 677  | A    | C5-C6-N1    | 5.28  | 120.34                 | 117.70              |
| 54  | BA    | 910  | A    | C4-C5-C6    | -5.28 | 114.36                 | 117.00              |
| 54  | BA    | 1221 | C    | O4'-C1'-N1  | 5.28  | 112.42                 | 108.20              |
| 54  | BA    | 1633 | G    | O4'-C1'-N9  | 5.28  | 112.42                 | 108.20              |
| 54  | BA    | 1723 | G    | N1-C6-O6    | -5.28 | 116.73                 | 119.90              |
| 54  | BA    | 2363 | G    | N3-C4-N9    | 5.28  | 129.17                 | 126.00              |
| 54  | BA    | 2709 | G    | C5-C6-N1    | 5.28  | 114.14                 | 111.50              |
| 55  | BB    | 106  | G    | N3-C4-C5    | -5.28 | 125.96                 | 128.60              |
| 54  | BA    | 99   | U    | N3-C2-O2    | -5.28 | 118.51                 | 122.20              |
| 54  | BA    | 309  | A    | C4-C5-C6    | -5.28 | 114.36                 | 117.00              |
| 54  | BA    | 574  | A    | C4-C5-C6    | -5.28 | 114.36                 | 117.00              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|-------------|-------|------------------------|---------------------|
| 54  | BA    | 1347 | A    | C4-C5-C6    | -5.28 | 114.36                 | 117.00              |
| 54  | BA    | 1433 | A    | N1-C6-N6    | -5.28 | 115.44                 | 118.60              |
| 54  | BA    | 2044 | C    | O4'-C1'-N1  | 5.28  | 112.42                 | 108.20              |
| 54  | BA    | 2200 | C    | N3-C2-O2    | -5.28 | 118.21                 | 121.90              |
| 54  | BA    | 2236 | U    | N3-C2-O2    | -5.28 | 118.51                 | 122.20              |
| 54  | BA    | 229  | C    | N1-C2-O2    | 5.27  | 122.06                 | 118.90              |
| 54  | BA    | 521  | U    | C5-C6-N1    | -5.27 | 120.06                 | 122.70              |
| 54  | BA    | 1418 | G    | N3-C4-C5    | -5.27 | 125.96                 | 128.60              |
| 54  | BA    | 1815 | A    | C5-C6-N1    | 5.27  | 120.34                 | 117.70              |
| 54  | BA    | 2618 | G    | N3-C4-C5    | -5.27 | 125.96                 | 128.60              |
| 21  | AA    | 821  | G    | N3-C4-C5    | -5.27 | 125.96                 | 128.60              |
| 21  | AA    | 1045 | C    | N1-C2-O2    | 5.27  | 122.06                 | 118.90              |
| 54  | BA    | 2442 | C    | O4'-C1'-N1  | 5.27  | 112.42                 | 108.20              |
| 54  | BA    | 2556 | C    | N3-C4-N4    | -5.27 | 114.31                 | 118.00              |
| 54  | BA    | 1272 | A    | C4-C5-C6    | -5.27 | 114.36                 | 117.00              |
| 54  | BA    | 2726 | A    | O4'-C1'-C2' | -5.27 | 100.53                 | 105.80              |
| 54  | BA    | 2804 | U    | O4'-C1'-N1  | 5.27  | 112.42                 | 108.20              |
| 21  | AA    | 1066 | C    | N3-C2-O2    | -5.27 | 118.21                 | 121.90              |
| 21  | AA    | 1216 | A    | C4'-C3'-C2' | -5.27 | 97.33                  | 102.60              |
| 21  | AA    | 1500 | A    | C5-C6-N1    | 5.27  | 120.33                 | 117.70              |
| 54  | BA    | 113  | U    | C5-C6-N1    | -5.27 | 120.06                 | 122.70              |
| 54  | BA    | 439  | A    | C2-N3-C4    | 5.27  | 113.23                 | 110.60              |
| 54  | BA    | 505  | A    | C4-C5-C6    | -5.27 | 114.36                 | 117.00              |
| 54  | BA    | 1086 | A    | C4-C5-C6    | -5.27 | 114.37                 | 117.00              |
| 54  | BA    | 2300 | C    | N1-C2-O2    | 5.27  | 122.06                 | 118.90              |
| 56  | B5    | 60   | ARG  | NE-CZ-NH1   | 5.27  | 122.94                 | 120.30              |
| 21  | AA    | 57   | G    | C5-C6-N1    | 5.27  | 114.13                 | 111.50              |
| 21  | AA    | 331  | G    | N7-C8-N9    | 5.27  | 115.73                 | 113.10              |
| 21  | AA    | 658  | C    | N3-C4-C5    | 5.27  | 124.01                 | 121.90              |
| 21  | AA    | 1232 | U    | N1-C2-N3    | 5.27  | 118.06                 | 114.90              |
| 24  | A3    | 48   | U    | C5'-C4'-C3' | -5.27 | 107.57                 | 116.00              |
| 39  | BQ    | 91   | ARG  | NH1-CZ-NH2  | -5.27 | 113.61                 | 119.40              |
| 54  | BA    | 35   | G    | C5-C6-N1    | 5.27  | 114.13                 | 111.50              |
| 54  | BA    | 234  | U    | O4'-C1'-N1  | 5.27  | 112.41                 | 108.20              |
| 54  | BA    | 243  | U    | O4'-C1'-N1  | 5.27  | 112.41                 | 108.20              |
| 54  | BA    | 437  | U    | N1-C2-N3    | 5.27  | 118.06                 | 114.90              |
| 54  | BA    | 817  | C    | N1-C2-O2    | 5.27  | 122.06                 | 118.90              |
| 54  | BA    | 1167 | C    | O4'-C1'-N1  | 5.27  | 112.41                 | 108.20              |
| 54  | BA    | 1210 | G    | C8-N9-C4    | -5.27 | 104.29                 | 106.40              |
| 54  | BA    | 2276 | G    | N1-C6-O6    | -5.27 | 116.74                 | 119.90              |
| 54  | BA    | 139  | U    | N1-C2-N3    | 5.27  | 118.06                 | 114.90              |
| 54  | BA    | 440  | C    | N3-C2-O2    | -5.27 | 118.21                 | 121.90              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 54  | BA    | 575  | A    | C5-C6-N1   | 5.27  | 120.33      | 117.70   |
| 54  | BA    | 583  | G    | N1-C6-O6   | -5.27 | 116.74      | 119.90   |
| 54  | BA    | 2038 | G    | C8-N9-C4   | -5.27 | 104.29      | 106.40   |
| 54  | BA    | 2038 | G    | N3-C4-C5   | -5.27 | 125.97      | 128.60   |
| 21  | AA    | 82   | G    | N1-C6-O6   | -5.26 | 116.74      | 119.90   |
| 21  | AA    | 111  | G    | N3-C4-C5   | -5.26 | 125.97      | 128.60   |
| 21  | AA    | 1038 | C    | N1-C2-O2   | 5.26  | 122.06      | 118.90   |
| 21  | AA    | 1056 | U    | N3-C2-O2   | -5.26 | 118.52      | 122.20   |
| 21  | AA    | 1070 | U    | C5-C6-N1   | -5.26 | 120.07      | 122.70   |
| 24  | A3    | 77   | A    | C4-C5-C6   | -5.26 | 114.37      | 117.00   |
| 36  | BN    | 46   | ARG  | NE-CZ-NH2  | -5.26 | 117.67      | 120.30   |
| 54  | BA    | 1831 | G    | N3-C4-C5   | -5.26 | 125.97      | 128.60   |
| 54  | BA    | 2619 | C    | N1-C2-O2   | 5.26  | 122.06      | 118.90   |
| 54  | BA    | 2709 | G    | N3-C4-C5   | -5.26 | 125.97      | 128.60   |
| 54  | BA    | 2767 | C    | O4'-C1'-N1 | 5.26  | 112.41      | 108.20   |
| 55  | BB    | 47   | C    | N3-C2-O2   | -5.26 | 118.22      | 121.90   |
| 10  | AK    | 35   | ASP  | CB-CG-OD2  | 5.26  | 123.04      | 118.30   |
| 21  | AA    | 147  | G    | O4'-C1'-N9 | 5.26  | 112.41      | 108.20   |
| 54  | BA    | 67   | U    | N1-C2-N3   | 5.26  | 118.06      | 114.90   |
| 55  | BB    | 98   | G    | N7-C8-N9   | 5.26  | 115.73      | 113.10   |
| 55  | BB    | 105  | G    | N9-C4-C5   | 5.26  | 107.50      | 105.40   |
| 21  | AA    | 1071 | C    | C2-N3-C4   | -5.26 | 117.27      | 119.90   |
| 22  | A1    | 71   | C    | N1-C2-O2   | 5.26  | 122.06      | 118.90   |
| 24  | A3    | 3    | C    | N1-C2-O2   | 5.26  | 122.06      | 118.90   |
| 54  | BA    | 87   | U    | N3-C2-O2   | -5.26 | 118.52      | 122.20   |
| 54  | BA    | 89   | A    | C4-C5-C6   | -5.26 | 114.37      | 117.00   |
| 54  | BA    | 652  | U    | N3-C2-O2   | -5.26 | 118.52      | 122.20   |
| 54  | BA    | 1761 | C    | C2-N3-C4   | -5.26 | 117.27      | 119.90   |
| 17  | AR    | 56   | ARG  | NH1-CZ-NH2 | -5.26 | 113.61      | 119.40   |
| 54  | BA    | 125  | A    | C2-N3-C4   | 5.26  | 113.23      | 110.60   |
| 54  | BA    | 607  | U    | C5-C6-N1   | -5.26 | 120.07      | 122.70   |
| 54  | BA    | 745  | G    | N1-C6-O6   | -5.26 | 116.74      | 119.90   |
| 54  | BA    | 784  | G    | N3-C4-C5   | -5.26 | 125.97      | 128.60   |
| 54  | BA    | 2239 | G    | C8-N9-C4   | -5.26 | 104.30      | 106.40   |
| 54  | BA    | 2707 | U    | N1-C2-N3   | 5.26  | 118.06      | 114.90   |
| 55  | BB    | 4    | C    | N1-C2-O2   | 5.26  | 122.06      | 118.90   |
| 21  | AA    | 1208 | C    | O4'-C1'-N1 | 5.26  | 112.41      | 108.20   |
| 54  | BA    | 188  | G    | C5-C6-N1   | 5.26  | 114.13      | 111.50   |
| 21  | AA    | 38   | G    | C5-C6-N1   | 5.26  | 114.13      | 111.50   |
| 21  | AA    | 348  | G    | N3-C4-C5   | -5.26 | 125.97      | 128.60   |
| 21  | AA    | 795  | C    | N1-C2-O2   | 5.26  | 122.05      | 118.90   |
| 21  | AA    | 1389 | C    | N3-C2-O2   | -5.26 | 118.22      | 121.90   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|-------------|-------|------------------------|---------------------|
| 21  | AA    | 1405 | G    | C4-C5-N7    | -5.26 | 108.70                 | 110.80              |
| 54  | BA    | 396  | G    | C5-C6-N1    | 5.26  | 114.13                 | 111.50              |
| 54  | BA    | 536  | G    | C8-N9-C4    | -5.26 | 104.30                 | 106.40              |
| 54  | BA    | 1389 | G    | O4'-C1'-N9  | 5.26  | 112.41                 | 108.20              |
| 54  | BA    | 1848 | A    | C4-C5-C6    | -5.26 | 114.37                 | 117.00              |
| 54  | BA    | 2334 | U    | O4'-C1'-N1  | 5.26  | 112.41                 | 108.20              |
| 54  | BA    | 2588 | G    | N3-C2-N2    | -5.26 | 116.22                 | 119.90              |
| 54  | BA    | 2683 | C    | N1-C2-O2    | 5.26  | 122.05                 | 118.90              |
| 21  | AA    | 1427 | C    | C6-N1-C2    | -5.25 | 118.20                 | 120.30              |
| 24  | A3    | 49   | C    | N1-C2-O2    | 5.25  | 122.05                 | 118.90              |
| 54  | BA    | 2049 | G    | C5-C6-N1    | 5.25  | 114.13                 | 111.50              |
| 54  | BA    | 2672 | U    | O4'-C1'-N1  | 5.25  | 112.40                 | 108.20              |
| 21  | AA    | 1367 | C    | C2-N3-C4    | -5.25 | 117.27                 | 119.90              |
| 25  | BC    | 100  | ARG  | NE-CZ-NH1   | 5.25  | 122.93                 | 120.30              |
| 54  | BA    | 209  | C    | N1-C2-O2    | 5.25  | 122.05                 | 118.90              |
| 54  | BA    | 371  | A    | C4-C5-C6    | -5.25 | 114.37                 | 117.00              |
| 54  | BA    | 431  | U    | N1-C2-N3    | 5.25  | 118.05                 | 114.90              |
| 54  | BA    | 1045 | C    | N3-C4-C5    | 5.25  | 124.00                 | 121.90              |
| 54  | BA    | 2425 | A    | C5-C6-N1    | 5.25  | 120.33                 | 117.70              |
| 21  | AA    | 8    | A    | O4'-C1'-N9  | 5.25  | 112.40                 | 108.20              |
| 21  | AA    | 993  | G    | O4'-C1'-N9  | 5.25  | 112.40                 | 108.20              |
| 21  | AA    | 1066 | C    | N1-C2-O2    | 5.25  | 122.05                 | 118.90              |
| 24  | A3    | 29   | C    | N1-C2-O2    | 5.25  | 122.05                 | 118.90              |
| 54  | BA    | 113  | U    | O4'-C1'-N1  | 5.25  | 112.40                 | 108.20              |
| 54  | BA    | 363  | G    | N1-C6-O6    | -5.25 | 116.75                 | 119.90              |
| 54  | BA    | 867  | C    | N3-C2-O2    | -5.25 | 118.22                 | 121.90              |
| 54  | BA    | 1171 | G    | O4'-C1'-N9  | 5.25  | 112.40                 | 108.20              |
| 54  | BA    | 2554 | U    | C5'-C4'-C3' | -5.25 | 107.60                 | 116.00              |
| 8   | AI    | 32   | ARG  | NE-CZ-NH1   | 5.25  | 122.92                 | 120.30              |
| 21  | AA    | 305  | G    | C4-C5-N7    | -5.25 | 108.70                 | 110.80              |
| 21  | AA    | 227  | G    | N1-C6-O6    | -5.25 | 116.75                 | 119.90              |
| 21  | AA    | 349  | A    | O4'-C1'-N9  | 5.25  | 112.40                 | 108.20              |
| 21  | AA    | 359  | G    | N1-C6-O6    | -5.25 | 116.75                 | 119.90              |
| 21  | AA    | 509  | A    | C2-N3-C4    | 5.25  | 113.22                 | 110.60              |
| 54  | BA    | 877  | A    | C4-C5-C6    | -5.25 | 114.38                 | 117.00              |
| 54  | BA    | 1449 | G    | C4'-C3'-C2' | -5.25 | 97.35                  | 102.60              |
| 54  | BA    | 1582 | C    | N1-C2-O2    | 5.25  | 122.05                 | 118.90              |
| 54  | BA    | 1729 | U    | C4-C5-C6    | 5.25  | 122.85                 | 119.70              |
| 54  | BA    | 1972 | G    | N7-C8-N9    | 5.25  | 115.72                 | 113.10              |
| 21  | AA    | 292  | G    | N7-C8-N9    | 5.25  | 115.72                 | 113.10              |
| 21  | AA    | 517  | G    | O4'-C1'-N9  | 5.25  | 112.40                 | 108.20              |
| 21  | AA    | 1406 | U    | O4'-C1'-N1  | 5.25  | 112.40                 | 108.20              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|-------------|-------|------------------------|---------------------|
| 24  | A3    | 68   | C    | C1'-O4'-C4' | -5.25 | 105.70                 | 109.90              |
| 54  | BA    | 2041 | U    | O4'-C1'-N1  | 5.25  | 112.40                 | 108.20              |
| 54  | BA    | 2282 | G    | N9-C4-C5    | 5.25  | 107.50                 | 105.40              |
| 21  | AA    | 883  | C    | N3-C2-O2    | -5.25 | 118.23                 | 121.90              |
| 21  | AA    | 1519 | A    | C6-C5-N7    | 5.25  | 135.97                 | 132.30              |
| 54  | BA    | 1063 | G    | O4'-C1'-N9  | 5.25  | 112.40                 | 108.20              |
| 54  | BA    | 1323 | C    | N1-C2-O2    | 5.25  | 122.05                 | 118.90              |
| 54  | BA    | 1481 | U    | N3-C2-O2    | -5.25 | 118.53                 | 122.20              |
| 21  | AA    | 151  | A    | C5-C6-N1    | 5.24  | 120.32                 | 117.70              |
| 21  | AA    | 792  | A    | C1'-O4'-C4' | -5.24 | 105.71                 | 109.90              |
| 21  | AA    | 1346 | A    | C6-C5-N7    | 5.24  | 135.97                 | 132.30              |
| 21  | AA    | 1524 | C    | N1-C2-O2    | 5.24  | 122.05                 | 118.90              |
| 24  | A3    | 64   | G    | C5-N7-C8    | -5.24 | 101.68                 | 104.30              |
| 54  | BA    | 693  | A    | C6-C5-N7    | 5.24  | 135.97                 | 132.30              |
| 54  | BA    | 2699 | C    | C2-N3-C4    | -5.24 | 117.28                 | 119.90              |
| 54  | BA    | 2820 | A    | N1-C6-N6    | -5.24 | 115.45                 | 118.60              |
| 21  | AA    | 6    | G    | N7-C8-N9    | 5.24  | 115.72                 | 113.10              |
| 21  | AA    | 741  | G    | N7-C8-N9    | 5.24  | 115.72                 | 113.10              |
| 21  | AA    | 793  | U    | N3-C2-O2    | -5.24 | 118.53                 | 122.20              |
| 20  | AU    | 16   | ARG  | NE-CZ-NH1   | 5.24  | 122.92                 | 120.30              |
| 21  | AA    | 222  | C    | N1-C2-O2    | 5.24  | 122.04                 | 118.90              |
| 21  | AA    | 304  | U    | C5-C6-N1    | -5.24 | 120.08                 | 122.70              |
| 21  | AA    | 643  | C    | N3-C2-O2    | -5.24 | 118.23                 | 121.90              |
| 21  | AA    | 709  | U    | N3-C2-O2    | -5.24 | 118.53                 | 122.20              |
| 21  | AA    | 1243 | C    | C6-N1-C2    | -5.24 | 118.20                 | 120.30              |
| 21  | AA    | 1472 | U    | C4-C5-C6    | 5.24  | 122.84                 | 119.70              |
| 23  | A2    | 93   | U    | N3-C2-O2    | -5.24 | 118.53                 | 122.20              |
| 54  | BA    | 973  | A    | C4-C5-C6    | -5.24 | 114.38                 | 117.00              |
| 54  | BA    | 1346 | G    | C4'-C3'-C2' | -5.24 | 97.36                  | 102.60              |
| 54  | BA    | 1555 | G    | C5-C6-N1    | 5.24  | 114.12                 | 111.50              |
| 54  | BA    | 1611 | C    | N1-C2-O2    | 5.24  | 122.04                 | 118.90              |
| 54  | BA    | 2080 | A    | C2-N3-C4    | 5.24  | 113.22                 | 110.60              |
| 54  | BA    | 2164 | C    | N1-C2-O2    | 5.24  | 122.04                 | 118.90              |
| 55  | BB    | 56   | G    | O4'-C4'-C3' | 5.24  | 110.29                 | 106.10              |
| 21  | AA    | 1085 | U    | N3-C2-O2    | -5.24 | 118.53                 | 122.20              |
| 21  | AA    | 1108 | G    | C8-N9-C4    | -5.24 | 104.31                 | 106.40              |
| 21  | AA    | 1312 | G    | N3-C4-C5    | -5.24 | 125.98                 | 128.60              |
| 54  | BA    | 467  | G    | N9-C4-C5    | 5.24  | 107.50                 | 105.40              |
| 54  | BA    | 1094 | U    | O4'-C1'-N1  | 5.24  | 112.39                 | 108.20              |
| 54  | BA    | 1531 | C    | O4'-C1'-N1  | 5.24  | 112.39                 | 108.20              |
| 55  | BB    | 100  | G    | N7-C8-N9    | 5.24  | 115.72                 | 113.10              |
| 54  | BA    | 731  | C    | O4'-C1'-N1  | 5.24  | 112.39                 | 108.20              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|------------|-------|------------------------|---------------------|
| 54  | BA    | 1736 | U    | C5-C6-N1   | -5.24 | 120.08                 | 122.70              |
| 54  | BA    | 2042 | A    | C5-C6-N1   | 5.24  | 120.32                 | 117.70              |
| 21  | AA    | 1345 | U    | O4'-C1'-N1 | 5.24  | 112.39                 | 108.20              |
| 21  | AA    | 1503 | A    | C4-C5-C6   | -5.24 | 114.38                 | 117.00              |
| 54  | BA    | 1521 | G    | C5-C6-N1   | 5.24  | 114.12                 | 111.50              |
| 54  | BA    | 1925 | C    | N3-C4-C5   | 5.24  | 124.00                 | 121.90              |
| 10  | AK    | 121  | ARG  | NE-CZ-NH2  | 5.23  | 122.92                 | 120.30              |
| 21  | AA    | 73   | C    | N1-C2-O2   | 5.23  | 122.04                 | 118.90              |
| 54  | BA    | 792  | A    | C2-N3-C4   | 5.23  | 113.22                 | 110.60              |
| 54  | BA    | 1185 | G    | O4'-C1'-N9 | 5.23  | 112.39                 | 108.20              |
| 54  | BA    | 2140 | G    | O4'-C1'-N9 | 5.23  | 112.39                 | 108.20              |
| 54  | BA    | 2790 | U    | C5-C6-N1   | -5.23 | 120.08                 | 122.70              |
| 21  | AA    | 220  | G    | C8-N9-C4   | -5.23 | 104.31                 | 106.40              |
| 21  | AA    | 1203 | C    | N1-C2-O2   | 5.23  | 122.04                 | 118.90              |
| 54  | BA    | 201  | C    | N1-C2-O2   | 5.23  | 122.04                 | 118.90              |
| 54  | BA    | 268  | C    | N3-C2-O2   | -5.23 | 118.24                 | 121.90              |
| 54  | BA    | 836  | G    | N3-C2-N2   | -5.23 | 116.24                 | 119.90              |
| 54  | BA    | 969  | G    | C8-N9-C4   | -5.23 | 104.31                 | 106.40              |
| 54  | BA    | 991  | C    | C6-N1-C2   | -5.23 | 118.21                 | 120.30              |
| 54  | BA    | 1454 | C    | N3-C4-C5   | 5.23  | 123.99                 | 121.90              |
| 54  | BA    | 2759 | G    | C8-N9-C4   | -5.23 | 104.31                 | 106.40              |
| 21  | AA    | 191  | G    | N3-C4-C5   | -5.23 | 125.98                 | 128.60              |
| 21  | AA    | 216  | U    | N3-C2-O2   | -5.23 | 118.54                 | 122.20              |
| 21  | AA    | 382  | A    | C6-C5-N7   | 5.23  | 135.96                 | 132.30              |
| 54  | BA    | 147  | C    | N3-C2-O2   | -5.23 | 118.24                 | 121.90              |
| 54  | BA    | 1118 | C    | N1-C2-O2   | 5.23  | 122.04                 | 118.90              |
| 54  | BA    | 1462 | C    | N3-C2-O2   | -5.23 | 118.24                 | 121.90              |
| 54  | BA    | 2209 | G    | C5-C6-N1   | 5.23  | 114.11                 | 111.50              |
| 55  | BB    | 46   | A    | C6-C5-N7   | 5.23  | 135.96                 | 132.30              |
| 54  | BA    | 2330 | G    | O4'-C1'-N9 | 5.23  | 112.38                 | 108.20              |
| 21  | AA    | 509  | A    | C6-C5-N7   | 5.23  | 135.96                 | 132.30              |
| 21  | AA    | 682  | G    | C5-C6-N1   | 5.23  | 114.11                 | 111.50              |
| 21  | AA    | 885  | G    | C5-C6-N1   | 5.23  | 114.11                 | 111.50              |
| 21  | AA    | 1183 | U    | N3-C2-O2   | -5.23 | 118.54                 | 122.20              |
| 21  | AA    | 1355 | G    | N9-C4-C5   | 5.23  | 107.49                 | 105.40              |
| 54  | BA    | 358  | U    | N3-C2-O2   | -5.23 | 118.54                 | 122.20              |
| 54  | BA    | 1826 | G    | P-O3'-C3'  | 5.23  | 125.97                 | 119.70              |
| 54  | BA    | 2050 | C    | O4'-C1'-N1 | 5.23  | 112.38                 | 108.20              |
| 54  | BA    | 2154 | A    | O4'-C1'-N9 | 5.23  | 112.38                 | 108.20              |
| 54  | BA    | 2256 | G    | N7-C8-N9   | 5.23  | 115.71                 | 113.10              |
| 54  | BA    | 2839 | G    | N3-C4-C5   | -5.23 | 125.99                 | 128.60              |
| 55  | BB    | 76   | G    | O4'-C1'-N9 | 5.23  | 112.38                 | 108.20              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|-------------|-------|------------------------|---------------------|
| 21  | AA    | 1401 | G    | N3-C4-N9    | 5.23  | 129.14                 | 126.00              |
| 54  | BA    | 1556 | C    | N3-C2-O2    | -5.23 | 118.24                 | 121.90              |
| 54  | BA    | 2715 | C    | C6-N1-C2    | -5.23 | 118.21                 | 120.30              |
| 54  | BA    | 2893 | A    | C4-C5-C6    | -5.23 | 114.39                 | 117.00              |
| 55  | BB    | 114  | C    | N3-C4-C5    | 5.23  | 123.99                 | 121.90              |
| 21  | AA    | 83   | C    | O4'-C1'-N1  | 5.22  | 112.38                 | 108.20              |
| 21  | AA    | 1355 | G    | N3-C4-C5    | -5.22 | 125.99                 | 128.60              |
| 54  | BA    | 104  | A    | C6-C5-N7    | 5.22  | 135.96                 | 132.30              |
| 54  | BA    | 208  | C    | C2-N3-C4    | -5.22 | 117.29                 | 119.90              |
| 54  | BA    | 607  | U    | N3-C2-O2    | -5.22 | 118.54                 | 122.20              |
| 54  | BA    | 617  | G    | N3-C4-C5    | -5.22 | 125.99                 | 128.60              |
| 54  | BA    | 968  | C    | N3-C2-O2    | -5.22 | 118.24                 | 121.90              |
| 54  | BA    | 998  | C    | N1-C2-O2    | 5.22  | 122.03                 | 118.90              |
| 54  | BA    | 1345 | C    | N1-C2-O2    | 5.22  | 122.03                 | 118.90              |
| 54  | BA    | 1707 | G    | C5-C6-N1    | 5.22  | 114.11                 | 111.50              |
| 54  | BA    | 1746 | A    | C6-C5-N7    | 5.22  | 135.96                 | 132.30              |
| 21  | AA    | 634  | C    | N1-C2-O2    | 5.22  | 122.03                 | 118.90              |
| 21  | AA    | 686  | U    | C4-C5-C6    | 5.22  | 122.83                 | 119.70              |
| 21  | AA    | 820  | U    | N1-C2-N3    | 5.22  | 118.03                 | 114.90              |
| 21  | AA    | 1192 | C    | N3-C2-O2    | -5.22 | 118.24                 | 121.90              |
| 21  | AA    | 1269 | A    | C4-C5-C6    | -5.22 | 114.39                 | 117.00              |
| 22  | A1    | 59   | U    | C3'-C2'-C1' | 5.22  | 105.68                 | 101.50              |
| 54  | BA    | 608  | A    | C2-N3-C4    | 5.22  | 113.21                 | 110.60              |
| 54  | BA    | 1180 | U    | O4'-C1'-N1  | 5.22  | 112.38                 | 108.20              |
| 54  | BA    | 2527 | C    | N1-C2-O2    | 5.22  | 122.03                 | 118.90              |
| 54  | BA    | 2620 | C    | O4'-C1'-N1  | 5.22  | 112.38                 | 108.20              |
| 54  | BA    | 2886 | A    | C8-N9-C4    | -5.22 | 103.71                 | 105.80              |
| 21  | AA    | 444  | G    | N3-C4-C5    | -5.22 | 125.99                 | 128.60              |
| 21  | AA    | 661  | G    | N3-C2-N2    | -5.22 | 116.25                 | 119.90              |
| 54  | BA    | 10   | A    | O4'-C1'-N9  | 5.22  | 112.38                 | 108.20              |
| 54  | BA    | 509  | C    | N1-C2-O2    | 5.22  | 122.03                 | 118.90              |
| 54  | BA    | 1194 | A    | N1-C6-N6    | -5.22 | 115.47                 | 118.60              |
| 54  | BA    | 2201 | G    | N9-C4-C5    | 5.22  | 107.49                 | 105.40              |
| 54  | BA    | 659  | G    | N1-C6-O6    | -5.22 | 116.77                 | 119.90              |
| 54  | BA    | 772  | C    | O4'-C1'-N1  | 5.22  | 112.38                 | 108.20              |
| 54  | BA    | 810  | U    | O4'-C1'-N1  | 5.22  | 112.38                 | 108.20              |
| 54  | BA    | 1288 | G    | N3-C4-C5    | -5.22 | 125.99                 | 128.60              |
| 54  | BA    | 2059 | A    | C5-C6-N1    | 5.22  | 120.31                 | 117.70              |
| 54  | BA    | 2337 | G    | N1-C6-O6    | -5.22 | 116.77                 | 119.90              |
| 54  | BA    | 2642 | G    | C4'-C3'-C2' | -5.22 | 97.38                  | 102.60              |
| 54  | BA    | 2807 | U    | N1-C2-N3    | 5.22  | 118.03                 | 114.90              |
| 13  | AN    | 65   | ARG  | NE-CZ-NH1   | 5.22  | 122.91                 | 120.30              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|-------------|-------|------------------------|---------------------|
| 21  | AA    | 886  | G    | O4'-C1'-N9  | 5.22  | 112.37                 | 108.20              |
| 21  | AA    | 1391 | U    | N3-C2-O2    | -5.22 | 118.55                 | 122.20              |
| 54  | BA    | 607  | U    | C5'-C4'-O4' | 5.22  | 115.36                 | 109.10              |
| 54  | BA    | 2071 | A    | C4-C5-C6    | -5.22 | 114.39                 | 117.00              |
| 54  | BA    | 2175 | C    | O4'-C1'-N1  | 5.22  | 112.37                 | 108.20              |
| 55  | BB    | 35   | C    | N1-C2-O2    | 5.22  | 122.03                 | 118.90              |
| 21  | AA    | 419  | C    | C1'-O4'-C4' | -5.22 | 105.73                 | 109.90              |
| 21  | AA    | 595  | A    | C3'-C2'-C1' | 5.22  | 105.67                 | 101.50              |
| 21  | AA    | 722  | G    | O4'-C1'-N9  | 5.22  | 112.37                 | 108.20              |
| 21  | AA    | 1298 | U    | O4'-C1'-N1  | 5.22  | 112.37                 | 108.20              |
| 21  | AA    | 1375 | A    | C6-C5-N7    | 5.22  | 135.95                 | 132.30              |
| 54  | BA    | 4    | U    | N3-C2-O2    | -5.22 | 118.55                 | 122.20              |
| 54  | BA    | 64   | A    | C6-C5-N7    | 5.22  | 135.95                 | 132.30              |
| 54  | BA    | 287  | G    | C5-C6-N1    | 5.22  | 114.11                 | 111.50              |
| 54  | BA    | 637  | A    | C5-C6-N1    | 5.22  | 120.31                 | 117.70              |
| 54  | BA    | 823  | C    | N3-C2-O2    | -5.22 | 118.25                 | 121.90              |
| 54  | BA    | 891  | G    | C8-N9-C4    | -5.22 | 104.31                 | 106.40              |
| 54  | BA    | 2301 | C    | N1-C2-O2    | 5.22  | 122.03                 | 118.90              |
| 54  | BA    | 2675 | A    | C4-C5-C6    | -5.22 | 114.39                 | 117.00              |
| 54  | BA    | 2818 | U    | N3-C2-O2    | -5.22 | 118.55                 | 122.20              |
| 21  | AA    | 746  | A    | C5-C6-N1    | 5.21  | 120.31                 | 117.70              |
| 42  | BT    | 3    | ARG  | NE-CZ-NH2   | -5.21 | 117.69                 | 120.30              |
| 54  | BA    | 658  | U    | N3-C2-O2    | -5.21 | 118.55                 | 122.20              |
| 54  | BA    | 883  | G    | C5-C6-N1    | 5.21  | 114.11                 | 111.50              |
| 54  | BA    | 1777 | U    | N3-C2-O2    | -5.21 | 118.55                 | 122.20              |
| 21  | AA    | 243  | A    | C4-C5-C6    | -5.21 | 114.39                 | 117.00              |
| 54  | BA    | 813  | U    | O4'-C1'-N1  | 5.21  | 112.37                 | 108.20              |
| 54  | BA    | 1056 | G    | C5-C6-N1    | 5.21  | 114.11                 | 111.50              |
| 54  | BA    | 1087 | G    | N1-C6-O6    | -5.21 | 116.77                 | 119.90              |
| 54  | BA    | 1237 | A    | C4-C5-C6    | -5.21 | 114.39                 | 117.00              |
| 54  | BA    | 2426 | A    | C6-C5-N7    | 5.21  | 135.95                 | 132.30              |
| 21  | AA    | 420  | U    | N1-C2-N3    | 5.21  | 118.03                 | 114.90              |
| 21  | AA    | 474  | G    | C5-C6-N1    | 5.21  | 114.11                 | 111.50              |
| 54  | BA    | 247  | G    | N1-C6-O6    | -5.21 | 116.77                 | 119.90              |
| 54  | BA    | 452  | G    | C5'-C4'-O4' | 5.21  | 115.35                 | 109.10              |
| 54  | BA    | 1364 | G    | C5-C6-N1    | 5.21  | 114.11                 | 111.50              |
| 54  | BA    | 1879 | C    | N1-C2-O2    | 5.21  | 122.03                 | 118.90              |
| 54  | BA    | 2563 | U    | N1-C2-N3    | 5.21  | 118.03                 | 114.90              |
| 55  | BB    | 85   | G    | N7-C8-N9    | 5.21  | 115.70                 | 113.10              |
| 21  | AA    | 33   | A    | C4-C5-C6    | -5.21 | 114.39                 | 117.00              |
| 54  | BA    | 127  | A    | C4-C5-C6    | -5.21 | 114.39                 | 117.00              |
| 54  | BA    | 1002 | G    | O4'-C1'-N9  | 5.21  | 112.37                 | 108.20              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|-------------|-------|------------------------|---------------------|
| 54  | BA    | 1081 | U    | N3-C2-O2    | -5.21 | 118.55                 | 122.20              |
| 54  | BA    | 1219 | U    | O4'-C1'-N1  | 5.21  | 112.37                 | 108.20              |
| 54  | BA    | 2331 | G    | N1-C6-O6    | -5.21 | 116.77                 | 119.90              |
| 21  | AA    | 1043 | G    | N3-C4-C5    | -5.21 | 126.00                 | 128.60              |
| 21  | AA    | 1056 | U    | C4-C5-C6    | 5.21  | 122.83                 | 119.70              |
| 21  | AA    | 1080 | A    | N7-C8-N9    | 5.21  | 116.40                 | 113.80              |
| 21  | AA    | 1458 | G    | N3-C4-C5    | -5.21 | 126.00                 | 128.60              |
| 24  | A3    | 45   | A    | C6-C5-N7    | 5.21  | 135.94                 | 132.30              |
| 54  | BA    | 584  | C    | N1-C2-O2    | 5.21  | 122.03                 | 118.90              |
| 54  | BA    | 1289 | C    | N1-C2-O2    | 5.21  | 122.03                 | 118.90              |
| 54  | BA    | 1835 | G    | N1-C6-O6    | -5.21 | 116.78                 | 119.90              |
| 54  | BA    | 2005 | A    | C4-C5-C6    | -5.21 | 114.39                 | 117.00              |
| 54  | BA    | 2240 | U    | N1-C2-N3    | 5.21  | 118.03                 | 114.90              |
| 54  | BA    | 2584 | U    | O4'-C1'-N1  | 5.21  | 112.37                 | 108.20              |
| 55  | BB    | 65   | U    | O4'-C1'-N1  | 5.21  | 112.37                 | 108.20              |
| 14  | AO    | 76   | ARG  | NH1-CZ-NH2  | -5.21 | 113.67                 | 119.40              |
| 21  | AA    | 641  | U    | N3-C2-O2    | -5.21 | 118.56                 | 122.20              |
| 21  | AA    | 1116 | U    | N3-C2-O2    | -5.21 | 118.56                 | 122.20              |
| 54  | BA    | 62   | U    | C4-C5-C6    | 5.21  | 122.82                 | 119.70              |
| 54  | BA    | 1008 | A    | C4-C5-C6    | -5.21 | 114.40                 | 117.00              |
| 54  | BA    | 1286 | A    | C4-C5-C6    | -5.21 | 114.40                 | 117.00              |
| 54  | BA    | 1529 | G    | C5-C6-N1    | 5.21  | 114.10                 | 111.50              |
| 54  | BA    | 1552 | A    | C1'-O4'-C4' | -5.21 | 105.73                 | 109.90              |
| 54  | BA    | 2221 | G    | N3-C4-C5    | -5.21 | 126.00                 | 128.60              |
| 54  | BA    | 2321 | U    | C4-C5-C6    | 5.21  | 122.82                 | 119.70              |
| 54  | BA    | 2388 | A    | N1-C6-N6    | -5.21 | 115.48                 | 118.60              |
| 54  | BA    | 2856 | A    | C6-C5-N7    | 5.21  | 135.94                 | 132.30              |
| 54  | BA    | 285  | G    | O4'-C1'-N9  | 5.21  | 112.36                 | 108.20              |
| 54  | BA    | 1658 | C    | N1-C2-O2    | 5.21  | 122.02                 | 118.90              |
| 54  | BA    | 1798 | U    | O4'-C1'-N1  | 5.21  | 112.36                 | 108.20              |
| 54  | BA    | 2099 | U    | N3-C2-O2    | -5.21 | 118.56                 | 122.20              |
| 21  | AA    | 882  | C    | N3-C4-C5    | 5.20  | 123.98                 | 121.90              |
| 21  | AA    | 1206 | G    | N7-C8-N9    | 5.20  | 115.70                 | 113.10              |
| 21  | AA    | 1448 | C    | N3-C2-O2    | -5.20 | 118.26                 | 121.90              |
| 49  | B0    | 39   | ARG  | NH1-CZ-NH2  | -5.20 | 113.68                 | 119.40              |
| 54  | BA    | 97   | C    | C5'-C4'-O4' | 5.20  | 115.34                 | 109.10              |
| 54  | BA    | 1933 | G    | N7-C8-N9    | 5.20  | 115.70                 | 113.10              |
| 54  | BA    | 1996 | C    | N3-C4-C5    | 5.20  | 123.98                 | 121.90              |
| 54  | BA    | 2078 | C    | C5'-C4'-O4' | 5.20  | 115.34                 | 109.10              |
| 54  | BA    | 2729 | G    | N3-C2-N2    | -5.20 | 116.26                 | 119.90              |
| 21  | AA    | 590  | U    | O4'-C1'-N1  | 5.20  | 112.36                 | 108.20              |
| 54  | BA    | 232  | G    | N3-C4-C5    | -5.20 | 126.00                 | 128.60              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|-------------|-------|------------------------|---------------------|
| 54  | BA    | 764  | A    | O4'-C1'-N9  | 5.20  | 112.36                 | 108.20              |
| 54  | BA    | 987  | C    | N3-C2-O2    | -5.20 | 118.26                 | 121.90              |
| 21  | AA    | 58   | C    | N3-C4-C5    | 5.20  | 123.98                 | 121.90              |
| 21  | AA    | 1458 | G    | N1-C6-O6    | -5.20 | 116.78                 | 119.90              |
| 54  | BA    | 212  | G    | N1-C6-O6    | -5.20 | 116.78                 | 119.90              |
| 54  | BA    | 594  | U    | C5-C6-N1    | -5.20 | 120.10                 | 122.70              |
| 54  | BA    | 1256 | G    | N3-C2-N2    | -5.20 | 116.26                 | 119.90              |
| 55  | BB    | 34   | A    | C4-C5-C6    | -5.20 | 114.40                 | 117.00              |
| 55  | BB    | 54   | G    | N3-C4-C5    | -5.20 | 126.00                 | 128.60              |
| 21  | AA    | 34   | C    | N3-C4-C5    | 5.20  | 123.98                 | 121.90              |
| 21  | AA    | 824  | G    | N3-C2-N2    | -5.20 | 116.26                 | 119.90              |
| 21  | AA    | 1026 | G    | N1-C6-O6    | -5.20 | 116.78                 | 119.90              |
| 21  | AA    | 1231 | G    | C8-N9-C4    | -5.20 | 104.32                 | 106.40              |
| 21  | AA    | 1231 | G    | N3-C2-N2    | -5.20 | 116.26                 | 119.90              |
| 21  | AA    | 1392 | G    | N1-C6-O6    | -5.20 | 116.78                 | 119.90              |
| 21  | AA    | 1435 | G    | C5-C6-N1    | 5.20  | 114.10                 | 111.50              |
| 54  | BA    | 116  | C    | N3-C4-N4    | -5.20 | 114.36                 | 118.00              |
| 54  | BA    | 346  | A    | C4-C5-C6    | -5.20 | 114.40                 | 117.00              |
| 54  | BA    | 2544 | G    | N7-C8-N9    | 5.20  | 115.70                 | 113.10              |
| 54  | BA    | 618  | G    | C5-C6-N1    | 5.20  | 114.10                 | 111.50              |
| 54  | BA    | 1122 | G    | N7-C8-N9    | 5.20  | 115.70                 | 113.10              |
| 54  | BA    | 2591 | C    | N1-C2-O2    | 5.20  | 122.02                 | 118.90              |
| 54  | BA    | 2610 | C    | N3-C4-C5    | 5.20  | 123.98                 | 121.90              |
| 54  | BA    | 2725 | A    | C5-C6-N1    | 5.20  | 120.30                 | 117.70              |
| 21  | AA    | 36   | C    | N1-C2-O2    | 5.20  | 122.02                 | 118.90              |
| 21  | AA    | 1182 | G    | N9-C4-C5    | 5.20  | 107.48                 | 105.40              |
| 54  | BA    | 114  | U    | N1-C2-N3    | 5.20  | 118.02                 | 114.90              |
| 54  | BA    | 544  | C    | O4'-C1'-N1  | 5.20  | 112.36                 | 108.20              |
| 54  | BA    | 586  | A    | C4-C5-C6    | -5.20 | 114.40                 | 117.00              |
| 54  | BA    | 1407 | G    | C4'-C3'-C2' | -5.20 | 97.41                  | 102.60              |
| 54  | BA    | 389  | G    | N9-C4-C5    | 5.19  | 107.48                 | 105.40              |
| 54  | BA    | 1068 | G    | C5-C6-N1    | 5.19  | 114.10                 | 111.50              |
| 54  | BA    | 1214 | A    | C4-C5-C6    | -5.19 | 114.40                 | 117.00              |
| 54  | BA    | 1651 | G    | O4'-C1'-N9  | 5.19  | 112.36                 | 108.20              |
| 54  | BA    | 1712 | U    | N3-C2-O2    | -5.19 | 118.56                 | 122.20              |
| 54  | BA    | 2142 | A    | C6-C5-N7    | 5.19  | 135.94                 | 132.30              |
| 54  | BA    | 2198 | A    | C6-C5-N7    | 5.19  | 135.94                 | 132.30              |
| 54  | BA    | 2372 | U    | C5'-C4'-O4' | 5.19  | 115.33                 | 109.10              |
| 21  | AA    | 1099 | G    | C5-C6-N1    | 5.19  | 114.10                 | 111.50              |
| 21  | AA    | 1318 | A    | C6-C5-N7    | 5.19  | 135.94                 | 132.30              |
| 21  | AA    | 1488 | G    | N1-C6-O6    | -5.19 | 116.78                 | 119.90              |
| 54  | BA    | 67   | U    | C5-C6-N1    | -5.19 | 120.10                 | 122.70              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|-------------|-------|------------------------|---------------------|
| 54  | BA    | 1585 | C    | N3-C4-C5    | 5.19  | 123.98                 | 121.90              |
| 21  | AA    | 129  | A    | C3'-C2'-C1' | 5.19  | 105.65                 | 101.50              |
| 54  | BA    | 123  | G    | O4'-C1'-N9  | 5.19  | 112.35                 | 108.20              |
| 54  | BA    | 908  | C    | N3-C4-C5    | 5.19  | 123.98                 | 121.90              |
| 54  | BA    | 1312 | U    | N3-C2-O2    | -5.19 | 118.57                 | 122.20              |
| 54  | BA    | 2289 | G    | N3-C4-C5    | -5.19 | 126.00                 | 128.60              |
| 54  | BA    | 2366 | A    | C5-C6-N1    | 5.19  | 120.30                 | 117.70              |
| 54  | BA    | 2806 | C    | N3-C2-O2    | -5.19 | 118.27                 | 121.90              |
| 54  | BA    | 2623 | G    | C8-N9-C4    | -5.19 | 104.32                 | 106.40              |
| 54  | BA    | 2664 | G    | C5-C6-N1    | 5.19  | 114.09                 | 111.50              |
| 21  | AA    | 498  | A    | C2-N3-C4    | 5.19  | 113.19                 | 110.60              |
| 21  | AA    | 605  | U    | O4'-C1'-N1  | 5.19  | 112.35                 | 108.20              |
| 54  | BA    | 33   | C    | N1-C2-O2    | 5.19  | 122.01                 | 118.90              |
| 54  | BA    | 58   | G    | N9-C4-C5    | 5.19  | 107.47                 | 105.40              |
| 54  | BA    | 837  | C    | C6-N1-C2    | -5.19 | 118.22                 | 120.30              |
| 54  | BA    | 1335 | C    | O4'-C1'-N1  | 5.19  | 112.35                 | 108.20              |
| 54  | BA    | 1671 | U    | C5-C6-N1    | -5.19 | 120.11                 | 122.70              |
| 54  | BA    | 2255 | G    | N1-C6-O6    | -5.19 | 116.79                 | 119.90              |
| 54  | BA    | 2398 | U    | N3-C2-O2    | -5.19 | 118.57                 | 122.20              |
| 54  | BA    | 2554 | U    | N1-C2-N3    | 5.19  | 118.01                 | 114.90              |
| 21  | AA    | 827  | U    | C5-C6-N1    | -5.19 | 120.11                 | 122.70              |
| 54  | BA    | 129  | C    | N1-C2-O2    | 5.19  | 122.01                 | 118.90              |
| 54  | BA    | 510  | C    | N3-C2-O2    | -5.19 | 118.27                 | 121.90              |
| 54  | BA    | 1207 | C    | N3-C2-O2    | -5.19 | 118.27                 | 121.90              |
| 21  | AA    | 220  | G    | N3-C4-C5    | -5.18 | 126.01                 | 128.60              |
| 21  | AA    | 522  | C    | C2-N3-C4    | -5.18 | 117.31                 | 119.90              |
| 21  | AA    | 564  | C    | N1-C2-O2    | 5.18  | 122.01                 | 118.90              |
| 21  | AA    | 1049 | U    | N3-C2-O2    | -5.18 | 118.57                 | 122.20              |
| 21  | AA    | 1063 | C    | N1-C2-O2    | 5.18  | 122.01                 | 118.90              |
| 54  | BA    | 322  | A    | C2-N3-C4    | 5.18  | 113.19                 | 110.60              |
| 54  | BA    | 844  | A    | C5-C6-N1    | 5.18  | 120.29                 | 117.70              |
| 54  | BA    | 1023 | U    | N3-C2-O2    | -5.18 | 118.57                 | 122.20              |
| 54  | BA    | 1674 | G    | N1-C6-O6    | -5.18 | 116.79                 | 119.90              |
| 54  | BA    | 1759 | A    | N9-C4-C5    | 5.18  | 107.87                 | 105.80              |
| 54  | BA    | 2362 | C    | C2-N3-C4    | -5.18 | 117.31                 | 119.90              |
| 21  | AA    | 79   | G    | N1-C6-O6    | -5.18 | 116.79                 | 119.90              |
| 21  | AA    | 123  | U    | N3-C2-O2    | -5.18 | 118.57                 | 122.20              |
| 21  | AA    | 310  | G    | N3-C2-N2    | -5.18 | 116.27                 | 119.90              |
| 21  | AA    | 527  | G    | N3-C4-C5    | -5.18 | 126.01                 | 128.60              |
| 21  | AA    | 1261 | A    | C4-C5-C6    | -5.18 | 114.41                 | 117.00              |
| 54  | BA    | 100  | U    | N3-C2-O2    | -5.18 | 118.57                 | 122.20              |
| 54  | BA    | 325  | G    | N3-C4-C5    | -5.18 | 126.01                 | 128.60              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 54  | BA    | 352  | A    | N9-C4-C5    | 5.18  | 107.87      | 105.80   |
| 54  | BA    | 1930 | G    | C5-C6-N1    | 5.18  | 114.09      | 111.50   |
| 54  | BA    | 2671 | G    | C5-C6-N1    | 5.18  | 114.09      | 111.50   |
| 55  | BB    | 36   | C    | N1-C2-O2    | 5.18  | 122.01      | 118.90   |
| 55  | BB    | 81   | G    | N1-C6-O6    | -5.18 | 116.79      | 119.90   |
| 54  | BA    | 2459 | A    | C4-C5-C6    | -5.18 | 114.41      | 117.00   |
| 54  | BA    | 2708 | G    | N3-C4-C5    | -5.18 | 126.01      | 128.60   |
| 21  | AA    | 370  | C    | C2-N3-C4    | -5.18 | 117.31      | 119.90   |
| 21  | AA    | 518  | C    | N1-C2-O2    | 5.18  | 122.01      | 118.90   |
| 21  | AA    | 675  | A    | C5-C6-N1    | 5.18  | 120.29      | 117.70   |
| 21  | AA    | 755  | G    | O4'-C4'-C3' | 5.18  | 110.24      | 106.10   |
| 21  | AA    | 1371 | G    | N3-C2-N2    | -5.18 | 116.28      | 119.90   |
| 21  | AA    | 1489 | G    | N3-C4-C5    | -5.18 | 126.01      | 128.60   |
| 54  | BA    | 1359 | A    | O4'-C1'-N9  | 5.18  | 112.34      | 108.20   |
| 54  | BA    | 2066 | C    | N3-C2-O2    | -5.18 | 118.27      | 121.90   |
| 54  | BA    | 447  | A    | C6-C5-N7    | 5.18  | 135.93      | 132.30   |
| 54  | BA    | 784  | G    | P-O3'-C3'   | 5.18  | 125.91      | 119.70   |
| 54  | BA    | 1246 | A    | C4-C5-C6    | -5.18 | 114.41      | 117.00   |
| 21  | AA    | 288  | A    | O4'-C1'-N9  | 5.18  | 112.34      | 108.20   |
| 21  | AA    | 328  | C    | N3-C4-C5    | 5.18  | 123.97      | 121.90   |
| 21  | AA    | 346  | G    | C2-N3-C4    | 5.18  | 114.49      | 111.90   |
| 54  | BA    | 307  | G    | C5-C6-N1    | 5.18  | 114.09      | 111.50   |
| 54  | BA    | 389  | G    | N1-C6-O6    | -5.18 | 116.79      | 119.90   |
| 54  | BA    | 604  | G    | C8-N9-C4    | -5.18 | 104.33      | 106.40   |
| 54  | BA    | 1464 | G    | C5-C6-N1    | 5.18  | 114.09      | 111.50   |
| 55  | BB    | 35   | C    | N3-C4-C5    | 5.18  | 123.97      | 121.90   |
| 21  | AA    | 1487 | G    | N3-C2-N2    | -5.17 | 116.28      | 119.90   |
| 54  | BA    | 299  | A    | C2-N3-C4    | 5.17  | 113.19      | 110.60   |
| 54  | BA    | 600  | G    | N3-C4-C5    | -5.17 | 126.01      | 128.60   |
| 54  | BA    | 1255 | U    | C1'-O4'-C4' | -5.17 | 105.76      | 109.90   |
| 54  | BA    | 1745 | A    | C4-C5-C6    | -5.17 | 114.41      | 117.00   |
| 54  | BA    | 1895 | C    | O4'-C1'-N1  | 5.17  | 112.34      | 108.20   |
| 54  | BA    | 2371 | G    | C8-N9-C4    | -5.17 | 104.33      | 106.40   |
| 54  | BA    | 2411 | A    | O4'-C1'-N9  | 5.17  | 112.34      | 108.20   |
| 54  | BA    | 2716 | C    | C5'-C4'-O4' | 5.17  | 115.31      | 109.10   |
| 54  | BA    | 2882 | A    | C6-C5-N7    | 5.17  | 135.92      | 132.30   |
| 54  | BA    | 1767 | G    | O4'-C1'-N9  | 5.17  | 112.34      | 108.20   |
| 54  | BA    | 1808 | A    | C6-C5-N7    | 5.17  | 135.92      | 132.30   |
| 54  | BA    | 1843 | C    | N3-C2-O2    | -5.17 | 118.28      | 121.90   |
| 21  | AA    | 38   | G    | N1-C6-O6    | -5.17 | 116.80      | 119.90   |
| 21  | AA    | 128  | G    | N1-C6-O6    | -5.17 | 116.80      | 119.90   |
| 21  | AA    | 580  | C    | N1-C2-O2    | 5.17  | 122.00      | 118.90   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|-------------|-------|------------------------|---------------------|
| 21  | AA    | 1049 | U    | C4-C5-C6    | 5.17  | 122.80                 | 119.70              |
| 21  | AA    | 1411 | C    | N1-C2-O2    | 5.17  | 122.00                 | 118.90              |
| 54  | BA    | 62   | U    | N1-C2-N3    | 5.17  | 118.00                 | 114.90              |
| 54  | BA    | 913  | U    | O4'-C1'-N1  | 5.17  | 112.34                 | 108.20              |
| 54  | BA    | 1363 | C    | C5'-C4'-O4' | 5.17  | 115.31                 | 109.10              |
| 54  | BA    | 1582 | C    | N3-C2-O2    | -5.17 | 118.28                 | 121.90              |
| 54  | BA    | 1663 | G    | N1-C6-O6    | -5.17 | 116.80                 | 119.90              |
| 54  | BA    | 1813 | G    | O4'-C1'-N9  | 5.17  | 112.34                 | 108.20              |
| 54  | BA    | 2103 | C    | C2-N3-C4    | -5.17 | 117.31                 | 119.90              |
| 54  | BA    | 2685 | G    | N3-C2-N2    | -5.17 | 116.28                 | 119.90              |
| 35  | BM    | 114  | ARG  | NE-CZ-NH2   | -5.17 | 117.72                 | 120.30              |
| 54  | BA    | 1756 | G    | C5-C6-N1    | 5.17  | 114.08                 | 111.50              |
| 54  | BA    | 1766 | G    | N1-C6-O6    | -5.17 | 116.80                 | 119.90              |
| 54  | BA    | 2079 | U    | N3-C2-O2    | -5.17 | 118.58                 | 122.20              |
| 54  | BA    | 2654 | A    | C6-C5-N7    | 5.17  | 135.92                 | 132.30              |
| 21  | AA    | 20   | U    | O4'-C1'-N1  | 5.17  | 112.33                 | 108.20              |
| 21  | AA    | 465  | A    | N7-C8-N9    | 5.17  | 116.39                 | 113.80              |
| 21  | AA    | 491  | G    | C5-C6-N1    | 5.17  | 114.08                 | 111.50              |
| 21  | AA    | 920  | U    | C5-C6-N1    | -5.17 | 120.12                 | 122.70              |
| 21  | AA    | 1064 | G    | N7-C8-N9    | 5.17  | 115.68                 | 113.10              |
| 21  | AA    | 1467 | C    | N1-C2-O2    | 5.17  | 122.00                 | 118.90              |
| 54  | BA    | 1446 | C    | C6-N1-C2    | -5.17 | 118.23                 | 120.30              |
| 54  | BA    | 2053 | G    | N9-C4-C5    | 5.17  | 107.47                 | 105.40              |
| 36  | BN    | 2    | ARG  | NE-CZ-NH1   | 5.17  | 122.88                 | 120.30              |
| 54  | BA    | 37   | C    | N1-C2-O2    | 5.17  | 122.00                 | 118.90              |
| 54  | BA    | 148  | U    | O4'-C1'-N1  | 5.17  | 112.33                 | 108.20              |
| 54  | BA    | 851  | C    | N3-C2-O2    | -5.17 | 118.28                 | 121.90              |
| 54  | BA    | 1873 | G    | N1-C6-O6    | -5.17 | 116.80                 | 119.90              |
| 54  | BA    | 2104 | C    | N3-C4-N4    | -5.17 | 114.38                 | 118.00              |
| 54  | BA    | 2109 | U    | N3-C2-O2    | -5.17 | 118.58                 | 122.20              |
| 54  | BA    | 2163 | A    | C4-C5-C6    | -5.17 | 114.42                 | 117.00              |
| 54  | BA    | 2501 | C    | N3-C2-O2    | -5.17 | 118.28                 | 121.90              |
| 5   | AF    | 91   | ARG  | NE-CZ-NH1   | 5.17  | 122.88                 | 120.30              |
| 21  | AA    | 520  | A    | C5-C6-N1    | 5.17  | 120.28                 | 117.70              |
| 21  | AA    | 1192 | C    | N3-C4-C5    | 5.17  | 123.97                 | 121.90              |
| 54  | BA    | 1613 | G    | N3-C2-N2    | -5.17 | 116.28                 | 119.90              |
| 54  | BA    | 2225 | A    | C5-C6-N1    | 5.17  | 120.28                 | 117.70              |
| 54  | BA    | 2686 | G    | C8-N9-C4    | -5.17 | 104.33                 | 106.40              |
| 21  | AA    | 908  | A    | N1-C6-N6    | -5.16 | 115.50                 | 118.60              |
| 39  | BQ    | 2    | ARG  | NE-CZ-NH1   | 5.16  | 122.88                 | 120.30              |
| 54  | BA    | 109  | C    | O4'-C1'-N1  | 5.16  | 112.33                 | 108.20              |
| 54  | BA    | 264  | C    | N1-C2-O2    | 5.16  | 122.00                 | 118.90              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|-------------|-------|------------------------|---------------------|
| 54  | BA    | 267  | C    | O4'-C1'-N1  | 5.16  | 112.33                 | 108.20              |
| 54  | BA    | 1317 | G    | C4-C5-N7    | -5.16 | 108.73                 | 110.80              |
| 54  | BA    | 2506 | U    | C5-C6-N1    | -5.16 | 120.12                 | 122.70              |
| 54  | BA    | 2539 | C    | N1-C2-O2    | 5.16  | 122.00                 | 118.90              |
| 21  | AA    | 596  | A    | C4-C5-C6    | -5.16 | 114.42                 | 117.00              |
| 21  | AA    | 1031 | C    | N3-C4-N4    | -5.16 | 114.39                 | 118.00              |
| 54  | BA    | 525  | U    | N3-C2-O2    | -5.16 | 118.59                 | 122.20              |
| 54  | BA    | 765  | C    | O4'-C1'-N1  | 5.16  | 112.33                 | 108.20              |
| 54  | BA    | 2580 | U    | O4'-C1'-N1  | 5.16  | 112.33                 | 108.20              |
| 55  | BB    | 62   | C    | N3-C2-O2    | -5.16 | 118.29                 | 121.90              |
| 55  | BB    | 82   | U    | O4'-C1'-N1  | 5.16  | 112.33                 | 108.20              |
| 21  | AA    | 516  | U    | O4'-C1'-N1  | 5.16  | 112.33                 | 108.20              |
| 22  | A1    | 3    | G    | C5-C6-N1    | 5.16  | 114.08                 | 111.50              |
| 54  | BA    | 98   | G    | N1-C6-O6    | -5.16 | 116.80                 | 119.90              |
| 54  | BA    | 545  | U    | N1-C2-N3    | 5.16  | 118.00                 | 114.90              |
| 54  | BA    | 1148 | U    | O4'-C1'-N1  | 5.16  | 112.33                 | 108.20              |
| 54  | BA    | 1963 | U    | C5-C6-N1    | -5.16 | 120.12                 | 122.70              |
| 54  | BA    | 2403 | C    | N1-C2-O2    | 5.16  | 122.00                 | 118.90              |
| 54  | BA    | 2818 | U    | N1-C2-N3    | 5.16  | 118.00                 | 114.90              |
| 21  | AA    | 1176 | A    | C5-C6-N1    | 5.16  | 120.28                 | 117.70              |
| 54  | BA    | 337  | C    | N1-C2-O2    | 5.16  | 122.00                 | 118.90              |
| 54  | BA    | 1468 | U    | C5-C6-N1    | -5.16 | 120.12                 | 122.70              |
| 55  | BB    | 62   | C    | N1-C2-O2    | 5.16  | 122.00                 | 118.90              |
| 21  | AA    | 574  | A    | C4-C5-C6    | -5.16 | 114.42                 | 117.00              |
| 32  | BJ    | 116  | ARG  | NE-CZ-NH2   | -5.16 | 117.72                 | 120.30              |
| 54  | BA    | 1645 | G    | N1-C6-O6    | -5.16 | 116.81                 | 119.90              |
| 54  | BA    | 1970 | A    | O4'-C1'-N9  | 5.16  | 112.33                 | 108.20              |
| 21  | AA    | 575  | G    | N3-C4-C5    | -5.16 | 126.02                 | 128.60              |
| 21  | AA    | 852  | G    | N9-C4-C5    | 5.16  | 107.46                 | 105.40              |
| 21  | AA    | 1294 | G    | N7-C8-N9    | 5.16  | 115.68                 | 113.10              |
| 21  | AA    | 1336 | C    | C2-N3-C4    | -5.16 | 117.32                 | 119.90              |
| 22  | A1    | 60   | C    | N3-C4-C5    | 5.16  | 123.96                 | 121.90              |
| 54  | BA    | 251  | A    | C4-C5-C6    | -5.16 | 114.42                 | 117.00              |
| 54  | BA    | 467  | G    | O4'-C1'-N9  | 5.16  | 112.33                 | 108.20              |
| 54  | BA    | 1097 | U    | C5-C6-N1    | -5.16 | 120.12                 | 122.70              |
| 54  | BA    | 1543 | G    | N1-C6-O6    | -5.16 | 116.81                 | 119.90              |
| 54  | BA    | 2557 | G    | C8-N9-C4    | -5.16 | 104.34                 | 106.40              |
| 54  | BA    | 2587 | A    | C6-C5-N7    | 5.16  | 135.91                 | 132.30              |
| 55  | BB    | 93   | C    | C4'-C3'-C2' | -5.16 | 97.44                  | 102.60              |
| 21  | AA    | 863  | U    | N1-C2-N3    | 5.15  | 117.99                 | 114.90              |
| 54  | BA    | 2578 | G    | C4'-C3'-C2' | -5.15 | 97.45                  | 102.60              |
| 55  | BB    | 118  | C    | O4'-C1'-N1  | 5.15  | 112.32                 | 108.20              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|-------------|-------|------------------------|---------------------|
| 21  | AA    | 267  | C    | N1-C2-O2    | 5.15  | 121.99                 | 118.90              |
| 21  | AA    | 470  | C    | N3-C4-C5    | 5.15  | 123.96                 | 121.90              |
| 21  | AA    | 518  | C    | N3-C4-N4    | -5.15 | 114.39                 | 118.00              |
| 21  | AA    | 532  | A    | O4'-C1'-N9  | 5.15  | 112.32                 | 108.20              |
| 21  | AA    | 1136 | C    | N3-C4-C5    | 5.15  | 123.96                 | 121.90              |
| 21  | AA    | 1490 | U    | N3-C2-O2    | -5.15 | 118.59                 | 122.20              |
| 21  | AA    | 1528 | U    | O4'-C1'-N1  | 5.15  | 112.32                 | 108.20              |
| 54  | BA    | 2    | G    | N3-C4-C5    | -5.15 | 126.02                 | 128.60              |
| 54  | BA    | 67   | U    | N3-C2-O2    | -5.15 | 118.59                 | 122.20              |
| 54  | BA    | 477  | A    | C4-C5-C6    | -5.15 | 114.42                 | 117.00              |
| 54  | BA    | 620  | G    | C8-N9-C4    | -5.15 | 104.34                 | 106.40              |
| 54  | BA    | 954  | G    | C5-C6-N1    | 5.15  | 114.08                 | 111.50              |
| 54  | BA    | 1169 | A    | C4-C5-C6    | -5.15 | 114.42                 | 117.00              |
| 54  | BA    | 2710 | C    | N1-C2-O2    | 5.15  | 121.99                 | 118.90              |
| 55  | BB    | 90   | C    | O4'-C1'-N1  | 5.15  | 112.32                 | 108.20              |
| 55  | BB    | 114  | C    | N1-C2-O2    | 5.15  | 121.99                 | 118.90              |
| 21  | AA    | 1092 | A    | N1-C6-N6    | -5.15 | 115.51                 | 118.60              |
| 21  | AA    | 1409 | C    | O4'-C1'-N1  | 5.15  | 112.32                 | 108.20              |
| 54  | BA    | 63   | A    | C6-C5-N7    | 5.15  | 135.91                 | 132.30              |
| 54  | BA    | 163  | C    | O4'-C1'-N1  | 5.15  | 112.32                 | 108.20              |
| 54  | BA    | 586  | A    | C5-C6-N1    | 5.15  | 120.28                 | 117.70              |
| 54  | BA    | 758  | C    | C4'-C3'-C2' | -5.15 | 97.45                  | 102.60              |
| 54  | BA    | 1256 | G    | N7-C8-N9    | 5.15  | 115.68                 | 113.10              |
| 54  | BA    | 1493 | C    | N1-C2-O2    | 5.15  | 121.99                 | 118.90              |
| 54  | BA    | 1726 | C    | O4'-C1'-N1  | 5.15  | 112.32                 | 108.20              |
| 54  | BA    | 1979 | U    | C5-C6-N1    | -5.15 | 120.12                 | 122.70              |
| 54  | BA    | 1981 | A    | C6-C5-N7    | 5.15  | 135.91                 | 132.30              |
| 54  | BA    | 2598 | A    | C6-C5-N7    | 5.15  | 135.91                 | 132.30              |
| 21  | AA    | 335  | C    | O4'-C1'-N1  | 5.15  | 112.32                 | 108.20              |
| 21  | AA    | 1439 | G    | C5-C6-N1    | 5.15  | 114.07                 | 111.50              |
| 54  | BA    | 317  | G    | C5-C6-N1    | 5.15  | 114.07                 | 111.50              |
| 54  | BA    | 2703 | C    | N3-C2-O2    | -5.15 | 118.30                 | 121.90              |
| 21  | AA    | 295  | C    | N3-C2-O2    | -5.15 | 118.30                 | 121.90              |
| 21  | AA    | 818  | G    | N1-C6-O6    | -5.15 | 116.81                 | 119.90              |
| 54  | BA    | 48   | G    | N3-C4-C5    | -5.15 | 126.03                 | 128.60              |
| 54  | BA    | 584  | C    | O4'-C1'-N1  | 5.15  | 112.32                 | 108.20              |
| 54  | BA    | 956  | G    | C5-C6-N1    | 5.15  | 114.07                 | 111.50              |
| 54  | BA    | 2238 | G    | P-O3'-C3'   | 5.15  | 125.88                 | 119.70              |
| 54  | BA    | 2851 | A    | C6-C5-N7    | 5.15  | 135.90                 | 132.30              |
| 54  | BA    | 2853 | C    | N3-C2-O2    | -5.15 | 118.30                 | 121.90              |
| 21  | AA    | 44   | A    | O4'-C1'-N9  | 5.15  | 112.32                 | 108.20              |
| 21  | AA    | 191  | G    | N1-C6-O6    | -5.15 | 116.81                 | 119.90              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 54  | BA    | 797  | G    | O4'-C1'-N9  | 5.15  | 112.32      | 108.20   |
| 54  | BA    | 1947 | C    | N3-C4-C5    | 5.15  | 123.96      | 121.90   |
| 55  | BB    | 8    | C    | N1-C2-O2    | 5.15  | 121.99      | 118.90   |
| 21  | AA    | 46   | G    | C5-C6-N1    | 5.14  | 114.07      | 111.50   |
| 21  | AA    | 68   | G    | C5-C6-N1    | 5.14  | 114.07      | 111.50   |
| 21  | AA    | 266  | G    | N3-C2-N2    | -5.14 | 116.30      | 119.90   |
| 21  | AA    | 419  | C    | N1-C2-O2    | 5.14  | 121.99      | 118.90   |
| 21  | AA    | 1022 | A    | C6-C5-N7    | 5.14  | 135.90      | 132.30   |
| 21  | AA    | 1108 | G    | N1-C6-O6    | -5.14 | 116.81      | 119.90   |
| 24  | A3    | 13   | C    | O4'-C1'-N1  | 5.14  | 112.31      | 108.20   |
| 25  | BC    | 216  | ARG  | NH1-CZ-NH2  | -5.14 | 113.74      | 119.40   |
| 25  | BC    | 269  | ARG  | NE-CZ-NH2   | -5.14 | 117.73      | 120.30   |
| 26  | BD    | 33   | ARG  | NE-CZ-NH1   | 5.14  | 122.87      | 120.30   |
| 54  | BA    | 318  | C    | N3-C2-O2    | -5.14 | 118.30      | 121.90   |
| 54  | BA    | 543  | G    | C5'-C4'-O4' | 5.14  | 115.27      | 109.10   |
| 54  | BA    | 825  | A    | C6-C5-N7    | 5.14  | 135.90      | 132.30   |
| 54  | BA    | 1232 | G    | C8-N9-C4    | -5.14 | 104.34      | 106.40   |
| 2   | AC    | 178  | ARG  | NE-CZ-NH1   | 5.14  | 122.87      | 120.30   |
| 21  | AA    | 119  | A    | C5-C6-N1    | 5.14  | 120.27      | 117.70   |
| 21  | AA    | 679  | C    | O4'-C1'-N1  | 5.14  | 112.31      | 108.20   |
| 21  | AA    | 713  | G    | N1-C6-O6    | -5.14 | 116.81      | 119.90   |
| 21  | AA    | 1164 | G    | C5-C6-N1    | 5.14  | 114.07      | 111.50   |
| 54  | BA    | 515  | A    | C6-C5-N7    | 5.14  | 135.90      | 132.30   |
| 54  | BA    | 1068 | G    | N1-C6-O6    | -5.14 | 116.81      | 119.90   |
| 54  | BA    | 1560 | G    | C8-N9-C4    | -5.14 | 104.34      | 106.40   |
| 54  | BA    | 2313 | C    | O4'-C1'-N1  | 5.14  | 112.31      | 108.20   |
| 54  | BA    | 2679 | A    | C4-C5-C6    | -5.14 | 114.43      | 117.00   |
| 55  | BB    | 114  | C    | N3-C2-O2    | -5.14 | 118.30      | 121.90   |
| 54  | BA    | 2073 | C    | C2-N3-C4    | -5.14 | 117.33      | 119.90   |
| 54  | BA    | 2179 | C    | O4'-C1'-N1  | 5.14  | 112.31      | 108.20   |
| 13  | AN    | 81   | ARG  | NE-CZ-NH1   | 5.14  | 122.87      | 120.30   |
| 21  | AA    | 177  | G    | O4'-C1'-N9  | 5.14  | 112.31      | 108.20   |
| 21  | AA    | 457  | G    | N9-C4-C5    | 5.14  | 107.46      | 105.40   |
| 21  | AA    | 554  | A    | C5-C6-N1    | 5.14  | 120.27      | 117.70   |
| 25  | BC    | 176  | ARG  | NH1-CZ-NH2  | -5.14 | 113.75      | 119.40   |
| 54  | BA    | 583  | G    | O4'-C1'-N9  | 5.14  | 112.31      | 108.20   |
| 54  | BA    | 626  | A    | C4-C5-C6    | -5.14 | 114.43      | 117.00   |
| 54  | BA    | 931  | U    | N3-C2-O2    | -5.14 | 118.60      | 122.20   |
| 54  | BA    | 942  | G    | N1-C6-O6    | -5.14 | 116.82      | 119.90   |
| 54  | BA    | 1264 | A    | C6-C5-N7    | 5.14  | 135.90      | 132.30   |
| 54  | BA    | 2817 | U    | N1-C2-N3    | 5.14  | 117.98      | 114.90   |
| 21  | AA    | 956  | U    | C5-C6-N1    | -5.14 | 120.13      | 122.70   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 21  | AA    | 1124 | G    | C1'-O4'-C4' | -5.14 | 105.79      | 109.90   |
| 36  | BN    | 8    | ARG  | NE-CZ-NH1   | 5.14  | 122.87      | 120.30   |
| 54  | BA    | 394  | C    | C4'-C3'-C2' | -5.14 | 97.46       | 102.60   |
| 54  | BA    | 1295 | C    | N3-C2-O2    | -5.14 | 118.30      | 121.90   |
| 54  | BA    | 2680 | U    | C4-C5-C6    | 5.14  | 122.78      | 119.70   |
| 19  | AT    | 28   | ARG  | NH1-CZ-NH2  | -5.14 | 113.75      | 119.40   |
| 21  | AA    | 83   | C    | N1-C2-O2    | 5.14  | 121.98      | 118.90   |
| 21  | AA    | 1422 | G    | C8-N9-C4    | -5.14 | 104.34      | 106.40   |
| 42  | BT    | 6    | ARG  | NE-CZ-NH1   | 5.14  | 122.87      | 120.30   |
| 54  | BA    | 666  | A    | C4-C5-C6    | -5.14 | 114.43      | 117.00   |
| 54  | BA    | 1469 | A    | N1-C6-N6    | -5.14 | 115.52      | 118.60   |
| 54  | BA    | 1720 | U    | C5-C6-N1    | -5.14 | 120.13      | 122.70   |
| 54  | BA    | 1822 | C    | N1-C2-O2    | 5.14  | 121.98      | 118.90   |
| 21  | AA    | 454  | G    | N3-C4-C5    | -5.13 | 126.03      | 128.60   |
| 21  | AA    | 1406 | U    | C4-C5-C6    | 5.13  | 122.78      | 119.70   |
| 54  | BA    | 193  | U    | N3-C2-O2    | -5.13 | 118.61      | 122.20   |
| 54  | BA    | 295  | G    | C5'-C4'-C3' | -5.13 | 107.78      | 116.00   |
| 54  | BA    | 370  | G    | C5-C6-N1    | 5.13  | 114.07      | 111.50   |
| 54  | BA    | 1128 | G    | C8-N9-C4    | -5.13 | 104.35      | 106.40   |
| 54  | BA    | 1427 | A    | C6-C5-N7    | 5.13  | 135.89      | 132.30   |
| 54  | BA    | 1580 | A    | C4-C5-C6    | -5.13 | 114.43      | 117.00   |
| 54  | BA    | 1903 | G    | N3-C2-N2    | -5.13 | 116.31      | 119.90   |
| 54  | BA    | 2497 | A    | C5-N7-C8    | -5.13 | 101.33      | 103.90   |
| 21  | AA    | 1488 | G    | C4-C5-N7    | -5.13 | 108.75      | 110.80   |
| 21  | AA    | 1518 | A    | C4-C5-C6    | -5.13 | 114.43      | 117.00   |
| 54  | BA    | 1735 | A    | C4-C5-C6    | -5.13 | 114.43      | 117.00   |
| 54  | BA    | 1954 | G    | N1-C6-O6    | -5.13 | 116.82      | 119.90   |
| 54  | BA    | 2122 | U    | O4'-C1'-N1  | 5.13  | 112.31      | 108.20   |
| 21  | AA    | 76   | G    | N7-C8-N9    | 5.13  | 115.67      | 113.10   |
| 54  | BA    | 49   | A    | C4-C5-C6    | -5.13 | 114.43      | 117.00   |
| 54  | BA    | 160  | A    | C4'-C3'-C2' | -5.13 | 97.47       | 102.60   |
| 54  | BA    | 341  | C    | N1-C2-O2    | 5.13  | 121.98      | 118.90   |
| 54  | BA    | 406  | G    | C5-C6-N1    | 5.13  | 114.07      | 111.50   |
| 54  | BA    | 684  | G    | C8-N9-C4    | -5.13 | 104.35      | 106.40   |
| 54  | BA    | 745  | G    | N3-C2-N2    | -5.13 | 116.31      | 119.90   |
| 54  | BA    | 1972 | G    | C8-N9-C4    | -5.13 | 104.35      | 106.40   |
| 12  | AM    | 91   | ARG  | NE-CZ-NH2   | -5.13 | 117.73      | 120.30   |
| 21  | AA    | 908  | A    | C4-C5-C6    | -5.13 | 114.44      | 117.00   |
| 21  | AA    | 974  | A    | C3'-C2'-C1' | 5.13  | 105.60      | 101.50   |
| 21  | AA    | 1292 | G    | N1-C6-O6    | -5.13 | 116.82      | 119.90   |
| 54  | BA    | 73   | A    | C1'-O4'-C4' | -5.13 | 105.80      | 109.90   |
| 54  | BA    | 254  | G    | N1-C6-O6    | -5.13 | 116.82      | 119.90   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|-------------|-------|------------------------|---------------------|
| 54  | BA    | 419  | U    | N1-C2-N3    | 5.13  | 117.98                 | 114.90              |
| 54  | BA    | 709  | U    | C4'-C3'-C2' | -5.13 | 97.47                  | 102.60              |
| 54  | BA    | 1100 | C    | C6-N1-C2    | -5.13 | 118.25                 | 120.30              |
| 54  | BA    | 1713 | A    | C4-C5-C6    | -5.13 | 114.44                 | 117.00              |
| 54  | BA    | 1943 | U    | N3-C2-O2    | -5.13 | 118.61                 | 122.20              |
| 54  | BA    | 2397 | G    | C5-C6-N1    | 5.13  | 114.06                 | 111.50              |
| 21  | AA    | 25   | C    | N1-C2-O2    | 5.13  | 121.98                 | 118.90              |
| 21  | AA    | 1114 | C    | N3-C2-O2    | -5.13 | 118.31                 | 121.90              |
| 52  | B3    | 29   | ARG  | NE-CZ-NH1   | 5.13  | 122.86                 | 120.30              |
| 54  | BA    | 701  | G    | N3-C4-C5    | -5.13 | 126.03                 | 128.60              |
| 54  | BA    | 1569 | A    | C4-C5-C6    | -5.13 | 114.44                 | 117.00              |
| 21  | AA    | 1230 | C    | N3-C2-O2    | -5.13 | 118.31                 | 121.90              |
| 21  | AA    | 1512 | U    | C5-C6-N1    | -5.13 | 120.14                 | 122.70              |
| 54  | BA    | 62   | U    | O4'-C1'-N1  | 5.13  | 112.30                 | 108.20              |
| 54  | BA    | 1007 | C    | N3-C2-O2    | -5.13 | 118.31                 | 121.90              |
| 54  | BA    | 1247 | A    | C4-C5-C6    | -5.13 | 114.44                 | 117.00              |
| 54  | BA    | 1505 | A    | C6-C5-N7    | 5.13  | 135.89                 | 132.30              |
| 54  | BA    | 1679 | A    | C6-C5-N7    | 5.13  | 135.89                 | 132.30              |
| 54  | BA    | 2604 | U    | N3-C2-O2    | -5.13 | 118.61                 | 122.20              |
| 21  | AA    | 289  | G    | C5-C6-N1    | 5.12  | 114.06                 | 111.50              |
| 21  | AA    | 363  | A    | N9-C4-C5    | 5.12  | 107.85                 | 105.80              |
| 54  | BA    | 437  | U    | C5-C6-N1    | -5.12 | 120.14                 | 122.70              |
| 54  | BA    | 1401 | G    | N3-C4-C5    | -5.12 | 126.04                 | 128.60              |
| 54  | BA    | 2087 | G    | N7-C8-N9    | 5.12  | 115.66                 | 113.10              |
| 54  | BA    | 2368 | C    | C2-N3-C4    | -5.12 | 117.34                 | 119.90              |
| 54  | BA    | 2641 | G    | C5-C6-N1    | 5.12  | 114.06                 | 111.50              |
| 21  | AA    | 355  | C    | O4'-C1'-N1  | 5.12  | 112.30                 | 108.20              |
| 21  | AA    | 604  | G    | C8-N9-C4    | -5.12 | 104.35                 | 106.40              |
| 22  | A1    | 20   | G    | N3-C4-C5    | -5.12 | 126.04                 | 128.60              |
| 54  | BA    | 541  | A    | C4'-C3'-C2' | -5.12 | 97.48                  | 102.60              |
| 54  | BA    | 651  | G    | N1-C6-O6    | -5.12 | 116.83                 | 119.90              |
| 54  | BA    | 1639 | C    | N3-C4-C5    | 5.12  | 123.95                 | 121.90              |
| 54  | BA    | 1695 | G    | N7-C8-N9    | 5.12  | 115.66                 | 113.10              |
| 54  | BA    | 2260 | C    | N3-C2-O2    | -5.12 | 118.31                 | 121.90              |
| 54  | BA    | 2391 | G    | N3-C4-C5    | -5.12 | 126.04                 | 128.60              |
| 54  | BA    | 2635 | A    | C6-C5-N7    | 5.12  | 135.89                 | 132.30              |
| 54  | BA    | 2718 | G    | C5-C6-N1    | 5.12  | 114.06                 | 111.50              |
| 21  | AA    | 122  | G    | C5-C6-N1    | 5.12  | 114.06                 | 111.50              |
| 54  | BA    | 141  | G    | N7-C8-N9    | 5.12  | 115.66                 | 113.10              |
| 54  | BA    | 2016 | U    | C5-C6-N1    | -5.12 | 120.14                 | 122.70              |
| 21  | AA    | 291  | U    | O4'-C1'-N1  | 5.12  | 112.30                 | 108.20              |
| 21  | AA    | 978  | A    | C4-C5-C6    | -5.12 | 114.44                 | 117.00              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 54  | BA    | 172  | A    | C4-C5-C6   | -5.12 | 114.44      | 117.00   |
| 54  | BA    | 1968 | G    | N7-C8-N9   | 5.12  | 115.66      | 113.10   |
| 54  | BA    | 2031 | A    | O4'-C1'-N9 | 5.12  | 112.30      | 108.20   |
| 21  | AA    | 21   | G    | C5-C6-N1   | 5.12  | 114.06      | 111.50   |
| 21  | AA    | 621  | A    | O4'-C1'-N9 | 5.12  | 112.30      | 108.20   |
| 54  | BA    | 203  | A    | C5-C6-N1   | 5.12  | 120.26      | 117.70   |
| 54  | BA    | 1249 | U    | C5-C6-N1   | -5.12 | 120.14      | 122.70   |
| 54  | BA    | 1975 | G    | N1-C6-O6   | -5.12 | 116.83      | 119.90   |
| 54  | BA    | 2092 | U    | O4'-C1'-N1 | 5.12  | 112.29      | 108.20   |
| 21  | AA    | 1503 | A    | C5-C6-N1   | 5.12  | 120.26      | 117.70   |
| 54  | BA    | 957  | C    | N3-C4-C5   | 5.12  | 123.95      | 121.90   |
| 54  | BA    | 2052 | A    | C4-C5-C6   | -5.12 | 114.44      | 117.00   |
| 54  | BA    | 2372 | U    | N1-C2-N3   | 5.12  | 117.97      | 114.90   |
| 21  | AA    | 705  | G    | C4-C5-N7   | -5.12 | 108.75      | 110.80   |
| 54  | BA    | 121  | G    | C8-N9-C4   | -5.12 | 104.35      | 106.40   |
| 54  | BA    | 267  | C    | N3-C2-O2   | -5.12 | 118.32      | 121.90   |
| 54  | BA    | 396  | G    | N3-C4-C5   | -5.12 | 126.04      | 128.60   |
| 54  | BA    | 458  | G    | C8-N9-C4   | -5.12 | 104.35      | 106.40   |
| 54  | BA    | 1520 | U    | O4'-C1'-N1 | 5.12  | 112.29      | 108.20   |
| 54  | BA    | 2116 | G    | N1-C6-O6   | -5.12 | 116.83      | 119.90   |
| 54  | BA    | 2177 | C    | O4'-C1'-N1 | 5.12  | 112.29      | 108.20   |
| 54  | BA    | 2381 | A    | N1-C2-N3   | -5.12 | 126.74      | 129.30   |
| 54  | BA    | 2614 | A    | C2-N3-C4   | 5.12  | 113.16      | 110.60   |
| 54  | BA    | 2753 | A    | C5-C6-N1   | 5.12  | 120.26      | 117.70   |
| 13  | AN    | 9    | ARG  | CD-NE-CZ   | 5.11  | 130.76      | 123.60   |
| 21  | AA    | 727  | G    | C5-C6-N1   | 5.11  | 114.06      | 111.50   |
| 21  | AA    | 800  | G    | N7-C8-N9   | 5.11  | 115.66      | 113.10   |
| 21  | AA    | 1140 | C    | N3-C4-C5   | 5.11  | 123.95      | 121.90   |
| 21  | AA    | 1161 | C    | N3-C2-O2   | -5.11 | 118.32      | 121.90   |
| 54  | BA    | 45   | G    | N3-C4-C5   | -5.11 | 126.04      | 128.60   |
| 54  | BA    | 116  | C    | N1-C2-O2   | 5.11  | 121.97      | 118.90   |
| 54  | BA    | 135  | U    | N3-C2-O2   | -5.11 | 118.62      | 122.20   |
| 54  | BA    | 1033 | U    | N3-C2-O2   | -5.11 | 118.62      | 122.20   |
| 54  | BA    | 1991 | U    | N1-C2-N3   | 5.11  | 117.97      | 114.90   |
| 2   | AC    | 106  | ARG  | NE-CZ-NH1  | 5.11  | 122.86      | 120.30   |
| 21  | AA    | 520  | A    | C5-C6-N6   | 5.11  | 127.79      | 123.70   |
| 21  | AA    | 959  | A    | C4-C5-C6   | -5.11 | 114.44      | 117.00   |
| 54  | BA    | 2039 | U    | N1-C2-N3   | 5.11  | 117.97      | 114.90   |
| 9   | AJ    | 9    | ARG  | NE-CZ-NH1  | 5.11  | 122.86      | 120.30   |
| 21  | AA    | 314  | C    | N3-C2-O2   | -5.11 | 118.32      | 121.90   |
| 52  | B3    | 39   | ARG  | NE-CZ-NH1  | 5.11  | 122.86      | 120.30   |
| 54  | BA    | 393  | C    | N3-C2-O2   | -5.11 | 118.32      | 121.90   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 54  | BA    | 798  | G    | C5-C6-N1    | 5.11  | 114.06      | 111.50   |
| 54  | BA    | 1050 | A    | C5'-C4'-O4' | 5.11  | 115.23      | 109.10   |
| 54  | BA    | 1750 | G    | C8-N9-C4    | -5.11 | 104.36      | 106.40   |
| 54  | BA    | 1971 | U    | C5'-C4'-C3' | -5.11 | 107.82      | 116.00   |
| 56  | B5    | 122  | ARG  | NH1-CZ-NH2  | -5.11 | 113.78      | 119.40   |
| 21  | AA    | 34   | C    | C3'-C2'-C1' | 5.11  | 105.59      | 101.50   |
| 49  | B0    | 16   | ARG  | NE-CZ-NH1   | 5.11  | 122.85      | 120.30   |
| 54  | BA    | 755  | U    | O4'-C1'-N1  | 5.11  | 112.29      | 108.20   |
| 54  | BA    | 1751 | U    | N1-C2-N3    | 5.11  | 117.97      | 114.90   |
| 54  | BA    | 1959 | G    | C4-C5-N7    | -5.11 | 108.76      | 110.80   |
| 54  | BA    | 2203 | U    | C5-C6-N1    | -5.11 | 120.15      | 122.70   |
| 54  | BA    | 2475 | C    | N3-C2-O2    | -5.11 | 118.33      | 121.90   |
| 55  | BB    | 24   | G    | C8-N9-C4    | -5.11 | 104.36      | 106.40   |
| 21  | AA    | 249  | U    | C3'-C2'-C1' | 5.11  | 105.58      | 101.50   |
| 21  | AA    | 1194 | U    | N3-C2-O2    | -5.11 | 118.63      | 122.20   |
| 54  | BA    | 113  | U    | C3'-C2'-C1' | 5.11  | 105.58      | 101.50   |
| 54  | BA    | 161  | A    | C2-N3-C4    | 5.11  | 113.15      | 110.60   |
| 54  | BA    | 567  | U    | N1-C2-N3    | 5.11  | 117.96      | 114.90   |
| 54  | BA    | 1746 | A    | C4-C5-C6    | -5.11 | 114.45      | 117.00   |
| 54  | BA    | 2021 | C    | C2-N3-C4    | -5.11 | 117.35      | 119.90   |
| 21  | AA    | 1177 | G    | N3-C2-N2    | -5.10 | 116.33      | 119.90   |
| 54  | BA    | 2192 | U    | N3-C2-O2    | -5.10 | 118.63      | 122.20   |
| 54  | BA    | 2366 | A    | N1-C6-N6    | -5.10 | 115.54      | 118.60   |
| 54  | BA    | 2649 | C    | N1-C2-O2    | 5.10  | 121.96      | 118.90   |
| 54  | BA    | 2696 | U    | O4'-C1'-N1  | 5.10  | 112.28      | 108.20   |
| 9   | AJ    | 72   | ARG  | CD-NE-CZ    | 5.10  | 130.75      | 123.60   |
| 21  | AA    | 1360 | A    | C6-C5-N7    | 5.10  | 135.87      | 132.30   |
| 22  | A1    | 71   | C    | O4'-C1'-N1  | 5.10  | 112.28      | 108.20   |
| 54  | BA    | 703  | U    | O4'-C1'-N1  | 5.10  | 112.28      | 108.20   |
| 54  | BA    | 984  | A    | P-O3'-C3'   | 5.10  | 125.82      | 119.70   |
| 54  | BA    | 1995 | U    | C4-C5-C6    | 5.10  | 122.76      | 119.70   |
| 54  | BA    | 2367 | G    | N9-C4-C5    | 5.10  | 107.44      | 105.40   |
| 54  | BA    | 2573 | C    | O4'-C1'-N1  | 5.10  | 112.28      | 108.20   |
| 21  | AA    | 1405 | G    | O4'-C1'-N9  | 5.10  | 112.28      | 108.20   |
| 54  | BA    | 343  | C    | N1-C2-O2    | 5.10  | 121.96      | 118.90   |
| 21  | AA    | 454  | G    | N1-C6-O6    | -5.10 | 116.84      | 119.90   |
| 21  | AA    | 1216 | A    | C4-C5-C6    | -5.10 | 114.45      | 117.00   |
| 21  | AA    | 1300 | G    | O4'-C1'-N9  | 5.10  | 112.28      | 108.20   |
| 21  | AA    | 1352 | C    | N1-C2-O2    | 5.10  | 121.96      | 118.90   |
| 21  | AA    | 1494 | G    | N7-C8-N9    | 5.10  | 115.65      | 113.10   |
| 54  | BA    | 61   | C    | N3-C4-C5    | 5.10  | 123.94      | 121.90   |
| 54  | BA    | 141  | G    | N3-C2-N2    | -5.10 | 116.33      | 119.90   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|-------------|-------|------------------------|---------------------|
| 54  | BA    | 632  | A    | C4-C5-C6    | -5.10 | 114.45                 | 117.00              |
| 54  | BA    | 735  | A    | C6-C5-N7    | 5.10  | 135.87                 | 132.30              |
| 54  | BA    | 2006 | C    | N1-C2-O2    | 5.10  | 121.96                 | 118.90              |
| 54  | BA    | 2783 | U    | C5-C6-N1    | -5.10 | 120.15                 | 122.70              |
| 54  | BA    | 2794 | C    | O4'-C1'-N1  | 5.10  | 112.28                 | 108.20              |
| 55  | BB    | 18   | G    | N9-C4-C5    | 5.10  | 107.44                 | 105.40              |
| 21  | AA    | 194  | C    | O4'-C4'-C3' | 5.10  | 110.18                 | 106.10              |
| 21  | AA    | 1070 | U    | C4-C5-C6    | 5.10  | 122.76                 | 119.70              |
| 21  | AA    | 1119 | C    | N3-C2-O2    | -5.10 | 118.33                 | 121.90              |
| 24  | A3    | 48   | U    | N3-C2-O2    | -5.10 | 118.63                 | 122.20              |
| 54  | BA    | 1662 | U    | C5-C6-N1    | -5.10 | 120.15                 | 122.70              |
| 54  | BA    | 2119 | A    | C4-C5-C6    | -5.10 | 114.45                 | 117.00              |
| 54  | BA    | 2266 | A    | C4-C5-C6    | -5.10 | 114.45                 | 117.00              |
| 55  | BB    | 5    | U    | C4'-C3'-C2' | -5.10 | 97.50                  | 102.60              |
| 21  | AA    | 701  | U    | O4'-C1'-N1  | 5.10  | 112.28                 | 108.20              |
| 54  | BA    | 357  | C    | N3-C2-O2    | -5.10 | 118.33                 | 121.90              |
| 54  | BA    | 1263 | U    | C5-C6-N1    | -5.10 | 120.15                 | 122.70              |
| 54  | BA    | 1442 | U    | N1-C2-N3    | 5.10  | 117.96                 | 114.90              |
| 54  | BA    | 1914 | C    | N1-C2-O2    | 5.10  | 121.96                 | 118.90              |
| 54  | BA    | 2074 | U    | N3-C2-O2    | -5.10 | 118.63                 | 122.20              |
| 54  | BA    | 2235 | G    | N3-C4-C5    | -5.10 | 126.05                 | 128.60              |
| 9   | AJ    | 41   | PRO  | C-N-CA      | 5.09  | 134.44                 | 121.70              |
| 14  | AO    | 63   | ARG  | NH1-CZ-NH2  | -5.09 | 113.80                 | 119.40              |
| 21  | AA    | 318  | G    | N1-C6-O6    | -5.09 | 116.84                 | 119.90              |
| 21  | AA    | 832  | G    | C5-C6-N1    | 5.09  | 114.05                 | 111.50              |
| 21  | AA    | 924  | C    | O4'-C1'-N1  | 5.09  | 112.28                 | 108.20              |
| 54  | BA    | 86   | G    | O4'-C1'-N9  | 5.09  | 112.28                 | 108.20              |
| 54  | BA    | 438  | G    | N3-C4-C5    | -5.09 | 126.05                 | 128.60              |
| 54  | BA    | 1729 | U    | O4'-C1'-N1  | 5.09  | 112.28                 | 108.20              |
| 54  | BA    | 2032 | G    | N3-C4-C5    | -5.09 | 126.05                 | 128.60              |
| 54  | BA    | 2495 | G    | C5'-C4'-C3' | -5.09 | 107.85                 | 116.00              |
| 21  | AA    | 593  | U    | N3-C2-O2    | -5.09 | 118.64                 | 122.20              |
| 54  | BA    | 559  | G    | N7-C8-N9    | 5.09  | 115.65                 | 113.10              |
| 54  | BA    | 653  | U    | C3'-C2'-C1' | 5.09  | 105.57                 | 101.50              |
| 54  | BA    | 1646 | C    | N1-C2-O2    | 5.09  | 121.96                 | 118.90              |
| 54  | BA    | 2035 | G    | O4'-C1'-N9  | 5.09  | 112.27                 | 108.20              |
| 54  | BA    | 2416 | C    | N1-C2-O2    | 5.09  | 121.96                 | 118.90              |
| 21  | AA    | 153  | C    | N1-C2-O2    | 5.09  | 121.95                 | 118.90              |
| 21  | AA    | 1086 | U    | N3-C2-O2    | -5.09 | 118.64                 | 122.20              |
| 21  | AA    | 1300 | G    | C5-C6-N1    | 5.09  | 114.05                 | 111.50              |
| 21  | AA    | 1448 | C    | O4'-C4'-C3' | 5.09  | 110.17                 | 106.10              |
| 54  | BA    | 384  | A    | C4-C5-C6    | -5.09 | 114.45                 | 117.00              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 54  | BA    | 1536 | C    | N3-C2-O2    | -5.09 | 118.34      | 121.90   |
| 54  | BA    | 1831 | G    | C5-C6-N1    | 5.09  | 114.05      | 111.50   |
| 54  | BA    | 2492 | U    | N3-C2-O2    | -5.09 | 118.64      | 122.20   |
| 54  | BA    | 2589 | A    | O4'-C1'-N9  | 5.09  | 112.27      | 108.20   |
| 55  | BB    | 89   | U    | N1-C2-N3    | 5.09  | 117.95      | 114.90   |
| 21  | AA    | 117  | G    | N1-C6-O6    | -5.09 | 116.85      | 119.90   |
| 54  | BA    | 715  | A    | C6-C5-N7    | 5.09  | 135.86      | 132.30   |
| 54  | BA    | 1071 | G    | N3-C4-C5    | -5.09 | 126.06      | 128.60   |
| 54  | BA    | 1380 | G    | N1-C6-O6    | -5.09 | 116.85      | 119.90   |
| 54  | BA    | 1528 | A    | C4-C5-C6    | -5.09 | 114.45      | 117.00   |
| 54  | BA    | 1636 | U    | C5-C6-N1    | -5.09 | 120.16      | 122.70   |
| 54  | BA    | 2186 | G    | C5-C6-N1    | 5.09  | 114.05      | 111.50   |
| 54  | BA    | 73   | A    | C5-C6-N1    | 5.09  | 120.24      | 117.70   |
| 54  | BA    | 313  | G    | N3-C2-N2    | -5.09 | 116.34      | 119.90   |
| 54  | BA    | 1075 | C    | N3-C4-C5    | 5.09  | 123.94      | 121.90   |
| 54  | BA    | 1234 | U    | O4'-C1'-N1  | 5.09  | 112.27      | 108.20   |
| 54  | BA    | 2178 | C    | N3-C2-O2    | -5.09 | 118.34      | 121.90   |
| 2   | AC    | 39   | ARG  | NE-CZ-NH2   | -5.09 | 117.76      | 120.30   |
| 21  | AA    | 175  | C    | N3-C4-N4    | -5.09 | 114.44      | 118.00   |
| 21  | AA    | 948  | C    | O4'-C1'-N1  | 5.09  | 112.27      | 108.20   |
| 22  | A1    | 61   | C    | N1-C2-O2    | 5.09  | 121.95      | 118.90   |
| 54  | BA    | 621  | A    | C4-C5-C6    | -5.09 | 114.46      | 117.00   |
| 54  | BA    | 1638 | C    | N1-C2-O2    | 5.09  | 121.95      | 118.90   |
| 54  | BA    | 1980 | G    | N3-C4-C5    | -5.09 | 126.06      | 128.60   |
| 54  | BA    | 2277 | G    | C5-C6-N1    | 5.09  | 114.04      | 111.50   |
| 54  | BA    | 2395 | C    | C6-N1-C2    | -5.09 | 118.27      | 120.30   |
| 6   | AG    | 2    | ARG  | NE-CZ-NH1   | 5.08  | 122.84      | 120.30   |
| 21  | AA    | 671  | G    | C5-C6-N1    | 5.08  | 114.04      | 111.50   |
| 21  | AA    | 1476 | A    | C5-C6-N1    | 5.08  | 120.24      | 117.70   |
| 54  | BA    | 620  | G    | N1-C6-O6    | -5.08 | 116.85      | 119.90   |
| 54  | BA    | 2532 | G    | N1-C6-O6    | -5.08 | 116.85      | 119.90   |
| 21  | AA    | 56   | U    | N3-C2-O2    | -5.08 | 118.64      | 122.20   |
| 21  | AA    | 129  | A    | O4'-C1'-N9  | 5.08  | 112.27      | 108.20   |
| 21  | AA    | 162  | A    | N1-C2-N3    | -5.08 | 126.76      | 129.30   |
| 21  | AA    | 942  | G    | N1-C6-O6    | -5.08 | 116.85      | 119.90   |
| 21  | AA    | 1528 | U    | N3-C2-O2    | -5.08 | 118.64      | 122.20   |
| 54  | BA    | 1358 | G    | C5-C6-N1    | 5.08  | 114.04      | 111.50   |
| 54  | BA    | 2825 | G    | C2-N3-C4    | 5.08  | 114.44      | 111.90   |
| 55  | BB    | 70   | C    | C5'-C4'-O4' | 5.08  | 115.20      | 109.10   |
| 21  | AA    | 619  | U    | N1-C2-N3    | 5.08  | 117.95      | 114.90   |
| 21  | AA    | 1240 | U    | C5-C6-N1    | -5.08 | 120.16      | 122.70   |
| 21  | AA    | 1293 | C    | O4'-C1'-N1  | 5.08  | 112.27      | 108.20   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 54  | BA    | 162  | U    | N3-C2-O2    | -5.08 | 118.64      | 122.20   |
| 54  | BA    | 277  | G    | N1-C6-O6    | -5.08 | 116.85      | 119.90   |
| 54  | BA    | 1451 | C    | C1'-O4'-C4' | -5.08 | 105.83      | 109.90   |
| 54  | BA    | 2180 | U    | C4-C5-C6    | 5.08  | 122.75      | 119.70   |
| 54  | BA    | 2271 | G    | C8-N9-C4    | -5.08 | 104.37      | 106.40   |
| 54  | BA    | 2376 | A    | O4'-C1'-N9  | 5.08  | 112.27      | 108.20   |
| 54  | BA    | 2752 | C    | N1-C2-O2    | 5.08  | 121.95      | 118.90   |
| 54  | BA    | 2807 | U    | C5-C6-N1    | -5.08 | 120.16      | 122.70   |
| 21  | AA    | 839  | C    | N1-C2-O2    | 5.08  | 121.95      | 118.90   |
| 21  | AA    | 1341 | U    | N1-C2-N3    | 5.08  | 117.95      | 114.90   |
| 54  | BA    | 437  | U    | O4'-C1'-N1  | 5.08  | 112.26      | 108.20   |
| 54  | BA    | 1566 | A    | C4-C5-C6    | -5.08 | 114.46      | 117.00   |
| 54  | BA    | 2842 | G    | N1-C6-O6    | -5.08 | 116.85      | 119.90   |
| 55  | BB    | 37   | C    | O4'-C1'-N1  | 5.08  | 112.26      | 108.20   |
| 21  | AA    | 183  | C    | O4'-C1'-N1  | 5.08  | 112.26      | 108.20   |
| 21  | AA    | 335  | C    | C2-N3-C4    | -5.08 | 117.36      | 119.90   |
| 54  | BA    | 685  | A    | C4-C5-C6    | -5.08 | 114.46      | 117.00   |
| 54  | BA    | 784  | G    | C3'-C2'-C1' | 5.08  | 105.56      | 101.50   |
| 54  | BA    | 1349 | C    | O4'-C1'-N1  | 5.08  | 112.26      | 108.20   |
| 54  | BA    | 2177 | C    | N3-C2-O2    | -5.08 | 118.34      | 121.90   |
| 55  | BB    | 18   | G    | C6-C5-N7    | 5.08  | 133.45      | 130.40   |
| 21  | AA    | 1527 | U    | N1-C2-N3    | 5.08  | 117.95      | 114.90   |
| 54  | BA    | 412  | A    | C5-C6-N1    | 5.08  | 120.24      | 117.70   |
| 54  | BA    | 476  | G    | N1-C6-O6    | -5.08 | 116.85      | 119.90   |
| 54  | BA    | 1111 | A    | C4-C5-C6    | -5.08 | 114.46      | 117.00   |
| 54  | BA    | 1792 | G    | N1-C6-O6    | -5.08 | 116.85      | 119.90   |
| 21  | AA    | 37   | U    | O4'-C1'-N1  | 5.08  | 112.26      | 108.20   |
| 21  | AA    | 734  | G    | N7-C8-N9    | 5.08  | 115.64      | 113.10   |
| 21  | AA    | 808  | C    | C1'-O4'-C4' | -5.08 | 105.84      | 109.90   |
| 54  | BA    | 33   | C    | N3-C4-C5    | 5.08  | 123.93      | 121.90   |
| 54  | BA    | 71   | A    | C2-N3-C4    | 5.08  | 113.14      | 110.60   |
| 54  | BA    | 465  | G    | N3-C2-N2    | -5.08 | 116.35      | 119.90   |
| 54  | BA    | 1105 | U    | N1-C2-N3    | 5.08  | 117.95      | 114.90   |
| 54  | BA    | 1478 | G    | C5-N7-C8    | -5.08 | 101.76      | 104.30   |
| 54  | BA    | 1774 | C    | N3-C4-C5    | 5.08  | 123.93      | 121.90   |
| 54  | BA    | 1864 | U    | C5-C6-N1    | -5.08 | 120.16      | 122.70   |
| 54  | BA    | 2347 | C    | N3-C2-O2    | -5.08 | 118.35      | 121.90   |
| 54  | BA    | 2420 | C    | N3-C4-C5    | 5.08  | 123.93      | 121.90   |
| 54  | BA    | 2559 | C    | N1-C2-O2    | 5.08  | 121.94      | 118.90   |
| 55  | BB    | 31   | C    | N3-C2-O2    | -5.08 | 118.35      | 121.90   |
| 21  | AA    | 155  | A    | C5-C6-N1    | 5.07  | 120.24      | 117.70   |
| 21  | AA    | 175  | C    | N3-C4-C5    | 5.07  | 123.93      | 121.90   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 21  | AA    | 287  | U    | O4'-C1'-N1  | 5.07  | 112.26      | 108.20   |
| 21  | AA    | 1446 | A    | C5-C6-N1    | 5.07  | 120.24      | 117.70   |
| 54  | BA    | 288  | U    | C5-C6-N1    | -5.07 | 120.16      | 122.70   |
| 54  | BA    | 336  | C    | N3-C2-O2    | -5.07 | 118.35      | 121.90   |
| 54  | BA    | 446  | G    | C3'-C2'-C1' | 5.07  | 105.56      | 101.50   |
| 54  | BA    | 1899 | A    | C4-C5-C6    | -5.07 | 114.46      | 117.00   |
| 54  | BA    | 2124 | G    | C4-C5-N7    | -5.07 | 108.77      | 110.80   |
| 54  | BA    | 2267 | A    | C2-N3-C4    | 5.07  | 113.14      | 110.60   |
| 54  | BA    | 2361 | G    | O4'-C1'-N9  | 5.07  | 112.26      | 108.20   |
| 54  | BA    | 2870 | C    | O4'-C1'-N1  | 5.07  | 112.26      | 108.20   |
| 54  | BA    | 2891 | U    | N3-C2-O2    | -5.07 | 118.65      | 122.20   |
| 55  | BB    | 109  | A    | C6-C5-N7    | 5.07  | 135.85      | 132.30   |
| 21  | AA    | 454  | G    | C5-C6-N1    | 5.07  | 114.04      | 111.50   |
| 21  | AA    | 777  | A    | C4-C5-C6    | -5.07 | 114.46      | 117.00   |
| 21  | AA    | 1006 | G    | C5-C6-N1    | 5.07  | 114.04      | 111.50   |
| 54  | BA    | 107  | G    | N9-C4-C5    | 5.07  | 107.43      | 105.40   |
| 54  | BA    | 2768 | U    | C4'-C3'-C2' | -5.07 | 97.53       | 102.60   |
| 21  | AA    | 1003 | G    | N1-C6-O6    | -5.07 | 116.86      | 119.90   |
| 21  | AA    | 1103 | C    | C6-N1-C2    | -5.07 | 118.27      | 120.30   |
| 21  | AA    | 1228 | C    | N3-C2-O2    | -5.07 | 118.35      | 121.90   |
| 54  | BA    | 1451 | C    | C6-N1-C2    | -5.07 | 118.27      | 120.30   |
| 54  | BA    | 1824 | G    | C5-C6-N1    | 5.07  | 114.03      | 111.50   |
| 21  | AA    | 912  | C    | N1-C2-O2    | 5.07  | 121.94      | 118.90   |
| 54  | BA    | 2734 | A    | C6-C5-N7    | 5.07  | 135.85      | 132.30   |
| 21  | AA    | 282  | A    | C5'-C4'-C3' | -5.07 | 107.89      | 116.00   |
| 21  | AA    | 1294 | G    | C8-N9-C4    | -5.07 | 104.37      | 106.40   |
| 34  | BL    | 132  | ARG  | NE-CZ-NH1   | 5.07  | 122.83      | 120.30   |
| 35  | BM    | 10   | ARG  | NE-CZ-NH1   | 5.07  | 122.83      | 120.30   |
| 54  | BA    | 1310 | G    | N1-C6-O6    | -5.07 | 116.86      | 119.90   |
| 54  | BA    | 1732 | C    | N3-C4-N4    | -5.07 | 114.45      | 118.00   |
| 54  | BA    | 1846 | G    | C5-C6-N1    | 5.07  | 114.03      | 111.50   |
| 55  | BB    | 68   | C    | N3-C2-O2    | -5.07 | 118.35      | 121.90   |
| 55  | BB    | 116  | G    | N7-C8-N9    | 5.07  | 115.63      | 113.10   |
| 11  | AL    | 85   | ARG  | NH1-CZ-NH2  | -5.07 | 113.83      | 119.40   |
| 54  | BA    | 479  | A    | P-O3'-C3'   | 5.07  | 125.78      | 119.70   |
| 54  | BA    | 741  | U    | N3-C2-O2    | -5.07 | 118.65      | 122.20   |
| 54  | BA    | 1633 | G    | N3-C4-C5    | -5.07 | 126.07      | 128.60   |
| 54  | BA    | 1681 | G    | C8-N9-C4    | -5.07 | 104.37      | 106.40   |
| 54  | BA    | 2083 | G    | C8-N9-C4    | -5.07 | 104.37      | 106.40   |
| 21  | AA    | 61   | G    | C5-C6-N1    | 5.06  | 114.03      | 111.50   |
| 21  | AA    | 680  | C    | N1-C2-O2    | 5.06  | 121.94      | 118.90   |
| 21  | AA    | 1184 | G    | N3-C4-C5    | -5.06 | 126.07      | 128.60   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|-------------|-------|------------------------|---------------------|
| 54  | BA    | 607  | U    | N1-C2-N3    | 5.06  | 117.94                 | 114.90              |
| 54  | BA    | 1397 | U    | N3-C2-O2    | -5.06 | 118.66                 | 122.20              |
| 54  | BA    | 1835 | G    | C5-C6-N1    | 5.06  | 114.03                 | 111.50              |
| 54  | BA    | 2250 | G    | C3'-C2'-C1' | 5.06  | 105.55                 | 101.50              |
| 54  | BA    | 2662 | A    | C5-C6-N1    | 5.06  | 120.23                 | 117.70              |
| 21  | AA    | 177  | G    | N3-C4-N9    | 5.06  | 129.04                 | 126.00              |
| 21  | AA    | 911  | U    | N3-C2-O2    | -5.06 | 118.66                 | 122.20              |
| 21  | AA    | 1082 | A    | C6-C5-N7    | 5.06  | 135.84                 | 132.30              |
| 21  | AA    | 1390 | U    | N3-C2-O2    | -5.06 | 118.66                 | 122.20              |
| 54  | BA    | 310  | A    | C4-C5-C6    | -5.06 | 114.47                 | 117.00              |
| 54  | BA    | 325  | G    | C5-C6-N1    | 5.06  | 114.03                 | 111.50              |
| 54  | BA    | 330  | A    | C4-C5-C6    | -5.06 | 114.47                 | 117.00              |
| 54  | BA    | 965  | C    | O4'-C1'-N1  | 5.06  | 112.25                 | 108.20              |
| 54  | BA    | 982  | C    | C6-N1-C1'   | -5.06 | 114.72                 | 120.80              |
| 54  | BA    | 1236 | G    | N9-C4-C5    | 5.06  | 107.42                 | 105.40              |
| 54  | BA    | 1765 | U    | C5-C6-N1    | -5.06 | 120.17                 | 122.70              |
| 54  | BA    | 2805 | C    | N1-C2-O2    | 5.06  | 121.94                 | 118.90              |
| 56  | B5    | 71   | ARG  | NE-CZ-NH2   | -5.06 | 117.77                 | 120.30              |
| 3   | AD    | 127  | ARG  | NH1-CZ-NH2  | -5.06 | 113.83                 | 119.40              |
| 25  | BC    | 86   | ARG  | CD-NE-CZ    | 5.06  | 130.69                 | 123.60              |
| 54  | BA    | 228  | C    | N1-C2-O2    | 5.06  | 121.94                 | 118.90              |
| 54  | BA    | 1708 | C    | N3-C2-O2    | -5.06 | 118.36                 | 121.90              |
| 54  | BA    | 2184 | A    | C5-C6-N1    | 5.06  | 120.23                 | 117.70              |
| 54  | BA    | 2538 | C    | O4'-C1'-N1  | 5.06  | 112.25                 | 108.20              |
| 21  | AA    | 641  | U    | P-O3'-C3'   | 5.06  | 125.77                 | 119.70              |
| 30  | BH    | 68   | ARG  | NE-CZ-NH2   | -5.06 | 117.77                 | 120.30              |
| 54  | BA    | 297  | G    | N3-C4-C5    | -5.06 | 126.07                 | 128.60              |
| 54  | BA    | 664  | G    | C5-C6-N1    | 5.06  | 114.03                 | 111.50              |
| 54  | BA    | 1763 | G    | N9-C1'-C2'  | -5.06 | 106.44                 | 112.00              |
| 54  | BA    | 1935 | G    | C5-C6-N1    | 5.06  | 114.03                 | 111.50              |
| 54  | BA    | 2150 | C    | N1-C2-O2    | 5.06  | 121.94                 | 118.90              |
| 55  | BB    | 33   | G    | N3-C2-N2    | -5.06 | 116.36                 | 119.90              |
| 21  | AA    | 802  | A    | C5-C6-N1    | 5.06  | 120.23                 | 117.70              |
| 21  | AA    | 1033 | G    | C5-C6-N1    | 5.06  | 114.03                 | 111.50              |
| 54  | BA    | 528  | A    | O4'-C1'-N9  | 5.06  | 112.25                 | 108.20              |
| 54  | BA    | 651  | G    | N9-C4-C5    | 5.06  | 107.42                 | 105.40              |
| 54  | BA    | 1964 | G    | N1-C6-O6    | -5.06 | 116.86                 | 119.90              |
| 54  | BA    | 2124 | G    | C5-C6-N1    | 5.06  | 114.03                 | 111.50              |
| 54  | BA    | 2592 | G    | C5-C6-N1    | 5.06  | 114.03                 | 111.50              |
| 54  | BA    | 2692 | G    | C8-N9-C4    | -5.06 | 104.38                 | 106.40              |
| 54  | BA    | 2759 | G    | N9-C4-C5    | 5.06  | 107.42                 | 105.40              |
| 21  | AA    | 22   | G    | C5-C6-N1    | 5.06  | 114.03                 | 111.50              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 21  | AA    | 1042 | A    | C4-C5-C6    | -5.06 | 114.47      | 117.00   |
| 54  | BA    | 355  | U    | C1'-O4'-C4' | -5.06 | 105.86      | 109.90   |
| 54  | BA    | 952  | G    | N9-C4-C5    | 5.06  | 107.42      | 105.40   |
| 54  | BA    | 2524 | G    | N1-C6-O6    | -5.06 | 116.87      | 119.90   |
| 54  | BA    | 2686 | G    | C4'-C3'-C2' | -5.06 | 97.54       | 102.60   |
| 7   | AH    | 53   | ASP  | C-N-CA      | 5.05  | 134.34      | 121.70   |
| 21  | AA    | 103  | U    | C1'-O4'-C4' | -5.05 | 105.86      | 109.90   |
| 21  | AA    | 212  | G    | C5-C6-N1    | 5.05  | 114.03      | 111.50   |
| 21  | AA    | 226  | G    | N9-C4-C5    | 5.05  | 107.42      | 105.40   |
| 21  | AA    | 490  | C    | N1-C2-O2    | 5.05  | 121.93      | 118.90   |
| 21  | AA    | 1070 | U    | N3-C2-O2    | -5.05 | 118.66      | 122.20   |
| 54  | BA    | 1008 | A    | C6-C5-N7    | 5.05  | 135.84      | 132.30   |
| 54  | BA    | 1202 | G    | C5-C6-N1    | 5.05  | 114.03      | 111.50   |
| 54  | BA    | 1435 | G    | C8-N9-C4    | -5.05 | 104.38      | 106.40   |
| 54  | BA    | 1456 | G    | C4'-C3'-C2' | -5.05 | 97.55       | 102.60   |
| 54  | BA    | 1793 | C    | C5'-C4'-O4' | 5.05  | 115.17      | 109.10   |
| 54  | BA    | 2130 | U    | N3-C2-O2    | -5.05 | 118.66      | 122.20   |
| 54  | BA    | 2406 | A    | C6-C5-N7    | 5.05  | 135.84      | 132.30   |
| 54  | BA    | 2794 | C    | N3-C4-C5    | 5.05  | 123.92      | 121.90   |
| 54  | BA    | 2841 | C    | O4'-C1'-N1  | 5.05  | 112.24      | 108.20   |
| 7   | AH    | 116  | ARG  | NE-CZ-NH2   | -5.05 | 117.77      | 120.30   |
| 21  | AA    | 180  | U    | N3-C2-O2    | -5.05 | 118.66      | 122.20   |
| 21  | AA    | 481  | G    | N9-C4-C5    | 5.05  | 107.42      | 105.40   |
| 24  | A3    | 53   | G    | C8-N9-C4    | -5.05 | 104.38      | 106.40   |
| 54  | BA    | 1795 | C    | O4'-C1'-N1  | 5.05  | 112.24      | 108.20   |
| 21  | AA    | 30   | U    | C5-C6-N1    | -5.05 | 120.17      | 122.70   |
| 21  | AA    | 141  | G    | N3-C4-C5    | -5.05 | 126.07      | 128.60   |
| 21  | AA    | 1512 | U    | N1-C2-N3    | 5.05  | 117.93      | 114.90   |
| 54  | BA    | 750  | A    | C6-C5-N7    | 5.05  | 135.84      | 132.30   |
| 54  | BA    | 1313 | U    | N3-C2-O2    | -5.05 | 118.66      | 122.20   |
| 54  | BA    | 2703 | C    | O4'-C1'-N1  | 5.05  | 112.24      | 108.20   |
| 54  | BA    | 2710 | C    | N3-C4-C5    | 5.05  | 123.92      | 121.90   |
| 55  | BB    | 23   | G    | N1-C6-O6    | -5.05 | 116.87      | 119.90   |
| 21  | AA    | 150  | U    | O4'-C4'-C3' | 5.05  | 110.14      | 106.10   |
| 54  | BA    | 288  | U    | N3-C2-O2    | -5.05 | 118.67      | 122.20   |
| 54  | BA    | 652  | U    | C4-C5-C6    | 5.05  | 122.73      | 119.70   |
| 54  | BA    | 1227 | G    | C5-C6-N1    | 5.05  | 114.03      | 111.50   |
| 54  | BA    | 1301 | A    | C4-C5-C6    | -5.05 | 114.47      | 117.00   |
| 54  | BA    | 2195 | U    | C4'-C3'-C2' | -5.05 | 97.55       | 102.60   |
| 54  | BA    | 2360 | G    | C5-N7-C8    | -5.05 | 101.78      | 104.30   |
| 54  | BA    | 2248 | C    | C4'-C3'-C2' | -5.05 | 97.55       | 102.60   |
| 54  | BA    | 2745 | C    | N1-C2-O2    | 5.05  | 121.93      | 118.90   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|-------------|-------|------------------------|---------------------|
| 21  | AA    | 169  | C    | N3-C2-O2    | -5.05 | 118.37                 | 121.90              |
| 21  | AA    | 545  | C    | N1-C2-O2    | 5.05  | 121.93                 | 118.90              |
| 21  | AA    | 1052 | U    | C1'-O4'-C4' | -5.05 | 105.86                 | 109.90              |
| 21  | AA    | 1422 | G    | N3-C4-C5    | -5.05 | 126.08                 | 128.60              |
| 54  | BA    | 364  | C    | N3-C4-C5    | 5.05  | 123.92                 | 121.90              |
| 54  | BA    | 664  | G    | O4'-C1'-N9  | 5.05  | 112.24                 | 108.20              |
| 54  | BA    | 677  | A    | O4'-C4'-C3' | 5.05  | 110.14                 | 106.10              |
| 54  | BA    | 1025 | G    | N3-C2-N2    | -5.05 | 116.37                 | 119.90              |
| 54  | BA    | 1196 | C    | N3-C2-O2    | -5.05 | 118.37                 | 121.90              |
| 54  | BA    | 1685 | C    | O4'-C1'-N1  | 5.05  | 112.24                 | 108.20              |
| 54  | BA    | 1916 | A    | C6-C5-N7    | 5.05  | 135.83                 | 132.30              |
| 54  | BA    | 2451 | A    | C6-C5-N7    | 5.05  | 135.83                 | 132.30              |
| 54  | BA    | 2615 | U    | C5-C6-N1    | -5.05 | 120.18                 | 122.70              |
| 21  | AA    | 128  | G    | N3-C4-C5    | -5.04 | 126.08                 | 128.60              |
| 21  | AA    | 687  | A    | C4-C5-C6    | -5.04 | 114.48                 | 117.00              |
| 21  | AA    | 725  | G    | C8-N9-C4    | -5.04 | 104.38                 | 106.40              |
| 21  | AA    | 1406 | U    | N3-C2-O2    | -5.04 | 118.67                 | 122.20              |
| 54  | BA    | 172  | A    | C6-C5-N7    | 5.04  | 135.83                 | 132.30              |
| 21  | AA    | 421  | U    | N3-C2-O2    | -5.04 | 118.67                 | 122.20              |
| 21  | AA    | 1038 | C    | N3-C2-O2    | -5.04 | 118.37                 | 121.90              |
| 21  | AA    | 1182 | G    | N3-C4-C5    | -5.04 | 126.08                 | 128.60              |
| 21  | AA    | 1259 | C    | C5'-C4'-O4' | 5.04  | 115.15                 | 109.10              |
| 54  | BA    | 303  | G    | C5-C6-N1    | 5.04  | 114.02                 | 111.50              |
| 54  | BA    | 393  | C    | N3-C4-C5    | 5.04  | 123.92                 | 121.90              |
| 54  | BA    | 516  | C    | N3-C4-C5    | 5.04  | 123.92                 | 121.90              |
| 54  | BA    | 1487 | U    | O4'-C1'-N1  | 5.04  | 112.23                 | 108.20              |
| 54  | BA    | 2244 | U    | O4'-C1'-N1  | 5.04  | 112.23                 | 108.20              |
| 54  | BA    | 2744 | G    | N1-C6-O6    | -5.04 | 116.87                 | 119.90              |
| 55  | BB    | 7    | G    | C8-N9-C4    | -5.04 | 104.38                 | 106.40              |
| 55  | BB    | 98   | G    | C8-N9-C4    | -5.04 | 104.38                 | 106.40              |
| 21  | AA    | 649  | A    | C4-C5-C6    | -5.04 | 114.48                 | 117.00              |
| 21  | AA    | 687  | A    | C6-C5-N7    | 5.04  | 135.83                 | 132.30              |
| 54  | BA    | 281  | C    | N1-C2-O2    | 5.04  | 121.92                 | 118.90              |
| 54  | BA    | 430  | A    | C6-C5-N7    | 5.04  | 135.83                 | 132.30              |
| 54  | BA    | 555  | G    | C5-C6-N1    | 5.04  | 114.02                 | 111.50              |
| 54  | BA    | 555  | G    | N1-C6-O6    | -5.04 | 116.88                 | 119.90              |
| 54  | BA    | 710  | U    | N1-C2-N3    | 5.04  | 117.92                 | 114.90              |
| 54  | BA    | 1154 | G    | N3-C4-C5    | -5.04 | 126.08                 | 128.60              |
| 54  | BA    | 1378 | A    | O4'-C4'-C3' | 5.04  | 110.13                 | 106.10              |
| 54  | BA    | 1940 | U    | C5-C6-N1    | -5.04 | 120.18                 | 122.70              |
| 54  | BA    | 2415 | G    | N3-C2-N2    | -5.04 | 116.37                 | 119.90              |
| 54  | BA    | 2670 | A    | C6-C5-N7    | 5.04  | 135.83                 | 132.30              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 55  | BB    | 95   | U    | O4'-C1'-N1  | 5.04  | 112.23      | 108.20   |
| 21  | AA    | 622  | A    | C6-C5-N7    | 5.04  | 135.83      | 132.30   |
| 21  | AA    | 1149 | C    | N3-C2-O2    | -5.04 | 118.37      | 121.90   |
| 54  | BA    | 363  | G    | N3-C4-C5    | -5.04 | 126.08      | 128.60   |
| 54  | BA    | 2159 | G    | O4'-C1'-N9  | 5.04  | 112.23      | 108.20   |
| 54  | BA    | 2597 | G    | N3-C4-C5    | -5.04 | 126.08      | 128.60   |
| 54  | BA    | 2752 | C    | C2-N3-C4    | -5.04 | 117.38      | 119.90   |
| 21  | AA    | 1248 | A    | C5'-C4'-O4' | 5.04  | 115.14      | 109.10   |
| 24  | A3    | 14   | A    | C4-C5-C6    | -5.04 | 114.48      | 117.00   |
| 50  | B1    | 43   | ARG  | NE-CZ-NH2   | -5.04 | 117.78      | 120.30   |
| 54  | BA    | 372  | G    | O4'-C1'-N9  | 5.04  | 112.23      | 108.20   |
| 54  | BA    | 596  | U    | C5-C6-N1    | -5.04 | 120.18      | 122.70   |
| 54  | BA    | 2132 | U    | N3-C2-O2    | -5.04 | 118.67      | 122.20   |
| 54  | BA    | 2668 | G    | O4'-C1'-N9  | 5.04  | 112.23      | 108.20   |
| 54  | BA    | 759  | G    | C8-N9-C4    | -5.04 | 104.39      | 106.40   |
| 54  | BA    | 939  | G    | C5-C6-N1    | 5.04  | 114.02      | 111.50   |
| 3   | AD    | 187  | ARG  | NE-CZ-NH1   | 5.04  | 122.82      | 120.30   |
| 21  | AA    | 343  | U    | C1'-O4'-C4' | -5.04 | 105.87      | 109.90   |
| 21  | AA    | 847  | G    | N3-C4-C5    | -5.04 | 126.08      | 128.60   |
| 21  | AA    | 1113 | C    | N1-C2-O2    | 5.04  | 121.92      | 118.90   |
| 21  | AA    | 1182 | G    | C6-N1-C2    | -5.04 | 122.08      | 125.10   |
| 54  | BA    | 71   | A    | C3'-C2'-C1' | 5.04  | 105.53      | 101.50   |
| 54  | BA    | 1122 | G    | N9-C4-C5    | 5.04  | 107.42      | 105.40   |
| 54  | BA    | 1390 | U    | C4-C5-C6    | 5.04  | 122.72      | 119.70   |
| 54  | BA    | 1399 | C    | N3-C2-O2    | -5.04 | 118.37      | 121.90   |
| 54  | BA    | 1779 | U    | N3-C2-O2    | -5.04 | 118.68      | 122.20   |
| 54  | BA    | 1927 | A    | C8-N9-C4    | -5.04 | 103.79      | 105.80   |
| 21  | AA    | 528  | C    | C2-N3-C4    | -5.03 | 117.38      | 119.90   |
| 21  | AA    | 1453 | G    | C8-N9-C4    | -5.03 | 104.39      | 106.40   |
| 54  | BA    | 250  | G    | O4'-C1'-N9  | 5.03  | 112.23      | 108.20   |
| 54  | BA    | 529  | A    | C2-N3-C4    | 5.03  | 113.12      | 110.60   |
| 54  | BA    | 1349 | C    | N1-C2-O2    | 5.03  | 121.92      | 118.90   |
| 54  | BA    | 1597 | A    | P-O3'-C3'   | 5.03  | 125.74      | 119.70   |
| 54  | BA    | 1996 | C    | N3-C4-N4    | -5.03 | 114.48      | 118.00   |
| 54  | BA    | 2272 | U    | C3'-C2'-C1' | 5.03  | 105.53      | 101.50   |
| 54  | BA    | 2899 | A    | O4'-C1'-N9  | 5.03  | 112.23      | 108.20   |
| 55  | BB    | 75   | G    | C8-N9-C4    | -5.03 | 104.39      | 106.40   |
| 21  | AA    | 826  | C    | O4'-C1'-N1  | 5.03  | 112.23      | 108.20   |
| 21  | AA    | 1001 | C    | N3-C2-O2    | -5.03 | 118.38      | 121.90   |
| 22  | A1    | 69   | A    | C4-C5-C6    | -5.03 | 114.48      | 117.00   |
| 54  | BA    | 435  | C    | N1-C2-O2    | 5.03  | 121.92      | 118.90   |
| 54  | BA    | 2388 | A    | C5-C6-N1    | 5.03  | 120.22      | 117.70   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 9   | AJ    | 45   | ARG  | NE-CZ-NH1   | 5.03  | 122.82      | 120.30   |
| 21  | AA    | 120  | A    | O4'-C4'-C3' | 5.03  | 110.12      | 106.10   |
| 21  | AA    | 412  | A    | C5-C6-N6    | 5.03  | 127.72      | 123.70   |
| 21  | AA    | 420  | U    | C1'-O4'-C4' | -5.03 | 105.88      | 109.90   |
| 54  | BA    | 1770 | G    | C4'-C3'-C2' | -5.03 | 97.57       | 102.60   |
| 54  | BA    | 1994 | C    | C6-N1-C2    | -5.03 | 118.29      | 120.30   |
| 54  | BA    | 2486 | C    | O4'-C1'-N1  | 5.03  | 112.22      | 108.20   |
| 54  | BA    | 2571 | U    | N3-C2-O2    | -5.03 | 118.68      | 122.20   |
| 54  | BA    | 2657 | A    | C5-C6-N1    | 5.03  | 120.22      | 117.70   |
| 55  | BB    | 85   | G    | N3-C2-N2    | -5.03 | 116.38      | 119.90   |
| 16  | AQ    | 76   | ARG  | NE-CZ-NH1   | 5.03  | 122.81      | 120.30   |
| 21  | AA    | 862  | C    | C6-N1-C2    | -5.03 | 118.29      | 120.30   |
| 54  | BA    | 54   | G    | N1-C6-O6    | -5.03 | 116.88      | 119.90   |
| 54  | BA    | 1306 | C    | O4'-C1'-N1  | 5.03  | 112.22      | 108.20   |
| 54  | BA    | 2836 | U    | O4'-C1'-N1  | 5.03  | 112.22      | 108.20   |
| 55  | BB    | 96   | G    | C5-C6-N1    | 5.03  | 114.01      | 111.50   |
| 21  | AA    | 365  | U    | O4'-C1'-N1  | 5.03  | 112.22      | 108.20   |
| 21  | AA    | 523  | A    | P-O3'-C3'   | 5.03  | 125.73      | 119.70   |
| 21  | AA    | 860  | A    | C6-C5-N7    | 5.03  | 135.82      | 132.30   |
| 46  | BX    | 2    | ARG  | NH1-CZ-NH2  | -5.03 | 113.87      | 119.40   |
| 54  | BA    | 107  | G    | C8-N9-C4    | -5.03 | 104.39      | 106.40   |
| 54  | BA    | 1301 | A    | O4'-C1'-N9  | 5.03  | 112.22      | 108.20   |
| 54  | BA    | 1349 | C    | C2-N3-C4    | -5.03 | 117.39      | 119.90   |
| 54  | BA    | 1472 | C    | N3-C4-C5    | 5.03  | 123.91      | 121.90   |
| 54  | BA    | 2155 | U    | C1'-O4'-C4' | -5.03 | 105.88      | 109.90   |
| 54  | BA    | 2629 | U    | C3'-C2'-C1' | 5.03  | 105.52      | 101.50   |
| 21  | AA    | 1049 | U    | O4'-C4'-C3' | 5.03  | 110.12      | 106.10   |
| 54  | BA    | 188  | G    | O4'-C1'-N9  | 5.03  | 112.22      | 108.20   |
| 54  | BA    | 809  | G    | N7-C8-N9    | 5.03  | 115.61      | 113.10   |
| 54  | BA    | 1269 | A    | C5-C6-N1    | 5.03  | 120.21      | 117.70   |
| 54  | BA    | 2029 | G    | N1-C6-O6    | -5.03 | 116.88      | 119.90   |
| 55  | BB    | 15   | A    | C1'-O4'-C4' | -5.03 | 105.88      | 109.90   |
| 21  | AA    | 1104 | G    | N1-C6-O6    | -5.02 | 116.89      | 119.90   |
| 21  | AA    | 1115 | U    | C4-C5-C6    | 5.02  | 122.72      | 119.70   |
| 38  | BP    | 38   | ARG  | NH1-CZ-NH2  | -5.02 | 113.87      | 119.40   |
| 54  | BA    | 55   | G    | O4'-C1'-N9  | 5.02  | 112.22      | 108.20   |
| 54  | BA    | 453  | A    | C4-C5-C6    | -5.02 | 114.49      | 117.00   |
| 54  | BA    | 2024 | G    | C5-C6-N1    | 5.02  | 114.01      | 111.50   |
| 55  | BB    | 37   | C    | C2-N3-C4    | -5.02 | 117.39      | 119.90   |
| 21  | AA    | 52   | C    | N1-C2-O2    | 5.02  | 121.91      | 118.90   |
| 21  | AA    | 508  | U    | N3-C2-O2    | -5.02 | 118.68      | 122.20   |
| 21  | AA    | 551  | U    | N1-C2-N3    | 5.02  | 117.91      | 114.90   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 21  | AA    | 557  | G    | N3-C4-C5    | -5.02 | 126.09      | 128.60   |
| 21  | AA    | 599  | C    | N1-C2-O2    | 5.02  | 121.91      | 118.90   |
| 54  | BA    | 377  | G    | N3-C4-C5    | -5.02 | 126.09      | 128.60   |
| 54  | BA    | 1718 | G    | N3-C4-C5    | -5.02 | 126.09      | 128.60   |
| 54  | BA    | 2787 | C    | C4'-C3'-C2' | -5.02 | 97.58       | 102.60   |
| 54  | BA    | 2830 | C    | N3-C2-O2    | -5.02 | 118.38      | 121.90   |
| 54  | BA    | 2858 | C    | C6-N1-C2    | -5.02 | 118.29      | 120.30   |
| 21  | AA    | 39   | G    | N3-C4-C5    | -5.02 | 126.09      | 128.60   |
| 21  | AA    | 269  | C    | N1-C2-O2    | 5.02  | 121.91      | 118.90   |
| 21  | AA    | 1048 | G    | N3-C4-C5    | -5.02 | 126.09      | 128.60   |
| 21  | AA    | 1386 | G    | C5-C6-N1    | 5.02  | 114.01      | 111.50   |
| 52  | B3    | 12   | ARG  | NH1-CZ-NH2  | -5.02 | 113.88      | 119.40   |
| 54  | BA    | 1324 | G    | C5-C6-N1    | 5.02  | 114.01      | 111.50   |
| 54  | BA    | 1494 | A    | C4-C5-C6    | -5.02 | 114.49      | 117.00   |
| 54  | BA    | 1674 | G    | O4'-C1'-N9  | 5.02  | 112.22      | 108.20   |
| 54  | BA    | 1896 | G    | C5-C6-N1    | 5.02  | 114.01      | 111.50   |
| 54  | BA    | 2251 | G    | N1-C6-O6    | -5.02 | 116.89      | 119.90   |
| 54  | BA    | 2486 | C    | N1-C2-O2    | 5.02  | 121.91      | 118.90   |
| 17  | AR    | 42   | ARG  | NE-CZ-NH1   | 5.02  | 122.81      | 120.30   |
| 21  | AA    | 521  | G    | C5-C6-N1    | 5.02  | 114.01      | 111.50   |
| 21  | AA    | 736  | C    | O4'-C1'-N1  | 5.02  | 112.22      | 108.20   |
| 21  | AA    | 1503 | A    | O4'-C1'-N9  | 5.02  | 112.22      | 108.20   |
| 54  | BA    | 69   | C    | N3-C4-C5    | 5.02  | 123.91      | 121.90   |
| 54  | BA    | 1191 | G    | N3-C4-C5    | -5.02 | 126.09      | 128.60   |
| 54  | BA    | 1382 | G    | N9-C4-C5    | 5.02  | 107.41      | 105.40   |
| 54  | BA    | 1743 | G    | C4'-C3'-C2' | -5.02 | 97.58       | 102.60   |
| 54  | BA    | 1787 | A    | C3'-C2'-C1' | 5.02  | 105.52      | 101.50   |
| 55  | BB    | 48   | U    | O4'-C1'-N1  | 5.02  | 112.22      | 108.20   |
| 21  | AA    | 20   | U    | C4-C5-C6    | 5.02  | 122.71      | 119.70   |
| 21  | AA    | 307  | C    | N3-C4-C5    | 5.02  | 123.91      | 121.90   |
| 21  | AA    | 733  | G    | C1'-O4'-C4' | -5.02 | 105.89      | 109.90   |
| 21  | AA    | 792  | A    | C6-C5-N7    | 5.02  | 135.81      | 132.30   |
| 21  | AA    | 942  | G    | N3-C4-C5    | -5.02 | 126.09      | 128.60   |
| 21  | AA    | 1287 | A    | C6-C5-N7    | 5.02  | 135.81      | 132.30   |
| 54  | BA    | 157  | C    | N3-C2-O2    | -5.02 | 118.39      | 121.90   |
| 54  | BA    | 1269 | A    | C4-C5-C6    | -5.02 | 114.49      | 117.00   |
| 54  | BA    | 2500 | U    | N3-C2-O2    | -5.02 | 118.69      | 122.20   |
| 54  | BA    | 2594 | C    | N3-C2-O2    | -5.02 | 118.39      | 121.90   |
| 54  | BA    | 2704 | C    | N3-C4-N4    | -5.02 | 114.49      | 118.00   |
| 55  | BB    | 75   | G    | N3-C4-C5    | -5.02 | 126.09      | 128.60   |
| 21  | AA    | 552  | U    | N3-C2-O2    | -5.02 | 118.69      | 122.20   |
| 21  | AA    | 702  | A    | O4'-C1'-N9  | 5.02  | 112.21      | 108.20   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 21  | AA    | 867  | G    | C5-C6-N1    | 5.02  | 114.01      | 111.50   |
| 54  | BA    | 591  | U    | O4'-C1'-N1  | 5.02  | 112.21      | 108.20   |
| 54  | BA    | 839  | U    | C3'-C2'-C1' | 5.02  | 105.51      | 101.50   |
| 54  | BA    | 1605 | C    | N3-C2-O2    | -5.02 | 118.39      | 121.90   |
| 54  | BA    | 1969 | A    | C6-C5-N7    | 5.02  | 135.81      | 132.30   |
| 54  | BA    | 2898 | U    | O4'-C1'-N1  | 5.02  | 112.21      | 108.20   |
| 21  | AA    | 1043 | G    | C5-C6-N1    | 5.01  | 114.01      | 111.50   |
| 21  | AA    | 1116 | U    | N1-C2-N3    | 5.01  | 117.91      | 114.90   |
| 21  | AA    | 1349 | A    | C5-C6-N1    | 5.01  | 120.21      | 117.70   |
| 33  | BK    | 105  | ARG  | NE-CZ-NH2   | -5.01 | 117.79      | 120.30   |
| 54  | BA    | 25   | U    | O4'-C1'-N1  | 5.01  | 112.21      | 108.20   |
| 54  | BA    | 101  | A    | C5-C6-N1    | 5.01  | 120.21      | 117.70   |
| 54  | BA    | 1711 | A    | C6-C5-N7    | 5.01  | 135.81      | 132.30   |
| 54  | BA    | 1788 | C    | C2-N3-C4    | -5.01 | 117.39      | 119.90   |
| 54  | BA    | 2154 | A    | C5-C6-N1    | 5.01  | 120.21      | 117.70   |
| 21  | AA    | 207  | C    | C6-N1-C2    | -5.01 | 118.30      | 120.30   |
| 21  | AA    | 405  | U    | O4'-C1'-N1  | 5.01  | 112.21      | 108.20   |
| 21  | AA    | 915  | A    | C6-C5-N7    | 5.01  | 135.81      | 132.30   |
| 21  | AA    | 1303 | C    | N1-C2-O2    | 5.01  | 121.91      | 118.90   |
| 54  | BA    | 1388 | G    | N7-C8-N9    | 5.01  | 115.61      | 113.10   |
| 54  | BA    | 1477 | A    | C2-N3-C4    | 5.01  | 113.11      | 110.60   |
| 54  | BA    | 1671 | U    | O4'-C1'-N1  | 5.01  | 112.21      | 108.20   |
| 54  | BA    | 1893 | C    | N1-C2-O2    | 5.01  | 121.91      | 118.90   |
| 54  | BA    | 2346 | A    | C6-C5-N7    | 5.01  | 135.81      | 132.30   |
| 54  | BA    | 2755 | C    | O4'-C4'-C3' | 5.01  | 110.11      | 106.10   |
| 54  | BA    | 2897 | U    | O4'-C1'-N1  | 5.01  | 112.21      | 108.20   |
| 21  | AA    | 107  | G    | C5-C6-N1    | 5.01  | 114.00      | 111.50   |
| 21  | AA    | 1382 | C    | N3-C2-O2    | -5.01 | 118.39      | 121.90   |
| 24  | A3    | 9    | G    | N1-C6-O6    | -5.01 | 116.89      | 119.90   |
| 54  | BA    | 1106 | G    | C5-C6-N1    | 5.01  | 114.00      | 111.50   |
| 54  | BA    | 1174 | U    | O4'-C1'-N1  | 5.01  | 112.21      | 108.20   |
| 54  | BA    | 1458 | U    | O4'-C1'-N1  | 5.01  | 112.21      | 108.20   |
| 54  | BA    | 1647 | U    | C5-C6-N1    | -5.01 | 120.20      | 122.70   |
| 54  | BA    | 1033 | U    | O4'-C1'-N1  | 5.01  | 112.21      | 108.20   |
| 54  | BA    | 2491 | U    | O4'-C1'-N1  | 5.01  | 112.21      | 108.20   |
| 21  | AA    | 359  | G    | N3-C2-N2    | -5.01 | 116.39      | 119.90   |
| 21  | AA    | 470  | C    | N1-C2-O2    | 5.01  | 121.90      | 118.90   |
| 21  | AA    | 508  | U    | C5-C6-N1    | -5.01 | 120.20      | 122.70   |
| 21  | AA    | 511  | C    | O4'-C1'-N1  | 5.01  | 112.20      | 108.20   |
| 21  | AA    | 710  | G    | C5-C6-N1    | 5.01  | 114.00      | 111.50   |
| 21  | AA    | 1445 | U    | N3-C2-O2    | -5.01 | 118.70      | 122.20   |
| 34  | BL    | 48   | ARG  | NE-CZ-NH1   | 5.01  | 122.80      | 120.30   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|-------------|-------|------------------------|---------------------|
| 54  | BA    | 810  | U    | C1'-O4'-C4' | -5.01 | 105.89                 | 109.90              |
| 54  | BA    | 1094 | U    | N1-C2-N3    | 5.01  | 117.90                 | 114.90              |
| 54  | BA    | 1426 | G    | N1-C6-O6    | -5.01 | 116.90                 | 119.90              |
| 54  | BA    | 1449 | G    | O4'-C1'-N9  | 5.01  | 112.20                 | 108.20              |
| 54  | BA    | 1541 | C    | O4'-C1'-N1  | 5.01  | 112.20                 | 108.20              |
| 54  | BA    | 2140 | G    | N9-C4-C5    | 5.01  | 107.40                 | 105.40              |
| 54  | BA    | 2395 | C    | P-O3'-C3'   | 5.01  | 125.71                 | 119.70              |
| 54  | BA    | 2446 | G    | C4'-C3'-C2' | -5.01 | 97.59                  | 102.60              |
| 55  | BB    | 64   | G    | C8-N9-C4    | -5.01 | 104.40                 | 106.40              |
| 21  | AA    | 45   | G    | C3'-C2'-C1' | 5.00  | 105.50                 | 101.50              |
| 54  | BA    | 1946 | U    | N3-C2-O2    | -5.00 | 118.70                 | 122.20              |
| 54  | BA    | 2398 | U    | C5-C6-N1    | -5.00 | 120.20                 | 122.70              |
| 54  | BA    | 2683 | C    | C2-N3-C4    | -5.00 | 117.40                 | 119.90              |
| 55  | BB    | 65   | U    | N1-C2-N3    | 5.00  | 117.90                 | 114.90              |
| 21  | AA    | 40   | C    | O4'-C1'-N1  | 5.00  | 112.20                 | 108.20              |
| 21  | AA    | 618  | C    | N3-C2-O2    | -5.00 | 118.40                 | 121.90              |
| 21  | AA    | 843  | U    | N3-C2-O2    | -5.00 | 118.70                 | 122.20              |
| 21  | AA    | 1471 | U    | N1-C2-N3    | 5.00  | 117.90                 | 114.90              |
| 33  | BK    | 70   | ARG  | NE-CZ-NH1   | 5.00  | 122.80                 | 120.30              |
| 54  | BA    | 669  | G    | O4'-C1'-N9  | 5.00  | 112.20                 | 108.20              |
| 54  | BA    | 752  | A    | C3'-C2'-C1' | -5.00 | 97.50                  | 101.50              |
| 54  | BA    | 2047 | C    | O4'-C1'-N1  | 5.00  | 112.20                 | 108.20              |
| 54  | BA    | 2692 | G    | N1-C6-O6    | -5.00 | 116.90                 | 119.90              |
| 21  | AA    | 122  | G    | N3-C2-N2    | -5.00 | 116.40                 | 119.90              |
| 21  | AA    | 543  | U    | O4'-C1'-N1  | 5.00  | 112.20                 | 108.20              |
| 21  | AA    | 642  | A    | C4-C5-C6    | -5.00 | 114.50                 | 117.00              |
| 21  | AA    | 846  | G    | C8-N9-C4    | -5.00 | 104.40                 | 106.40              |
| 21  | AA    | 985  | C    | N1-C2-O2    | 5.00  | 121.90                 | 118.90              |
| 21  | AA    | 1126 | U    | C5-C6-N1    | -5.00 | 120.20                 | 122.70              |
| 21  | AA    | 1390 | U    | C3'-C2'-C1' | 5.00  | 105.50                 | 101.50              |
| 21  | AA    | 1421 | G    | O4'-C1'-N9  | 5.00  | 112.20                 | 108.20              |
| 54  | BA    | 39   | G    | N9-C4-C5    | 5.00  | 107.40                 | 105.40              |
| 54  | BA    | 1625 | C    | N1-C2-O2    | 5.00  | 121.90                 | 118.90              |
| 54  | BA    | 1988 | G    | C5-C6-N1    | 5.00  | 114.00                 | 111.50              |
| 54  | BA    | 2780 | G    | N3-C4-C5    | -5.00 | 126.10                 | 128.60              |

There are no chirality outliers.

All (1094) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 22  | A1    | 23  | A    | Sidechain |
| 22  | A1    | 26  | A    | Sidechain |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 22  | A1    | 31   | C    | Sidechain |
| 22  | A1    | 45   | G    | Sidechain |
| 22  | A1    | 49   | G    | Sidechain |
| 22  | A1    | 57   | G    | Sidechain |
| 22  | A1    | 59   | U    | Sidechain |
| 22  | A1    | 70   | C    | Sidechain |
| 22  | A1    | 72   | C    | Sidechain |
| 22  | A1    | 74   | C    | Sidechain |
| 23  | A2    | 81   | U    | Sidechain |
| 24  | A3    | 11   | A    | Sidechain |
| 24  | A3    | 24   | C    | Sidechain |
| 24  | A3    | 25   | U    | Sidechain |
| 24  | A3    | 27   | G    | Sidechain |
| 24  | A3    | 32   | G    | Sidechain |
| 24  | A3    | 34   | U    | Sidechain |
| 24  | A3    | 37   | U    | Sidechain |
| 24  | A3    | 47   | G    | Sidechain |
| 24  | A3    | 57   | C    | Sidechain |
| 24  | A3    | 71   | G    | Sidechain |
| 24  | A3    | 73   | A    | Sidechain |
| 24  | A3    | 76   | C    | Sidechain |
| 24  | A3    | 77   | A    | Sidechain |
| 24  | A3    | 9    | G    | Sidechain |
| 21  | AA    | 100  | G    | Sidechain |
| 21  | AA    | 1002 | G    | Sidechain |
| 21  | AA    | 1010 | U    | Sidechain |
| 21  | AA    | 1013 | G    | Sidechain |
| 21  | AA    | 1021 | A    | Sidechain |
| 21  | AA    | 1025 | U    | Sidechain |
| 21  | AA    | 1045 | C    | Sidechain |
| 21  | AA    | 1049 | U    | Sidechain |
| 21  | AA    | 1054 | C    | Sidechain |
| 21  | AA    | 1058 | G    | Sidechain |
| 21  | AA    | 1059 | C    | Sidechain |
| 21  | AA    | 1067 | A    | Sidechain |
| 21  | AA    | 107  | G    | Sidechain |
| 21  | AA    | 1077 | G    | Sidechain |
| 21  | AA    | 1085 | U    | Sidechain |
| 21  | AA    | 109  | A    | Sidechain |
| 21  | AA    | 1091 | U    | Sidechain |
| 21  | AA    | 1093 | A    | Sidechain |
| 21  | AA    | 110  | C    | Sidechain |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 21  | AA    | 1103 | C    | Sidechain |
| 21  | AA    | 1106 | G    | Sidechain |
| 21  | AA    | 1107 | C    | Sidechain |
| 21  | AA    | 1108 | G    | Sidechain |
| 21  | AA    | 111  | G    | Sidechain |
| 21  | AA    | 1112 | C    | Sidechain |
| 21  | AA    | 1115 | U    | Sidechain |
| 21  | AA    | 1118 | U    | Sidechain |
| 21  | AA    | 1120 | C    | Sidechain |
| 21  | AA    | 1126 | U    | Sidechain |
| 21  | AA    | 1131 | G    | Sidechain |
| 21  | AA    | 1133 | G    | Sidechain |
| 21  | AA    | 1136 | C    | Sidechain |
| 21  | AA    | 114  | U    | Sidechain |
| 21  | AA    | 1142 | G    | Sidechain |
| 21  | AA    | 1146 | A    | Sidechain |
| 21  | AA    | 1159 | U    | Sidechain |
| 21  | AA    | 116  | A    | Sidechain |
| 21  | AA    | 1160 | G    | Sidechain |
| 21  | AA    | 1162 | C    | Sidechain |
| 21  | AA    | 1165 | U    | Sidechain |
| 21  | AA    | 1168 | U    | Sidechain |
| 21  | AA    | 117  | G    | Sidechain |
| 21  | AA    | 1170 | A    | Sidechain |
| 21  | AA    | 1178 | G    | Sidechain |
| 21  | AA    | 1189 | U    | Sidechain |
| 21  | AA    | 119  | A    | Sidechain |
| 21  | AA    | 1191 | A    | Sidechain |
| 21  | AA    | 1194 | U    | Sidechain |
| 21  | AA    | 1201 | A    | Sidechain |
| 21  | AA    | 1204 | A    | Sidechain |
| 21  | AA    | 1211 | U    | Sidechain |
| 21  | AA    | 1215 | G    | Sidechain |
| 21  | AA    | 122  | G    | Sidechain |
| 21  | AA    | 1221 | G    | Sidechain |
| 21  | AA    | 1223 | C    | Sidechain |
| 21  | AA    | 1224 | U    | Sidechain |
| 21  | AA    | 1227 | A    | Sidechain |
| 21  | AA    | 123  | U    | Sidechain |
| 21  | AA    | 1231 | G    | Sidechain |
| 21  | AA    | 1234 | C    | Sidechain |
| 21  | AA    | 1249 | C    | Sidechain |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 21  | AA    | 125  | U    | Sidechain |
| 21  | AA    | 1257 | A    | Sidechain |
| 21  | AA    | 1263 | C    | Sidechain |
| 21  | AA    | 1264 | U    | Sidechain |
| 21  | AA    | 1266 | G    | Sidechain |
| 21  | AA    | 1267 | C    | Sidechain |
| 21  | AA    | 1270 | G    | Sidechain |
| 21  | AA    | 1271 | A    | Sidechain |
| 21  | AA    | 1276 | G    | Sidechain |
| 21  | AA    | 1279 | G    | Sidechain |
| 21  | AA    | 1281 | C    | Sidechain |
| 21  | AA    | 1283 | U    | Sidechain |
| 21  | AA    | 1289 | A    | Sidechain |
| 21  | AA    | 1296 | C    | Sidechain |
| 21  | AA    | 130  | A    | Sidechain |
| 21  | AA    | 1300 | G    | Sidechain |
| 21  | AA    | 1303 | C    | Sidechain |
| 21  | AA    | 1305 | G    | Sidechain |
| 21  | AA    | 1307 | U    | Sidechain |
| 21  | AA    | 1308 | U    | Sidechain |
| 21  | AA    | 1309 | G    | Sidechain |
| 21  | AA    | 1311 | A    | Sidechain |
| 21  | AA    | 1312 | G    | Sidechain |
| 21  | AA    | 1316 | G    | Sidechain |
| 21  | AA    | 1319 | A    | Sidechain |
| 21  | AA    | 1336 | C    | Sidechain |
| 21  | AA    | 1339 | A    | Sidechain |
| 21  | AA    | 1342 | C    | Sidechain |
| 21  | AA    | 1343 | G    | Sidechain |
| 21  | AA    | 1345 | U    | Sidechain |
| 21  | AA    | 1347 | G    | Sidechain |
| 21  | AA    | 1351 | U    | Sidechain |
| 21  | AA    | 1356 | G    | Sidechain |
| 21  | AA    | 1358 | U    | Sidechain |
| 21  | AA    | 1360 | A    | Sidechain |
| 21  | AA    | 1361 | G    | Sidechain |
| 21  | AA    | 1363 | A    | Sidechain |
| 21  | AA    | 1370 | G    | Sidechain |
| 21  | AA    | 1377 | A    | Sidechain |
| 21  | AA    | 1378 | C    | Sidechain |
| 21  | AA    | 1380 | U    | Sidechain |
| 21  | AA    | 1387 | G    | Sidechain |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 21  | AA    | 1388 | C    | Sidechain |
| 21  | AA    | 139  | A    | Sidechain |
| 21  | AA    | 1397 | C    | Sidechain |
| 21  | AA    | 1405 | G    | Sidechain |
| 21  | AA    | 1414 | U    | Sidechain |
| 21  | AA    | 1415 | G    | Sidechain |
| 21  | AA    | 1416 | G    | Sidechain |
| 21  | AA    | 1417 | G    | Sidechain |
| 21  | AA    | 1420 | U    | Sidechain |
| 21  | AA    | 1421 | G    | Sidechain |
| 21  | AA    | 1423 | G    | Sidechain |
| 21  | AA    | 1427 | C    | Sidechain |
| 21  | AA    | 1430 | A    | Sidechain |
| 21  | AA    | 1431 | A    | Sidechain |
| 21  | AA    | 1438 | G    | Sidechain |
| 21  | AA    | 1441 | A    | Sidechain |
| 21  | AA    | 1442 | G    | Sidechain |
| 21  | AA    | 1446 | A    | Sidechain |
| 21  | AA    | 1449 | C    | Sidechain |
| 21  | AA    | 1451 | U    | Sidechain |
| 21  | AA    | 1455 | G    | Sidechain |
| 21  | AA    | 1459 | G    | Sidechain |
| 21  | AA    | 1460 | C    | Sidechain |
| 21  | AA    | 1461 | G    | Sidechain |
| 21  | AA    | 1464 | U    | Sidechain |
| 21  | AA    | 1470 | U    | Sidechain |
| 21  | AA    | 1479 | C    | Sidechain |
| 21  | AA    | 148  | G    | Sidechain |
| 21  | AA    | 1485 | U    | Sidechain |
| 21  | AA    | 1496 | C    | Sidechain |
| 21  | AA    | 150  | U    | Sidechain |
| 21  | AA    | 1503 | A    | Sidechain |
| 21  | AA    | 151  | A    | Sidechain |
| 21  | AA    | 1516 | G    | Sidechain |
| 21  | AA    | 1519 | A    | Sidechain |
| 21  | AA    | 1525 | G    | Sidechain |
| 21  | AA    | 1526 | G    | Sidechain |
| 21  | AA    | 1529 | G    | Sidechain |
| 21  | AA    | 1530 | G    | Sidechain |
| 21  | AA    | 1532 | U    | Sidechain |
| 21  | AA    | 1534 | A    | Sidechain |
| 21  | AA    | 163  | C    | Sidechain |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 21  | AA    | 164 | G    | Sidechain |
| 21  | AA    | 165 | G    | Sidechain |
| 21  | AA    | 169 | C    | Sidechain |
| 21  | AA    | 173 | U    | Sidechain |
| 21  | AA    | 183 | C    | Sidechain |
| 21  | AA    | 187 | G    | Sidechain |
| 21  | AA    | 188 | C    | Sidechain |
| 21  | AA    | 195 | A    | Sidechain |
| 21  | AA    | 196 | A    | Sidechain |
| 21  | AA    | 20  | U    | Sidechain |
| 21  | AA    | 205 | A    | Sidechain |
| 21  | AA    | 210 | C    | Sidechain |
| 21  | AA    | 211 | G    | Sidechain |
| 21  | AA    | 215 | C    | Sidechain |
| 21  | AA    | 217 | C    | Sidechain |
| 21  | AA    | 218 | U    | Sidechain |
| 21  | AA    | 219 | U    | Sidechain |
| 21  | AA    | 232 | G    | Sidechain |
| 21  | AA    | 234 | C    | Sidechain |
| 21  | AA    | 235 | C    | Sidechain |
| 21  | AA    | 242 | G    | Sidechain |
| 21  | AA    | 245 | U    | Sidechain |
| 21  | AA    | 25  | C    | Sidechain |
| 21  | AA    | 256 | U    | Sidechain |
| 21  | AA    | 259 | G    | Sidechain |
| 21  | AA    | 261 | U    | Sidechain |
| 21  | AA    | 262 | A    | Sidechain |
| 21  | AA    | 263 | A    | Sidechain |
| 21  | AA    | 267 | C    | Sidechain |
| 21  | AA    | 27  | G    | Sidechain |
| 21  | AA    | 278 | G    | Sidechain |
| 21  | AA    | 280 | C    | Sidechain |
| 21  | AA    | 281 | G    | Sidechain |
| 21  | AA    | 29  | U    | Sidechain |
| 21  | AA    | 297 | G    | Sidechain |
| 21  | AA    | 309 | A    | Sidechain |
| 21  | AA    | 31  | G    | Sidechain |
| 21  | AA    | 313 | A    | Sidechain |
| 21  | AA    | 319 | G    | Sidechain |
| 21  | AA    | 321 | A    | Sidechain |
| 21  | AA    | 324 | G    | Sidechain |
| 21  | AA    | 326 | G    | Sidechain |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 21  | AA    | 328 | C    | Sidechain |
| 21  | AA    | 330 | C    | Sidechain |
| 21  | AA    | 331 | G    | Sidechain |
| 21  | AA    | 338 | A    | Sidechain |
| 21  | AA    | 340 | U    | Sidechain |
| 21  | AA    | 343 | U    | Sidechain |
| 21  | AA    | 346 | G    | Sidechain |
| 21  | AA    | 347 | G    | Sidechain |
| 21  | AA    | 349 | A    | Sidechain |
| 21  | AA    | 350 | G    | Sidechain |
| 21  | AA    | 353 | A    | Sidechain |
| 21  | AA    | 36  | C    | Sidechain |
| 21  | AA    | 362 | G    | Sidechain |
| 21  | AA    | 363 | A    | Sidechain |
| 21  | AA    | 37  | U    | Sidechain |
| 21  | AA    | 372 | C    | Sidechain |
| 21  | AA    | 375 | U    | Sidechain |
| 21  | AA    | 380 | G    | Sidechain |
| 21  | AA    | 389 | A    | Sidechain |
| 21  | AA    | 390 | U    | Sidechain |
| 21  | AA    | 397 | A    | Sidechain |
| 21  | AA    | 399 | G    | Sidechain |
| 21  | AA    | 400 | C    | Sidechain |
| 21  | AA    | 402 | G    | Sidechain |
| 21  | AA    | 408 | A    | Sidechain |
| 21  | AA    | 413 | G    | Sidechain |
| 21  | AA    | 429 | U    | Sidechain |
| 21  | AA    | 431 | A    | Sidechain |
| 21  | AA    | 432 | A    | Sidechain |
| 21  | AA    | 436 | C    | Sidechain |
| 21  | AA    | 439 | U    | Sidechain |
| 21  | AA    | 448 | A    | Sidechain |
| 21  | AA    | 449 | G    | Sidechain |
| 21  | AA    | 458 | U    | Sidechain |
| 21  | AA    | 461 | A    | Sidechain |
| 21  | AA    | 465 | A    | Sidechain |
| 21  | AA    | 466 | A    | Sidechain |
| 21  | AA    | 475 | C    | Sidechain |
| 21  | AA    | 479 | U    | Sidechain |
| 21  | AA    | 483 | C    | Sidechain |
| 21  | AA    | 484 | G    | Sidechain |
| 21  | AA    | 485 | U    | Sidechain |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 21  | AA    | 497 | G    | Sidechain |
| 21  | AA    | 499 | A    | Sidechain |
| 21  | AA    | 507 | C    | Sidechain |
| 21  | AA    | 511 | C    | Sidechain |
| 21  | AA    | 515 | G    | Sidechain |
| 21  | AA    | 517 | G    | Sidechain |
| 21  | AA    | 518 | C    | Sidechain |
| 21  | AA    | 519 | C    | Sidechain |
| 21  | AA    | 520 | A    | Sidechain |
| 21  | AA    | 527 | G    | Sidechain |
| 21  | AA    | 529 | G    | Sidechain |
| 21  | AA    | 530 | G    | Sidechain |
| 21  | AA    | 533 | A    | Sidechain |
| 21  | AA    | 54  | C    | Sidechain |
| 21  | AA    | 542 | G    | Sidechain |
| 21  | AA    | 549 | C    | Sidechain |
| 21  | AA    | 55  | A    | Sidechain |
| 21  | AA    | 555 | U    | Sidechain |
| 21  | AA    | 562 | U    | Sidechain |
| 21  | AA    | 563 | A    | Sidechain |
| 21  | AA    | 564 | C    | Sidechain |
| 21  | AA    | 566 | G    | Sidechain |
| 21  | AA    | 568 | G    | Sidechain |
| 21  | AA    | 586 | C    | Sidechain |
| 21  | AA    | 588 | G    | Sidechain |
| 21  | AA    | 591 | U    | Sidechain |
| 21  | AA    | 6   | G    | Sidechain |
| 21  | AA    | 60  | A    | Sidechain |
| 21  | AA    | 600 | A    | Sidechain |
| 21  | AA    | 61  | G    | Sidechain |
| 21  | AA    | 610 | U    | Sidechain |
| 21  | AA    | 615 | G    | Sidechain |
| 21  | AA    | 618 | C    | Sidechain |
| 21  | AA    | 621 | A    | Sidechain |
| 21  | AA    | 623 | C    | Sidechain |
| 21  | AA    | 634 | C    | Sidechain |
| 21  | AA    | 639 | G    | Sidechain |
| 21  | AA    | 650 | G    | Sidechain |
| 21  | AA    | 653 | U    | Sidechain |
| 21  | AA    | 654 | G    | Sidechain |
| 21  | AA    | 656 | G    | Sidechain |
| 21  | AA    | 660 | C    | Sidechain |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 21  | AA    | 664 | G    | Sidechain |
| 21  | AA    | 666 | G    | Sidechain |
| 21  | AA    | 669 | G    | Sidechain |
| 21  | AA    | 678 | U    | Sidechain |
| 21  | AA    | 68  | G    | Sidechain |
| 21  | AA    | 682 | G    | Sidechain |
| 21  | AA    | 683 | G    | Sidechain |
| 21  | AA    | 689 | C    | Sidechain |
| 21  | AA    | 69  | G    | Sidechain |
| 21  | AA    | 691 | G    | Sidechain |
| 21  | AA    | 695 | A    | Sidechain |
| 21  | AA    | 698 | G    | Sidechain |
| 21  | AA    | 700 | G    | Sidechain |
| 21  | AA    | 701 | U    | Sidechain |
| 21  | AA    | 702 | A    | Sidechain |
| 21  | AA    | 704 | A    | Sidechain |
| 21  | AA    | 705 | G    | Sidechain |
| 21  | AA    | 717 | U    | Sidechain |
| 21  | AA    | 725 | G    | Sidechain |
| 21  | AA    | 727 | G    | Sidechain |
| 21  | AA    | 730 | G    | Sidechain |
| 21  | AA    | 734 | G    | Sidechain |
| 21  | AA    | 743 | A    | Sidechain |
| 21  | AA    | 75  | G    | Sidechain |
| 21  | AA    | 752 | G    | Sidechain |
| 21  | AA    | 753 | A    | Sidechain |
| 21  | AA    | 76  | G    | Sidechain |
| 21  | AA    | 760 | G    | Sidechain |
| 21  | AA    | 761 | G    | Sidechain |
| 21  | AA    | 763 | G    | Sidechain |
| 21  | AA    | 764 | C    | Sidechain |
| 21  | AA    | 765 | G    | Sidechain |
| 21  | AA    | 772 | U    | Sidechain |
| 21  | AA    | 774 | G    | Sidechain |
| 21  | AA    | 778 | G    | Sidechain |
| 21  | AA    | 796 | C    | Sidechain |
| 21  | AA    | 81  | A    | Sidechain |
| 21  | AA    | 810 | C    | Sidechain |
| 21  | AA    | 811 | C    | Sidechain |
| 21  | AA    | 812 | G    | Sidechain |
| 21  | AA    | 818 | G    | Sidechain |
| 21  | AA    | 820 | U    | Sidechain |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 21  | AA    | 826 | C    | Sidechain |
| 21  | AA    | 827 | U    | Sidechain |
| 21  | AA    | 834 | U    | Sidechain |
| 21  | AA    | 836 | G    | Sidechain |
| 21  | AA    | 84  | U    | Sidechain |
| 21  | AA    | 841 | C    | Sidechain |
| 21  | AA    | 842 | U    | Sidechain |
| 21  | AA    | 849 | G    | Sidechain |
| 21  | AA    | 855 | U    | Sidechain |
| 21  | AA    | 858 | G    | Sidechain |
| 21  | AA    | 859 | G    | Sidechain |
| 21  | AA    | 863 | U    | Sidechain |
| 21  | AA    | 866 | C    | Sidechain |
| 21  | AA    | 869 | G    | Sidechain |
| 21  | AA    | 871 | U    | Sidechain |
| 21  | AA    | 88  | U    | Sidechain |
| 21  | AA    | 887 | G    | Sidechain |
| 21  | AA    | 888 | G    | Sidechain |
| 21  | AA    | 890 | G    | Sidechain |
| 21  | AA    | 891 | U    | Sidechain |
| 21  | AA    | 895 | G    | Sidechain |
| 21  | AA    | 898 | G    | Sidechain |
| 21  | AA    | 9   | G    | Sidechain |
| 21  | AA    | 903 | G    | Sidechain |
| 21  | AA    | 905 | U    | Sidechain |
| 21  | AA    | 91  | U    | Sidechain |
| 21  | AA    | 911 | U    | Sidechain |
| 21  | AA    | 916 | U    | Sidechain |
| 21  | AA    | 919 | A    | Sidechain |
| 21  | AA    | 921 | U    | Sidechain |
| 21  | AA    | 927 | G    | Sidechain |
| 21  | AA    | 931 | C    | Sidechain |
| 21  | AA    | 936 | C    | Sidechain |
| 21  | AA    | 937 | A    | Sidechain |
| 21  | AA    | 938 | A    | Sidechain |
| 21  | AA    | 941 | G    | Sidechain |
| 21  | AA    | 944 | G    | Sidechain |
| 21  | AA    | 951 | G    | Sidechain |
| 21  | AA    | 957 | U    | Sidechain |
| 21  | AA    | 960 | U    | Sidechain |
| 21  | AA    | 961 | U    | Sidechain |
| 21  | AA    | 962 | C    | Sidechain |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 21  | AA    | 968  | A    | Sidechain |
| 21  | AA    | 976  | G    | Sidechain |
| 21  | AA    | 977  | A    | Sidechain |
| 21  | AA    | 978  | A    | Sidechain |
| 21  | AA    | 982  | U    | Sidechain |
| 21  | AA    | 985  | C    | Sidechain |
| 21  | AA    | 989  | U    | Sidechain |
| 21  | AA    | 992  | U    | Sidechain |
| 21  | AA    | 995  | C    | Sidechain |
| 21  | AA    | 997  | U    | Sidechain |
| 2   | AC    | 168  | ARG  | Sidechain |
| 2   | AC    | 172  | VAL  | Peptide   |
| 8   | AI    | 124  | PRO  | Peptide   |
| 10  | AK    | 115  | ILE  | Peptide   |
| 54  | BA    | 10   | A    | Sidechain |
| 54  | BA    | 100  | U    | Sidechain |
| 54  | BA    | 1000 | A    | Sidechain |
| 54  | BA    | 1006 | C    | Sidechain |
| 54  | BA    | 1009 | A    | Sidechain |
| 54  | BA    | 1020 | A    | Sidechain |
| 54  | BA    | 1025 | G    | Sidechain |
| 54  | BA    | 1026 | G    | Sidechain |
| 54  | BA    | 103  | A    | Sidechain |
| 54  | BA    | 1042 | G    | Sidechain |
| 54  | BA    | 1046 | A    | Sidechain |
| 54  | BA    | 1047 | G    | Sidechain |
| 54  | BA    | 1050 | A    | Sidechain |
| 54  | BA    | 1056 | G    | Sidechain |
| 54  | BA    | 106  | C    | Sidechain |
| 54  | BA    | 1066 | U    | Sidechain |
| 54  | BA    | 1069 | A    | Sidechain |
| 54  | BA    | 1074 | G    | Sidechain |
| 54  | BA    | 1079 | C    | Sidechain |
| 54  | BA    | 1086 | A    | Sidechain |
| 54  | BA    | 1088 | A    | Sidechain |
| 54  | BA    | 1095 | A    | Sidechain |
| 54  | BA    | 1098 | A    | Sidechain |
| 54  | BA    | 1101 | U    | Sidechain |
| 54  | BA    | 1106 | G    | Sidechain |
| 54  | BA    | 1127 | A    | Sidechain |
| 54  | BA    | 1130 | U    | Sidechain |
| 54  | BA    | 1131 | G    | Sidechain |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 54  | BA    | 1132 | U    | Sidechain |
| 54  | BA    | 1133 | A    | Sidechain |
| 54  | BA    | 1135 | C    | Sidechain |
| 54  | BA    | 1138 | G    | Sidechain |
| 54  | BA    | 1139 | G    | Sidechain |
| 54  | BA    | 1140 | C    | Sidechain |
| 54  | BA    | 1160 | G    | Sidechain |
| 54  | BA    | 117  | G    | Sidechain |
| 54  | BA    | 1179 | G    | Sidechain |
| 54  | BA    | 1188 | U    | Sidechain |
| 54  | BA    | 119  | A    | Sidechain |
| 54  | BA    | 1191 | G    | Sidechain |
| 54  | BA    | 1193 | G    | Sidechain |
| 54  | BA    | 1199 | U    | Sidechain |
| 54  | BA    | 1200 | C    | Sidechain |
| 54  | BA    | 1203 | U    | Sidechain |
| 54  | BA    | 1209 | U    | Sidechain |
| 54  | BA    | 1210 | G    | Sidechain |
| 54  | BA    | 1212 | G    | Sidechain |
| 54  | BA    | 1215 | G    | Sidechain |
| 54  | BA    | 1224 | U    | Sidechain |
| 54  | BA    | 1225 | G    | Sidechain |
| 54  | BA    | 1226 | A    | Sidechain |
| 54  | BA    | 1232 | G    | Sidechain |
| 54  | BA    | 1233 | C    | Sidechain |
| 54  | BA    | 1235 | G    | Sidechain |
| 54  | BA    | 1236 | G    | Sidechain |
| 54  | BA    | 1237 | A    | Sidechain |
| 54  | BA    | 1244 | A    | Sidechain |
| 54  | BA    | 1248 | G    | Sidechain |
| 54  | BA    | 1251 | C    | Sidechain |
| 54  | BA    | 1253 | A    | Sidechain |
| 54  | BA    | 1256 | G    | Sidechain |
| 54  | BA    | 1259 | G    | Sidechain |
| 54  | BA    | 1266 | G    | Sidechain |
| 54  | BA    | 1268 | A    | Sidechain |
| 54  | BA    | 1270 | C    | Sidechain |
| 54  | BA    | 1272 | A    | Sidechain |
| 54  | BA    | 1276 | A    | Sidechain |
| 54  | BA    | 1283 | G    | Sidechain |
| 54  | BA    | 1287 | A    | Sidechain |
| 54  | BA    | 1288 | G    | Sidechain |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 54  | BA    | 1291 | C    | Sidechain |
| 54  | BA    | 1292 | G    | Sidechain |
| 54  | BA    | 1293 | C    | Sidechain |
| 54  | BA    | 1297 | C    | Sidechain |
| 54  | BA    | 13   | A    | Sidechain |
| 54  | BA    | 1300 | G    | Sidechain |
| 54  | BA    | 1302 | A    | Sidechain |
| 54  | BA    | 1308 | A    | Sidechain |
| 54  | BA    | 1310 | G    | Sidechain |
| 54  | BA    | 1314 | C    | Sidechain |
| 54  | BA    | 1315 | C    | Sidechain |
| 54  | BA    | 1317 | G    | Sidechain |
| 54  | BA    | 1319 | C    | Sidechain |
| 54  | BA    | 1320 | C    | Sidechain |
| 54  | BA    | 1324 | G    | Sidechain |
| 54  | BA    | 1326 | U    | Sidechain |
| 54  | BA    | 1327 | A    | Sidechain |
| 54  | BA    | 1330 | C    | Sidechain |
| 54  | BA    | 1334 | G    | Sidechain |
| 54  | BA    | 1340 | U    | Sidechain |
| 54  | BA    | 1342 | A    | Sidechain |
| 54  | BA    | 1347 | A    | Sidechain |
| 54  | BA    | 1350 | C    | Sidechain |
| 54  | BA    | 1356 | G    | Sidechain |
| 54  | BA    | 1360 | G    | Sidechain |
| 54  | BA    | 1364 | G    | Sidechain |
| 54  | BA    | 1370 | C    | Sidechain |
| 54  | BA    | 1374 | G    | Sidechain |
| 54  | BA    | 1376 | C    | Sidechain |
| 54  | BA    | 1382 | G    | Sidechain |
| 54  | BA    | 1387 | A    | Sidechain |
| 54  | BA    | 1389 | G    | Sidechain |
| 54  | BA    | 1390 | U    | Sidechain |
| 54  | BA    | 1391 | U    | Sidechain |
| 54  | BA    | 1394 | U    | Sidechain |
| 54  | BA    | 1399 | C    | Sidechain |
| 54  | BA    | 1403 | A    | Sidechain |
| 54  | BA    | 1411 | U    | Sidechain |
| 54  | BA    | 1412 | U    | Sidechain |
| 54  | BA    | 1418 | G    | Sidechain |
| 54  | BA    | 1419 | A    | Sidechain |
| 54  | BA    | 1421 | G    | Sidechain |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 54  | BA    | 1425 | G    | Sidechain |
| 54  | BA    | 1431 | A    | Sidechain |
| 54  | BA    | 1432 | G    | Sidechain |
| 54  | BA    | 1441 | G    | Sidechain |
| 54  | BA    | 1445 | G    | Sidechain |
| 54  | BA    | 1452 | G    | Sidechain |
| 54  | BA    | 1453 | A    | Sidechain |
| 54  | BA    | 1454 | C    | Sidechain |
| 54  | BA    | 1460 | U    | Sidechain |
| 54  | BA    | 1464 | G    | Sidechain |
| 54  | BA    | 147  | C    | Sidechain |
| 54  | BA    | 1470 | A    | Sidechain |
| 54  | BA    | 1483 | G    | Sidechain |
| 54  | BA    | 1484 | U    | Sidechain |
| 54  | BA    | 1492 | G    | Sidechain |
| 54  | BA    | 1498 | C    | Sidechain |
| 54  | BA    | 1505 | A    | Sidechain |
| 54  | BA    | 1510 | G    | Sidechain |
| 54  | BA    | 1519 | G    | Sidechain |
| 54  | BA    | 152  | A    | Sidechain |
| 54  | BA    | 1520 | U    | Sidechain |
| 54  | BA    | 1522 | A    | Sidechain |
| 54  | BA    | 1525 | A    | Sidechain |
| 54  | BA    | 1526 | C    | Sidechain |
| 54  | BA    | 1529 | G    | Sidechain |
| 54  | BA    | 153  | U    | Sidechain |
| 54  | BA    | 1536 | C    | Sidechain |
| 54  | BA    | 1537 | G    | Sidechain |
| 54  | BA    | 1539 | U    | Sidechain |
| 54  | BA    | 154  | U    | Sidechain |
| 54  | BA    | 1546 | G    | Sidechain |
| 54  | BA    | 1547 | C    | Sidechain |
| 54  | BA    | 1552 | A    | Sidechain |
| 54  | BA    | 1554 | U    | Sidechain |
| 54  | BA    | 1555 | G    | Sidechain |
| 54  | BA    | 156  | A    | Sidechain |
| 54  | BA    | 1560 | G    | Sidechain |
| 54  | BA    | 1561 | C    | Sidechain |
| 54  | BA    | 1562 | U    | Sidechain |
| 54  | BA    | 1567 | G    | Sidechain |
| 54  | BA    | 1581 | G    | Sidechain |
| 54  | BA    | 1585 | C    | Sidechain |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 54  | BA    | 1595 | C    | Sidechain |
| 54  | BA    | 1600 | C    | Sidechain |
| 54  | BA    | 1601 | G    | Sidechain |
| 54  | BA    | 1602 | U    | Sidechain |
| 54  | BA    | 1618 | A    | Sidechain |
| 54  | BA    | 1621 | U    | Sidechain |
| 54  | BA    | 1632 | A    | Sidechain |
| 54  | BA    | 1633 | G    | Sidechain |
| 54  | BA    | 1636 | U    | Sidechain |
| 54  | BA    | 1641 | A    | Sidechain |
| 54  | BA    | 1642 | G    | Sidechain |
| 54  | BA    | 1651 | G    | Sidechain |
| 54  | BA    | 1653 | G    | Sidechain |
| 54  | BA    | 1655 | A    | Sidechain |
| 54  | BA    | 1656 | C    | Sidechain |
| 54  | BA    | 1657 | U    | Sidechain |
| 54  | BA    | 1664 | A    | Sidechain |
| 54  | BA    | 1665 | A    | Sidechain |
| 54  | BA    | 1667 | G    | Sidechain |
| 54  | BA    | 1672 | A    | Sidechain |
| 54  | BA    | 1682 | G    | Sidechain |
| 54  | BA    | 1688 | U    | Sidechain |
| 54  | BA    | 1705 | A    | Sidechain |
| 54  | BA    | 172  | A    | Sidechain |
| 54  | BA    | 1729 | U    | Sidechain |
| 54  | BA    | 1737 | G    | Sidechain |
| 54  | BA    | 1738 | G    | Sidechain |
| 54  | BA    | 1739 | A    | Sidechain |
| 54  | BA    | 1740 | G    | Sidechain |
| 54  | BA    | 1743 | G    | Sidechain |
| 54  | BA    | 1747 | U    | Sidechain |
| 54  | BA    | 1750 | G    | Sidechain |
| 54  | BA    | 1753 | G    | Sidechain |
| 54  | BA    | 1758 | U    | Sidechain |
| 54  | BA    | 1760 | C    | Sidechain |
| 54  | BA    | 1763 | G    | Sidechain |
| 54  | BA    | 1774 | C    | Sidechain |
| 54  | BA    | 1788 | C    | Sidechain |
| 54  | BA    | 1789 | A    | Sidechain |
| 54  | BA    | 1792 | G    | Sidechain |
| 54  | BA    | 1793 | C    | Sidechain |
| 54  | BA    | 1797 | G    | Sidechain |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 54  | BA    | 1799 | G    | Sidechain |
| 54  | BA    | 1802 | A    | Sidechain |
| 54  | BA    | 1807 | G    | Sidechain |
| 54  | BA    | 181  | A    | Sidechain |
| 54  | BA    | 1814 | G    | Sidechain |
| 54  | BA    | 1817 | G    | Sidechain |
| 54  | BA    | 1821 | A    | Sidechain |
| 54  | BA    | 1825 | U    | Sidechain |
| 54  | BA    | 1827 | U    | Sidechain |
| 54  | BA    | 1831 | G    | Sidechain |
| 54  | BA    | 1833 | C    | Sidechain |
| 54  | BA    | 1835 | G    | Sidechain |
| 54  | BA    | 1838 | C    | Sidechain |
| 54  | BA    | 1839 | G    | Sidechain |
| 54  | BA    | 1843 | C    | Sidechain |
| 54  | BA    | 1849 | G    | Sidechain |
| 54  | BA    | 185  | G    | Sidechain |
| 54  | BA    | 1857 | G    | Sidechain |
| 54  | BA    | 1858 | A    | Sidechain |
| 54  | BA    | 1860 | G    | Sidechain |
| 54  | BA    | 1863 | G    | Sidechain |
| 54  | BA    | 1864 | U    | Sidechain |
| 54  | BA    | 1865 | U    | Sidechain |
| 54  | BA    | 1869 | G    | Sidechain |
| 54  | BA    | 1883 | U    | Sidechain |
| 54  | BA    | 1884 | G    | Sidechain |
| 54  | BA    | 1885 | A    | Sidechain |
| 54  | BA    | 1886 | U    | Sidechain |
| 54  | BA    | 1887 | C    | Sidechain |
| 54  | BA    | 1902 | C    | Sidechain |
| 54  | BA    | 1903 | G    | Sidechain |
| 54  | BA    | 1906 | G    | Sidechain |
| 54  | BA    | 1910 | G    | Sidechain |
| 54  | BA    | 1918 | A    | Sidechain |
| 54  | BA    | 1920 | C    | Sidechain |
| 54  | BA    | 1924 | C    | Sidechain |
| 54  | BA    | 1932 | A    | Sidechain |
| 54  | BA    | 1941 | C    | Sidechain |
| 54  | BA    | 1944 | U    | Sidechain |
| 54  | BA    | 1945 | G    | Sidechain |
| 54  | BA    | 1948 | G    | Sidechain |
| 54  | BA    | 1949 | G    | Sidechain |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 54  | BA    | 1952 | A    | Sidechain |
| 54  | BA    | 1957 | C    | Sidechain |
| 54  | BA    | 196  | A    | Sidechain |
| 54  | BA    | 1960 | A    | Sidechain |
| 54  | BA    | 1962 | C    | Sidechain |
| 54  | BA    | 1966 | A    | Sidechain |
| 54  | BA    | 1969 | A    | Sidechain |
| 54  | BA    | 1976 | U    | Sidechain |
| 54  | BA    | 1978 | A    | Sidechain |
| 54  | BA    | 1983 | G    | Sidechain |
| 54  | BA    | 200  | U    | Sidechain |
| 54  | BA    | 2003 | A    | Sidechain |
| 54  | BA    | 2008 | C    | Sidechain |
| 54  | BA    | 2011 | U    | Sidechain |
| 54  | BA    | 2013 | A    | Sidechain |
| 54  | BA    | 2014 | A    | Sidechain |
| 54  | BA    | 2015 | A    | Sidechain |
| 54  | BA    | 2019 | A    | Sidechain |
| 54  | BA    | 202  | U    | Sidechain |
| 54  | BA    | 2028 | U    | Sidechain |
| 54  | BA    | 203  | A    | Sidechain |
| 54  | BA    | 2030 | A    | Sidechain |
| 54  | BA    | 2031 | A    | Sidechain |
| 54  | BA    | 2035 | G    | Sidechain |
| 54  | BA    | 2040 | G    | Sidechain |
| 54  | BA    | 2042 | A    | Sidechain |
| 54  | BA    | 2048 | G    | Sidechain |
| 54  | BA    | 206  | U    | Sidechain |
| 54  | BA    | 2065 | C    | Sidechain |
| 54  | BA    | 2066 | C    | Sidechain |
| 54  | BA    | 2069 | G    | Sidechain |
| 54  | BA    | 2074 | U    | Sidechain |
| 54  | BA    | 2075 | U    | Sidechain |
| 54  | BA    | 2077 | A    | Sidechain |
| 54  | BA    | 2079 | U    | Sidechain |
| 54  | BA    | 208  | C    | Sidechain |
| 54  | BA    | 2093 | G    | Sidechain |
| 54  | BA    | 2094 | A    | Sidechain |
| 54  | BA    | 2097 | A    | Sidechain |
| 54  | BA    | 2099 | U    | Sidechain |
| 54  | BA    | 2100 | G    | Sidechain |
| 54  | BA    | 2104 | C    | Sidechain |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 54  | BA    | 2108 | A    | Sidechain |
| 54  | BA    | 2116 | G    | Sidechain |
| 54  | BA    | 2125 | G    | Sidechain |
| 54  | BA    | 2141 | G    | Sidechain |
| 54  | BA    | 2145 | C    | Sidechain |
| 54  | BA    | 2155 | U    | Sidechain |
| 54  | BA    | 2163 | A    | Sidechain |
| 54  | BA    | 2168 | G    | Sidechain |
| 54  | BA    | 2178 | C    | Sidechain |
| 54  | BA    | 2180 | U    | Sidechain |
| 54  | BA    | 2183 | A    | Sidechain |
| 54  | BA    | 2188 | U    | Sidechain |
| 54  | BA    | 2190 | G    | Sidechain |
| 54  | BA    | 2196 | C    | Sidechain |
| 54  | BA    | 2201 | G    | Sidechain |
| 54  | BA    | 2203 | U    | Sidechain |
| 54  | BA    | 2205 | A    | Sidechain |
| 54  | BA    | 2221 | G    | Sidechain |
| 54  | BA    | 2223 | G    | Sidechain |
| 54  | BA    | 2224 | G    | Sidechain |
| 54  | BA    | 2227 | A    | Sidechain |
| 54  | BA    | 2228 | G    | Sidechain |
| 54  | BA    | 2233 | U    | Sidechain |
| 54  | BA    | 2238 | G    | Sidechain |
| 54  | BA    | 2249 | U    | Sidechain |
| 54  | BA    | 2252 | G    | Sidechain |
| 54  | BA    | 2255 | G    | Sidechain |
| 54  | BA    | 2259 | U    | Sidechain |
| 54  | BA    | 226  | A    | Sidechain |
| 54  | BA    | 2260 | C    | Sidechain |
| 54  | BA    | 2262 | U    | Sidechain |
| 54  | BA    | 2269 | G    | Sidechain |
| 54  | BA    | 2272 | U    | Sidechain |
| 54  | BA    | 2273 | A    | Sidechain |
| 54  | BA    | 2278 | A    | Sidechain |
| 54  | BA    | 2279 | G    | Sidechain |
| 54  | BA    | 2280 | G    | Sidechain |
| 54  | BA    | 2282 | G    | Sidechain |
| 54  | BA    | 2295 | C    | Sidechain |
| 54  | BA    | 2299 | U    | Sidechain |
| 54  | BA    | 2301 | C    | Sidechain |
| 54  | BA    | 2304 | G    | Sidechain |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 54  | BA    | 2309 | A    | Sidechain |
| 54  | BA    | 2312 | U    | Sidechain |
| 54  | BA    | 2325 | G    | Sidechain |
| 54  | BA    | 2327 | A    | Sidechain |
| 54  | BA    | 2332 | C    | Sidechain |
| 54  | BA    | 2345 | G    | Sidechain |
| 54  | BA    | 235  | U    | Sidechain |
| 54  | BA    | 2354 | C    | Sidechain |
| 54  | BA    | 2357 | G    | Sidechain |
| 54  | BA    | 2358 | A    | Sidechain |
| 54  | BA    | 2375 | G    | Sidechain |
| 54  | BA    | 238  | C    | Sidechain |
| 54  | BA    | 2383 | G    | Sidechain |
| 54  | BA    | 2384 | U    | Sidechain |
| 54  | BA    | 2385 | C    | Sidechain |
| 54  | BA    | 2388 | A    | Sidechain |
| 54  | BA    | 2389 | G    | Sidechain |
| 54  | BA    | 2391 | G    | Sidechain |
| 54  | BA    | 2396 | G    | Sidechain |
| 54  | BA    | 240  | C    | Sidechain |
| 54  | BA    | 2406 | A    | Sidechain |
| 54  | BA    | 2413 | G    | Sidechain |
| 54  | BA    | 2421 | G    | Sidechain |
| 54  | BA    | 2424 | C    | Sidechain |
| 54  | BA    | 2427 | C    | Sidechain |
| 54  | BA    | 2428 | G    | Sidechain |
| 54  | BA    | 2430 | A    | Sidechain |
| 54  | BA    | 2432 | A    | Sidechain |
| 54  | BA    | 2437 | G    | Sidechain |
| 54  | BA    | 2440 | C    | Sidechain |
| 54  | BA    | 2442 | C    | Sidechain |
| 54  | BA    | 2445 | G    | Sidechain |
| 54  | BA    | 2446 | G    | Sidechain |
| 54  | BA    | 2447 | G    | Sidechain |
| 54  | BA    | 2453 | A    | Sidechain |
| 54  | BA    | 2455 | G    | Sidechain |
| 54  | BA    | 2460 | U    | Sidechain |
| 54  | BA    | 2466 | C    | Sidechain |
| 54  | BA    | 2468 | A    | Sidechain |
| 54  | BA    | 2470 | G    | Sidechain |
| 54  | BA    | 2475 | C    | Sidechain |
| 54  | BA    | 2478 | A    | Sidechain |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 54  | BA    | 2488 | G    | Sidechain |
| 54  | BA    | 2489 | U    | Sidechain |
| 54  | BA    | 249  | C    | Sidechain |
| 54  | BA    | 2491 | U    | Sidechain |
| 54  | BA    | 2494 | G    | Sidechain |
| 54  | BA    | 2498 | C    | Sidechain |
| 54  | BA    | 25   | U    | Sidechain |
| 54  | BA    | 250  | G    | Sidechain |
| 54  | BA    | 2502 | G    | Sidechain |
| 54  | BA    | 2506 | U    | Sidechain |
| 54  | BA    | 2510 | C    | Sidechain |
| 54  | BA    | 2516 | A    | Sidechain |
| 54  | BA    | 2517 | C    | Sidechain |
| 54  | BA    | 2520 | C    | Sidechain |
| 54  | BA    | 2523 | G    | Sidechain |
| 54  | BA    | 2530 | A    | Sidechain |
| 54  | BA    | 2534 | A    | Sidechain |
| 54  | BA    | 2540 | C    | Sidechain |
| 54  | BA    | 2543 | G    | Sidechain |
| 54  | BA    | 2544 | G    | Sidechain |
| 54  | BA    | 2545 | G    | Sidechain |
| 54  | BA    | 2553 | G    | Sidechain |
| 54  | BA    | 2554 | U    | Sidechain |
| 54  | BA    | 256  | A    | Sidechain |
| 54  | BA    | 2564 | A    | Sidechain |
| 54  | BA    | 2574 | G    | Sidechain |
| 54  | BA    | 2576 | G    | Sidechain |
| 54  | BA    | 2577 | A    | Sidechain |
| 54  | BA    | 2578 | G    | Sidechain |
| 54  | BA    | 2579 | C    | Sidechain |
| 54  | BA    | 2580 | U    | Sidechain |
| 54  | BA    | 2585 | U    | Sidechain |
| 54  | BA    | 2587 | A    | Sidechain |
| 54  | BA    | 2588 | G    | Sidechain |
| 54  | BA    | 2589 | A    | Sidechain |
| 54  | BA    | 2590 | A    | Sidechain |
| 54  | BA    | 2591 | C    | Sidechain |
| 54  | BA    | 2594 | C    | Sidechain |
| 54  | BA    | 2595 | G    | Sidechain |
| 54  | BA    | 2596 | U    | Sidechain |
| 54  | BA    | 2597 | G    | Sidechain |
| 54  | BA    | 2602 | A    | Sidechain |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 54  | BA    | 2603 | G    | Sidechain |
| 54  | BA    | 2608 | G    | Sidechain |
| 54  | BA    | 2609 | U    | Sidechain |
| 54  | BA    | 261  | G    | Sidechain |
| 54  | BA    | 2614 | A    | Sidechain |
| 54  | BA    | 2615 | U    | Sidechain |
| 54  | BA    | 2621 | G    | Sidechain |
| 54  | BA    | 2625 | G    | Sidechain |
| 54  | BA    | 2627 | G    | Sidechain |
| 54  | BA    | 2629 | U    | Sidechain |
| 54  | BA    | 2635 | A    | Sidechain |
| 54  | BA    | 2636 | C    | Sidechain |
| 54  | BA    | 2637 | U    | Sidechain |
| 54  | BA    | 2639 | A    | Sidechain |
| 54  | BA    | 2644 | G    | Sidechain |
| 54  | BA    | 2645 | G    | Sidechain |
| 54  | BA    | 265  | A    | Sidechain |
| 54  | BA    | 2651 | C    | Sidechain |
| 54  | BA    | 2653 | U    | Sidechain |
| 54  | BA    | 2659 | G    | Sidechain |
| 54  | BA    | 2661 | G    | Sidechain |
| 54  | BA    | 2662 | A    | Sidechain |
| 54  | BA    | 2664 | G    | Sidechain |
| 54  | BA    | 2680 | U    | Sidechain |
| 54  | BA    | 2699 | C    | Sidechain |
| 54  | BA    | 2700 | A    | Sidechain |
| 54  | BA    | 2705 | A    | Sidechain |
| 54  | BA    | 2713 | U    | Sidechain |
| 54  | BA    | 272  | A    | Sidechain |
| 54  | BA    | 2721 | A    | Sidechain |
| 54  | BA    | 2722 | G    | Sidechain |
| 54  | BA    | 2725 | A    | Sidechain |
| 54  | BA    | 2730 | C    | Sidechain |
| 54  | BA    | 2731 | G    | Sidechain |
| 54  | BA    | 2739 | U    | Sidechain |
| 54  | BA    | 2743 | U    | Sidechain |
| 54  | BA    | 2751 | G    | Sidechain |
| 54  | BA    | 2753 | A    | Sidechain |
| 54  | BA    | 2759 | G    | Sidechain |
| 54  | BA    | 2765 | A    | Sidechain |
| 54  | BA    | 2780 | G    | Sidechain |
| 54  | BA    | 2782 | G    | Sidechain |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 54  | BA    | 2783 | U    | Sidechain |
| 54  | BA    | 2786 | U    | Sidechain |
| 54  | BA    | 2790 | U    | Sidechain |
| 54  | BA    | 2794 | C    | Sidechain |
| 54  | BA    | 2796 | U    | Sidechain |
| 54  | BA    | 2799 | A    | Sidechain |
| 54  | BA    | 2801 | G    | Sidechain |
| 54  | BA    | 2805 | C    | Sidechain |
| 54  | BA    | 2808 | G    | Sidechain |
| 54  | BA    | 2816 | G    | Sidechain |
| 54  | BA    | 2819 | G    | Sidechain |
| 54  | BA    | 282  | A    | Sidechain |
| 54  | BA    | 2824 | C    | Sidechain |
| 54  | BA    | 2827 | C    | Sidechain |
| 54  | BA    | 2840 | C    | Sidechain |
| 54  | BA    | 2841 | C    | Sidechain |
| 54  | BA    | 2842 | G    | Sidechain |
| 54  | BA    | 2845 | U    | Sidechain |
| 54  | BA    | 2848 | G    | Sidechain |
| 54  | BA    | 2850 | A    | Sidechain |
| 54  | BA    | 2856 | A    | Sidechain |
| 54  | BA    | 2857 | G    | Sidechain |
| 54  | BA    | 2859 | G    | Sidechain |
| 54  | BA    | 2863 | C    | Sidechain |
| 54  | BA    | 2864 | G    | Sidechain |
| 54  | BA    | 2866 | U    | Sidechain |
| 54  | BA    | 2868 | A    | Sidechain |
| 54  | BA    | 2869 | G    | Sidechain |
| 54  | BA    | 2871 | U    | Sidechain |
| 54  | BA    | 2873 | A    | Sidechain |
| 54  | BA    | 2876 | G    | Sidechain |
| 54  | BA    | 2877 | G    | Sidechain |
| 54  | BA    | 2879 | A    | Sidechain |
| 54  | BA    | 2889 | C    | Sidechain |
| 54  | BA    | 2891 | U    | Sidechain |
| 54  | BA    | 2893 | A    | Sidechain |
| 54  | BA    | 2896 | C    | Sidechain |
| 54  | BA    | 298  | G    | Sidechain |
| 54  | BA    | 302  | C    | Sidechain |
| 54  | BA    | 303  | G    | Sidechain |
| 54  | BA    | 307  | G    | Sidechain |
| 54  | BA    | 313  | G    | Sidechain |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 54  | BA    | 315 | G    | Sidechain |
| 54  | BA    | 323 | C    | Sidechain |
| 54  | BA    | 325 | G    | Sidechain |
| 54  | BA    | 326 | G    | Sidechain |
| 54  | BA    | 327 | G    | Sidechain |
| 54  | BA    | 328 | U    | Sidechain |
| 54  | BA    | 333 | G    | Sidechain |
| 54  | BA    | 335 | C    | Sidechain |
| 54  | BA    | 339 | U    | Sidechain |
| 54  | BA    | 347 | A    | Sidechain |
| 54  | BA    | 354 | A    | Sidechain |
| 54  | BA    | 355 | U    | Sidechain |
| 54  | BA    | 357 | C    | Sidechain |
| 54  | BA    | 359 | G    | Sidechain |
| 54  | BA    | 361 | G    | Sidechain |
| 54  | BA    | 362 | A    | Sidechain |
| 54  | BA    | 384 | A    | Sidechain |
| 54  | BA    | 389 | G    | Sidechain |
| 54  | BA    | 39  | G    | Sidechain |
| 54  | BA    | 392 | U    | Sidechain |
| 54  | BA    | 395 | U    | Sidechain |
| 54  | BA    | 400 | G    | Sidechain |
| 54  | BA    | 401 | A    | Sidechain |
| 54  | BA    | 410 | G    | Sidechain |
| 54  | BA    | 412 | A    | Sidechain |
| 54  | BA    | 415 | A    | Sidechain |
| 54  | BA    | 416 | U    | Sidechain |
| 54  | BA    | 417 | C    | Sidechain |
| 54  | BA    | 418 | C    | Sidechain |
| 54  | BA    | 419 | U    | Sidechain |
| 54  | BA    | 420 | C    | Sidechain |
| 54  | BA    | 422 | A    | Sidechain |
| 54  | BA    | 426 | C    | Sidechain |
| 54  | BA    | 43  | G    | Sidechain |
| 54  | BA    | 432 | A    | Sidechain |
| 54  | BA    | 434 | U    | Sidechain |
| 54  | BA    | 442 | G    | Sidechain |
| 54  | BA    | 446 | G    | Sidechain |
| 54  | BA    | 449 | A    | Sidechain |
| 54  | BA    | 456 | C    | Sidechain |
| 54  | BA    | 458 | G    | Sidechain |
| 54  | BA    | 463 | G    | Sidechain |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 54  | BA    | 464 | U    | Sidechain |
| 54  | BA    | 470 | A    | Sidechain |
| 54  | BA    | 48  | G    | Sidechain |
| 54  | BA    | 489 | G    | Sidechain |
| 54  | BA    | 490 | C    | Sidechain |
| 54  | BA    | 491 | G    | Sidechain |
| 54  | BA    | 493 | G    | Sidechain |
| 54  | BA    | 494 | G    | Sidechain |
| 54  | BA    | 498 | G    | Sidechain |
| 54  | BA    | 500 | G    | Sidechain |
| 54  | BA    | 501 | A    | Sidechain |
| 54  | BA    | 503 | A    | Sidechain |
| 54  | BA    | 51  | G    | Sidechain |
| 54  | BA    | 511 | U    | Sidechain |
| 54  | BA    | 512 | G    | Sidechain |
| 54  | BA    | 514 | A    | Sidechain |
| 54  | BA    | 515 | A    | Sidechain |
| 54  | BA    | 528 | A    | Sidechain |
| 54  | BA    | 529 | A    | Sidechain |
| 54  | BA    | 533 | G    | Sidechain |
| 54  | BA    | 541 | A    | Sidechain |
| 54  | BA    | 544 | C    | Sidechain |
| 54  | BA    | 551 | G    | Sidechain |
| 54  | BA    | 556 | A    | Sidechain |
| 54  | BA    | 561 | G    | Sidechain |
| 54  | BA    | 562 | U    | Sidechain |
| 54  | BA    | 563 | A    | Sidechain |
| 54  | BA    | 569 | U    | Sidechain |
| 54  | BA    | 571 | U    | Sidechain |
| 54  | BA    | 572 | A    | Sidechain |
| 54  | BA    | 578 | G    | Sidechain |
| 54  | BA    | 579 | G    | Sidechain |
| 54  | BA    | 580 | U    | Sidechain |
| 54  | BA    | 581 | C    | Sidechain |
| 54  | BA    | 582 | A    | Sidechain |
| 54  | BA    | 587 | C    | Sidechain |
| 54  | BA    | 588 | U    | Sidechain |
| 54  | BA    | 589 | U    | Sidechain |
| 54  | BA    | 595 | C    | Sidechain |
| 54  | BA    | 608 | A    | Sidechain |
| 54  | BA    | 612 | G    | Sidechain |
| 54  | BA    | 617 | G    | Sidechain |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 54  | BA    | 624 | C    | Sidechain |
| 54  | BA    | 633 | A    | Sidechain |
| 54  | BA    | 636 | G    | Sidechain |
| 54  | BA    | 637 | A    | Sidechain |
| 54  | BA    | 644 | A    | Sidechain |
| 54  | BA    | 649 | G    | Sidechain |
| 54  | BA    | 653 | U    | Sidechain |
| 54  | BA    | 657 | U    | Sidechain |
| 54  | BA    | 659 | G    | Sidechain |
| 54  | BA    | 667 | U    | Sidechain |
| 54  | BA    | 669 | G    | Sidechain |
| 54  | BA    | 671 | C    | Sidechain |
| 54  | BA    | 680 | C    | Sidechain |
| 54  | BA    | 683 | U    | Sidechain |
| 54  | BA    | 686 | U    | Sidechain |
| 54  | BA    | 699 | A    | Sidechain |
| 54  | BA    | 703 | U    | Sidechain |
| 54  | BA    | 704 | G    | Sidechain |
| 54  | BA    | 707 | G    | Sidechain |
| 54  | BA    | 708 | G    | Sidechain |
| 54  | BA    | 711 | G    | Sidechain |
| 54  | BA    | 714 | U    | Sidechain |
| 54  | BA    | 715 | A    | Sidechain |
| 54  | BA    | 716 | A    | Sidechain |
| 54  | BA    | 718 | A    | Sidechain |
| 54  | BA    | 723 | C    | Sidechain |
| 54  | BA    | 724 | U    | Sidechain |
| 54  | BA    | 725 | G    | Sidechain |
| 54  | BA    | 726 | G    | Sidechain |
| 54  | BA    | 727 | A    | Sidechain |
| 54  | BA    | 728 | G    | Sidechain |
| 54  | BA    | 73  | A    | Sidechain |
| 54  | BA    | 739 | A    | Sidechain |
| 54  | BA    | 74  | A    | Sidechain |
| 54  | BA    | 743 | A    | Sidechain |
| 54  | BA    | 746 | U    | Sidechain |
| 54  | BA    | 754 | U    | Sidechain |
| 54  | BA    | 758 | C    | Sidechain |
| 54  | BA    | 759 | G    | Sidechain |
| 54  | BA    | 772 | C    | Sidechain |
| 54  | BA    | 774 | G    | Sidechain |
| 54  | BA    | 775 | G    | Sidechain |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 54  | BA    | 776 | G    | Sidechain |
| 54  | BA    | 782 | A    | Sidechain |
| 54  | BA    | 784 | G    | Sidechain |
| 54  | BA    | 785 | G    | Sidechain |
| 54  | BA    | 79  | C    | Sidechain |
| 54  | BA    | 801 | G    | Sidechain |
| 54  | BA    | 804 | A    | Sidechain |
| 54  | BA    | 810 | U    | Sidechain |
| 54  | BA    | 811 | U    | Sidechain |
| 54  | BA    | 816 | C    | Sidechain |
| 54  | BA    | 827 | U    | Sidechain |
| 54  | BA    | 828 | U    | Sidechain |
| 54  | BA    | 837 | C    | Sidechain |
| 54  | BA    | 84  | A    | Sidechain |
| 54  | BA    | 841 | G    | Sidechain |
| 54  | BA    | 851 | C    | Sidechain |
| 54  | BA    | 852 | U    | Sidechain |
| 54  | BA    | 856 | G    | Sidechain |
| 54  | BA    | 858 | G    | Sidechain |
| 54  | BA    | 859 | G    | Sidechain |
| 54  | BA    | 861 | A    | Sidechain |
| 54  | BA    | 864 | G    | Sidechain |
| 54  | BA    | 868 | U    | Sidechain |
| 54  | BA    | 882 | G    | Sidechain |
| 54  | BA    | 886 | A    | Sidechain |
| 54  | BA    | 891 | G    | Sidechain |
| 54  | BA    | 897 | C    | Sidechain |
| 54  | BA    | 9   | G    | Sidechain |
| 54  | BA    | 900 | A    | Sidechain |
| 54  | BA    | 904 | G    | Sidechain |
| 54  | BA    | 91  | A    | Sidechain |
| 54  | BA    | 910 | A    | Sidechain |
| 54  | BA    | 912 | C    | Sidechain |
| 54  | BA    | 917 | A    | Sidechain |
| 54  | BA    | 918 | A    | Sidechain |
| 54  | BA    | 92  | U    | Sidechain |
| 54  | BA    | 923 | G    | Sidechain |
| 54  | BA    | 932 | U    | Sidechain |
| 54  | BA    | 940 | G    | Sidechain |
| 54  | BA    | 950 | G    | Sidechain |
| 54  | BA    | 953 | G    | Sidechain |
| 54  | BA    | 955 | U    | Sidechain |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 54  | BA    | 957 | C    | Sidechain |
| 54  | BA    | 959 | A    | Sidechain |
| 54  | BA    | 966 | G    | Sidechain |
| 54  | BA    | 969 | G    | Sidechain |
| 54  | BA    | 975 | A    | Sidechain |
| 54  | BA    | 980 | A    | Sidechain |
| 54  | BA    | 983 | A    | Sidechain |
| 54  | BA    | 99  | U    | Sidechain |
| 55  | BB    | 10  | G    | Sidechain |
| 55  | BB    | 105 | G    | Sidechain |
| 55  | BB    | 106 | G    | Sidechain |
| 55  | BB    | 107 | G    | Sidechain |
| 55  | BB    | 117 | G    | Sidechain |
| 55  | BB    | 13  | G    | Sidechain |
| 55  | BB    | 14  | U    | Sidechain |
| 55  | BB    | 15  | A    | Sidechain |
| 55  | BB    | 2   | G    | Sidechain |
| 55  | BB    | 24  | G    | Sidechain |
| 55  | BB    | 25  | U    | Sidechain |
| 55  | BB    | 29  | A    | Sidechain |
| 55  | BB    | 33  | G    | Sidechain |
| 55  | BB    | 36  | C    | Sidechain |
| 55  | BB    | 40  | U    | Sidechain |
| 55  | BB    | 47  | C    | Sidechain |
| 55  | BB    | 48  | U    | Sidechain |
| 55  | BB    | 64  | G    | Sidechain |
| 55  | BB    | 66  | A    | Sidechain |
| 55  | BB    | 69  | G    | Sidechain |
| 55  | BB    | 7   | G    | Sidechain |
| 55  | BB    | 73  | A    | Sidechain |
| 55  | BB    | 75  | G    | Sidechain |
| 55  | BB    | 83  | G    | Sidechain |
| 55  | BB    | 85  | G    | Sidechain |
| 55  | BB    | 9   | G    | Sidechain |
| 55  | BB    | 91  | C    | Sidechain |
| 55  | BB    | 93  | C    | Sidechain |
| 55  | BB    | 94  | A    | Sidechain |
| 55  | BB    | 96  | G    | Sidechain |
| 25  | BC    | 142 | ASN  | Peptide   |
| 25  | BC    | 62  | ARG  | Sidechain |
| 33  | BK    | 105 | ARG  | Sidechain |
| 34  | BL    | 123 | ARG  | Sidechain |

## 5.2 Too-close contacts [\(i\)](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | AB    | 1708  | 0        | 1736     | 2       | 0            |
| 2   | AC    | 1625  | 0        | 1699     | 0       | 0            |
| 3   | AD    | 1643  | 0        | 1710     | 0       | 0            |
| 4   | AE    | 1109  | 0        | 1152     | 0       | 0            |
| 5   | AF    | 818   | 0        | 808      | 0       | 0            |
| 6   | AG    | 1178  | 0        | 1234     | 0       | 0            |
| 7   | AH    | 979   | 0        | 1034     | 0       | 0            |
| 8   | AI    | 1025  | 0        | 1074     | 0       | 0            |
| 9   | AJ    | 790   | 0        | 832      | 1       | 0            |
| 10  | AK    | 880   | 0        | 891      | 0       | 0            |
| 11  | AL    | 955   | 0        | 1019     | 0       | 0            |
| 12  | AM    | 877   | 0        | 937      | 0       | 0            |
| 13  | AN    | 805   | 0        | 844      | 0       | 0            |
| 14  | AO    | 714   | 0        | 737      | 0       | 0            |
| 15  | AP    | 639   | 0        | 656      | 0       | 0            |
| 16  | AQ    | 652   | 0        | 695      | 0       | 0            |
| 17  | AR    | 459   | 0        | 482      | 0       | 0            |
| 18  | AS    | 641   | 0        | 669      | 1       | 0            |
| 19  | AT    | 668   | 0        | 718      | 2       | 0            |
| 20  | AU    | 429   | 0        | 453      | 0       | 0            |
| 21  | AA    | 32828 | 0        | 15886    | 9       | 0            |
| 22  | A1    | 1627  | 0        | 798      | 0       | 0            |
| 23  | A2    | 309   | 0        | 156      | 0       | 0            |
| 24  | A3    | 1642  | 0        | 801      | 1       | 0            |
| 25  | BC    | 2083  | 0        | 2157     | 2       | 0            |
| 26  | BD    | 1565  | 0        | 1616     | 3       | 0            |
| 27  | BE    | 1552  | 0        | 1619     | 1       | 0            |
| 28  | BF    | 1420  | 0        | 1460     | 0       | 0            |
| 29  | BG    | 1323  | 0        | 1374     | 0       | 0            |
| 30  | BH    | 1111  | 0        | 1148     | 0       | 0            |
| 31  | BI    | 1032  | 0        | 1088     | 0       | 0            |
| 32  | BJ    | 1129  | 0        | 1162     | 0       | 0            |
| 33  | BK    | 939   | 0        | 1012     | 2       | 0            |
| 34  | BL    | 1045  | 0        | 1117     | 1       | 0            |
| 35  | BM    | 1074  | 0        | 1157     | 0       | 0            |
| 36  | BN    | 961   | 0        | 1000     | 0       | 0            |
| 37  | BO    | 892   | 0        | 923      | 1       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 38  | BP    | 917    | 0        | 965      | 0       | 0            |
| 39  | BQ    | 947    | 0        | 1022     | 0       | 0            |
| 40  | BR    | 816    | 0        | 839      | 0       | 0            |
| 41  | BS    | 857    | 0        | 922      | 0       | 0            |
| 42  | BT    | 739    | 0        | 807      | 0       | 0            |
| 43  | BU    | 780    | 0        | 834      | 0       | 0            |
| 44  | BV    | 753    | 0        | 780      | 0       | 0            |
| 45  | BW    | 599    | 0        | 614      | 1       | 0            |
| 46  | BX    | 625    | 0        | 655      | 0       | 0            |
| 47  | BY    | 509    | 0        | 543      | 0       | 0            |
| 48  | BZ    | 449    | 0        | 491      | 1       | 0            |
| 49  | B0    | 444    | 0        | 461      | 0       | 0            |
| 50  | B1    | 413    | 0        | 444      | 1       | 0            |
| 51  | B2    | 377    | 0        | 418      | 1       | 0            |
| 52  | B3    | 504    | 0        | 574      | 0       | 0            |
| 53  | B4    | 302    | 0        | 343      | 0       | 0            |
| 54  | BA    | 62317  | 0        | 30186    | 21      | 0            |
| 55  | BB    | 2504   | 0        | 1181     | 0       | 0            |
| 56  | B5    | 1658   | 0        | 1751     | 0       | 0            |
| 57  | A1    | 7      | 0        | 8        | 0       | 0            |
| 58  | BA    | 10     | 0        | 10       | 0       | 0            |
| All | All   | 147653 | 0        | 97702    | 45      | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 0.

All (45) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 19:AT:40:ALA:HB1  | 19:AT:41:GLY:HA2  | 1.81                     | 0.62              |
| 48:BZ:28:LEU:H    | 48:BZ:28:LEU:HD23 | 1.76                     | 0.51              |
| 26:BD:154:LYS:HE3 | 26:BD:156:PHE:CE1 | 2.46                     | 0.51              |
| 54:BA:931:U:C5    | 54:BA:1167:C:H1'  | 2.46                     | 0.50              |
| 21:AA:5:U:H4'     | 21:AA:6:G:C6      | 2.46                     | 0.50              |
| 54:BA:1021:A:N6   | 54:BA:1142:A:H62  | 2.11                     | 0.49              |
| 54:BA:1025:G:C4   | 54:BA:1135:C:H1'  | 2.48                     | 0.48              |
| 26:BD:58:ASN:H    | 26:BD:59:ARG:HB2  | 1.79                     | 0.46              |
| 54:BA:1451:C:H4'  | 54:BA:1452:G:C4   | 2.50                     | 0.46              |
| 54:BA:36:G:H4'    | 54:BA:451:U:C4    | 2.50                     | 0.46              |
| 54:BA:561:G:H2'   | 54:BA:562:U:H5"   | 1.98                     | 0.45              |
| 45:BW:11:ASN:ND2  | 54:BA:2264:C:H41  | 2.14                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 21:AA:1533:C:H3'   | 21:AA:1534:A:H5"  | 1.98                     | 0.44              |
| 24:A3:76:C:H1'     | 54:BA:2252:G:N2   | 2.33                     | 0.44              |
| 21:AA:87:C:H2'     | 21:AA:88:U:C6     | 2.52                     | 0.44              |
| 54:BA:2144:G:H2'   | 54:BA:2146:C:C5   | 2.52                     | 0.44              |
| 33:BK:103:VAL:HG12 | 33:BK:104:THR:H   | 1.82                     | 0.44              |
| 54:BA:2557:G:H2'   | 54:BA:2558:C:C6   | 2.53                     | 0.44              |
| 33:BK:103:VAL:HG12 | 33:BK:104:THR:N   | 2.34                     | 0.43              |
| 54:BA:783:A:C4     | 54:BA:785:G:H1'   | 2.54                     | 0.43              |
| 27:BE:165:HIS:HA   | 54:BA:1205:A:C5   | 2.54                     | 0.43              |
| 54:BA:1826:G:H2'   | 54:BA:1827:U:C6   | 2.54                     | 0.43              |
| 19:AT:40:ALA:HB1   | 19:AT:41:GLY:CA   | 2.47                     | 0.42              |
| 51:B2:37:LYS:HE3   | 54:BA:458:G:N7    | 2.34                     | 0.42              |
| 54:BA:532:A:C8     | 54:BA:2021:C:C4   | 3.07                     | 0.42              |
| 50:B1:20:TYR:CE1   | 50:B1:37:LYS:HE3  | 2.55                     | 0.42              |
| 1:AB:162:VAL:HG22  | 1:AB:164:ASP:H    | 1.85                     | 0.42              |
| 21:AA:5:U:H4'      | 21:AA:6:G:C5      | 2.54                     | 0.42              |
| 9:AJ:71:LEU:HD23   | 9:AJ:72:ARG:N     | 2.35                     | 0.42              |
| 54:BA:2440:C:C5    | 54:BA:2441:U:H1'  | 2.55                     | 0.41              |
| 25:BC:222:THR:HG22 | 54:BA:1826:G:H5"  | 2.03                     | 0.41              |
| 54:BA:61:C:H3'     | 54:BA:62:U:H5"    | 2.03                     | 0.41              |
| 26:BD:106:LYS:HE3  | 26:BD:206:ALA:O   | 2.20                     | 0.41              |
| 54:BA:1729:U:C5    | 54:BA:1730:C:H1'  | 2.55                     | 0.41              |
| 1:AB:30:ILE:HG22   | 1:AB:32:GLY:H     | 1.86                     | 0.41              |
| 54:BA:1631:G:C2    | 54:BA:1633:G:H5"  | 2.56                     | 0.41              |
| 18:AS:5:LYS:HE2    | 21:AA:1312:G:H5'  | 2.02                     | 0.41              |
| 21:AA:6:G:H2'      | 21:AA:6:G:N3      | 2.36                     | 0.41              |
| 21:AA:765:G:C8     | 21:AA:813:U:C4    | 3.08                     | 0.41              |
| 21:AA:35:G:H1'     | 21:AA:36:C:C6     | 2.56                     | 0.41              |
| 37:BO:40:ILE:N     | 37:BO:40:ILE:HD12 | 2.36                     | 0.41              |
| 21:AA:410:G:H2'    | 21:AA:429:U:C4    | 2.56                     | 0.40              |
| 54:BA:1712:U:H3'   | 54:BA:1713:A:H3'  | 2.03                     | 0.40              |
| 25:BC:75:ALA:HB2   | 25:BC:95:TYR:CD2  | 2.57                     | 0.40              |
| 34:BL:70:LYS:HE2   | 34:BL:107:PHE:CZ  | 2.56                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [\(i\)](#)

### 5.3.1 Protein backbone [\(i\)](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |
|-----|-------|---------------|-----------|----------|----------|-------------|
| 1   | AB    | 218/220 (99%) | 195 (89%) | 22 (10%) | 1 (0%)   | 29 69       |
| 2   | AC    | 205/208 (99%) | 191 (93%) | 12 (6%)  | 2 (1%)   | 15 55       |
| 3   | AD    | 203/206 (98%) | 185 (91%) | 15 (7%)  | 3 (2%)   | 10 46       |
| 4   | AE    | 150/152 (99%) | 134 (89%) | 9 (6%)   | 7 (5%)   | 2 21        |
| 5   | AF    | 99/101 (98%)  | 86 (87%)  | 6 (6%)   | 7 (7%)   | 1 14        |
| 6   | AG    | 150/152 (99%) | 143 (95%) | 7 (5%)   | 0        | 100 100     |
| 7   | AH    | 127/130 (98%) | 118 (93%) | 9 (7%)   | 0        | 100 100     |
| 8   | AI    | 126/128 (98%) | 110 (87%) | 12 (10%) | 4 (3%)   | 4 26        |
| 9   | AJ    | 98/100 (98%)  | 88 (90%)  | 5 (5%)   | 5 (5%)   | 2 19        |
| 10  | AK    | 116/118 (98%) | 110 (95%) | 5 (4%)   | 1 (1%)   | 17 57       |
| 11  | AL    | 121/124 (98%) | 111 (92%) | 10 (8%)  | 0        | 100 100     |
| 12  | AM    | 112/115 (97%) | 98 (88%)  | 12 (11%) | 2 (2%)   | 8 40        |
| 13  | AN    | 98/101 (97%)  | 90 (92%)  | 7 (7%)   | 1 (1%)   | 15 55       |
| 14  | AO    | 86/89 (97%)   | 78 (91%)  | 7 (8%)   | 1 (1%)   | 13 50       |
| 15  | AP    | 79/81 (98%)   | 68 (86%)  | 7 (9%)   | 4 (5%)   | 2 19        |
| 16  | AQ    | 80/82 (98%)   | 71 (89%)  | 7 (9%)   | 2 (2%)   | 5 32        |
| 17  | AR    | 55/57 (96%)   | 52 (94%)  | 2 (4%)   | 1 (2%)   | 8 40        |
| 18  | AS    | 79/81 (98%)   | 73 (92%)  | 6 (8%)   | 0        | 100 100     |
| 19  | AT    | 84/86 (98%)   | 74 (88%)  | 8 (10%)  | 2 (2%)   | 6 33        |
| 20  | AU    | 51/53 (96%)   | 27 (53%)  | 14 (28%) | 10 (20%) | 0 2         |
| 25  | BC    | 270/273 (99%) | 238 (88%) | 21 (8%)  | 11 (4%)  | 3 23        |
| 26  | BD    | 207/209 (99%) | 178 (86%) | 18 (9%)  | 11 (5%)  | 2 19        |
| 27  | BE    | 199/201 (99%) | 177 (89%) | 17 (8%)  | 5 (2%)   | 5 32        |
| 28  | BF    | 176/179 (98%) | 151 (86%) | 21 (12%) | 4 (2%)   | 6 34        |
| 29  | BG    | 174/177 (98%) | 152 (87%) | 13 (8%)  | 9 (5%)   | 2 19        |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |
|-----|-------|-----------------|------------|----------|----------|-------------|
| 30  | BH    | 147/149 (99%)   | 132 (90%)  | 13 (9%)  | 2 (1%)   | 11 46       |
| 31  | BI    | 139/142 (98%)   | 125 (90%)  | 10 (7%)  | 4 (3%)   | 4 29        |
| 32  | BJ    | 140/142 (99%)   | 125 (89%)  | 8 (6%)   | 7 (5%)   | 2 20        |
| 33  | BK    | 121/123 (98%)   | 106 (88%)  | 12 (10%) | 3 (2%)   | 5 32        |
| 34  | BL    | 141/144 (98%)   | 117 (83%)  | 12 (8%)  | 12 (8%)  | 1 12        |
| 35  | BM    | 134/136 (98%)   | 117 (87%)  | 12 (9%)  | 5 (4%)   | 3 24        |
| 36  | BN    | 119/121 (98%)   | 107 (90%)  | 10 (8%)  | 2 (2%)   | 9 42        |
| 37  | BO    | 114/117 (97%)   | 111 (97%)  | 3 (3%)   | 0        | 100 100     |
| 38  | BP    | 112/115 (97%)   | 91 (81%)   | 15 (13%) | 6 (5%)   | 2 19        |
| 39  | BQ    | 115/118 (98%)   | 100 (87%)  | 15 (13%) | 0        | 100 100     |
| 40  | BR    | 101/103 (98%)   | 94 (93%)   | 3 (3%)   | 4 (4%)   | 3 23        |
| 41  | BS    | 108/110 (98%)   | 100 (93%)  | 6 (6%)   | 2 (2%)   | 8 38        |
| 42  | BT    | 92/94 (98%)     | 78 (85%)   | 11 (12%) | 3 (3%)   | 4 26        |
| 43  | BU    | 101/104 (97%)   | 85 (84%)   | 12 (12%) | 4 (4%)   | 3 23        |
| 44  | BV    | 92/94 (98%)     | 88 (96%)   | 4 (4%)   | 0        | 100 100     |
| 45  | BW    | 78/80 (98%)     | 65 (83%)   | 6 (8%)   | 7 (9%)   | 1 11        |
| 46  | BX    | 75/79 (95%)     | 70 (93%)   | 3 (4%)   | 2 (3%)   | 5 31        |
| 47  | BY    | 61/63 (97%)     | 56 (92%)   | 4 (7%)   | 1 (2%)   | 9 44        |
| 48  | BZ    | 56/59 (95%)     | 50 (89%)   | 4 (7%)   | 2 (4%)   | 3 25        |
| 49  | B0    | 54/57 (95%)     | 48 (89%)   | 5 (9%)   | 1 (2%)   | 8 38        |
| 50  | B1    | 50/52 (96%)     | 43 (86%)   | 3 (6%)   | 4 (8%)   | 1 12        |
| 51  | B2    | 44/46 (96%)     | 41 (93%)   | 3 (7%)   | 0        | 100 100     |
| 52  | B3    | 62/65 (95%)     | 58 (94%)   | 2 (3%)   | 2 (3%)   | 4 26        |
| 53  | B4    | 36/38 (95%)     | 34 (94%)   | 2 (6%)   | 0        | 100 100     |
| 56  | B5    | 221/234 (94%)   | 210 (95%)  | 8 (4%)   | 3 (1%)   | 11 46       |
| All | All   | 5876/6008 (98%) | 5249 (89%) | 458 (8%) | 169 (3%) | 7 29        |

All (169) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | AE    | 149 | PRO  |
| 8   | AI    | 44  | ARG  |
| 16  | AQ    | 80  | LYS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20  | AU    | 6   | ARG  |
| 20  | AU    | 9   | GLU  |
| 20  | AU    | 13  | VAL  |
| 25  | BC    | 141 | HIS  |
| 26  | BD    | 80  | TRP  |
| 27  | BE    | 31  | VAL  |
| 33  | BK    | 71  | ARG  |
| 33  | BK    | 103 | VAL  |
| 34  | BL    | 55  | MET  |
| 34  | BL    | 66  | PHE  |
| 35  | BM    | 21  | ALA  |
| 35  | BM    | 110 | GLU  |
| 43  | BU    | 70  | ALA  |
| 49  | B0    | 39  | ARG  |
| 2   | AC    | 195 | ILE  |
| 3   | AD    | 47  | LEU  |
| 4   | AE    | 54  | GLU  |
| 4   | AE    | 104 | ILE  |
| 4   | AE    | 105 | ILE  |
| 5   | AF    | 10  | VAL  |
| 5   | AF    | 59  | TYR  |
| 8   | AI    | 119 | LYS  |
| 12  | AM    | 22  | TYR  |
| 12  | AM    | 42  | VAL  |
| 15  | AP    | 17  | TYR  |
| 19  | AT    | 42  | ASP  |
| 20  | AU    | 22  | CYS  |
| 20  | AU    | 48  | LYS  |
| 25  | BC    | 161 | VAL  |
| 25  | BC    | 185 | ALA  |
| 26  | BD    | 51  | THR  |
| 26  | BD    | 60  | VAL  |
| 26  | BD    | 75  | ALA  |
| 27  | BE    | 96  | VAL  |
| 28  | BF    | 103 | ILE  |
| 29  | BG    | 46  | ASP  |
| 29  | BG    | 167 | VAL  |
| 29  | BG    | 174 | LYS  |
| 31  | BI    | 10  | LEU  |
| 31  | BI    | 119 | ALA  |
| 32  | BJ    | 15  | TRP  |
| 33  | BK    | 25  | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34  | BL    | 82  | LEU  |
| 34  | BL    | 83  | ALA  |
| 34  | BL    | 101 | ILE  |
| 36  | BN    | 47  | VAL  |
| 38  | BP    | 69  | VAL  |
| 40  | BR    | 29  | THR  |
| 40  | BR    | 53  | PHE  |
| 45  | BW    | 10  | ARG  |
| 45  | BW    | 14  | ASP  |
| 45  | BW    | 23  | LYS  |
| 46  | BX    | 27  | ARG  |
| 50  | B1    | 36  | LYS  |
| 52  | B3    | 46  | LYS  |
| 4   | AE    | 43  | GLY  |
| 5   | AF    | 6   | ILE  |
| 5   | AF    | 86  | ARG  |
| 8   | AI    | 120 | ALA  |
| 9   | AJ    | 41  | PRO  |
| 9   | AJ    | 57  | VAL  |
| 9   | AJ    | 75  | ASP  |
| 10  | AK    | 16  | SER  |
| 20  | AU    | 20  | ARG  |
| 20  | AU    | 34  | ARG  |
| 25  | BC    | 13  | ARG  |
| 25  | BC    | 36  | ASN  |
| 26  | BD    | 34  | VAL  |
| 26  | BD    | 86  | GLU  |
| 26  | BD    | 136 | ASN  |
| 28  | BF    | 77  | LYS  |
| 29  | BG    | 39  | ALA  |
| 29  | BG    | 59  | ASP  |
| 30  | BH    | 10  | ALA  |
| 32  | BJ    | 81  | ILE  |
| 34  | BL    | 15  | ALA  |
| 34  | BL    | 44  | GLY  |
| 38  | BP    | 26  | GLU  |
| 38  | BP    | 50  | ARG  |
| 38  | BP    | 64  | SER  |
| 40  | BR    | 30  | GLY  |
| 42  | BT    | 11  | LEU  |
| 43  | BU    | 5   | ARG  |
| 45  | BW    | 41  | GLY  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 45  | BW    | 74  | LYS  |
| 50  | B1    | 45  | HIS  |
| 56  | B5    | 109 | MET  |
| 1   | AB    | 18  | GLN  |
| 5   | AF    | 90  | MET  |
| 8   | AI    | 122 | ARG  |
| 15  | AP    | 9   | HIS  |
| 15  | AP    | 79  | ASN  |
| 16  | AQ    | 17  | GLU  |
| 19  | AT    | 65  | LEU  |
| 20  | AU    | 21  | SER  |
| 25  | BC    | 189 | ALA  |
| 25  | BC    | 196 | ASN  |
| 26  | BD    | 95  | SER  |
| 26  | BD    | 114 | LYS  |
| 27  | BE    | 94  | GLN  |
| 27  | BE    | 97  | ASN  |
| 27  | BE    | 123 | LYS  |
| 28  | BF    | 136 | ILE  |
| 29  | BG    | 22  | VAL  |
| 29  | BG    | 151 | ARG  |
| 30  | BH    | 88  | GLY  |
| 31  | BI    | 135 | MET  |
| 32  | BJ    | 44  | TYR  |
| 32  | BJ    | 45  | THR  |
| 34  | BL    | 5   | THR  |
| 34  | BL    | 29  | LYS  |
| 34  | BL    | 30  | THR  |
| 35  | BM    | 36  | VAL  |
| 35  | BM    | 58  | LYS  |
| 38  | BP    | 32  | VAL  |
| 42  | BT    | 78  | SER  |
| 45  | BW    | 11  | ASN  |
| 47  | BY    | 61  | ALA  |
| 48  | BZ    | 3   | THR  |
| 50  | B1    | 24  | LYS  |
| 52  | B3    | 25  | HIS  |
| 3   | AD    | 26  | ALA  |
| 3   | AD    | 84  | ASN  |
| 4   | AE    | 106 | ALA  |
| 5   | AF    | 92  | THR  |
| 5   | AF    | 98  | GLU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | AJ    | 42  | LEU  |
| 9   | AJ    | 92  | LEU  |
| 15  | AP    | 13  | LYS  |
| 20  | AU    | 28  | LEU  |
| 25  | BC    | 153 | LEU  |
| 26  | BD    | 15  | PHE  |
| 28  | BF    | 107 | VAL  |
| 31  | BI    | 64  | ARG  |
| 32  | BJ    | 53  | TYR  |
| 34  | BL    | 17  | LYS  |
| 34  | BL    | 69  | ARG  |
| 36  | BN    | 10  | LEU  |
| 41  | BS    | 90  | LYS  |
| 43  | BU    | 12  | VAL  |
| 45  | BW    | 44  | PHE  |
| 46  | BX    | 53  | LYS  |
| 4   | AE    | 158 | LYS  |
| 13  | AN    | 70  | PRO  |
| 20  | AU    | 23  | GLU  |
| 25  | BC    | 169 | ALA  |
| 25  | BC    | 235 | GLU  |
| 26  | BD    | 119 | ALA  |
| 32  | BJ    | 42  | ALA  |
| 35  | BM    | 80  | VAL  |
| 42  | BT    | 9   | LYS  |
| 50  | B1    | 4   | ILE  |
| 32  | BJ    | 112 | GLY  |
| 56  | B5    | 91  | GLY  |
| 56  | B5    | 107 | GLY  |
| 38  | BP    | 31  | VAL  |
| 2   | AC    | 14  | VAL  |
| 25  | BC    | 9   | SER  |
| 29  | BG    | 112 | VAL  |
| 48  | BZ    | 31  | ILE  |
| 14  | AO    | 40  | GLY  |
| 17  | AR    | 20  | ILE  |
| 40  | BR    | 27  | ILE  |
| 41  | BS    | 29  | VAL  |
| 43  | BU    | 19  | GLY  |
| 29  | BG    | 97  | VAL  |

### 5.3.2 Protein sidechains [\(i\)](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |
|-----|-------|----------------|------------|----------|-------------|
| 1   | AB    | 180/180 (100%) | 177 (98%)  | 3 (2%)   | 60 78       |
| 2   | AC    | 170/171 (99%)  | 167 (98%)  | 3 (2%)   | 59 77       |
| 3   | AD    | 172/173 (99%)  | 168 (98%)  | 4 (2%)   | 50 70       |
| 4   | AE    | 113/113 (100%) | 110 (97%)  | 3 (3%)   | 44 65       |
| 5   | AF    | 87/87 (100%)   | 86 (99%)   | 1 (1%)   | 73 84       |
| 6   | AG    | 123/123 (100%) | 123 (100%) | 0        | 100 100     |
| 7   | AH    | 104/105 (99%)  | 102 (98%)  | 2 (2%)   | 57 75       |
| 8   | AI    | 105/105 (100%) | 105 (100%) | 0        | 100 100     |
| 9   | AJ    | 86/86 (100%)   | 82 (95%)   | 4 (5%)   | 26 51       |
| 10  | AK    | 90/90 (100%)   | 88 (98%)   | 2 (2%)   | 52 71       |
| 11  | AL    | 103/104 (99%)  | 102 (99%)  | 1 (1%)   | 76 86       |
| 12  | AM    | 91/92 (99%)    | 88 (97%)   | 3 (3%)   | 38 61       |
| 13  | AN    | 83/84 (99%)    | 81 (98%)   | 2 (2%)   | 49 69       |
| 14  | AO    | 76/77 (99%)    | 76 (100%)  | 0        | 100 100     |
| 15  | AP    | 65/65 (100%)   | 65 (100%)  | 0        | 100 100     |
| 16  | AQ    | 74/74 (100%)   | 74 (100%)  | 0        | 100 100     |
| 17  | AR    | 48/48 (100%)   | 47 (98%)   | 1 (2%)   | 53 72       |
| 18  | AS    | 70/70 (100%)   | 70 (100%)  | 0        | 100 100     |
| 19  | AT    | 65/65 (100%)   | 62 (95%)   | 3 (5%)   | 27 52       |
| 20  | AU    | 44/44 (100%)   | 44 (100%)  | 0        | 100 100     |
| 25  | BC    | 216/217 (100%) | 210 (97%)  | 6 (3%)   | 43 65       |
| 26  | BD    | 164/164 (100%) | 161 (98%)  | 3 (2%)   | 59 77       |
| 27  | BE    | 165/165 (100%) | 163 (99%)  | 2 (1%)   | 71 83       |
| 28  | BF    | 149/150 (99%)  | 148 (99%)  | 1 (1%)   | 84 90       |
| 29  | BG    | 137/138 (99%)  | 134 (98%)  | 3 (2%)   | 52 71       |
| 30  | BH    | 114/114 (100%) | 113 (99%)  | 1 (1%)   | 78 87       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 31  | BI    | 109/110 (99%)   | 106 (97%)  | 3 (3%)   | 43          | 65  |
| 32  | BJ    | 116/116 (100%)  | 114 (98%)  | 2 (2%)   | 60          | 78  |
| 33  | BK    | 103/103 (100%)  | 99 (96%)   | 4 (4%)   | 32          | 56  |
| 34  | BL    | 102/103 (99%)   | 101 (99%)  | 1 (1%)   | 76          | 86  |
| 35  | BM    | 109/109 (100%)  | 106 (97%)  | 3 (3%)   | 43          | 65  |
| 36  | BN    | 100/100 (100%)  | 99 (99%)   | 1 (1%)   | 76          | 86  |
| 37  | BO    | 86/87 (99%)     | 85 (99%)   | 1 (1%)   | 71          | 83  |
| 38  | BP    | 99/100 (99%)    | 95 (96%)   | 4 (4%)   | 31          | 55  |
| 39  | BQ    | 89/90 (99%)     | 88 (99%)   | 1 (1%)   | 73          | 84  |
| 40  | BR    | 84/84 (100%)    | 83 (99%)   | 1 (1%)   | 71          | 83  |
| 41  | BS    | 93/93 (100%)    | 90 (97%)   | 3 (3%)   | 39          | 61  |
| 42  | BT    | 80/80 (100%)    | 80 (100%)  | 0        | 100         | 100 |
| 43  | BU    | 83/84 (99%)     | 83 (100%)  | 0        | 100         | 100 |
| 44  | BV    | 78/78 (100%)    | 76 (97%)   | 2 (3%)   | 46          | 66  |
| 45  | BW    | 59/59 (100%)    | 55 (93%)   | 4 (7%)   | 16          | 41  |
| 46  | BX    | 67/68 (98%)     | 67 (100%)  | 0        | 100         | 100 |
| 47  | BY    | 55/55 (100%)    | 55 (100%)  | 0        | 100         | 100 |
| 48  | BZ    | 48/49 (98%)     | 48 (100%)  | 0        | 100         | 100 |
| 49  | B0    | 47/48 (98%)     | 45 (96%)   | 2 (4%)   | 29          | 53  |
| 50  | B1    | 45/45 (100%)    | 45 (100%)  | 0        | 100         | 100 |
| 51  | B2    | 38/38 (100%)    | 37 (97%)   | 1 (3%)   | 46          | 66  |
| 52  | B3    | 51/52 (98%)     | 50 (98%)   | 1 (2%)   | 55          | 74  |
| 53  | B4    | 34/34 (100%)    | 33 (97%)   | 1 (3%)   | 42          | 64  |
| 56  | B5    | 173/181 (96%)   | 170 (98%)  | 3 (2%)   | 60          | 78  |
| All | All   | 4842/4870 (99%) | 4756 (98%) | 86 (2%)  | 61          | 77  |

All (86) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AB    | 22  | TRP  |
| 1   | AB    | 88  | GLN  |
| 1   | AB    | 164 | ASP  |
| 2   | AC    | 35  | ASP  |
| 2   | AC    | 128 | MET  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | AC    | 175 | HIS  |
| 3   | AD    | 39  | GLN  |
| 3   | AD    | 40  | HIS  |
| 3   | AD    | 169 | TRP  |
| 3   | AD    | 197 | HIS  |
| 4   | AE    | 30  | PHE  |
| 4   | AE    | 47  | PHE  |
| 4   | AE    | 151 | MET  |
| 5   | AF    | 52  | ASN  |
| 7   | AH    | 76  | ARG  |
| 7   | AH    | 104 | SER  |
| 9   | AJ    | 42  | LEU  |
| 9   | AJ    | 48  | ARG  |
| 9   | AJ    | 49  | PHE  |
| 9   | AJ    | 59  | LYS  |
| 10  | AK    | 52  | ARG  |
| 10  | AK    | 121 | ARG  |
| 11  | AL    | 4   | ASN  |
| 12  | AM    | 3   | ILE  |
| 12  | AM    | 18  | LEU  |
| 12  | AM    | 54  | THR  |
| 13  | AN    | 62  | ASN  |
| 13  | AN    | 71  | HIS  |
| 17  | AR    | 34  | GLU  |
| 19  | AT    | 22  | SER  |
| 19  | AT    | 35  | TYR  |
| 19  | AT    | 67  | HIS  |
| 25  | BC    | 80  | LEU  |
| 25  | BC    | 173 | LEU  |
| 25  | BC    | 188 | ARG  |
| 25  | BC    | 190 | THR  |
| 25  | BC    | 200 | MET  |
| 25  | BC    | 235 | GLU  |
| 26  | BD    | 33  | ARG  |
| 26  | BD    | 67  | HIS  |
| 26  | BD    | 124 | ARG  |
| 27  | BE    | 78  | TRP  |
| 27  | BE    | 116 | ASP  |
| 28  | BF    | 162 | ASP  |
| 29  | BG    | 59  | ASP  |
| 29  | BG    | 66  | THR  |
| 29  | BG    | 162 | ARG  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30  | BH    | 137 | GLU  |
| 31  | BI    | 22  | PRO  |
| 31  | BI    | 34  | ILE  |
| 31  | BI    | 87  | SER  |
| 32  | BJ    | 1   | MET  |
| 32  | BJ    | 135 | GLN  |
| 33  | BK    | 32  | TYR  |
| 33  | BK    | 65  | THR  |
| 33  | BK    | 84  | CYS  |
| 33  | BK    | 105 | ARG  |
| 34  | BL    | 46  | VAL  |
| 35  | BM    | 57  | VAL  |
| 35  | BM    | 97  | GLN  |
| 35  | BM    | 131 | VAL  |
| 36  | BN    | 4   | ARG  |
| 37  | BO    | 9   | ARG  |
| 38  | BP    | 32  | VAL  |
| 38  | BP    | 64  | SER  |
| 38  | BP    | 67  | GLU  |
| 38  | BP    | 98  | TYR  |
| 39  | BQ    | 32  | ARG  |
| 40  | BR    | 32  | THR  |
| 41  | BS    | 1   | MET  |
| 41  | BS    | 3   | THR  |
| 41  | BS    | 15  | GLN  |
| 44  | BV    | 24  | ASN  |
| 44  | BV    | 51  | GLN  |
| 45  | BW    | 31  | LEU  |
| 45  | BW    | 38  | ARG  |
| 45  | BW    | 39  | GLN  |
| 45  | BW    | 40  | ARG  |
| 49  | B0    | 26  | SER  |
| 49  | B0    | 45  | ASP  |
| 51  | B2    | 16  | HIS  |
| 52  | B3    | 25  | HIS  |
| 53  | B4    | 19  | ARG  |
| 56  | B5    | 109 | MET  |
| 56  | B5    | 129 | GLN  |
| 56  | B5    | 180 | PHE  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AB    | 145 | ASN  |
| 13  | AN    | 62  | ASN  |
| 18  | AS    | 51  | HIS  |
| 18  | AS    | 56  | HIS  |
| 26  | BD    | 134 | HIS  |
| 32  | BJ    | 77  | HIS  |

### 5.3.3 RNA [\(i\)](#)

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 21  | AA    | 1529/1533 (99%) | 250 (16%)         | 72 (4%)         |
| 22  | A1    | 73/76 (96%)     | 8 (10%)           | 6 (8%)          |
| 23  | A2    | 14/15 (93%)     | 3 (21%)           | 1 (7%)          |
| 24  | A3    | 76/77 (98%)     | 9 (11%)           | 6 (7%)          |
| 54  | BA    | 2902/2903 (99%) | 460 (15%)         | 132 (4%)        |
| 55  | BB    | 116/118 (98%)   | 17 (14%)          | 3 (2%)          |
| All | All   | 4710/4722 (99%) | 747 (15%)         | 220 (4%)        |

All (747) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21  | AA    | 7   | A    |
| 21  | AA    | 8   | A    |
| 21  | AA    | 9   | G    |
| 21  | AA    | 13  | U    |
| 21  | AA    | 14  | U    |
| 21  | AA    | 16  | A    |
| 21  | AA    | 27  | G    |
| 21  | AA    | 31  | G    |
| 21  | AA    | 32  | A    |
| 21  | AA    | 34  | C    |
| 21  | AA    | 35  | G    |
| 21  | AA    | 39  | G    |
| 21  | AA    | 46  | G    |
| 21  | AA    | 48  | C    |
| 21  | AA    | 51  | A    |
| 21  | AA    | 65  | A    |
| 21  | AA    | 66  | A    |
| 21  | AA    | 69  | G    |
| 21  | AA    | 71  | A    |
| 21  | AA    | 72  | A    |
| 21  | AA    | 83  | C    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21  | AA    | 84  | U    |
| 21  | AA    | 85  | U    |
| 21  | AA    | 86  | G    |
| 21  | AA    | 87  | C    |
| 21  | AA    | 95  | C    |
| 21  | AA    | 110 | C    |
| 21  | AA    | 121 | U    |
| 21  | AA    | 130 | A    |
| 21  | AA    | 132 | C    |
| 21  | AA    | 133 | U    |
| 21  | AA    | 144 | G    |
| 21  | AA    | 159 | G    |
| 21  | AA    | 160 | A    |
| 21  | AA    | 163 | C    |
| 21  | AA    | 165 | G    |
| 21  | AA    | 182 | A    |
| 21  | AA    | 183 | C    |
| 21  | AA    | 195 | A    |
| 21  | AA    | 197 | A    |
| 21  | AA    | 198 | G    |
| 21  | AA    | 211 | G    |
| 21  | AA    | 212 | G    |
| 21  | AA    | 239 | U    |
| 21  | AA    | 240 | G    |
| 21  | AA    | 243 | A    |
| 21  | AA    | 244 | U    |
| 21  | AA    | 246 | A    |
| 21  | AA    | 249 | U    |
| 21  | AA    | 250 | A    |
| 21  | AA    | 251 | G    |
| 21  | AA    | 252 | U    |
| 21  | AA    | 272 | C    |
| 21  | AA    | 275 | G    |
| 21  | AA    | 282 | A    |
| 21  | AA    | 285 | C    |
| 21  | AA    | 289 | G    |
| 21  | AA    | 293 | G    |
| 21  | AA    | 306 | A    |
| 21  | AA    | 309 | A    |
| 21  | AA    | 310 | G    |
| 21  | AA    | 316 | C    |
| 21  | AA    | 317 | U    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21  | AA    | 328 | C    |
| 21  | AA    | 329 | A    |
| 21  | AA    | 330 | C    |
| 21  | AA    | 340 | U    |
| 21  | AA    | 341 | C    |
| 21  | AA    | 347 | G    |
| 21  | AA    | 348 | G    |
| 21  | AA    | 352 | C    |
| 21  | AA    | 354 | G    |
| 21  | AA    | 355 | C    |
| 21  | AA    | 367 | U    |
| 21  | AA    | 381 | C    |
| 21  | AA    | 382 | A    |
| 21  | AA    | 383 | A    |
| 21  | AA    | 397 | A    |
| 21  | AA    | 398 | U    |
| 21  | AA    | 412 | A    |
| 21  | AA    | 413 | G    |
| 21  | AA    | 415 | A    |
| 21  | AA    | 421 | U    |
| 21  | AA    | 422 | C    |
| 21  | AA    | 424 | G    |
| 21  | AA    | 428 | G    |
| 21  | AA    | 429 | U    |
| 21  | AA    | 452 | A    |
| 21  | AA    | 456 | A    |
| 21  | AA    | 461 | A    |
| 21  | AA    | 467 | U    |
| 21  | AA    | 468 | A    |
| 21  | AA    | 470 | C    |
| 21  | AA    | 484 | G    |
| 21  | AA    | 485 | U    |
| 21  | AA    | 493 | A    |
| 21  | AA    | 496 | A    |
| 21  | AA    | 497 | G    |
| 21  | AA    | 504 | C    |
| 21  | AA    | 505 | G    |
| 21  | AA    | 506 | G    |
| 21  | AA    | 509 | A    |
| 21  | AA    | 510 | A    |
| 21  | AA    | 511 | C    |
| 21  | AA    | 523 | A    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21  | AA    | 527 | G    |
| 21  | AA    | 532 | A    |
| 21  | AA    | 533 | A    |
| 21  | AA    | 534 | U    |
| 21  | AA    | 547 | A    |
| 21  | AA    | 550 | G    |
| 21  | AA    | 562 | U    |
| 21  | AA    | 564 | C    |
| 21  | AA    | 572 | A    |
| 21  | AA    | 573 | A    |
| 21  | AA    | 575 | G    |
| 21  | AA    | 576 | C    |
| 21  | AA    | 577 | G    |
| 21  | AA    | 610 | U    |
| 21  | AA    | 618 | C    |
| 21  | AA    | 619 | U    |
| 21  | AA    | 642 | A    |
| 21  | AA    | 649 | A    |
| 21  | AA    | 653 | U    |
| 21  | AA    | 660 | C    |
| 21  | AA    | 675 | A    |
| 21  | AA    | 700 | G    |
| 21  | AA    | 722 | G    |
| 21  | AA    | 723 | U    |
| 21  | AA    | 724 | G    |
| 21  | AA    | 731 | G    |
| 21  | AA    | 734 | G    |
| 21  | AA    | 735 | C    |
| 21  | AA    | 755 | G    |
| 21  | AA    | 767 | A    |
| 21  | AA    | 777 | A    |
| 21  | AA    | 794 | A    |
| 21  | AA    | 808 | C    |
| 21  | AA    | 811 | C    |
| 21  | AA    | 812 | G    |
| 21  | AA    | 819 | A    |
| 21  | AA    | 841 | C    |
| 21  | AA    | 842 | U    |
| 21  | AA    | 843 | U    |
| 21  | AA    | 846 | G    |
| 21  | AA    | 867 | G    |
| 21  | AA    | 872 | A    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 21  | AA    | 885  | G    |
| 21  | AA    | 891  | U    |
| 21  | AA    | 892  | A    |
| 21  | AA    | 893  | C    |
| 21  | AA    | 914  | A    |
| 21  | AA    | 926  | G    |
| 21  | AA    | 927  | G    |
| 21  | AA    | 929  | G    |
| 21  | AA    | 934  | C    |
| 21  | AA    | 939  | G    |
| 21  | AA    | 960  | U    |
| 21  | AA    | 961  | U    |
| 21  | AA    | 968  | A    |
| 21  | AA    | 969  | A    |
| 21  | AA    | 974  | A    |
| 21  | AA    | 976  | G    |
| 21  | AA    | 978  | A    |
| 21  | AA    | 980  | C    |
| 21  | AA    | 981  | U    |
| 21  | AA    | 983  | A    |
| 21  | AA    | 992  | U    |
| 21  | AA    | 993  | G    |
| 21  | AA    | 994  | A    |
| 21  | AA    | 1004 | A    |
| 21  | AA    | 1030 | U    |
| 21  | AA    | 1031 | C    |
| 21  | AA    | 1033 | G    |
| 21  | AA    | 1053 | G    |
| 21  | AA    | 1054 | C    |
| 21  | AA    | 1055 | A    |
| 21  | AA    | 1056 | U    |
| 21  | AA    | 1065 | U    |
| 21  | AA    | 1068 | G    |
| 21  | AA    | 1094 | G    |
| 21  | AA    | 1095 | U    |
| 21  | AA    | 1101 | A    |
| 21  | AA    | 1102 | A    |
| 21  | AA    | 1124 | G    |
| 21  | AA    | 1125 | U    |
| 21  | AA    | 1137 | C    |
| 21  | AA    | 1139 | G    |
| 21  | AA    | 1152 | A    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 21  | AA    | 1157 | A    |
| 21  | AA    | 1159 | U    |
| 21  | AA    | 1160 | G    |
| 21  | AA    | 1161 | C    |
| 21  | AA    | 1167 | A    |
| 21  | AA    | 1183 | U    |
| 21  | AA    | 1189 | U    |
| 21  | AA    | 1190 | G    |
| 21  | AA    | 1191 | A    |
| 21  | AA    | 1196 | A    |
| 21  | AA    | 1201 | A    |
| 21  | AA    | 1202 | U    |
| 21  | AA    | 1204 | A    |
| 21  | AA    | 1213 | A    |
| 21  | AA    | 1217 | C    |
| 21  | AA    | 1222 | G    |
| 21  | AA    | 1225 | A    |
| 21  | AA    | 1227 | A    |
| 21  | AA    | 1228 | C    |
| 21  | AA    | 1241 | G    |
| 21  | AA    | 1256 | A    |
| 21  | AA    | 1257 | A    |
| 21  | AA    | 1258 | G    |
| 21  | AA    | 1266 | G    |
| 21  | AA    | 1280 | A    |
| 21  | AA    | 1281 | C    |
| 21  | AA    | 1286 | U    |
| 21  | AA    | 1301 | U    |
| 21  | AA    | 1302 | C    |
| 21  | AA    | 1304 | G    |
| 21  | AA    | 1305 | G    |
| 21  | AA    | 1312 | G    |
| 21  | AA    | 1317 | C    |
| 21  | AA    | 1318 | A    |
| 21  | AA    | 1322 | C    |
| 21  | AA    | 1329 | A    |
| 21  | AA    | 1336 | C    |
| 21  | AA    | 1337 | G    |
| 21  | AA    | 1338 | G    |
| 21  | AA    | 1345 | U    |
| 21  | AA    | 1346 | A    |
| 21  | AA    | 1360 | A    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 21  | AA    | 1363 | A    |
| 21  | AA    | 1381 | U    |
| 21  | AA    | 1397 | C    |
| 21  | AA    | 1398 | A    |
| 21  | AA    | 1419 | G    |
| 21  | AA    | 1432 | G    |
| 21  | AA    | 1446 | A    |
| 21  | AA    | 1447 | A    |
| 21  | AA    | 1448 | C    |
| 21  | AA    | 1470 | U    |
| 21  | AA    | 1493 | A    |
| 21  | AA    | 1494 | G    |
| 21  | AA    | 1497 | G    |
| 21  | AA    | 1503 | A    |
| 21  | AA    | 1506 | U    |
| 21  | AA    | 1529 | G    |
| 21  | AA    | 1530 | G    |
| 21  | AA    | 1533 | C    |
| 21  | AA    | 1534 | A    |
| 22  | A1    | 10   | G    |
| 22  | A1    | 11   | C    |
| 22  | A1    | 17   | U    |
| 22  | A1    | 48   | C    |
| 22  | A1    | 57   | G    |
| 22  | A1    | 60   | C    |
| 22  | A1    | 61   | C    |
| 22  | A1    | 75   | C    |
| 23  | A2    | 89   | U    |
| 23  | A2    | 90   | U    |
| 23  | A2    | 91   | A    |
| 24  | A3    | 9    | G    |
| 24  | A3    | 16   | C    |
| 24  | A3    | 17   | C    |
| 24  | A3    | 18   | U    |
| 24  | A3    | 48   | U    |
| 24  | A3    | 49   | C    |
| 24  | A3    | 62   | C    |
| 24  | A3    | 63   | C    |
| 24  | A3    | 73   | A    |
| 54  | BA    | 10   | A    |
| 54  | BA    | 11   | C    |
| 54  | BA    | 34   | U    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 54  | BA    | 48  | G    |
| 54  | BA    | 52  | A    |
| 54  | BA    | 61  | C    |
| 54  | BA    | 62  | U    |
| 54  | BA    | 71  | A    |
| 54  | BA    | 72  | U    |
| 54  | BA    | 73  | A    |
| 54  | BA    | 75  | G    |
| 54  | BA    | 84  | A    |
| 54  | BA    | 100 | U    |
| 54  | BA    | 101 | A    |
| 54  | BA    | 102 | U    |
| 54  | BA    | 118 | A    |
| 54  | BA    | 119 | A    |
| 54  | BA    | 120 | U    |
| 54  | BA    | 122 | G    |
| 54  | BA    | 142 | A    |
| 54  | BA    | 143 | C    |
| 54  | BA    | 149 | A    |
| 54  | BA    | 162 | U    |
| 54  | BA    | 181 | A    |
| 54  | BA    | 196 | A    |
| 54  | BA    | 199 | A    |
| 54  | BA    | 205 | G    |
| 54  | BA    | 216 | A    |
| 54  | BA    | 222 | A    |
| 54  | BA    | 225 | C    |
| 54  | BA    | 233 | A    |
| 54  | BA    | 248 | G    |
| 54  | BA    | 249 | C    |
| 54  | BA    | 250 | G    |
| 54  | BA    | 263 | G    |
| 54  | BA    | 271 | G    |
| 54  | BA    | 272 | A    |
| 54  | BA    | 273 | G    |
| 54  | BA    | 279 | A    |
| 54  | BA    | 280 | U    |
| 54  | BA    | 295 | G    |
| 54  | BA    | 317 | G    |
| 54  | BA    | 323 | C    |
| 54  | BA    | 324 | A    |
| 54  | BA    | 326 | G    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 54  | BA    | 327 | G    |
| 54  | BA    | 329 | G    |
| 54  | BA    | 330 | A    |
| 54  | BA    | 331 | C    |
| 54  | BA    | 332 | A    |
| 54  | BA    | 345 | A    |
| 54  | BA    | 346 | A    |
| 54  | BA    | 370 | G    |
| 54  | BA    | 372 | G    |
| 54  | BA    | 386 | G    |
| 54  | BA    | 404 | A    |
| 54  | BA    | 405 | U    |
| 54  | BA    | 406 | G    |
| 54  | BA    | 412 | A    |
| 54  | BA    | 428 | A    |
| 54  | BA    | 430 | A    |
| 54  | BA    | 443 | A    |
| 54  | BA    | 449 | A    |
| 54  | BA    | 451 | U    |
| 54  | BA    | 452 | G    |
| 54  | BA    | 453 | A    |
| 54  | BA    | 454 | A    |
| 54  | BA    | 456 | C    |
| 54  | BA    | 457 | A    |
| 54  | BA    | 458 | G    |
| 54  | BA    | 473 | G    |
| 54  | BA    | 478 | A    |
| 54  | BA    | 479 | A    |
| 54  | BA    | 480 | A    |
| 54  | BA    | 481 | G    |
| 54  | BA    | 484 | C    |
| 54  | BA    | 491 | G    |
| 54  | BA    | 504 | A    |
| 54  | BA    | 505 | A    |
| 54  | BA    | 520 | G    |
| 54  | BA    | 526 | A    |
| 54  | BA    | 527 | C    |
| 54  | BA    | 529 | A    |
| 54  | BA    | 531 | C    |
| 54  | BA    | 532 | A    |
| 54  | BA    | 533 | G    |
| 54  | BA    | 544 | C    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 54  | BA    | 546 | U    |
| 54  | BA    | 547 | A    |
| 54  | BA    | 548 | G    |
| 54  | BA    | 573 | U    |
| 54  | BA    | 575 | A    |
| 54  | BA    | 586 | A    |
| 54  | BA    | 587 | C    |
| 54  | BA    | 603 | A    |
| 54  | BA    | 607 | U    |
| 54  | BA    | 612 | G    |
| 54  | BA    | 613 | A    |
| 54  | BA    | 614 | A    |
| 54  | BA    | 615 | U    |
| 54  | BA    | 620 | G    |
| 54  | BA    | 627 | A    |
| 54  | BA    | 631 | A    |
| 54  | BA    | 632 | A    |
| 54  | BA    | 637 | A    |
| 54  | BA    | 646 | U    |
| 54  | BA    | 653 | U    |
| 54  | BA    | 654 | A    |
| 54  | BA    | 671 | C    |
| 54  | BA    | 672 | C    |
| 54  | BA    | 685 | A    |
| 54  | BA    | 686 | U    |
| 54  | BA    | 715 | A    |
| 54  | BA    | 716 | A    |
| 54  | BA    | 719 | C    |
| 54  | BA    | 727 | A    |
| 54  | BA    | 730 | A    |
| 54  | BA    | 747 | U    |
| 54  | BA    | 751 | A    |
| 54  | BA    | 758 | C    |
| 54  | BA    | 759 | G    |
| 54  | BA    | 763 | G    |
| 54  | BA    | 775 | G    |
| 54  | BA    | 781 | A    |
| 54  | BA    | 782 | A    |
| 54  | BA    | 783 | A    |
| 54  | BA    | 784 | G    |
| 54  | BA    | 785 | G    |
| 54  | BA    | 791 | C    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 54  | BA    | 792  | A    |
| 54  | BA    | 794  | A    |
| 54  | BA    | 805  | G    |
| 54  | BA    | 809  | G    |
| 54  | BA    | 812  | C    |
| 54  | BA    | 847  | U    |
| 54  | BA    | 848  | C    |
| 54  | BA    | 858  | G    |
| 54  | BA    | 866  | A    |
| 54  | BA    | 889  | C    |
| 54  | BA    | 890  | C    |
| 54  | BA    | 891  | G    |
| 54  | BA    | 896  | A    |
| 54  | BA    | 897  | C    |
| 54  | BA    | 907  | G    |
| 54  | BA    | 910  | A    |
| 54  | BA    | 914  | G    |
| 54  | BA    | 915  | C    |
| 54  | BA    | 931  | U    |
| 54  | BA    | 941  | A    |
| 54  | BA    | 946  | C    |
| 54  | BA    | 955  | U    |
| 54  | BA    | 959  | A    |
| 54  | BA    | 961  | C    |
| 54  | BA    | 972  | A    |
| 54  | BA    | 974  | G    |
| 54  | BA    | 975  | A    |
| 54  | BA    | 980  | A    |
| 54  | BA    | 982  | C    |
| 54  | BA    | 983  | A    |
| 54  | BA    | 985  | C    |
| 54  | BA    | 990  | A    |
| 54  | BA    | 995  | C    |
| 54  | BA    | 996  | A    |
| 54  | BA    | 1012 | U    |
| 54  | BA    | 1013 | C    |
| 54  | BA    | 1021 | A    |
| 54  | BA    | 1022 | G    |
| 54  | BA    | 1024 | G    |
| 54  | BA    | 1025 | G    |
| 54  | BA    | 1033 | U    |
| 54  | BA    | 1044 | C    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 54  | BA    | 1048 | A    |
| 54  | BA    | 1060 | U    |
| 54  | BA    | 1062 | G    |
| 54  | BA    | 1063 | G    |
| 54  | BA    | 1067 | A    |
| 54  | BA    | 1068 | G    |
| 54  | BA    | 1070 | A    |
| 54  | BA    | 1071 | G    |
| 54  | BA    | 1073 | A    |
| 54  | BA    | 1076 | C    |
| 54  | BA    | 1078 | U    |
| 54  | BA    | 1079 | C    |
| 54  | BA    | 1088 | A    |
| 54  | BA    | 1089 | A    |
| 54  | BA    | 1090 | A    |
| 54  | BA    | 1094 | U    |
| 54  | BA    | 1096 | A    |
| 54  | BA    | 1112 | G    |
| 54  | BA    | 1126 | A    |
| 54  | BA    | 1128 | G    |
| 54  | BA    | 1129 | A    |
| 54  | BA    | 1132 | U    |
| 54  | BA    | 1134 | A    |
| 54  | BA    | 1135 | C    |
| 54  | BA    | 1143 | A    |
| 54  | BA    | 1155 | A    |
| 54  | BA    | 1175 | A    |
| 54  | BA    | 1176 | U    |
| 54  | BA    | 1186 | G    |
| 54  | BA    | 1210 | G    |
| 54  | BA    | 1211 | C    |
| 54  | BA    | 1225 | G    |
| 54  | BA    | 1242 | U    |
| 54  | BA    | 1247 | A    |
| 54  | BA    | 1251 | C    |
| 54  | BA    | 1253 | A    |
| 54  | BA    | 1255 | U    |
| 54  | BA    | 1256 | G    |
| 54  | BA    | 1265 | A    |
| 54  | BA    | 1266 | G    |
| 54  | BA    | 1267 | U    |
| 54  | BA    | 1272 | A    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 54  | BA    | 1273 | U    |
| 54  | BA    | 1275 | A    |
| 54  | BA    | 1276 | A    |
| 54  | BA    | 1287 | A    |
| 54  | BA    | 1291 | C    |
| 54  | BA    | 1300 | G    |
| 54  | BA    | 1301 | A    |
| 54  | BA    | 1314 | C    |
| 54  | BA    | 1319 | C    |
| 54  | BA    | 1320 | C    |
| 54  | BA    | 1326 | U    |
| 54  | BA    | 1328 | A    |
| 54  | BA    | 1332 | G    |
| 54  | BA    | 1341 | G    |
| 54  | BA    | 1365 | A    |
| 54  | BA    | 1374 | G    |
| 54  | BA    | 1379 | U    |
| 54  | BA    | 1383 | A    |
| 54  | BA    | 1385 | A    |
| 54  | BA    | 1386 | C    |
| 54  | BA    | 1390 | U    |
| 54  | BA    | 1394 | U    |
| 54  | BA    | 1396 | U    |
| 54  | BA    | 1397 | U    |
| 54  | BA    | 1416 | G    |
| 54  | BA    | 1420 | A    |
| 54  | BA    | 1421 | G    |
| 54  | BA    | 1427 | A    |
| 54  | BA    | 1428 | C    |
| 54  | BA    | 1440 | U    |
| 54  | BA    | 1452 | G    |
| 54  | BA    | 1453 | A    |
| 54  | BA    | 1454 | C    |
| 54  | BA    | 1458 | U    |
| 54  | BA    | 1459 | G    |
| 54  | BA    | 1461 | C    |
| 54  | BA    | 1466 | U    |
| 54  | BA    | 1482 | G    |
| 54  | BA    | 1490 | A    |
| 54  | BA    | 1493 | C    |
| 54  | BA    | 1524 | G    |
| 54  | BA    | 1535 | A    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 54  | BA    | 1536 | C    |
| 54  | BA    | 1537 | G    |
| 54  | BA    | 1538 | G    |
| 54  | BA    | 1539 | U    |
| 54  | BA    | 1540 | G    |
| 54  | BA    | 1550 | C    |
| 54  | BA    | 1560 | G    |
| 54  | BA    | 1569 | A    |
| 54  | BA    | 1584 | U    |
| 54  | BA    | 1598 | A    |
| 54  | BA    | 1599 | U    |
| 54  | BA    | 1607 | C    |
| 54  | BA    | 1608 | A    |
| 54  | BA    | 1618 | A    |
| 54  | BA    | 1625 | C    |
| 54  | BA    | 1626 | A    |
| 54  | BA    | 1629 | U    |
| 54  | BA    | 1633 | G    |
| 54  | BA    | 1634 | A    |
| 54  | BA    | 1635 | A    |
| 54  | BA    | 1648 | U    |
| 54  | BA    | 1652 | A    |
| 54  | BA    | 1656 | C    |
| 54  | BA    | 1674 | G    |
| 54  | BA    | 1675 | C    |
| 54  | BA    | 1707 | G    |
| 54  | BA    | 1712 | U    |
| 54  | BA    | 1714 | U    |
| 54  | BA    | 1730 | C    |
| 54  | BA    | 1758 | U    |
| 54  | BA    | 1764 | C    |
| 54  | BA    | 1773 | A    |
| 54  | BA    | 1800 | C    |
| 54  | BA    | 1808 | A    |
| 54  | BA    | 1816 | C    |
| 54  | BA    | 1821 | A    |
| 54  | BA    | 1827 | U    |
| 54  | BA    | 1833 | C    |
| 54  | BA    | 1847 | A    |
| 54  | BA    | 1873 | G    |
| 54  | BA    | 1888 | G    |
| 54  | BA    | 1900 | A    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 54  | BA    | 1901 | A    |
| 54  | BA    | 1906 | G    |
| 54  | BA    | 1913 | A    |
| 54  | BA    | 1914 | C    |
| 54  | BA    | 1929 | G    |
| 54  | BA    | 1930 | G    |
| 54  | BA    | 1937 | A    |
| 54  | BA    | 1938 | A    |
| 54  | BA    | 1939 | U    |
| 54  | BA    | 1940 | U    |
| 54  | BA    | 1941 | C    |
| 54  | BA    | 1943 | U    |
| 54  | BA    | 1944 | U    |
| 54  | BA    | 1946 | U    |
| 54  | BA    | 1955 | U    |
| 54  | BA    | 1970 | A    |
| 54  | BA    | 1971 | U    |
| 54  | BA    | 1972 | G    |
| 54  | BA    | 1981 | A    |
| 54  | BA    | 1993 | U    |
| 54  | BA    | 1997 | C    |
| 54  | BA    | 2002 | G    |
| 54  | BA    | 2003 | A    |
| 54  | BA    | 2018 | G    |
| 54  | BA    | 2020 | A    |
| 54  | BA    | 2030 | A    |
| 54  | BA    | 2031 | A    |
| 54  | BA    | 2032 | G    |
| 54  | BA    | 2043 | C    |
| 54  | BA    | 2055 | C    |
| 54  | BA    | 2058 | A    |
| 54  | BA    | 2061 | G    |
| 54  | BA    | 2069 | G    |
| 54  | BA    | 2076 | U    |
| 54  | BA    | 2093 | G    |
| 54  | BA    | 2112 | G    |
| 54  | BA    | 2113 | U    |
| 54  | BA    | 2115 | G    |
| 54  | BA    | 2117 | A    |
| 54  | BA    | 2119 | A    |
| 54  | BA    | 2126 | A    |
| 54  | BA    | 2127 | G    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 54  | BA    | 2133 | G    |
| 54  | BA    | 2135 | A    |
| 54  | BA    | 2137 | U    |
| 54  | BA    | 2138 | G    |
| 54  | BA    | 2155 | U    |
| 54  | BA    | 2157 | G    |
| 54  | BA    | 2159 | G    |
| 54  | BA    | 2160 | C    |
| 54  | BA    | 2169 | A    |
| 54  | BA    | 2172 | U    |
| 54  | BA    | 2173 | A    |
| 54  | BA    | 2181 | U    |
| 54  | BA    | 2198 | A    |
| 54  | BA    | 2203 | U    |
| 54  | BA    | 2211 | A    |
| 54  | BA    | 2212 | A    |
| 54  | BA    | 2213 | U    |
| 54  | BA    | 2216 | G    |
| 54  | BA    | 2226 | C    |
| 54  | BA    | 2238 | G    |
| 54  | BA    | 2250 | G    |
| 54  | BA    | 2251 | G    |
| 54  | BA    | 2267 | A    |
| 54  | BA    | 2276 | G    |
| 54  | BA    | 2283 | C    |
| 54  | BA    | 2296 | U    |
| 54  | BA    | 2297 | A    |
| 54  | BA    | 2305 | U    |
| 54  | BA    | 2307 | G    |
| 54  | BA    | 2308 | G    |
| 54  | BA    | 2313 | C    |
| 54  | BA    | 2320 | U    |
| 54  | BA    | 2321 | U    |
| 54  | BA    | 2324 | U    |
| 54  | BA    | 2325 | G    |
| 54  | BA    | 2333 | A    |
| 54  | BA    | 2334 | U    |
| 54  | BA    | 2335 | A    |
| 54  | BA    | 2339 | C    |
| 54  | BA    | 2347 | C    |
| 54  | BA    | 2350 | C    |
| 54  | BA    | 2352 | A    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 54  | BA    | 2353 | G    |
| 54  | BA    | 2383 | G    |
| 54  | BA    | 2385 | C    |
| 54  | BA    | 2389 | G    |
| 54  | BA    | 2391 | G    |
| 54  | BA    | 2392 | A    |
| 54  | BA    | 2396 | G    |
| 54  | BA    | 2402 | U    |
| 54  | BA    | 2406 | A    |
| 54  | BA    | 2407 | A    |
| 54  | BA    | 2409 | G    |
| 54  | BA    | 2419 | U    |
| 54  | BA    | 2425 | A    |
| 54  | BA    | 2429 | G    |
| 54  | BA    | 2430 | A    |
| 54  | BA    | 2431 | U    |
| 54  | BA    | 2432 | A    |
| 54  | BA    | 2433 | A    |
| 54  | BA    | 2441 | U    |
| 54  | BA    | 2447 | G    |
| 54  | BA    | 2448 | A    |
| 54  | BA    | 2476 | A    |
| 54  | BA    | 2491 | U    |
| 54  | BA    | 2495 | G    |
| 54  | BA    | 2498 | C    |
| 54  | BA    | 2501 | C    |
| 54  | BA    | 2502 | G    |
| 54  | BA    | 2503 | A    |
| 54  | BA    | 2505 | G    |
| 54  | BA    | 2514 | U    |
| 54  | BA    | 2518 | A    |
| 54  | BA    | 2529 | G    |
| 54  | BA    | 2531 | A    |
| 54  | BA    | 2540 | C    |
| 54  | BA    | 2544 | G    |
| 54  | BA    | 2554 | U    |
| 54  | BA    | 2566 | A    |
| 54  | BA    | 2573 | C    |
| 54  | BA    | 2576 | G    |
| 54  | BA    | 2578 | G    |
| 54  | BA    | 2581 | G    |
| 54  | BA    | 2609 | U    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 54  | BA    | 2613 | U    |
| 54  | BA    | 2614 | A    |
| 54  | BA    | 2628 | C    |
| 54  | BA    | 2629 | U    |
| 54  | BA    | 2630 | G    |
| 54  | BA    | 2631 | G    |
| 54  | BA    | 2645 | G    |
| 54  | BA    | 2646 | C    |
| 54  | BA    | 2647 | U    |
| 54  | BA    | 2655 | G    |
| 54  | BA    | 2660 | A    |
| 54  | BA    | 2683 | C    |
| 54  | BA    | 2689 | U    |
| 54  | BA    | 2690 | U    |
| 54  | BA    | 2691 | C    |
| 54  | BA    | 2721 | A    |
| 54  | BA    | 2726 | A    |
| 54  | BA    | 2744 | G    |
| 54  | BA    | 2751 | G    |
| 54  | BA    | 2757 | A    |
| 54  | BA    | 2765 | A    |
| 54  | BA    | 2778 | A    |
| 54  | BA    | 2779 | U    |
| 54  | BA    | 2791 | G    |
| 54  | BA    | 2797 | U    |
| 54  | BA    | 2798 | U    |
| 54  | BA    | 2821 | A    |
| 54  | BA    | 2823 | A    |
| 54  | BA    | 2824 | C    |
| 54  | BA    | 2833 | U    |
| 54  | BA    | 2846 | G    |
| 54  | BA    | 2858 | C    |
| 54  | BA    | 2859 | G    |
| 54  | BA    | 2867 | G    |
| 54  | BA    | 2868 | A    |
| 54  | BA    | 2880 | C    |
| 54  | BA    | 2884 | U    |
| 55  | BB    | 9    | G    |
| 55  | BB    | 13   | G    |
| 55  | BB    | 16   | G    |
| 55  | BB    | 37   | C    |
| 55  | BB    | 41   | G    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 55  | BB    | 44  | G    |
| 55  | BB    | 45  | A    |
| 55  | BB    | 52  | A    |
| 55  | BB    | 56  | G    |
| 55  | BB    | 57  | A    |
| 55  | BB    | 58  | A    |
| 55  | BB    | 67  | G    |
| 55  | BB    | 70  | C    |
| 55  | BB    | 74  | U    |
| 55  | BB    | 87  | U    |
| 55  | BB    | 90  | C    |
| 55  | BB    | 109 | A    |

All (220) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21  | AA    | 13  | U    |
| 21  | AA    | 34  | C    |
| 21  | AA    | 46  | G    |
| 21  | AA    | 65  | A    |
| 21  | AA    | 85  | U    |
| 21  | AA    | 109 | A    |
| 21  | AA    | 132 | C    |
| 21  | AA    | 173 | U    |
| 21  | AA    | 194 | C    |
| 21  | AA    | 211 | G    |
| 21  | AA    | 243 | A    |
| 21  | AA    | 251 | G    |
| 21  | AA    | 281 | G    |
| 21  | AA    | 309 | A    |
| 21  | AA    | 316 | C    |
| 21  | AA    | 328 | C    |
| 21  | AA    | 340 | U    |
| 21  | AA    | 350 | G    |
| 21  | AA    | 354 | G    |
| 21  | AA    | 366 | A    |
| 21  | AA    | 382 | A    |
| 21  | AA    | 383 | A    |
| 21  | AA    | 414 | A    |
| 21  | AA    | 451 | A    |
| 21  | AA    | 496 | A    |
| 21  | AA    | 504 | C    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 21  | AA    | 509  | A    |
| 21  | AA    | 527  | G    |
| 21  | AA    | 532  | A    |
| 21  | AA    | 535  | A    |
| 21  | AA    | 575  | G    |
| 21  | AA    | 641  | U    |
| 21  | AA    | 653  | U    |
| 21  | AA    | 675  | A    |
| 21  | AA    | 733  | G    |
| 21  | AA    | 734  | G    |
| 21  | AA    | 792  | A    |
| 21  | AA    | 811  | C    |
| 21  | AA    | 840  | C    |
| 21  | AA    | 891  | U    |
| 21  | AA    | 892  | A    |
| 21  | AA    | 925  | G    |
| 21  | AA    | 965  | U    |
| 21  | AA    | 983  | A    |
| 21  | AA    | 1029 | U    |
| 21  | AA    | 1030 | U    |
| 21  | AA    | 1049 | U    |
| 21  | AA    | 1101 | A    |
| 21  | AA    | 1124 | G    |
| 21  | AA    | 1139 | G    |
| 21  | AA    | 1151 | A    |
| 21  | AA    | 1166 | G    |
| 21  | AA    | 1190 | G    |
| 21  | AA    | 1196 | A    |
| 21  | AA    | 1201 | A    |
| 21  | AA    | 1225 | A    |
| 21  | AA    | 1226 | C    |
| 21  | AA    | 1227 | A    |
| 21  | AA    | 1231 | G    |
| 21  | AA    | 1233 | G    |
| 21  | AA    | 1257 | A    |
| 21  | AA    | 1298 | U    |
| 21  | AA    | 1300 | G    |
| 21  | AA    | 1304 | G    |
| 21  | AA    | 1305 | G    |
| 21  | AA    | 1336 | C    |
| 21  | AA    | 1345 | U    |
| 21  | AA    | 1381 | U    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 21  | AA    | 1429 | A    |
| 21  | AA    | 1431 | A    |
| 21  | AA    | 1447 | A    |
| 21  | AA    | 1469 | C    |
| 22  | A1    | 10   | G    |
| 22  | A1    | 46   | 7MG  |
| 22  | A1    | 47   | U    |
| 22  | A1    | 59   | U    |
| 22  | A1    | 60   | C    |
| 22  | A1    | 74   | C    |
| 23  | A2    | 90   | U    |
| 24  | A3    | 9    | G    |
| 24  | A3    | 16   | C    |
| 24  | A3    | 17   | C    |
| 24  | A3    | 19   | G    |
| 24  | A3    | 48   | U    |
| 24  | A3    | 62   | C    |
| 54  | BA    | 10   | A    |
| 54  | BA    | 60   | G    |
| 54  | BA    | 71   | A    |
| 54  | BA    | 72   | U    |
| 54  | BA    | 74   | A    |
| 54  | BA    | 101  | A    |
| 54  | BA    | 149  | A    |
| 54  | BA    | 196  | A    |
| 54  | BA    | 249  | C    |
| 54  | BA    | 279  | A    |
| 54  | BA    | 322  | A    |
| 54  | BA    | 323  | C    |
| 54  | BA    | 329  | G    |
| 54  | BA    | 345  | A    |
| 54  | BA    | 384  | A    |
| 54  | BA    | 387  | U    |
| 54  | BA    | 388  | G    |
| 54  | BA    | 405  | U    |
| 54  | BA    | 411  | G    |
| 54  | BA    | 428  | A    |
| 54  | BA    | 442  | G    |
| 54  | BA    | 455  | C    |
| 54  | BA    | 456  | C    |
| 54  | BA    | 457  | A    |
| 54  | BA    | 506  | G    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 54  | BA    | 547  | A    |
| 54  | BA    | 548  | G    |
| 54  | BA    | 613  | A    |
| 54  | BA    | 627  | A    |
| 54  | BA    | 631  | A    |
| 54  | BA    | 651  | G    |
| 54  | BA    | 654  | A    |
| 54  | BA    | 656  | G    |
| 54  | BA    | 670  | A    |
| 54  | BA    | 675  | A    |
| 54  | BA    | 685  | A    |
| 54  | BA    | 715  | A    |
| 54  | BA    | 762  | U    |
| 54  | BA    | 764  | A    |
| 54  | BA    | 782  | A    |
| 54  | BA    | 790  | U    |
| 54  | BA    | 846  | U    |
| 54  | BA    | 847  | U    |
| 54  | BA    | 866  | A    |
| 54  | BA    | 931  | U    |
| 54  | BA    | 973  | A    |
| 54  | BA    | 989  | G    |
| 54  | BA    | 1008 | A    |
| 54  | BA    | 1021 | A    |
| 54  | BA    | 1089 | A    |
| 54  | BA    | 1128 | G    |
| 54  | BA    | 1132 | U    |
| 54  | BA    | 1134 | A    |
| 54  | BA    | 1142 | A    |
| 54  | BA    | 1224 | U    |
| 54  | BA    | 1254 | A    |
| 54  | BA    | 1266 | G    |
| 54  | BA    | 1288 | G    |
| 54  | BA    | 1300 | G    |
| 54  | BA    | 1320 | C    |
| 54  | BA    | 1325 | U    |
| 54  | BA    | 1332 | G    |
| 54  | BA    | 1378 | A    |
| 54  | BA    | 1385 | A    |
| 54  | BA    | 1396 | U    |
| 54  | BA    | 1397 | U    |
| 54  | BA    | 1420 | A    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 54  | BA    | 1427 | A    |
| 54  | BA    | 1453 | A    |
| 54  | BA    | 1465 | G    |
| 54  | BA    | 1490 | A    |
| 54  | BA    | 1535 | A    |
| 54  | BA    | 1539 | U    |
| 54  | BA    | 1607 | C    |
| 54  | BA    | 1625 | C    |
| 54  | BA    | 1634 | A    |
| 54  | BA    | 1651 | G    |
| 54  | BA    | 1674 | G    |
| 54  | BA    | 1706 | C    |
| 54  | BA    | 1711 | A    |
| 54  | BA    | 1713 | A    |
| 54  | BA    | 1769 | U    |
| 54  | BA    | 1783 | A    |
| 54  | BA    | 1787 | A    |
| 54  | BA    | 1826 | G    |
| 54  | BA    | 1913 | A    |
| 54  | BA    | 1936 | A    |
| 54  | BA    | 1938 | A    |
| 54  | BA    | 1940 | U    |
| 54  | BA    | 1943 | U    |
| 54  | BA    | 1945 | G    |
| 54  | BA    | 1955 | U    |
| 54  | BA    | 1971 | U    |
| 54  | BA    | 1980 | G    |
| 54  | BA    | 2002 | G    |
| 54  | BA    | 2030 | A    |
| 54  | BA    | 2031 | A    |
| 54  | BA    | 2060 | A    |
| 54  | BA    | 2126 | A    |
| 54  | BA    | 2150 | C    |
| 54  | BA    | 2172 | U    |
| 54  | BA    | 2197 | U    |
| 54  | BA    | 2212 | A    |
| 54  | BA    | 2225 | A    |
| 54  | BA    | 2249 | U    |
| 54  | BA    | 2286 | G    |
| 54  | BA    | 2296 | U    |
| 54  | BA    | 2324 | U    |
| 54  | BA    | 2343 | U    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 54  | BA    | 2389 | G    |
| 54  | BA    | 2391 | G    |
| 54  | BA    | 2429 | G    |
| 54  | BA    | 2447 | G    |
| 54  | BA    | 2453 | A    |
| 54  | BA    | 2494 | G    |
| 54  | BA    | 2497 | A    |
| 54  | BA    | 2503 | A    |
| 54  | BA    | 2513 | A    |
| 54  | BA    | 2529 | G    |
| 54  | BA    | 2572 | A    |
| 54  | BA    | 2576 | G    |
| 54  | BA    | 2609 | U    |
| 54  | BA    | 2628 | C    |
| 54  | BA    | 2630 | G    |
| 54  | BA    | 2720 | U    |
| 54  | BA    | 2721 | A    |
| 54  | BA    | 2726 | A    |
| 54  | BA    | 2751 | G    |
| 54  | BA    | 2756 | U    |
| 54  | BA    | 2788 | C    |
| 54  | BA    | 2790 | U    |
| 54  | BA    | 2823 | A    |
| 55  | BB    | 12   | C    |
| 55  | BB    | 56   | G    |
| 55  | BB    | 57   | A    |

## 5.4 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

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

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 24  | H2U  | A3    | 21  | 24   | 18,21,22     | 1.40 | 2 (11%)  | 21,30,33    | 1.11 | 3 (14%)  |
| 24  | 5MU  | A3    | 55  | 24   | 19,22,23     | 0.97 | 1 (5%)   | 28,32,35    | 1.52 | 4 (14%)  |

| Mol | Type | Chain | Res | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 22  | 5MU  | A1    | 54  | 22    | 19,22,23     | 0.85 | 0        | 28,32,35    | 1.59 | 6 (21%)  |
| 22  | 4SU  | A1    | 7   | 22    | 18,21,22     | 1.51 | 2 (11%)  | 26,30,33    | 1.11 | 2 (7%)   |
| 22  | 6MZ  | A1    | 37  | 22    | 18,25,26     | 0.94 | 1 (5%)   | 16,36,39    | 1.74 | 2 (12%)  |
| 24  | 4SU  | A3    | 8   | 24    | 18,21,22     | 1.61 | 3 (16%)  | 26,30,33    | 0.83 | 1 (3%)   |
| 24  | PSU  | A3    | 56  | 24    | 18,21,22     | 1.08 | 1 (5%)   | 22,30,33    | 1.58 | 4 (18%)  |
| 22  | PSU  | A1    | 55  | 22    | 18,21,22     | 1.03 | 1 (5%)   | 22,30,33    | 1.33 | 2 (9%)   |
| 24  | OMC  | A3    | 33  | 24    | 19,22,23     | 0.96 | 0        | 26,31,34    | 1.14 | 2 (7%)   |
| 22  | CM0  | A1    | 34  | 23,22 | 22,26,27     | 1.50 | 3 (13%)  | 28,37,40    | 1.30 | 3 (10%)  |
| 22  | 7MG  | A1    | 46  | 22    | 22,26,27     | 4.94 | 2 (9%)   | 29,39,42    | 1.50 | 2 (6%)   |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link  | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|-------|---------|------------|---------|
| 24  | H2U  | A3    | 21  | 24    | -       | 0/7/38/39  | 0/2/2/2 |
| 24  | 5MU  | A3    | 55  | 24    | -       | 0/7/25/26  | 0/2/2/2 |
| 22  | 5MU  | A1    | 54  | 22    | -       | 0/7/25/26  | 0/2/2/2 |
| 22  | 4SU  | A1    | 7   | 22    | -       | 0/7/25/26  | 0/2/2/2 |
| 22  | 6MZ  | A1    | 37  | 22    | -       | 0/5/27/28  | 0/3/3/3 |
| 24  | 4SU  | A3    | 8   | 24    | -       | 0/7/25/26  | 0/2/2/2 |
| 24  | PSU  | A3    | 56  | 24    | -       | 2/7/25/26  | 0/2/2/2 |
| 22  | PSU  | A1    | 55  | 22    | -       | 2/7/25/26  | 0/2/2/2 |
| 24  | OMC  | A3    | 33  | 24    | -       | 0/9/27/28  | 0/2/2/2 |
| 22  | CM0  | A1    | 34  | 23,22 | -       | 2/12/30/31 | 0/2/2/2 |
| 22  | 7MG  | A1    | 46  | 22    | -       | 1/7/37/38  | 0/3/3/3 |

All (16) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 22  | A1    | 46  | 7MG  | C8-N9   | -22.83 | 1.33        | 1.46     |
| 24  | A3    | 8   | 4SU  | C5-C4   | -5.34  | 1.35        | 1.42     |
| 22  | A1    | 34  | CM0  | O5-C5   | -5.14  | 1.24        | 1.36     |
| 22  | A1    | 7   | 4SU  | C5-C4   | -4.77  | 1.36        | 1.42     |
| 24  | A3    | 21  | H2U  | C2-N3   | -3.58  | 1.31        | 1.38     |
| 24  | A3    | 21  | H2U  | C4-N3   | -3.09  | 1.32        | 1.37     |
| 22  | A1    | 55  | PSU  | O4'-C1' | -2.70  | 1.40        | 1.43     |
| 22  | A1    | 46  | 7MG  | O5'-C5' | -2.45  | 1.38        | 1.44     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24  | A3    | 56  | PSU  | C4-N3   | -2.40 | 1.34        | 1.38     |
| 22  | A1    | 7   | 4SU  | C4-S4   | -2.38 | 1.63        | 1.68     |
| 24  | A3    | 8   | 4SU  | O4'-C4' | -2.35 | 1.39        | 1.45     |
| 24  | A3    | 8   | 4SU  | C4-S4   | -2.32 | 1.64        | 1.68     |
| 22  | A1    | 34  | CM0  | O8-C8   | -2.27 | 1.23        | 1.30     |
| 24  | A3    | 55  | 5MU  | O5'-C5' | -2.26 | 1.39        | 1.44     |
| 22  | A1    | 34  | CM0  | O5'-C5' | -2.11 | 1.39        | 1.44     |
| 22  | A1    | 37  | 6MZ  | C8-N7   | -2.02 | 1.31        | 1.34     |

All (31) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | A1    | 46  | 7MG  | N9-C8-N7    | 6.33  | 112.43      | 103.38   |
| 22  | A1    | 37  | 6MZ  | C9-N6-C6    | 5.36  | 127.49      | 122.87   |
| 22  | A1    | 54  | 5MU  | C5M-C5-C6   | -4.17 | 117.27      | 122.85   |
| 24  | A3    | 55  | 5MU  | C5M-C5-C6   | -4.13 | 117.34      | 122.85   |
| 22  | A1    | 55  | PSU  | C6-C5-C4    | 3.99  | 120.99      | 118.20   |
| 22  | A1    | 34  | CM0  | C7-O5-C5    | 3.96  | 122.76      | 117.58   |
| 24  | A3    | 56  | PSU  | C6-C5-C4    | 3.78  | 120.84      | 118.20   |
| 22  | A1    | 54  | 5MU  | C6-C5-C4    | 3.56  | 121.00      | 118.03   |
| 24  | A3    | 55  | 5MU  | C5M-C5-C4   | 3.20  | 122.29      | 118.77   |
| 22  | A1    | 54  | 5MU  | C5-C6-N1    | -3.14 | 120.11      | 123.34   |
| 24  | A3    | 33  | OMC  | O2-C2-N3    | -3.10 | 117.29      | 122.33   |
| 22  | A1    | 37  | 6MZ  | C2-N1-C6    | 3.01  | 119.17      | 116.59   |
| 22  | A1    | 7   | 4SU  | C6-C5-C4    | 2.99  | 122.54      | 119.95   |
| 24  | A3    | 55  | 5MU  | C6-C5-C4    | 2.78  | 120.36      | 118.03   |
| 24  | A3    | 21  | H2U  | N3-C2-N1    | 2.74  | 119.55      | 116.65   |
| 24  | A3    | 56  | PSU  | O4'-C1'-C2' | 2.71  | 108.97      | 105.14   |
| 22  | A1    | 54  | 5MU  | C5M-C5-C4   | 2.68  | 121.72      | 118.77   |
| 24  | A3    | 56  | PSU  | N1-C2-N3    | 2.67  | 118.15      | 115.13   |
| 24  | A3    | 55  | 5MU  | C5-C6-N1    | -2.52 | 120.75      | 123.34   |
| 24  | A3    | 33  | OMC  | C2'-C1'-N1  | -2.46 | 109.45      | 114.22   |
| 22  | A1    | 7   | 4SU  | O4'-C1'-N1  | 2.44  | 113.93      | 108.36   |
| 22  | A1    | 54  | 5MU  | C4-N3-C2    | -2.34 | 124.32      | 127.35   |
| 22  | A1    | 55  | PSU  | O4'-C1'-C2' | 2.25  | 108.32      | 105.14   |
| 24  | A3    | 21  | H2U  | C5-C4-N3    | 2.24  | 119.17      | 116.65   |
| 24  | A3    | 21  | H2U  | O2-C2-N3    | -2.19 | 117.42      | 121.50   |
| 22  | A1    | 54  | 5MU  | N3-C2-N1    | 2.14  | 117.73      | 114.89   |
| 22  | A1    | 46  | 7MG  | O4'-C4'-C3' | 2.06  | 109.18      | 105.11   |
| 24  | A3    | 56  | PSU  | O4-C4-N3    | -2.05 | 116.19      | 120.12   |
| 22  | A1    | 34  | CM0  | O2-C2-N3    | -2.01 | 117.75      | 121.50   |
| 22  | A1    | 34  | CM0  | O2-C2-N1    | 2.01  | 125.46      | 122.79   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 24  | A3    | 8   | 4SU  | C6-C5-C4 | 2.01 | 121.69      | 119.95   |

There are no chirality outliers.

All (7) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | A1    | 55  | PSU  | C2'-C1'-C5-C6   |
| 24  | A3    | 56  | PSU  | O4'-C1'-C5-C4   |
| 24  | A3    | 56  | PSU  | O4'-C1'-C5-C6   |
| 22  | A1    | 34  | CM0  | O5-C7-C8-O8     |
| 22  | A1    | 34  | CM0  | O5-C7-C8-O9     |
| 22  | A1    | 46  | 7MG  | C3'-C4'-C5'-O5' |
| 22  | A1    | 55  | PSU  | O4'-C1'-C5-C6   |

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [\(i\)](#)

2 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 58  | FME  | BA    | 3001 | 57    | 8,9,10       | 0.82 | 0        | 7,9,11      | 1.10 | 0        |
| 57  | VAL  | A1    | 101  | 22,58 | 4,6,7        | 0.77 | 0        | 6,7,9       | 1.08 | 1 (16%)  |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.  
'-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res  | Link  | Chirals | Torsions | Rings |
|-----|------|-------|------|-------|---------|----------|-------|
| 58  | FME  | BA    | 3001 | 57    | -       | 1/7/9/11 | -     |
| 57  | VAL  | A1    | 101  | 22,58 | -       | 0/5/6/8  | -     |

There are no bond length outliers.

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|-----|------|--------|-------|------------------------|---------------------|
| 57  | A1    | 101 | VAL  | O-C-CA | -2.62 | 117.91                 | 124.78              |

There are no chirality outliers.

All (1) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms      |
|-----|-------|------|------|------------|
| 58  | BA    | 3001 | FME  | O1-CN-N-CA |

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

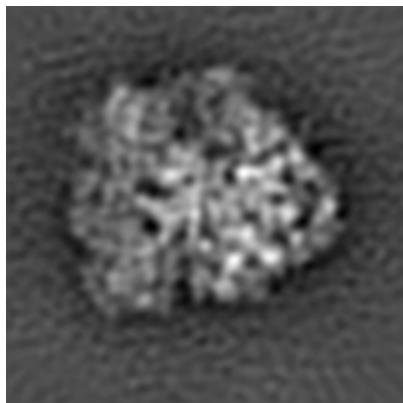
## 6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-2472. These allow visual inspection of the internal detail of the map and identification of artifacts.

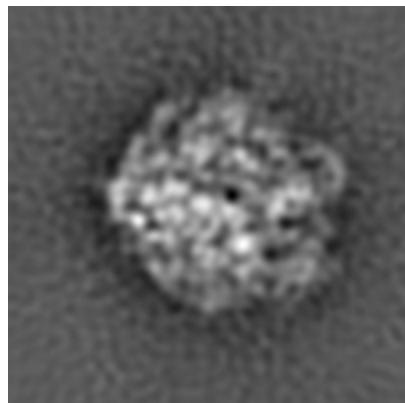
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections (i)

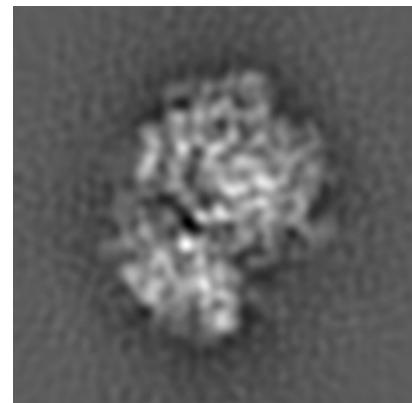
#### 6.1.1 Primary map



X



Y

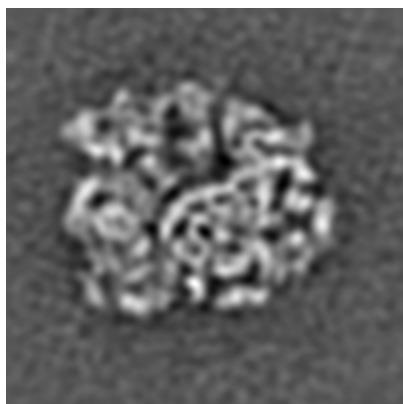


Z

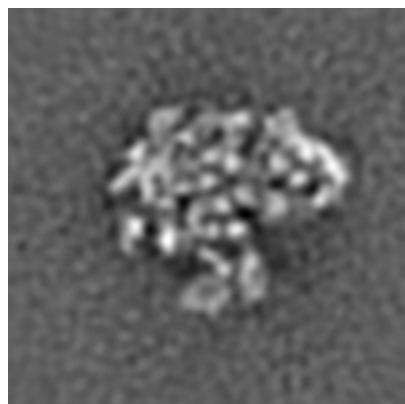
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices (i)

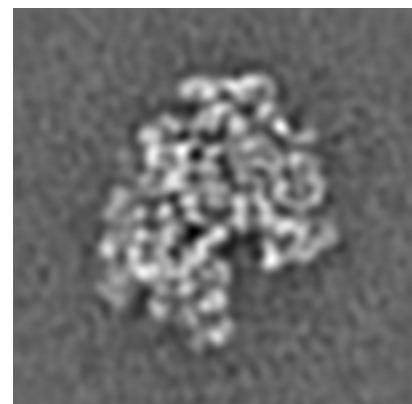
#### 6.2.1 Primary map



X Index: 64



Y Index: 64

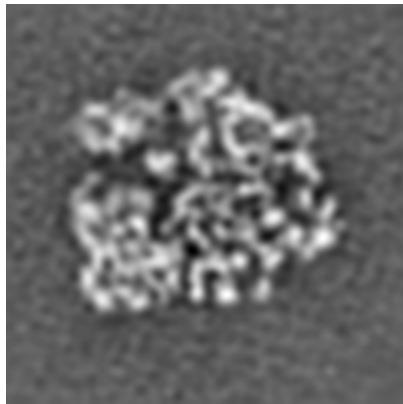


Z Index: 64

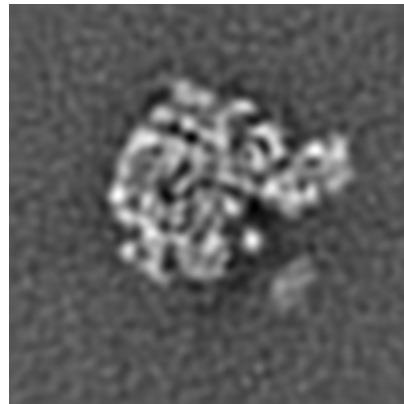
The images above show central slices of the map in three orthogonal directions.

### 6.3 Largest variance slices [\(i\)](#)

#### 6.3.1 Primary map



X Index: 67



Y Index: 71

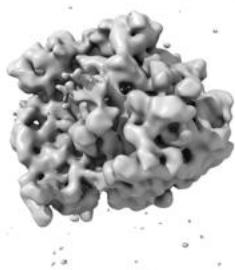


Z Index: 61

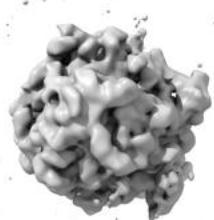
The images above show the largest variance slices of the map in three orthogonal directions.

### 6.4 Orthogonal surface views [\(i\)](#)

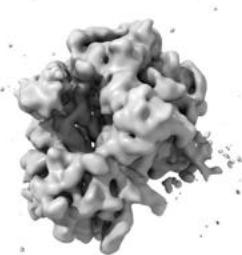
#### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 25.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

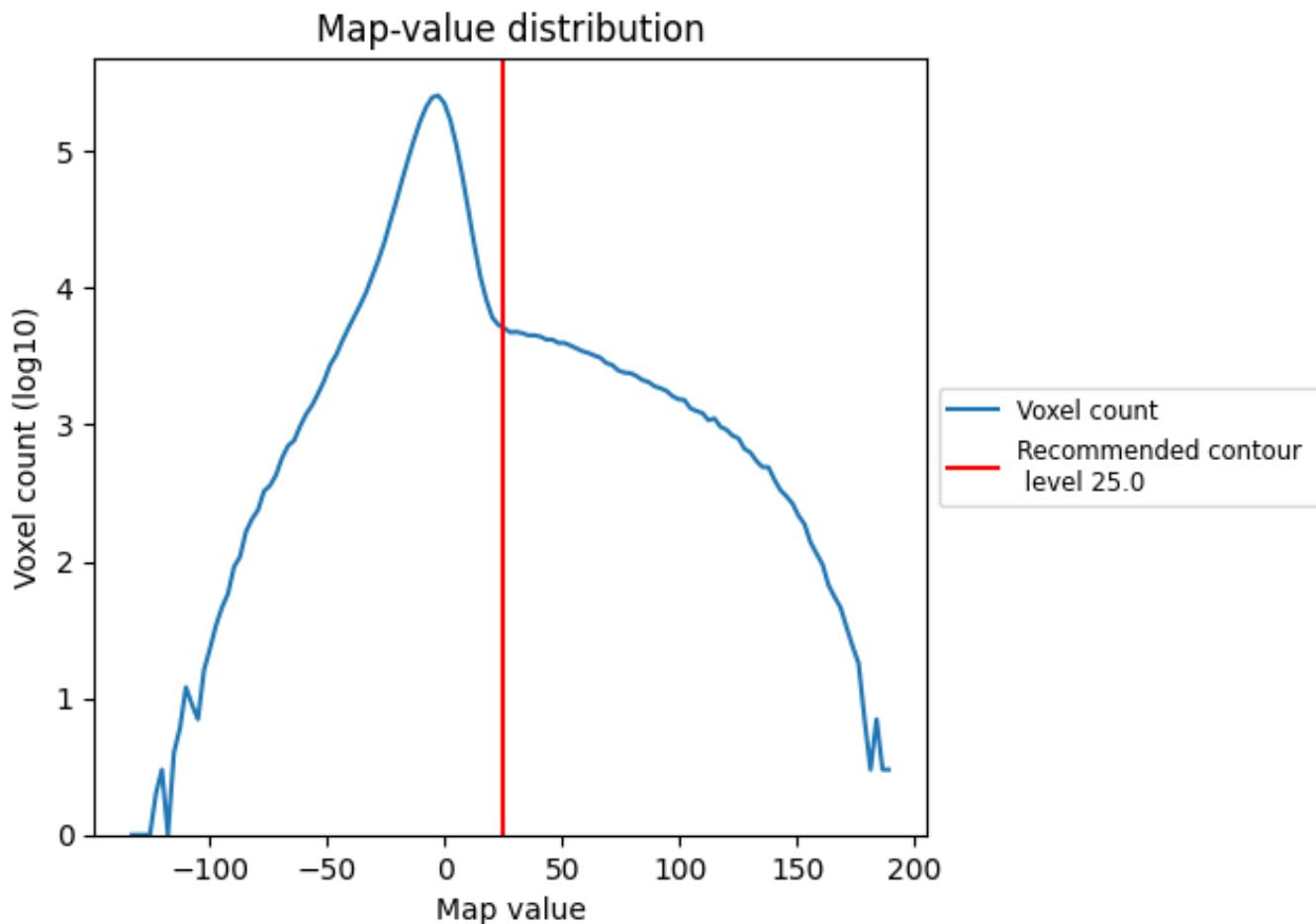
## 6.5 Mask visualisation

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

## 7 Map analysis (i)

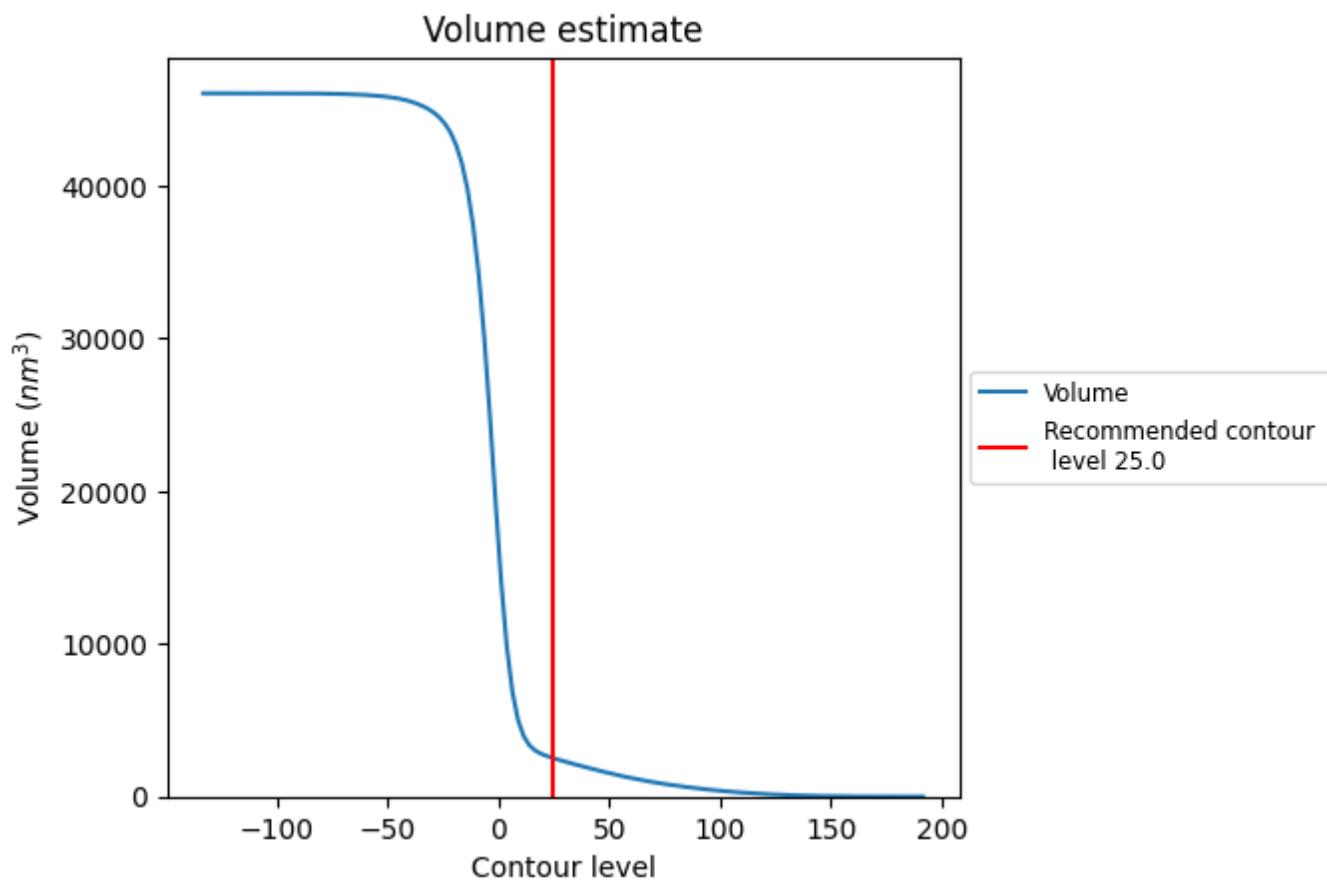
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution (i)



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

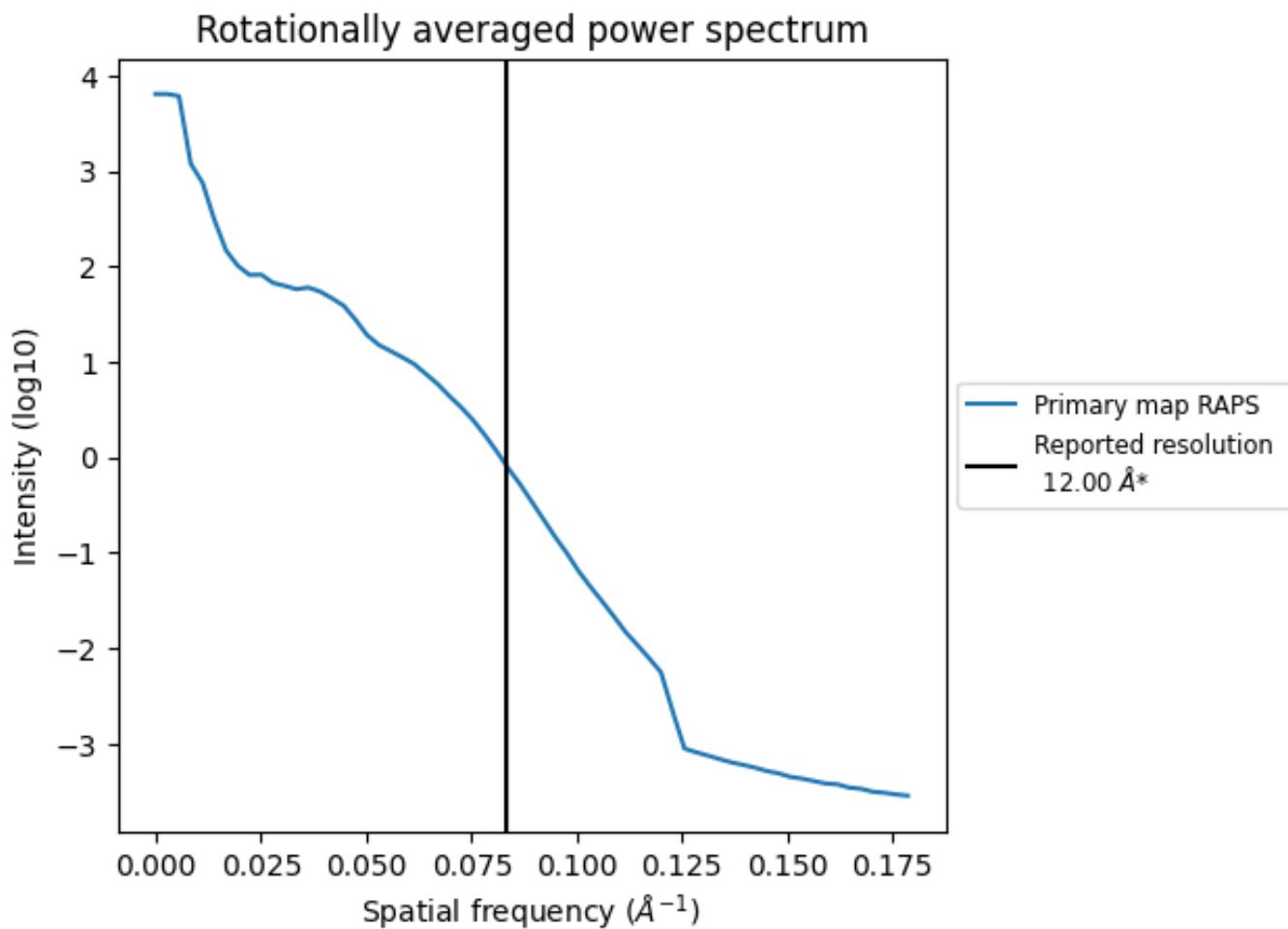
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is  $2507 \text{ nm}^3$ ; this corresponds to an approximate mass of 2264 kDa.

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

### 7.3 Rotationally averaged power spectrum [\(i\)](#)



\*Reported resolution corresponds to spatial frequency of  $0.083 \text{ \AA}^{-1}$

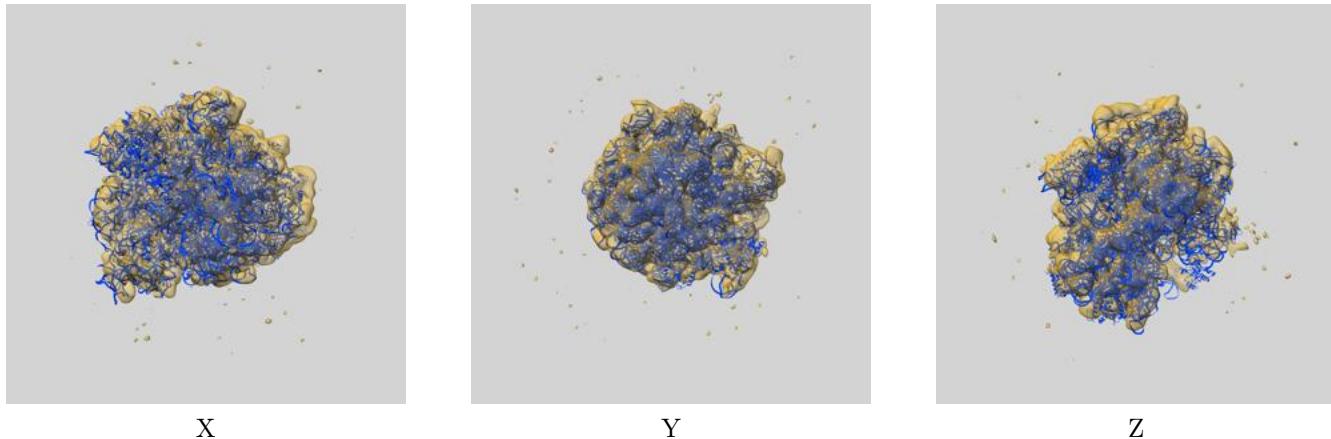
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit (i)

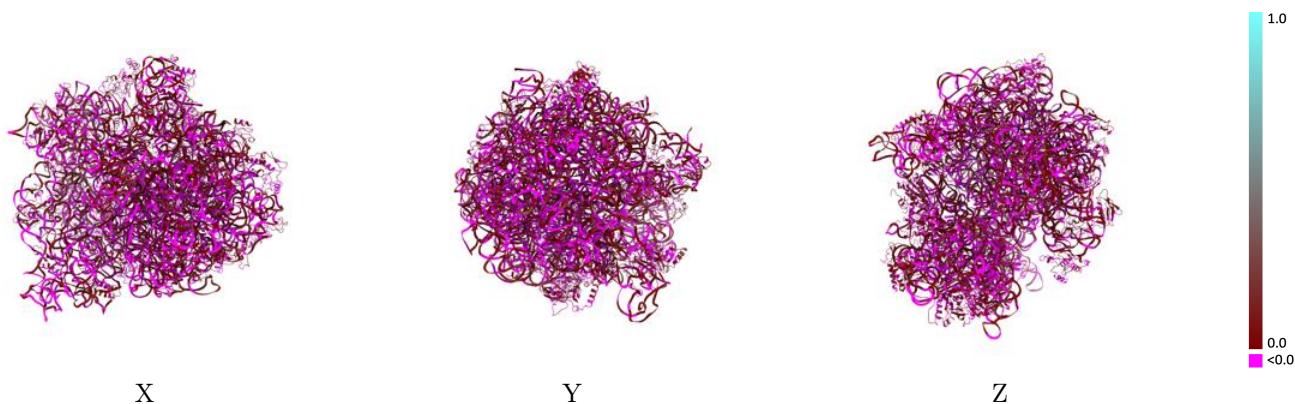
This section contains information regarding the fit between EMDB map EMD-2472 and PDB model 4V6Z. Per-residue inclusion information can be found in section 3 on page 17.

### 9.1 Map-model overlay (i)



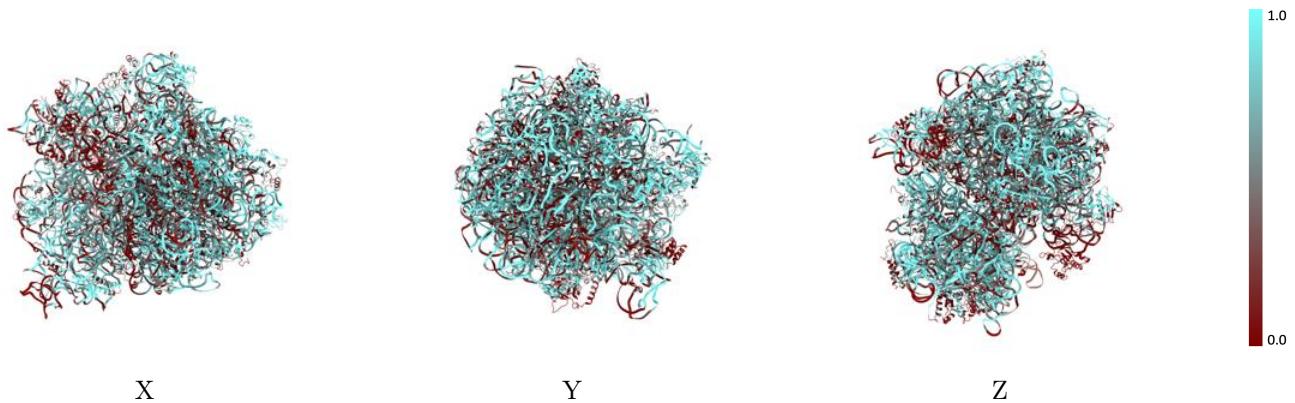
The images above show the 3D surface view of the map at the recommended contour level 25.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



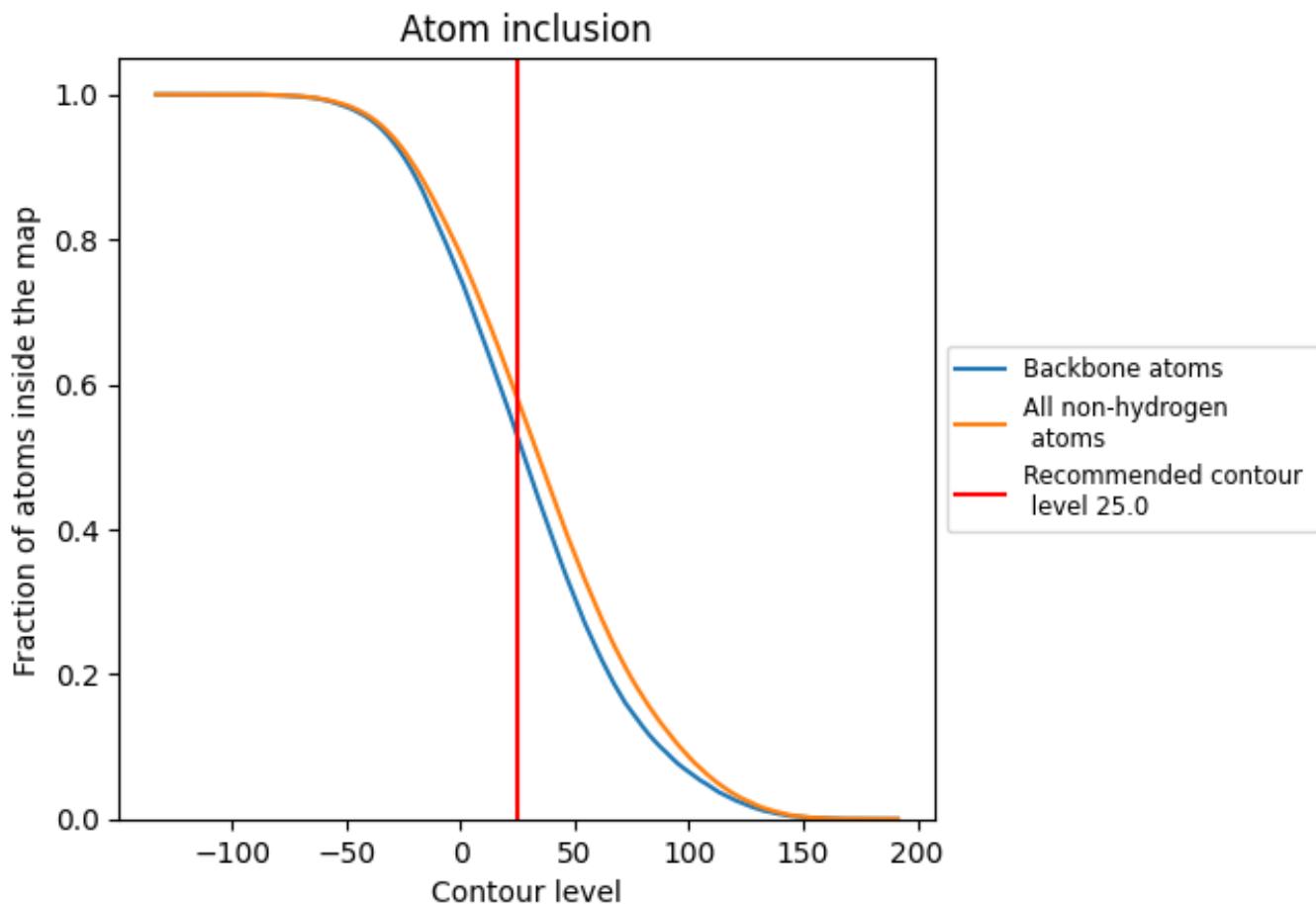
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (25.0).

## 9.4 Atom inclusion [\(i\)](#)



At the recommended contour level, 53% of all backbone atoms, 58% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (25.0) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|----------------|---------|
| All   | 0.5805         | 0.0150  |
| A1    | 0.5165         | 0.0210  |
| A2    | 0.4757         | <0.0    |
| A3    | 0.3831         | <0.0    |
| AA    | 0.6608         | 0.0230  |
| AB    | 0.4762         | 0.0520  |
| AC    | 0.5206         | 0.0090  |
| AD    | 0.4340         | 0.0110  |
| AE    | 0.5203         | 0.0300  |
| AF    | 0.7139         | 0.0380  |
| AG    | 0.5947         | 0.0120  |
| AH    | 0.5115         | 0.0070  |
| AI    | 0.7074         | 0.0030  |
| AJ    | 0.4241         | 0.0030  |
| AK    | 0.6725         | 0.0330  |
| AL    | 0.6298         | 0.0140  |
| AM    | 0.6533         | 0.0320  |
| AN    | 0.3424         | <0.0    |
| AO    | 0.7130         | 0.0190  |
| AP    | 0.4344         | 0.0050  |
| AQ    | 0.5449         | 0.0230  |
| AR    | 0.5809         | 0.0020  |
| AS    | 0.6651         | 0.0190  |
| AT    | 0.7025         | 0.0010  |
| AU    | 0.5819         | 0.0460  |
| B0    | 0.7103         | 0.0380  |
| B1    | 0.5124         | 0.0350  |
| B2    | 0.4169         | <0.0    |
| B3    | 0.4134         | <0.0    |
| B4    | 0.5103         | <0.0    |
| B5    | 0.3460         | <0.0    |
| BA    | 0.5875         | 0.0150  |
| BB    | 0.7177         | 0.0320  |
| BC    | 0.4313         | <0.0    |
| BD    | 0.4714         | 0.0100  |



*Continued on next page...*

Continued from previous page...

| Chain | Atom inclusion | Q-score |
|-------|----------------|---------|
| BE    | 0.5908         | -0.0060 |
| BF    | 0.5842         | 0.0210  |
| BG    | 0.4588         | 0.0220  |
| BH    | 0.2245         | 0.0250  |
| BI    | 0.0000         | -0.0030 |
| BJ    | 0.4791         | -0.0040 |
| BK    | 0.4540         | 0.0030  |
| BL    | 0.6083         | -0.0140 |
| BM    | 0.4261         | 0.0170  |
| BN    | 0.5742         | -0.0180 |
| BO    | 0.8413         | 0.0280  |
| BP    | 0.4291         | -0.0060 |
| BQ    | 0.5297         | -0.0060 |
| BR    | 0.6136         | -0.0070 |
| BS    | 0.4797         | 0.0010  |
| BT    | 0.6279         | -0.0100 |
| BU    | 0.5690         | 0.0050  |
| BV    | 0.6314         | 0.0560  |
| BW    | 0.6220         | 0.0220  |
| BX    | 0.4459         | -0.0480 |
| BY    | 0.5493         | 0.0070  |
| BZ    | 0.4462         | 0.0020  |