# Full wwPDB EM Validation Report (i)

Feb 22, 2024 – 02:06 PM EST

| | | |
|---|---|---|
| PDB ID | : | 4V6V |
| EMDB ID | : | EMD-5562 |
| Title | : | Tetracycline resistance protein Tet(O) bound to the ribosome |
| Authors | : | Li, W.; Atkinson, G.C.; Thakor, N.S.; Allas, U.; Lu, C.; Chan, K.Y.; Tenson, T.; Schulten, K.; Wilson, K.S.; Hauryliuk, V.; Frank, J. |
| Deposited on | : | 2013-02-25 |
| Resolution | : | 9.80 Å(reported) |
| Based on initial models | : | 2I2U, 2I2V |

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (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:

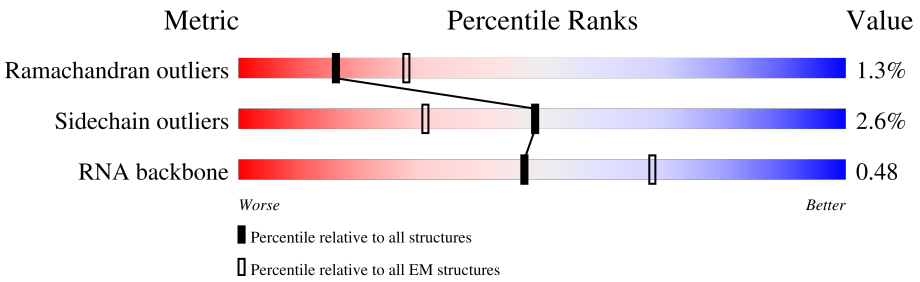
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev70 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | 1.9.13 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.36 |

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 9.80 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) |
|---|---|---|
| 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 >=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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | AJ | 103 | 89% 10% • |
| 2 | AK | 128 | 8% 91% 8% • |
| 3 | AL | 123 | 89% 9% • |
| 4 | AM | 117 | 87% 13% |
| 5 | AN | 100 | 89% 11% |
| 6 | AO | 88 | 91% 7% •• |
| 7 | AP | 82 | 88% 11% • |
| 8 | AQ | 83 | 93% 6% • |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 9 | AR | 74 | 7% 82% 16% |
| 10 | AS | 91 | 87% 13% |
| 11 | AB | 240 | 95% 5% |
| 12 | AT | 86 | 93% 7% |
| 13 | AU | 70 | 6% 77% 20% |
| 14 | AC | 232 | 91% 9% |
| 15 | AD | 205 | 90% 9% |
| 16 | AE | 166 | 92% 8% |
| 17 | AF | 135 | 17% 90% 9% |
| 18 | AG | 178 | 90% 9% |
| 19 | AH | 129 | 93% 6% |
| 20 | AI | 129 | 87% 12% |
| 21 | A1 | 639 | 94% 6% |
| 22 | AA | 1542 | 15% 58% 24% |
| 23 | A2 | 47 | 47% 23% 51% 26% |
| 24 | A3 | 77 | 12% 61% 27% |
| 25 | BC | 234 | 10% 95% 5% |
| 26 | BJ | 164 | 7% 93% 5% |
| 27 | BK | 141 | 95% 5% |
| 28 | BN | 142 | 87% 12% |
| 29 | BO | 123 | 84% 13% |
| 30 | BP | 144 | 88% 10% |
| 31 | BQ | 136 | 87% 13% |
| 32 | BR | 127 | 84% 15% |
| 33 | BS | 117 | 91% 9% |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 34 | BT | 114 | 89% 11% |
| 35 | BD | 272 | 88% 11% |
| 36 | BU | 117 | 85% 13% |
| 37 | BV | 103 | 88% 12% |
| 38 | BW | 110 | 90% 8% |
| 39 | BX | 100 | 94% 5% |
| 40 | BY | 103 | 94% 5% |
| 41 | BZ | 94 | 94% 6% |
| 42 | B0 | 84 | 7% 85% 12% |
| 43 | B1 | 77 | 87% 10% |
| 44 | B2 | 63 | 92% 6% |
| 45 | BE | 209 | 92% 7% |
| 46 | B3 | 58 | 90% 10% |
| 47 | B4 | 70 | 10% 93% 6% |
| 48 | B5 | 56 | 82% 18% |
| 49 | B6 | 54 | 94% 6% |
| 50 | B7 | 46 | 80% 20% |
| 51 | B8 | 64 | 89% 9% |
| 52 | B9 | 38 | 87% 13% |
| 53 | BF | 201 | 92% 7% |
| 54 | BG | 178 | 88% 11% |
| 55 | BH | 176 | 92% 6% |
| 56 | BL | 149 | 18% 95% 5% |
| 57 | BA | 2904 | 15% 58% 24% |
| 58 | Ba | 120 | 18% 64% 17% |

# 2 Entry composition (i)

There are 58 unique types of molecules in this entry. The entry contains 154956 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 S10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 1 | AJ | 103 | 794 | 483 | 158 | 151 | 2 | 0 | 0 |

- Molecule 2 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 2 | AK | 128 | 923 | 553 | 196 | 171 | 3 | 0 | 0 |

- Molecule 3 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 3 | AL | 123 | 923 | 558 | 196 | 165 | 4 | 0 | 0 |

- Molecule 4 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 4 | AM | 117 | 876 | 530 | 183 | 160 | 3 | 0 | 0 |

- Molecule 5 is a protein called 30S ribosomal protein S14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 5 | AN | 100 | 771 | 465 | 164 | 139 | 3 | 0 | 0 |

- Molecule 6 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 6 | AO | 88 | 690 | 414 | 146 | 129 | 1 | 0 | 0 |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| AO | 79 | ARG | GLN | conflict | UNP P0ADZ4 |

- Molecule 7 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 7 | AP | 82 | 620 | 377 | 128 | 114 | 1 | 0 | 0 |

- Molecule 8 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 8 | AQ | 83 | 657 | 410 | 124 | 120 | 3 | 0 | 0 |

- Molecule 9 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 9 | AR | 74 | 603 | 372 | 123 | 107 | 1 | 0 | 0 |

- Molecule 10 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 10 | AS | 91 | 708 | 445 | 139 | 122 | 2 | 0 | 0 |

- Molecule 11 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 11 | AB | 240 | 1805 | 1113 | 332 | 352 | 8 | 0 | 0 |

- Molecule 12 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 12 | AT | 86 | 636 | 380 | 138 | 115 | 3 | 0 | 0 |

- Molecule 13 is a protein called 30S ribosomal protein S21.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 13 | AU | 70 | 564 | 340 | 125 | 98 | 1 | 0 | 0 |

- Molecule 14 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 14 | AC | 232 | 1761 | 1088 | 346 | 323 | 4 | 0 | 0 |

- Molecule 15 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 15 | AD | 205 | 1587 | 970 | 315 | 298 | 4 | 0 | 0 |

- Molecule 16 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 16 | AE | 166 | 1182 | 718 | 232 | 226 | 6 | 0 | 0 |

- Molecule 17 is a protein called 30S ribosomal protein S6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 17 | AF | 135 | 1061 | 637 | 198 | 219 | 7 | 0 | 0 |

- Molecule 18 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 18 | AG | 178 | 1347 | 821 | 269 | 253 | 4 | 0 | 0 |

- Molecule 19 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 19 | AH | 129 | 948 | 585 | 173 | 184 | 6 | 0 | 0 |

- Molecule 20 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 20 | AI | 129 | 1000 | 606 | 208 | 183 | 3 | 0 | 0 |

- Molecule 21 is a protein called Tetracycline resistance protein TetO.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 21 | A1 | 639 | 4989 | 3146 | 850 | 966 | 27 | 0 | 0 |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A1 | 227 | ILE | THR | conflict | UNP P10952 |

- Molecule 22 is a RNA chain called 16S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 22 | AA | 1542 | 33089 | 14767 | 6064 | 10717 | 1541 | 0 | 0 |

- Molecule 23 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 23 | A2 | 47 | 993 | 445 | 167 | 335 | 46 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | S | | |
| 24 | A3 | 77 | 1640 | 734 | 297 | 533 | 75 | 1 | 0 | 0 |

- Molecule 25 is a protein called 50S ribosomal protein L1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 25 | BC | 234 | 1733 | 1081 | 315 | 330 | 7 | 0 | 0 |

- Molecule 26 is a protein called 50S ribosomal protein L10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 26 | BJ | 164 | 1233 | 776 | 220 | 231 | 6 | 0 | 0 |

- Molecule 27 is a protein called 50S ribosomal protein L11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 27 | BK | 141 | 1032 | 651 | 179 | 196 | 6 | 0 | 0 |

- Molecule 28 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 28 | BN | 142 | 1129 | 714 | 212 | 199 | 4 | 0 | 0 |

- Molecule 29 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 29 | BO | 123 | 947 | 593 | 181 | 167 | 6 | 0 | 0 |

- Molecule 30 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 30 | BP | 144 | 1053 | 654 | 207 | 190 | 2 | 0 | 0 |

- Molecule 31 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 31 | BQ | 136 | 1074 | 686 | 205 | 177 | 6 | 0 | 0 |

- Molecule 32 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 32 | BR | 127 | 1008 | 621 | 204 | 178 | 5 | 0 | 0 |

- Molecule 33 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 33 | BS | 117 | 900 | 557 | 179 | 163 | 1 | 0 | 0 |

- Molecule 34 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 34 | BT | 114 | 917 | 574 | 179 | 163 | 1 | 0 | 0 |

- Molecule 35 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 35 | BD | 272 | 2092 | 1294 | 425 | 366 | 7 | 0 | 0 |

- Molecule 36 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 36 | BU | 117 | 947 | 604 | 192 | 151 | 0 | 0 |

- Molecule 37 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 37 | BV | 103 | 816 | 516 | 153 | 145 | 2 | 0 | 0 |

- Molecule 38 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 38 | BW | 110 | 857 | 532 | 166 | 156 | 3 | 0 | 0 |

- Molecule 39 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 39 | BX | 100 | 787 | 496 | 146 | 143 | 2 | 0 | 0 |

- Molecule 40 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 40 | BY | 103 | 789 | 498 | 148 | 143 | 0 | 0 |

- Molecule 41 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 41 | BZ | 94 | 753 | 479 | 137 | 134 | 3 | 0 | 0 |

- Molecule 42 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 42 | B0 | 84 | 634 | 391 | 129 | 113 | 1 | 0 | 0 |

- Molecule 43 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 43 | B1 | 77 | 625 | 388 | 129 | 106 | 2 | 0 | 0 |

- Molecule 44 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 44 | B2 | 63 | 509 | 313 | 99 | 95 | 2 | 0 | 0 |

- Molecule 45 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 45 | BE | 209 | 1565 | 979 | 288 | 294 | 4 | 0 | 0 |

- Molecule 46 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 46 | B3 | 58 | 449 | 281 | 87 | 79 | 2 | 0 | 0 |

- Molecule 47 is a protein called 50S ribosomal protein L31.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 47 | B4 | 70 | 549 | 339 | 104 | 100 | 6 | 0 | 0 |

- Molecule 48 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 48 | B5 | 56 | 444 | 269 | 94 | 80 | 1 | 0 | 0 |

- Molecule 49 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 49 | B6 | 54 | 441 | 284 | 81 | 76 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 50 | B7 | 46 | 377 | 228 | 90 | 57 | 2 | 0 | 0 |

- Molecule 51 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 51 | B8 | 64 | 504 | 323 | 105 | 74 | 2 | 0 | 0 |

- Molecule 52 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 52 | B9 | 38 | 302 | 185 | 65 | 48 | 4 | 0 | 0 |

- Molecule 53 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 53 | BF | 201 | 1552 | 974 | 283 | 290 | 5 | 0 | 0 |

- Molecule 54 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 54 | BG | 178 | 1420 | 905 | 251 | 258 | 6 | 0 | 0 |

- Molecule 55 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 55 | BH | 176 | 1323 | 832 | 243 | 246 | 2 | 0 | 0 |

- Molecule 56 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 56 | BL | 149 | 1111 | 699 | 197 | 214 | 1 | 0 | 0 |

- Molecule 57 is a RNA chain called 23S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 57 | BA | 2904 | 62351 | 27824 | 11469 | 20155 | 2903 | 0 | 0 |

- Molecule 58 is a RNA chain called 5S ribosomal RNA.

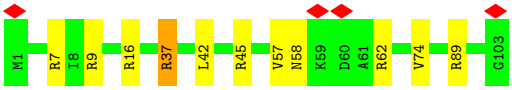
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 58 | Ba | 120 | 2566 | 1144 | 468 | 835 | 119 | 0 | 0 |

# 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.

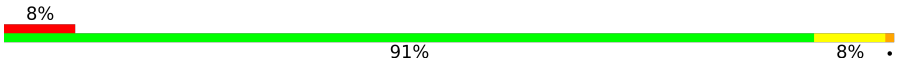
• Molecule 1: 30S ribosomal protein S10

Chain AJ:



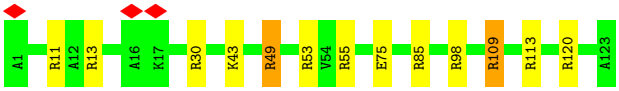

• Molecule 2: 30S ribosomal protein S11

Chain AK:



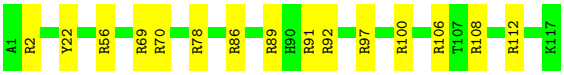
• Molecule 3: 30S ribosomal protein S12

Chain AL:



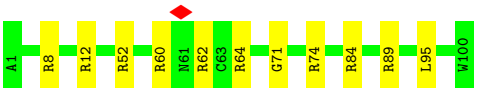

• Molecule 4: 30S ribosomal protein S13

Chain AM:




• Molecule 5: 30S ribosomal protein S14

Chain AN:

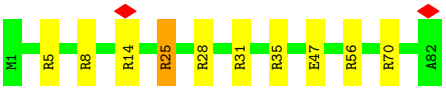


• Molecule 6: 30S ribosomal protein S15

Chain AO: 91% 7%

• Molecule 7: 30S ribosomal protein S16

Chain AP: 88% 11%




• Molecule 8: 30S ribosomal protein S17

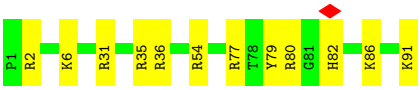
Chain AQ: 93% 6%

• Molecule 9: 30S ribosomal protein S18

Chain AR: 7% 82% 16%

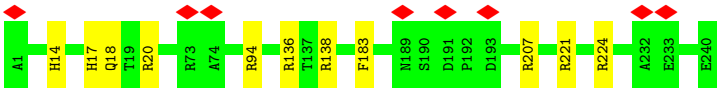
• Molecule 10: 30S ribosomal protein S19

Chain AS: 87% 13%



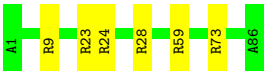

• Molecule 11: 30S ribosomal protein S2

Chain AB: 95% 5%



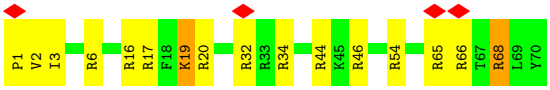

• Molecule 12: 30S ribosomal protein S20

Chain AT: 93% 7%




• Molecule 13: 30S ribosomal protein S21

Chain AU:




• Molecule 14: 30S ribosomal protein S3

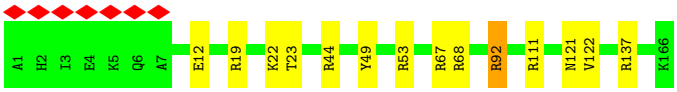
Chain AC:

• Molecule 15: 30S ribosomal protein S4

Chain AD:

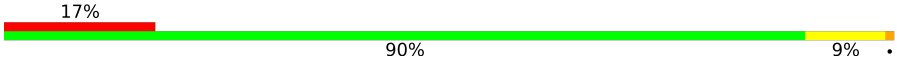
• Molecule 16: 30S ribosomal protein S5

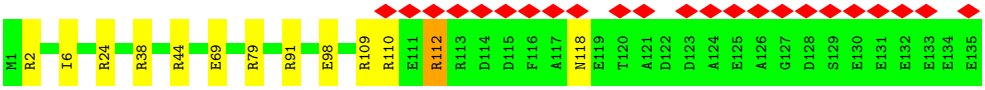
Chain AE:




• Molecule 17: 30S ribosomal protein S6

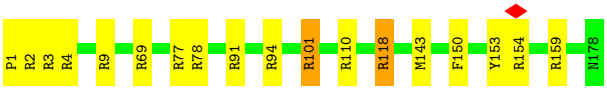
Chain AF:



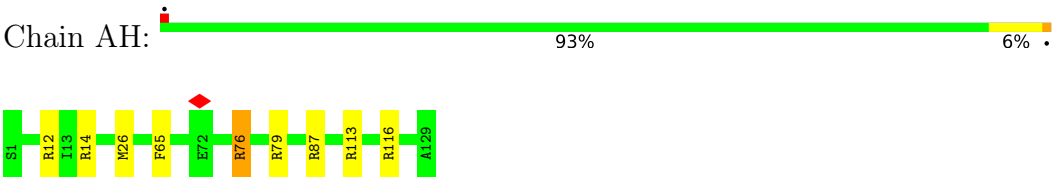

• Molecule 18: 30S ribosomal protein S7

Chain AG:



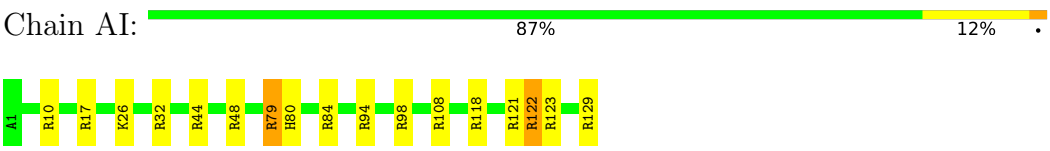

• Molecule 19: 30S ribosomal protein S8

Chain AH:



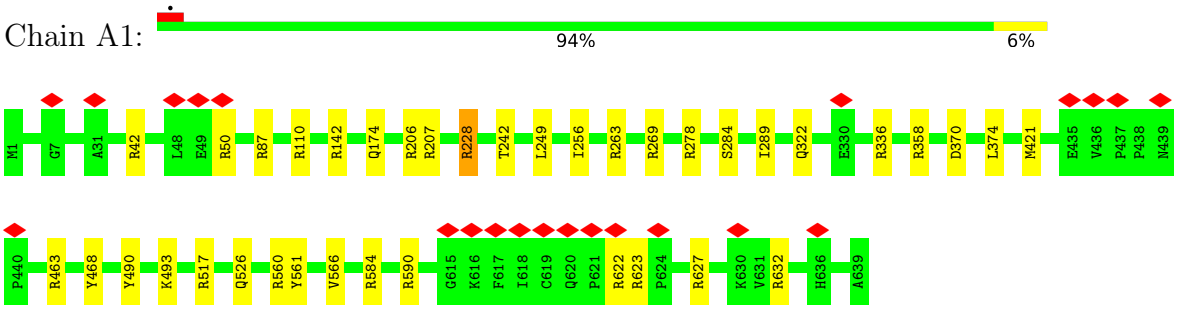

• Molecule 20: 30S ribosomal protein S9

Chain AI:



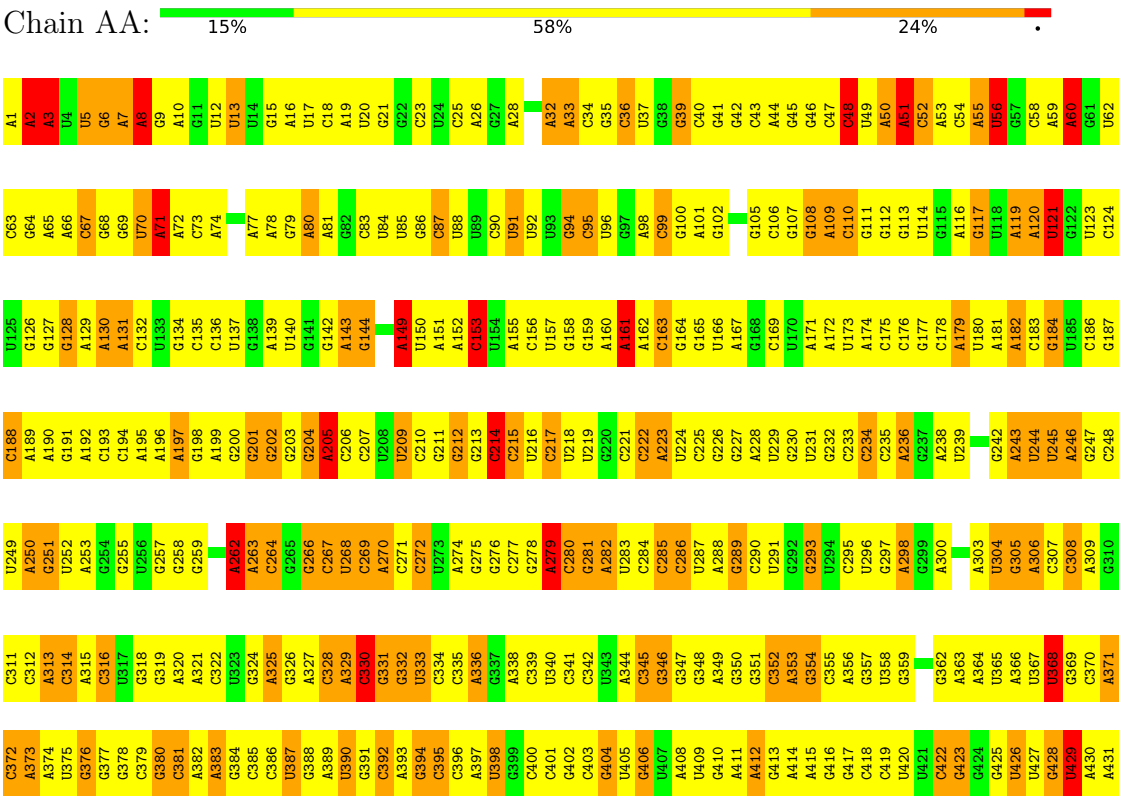

• Molecule 21: Tetracycline resistance protein TetO

Chain A1:

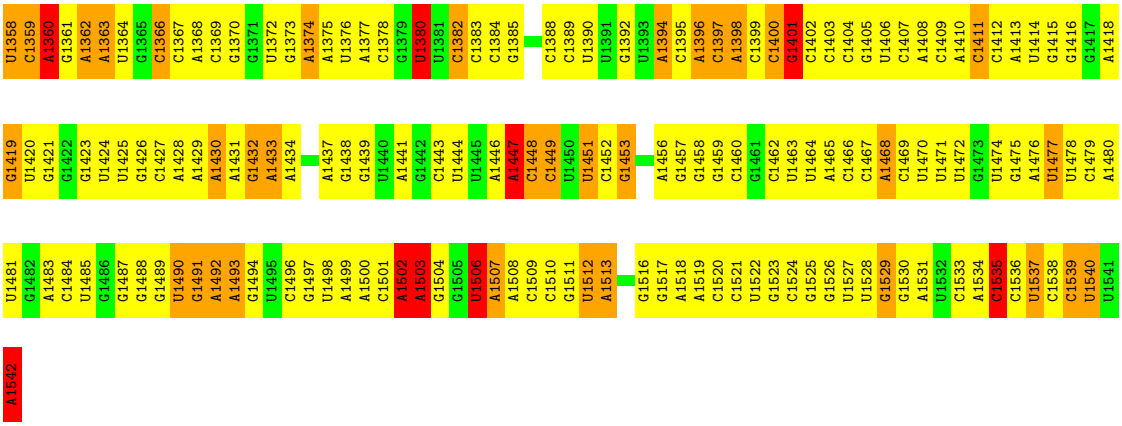



• Molecule 22: 16S ribosomal RNA

Chain AA:

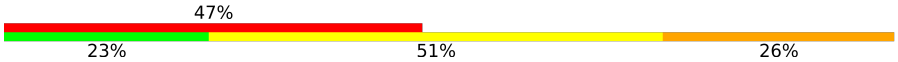


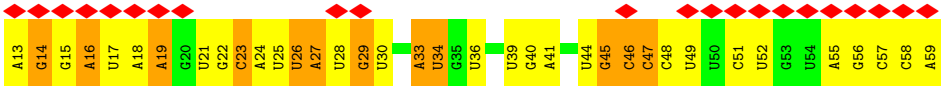
G1297 U1298 A1299 G1300 U1301 C1302 C1303 G1304 G1305 A1306 U1307 U1308 A1311 G1312 U1313 C1314 U1315 G1316 C1317 A1318 A1319 C1320 U1321 C1322 G1323 A1324 C1325 U1326 C1327 C1328 A1329 U1330 G1331 A1332 A1333 G1334 U1335 C1336 G1337 G1338 A1339 A1340 U1341 C1342 G1343 C1344 U1345 A1346 G1347 U1348 A1349 A1350 U1351 C1352 G1353 U1354 G1355 G1356 A1357
C1237 A1238 A1239 U1240 G1241 G1242 C1243 G1244 C1245 A1246 U1247 A1248 C1249 A1250 A1251 A1252 G1253 A1254 G1255 A1256 A1257 G1258 C1259 G1260 A1261 C1262 C1263 U1264 C1265 G1266 C1267 G1268 A1269 G1270 A1271 G1272 C1273 A1274 A1275 G1276 C1277 G1278 G1279 A1280 C1281 C1282 U1283 C1284 A1285 U1286 A1287 A1288 A1289 G1290 U1291 G1292 C1293 G1294 U1295 C1296
A1176 G1177 G1178 A1179 A1180 U1183 G1184 G1185 G1186 G1187 A1188 U1189 G1190 A1191 C1192 G1193 U1194 C1195 A1196 A1197 G1198 C1199 C1200 A1201 U1202 C1203 A1204 U1205 G1206 G1207 C1208 C1209 C1210 U1211 U1212 A1213 C1214 G1215 A1216 C1217 C1218 A1219 G1220 G1221 G1222 C1223 U1224 A1225 C1226 A1227 C1228 A1229 C1230 G1231 U1232 G1233 C1234 U1235 A1236
C1113 C1114 U1115 U1116 A1117 U1118 C1119 C1120 U1121 U1122 U1123 G1124 C1128 C1129 A1130 G1131 C1132 G1133 C1136 C1137 G1138 G1139 C1140 C1141 G1142 G1143 G1144 A1145 A1146 C1147 U1148 C1149 A1150 A1151 A1152 G1153 G1154 A1155 G1156 A1157 C1158 U1159 G1160 C1161 C1162 A1163 G1164 U1165 G1166 A1167 U1168 A1169 A1170 A1171 C1172 U1173 G1174 G1175
G1050 G1051 U1052 G1053 C1054 A1055 U1056 C1059 U1060 C1063 G1064 U1065 C1066 A1067 G1068 C1069 U1070 C1071 G1072 U1073 G1074 U1075 U1076 G1077 A1080 A1081 A1082 U1083 G1084 U1085 U1086 G1087 G1088 G1089 U1090 U1091 A1092 A1093 G1094 U1095 C1096 C1097 C1098 G1099 C1100 A1101 A1102 C1103 G1104 A1105 G1106 C1107 G1108 C1109 A1110 A1111 C1112
G988 U989 C990 U991 U992 G993 A994 C995 A996 U997 C998 C999 A1000 C1001 A1004 A1005 G1006 U1007 U1008 U1009 U1010 C1011 U1012 A1013 G1015 A1016 U1017 G1018 A1019 G1020 A1021 A1022 U1023 G1024 U1025 G1026 C1027 C1028 U1029 U1030 C1031 G1032 G1033 G1034 A1035 A1036 C1037 C1038 G1039 U1040 G1041 A1042 G1043 A1044 C1045 A1046 G1047
G927 C930 C931 C932 G933 C934 A935 C936 A937 A938 G939 C940 G941 G942 U943 G944 G945 A946 G947 C948 A949 U950 C951 U952 G953 G954 U955 U956 U957 A958 A959 U960 U961 C962 G963 A964 U965 G966 C967 A968 A969 C970 G971 C972 G973 A974 A975 G976 A977 A978 C979 C980 U981 U982 A983 C984 C985 U986 G987
C866 G867 C868 G869 U870 U871 A872 A873 G874 U875 C876 C877 A878 C879 C880 G881 C882 C883 U884 G885 G886 G887 G888 A889 G890 U891 A892 C893 G894 G895 C896 C897 G898 C899 A900 A901 G902 G903 U904 U905 A906 A907 A908 A909 C910 U911 C912 A913 A914 A915 A918 A919 U920 U921 G922 A923 C924 G925 G926
C805 C806 A807 C808 G809 C810 C811 G812 U813 A814 A815 A816 C817 G818 A819 U820 G821 U822 C823 G824 A825 C826 U827 U828 G829 G830 A831 G832 G833 U834 U835 G836 U837 G838 C839 C840 C841 U842 U843 G844 A845 G846 G847 C848 G849 G852 C853 U854 U855 C856 C857 G858 G859 A860 G861 C862 U863 A864 A865
C744 G745 A746 A747 G748 A749 C750 U751 G752 G753 A754 G755 C756 U757 C758 A759 G760 G761 U762 G763 C764 G765 A766 A767 A768 G769 C770 G771 U772 G773 G774 G775 G776 A777 G778 C779 A780 A781 A782 C783 A784 G785 G786 A787 U788 U789 A790 G791 A792 U793 A794 C795 C796 C797 U798 G799 G800 U801 A802
G683 U686 A687 G688 C689 G690 G691 U692 G693 A694 A695 A696 U697 G698 C699 G700 U701 A702 G703 A704 G705 A706 U707 C708 U709 G710 G711 A712 G713 G714 A715 A716 U717 A718 C719 C720 G721 G722 U723 G724 G725 C726 G727 A728 A729 G730 G731 C732 G733 G734 C735 C736 G737 C738 C739 U740 G741 G742 A743
U619 C620 A621 A622 C623 C624 U625 G626 G627 G628 A629 A630 C631 U632 G633 C634 A635 U636 C637 U638 G639 A640 U641 A642 C643 U644 G645 G646 C647 A648 A649 G650 C651 G654 A655 C658 U659 C660 G661 U662 A663 G664 A665 G666 G670 G671 U672 A673 G674 A675 A676 U677 U678 C679 C680 A681 G682
U555 C556 G557 G558 A559 A560 U561 U562 A563 C564 U565 G566 G567 G568 C569 G570 U571 A572 A573 A574 G575 G576 G577 C578 A579 C580 G581 C582 A583 G584 G585 C586 U590 U591 G592 U593 U594 A595 A596 G597 U598 C599 A600 G601 A602 U603 A607 A608 A609 U610 C611 C612 C613 C614 G615 G616 G617 C618
G494 A495 A496 G497 A498 A499 G500 C501 A502 C503 C504 G505 G506 C507 U508 A509 A510 C511 U512 C513 C514 G515 U516 G517 C518 U519 A520 G521 G522 A523 G524 C525 C526 G527 C528 G529 G530 U531 A532 A533 U534 A535 C536 A539 G540 G541 G542 U543 G544 C545 A546 A547 G548 C549 G550 U551 U552 A553 A554
A432 G433 U434 A435 C436 U437 U438 U439 C440 A441 G442 C443 G444 G445 G446 G447 A448 A451 A452 G455 A456 G457 U458 A459 A460 A461 G462 U463 U464 A465 A466 U467 A468 C469 C470 U471 U472 U473 G474 C475 U476 C477 A478 U479 U480 G481 A482 C483 G484 U485 U486 A487 C488 C489 C490 G491 C492 A493




- Molecule 23: mRNA

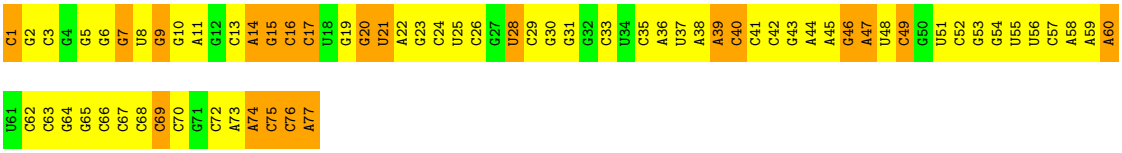
Chain A2:



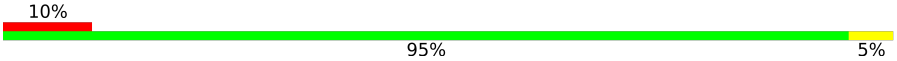

- Molecule 24: P-tRNA

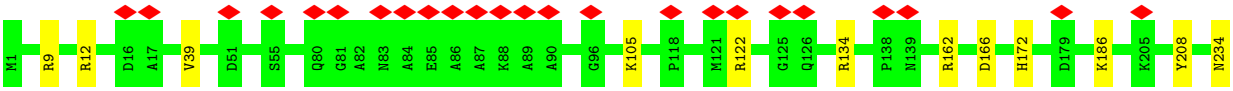
Chain A3:




- Molecule 25: 50S ribosomal protein L1

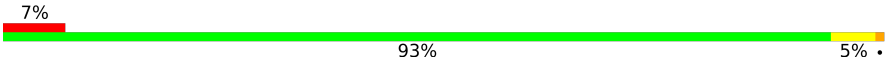
Chain BC:

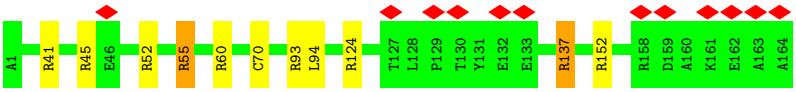



- Molecule 26: 50S ribosomal protein L10

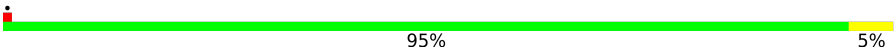
Chain BJ:

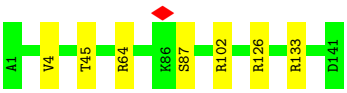



- Molecule 27: 50S ribosomal protein L11

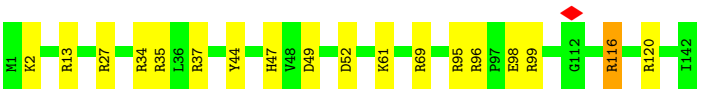
Chain BK:





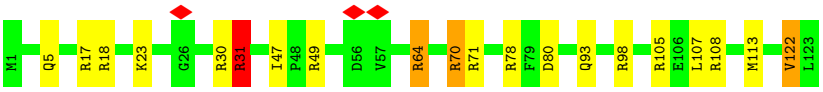

• Molecule 28: 50S ribosomal protein L13

Chain BN:



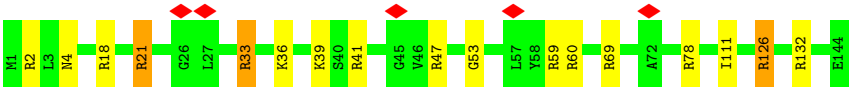

• Molecule 29: 50S ribosomal protein L14

Chain BO:



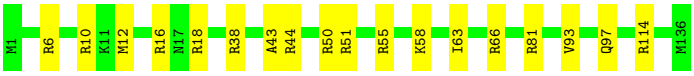

• Molecule 30: 50S ribosomal protein L15

Chain BP:



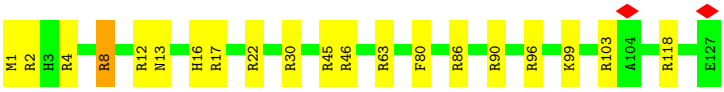

• Molecule 31: 50S ribosomal protein L16

Chain BQ:




• Molecule 32: 50S ribosomal protein L17

Chain BR:

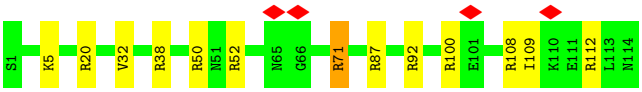



• Molecule 33: 50S ribosomal protein L18

Chain BS:

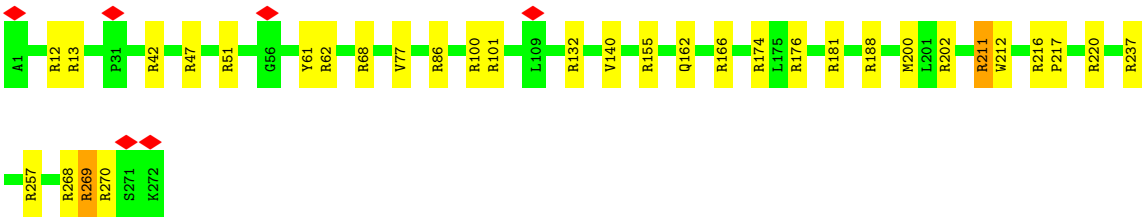
• Molecule 34: 50S ribosomal protein L19

Chain BT: 89% 11%




• Molecule 35: 50S ribosomal protein L2

Chain BD: 88% 11%

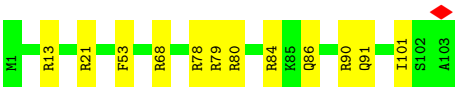



• Molecule 36: 50S ribosomal protein L20

Chain BU: 85% 13%

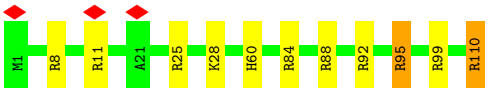
• Molecule 37: 50S ribosomal protein L21

Chain BV: 88% 12%



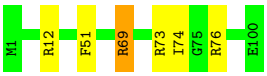

• Molecule 38: 50S ribosomal protein L22

Chain BW: 90% 8%



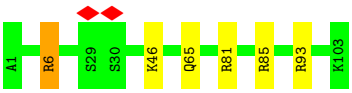

• Molecule 39: 50S ribosomal protein L23

Chain BX: 94% 5%

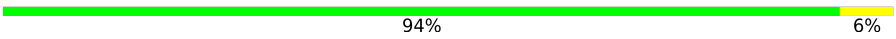



• Molecule 40: 50S ribosomal protein L24

Chain BY: 94% 5%

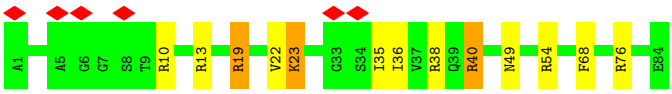



• Molecule 41: 50S ribosomal protein L25

Chain BZ: 

• Molecule 42: 50S ribosomal protein L27

Chain B0:

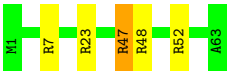




• Molecule 43: 50S ribosomal protein L28

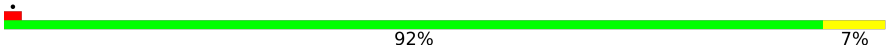
Chain B1:

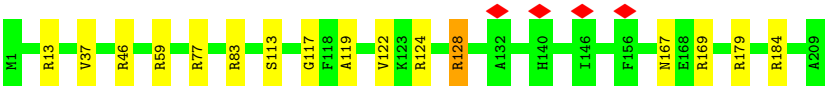

• Molecule 44: 50S ribosomal protein L29

Chain B2:


• Molecule 45: 50S ribosomal protein L3

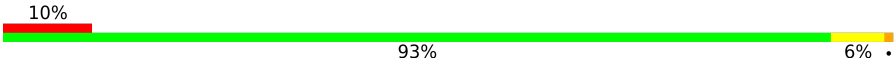
Chain BE: 

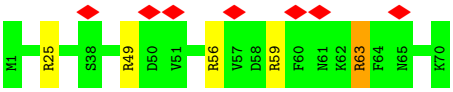




• Molecule 46: 50S ribosomal protein L30

Chain B3:

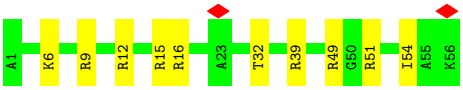

• Molecule 47: 50S ribosomal protein L31

Chain B4: 

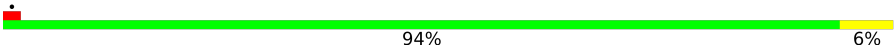




- Molecule 48: 50S ribosomal protein L32

Chain B5:


- Molecule 49: 50S ribosomal protein L33

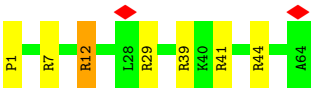
Chain B6: 

- Molecule 50: 50S ribosomal protein L34

Chain B7:


- Molecule 51: 50S ribosomal protein L35

Chain B8:

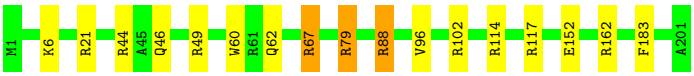




- Molecule 52: 50S ribosomal protein L36

Chain B9:


- Molecule 53: 50S ribosomal protein L4

Chain BF:


- Molecule 54: 50S ribosomal protein L5

Chain BG: 88% 11%

A1 R29 T34 L35 L65 R70 R79 Q80 G81 V88 R91 R94 R101 L102 I103 R109 I110 R111 K119 R132 E133 Q134 R147 V148 R149 R166 R177 K178

- Molecule 55: 50S ribosomal protein L6

Chain BH: 92% 6%

S1 R2 N29 D46 Y57 R68 R94 L104 R148 R151 R152 P153 E154 E166 R169 K175 K176

- Molecule 56: 50S ribosomal protein L9

Chain BL: 18% 95% 5%

M1 K8 K35 K41 K42 N43 R50 R51 L62 N66 A67 R68 A74 A81 S82 K83 A84 G85 D86 R97 D101 E109 V110 A111 K112 R116 L117 P118 N119 G120 V121 L122 R123 S136 E137 V147 A148 E149

- Molecule 57: 23S ribosomal RNA

Chain BA: 15% 58% 24%

G1 G2 U3 U4 A5 A6 G7 C8 G9 A10 C11 U12 A13 A14 G15 C16 G17 U18 A19 C20 A21 C22 G23 G24 U25 G26 G27 A28 U29 G30 C31 C32 C33 U34 G35 G36 C37 A38 G39 U40 C41 A42 G43 A44 G45 G46 C47 G48 A49 U50 G51 A52 A53 G54 G55 A56 C57 G58 U59 G60

C61 U62 A63 A64 U65 C66 C69 G70 A71 U72 A73 A74 G75 C76 G77 U78 C79 G80 G81 U82 A83 A84 G85 G86 U87 G88 A89 U90 A91 U92 G93 A94 A95 C96 C97 G98 U99 U100 A101 U102 A103 A104 C105 C106 G107 G108 C109 G110 A111 U112 U113 U114 C115 C116 G117 A118 A119 U120 G121

G122 G123 G124 A125 A126 A127 C128 C129 C130 A131 G132 U133 G134 U135 U138 U139 C140 G141 A142 C143 A144 A145 A146 C147 U148 A149 U150 C151 A152 U153 U154 A155 A156 C157 U158 G159 A160 A161 U162 C163 C164 A165 U166 A167 G168 G169 U170 U171 A172 A173 U174 G175 A176 G177 G178 C179 G180 A181 A182

C183 C184 G187 G188 G189 A190 A191 C192 U193 G194 A195 A196 A197 C198 A199 U200 C201 U202 A203 A204 G205 U206 A207 C208 C209 C210 C211 G212 A213 G214 G215 A216 A217 A218 A219 G220 A221 A222 A223 U224 C225 A226 A227 C228 C229 G230 A231 G232 A233 U234 U235 C236 C237 C238 C239 C240 A241 G242 U243

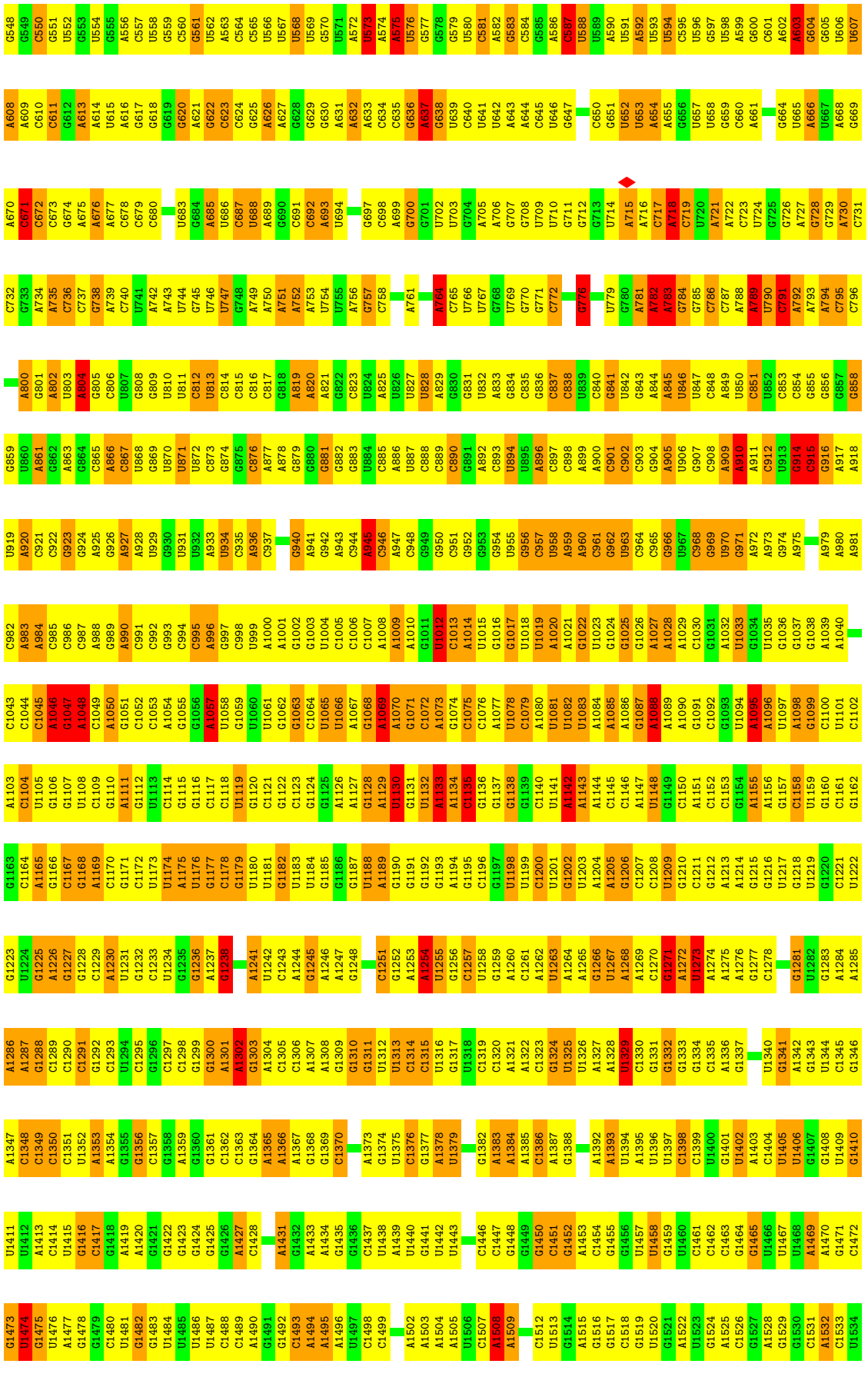
A244 G245 C246 G247 G248 C249 G250 A251 A252 C253 G254 A255 A256 C257 G261 A262 C263 C264 A265 C266 C267 C268 C269 A270 G271 A272 G273 C274 C275 U276 G277 G278 A279 U280 C281 A282 G283 U284 G285 U286 G287 U288 G289 U290 G291 U292 U293 A294 G295 U296 G297 G298 A299 A300 G301 C302 G303 U304 C305

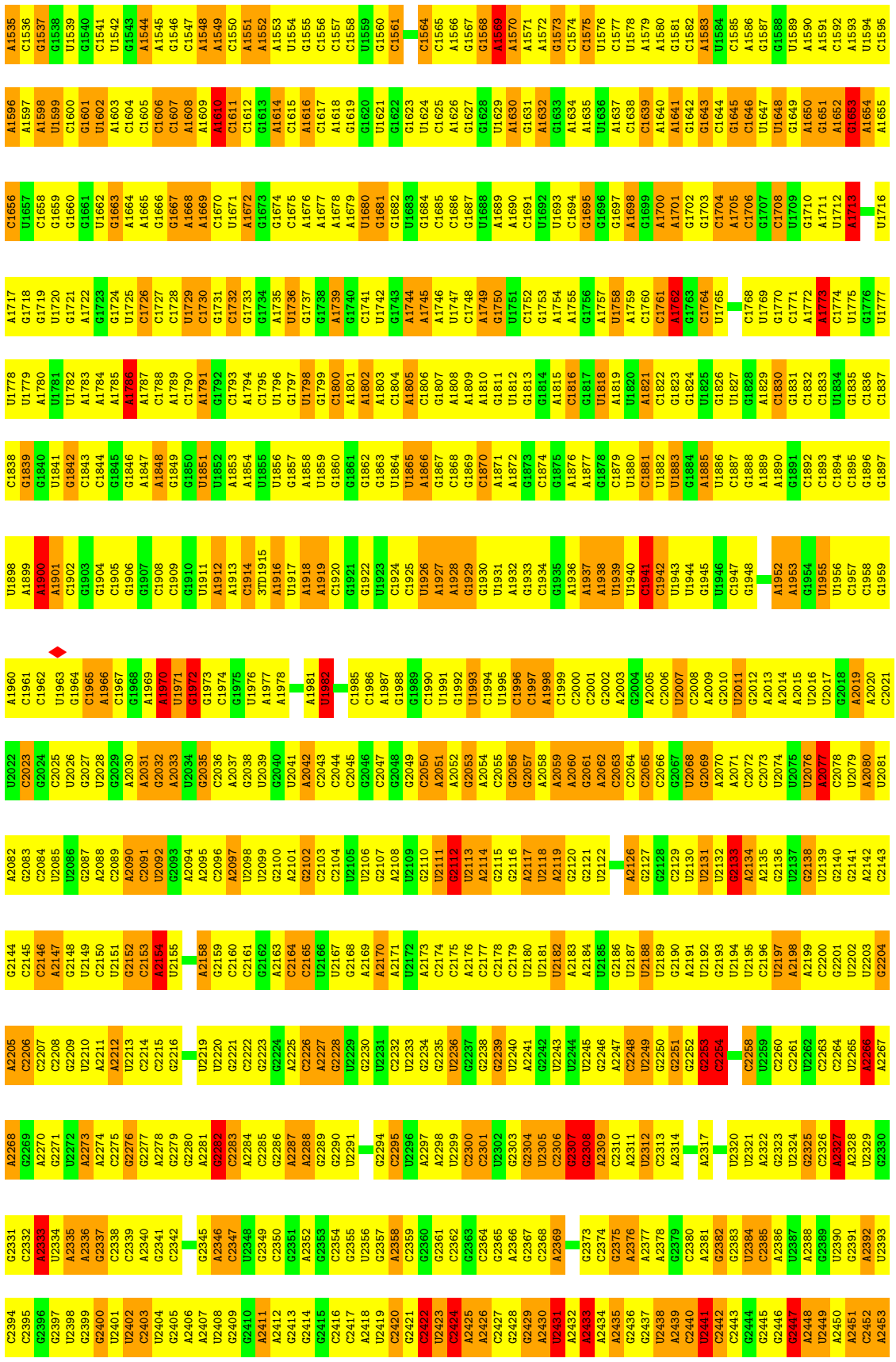
U306 G307 G308 A309 A310 A311 G312 G313 C314 G315 C316 G317 C318 G319 A320 U321 A322 C323 A324 G325 G326 G327 A330 C331 A332 G333 C334 C335 C336 C337 G338 U339 A340 C341 A342 C343 A344 A345 A346 A347 A348 U349 G350 C351 A352 C353 A354 U355 G356 C357 U358 G359 U360 G361 A362 G363 C364 U365 C366

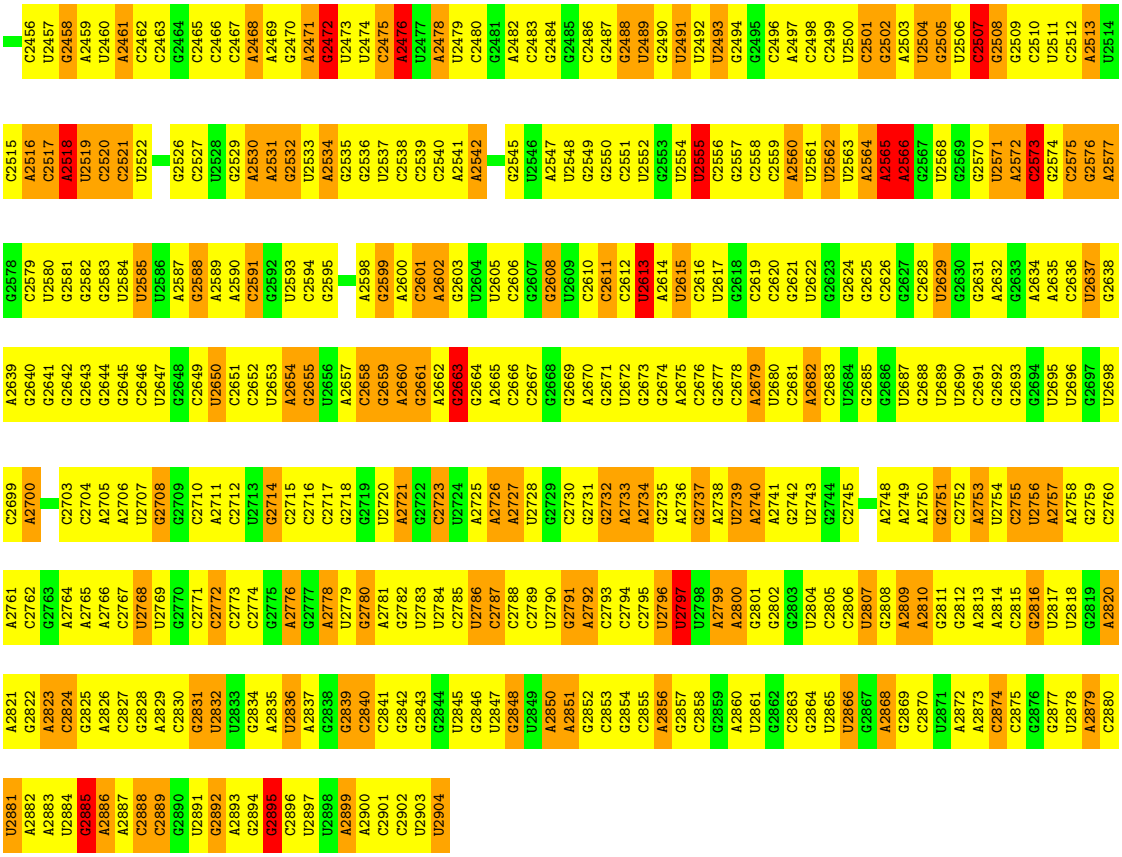
G367 A368 U369 G370 A371 G372 U373 A374 G375 G376 G377 C378 G379 G380 G381 A382 C383 A384 C385 G386 U387 G388 G389 U390 A391 U392 C393 C394 U395 G396 U397 C398 U399 G400 A401 A402 U403 A404 U405 G406 G407 G408 G409 G410 G411 A412 C413 C414 A415 U416 C417 C418 U419 C420 C421 A422 A423 G424 G425 C426

U427 A428 A429 A430 U431 A432 C433 U434 C435 C436 U437 G438 A439 C440 U441 G442 A443 C444 C445 G446 A447 U448 A449 G450 U451 G452 A453 A454 C455 C456 A457 C458 U459 A460 C461 C462 G463 U464 G465 A466 G467 G468 G469 A470 A471 A472 G473 G474 C475 G476 A477 A478 A479 A480 G481 A482 A483 C484 C485 C486

C487 G488 G489 C490 G491 A492 G493 G496 A497 G498 U499 G500 A501 A502 A503 A504 A505 G506 A507 A508 C509 C510 U511 G512 A513 A514 A515 C516 C517 G518 U519 G520 U521 A522 C523 G524 U525 A526 C527 A528 A529 G530 C531 A532 G533 U534 G535 G536 G537 A538 G539 C540 A541 C542 G543 G544 U545 U546 A547

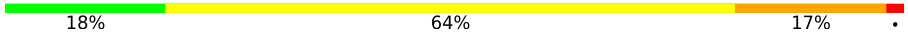


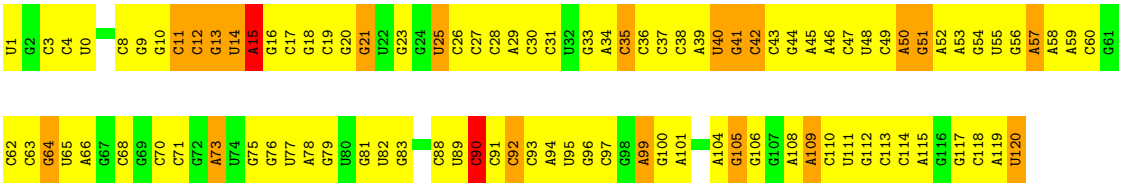





- Molecule 58: 5S ribosomal RNA

Chain Ba:



# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of particles used | 98000 | Depositor |
| Resolution determination method | FSC | Depositor |
| CTF correction method | group defocus | Depositor |
| Microscope | FEI TECNAI F20 | Depositor |
| Voltage (kV) | 200 | Depositor |
| Electron dose ($e^-/Å^2$) | 10 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | Not provided | |
| Image detector | Not provided | |
| Maximum map value | 253.190 | Depositor |
| Minimum map value | -113.794 | Depositor |
| Average map value | 4.829 | Depositor |
| Map value standard deviation | 25.951 | Depositor |
| Recommended contour level | 22.0 | Depositor |
| Map size (Å) | 365.85, 365.85, 365.85 | wwPDB |
| Map dimensions | 135, 135, 135 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 2.71, 2.71, 2.71 | 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: 5MC, 1MG, UR3, 3TD, OMC, H2U, 2MA, OMG, 5MU, 4SU, PSU, 4OC, 2MG, 7MG, 6MZ, MA6, OMU

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 | AJ | 0.75 | 0/742 | 1.26 | 7/941 (0.7%) |
| 2 | AK | 0.79 | 0/856 | 1.39 | 14/1069 (1.3%) |
| 3 | AL | 0.79 | 0/873 | 1.30 | 12/1110 (1.1%) |
| 4 | AM | 0.79 | 0/817 | 1.45 | 20/1022 (2.0%) |
| 5 | AN | 0.82 | 0/715 | 1.37 | 10/883 (1.1%) |
| 6 | AO | 0.76 | 0/646 | 1.22 | 8/813 (1.0%) |
| 7 | AP | 0.83 | 0/572 | 1.39 | 11/711 (1.5%) |
| 8 | AQ | 0.72 | 0/636 | 1.16 | 6/822 (0.7%) |
| 9 | AR | 0.92 | 0/568 | 1.46 | 12/713 (1.7%) |
| 10 | AS | 0.77 | 0/687 | 1.27 | 10/880 (1.1%) |
| 11 | AB | 0.74 | 0/1703 | 1.07 | 9/2161 (0.4%) |
| 12 | AT | 0.75 | 0/574 | 1.25 | 12/694 (1.7%) |
| 13 | AU | 0.94 | 0/520 | 1.61 | 15/636 (2.4%) |
| 14 | AC | 0.75 | 0/1669 | 1.15 | 16/2122 (0.8%) |
| 15 | AD | 0.80 | 0/1497 | 1.29 | 19/1890 (1.0%) |
| 16 | AE | 0.73 | 0/1110 | 1.14 | 9/1405 (0.6%) |
| 17 | AF | 0.79 | 0/1001 | 1.23 | 11/1268 (0.9%) |
| 18 | AG | 0.79 | 0/1263 | 1.33 | 16/1590 (1.0%) |
| 19 | AH | 0.72 | 0/896 | 1.11 | 7/1141 (0.6%) |
| 20 | AI | 0.85 | 0/940 | 1.37 | 19/1180 (1.6%) |
| 21 | A1 | 0.76 | 0/4864 | 1.12 | 24/6363 (0.4%) |
| 22 | AA | 1.47 | 6/36769 (0.0%) | 2.38 | 2673/57354 (4.7%) |
| 23 | A2 | 1.48 | 0/1108 | 2.31 | 71/1724 (4.1%) |
| 24 | A3 | 1.49 | 0/1717 | 2.41 | 129/2675 (4.8%) |
| 25 | BC | 0.68 | 0/1748 | 0.98 | 4/2355 (0.2%) |
| 26 | BJ | 0.73 | 0/1247 | 1.15 | 10/1679 (0.6%) |
| 27 | BK | 0.67 | 0/1046 | 1.00 | 4/1410 (0.3%) |
| 28 | BN | 0.75 | 0/1152 | 1.11 | 11/1551 (0.7%) |
| 29 | BO | 0.74 | 0/956 | 1.20 | 13/1279 (1.0%) |
| 30 | BP | 0.79 | 0/1062 | 1.36 | 15/1413 (1.1%) |
| 31 | BQ | 0.78 | 0/1093 | 1.24 | 13/1460 (0.9%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 32 | BR | 0.79 | 0/1021 | 1.35 | 17/1364 (1.2%) |
| 33 | BS | 0.76 | 0/910 | 1.23 | 14/1219 (1.1%) |
| 34 | BT | 0.77 | 0/929 | 1.25 | 10/1242 (0.8%) |
| 35 | BD | 0.75 | 0/2131 | 1.25 | 32/2863 (1.1%) |
| 36 | BU | 0.80 | 0/960 | 1.29 | 15/1278 (1.2%) |
| 37 | BV | 0.76 | 0/829 | 1.18 | 9/1107 (0.8%) |
| 38 | BW | 0.67 | 0/864 | 1.10 | 12/1156 (1.0%) |
| 39 | BX | 0.69 | 0/794 | 1.10 | 3/1060 (0.3%) |
| 40 | BY | 0.69 | 0/797 | 1.04 | 4/1062 (0.4%) |
| 41 | BZ | 0.73 | 0/766 | 1.11 | 6/1025 (0.6%) |
| 42 | B0 | 0.79 | 0/642 | 1.25 | 8/848 (0.9%) |
| 43 | B1 | 0.79 | 0/635 | 1.37 | 13/848 (1.5%) |
| 44 | B2 | 0.71 | 0/510 | 1.17 | 6/677 (0.9%) |
| 45 | BE | 0.72 | 0/1586 | 1.14 | 15/2134 (0.7%) |
| 46 | B3 | 0.72 | 0/453 | 1.29 | 9/605 (1.5%) |
| 47 | B4 | 0.75 | 0/559 | 1.06 | 5/745 (0.7%) |
| 48 | B5 | 0.79 | 0/450 | 1.38 | 9/599 (1.5%) |
| 49 | B6 | 0.73 | 0/448 | 1.02 | 3/594 (0.5%) |
| 50 | B7 | 0.84 | 0/380 | 1.47 | 10/498 (2.0%) |
| 51 | B8 | 0.76 | 0/513 | 1.28 | 9/676 (1.3%) |
| 52 | B9 | 0.71 | 0/303 | 1.16 | 3/397 (0.8%) |
| 53 | BF | 0.71 | 0/1571 | 1.09 | 13/2113 (0.6%) |
| 54 | BG | 0.77 | 0/1444 | 1.18 | 10/1937 (0.5%) |
| 55 | BH | 0.72 | 0/1343 | 1.08 | 7/1816 (0.4%) |
| 56 | BL | 0.70 | 0/1122 | 1.05 | 8/1515 (0.5%) |
| 57 | BA | 1.47 | 5/69280 (0.0%) | 2.39 | 5083/108078 (4.7%) |
| 58 | Ba | 1.46 | 0/2869 | 2.35 | 208/4474 (4.6%) |
| All | All | 1.28 | 11/165156 (0.0%) | 2.11 | 8751/244244 (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 |
|---|---|---|---|
| 3 | AL | 0 | 1 |
| 6 | AO | 0 | 1 |
| 7 | AP | 0 | 1 |
| 9 | AR | 0 | 1 |
| 10 | AS | 0 | 1 |
| 15 | AD | 0 | 1 |
| 18 | AG | 0 | 2 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 21 | A1 | 0 | 2 |
| 22 | AA | 0 | 350 |
| 23 | A2 | 0 | 5 |
| 24 | A3 | 0 | 15 |
| 26 | BJ | 0 | 1 |
| 28 | BN | 0 | 2 |
| 29 | BO | 0 | 1 |
| 32 | BR | 0 | 1 |
| 34 | BT | 0 | 1 |
| 35 | BD | 0 | 1 |
| 36 | BU | 0 | 2 |
| 38 | BW | 0 | 1 |
| 40 | BY | 0 | 1 |
| 42 | B0 | 0 | 1 |
| 51 | B8 | 0 | 1 |
| 55 | BH | 0 | 2 |
| 57 | BA | 0 | 660 |
| 58 | Ba | 0 | 15 |
| All | All | 0 | 1070 |

All (11) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 22 | AA | 1223 | C | C4-N4 | -5.72 | 1.28 | 1.33 |
| 22 | AA | 1226 | C | O3'-P | -5.66 | 1.54 | 1.61 |
| 22 | AA | 1432 | G | C2-N2 | -5.45 | 1.29 | 1.34 |
| 57 | BA | 823 | C | C4-N4 | -5.35 | 1.29 | 1.33 |
| 22 | AA | 1497 | G | C2-N2 | -5.32 | 1.29 | 1.34 |
| 57 | BA | 1568 | G | C2-N2 | -5.22 | 1.29 | 1.34 |
| 57 | BA | 750 | A | P-O5' | 5.17 | 1.65 | 1.59 |
| 22 | AA | 326 | G | C2-N2 | -5.16 | 1.29 | 1.34 |
| 57 | BA | 2500 | U | P-O5' | 5.12 | 1.64 | 1.59 |
| 57 | BA | 2667 | C | C4-N4 | -5.11 | 1.29 | 1.33 |
| 22 | AA | 566 | G | C2-N2 | -5.02 | 1.29 | 1.34 |

All (8751) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 16 | AE | 111 | ARG | NE-CZ-NH1 | 15.27 | 127.93 | 120.30 |
| 57 | BA | 1073 | A | N1-C6-N6 | -14.45 | 109.93 | 118.60 |
| 26 | BJ | 55 | ARG | NE-CZ-NH1 | 14.31 | 127.46 | 120.30 |
| 57 | BA | 423 | A | N1-C6-N6 | -14.03 | 110.18 | 118.60 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 7 | AP | 70 | ARG | NE-CZ-NH1 | 13.34 | 126.97 | 120.30 |
| 13 | AU | 34 | ARG | NE-CZ-NH1 | 13.01 | 126.81 | 120.30 |
| 57 | BA | 346 | A | O4'-C1'-N9 | 12.88 | 118.50 | 108.20 |
| 30 | BP | 33 | ARG | NE-CZ-NH1 | 12.79 | 126.69 | 120.30 |
| 31 | BQ | 81 | ARG | NE-CZ-NH1 | 12.79 | 126.69 | 120.30 |
| 57 | BA | 2882 | A | N1-C6-N6 | -12.70 | 110.98 | 118.60 |
| 22 | AA | 573 | A | N1-C6-N6 | -12.56 | 111.06 | 118.60 |
| 22 | AA | 983 | A | N1-C6-N6 | -12.53 | 111.08 | 118.60 |
| 22 | AA | 704 | A | N1-C6-N6 | -12.52 | 111.09 | 118.60 |
| 57 | BA | 877 | A | N1-C6-N6 | -12.32 | 111.21 | 118.60 |
| 22 | AA | 1513 | A | N1-C6-N6 | -12.20 | 111.28 | 118.60 |
| 58 | Ba | 46 | A | N1-C6-N6 | -12.20 | 111.28 | 118.60 |
| 22 | AA | 793 | U | O4'-C1'-N1 | 12.17 | 117.93 | 108.20 |
| 22 | AA | 325 | A | N1-C6-N6 | -12.12 | 111.33 | 118.60 |
| 18 | AG | 101 | ARG | NE-CZ-NH1 | 12.09 | 126.34 | 120.30 |
| 22 | AA | 523 | A | N1-C6-N6 | -12.07 | 111.36 | 118.60 |
| 57 | BA | 219 | A | N1-C6-N6 | -12.07 | 111.36 | 118.60 |
| 22 | AA | 815 | A | N1-C6-N6 | -12.03 | 111.39 | 118.60 |
| 57 | BA | 99 | U | O4'-C1'-N1 | 12.02 | 117.81 | 108.20 |
| 57 | BA | 1204 | A | N1-C6-N6 | -11.98 | 111.41 | 118.60 |
| 22 | AA | 622 | A | N1-C6-N6 | -11.92 | 111.45 | 118.60 |
| 57 | BA | 1515 | A | N1-C6-N6 | -11.87 | 111.48 | 118.60 |
| 57 | BA | 84 | A | N1-C6-N6 | -11.83 | 111.50 | 118.60 |
| 57 | BA | 299 | A | N1-C6-N6 | -11.81 | 111.51 | 118.60 |
| 57 | BA | 2476 | A | N1-C6-N6 | -11.79 | 111.52 | 118.60 |
| 22 | AA | 563 | A | N1-C6-N6 | -11.79 | 111.53 | 118.60 |
| 57 | BA | 1672 | A | N1-C6-N6 | -11.79 | 111.53 | 118.60 |
| 30 | BP | 18 | ARG | NE-CZ-NH1 | 11.76 | 126.18 | 120.30 |
| 36 | BU | 57 | ARG | NE-CZ-NH1 | 11.75 | 126.18 | 120.30 |
| 22 | AA | 415 | A | O4'-C1'-N9 | 11.74 | 117.59 | 108.20 |
| 57 | BA | 1427 | A | N1-C6-N6 | -11.71 | 111.57 | 118.60 |
| 57 | BA | 278 | A | N1-C6-N6 | -11.70 | 111.58 | 118.60 |
| 57 | BA | 1284 | A | N1-C6-N6 | -11.69 | 111.59 | 118.60 |
| 20 | AI | 129 | ARG | NE-CZ-NH1 | 11.68 | 126.14 | 120.30 |
| 57 | BA | 1943 | U | O4'-C1'-N1 | 11.68 | 117.54 | 108.20 |
| 22 | AA | 1191 | A | N1-C6-N6 | -11.63 | 111.62 | 118.60 |
| 22 | AA | 160 | A | N1-C6-N6 | -11.62 | 111.63 | 118.60 |
| 57 | BA | 2576 | G | O4'-C1'-N9 | 11.62 | 117.50 | 108.20 |
| 24 | A3 | 9 | G | O4'-C1'-N9 | 11.61 | 117.49 | 108.20 |
| 22 | AA | 765 | G | O4'-C1'-N9 | 11.61 | 117.49 | 108.20 |
| 57 | BA | 74 | A | N1-C6-N6 | -11.59 | 111.65 | 118.60 |
| 22 | AA | 899 | C | O4'-C1'-N1 | 11.57 | 117.46 | 108.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 58 | Ba | 15 | A | O4'-C1'-N9 | 11.55 | 117.44 | 108.20 |
| 22 | AA | 448 | A | N1-C6-N6 | -11.53 | 111.68 | 118.60 |
| 48 | B5 | 9 | ARG | NE-CZ-NH2 | 11.53 | 126.06 | 120.30 |
| 57 | BA | 1552 | A | O4'-C1'-N9 | 11.51 | 117.40 | 108.20 |
| 22 | AA | 728 | A | N1-C6-N6 | -11.50 | 111.70 | 118.60 |
| 22 | AA | 108 | G | O4'-C1'-N9 | 11.47 | 117.38 | 108.20 |
| 22 | AA | 1204 | A | N1-C6-N6 | -11.45 | 111.73 | 118.60 |
| 57 | BA | 294 | A | N1-C6-N6 | -11.42 | 111.75 | 118.60 |
| 21 | A1 | 87 | ARG | NE-CZ-NH1 | 11.41 | 126.01 | 120.30 |
| 22 | AA | 422 | C | O4'-C1'-N1 | 11.40 | 117.32 | 108.20 |
| 22 | AA | 151 | A | N1-C6-N6 | -11.40 | 111.76 | 118.60 |
| 57 | BA | 1127 | A | N1-C6-N6 | -11.38 | 111.78 | 118.60 |
| 2 | AK | 121 | ARG | NE-CZ-NH1 | 11.37 | 125.98 | 120.30 |
| 23 | A2 | 24 | A | N1-C6-N6 | -11.35 | 111.79 | 118.60 |
| 22 | AA | 498 | A | N1-C6-N6 | -11.35 | 111.79 | 118.60 |
| 22 | AA | 766 | A | N1-C6-N6 | -11.33 | 111.80 | 118.60 |
| 57 | BA | 404 | A | N1-C6-N6 | -11.31 | 111.81 | 118.60 |
| 57 | BA | 479 | A | N1-C6-N6 | -11.30 | 111.82 | 118.60 |
| 22 | AA | 1286 | U | O4'-C1'-N1 | 11.25 | 117.20 | 108.20 |
| 57 | BA | 13 | A | N1-C6-N6 | -11.24 | 111.85 | 118.60 |
| 57 | BA | 1155 | A | N1-C6-N6 | -11.24 | 111.85 | 118.60 |
| 22 | AA | 171 | A | N1-C6-N6 | -11.23 | 111.86 | 118.60 |
| 57 | BA | 2241 | A | N1-C6-N6 | -11.22 | 111.86 | 118.60 |
| 57 | BA | 1755 | A | N1-C6-N6 | -11.19 | 111.89 | 118.60 |
| 57 | BA | 1783 | A | N1-C6-N6 | -11.18 | 111.89 | 118.60 |
| 57 | BA | 1378 | A | N1-C6-N6 | -11.12 | 111.93 | 118.60 |
| 18 | AG | 4 | ARG | NE-CZ-NH1 | 11.12 | 125.86 | 120.30 |
| 22 | AA | 493 | A | N1-C6-N6 | -11.12 | 111.93 | 118.60 |
| 34 | BT | 112 | ARG | NE-CZ-NH1 | 11.11 | 125.86 | 120.30 |
| 2 | AK | 126 | ARG | NE-CZ-NH1 | 11.11 | 125.85 | 120.30 |
| 22 | AA | 665 | A | N1-C6-N6 | -11.09 | 111.95 | 118.60 |
| 57 | BA | 2054 | A | N1-C6-N6 | -11.08 | 111.95 | 118.60 |
| 57 | BA | 896 | A | N1-C6-N6 | -11.08 | 111.95 | 118.60 |
| 22 | AA | 1238 | A | N1-C6-N6 | -11.07 | 111.96 | 118.60 |
| 57 | BA | 508 | A | N1-C6-N6 | -11.06 | 111.96 | 118.60 |
| 57 | BA | 2425 | A | N1-C6-N6 | -11.06 | 111.96 | 118.60 |
| 57 | BA | 119 | A | N1-C6-N6 | -11.06 | 111.97 | 118.60 |
| 57 | BA | 217 | A | N1-C6-N6 | -11.05 | 111.97 | 118.60 |
| 57 | BA | 196 | A | N1-C6-N6 | -11.04 | 111.97 | 118.60 |
| 22 | AA | 532 | A | N1-C6-N6 | -11.03 | 111.98 | 118.60 |
| 22 | AA | 610 | U | O4'-C1'-N1 | 11.03 | 117.02 | 108.20 |
| 22 | AA | 1433 | A | N1-C6-N6 | -11.01 | 111.99 | 118.60 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 2600 | A | N1-C6-N6 | -11.00 | 112.00 | 118.60 |
| 57 | BA | 910 | A | N1-C6-N6 | -10.99 | 112.00 | 118.60 |
| 57 | BA | 2274 | A | N1-C6-N6 | -10.96 | 112.02 | 118.60 |
| 57 | BA | 1580 | A | N1-C6-N6 | -10.93 | 112.04 | 118.60 |
| 57 | BA | 2450 | A | N1-C6-N6 | -10.92 | 112.05 | 118.60 |
| 57 | BA | 1739 | A | N1-C6-N6 | -10.91 | 112.05 | 118.60 |
| 57 | BA | 1569 | A | N1-C6-N6 | -10.88 | 112.07 | 118.60 |
| 57 | BA | 1129 | A | N1-C6-N6 | -10.86 | 112.08 | 118.60 |
| 57 | BA | 2266 | A | N1-C6-N6 | -10.84 | 112.09 | 118.60 |
| 4 | AM | 89 | ARG | NE-CZ-NH1 | 10.83 | 125.72 | 120.30 |
| 57 | BA | 2750 | A | N1-C6-N6 | -10.83 | 112.10 | 118.60 |
| 57 | BA | 1853 | A | N1-C6-N6 | -10.83 | 112.10 | 118.60 |
| 22 | AA | 152 | A | N1-C6-N6 | -10.81 | 112.11 | 118.60 |
| 57 | BA | 1635 | A | N1-C6-N6 | -10.78 | 112.13 | 118.60 |
| 57 | BA | 990 | A | N1-C6-N6 | -10.77 | 112.14 | 118.60 |
| 57 | BA | 2733 | A | N1-C6-N6 | -10.76 | 112.14 | 118.60 |
| 57 | BA | 575 | A | N1-C6-N6 | -10.76 | 112.14 | 118.60 |
| 57 | BA | 2851 | A | N1-C6-N6 | -10.74 | 112.16 | 118.60 |
| 57 | BA | 2327 | A | N1-C6-N6 | -10.73 | 112.16 | 118.60 |
| 57 | BA | 1096 | A | N1-C6-N6 | -10.72 | 112.17 | 118.60 |
| 57 | BA | 1952 | A | N1-C6-N6 | -10.71 | 112.17 | 118.60 |
| 2 | AK | 127 | ARG | NE-CZ-NH1 | 10.71 | 125.66 | 120.30 |
| 22 | AA | 274 | A | N1-C6-N6 | -10.71 | 112.17 | 118.60 |
| 57 | BA | 2062 | A | N1-C6-N6 | -10.70 | 112.18 | 118.60 |
| 57 | BA | 91 | A | N1-C6-N6 | -10.70 | 112.18 | 118.60 |
| 57 | BA | 1566 | A | O4'-C1'-N9 | 10.69 | 116.75 | 108.20 |
| 22 | AA | 195 | A | N1-C6-N6 | -10.69 | 112.19 | 118.60 |
| 22 | AA | 196 | A | N1-C6-N6 | -10.69 | 112.19 | 118.60 |
| 57 | BA | 2386 | A | N1-C6-N6 | -10.65 | 112.21 | 118.60 |
| 57 | BA | 2675 | A | N1-C6-N6 | -10.64 | 112.21 | 118.60 |
| 57 | BA | 1918 | A | N1-C6-N6 | -10.64 | 112.22 | 118.60 |
| 22 | AA | 262 | A | N1-C6-N6 | -10.63 | 112.22 | 118.60 |
| 57 | BA | 1650 | A | N1-C6-N6 | -10.63 | 112.22 | 118.60 |
| 22 | AA | 1502 | A | O4'-C1'-N9 | 10.63 | 116.70 | 108.20 |
| 22 | AA | 109 | A | N1-C6-N6 | -10.62 | 112.23 | 118.60 |
| 36 | BU | 5 | ARG | NE-CZ-NH2 | 10.62 | 125.61 | 120.30 |
| 57 | BA | 1353 | A | N1-C6-N6 | -10.61 | 112.23 | 118.60 |
| 57 | BA | 1566 | A | N1-C6-N6 | -10.61 | 112.23 | 118.60 |
| 22 | AA | 1349 | A | N1-C6-N6 | -10.61 | 112.24 | 118.60 |
| 57 | BA | 1801 | A | N1-C6-N6 | -10.60 | 112.24 | 118.60 |
| 22 | AA | 1362 | A | N1-C6-N6 | -10.59 | 112.24 | 118.60 |
| 22 | AA | 465 | A | O4'-C1'-N9 | 10.58 | 116.66 | 108.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 790 | U | O4'-C1'-N1 | 10.58 | 116.66 | 108.20 |
| 22 | AA | 423 | G | O4'-C1'-N9 | 10.55 | 116.64 | 108.20 |
| 22 | AA | 315 | A | N1-C6-N6 | -10.55 | 112.27 | 118.60 |
| 22 | AA | 977 | A | N1-C6-N6 | -10.55 | 112.27 | 118.60 |
| 57 | BA | 1494 | A | N1-C6-N6 | -10.54 | 112.28 | 118.60 |
| 57 | BA | 1665 | A | N1-C6-N6 | -10.54 | 112.28 | 118.60 |
| 57 | BA | 941 | A | N1-C6-N6 | -10.51 | 112.30 | 118.60 |
| 22 | AA | 608 | A | N1-C6-N6 | -10.51 | 112.30 | 118.60 |
| 57 | BA | 2054 | A | C5-C6-N1 | 10.51 | 122.95 | 117.70 |
| 57 | BA | 1579 | A | N1-C6-N6 | -10.50 | 112.30 | 118.60 |
| 2 | AK | 10 | ARG | NE-CZ-NH1 | 10.49 | 125.55 | 120.30 |
| 22 | AA | 16 | A | N1-C6-N6 | -10.47 | 112.32 | 118.60 |
| 57 | BA | 603 | A | N1-C6-N6 | -10.47 | 112.32 | 118.60 |
| 57 | BA | 71 | A | N1-C6-N6 | -10.45 | 112.33 | 118.60 |
| 57 | BA | 1205 | A | N1-C6-N6 | -10.45 | 112.33 | 118.60 |
| 57 | BA | 197 | A | N1-C6-N6 | -10.45 | 112.33 | 118.60 |
| 22 | AA | 1067 | A | N1-C6-N6 | -10.44 | 112.34 | 118.60 |
| 22 | AA | 1111 | A | N1-C6-N6 | -10.44 | 112.34 | 118.60 |
| 22 | AA | 139 | A | N1-C6-N6 | -10.43 | 112.34 | 118.60 |
| 57 | BA | 428 | A | N1-C6-N6 | -10.41 | 112.35 | 118.60 |
| 54 | BG | 29 | ARG | NE-CZ-NH1 | 10.40 | 125.50 | 120.30 |
| 22 | AA | 465 | A | C5-C6-N1 | 10.39 | 122.90 | 117.70 |
| 51 | B8 | 44 | ARG | NE-CZ-NH1 | 10.39 | 125.50 | 120.30 |
| 57 | BA | 2799 | A | N1-C6-N6 | -10.39 | 112.36 | 118.60 |
| 57 | BA | 2439 | A | N1-C6-N6 | -10.39 | 112.37 | 118.60 |
| 57 | BA | 1301 | A | N1-C6-N6 | -10.38 | 112.37 | 118.60 |
| 22 | AA | 161 | A | N1-C6-N6 | -10.37 | 112.38 | 118.60 |
| 22 | AA | 938 | A | N1-C6-N6 | -10.36 | 112.38 | 118.60 |
| 57 | BA | 1327 | A | N1-C6-N6 | -10.36 | 112.38 | 118.60 |
| 57 | BA | 38 | A | N1-C6-N6 | -10.36 | 112.38 | 118.60 |
| 57 | BA | 1000 | A | N1-C6-N6 | -10.36 | 112.38 | 118.60 |
| 22 | AA | 129 | A | N1-C6-N6 | -10.36 | 112.39 | 118.60 |
| 15 | AD | 12 | ARG | NE-CZ-NH1 | 10.35 | 125.48 | 120.30 |
| 57 | BA | 2726 | A | N1-C6-N6 | -10.35 | 112.39 | 118.60 |
| 57 | BA | 1640 | A | N1-C6-N6 | -10.35 | 112.39 | 118.60 |
| 57 | BA | 1419 | A | N1-C6-N6 | -10.34 | 112.39 | 118.60 |
| 57 | BA | 592 | A | N1-C6-N6 | -10.33 | 112.40 | 118.60 |
| 57 | BA | 2108 | A | N1-C6-N6 | -10.32 | 112.41 | 118.60 |
| 57 | BA | 825 | A | N1-C6-N6 | -10.31 | 112.41 | 118.60 |
| 22 | AA | 1105 | A | N1-C6-N6 | -10.31 | 112.42 | 118.60 |
| 20 | AI | 17 | ARG | NE-CZ-NH1 | 10.30 | 125.45 | 120.30 |
| 22 | AA | 1441 | A | N1-C6-N6 | -10.28 | 112.43 | 118.60 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 41 | BZ | 18 | ARG | NE-CZ-NH1 | 10.28 | 125.44 | 120.30 |
| 22 | AA | 353 | A | N1-C6-N6 | -10.27 | 112.44 | 118.60 |
| 57 | BA | 788 | A | N1-C6-N6 | -10.27 | 112.44 | 118.60 |
| 57 | BA | 781 | A | N1-C6-N6 | -10.26 | 112.44 | 118.60 |
| 57 | BA | 1490 | A | N1-C6-N6 | -10.25 | 112.45 | 118.60 |
| 22 | AA | 559 | A | N1-C6-N6 | -10.25 | 112.45 | 118.60 |
| 57 | BA | 95 | A | N1-C6-N6 | -10.24 | 112.46 | 118.60 |
| 22 | AA | 1213 | A | N1-C6-N6 | -10.24 | 112.46 | 118.60 |
| 57 | BA | 2764 | A | N1-C6-N6 | -10.23 | 112.46 | 118.60 |
| 57 | BA | 631 | A | N1-C6-N6 | -10.23 | 112.47 | 118.60 |
| 22 | AA | 389 | A | N1-C6-N6 | -10.22 | 112.47 | 118.60 |
| 22 | AA | 864 | A | N1-C6-N6 | -10.22 | 112.47 | 118.60 |
| 57 | BA | 529 | A | N1-C6-N6 | -10.21 | 112.47 | 118.60 |
| 57 | BA | 1664 | A | N1-C6-N6 | -10.21 | 112.47 | 118.60 |
| 57 | BA | 2080 | A | N1-C6-N6 | -10.21 | 112.47 | 118.60 |
| 57 | BA | 1142 | A | N1-C6-N6 | -10.20 | 112.48 | 118.60 |
| 57 | BA | 1717 | A | N1-C6-N6 | -10.19 | 112.48 | 118.60 |
| 57 | BA | 2287 | A | N1-C6-N6 | -10.19 | 112.49 | 118.60 |
| 22 | AA | 872 | A | N1-C6-N6 | -10.19 | 112.49 | 118.60 |
| 57 | BA | 2872 | A | N1-C6-N6 | -10.18 | 112.49 | 118.60 |
| 57 | BA | 2225 | A | N1-C6-N6 | -10.18 | 112.49 | 118.60 |
| 57 | BA | 2478 | A | N1-C6-N6 | -10.18 | 112.49 | 118.60 |
| 57 | BA | 2433 | A | N1-C6-N6 | -10.17 | 112.50 | 118.60 |
| 22 | AA | 414 | A | N1-C6-N6 | -10.17 | 112.50 | 118.60 |
| 24 | A3 | 39 | A | N1-C6-N6 | -10.17 | 112.50 | 118.60 |
| 58 | Ba | 78 | A | N1-C6-N6 | -10.17 | 112.50 | 118.60 |
| 57 | BA | 412 | A | N1-C6-N6 | -10.16 | 112.50 | 118.60 |
| 57 | BA | 1133 | A | N1-C6-N6 | -10.16 | 112.50 | 118.60 |
| 57 | BA | 2253 | G | O4'-C1'-N9 | 10.16 | 116.33 | 108.20 |
| 5 | AN | 84 | ARG | NE-CZ-NH1 | 10.15 | 125.38 | 120.30 |
| 24 | A3 | 22 | A | N1-C6-N6 | -10.14 | 112.52 | 118.60 |
| 57 | BA | 685 | A | N1-C6-N6 | -10.14 | 112.52 | 118.60 |
| 57 | BA | 1614 | A | N1-C6-N6 | -10.14 | 112.52 | 118.60 |
| 57 | BA | 1913 | A | N1-C6-N6 | -10.13 | 112.52 | 118.60 |
| 57 | BA | 2134 | A | O4'-C1'-N9 | 10.13 | 116.31 | 108.20 |
| 32 | BR | 12 | ARG | NE-CZ-NH1 | 10.12 | 125.36 | 120.30 |
| 22 | AA | 1311 | A | N1-C6-N6 | -10.12 | 112.53 | 118.60 |
| 22 | AA | 1269 | A | N1-C6-N6 | -10.12 | 112.53 | 118.60 |
| 57 | BA | 2721 | A | N1-C6-N6 | -10.12 | 112.53 | 118.60 |
| 57 | BA | 1175 | A | N1-C6-N6 | -10.11 | 112.53 | 118.60 |
| 22 | AA | 1329 | A | N1-C6-N6 | -10.11 | 112.54 | 118.60 |
| 57 | BA | 2335 | A | N1-C6-N6 | -10.10 | 112.54 | 118.60 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 2198 | A | N1-C6-N6 | -10.09 | 112.55 | 118.60 |
| 57 | BA | 2309 | A | N1-C6-N6 | -10.08 | 112.55 | 118.60 |
| 22 | AA | 572 | A | N1-C6-N6 | -10.08 | 112.55 | 118.60 |
| 57 | BA | 1285 | A | N1-C6-N6 | -10.08 | 112.55 | 118.60 |
| 57 | BA | 666 | A | N1-C6-N6 | -10.08 | 112.55 | 118.60 |
| 57 | BA | 905 | A | N1-C6-N6 | -10.08 | 112.55 | 118.60 |
| 57 | BA | 829 | A | N1-C6-N6 | -10.08 | 112.56 | 118.60 |
| 22 | AA | 547 | A | N1-C6-N6 | -10.07 | 112.56 | 118.60 |
| 9 | AR | 42 | ARG | NE-CZ-NH1 | 10.07 | 125.34 | 120.30 |
| 57 | BA | 2311 | A | N1-C6-N6 | -10.07 | 112.56 | 118.60 |
| 57 | BA | 1103 | A | N1-C6-N6 | -10.06 | 112.56 | 118.60 |
| 57 | BA | 2711 | A | N1-C6-N6 | -10.06 | 112.56 | 118.60 |
| 22 | AA | 1248 | A | N1-C6-N6 | -10.06 | 112.57 | 118.60 |
| 32 | BR | 4 | ARG | NE-CZ-NH1 | 10.06 | 125.33 | 120.30 |
| 57 | BA | 2886 | A | N1-C6-N6 | -10.05 | 112.57 | 118.60 |
| 57 | BA | 1553 | A | N1-C6-N6 | -10.05 | 112.57 | 118.60 |
| 22 | AA | 101 | A | N1-C6-N6 | -10.04 | 112.58 | 118.60 |
| 22 | AA | 1271 | A | N1-C6-N6 | -10.04 | 112.58 | 118.60 |
| 57 | BA | 1810 | A | N1-C6-N6 | -10.03 | 112.58 | 118.60 |
| 57 | BA | 2541 | A | N1-C6-N6 | -10.03 | 112.58 | 118.60 |
| 1 | AJ | 37 | ARG | NE-CZ-NH1 | 10.03 | 125.31 | 120.30 |
| 57 | BA | 1048 | A | N1-C6-N6 | -10.03 | 112.58 | 118.60 |
| 57 | BA | 223 | A | N1-C6-N6 | -10.02 | 112.59 | 118.60 |
| 57 | BA | 1307 | A | N1-C6-N6 | -10.02 | 112.59 | 118.60 |
| 57 | BA | 1508 | A | O4'-C1'-N9 | 10.02 | 116.21 | 108.20 |
| 57 | BA | 2661 | G | C1'-O4'-C4' | -10.02 | 101.89 | 109.90 |
| 57 | BA | 2471 | A | N1-C6-N6 | -10.01 | 112.59 | 118.60 |
| 22 | AA | 460 | A | N1-C6-N6 | -10.01 | 112.59 | 118.60 |
| 57 | BA | 2059 | A | N1-C6-N6 | -10.01 | 112.59 | 118.60 |
| 22 | AA | 451 | A | N1-C6-N6 | -10.00 | 112.60 | 118.60 |
| 57 | BA | 382 | A | N1-C6-N6 | -10.00 | 112.60 | 118.60 |
| 22 | AA | 459 | A | N1-C6-N6 | -9.99 | 112.61 | 118.60 |
| 24 | A3 | 16 | C | O4'-C1'-N1 | 9.99 | 116.19 | 108.20 |
| 22 | AA | 1346 | A | N1-C6-N6 | -9.98 | 112.61 | 118.60 |
| 57 | BA | 430 | A | N1-C6-N6 | -9.98 | 112.61 | 118.60 |
| 22 | AA | 381 | C | O4'-C1'-N1 | 9.98 | 116.18 | 108.20 |
| 22 | AA | 716 | A | N1-C6-N6 | -9.97 | 112.62 | 118.60 |
| 57 | BA | 1067 | A | N1-C6-N6 | -9.96 | 112.62 | 118.60 |
| 58 | Ba | 104 | A | N1-C6-N6 | -9.96 | 112.62 | 118.60 |
| 22 | AA | 1289 | A | N1-C6-N6 | -9.95 | 112.63 | 118.60 |
| 57 | BA | 492 | A | N1-C6-N6 | -9.95 | 112.63 | 118.60 |
| 22 | AA | 899 | C | N3-C2-O2 | -9.95 | 114.94 | 121.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 2448 | A | N1-C6-N6 | -9.94 | 112.63 | 118.60 |
| 57 | BA | 1247 | A | N1-C6-N6 | -9.94 | 112.64 | 118.60 |
| 22 | AA | 965 | U | O4'-C1'-N1 | 9.94 | 116.15 | 108.20 |
| 57 | BA | 716 | A | N1-C6-N6 | -9.93 | 112.64 | 118.60 |
| 57 | BA | 945 | A | N1-C6-N6 | -9.92 | 112.65 | 118.60 |
| 57 | BA | 2451 | A | N1-C6-N6 | -9.92 | 112.65 | 118.60 |
| 22 | AA | 900 | A | N1-C6-N6 | -9.91 | 112.65 | 118.60 |
| 22 | AA | 718 | A | N1-C6-N6 | -9.90 | 112.66 | 118.60 |
| 57 | BA | 900 | A | N1-C6-N6 | -9.90 | 112.66 | 118.60 |
| 22 | AA | 251 | G | O4'-C1'-N9 | 9.90 | 116.12 | 108.20 |
| 57 | BA | 309 | A | N1-C6-N6 | -9.90 | 112.66 | 118.60 |
| 57 | BA | 2432 | A | N1-C6-N6 | -9.88 | 112.67 | 118.60 |
| 32 | BR | 17 | ARG | NE-CZ-NH1 | 9.88 | 125.24 | 120.30 |
| 57 | BA | 2278 | A | N1-C6-N6 | -9.88 | 112.67 | 118.60 |
| 57 | BA | 2434 | A | N1-C6-N6 | -9.88 | 112.67 | 118.60 |
| 57 | BA | 190 | A | N1-C6-N6 | -9.87 | 112.68 | 118.60 |
| 57 | BA | 454 | A | N1-C6-N6 | -9.87 | 112.68 | 118.60 |
| 57 | BA | 1509 | A | N1-C6-N6 | -9.87 | 112.68 | 118.60 |
| 22 | AA | 918 | A | N1-C6-N6 | -9.86 | 112.68 | 118.60 |
| 23 | A2 | 19 | A | N1-C6-N6 | -9.86 | 112.68 | 118.60 |
| 57 | BA | 1495 | A | N1-C6-N6 | -9.86 | 112.68 | 118.60 |
| 15 | AD | 114 | ARG | NE-CZ-NH1 | 9.86 | 125.23 | 120.30 |
| 22 | AA | 309 | A | N1-C6-N6 | -9.86 | 112.68 | 118.60 |
| 22 | AA | 792 | A | N1-C6-N6 | -9.86 | 112.69 | 118.60 |
| 5 | AN | 74 | ARG | NE-CZ-NH1 | 9.86 | 125.23 | 120.30 |
| 6 | AO | 53 | ARG | NE-CZ-NH1 | 9.85 | 125.23 | 120.30 |
| 22 | AA | 499 | A | N1-C6-N6 | -9.85 | 112.69 | 118.60 |
| 22 | AA | 1285 | A | N1-C6-N6 | -9.85 | 112.69 | 118.60 |
| 22 | AA | 155 | A | N1-C6-N6 | -9.84 | 112.69 | 118.60 |
| 22 | AA | 915 | A | N1-C6-N6 | -9.84 | 112.69 | 118.60 |
| 57 | BA | 532 | A | N1-C6-N6 | -9.84 | 112.69 | 118.60 |
| 34 | BT | 87 | ARG | NE-CZ-NH1 | 9.84 | 125.22 | 120.30 |
| 22 | AA | 74 | A | N1-C6-N6 | -9.84 | 112.70 | 118.60 |
| 57 | BA | 42 | A | N1-C6-N6 | -9.84 | 112.70 | 118.60 |
| 57 | BA | 64 | A | N1-C6-N6 | -9.84 | 112.70 | 118.60 |
| 22 | AA | 1288 | A | N1-C6-N6 | -9.83 | 112.70 | 118.60 |
| 57 | BA | 2654 | A | N1-C6-N6 | -9.83 | 112.70 | 118.60 |
| 9 | AR | 56 | ARG | NE-CZ-NH1 | 9.82 | 125.21 | 120.30 |
| 37 | BV | 68 | ARG | NE-CZ-NH2 | 9.82 | 125.21 | 120.30 |
| 22 | AA | 781 | A | N1-C6-N6 | -9.81 | 112.71 | 118.60 |
| 57 | BA | 2577 | A | N1-C6-N6 | -9.81 | 112.71 | 118.60 |
| 57 | BA | 161 | A | N1-C6-N6 | -9.81 | 112.71 | 118.60 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 1010 | A | N1-C6-N6 | -9.80 | 112.72 | 118.60 |
| 57 | BA | 1735 | A | N1-C6-N6 | -9.80 | 112.72 | 118.60 |
| 57 | BA | 1194 | A | N1-C6-N6 | -9.80 | 112.72 | 118.60 |
| 57 | BA | 582 | A | N1-C6-N6 | -9.80 | 112.72 | 118.60 |
| 57 | BA | 2531 | A | N1-C6-N6 | -9.80 | 112.72 | 118.60 |
| 22 | AA | 958 | A | N1-C6-N6 | -9.79 | 112.72 | 118.60 |
| 4 | AM | 70 | ARG | NE-CZ-NH1 | 9.79 | 125.19 | 120.30 |
| 57 | BA | 590 | A | N1-C6-N6 | -9.78 | 112.73 | 118.60 |
| 58 | Ba | 15 | A | N1-C6-N6 | -9.78 | 112.73 | 118.60 |
| 57 | BA | 126 | A | N1-C6-N6 | -9.78 | 112.73 | 118.60 |
| 22 | AA | 364 | A | N1-C6-N6 | -9.77 | 112.74 | 118.60 |
| 22 | AA | 675 | A | N1-C6-N6 | -9.77 | 112.74 | 118.60 |
| 22 | AA | 1363 | A | N1-C6-N6 | -9.76 | 112.74 | 118.60 |
| 57 | BA | 270 | A | N1-C6-N6 | -9.76 | 112.74 | 118.60 |
| 22 | AA | 1170 | A | N1-C6-N6 | -9.76 | 112.75 | 118.60 |
| 57 | BA | 1395 | A | N1-C6-N6 | -9.76 | 112.75 | 118.60 |
| 57 | BA | 216 | A | N1-C6-N6 | -9.75 | 112.75 | 118.60 |
| 22 | AA | 1021 | A | N1-C6-N6 | -9.74 | 112.75 | 118.60 |
| 57 | BA | 2270 | A | N1-C6-N6 | -9.74 | 112.76 | 118.60 |
| 57 | BA | 2879 | A | N1-C6-N6 | -9.73 | 112.76 | 118.60 |
| 26 | BJ | 137 | ARG | NE-CZ-NH1 | 9.73 | 125.16 | 120.30 |
| 24 | A3 | 38 | A | N1-C6-N6 | -9.72 | 112.77 | 118.60 |
| 57 | BA | 1262 | A | N1-C6-N6 | -9.72 | 112.77 | 118.60 |
| 12 | AT | 24 | ARG | NE-CZ-NH1 | 9.72 | 125.16 | 120.30 |
| 22 | AA | 431 | A | N1-C6-N6 | -9.72 | 112.77 | 118.60 |
| 22 | AA | 746 | A | N1-C6-N6 | -9.71 | 112.77 | 118.60 |
| 35 | BD | 220 | ARG | NE-CZ-NH1 | 9.71 | 125.15 | 120.30 |
| 57 | BA | 1877 | A | N1-C6-N6 | -9.70 | 112.78 | 118.60 |
| 22 | AA | 937 | A | N1-C6-N6 | -9.70 | 112.78 | 118.60 |
| 57 | BA | 1237 | A | N1-C6-N6 | -9.70 | 112.78 | 118.60 |
| 57 | BA | 2031 | A | N1-C6-N6 | -9.70 | 112.78 | 118.60 |
| 57 | BA | 2033 | A | N1-C6-N6 | -9.70 | 112.78 | 118.60 |
| 57 | BA | 2530 | A | N1-C6-N6 | -9.70 | 112.78 | 118.60 |
| 1 | AJ | 16 | ARG | NE-CZ-NH1 | 9.69 | 125.15 | 120.30 |
| 35 | BD | 51 | ARG | NE-CZ-NH1 | 9.69 | 125.15 | 120.30 |
| 22 | AA | 1227 | A | N1-C6-N6 | -9.68 | 112.79 | 118.60 |
| 57 | BA | 1321 | A | N1-C6-N6 | -9.68 | 112.79 | 118.60 |
| 57 | BA | 975 | A | N1-C6-N6 | -9.68 | 112.79 | 118.60 |
| 57 | BA | 2781 | A | N1-C6-N6 | -9.68 | 112.79 | 118.60 |
| 22 | AA | 1322 | C | O4'-C1'-N1 | 9.68 | 115.94 | 108.20 |
| 10 | AS | 77 | ARG | NE-CZ-NH1 | 9.67 | 125.14 | 120.30 |
| 57 | BA | 1932 | A | N1-C6-N6 | -9.67 | 112.80 | 118.60 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 2388 | A | N1-C6-N6 | -9.67 | 112.80 | 118.60 |
| 5 | AN | 52 | ARG | NE-CZ-NH1 | 9.67 | 125.13 | 120.30 |
| 57 | BA | 1632 | A | N1-C6-N6 | -9.66 | 112.80 | 118.60 |
| 57 | BA | 2212 | A | N1-C6-N6 | -9.66 | 112.81 | 118.60 |
| 22 | AA | 1117 | A | N1-C6-N6 | -9.66 | 112.81 | 118.60 |
| 57 | BA | 1786 | A | N1-C6-N6 | -9.65 | 112.81 | 118.60 |
| 10 | AS | 80 | ARG | NE-CZ-NH1 | 9.65 | 125.12 | 120.30 |
| 22 | AA | 452 | A | N1-C6-N6 | -9.65 | 112.81 | 118.60 |
| 22 | AA | 842 | U | O4'-C1'-N1 | 9.65 | 115.92 | 108.20 |
| 57 | BA | 1746 | A | N1-C6-N6 | -9.64 | 112.81 | 118.60 |
| 22 | AA | 640 | A | N1-C6-N6 | -9.64 | 112.82 | 118.60 |
| 22 | AA | 1036 | A | N1-C6-N6 | -9.63 | 112.82 | 118.60 |
| 57 | BA | 2682 | A | N1-C6-N6 | -9.64 | 112.82 | 118.60 |
| 22 | AA | 807 | A | N1-C6-N6 | -9.63 | 112.82 | 118.60 |
| 57 | BA | 74 | A | C5-C6-N1 | 9.63 | 122.52 | 117.70 |
| 57 | BA | 925 | A | N1-C6-N6 | -9.63 | 112.82 | 118.60 |
| 22 | AA | 816 | A | N1-C6-N6 | -9.63 | 112.82 | 118.60 |
| 57 | BA | 2418 | A | N1-C6-N6 | -9.63 | 112.82 | 118.60 |
| 22 | AA | 533 | A | C5-C6-N1 | 9.62 | 122.51 | 117.70 |
| 57 | BA | 2662 | A | N1-C6-N6 | -9.62 | 112.83 | 118.60 |
| 4 | AM | 86 | ARG | NE-CZ-NH1 | 9.62 | 125.11 | 120.30 |
| 22 | AA | 843 | U | O4'-C1'-N1 | 9.62 | 115.89 | 108.20 |
| 57 | BA | 718 | A | N1-C6-N6 | -9.62 | 112.83 | 118.60 |
| 41 | BZ | 19 | ARG | NE-CZ-NH1 | 9.62 | 125.11 | 120.30 |
| 57 | BA | 1829 | A | N1-C6-N6 | -9.61 | 112.83 | 118.60 |
| 57 | BA | 2171 | A | N1-C6-N6 | -9.61 | 112.83 | 118.60 |
| 57 | BA | 2572 | A | N1-C6-N6 | -9.61 | 112.83 | 118.60 |
| 57 | BA | 2810 | A | N1-C6-N6 | -9.61 | 112.83 | 118.60 |
| 57 | BA | 2376 | A | N1-C6-N6 | -9.61 | 112.83 | 118.60 |
| 22 | AA | 1396 | A | N1-C6-N6 | -9.61 | 112.84 | 118.60 |
| 57 | BA | 1147 | A | N1-C6-N6 | -9.61 | 112.84 | 118.60 |
| 22 | AA | 975 | A | N1-C6-N6 | -9.60 | 112.84 | 118.60 |
| 44 | B2 | 7 | ARG | NE-CZ-NH1 | 9.60 | 125.10 | 120.30 |
| 57 | BA | 1453 | A | N1-C6-N6 | -9.59 | 112.85 | 118.60 |
| 57 | BA | 1919 | A | N1-C6-N6 | -9.59 | 112.85 | 118.60 |
| 57 | BA | 2575 | C | N1-C2-O2 | 9.58 | 124.65 | 118.90 |
| 34 | BT | 38 | ARG | NE-CZ-NH2 | 9.58 | 125.09 | 120.30 |
| 57 | BA | 429 | A | N1-C6-N6 | -9.58 | 112.85 | 118.60 |
| 57 | BA | 2333 | A | N1-C6-N6 | -9.58 | 112.85 | 118.60 |
| 57 | BA | 1610 | A | N1-C6-N6 | -9.57 | 112.86 | 118.60 |
| 57 | BA | 909 | A | N1-C6-N6 | -9.57 | 112.86 | 118.60 |
| 57 | BA | 2126 | A | N1-C6-N6 | -9.57 | 112.86 | 118.60 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 2346 | A | N1-C6-N6 | -9.57 | 112.86 | 118.60 |
| 22 | AA | 50 | A | N1-C6-N6 | -9.56 | 112.86 | 118.60 |
| 57 | BA | 1669 | A | N1-C6-N6 | -9.56 | 112.86 | 118.60 |
| 57 | BA | 793 | A | N1-C6-N6 | -9.56 | 112.86 | 118.60 |
| 57 | BA | 1014 | A | N1-C6-N6 | -9.56 | 112.86 | 118.60 |
| 57 | BA | 2813 | A | N1-C6-N6 | -9.56 | 112.86 | 118.60 |
| 30 | BP | 2 | ARG | NE-CZ-NH1 | 9.56 | 125.08 | 120.30 |
| 22 | AA | 554 | A | N1-C6-N6 | -9.56 | 112.86 | 118.60 |
| 57 | BA | 668 | A | N1-C6-N6 | -9.56 | 112.86 | 118.60 |
| 57 | BA | 1586 | A | N1-C6-N6 | -9.56 | 112.86 | 118.60 |
| 57 | BA | 1900 | A | N1-C6-N6 | -9.56 | 112.86 | 118.60 |
| 57 | BA | 1901 | A | N1-C6-N6 | -9.55 | 112.87 | 118.60 |
| 57 | BA | 538 | A | N1-C6-N6 | -9.55 | 112.87 | 118.60 |
| 57 | BA | 2134 | A | N1-C6-N6 | -9.55 | 112.87 | 118.60 |
| 57 | BA | 1050 | A | N1-C6-N6 | -9.55 | 112.87 | 118.60 |
| 57 | BA | 371 | A | N1-C6-N6 | -9.54 | 112.88 | 118.60 |
| 57 | BA | 526 | A | N1-C6-N6 | -9.54 | 112.88 | 118.60 |
| 57 | BA | 1608 | A | N1-C6-N6 | -9.53 | 112.88 | 118.60 |
| 57 | BA | 689 | A | N1-C6-N6 | -9.53 | 112.88 | 118.60 |
| 57 | BA | 1434 | A | N1-C6-N6 | -9.53 | 112.88 | 118.60 |
| 7 | AP | 25 | ARG | NE-CZ-NH1 | 9.52 | 125.06 | 120.30 |
| 22 | AA | 1493 | A | N1-C6-N6 | -9.52 | 112.89 | 118.60 |
| 22 | AA | 1502 | A | N1-C6-N6 | -9.52 | 112.89 | 118.60 |
| 57 | BA | 347 | A | N1-C6-N6 | -9.52 | 112.89 | 118.60 |
| 57 | BA | 2453 | A | N1-C6-N6 | -9.52 | 112.89 | 118.60 |
| 57 | BA | 165 | A | N1-C6-N6 | -9.52 | 112.89 | 118.60 |
| 22 | AA | 1180 | A | N1-C6-N6 | -9.52 | 112.89 | 118.60 |
| 57 | BA | 804 | A | N1-C6-N6 | -9.52 | 112.89 | 118.60 |
| 57 | BA | 1937 | A | N1-C6-N6 | -9.52 | 112.89 | 118.60 |
| 57 | BA | 849 | A | N1-C6-N6 | -9.51 | 112.89 | 118.60 |
| 23 | A2 | 16 | A | N1-C6-N6 | -9.51 | 112.89 | 118.60 |
| 57 | BA | 1354 | A | N1-C6-N6 | -9.51 | 112.89 | 118.60 |
| 57 | BA | 2740 | A | N1-C6-N6 | -9.50 | 112.90 | 118.60 |
| 57 | BA | 608 | A | N1-C6-N6 | -9.50 | 112.90 | 118.60 |
| 22 | AA | 412 | A | N1-C6-N6 | -9.49 | 112.91 | 118.60 |
| 22 | AA | 1257 | A | N1-C6-N6 | -9.48 | 112.91 | 118.60 |
| 35 | BD | 216 | ARG | NE-CZ-NH1 | 9.48 | 125.04 | 120.30 |
| 57 | BA | 1981 | A | N1-C6-N6 | -9.48 | 112.91 | 118.60 |
| 57 | BA | 2273 | A | N1-C6-N6 | -9.48 | 112.91 | 118.60 |
| 5 | AN | 89 | ARG | NE-CZ-NH1 | 9.47 | 125.04 | 120.30 |
| 57 | BA | 227 | A | N1-C6-N6 | -9.47 | 112.92 | 118.60 |
| 57 | BA | 504 | A | N1-C6-N6 | -9.47 | 112.92 | 118.60 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 2614 | A | N1-C6-N6 | -9.47 | 112.92 | 118.60 |
| 22 | AA | 177 | G | O4'-C1'-N9 | 9.47 | 115.78 | 108.20 |
| 22 | AA | 676 | A | N1-C6-N6 | -9.47 | 112.92 | 118.60 |
| 57 | BA | 1503 | A | N1-C6-N6 | -9.47 | 112.92 | 118.60 |
| 22 | AA | 1339 | A | N1-C6-N6 | -9.47 | 112.92 | 118.60 |
| 22 | AA | 1239 | A | N1-C6-N6 | -9.46 | 112.92 | 118.60 |
| 22 | AA | 167 | A | N1-C6-N6 | -9.46 | 112.92 | 118.60 |
| 57 | BA | 2778 | A | N1-C6-N6 | -9.46 | 112.92 | 118.60 |
| 23 | A2 | 41 | A | N1-C6-N6 | -9.45 | 112.93 | 118.60 |
| 38 | BW | 95 | ARG | NE-CZ-NH2 | 9.45 | 125.03 | 120.30 |
| 22 | AA | 262 | A | C5-C6-N1 | 9.45 | 122.42 | 117.70 |
| 22 | AA | 777 | A | N1-C6-N6 | -9.45 | 112.93 | 118.60 |
| 22 | AA | 1280 | A | N1-C6-N6 | -9.45 | 112.93 | 118.60 |
| 57 | BA | 1304 | A | N1-C6-N6 | -9.45 | 112.93 | 118.60 |
| 57 | BA | 2792 | A | N1-C6-N6 | -9.45 | 112.93 | 118.60 |
| 22 | AA | 712 | A | N1-C6-N6 | -9.44 | 112.94 | 118.60 |
| 57 | BA | 262 | A | N1-C6-N6 | -9.44 | 112.94 | 118.60 |
| 57 | BA | 752 | A | N1-C6-N6 | -9.44 | 112.94 | 118.60 |
| 57 | BA | 1077 | A | N1-C6-N6 | -9.44 | 112.94 | 118.60 |
| 57 | BA | 1505 | A | N1-C6-N6 | -9.44 | 112.94 | 118.60 |
| 22 | AA | 533 | A | N1-C6-N6 | -9.44 | 112.94 | 118.60 |
| 57 | BA | 181 | A | N1-C6-N6 | -9.44 | 112.94 | 118.60 |
| 57 | BA | 502 | A | N1-C6-N6 | -9.43 | 112.94 | 118.60 |
| 57 | BA | 1274 | A | N1-C6-N6 | -9.43 | 112.94 | 118.60 |
| 57 | BA | 1085 | A | N1-C6-N6 | -9.43 | 112.94 | 118.60 |
| 22 | AA | 913 | A | N1-C6-N6 | -9.42 | 112.95 | 118.60 |
| 22 | AA | 1447 | A | N1-C6-N6 | -9.42 | 112.95 | 118.60 |
| 30 | BP | 126 | ARG | NE-CZ-NH1 | 9.42 | 125.01 | 120.30 |
| 14 | AC | 53 | ARG | NE-CZ-NH1 | 9.42 | 125.01 | 120.30 |
| 22 | AA | 1 | A | N1-C6-N6 | -9.41 | 112.95 | 118.60 |
| 57 | BA | 1711 | A | N1-C6-N6 | -9.41 | 112.95 | 118.60 |
| 58 | Ba | 34 | A | N1-C6-N6 | -9.41 | 112.96 | 118.60 |
| 15 | AD | 62 | ARG | NE-CZ-NH1 | 9.40 | 125.00 | 120.30 |
| 57 | BA | 2163 | A | N1-C6-N6 | -9.40 | 112.96 | 118.60 |
| 22 | AA | 1377 | A | N1-C6-N6 | -9.40 | 112.96 | 118.60 |
| 57 | BA | 1403 | A | N1-C6-N6 | -9.40 | 112.96 | 118.60 |
| 30 | BP | 60 | ARG | NE-CZ-NH1 | 9.39 | 125.00 | 120.30 |
| 57 | BA | 1226 | A | N1-C6-N6 | -9.38 | 112.97 | 118.60 |
| 22 | AA | 889 | A | N1-C6-N6 | -9.38 | 112.97 | 118.60 |
| 57 | BA | 979 | A | N1-C6-N6 | -9.38 | 112.97 | 118.60 |
| 22 | AA | 819 | A | N1-C6-N6 | -9.38 | 112.97 | 118.60 |
| 37 | BV | 84 | ARG | NE-CZ-NH2 | 9.38 | 124.99 | 120.30 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 300 | A | N1-C6-N6 | -9.38 | 112.97 | 118.60 |
| 57 | BA | 1532 | A | N1-C6-N6 | -9.37 | 112.98 | 118.60 |
| 22 | AA | 935 | A | N1-C6-N6 | -9.37 | 112.98 | 118.60 |
| 57 | BA | 10 | A | N1-C6-N6 | -9.37 | 112.98 | 118.60 |
| 57 | BA | 2666 | C | N3-C2-O2 | -9.37 | 115.34 | 121.90 |
| 22 | AA | 1179 | A | N1-C6-N6 | -9.36 | 112.98 | 118.60 |
| 22 | AA | 1216 | A | N1-C6-N6 | -9.36 | 112.98 | 118.60 |
| 57 | BA | 1876 | A | N1-C6-N6 | -9.36 | 112.98 | 118.60 |
| 23 | A2 | 59 | A | N1-C6-N6 | -9.36 | 112.98 | 118.60 |
| 57 | BA | 654 | A | N1-C6-N6 | -9.36 | 112.99 | 118.60 |
| 57 | BA | 1477 | A | N1-C6-N6 | -9.36 | 112.99 | 118.60 |
| 22 | AA | 422 | C | N3-C2-O2 | -9.35 | 115.35 | 121.90 |
| 57 | BA | 73 | A | N1-C6-N6 | -9.35 | 112.99 | 118.60 |
| 57 | BA | 324 | A | N1-C6-N6 | -9.35 | 112.99 | 118.60 |
| 57 | BA | 348 | A | N1-C6-N6 | -9.35 | 112.99 | 118.60 |
| 57 | BA | 2392 | A | N1-C6-N6 | -9.35 | 112.99 | 118.60 |
| 57 | BA | 1679 | A | N1-C6-N6 | -9.34 | 113.00 | 118.60 |
| 57 | BA | 2679 | A | N1-C6-N6 | -9.34 | 113.00 | 118.60 |
| 57 | BA | 2736 | A | N1-C6-N6 | -9.34 | 113.00 | 118.60 |
| 57 | BA | 878 | A | N1-C6-N6 | -9.33 | 113.00 | 118.60 |
| 22 | AA | 466 | A | N1-C6-N6 | -9.33 | 113.00 | 118.60 |
| 24 | A3 | 74 | A | N1-C6-N6 | -9.33 | 113.00 | 118.60 |
| 57 | BA | 2566 | A | N1-C6-N6 | -9.33 | 113.00 | 118.60 |
| 22 | AA | 520 | A | N1-C6-N6 | -9.32 | 113.00 | 118.60 |
| 22 | AA | 1492 | A | N1-C6-N6 | -9.32 | 113.01 | 118.60 |
| 57 | BA | 527 | C | O4'-C1'-N1 | 9.32 | 115.66 | 108.20 |
| 57 | BA | 1762 | A | N1-C6-N6 | -9.32 | 113.01 | 118.60 |
| 22 | AA | 344 | A | N1-C6-N6 | -9.32 | 113.01 | 118.60 |
| 57 | BA | 1308 | A | N1-C6-N6 | -9.32 | 113.01 | 118.60 |
| 22 | AA | 1151 | A | N1-C6-N6 | -9.31 | 113.01 | 118.60 |
| 57 | BA | 750 | A | N1-C6-N6 | -9.31 | 113.01 | 118.60 |
| 57 | BA | 2211 | A | N1-C6-N6 | -9.31 | 113.01 | 118.60 |
| 57 | BA | 503 | A | N1-C6-N6 | -9.31 | 113.01 | 118.60 |
| 57 | BA | 368 | A | N1-C6-N6 | -9.31 | 113.01 | 118.60 |
| 22 | AA | 181 | A | N1-C6-N6 | -9.31 | 113.02 | 118.60 |
| 22 | AA | 702 | A | N1-C6-N6 | -9.31 | 113.02 | 118.60 |
| 58 | Ba | 50 | A | N1-C6-N6 | -9.31 | 113.02 | 118.60 |
| 57 | BA | 866 | A | C5-C6-N1 | 9.31 | 122.35 | 117.70 |
| 57 | BA | 125 | A | N1-C6-N6 | -9.30 | 113.02 | 118.60 |
| 22 | AA | 3 | A | N1-C6-N6 | -9.30 | 113.02 | 118.60 |
| 22 | AA | 1446 | A | N1-C6-N6 | -9.30 | 113.02 | 118.60 |
| 57 | BA | 1020 | A | N1-C6-N6 | -9.30 | 113.02 | 118.60 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 2602 | A | N1-C6-N6 | -9.30 | 113.02 | 118.60 |
| 57 | BA | 2766 | A | C5-C6-N1 | 9.30 | 122.35 | 117.70 |
| 22 | AA | 1176 | A | N1-C6-N6 | -9.29 | 113.02 | 118.60 |
| 22 | AA | 493 | A | O4'-C1'-N9 | 9.29 | 115.64 | 108.20 |
| 22 | AA | 509 | A | N1-C6-N6 | -9.29 | 113.03 | 118.60 |
| 57 | BA | 2225 | A | C5-C6-N1 | 9.29 | 122.34 | 117.70 |
| 22 | AA | 715 | A | N1-C6-N6 | -9.29 | 113.03 | 118.60 |
| 57 | BA | 83 | A | N1-C6-N6 | -9.29 | 113.03 | 118.60 |
| 57 | BA | 320 | A | N1-C6-N6 | -9.28 | 113.03 | 118.60 |
| 22 | AA | 1019 | A | N1-C6-N6 | -9.28 | 113.03 | 118.60 |
| 57 | BA | 927 | A | N1-C6-N6 | -9.28 | 113.03 | 118.60 |
| 58 | Ba | 58 | A | N1-C6-N6 | -9.28 | 113.03 | 118.60 |
| 22 | AA | 1246 | A | N1-C6-N6 | -9.28 | 113.03 | 118.60 |
| 57 | BA | 980 | A | N1-C6-N6 | -9.28 | 113.03 | 118.60 |
| 57 | BA | 439 | A | N1-C6-N6 | -9.28 | 113.03 | 118.60 |
| 22 | AA | 1022 | A | N1-C6-N6 | -9.27 | 113.03 | 118.60 |
| 57 | BA | 2199 | A | N1-C6-N6 | -9.27 | 113.04 | 118.60 |
| 57 | BA | 432 | A | N1-C6-N6 | -9.27 | 113.04 | 118.60 |
| 57 | BA | 111 | A | N1-C6-N6 | -9.26 | 113.04 | 118.60 |
| 57 | BA | 1276 | A | N1-C6-N6 | -9.26 | 113.04 | 118.60 |
| 22 | AA | 456 | A | N1-C6-N6 | -9.26 | 113.04 | 118.60 |
| 22 | AA | 461 | A | N1-C6-N6 | -9.26 | 113.04 | 118.60 |
| 57 | BA | 614 | A | N1-C6-N6 | -9.26 | 113.04 | 118.60 |
| 57 | BA | 685 | A | C5-C6-N1 | 9.26 | 122.33 | 117.70 |
| 57 | BA | 692 | C | N3-C2-O2 | -9.26 | 115.42 | 121.90 |
| 57 | BA | 1420 | A | N1-C6-N6 | -9.26 | 113.04 | 118.60 |
| 57 | BA | 2873 | A | N1-C6-N6 | -9.26 | 113.05 | 118.60 |
| 22 | AA | 51 | A | N1-C6-N6 | -9.25 | 113.05 | 118.60 |
| 57 | BA | 1253 | A | N1-C6-N6 | -9.25 | 113.05 | 118.60 |
| 57 | BA | 1847 | A | N1-C6-N6 | -9.25 | 113.05 | 118.60 |
| 22 | AA | 1480 | A | N1-C6-N6 | -9.25 | 113.05 | 118.60 |
| 57 | BA | 1469 | A | N1-C6-N6 | -9.25 | 113.05 | 118.60 |
| 57 | BA | 1616 | A | N1-C6-N6 | -9.25 | 113.05 | 118.60 |
| 22 | AA | 119 | A | N1-C6-N6 | -9.24 | 113.06 | 118.60 |
| 57 | BA | 988 | A | N1-C6-N6 | -9.24 | 113.05 | 118.60 |
| 57 | BA | 1960 | A | N1-C6-N6 | -9.24 | 113.06 | 118.60 |
| 22 | AA | 845 | A | N1-C6-N6 | -9.24 | 113.06 | 118.60 |
| 22 | AA | 1093 | A | N1-C6-N6 | -9.24 | 113.06 | 118.60 |
| 57 | BA | 322 | A | N1-C6-N6 | -9.24 | 113.06 | 118.60 |
| 57 | BA | 2856 | A | N1-C6-N6 | -9.24 | 113.06 | 118.60 |
| 57 | BA | 2169 | A | N1-C6-N6 | -9.23 | 113.06 | 118.60 |
| 57 | BA | 2020 | 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($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 1359 | A | C5-C6-N1 | 9.23 | 122.31 | 117.70 |
| 57 | BA | 1890 | A | N1-C6-N6 | -9.23 | 113.06 | 118.60 |
| 22 | AA | 374 | A | C5-C6-N1 | 9.23 | 122.31 | 117.70 |
| 22 | AA | 397 | A | C5-C6-N1 | 9.23 | 122.31 | 117.70 |
| 57 | BA | 2887 | A | N1-C6-N6 | -9.23 | 113.06 | 118.60 |
| 57 | BA | 1927 | A | N1-C6-N6 | -9.23 | 113.06 | 118.60 |
| 22 | AA | 969 | A | N1-C6-N6 | -9.22 | 113.06 | 118.60 |
| 57 | BA | 2267 | A | N1-C6-N6 | -9.22 | 113.07 | 118.60 |
| 22 | AA | 197 | A | N1-C6-N6 | -9.22 | 113.07 | 118.60 |
| 57 | BA | 127 | A | N1-C6-N6 | -9.22 | 113.07 | 118.60 |
| 57 | BA | 344 | A | N1-C6-N6 | -9.22 | 113.07 | 118.60 |
| 57 | BA | 984 | A | N1-C6-N6 | -9.22 | 113.07 | 118.60 |
| 57 | BA | 1603 | A | N1-C6-N6 | -9.22 | 113.07 | 118.60 |
| 57 | BA | 2005 | A | N1-C6-N6 | -9.22 | 113.07 | 118.60 |
| 57 | BA | 2461 | A | N1-C6-N6 | -9.22 | 113.07 | 118.60 |
| 57 | BA | 2534 | A | N1-C6-N6 | -9.22 | 113.07 | 118.60 |
| 57 | BA | 204 | A | N1-C6-N6 | -9.22 | 113.07 | 118.60 |
| 22 | AA | 996 | A | N1-C6-N6 | -9.22 | 113.07 | 118.60 |
| 57 | BA | 914 | G | O4'-C1'-N9 | 9.21 | 115.57 | 108.20 |
| 57 | BA | 101 | A | N1-C6-N6 | -9.21 | 113.08 | 118.60 |
| 57 | BA | 1095 | A | O4'-C1'-N9 | 9.21 | 115.56 | 108.20 |
| 57 | BA | 1609 | A | N1-C6-N6 | -9.20 | 113.08 | 118.60 |
| 22 | AA | 26 | A | N1-C6-N6 | -9.20 | 113.08 | 118.60 |
| 57 | BA | 613 | A | N1-C6-N6 | -9.20 | 113.08 | 118.60 |
| 22 | AA | 1155 | A | N1-C6-N6 | -9.20 | 113.08 | 118.60 |
| 57 | BA | 14 | A | N1-C6-N6 | -9.19 | 113.08 | 118.60 |
| 57 | BA | 547 | A | N1-C6-N6 | -9.19 | 113.09 | 118.60 |
| 57 | BA | 443 | A | N1-C6-N6 | -9.19 | 113.09 | 118.60 |
| 57 | BA | 1241 | A | N1-C6-N6 | -9.19 | 113.09 | 118.60 |
| 57 | BA | 1815 | A | N1-C6-N6 | -9.18 | 113.09 | 118.60 |
| 57 | BA | 1446 | C | N3-C2-O2 | -9.18 | 115.48 | 121.90 |
| 57 | BA | 1080 | A | N1-C6-N6 | -9.17 | 113.10 | 118.60 |
| 57 | BA | 1134 | A | N1-C6-N6 | -9.17 | 113.10 | 118.60 |
| 57 | BA | 2670 | A | N1-C6-N6 | -9.17 | 113.10 | 118.60 |
| 57 | BA | 1244 | A | N1-C6-N6 | -9.17 | 113.10 | 118.60 |
| 57 | BA | 1365 | A | N1-C6-N6 | -9.17 | 113.10 | 118.60 |
| 22 | AA | 665 | A | C5-C6-N1 | 9.17 | 122.28 | 117.70 |
| 32 | BR | 86 | ARG | NE-CZ-NH1 | 9.16 | 124.88 | 120.30 |
| 22 | AA | 782 | A | N1-C6-N6 | -9.16 | 113.10 | 118.60 |
| 23 | A2 | 13 | A | N1-C6-N6 | -9.16 | 113.10 | 118.60 |
| 57 | BA | 1598 | A | N1-C6-N6 | -9.15 | 113.11 | 118.60 |
| 57 | BA | 1821 | A | N1-C6-N6 | -9.15 | 113.11 | 118.60 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 2176 | A | N1-C6-N6 | -9.15 | 113.11 | 118.60 |
| 57 | BA | 2424 | C | O4'-C1'-N1 | 9.15 | 115.52 | 108.20 |
| 22 | AA | 936 | C | N3-C2-O2 | -9.15 | 115.50 | 121.90 |
| 57 | BA | 866 | A | N1-C6-N6 | -9.15 | 113.11 | 118.60 |
| 57 | BA | 2426 | A | N1-C6-N6 | -9.15 | 113.11 | 118.60 |
| 57 | BA | 2825 | G | O4'-C1'-N9 | 9.15 | 115.52 | 108.20 |
| 57 | BA | 2513 | A | N1-C6-N6 | -9.14 | 113.11 | 118.60 |
| 57 | BA | 2829 | A | N1-C6-N6 | -9.14 | 113.11 | 118.60 |
| 57 | BA | 602 | A | N1-C6-N6 | -9.14 | 113.11 | 118.60 |
| 57 | BA | 384 | A | N1-C6-N6 | -9.14 | 113.12 | 118.60 |
| 57 | BA | 858 | G | O4'-C1'-N9 | 9.14 | 115.51 | 108.20 |
| 57 | BA | 2800 | A | N1-C6-N6 | -9.13 | 113.12 | 118.60 |
| 57 | BA | 2435 | A | N1-C6-N6 | -9.13 | 113.12 | 118.60 |
| 22 | AA | 7 | A | N1-C6-N6 | -9.13 | 113.12 | 118.60 |
| 22 | AA | 162 | A | N1-C6-N6 | -9.13 | 113.12 | 118.60 |
| 57 | BA | 1384 | A | N1-C6-N6 | -9.12 | 113.13 | 118.60 |
| 22 | AA | 8 | A | N1-C6-N6 | -9.12 | 113.13 | 118.60 |
| 22 | AA | 353 | A | O4'-C1'-N9 | 9.12 | 115.50 | 108.20 |
| 22 | AA | 767 | A | N1-C6-N6 | -9.12 | 113.13 | 118.60 |
| 57 | BA | 453 | A | N1-C6-N6 | -9.12 | 113.13 | 118.60 |
| 22 | AA | 1542 | A | N1-C6-N6 | -9.12 | 113.13 | 118.60 |
| 57 | BA | 2589 | A | N1-C6-N6 | -9.12 | 113.13 | 118.60 |
| 57 | BA | 1787 | A | N1-C6-N6 | -9.12 | 113.13 | 118.60 |
| 22 | AA | 1410 | A | N1-C6-N6 | -9.11 | 113.13 | 118.60 |
| 57 | BA | 1046 | A | N1-C6-N6 | -9.11 | 113.13 | 118.60 |
| 57 | BA | 2734 | A | N1-C6-N6 | -9.11 | 113.13 | 118.60 |
| 57 | BA | 2634 | A | N1-C6-N6 | -9.11 | 113.13 | 118.60 |
| 22 | AA | 270 | A | N1-C6-N6 | -9.11 | 113.14 | 118.60 |
| 22 | AA | 1188 | A | N1-C6-N6 | -9.11 | 113.14 | 118.60 |
| 57 | BA | 2314 | A | N1-C6-N6 | -9.11 | 113.13 | 118.60 |
| 57 | BA | 2660 | A | N1-C6-N6 | -9.11 | 113.13 | 118.60 |
| 57 | BA | 2886 | A | O4'-C1'-N9 | 9.11 | 115.49 | 108.20 |
| 57 | BA | 1535 | A | N1-C6-N6 | -9.10 | 113.14 | 118.60 |
| 22 | AA | 831 | A | N1-C6-N6 | -9.10 | 113.14 | 118.60 |
| 22 | AA | 968 | A | N1-C6-N6 | -9.10 | 113.14 | 118.60 |
| 57 | BA | 142 | A | N1-C6-N6 | -9.09 | 113.14 | 118.60 |
| 57 | BA | 1641 | A | N1-C6-N6 | -9.09 | 113.14 | 118.60 |
| 22 | AA | 2 | A | N1-C6-N6 | -9.09 | 113.15 | 118.60 |
| 22 | AA | 649 | A | N1-C6-N6 | -9.09 | 113.15 | 118.60 |
| 57 | BA | 2114 | A | N1-C6-N6 | -9.09 | 113.15 | 118.60 |
| 57 | BA | 2058 | A | N1-C6-N6 | -9.08 | 113.15 | 118.60 |
| 22 | AA | 415 | A | C5-C6-N1 | 9.08 | 122.24 | 117.70 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 58 | Ba | 29 | A | N1-C6-N6 | -9.08 | 113.15 | 118.60 |
| 57 | BA | 675 | A | N1-C6-N6 | -9.07 | 113.16 | 118.60 |
| 22 | AA | 1360 | A | C5-C6-N1 | 9.07 | 122.24 | 117.70 |
| 57 | BA | 2765 | A | N1-C6-N6 | -9.07 | 113.16 | 118.60 |
| 22 | AA | 422 | C | N1-C2-O2 | 9.07 | 124.34 | 118.90 |
| 57 | BA | 715 | A | N1-C6-N6 | -9.07 | 113.16 | 118.60 |
| 18 | AG | 3 | ARG | NE-CZ-NH1 | 9.07 | 124.83 | 120.30 |
| 22 | AA | 411 | A | C5-C6-N1 | 9.07 | 122.23 | 117.70 |
| 22 | AA | 1431 | A | N1-C6-N6 | -9.07 | 113.16 | 118.60 |
| 22 | AA | 1430 | A | N1-C6-N6 | -9.07 | 113.16 | 118.60 |
| 57 | BA | 918 | A | N1-C6-N6 | -9.06 | 113.16 | 118.60 |
| 57 | BA | 2748 | A | N1-C6-N6 | -9.06 | 113.16 | 118.60 |
| 22 | AA | 411 | A | N1-C6-N6 | -9.06 | 113.17 | 118.60 |
| 57 | BA | 802 | A | N1-C6-N6 | -9.06 | 113.17 | 118.60 |
| 22 | AA | 609 | A | N1-C6-N6 | -9.05 | 113.17 | 118.60 |
| 23 | A2 | 55 | A | N1-C6-N6 | -9.05 | 113.17 | 118.60 |
| 57 | BA | 2814 | A | N1-C6-N6 | -9.05 | 113.17 | 118.60 |
| 22 | AA | 600 | A | N1-C6-N6 | -9.05 | 113.17 | 118.60 |
| 57 | BA | 2441 | U | O4'-C1'-N1 | 9.05 | 115.44 | 108.20 |
| 57 | BA | 1717 | A | C5-C6-N1 | 9.05 | 122.22 | 117.70 |
| 22 | AA | 621 | A | N1-C6-N6 | -9.04 | 113.17 | 118.60 |
| 57 | BA | 2835 | A | N1-C6-N6 | -9.04 | 113.17 | 118.60 |
| 57 | BA | 401 | A | N1-C6-N6 | -9.04 | 113.17 | 118.60 |
| 57 | BA | 1785 | A | N1-C6-N6 | -9.04 | 113.17 | 118.60 |
| 57 | BA | 886 | A | N1-C6-N6 | -9.04 | 113.18 | 118.60 |
| 57 | BA | 1427 | A | C5-C6-N1 | 9.04 | 122.22 | 117.70 |
| 57 | BA | 1508 | A | N1-C6-N6 | -9.04 | 113.18 | 118.60 |
| 22 | AA | 363 | A | N1-C6-N6 | -9.03 | 113.18 | 118.60 |
| 22 | AA | 1000 | A | N1-C6-N6 | -9.04 | 113.18 | 118.60 |
| 57 | BA | 1744 | A | N1-C6-N6 | -9.03 | 113.18 | 118.60 |
| 22 | AA | 1398 | A | N1-C6-N6 | -9.03 | 113.18 | 118.60 |
| 57 | BA | 2055 | C | O4'-C1'-N1 | 9.03 | 115.43 | 108.20 |
| 57 | BA | 2406 | A | N1-C6-N6 | -9.03 | 113.18 | 118.60 |
| 57 | BA | 1502 | A | N1-C6-N6 | -9.03 | 113.18 | 118.60 |
| 57 | BA | 2590 | A | N1-C6-N6 | -9.03 | 113.18 | 118.60 |
| 22 | AA | 1130 | A | C5-C6-N1 | 9.03 | 122.21 | 117.70 |
| 57 | BA | 1545 | A | N1-C6-N6 | -9.03 | 113.18 | 118.60 |
| 29 | BO | 30 | ARG | NE-CZ-NH1 | 9.02 | 124.81 | 120.30 |
| 57 | BA | 1275 | A | C5-C6-N1 | 9.02 | 122.21 | 117.70 |
| 22 | AA | 860 | A | N1-C6-N6 | -9.02 | 113.19 | 118.60 |
| 24 | A3 | 60 | A | N1-C6-N6 | -9.02 | 113.19 | 118.60 |
| 33 | BS | 9 | ARG | NE-CZ-NH1 | 9.02 | 124.81 | 120.30 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 58 | Ba | 52 | A | N1-C6-N6 | -9.02 | 113.19 | 118.60 |
| 58 | Ba | 78 | A | C5-C6-N1 | 9.02 | 122.21 | 117.70 |
| 35 | BD | 211 | ARG | NE-CZ-NH1 | 9.02 | 124.81 | 120.30 |
| 57 | BA | 2407 | A | N1-C6-N6 | -9.01 | 113.19 | 118.60 |
| 22 | AA | 1256 | A | N1-C6-N6 | -9.01 | 113.19 | 118.60 |
| 57 | BA | 1889 | A | N1-C6-N6 | -9.01 | 113.19 | 118.60 |
| 57 | BA | 2003 | A | N1-C6-N6 | -9.01 | 113.20 | 118.60 |
| 57 | BA | 892 | A | N1-C6-N6 | -9.00 | 113.20 | 118.60 |
| 22 | AA | 1434 | A | N1-C6-N6 | -9.00 | 113.20 | 118.60 |
| 57 | BA | 789 | A | C5-C6-N1 | 9.00 | 122.20 | 117.70 |
| 57 | BA | 2657 | A | N1-C6-N6 | -9.00 | 113.20 | 118.60 |
| 22 | AA | 85 | U | O4'-C1'-N1 | 8.99 | 115.39 | 108.20 |
| 34 | BT | 52 | ARG | NE-CZ-NH1 | 8.99 | 124.80 | 120.30 |
| 57 | BA | 1089 | A | N1-C6-N6 | -8.99 | 113.20 | 118.60 |
| 57 | BA | 1393 | A | N1-C6-N6 | -8.99 | 113.20 | 118.60 |
| 57 | BA | 2468 | A | N1-C6-N6 | -8.99 | 113.20 | 118.60 |
| 57 | BA | 1928 | A | N1-C6-N6 | -8.99 | 113.21 | 118.60 |
| 22 | AA | 382 | A | N1-C6-N6 | -8.99 | 113.21 | 118.60 |
| 57 | BA | 514 | A | N1-C6-N6 | -8.98 | 113.21 | 118.60 |
| 57 | BA | 1213 | A | N1-C6-N6 | -8.98 | 113.21 | 118.60 |
| 57 | BA | 2117 | A | N1-C6-N6 | -8.98 | 113.21 | 118.60 |
| 57 | BA | 2749 | A | N1-C6-N6 | -8.98 | 113.21 | 118.60 |
| 57 | BA | 472 | A | N1-C6-N6 | -8.98 | 113.21 | 118.60 |
| 57 | BA | 2761 | A | N1-C6-N6 | -8.98 | 113.21 | 118.60 |
| 22 | AA | 130 | A | C5-C6-N1 | 8.98 | 122.19 | 117.70 |
| 22 | AA | 374 | A | N1-C6-N6 | -8.98 | 113.21 | 118.60 |
| 57 | BA | 2598 | A | N1-C6-N6 | -8.98 | 113.21 | 118.60 |
| 57 | BA | 278 | A | C5-C6-N1 | 8.97 | 122.19 | 117.70 |
| 57 | BA | 2090 | A | N1-C6-N6 | -8.97 | 113.22 | 118.60 |
| 22 | AA | 899 | C | N1-C2-O2 | 8.97 | 124.28 | 118.90 |
| 57 | BA | 345 | A | N1-C6-N6 | -8.97 | 113.22 | 118.60 |
| 57 | BA | 782 | A | N1-C6-N6 | -8.97 | 113.22 | 118.60 |
| 57 | BA | 2727 | A | N1-C6-N6 | -8.97 | 113.22 | 118.60 |
| 22 | AA | 279 | A | N1-C6-N6 | -8.97 | 113.22 | 118.60 |
| 32 | BR | 63 | ARG | NE-CZ-NH1 | 8.96 | 124.78 | 120.30 |
| 57 | BA | 1393 | A | C5-C6-N1 | 8.96 | 122.18 | 117.70 |
| 57 | BA | 2173 | A | N1-C6-N6 | -8.96 | 113.22 | 118.60 |
| 57 | BA | 89 | A | N1-C6-N6 | -8.96 | 113.22 | 118.60 |
| 57 | BA | 244 | A | N1-C6-N6 | -8.96 | 113.23 | 118.60 |
| 22 | AA | 131 | A | N1-C6-N6 | -8.96 | 113.23 | 118.60 |
| 57 | BA | 497 | A | N1-C6-N6 | -8.95 | 113.23 | 118.60 |
| 22 | AA | 179 | A | N1-C6-N6 | -8.95 | 113.23 | 118.60 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | AA | 602 | A | N1-C6-N6 | -8.95 | 113.23 | 118.60 |
| 57 | BA | 332 | A | N1-C6-N6 | -8.95 | 113.23 | 118.60 |
| 57 | BA | 1392 | A | N1-C6-N6 | -8.95 | 113.23 | 118.60 |
| 35 | BD | 269 | ARG | NE-CZ-NH1 | 8.94 | 124.77 | 120.30 |
| 57 | BA | 2635 | A | N1-C6-N6 | -8.95 | 113.23 | 118.60 |
| 57 | BA | 362 | A | N1-C6-N6 | -8.94 | 113.23 | 118.60 |
| 57 | BA | 1342 | A | N1-C6-N6 | -8.94 | 113.23 | 118.60 |
| 22 | AA | 243 | A | N1-C6-N6 | -8.94 | 113.23 | 118.60 |
| 57 | BA | 1668 | A | N1-C6-N6 | -8.94 | 113.23 | 118.60 |
| 22 | AA | 964 | A | N1-C6-N6 | -8.94 | 113.24 | 118.60 |
| 57 | BA | 1953 | A | N1-C6-N6 | -8.94 | 113.24 | 118.60 |
| 23 | A2 | 27 | A | N1-C6-N6 | -8.93 | 113.24 | 118.60 |
| 57 | BA | 1759 | A | N1-C6-N6 | -8.93 | 113.24 | 118.60 |
| 57 | BA | 972 | A | N1-C6-N6 | -8.93 | 113.24 | 118.60 |
| 57 | BA | 2135 | A | N1-C6-N6 | -8.93 | 113.24 | 118.60 |
| 18 | AG | 91 | ARG | NE-CZ-NH1 | 8.93 | 124.77 | 120.30 |
| 22 | AA | 964 | A | C5-C6-N1 | 8.93 | 122.16 | 117.70 |
| 24 | A3 | 16 | C | N3-C2-O2 | -8.93 | 115.65 | 121.90 |
| 57 | BA | 1854 | A | N1-C6-N6 | -8.93 | 113.24 | 118.60 |
| 22 | AA | 1152 | A | N1-C6-N6 | -8.93 | 113.24 | 118.60 |
| 57 | BA | 821 | A | N1-C6-N6 | -8.93 | 113.25 | 118.60 |
| 22 | AA | 974 | A | N1-C6-N6 | -8.92 | 113.25 | 118.60 |
| 57 | BA | 1757 | A | N1-C6-N6 | -8.92 | 113.25 | 118.60 |
| 22 | AA | 1163 | A | N1-C6-N6 | -8.92 | 113.25 | 118.60 |
| 22 | AA | 983 | A | C5-C6-N1 | 8.92 | 122.16 | 117.70 |
| 57 | BA | 310 | A | N1-C6-N6 | -8.92 | 113.25 | 118.60 |
| 57 | BA | 2059 | A | C5-C6-N1 | 8.92 | 122.16 | 117.70 |
| 46 | B3 | 44 | ARG | NE-CZ-NH2 | 8.91 | 124.76 | 120.30 |
| 57 | BA | 470 | A | N1-C6-N6 | -8.91 | 113.25 | 118.60 |
| 22 | AA | 704 | A | C5-C6-N1 | 8.91 | 122.16 | 117.70 |
| 57 | BA | 1008 | A | N1-C6-N6 | -8.91 | 113.25 | 118.60 |
| 57 | BA | 2868 | A | N1-C6-N6 | -8.91 | 113.26 | 118.60 |
| 57 | BA | 1287 | A | N1-C6-N6 | -8.90 | 113.26 | 118.60 |
| 57 | BA | 2317 | A | N1-C6-N6 | -8.90 | 113.26 | 118.60 |
| 57 | BA | 481 | G | O4'-C1'-N9 | 8.90 | 115.32 | 108.20 |
| 22 | AA | 468 | A | N1-C6-N6 | -8.90 | 113.26 | 118.60 |
| 58 | Ba | 109 | A | N1-C6-N6 | -8.90 | 113.26 | 118.60 |
| 22 | AA | 313 | A | N1-C6-N6 | -8.90 | 113.26 | 118.60 |
| 57 | BA | 1454 | C | O4'-C1'-N1 | 8.90 | 115.32 | 108.20 |
| 22 | AA | 120 | A | N1-C6-N6 | -8.90 | 113.26 | 118.60 |
| 57 | BA | 1086 | A | N1-C6-N6 | -8.90 | 113.26 | 118.60 |
| 45 | BE | 83 | ARG | NE-CZ-NH2 | 8.89 | 124.75 | 120.30 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | AA | 172 | A | N1-C6-N6 | -8.89 | 113.27 | 118.60 |
| 22 | AA | 495 | A | N1-C6-N6 | -8.89 | 113.27 | 118.60 |
| 22 | AA | 397 | A | N1-C6-N6 | -8.88 | 113.27 | 118.60 |
| 57 | BA | 2097 | A | N1-C6-N6 | -8.88 | 113.27 | 118.60 |
| 57 | BA | 2850 | A | N1-C6-N6 | -8.89 | 113.27 | 118.60 |
| 58 | Ba | 99 | A | N1-C6-N6 | -8.88 | 113.27 | 118.60 |
| 22 | AA | 673 | A | N1-C6-N6 | -8.88 | 113.27 | 118.60 |
| 57 | BA | 323 | C | N3-C2-O2 | -8.88 | 115.68 | 121.90 |
| 57 | BA | 626 | A | N1-C6-N6 | -8.88 | 113.27 | 118.60 |
| 57 | BA | 676 | A | N1-C6-N6 | -8.88 | 113.27 | 118.60 |
| 57 | BA | 1366 | A | N1-C6-N6 | -8.88 | 113.27 | 118.60 |
| 57 | BA | 1966 | A | N1-C6-N6 | -8.88 | 113.27 | 118.60 |
| 23 | A2 | 59 | A | O4'-C1'-N9 | 8.88 | 115.30 | 108.20 |
| 24 | A3 | 73 | A | N1-C6-N6 | -8.88 | 113.27 | 118.60 |
| 57 | BA | 2147 | A | O4'-C1'-N9 | 8.88 | 115.30 | 108.20 |
| 22 | AA | 1055 | A | N1-C6-N6 | -8.88 | 113.28 | 118.60 |
| 4 | AM | 78 | ARG | NE-CZ-NH1 | 8.87 | 124.74 | 120.30 |
| 22 | AA | 648 | A | N1-C6-N6 | -8.87 | 113.28 | 118.60 |
| 22 | AA | 59 | A | N1-C6-N6 | -8.87 | 113.28 | 118.60 |
| 57 | BA | 104 | A | N1-C6-N6 | -8.86 | 113.28 | 118.60 |
| 22 | AA | 1171 | A | N1-C6-N6 | -8.86 | 113.28 | 118.60 |
| 54 | BG | 149 | ARG | NE-CZ-NH1 | 8.86 | 124.73 | 120.30 |
| 22 | AA | 560 | A | N1-C6-N6 | -8.86 | 113.28 | 118.60 |
| 57 | BA | 739 | A | N1-C6-N6 | -8.86 | 113.28 | 118.60 |
| 57 | BA | 1912 | A | N1-C6-N6 | -8.86 | 113.28 | 118.60 |
| 57 | BA | 2336 | A | N1-C6-N6 | -8.85 | 113.29 | 118.60 |
| 58 | Ba | 39 | A | N1-C6-N6 | -8.85 | 113.29 | 118.60 |
| 58 | Ba | 88 | C | O4'-C1'-N1 | 8.85 | 115.28 | 108.20 |
| 22 | AA | 1250 | A | N1-C6-N6 | -8.85 | 113.29 | 118.60 |
| 57 | BA | 233 | A | C5-C6-N1 | 8.85 | 122.12 | 117.70 |
| 58 | Ba | 45 | A | N1-C6-N6 | -8.85 | 113.29 | 118.60 |
| 22 | AA | 182 | A | N1-C6-N6 | -8.85 | 113.29 | 118.60 |
| 57 | BA | 527 | C | N3-C2-O2 | -8.85 | 115.71 | 121.90 |
| 57 | BA | 2019 | A | N1-C6-N6 | -8.85 | 113.29 | 118.60 |
| 22 | AA | 238 | A | N1-C6-N6 | -8.84 | 113.30 | 118.60 |
| 54 | BG | 166 | ARG | NE-CZ-NH1 | 8.84 | 124.72 | 120.30 |
| 57 | BA | 2060 | A | N1-C6-N6 | -8.84 | 113.30 | 118.60 |
| 22 | AA | 263 | A | N1-C6-N6 | -8.83 | 113.30 | 118.60 |
| 22 | AA | 1080 | A | N1-C6-N6 | -8.83 | 113.30 | 118.60 |
| 22 | AA | 1158 | C | N3-C2-O2 | -8.83 | 115.72 | 121.90 |
| 57 | BA | 2322 | A | N1-C6-N6 | -8.83 | 113.30 | 118.60 |
| 57 | BA | 2706 | A | N1-C6-N6 | -8.83 | 113.30 | 118.60 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 1165 | A | N1-C6-N6 | -8.83 | 113.30 | 118.60 |
| 57 | BA | 2313 | C | N3-C2-O2 | -8.83 | 115.72 | 121.90 |
| 50 | B7 | 34 | ARG | NE-CZ-NH1 | 8.83 | 124.71 | 120.30 |
| 57 | BA | 1626 | A | N1-C6-N6 | -8.83 | 113.31 | 118.60 |
| 22 | AA | 58 | C | N3-C2-O2 | -8.82 | 115.72 | 121.90 |
| 57 | BA | 447 | A | N1-C6-N6 | -8.82 | 113.31 | 118.60 |
| 57 | BA | 1253 | A | C5-C6-N1 | 8.82 | 122.11 | 117.70 |
| 57 | BA | 1700 | A | N1-C6-N6 | -8.82 | 113.31 | 118.60 |
| 57 | BA | 2765 | A | C5-C6-N1 | 8.82 | 122.11 | 117.70 |
| 22 | AA | 1322 | C | N3-C2-O2 | -8.81 | 115.73 | 121.90 |
| 23 | A2 | 45 | G | O4'-C1'-N9 | 8.81 | 115.25 | 108.20 |
| 33 | BS | 10 | ARG | NE-CZ-NH1 | 8.81 | 124.71 | 120.30 |
| 35 | BD | 86 | ARG | NE-CZ-NH1 | 8.81 | 124.70 | 120.30 |
| 57 | BA | 1230 | A | N1-C6-N6 | -8.81 | 113.31 | 118.60 |
| 57 | BA | 1773 | A | N1-C6-N6 | -8.81 | 113.31 | 118.60 |
| 22 | AA | 152 | A | C5-C6-N1 | 8.81 | 122.10 | 117.70 |
| 22 | AA | 298 | A | N1-C6-N6 | -8.80 | 113.32 | 118.60 |
| 22 | AA | 1374 | A | N1-C6-N6 | -8.80 | 113.32 | 118.60 |
| 57 | BA | 1057 | A | N1-C6-N6 | -8.80 | 113.32 | 118.60 |
| 22 | AA | 250 | A | N1-C6-N6 | -8.80 | 113.32 | 118.60 |
| 57 | BA | 515 | A | C5-C6-N1 | 8.80 | 122.10 | 117.70 |
| 57 | BA | 1084 | A | C5-C6-N1 | 8.80 | 122.10 | 117.70 |
| 57 | BA | 2076 | U | O4'-C1'-N1 | 8.80 | 115.24 | 108.20 |
| 57 | BA | 670 | A | N1-C6-N6 | -8.80 | 113.32 | 118.60 |
| 57 | BA | 1987 | A | N1-C6-N6 | -8.80 | 113.32 | 118.60 |
| 21 | A1 | 463 | ARG | NE-CZ-NH1 | 8.79 | 124.70 | 120.30 |
| 22 | AA | 81 | A | N1-C6-N6 | -8.79 | 113.33 | 118.60 |
| 22 | AA | 1279 | G | O4'-C1'-N9 | 8.79 | 115.23 | 108.20 |
| 57 | BA | 146 | A | N1-C6-N6 | -8.79 | 113.33 | 118.60 |
| 57 | BA | 936 | A | N1-C6-N6 | -8.78 | 113.33 | 118.60 |
| 57 | BA | 2432 | A | O4'-C1'-N9 | 8.78 | 115.22 | 108.20 |
| 22 | AA | 794 | A | N1-C6-N6 | -8.78 | 113.33 | 118.60 |
| 57 | BA | 2358 | A | N1-C6-N6 | -8.78 | 113.33 | 118.60 |
| 24 | A3 | 58 | A | N1-C6-N6 | -8.78 | 113.33 | 118.60 |
| 57 | BA | 2183 | A | N1-C6-N6 | -8.78 | 113.33 | 118.60 |
| 22 | AA | 814 | A | C5-C6-N1 | 8.77 | 122.09 | 117.70 |
| 57 | BA | 1246 | A | N1-C6-N6 | -8.77 | 113.34 | 118.60 |
| 57 | BA | 1548 | A | N1-C6-N6 | -8.77 | 113.34 | 118.60 |
| 22 | AA | 759 | A | N1-C6-N6 | -8.77 | 113.34 | 118.60 |
| 22 | AA | 366 | A | N1-C6-N6 | -8.77 | 113.34 | 118.60 |
| 57 | BA | 2741 | A | N1-C6-N6 | -8.76 | 113.34 | 118.60 |
| 23 | A2 | 18 | A | N1-C6-N6 | -8.76 | 113.34 | 118.60 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|---|---|---|---|---|---|---|---|
| 22 | AA | 215 | C | N3-C2-O2 | -8.76 | 115.77 | 121.90 |
| 22 | AA | 693 | G | O4'-C1'-N9 | 8.76 | 115.21 | 108.20 |
| 57 | BA | 1808 | A | N1-C6-N6 | -8.76 | 113.34 | 118.60 |
| 4 | AM | 69 | ARG | NE-CZ-NH1 | 8.76 | 124.68 | 120.30 |
| 23 | A2 | 29 | G | O4'-C1'-N9 | 8.75 | 115.20 | 108.20 |
| 57 | BA | 1086 | A | C5-C6-N1 | 8.74 | 122.07 | 117.70 |
| 57 | BA | 2518 | A | N1-C6-N6 | -8.74 | 113.36 | 118.60 |
| 22 | AA | 510 | A | N1-C6-N6 | -8.74 | 113.36 | 118.60 |
| 22 | AA | 1005 | A | N1-C6-N6 | -8.74 | 113.36 | 118.60 |
| 22 | AA | 1146 | A | N1-C6-N6 | -8.74 | 113.36 | 118.60 |
| 22 | AA | 574 | A | N1-C6-N6 | -8.73 | 113.36 | 118.60 |
| 57 | BA | 586 | A | N1-C6-N6 | -8.73 | 113.36 | 118.60 |
| 57 | BA | 1676 | A | C5-C6-N1 | 8.73 | 122.06 | 117.70 |
| 22 | AA | 65 | A | N1-C6-N6 | -8.72 | 113.37 | 118.60 |
| 22 | AA | 1408 | A | N1-C6-N6 | -8.72 | 113.36 | 118.60 |
| 22 | AA | 1429 | A | N1-C6-N6 | -8.72 | 113.36 | 118.60 |
| 57 | BA | 1413 | A | N1-C6-N6 | -8.72 | 113.37 | 118.60 |
| 57 | BA | 582 | A | C5-C6-N1 | 8.72 | 122.06 | 117.70 |
| 57 | BA | 1630 | A | N1-C6-N6 | -8.72 | 113.37 | 118.60 |
| 57 | BA | 1504 | A | N1-C6-N6 | -8.72 | 113.37 | 118.60 |
| 57 | BA | 1522 | A | N1-C6-N6 | -8.72 | 113.37 | 118.60 |
| 57 | BA | 2328 | A | N1-C6-N6 | -8.71 | 113.37 | 118.60 |
| 57 | BA | 2721 | A | C5-C6-N1 | 8.71 | 122.06 | 117.70 |
| 57 | BA | 1936 | A | N1-C6-N6 | -8.71 | 113.37 | 118.60 |
| 57 | BA | 2700 | A | N1-C6-N6 | -8.71 | 113.37 | 118.60 |
| 57 | BA | 750 | A | C5-C6-N1 | 8.71 | 122.06 | 117.70 |
| 57 | BA | 1525 | A | N1-C6-N6 | -8.71 | 113.38 | 118.60 |
| 45 | BE | 128 | ARG | NE-CZ-NH1 | 8.70 | 124.65 | 120.30 |
| 57 | BA | 2170 | A | N1-C6-N6 | -8.70 | 113.38 | 118.60 |
| 17 | AF | 91 | ARG | NE-CZ-NH1 | 8.70 | 124.65 | 120.30 |
| 22 | AA | 535 | A | N1-C6-N6 | -8.70 | 113.38 | 118.60 |
| 57 | BA | 981 | A | C5-C6-N1 | 8.70 | 122.05 | 117.70 |
| 57 | BA | 1385 | A | N1-C6-N6 | -8.70 | 113.38 | 118.60 |
| 57 | BA | 1677 | A | N1-C6-N6 | -8.70 | 113.38 | 118.60 |
| 22 | AA | 78 | A | N1-C6-N6 | -8.70 | 113.38 | 118.60 |
| 57 | BA | 637 | A | N1-C6-N6 | -8.70 | 113.38 | 118.60 |
| 18 | AG | 110 | ARG | NE-CZ-NH1 | 8.69 | 124.65 | 120.30 |
| 22 | AA | 1014 | A | C5-C6-N1 | 8.69 | 122.05 | 117.70 |
| 57 | BA | 516 | C | N3-C2-O2 | -8.69 | 115.81 | 121.90 |
| 57 | BA | 621 | A | N1-C6-N6 | -8.69 | 113.39 | 118.60 |
| 57 | BA | 2014 | A | N1-C6-N6 | -8.69 | 113.39 | 118.60 |
| 22 | AA | 228 | A | N1-C6-N6 | -8.69 | 113.39 | 118.60 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 1347 | A | C5-C6-N1 | 8.69 | 122.04 | 117.70 |
| 22 | AA | 371 | A | N1-C6-N6 | -8.69 | 113.39 | 118.60 |
| 22 | AA | 432 | A | N1-C6-N6 | -8.68 | 113.39 | 118.60 |
| 57 | BA | 507 | A | N1-C6-N6 | -8.68 | 113.39 | 118.60 |
| 22 | AA | 1363 | A | C5-C6-N1 | 8.68 | 122.04 | 117.70 |
| 57 | BA | 52 | A | N1-C6-N6 | -8.68 | 113.39 | 118.60 |
| 57 | BA | 1419 | A | C5-C6-N1 | 8.68 | 122.04 | 117.70 |
| 57 | BA | 1070 | A | N1-C6-N6 | -8.68 | 113.39 | 118.60 |
| 57 | BA | 2288 | A | N1-C6-N6 | -8.68 | 113.39 | 118.60 |
| 57 | BA | 2450 | A | C5-C6-N1 | 8.68 | 122.04 | 117.70 |
| 57 | BA | 2432 | A | C5-C6-N1 | 8.68 | 122.04 | 117.70 |
| 57 | BA | 63 | A | N1-C6-N6 | -8.67 | 113.40 | 118.60 |
| 57 | BA | 2342 | C | N3-C2-O2 | -8.67 | 115.83 | 121.90 |
| 22 | AA | 223 | A | N1-C6-N6 | -8.67 | 113.40 | 118.60 |
| 22 | AA | 246 | A | N1-C6-N6 | -8.67 | 113.40 | 118.60 |
| 22 | AA | 1238 | A | C5-C6-N1 | 8.67 | 122.03 | 117.70 |
| 24 | A3 | 36 | A | N1-C6-N6 | -8.67 | 113.40 | 118.60 |
| 57 | BA | 1583 | A | N1-C6-N6 | -8.67 | 113.40 | 118.60 |
| 20 | AI | 123 | ARG | NE-CZ-NH1 | 8.67 | 124.63 | 120.30 |
| 24 | A3 | 59 | A | N1-C6-N6 | -8.67 | 113.40 | 118.60 |
| 57 | BA | 53 | A | N1-C6-N6 | -8.67 | 113.40 | 118.60 |
| 57 | BA | 2070 | A | N1-C6-N6 | -8.67 | 113.40 | 118.60 |
| 57 | BA | 1012 | U | O4'-C1'-N1 | 8.66 | 115.13 | 108.20 |
| 57 | BA | 899 | A | N1-C6-N6 | -8.66 | 113.40 | 118.60 |
| 57 | BA | 911 | A | C5-C6-N1 | 8.66 | 122.03 | 117.70 |
| 57 | BA | 1275 | A | O4'-C1'-N9 | 8.66 | 115.13 | 108.20 |
| 57 | BA | 2101 | A | N1-C6-N6 | -8.66 | 113.40 | 118.60 |
| 22 | AA | 934 | C | N3-C2-O2 | -8.66 | 115.84 | 121.90 |
| 57 | BA | 574 | A | N1-C6-N6 | -8.66 | 113.41 | 118.60 |
| 57 | BA | 2632 | A | N1-C6-N6 | -8.65 | 113.41 | 118.60 |
| 57 | BA | 2835 | A | C5-C6-N1 | 8.65 | 122.03 | 117.70 |
| 57 | BA | 352 | A | N1-C6-N6 | -8.65 | 113.41 | 118.60 |
| 15 | AD | 183 | ARG | NE-CZ-NH1 | 8.65 | 124.62 | 120.30 |
| 57 | BA | 2095 | A | N1-C6-N6 | -8.65 | 113.41 | 118.60 |
| 57 | BA | 160 | A | N1-C6-N6 | -8.64 | 113.41 | 118.60 |
| 22 | AA | 349 | A | N1-C6-N6 | -8.64 | 113.41 | 118.60 |
| 22 | AA | 1157 | A | C5-C6-N1 | 8.64 | 122.02 | 117.70 |
| 57 | BA | 980 | A | C5-C6-N1 | 8.64 | 122.02 | 117.70 |
| 22 | AA | 461 | A | C5-C6-N1 | 8.63 | 122.02 | 117.70 |
| 22 | AA | 1275 | A | N1-C6-N6 | -8.63 | 113.42 | 118.60 |
| 57 | BA | 38 | A | C5-C6-N1 | 8.63 | 122.02 | 117.70 |
| 22 | AA | 1252 | A | N1-C6-N6 | -8.63 | 113.42 | 118.60 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 182 | A | N1-C6-N6 | -8.62 | 113.42 | 118.60 |
| 57 | BA | 2614 | A | C5-C6-N1 | 8.63 | 122.01 | 117.70 |
| 22 | AA | 872 | A | C5-C6-N1 | 8.62 | 122.01 | 117.70 |
| 57 | BA | 1871 | A | N1-C6-N6 | -8.62 | 113.43 | 118.60 |
| 57 | BA | 2797 | U | O4'-C1'-N1 | 8.62 | 115.10 | 108.20 |
| 14 | AC | 231 | ARG | NE-CZ-NH2 | 8.62 | 124.61 | 120.30 |
| 57 | BA | 1268 | A | N1-C6-N6 | -8.62 | 113.43 | 118.60 |
| 57 | BA | 1322 | A | N1-C6-N6 | -8.62 | 113.43 | 118.60 |
| 22 | AA | 189 | A | N1-C6-N6 | -8.62 | 113.43 | 118.60 |
| 57 | BA | 222 | A | N1-C6-N6 | -8.62 | 113.43 | 118.60 |
| 57 | BA | 635 | C | N3-C2-O2 | -8.62 | 115.87 | 121.90 |
| 57 | BA | 1805 | A | N1-C6-N6 | -8.62 | 113.43 | 118.60 |
| 57 | BA | 2008 | C | N3-C2-O2 | -8.61 | 115.87 | 121.90 |
| 57 | BA | 2247 | A | N1-C6-N6 | -8.61 | 113.43 | 118.60 |
| 22 | AA | 1287 | A | N1-C6-N6 | -8.61 | 113.43 | 118.60 |
| 57 | BA | 1678 | A | N1-C6-N6 | -8.61 | 113.43 | 118.60 |
| 57 | BA | 1938 | A | N1-C6-N6 | -8.61 | 113.43 | 118.60 |
| 24 | A3 | 14 | A | N1-C6-N6 | -8.61 | 113.44 | 118.60 |
| 48 | B5 | 49 | ARG | NE-CZ-NH1 | 8.61 | 124.60 | 120.30 |
| 57 | BA | 226 | A | N1-C6-N6 | -8.61 | 113.44 | 118.60 |
| 22 | AA | 1046 | A | N1-C6-N6 | -8.61 | 113.44 | 118.60 |
| 22 | AA | 1167 | A | N1-C6-N6 | -8.61 | 113.44 | 118.60 |
| 57 | BA | 1932 | A | C5-C6-N1 | 8.61 | 122.00 | 117.70 |
| 57 | BA | 1009 | A | N1-C6-N6 | -8.60 | 113.44 | 118.60 |
| 57 | BA | 1912 | A | C5-C6-N1 | 8.60 | 122.00 | 117.70 |
| 57 | BA | 2732 | G | O4'-C1'-N9 | 8.60 | 115.08 | 108.20 |
| 22 | AA | 315 | A | C5-C6-N1 | 8.60 | 122.00 | 117.70 |
| 30 | BP | 78 | ARG | NE-CZ-NH1 | 8.60 | 124.60 | 120.30 |
| 57 | BA | 765 | C | N3-C2-O2 | -8.60 | 115.88 | 121.90 |
| 57 | BA | 838 | C | N3-C2-O2 | -8.60 | 115.88 | 121.90 |
| 22 | AA | 499 | A | C5-C6-N1 | 8.60 | 122.00 | 117.70 |
| 57 | BA | 1040 | A | N1-C6-N6 | -8.60 | 113.44 | 118.60 |
| 57 | BA | 2560 | A | N1-C6-N6 | -8.60 | 113.44 | 118.60 |
| 57 | BA | 943 | A | N1-C6-N6 | -8.60 | 113.44 | 118.60 |
| 57 | BA | 794 | A | N1-C6-N6 | -8.59 | 113.44 | 118.60 |
| 57 | BA | 1268 | A | C5-C6-N1 | 8.59 | 122.00 | 117.70 |
| 22 | AA | 579 | A | N1-C6-N6 | -8.59 | 113.44 | 118.60 |
| 22 | AA | 1004 | A | N1-C6-N6 | -8.59 | 113.45 | 118.60 |
| 57 | BA | 947 | A | C5-C6-N1 | 8.59 | 122.00 | 117.70 |
| 57 | BA | 2758 | A | N1-C6-N6 | -8.59 | 113.45 | 118.60 |
| 3 | AL | 85 | ARG | NE-CZ-NH1 | 8.59 | 124.59 | 120.30 |
| 22 | AA | 1092 | A | N1-C6-N6 | -8.59 | 113.45 | 118.60 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 1786 | A | C5-C6-N1 | 8.59 | 121.99 | 117.70 |
| 57 | BA | 103 | A | N1-C6-N6 | -8.58 | 113.45 | 118.60 |
| 57 | BA | 1204 | A | C5-C6-N1 | 8.58 | 121.99 | 117.70 |
| 22 | AA | 77 | A | N1-C6-N6 | -8.58 | 113.45 | 118.60 |
| 57 | BA | 572 | A | C5-C6-N1 | 8.57 | 121.99 | 117.70 |
| 57 | BA | 13 | A | C5-C6-N1 | 8.57 | 121.99 | 117.70 |
| 22 | AA | 696 | A | N1-C6-N6 | -8.57 | 113.46 | 118.60 |
| 22 | AA | 1394 | A | N1-C6-N6 | -8.57 | 113.46 | 118.60 |
| 8 | AQ | 10 | ARG | NE-CZ-NH1 | 8.57 | 124.58 | 120.30 |
| 22 | AA | 530 | G | O4'-C1'-N9 | 8.57 | 115.05 | 108.20 |
| 57 | BA | 1496 | A | N1-C6-N6 | -8.56 | 113.46 | 118.60 |
| 22 | AA | 327 | A | N1-C6-N6 | -8.56 | 113.46 | 118.60 |
| 22 | AA | 1433 | A | C5-C6-N1 | 8.56 | 121.98 | 117.70 |
| 57 | BA | 1302 | A | C5-C6-N1 | 8.56 | 121.98 | 117.70 |
| 43 | B1 | 73 | ARG | NE-CZ-NH2 | 8.56 | 124.58 | 120.30 |
| 57 | BA | 73 | A | C5-C6-N1 | 8.56 | 121.98 | 117.70 |
| 57 | BA | 155 | A | N1-C6-N6 | -8.56 | 113.46 | 118.60 |
| 57 | BA | 265 | A | N1-C6-N6 | -8.56 | 113.46 | 118.60 |
| 22 | AA | 781 | A | C5-C6-N1 | 8.56 | 121.98 | 117.70 |
| 57 | BA | 199 | A | N1-C6-N6 | -8.56 | 113.46 | 118.60 |
| 57 | BA | 2071 | A | C5-C6-N1 | 8.56 | 121.98 | 117.70 |
| 57 | BA | 1544 | A | N1-C6-N6 | -8.55 | 113.47 | 118.60 |
| 57 | BA | 960 | A | N1-C6-N6 | -8.55 | 113.47 | 118.60 |
| 57 | BA | 1383 | A | N1-C6-N6 | -8.55 | 113.47 | 118.60 |
| 57 | BA | 1454 | C | N3-C2-O2 | -8.55 | 115.91 | 121.90 |
| 42 | B0 | 38 | ARG | NE-CZ-NH1 | 8.55 | 124.58 | 120.30 |
| 57 | BA | 844 | A | N1-C6-N6 | -8.55 | 113.47 | 118.60 |
| 57 | BA | 514 | A | C5-C6-N1 | 8.55 | 121.97 | 117.70 |
| 57 | BA | 751 | A | N1-C6-N6 | -8.55 | 113.47 | 118.60 |
| 57 | BA | 2882 | A | C5-C6-N1 | 8.55 | 121.97 | 117.70 |
| 57 | BA | 294 | A | C5-C6-N1 | 8.55 | 121.97 | 117.70 |
| 22 | AA | 630 | A | N1-C6-N6 | -8.54 | 113.47 | 118.60 |
| 22 | AA | 729 | A | N1-C6-N6 | -8.54 | 113.47 | 118.60 |
| 57 | BA | 2184 | A | N1-C6-N6 | -8.54 | 113.47 | 118.60 |
| 57 | BA | 2278 | A | C5-C6-N1 | 8.54 | 121.97 | 117.70 |
| 57 | BA | 2534 | A | C5-C6-N1 | 8.54 | 121.97 | 117.70 |
| 57 | BA | 2883 | A | N1-C6-N6 | -8.54 | 113.47 | 118.60 |
| 20 | AI | 32 | ARG | NE-CZ-NH1 | 8.54 | 124.57 | 120.30 |
| 57 | BA | 269 | C | O4'-C1'-N1 | 8.54 | 115.03 | 108.20 |
| 4 | AM | 91 | ARG | NE-CZ-NH1 | 8.54 | 124.57 | 120.30 |
| 10 | AS | 36 | ARG | NE-CZ-NH1 | 8.54 | 124.57 | 120.30 |
| 22 | AA | 282 | A | N1-C6-N6 | -8.54 | 113.48 | 118.60 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 1597 | A | N1-C6-N6 | -8.54 | 113.48 | 118.60 |
| 57 | BA | 2781 | A | C5-C6-N1 | 8.53 | 121.97 | 117.70 |
| 22 | AA | 1042 | A | N1-C6-N6 | -8.53 | 113.48 | 118.60 |
| 22 | AA | 583 | A | N1-C6-N6 | -8.53 | 113.48 | 118.60 |
| 57 | BA | 1665 | A | C5-C6-N1 | 8.53 | 121.96 | 117.70 |
| 57 | BA | 2639 | A | N1-C6-N6 | -8.53 | 113.48 | 118.60 |
| 22 | AA | 681 | A | N1-C6-N6 | -8.53 | 113.48 | 118.60 |
| 22 | AA | 747 | A | N1-C6-N6 | -8.52 | 113.49 | 118.60 |
| 57 | BA | 661 | A | C5-C6-N1 | 8.52 | 121.96 | 117.70 |
| 57 | BA | 1652 | A | N1-C6-N6 | -8.52 | 113.49 | 118.60 |
| 22 | AA | 695 | A | C5-C6-N1 | 8.52 | 121.96 | 117.70 |
| 57 | BA | 2266 | A | C5-C6-N1 | 8.52 | 121.96 | 117.70 |
| 57 | BA | 176 | A | N1-C6-N6 | -8.52 | 113.49 | 118.60 |
| 57 | BA | 1275 | A | N1-C6-N6 | -8.52 | 113.49 | 118.60 |
| 57 | BA | 1286 | A | N1-C6-N6 | -8.51 | 113.49 | 118.60 |
| 22 | AA | 211 | G | O4'-C1'-N9 | 8.51 | 115.01 | 108.20 |
| 22 | AA | 1299 | A | N1-C6-N6 | -8.51 | 113.50 | 118.60 |
| 57 | BA | 478 | A | N1-C6-N6 | -8.51 | 113.49 | 118.60 |
| 57 | BA | 1084 | A | N1-C6-N6 | -8.51 | 113.50 | 118.60 |
| 57 | BA | 2154 | A | N1-C6-N6 | -8.51 | 113.50 | 118.60 |
| 57 | BA | 2119 | A | N1-C6-N6 | -8.51 | 113.50 | 118.60 |
| 22 | AA | 1093 | A | C5-C6-N1 | 8.50 | 121.95 | 117.70 |
| 22 | AA | 28 | A | N1-C6-N6 | -8.50 | 113.50 | 118.60 |
| 57 | BA | 1434 | A | O4'-C1'-N9 | 8.50 | 115.00 | 108.20 |
| 22 | AA | 621 | A | C5-C6-N1 | 8.50 | 121.95 | 117.70 |
| 57 | BA | 1528 | A | N1-C6-N6 | -8.50 | 113.50 | 118.60 |
| 57 | BA | 1899 | A | N1-C6-N6 | -8.50 | 113.50 | 118.60 |
| 57 | BA | 2275 | C | O4'-C1'-N1 | 8.49 | 115.00 | 108.20 |
| 22 | AA | 1169 | A | N1-C6-N6 | -8.49 | 113.50 | 118.60 |
| 22 | AA | 1368 | A | N1-C6-N6 | -8.49 | 113.50 | 118.60 |
| 48 | B5 | 39 | ARG | NE-CZ-NH1 | 8.49 | 124.55 | 120.30 |
| 57 | BA | 423 | A | C5-C6-N1 | 8.49 | 121.95 | 117.70 |
| 18 | AG | 2 | ARG | NE-CZ-NH1 | 8.49 | 124.54 | 120.30 |
| 57 | BA | 119 | A | C5-C6-N1 | 8.49 | 121.94 | 117.70 |
| 22 | AA | 787 | A | N1-C6-N6 | -8.49 | 113.51 | 118.60 |
| 22 | AA | 572 | A | C5-C6-N1 | 8.48 | 121.94 | 117.70 |
| 57 | BA | 94 | A | N1-C6-N6 | -8.48 | 113.51 | 118.60 |
| 22 | AA | 109 | A | C5-C6-N1 | 8.48 | 121.94 | 117.70 |
| 57 | BA | 301 | G | O4'-C1'-N9 | 8.48 | 114.98 | 108.20 |
| 57 | BA | 1069 | A | N1-C6-N6 | -8.48 | 113.51 | 118.60 |
| 57 | BA | 131 | A | N1-C6-N6 | -8.48 | 113.51 | 118.60 |
| 57 | BA | 2738 | A | N1-C6-N6 | -8.48 | 113.51 | 118.60 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 2893 | A | N1-C6-N6 | -8.48 | 113.51 | 118.60 |
| 57 | BA | 655 | A | C5-C6-N1 | 8.47 | 121.94 | 117.70 |
| 22 | AA | 1456 | A | N1-C6-N6 | -8.47 | 113.52 | 118.60 |
| 57 | BA | 2810 | A | C5-C6-N1 | 8.47 | 121.94 | 117.70 |
| 22 | AA | 393 | A | N1-C6-N6 | -8.47 | 113.52 | 118.60 |
| 57 | BA | 906 | U | O4'-C1'-N1 | 8.47 | 114.98 | 108.20 |
| 22 | AA | 106 | C | N3-C2-O2 | -8.47 | 115.97 | 121.90 |
| 24 | A3 | 77 | A | N1-C6-N6 | -8.47 | 113.52 | 118.60 |
| 57 | BA | 221 | A | N1-C6-N6 | -8.47 | 113.52 | 118.60 |
| 57 | BA | 845 | A | N1-C6-N6 | -8.47 | 113.52 | 118.60 |
| 57 | BA | 1111 | A | N1-C6-N6 | -8.47 | 113.52 | 118.60 |
| 57 | BA | 2705 | A | N1-C6-N6 | -8.47 | 113.52 | 118.60 |
| 22 | AA | 1155 | A | C5-C6-N1 | 8.47 | 121.93 | 117.70 |
| 22 | AA | 914 | A | N1-C6-N6 | -8.46 | 113.52 | 118.60 |
| 22 | AA | 408 | A | N1-C6-N6 | -8.46 | 113.52 | 118.60 |
| 57 | BA | 1990 | C | N3-C2-O2 | -8.46 | 115.98 | 121.90 |
| 57 | BA | 2662 | A | C5-C6-N1 | 8.46 | 121.93 | 117.70 |
| 22 | AA | 687 | A | N1-C6-N6 | -8.46 | 113.53 | 118.60 |
| 53 | BF | 102 | ARG | NE-CZ-NH2 | 8.46 | 124.53 | 120.30 |
| 22 | AA | 303 | A | N1-C6-N6 | -8.46 | 113.53 | 118.60 |
| 57 | BA | 131 | A | C5-C6-N1 | 8.45 | 121.93 | 117.70 |
| 57 | BA | 2202 | U | O4'-C1'-N1 | 8.46 | 114.96 | 108.20 |
| 22 | AA | 501 | C | N3-C2-O2 | -8.45 | 115.98 | 121.90 |
| 22 | AA | 1014 | A | N1-C6-N6 | -8.45 | 113.53 | 118.60 |
| 57 | BA | 718 | A | C5-C6-N1 | 8.45 | 121.93 | 117.70 |
| 22 | AA | 873 | A | N1-C6-N6 | -8.45 | 113.53 | 118.60 |
| 22 | AA | 1441 | A | C5-C6-N1 | 8.45 | 121.92 | 117.70 |
| 22 | AA | 1167 | A | C5-C6-N1 | 8.44 | 121.92 | 117.70 |
| 57 | BA | 1367 | A | N1-C6-N6 | -8.44 | 113.53 | 118.60 |
| 57 | BA | 2542 | A | N1-C6-N6 | -8.44 | 113.53 | 118.60 |
| 57 | BA | 981 | A | N1-C6-N6 | -8.44 | 113.54 | 118.60 |
| 57 | BA | 1433 | A | C5-C6-N1 | 8.44 | 121.92 | 117.70 |
| 47 | B4 | 49 | ARG | NE-CZ-NH1 | 8.44 | 124.52 | 120.30 |
| 22 | AA | 728 | A | C5-C6-N1 | 8.44 | 121.92 | 117.70 |
| 22 | AA | 1150 | A | N1-C6-N6 | -8.44 | 113.54 | 118.60 |
| 57 | BA | 668 | A | C5-C6-N1 | 8.44 | 121.92 | 117.70 |
| 22 | AA | 1499 | A | C5-C6-N1 | 8.44 | 121.92 | 117.70 |
| 22 | AA | 814 | A | N1-C6-N6 | -8.43 | 113.54 | 118.60 |
| 22 | AA | 1197 | A | C5-C6-N1 | 8.43 | 121.92 | 117.70 |
| 57 | BA | 1783 | A | C5-C6-N1 | 8.43 | 121.92 | 117.70 |
| 57 | BA | 756 | A | N1-C6-N6 | -8.43 | 113.54 | 118.60 |
| 57 | BA | 2860 | A | N1-C6-N6 | -8.43 | 113.54 | 118.60 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | AA | 71 | A | C5-C6-N1 | 8.43 | 121.91 | 117.70 |
| 57 | BA | 152 | A | N1-C6-N6 | -8.43 | 113.54 | 118.60 |
| 57 | BA | 2281 | A | N1-C6-N6 | -8.42 | 113.55 | 118.60 |
| 57 | BA | 631 | A | C5-C6-N1 | 8.42 | 121.91 | 117.70 |
| 57 | BA | 490 | C | N3-C2-O2 | -8.42 | 116.01 | 121.90 |
| 57 | BA | 1635 | A | C5-C6-N1 | 8.42 | 121.91 | 117.70 |
| 4 | AM | 112 | ARG | NE-CZ-NH1 | 8.41 | 124.51 | 120.30 |
| 22 | AA | 553 | A | N1-C6-N6 | -8.41 | 113.55 | 118.60 |
| 22 | AA | 1050 | G | O4'-C1'-N9 | 8.41 | 114.93 | 108.20 |
| 57 | BA | 322 | A | C5-C6-N1 | 8.41 | 121.91 | 117.70 |
| 22 | AA | 328 | C | N3-C2-O2 | -8.41 | 116.01 | 121.90 |
| 22 | AA | 1333 | A | N1-C6-N6 | -8.41 | 113.56 | 118.60 |
| 22 | AA | 1035 | A | N1-C6-N6 | -8.41 | 113.56 | 118.60 |
| 57 | BA | 1551 | A | C5-C6-N1 | 8.40 | 121.90 | 117.70 |
| 57 | BA | 1800 | C | N3-C2-O2 | -8.40 | 116.02 | 121.90 |
| 57 | BA | 2054 | A | C4-C5-C6 | -8.40 | 112.80 | 117.00 |
| 24 | A3 | 38 | A | C5-C6-N1 | 8.40 | 121.90 | 117.70 |
| 57 | BA | 2297 | A | N1-C6-N6 | -8.40 | 113.56 | 118.60 |
| 57 | BA | 1070 | A | C5-C6-N1 | 8.40 | 121.90 | 117.70 |
| 57 | BA | 1213 | A | C5-C6-N1 | 8.40 | 121.90 | 117.70 |
| 22 | AA | 1201 | A | N1-C6-N6 | -8.40 | 113.56 | 118.60 |
| 57 | BA | 2381 | A | N1-C6-N6 | -8.40 | 113.56 | 118.60 |
| 58 | Ba | 108 | A | C5-C6-N1 | 8.40 | 121.90 | 117.70 |
| 57 | BA | 480 | A | N1-C6-N6 | -8.39 | 113.56 | 118.60 |
| 22 | AA | 532 | A | C5-C6-N1 | 8.39 | 121.90 | 117.70 |
| 22 | AA | 622 | A | C5-C6-N1 | 8.39 | 121.90 | 117.70 |
| 23 | A2 | 18 | A | C5-C6-N1 | 8.39 | 121.89 | 117.70 |
| 57 | BA | 279 | A | N1-C6-N6 | -8.39 | 113.56 | 118.60 |
| 57 | BA | 1847 | A | O4'-C1'-N9 | 8.39 | 114.91 | 108.20 |
| 57 | BA | 2412 | A | N1-C6-N6 | -8.39 | 113.56 | 118.60 |
| 22 | AA | 949 | A | N1-C6-N6 | -8.39 | 113.57 | 118.60 |
| 22 | AA | 234 | C | N3-C2-O2 | -8.38 | 116.03 | 121.90 |
| 57 | BA | 249 | C | N3-C2-O2 | -8.39 | 116.03 | 121.90 |
| 57 | BA | 743 | A | N1-C6-N6 | -8.38 | 113.57 | 118.60 |
| 57 | BA | 1129 | A | C5-C6-N1 | 8.38 | 121.89 | 117.70 |
| 57 | BA | 1689 | A | N1-C6-N6 | -8.38 | 113.57 | 118.60 |
| 57 | BA | 2158 | A | N1-C6-N6 | -8.38 | 113.57 | 118.60 |
| 22 | AA | 10 | A | N1-C6-N6 | -8.38 | 113.57 | 118.60 |
| 22 | AA | 327 | A | C5-C6-N1 | 8.38 | 121.89 | 117.70 |
| 57 | BA | 192 | C | O4'-C1'-N1 | 8.38 | 114.90 | 108.20 |
| 57 | BA | 222 | A | C5-C6-N1 | 8.38 | 121.89 | 117.70 |
| 57 | BA | 1439 | A | N1-C6-N6 | -8.38 | 113.57 | 118.60 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 2861 | U | O4'-C1'-N1 | 8.38 | 114.90 | 108.20 |
| 22 | AA | 1274 | A | N1-C6-N6 | -8.38 | 113.57 | 118.60 |
| 57 | BA | 457 | A | N1-C6-N6 | -8.38 | 113.58 | 118.60 |
| 57 | BA | 1156 | A | N1-C6-N6 | -8.38 | 113.58 | 118.60 |
| 57 | BA | 1515 | A | C5-C6-N1 | 8.37 | 121.89 | 117.70 |
| 22 | AA | 1196 | A | N1-C6-N6 | -8.37 | 113.58 | 118.60 |
| 57 | BA | 126 | A | C5-C6-N1 | 8.37 | 121.88 | 117.70 |
| 57 | BA | 1359 | A | N1-C6-N6 | -8.37 | 113.58 | 118.60 |
| 57 | BA | 1952 | A | C5-C6-N1 | 8.37 | 121.88 | 117.70 |
| 57 | BA | 2411 | A | C5-C6-N1 | 8.37 | 121.88 | 117.70 |
| 58 | Ba | 53 | A | C5-C6-N1 | 8.37 | 121.89 | 117.70 |
| 57 | BA | 330 | A | C5-C6-N1 | 8.37 | 121.88 | 117.70 |
| 57 | BA | 752 | A | O4'-C1'-N9 | 8.37 | 114.89 | 108.20 |
| 57 | BA | 2284 | A | C5-C6-N1 | 8.37 | 121.88 | 117.70 |
| 57 | BA | 2497 | A | N1-C6-N6 | -8.37 | 113.58 | 118.60 |
| 57 | BA | 2531 | A | C5-C6-N1 | 8.37 | 121.88 | 117.70 |
| 57 | BA | 21 | A | N1-C6-N6 | -8.36 | 113.58 | 118.60 |
| 57 | BA | 1260 | A | N1-C6-N6 | -8.36 | 113.58 | 118.60 |
| 57 | BA | 1676 | A | N1-C6-N6 | -8.36 | 113.58 | 118.60 |
| 57 | BA | 101 | A | C5-C6-N1 | 8.36 | 121.88 | 117.70 |
| 57 | BA | 925 | A | C5-C6-N1 | 8.36 | 121.88 | 117.70 |
| 57 | BA | 753 | A | N1-C6-N6 | -8.36 | 113.59 | 118.60 |
| 57 | BA | 1189 | A | N1-C6-N6 | -8.36 | 113.59 | 118.60 |
| 57 | BA | 1713 | A | N1-C6-N6 | -8.36 | 113.59 | 118.60 |
| 57 | BA | 1997 | C | O4'-C1'-N1 | 8.36 | 114.88 | 108.20 |
| 22 | AA | 1257 | A | O4'-C1'-N9 | 8.35 | 114.88 | 108.20 |
| 57 | BA | 342 | A | N1-C6-N6 | -8.35 | 113.59 | 118.60 |
| 22 | AA | 1339 | A | C5-C6-N1 | 8.35 | 121.88 | 117.70 |
| 22 | AA | 1396 | A | C5-C6-N1 | 8.35 | 121.88 | 117.70 |
| 57 | BA | 730 | A | C5-C6-N1 | 8.35 | 121.87 | 117.70 |
| 57 | BA | 1205 | A | C5-C6-N1 | 8.35 | 121.87 | 117.70 |
| 57 | BA | 2434 | A | C5-C6-N1 | 8.35 | 121.87 | 117.70 |
| 57 | BA | 1916 | A | N1-C6-N6 | -8.34 | 113.59 | 118.60 |
| 22 | AA | 499 | A | C4-C5-C6 | -8.34 | 112.83 | 117.00 |
| 22 | AA | 493 | A | C5-C6-N1 | 8.34 | 121.87 | 117.70 |
| 57 | BA | 1580 | A | C5-C6-N1 | 8.34 | 121.87 | 117.70 |
| 22 | AA | 640 | A | C5-C6-N1 | 8.34 | 121.87 | 117.70 |
| 22 | AA | 1200 | C | N3-C2-O2 | -8.34 | 116.06 | 121.90 |
| 57 | BA | 727 | A | N1-C6-N6 | -8.34 | 113.60 | 118.60 |
| 57 | BA | 920 | A | N1-C6-N6 | -8.34 | 113.60 | 118.60 |
| 57 | BA | 1791 | A | C5-C6-N1 | 8.34 | 121.87 | 117.70 |
| 57 | BA | 975 | A | C5-C6-N1 | 8.34 | 121.87 | 117.70 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 15 | AD | 80 | ARG | NE-CZ-NH1 | 8.33 | 124.47 | 120.30 |
| 57 | BA | 1978 | A | N1-C6-N6 | -8.33 | 113.60 | 118.60 |
| 22 | AA | 1096 | C | N3-C2-O2 | -8.33 | 116.07 | 121.90 |
| 46 | B3 | 10 | ARG | NE-CZ-NH2 | 8.33 | 124.47 | 120.30 |
| 57 | BA | 556 | A | N1-C6-N6 | -8.33 | 113.60 | 118.60 |
| 58 | Ba | 119 | A | N1-C6-N6 | -8.33 | 113.60 | 118.60 |
| 57 | BA | 71 | A | C5-C6-N1 | 8.33 | 121.86 | 117.70 |
| 57 | BA | 730 | A | N1-C6-N6 | -8.33 | 113.60 | 118.60 |
| 17 | AF | 112 | ARG | NE-CZ-NH1 | 8.32 | 124.46 | 120.30 |
| 22 | AA | 161 | A | C5-C6-N1 | 8.32 | 121.86 | 117.70 |
| 24 | A3 | 47 | A | N1-C6-N6 | -8.32 | 113.61 | 118.60 |
| 39 | BX | 73 | ARG | NE-CZ-NH1 | 8.32 | 124.46 | 120.30 |
| 57 | BA | 466 | A | N1-C6-N6 | -8.32 | 113.61 | 118.60 |
| 22 | AA | 977 | A | C5-C6-N1 | 8.32 | 121.86 | 117.70 |
| 57 | BA | 677 | A | N1-C6-N6 | -8.32 | 113.61 | 118.60 |
| 57 | BA | 792 | A | N1-C6-N6 | -8.32 | 113.61 | 118.60 |
| 57 | BA | 2766 | A | N1-C6-N6 | -8.32 | 113.61 | 118.60 |
| 57 | BA | 223 | A | C5-C6-N1 | 8.31 | 121.86 | 117.70 |
| 57 | BA | 231 | A | N1-C6-N6 | -8.31 | 113.61 | 118.60 |
| 57 | BA | 2872 | A | C5-C6-N1 | 8.31 | 121.86 | 117.70 |
| 57 | BA | 1893 | C | N3-C2-O2 | -8.31 | 116.08 | 121.90 |
| 22 | AA | 53 | A | N1-C6-N6 | -8.31 | 113.61 | 118.60 |
| 37 | BV | 80 | ARG | NE-CZ-NH1 | 8.31 | 124.45 | 120.30 |
| 57 | BA | 354 | A | N1-C6-N6 | -8.31 | 113.61 | 118.60 |
| 57 | BA | 2191 | A | N1-C6-N6 | -8.31 | 113.61 | 118.60 |
| 22 | AA | 825 | A | N1-C6-N6 | -8.31 | 113.62 | 118.60 |
| 22 | AA | 1306 | A | C5-C6-N1 | 8.31 | 121.85 | 117.70 |
| 57 | BA | 167 | A | N1-C6-N6 | -8.31 | 113.62 | 118.60 |
| 57 | BA | 2369 | A | N1-C6-N6 | -8.31 | 113.62 | 118.60 |
| 22 | AA | 1368 | A | C5-C6-N1 | 8.31 | 121.85 | 117.70 |
| 57 | BA | 941 | A | C5-C6-N1 | 8.31 | 121.85 | 117.70 |
| 53 | BF | 49 | ARG | NE-CZ-NH2 | 8.30 | 124.45 | 120.30 |
| 57 | BA | 244 | A | C5-C6-N1 | 8.30 | 121.85 | 117.70 |
| 57 | BA | 920 | A | C5-C6-N1 | 8.30 | 121.85 | 117.70 |
| 57 | BA | 1085 | A | C5-C6-N1 | 8.30 | 121.85 | 117.70 |
| 22 | AA | 892 | A | N1-C6-N6 | -8.30 | 113.62 | 118.60 |
| 22 | AA | 236 | A | N1-C6-N6 | -8.30 | 113.62 | 118.60 |
| 57 | BA | 1336 | A | N1-C6-N6 | -8.30 | 113.62 | 118.60 |
| 22 | AA | 400 | C | N3-C2-O2 | -8.30 | 116.09 | 121.90 |
| 57 | BA | 340 | A | N1-C6-N6 | -8.30 | 113.62 | 118.60 |
| 57 | BA | 449 | A | C5-C6-N1 | 8.30 | 121.85 | 117.70 |
| 57 | BA | 1048 | A | C5-C6-N1 | 8.30 | 121.85 | 117.70 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 31 | BQ | 6 | ARG | NE-CZ-NH1 | 8.30 | 124.45 | 120.30 |
| 57 | BA | 644 | A | N1-C6-N6 | -8.29 | 113.62 | 118.60 |
| 57 | BA | 800 | A | N1-C6-N6 | -8.29 | 113.62 | 118.60 |
| 57 | BA | 1590 | A | N1-C6-N6 | -8.29 | 113.62 | 118.60 |
| 22 | AA | 798 | U | O4'-C1'-N1 | 8.29 | 114.83 | 108.20 |
| 57 | BA | 5 | A | C5-C6-N1 | 8.29 | 121.85 | 117.70 |
| 57 | BA | 699 | A | N1-C6-N6 | -8.29 | 113.62 | 118.60 |
| 57 | BA | 505 | A | C5-C6-N1 | 8.29 | 121.84 | 117.70 |
| 57 | BA | 933 | A | N1-C6-N6 | -8.29 | 113.63 | 118.60 |
| 57 | BA | 2809 | A | C5-C6-N1 | 8.29 | 121.84 | 117.70 |
| 57 | BA | 2883 | A | C5-C6-N1 | 8.29 | 121.84 | 117.70 |
| 42 | B0 | 76 | ARG | NE-CZ-NH1 | 8.29 | 124.44 | 120.30 |
| 57 | BA | 1065 | U | O4'-C1'-N1 | 8.28 | 114.83 | 108.20 |
| 57 | BA | 2126 | A | C5-C6-N1 | 8.28 | 121.84 | 117.70 |
| 57 | BA | 1133 | A | C5-C6-N1 | 8.28 | 121.84 | 117.70 |
| 5 | AN | 12 | ARG | NE-CZ-NH1 | 8.28 | 124.44 | 120.30 |
| 57 | BA | 1427 | A | C4-C5-C6 | -8.28 | 112.86 | 117.00 |
| 57 | BA | 1654 | A | C5-C6-N1 | 8.28 | 121.84 | 117.70 |
| 22 | AA | 199 | A | C5-C6-N1 | 8.28 | 121.84 | 117.70 |
| 22 | AA | 1254 | A | N1-C6-N6 | -8.28 | 113.63 | 118.60 |
| 57 | BA | 1395 | A | C5-C6-N1 | 8.28 | 121.84 | 117.70 |
| 57 | BA | 1829 | A | C5-C6-N1 | 8.28 | 121.84 | 117.70 |
| 57 | BA | 2435 | A | C5-C6-N1 | 8.28 | 121.84 | 117.70 |
| 57 | BA | 305 | C | N3-C2-O2 | -8.28 | 116.11 | 121.90 |
| 57 | BA | 1919 | A | C5-C6-N1 | 8.28 | 121.84 | 117.70 |
| 22 | AA | 55 | A | N1-C6-N6 | -8.27 | 113.64 | 118.60 |
| 22 | AA | 1111 | A | C5-C6-N1 | 8.27 | 121.84 | 117.70 |
| 22 | AA | 160 | A | C5-C6-N1 | 8.27 | 121.83 | 117.70 |
| 22 | AA | 938 | A | C5-C6-N1 | 8.27 | 121.83 | 117.70 |
| 22 | AA | 1468 | A | N1-C6-N6 | -8.27 | 113.64 | 118.60 |
| 57 | BA | 928 | A | N1-C6-N6 | -8.27 | 113.64 | 118.60 |
| 57 | BA | 2297 | A | C5-C6-N1 | 8.27 | 121.84 | 117.70 |
| 57 | BA | 1032 | A | C5-C6-N1 | 8.27 | 121.83 | 117.70 |
| 57 | BA | 1611 | C | N3-C2-O2 | -8.27 | 116.11 | 121.90 |
| 58 | Ba | 15 | A | C5-C6-N1 | 8.27 | 121.83 | 117.70 |
| 57 | BA | 237 | C | N3-C2-O2 | -8.27 | 116.11 | 121.90 |
| 57 | BA | 1143 | A | C5-C6-N1 | 8.27 | 121.83 | 117.70 |
| 22 | AA | 972 | C | N3-C2-O2 | -8.26 | 116.11 | 121.90 |
| 22 | AA | 749 | A | N1-C6-N6 | -8.26 | 113.64 | 118.60 |
| 22 | AA | 174 | A | N1-C6-N6 | -8.26 | 113.64 | 118.60 |
| 22 | AA | 1219 | A | C5-C6-N1 | 8.26 | 121.83 | 117.70 |
| 57 | BA | 1669 | 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($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | AA | 1377 | A | C5-C6-N1 | 8.26 | 121.83 | 117.70 |
| 3 | AL | 113 | ARG | NE-CZ-NH1 | 8.26 | 124.43 | 120.30 |
| 33 | BS | 102 | ARG | NE-CZ-NH1 | 8.26 | 124.43 | 120.30 |
| 22 | AA | 1180 | A | C5-C6-N1 | 8.25 | 121.83 | 117.70 |
| 57 | BA | 886 | A | C5-C6-N1 | 8.25 | 121.83 | 117.70 |
| 57 | BA | 1434 | A | C5-C6-N1 | 8.25 | 121.83 | 117.70 |
| 22 | AA | 1340 | A | N1-C6-N6 | -8.25 | 113.65 | 118.60 |
| 22 | AA | 1531 | A | N1-C6-N6 | -8.25 | 113.65 | 118.60 |
| 57 | BA | 340 | A | C5-C6-N1 | 8.25 | 121.83 | 117.70 |
| 57 | BA | 2655 | G | O4'-C1'-N9 | 8.25 | 114.80 | 108.20 |
| 22 | AA | 983 | A | C4-C5-C6 | -8.25 | 112.88 | 117.00 |
| 22 | AA | 629 | A | N1-C6-N6 | -8.25 | 113.65 | 118.60 |
| 22 | AA | 906 | A | N1-C6-N6 | -8.25 | 113.65 | 118.60 |
| 57 | BA | 2660 | A | C5-C6-N1 | 8.25 | 121.82 | 117.70 |
| 57 | BA | 964 | C | N3-C2-O2 | -8.25 | 116.13 | 121.90 |
| 57 | BA | 83 | A | C5-C6-N1 | 8.24 | 121.82 | 117.70 |
| 57 | BA | 2376 | A | C5-C6-N1 | 8.24 | 121.82 | 117.70 |
| 57 | BA | 1598 | A | O4'-C1'-N9 | 8.24 | 114.79 | 108.20 |
| 57 | BA | 1940 | U | O4'-C1'-N1 | 8.24 | 114.79 | 108.20 |
| 57 | BA | 2587 | A | C5-C6-N1 | 8.24 | 121.82 | 117.70 |
| 22 | AA | 743 | A | N1-C6-N6 | -8.24 | 113.66 | 118.60 |
| 57 | BA | 197 | A | C5-C6-N1 | 8.24 | 121.82 | 117.70 |
| 57 | BA | 49 | A | C5-C6-N1 | 8.23 | 121.82 | 117.70 |
| 57 | BA | 323 | C | O4'-C1'-N1 | 8.23 | 114.79 | 108.20 |
| 57 | BA | 391 | A | C5-C6-N1 | 8.23 | 121.82 | 117.70 |
| 1 | AJ | 45 | ARG | NE-CZ-NH1 | 8.23 | 124.42 | 120.30 |
| 57 | BA | 945 | A | C5-C6-N1 | 8.23 | 121.81 | 117.70 |
| 22 | AA | 98 | A | N1-C6-N6 | -8.23 | 113.66 | 118.60 |
| 22 | AA | 121 | U | O4'-C1'-N1 | 8.23 | 114.78 | 108.20 |
| 57 | BA | 2211 | A | C5-C6-N1 | 8.23 | 121.81 | 117.70 |
| 57 | BA | 2565 | A | N1-C6-N6 | -8.23 | 113.66 | 118.60 |
| 57 | BA | 2886 | A | C5-C6-N1 | 8.23 | 121.81 | 117.70 |
| 22 | AA | 50 | A | C5-C6-N1 | 8.22 | 121.81 | 117.70 |
| 22 | AA | 777 | A | C5-C6-N1 | 8.22 | 121.81 | 117.70 |
| 57 | BA | 783 | A | O4'-C1'-N9 | 8.22 | 114.78 | 108.20 |
| 21 | A1 | 560 | ARG | NE-CZ-NH1 | 8.22 | 124.41 | 120.30 |
| 12 | AT | 73 | ARG | NE-CZ-NH1 | 8.22 | 124.41 | 120.30 |
| 22 | AA | 1349 | A | C5-C6-N1 | 8.22 | 121.81 | 117.70 |
| 57 | BA | 1269 | A | N1-C6-N6 | -8.22 | 113.67 | 118.60 |
| 22 | AA | 1213 | A | C4-C5-C6 | -8.21 | 112.89 | 117.00 |
| 57 | BA | 2646 | C | N3-C2-O2 | -8.21 | 116.15 | 121.90 |
| 57 | BA | 2868 | A | C5-C6-N1 | 8.21 | 121.81 | 117.70 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | AA | 143 | A | C5-C6-N1 | 8.21 | 121.81 | 117.70 |
| 22 | AA | 502 | A | C5-C6-N1 | 8.21 | 121.81 | 117.70 |
| 57 | BA | 1956 | U | O4'-C1'-N1 | 8.21 | 114.77 | 108.20 |
| 58 | Ba | 94 | A | N1-C6-N6 | -8.21 | 113.67 | 118.60 |
| 57 | BA | 528 | A | N1-C6-N6 | -8.21 | 113.67 | 118.60 |
| 57 | BA | 650 | C | N3-C2-O2 | -8.21 | 116.15 | 121.90 |
| 22 | AA | 26 | A | C5-C6-N1 | 8.21 | 121.80 | 117.70 |
| 33 | BS | 16 | ARG | NE-CZ-NH1 | 8.21 | 124.40 | 120.30 |
| 22 | AA | 101 | A | C5-C6-N1 | 8.21 | 121.80 | 117.70 |
| 22 | AA | 878 | A | C5-C6-N1 | 8.21 | 121.80 | 117.70 |
| 22 | AA | 915 | A | C5-C6-N1 | 8.20 | 121.80 | 117.70 |
| 57 | BA | 49 | A | N1-C6-N6 | -8.20 | 113.68 | 118.60 |
| 22 | AA | 1399 | C | N3-C2-O2 | -8.20 | 116.16 | 121.90 |
| 57 | BA | 28 | A | C5-C6-N1 | 8.20 | 121.80 | 117.70 |
| 57 | BA | 1301 | A | C5-C6-N1 | 8.20 | 121.80 | 117.70 |
| 57 | BA | 1788 | C | N3-C2-O2 | -8.20 | 116.16 | 121.90 |
| 22 | AA | 648 | A | C5-C6-N1 | 8.20 | 121.80 | 117.70 |
| 57 | BA | 1028 | A | C5-C6-N1 | 8.20 | 121.80 | 117.70 |
| 57 | BA | 2374 | C | N3-C2-O2 | -8.20 | 116.16 | 121.90 |
| 22 | AA | 1251 | A | C5-C6-N1 | 8.19 | 121.80 | 117.70 |
| 22 | AA | 539 | A | N1-C6-N6 | -8.19 | 113.68 | 118.60 |
| 57 | BA | 2518 | A | C5-C6-N1 | 8.19 | 121.80 | 117.70 |
| 10 | AS | 2 | ARG | NE-CZ-NH1 | 8.19 | 124.39 | 120.30 |
| 22 | AA | 129 | A | C5-C6-N1 | 8.19 | 121.79 | 117.70 |
| 22 | AA | 1236 | A | C5-C6-N1 | 8.19 | 121.80 | 117.70 |
| 48 | B5 | 51 | ARG | NE-CZ-NH2 | 8.19 | 124.39 | 120.30 |
| 57 | BA | 677 | A | C5-C6-N1 | 8.19 | 121.79 | 117.70 |
| 22 | AA | 574 | A | C5-C6-N1 | 8.19 | 121.79 | 117.70 |
| 57 | BA | 1143 | A | N1-C6-N6 | -8.19 | 113.69 | 118.60 |
| 57 | BA | 426 | C | N3-C2-O2 | -8.18 | 116.17 | 121.90 |
| 57 | BA | 2750 | A | C5-C6-N1 | 8.18 | 121.79 | 117.70 |
| 22 | AA | 300 | A | N1-C6-N6 | -8.18 | 113.69 | 118.60 |
| 22 | AA | 116 | A | C5-C6-N1 | 8.18 | 121.79 | 117.70 |
| 22 | AA | 149 | A | N1-C6-N6 | -8.18 | 113.69 | 118.60 |
| 22 | AA | 1016 | A | N1-C6-N6 | -8.18 | 113.69 | 118.60 |
| 57 | BA | 56 | A | C5-C6-N1 | 8.18 | 121.79 | 117.70 |
| 57 | BA | 1616 | A | C5-C6-N1 | 8.18 | 121.79 | 117.70 |
| 57 | BA | 1526 | C | N3-C2-O2 | -8.18 | 116.18 | 121.90 |
| 22 | AA | 2 | A | C5-C6-N1 | 8.17 | 121.79 | 117.70 |
| 57 | BA | 544 | C | N3-C2-O2 | -8.17 | 116.18 | 121.90 |
| 29 | BO | 108 | ARG | NE-CZ-NH1 | 8.17 | 124.39 | 120.30 |
| 57 | BA | 1103 | A | C5-C6-N1 | 8.17 | 121.78 | 117.70 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 1537 | G | O4'-C1'-N9 | 8.17 | 114.73 | 108.20 |
| 4 | AM | 100 | ARG | NE-CZ-NH1 | 8.17 | 124.38 | 120.30 |
| 21 | A1 | 207 | ARG | NE-CZ-NH1 | 8.17 | 124.38 | 120.30 |
| 57 | BA | 787 | C | N3-C2-O2 | -8.17 | 116.18 | 121.90 |
| 57 | BA | 2433 | A | C5-C6-N1 | 8.17 | 121.78 | 117.70 |
| 22 | AA | 726 | C | N3-C2-O2 | -8.17 | 116.18 | 121.90 |
| 57 | BA | 2378 | A | N1-C6-N6 | -8.16 | 113.70 | 118.60 |
| 57 | BA | 2380 | C | N3-C2-O2 | -8.16 | 116.18 | 121.90 |
| 22 | AA | 336 | A | N1-C6-N6 | -8.16 | 113.70 | 118.60 |
| 57 | BA | 2288 | A | C5-C6-N1 | 8.16 | 121.78 | 117.70 |
| 13 | AU | 65 | ARG | NE-CZ-NH1 | 8.16 | 124.38 | 120.30 |
| 57 | BA | 1579 | A | C5-C6-N1 | 8.16 | 121.78 | 117.70 |
| 22 | AA | 356 | A | C5-C6-N1 | 8.16 | 121.78 | 117.70 |
| 57 | BA | 1001 | A | N1-C6-N6 | -8.15 | 113.71 | 118.60 |
| 22 | AA | 468 | A | C5-C6-N1 | 8.15 | 121.78 | 117.70 |
| 24 | A3 | 57 | C | N3-C2-O2 | -8.15 | 116.19 | 121.90 |
| 57 | BA | 933 | A | C5-C6-N1 | 8.15 | 121.78 | 117.70 |
| 22 | AA | 197 | A | C5-C6-N1 | 8.15 | 121.77 | 117.70 |
| 22 | AA | 1332 | A | C5-C6-N1 | 8.15 | 121.78 | 117.70 |
| 50 | B7 | 34 | ARG | NE-CZ-NH2 | -8.15 | 116.23 | 120.30 |
| 57 | BA | 268 | C | N3-C2-O2 | -8.15 | 116.20 | 121.90 |
| 57 | BA | 1021 | A | N1-C6-N6 | -8.15 | 113.71 | 118.60 |
| 57 | BA | 1664 | A | C5-C6-N1 | 8.15 | 121.77 | 117.70 |
| 57 | BA | 2879 | A | C5-C6-N1 | 8.15 | 121.77 | 117.70 |
| 58 | Ba | 99 | A | C5-C6-N1 | 8.15 | 121.78 | 117.70 |
| 57 | BA | 1705 | A | N1-C6-N6 | -8.15 | 113.71 | 118.60 |
| 57 | BA | 1067 | A | C5-C6-N1 | 8.14 | 121.77 | 117.70 |
| 57 | BA | 2483 | C | N3-C2-O2 | -8.14 | 116.20 | 121.90 |
| 57 | BA | 1327 | A | C5-C6-N1 | 8.14 | 121.77 | 117.70 |
| 22 | AA | 1465 | A | N1-C6-N6 | -8.14 | 113.72 | 118.60 |
| 57 | BA | 1745 | A | N1-C6-N6 | -8.14 | 113.72 | 118.60 |
| 58 | Ba | 53 | A | N1-C6-N6 | -8.13 | 113.72 | 118.60 |
| 57 | BA | 420 | C | N3-C2-O2 | -8.13 | 116.21 | 121.90 |
| 57 | BA | 783 | A | N1-C6-N6 | -8.13 | 113.72 | 118.60 |
| 57 | BA | 1717 | A | C4-C5-C6 | -8.13 | 112.93 | 117.00 |
| 58 | Ba | 104 | A | C5-C6-N1 | 8.13 | 121.77 | 117.70 |
| 57 | BA | 2710 | C | N3-C2-O2 | -8.13 | 116.21 | 121.90 |
| 57 | BA | 1307 | A | C5-C6-N1 | 8.13 | 121.76 | 117.70 |
| 57 | BA | 1370 | C | N3-C2-O2 | -8.13 | 116.21 | 121.90 |
| 57 | BA | 2019 | A | C5-C6-N1 | 8.13 | 121.76 | 117.70 |
| 22 | AA | 205 | A | N1-C6-N6 | -8.12 | 113.72 | 118.60 |
| 57 | BA | 753 | 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($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | AA | 496 | A | N1-C6-N6 | -8.12 | 113.73 | 118.60 |
| 57 | BA | 1998 | A | N1-C6-N6 | -8.12 | 113.73 | 118.60 |
| 22 | AA | 635 | A | N1-C6-N6 | -8.12 | 113.73 | 118.60 |
| 22 | AA | 151 | A | C5-C6-N1 | 8.12 | 121.76 | 117.70 |
| 22 | AA | 205 | A | C5-C6-N1 | 8.12 | 121.76 | 117.70 |
| 57 | BA | 1879 | C | N3-C2-O2 | -8.12 | 116.22 | 121.90 |
| 22 | AA | 560 | A | C5-C6-N1 | 8.12 | 121.76 | 117.70 |
| 57 | BA | 2826 | A | N1-C6-N6 | -8.12 | 113.73 | 118.60 |
| 57 | BA | 849 | A | C5-C6-N1 | 8.11 | 121.76 | 117.70 |
| 22 | AA | 385 | C | N3-C2-O2 | -8.11 | 116.22 | 121.90 |
| 22 | AA | 509 | A | C5-C6-N1 | 8.11 | 121.76 | 117.70 |
| 57 | BA | 1095 | A | C5-C6-N1 | 8.11 | 121.76 | 117.70 |
| 57 | BA | 624 | C | N3-C2-O2 | -8.11 | 116.22 | 121.90 |
| 22 | AA | 3 | A | C5-C6-N1 | 8.11 | 121.75 | 117.70 |
| 22 | AA | 59 | A | C5-C6-N1 | 8.11 | 121.75 | 117.70 |
| 22 | AA | 321 | A | C5-C6-N1 | 8.11 | 121.75 | 117.70 |
| 22 | AA | 1188 | A | C5-C6-N1 | 8.11 | 121.75 | 117.70 |
| 57 | BA | 1027 | A | C5-C6-N1 | 8.11 | 121.75 | 117.70 |
| 57 | BA | 581 | C | N3-C2-O2 | -8.11 | 116.22 | 121.90 |
| 57 | BA | 1366 | A | C5-C6-N1 | 8.11 | 121.75 | 117.70 |
| 22 | AA | 403 | C | N3-C2-O2 | -8.11 | 116.22 | 121.90 |
| 22 | AA | 768 | A | N1-C6-N6 | -8.11 | 113.74 | 118.60 |
| 17 | AF | 2 | ARG | NE-CZ-NH1 | 8.11 | 124.35 | 120.30 |
| 57 | BA | 457 | A | C5-C6-N1 | 8.11 | 121.75 | 117.70 |
| 57 | BA | 1090 | A | C5-C6-N1 | 8.11 | 121.75 | 117.70 |
| 57 | BA | 2062 | A | C5-C6-N1 | 8.11 | 121.75 | 117.70 |
| 20 | AI | 94 | ARG | NE-CZ-NH1 | 8.10 | 124.35 | 120.30 |
| 57 | BA | 764 | A | N1-C6-N6 | -8.10 | 113.74 | 118.60 |
| 57 | BA | 1503 | A | C5-C6-N1 | 8.10 | 121.75 | 117.70 |
| 22 | AA | 356 | A | N1-C6-N6 | -8.10 | 113.74 | 118.60 |
| 22 | AA | 718 | A | C5-C6-N1 | 8.10 | 121.75 | 117.70 |
| 57 | BA | 1958 | C | N3-C2-O2 | -8.10 | 116.23 | 121.90 |
| 22 | AA | 1256 | A | O4'-C1'-N9 | 8.10 | 114.68 | 108.20 |
| 23 | A2 | 19 | A | C5-C6-N1 | 8.10 | 121.75 | 117.70 |
| 35 | BD | 237 | ARG | NE-CZ-NH2 | -8.10 | 116.25 | 120.30 |
| 57 | BA | 116 | C | N3-C2-O2 | -8.10 | 116.23 | 121.90 |
| 57 | BA | 423 | A | C4-C5-C6 | -8.10 | 112.95 | 117.00 |
| 57 | BA | 601 | C | N3-C2-O2 | -8.10 | 116.23 | 121.90 |
| 57 | BA | 1151 | A | C5-C6-N1 | 8.10 | 121.75 | 117.70 |
| 57 | BA | 1384 | A | C5-C6-N1 | 8.10 | 121.75 | 117.70 |
| 57 | BA | 239 | C | N3-C2-O2 | -8.09 | 116.23 | 121.90 |
| 57 | BA | 633 | A | N1-C6-N6 | -8.09 | 113.74 | 118.60 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | AA | 482 | A | N1-C6-N6 | -8.09 | 113.75 | 118.60 |
| 41 | BZ | 79 | ARG | NE-CZ-NH1 | 8.09 | 124.34 | 120.30 |
| 57 | BA | 1759 | A | C5-C6-N1 | 8.09 | 121.75 | 117.70 |
| 57 | BA | 1982 | U | O4'-C1'-N1 | 8.09 | 114.67 | 108.20 |
| 57 | BA | 2658 | C | C4'-C3'-C2' | -8.09 | 94.51 | 102.60 |
| 57 | BA | 2850 | A | C5-C6-N1 | 8.09 | 121.75 | 117.70 |
| 57 | BA | 118 | A | N1-C6-N6 | -8.09 | 113.75 | 118.60 |
| 57 | BA | 2753 | A | N1-C6-N6 | -8.09 | 113.75 | 118.60 |
| 22 | AA | 325 | A | C5-C6-N1 | 8.08 | 121.74 | 117.70 |
| 22 | AA | 919 | A | N1-C6-N6 | -8.08 | 113.75 | 118.60 |
| 22 | AA | 1158 | C | N1-C2-O2 | 8.08 | 123.75 | 118.90 |
| 57 | BA | 1490 | A | C5-C6-N1 | 8.08 | 121.74 | 117.70 |
| 57 | BA | 2847 | U | O4'-C1'-N1 | 8.08 | 114.67 | 108.20 |
| 22 | AA | 689 | C | N3-C2-O2 | -8.08 | 116.24 | 121.90 |
| 22 | AA | 889 | A | C5-C6-N1 | 8.08 | 121.74 | 117.70 |
| 57 | BA | 1378 | A | C5-C6-N1 | 8.08 | 121.74 | 117.70 |
| 57 | BA | 1705 | A | C5-C6-N1 | 8.08 | 121.74 | 117.70 |
| 22 | AA | 1044 | A | N1-C6-N6 | -8.08 | 113.75 | 118.60 |
| 57 | BA | 191 | A | N1-C6-N6 | -8.08 | 113.75 | 118.60 |
| 57 | BA | 1142 | A | C5-C6-N1 | 8.08 | 121.74 | 117.70 |
| 57 | BA | 2094 | A | N1-C6-N6 | -8.08 | 113.75 | 118.60 |
| 22 | AA | 1476 | A | N1-C6-N6 | -8.07 | 113.75 | 118.60 |
| 57 | BA | 433 | C | N3-C2-O2 | -8.07 | 116.25 | 121.90 |
| 22 | AA | 161 | A | O4'-C1'-N9 | 8.07 | 114.66 | 108.20 |
| 22 | AA | 1434 | A | C5-C6-N1 | 8.07 | 121.73 | 117.70 |
| 57 | BA | 216 | A | C5-C6-N1 | 8.07 | 121.74 | 117.70 |
| 57 | BA | 1848 | A | C5-C6-N1 | 8.07 | 121.73 | 117.70 |
| 57 | BA | 2634 | A | C5-C6-N1 | 8.07 | 121.73 | 117.70 |
| 22 | AA | 665 | A | C4-C5-C6 | -8.07 | 112.97 | 117.00 |
| 22 | AA | 1384 | C | N3-C2-O2 | -8.07 | 116.25 | 121.90 |
| 57 | BA | 2660 | A | O4'-C1'-N9 | 8.07 | 114.65 | 108.20 |
| 22 | AA | 1101 | A | C5-C6-N1 | 8.06 | 121.73 | 117.70 |
| 57 | BA | 854 | C | N3-C2-O2 | -8.06 | 116.25 | 121.90 |
| 57 | BA | 1713 | A | C5-C6-N1 | 8.06 | 121.73 | 117.70 |
| 57 | BA | 2478 | A | C5-C6-N1 | 8.06 | 121.73 | 117.70 |
| 22 | AA | 288 | A | C5-C6-N1 | 8.06 | 121.73 | 117.70 |
| 57 | BA | 795 | C | N3-C2-O2 | -8.06 | 116.26 | 121.90 |
| 57 | BA | 918 | A | C5-C6-N1 | 8.06 | 121.73 | 117.70 |
| 57 | BA | 1069 | A | C5-C6-N1 | 8.06 | 121.73 | 117.70 |
| 57 | BA | 1803 | A | C5-C6-N1 | 8.06 | 121.73 | 117.70 |
| 57 | BA | 1847 | A | C5-C6-N1 | 8.06 | 121.73 | 117.70 |
| 57 | BA | 2564 | A | C5-C6-N1 | 8.06 | 121.73 | 117.70 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 2900 | A | N1-C6-N6 | -8.06 | 113.77 | 118.60 |
| 22 | AA | 1413 | A | N1-C6-N6 | -8.06 | 113.77 | 118.60 |
| 57 | BA | 2734 | A | C5-C6-N1 | 8.06 | 121.73 | 117.70 |
| 57 | BA | 13 | A | C4-C5-C6 | -8.05 | 112.97 | 117.00 |
| 57 | BA | 802 | A | C5-C6-N1 | 8.05 | 121.73 | 117.70 |
| 57 | BA | 819 | A | N1-C6-N6 | -8.05 | 113.77 | 118.60 |
| 57 | BA | 1167 | C | N3-C2-O2 | -8.05 | 116.26 | 121.90 |
| 57 | BA | 2273 | A | C5-C6-N1 | 8.05 | 121.73 | 117.70 |
| 22 | AA | 1124 | G | O4'-C1'-N9 | 8.05 | 114.64 | 108.20 |
| 57 | BA | 1054 | A | C5-C6-N1 | 8.05 | 121.73 | 117.70 |
| 22 | AA | 1534 | A | N1-C6-N6 | -8.05 | 113.77 | 118.60 |
| 57 | BA | 1570 | A | C5-C6-N1 | 8.05 | 121.73 | 117.70 |
| 57 | BA | 1937 | A | C5-C6-N1 | 8.05 | 121.73 | 117.70 |
| 57 | BA | 2882 | A | C4-C5-C6 | -8.05 | 112.97 | 117.00 |
| 57 | BA | 2778 | A | C5-C6-N1 | 8.05 | 121.72 | 117.70 |
| 22 | AA | 547 | A | C5-C6-N1 | 8.05 | 121.72 | 117.70 |
| 57 | BA | 91 | A | C5-C6-N1 | 8.05 | 121.72 | 117.70 |
| 22 | AA | 909 | A | N1-C6-N6 | -8.05 | 113.77 | 118.60 |
| 43 | B1 | 44 | ARG | NE-CZ-NH1 | 8.05 | 124.32 | 120.30 |
| 57 | BA | 1241 | A | O4'-C1'-N9 | 8.05 | 114.64 | 108.20 |
| 57 | BA | 2327 | A | C5-C6-N1 | 8.05 | 121.72 | 117.70 |
| 22 | AA | 179 | A | C5-C6-N1 | 8.05 | 121.72 | 117.70 |
| 22 | AA | 614 | C | N3-C2-O2 | -8.05 | 116.27 | 121.90 |
| 57 | BA | 1155 | A | C5-C6-N1 | 8.05 | 121.72 | 117.70 |
| 57 | BA | 1637 | A | N1-C6-N6 | -8.05 | 113.77 | 118.60 |
| 57 | BA | 2358 | A | C5-C6-N1 | 8.05 | 121.72 | 117.70 |
| 49 | B6 | 43 | ARG | NE-CZ-NH1 | 8.04 | 124.32 | 120.30 |
| 22 | AA | 132 | C | N3-C2-O2 | -8.04 | 116.27 | 121.90 |
| 57 | BA | 127 | A | C5-C6-N1 | 8.04 | 121.72 | 117.70 |
| 57 | BA | 896 | A | C5-C6-N1 | 8.04 | 121.72 | 117.70 |
| 57 | BA | 1262 | A | C5-C6-N1 | 8.04 | 121.72 | 117.70 |
| 22 | AA | 65 | A | C5-C6-N1 | 8.04 | 121.72 | 117.70 |
| 22 | AA | 790 | A | N1-C6-N6 | -8.04 | 113.78 | 118.60 |
| 23 | A2 | 27 | A | C5-C6-N1 | 8.04 | 121.72 | 117.70 |
| 57 | BA | 309 | A | C5-C6-N1 | 8.04 | 121.72 | 117.70 |
| 57 | BA | 199 | A | C5-C6-N1 | 8.04 | 121.72 | 117.70 |
| 57 | BA | 378 | C | N3-C2-O2 | -8.04 | 116.27 | 121.90 |
| 57 | BA | 735 | A | N1-C6-N6 | -8.04 | 113.78 | 118.60 |
| 57 | BA | 1073 | A | C5-C6-N1 | 8.04 | 121.72 | 117.70 |
| 57 | BA | 1095 | A | N1-C6-N6 | -8.03 | 113.78 | 118.60 |
| 57 | BA | 2042 | A | N1-C6-N6 | -8.04 | 113.78 | 118.60 |
| 57 | BA | 2800 | 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($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | AA | 363 | A | C5-C6-N1 | 8.03 | 121.72 | 117.70 |
| 57 | BA | 1819 | A | N1-C6-N6 | -8.03 | 113.78 | 118.60 |
| 22 | AA | 435 | A | N1-C6-N6 | -8.03 | 113.78 | 118.60 |
| 22 | AA | 1428 | A | C5-C6-N1 | 8.03 | 121.72 | 117.70 |
| 57 | BA | 1265 | A | N1-C6-N6 | -8.03 | 113.78 | 118.60 |
| 22 | AA | 712 | A | C5-C6-N1 | 8.03 | 121.71 | 117.70 |
| 53 | BF | 102 | ARG | NE-CZ-NH1 | -8.03 | 116.29 | 120.30 |
| 57 | BA | 788 | A | C5-C6-N1 | 8.03 | 121.71 | 117.70 |
| 57 | BA | 2078 | C | N3-C2-O2 | -8.03 | 116.28 | 121.90 |
| 22 | AA | 1012 | A | N1-C6-N6 | -8.03 | 113.78 | 118.60 |
| 22 | AA | 1225 | A | C5-C6-N1 | 8.03 | 121.71 | 117.70 |
| 57 | BA | 727 | A | C5-C6-N1 | 8.03 | 121.71 | 117.70 |
| 58 | Ba | 66 | A | C5-C6-N1 | 8.03 | 121.71 | 117.70 |
| 57 | BA | 183 | C | N3-C2-O2 | -8.02 | 116.28 | 121.90 |
| 57 | BA | 1987 | A | C5-C6-N1 | 8.02 | 121.71 | 117.70 |
| 22 | AA | 974 | A | C5-C6-N1 | 8.02 | 121.71 | 117.70 |
| 22 | AA | 1324 | A | N1-C6-N6 | -8.02 | 113.79 | 118.60 |
| 57 | BA | 749 | A | N1-C6-N6 | -8.02 | 113.79 | 118.60 |
| 22 | AA | 1346 | A | C5-C6-N1 | 8.02 | 121.71 | 117.70 |
| 57 | BA | 1997 | C | N3-C2-O2 | -8.02 | 116.29 | 121.90 |
| 4 | AM | 2 | ARG | NE-CZ-NH1 | 8.02 | 124.31 | 120.30 |
| 8 | AQ | 64 | ARG | NE-CZ-NH1 | 8.02 | 124.31 | 120.30 |
| 22 | AA | 1447 | A | C5-C6-N1 | 8.02 | 121.71 | 117.70 |
| 35 | BD | 237 | ARG | NE-CZ-NH1 | 8.02 | 124.31 | 120.30 |
| 57 | BA | 905 | A | C5-C6-N1 | 8.02 | 121.71 | 117.70 |
| 16 | AE | 111 | ARG | NH1-CZ-NH2 | -8.02 | 110.58 | 119.40 |
| 22 | AA | 19 | A | N1-C6-N6 | -8.02 | 113.79 | 118.60 |
| 57 | BA | 603 | A | C5-C6-N1 | 8.02 | 121.71 | 117.70 |
| 22 | AA | 1227 | A | C5-C6-N1 | 8.02 | 121.71 | 117.70 |
| 57 | BA | 1098 | A | N1-C6-N6 | -8.02 | 113.79 | 118.60 |
| 57 | BA | 2764 | A | C5-C6-N1 | 8.02 | 121.71 | 117.70 |
| 22 | AA | 80 | A | N1-C6-N6 | -8.01 | 113.79 | 118.60 |
| 57 | BA | 1247 | A | C5-C6-N1 | 8.01 | 121.71 | 117.70 |
| 57 | BA | 1398 | C | N3-C2-O2 | -8.01 | 116.29 | 121.90 |
| 57 | BA | 2333 | A | C5-C6-N1 | 8.01 | 121.71 | 117.70 |
| 57 | BA | 1039 | A | C5-C6-N1 | 8.01 | 121.71 | 117.70 |
| 57 | BA | 1722 | A | N1-C6-N6 | -8.01 | 113.79 | 118.60 |
| 57 | BA | 204 | A | C5-C6-N1 | 8.01 | 121.70 | 117.70 |
| 22 | AA | 1303 | C | N3-C2-O2 | -8.01 | 116.29 | 121.90 |
| 57 | BA | 172 | A | N1-C6-N6 | -8.01 | 113.79 | 118.60 |
| 57 | BA | 2870 | C | N3-C2-O2 | -8.01 | 116.30 | 121.90 |
| 22 | AA | 1513 | A | C5-C6-N1 | 8.01 | 121.70 | 117.70 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 1403 | A | C5-C6-N1 | 8.01 | 121.70 | 117.70 |
| 57 | BA | 2516 | A | N1-C6-N6 | -8.01 | 113.80 | 118.60 |
| 22 | AA | 60 | A | N1-C6-N6 | -8.00 | 113.80 | 118.60 |
| 22 | AA | 311 | C | N3-C2-O2 | -8.00 | 116.30 | 121.90 |
| 22 | AA | 624 | C | N3-C2-O2 | -8.00 | 116.30 | 121.90 |
| 57 | BA | 1153 | C | N3-C2-O2 | -8.00 | 116.30 | 121.90 |
| 57 | BA | 95 | A | C5-C6-N1 | 8.00 | 121.70 | 117.70 |
| 24 | A3 | 11 | A | N1-C6-N6 | -8.00 | 113.80 | 118.60 |
| 57 | BA | 2258 | C | N3-C2-O2 | -8.00 | 116.30 | 121.90 |
| 57 | BA | 156 | A | N1-C6-N6 | -8.00 | 113.80 | 118.60 |
| 57 | BA | 1010 | A | C5-C6-N1 | 8.00 | 121.70 | 117.70 |
| 57 | BA | 705 | A | C5-C6-N1 | 8.00 | 121.70 | 117.70 |
| 57 | BA | 1342 | A | C5-C6-N1 | 8.00 | 121.70 | 117.70 |
| 57 | BA | 2134 | A | C5-C6-N1 | 8.00 | 121.70 | 117.70 |
| 57 | BA | 2459 | A | C5-C6-N1 | 8.00 | 121.70 | 117.70 |
| 57 | BA | 2851 | A | C5-C6-N1 | 8.00 | 121.70 | 117.70 |
| 22 | AA | 1325 | C | N3-C2-O2 | -7.99 | 116.31 | 121.90 |
| 22 | AA | 1428 | A | N1-C6-N6 | -7.99 | 113.80 | 118.60 |
| 22 | AA | 430 | A | C5-C6-N1 | 7.99 | 121.70 | 117.70 |
| 57 | BA | 1598 | A | C5-C6-N1 | 7.99 | 121.70 | 117.70 |
| 22 | AA | 608 | A | C5-C6-N1 | 7.99 | 121.69 | 117.70 |
| 22 | AA | 767 | A | C5-C6-N1 | 7.99 | 121.69 | 117.70 |
| 57 | BA | 2679 | A | C5-C6-N1 | 7.99 | 121.69 | 117.70 |
| 57 | BA | 1593 | A | N1-C6-N6 | -7.99 | 113.81 | 118.60 |
| 57 | BA | 257 | C | O4'-C1'-N1 | 7.99 | 114.59 | 108.20 |
| 57 | BA | 1549 | A | N1-C6-N6 | -7.99 | 113.81 | 118.60 |
| 57 | BA | 2541 | A | C5-C6-N1 | 7.99 | 121.69 | 117.70 |
| 57 | BA | 2573 | C | O4'-C1'-N1 | 7.99 | 114.59 | 108.20 |
| 22 | AA | 430 | A | N1-C6-N6 | -7.99 | 113.81 | 118.60 |
| 22 | AA | 1502 | A | C5-C6-N1 | 7.99 | 121.69 | 117.70 |
| 56 | BL | 123 | ARG | NE-CZ-NH1 | 7.99 | 124.29 | 120.30 |
| 57 | BA | 960 | A | C5-C6-N1 | 7.99 | 121.69 | 117.70 |
| 57 | BA | 2287 | A | C5-C6-N1 | 7.99 | 121.69 | 117.70 |
| 57 | BA | 282 | A | N1-C6-N6 | -7.98 | 113.81 | 118.60 |
| 57 | BA | 2283 | C | N3-C2-O2 | -7.98 | 116.31 | 121.90 |
| 57 | BA | 2309 | A | C5-C6-N1 | 7.98 | 121.69 | 117.70 |
| 57 | BA | 2450 | A | C4-C5-C6 | -7.98 | 113.01 | 117.00 |
| 22 | AA | 353 | A | C5-C6-N1 | 7.98 | 121.69 | 117.70 |
| 57 | BA | 783 | A | C5-C6-N1 | 7.98 | 121.69 | 117.70 |
| 57 | BA | 903 | C | N3-C2-O2 | -7.98 | 116.31 | 121.90 |
| 57 | BA | 2579 | C | O4'-C1'-N1 | 7.98 | 114.58 | 108.20 |
| 57 | BA | 272 | A | C5-C6-N1 | 7.98 | 121.69 | 117.70 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | AA | 441 | A | N1-C6-N6 | -7.98 | 113.81 | 118.60 |
| 22 | AA | 732 | C | N3-C2-O2 | -7.98 | 116.31 | 121.90 |
| 42 | B0 | 10 | ARG | NE-CZ-NH1 | 7.98 | 124.29 | 120.30 |
| 57 | BA | 896 | A | O4'-C1'-N9 | 7.98 | 114.58 | 108.20 |
| 43 | B1 | 49 | ARG | NE-CZ-NH2 | 7.98 | 124.29 | 120.30 |
| 57 | BA | 2212 | A | C5-C6-N1 | 7.98 | 121.69 | 117.70 |
| 22 | AA | 1542 | A | O4'-C1'-N9 | 7.97 | 114.58 | 108.20 |
| 24 | A3 | 41 | C | N3-C2-O2 | -7.97 | 116.32 | 121.90 |
| 57 | BA | 173 | A | N1-C6-N6 | -7.97 | 113.81 | 118.60 |
| 57 | BA | 531 | C | N3-C2-O2 | -7.97 | 116.32 | 121.90 |
| 57 | BA | 2101 | A | C5-C6-N1 | 7.97 | 121.69 | 117.70 |
| 22 | AA | 1261 | A | C5-C6-N1 | 7.97 | 121.69 | 117.70 |
| 57 | BA | 761 | A | N1-C6-N6 | -7.97 | 113.82 | 118.60 |
| 57 | BA | 2225 | A | C4-C5-C6 | -7.97 | 113.01 | 117.00 |
| 57 | BA | 1238 | G | O4'-C1'-N9 | 7.97 | 114.58 | 108.20 |
| 57 | BA | 1640 | A | C5-C6-N1 | 7.97 | 121.69 | 117.70 |
| 57 | BA | 1969 | A | N1-C6-N6 | -7.97 | 113.82 | 118.60 |
| 58 | Ba | 115 | A | N1-C6-N6 | -7.97 | 113.82 | 118.60 |
| 57 | BA | 1009 | A | C5-C6-N1 | 7.97 | 121.68 | 117.70 |
| 22 | AA | 130 | A | N1-C6-N6 | -7.97 | 113.82 | 118.60 |
| 22 | AA | 495 | A | C5-C6-N1 | 7.97 | 121.68 | 117.70 |
| 57 | BA | 812 | C | O4'-C1'-N1 | 7.97 | 114.57 | 108.20 |
| 57 | BA | 2417 | C | N3-C2-O2 | -7.97 | 116.32 | 121.90 |
| 57 | BA | 1872 | A | N1-C6-N6 | -7.96 | 113.82 | 118.60 |
| 57 | BA | 2542 | A | C5-C6-N1 | 7.96 | 121.68 | 117.70 |
| 22 | AA | 320 | A | N1-C6-N6 | -7.96 | 113.82 | 118.60 |
| 22 | AA | 233 | C | N3-C2-O2 | -7.96 | 116.33 | 121.90 |
| 23 | A2 | 26 | U | O4'-C1'-N1 | 7.96 | 114.57 | 108.20 |
| 57 | BA | 5 | A | N1-C6-N6 | -7.96 | 113.82 | 118.60 |
| 22 | AA | 1513 | A | C4-C5-C6 | -7.96 | 113.02 | 117.00 |
| 57 | BA | 2322 | A | C5-C6-N1 | 7.96 | 121.68 | 117.70 |
| 57 | BA | 1507 | C | N3-C2-O2 | -7.96 | 116.33 | 121.90 |
| 22 | AA | 878 | A | N1-C6-N6 | -7.96 | 113.83 | 118.60 |
| 22 | AA | 1110 | A | N1-C6-N6 | -7.96 | 113.83 | 118.60 |
| 57 | BA | 2051 | A | N1-C6-N6 | -7.96 | 113.83 | 118.60 |
| 57 | BA | 2088 | A | C5-C6-N1 | 7.96 | 121.68 | 117.70 |
| 22 | AA | 53 | A | C5-C6-N1 | 7.95 | 121.68 | 117.70 |
| 22 | AA | 320 | A | C5-C6-N1 | 7.95 | 121.68 | 117.70 |
| 22 | AA | 826 | C | N3-C2-O2 | -7.95 | 116.33 | 121.90 |
| 57 | BA | 752 | A | C5-C6-N1 | 7.95 | 121.68 | 117.70 |
| 22 | AA | 1542 | A | C5-C6-N1 | 7.95 | 121.67 | 117.70 |
| 57 | BA | 213 | A | C5-C6-N1 | 7.95 | 121.67 | 117.70 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 515 | A | N1-C6-N6 | -7.95 | 113.83 | 118.60 |
| 57 | BA | 1000 | A | C5-C6-N1 | 7.95 | 121.67 | 117.70 |
| 57 | BA | 1328 | A | C5-C6-N1 | 7.95 | 121.68 | 117.70 |
| 57 | BA | 2088 | A | N1-C6-N6 | -7.95 | 113.83 | 118.60 |
| 57 | BA | 2497 | A | C5-C6-N1 | 7.95 | 121.67 | 117.70 |
| 22 | AA | 119 | A | C5-C6-N1 | 7.95 | 121.67 | 117.70 |
| 22 | AA | 475 | C | N3-C2-O2 | -7.95 | 116.34 | 121.90 |
| 22 | AA | 906 | A | C5-C6-N1 | 7.95 | 121.67 | 117.70 |
| 57 | BA | 382 | A | C5-C6-N1 | 7.95 | 121.67 | 117.70 |
| 57 | BA | 1900 | A | C5-C6-N1 | 7.95 | 121.67 | 117.70 |
| 57 | BA | 722 | A | N1-C6-N6 | -7.95 | 113.83 | 118.60 |
| 57 | BA | 1970 | A | N1-C6-N6 | -7.95 | 113.83 | 118.60 |
| 57 | BA | 1966 | A | C5-C6-N1 | 7.94 | 121.67 | 117.70 |
| 57 | BA | 2378 | A | C5-C6-N1 | 7.94 | 121.67 | 117.70 |
| 22 | AA | 1081 | A | N1-C6-N6 | -7.94 | 113.83 | 118.60 |
| 57 | BA | 130 | C | N3-C2-O2 | -7.94 | 116.34 | 121.90 |
| 57 | BA | 342 | A | C5-C6-N1 | 7.94 | 121.67 | 117.70 |
| 57 | BA | 602 | A | C5-C6-N1 | 7.94 | 121.67 | 117.70 |
| 57 | BA | 1610 | A | C5-C6-N1 | 7.94 | 121.67 | 117.70 |
| 9 | AR | 5 | ARG | NE-CZ-NH1 | 7.94 | 124.27 | 120.30 |
| 22 | AA | 996 | A | C5-C6-N1 | 7.94 | 121.67 | 117.70 |
| 57 | BA | 2412 | A | C5-C6-N1 | 7.94 | 121.67 | 117.70 |
| 57 | BA | 2564 | A | N1-C6-N6 | -7.94 | 113.84 | 118.60 |
| 22 | AA | 1507 | A | C5-C6-N1 | 7.94 | 121.67 | 117.70 |
| 22 | AA | 1004 | A | C5-C6-N1 | 7.94 | 121.67 | 117.70 |
| 22 | AA | 1499 | A | N1-C6-N6 | -7.94 | 113.84 | 118.60 |
| 57 | BA | 1439 | A | C5-C6-N1 | 7.94 | 121.67 | 117.70 |
| 58 | Ba | 29 | A | C5-C6-N1 | 7.94 | 121.67 | 117.70 |
| 57 | BA | 2468 | A | C5-C6-N1 | 7.94 | 121.67 | 117.70 |
| 57 | BA | 2507 | C | N3-C2-O2 | -7.94 | 116.34 | 121.90 |
| 57 | BA | 2602 | A | C5-C6-N1 | 7.94 | 121.67 | 117.70 |
| 57 | BA | 2814 | A | C5-C6-N1 | 7.94 | 121.67 | 117.70 |
| 22 | AA | 195 | A | C5-C6-N1 | 7.93 | 121.67 | 117.70 |
| 22 | AA | 663 | A | N1-C6-N6 | -7.93 | 113.84 | 118.60 |
| 22 | AA | 253 | A | C5-C6-N1 | 7.93 | 121.67 | 117.70 |
| 57 | BA | 251 | A | N1-C6-N6 | -7.93 | 113.84 | 118.60 |
| 57 | BA | 371 | A | C5-C6-N1 | 7.93 | 121.67 | 117.70 |
| 57 | BA | 415 | A | N1-C6-N6 | -7.93 | 113.84 | 118.60 |
| 57 | BA | 821 | A | C5-C6-N1 | 7.93 | 121.67 | 117.70 |
| 57 | BA | 972 | A | C5-C6-N1 | 7.93 | 121.67 | 117.70 |
| 57 | BA | 1287 | A | C5-C6-N1 | 7.93 | 121.67 | 117.70 |
| 57 | BA | 541 | A | N1-C6-N6 | -7.93 | 113.84 | 118.60 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 1050 | A | C5-C6-N1 | 7.93 | 121.67 | 117.70 |
| 57 | BA | 1827 | U | O4'-C1'-N1 | 7.93 | 114.55 | 108.20 |
| 57 | BA | 1833 | C | N3-C2-O2 | -7.93 | 116.35 | 121.90 |
| 22 | AA | 968 | A | C5-C6-N1 | 7.93 | 121.67 | 117.70 |
| 22 | AA | 1282 | C | N3-C2-O2 | -7.93 | 116.35 | 121.90 |
| 57 | BA | 191 | A | C5-C6-N1 | 7.93 | 121.67 | 117.70 |
| 57 | BA | 2758 | A | C5-C6-N1 | 7.93 | 121.67 | 117.70 |
| 22 | AA | 1492 | A | C5-C6-N1 | 7.93 | 121.66 | 117.70 |
| 57 | BA | 1986 | C | N3-C2-O2 | -7.93 | 116.35 | 121.90 |
| 57 | BA | 654 | A | C5-C6-N1 | 7.93 | 121.66 | 117.70 |
| 57 | BA | 1981 | A | C5-C6-N1 | 7.93 | 121.66 | 117.70 |
| 57 | BA | 2214 | C | N3-C2-O2 | -7.93 | 116.35 | 121.90 |
| 4 | AM | 97 | ARG | NE-CZ-NH1 | 7.92 | 124.26 | 120.30 |
| 21 | A1 | 632 | ARG | NE-CZ-NH1 | 7.92 | 124.26 | 120.30 |
| 22 | AA | 596 | A | C5-C6-N1 | 7.92 | 121.66 | 117.70 |
| 22 | AA | 1261 | A | N1-C6-N6 | -7.92 | 113.85 | 118.60 |
| 57 | BA | 1755 | A | C5-C6-N1 | 7.92 | 121.66 | 117.70 |
| 57 | BA | 2388 | A | C5-C6-N1 | 7.92 | 121.66 | 117.70 |
| 22 | AA | 28 | A | C5-C6-N1 | 7.92 | 121.66 | 117.70 |
| 57 | BA | 44 | A | N1-C6-N6 | -7.92 | 113.85 | 118.60 |
| 22 | AA | 175 | C | N3-C2-O2 | -7.92 | 116.36 | 121.90 |
| 22 | AA | 622 | A | C4-C5-C6 | -7.92 | 113.04 | 117.00 |
| 22 | AA | 743 | A | C5-C6-N1 | 7.92 | 121.66 | 117.70 |
| 57 | BA | 207 | A | C5-C6-N1 | 7.92 | 121.66 | 117.70 |
| 57 | BA | 2031 | A | C5-C6-N1 | 7.92 | 121.66 | 117.70 |
| 22 | AA | 1069 | C | N3-C2-O2 | -7.92 | 116.36 | 121.90 |
| 57 | BA | 1264 | A | C5-C6-N1 | 7.92 | 121.66 | 117.70 |
| 22 | AA | 749 | A | C5-C6-N1 | 7.92 | 121.66 | 117.70 |
| 22 | AA | 857 | C | N3-C2-O2 | -7.92 | 116.36 | 121.90 |
| 22 | AA | 907 | A | N1-C6-N6 | -7.92 | 113.85 | 118.60 |
| 57 | BA | 1089 | A | C5-C6-N1 | 7.92 | 121.66 | 117.70 |
| 22 | AA | 267 | C | N3-C2-O2 | -7.92 | 116.36 | 121.90 |
| 57 | BA | 1079 | C | N3-C2-O2 | -7.92 | 116.36 | 121.90 |
| 57 | BA | 1175 | A | C5-C6-N1 | 7.92 | 121.66 | 117.70 |
| 57 | BA | 2823 | A | C5-C6-N1 | 7.92 | 121.66 | 117.70 |
| 22 | AA | 815 | A | C5-C6-N1 | 7.92 | 121.66 | 117.70 |
| 57 | BA | 526 | A | C5-C6-N1 | 7.92 | 121.66 | 117.70 |
| 57 | BA | 2723 | C | N3-C2-O2 | -7.92 | 116.36 | 121.90 |
| 22 | AA | 358 | U | O4'-C1'-N1 | 7.91 | 114.53 | 108.20 |
| 57 | BA | 988 | A | C5-C6-N1 | 7.91 | 121.66 | 117.70 |
| 57 | BA | 2169 | A | C5-C6-N1 | 7.91 | 121.66 | 117.70 |
| 22 | AA | 312 | C | N3-C2-O2 | -7.91 | 116.36 | 121.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | AA | 72 | A | C5-C6-N1 | 7.91 | 121.66 | 117.70 |
| 22 | AA | 95 | C | N3-C2-O2 | -7.91 | 116.36 | 121.90 |
| 23 | A2 | 27 | A | O4'-C1'-N9 | 7.91 | 114.53 | 108.20 |
| 57 | BA | 430 | A | C5-C6-N1 | 7.91 | 121.66 | 117.70 |
| 57 | BA | 699 | A | C5-C6-N1 | 7.91 | 121.66 | 117.70 |
| 57 | BA | 1040 | A | C5-C6-N1 | 7.91 | 121.66 | 117.70 |
| 22 | AA | 306 | A | N1-C6-N6 | -7.91 | 113.86 | 118.60 |
| 22 | AA | 398 | U | O4'-C1'-N1 | 7.91 | 114.53 | 108.20 |
| 22 | AA | 610 | U | N3-C2-O2 | -7.91 | 116.66 | 122.20 |
| 22 | AA | 1146 | A | C5-C6-N1 | 7.91 | 121.65 | 117.70 |
| 57 | BA | 1226 | A | C5-C6-N1 | 7.91 | 121.65 | 117.70 |
| 57 | BA | 1614 | A | C5-C6-N1 | 7.91 | 121.65 | 117.70 |
| 57 | BA | 1678 | A | C5-C6-N1 | 7.91 | 121.65 | 117.70 |
| 57 | BA | 2590 | A | C4-C5-C6 | -7.91 | 113.05 | 117.00 |
| 22 | AA | 1503 | A | N1-C6-N6 | -7.91 | 113.86 | 118.60 |
| 22 | AA | 190 | A | N1-C6-N6 | -7.91 | 113.86 | 118.60 |
| 57 | BA | 1749 | A | N1-C6-N6 | -7.91 | 113.86 | 118.60 |
| 57 | BA | 2510 | C | N3-C2-O2 | -7.91 | 116.37 | 121.90 |
| 22 | AA | 559 | A | C5-C6-N1 | 7.90 | 121.65 | 117.70 |
| 57 | BA | 368 | A | C5-C6-N1 | 7.90 | 121.65 | 117.70 |
| 57 | BA | 1021 | A | C5-C6-N1 | 7.90 | 121.65 | 117.70 |
| 57 | BA | 2052 | A | N1-C6-N6 | -7.90 | 113.86 | 118.60 |
| 57 | BA | 2711 | A | C5-C6-N1 | 7.90 | 121.65 | 117.70 |
| 22 | AA | 1346 | A | C4-C5-C6 | -7.90 | 113.05 | 117.00 |
| 37 | BV | 90 | ARG | NE-CZ-NH1 | 7.90 | 124.25 | 120.30 |
| 57 | BA | 1583 | A | C5-C6-N1 | 7.90 | 121.65 | 117.70 |
| 57 | BA | 2005 | A | C5-C6-N1 | 7.90 | 121.65 | 117.70 |
| 56 | BL | 97 | ARG | NE-CZ-NH1 | 7.90 | 124.25 | 120.30 |
| 22 | AA | 176 | C | N3-C2-O2 | -7.90 | 116.37 | 121.90 |
| 22 | AA | 243 | A | C5-C6-N1 | 7.90 | 121.65 | 117.70 |
| 57 | BA | 693 | A | C5-C6-N1 | 7.90 | 121.65 | 117.70 |
| 57 | BA | 1134 | A | C5-C6-N1 | 7.90 | 121.65 | 117.70 |
| 58 | Ba | 4 | C | N3-C2-O2 | -7.90 | 116.37 | 121.90 |
| 57 | BA | 1794 | A | C5-C6-N1 | 7.90 | 121.65 | 117.70 |
| 22 | AA | 120 | A | C5-C6-N1 | 7.89 | 121.65 | 117.70 |
| 22 | AA | 1289 | A | C5-C6-N1 | 7.89 | 121.65 | 117.70 |
| 57 | BA | 1499 | C | N3-C2-O2 | -7.89 | 116.37 | 121.90 |
| 57 | BA | 323 | C | N1-C2-O2 | 7.89 | 123.64 | 118.90 |
| 57 | BA | 503 | A | C5-C6-N1 | 7.89 | 121.65 | 117.70 |
| 57 | BA | 825 | A | C5-C6-N1 | 7.89 | 121.65 | 117.70 |
| 57 | BA | 863 | A | C5-C6-N1 | 7.89 | 121.65 | 117.70 |
| 57 | BA | 2033 | A | C5-C6-N1 | 7.89 | 121.65 | 117.70 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 2094 | A | C5-C6-N1 | 7.89 | 121.65 | 117.70 |
| 21 | A1 | 228 | ARG | NE-CZ-NH1 | 7.89 | 124.25 | 120.30 |
| 22 | AA | 792 | A | C5-C6-N1 | 7.89 | 121.65 | 117.70 |
| 57 | BA | 1977 | A | N1-C6-N6 | -7.89 | 113.87 | 118.60 |
| 22 | AA | 373 | A | C5-C6-N1 | 7.89 | 121.64 | 117.70 |
| 57 | BA | 718 | A | O4'-C1'-N9 | 7.89 | 114.51 | 108.20 |
| 57 | BA | 1961 | C | N3-C2-O2 | -7.89 | 116.38 | 121.90 |
| 57 | BA | 2366 | A | C5-C6-N1 | 7.89 | 121.64 | 117.70 |
| 22 | AA | 1503 | A | C5-C6-N1 | 7.89 | 121.64 | 117.70 |
| 57 | BA | 144 | A | N1-C6-N6 | -7.89 | 113.87 | 118.60 |
| 57 | BA | 1387 | A | C5-C6-N1 | 7.89 | 121.64 | 117.70 |
| 57 | BA | 829 | A | C5-C6-N1 | 7.88 | 121.64 | 117.70 |
| 57 | BA | 1544 | A | C5-C6-N1 | 7.88 | 121.64 | 117.70 |
| 57 | BA | 2170 | A | C5-C6-N1 | 7.88 | 121.64 | 117.70 |
| 57 | BA | 2521 | C | N3-C2-O2 | -7.88 | 116.38 | 121.90 |
| 58 | Ba | 59 | A | N1-C6-N6 | -7.88 | 113.87 | 118.60 |
| 57 | BA | 671 | C | N3-C2-O2 | -7.88 | 116.38 | 121.90 |
| 57 | BA | 1169 | A | N1-C6-N6 | -7.88 | 113.87 | 118.60 |
| 57 | BA | 1639 | C | O4'-C1'-N1 | 7.88 | 114.50 | 108.20 |
| 57 | BA | 1677 | A | C5-C6-N1 | 7.88 | 121.64 | 117.70 |
| 57 | BA | 2439 | A | C5-C6-N1 | 7.88 | 121.64 | 117.70 |
| 22 | AA | 546 | A | N1-C6-N6 | -7.88 | 113.87 | 118.60 |
| 22 | AA | 595 | A | N1-C6-N6 | -7.88 | 113.87 | 118.60 |
| 57 | BA | 1274 | A | C5-C6-N1 | 7.88 | 121.64 | 117.70 |
| 57 | BA | 1328 | A | N1-C6-N6 | -7.88 | 113.87 | 118.60 |
| 57 | BA | 1575 | C | N3-C2-O2 | -7.88 | 116.38 | 121.90 |
| 57 | BA | 2579 | C | N3-C2-O2 | -7.88 | 116.38 | 121.90 |
| 57 | BA | 2771 | C | N3-C2-O2 | -7.88 | 116.38 | 121.90 |
| 22 | AA | 962 | C | N3-C2-O2 | -7.88 | 116.39 | 121.90 |
| 22 | AA | 1480 | A | C5-C6-N1 | 7.88 | 121.64 | 117.70 |
| 57 | BA | 538 | A | C5-C6-N1 | 7.88 | 121.64 | 117.70 |
| 57 | BA | 2001 | C | N3-C2-O2 | -7.88 | 116.39 | 121.90 |
| 57 | BA | 2347 | C | N3-C2-O2 | -7.88 | 116.39 | 121.90 |
| 57 | BA | 2611 | C | N3-C2-O2 | -7.88 | 116.39 | 121.90 |
| 23 | A2 | 16 | A | C5-C6-N1 | 7.88 | 121.64 | 117.70 |
| 57 | BA | 1244 | A | C5-C6-N1 | 7.88 | 121.64 | 117.70 |
| 58 | Ba | 88 | C | N3-C2-O2 | -7.88 | 116.39 | 121.90 |
| 22 | AA | 73 | C | N3-C2-O2 | -7.88 | 116.39 | 121.90 |
| 57 | BA | 225 | C | N3-C2-O2 | -7.88 | 116.39 | 121.90 |
| 57 | BA | 1237 | A | C5-C6-N1 | 7.88 | 121.64 | 117.70 |
| 22 | AA | 131 | A | O4'-C1'-N9 | 7.87 | 114.50 | 108.20 |
| 22 | AA | 600 | A | C5-C6-N1 | 7.87 | 121.64 | 117.70 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 21 | A1 | 590 | ARG | NE-CZ-NH1 | 7.87 | 124.23 | 120.30 |
| 22 | AA | 178 | C | N3-C2-O2 | -7.87 | 116.39 | 121.90 |
| 57 | BA | 394 | C | N3-C2-O2 | -7.87 | 116.39 | 121.90 |
| 57 | BA | 1528 | A | C5-C6-N1 | 7.87 | 121.64 | 117.70 |
| 57 | BA | 2427 | C | N3-C2-O2 | -7.87 | 116.39 | 121.90 |
| 58 | Ba | 39 | A | C5-C6-N1 | 7.87 | 121.63 | 117.70 |
| 57 | BA | 2813 | A | C5-C6-N1 | 7.87 | 121.63 | 117.70 |
| 57 | BA | 2266 | A | C4-C5-C6 | -7.87 | 113.07 | 117.00 |
| 43 | B1 | 26 | ARG | NE-CZ-NH1 | 7.86 | 124.23 | 120.30 |
| 55 | BH | 94 | ARG | NE-CZ-NH1 | 7.86 | 124.23 | 120.30 |
| 57 | BA | 269 | C | N3-C2-O2 | -7.86 | 116.39 | 121.90 |
| 22 | AA | 412 | A | C5-C6-N1 | 7.86 | 121.63 | 117.70 |
| 54 | BG | 101 | ARG | NE-CZ-NH2 | 7.86 | 124.23 | 120.30 |
| 57 | BA | 689 | A | C5-C6-N1 | 7.86 | 121.63 | 117.70 |
| 57 | BA | 990 | A | C5-C6-N1 | 7.86 | 121.63 | 117.70 |
| 22 | AA | 630 | A | C5-C6-N1 | 7.86 | 121.63 | 117.70 |
| 57 | BA | 227 | A | C4-C5-C6 | -7.86 | 113.07 | 117.00 |
| 57 | BA | 1090 | A | N1-C6-N6 | -7.86 | 113.89 | 118.60 |
| 22 | AA | 395 | C | N3-C2-O2 | -7.86 | 116.40 | 121.90 |
| 22 | AA | 1299 | A | C5-C6-N1 | 7.86 | 121.63 | 117.70 |
| 22 | AA | 1508 | A | C5-C6-N1 | 7.86 | 121.63 | 117.70 |
| 57 | BA | 53 | A | C5-C6-N1 | 7.86 | 121.63 | 117.70 |
| 58 | Ba | 25 | U | O4'-C1'-N1 | 7.86 | 114.49 | 108.20 |
| 2 | AK | 126 | ARG | NE-CZ-NH2 | -7.86 | 116.37 | 120.30 |
| 22 | AA | 174 | A | C5-C6-N1 | 7.86 | 121.63 | 117.70 |
| 22 | AA | 865 | A | N1-C6-N6 | -7.86 | 113.89 | 118.60 |
| 22 | AA | 1169 | A | C5-C6-N1 | 7.86 | 121.63 | 117.70 |
| 57 | BA | 63 | A | C5-C6-N1 | 7.85 | 121.63 | 117.70 |
| 22 | AA | 536 | C | N3-C2-O2 | -7.85 | 116.40 | 121.90 |
| 26 | BJ | 45 | ARG | NE-CZ-NH1 | 7.85 | 124.23 | 120.30 |
| 57 | BA | 998 | C | N3-C2-O2 | -7.85 | 116.40 | 121.90 |
| 57 | BA | 1308 | A | C5-C6-N1 | 7.85 | 121.63 | 117.70 |
| 57 | BA | 2717 | C | N3-C2-O2 | -7.85 | 116.40 | 121.90 |
| 57 | BA | 412 | A | C5-C6-N1 | 7.85 | 121.63 | 117.70 |
| 57 | BA | 1591 | A | N1-C6-N6 | -7.85 | 113.89 | 118.60 |
| 57 | BA | 2215 | C | N3-C2-O2 | -7.85 | 116.40 | 121.90 |
| 22 | AA | 1005 | A | C5-C6-N1 | 7.85 | 121.62 | 117.70 |
| 23 | A2 | 16 | A | O4'-C1'-N9 | 7.85 | 114.48 | 108.20 |
| 23 | A2 | 59 | A | C5-C6-N1 | 7.85 | 121.62 | 117.70 |
| 54 | BG | 109 | ARG | NE-CZ-NH2 | 7.85 | 124.22 | 120.30 |
| 57 | BA | 1772 | A | C5-C6-N1 | 7.85 | 121.62 | 117.70 |
| 22 | AA | 1114 | C | N3-C2-O2 | -7.85 | 116.41 | 121.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 1286 | A | C5-C6-N1 | 7.85 | 121.62 | 117.70 |
| 58 | Ba | 78 | A | C4-C5-C6 | -7.85 | 113.08 | 117.00 |
| 57 | BA | 1453 | A | C5-C6-N1 | 7.85 | 121.62 | 117.70 |
| 18 | AG | 94 | ARG | NE-CZ-NH1 | 7.84 | 124.22 | 120.30 |
| 57 | BA | 2147 | A | N1-C6-N6 | -7.84 | 113.89 | 118.60 |
| 24 | A3 | 16 | C | N1-C2-O2 | 7.84 | 123.61 | 118.90 |
| 57 | BA | 1564 | C | N3-C2-O2 | -7.84 | 116.41 | 121.90 |
| 22 | AA | 607 | A | C5-C6-N1 | 7.84 | 121.62 | 117.70 |
| 22 | AA | 1118 | U | C5'-C4'-C3' | -7.84 | 103.45 | 116.00 |
| 57 | BA | 1634 | A | N1-C6-N6 | -7.84 | 113.89 | 118.60 |
| 57 | BA | 487 | C | N3-C2-O2 | -7.84 | 116.41 | 121.90 |
| 57 | BA | 2620 | C | N3-C2-O2 | -7.84 | 116.41 | 121.90 |
| 18 | AG | 69 | ARG | NE-CZ-NH1 | 7.84 | 124.22 | 120.30 |
| 22 | AA | 872 | A | O4'-C1'-N9 | 7.84 | 114.47 | 108.20 |
| 57 | BA | 900 | A | C5-C6-N1 | 7.84 | 121.62 | 117.70 |
| 22 | AA | 308 | C | N3-C2-O2 | -7.83 | 116.42 | 121.90 |
| 57 | BA | 141 | G | O4'-C1'-N9 | 7.83 | 114.47 | 108.20 |
| 22 | AA | 274 | A | C5-C6-N1 | 7.83 | 121.62 | 117.70 |
| 57 | BA | 94 | A | C5-C6-N1 | 7.83 | 121.62 | 117.70 |
| 57 | BA | 522 | A | N1-C6-N6 | -7.83 | 113.90 | 118.60 |
| 57 | BA | 706 | A | N1-C6-N6 | -7.83 | 113.90 | 118.60 |
| 22 | AA | 1035 | A | C5-C6-N1 | 7.83 | 121.62 | 117.70 |
| 43 | B1 | 36 | ARG | NE-CZ-NH2 | 7.83 | 124.22 | 120.30 |
| 57 | BA | 300 | A | C5-C6-N1 | 7.83 | 121.62 | 117.70 |
| 22 | AA | 382 | A | C5-C6-N1 | 7.83 | 121.61 | 117.70 |
| 57 | BA | 483 | A | N1-C6-N6 | -7.83 | 113.90 | 118.60 |
| 57 | BA | 2899 | A | C5-C6-N1 | 7.83 | 121.61 | 117.70 |
| 15 | AD | 153 | ARG | NE-CZ-NH1 | 7.83 | 124.21 | 120.30 |
| 22 | AA | 864 | A | C5-C6-N1 | 7.83 | 121.61 | 117.70 |
| 22 | AA | 149 | A | C5-C6-N1 | 7.83 | 121.61 | 117.70 |
| 22 | AA | 583 | A | C5-C6-N1 | 7.83 | 121.61 | 117.70 |
| 22 | AA | 1163 | A | C5-C6-N1 | 7.83 | 121.61 | 117.70 |
| 57 | BA | 574 | A | C5-C6-N1 | 7.83 | 121.61 | 117.70 |
| 57 | BA | 987 | C | N3-C2-O2 | -7.83 | 116.42 | 121.90 |
| 57 | BA | 2448 | A | C5-C6-N1 | 7.83 | 121.61 | 117.70 |
| 22 | AA | 1141 | C | N3-C2-O2 | -7.82 | 116.42 | 121.90 |
| 57 | BA | 2632 | A | C5-C6-N1 | 7.82 | 121.61 | 117.70 |
| 23 | A2 | 17 | U | O4'-C1'-N1 | 7.82 | 114.46 | 108.20 |
| 57 | BA | 944 | C | O4'-C1'-N1 | 7.82 | 114.46 | 108.20 |
| 57 | BA | 2122 | U | O4'-C1'-N1 | 7.82 | 114.46 | 108.20 |
| 22 | AA | 840 | C | N3-C2-O2 | -7.82 | 116.43 | 121.90 |
| 22 | AA | 1394 | A | C5-C6-N1 | 7.82 | 121.61 | 117.70 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 181 | A | C5-C6-N1 | 7.82 | 121.61 | 117.70 |
| 57 | BA | 1801 | A | C5-C6-N1 | 7.82 | 121.61 | 117.70 |
| 57 | BA | 1336 | A | C5-C6-N1 | 7.82 | 121.61 | 117.70 |
| 57 | BA | 2060 | A | C5-C6-N1 | 7.82 | 121.61 | 117.70 |
| 57 | BA | 2443 | C | N3-C2-O2 | -7.82 | 116.43 | 121.90 |
| 22 | AA | 284 | C | N3-C2-O2 | -7.82 | 116.43 | 121.90 |
| 57 | BA | 203 | A | N1-C6-N6 | -7.82 | 113.91 | 118.60 |
| 57 | BA | 2547 | A | N1-C6-N6 | -7.82 | 113.91 | 118.60 |
| 22 | AA | 706 | A | C5-C6-N1 | 7.81 | 121.61 | 117.70 |
| 57 | BA | 873 | C | N3-C2-O2 | -7.81 | 116.43 | 121.90 |
| 57 | BA | 2009 | A | N1-C6-N6 | -7.81 | 113.91 | 118.60 |
| 22 | AA | 546 | A | C5-C6-N1 | 7.81 | 121.61 | 117.70 |
| 58 | Ba | 90 | C | N3-C2-O2 | -7.81 | 116.43 | 121.90 |
| 57 | BA | 1382 | G | O4'-C1'-N9 | 7.81 | 114.45 | 108.20 |
| 22 | AA | 66 | A | C5-C6-N1 | 7.81 | 121.61 | 117.70 |
| 22 | AA | 1322 | C | N1-C2-O2 | 7.81 | 123.58 | 118.90 |
| 57 | BA | 210 | C | N3-C2-O2 | -7.81 | 116.43 | 121.90 |
| 57 | BA | 1273 | U | O4'-C1'-N1 | 7.81 | 114.45 | 108.20 |
| 57 | BA | 1569 | A | C4-C5-C6 | -7.81 | 113.09 | 117.00 |
| 2 | AK | 55 | ARG | NE-CZ-NH1 | 7.81 | 124.20 | 120.30 |
| 22 | AA | 704 | A | C4-C5-C6 | -7.81 | 113.10 | 117.00 |
| 57 | BA | 1732 | C | N3-C2-O2 | -7.81 | 116.44 | 121.90 |
| 22 | AA | 1446 | A | C5-C6-N1 | 7.81 | 121.60 | 117.70 |
| 57 | BA | 497 | A | C5-C6-N1 | 7.81 | 121.60 | 117.70 |
| 57 | BA | 104 | A | C5-C6-N1 | 7.80 | 121.60 | 117.70 |
| 57 | BA | 2773 | C | N3-C2-O2 | -7.80 | 116.44 | 121.90 |
| 22 | AA | 236 | A | C5-C6-N1 | 7.80 | 121.60 | 117.70 |
| 29 | BO | 98 | ARG | NE-CZ-NH1 | 7.80 | 124.20 | 120.30 |
| 22 | AA | 1296 | C | N3-C2-O2 | -7.80 | 116.44 | 121.90 |
| 57 | BA | 1365 | A | C5-C6-N1 | 7.80 | 121.60 | 117.70 |
| 22 | AA | 1501 | C | N3-C2-O2 | -7.80 | 116.44 | 121.90 |
| 58 | Ba | 93 | C | N3-C2-O2 | -7.80 | 116.44 | 121.90 |
| 22 | AA | 675 | A | C5-C6-N1 | 7.80 | 121.60 | 117.70 |
| 22 | AA | 998 | C | N3-C2-O2 | -7.80 | 116.44 | 121.90 |
| 57 | BA | 2366 | A | N1-C6-N6 | -7.80 | 113.92 | 118.60 |
| 22 | AA | 1251 | A | N1-C6-N6 | -7.80 | 113.92 | 118.60 |
| 57 | BA | 161 | A | C5-C6-N1 | 7.80 | 121.60 | 117.70 |
| 57 | BA | 627 | A | N1-C6-N6 | -7.80 | 113.92 | 118.60 |
| 57 | BA | 740 | C | N3-C2-O2 | -7.79 | 116.44 | 121.90 |
| 57 | BA | 742 | A | N1-C6-N6 | -7.79 | 113.92 | 118.60 |
| 57 | BA | 814 | C | N3-C2-O2 | -7.79 | 116.44 | 121.90 |
| 57 | BA | 1029 | A | N1-C6-N6 | -7.79 | 113.92 | 118.60 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | AA | 511 | C | N3-C2-O2 | -7.79 | 116.45 | 121.90 |
| 57 | BA | 270 | A | C5-C6-N1 | 7.79 | 121.60 | 117.70 |
| 57 | BA | 482 | A | N1-C6-N6 | -7.79 | 113.92 | 118.60 |
| 23 | A2 | 13 | A | C5-C6-N1 | 7.79 | 121.59 | 117.70 |
| 57 | BA | 1305 | C | O4'-C1'-N1 | 7.79 | 114.43 | 108.20 |
| 57 | BA | 14 | A | C5-C6-N1 | 7.79 | 121.59 | 117.70 |
| 57 | BA | 1552 | A | C5-C6-N1 | 7.79 | 121.59 | 117.70 |
| 57 | BA | 1605 | C | N3-C2-O2 | -7.79 | 116.45 | 121.90 |
| 57 | BA | 1638 | C | N3-C2-O2 | -7.79 | 116.45 | 121.90 |
| 22 | AA | 1042 | A | C5-C6-N1 | 7.79 | 121.59 | 117.70 |
| 22 | AA | 1520 | C | N3-C2-O2 | -7.79 | 116.45 | 121.90 |
| 22 | AA | 1524 | C | N3-C2-O2 | -7.79 | 116.45 | 121.90 |
| 22 | AA | 329 | A | N1-C6-N6 | -7.79 | 113.93 | 118.60 |
| 57 | BA | 1890 | A | C5-C6-N1 | 7.79 | 121.59 | 117.70 |
| 57 | BA | 2416 | C | N3-C2-O2 | -7.79 | 116.45 | 121.90 |
| 22 | AA | 152 | A | C4-C5-C6 | -7.78 | 113.11 | 117.00 |
| 22 | AA | 448 | A | C5-C6-N1 | 7.78 | 121.59 | 117.70 |
| 24 | A3 | 75 | C | N3-C2-O2 | -7.78 | 116.45 | 121.90 |
| 57 | BA | 262 | A | C5-C6-N1 | 7.78 | 121.59 | 117.70 |
| 57 | BA | 623 | C | N3-C2-O2 | -7.78 | 116.45 | 121.90 |
| 57 | BA | 761 | A | C5-C6-N1 | 7.78 | 121.59 | 117.70 |
| 57 | BA | 1596 | A | C5-C6-N1 | 7.78 | 121.59 | 117.70 |
| 58 | Ba | 50 | A | C5-C6-N1 | 7.78 | 121.59 | 117.70 |
| 22 | AA | 432 | A | C5-C6-N1 | 7.78 | 121.59 | 117.70 |
| 22 | AA | 845 | A | C5-C6-N1 | 7.78 | 121.59 | 117.70 |
| 22 | AA | 969 | A | C5-C6-N1 | 7.78 | 121.59 | 117.70 |
| 22 | AA | 1036 | A | C5-C6-N1 | 7.78 | 121.59 | 117.70 |
| 57 | BA | 1938 | A | C5-C6-N1 | 7.78 | 121.59 | 117.70 |
| 22 | AA | 143 | A | N1-C6-N6 | -7.78 | 113.93 | 118.60 |
| 22 | AA | 163 | C | N3-C2-O2 | -7.78 | 116.46 | 121.90 |
| 57 | BA | 614 | A | C5-C6-N1 | 7.78 | 121.59 | 117.70 |
| 57 | BA | 2565 | A | C5-C6-N1 | 7.78 | 121.59 | 117.70 |
| 57 | BA | 2761 | A | C5-C6-N1 | 7.78 | 121.59 | 117.70 |
| 21 | A1 | 622 | ARG | NE-CZ-NH1 | 7.78 | 124.19 | 120.30 |
| 57 | BA | 666 | A | C5-C6-N1 | 7.78 | 121.59 | 117.70 |
| 57 | BA | 1054 | A | N1-C6-N6 | -7.78 | 113.94 | 118.60 |
| 58 | Ba | 66 | A | N1-C6-N6 | -7.78 | 113.93 | 118.60 |
| 22 | AA | 466 | A | C5-C6-N1 | 7.77 | 121.59 | 117.70 |
| 22 | AA | 913 | A | C5-C6-N1 | 7.77 | 121.59 | 117.70 |
| 22 | AA | 1418 | A | N1-C6-N6 | -7.77 | 113.94 | 118.60 |
| 22 | AA | 1443 | C | N3-C2-O2 | -7.77 | 116.46 | 121.90 |
| 57 | BA | 1151 | A | N1-C6-N6 | -7.77 | 113.94 | 118.60 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 1578 | U | O4'-C1'-N1 | 7.77 | 114.42 | 108.20 |
| 57 | BA | 2207 | C | N3-C2-O2 | -7.77 | 116.46 | 121.90 |
| 22 | AA | 873 | A | C5-C6-N1 | 7.77 | 121.58 | 117.70 |
| 57 | BA | 2095 | A | C5-C6-N1 | 7.77 | 121.59 | 117.70 |
| 22 | AA | 510 | A | C5-C6-N1 | 7.77 | 121.58 | 117.70 |
| 24 | A3 | 73 | A | C5-C6-N1 | 7.77 | 121.58 | 117.70 |
| 57 | BA | 986 | C | N3-C2-O2 | -7.77 | 116.46 | 121.90 |
| 57 | BA | 1794 | A | N1-C6-N6 | -7.77 | 113.94 | 118.60 |
| 57 | BA | 1808 | A | C5-C6-N1 | 7.77 | 121.58 | 117.70 |
| 22 | AA | 994 | A | N1-C6-N6 | -7.77 | 113.94 | 118.60 |
| 57 | BA | 1745 | A | C5-C6-N1 | 7.77 | 121.58 | 117.70 |
| 22 | AA | 1496 | C | N3-C2-O2 | -7.76 | 116.46 | 121.90 |
| 26 | BJ | 152 | ARG | NE-CZ-NH1 | 7.76 | 124.18 | 120.30 |
| 57 | BA | 428 | A | C5-C6-N1 | 7.76 | 121.58 | 117.70 |
| 57 | BA | 575 | A | C4-C5-C6 | -7.76 | 113.12 | 117.00 |
| 57 | BA | 846 | U | O4'-C1'-N1 | 7.76 | 114.41 | 108.20 |
| 57 | BA | 1502 | A | C5-C6-N1 | 7.76 | 121.58 | 117.70 |
| 22 | AA | 492 | C | N3-C2-O2 | -7.76 | 116.47 | 121.90 |
| 57 | BA | 1254 | A | C5-C6-N1 | 7.76 | 121.58 | 117.70 |
| 57 | BA | 1354 | A | C5-C6-N1 | 7.76 | 121.58 | 117.70 |
| 57 | BA | 1970 | A | C5-C6-N1 | 7.76 | 121.58 | 117.70 |
| 57 | BA | 2475 | C | N3-C2-O2 | -7.76 | 116.47 | 121.90 |
| 22 | AA | 44 | A | N1-C6-N6 | -7.76 | 113.94 | 118.60 |
| 22 | AA | 279 | A | C5-C6-N1 | 7.76 | 121.58 | 117.70 |
| 57 | BA | 1321 | A | C5-C6-N1 | 7.76 | 121.58 | 117.70 |
| 57 | BA | 1632 | A | C5-C6-N1 | 7.76 | 121.58 | 117.70 |
| 58 | Ba | 46 | A | C5-C6-N1 | 7.76 | 121.58 | 117.70 |
| 57 | BA | 676 | A | C5-C6-N1 | 7.76 | 121.58 | 117.70 |
| 57 | BA | 1032 | A | N1-C6-N6 | -7.76 | 113.94 | 118.60 |
| 57 | BA | 1967 | C | N3-C2-O2 | -7.76 | 116.47 | 121.90 |
| 57 | BA | 2346 | A | C5-C6-N1 | 7.76 | 121.58 | 117.70 |
| 57 | BA | 2665 | A | N1-C6-N6 | -7.76 | 113.94 | 118.60 |
| 57 | BA | 739 | A | C5-C6-N1 | 7.76 | 121.58 | 117.70 |
| 57 | BA | 2008 | C | O4'-C1'-N1 | 7.76 | 114.41 | 108.20 |
| 22 | AA | 139 | A | C5-C6-N1 | 7.76 | 121.58 | 117.70 |
| 22 | AA | 643 | C | N3-C2-O2 | -7.76 | 116.47 | 121.90 |
| 57 | BA | 227 | A | C5-C6-N1 | 7.76 | 121.58 | 117.70 |
| 57 | BA | 995 | C | N3-C2-O2 | -7.76 | 116.47 | 121.90 |
| 57 | BA | 2307 | G | O4'-C1'-N9 | 7.76 | 114.41 | 108.20 |
| 57 | BA | 1885 | A | N1-C6-N6 | -7.75 | 113.95 | 118.60 |
| 22 | AA | 1219 | A | N1-C6-N6 | -7.75 | 113.95 | 118.60 |
| 57 | BA | 190 | A | C5-C6-N1 | 7.75 | 121.58 | 117.70 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 2725 | A | N1-C6-N6 | -7.75 | 113.95 | 118.60 |
| 25 | BC | 12 | ARG | NE-CZ-NH1 | 7.75 | 124.17 | 120.30 |
| 57 | BA | 1876 | A | C5-C6-N1 | 7.75 | 121.58 | 117.70 |
| 22 | AA | 1252 | A | C5-C6-N1 | 7.75 | 121.58 | 117.70 |
| 23 | A2 | 41 | A | C5-C6-N1 | 7.75 | 121.58 | 117.70 |
| 57 | BA | 1092 | C | N3-C2-O2 | -7.75 | 116.47 | 121.90 |
| 57 | BA | 1508 | A | C5-C6-N1 | 7.75 | 121.58 | 117.70 |
| 57 | BA | 1553 | A | C5-C6-N1 | 7.75 | 121.58 | 117.70 |
| 57 | BA | 1773 | A | C5-C6-N1 | 7.75 | 121.58 | 117.70 |
| 24 | A3 | 59 | A | C5-C6-N1 | 7.75 | 121.58 | 117.70 |
| 57 | BA | 608 | A | C5-C6-N1 | 7.75 | 121.57 | 117.70 |
| 57 | BA | 947 | A | N1-C6-N6 | -7.75 | 113.95 | 118.60 |
| 57 | BA | 1509 | A | C5-C6-N1 | 7.75 | 121.57 | 117.70 |
| 19 | AH | 76 | ARG | NE-CZ-NH1 | 7.75 | 124.17 | 120.30 |
| 57 | BA | 144 | A | C5-C6-N1 | 7.75 | 121.57 | 117.70 |
| 22 | AA | 123 | U | O4'-C1'-N1 | 7.75 | 114.40 | 108.20 |
| 57 | BA | 2222 | C | N3-C2-O2 | -7.75 | 116.48 | 121.90 |
| 24 | A3 | 70 | C | N3-C2-O2 | -7.74 | 116.48 | 121.90 |
| 50 | B7 | 19 | ARG | NE-CZ-NH2 | 7.74 | 124.17 | 120.30 |
| 57 | BA | 724 | U | O4'-C1'-N1 | 7.74 | 114.40 | 108.20 |
| 57 | BA | 2014 | A | C5-C6-N1 | 7.74 | 121.57 | 117.70 |
| 22 | AA | 167 | A | C5-C6-N1 | 7.74 | 121.57 | 117.70 |
| 57 | BA | 299 | A | C5-C6-N1 | 7.74 | 121.57 | 117.70 |
| 57 | BA | 195 | A | C5-C6-N1 | 7.74 | 121.57 | 117.70 |
| 57 | BA | 1936 | A | C5-C6-N1 | 7.74 | 121.57 | 117.70 |
| 57 | BA | 2661 | G | O4'-C1'-N9 | 7.74 | 114.39 | 108.20 |
| 57 | BA | 2873 | A | C5-C6-N1 | 7.74 | 121.57 | 117.70 |
| 57 | BA | 2873 | A | O4'-C1'-N9 | 7.74 | 114.39 | 108.20 |
| 22 | AA | 1059 | C | N3-C2-O2 | -7.74 | 116.48 | 121.90 |
| 22 | AA | 802 | A | C5-C6-N1 | 7.74 | 121.57 | 117.70 |
| 22 | AA | 1229 | A | C5-C6-N1 | 7.74 | 121.57 | 117.70 |
| 24 | A3 | 13 | C | N3-C2-O2 | -7.74 | 116.48 | 121.90 |
| 57 | BA | 2856 | A | C5-C6-N1 | 7.74 | 121.57 | 117.70 |
| 22 | AA | 901 | A | C5-C6-N1 | 7.74 | 121.57 | 117.70 |
| 22 | AA | 1132 | C | N3-C2-O2 | -7.74 | 116.48 | 121.90 |
| 22 | AA | 1201 | A | C5-C6-N1 | 7.74 | 121.57 | 117.70 |
| 22 | AA | 1493 | A | C5-C6-N1 | 7.74 | 121.57 | 117.70 |
| 24 | A3 | 60 | A | C5-C6-N1 | 7.74 | 121.57 | 117.70 |
| 24 | A3 | 72 | C | N3-C2-O2 | -7.74 | 116.48 | 121.90 |
| 57 | BA | 179 | C | N3-C2-O2 | -7.74 | 116.48 | 121.90 |
| 57 | BA | 482 | A | C5-C6-N1 | 7.74 | 121.57 | 117.70 |
| 57 | BA | 996 | A | N1-C6-N6 | -7.74 | 113.96 | 118.60 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 1118 | C | N3-C2-O2 | -7.74 | 116.48 | 121.90 |
| 57 | BA | 1133 | A | C4-C5-C6 | -7.74 | 113.13 | 117.00 |
| 57 | BA | 2406 | A | C5-C6-N1 | 7.74 | 121.57 | 117.70 |
| 57 | BA | 2736 | A | C5-C6-N1 | 7.74 | 121.57 | 117.70 |
| 24 | A3 | 45 | A | C5-C6-N1 | 7.73 | 121.57 | 117.70 |
| 57 | BA | 820 | A | C5-C6-N1 | 7.73 | 121.57 | 117.70 |
| 22 | AA | 841 | C | N3-C2-O2 | -7.73 | 116.49 | 121.90 |
| 22 | AA | 1408 | A | C5-C6-N1 | 7.73 | 121.57 | 117.70 |
| 57 | BA | 422 | A | C5-C6-N1 | 7.73 | 121.57 | 117.70 |
| 57 | BA | 693 | A | N1-C6-N6 | -7.73 | 113.96 | 118.60 |
| 57 | BA | 921 | C | N3-C2-O2 | -7.73 | 116.49 | 121.90 |
| 57 | BA | 1156 | A | C5-C6-N1 | 7.73 | 121.57 | 117.70 |
| 57 | BA | 1264 | A | N1-C6-N6 | -7.73 | 113.96 | 118.60 |
| 57 | BA | 6 | A | N1-C6-N6 | -7.73 | 113.96 | 118.60 |
| 22 | AA | 819 | A | C5-C6-N1 | 7.73 | 121.56 | 117.70 |
| 57 | BA | 817 | C | N3-C2-O2 | -7.73 | 116.49 | 121.90 |
| 24 | A3 | 39 | A | C5-C6-N1 | 7.73 | 121.56 | 117.70 |
| 57 | BA | 362 | A | C5-C6-N1 | 7.73 | 121.56 | 117.70 |
| 57 | BA | 453 | A | C5-C6-N1 | 7.73 | 121.56 | 117.70 |
| 22 | AA | 52 | C | N3-C2-O2 | -7.73 | 116.49 | 121.90 |
| 22 | AA | 1465 | A | C5-C6-N1 | 7.73 | 121.56 | 117.70 |
| 22 | AA | 514 | C | N3-C2-O2 | -7.72 | 116.49 | 121.90 |
| 57 | BA | 219 | A | C5-C6-N1 | 7.72 | 121.56 | 117.70 |
| 22 | AA | 655 | A | N1-C6-N6 | -7.72 | 113.97 | 118.60 |
| 30 | BP | 59 | ARG | NE-CZ-NH1 | 7.72 | 124.16 | 120.30 |
| 22 | AA | 1082 | A | N1-C6-N6 | -7.72 | 113.97 | 118.60 |
| 24 | A3 | 47 | A | C5-C6-N1 | 7.72 | 121.56 | 117.70 |
| 57 | BA | 84 | A | C5-C6-N1 | 7.72 | 121.56 | 117.70 |
| 22 | AA | 7 | A | C5-C6-N1 | 7.72 | 121.56 | 117.70 |
| 22 | AA | 223 | A | C5-C6-N1 | 7.72 | 121.56 | 117.70 |
| 22 | AA | 418 | C | N3-C2-O2 | -7.72 | 116.50 | 121.90 |
| 22 | AA | 477 | C | N3-C2-O2 | -7.72 | 116.50 | 121.90 |
| 22 | AA | 286 | C | N3-C2-O2 | -7.71 | 116.50 | 121.90 |
| 22 | AA | 419 | C | N3-C2-O2 | -7.71 | 116.50 | 121.90 |
| 22 | AA | 1314 | C | N3-C2-O2 | -7.71 | 116.50 | 121.90 |
| 24 | A3 | 1 | C | O4'-C1'-N1 | 7.71 | 114.37 | 108.20 |
| 24 | A3 | 44 | A | C5-C6-N1 | 7.71 | 121.56 | 117.70 |
| 57 | BA | 848 | C | N3-C2-O2 | -7.71 | 116.50 | 121.90 |
| 22 | AA | 1479 | C | N3-C2-O2 | -7.71 | 116.50 | 121.90 |
| 57 | BA | 316 | C | N3-C2-O2 | -7.71 | 116.50 | 121.90 |
| 57 | BA | 2160 | C | N3-C2-O2 | -7.71 | 116.50 | 121.90 |
| 57 | BA | 1241 | A | C5-C6-N1 | 7.71 | 121.56 | 117.70 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 1323 | C | O4'-C1'-N1 | 7.71 | 114.37 | 108.20 |
| 57 | BA | 2740 | A | C5-C6-N1 | 7.71 | 121.56 | 117.70 |
| 24 | A3 | 58 | A | C5-C6-N1 | 7.71 | 121.56 | 117.70 |
| 22 | AA | 78 | A | C5-C6-N1 | 7.71 | 121.55 | 117.70 |
| 22 | AA | 1218 | C | N3-C2-O2 | -7.71 | 116.50 | 121.90 |
| 22 | AA | 1389 | C | N3-C2-O2 | -7.71 | 116.50 | 121.90 |
| 57 | BA | 255 | A | N1-C6-N6 | -7.71 | 113.97 | 118.60 |
| 57 | BA | 790 | U | N3-C2-O2 | -7.71 | 116.80 | 122.20 |
| 22 | AA | 478 | A | N1-C6-N6 | -7.71 | 113.98 | 118.60 |
| 22 | AA | 595 | A | C5-C6-N1 | 7.71 | 121.55 | 117.70 |
| 22 | AA | 1105 | A | C5-C6-N1 | 7.71 | 121.55 | 117.70 |
| 22 | AA | 1362 | A | C5-C6-N1 | 7.71 | 121.55 | 117.70 |
| 57 | BA | 479 | A | C5-C6-N1 | 7.71 | 121.55 | 117.70 |
| 57 | BA | 816 | C | N3-C2-O2 | -7.71 | 116.51 | 121.90 |
| 57 | BA | 532 | A | C5-C6-N1 | 7.71 | 121.55 | 117.70 |
| 57 | BA | 2707 | U | O4'-C1'-N1 | 7.71 | 114.36 | 108.20 |
| 57 | BA | 118 | A | C5-C6-N1 | 7.70 | 121.55 | 117.70 |
| 57 | BA | 1535 | A | C5-C6-N1 | 7.70 | 121.55 | 117.70 |
| 57 | BA | 2176 | A | C5-C6-N1 | 7.70 | 121.55 | 117.70 |
| 57 | BA | 2547 | A | C5-C6-N1 | 7.70 | 121.55 | 117.70 |
| 22 | AA | 919 | A | C5-C6-N1 | 7.70 | 121.55 | 117.70 |
| 22 | AA | 1038 | C | N3-C2-O2 | -7.70 | 116.51 | 121.90 |
| 22 | AA | 1256 | A | C5-C6-N1 | 7.70 | 121.55 | 117.70 |
| 44 | B2 | 52 | ARG | NE-CZ-NH2 | 7.70 | 124.15 | 120.30 |
| 57 | BA | 443 | A | C5-C6-N1 | 7.70 | 121.55 | 117.70 |
| 57 | BA | 547 | A | C5-C6-N1 | 7.70 | 121.55 | 117.70 |
| 57 | BA | 1013 | C | N3-C2-O2 | -7.70 | 116.51 | 121.90 |
| 57 | BA | 1454 | C | N1-C2-O2 | 7.70 | 123.52 | 118.90 |
| 57 | BA | 1746 | A | C5-C6-N1 | 7.70 | 121.55 | 117.70 |
| 57 | BA | 2772 | C | N3-C2-O2 | -7.70 | 116.51 | 121.90 |
| 22 | AA | 414 | A | C5-C6-N1 | 7.70 | 121.55 | 117.70 |
| 22 | AA | 441 | A | C5-C6-N1 | 7.70 | 121.55 | 117.70 |
| 23 | A2 | 55 | A | C5-C6-N1 | 7.70 | 121.55 | 117.70 |
| 57 | BA | 1420 | A | C5-C6-N1 | 7.70 | 121.55 | 117.70 |
| 57 | BA | 1270 | C | N3-C2-O2 | -7.70 | 116.51 | 121.90 |
| 22 | AA | 1148 | U | O4'-C1'-N1 | 7.70 | 114.36 | 108.20 |
| 57 | BA | 2496 | C | N3-C2-O2 | -7.70 | 116.51 | 121.90 |
| 11 | AB | 20 | ARG | NE-CZ-NH1 | 7.69 | 124.15 | 120.30 |
| 22 | AA | 907 | A | C5-C6-N1 | 7.69 | 121.55 | 117.70 |
| 57 | BA | 2820 | A | N1-C6-N6 | -7.69 | 113.98 | 118.60 |
| 22 | AA | 574 | A | C4-C5-C6 | -7.69 | 113.16 | 117.00 |
| 57 | BA | 156 | A | C5-C6-N1 | 7.69 | 121.54 | 117.70 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 927 | A | C5-C6-N1 | 7.69 | 121.54 | 117.70 |
| 57 | BA | 1221 | C | N3-C2-O2 | -7.69 | 116.52 | 121.90 |
| 57 | BA | 1630 | A | C5-C6-N1 | 7.69 | 121.54 | 117.70 |
| 57 | BA | 2675 | A | C5-C6-N1 | 7.69 | 121.54 | 117.70 |
| 1 | AJ | 9 | ARG | NE-CZ-NH1 | 7.69 | 124.14 | 120.30 |
| 22 | AA | 522 | C | N3-C2-O2 | -7.69 | 116.52 | 121.90 |
| 57 | BA | 2364 | C | N3-C2-O2 | -7.69 | 116.52 | 121.90 |
| 58 | Ba | 31 | C | N3-C2-O2 | -7.69 | 116.52 | 121.90 |
| 22 | AA | 503 | C | N3-C2-O2 | -7.68 | 116.52 | 121.90 |
| 22 | AA | 535 | A | C5-C6-N1 | 7.68 | 121.54 | 117.70 |
| 22 | AA | 1067 | A | C4-C5-C6 | -7.68 | 113.16 | 117.00 |
| 22 | AA | 1170 | A | C5-C6-N1 | 7.68 | 121.54 | 117.70 |
| 22 | AA | 816 | A | C5-C6-N1 | 7.68 | 121.54 | 117.70 |
| 57 | BA | 1127 | A | C5-C6-N1 | 7.68 | 121.54 | 117.70 |
| 57 | BA | 1155 | A | C4-C5-C6 | -7.68 | 113.16 | 117.00 |
| 57 | BA | 246 | C | N3-C2-O2 | -7.68 | 116.52 | 121.90 |
| 22 | AA | 790 | A | C5-C6-N1 | 7.68 | 121.54 | 117.70 |
| 57 | BA | 348 | A | C5-C6-N1 | 7.68 | 121.54 | 117.70 |
| 57 | BA | 1541 | C | N3-C2-O2 | -7.68 | 116.53 | 121.90 |
| 57 | BA | 2037 | A | N1-C6-N6 | -7.68 | 113.99 | 118.60 |
| 57 | BA | 2301 | C | N3-C2-O2 | -7.68 | 116.53 | 121.90 |
| 22 | AA | 8 | A | C5-C6-N1 | 7.68 | 121.54 | 117.70 |
| 57 | BA | 1561 | C | N3-C2-O2 | -7.68 | 116.53 | 121.90 |
| 57 | BA | 2066 | C | N3-C2-O2 | -7.68 | 116.53 | 121.90 |
| 57 | BA | 2278 | A | C4-C5-C6 | -7.68 | 113.16 | 117.00 |
| 22 | AA | 706 | A | N1-C6-N6 | -7.68 | 113.99 | 118.60 |
| 57 | BA | 1864 | U | O4'-C1'-N1 | 7.68 | 114.34 | 108.20 |
| 57 | BA | 2456 | C | N3-C2-O2 | -7.68 | 116.53 | 121.90 |
| 57 | BA | 2591 | C | N3-C2-O2 | -7.68 | 116.53 | 121.90 |
| 57 | BA | 2598 | A | C5-C6-N1 | 7.68 | 121.54 | 117.70 |
| 22 | AA | 923 | A | C5-C6-N1 | 7.67 | 121.54 | 117.70 |
| 22 | AA | 1500 | A | C5-C6-N1 | 7.67 | 121.54 | 117.70 |
| 24 | A3 | 45 | A | N1-C6-N6 | -7.67 | 114.00 | 118.60 |
| 57 | BA | 404 | A | C5-C6-N1 | 7.67 | 121.54 | 117.70 |
| 57 | BA | 716 | A | C5-C6-N1 | 7.67 | 121.54 | 117.70 |
| 57 | BA | 2163 | A | C5-C6-N1 | 7.67 | 121.54 | 117.70 |
| 57 | BA | 2540 | C | N3-C2-O2 | -7.67 | 116.53 | 121.90 |
| 58 | Ba | 11 | C | O4'-C1'-N1 | 7.67 | 114.34 | 108.20 |
| 58 | Ba | 60 | C | N3-C2-O2 | -7.67 | 116.53 | 121.90 |
| 57 | BA | 877 | A | C5-C6-N1 | 7.67 | 121.54 | 117.70 |
| 57 | BA | 2298 | A | N1-C6-N6 | -7.67 | 114.00 | 118.60 |
| 22 | AA | 556 | C | N3-C2-O2 | -7.67 | 116.53 | 121.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 528 | A | C5-C6-N1 | 7.67 | 121.54 | 117.70 |
| 57 | BA | 2458 | G | O4'-C1'-N9 | 7.67 | 114.34 | 108.20 |
| 58 | Ba | 94 | A | C5-C6-N1 | 7.67 | 121.54 | 117.70 |
| 22 | AA | 190 | A | C5-C6-N1 | 7.67 | 121.53 | 117.70 |
| 22 | AA | 1328 | C | N3-C2-O2 | -7.67 | 116.53 | 121.90 |
| 10 | AS | 35 | ARG | NE-CZ-NH1 | 7.67 | 124.13 | 120.30 |
| 22 | AA | 1019 | A | C5-C6-N1 | 7.67 | 121.53 | 117.70 |
| 22 | AA | 1466 | C | N3-C2-O2 | -7.67 | 116.53 | 121.90 |
| 57 | BA | 781 | A | C5-C6-N1 | 7.67 | 121.53 | 117.70 |
| 57 | BA | 2114 | A | C5-C6-N1 | 7.67 | 121.53 | 117.70 |
| 22 | AA | 523 | A | C4-C5-C6 | -7.67 | 113.17 | 117.00 |
| 22 | AA | 1199 | U | O4'-C1'-N1 | 7.67 | 114.33 | 108.20 |
| 22 | AA | 1237 | C | O4'-C1'-N1 | 7.67 | 114.33 | 108.20 |
| 57 | BA | 432 | A | C5-C6-N1 | 7.67 | 121.53 | 117.70 |
| 57 | BA | 928 | A | C5-C6-N1 | 7.67 | 121.53 | 117.70 |
| 57 | BA | 2403 | C | N3-C2-O2 | -7.67 | 116.53 | 121.90 |
| 57 | BA | 2572 | A | C5-C6-N1 | 7.67 | 121.53 | 117.70 |
| 57 | BA | 1462 | C | N3-C2-O2 | -7.67 | 116.53 | 121.90 |
| 58 | Ba | 52 | A | C5-C6-N1 | 7.67 | 121.53 | 117.70 |
| 21 | A1 | 110 | ARG | NE-CZ-NH1 | 7.66 | 124.13 | 120.30 |
| 22 | AA | 452 | A | C5-C6-N1 | 7.66 | 121.53 | 117.70 |
| 57 | BA | 749 | A | C5-C6-N1 | 7.66 | 121.53 | 117.70 |
| 57 | BA | 2741 | A | C5-C6-N1 | 7.66 | 121.53 | 117.70 |
| 22 | AA | 451 | A | C5-C6-N1 | 7.66 | 121.53 | 117.70 |
| 22 | AA | 1369 | C | N3-C2-O2 | -7.66 | 116.54 | 121.90 |
| 32 | BR | 90 | ARG | NE-CZ-NH1 | 7.66 | 124.13 | 120.30 |
| 43 | B1 | 27 | ARG | NE-CZ-NH1 | 7.66 | 124.13 | 120.30 |
| 22 | AA | 25 | C | N3-C2-O2 | -7.66 | 116.54 | 121.90 |
| 22 | AA | 554 | A | C5-C6-N1 | 7.66 | 121.53 | 117.70 |
| 22 | AA | 580 | C | N3-C2-O2 | -7.66 | 116.54 | 121.90 |
| 55 | BH | 2 | ARG | NE-CZ-NH2 | 7.66 | 124.13 | 120.30 |
| 57 | BA | 1126 | A | C5-C6-N1 | 7.66 | 121.53 | 117.70 |
| 57 | BA | 2045 | C | N3-C2-O2 | -7.66 | 116.54 | 121.90 |
| 57 | BA | 2267 | A | C5-C6-N1 | 7.66 | 121.53 | 117.70 |
| 22 | AA | 344 | A | C5-C6-N1 | 7.66 | 121.53 | 117.70 |
| 57 | BA | 1877 | A | C5-C6-N1 | 7.66 | 121.53 | 117.70 |
| 22 | AA | 1317 | C | N3-C4-C5 | 7.65 | 124.96 | 121.90 |
| 57 | BA | 563 | A | C5-C6-N1 | 7.65 | 121.53 | 117.70 |
| 57 | BA | 2749 | A | C5-C6-N1 | 7.65 | 121.53 | 117.70 |
| 22 | AA | 1398 | A | C5-C6-N1 | 7.65 | 121.53 | 117.70 |
| 24 | A3 | 22 | A | C5-C6-N1 | 7.65 | 121.53 | 117.70 |
| 57 | BA | 1417 | C | N3-C2-O2 | -7.65 | 116.54 | 121.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | AA | 897 | C | N3-C2-O2 | -7.65 | 116.55 | 121.90 |
| 57 | BA | 504 | A | C5-C6-N1 | 7.65 | 121.53 | 117.70 |
| 57 | BA | 1943 | U | N3-C2-O2 | -7.65 | 116.84 | 122.20 |
| 57 | BA | 155 | A | C5-C6-N1 | 7.65 | 121.52 | 117.70 |
| 57 | BA | 878 | A | C5-C6-N1 | 7.65 | 121.52 | 117.70 |
| 57 | BA | 1853 | A | C4-C5-C6 | -7.65 | 113.17 | 117.00 |
| 57 | BA | 756 | A | C5-C6-N1 | 7.65 | 121.52 | 117.70 |
| 57 | BA | 984 | A | C5-C6-N1 | 7.65 | 121.52 | 117.70 |
| 22 | AA | 274 | A | C4-C5-C6 | -7.65 | 113.18 | 117.00 |
| 57 | BA | 1741 | C | N3-C2-O2 | -7.65 | 116.55 | 121.90 |
| 22 | AA | 779 | C | N3-C2-O2 | -7.64 | 116.55 | 121.90 |
| 57 | BA | 1383 | A | C5-C6-N1 | 7.64 | 121.52 | 117.70 |
| 57 | BA | 1772 | A | N1-C6-N6 | -7.64 | 114.01 | 118.60 |
| 57 | BA | 2147 | A | C5-C6-N1 | 7.64 | 121.52 | 117.70 |
| 22 | AA | 228 | A | C5-C6-N1 | 7.64 | 121.52 | 117.70 |
| 22 | AA | 456 | A | C5-C6-N1 | 7.64 | 121.52 | 117.70 |
| 22 | AA | 918 | A | C5-C6-N1 | 7.64 | 121.52 | 117.70 |
| 43 | B1 | 17 | ARG | NE-CZ-NH2 | 7.64 | 124.12 | 120.30 |
| 57 | BA | 160 | A | C5-C6-N1 | 7.64 | 121.52 | 117.70 |
| 57 | BA | 2020 | A | C5-C6-N1 | 7.64 | 121.52 | 117.70 |
| 22 | AA | 937 | A | C5-C6-N1 | 7.64 | 121.52 | 117.70 |
| 57 | BA | 1686 | C | N3-C2-O2 | -7.64 | 116.55 | 121.90 |
| 22 | AA | 136 | C | N3-C2-O2 | -7.64 | 116.55 | 121.90 |
| 22 | AA | 794 | A | C5-C6-N1 | 7.64 | 121.52 | 117.70 |
| 57 | BA | 1077 | A | C5-C6-N1 | 7.64 | 121.52 | 117.70 |
| 57 | BA | 1140 | C | N3-C2-O2 | -7.64 | 116.55 | 121.90 |
| 57 | BA | 2191 | A | C5-C6-N1 | 7.64 | 121.52 | 117.70 |
| 57 | BA | 2860 | A | C5-C6-N1 | 7.64 | 121.52 | 117.70 |
| 22 | AA | 181 | A | C5-C6-N1 | 7.64 | 121.52 | 117.70 |
| 22 | AA | 1055 | A | C5-C6-N1 | 7.64 | 121.52 | 117.70 |
| 22 | AA | 1234 | C | N3-C2-O2 | -7.64 | 116.55 | 121.90 |
| 57 | BA | 346 | A | N1-C6-N6 | -7.64 | 114.02 | 118.60 |
| 57 | BA | 672 | C | N3-C2-O2 | -7.64 | 116.55 | 121.90 |
| 57 | BA | 1272 | A | N1-C6-N6 | -7.64 | 114.02 | 118.60 |
| 57 | BA | 1489 | C | N3-C2-O2 | -7.64 | 116.55 | 121.90 |
| 57 | BA | 19 | A | N1-C6-N6 | -7.63 | 114.02 | 118.60 |
| 57 | BA | 680 | C | N3-C2-O2 | -7.63 | 116.56 | 121.90 |
| 57 | BA | 833 | A | N1-C6-N6 | -7.63 | 114.02 | 118.60 |
| 57 | BA | 2560 | A | C5-C6-N1 | 7.63 | 121.52 | 117.70 |
| 22 | AA | 1274 | A | C5-C6-N1 | 7.63 | 121.52 | 117.70 |
| 22 | AA | 1484 | C | N3-C2-O2 | -7.63 | 116.56 | 121.90 |
| 35 | BD | 216 | ARG | NE-CZ-NH2 | -7.63 | 116.48 | 120.30 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 734 | A | N1-C6-N6 | -7.63 | 114.02 | 118.60 |
| 57 | BA | 1144 | A | N1-C6-N6 | -7.63 | 114.02 | 118.60 |
| 57 | BA | 1170 | C | N3-C2-O2 | -7.63 | 116.56 | 121.90 |
| 57 | BA | 157 | C | N3-C2-O2 | -7.63 | 116.56 | 121.90 |
| 57 | BA | 320 | A | C5-C6-N1 | 7.63 | 121.51 | 117.70 |
| 57 | BA | 1386 | C | N3-C2-O2 | -7.63 | 116.56 | 121.90 |
| 57 | BA | 1771 | C | N3-C2-O2 | -7.63 | 116.56 | 121.90 |
| 24 | A3 | 77 | A | C5-C6-N1 | 7.63 | 121.51 | 117.70 |
| 57 | BA | 75 | G | O4'-C1'-N9 | 7.63 | 114.30 | 108.20 |
| 57 | BA | 1008 | A | C5-C6-N1 | 7.63 | 121.51 | 117.70 |
| 35 | BD | 13 | ARG | NE-CZ-NH1 | 7.62 | 124.11 | 120.30 |
| 57 | BA | 766 | U | O4'-C1'-N1 | 7.62 | 114.30 | 108.20 |
| 57 | BA | 1123 | C | N3-C2-O2 | -7.62 | 116.56 | 121.90 |
| 57 | BA | 1387 | A | N1-C6-N6 | -7.62 | 114.03 | 118.60 |
| 57 | BA | 351 | C | N3-C2-O2 | -7.62 | 116.56 | 121.90 |
| 57 | BA | 1102 | C | N3-C2-O2 | -7.62 | 116.56 | 121.90 |
| 57 | BA | 1793 | C | N3-C2-O2 | -7.62 | 116.56 | 121.90 |
| 57 | BA | 2776 | A | C5-C6-N1 | 7.62 | 121.51 | 117.70 |
| 57 | BA | 2853 | C | N3-C2-O2 | -7.62 | 116.56 | 121.90 |
| 22 | AA | 948 | C | N3-C2-O2 | -7.62 | 116.56 | 121.90 |
| 22 | AA | 1203 | C | N3-C2-O2 | -7.62 | 116.56 | 121.90 |
| 22 | AA | 1271 | A | C5-C6-N1 | 7.62 | 121.51 | 117.70 |
| 57 | BA | 404 | A | C4-C5-C6 | -7.62 | 113.19 | 117.00 |
| 22 | AA | 1152 | A | C5-C6-N1 | 7.62 | 121.51 | 117.70 |
| 57 | BA | 959 | A | C5-C6-N1 | 7.62 | 121.51 | 117.70 |
| 57 | BA | 1314 | C | N3-C2-O2 | -7.62 | 116.57 | 121.90 |
| 57 | BA | 1419 | A | C4-C5-C6 | -7.62 | 113.19 | 117.00 |
| 22 | AA | 386 | C | N3-C2-O2 | -7.62 | 116.57 | 121.90 |
| 22 | AA | 935 | A | C5-C6-N1 | 7.62 | 121.51 | 117.70 |
| 57 | BA | 196 | A | C5-C6-N1 | 7.62 | 121.51 | 117.70 |
| 57 | BA | 2613 | U | O4'-C1'-N1 | 7.62 | 114.30 | 108.20 |
| 22 | AA | 526 | C | N3-C2-O2 | -7.62 | 116.57 | 121.90 |
| 57 | BA | 505 | A | N1-C6-N6 | -7.62 | 114.03 | 118.60 |
| 22 | AA | 77 | A | C5-C6-N1 | 7.62 | 121.51 | 117.70 |
| 57 | BA | 983 | A | C5-C6-N1 | 7.62 | 121.51 | 117.70 |
| 57 | BA | 1214 | A | N1-C6-N6 | -7.62 | 114.03 | 118.60 |
| 57 | BA | 1899 | A | C5-C6-N1 | 7.62 | 121.51 | 117.70 |
| 22 | AA | 221 | C | N3-C2-O2 | -7.61 | 116.57 | 121.90 |
| 22 | AA | 787 | A | C5-C6-N1 | 7.61 | 121.51 | 117.70 |
| 22 | AA | 890 | G | O4'-C1'-N9 | 7.61 | 114.29 | 108.20 |
| 22 | AA | 1229 | A | N1-C6-N6 | -7.61 | 114.03 | 118.60 |
| 57 | BA | 61 | 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($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | AA | 321 | A | N1-C6-N6 | -7.61 | 114.03 | 118.60 |
| 22 | AA | 1191 | A | C5-C6-N1 | 7.61 | 121.51 | 117.70 |
| 22 | AA | 1248 | A | C5-C6-N1 | 7.61 | 121.51 | 117.70 |
| 22 | AA | 298 | A | C5-C6-N1 | 7.61 | 121.50 | 117.70 |
| 22 | AA | 1456 | A | C5-C6-N1 | 7.61 | 121.50 | 117.70 |
| 22 | AA | 1102 | A | N1-C6-N6 | -7.61 | 114.03 | 118.60 |
| 57 | BA | 2336 | A | C5-C6-N1 | 7.61 | 121.50 | 117.70 |
| 58 | Ba | 30 | C | N3-C2-O2 | -7.61 | 116.58 | 121.90 |
| 58 | Ba | 115 | A | C5-C6-N1 | 7.61 | 121.50 | 117.70 |
| 57 | BA | 10 | A | C5-C6-N1 | 7.61 | 121.50 | 117.70 |
| 57 | BA | 595 | C | N3-C2-O2 | -7.61 | 116.58 | 121.90 |
| 57 | BA | 1978 | A | C5-C6-N1 | 7.61 | 121.50 | 117.70 |
| 57 | BA | 2698 | U | O4'-C1'-N1 | 7.61 | 114.28 | 108.20 |
| 58 | Ba | 73 | A | N1-C6-N6 | -7.61 | 114.04 | 118.60 |
| 57 | BA | 999 | U | O4'-C1'-N1 | 7.60 | 114.28 | 108.20 |
| 57 | BA | 2426 | A | C5-C6-N1 | 7.60 | 121.50 | 117.70 |
| 22 | AA | 946 | A | N1-C6-N6 | -7.60 | 114.04 | 118.60 |
| 22 | AA | 978 | A | N1-C6-N6 | -7.60 | 114.04 | 118.60 |
| 57 | BA | 324 | A | C5-C6-N1 | 7.60 | 121.50 | 117.70 |
| 57 | BA | 1748 | C | N3-C2-O2 | -7.60 | 116.58 | 121.90 |
| 57 | BA | 1832 | C | N3-C2-O2 | -7.60 | 116.58 | 121.90 |
| 57 | BA | 2480 | C | O4'-C1'-N1 | 7.60 | 114.28 | 108.20 |
| 19 | AH | 116 | ARG | NE-CZ-NH1 | 7.60 | 124.10 | 120.30 |
| 22 | AA | 802 | A | N1-C6-N6 | -7.60 | 114.04 | 118.60 |
| 22 | AA | 1257 | A | C5-C6-N1 | 7.60 | 121.50 | 117.70 |
| 57 | BA | 1595 | C | N3-C2-O2 | -7.60 | 116.58 | 121.90 |
| 22 | AA | 238 | A | C5-C6-N1 | 7.60 | 121.50 | 117.70 |
| 22 | AA | 1449 | C | N3-C2-O2 | -7.60 | 116.58 | 121.90 |
| 57 | BA | 97 | C | N3-C2-O2 | -7.60 | 116.58 | 121.90 |
| 57 | BA | 2129 | C | N3-C2-O2 | -7.60 | 116.58 | 121.90 |
| 22 | AA | 116 | A | N1-C6-N6 | -7.60 | 114.04 | 118.60 |
| 57 | BA | 415 | A | C5-C6-N1 | 7.60 | 121.50 | 117.70 |
| 57 | BA | 1233 | C | N3-C2-O2 | -7.60 | 116.58 | 121.90 |
| 57 | BA | 1701 | A | N1-C6-N6 | -7.60 | 114.04 | 118.60 |
| 57 | BA | 217 | A | C5-C6-N1 | 7.59 | 121.50 | 117.70 |
| 57 | BA | 1064 | C | N3-C2-O2 | -7.59 | 116.58 | 121.90 |
| 57 | BA | 1494 | A | C5-C6-N1 | 7.59 | 121.50 | 117.70 |
| 57 | BA | 1572 | A | N1-C6-N6 | -7.59 | 114.04 | 118.60 |
| 13 | AU | 32 | ARG | NE-CZ-NH1 | 7.59 | 124.10 | 120.30 |
| 22 | AA | 1531 | A | C5-C6-N1 | 7.59 | 121.50 | 117.70 |
| 57 | BA | 2142 | A | C5-C6-N1 | 7.59 | 121.50 | 117.70 |
| 20 | AI | 118 | ARG | NE-CZ-NH1 | 7.59 | 124.09 | 120.30 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | AA | 498 | A | C5-C6-N1 | 7.59 | 121.50 | 117.70 |
| 22 | AA | 768 | A | C5-C6-N1 | 7.59 | 121.50 | 117.70 |
| 22 | AA | 1418 | A | C5-C6-N1 | 7.59 | 121.50 | 117.70 |
| 36 | BU | 52 | ARG | NE-CZ-NH1 | 7.59 | 124.10 | 120.30 |
| 57 | BA | 56 | A | N1-C6-N6 | -7.59 | 114.05 | 118.60 |
| 57 | BA | 853 | C | N3-C2-O2 | -7.59 | 116.59 | 121.90 |
| 57 | BA | 1447 | C | N3-C2-O2 | -7.59 | 116.59 | 121.90 |
| 57 | BA | 2051 | A | C5-C6-N1 | 7.59 | 121.50 | 117.70 |
| 57 | BA | 2829 | A | C5-C6-N1 | 7.59 | 121.50 | 117.70 |
| 22 | AA | 155 | A | C5-C6-N1 | 7.59 | 121.49 | 117.70 |
| 22 | AA | 272 | C | N3-C2-O2 | -7.59 | 116.59 | 121.90 |
| 22 | AA | 1150 | A | C5-C6-N1 | 7.59 | 121.49 | 117.70 |
| 57 | BA | 1609 | A | C5-C6-N1 | 7.59 | 121.50 | 117.70 |
| 57 | BA | 1658 | C | N3-C2-O2 | -7.59 | 116.59 | 121.90 |
| 57 | BA | 2715 | C | N3-C2-O2 | -7.59 | 116.59 | 121.90 |
| 57 | BA | 2720 | U | O4'-C1'-N1 | 7.59 | 114.27 | 108.20 |
| 22 | AA | 1204 | A | C4-C5-C6 | -7.59 | 113.21 | 117.00 |
| 57 | BA | 2058 | A | C5-C6-N1 | 7.59 | 121.49 | 117.70 |
| 58 | Ba | 28 | C | N3-C2-O2 | -7.59 | 116.59 | 121.90 |
| 46 | B3 | 29 | ARG | NE-CZ-NH2 | 7.59 | 124.09 | 120.30 |
| 57 | BA | 1082 | U | O4'-C1'-N1 | 7.59 | 114.27 | 108.20 |
| 57 | BA | 1194 | A | C5-C6-N1 | 7.59 | 121.49 | 117.70 |
| 22 | AA | 300 | A | C5-C6-N1 | 7.58 | 121.49 | 117.70 |
| 42 | B0 | 13 | ARG | NE-CZ-NH1 | 7.58 | 124.09 | 120.30 |
| 57 | BA | 786 | C | N3-C2-O2 | -7.58 | 116.59 | 121.90 |
| 22 | AA | 32 | A | C5-C6-N1 | 7.58 | 121.49 | 117.70 |
| 57 | BA | 332 | A | C5-C6-N1 | 7.58 | 121.49 | 117.70 |
| 22 | AA | 1140 | C | N3-C2-O2 | -7.58 | 116.59 | 121.90 |
| 57 | BA | 460 | A | N1-C6-N6 | -7.58 | 114.05 | 118.60 |
| 57 | BA | 621 | A | C5-C6-N1 | 7.58 | 121.49 | 117.70 |
| 17 | AF | 38 | ARG | NE-CZ-NH1 | 7.58 | 124.09 | 120.30 |
| 22 | AA | 680 | C | N3-C2-O2 | -7.58 | 116.60 | 121.90 |
| 32 | BR | 22 | ARG | NE-CZ-NH1 | 7.58 | 124.09 | 120.30 |
| 57 | BA | 6 | A | C5-C6-N1 | 7.58 | 121.49 | 117.70 |
| 57 | BA | 1749 | A | C5-C6-N1 | 7.58 | 121.49 | 117.70 |
| 57 | BA | 1768 | C | N3-C2-O2 | -7.58 | 116.59 | 121.90 |
| 57 | BA | 2208 | C | N3-C2-O2 | -7.58 | 116.59 | 121.90 |
| 57 | BA | 2654 | A | C5-C6-N1 | 7.58 | 121.49 | 117.70 |
| 22 | AA | 1250 | A | C5-C6-N1 | 7.58 | 121.49 | 117.70 |
| 57 | BA | 149 | A | C5-C6-N1 | 7.58 | 121.49 | 117.70 |
| 57 | BA | 480 | A | C5-C6-N1 | 7.58 | 121.49 | 117.70 |
| 57 | BA | 1142 | A | C4-C5-C6 | -7.58 | 113.21 | 117.00 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | AA | 979 | C | N3-C2-O2 | -7.57 | 116.60 | 121.90 |
| 22 | AA | 1311 | A | C5-C6-N1 | 7.57 | 121.49 | 117.70 |
| 57 | BA | 337 | C | N3-C2-O2 | -7.57 | 116.60 | 121.90 |
| 57 | BA | 1305 | C | N3-C2-O2 | -7.57 | 116.60 | 121.90 |
| 57 | BA | 1787 | A | C5-C6-N1 | 7.57 | 121.49 | 117.70 |
| 22 | AA | 1243 | C | N3-C2-O2 | -7.57 | 116.60 | 121.90 |
| 22 | AA | 1397 | C | N3-C2-O2 | -7.57 | 116.60 | 121.90 |
| 57 | BA | 613 | A | C5-C6-N1 | 7.57 | 121.48 | 117.70 |
| 22 | AA | 1367 | C | N3-C2-O2 | -7.57 | 116.60 | 121.90 |
| 57 | BA | 996 | A | C5-C6-N1 | 7.57 | 121.48 | 117.70 |
| 57 | BA | 2265 | U | O4'-C1'-N1 | 7.57 | 114.25 | 108.20 |
| 57 | BA | 2647 | U | O4'-C1'-N1 | 7.57 | 114.25 | 108.20 |
| 22 | AA | 596 | A | N1-C6-N6 | -7.57 | 114.06 | 118.60 |
| 22 | AA | 1427 | C | N3-C2-O2 | -7.57 | 116.61 | 121.90 |
| 57 | BA | 951 | C | N3-C2-O2 | -7.57 | 116.61 | 121.90 |
| 57 | BA | 1795 | C | O4'-C1'-N1 | 7.57 | 114.25 | 108.20 |
| 57 | BA | 2678 | C | N3-C2-O2 | -7.57 | 116.60 | 121.90 |
| 22 | AA | 1045 | C | N3-C2-O2 | -7.56 | 116.61 | 121.90 |
| 22 | AA | 1437 | A | N1-C6-N6 | -7.56 | 114.06 | 118.60 |
| 22 | AA | 1228 | C | N3-C2-O2 | -7.56 | 116.61 | 121.90 |
| 57 | BA | 744 | U | O4'-C1'-N1 | 7.56 | 114.25 | 108.20 |
| 57 | BA | 1706 | C | N3-C2-O2 | -7.56 | 116.61 | 121.90 |
| 22 | AA | 1397 | C | O4'-C1'-N1 | 7.56 | 114.25 | 108.20 |
| 57 | BA | 1246 | A | C5-C6-N1 | 7.56 | 121.48 | 117.70 |
| 57 | BA | 2899 | A | N1-C6-N6 | -7.56 | 114.06 | 118.60 |
| 21 | A1 | 517 | ARG | NE-CZ-NH1 | 7.56 | 124.08 | 120.30 |
| 22 | AA | 217 | C | N3-C2-O2 | -7.56 | 116.61 | 121.90 |
| 22 | AA | 231 | U | O4'-C1'-N1 | 7.56 | 114.25 | 108.20 |
| 57 | BA | 145 | C | N3-C2-O2 | -7.56 | 116.61 | 121.90 |
| 57 | BA | 1315 | C | N3-C2-O2 | -7.56 | 116.61 | 121.90 |
| 57 | BA | 2084 | C | N3-C2-O2 | -7.56 | 116.61 | 121.90 |
| 13 | AU | 54 | ARG | NE-CZ-NH1 | 7.56 | 124.08 | 120.30 |
| 22 | AA | 478 | A | C5-C6-N1 | 7.56 | 121.48 | 117.70 |
| 33 | BS | 94 | ARG | NE-CZ-NH1 | 7.56 | 124.08 | 120.30 |
| 57 | BA | 422 | A | N1-C6-N6 | -7.56 | 114.07 | 118.60 |
| 57 | BA | 2635 | A | C5-C6-N1 | 7.56 | 121.48 | 117.70 |
| 57 | BA | 529 | A | C5-C6-N1 | 7.56 | 121.48 | 117.70 |
| 57 | BA | 1650 | A | C5-C6-N1 | 7.56 | 121.48 | 117.70 |
| 58 | Ba | 119 | A | C5-C6-N1 | 7.56 | 121.48 | 117.70 |
| 22 | AA | 655 | A | C5-C6-N1 | 7.55 | 121.48 | 117.70 |
| 33 | BS | 25 | ARG | NE-CZ-NH1 | 7.55 | 124.08 | 120.30 |
| 57 | BA | 540 | C | N3-C2-O2 | -7.55 | 116.61 | 121.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 985 | C | N3-C2-O2 | -7.55 | 116.61 | 121.90 |
| 57 | BA | 2077 | A | C5-C6-N1 | 7.55 | 121.48 | 117.70 |
| 57 | BA | 2752 | C | O4'-C1'-N1 | 7.55 | 114.24 | 108.20 |
| 22 | AA | 1021 | A | C5-C6-N1 | 7.55 | 121.48 | 117.70 |
| 57 | BA | 626 | A | C5-C6-N1 | 7.55 | 121.48 | 117.70 |
| 57 | BA | 1784 | A | C5-C6-N1 | 7.55 | 121.48 | 117.70 |
| 22 | AA | 151 | A | C4-C5-C6 | -7.55 | 113.22 | 117.00 |
| 22 | AA | 932 | C | N3-C2-O2 | -7.55 | 116.61 | 121.90 |
| 53 | BF | 162 | ARG | NE-CZ-NH2 | 7.55 | 124.08 | 120.30 |
| 57 | BA | 318 | C | N3-C2-O2 | -7.55 | 116.61 | 121.90 |
| 57 | BA | 633 | A | C5-C6-N1 | 7.55 | 121.47 | 117.70 |
| 57 | BA | 804 | A | C5-C6-N1 | 7.55 | 121.48 | 117.70 |
| 57 | BA | 915 | C | N3-C2-O2 | -7.55 | 116.61 | 121.90 |
| 57 | BA | 1027 | A | N1-C6-N6 | -7.55 | 114.07 | 118.60 |
| 57 | BA | 1378 | A | C4-C5-C6 | -7.55 | 113.22 | 117.00 |
| 57 | BA | 2089 | C | N3-C2-O2 | -7.55 | 116.61 | 121.90 |
| 57 | BA | 2199 | A | C5-C6-N1 | 7.55 | 121.47 | 117.70 |
| 57 | BA | 2275 | C | N3-C2-O2 | -7.55 | 116.61 | 121.90 |
| 57 | BA | 2815 | C | N3-C2-O2 | -7.55 | 116.61 | 121.90 |
| 57 | BA | 362 | A | O4'-C1'-N9 | 7.55 | 114.24 | 108.20 |
| 57 | BA | 943 | A | C5-C6-N1 | 7.55 | 121.47 | 117.70 |
| 57 | BA | 2551 | C | N3-C2-O2 | -7.55 | 116.62 | 121.90 |
| 22 | AA | 452 | A | C4-C5-C6 | -7.55 | 113.23 | 117.00 |
| 57 | BA | 861 | A | C5-C6-N1 | 7.55 | 121.47 | 117.70 |
| 57 | BA | 1323 | C | N3-C2-O2 | -7.55 | 116.62 | 121.90 |
| 57 | BA | 1569 | A | C5-C6-N1 | 7.55 | 121.47 | 117.70 |
| 22 | AA | 250 | A | C5-C6-N1 | 7.55 | 121.47 | 117.70 |
| 22 | AA | 1217 | C | N3-C2-O2 | -7.55 | 116.62 | 121.90 |
| 57 | BA | 2037 | A | C5-C6-N1 | 7.55 | 121.47 | 117.70 |
| 57 | BA | 2367 | G | O4'-C1'-N9 | 7.55 | 114.24 | 108.20 |
| 22 | AA | 1430 | A | C5-C6-N1 | 7.54 | 121.47 | 117.70 |
| 57 | BA | 440 | C | N3-C2-O2 | -7.54 | 116.62 | 121.90 |
| 57 | BA | 1928 | A | C5-C6-N1 | 7.54 | 121.47 | 117.70 |
| 22 | AA | 796 | C | N3-C2-O2 | -7.54 | 116.62 | 121.90 |
| 22 | AA | 815 | A | C4-C5-C6 | -7.54 | 113.23 | 117.00 |
| 57 | BA | 345 | A | C5-C6-N1 | 7.54 | 121.47 | 117.70 |
| 57 | BA | 835 | C | N3-C2-O2 | -7.54 | 116.62 | 121.90 |
| 57 | BA | 1918 | A | C5-C6-N1 | 7.54 | 121.47 | 117.70 |
| 22 | AA | 1081 | A | C5-C6-N1 | 7.54 | 121.47 | 117.70 |
| 57 | BA | 2328 | A | C5-C6-N1 | 7.54 | 121.47 | 117.70 |
| 57 | BA | 2270 | A | C5-C6-N1 | 7.54 | 121.47 | 117.70 |
| 22 | AA | 1324 | 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($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 1353 | A | C5-C6-N1 | 7.54 | 121.47 | 117.70 |
| 57 | BA | 1577 | C | N3-C2-O2 | -7.54 | 116.62 | 121.90 |
| 57 | BA | 1872 | A | C5-C6-N1 | 7.54 | 121.47 | 117.70 |
| 22 | AA | 1350 | A | C5-C6-N1 | 7.54 | 121.47 | 117.70 |
| 22 | AA | 87 | C | N3-C2-O2 | -7.54 | 116.63 | 121.90 |
| 57 | BA | 310 | A | C5-C6-N1 | 7.54 | 121.47 | 117.70 |
| 57 | BA | 509 | C | N3-C2-O2 | -7.54 | 116.62 | 121.90 |
| 22 | AA | 766 | A | C5-C6-N1 | 7.53 | 121.47 | 117.70 |
| 22 | AA | 539 | A | C5-C6-N1 | 7.53 | 121.47 | 117.70 |
| 57 | BA | 1556 | C | N3-C2-O2 | -7.53 | 116.63 | 121.90 |
| 22 | AA | 573 | A | C4-C5-C6 | -7.53 | 113.23 | 117.00 |
| 57 | BA | 522 | A | C5-C6-N1 | 7.53 | 121.47 | 117.70 |
| 22 | AA | 1082 | A | C5-C6-N1 | 7.53 | 121.47 | 117.70 |
| 57 | BA | 1126 | A | N1-C6-N6 | -7.53 | 114.08 | 118.60 |
| 57 | BA | 1755 | A | C4-C5-C6 | -7.53 | 113.24 | 117.00 |
| 57 | BA | 2705 | A | C5-C6-N1 | 7.53 | 121.47 | 117.70 |
| 15 | AD | 25 | ARG | NE-CZ-NH1 | 7.53 | 124.06 | 120.30 |
| 57 | BA | 917 | A | N1-C6-N6 | -7.53 | 114.08 | 118.60 |
| 57 | BA | 1052 | C | N3-C2-O2 | -7.53 | 116.63 | 121.90 |
| 57 | BA | 2311 | A | C5-C6-N1 | 7.53 | 121.46 | 117.70 |
| 15 | AD | 145 | ARG | NE-CZ-NH1 | 7.53 | 124.06 | 120.30 |
| 22 | AA | 1080 | A | C5-C6-N1 | 7.53 | 121.46 | 117.70 |
| 24 | A3 | 74 | A | C5-C6-N1 | 7.53 | 121.46 | 117.70 |
| 57 | BA | 384 | A | C5-C6-N1 | 7.53 | 121.46 | 117.70 |
| 57 | BA | 973 | A | C5-C6-N1 | 7.53 | 121.46 | 117.70 |
| 57 | BA | 1272 | A | C5-C6-N1 | 7.53 | 121.46 | 117.70 |
| 57 | BA | 1376 | C | N3-C2-O2 | -7.53 | 116.63 | 121.90 |
| 57 | BA | 1913 | A | C5-C6-N1 | 7.53 | 121.46 | 117.70 |
| 57 | BA | 466 | A | C5-C6-N1 | 7.52 | 121.46 | 117.70 |
| 22 | AA | 1046 | A | C4-C5-C6 | -7.52 | 113.24 | 117.00 |
| 50 | B7 | 41 | ARG | NE-CZ-NH2 | 7.52 | 124.06 | 120.30 |
| 57 | BA | 2482 | A | N1-C6-N6 | -7.52 | 114.09 | 118.60 |
| 57 | BA | 2727 | A | C5-C6-N1 | 7.52 | 121.46 | 117.70 |
| 57 | BA | 1512 | C | N3-C2-O2 | -7.52 | 116.64 | 121.90 |
| 22 | AA | 408 | A | C5-C6-N1 | 7.52 | 121.46 | 117.70 |
| 22 | AA | 702 | A | C5-C6-N1 | 7.52 | 121.46 | 117.70 |
| 57 | BA | 1549 | A | C5-C6-N1 | 7.52 | 121.46 | 117.70 |
| 57 | BA | 1593 | A | C5-C6-N1 | 7.52 | 121.46 | 117.70 |
| 57 | BA | 2516 | A | C5-C6-N1 | 7.52 | 121.46 | 117.70 |
| 22 | AA | 459 | A | C4-C5-C6 | -7.51 | 113.24 | 117.00 |
| 22 | AA | 914 | A | C5-C6-N1 | 7.51 | 121.46 | 117.70 |
| 57 | BA | 2750 | A | C4-C5-C6 | -7.51 | 113.24 | 117.00 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | AA | 156 | C | N3-C2-O2 | -7.51 | 116.64 | 121.90 |
| 22 | AA | 371 | A | C5-C6-N1 | 7.51 | 121.46 | 117.70 |
| 22 | AA | 1510 | C | N3-C2-O2 | -7.51 | 116.64 | 121.90 |
| 58 | Ba | 109 | A | C5-C6-N1 | 7.51 | 121.45 | 117.70 |
| 11 | AB | 224 | ARG | NE-CZ-NH1 | 7.51 | 124.06 | 120.30 |
| 57 | BA | 403 | U | O4'-C1'-N1 | 7.51 | 114.21 | 108.20 |
| 57 | BA | 1080 | A | C5-C6-N1 | 7.51 | 121.45 | 117.70 |
| 22 | AA | 609 | A | C5-C6-N1 | 7.51 | 121.45 | 117.70 |
| 22 | AA | 910 | C | N3-C2-O2 | -7.51 | 116.64 | 121.90 |
| 22 | AA | 1246 | A | C5-C6-N1 | 7.51 | 121.45 | 117.70 |
| 57 | BA | 2232 | C | N3-C2-O2 | -7.51 | 116.64 | 121.90 |
| 57 | BA | 2841 | C | N3-C2-O2 | -7.51 | 116.64 | 121.90 |
| 22 | AA | 1067 | A | C5-C6-N1 | 7.51 | 121.45 | 117.70 |
| 57 | BA | 105 | C | N3-C2-O2 | -7.51 | 116.65 | 121.90 |
| 57 | BA | 542 | C | N3-C2-O2 | -7.51 | 116.65 | 121.90 |
| 57 | BA | 603 | A | C4-C5-C6 | -7.51 | 113.25 | 117.00 |
| 57 | BA | 611 | C | N3-C2-O2 | -7.51 | 116.65 | 121.90 |
| 57 | BA | 772 | C | N3-C2-O2 | -7.51 | 116.64 | 121.90 |
| 22 | AA | 366 | A | C5-C6-N1 | 7.50 | 121.45 | 117.70 |
| 57 | BA | 1104 | C | N3-C2-O2 | -7.50 | 116.65 | 121.90 |
| 58 | Ba | 62 | C | N3-C2-O2 | -7.50 | 116.65 | 121.90 |
| 57 | BA | 968 | C | N3-C2-O2 | -7.50 | 116.65 | 121.90 |
| 57 | BA | 1194 | A | C4-C5-C6 | -7.50 | 113.25 | 117.00 |
| 57 | BA | 2792 | A | C5-C6-N1 | 7.50 | 121.45 | 117.70 |
| 17 | AF | 44 | ARG | NE-CZ-NH1 | 7.50 | 124.05 | 120.30 |
| 22 | AA | 1441 | A | C4-C5-C6 | -7.50 | 113.25 | 117.00 |
| 57 | BA | 510 | C | N3-C2-O2 | -7.50 | 116.65 | 121.90 |
| 57 | BA | 2139 | U | O4'-C1'-N1 | 7.50 | 114.20 | 108.20 |
| 57 | BA | 2471 | A | C5-C6-N1 | 7.50 | 121.45 | 117.70 |
| 57 | BA | 42 | A | C5-C6-N1 | 7.50 | 121.45 | 117.70 |
| 57 | BA | 253 | C | N3-C2-O2 | -7.50 | 116.65 | 121.90 |
| 22 | AA | 1063 | C | N3-C2-O2 | -7.50 | 116.65 | 121.90 |
| 22 | AA | 1375 | A | C5-C6-N1 | 7.50 | 121.45 | 117.70 |
| 57 | BA | 1367 | A | C5-C6-N1 | 7.50 | 121.45 | 117.70 |
| 57 | BA | 1819 | A | C5-C6-N1 | 7.50 | 121.45 | 117.70 |
| 57 | BA | 57 | C | O4'-C1'-N1 | 7.50 | 114.20 | 108.20 |
| 57 | BA | 1189 | A | C5-C6-N1 | 7.50 | 121.45 | 117.70 |
| 22 | AA | 883 | C | N3-C2-O2 | -7.50 | 116.65 | 121.90 |
| 57 | BA | 226 | A | C5-C6-N1 | 7.50 | 121.45 | 117.70 |
| 22 | AA | 784 | A | C5-C6-N1 | 7.49 | 121.45 | 117.70 |
| 24 | A3 | 52 | C | N3-C2-O2 | -7.49 | 116.65 | 121.90 |
| 57 | BA | 45 | G | O4'-C1'-N9 | 7.49 | 114.19 | 108.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 213 | A | N1-C6-N6 | -7.49 | 114.10 | 118.60 |
| 57 | BA | 1789 | A | N1-C6-N6 | -7.49 | 114.10 | 118.60 |
| 24 | A3 | 1 | C | N3-C2-O2 | -7.49 | 116.66 | 121.90 |
| 57 | BA | 2317 | A | C5-C6-N1 | 7.49 | 121.45 | 117.70 |
| 57 | BA | 2896 | C | N3-C2-O2 | -7.49 | 116.66 | 121.90 |
| 22 | AA | 411 | A | C4-C5-C6 | -7.49 | 113.25 | 117.00 |
| 22 | AA | 1117 | A | C5-C6-N1 | 7.49 | 121.44 | 117.70 |
| 57 | BA | 806 | C | N3-C2-O2 | -7.49 | 116.66 | 121.90 |
| 57 | BA | 1214 | A | C5-C6-N1 | 7.49 | 121.44 | 117.70 |
| 57 | BA | 1652 | A | C5-C6-N1 | 7.49 | 121.44 | 117.70 |
| 22 | AA | 839 | C | O4'-C1'-N1 | 7.49 | 114.19 | 108.20 |
| 57 | BA | 173 | A | C5-C6-N1 | 7.49 | 121.44 | 117.70 |
| 22 | AA | 131 | A | C5-C6-N1 | 7.49 | 121.44 | 117.70 |
| 22 | AA | 1176 | A | C5-C6-N1 | 7.49 | 121.44 | 117.70 |
| 57 | BA | 125 | A | C5-C6-N1 | 7.49 | 121.44 | 117.70 |
| 57 | BA | 294 | A | C4-C5-C6 | -7.49 | 113.26 | 117.00 |
| 57 | BA | 2392 | A | C5-C6-N1 | 7.49 | 121.44 | 117.70 |
| 57 | BA | 2425 | A | C5-C6-N1 | 7.49 | 121.44 | 117.70 |
| 57 | BA | 1121 | C | N3-C2-O2 | -7.48 | 116.66 | 121.90 |
| 57 | BA | 1881 | C | N3-C2-O2 | -7.48 | 116.66 | 121.90 |
| 22 | AA | 586 | C | N3-C2-O2 | -7.48 | 116.66 | 121.90 |
| 22 | AA | 716 | A | C5-C6-N1 | 7.48 | 121.44 | 117.70 |
| 22 | AA | 879 | C | N3-C2-O2 | -7.48 | 116.66 | 121.90 |
| 22 | AA | 1255 | G | O4'-C1'-N9 | 7.48 | 114.19 | 108.20 |
| 57 | BA | 590 | A | C5-C6-N1 | 7.48 | 121.44 | 117.70 |
| 57 | BA | 691 | C | N3-C2-O2 | -7.48 | 116.66 | 121.90 |
| 57 | BA | 1306 | C | N3-C2-O2 | -7.48 | 116.66 | 121.90 |
| 57 | BA | 2117 | A | C5-C6-N1 | 7.48 | 121.44 | 117.70 |
| 57 | BA | 302 | C | N3-C2-O2 | -7.48 | 116.66 | 121.90 |
| 57 | BA | 2733 | A | C4-C5-C6 | -7.48 | 113.26 | 117.00 |
| 58 | Ba | 45 | A | C5-C6-N1 | 7.48 | 121.44 | 117.70 |
| 22 | AA | 199 | A | N1-C6-N6 | -7.48 | 114.11 | 118.60 |
| 22 | AA | 263 | A | C5-C6-N1 | 7.48 | 121.44 | 117.70 |
| 22 | AA | 958 | A | C5-C6-N1 | 7.48 | 121.44 | 117.70 |
| 57 | BA | 1386 | C | O4'-C1'-N1 | 7.48 | 114.18 | 108.20 |
| 57 | BA | 2430 | A | C5-C6-N1 | 7.48 | 121.44 | 117.70 |
| 57 | BA | 1496 | A | C5-C6-N1 | 7.48 | 121.44 | 117.70 |
| 57 | BA | 1810 | A | C5-C6-N1 | 7.48 | 121.44 | 117.70 |
| 57 | BA | 2420 | C | N3-C2-O2 | -7.48 | 116.67 | 121.90 |
| 57 | BA | 2721 | A | C4-C5-C6 | -7.48 | 113.26 | 117.00 |
| 24 | A3 | 26 | C | N3-C2-O2 | -7.48 | 116.67 | 121.90 |
| 57 | BA | 1708 | C | N3-C2-O2 | -7.48 | 116.67 | 121.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 1789 | A | C5-C6-N1 | 7.48 | 121.44 | 117.70 |
| 57 | BA | 2855 | C | N3-C2-O2 | -7.48 | 116.67 | 121.90 |
| 58 | Ba | 90 | C | N1-C2-O2 | 7.48 | 123.39 | 118.90 |
| 22 | AA | 753 | A | N1-C6-N6 | -7.47 | 114.12 | 118.60 |
| 22 | AA | 1284 | C | N3-C2-O2 | -7.47 | 116.67 | 121.90 |
| 57 | BA | 22 | C | N3-C2-O2 | -7.47 | 116.67 | 121.90 |
| 57 | BA | 1147 | A | C5-C6-N1 | 7.47 | 121.44 | 117.70 |
| 57 | BA | 1357 | C | N3-C2-O2 | -7.47 | 116.67 | 121.90 |
| 57 | BA | 1586 | A | C5-C6-N1 | 7.47 | 121.44 | 117.70 |
| 57 | BA | 2295 | C | N3-C2-O2 | -7.47 | 116.67 | 121.90 |
| 22 | AA | 435 | A | C4-C5-C6 | -7.47 | 113.26 | 117.00 |
| 22 | AA | 637 | C | N3-C2-O2 | -7.47 | 116.67 | 121.90 |
| 24 | A3 | 42 | C | N3-C2-O2 | -7.47 | 116.67 | 121.90 |
| 57 | BA | 344 | A | C5-C6-N1 | 7.47 | 121.44 | 117.70 |
| 57 | BA | 2764 | A | C4-C5-C6 | -7.47 | 113.26 | 117.00 |
| 22 | AA | 36 | C | N3-C2-O2 | -7.47 | 116.67 | 121.90 |
| 57 | BA | 1117 | C | N3-C2-O2 | -7.47 | 116.67 | 121.90 |
| 57 | BA | 1146 | C | N3-C2-O2 | -7.47 | 116.67 | 121.90 |
| 57 | BA | 2274 | A | C5-C6-N1 | 7.47 | 121.44 | 117.70 |
| 57 | BA | 1866 | A | N1-C6-N6 | -7.47 | 114.12 | 118.60 |
| 22 | AA | 1196 | A | C5-C6-N1 | 7.47 | 121.43 | 117.70 |
| 57 | BA | 723 | C | N3-C2-O2 | -7.47 | 116.67 | 121.90 |
| 57 | BA | 2733 | A | C5-C6-N1 | 7.47 | 121.43 | 117.70 |
| 57 | BA | 374 | A | N1-C6-N6 | -7.47 | 114.12 | 118.60 |
| 57 | BA | 737 | C | N3-C2-O2 | -7.47 | 116.67 | 121.90 |
| 57 | BA | 1596 | A | N1-C6-N6 | -7.47 | 114.12 | 118.60 |
| 22 | AA | 735 | C | N3-C2-O2 | -7.46 | 116.67 | 121.90 |
| 22 | AA | 1374 | A | C5-C6-N1 | 7.46 | 121.43 | 117.70 |
| 23 | A2 | 24 | A | C5-C6-N1 | 7.46 | 121.43 | 117.70 |
| 57 | BA | 563 | A | N1-C6-N6 | -7.46 | 114.12 | 118.60 |
| 57 | BA | 2015 | A | C5-C6-N1 | 7.46 | 121.43 | 117.70 |
| 22 | AA | 269 | C | N3-C2-O2 | -7.46 | 116.68 | 121.90 |
| 22 | AA | 341 | C | N3-C2-O2 | -7.46 | 116.68 | 121.90 |
| 57 | BA | 508 | A | C5-C6-N1 | 7.46 | 121.43 | 117.70 |
| 57 | BA | 2015 | A | N1-C6-N6 | -7.46 | 114.12 | 118.60 |
| 57 | BA | 2260 | C | O4'-C1'-N1 | 7.46 | 114.17 | 108.20 |
| 57 | BA | 2395 | C | N3-C2-O2 | -7.46 | 116.68 | 121.90 |
| 22 | AA | 716 | A | C4-C5-C6 | -7.46 | 113.27 | 117.00 |
| 57 | BA | 401 | A | C4-C5-C6 | -7.46 | 113.27 | 117.00 |
| 57 | BA | 1057 | A | C4-C5-C6 | -7.46 | 113.27 | 117.00 |
| 57 | BA | 2150 | C | N3-C2-O2 | -7.46 | 116.68 | 121.90 |
| 57 | BA | 2241 | A | C5-C6-N1 | 7.46 | 121.43 | 117.70 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 2805 | C | N3-C2-O2 | -7.46 | 116.68 | 121.90 |
| 22 | AA | 443 | C | N3-C2-O2 | -7.46 | 116.68 | 121.90 |
| 57 | BA | 357 | C | N3-C2-O2 | -7.46 | 116.68 | 121.90 |
| 57 | BA | 643 | A | N1-C6-N6 | -7.46 | 114.12 | 118.60 |
| 22 | AA | 160 | A | C4-C5-C6 | -7.46 | 113.27 | 117.00 |
| 22 | AA | 1210 | C | N3-C2-O2 | -7.46 | 116.68 | 121.90 |
| 57 | BA | 279 | A | C5-C6-N1 | 7.46 | 121.43 | 117.70 |
| 57 | BA | 640 | C | N3-C2-O2 | -7.46 | 116.68 | 121.90 |
| 57 | BA | 1927 | A | C5-C6-N1 | 7.46 | 121.43 | 117.70 |
| 22 | AA | 1103 | C | N3-C2-O2 | -7.46 | 116.68 | 121.90 |
| 30 | BP | 132 | ARG | NE-CZ-NH1 | 7.46 | 124.03 | 120.30 |
| 57 | BA | 152 | A | C5-C6-N1 | 7.46 | 121.43 | 117.70 |
| 57 | BA | 2171 | A | C4-C5-C6 | -7.46 | 113.27 | 117.00 |
| 57 | BA | 2676 | C | N3-C2-O2 | -7.46 | 116.68 | 121.90 |
| 58 | Ba | 101 | A | C5-C6-N1 | 7.46 | 121.43 | 117.70 |
| 22 | AA | 754 | C | N3-C2-O2 | -7.46 | 116.68 | 121.90 |
| 57 | BA | 1974 | C | N3-C2-O2 | -7.46 | 116.68 | 121.90 |
| 57 | BA | 2097 | A | C5-C6-N1 | 7.46 | 121.43 | 117.70 |
| 57 | BA | 2227 | A | C5-C6-N1 | 7.46 | 121.43 | 117.70 |
| 57 | BA | 2606 | C | N3-C2-O2 | -7.46 | 116.68 | 121.90 |
| 57 | BA | 1711 | A | C5-C6-N1 | 7.45 | 121.43 | 117.70 |
| 57 | BA | 893 | C | N3-C2-O2 | -7.45 | 116.68 | 121.90 |
| 22 | AA | 60 | A | C5-C6-N1 | 7.45 | 121.42 | 117.70 |
| 22 | AA | 862 | C | N3-C2-O2 | -7.45 | 116.69 | 121.90 |
| 22 | AA | 969 | A | O4'-C1'-N9 | 7.45 | 114.16 | 108.20 |
| 57 | BA | 462 | C | N3-C2-O2 | -7.45 | 116.69 | 121.90 |
| 57 | BA | 632 | A | N1-C6-N6 | -7.45 | 114.13 | 118.60 |
| 57 | BA | 1853 | A | C5-C6-N1 | 7.45 | 121.42 | 117.70 |
| 57 | BA | 2044 | C | N3-C2-O2 | -7.45 | 116.68 | 121.90 |
| 57 | BA | 2418 | A | C5-C6-N1 | 7.45 | 121.42 | 117.70 |
| 22 | AA | 489 | C | N3-C2-O2 | -7.45 | 116.69 | 121.90 |
| 22 | AA | 663 | A | C5-C6-N1 | 7.45 | 121.42 | 117.70 |
| 22 | AA | 839 | C | N3-C2-O2 | -7.45 | 116.69 | 121.90 |
| 22 | AA | 1129 | C | N3-C2-O2 | -7.45 | 116.69 | 121.90 |
| 57 | BA | 501 | A | C5-C6-N1 | 7.45 | 121.42 | 117.70 |
| 57 | BA | 564 | C | N3-C2-O2 | -7.45 | 116.69 | 121.90 |
| 57 | BA | 128 | C | N3-C2-O2 | -7.45 | 116.69 | 121.90 |
| 57 | BA | 517 | C | N3-C2-O2 | -7.45 | 116.69 | 121.90 |
| 20 | AI | 98 | ARG | NE-CZ-NH1 | 7.45 | 124.02 | 120.30 |
| 22 | AA | 649 | A | C5-C6-N1 | 7.45 | 121.42 | 117.70 |
| 22 | AA | 1521 | C | N3-C2-O2 | -7.45 | 116.69 | 121.90 |
| 57 | BA | 515 | A | C4-C5-C6 | -7.45 | 113.28 | 117.00 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 1169 | A | C5-C6-N1 | 7.45 | 121.42 | 117.70 |
| 15 | AD | 69 | ARG | NE-CZ-NH1 | 7.44 | 124.02 | 120.30 |
| 57 | BA | 1350 | C | N3-C2-O2 | -7.44 | 116.69 | 121.90 |
| 57 | BA | 1698 | A | C5-C6-N1 | 7.44 | 121.42 | 117.70 |
| 57 | BA | 2291 | U | O4'-C1'-N1 | 7.44 | 114.16 | 108.20 |
| 22 | AA | 1153 | G | O4'-C1'-N9 | 7.44 | 114.15 | 108.20 |
| 57 | BA | 1328 | A | C4-C5-C6 | -7.44 | 113.28 | 117.00 |
| 57 | BA | 2376 | A | C4-C5-C6 | -7.44 | 113.28 | 117.00 |
| 22 | AA | 313 | A | C5-C6-N1 | 7.44 | 121.42 | 117.70 |
| 22 | AA | 1410 | A | C5-C6-N1 | 7.44 | 121.42 | 117.70 |
| 57 | BA | 147 | C | N3-C2-O2 | -7.44 | 116.69 | 121.90 |
| 57 | BA | 1284 | A | C5-C6-N1 | 7.44 | 121.42 | 117.70 |
| 57 | BA | 418 | C | N3-C2-O2 | -7.44 | 116.69 | 121.90 |
| 22 | AA | 1269 | A | C5-C6-N1 | 7.44 | 121.42 | 117.70 |
| 57 | BA | 278 | A | C4-C5-C6 | -7.44 | 113.28 | 117.00 |
| 57 | BA | 1996 | C | N3-C2-O2 | -7.44 | 116.69 | 121.90 |
| 57 | BA | 2200 | C | N3-C2-O2 | -7.44 | 116.69 | 121.90 |
| 22 | AA | 1071 | C | N3-C2-O2 | -7.44 | 116.69 | 121.90 |
| 57 | BA | 1901 | A | C5-C6-N1 | 7.44 | 121.42 | 117.70 |
| 57 | BA | 2575 | C | C2-N3-C4 | 7.44 | 123.62 | 119.90 |
| 57 | BA | 205 | G | O4'-C1'-N9 | 7.43 | 114.15 | 108.20 |
| 57 | BA | 1276 | A | C5-C6-N1 | 7.43 | 121.42 | 117.70 |
| 57 | BA | 1780 | A | N1-C6-N6 | -7.43 | 114.14 | 118.60 |
| 57 | BA | 1844 | C | N3-C2-O2 | -7.43 | 116.70 | 121.90 |
| 57 | BA | 2340 | A | C5-C6-N1 | 7.43 | 121.42 | 117.70 |
| 22 | AA | 759 | A | C5-C6-N1 | 7.43 | 121.42 | 117.70 |
| 22 | AA | 880 | C | N3-C2-O2 | -7.43 | 116.70 | 121.90 |
| 22 | AA | 1012 | A | C5-C6-N1 | 7.43 | 121.42 | 117.70 |
| 57 | BA | 2704 | C | N3-C2-O2 | -7.43 | 116.70 | 121.90 |
| 22 | AA | 342 | C | N3-C2-O2 | -7.43 | 116.70 | 121.90 |
| 22 | AA | 1506 | U | O4'-C1'-N1 | 7.43 | 114.14 | 108.20 |
| 57 | BA | 231 | A | C5-C6-N1 | 7.43 | 121.42 | 117.70 |
| 57 | BA | 751 | A | C5-C6-N1 | 7.43 | 121.42 | 117.70 |
| 57 | BA | 1566 | A | C5-C6-N1 | 7.43 | 121.42 | 117.70 |
| 57 | BA | 2135 | A | C5-C6-N1 | 7.43 | 121.42 | 117.70 |
| 22 | AA | 192 | A | C5-C6-N1 | 7.43 | 121.42 | 117.70 |
| 22 | AA | 483 | C | O4'-C1'-N1 | 7.43 | 114.14 | 108.20 |
| 57 | BA | 470 | A | C5-C6-N1 | 7.43 | 121.41 | 117.70 |
| 57 | BA | 732 | C | N3-C2-O2 | -7.43 | 116.70 | 121.90 |
| 57 | BA | 936 | A | C5-C6-N1 | 7.43 | 121.42 | 117.70 |
| 57 | BA | 1404 | C | N3-C2-O2 | -7.43 | 116.70 | 121.90 |
| 57 | BA | 1550 | C | N3-C2-O2 | -7.43 | 116.70 | 121.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 2184 | A | C5-C6-N1 | 7.43 | 121.42 | 117.70 |
| 22 | AA | 26 | A | C4-C5-C6 | -7.43 | 113.29 | 117.00 |
| 57 | BA | 2070 | A | C5-C6-N1 | 7.43 | 121.41 | 117.70 |
| 22 | AA | 285 | C | N3-C2-O2 | -7.43 | 116.70 | 121.90 |
| 57 | BA | 1205 | A | C4-C5-C6 | -7.43 | 113.29 | 117.00 |
| 3 | AL | 109 | ARG | NE-CZ-NH1 | 7.42 | 124.01 | 120.30 |
| 21 | A1 | 584 | ARG | NE-CZ-NH1 | 7.42 | 124.01 | 120.30 |
| 22 | AA | 290 | C | N3-C2-O2 | -7.42 | 116.70 | 121.90 |
| 22 | AA | 853 | C | N3-C2-O2 | -7.42 | 116.70 | 121.90 |
| 22 | AA | 1113 | C | N3-C2-O2 | -7.42 | 116.70 | 121.90 |
| 57 | BA | 734 | A | C5-C6-N1 | 7.42 | 121.41 | 117.70 |
| 57 | BA | 1100 | C | N3-C2-O2 | -7.42 | 116.70 | 121.90 |
| 22 | AA | 750 | C | N3-C2-O2 | -7.42 | 116.70 | 121.90 |
| 22 | AA | 1239 | A | C5-C6-N1 | 7.42 | 121.41 | 117.70 |
| 22 | AA | 1285 | A | C5-C6-N1 | 7.42 | 121.41 | 117.70 |
| 57 | BA | 2527 | C | N3-C2-O2 | -7.42 | 116.70 | 121.90 |
| 57 | BA | 2757 | A | C5-C6-N1 | 7.42 | 121.41 | 117.70 |
| 57 | BA | 2827 | C | N3-C2-O2 | -7.42 | 116.70 | 121.90 |
| 42 | B0 | 38 | ARG | NE-CZ-NH2 | -7.42 | 116.59 | 120.30 |
| 22 | AA | 856 | C | N3-C2-O2 | -7.42 | 116.71 | 121.90 |
| 22 | AA | 1044 | A | C5-C6-N1 | 7.42 | 121.41 | 117.70 |
| 57 | BA | 610 | C | N3-C2-O2 | -7.42 | 116.71 | 121.90 |
| 57 | BA | 2767 | C | N3-C2-O2 | -7.42 | 116.71 | 121.90 |
| 22 | AA | 207 | C | N3-C2-O2 | -7.42 | 116.71 | 121.90 |
| 57 | BA | 503 | A | C4-C5-C6 | -7.42 | 113.29 | 117.00 |
| 57 | BA | 937 | C | N3-C2-O2 | -7.42 | 116.71 | 121.90 |
| 57 | BA | 1204 | A | C4-C5-C6 | -7.42 | 113.29 | 117.00 |
| 57 | BA | 1505 | A | C4-C5-C6 | -7.42 | 113.29 | 117.00 |
| 57 | BA | 2534 | A | C4-C5-C6 | -7.42 | 113.29 | 117.00 |
| 57 | BA | 2787 | C | N3-C2-O2 | -7.42 | 116.71 | 121.90 |
| 57 | BA | 2880 | C | N3-C2-O2 | -7.42 | 116.71 | 121.90 |
| 57 | BA | 678 | C | N3-C2-O2 | -7.42 | 116.71 | 121.90 |
| 57 | BA | 2264 | C | N3-C2-O2 | -7.42 | 116.71 | 121.90 |
| 34 | BT | 108 | ARG | NE-CZ-NH2 | 7.41 | 124.01 | 120.30 |
| 57 | BA | 2653 | U | O4'-C1'-N1 | 7.41 | 114.13 | 108.20 |
| 57 | BA | 2762 | C | N3-C2-O2 | -7.41 | 116.71 | 121.90 |
| 22 | AA | 578 | C | N3-C2-O2 | -7.41 | 116.71 | 121.90 |
| 57 | BA | 944 | C | N3-C2-O2 | -7.41 | 116.71 | 121.90 |
| 57 | BA | 1739 | A | C5-C6-N1 | 7.41 | 121.41 | 117.70 |
| 58 | Ba | 57 | A | N1-C6-N6 | -7.41 | 114.15 | 118.60 |
| 22 | AA | 80 | A | C5-C6-N1 | 7.41 | 121.41 | 117.70 |
| 22 | AA | 1151 | A | C4-C5-C6 | -7.41 | 113.30 | 117.00 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 2711 | A | C4-C5-C6 | -7.41 | 113.30 | 117.00 |
| 57 | BA | 1545 | A | C5-C6-N1 | 7.41 | 121.40 | 117.70 |
| 57 | BA | 1809 | A | C5-C6-N1 | 7.41 | 121.40 | 117.70 |
| 57 | BA | 2821 | A | N1-C6-N6 | -7.41 | 114.15 | 118.60 |
| 57 | BA | 103 | A | C5-C6-N1 | 7.41 | 121.40 | 117.70 |
| 57 | BA | 1046 | A | C5-C6-N1 | 7.41 | 121.40 | 117.70 |
| 57 | BA | 1806 | C | N3-C2-O2 | -7.41 | 116.72 | 121.90 |
| 22 | AA | 756 | C | N3-C2-O2 | -7.41 | 116.72 | 121.90 |
| 22 | AA | 1254 | A | C5-C6-N1 | 7.41 | 121.40 | 117.70 |
| 57 | BA | 973 | A | N1-C6-N6 | -7.41 | 114.16 | 118.60 |
| 57 | BA | 1437 | C | N3-C2-O2 | -7.41 | 116.72 | 121.90 |
| 57 | BA | 1679 | A | C5-C6-N1 | 7.41 | 121.40 | 117.70 |
| 22 | AA | 1411 | C | N3-C2-O2 | -7.40 | 116.72 | 121.90 |
| 57 | BA | 486 | C | N3-C2-O2 | -7.40 | 116.72 | 121.90 |
| 22 | AA | 1412 | C | N3-C2-O2 | -7.40 | 116.72 | 121.90 |
| 57 | BA | 513 | A | C5-C6-N1 | 7.40 | 121.40 | 117.70 |
| 57 | BA | 2407 | A | C5-C6-N1 | 7.40 | 121.40 | 117.70 |
| 58 | Ba | 68 | C | N3-C2-O2 | -7.40 | 116.72 | 121.90 |
| 22 | AA | 182 | A | C5-C6-N1 | 7.40 | 121.40 | 117.70 |
| 22 | AA | 295 | C | N3-C2-O2 | -7.40 | 116.72 | 121.90 |
| 22 | AA | 1119 | C | N3-C2-O2 | -7.40 | 116.72 | 121.90 |
| 30 | BP | 21 | ARG | NE-CZ-NH1 | 7.40 | 124.00 | 120.30 |
| 51 | B8 | 7 | ARG | NE-CZ-NH1 | 7.40 | 124.00 | 120.30 |
| 57 | BA | 1103 | A | C4-C5-C6 | -7.40 | 113.30 | 117.00 |
| 57 | BA | 2433 | A | C4-C5-C6 | -7.40 | 113.30 | 117.00 |
| 57 | BA | 73 | A | C4-C5-C6 | -7.40 | 113.30 | 117.00 |
| 57 | BA | 2354 | C | N3-C2-O2 | -7.40 | 116.72 | 121.90 |
| 57 | BA | 151 | C | N3-C2-O2 | -7.40 | 116.72 | 121.90 |
| 57 | BA | 314 | C | N3-C2-O2 | -7.40 | 116.72 | 121.90 |
| 57 | BA | 1672 | A | C5-C6-N1 | 7.40 | 121.40 | 117.70 |
| 22 | AA | 1016 | A | C5-C6-N1 | 7.40 | 121.40 | 117.70 |
| 22 | AA | 1172 | C | N3-C2-O2 | -7.40 | 116.72 | 121.90 |
| 57 | BA | 1960 | A | C5-C6-N1 | 7.40 | 121.40 | 117.70 |
| 22 | AA | 99 | C | N3-C2-O2 | -7.39 | 116.72 | 121.90 |
| 57 | BA | 52 | A | C5-C6-N1 | 7.39 | 121.40 | 117.70 |
| 22 | AA | 186 | C | N3-C2-O2 | -7.39 | 116.73 | 121.90 |
| 22 | AA | 860 | A | C5-C6-N1 | 7.39 | 121.40 | 117.70 |
| 48 | B5 | 15 | ARG | NE-CZ-NH2 | 7.39 | 124.00 | 120.30 |
| 57 | BA | 31 | C | N3-C2-O2 | -7.39 | 116.72 | 121.90 |
| 57 | BA | 742 | A | C5-C6-N1 | 7.39 | 121.40 | 117.70 |
| 57 | BA | 844 | A | C5-C6-N1 | 7.39 | 121.40 | 117.70 |
| 57 | BA | 1164 | C | N3-C2-O2 | -7.39 | 116.72 | 121.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 1909 | C | N3-C2-O2 | -7.39 | 116.72 | 121.90 |
| 57 | BA | 1319 | C | N3-C2-O2 | -7.39 | 116.73 | 121.90 |
| 22 | AA | 47 | C | N3-C2-O2 | -7.39 | 116.73 | 121.90 |
| 36 | BU | 32 | ARG | NE-CZ-NH2 | 7.39 | 124.00 | 120.30 |
| 57 | BA | 1639 | C | N3-C2-O2 | -7.39 | 116.73 | 121.90 |
| 57 | BA | 2377 | A | N1-C6-N6 | -7.39 | 114.17 | 118.60 |
| 57 | BA | 2652 | C | N3-C2-O2 | -7.39 | 116.73 | 121.90 |
| 57 | BA | 76 | C | N3-C2-O2 | -7.39 | 116.73 | 121.90 |
| 24 | A3 | 63 | C | N3-C2-O2 | -7.39 | 116.73 | 121.90 |
| 57 | BA | 225 | C | O4'-C1'-N1 | 7.39 | 114.11 | 108.20 |
| 22 | AA | 958 | A | C4-C5-C6 | -7.38 | 113.31 | 117.00 |
| 35 | BD | 181 | ARG | NE-CZ-NH1 | 7.38 | 123.99 | 120.30 |
| 57 | BA | 815 | C | N3-C2-O2 | -7.38 | 116.73 | 121.90 |
| 57 | BA | 979 | A | C5-C6-N1 | 7.38 | 121.39 | 117.70 |
| 57 | BA | 1007 | C | N3-C2-O2 | -7.38 | 116.73 | 121.90 |
| 57 | BA | 1345 | C | N3-C2-O2 | -7.38 | 116.73 | 121.90 |
| 57 | BA | 1488 | C | N3-C2-O2 | -7.38 | 116.73 | 121.90 |
| 57 | BA | 2042 | A | C5-C6-N1 | 7.38 | 121.39 | 117.70 |
| 57 | BA | 2559 | C | N3-C2-O2 | -7.38 | 116.73 | 121.90 |
| 22 | AA | 196 | A | C5-C6-N1 | 7.38 | 121.39 | 117.70 |
| 22 | AA | 270 | A | C5-C6-N1 | 7.38 | 121.39 | 117.70 |
| 57 | BA | 592 | A | C5-C6-N1 | 7.38 | 121.39 | 117.70 |
| 57 | BA | 1757 | A | C5-C6-N1 | 7.38 | 121.39 | 117.70 |
| 22 | AA | 1203 | C | O4'-C1'-N1 | 7.38 | 114.11 | 108.20 |
| 57 | BA | 2726 | A | C4-C5-C6 | -7.38 | 113.31 | 117.00 |
| 57 | BA | 2730 | C | N3-C2-O2 | -7.38 | 116.73 | 121.90 |
| 57 | BA | 2837 | A | C5-C6-N1 | 7.38 | 121.39 | 117.70 |
| 57 | BA | 2856 | A | C4-C5-C6 | -7.38 | 113.31 | 117.00 |
| 10 | AS | 54 | ARG | NE-CZ-NH1 | 7.38 | 123.99 | 120.30 |
| 24 | A3 | 14 | A | C5-C6-N1 | 7.38 | 121.39 | 117.70 |
| 57 | BA | 715 | A | C5-C6-N1 | 7.38 | 121.39 | 117.70 |
| 57 | BA | 991 | C | N3-C2-O2 | -7.38 | 116.73 | 121.90 |
| 57 | BA | 1144 | A | C5-C6-N1 | 7.38 | 121.39 | 117.70 |
| 57 | BA | 2806 | C | N3-C2-O2 | -7.38 | 116.74 | 121.90 |
| 22 | AA | 282 | A | C5-C6-N1 | 7.38 | 121.39 | 117.70 |
| 22 | AA | 676 | A | C5-C6-N1 | 7.38 | 121.39 | 117.70 |
| 22 | AA | 994 | A | C5-C6-N1 | 7.38 | 121.39 | 117.70 |
| 22 | AA | 1180 | A | C4-C5-C6 | -7.38 | 113.31 | 117.00 |
| 57 | BA | 21 | A | C5-C6-N1 | 7.38 | 121.39 | 117.70 |
| 57 | BA | 2153 | C | N3-C2-O2 | -7.38 | 116.74 | 121.90 |
| 22 | AA | 549 | C | N3-C2-O2 | -7.38 | 116.74 | 121.90 |
| 57 | BA | 922 | C | O4'-C1'-N1 | 7.38 | 114.10 | 108.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 343 | C | N3-C2-O2 | -7.37 | 116.74 | 121.90 |
| 57 | BA | 382 | A | C4-C5-C6 | -7.37 | 113.31 | 117.00 |
| 57 | BA | 1597 | A | C5-C6-N1 | 7.37 | 121.39 | 117.70 |
| 57 | BA | 1796 | U | O4'-C1'-N1 | 7.37 | 114.10 | 108.20 |
| 22 | AA | 189 | A | C5-C6-N1 | 7.37 | 121.39 | 117.70 |
| 22 | AA | 1011 | C | N3-C2-O2 | -7.37 | 116.74 | 121.90 |
| 22 | AA | 1448 | C | N3-C2-O2 | -7.37 | 116.74 | 121.90 |
| 57 | BA | 910 | A | C5-C6-N1 | 7.37 | 121.39 | 117.70 |
| 57 | BA | 1302 | A | N1-C6-N6 | -7.37 | 114.18 | 118.60 |
| 57 | BA | 1347 | A | N1-C6-N6 | -7.37 | 114.18 | 118.60 |
| 57 | BA | 1668 | A | C5-C6-N1 | 7.37 | 121.39 | 117.70 |
| 22 | AA | 23 | C | N3-C2-O2 | -7.37 | 116.74 | 121.90 |
| 22 | AA | 673 | A | C5-C6-N1 | 7.37 | 121.39 | 117.70 |
| 22 | AA | 553 | A | C5-C6-N1 | 7.37 | 121.38 | 117.70 |
| 57 | BA | 2263 | C | N3-C2-O2 | -7.37 | 116.74 | 121.90 |
| 57 | BA | 2469 | A | C5-C6-N1 | 7.37 | 121.39 | 117.70 |
| 22 | AA | 1409 | C | N3-C2-O2 | -7.37 | 116.74 | 121.90 |
| 22 | AA | 908 | A | N1-C6-N6 | -7.37 | 114.18 | 118.60 |
| 57 | BA | 523 | C | N3-C2-O2 | -7.37 | 116.74 | 121.90 |
| 57 | BA | 792 | A | C5-C6-N1 | 7.37 | 121.38 | 117.70 |
| 57 | BA | 1752 | C | N3-C2-O2 | -7.37 | 116.74 | 121.90 |
| 57 | BA | 2154 | A | C5-C6-N1 | 7.37 | 121.38 | 117.70 |
| 57 | BA | 2774 | C | N3-C2-O2 | -7.37 | 116.75 | 121.90 |
| 3 | AL | 30 | ARG | NE-CZ-NH1 | 7.36 | 123.98 | 120.30 |
| 57 | BA | 364 | C | N3-C2-O2 | -7.36 | 116.75 | 121.90 |
| 57 | BA | 2340 | A | N1-C6-N6 | -7.36 | 114.18 | 118.60 |
| 22 | AA | 381 | C | N3-C2-O2 | -7.36 | 116.75 | 121.90 |
| 57 | BA | 1268 | A | C4-C5-C6 | -7.36 | 113.32 | 117.00 |
| 22 | AA | 71 | A | N1-C6-N6 | -7.36 | 114.18 | 118.60 |
| 22 | AA | 1245 | C | N3-C2-O2 | -7.36 | 116.75 | 121.90 |
| 57 | BA | 281 | C | N3-C2-O2 | -7.36 | 116.75 | 121.90 |
| 57 | BA | 1637 | A | C5-C6-N1 | 7.36 | 121.38 | 117.70 |
| 57 | BA | 1985 | C | N3-C2-O2 | -7.36 | 116.75 | 121.90 |
| 22 | AA | 513 | C | N3-C2-O2 | -7.36 | 116.75 | 121.90 |
| 57 | BA | 885 | C | N3-C2-O2 | -7.36 | 116.75 | 121.90 |
| 57 | BA | 1547 | C | N3-C2-O2 | -7.36 | 116.75 | 121.90 |
| 57 | BA | 781 | A | C4-C5-C6 | -7.36 | 113.32 | 117.00 |
| 45 | BE | 83 | ARG | NE-CZ-NH1 | -7.36 | 116.62 | 120.30 |
| 54 | BG | 91 | ARG | NE-CZ-NH2 | 7.36 | 123.98 | 120.30 |
| 57 | BA | 1918 | A | C4-C5-C6 | -7.36 | 113.32 | 117.00 |
| 57 | BA | 2440 | C | N3-C2-O2 | -7.36 | 116.75 | 121.90 |
| 57 | BA | 2670 | A | C5-C6-N1 | 7.36 | 121.38 | 117.70 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | AA | 882 | C | N3-C2-O2 | -7.35 | 116.75 | 121.90 |
| 22 | AA | 889 | A | C4-C5-C6 | -7.35 | 113.32 | 117.00 |
| 22 | AA | 379 | C | N3-C2-O2 | -7.35 | 116.75 | 121.90 |
| 57 | BA | 224 | U | O4'-C1'-N1 | 7.35 | 114.08 | 108.20 |
| 57 | BA | 1335 | C | N3-C2-O2 | -7.35 | 116.75 | 121.90 |
| 57 | BA | 1548 | A | C5-C6-N1 | 7.35 | 121.38 | 117.70 |
| 57 | BA | 1744 | A | C5-C6-N1 | 7.35 | 121.38 | 117.70 |
| 57 | BA | 2036 | C | N3-C2-O2 | -7.35 | 116.75 | 121.90 |
| 22 | AA | 651 | C | N3-C2-O2 | -7.35 | 116.75 | 121.90 |
| 22 | AA | 806 | C | N3-C2-O2 | -7.35 | 116.75 | 121.90 |
| 22 | AA | 975 | A | C5-C6-N1 | 7.35 | 121.38 | 117.70 |
| 57 | BA | 1505 | A | C5-C6-N1 | 7.35 | 121.38 | 117.70 |
| 22 | AA | 44 | A | C5-C6-N1 | 7.35 | 121.37 | 117.70 |
| 22 | AA | 694 | A | C5-C6-N1 | 7.35 | 121.37 | 117.70 |
| 22 | AA | 793 | U | N3-C2-O2 | -7.35 | 117.06 | 122.20 |
| 57 | BA | 66 | C | N3-C2-O2 | -7.35 | 116.76 | 121.90 |
| 57 | BA | 204 | A | C4-C5-C6 | -7.35 | 113.33 | 117.00 |
| 57 | BA | 541 | A | C5-C6-N1 | 7.35 | 121.37 | 117.70 |
| 57 | BA | 1518 | C | N3-C2-O2 | -7.35 | 116.76 | 121.90 |
| 57 | BA | 2442 | C | N3-C2-O2 | -7.35 | 116.76 | 121.90 |
| 57 | BA | 2639 | A | C5-C6-N1 | 7.35 | 121.37 | 117.70 |
| 22 | AA | 315 | A | C4-C5-C6 | -7.35 | 113.33 | 117.00 |
| 22 | AA | 1216 | A | C5-C6-N1 | 7.35 | 121.37 | 117.70 |
| 22 | AA | 431 | A | C5-C6-N1 | 7.34 | 121.37 | 117.70 |
| 22 | AA | 931 | C | N3-C2-O2 | -7.34 | 116.76 | 121.90 |
| 50 | B7 | 12 | ARG | NE-CZ-NH2 | 7.34 | 123.97 | 120.30 |
| 57 | BA | 119 | A | C4-C5-C6 | -7.34 | 113.33 | 117.00 |
| 57 | BA | 1327 | A | C4-C5-C6 | -7.34 | 113.33 | 117.00 |
| 57 | BA | 1414 | C | N3-C2-O2 | -7.34 | 116.76 | 121.90 |
| 57 | BA | 706 | A | C5-C6-N1 | 7.34 | 121.37 | 117.70 |
| 57 | BA | 2281 | A | C4-C5-C6 | -7.34 | 113.33 | 117.00 |
| 22 | AA | 1130 | A | N1-C6-N6 | -7.34 | 114.19 | 118.60 |
| 57 | BA | 670 | A | C5-C6-N1 | 7.34 | 121.37 | 117.70 |
| 57 | BA | 2177 | C | N3-C2-O2 | -7.34 | 116.76 | 121.90 |
| 57 | BA | 2691 | C | N3-C2-O2 | -7.34 | 116.76 | 121.90 |
| 22 | AA | 373 | A | N1-C6-N6 | -7.34 | 114.20 | 118.60 |
| 22 | AA | 487 | A | N1-C6-N6 | -7.34 | 114.20 | 118.60 |
| 57 | BA | 1815 | A | C5-C6-N1 | 7.34 | 121.37 | 117.70 |
| 57 | BA | 2753 | A | C5-C6-N1 | 7.34 | 121.37 | 117.70 |
| 22 | AA | 1223 | C | N3-C2-O2 | -7.34 | 116.76 | 121.90 |
| 24 | A3 | 35 | C | N3-C2-O2 | -7.34 | 116.76 | 121.90 |
| 57 | BA | 1359 | A | C4-C5-C6 | -7.34 | 113.33 | 117.00 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | AA | 1179 | A | C4-C5-C6 | -7.34 | 113.33 | 117.00 |
| 57 | BA | 1254 | A | N1-C6-N6 | -7.34 | 114.20 | 118.60 |
| 57 | BA | 2482 | A | C5-C6-N1 | 7.34 | 121.37 | 117.70 |
| 57 | BA | 2558 | C | N3-C2-O2 | -7.34 | 116.76 | 121.90 |
| 57 | BA | 2820 | A | C5-C6-N1 | 7.34 | 121.37 | 117.70 |
| 22 | AA | 383 | A | N1-C6-N6 | -7.33 | 114.20 | 118.60 |
| 22 | AA | 396 | C | N3-C2-O2 | -7.33 | 116.77 | 121.90 |
| 57 | BA | 143 | C | N3-C2-O2 | -7.33 | 116.77 | 121.90 |
| 31 | BQ | 44 | ARG | NE-CZ-NH2 | 7.33 | 123.97 | 120.30 |
| 57 | BA | 794 | A | C5-C6-N1 | 7.33 | 121.37 | 117.70 |
| 57 | BA | 1625 | C | N3-C2-O2 | -7.33 | 116.77 | 121.90 |
| 22 | AA | 1275 | A | C5-C6-N1 | 7.33 | 121.36 | 117.70 |
| 57 | BA | 354 | A | C5-C6-N1 | 7.33 | 121.37 | 117.70 |
| 22 | AA | 738 | C | N3-C2-O2 | -7.33 | 116.77 | 121.90 |
| 57 | BA | 161 | A | C4-C5-C6 | -7.33 | 113.33 | 117.00 |
| 57 | BA | 731 | C | N3-C2-O2 | -7.33 | 116.77 | 121.90 |
| 57 | BA | 2039 | U | O4'-C1'-N1 | 7.33 | 114.06 | 108.20 |
| 22 | AA | 808 | C | N3-C2-O2 | -7.33 | 116.77 | 121.90 |
| 22 | AA | 1380 | U | O4'-C1'-N1 | 7.33 | 114.06 | 108.20 |
| 57 | BA | 2082 | A | C5-C6-N1 | 7.33 | 121.36 | 117.70 |
| 57 | BA | 2267 | A | C4-C5-C6 | -7.33 | 113.34 | 117.00 |
| 22 | AA | 448 | A | C4-C5-C6 | -7.33 | 113.34 | 117.00 |
| 57 | BA | 1230 | A | C5-C6-N1 | 7.33 | 121.36 | 117.70 |
| 57 | BA | 2467 | C | N3-C2-O2 | -7.33 | 116.77 | 121.90 |
| 22 | AA | 1037 | C | N3-C2-O2 | -7.33 | 116.77 | 121.90 |
| 57 | BA | 37 | C | N3-C2-O2 | -7.33 | 116.77 | 121.90 |
| 57 | BA | 675 | A | C5-C6-N1 | 7.33 | 121.36 | 117.70 |
| 22 | AA | 328 | C | N1-C2-O2 | 7.32 | 123.29 | 118.90 |
| 22 | AA | 1293 | C | N3-C2-O2 | -7.32 | 116.77 | 121.90 |
| 22 | AA | 1318 | A | N1-C6-N6 | -7.32 | 114.21 | 118.60 |
| 57 | BA | 255 | A | C5-C6-N1 | 7.32 | 121.36 | 117.70 |
| 57 | BA | 1999 | C | N3-C2-O2 | -7.32 | 116.77 | 121.90 |
| 57 | BA | 2893 | A | C5-C6-N1 | 7.32 | 121.36 | 117.70 |
| 57 | BA | 1096 | A | C5-C6-N1 | 7.32 | 121.36 | 117.70 |
| 21 | A1 | 358 | ARG | NE-CZ-NH1 | 7.32 | 123.96 | 120.30 |
| 22 | AA | 325 | A | C4-C5-C6 | -7.32 | 113.34 | 117.00 |
| 22 | AA | 681 | A | C5-C6-N1 | 7.32 | 121.36 | 117.70 |
| 57 | BA | 1165 | A | C5-C6-N1 | 7.32 | 121.36 | 117.70 |
| 57 | BA | 2451 | A | C4-C5-C6 | -7.32 | 113.34 | 117.00 |
| 57 | BA | 311 | A | C5-C6-N1 | 7.32 | 121.36 | 117.70 |
| 57 | BA | 1152 | C | N3-C2-O2 | -7.32 | 116.78 | 121.90 |
| 57 | BA | 1480 | C | N3-C2-O2 | -7.32 | 116.78 | 121.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 917 | A | C5-C6-N1 | 7.32 | 121.36 | 117.70 |
| 57 | BA | 1020 | A | C5-C6-N1 | 7.32 | 121.36 | 117.70 |
| 22 | AA | 1179 | A | C5-C6-N1 | 7.32 | 121.36 | 117.70 |
| 57 | BA | 1854 | A | C5-C6-N1 | 7.32 | 121.36 | 117.70 |
| 57 | BA | 2023 | C | N3-C2-O2 | -7.32 | 116.78 | 121.90 |
| 57 | BA | 899 | A | C5-C6-N1 | 7.31 | 121.36 | 117.70 |
| 22 | AA | 780 | A | C5-C6-N1 | 7.31 | 121.36 | 117.70 |
| 57 | BA | 102 | U | O4'-C1'-N1 | 7.31 | 114.05 | 108.20 |
| 57 | BA | 111 | A | C5-C6-N1 | 7.31 | 121.36 | 117.70 |
| 57 | BA | 346 | A | C5-C6-N1 | 7.31 | 121.36 | 117.70 |
| 57 | BA | 592 | A | C4-C5-C6 | -7.31 | 113.34 | 117.00 |
| 22 | AA | 55 | A | C5-C6-N1 | 7.31 | 121.36 | 117.70 |
| 22 | AA | 1497 | G | N1-C6-O6 | -7.31 | 115.51 | 119.90 |
| 24 | A3 | 38 | A | C4-C5-C6 | -7.31 | 113.35 | 117.00 |
| 57 | BA | 660 | C | N3-C2-O2 | -7.31 | 116.78 | 121.90 |
| 57 | BA | 2368 | C | N3-C2-O2 | -7.31 | 116.78 | 121.90 |
| 57 | BA | 2515 | C | N3-C2-O2 | -7.31 | 116.78 | 121.90 |
| 22 | AA | 1171 | A | C5-C6-N1 | 7.31 | 121.35 | 117.70 |
| 57 | BA | 20 | C | N3-C2-O2 | -7.31 | 116.78 | 121.90 |
| 57 | BA | 336 | C | N3-C2-O2 | -7.31 | 116.78 | 121.90 |
| 57 | BA | 1001 | A | C5-C6-N1 | 7.31 | 121.35 | 117.70 |
| 57 | BA | 2006 | C | N3-C2-O2 | -7.31 | 116.78 | 121.90 |
| 57 | BA | 2785 | C | N3-C2-O2 | -7.31 | 116.78 | 121.90 |
| 22 | AA | 807 | A | C5-C6-N1 | 7.31 | 121.35 | 117.70 |
| 57 | BA | 2649 | C | N3-C2-O2 | -7.31 | 116.78 | 121.90 |
| 22 | AA | 1092 | A | C5-C6-N1 | 7.30 | 121.35 | 117.70 |
| 22 | AA | 1311 | A | C4-C5-C6 | -7.30 | 113.35 | 117.00 |
| 57 | BA | 485 | C | N3-C2-O2 | -7.30 | 116.79 | 121.90 |
| 57 | BA | 1150 | C | N3-C2-O2 | -7.30 | 116.79 | 121.90 |
| 57 | BA | 2799 | A | C5-C6-N1 | 7.30 | 121.35 | 117.70 |
| 22 | AA | 370 | C | N3-C2-O2 | -7.30 | 116.79 | 121.90 |
| 57 | BA | 479 | A | C4-C5-C6 | -7.30 | 113.35 | 117.00 |
| 57 | BA | 1504 | A | C4-C5-C6 | -7.30 | 113.35 | 117.00 |
| 57 | BA | 1893 | C | O4'-C1'-N1 | 7.30 | 114.04 | 108.20 |
| 57 | BA | 2248 | C | N3-C2-O2 | -7.30 | 116.79 | 121.90 |
| 22 | AA | 401 | C | N3-C2-O2 | -7.30 | 116.79 | 121.90 |
| 54 | BG | 177 | ARG | NE-CZ-NH1 | 7.30 | 123.95 | 120.30 |
| 24 | A3 | 24 | C | N3-C2-O2 | -7.30 | 116.79 | 121.90 |
| 57 | BA | 176 | A | C5-C6-N1 | 7.30 | 121.35 | 117.70 |
| 57 | BA | 668 | A | C4-C5-C6 | -7.30 | 113.35 | 117.00 |
| 58 | Ba | 110 | C | N3-C2-O2 | -7.30 | 116.79 | 121.90 |
| 22 | AA | 1349 | A | C4-C5-C6 | -7.30 | 113.35 | 117.00 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 1735 | A | C5-C6-N1 | 7.30 | 121.35 | 117.70 |
| 22 | AA | 1028 | C | N3-C2-O2 | -7.29 | 116.79 | 121.90 |
| 57 | BA | 1114 | C | N3-C2-O2 | -7.29 | 116.79 | 121.90 |
| 57 | BA | 2636 | C | O4'-C1'-N1 | 7.29 | 114.04 | 108.20 |
| 22 | AA | 98 | A | C5-C6-N1 | 7.29 | 121.35 | 117.70 |
| 22 | AA | 1413 | A | C5-C6-N1 | 7.29 | 121.35 | 117.70 |
| 24 | A3 | 69 | C | N3-C2-O2 | -7.29 | 116.80 | 121.90 |
| 57 | BA | 172 | A | C5-C6-N1 | 7.29 | 121.35 | 117.70 |
| 57 | BA | 1399 | C | N3-C2-O2 | -7.29 | 116.80 | 121.90 |
| 57 | BA | 1732 | C | O4'-C1'-N1 | 7.29 | 114.03 | 108.20 |
| 22 | AA | 81 | A | C5-C6-N1 | 7.29 | 121.34 | 117.70 |
| 57 | BA | 833 | A | C5-C6-N1 | 7.29 | 121.34 | 117.70 |
| 57 | BA | 1291 | C | N3-C2-O2 | -7.29 | 116.80 | 121.90 |
| 57 | BA | 2091 | C | N3-C2-O2 | -7.29 | 116.80 | 121.90 |
| 22 | AA | 338 | A | C5-C6-N1 | 7.29 | 121.34 | 117.70 |
| 22 | AA | 1109 | C | N3-C2-O2 | -7.29 | 116.80 | 121.90 |
| 57 | BA | 1977 | A | C5-C6-N1 | 7.29 | 121.34 | 117.70 |
| 57 | BA | 2326 | C | N3-C2-O2 | -7.29 | 116.80 | 121.90 |
| 57 | BA | 1532 | A | C4-C5-C6 | -7.29 | 113.36 | 117.00 |
| 57 | BA | 2486 | C | N3-C2-O2 | -7.29 | 116.80 | 121.90 |
| 22 | AA | 451 | A | C4-C5-C6 | -7.28 | 113.36 | 117.00 |
| 22 | AA | 460 | A | C4-C5-C6 | -7.28 | 113.36 | 117.00 |
| 22 | AA | 915 | A | C4-C5-C6 | -7.28 | 113.36 | 117.00 |
| 46 | B3 | 15 | ARG | NE-CZ-NH2 | 7.28 | 123.94 | 120.30 |
| 57 | BA | 1522 | A | C5-C6-N1 | 7.28 | 121.34 | 117.70 |
| 58 | Ba | 3 | C | N3-C2-O2 | -7.28 | 116.80 | 121.90 |
| 57 | BA | 800 | A | C5-C6-N1 | 7.28 | 121.34 | 117.70 |
| 57 | BA | 1533 | C | N3-C2-O2 | -7.28 | 116.80 | 121.90 |
| 22 | AA | 33 | A | C5-C6-N1 | 7.28 | 121.34 | 117.70 |
| 22 | AA | 634 | C | N3-C2-O2 | -7.28 | 116.80 | 121.90 |
| 57 | BA | 366 | C | N3-C2-O2 | -7.28 | 116.80 | 121.90 |
| 57 | BA | 743 | A | C5-C6-N1 | 7.28 | 121.34 | 117.70 |
| 57 | BA | 1158 | C | N3-C2-O2 | -7.28 | 116.80 | 121.90 |
| 57 | BA | 1363 | C | N3-C2-O2 | -7.28 | 116.80 | 121.90 |
| 57 | BA | 1431 | A | C5-C6-N1 | 7.28 | 121.34 | 117.70 |
| 57 | BA | 1727 | C | N3-C2-O2 | -7.28 | 116.80 | 121.90 |
| 22 | AA | 171 | A | C5-C6-N1 | 7.28 | 121.34 | 117.70 |
| 58 | Ba | 101 | A | N1-C6-N6 | -7.28 | 114.23 | 118.60 |
| 22 | AA | 662 | U | O4'-C1'-N1 | 7.28 | 114.02 | 108.20 |
| 57 | BA | 1469 | A | C5-C6-N1 | 7.28 | 121.34 | 117.70 |
| 57 | BA | 2418 | A | C4-C5-C6 | -7.28 | 113.36 | 117.00 |
| 22 | AA | 523 | A | C5-C6-N1 | 7.28 | 121.34 | 117.70 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 256 | A | C5-C6-N1 | 7.28 | 121.34 | 117.70 |
| 57 | BA | 1196 | C | N3-C2-O2 | -7.28 | 116.81 | 121.90 |
| 22 | AA | 658 | C | N3-C2-O2 | -7.27 | 116.81 | 121.90 |
| 13 | AU | 16 | ARG | NE-CZ-NH1 | 7.27 | 123.94 | 120.30 |
| 22 | AA | 747 | A | C5-C6-N1 | 7.27 | 121.34 | 117.70 |
| 57 | BA | 644 | A | C5-C6-N1 | 7.27 | 121.34 | 117.70 |
| 57 | BA | 1265 | A | C5-C6-N1 | 7.27 | 121.34 | 117.70 |
| 57 | BA | 1868 | C | N3-C2-O2 | -7.27 | 116.81 | 121.90 |
| 22 | AA | 784 | A | N1-C6-N6 | -7.27 | 114.24 | 118.60 |
| 27 | BK | 133 | ARG | NE-CZ-NH1 | 7.27 | 123.94 | 120.30 |
| 22 | AA | 848 | C | N3-C2-O2 | -7.27 | 116.81 | 121.90 |
| 22 | AA | 1429 | A | C5-C6-N1 | 7.27 | 121.33 | 117.70 |
| 22 | AA | 1431 | A | C5-C6-N1 | 7.27 | 121.33 | 117.70 |
| 57 | BA | 2776 | A | N1-C6-N6 | -7.27 | 114.24 | 118.60 |
| 57 | BA | 2469 | A | N1-C6-N6 | -7.27 | 114.24 | 118.60 |
| 22 | AA | 1 | A | C5-C6-N1 | 7.27 | 121.33 | 117.70 |
| 57 | BA | 2451 | A | C5-C6-N1 | 7.26 | 121.33 | 117.70 |
| 58 | Ba | 63 | C | N3-C2-O2 | -7.26 | 116.81 | 121.90 |
| 22 | AA | 1280 | A | C5-C6-N1 | 7.26 | 121.33 | 117.70 |
| 57 | BA | 1711 | A | C4-C5-C6 | -7.26 | 113.37 | 117.00 |
| 57 | BA | 2043 | C | N3-C2-O2 | -7.26 | 116.82 | 121.90 |
| 57 | BA | 1269 | A | C5-C6-N1 | 7.26 | 121.33 | 117.70 |
| 57 | BA | 2682 | A | C5-C6-N1 | 7.26 | 121.33 | 117.70 |
| 58 | Ba | 58 | A | C4-C5-C6 | -7.26 | 113.37 | 117.00 |
| 22 | AA | 225 | C | N3-C2-O2 | -7.26 | 116.82 | 121.90 |
| 22 | AA | 912 | C | N3-C2-O2 | -7.26 | 116.82 | 121.90 |
| 23 | A2 | 58 | C | N3-C2-O2 | -7.26 | 116.82 | 121.90 |
| 24 | A3 | 22 | A | C4-C5-C6 | -7.26 | 113.37 | 117.00 |
| 45 | BE | 59 | ARG | NE-CZ-NH2 | 7.26 | 123.93 | 120.30 |
| 57 | BA | 609 | A | N1-C6-N6 | -7.26 | 114.24 | 118.60 |
| 57 | BA | 1384 | A | C4-C5-C6 | -7.26 | 113.37 | 117.00 |
| 57 | BA | 1685 | C | N3-C2-O2 | -7.26 | 116.82 | 121.90 |
| 58 | Ba | 71 | C | N3-C2-O2 | -7.26 | 116.82 | 121.90 |
| 57 | BA | 922 | C | N3-C2-O2 | -7.26 | 116.82 | 121.90 |
| 57 | BA | 2739 | U | O4'-C1'-N1 | 7.26 | 114.01 | 108.20 |
| 58 | Ba | 46 | A | C4-C5-C6 | -7.26 | 113.37 | 117.00 |
| 22 | AA | 303 | A | C5-C6-N1 | 7.26 | 121.33 | 117.70 |
| 57 | BA | 1161 | C | N3-C2-O2 | -7.26 | 116.82 | 121.90 |
| 57 | BA | 1472 | C | N3-C2-O2 | -7.26 | 116.82 | 121.90 |
| 57 | BA | 1571 | A | N1-C6-N6 | -7.26 | 114.25 | 118.60 |
| 22 | AA | 573 | A | C5-C6-N1 | 7.25 | 121.33 | 117.70 |
| 57 | BA | 2317 | A | C4-C5-C6 | -7.25 | 113.37 | 117.00 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | AA | 1388 | C | N3-C2-O2 | -7.25 | 116.82 | 121.90 |
| 24 | A3 | 15 | G | O4'-C1'-N9 | 7.25 | 114.00 | 108.20 |
| 22 | AA | 1329 | A | C5-C6-N1 | 7.25 | 121.33 | 117.70 |
| 57 | BA | 472 | A | C5-C6-N1 | 7.25 | 121.33 | 117.70 |
| 57 | BA | 1991 | U | O4'-C1'-N1 | 7.25 | 114.00 | 108.20 |
| 22 | AA | 465 | A | N1-C6-N6 | -7.25 | 114.25 | 118.60 |
| 57 | BA | 1969 | A | C5-C6-N1 | 7.25 | 121.33 | 117.70 |
| 22 | AA | 490 | C | N3-C2-O2 | -7.25 | 116.83 | 121.90 |
| 57 | BA | 1902 | C | N3-C2-O2 | -7.25 | 116.83 | 121.90 |
| 22 | AA | 40 | C | N3-C2-O2 | -7.25 | 116.83 | 121.90 |
| 32 | BR | 118 | ARG | NE-CZ-NH1 | 7.25 | 123.92 | 120.30 |
| 22 | AA | 74 | A | C5-C6-N1 | 7.25 | 121.32 | 117.70 |
| 57 | BA | 393 | C | N3-C2-O2 | -7.25 | 116.83 | 121.90 |
| 57 | BA | 599 | A | C5-C6-N1 | 7.25 | 121.32 | 117.70 |
| 57 | BA | 1947 | C | N3-C2-O2 | -7.25 | 116.83 | 121.90 |
| 58 | Ba | 49 | C | N3-C2-O2 | -7.25 | 116.83 | 121.90 |
| 22 | AA | 329 | A | C5-C6-N1 | 7.24 | 121.32 | 117.70 |
| 22 | AA | 334 | C | N3-C2-O2 | -7.24 | 116.83 | 121.90 |
| 22 | AA | 602 | A | C4-C5-C6 | -7.24 | 113.38 | 117.00 |
| 22 | AA | 946 | A | C5-C6-N1 | 7.24 | 121.32 | 117.70 |
| 22 | AA | 1046 | A | C5-C6-N1 | 7.24 | 121.32 | 117.70 |
| 50 | B7 | 39 | ARG | NE-CZ-NH1 | 7.24 | 123.92 | 120.30 |
| 57 | BA | 455 | C | N3-C2-O2 | -7.24 | 116.83 | 121.90 |
| 57 | BA | 1261 | C | N3-C2-O2 | -7.24 | 116.83 | 121.90 |
| 57 | BA | 1701 | A | C5-C6-N1 | 7.24 | 121.32 | 117.70 |
| 57 | BA | 2175 | C | N3-C2-O2 | -7.24 | 116.83 | 121.90 |
| 57 | BA | 2888 | C | N3-C2-O2 | -7.24 | 116.83 | 121.90 |
| 22 | AA | 1318 | A | C5-C6-N1 | 7.24 | 121.32 | 117.70 |
| 57 | BA | 1580 | A | C4-C5-C6 | -7.24 | 113.38 | 117.00 |
| 57 | BA | 1722 | A | C5-C6-N1 | 7.24 | 121.32 | 117.70 |
| 57 | BA | 265 | A | C5-C6-N1 | 7.24 | 121.32 | 117.70 |
| 57 | BA | 1247 | A | C4-C5-C6 | -7.24 | 113.38 | 117.00 |
| 57 | BA | 1330 | C | N3-C2-O2 | -7.24 | 116.83 | 121.90 |
| 57 | BA | 1804 | C | N3-C2-O2 | -7.24 | 116.83 | 121.90 |
| 57 | BA | 2863 | C | N3-C2-O2 | -7.24 | 116.83 | 121.90 |
| 22 | AA | 316 | C | N3-C2-O2 | -7.24 | 116.83 | 121.90 |
| 57 | BA | 1848 | A | C4-C5-C6 | -7.24 | 113.38 | 117.00 |
| 57 | BA | 2521 | C | N1-C2-O2 | 7.24 | 123.24 | 118.90 |
| 57 | BA | 428 | A | C4-C5-C6 | -7.24 | 113.38 | 117.00 |
| 57 | BA | 2369 | A | C5-C6-N1 | 7.24 | 121.32 | 117.70 |
| 22 | AA | 415 | A | N1-C6-N6 | -7.23 | 114.26 | 118.60 |
| 22 | AA | 1476 | A | C5-C6-N1 | 7.23 | 121.32 | 117.70 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | AA | 696 | A | C5-C6-N1 | 7.23 | 121.32 | 117.70 |
| 57 | BA | 115 | C | N3-C2-O2 | -7.23 | 116.84 | 121.90 |
| 57 | BA | 238 | C | N3-C2-O2 | -7.23 | 116.84 | 121.90 |
| 57 | BA | 253 | C | O4'-C1'-N1 | 7.23 | 113.99 | 108.20 |
| 57 | BA | 1392 | A | C5-C6-N1 | 7.23 | 121.32 | 117.70 |
| 57 | BA | 2003 | A | C5-C6-N1 | 7.23 | 121.32 | 117.70 |
| 58 | Ba | 113 | C | N3-C2-O2 | -7.23 | 116.84 | 121.90 |
| 22 | AA | 805 | C | N3-C2-O2 | -7.23 | 116.84 | 121.90 |
| 24 | A3 | 66 | C | N3-C2-O2 | -7.23 | 116.84 | 121.90 |
| 57 | BA | 2486 | C | O4'-C1'-N1 | 7.23 | 113.98 | 108.20 |
| 57 | BA | 1243 | C | N3-C2-O2 | -7.23 | 116.84 | 121.90 |
| 57 | BA | 1494 | A | C4-C5-C6 | -7.23 | 113.39 | 117.00 |
| 57 | BA | 1551 | A | N1-C6-N6 | -7.23 | 114.26 | 118.60 |
| 22 | AA | 321 | A | C4-C5-C6 | -7.23 | 113.39 | 117.00 |
| 22 | AA | 1434 | A | C4-C5-C6 | -7.23 | 113.39 | 117.00 |
| 24 | A3 | 40 | C | N3-C2-O2 | -7.23 | 116.84 | 121.90 |
| 57 | BA | 2600 | A | C5-C6-N1 | 7.23 | 121.31 | 117.70 |
| 58 | Ba | 118 | C | N3-C2-O2 | -7.23 | 116.84 | 121.90 |
| 57 | BA | 2439 | A | O4'-C1'-N9 | 7.23 | 113.98 | 108.20 |
| 22 | AA | 349 | A | C5-C6-N1 | 7.22 | 121.31 | 117.70 |
| 57 | BA | 340 | A | C4-C5-C6 | -7.22 | 113.39 | 117.00 |
| 57 | BA | 1503 | A | C4-C5-C6 | -7.22 | 113.39 | 117.00 |
| 57 | BA | 2129 | C | O4'-C1'-N1 | 7.22 | 113.98 | 108.20 |
| 22 | AA | 896 | C | N3-C2-O2 | -7.22 | 116.84 | 121.90 |
| 22 | AA | 1032 | G | O4'-C1'-N9 | 7.22 | 113.98 | 108.20 |
| 57 | BA | 1495 | A | C5-C6-N1 | 7.22 | 121.31 | 117.70 |
| 57 | BA | 1821 | A | C4-C5-C6 | -7.22 | 113.39 | 117.00 |
| 22 | AA | 1280 | A | C4-C5-C6 | -7.22 | 113.39 | 117.00 |
| 57 | BA | 516 | C | O4'-C1'-N1 | 7.22 | 113.98 | 108.20 |
| 57 | BA | 929 | U | O4'-C1'-N1 | 7.22 | 113.98 | 108.20 |
| 57 | BA | 2566 | A | C5-C6-N1 | 7.22 | 121.31 | 117.70 |
| 57 | BA | 723 | C | O4'-C1'-N1 | 7.22 | 113.97 | 108.20 |
| 57 | BA | 784 | G | O4'-C1'-N9 | 7.22 | 113.97 | 108.20 |
| 57 | BA | 1229 | C | N3-C2-O2 | -7.22 | 116.85 | 121.90 |
| 57 | BA | 1600 | C | N3-C2-O2 | -7.22 | 116.85 | 121.90 |
| 57 | BA | 2657 | A | C5-C6-N1 | 7.22 | 121.31 | 117.70 |
| 22 | AA | 1437 | A | C5-C6-N1 | 7.21 | 121.31 | 117.70 |
| 24 | A3 | 68 | C | N3-C2-O2 | -7.21 | 116.85 | 121.90 |
| 57 | BA | 244 | A | C4-C5-C6 | -7.21 | 113.39 | 117.00 |
| 57 | BA | 449 | A | N1-C6-N6 | -7.21 | 114.27 | 118.60 |
| 57 | BA | 1403 | A | C4-C5-C6 | -7.21 | 113.39 | 117.00 |
| 57 | BA | 1874 | C | N3-C2-O2 | -7.21 | 116.85 | 121.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 58 | Ba | 59 | A | C5-C6-N1 | 7.21 | 121.31 | 117.70 |
| 9 | AR | 2 | ARG | NE-CZ-NH1 | 7.21 | 123.91 | 120.30 |
| 22 | AA | 90 | C | N3-C2-O2 | -7.21 | 116.85 | 121.90 |
| 57 | BA | 2196 | C | N3-C2-O2 | -7.21 | 116.85 | 121.90 |
| 22 | AA | 389 | A | C5-C6-N1 | 7.21 | 121.31 | 117.70 |
| 22 | AA | 1306 | A | N1-C6-N6 | -7.21 | 114.27 | 118.60 |
| 24 | A3 | 36 | A | C5-C6-N1 | 7.21 | 121.31 | 117.70 |
| 57 | BA | 92 | U | O4'-C1'-N1 | 7.21 | 113.97 | 108.20 |
| 57 | BA | 492 | A | C5-C6-N1 | 7.21 | 121.31 | 117.70 |
| 57 | BA | 990 | A | C4-C5-C6 | -7.21 | 113.39 | 117.00 |
| 57 | BA | 1532 | A | C5-C6-N1 | 7.21 | 121.31 | 117.70 |
| 57 | BA | 677 | A | C4-C5-C6 | -7.21 | 113.39 | 117.00 |
| 57 | BA | 840 | C | N3-C2-O2 | -7.21 | 116.85 | 121.90 |
| 22 | AA | 486 | U | O4'-C1'-N1 | 7.21 | 113.97 | 108.20 |
| 22 | AA | 1197 | A | N1-C6-N6 | -7.21 | 114.28 | 118.60 |
| 57 | BA | 572 | A | N1-C6-N6 | -7.21 | 114.28 | 118.60 |
| 57 | BA | 1531 | C | N3-C2-O2 | -7.21 | 116.85 | 121.90 |
| 58 | Ba | 19 | C | N3-C2-O2 | -7.21 | 116.85 | 121.90 |
| 22 | AA | 488 | C | N3-C2-O2 | -7.21 | 116.86 | 121.90 |
| 22 | AA | 572 | A | C4-C5-C6 | -7.21 | 113.40 | 117.00 |
| 57 | BA | 1290 | C | N3-C2-O2 | -7.21 | 116.86 | 121.90 |
| 22 | AA | 74 | A | C4-C5-C6 | -7.20 | 113.40 | 117.00 |
| 22 | AA | 392 | C | N3-C2-O2 | -7.20 | 116.86 | 121.90 |
| 22 | AA | 892 | A | C5-C6-N1 | 7.20 | 121.30 | 117.70 |
| 22 | AA | 1344 | C | N3-C2-O2 | -7.20 | 116.86 | 121.90 |
| 57 | BA | 209 | C | N3-C2-O2 | -7.20 | 116.86 | 121.90 |
| 57 | BA | 2119 | A | C5-C6-N1 | 7.20 | 121.30 | 117.70 |
| 57 | BA | 201 | C | N3-C2-O2 | -7.20 | 116.86 | 121.90 |
| 57 | BA | 2751 | G | O4'-C1'-N9 | 7.20 | 113.96 | 108.20 |
| 22 | AA | 699 | C | N3-C2-O2 | -7.20 | 116.86 | 121.90 |
| 22 | AA | 739 | C | N3-C2-O2 | -7.20 | 116.86 | 121.90 |
| 22 | AA | 1462 | C | N3-C2-O2 | -7.20 | 116.86 | 121.90 |
| 57 | BA | 385 | C | N3-C2-O2 | -7.20 | 116.86 | 121.90 |
| 57 | BA | 1916 | A | C5-C6-N1 | 7.20 | 121.30 | 117.70 |
| 57 | BA | 2206 | C | N3-C2-O2 | -7.20 | 116.86 | 121.90 |
| 9 | AR | 47 | ARG | NE-CZ-NH1 | 7.20 | 123.90 | 120.30 |
| 57 | BA | 959 | A | N1-C6-N6 | -7.20 | 114.28 | 118.60 |
| 57 | BA | 1612 | C | N3-C2-O2 | -7.20 | 116.86 | 121.90 |
| 58 | Ba | 0 | U | O4'-C1'-N1 | 7.20 | 113.96 | 108.20 |
| 22 | AA | 364 | A | C5-C6-N1 | 7.20 | 121.30 | 117.70 |
| 57 | BA | 1728 | C | N3-C2-O2 | -7.20 | 116.86 | 121.90 |
| 57 | BA | 2381 | A | C4-C5-C6 | -7.20 | 113.40 | 117.00 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | AA | 67 | C | N3-C2-O2 | -7.20 | 116.86 | 121.90 |
| 22 | AA | 153 | C | N3-C2-O2 | -7.20 | 116.86 | 121.90 |
| 22 | AA | 1001 | C | N3-C2-O2 | -7.20 | 116.86 | 121.90 |
| 57 | BA | 634 | C | N3-C2-O2 | -7.20 | 116.86 | 121.90 |
| 57 | BA | 870 | U | O4'-C1'-N1 | 7.19 | 113.96 | 108.20 |
| 22 | AA | 1236 | A | N1-C6-N6 | -7.19 | 114.28 | 118.60 |
| 57 | BA | 290 | U | O4'-C1'-N1 | 7.19 | 113.95 | 108.20 |
| 57 | BA | 436 | C | N3-C2-O2 | -7.19 | 116.86 | 121.90 |
| 57 | BA | 1726 | C | N3-C2-O2 | -7.19 | 116.86 | 121.90 |
| 57 | BA | 2716 | C | N3-C2-O2 | -7.19 | 116.86 | 121.90 |
| 22 | AA | 34 | C | N3-C2-O2 | -7.19 | 116.87 | 121.90 |
| 57 | BA | 221 | A | C5-C6-N1 | 7.19 | 121.30 | 117.70 |
| 57 | BA | 2003 | A | C4-C5-C6 | -7.19 | 113.41 | 117.00 |
| 58 | Ba | 17 | C | N3-C2-O2 | -7.19 | 116.87 | 121.90 |
| 58 | Ba | 114 | C | N3-C2-O2 | -7.19 | 116.87 | 121.90 |
| 22 | AA | 393 | A | C4-C5-C6 | -7.19 | 113.41 | 117.00 |
| 22 | AA | 1329 | A | C4-C5-C6 | -7.19 | 113.41 | 117.00 |
| 57 | BA | 945 | A | C4-C5-C6 | -7.19 | 113.41 | 117.00 |
| 57 | BA | 1704 | C | N3-C2-O2 | -7.19 | 116.87 | 121.90 |
| 57 | BA | 1608 | A | C5-C6-N1 | 7.19 | 121.29 | 117.70 |
| 22 | AA | 1302 | C | N3-C2-O2 | -7.19 | 116.87 | 121.90 |
| 24 | A3 | 62 | C | N3-C2-O2 | -7.18 | 116.87 | 121.90 |
| 57 | BA | 32 | C | N3-C2-O2 | -7.18 | 116.87 | 121.90 |
| 57 | BA | 1014 | A | C5-C6-N1 | 7.18 | 121.29 | 117.70 |
| 22 | AA | 374 | A | C4-C5-C6 | -7.18 | 113.41 | 117.00 |
| 22 | AA | 1195 | C | N3-C2-O2 | -7.18 | 116.87 | 121.90 |
| 57 | BA | 414 | C | N3-C2-O2 | -7.18 | 116.87 | 121.90 |
| 57 | BA | 793 | A | C5-C6-N1 | 7.18 | 121.29 | 117.70 |
| 57 | BA | 2513 | A | C5-C6-N1 | 7.18 | 121.29 | 117.70 |
| 21 | A1 | 50 | ARG | NE-CZ-NH1 | 7.18 | 123.89 | 120.30 |
| 57 | BA | 2463 | C | N3-C2-O2 | -7.18 | 116.87 | 121.90 |
| 13 | AU | 68 | ARG | NE-CZ-NH1 | 7.18 | 123.89 | 120.30 |
| 22 | AA | 1273 | C | N3-C2-O2 | -7.18 | 116.87 | 121.90 |
| 57 | BA | 505 | A | C4-C5-C6 | -7.18 | 113.41 | 117.00 |
| 57 | BA | 758 | C | N3-C2-O2 | -7.18 | 116.88 | 121.90 |
| 57 | BA | 2063 | C | N3-C2-O2 | -7.18 | 116.88 | 121.90 |
| 57 | BA | 2902 | C | N3-C2-O2 | -7.18 | 116.88 | 121.90 |
| 22 | AA | 277 | C | N3-C2-O2 | -7.18 | 116.88 | 121.90 |
| 22 | AA | 1136 | C | N3-C2-O2 | -7.18 | 116.88 | 121.90 |
| 57 | BA | 203 | A | C5-C6-N1 | 7.18 | 121.29 | 117.70 |
| 57 | BA | 211 | C | N3-C2-O2 | -7.18 | 116.88 | 121.90 |
| 57 | BA | 1001 | A | C4-C5-C6 | -7.18 | 113.41 | 117.00 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 1572 | A | C5-C6-N1 | 7.18 | 121.29 | 117.70 |
| 57 | BA | 1591 | A | C5-C6-N1 | 7.18 | 121.29 | 117.70 |
| 57 | BA | 2636 | C | N3-C2-O2 | -7.18 | 116.88 | 121.90 |
| 22 | AA | 900 | A | C5-C6-N1 | 7.17 | 121.29 | 117.70 |
| 57 | BA | 1172 | C | N3-C2-O2 | -7.17 | 116.88 | 121.90 |
| 43 | B1 | 10 | ARG | NE-CZ-NH2 | 7.17 | 123.89 | 120.30 |
| 57 | BA | 1237 | A | C4-C5-C6 | -7.17 | 113.41 | 117.00 |
| 57 | BA | 2112 | G | O4'-C1'-N9 | 7.17 | 113.94 | 108.20 |
| 57 | BA | 1998 | A | C5-C6-N1 | 7.17 | 121.29 | 117.70 |
| 57 | BA | 2103 | C | N3-C2-O2 | -7.17 | 116.88 | 121.90 |
| 58 | Ba | 26 | C | N3-C2-O2 | -7.17 | 116.88 | 121.90 |
| 57 | BA | 331 | C | N3-C2-O2 | -7.17 | 116.88 | 121.90 |
| 57 | BA | 2795 | C | N3-C2-O2 | -7.17 | 116.88 | 121.90 |
| 22 | AA | 63 | C | N3-C2-O2 | -7.17 | 116.88 | 121.90 |
| 22 | AA | 339 | C | N3-C2-O2 | -7.17 | 116.88 | 121.90 |
| 22 | AA | 930 | C | N3-C2-O2 | -7.17 | 116.88 | 121.90 |
| 22 | AA | 206 | C | N3-C2-O2 | -7.17 | 116.88 | 121.90 |
| 22 | AA | 1357 | A | C5-C6-N1 | 7.17 | 121.28 | 117.70 |
| 22 | AA | 1366 | C | N3-C2-O2 | -7.17 | 116.88 | 121.90 |
| 57 | BA | 1005 | C | N3-C2-O2 | -7.17 | 116.88 | 121.90 |
| 57 | BA | 2826 | A | C5-C6-N1 | 7.17 | 121.28 | 117.70 |
| 57 | BA | 679 | C | N3-C2-O2 | -7.16 | 116.89 | 121.90 |
| 57 | BA | 958 | U | O4'-C1'-N1 | 7.16 | 113.93 | 108.20 |
| 57 | BA | 1920 | C | N3-C2-O2 | -7.16 | 116.89 | 121.90 |
| 57 | BA | 2837 | A | N1-C6-N6 | -7.16 | 114.30 | 118.60 |
| 22 | AA | 1340 | A | C4-C5-C6 | -7.16 | 113.42 | 117.00 |
| 22 | AA | 282 | A | C4-C5-C6 | -7.16 | 113.42 | 117.00 |
| 22 | AA | 1396 | A | C4-C5-C6 | -7.16 | 113.42 | 117.00 |
| 57 | BA | 445 | C | N3-C2-O2 | -7.16 | 116.89 | 121.90 |
| 57 | BA | 1848 | A | N1-C6-N6 | -7.16 | 114.31 | 118.60 |
| 57 | BA | 2080 | A | C5-C6-N1 | 7.16 | 121.28 | 117.70 |
| 57 | BA | 2520 | C | N3-C2-O2 | -7.16 | 116.89 | 121.90 |
| 57 | BA | 2830 | C | N3-C2-O2 | -7.16 | 116.89 | 121.90 |
| 7 | AP | 31 | ARG | NE-CZ-NH1 | 7.16 | 123.88 | 120.30 |
| 57 | BA | 2198 | A | C5-C6-N1 | 7.16 | 121.28 | 117.70 |
| 57 | BA | 2338 | C | N3-C2-O2 | -7.16 | 116.89 | 121.90 |
| 3 | AL | 98 | ARG | NE-CZ-NH1 | 7.16 | 123.88 | 120.30 |
| 57 | BA | 1298 | C | N3-C2-O2 | -7.16 | 116.89 | 121.90 |
| 57 | BA | 2670 | A | C4-C5-C6 | -7.16 | 113.42 | 117.00 |
| 22 | AA | 1045 | C | O4'-C1'-N1 | 7.15 | 113.92 | 108.20 |
| 57 | BA | 877 | A | C4-C5-C6 | -7.15 | 113.42 | 117.00 |
| 18 | AG | 154 | ARG | NE-CZ-NH1 | 7.15 | 123.88 | 120.30 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 43 | B1 | 73 | ARG | NE-CZ-NH1 | -7.15 | 116.72 | 120.30 |
| 57 | BA | 2108 | A | C5-C6-N1 | 7.15 | 121.28 | 117.70 |
| 57 | BA | 2171 | A | C5-C6-N1 | 7.15 | 121.28 | 117.70 |
| 57 | BA | 341 | C | N3-C2-O2 | -7.15 | 116.89 | 121.90 |
| 57 | BA | 1366 | A | C4-C5-C6 | -7.15 | 113.42 | 117.00 |
| 57 | BA | 2874 | C | N3-C2-O2 | -7.15 | 116.90 | 121.90 |
| 22 | AA | 66 | A | N1-C6-N6 | -7.15 | 114.31 | 118.60 |
| 22 | AA | 83 | C | N3-C2-O2 | -7.15 | 116.90 | 121.90 |
| 35 | BD | 202 | ARG | NE-CZ-NH1 | 7.15 | 123.87 | 120.30 |
| 57 | BA | 1278 | C | N3-C2-O2 | -7.15 | 116.90 | 121.90 |
| 57 | BA | 13 | A | C1'-O4'-C4' | -7.15 | 104.18 | 109.90 |
| 57 | BA | 2335 | A | C5-C6-N1 | 7.15 | 121.27 | 117.70 |
| 22 | AA | 520 | A | O4'-C1'-N9 | 7.14 | 113.92 | 108.20 |
| 22 | AA | 1163 | A | C4-C5-C6 | -7.14 | 113.43 | 117.00 |
| 24 | A3 | 11 | A | C5-C6-N1 | 7.14 | 121.27 | 117.70 |
| 36 | BU | 54 | ARG | NE-CZ-NH1 | 7.14 | 123.87 | 120.30 |
| 57 | BA | 616 | A | C5-C6-N1 | 7.14 | 121.27 | 117.70 |
| 57 | BA | 1552 | A | C1'-O4'-C4' | -7.14 | 104.18 | 109.90 |
| 57 | BA | 2270 | A | C4-C5-C6 | -7.14 | 113.43 | 117.00 |
| 57 | BA | 2419 | U | O4'-C1'-N1 | 7.14 | 113.92 | 108.20 |
| 22 | AA | 271 | C | N3-C2-O2 | -7.14 | 116.90 | 121.90 |
| 57 | BA | 1351 | C | N3-C2-O2 | -7.14 | 116.90 | 121.90 |
| 57 | BA | 2872 | A | C4-C5-C6 | -7.14 | 113.43 | 117.00 |
| 22 | AA | 909 | A | C5-C6-N1 | 7.14 | 121.27 | 117.70 |
| 22 | AA | 1342 | C | N3-C2-O2 | -7.14 | 116.90 | 121.90 |
| 22 | AA | 1404 | C | N3-C2-O2 | -7.14 | 116.90 | 121.90 |
| 57 | BA | 1284 | A | C4-C5-C6 | -7.14 | 113.43 | 117.00 |
| 57 | BA | 1545 | A | C4-C5-C6 | -7.14 | 113.43 | 117.00 |
| 57 | BA | 2471 | A | C4-C5-C6 | -7.14 | 113.43 | 117.00 |
| 20 | AI | 108 | ARG | NE-CZ-NH1 | 7.14 | 123.87 | 120.30 |
| 31 | BQ | 10 | ARG | NE-CZ-NH2 | 7.14 | 123.87 | 120.30 |
| 57 | BA | 8 | C | N3-C2-O2 | -7.14 | 116.90 | 121.90 |
| 57 | BA | 84 | A | C4-C5-C6 | -7.14 | 113.43 | 117.00 |
| 57 | BA | 2033 | A | C4-C5-C6 | -7.14 | 113.43 | 117.00 |
| 57 | BA | 2632 | A | C4-C5-C6 | -7.14 | 113.43 | 117.00 |
| 57 | BA | 2738 | A | C5-C6-N1 | 7.14 | 121.27 | 117.70 |
| 22 | AA | 600 | A | C4-C5-C6 | -7.14 | 113.43 | 117.00 |
| 40 | BY | 6 | ARG | NE-CZ-NH1 | 7.14 | 123.87 | 120.30 |
| 57 | BA | 2703 | C | N3-C2-O2 | -7.14 | 116.90 | 121.90 |
| 22 | AA | 19 | A | C5-C6-N1 | 7.14 | 121.27 | 117.70 |
| 22 | AA | 309 | A | C4-C5-C6 | -7.14 | 113.43 | 117.00 |
| 57 | BA | 719 | C | N3-C2-O2 | -7.14 | 116.91 | 121.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 912 | C | N3-C2-O2 | -7.14 | 116.91 | 121.90 |
| 57 | BA | 1178 | C | N3-C2-O2 | -7.14 | 116.90 | 121.90 |
| 57 | BA | 2300 | C | N3-C2-O2 | -7.14 | 116.90 | 121.90 |
| 57 | BA | 2783 | U | O4'-C1'-N1 | 7.14 | 113.91 | 108.20 |
| 22 | AA | 681 | A | C4-C5-C6 | -7.13 | 113.43 | 117.00 |
| 22 | AA | 1022 | A | C4-C5-C6 | -7.13 | 113.43 | 117.00 |
| 22 | AA | 1339 | A | C4-C5-C6 | -7.13 | 113.43 | 117.00 |
| 22 | AA | 712 | A | C4-C5-C6 | -7.13 | 113.43 | 117.00 |
| 22 | AA | 1000 | A | C5-C6-N1 | 7.13 | 121.27 | 117.70 |
| 57 | BA | 19 | A | C5-C6-N1 | 7.13 | 121.27 | 117.70 |
| 57 | BA | 1072 | C | N3-C2-O2 | -7.13 | 116.91 | 121.90 |
| 57 | BA | 2666 | C | N1-C2-O2 | 7.13 | 123.18 | 118.90 |
| 22 | AA | 607 | A | C4-C5-C6 | -7.13 | 113.43 | 117.00 |
| 22 | AA | 1360 | A | N1-C6-N6 | -7.13 | 114.32 | 118.60 |
| 57 | BA | 129 | C | N3-C2-O2 | -7.13 | 116.91 | 121.90 |
| 57 | BA | 2072 | C | N3-C2-O2 | -7.13 | 116.91 | 121.90 |
| 57 | BA | 2594 | C | N3-C2-O2 | -7.13 | 116.91 | 121.90 |
| 22 | AA | 51 | A | C5-C6-N1 | 7.13 | 121.27 | 117.70 |
| 22 | AA | 746 | A | C5-C6-N1 | 7.13 | 121.27 | 117.70 |
| 38 | BW | 11 | ARG | NE-CZ-NH1 | 7.13 | 123.86 | 120.30 |
| 57 | BA | 1129 | A | C4-C5-C6 | -7.13 | 113.44 | 117.00 |
| 22 | AA | 16 | A | C5-C6-N1 | 7.13 | 121.26 | 117.70 |
| 57 | BA | 429 | A | C4-C5-C6 | -7.13 | 113.44 | 117.00 |
| 57 | BA | 1784 | A | N1-C6-N6 | -7.13 | 114.32 | 118.60 |
| 57 | BA | 1908 | C | N3-C2-O2 | -7.13 | 116.91 | 121.90 |
| 57 | BA | 2035 | G | O4'-C1'-N9 | 7.13 | 113.90 | 108.20 |
| 57 | BA | 2339 | C | N3-C2-O2 | -7.13 | 116.91 | 121.90 |
| 57 | BA | 2466 | C | N3-C2-O2 | -7.13 | 116.91 | 121.90 |
| 57 | BA | 2700 | A | C4-C5-C6 | -7.13 | 113.44 | 117.00 |
| 58 | Ba | 51 | G | N1-C6-O6 | -7.13 | 115.62 | 119.90 |
| 22 | AA | 1200 | C | N1-C2-O2 | 7.13 | 123.18 | 118.90 |
| 53 | BF | 88 | ARG | NE-CZ-NH2 | 7.13 | 123.86 | 120.30 |
| 57 | BA | 892 | A | C5-C6-N1 | 7.13 | 121.26 | 117.70 |
| 57 | BA | 908 | C | N3-C2-O2 | -7.13 | 116.91 | 121.90 |
| 22 | AA | 642 | A | C5-C6-N1 | 7.12 | 121.26 | 117.70 |
| 22 | AA | 1230 | C | N3-C2-O2 | -7.12 | 116.91 | 121.90 |
| 52 | B9 | 4 | ARG | NE-CZ-NH1 | 7.12 | 123.86 | 120.30 |
| 57 | BA | 64 | A | C5-C6-N1 | 7.12 | 121.26 | 117.70 |
| 57 | BA | 353 | C | N3-C2-O2 | -7.12 | 116.91 | 121.90 |
| 57 | BA | 2017 | U | N3-C2-O2 | -7.12 | 117.21 | 122.20 |
| 18 | AG | 118 | ARG | NE-CZ-NH1 | 7.12 | 123.86 | 120.30 |
| 57 | BA | 1244 | A | C4-C5-C6 | -7.12 | 113.44 | 117.00 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 2009 | A | C4-C5-C6 | -7.12 | 113.44 | 117.00 |
| 57 | BA | 2794 | C | N3-C2-O2 | -7.12 | 116.91 | 121.90 |
| 57 | BA | 2900 | A | C5-C6-N1 | 7.12 | 121.26 | 117.70 |
| 22 | AA | 101 | A | C4-C5-C6 | -7.12 | 113.44 | 117.00 |
| 57 | BA | 2096 | C | N3-C2-O2 | -7.12 | 116.92 | 121.90 |
| 57 | BA | 2146 | C | N3-C2-O2 | -7.12 | 116.92 | 121.90 |
| 12 | AT | 23 | ARG | NE-CZ-NH1 | 7.12 | 123.86 | 120.30 |
| 22 | AA | 243 | A | C4-C5-C6 | -7.12 | 113.44 | 117.00 |
| 22 | AA | 708 | C | N3-C2-O2 | -7.12 | 116.92 | 121.90 |
| 57 | BA | 1278 | C | O4'-C1'-N1 | 7.12 | 113.89 | 108.20 |
| 57 | BA | 2362 | C | N3-C2-O2 | -7.12 | 116.92 | 121.90 |
| 57 | BA | 2654 | A | C4-C5-C6 | -7.12 | 113.44 | 117.00 |
| 22 | AA | 635 | A | C5-C6-N1 | 7.12 | 121.26 | 117.70 |
| 22 | AA | 990 | C | N3-C2-O2 | -7.12 | 116.92 | 121.90 |
| 57 | BA | 1836 | C | N3-C2-O2 | -7.12 | 116.92 | 121.90 |
| 24 | A3 | 76 | C | N3-C2-O2 | -7.12 | 116.92 | 121.90 |
| 37 | BV | 78 | ARG | NE-CZ-NH2 | 7.12 | 123.86 | 120.30 |
| 45 | BE | 169 | ARG | NE-CZ-NH2 | 7.12 | 123.86 | 120.30 |
| 57 | BA | 44 | A | C4-C5-C6 | -7.12 | 113.44 | 117.00 |
| 57 | BA | 1044 | C | N3-C2-O2 | -7.12 | 116.92 | 121.90 |
| 57 | BA | 1304 | A | C4-C5-C6 | -7.12 | 113.44 | 117.00 |
| 57 | BA | 2377 | A | O4'-C1'-N9 | 7.12 | 113.89 | 108.20 |
| 22 | AA | 728 | A | C4-C5-C6 | -7.11 | 113.44 | 117.00 |
| 57 | BA | 1463 | C | N3-C2-O2 | -7.11 | 116.92 | 121.90 |
| 57 | BA | 2050 | C | N3-C2-O2 | -7.11 | 116.92 | 121.90 |
| 22 | AA | 715 | A | C4-C5-C6 | -7.11 | 113.44 | 117.00 |
| 22 | AA | 940 | C | N3-C2-O2 | -7.11 | 116.92 | 121.90 |
| 22 | AA | 1204 | A | C5-C6-N1 | 7.11 | 121.25 | 117.70 |
| 22 | AA | 1460 | C | N3-C2-O2 | -7.11 | 116.92 | 121.90 |
| 23 | A2 | 22 | G | O4'-C1'-N9 | 7.11 | 113.89 | 108.20 |
| 23 | A2 | 33 | A | N1-C6-N6 | -7.11 | 114.33 | 118.60 |
| 57 | BA | 655 | A | C4-C5-C6 | -7.11 | 113.44 | 117.00 |
| 57 | BA | 2821 | A | C5-C6-N1 | 7.11 | 121.25 | 117.70 |
| 22 | AA | 309 | A | C5-C6-N1 | 7.11 | 121.25 | 117.70 |
| 32 | BR | 2 | ARG | NE-CZ-NH1 | 7.11 | 123.86 | 120.30 |
| 57 | BA | 282 | A | C5-C6-N1 | 7.11 | 121.25 | 117.70 |
| 57 | BA | 2158 | A | C5-C6-N1 | 7.11 | 121.25 | 117.70 |
| 22 | AA | 356 | A | C4-C5-C6 | -7.11 | 113.45 | 117.00 |
| 22 | AA | 1378 | C | N3-C2-O2 | -7.11 | 116.92 | 121.90 |
| 57 | BA | 41 | C | N3-C2-O2 | -7.11 | 116.92 | 121.90 |
| 57 | BA | 1805 | A | C5-C6-N1 | 7.11 | 121.25 | 117.70 |
| 57 | BA | 1039 | A | N1-C6-N6 | -7.11 | 114.34 | 118.60 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 1145 | C | N3-C2-O2 | -7.11 | 116.93 | 121.90 |
| 57 | BA | 1653 | G | O4'-C1'-N9 | 7.11 | 113.88 | 108.20 |
| 57 | BA | 2501 | C | N3-C2-O2 | -7.11 | 116.93 | 121.90 |
| 22 | AA | 579 | A | C4-C5-C6 | -7.10 | 113.45 | 117.00 |
| 22 | AA | 629 | A | C5-C6-N1 | 7.10 | 121.25 | 117.70 |
| 22 | AA | 1093 | A | C4-C5-C6 | -7.10 | 113.45 | 117.00 |
| 22 | AA | 1128 | C | N3-C2-O2 | -7.10 | 116.93 | 121.90 |
| 22 | AA | 336 | A | C4-C5-C6 | -7.10 | 113.45 | 117.00 |
| 22 | AA | 1022 | A | C5-C6-N1 | 7.10 | 121.25 | 117.70 |
| 57 | BA | 492 | A | C4-C5-C6 | -7.10 | 113.45 | 117.00 |
| 57 | BA | 1148 | U | O4'-C1'-N1 | 7.10 | 113.88 | 108.20 |
| 57 | BA | 1516 | G | O4'-C1'-N9 | 7.10 | 113.88 | 108.20 |
| 57 | BA | 1889 | A | C5-C6-N1 | 7.10 | 121.25 | 117.70 |
| 22 | AA | 368 | U | N3-C2-O2 | -7.10 | 117.23 | 122.20 |
| 57 | BA | 1184 | U | O4'-C1'-N1 | 7.10 | 113.88 | 108.20 |
| 57 | BA | 142 | A | C5-C6-N1 | 7.10 | 121.25 | 117.70 |
| 57 | BA | 702 | U | O4'-C1'-N1 | 7.10 | 113.88 | 108.20 |
| 57 | BA | 2025 | C | N3-C2-O2 | -7.10 | 116.93 | 121.90 |
| 57 | BA | 2377 | A | C5-C6-N1 | 7.10 | 121.25 | 117.70 |
| 57 | BA | 2626 | C | N3-C2-O2 | -7.10 | 116.93 | 121.90 |
| 22 | AA | 842 | U | N3-C2-O2 | -7.10 | 117.23 | 122.20 |
| 58 | Ba | 34 | A | C5-C6-N1 | 7.10 | 121.25 | 117.70 |
| 22 | AA | 83 | C | O4'-C1'-N1 | 7.09 | 113.88 | 108.20 |
| 22 | AA | 129 | A | C4-C5-C6 | -7.09 | 113.45 | 117.00 |
| 22 | AA | 355 | C | N3-C2-O2 | -7.09 | 116.93 | 121.90 |
| 22 | AA | 868 | C | N3-C2-O2 | -7.09 | 116.93 | 121.90 |
| 28 | BN | 120 | ARG | NE-CZ-NH2 | 7.09 | 123.85 | 120.30 |
| 57 | BA | 1030 | C | N3-C2-O2 | -7.09 | 116.93 | 121.90 |
| 57 | BA | 1592 | C | N3-C2-O2 | -7.09 | 116.93 | 121.90 |
| 57 | BA | 2220 | U | O4'-C1'-N1 | 7.09 | 113.87 | 108.20 |
| 57 | BA | 89 | A | C4-C5-C6 | -7.09 | 113.45 | 117.00 |
| 57 | BA | 942 | G | C8-N9-C4 | -7.09 | 103.56 | 106.40 |
| 22 | AA | 383 | A | C5-C6-N1 | 7.09 | 121.25 | 117.70 |
| 22 | AA | 729 | A | C5-C6-N1 | 7.09 | 121.25 | 117.70 |
| 22 | AA | 1287 | A | C5-C6-N1 | 7.09 | 121.25 | 117.70 |
| 22 | AA | 1483 | A | N1-C6-N6 | -7.09 | 114.35 | 118.60 |
| 57 | BA | 1955 | U | O4'-C1'-N1 | 7.09 | 113.87 | 108.20 |
| 57 | BA | 2424 | C | C3'-C2'-C1' | 7.09 | 107.17 | 101.50 |
| 22 | AA | 1263 | C | N3-C2-O2 | -7.09 | 116.94 | 121.90 |
| 57 | BA | 236 | C | N3-C2-O2 | -7.09 | 116.94 | 121.90 |
| 57 | BA | 1251 | C | N3-C2-O2 | -7.09 | 116.94 | 121.90 |
| 22 | AA | 280 | C | N3-C2-O2 | -7.09 | 116.94 | 121.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | AA | 602 | A | C5-C6-N1 | 7.09 | 121.24 | 117.70 |
| 57 | BA | 1957 | C | N3-C2-O2 | -7.09 | 116.94 | 121.90 |
| 57 | BA | 2065 | C | N3-C2-O2 | -7.09 | 116.94 | 121.90 |
| 22 | AA | 810 | C | N3-C2-O2 | -7.08 | 116.94 | 121.90 |
| 22 | AA | 923 | A | N1-C6-N6 | -7.08 | 114.35 | 118.60 |
| 22 | AA | 414 | A | C4-C5-C6 | -7.08 | 113.46 | 117.00 |
| 57 | BA | 1174 | U | O4'-C1'-N1 | 7.08 | 113.87 | 108.20 |
| 22 | AA | 908 | A | C5-C6-N1 | 7.08 | 121.24 | 117.70 |
| 57 | BA | 1934 | C | N3-C2-O2 | -7.08 | 116.94 | 121.90 |
| 57 | BA | 2614 | A | C4-C5-C6 | -7.08 | 113.46 | 117.00 |
| 57 | BA | 2752 | C | N3-C4-C5 | 7.08 | 124.73 | 121.90 |
| 22 | AA | 1368 | A | C4-C5-C6 | -7.08 | 113.46 | 117.00 |
| 22 | AA | 10 | A | C5-C6-N1 | 7.08 | 121.24 | 117.70 |
| 22 | AA | 412 | A | O4'-C1'-N9 | 7.08 | 113.86 | 108.20 |
| 22 | AA | 694 | A | N1-C6-N6 | -7.08 | 114.35 | 118.60 |
| 22 | AA | 1317 | C | N3-C2-O2 | -7.08 | 116.94 | 121.90 |
| 57 | BA | 146 | A | C5-C6-N1 | 7.08 | 121.24 | 117.70 |
| 57 | BA | 372 | G | O4'-C1'-N9 | 7.08 | 113.86 | 108.20 |
| 57 | BA | 1843 | C | N3-C2-O2 | -7.08 | 116.94 | 121.90 |
| 57 | BA | 2662 | A | C3'-C2'-C1' | 7.08 | 107.16 | 101.50 |
| 57 | BA | 1413 | A | C5-C6-N1 | 7.08 | 121.24 | 117.70 |
| 22 | AA | 783 | C | N3-C2-O2 | -7.08 | 116.95 | 121.90 |
| 24 | A3 | 44 | A | N1-C6-N6 | -7.08 | 114.36 | 118.60 |
| 57 | BA | 126 | A | C4-C5-C6 | -7.08 | 113.46 | 117.00 |
| 57 | BA | 216 | A | C4-C5-C6 | -7.08 | 113.46 | 117.00 |
| 57 | BA | 1200 | C | N3-C2-O2 | -7.08 | 116.95 | 121.90 |
| 57 | BA | 1895 | C | N3-C2-O2 | -7.08 | 116.95 | 121.90 |
| 2 | AK | 36 | ARG | NE-CZ-NH1 | 7.07 | 123.84 | 120.30 |
| 22 | AA | 1111 | A | C4-C5-C6 | -7.07 | 113.46 | 117.00 |
| 57 | BA | 96 | C | N3-C2-O2 | -7.07 | 116.95 | 121.90 |
| 57 | BA | 241 | A | C5-C6-N1 | 7.07 | 121.24 | 117.70 |
| 57 | BA | 1924 | C | N3-C2-O2 | -7.07 | 116.95 | 121.90 |
| 57 | BA | 2796 | U | O4'-C1'-N1 | 7.07 | 113.86 | 108.20 |
| 57 | BA | 2840 | C | N3-C2-O2 | -7.07 | 116.95 | 121.90 |
| 57 | BA | 898 | C | N3-C2-O2 | -7.07 | 116.95 | 121.90 |
| 57 | BA | 1057 | A | C5-C6-N1 | 7.07 | 121.24 | 117.70 |
| 57 | BA | 1053 | C | N3-C2-O2 | -7.07 | 116.95 | 121.90 |
| 57 | BA | 1871 | A | C5-C6-N1 | 7.07 | 121.23 | 117.70 |
| 57 | BA | 2448 | A | C4-C5-C6 | -7.07 | 113.47 | 117.00 |
| 57 | BA | 632 | A | C5-C6-N1 | 7.07 | 121.23 | 117.70 |
| 57 | BA | 1260 | A | C5-C6-N1 | 7.07 | 121.23 | 117.70 |
| 22 | AA | 2 | A | C4-C5-C6 | -7.07 | 113.47 | 117.00 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | AA | 1265 | C | N3-C2-O2 | -7.07 | 116.95 | 121.90 |
| 57 | BA | 374 | A | C5-C6-N1 | 7.07 | 121.23 | 117.70 |
| 21 | A1 | 269 | ARG | NE-CZ-NH1 | 7.07 | 123.83 | 120.30 |
| 57 | BA | 95 | A | C4-C5-C6 | -7.07 | 113.47 | 117.00 |
| 57 | BA | 1821 | A | C5-C6-N1 | 7.07 | 121.23 | 117.70 |
| 57 | BA | 2901 | C | N3-C2-O2 | -7.07 | 116.95 | 121.90 |
| 22 | AA | 183 | C | N3-C2-O2 | -7.06 | 116.95 | 121.90 |
| 22 | AA | 792 | A | C4-C5-C6 | -7.06 | 113.47 | 117.00 |
| 22 | AA | 1433 | A | C4-C5-C6 | -7.06 | 113.47 | 117.00 |
| 57 | BA | 106 | C | N3-C2-O2 | -7.06 | 116.96 | 121.90 |
| 57 | BA | 2020 | A | C4-C5-C6 | -7.06 | 113.47 | 117.00 |
| 57 | BA | 2461 | A | C5-C6-N1 | 7.06 | 121.23 | 117.70 |
| 58 | Ba | 104 | A | C4-C5-C6 | -7.06 | 113.47 | 117.00 |
| 57 | BA | 274 | C | N3-C2-O2 | -7.06 | 116.96 | 121.90 |
| 57 | BA | 1088 | A | C5-C6-N1 | 7.06 | 121.23 | 117.70 |
| 57 | BA | 2793 | C | N3-C2-O2 | -7.06 | 116.96 | 121.90 |
| 58 | Ba | 8 | C | N3-C2-O2 | -7.06 | 116.96 | 121.90 |
| 22 | AA | 124 | C | N3-C2-O2 | -7.06 | 116.96 | 121.90 |
| 22 | AA | 248 | C | N3-C2-O2 | -7.06 | 116.96 | 121.90 |
| 22 | AA | 1167 | A | C4-C5-C6 | -7.06 | 113.47 | 117.00 |
| 57 | BA | 756 | A | C4-C5-C6 | -7.06 | 113.47 | 117.00 |
| 57 | BA | 2061 | G | P-O3'-C3' | 7.06 | 128.17 | 119.70 |
| 57 | BA | 2350 | C | N3-C2-O2 | -7.06 | 116.96 | 121.90 |
| 58 | Ba | 58 | A | C5-C6-N1 | 7.06 | 121.23 | 117.70 |
| 22 | AA | 1027 | C | N3-C2-O2 | -7.06 | 116.96 | 121.90 |
| 22 | AA | 1214 | C | N3-C2-O2 | -7.06 | 116.96 | 121.90 |
| 38 | BW | 88 | ARG | NE-CZ-NH2 | 7.06 | 123.83 | 120.30 |
| 57 | BA | 1307 | A | C4-C5-C6 | -7.06 | 113.47 | 117.00 |
| 57 | BA | 1731 | G | O4'-C1'-N9 | 7.06 | 113.85 | 108.20 |
| 57 | BA | 2064 | C | N3-C2-O2 | -7.06 | 116.96 | 121.90 |
| 22 | AA | 918 | A | C4-C5-C6 | -7.06 | 113.47 | 117.00 |
| 57 | BA | 845 | A | C4-C5-C6 | -7.06 | 113.47 | 117.00 |
| 57 | BA | 1357 | C | O4'-C1'-N1 | 7.06 | 113.84 | 108.20 |
| 57 | BA | 1712 | U | O4'-C1'-N1 | 7.06 | 113.84 | 108.20 |
| 57 | BA | 2465 | C | N3-C2-O2 | -7.06 | 116.96 | 121.90 |
| 22 | AA | 528 | C | N3-C2-O2 | -7.05 | 116.96 | 121.90 |
| 57 | BA | 965 | C | N3-C2-O2 | -7.05 | 116.96 | 121.90 |
| 57 | BA | 2241 | A | C4-C5-C6 | -7.05 | 113.47 | 117.00 |
| 57 | BA | 1048 | A | C4-C5-C6 | -7.05 | 113.47 | 117.00 |
| 22 | AA | 172 | A | C5-C6-N1 | 7.05 | 121.22 | 117.70 |
| 22 | AA | 545 | C | N3-C2-O2 | -7.05 | 116.96 | 121.90 |
| 22 | AA | 167 | A | C4-C5-C6 | -7.05 | 113.47 | 117.00 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | AA | 825 | A | C5-C6-N1 | 7.05 | 121.22 | 117.70 |
| 22 | AA | 1161 | C | N3-C2-O2 | -7.05 | 116.97 | 121.90 |
| 24 | A3 | 3 | C | N3-C2-O2 | -7.05 | 116.97 | 121.90 |
| 57 | BA | 1579 | A | C4-C5-C6 | -7.05 | 113.47 | 117.00 |
| 57 | BA | 1838 | C | N3-C2-O2 | -7.05 | 116.97 | 121.90 |
| 57 | BA | 2792 | A | C4-C5-C6 | -7.05 | 113.48 | 117.00 |
| 22 | AA | 941 | G | O4'-C1'-N9 | 7.05 | 113.84 | 108.20 |
| 57 | BA | 167 | A | C5-C6-N1 | 7.05 | 121.22 | 117.70 |
| 57 | BA | 417 | C | O4'-C1'-N1 | 7.05 | 113.84 | 108.20 |
| 57 | BA | 591 | U | O4'-C1'-N1 | 7.05 | 113.84 | 108.20 |
| 57 | BA | 1322 | A | C5-C6-N1 | 7.05 | 121.22 | 117.70 |
| 57 | BA | 2875 | C | N3-C2-O2 | -7.05 | 116.97 | 121.90 |
| 22 | AA | 612 | C | N3-C2-O2 | -7.04 | 116.97 | 121.90 |
| 29 | BO | 17 | ARG | NE-CZ-NH1 | 7.04 | 123.82 | 120.30 |
| 57 | BA | 2512 | C | N3-C2-O2 | -7.04 | 116.97 | 121.90 |
| 22 | AA | 807 | A | C4-C5-C6 | -7.04 | 113.48 | 117.00 |
| 24 | A3 | 36 | A | C4-C5-C6 | -7.04 | 113.48 | 117.00 |
| 22 | AA | 579 | A | C5-C6-N1 | 7.04 | 121.22 | 117.70 |
| 22 | AA | 1237 | C | N3-C2-O2 | -7.04 | 116.97 | 121.90 |
| 57 | BA | 422 | A | C4-C5-C6 | -7.04 | 113.48 | 117.00 |
| 57 | BA | 800 | A | C4-C5-C6 | -7.04 | 113.48 | 117.00 |
| 57 | BA | 2327 | A | C4-C5-C6 | -7.04 | 113.48 | 117.00 |
| 57 | BA | 2450 | A | O4'-C1'-N9 | 7.04 | 113.83 | 108.20 |
| 22 | AA | 1289 | A | C4-C5-C6 | -7.04 | 113.48 | 117.00 |
| 30 | BP | 41 | ARG | NE-CZ-NH1 | 7.04 | 123.82 | 120.30 |
| 57 | BA | 2480 | C | N3-C2-O2 | -7.04 | 116.97 | 121.90 |
| 22 | AA | 974 | A | C4-C5-C6 | -7.04 | 113.48 | 117.00 |
| 22 | AA | 1055 | A | C4-C5-C6 | -7.04 | 113.48 | 117.00 |
| 22 | AA | 1080 | A | C4-C5-C6 | -7.04 | 113.48 | 117.00 |
| 22 | AA | 1120 | C | N3-C2-O2 | -7.04 | 116.97 | 121.90 |
| 57 | BA | 460 | A | C5-C6-N1 | 7.04 | 121.22 | 117.70 |
| 57 | BA | 782 | A | C5-C6-N1 | 7.04 | 121.22 | 117.70 |
| 57 | BA | 1539 | U | O4'-C1'-N1 | 7.04 | 113.83 | 108.20 |
| 57 | BA | 1590 | A | C5-C6-N1 | 7.04 | 121.22 | 117.70 |
| 22 | AA | 78 | A | C4-C5-C6 | -7.03 | 113.48 | 117.00 |
| 22 | AA | 502 | A | N1-C6-N6 | -7.03 | 114.38 | 118.60 |
| 22 | AA | 865 | A | C5-C6-N1 | 7.03 | 121.22 | 117.70 |
| 22 | AA | 937 | A | C4-C5-C6 | -7.03 | 113.48 | 117.00 |
| 22 | AA | 1239 | A | C4-C5-C6 | -7.03 | 113.48 | 117.00 |
| 57 | BA | 796 | C | N3-C2-O2 | -7.03 | 116.98 | 121.90 |
| 57 | BA | 981 | A | C4-C5-C6 | -7.03 | 113.48 | 117.00 |
| 57 | BA | 1700 | A | C5-C6-N1 | 7.03 | 121.22 | 117.70 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 2284 | A | N1-C6-N6 | -7.03 | 114.38 | 118.60 |
| 22 | AA | 959 | A | N1-C6-N6 | -7.03 | 114.38 | 118.60 |
| 57 | BA | 544 | C | N1-C2-O2 | 7.03 | 123.12 | 118.90 |
| 57 | BA | 2381 | A | C5-C6-N1 | 7.03 | 121.22 | 117.70 |
| 57 | BA | 2699 | C | N3-C2-O2 | -7.03 | 116.98 | 121.90 |
| 57 | BA | 352 | A | C5-C6-N1 | 7.03 | 121.21 | 117.70 |
| 57 | BA | 2311 | A | C4-C5-C6 | -7.03 | 113.49 | 117.00 |
| 22 | AA | 461 | A | C4-C5-C6 | -7.03 | 113.49 | 117.00 |
| 57 | BA | 554 | U | O4'-C1'-N1 | 7.03 | 113.82 | 108.20 |
| 57 | BA | 1014 | A | C4-C5-C6 | -7.03 | 113.49 | 117.00 |
| 22 | AA | 174 | A | C4-C5-C6 | -7.02 | 113.49 | 117.00 |
| 57 | BA | 1780 | A | C5-C6-N1 | 7.02 | 121.21 | 117.70 |
| 22 | AA | 736 | C | N3-C2-O2 | -7.02 | 116.98 | 121.90 |
| 24 | A3 | 49 | C | N3-C2-O2 | -7.02 | 116.98 | 121.90 |
| 24 | A3 | 67 | C | N3-C2-O2 | -7.02 | 116.98 | 121.90 |
| 57 | BA | 1477 | A | C5-C6-N1 | 7.02 | 121.21 | 117.70 |
| 57 | BA | 1902 | C | O4'-C1'-N1 | 7.02 | 113.82 | 108.20 |
| 57 | BA | 2260 | C | N3-C2-O2 | -7.02 | 116.99 | 121.90 |
| 22 | AA | 647 | C | N3-C2-O2 | -7.02 | 116.99 | 121.90 |
| 22 | AA | 436 | C | N3-C2-O2 | -7.02 | 116.99 | 121.90 |
| 22 | AA | 1395 | C | N3-C2-O2 | -7.02 | 116.99 | 121.90 |
| 22 | AA | 1102 | A | C5-C6-N1 | 7.01 | 121.21 | 117.70 |
| 57 | BA | 231 | A | C4-C5-C6 | -7.01 | 113.49 | 117.00 |
| 57 | BA | 2143 | C | N3-C2-O2 | -7.01 | 116.99 | 121.90 |
| 57 | BA | 42 | A | C4-C5-C6 | -7.01 | 113.49 | 117.00 |
| 57 | BA | 398 | C | N3-C2-O2 | -7.01 | 116.99 | 121.90 |
| 57 | BA | 918 | A | C4-C5-C6 | -7.01 | 113.49 | 117.00 |
| 57 | BA | 1794 | A | C4-C5-C6 | -7.01 | 113.49 | 117.00 |
| 22 | AA | 938 | A | C4-C5-C6 | -7.01 | 113.49 | 117.00 |
| 22 | AA | 989 | U | O4'-C1'-N1 | 7.01 | 113.81 | 108.20 |
| 22 | AA | 1107 | C | N3-C2-O2 | -7.01 | 116.99 | 121.90 |
| 57 | BA | 179 | C | O4'-C1'-N1 | 7.01 | 113.81 | 108.20 |
| 57 | BA | 242 | G | C1'-O4'-C4' | -7.01 | 104.29 | 109.90 |
| 57 | BA | 1091 | G | O4'-C1'-N9 | 7.01 | 113.81 | 108.20 |
| 57 | BA | 1941 | C | O4'-C1'-N1 | 7.01 | 113.81 | 108.20 |
| 57 | BA | 2297 | A | C4-C5-C6 | -7.01 | 113.50 | 117.00 |
| 57 | BA | 584 | C | N3-C2-O2 | -7.01 | 116.99 | 121.90 |
| 22 | AA | 456 | A | C4-C5-C6 | -7.01 | 113.50 | 117.00 |
| 23 | A2 | 57 | C | N3-C2-O2 | -7.01 | 117.00 | 121.90 |
| 57 | BA | 1181 | U | O4'-C1'-N1 | 7.01 | 113.81 | 108.20 |
| 57 | BA | 1764 | C | N3-C2-O2 | -7.01 | 117.00 | 121.90 |
| 57 | BA | 2404 | U | O4'-C1'-N1 | 7.01 | 113.81 | 108.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 2476 | A | C4-C5-C6 | -7.01 | 113.50 | 117.00 |
| 57 | BA | 909 | A | C5-C6-N1 | 7.00 | 121.20 | 117.70 |
| 57 | BA | 2755 | C | N3-C2-O2 | -7.00 | 117.00 | 121.90 |
| 58 | Ba | 27 | C | N3-C2-O2 | -7.00 | 117.00 | 121.90 |
| 22 | AA | 623 | C | N3-C2-O2 | -7.00 | 117.00 | 121.90 |
| 57 | BA | 109 | C | N3-C2-O2 | -7.00 | 117.00 | 121.90 |
| 22 | AA | 901 | A | N1-C6-N6 | -7.00 | 114.40 | 118.60 |
| 22 | AA | 1327 | C | N3-C2-O2 | -7.00 | 117.00 | 121.90 |
| 57 | BA | 1574 | C | N3-C2-O2 | -7.00 | 117.00 | 121.90 |
| 15 | AD | 46 | ARG | NE-CZ-NH1 | 7.00 | 123.80 | 120.30 |
| 22 | AA | 1146 | A | C4-C5-C6 | -7.00 | 113.50 | 117.00 |
| 22 | AA | 1354 | U | O4'-C1'-N1 | 7.00 | 113.80 | 108.20 |
| 57 | BA | 64 | A | C4-C5-C6 | -7.00 | 113.50 | 117.00 |
| 19 | AH | 113 | ARG | NE-CZ-NH1 | 7.00 | 123.80 | 120.30 |
| 24 | A3 | 13 | C | O4'-C1'-N1 | 7.00 | 113.80 | 108.20 |
| 57 | BA | 2080 | A | C4-C5-C6 | -7.00 | 113.50 | 117.00 |
| 20 | AI | 121 | ARG | NE-CZ-NH1 | 7.00 | 123.80 | 120.30 |
| 22 | AA | 831 | A | C5-C6-N1 | 7.00 | 121.20 | 117.70 |
| 57 | BA | 1509 | A | C4-C5-C6 | -7.00 | 113.50 | 117.00 |
| 57 | BA | 2804 | U | O4'-C1'-N1 | 7.00 | 113.80 | 108.20 |
| 57 | BA | 16 | C | N3-C2-O2 | -6.99 | 117.00 | 121.90 |
| 57 | BA | 1289 | C | N3-C2-O2 | -6.99 | 117.00 | 121.90 |
| 57 | BA | 490 | C | N1-C2-O2 | 6.99 | 123.09 | 118.90 |
| 58 | Ba | 52 | A | C4-C5-C6 | -6.99 | 113.50 | 117.00 |
| 22 | AA | 96 | U | O4'-C1'-N1 | 6.99 | 113.79 | 108.20 |
| 22 | AA | 782 | A | C5-C6-N1 | 6.99 | 121.20 | 117.70 |
| 57 | BA | 861 | A | N1-C6-N6 | -6.99 | 114.41 | 118.60 |
| 57 | BA | 1147 | A | C4-C5-C6 | -6.99 | 113.50 | 117.00 |
| 57 | BA | 2052 | A | C5-C6-N1 | 6.99 | 121.20 | 117.70 |
| 57 | BA | 2738 | A | C4-C5-C6 | -6.99 | 113.50 | 117.00 |
| 2 | AK | 12 | ARG | NE-CZ-NH1 | 6.99 | 123.80 | 120.30 |
| 57 | BA | 735 | A | C5-C6-N1 | 6.99 | 121.19 | 117.70 |
| 57 | BA | 2314 | A | C5-C6-N1 | 6.99 | 121.19 | 117.70 |
| 57 | BA | 2519 | U | O4'-C1'-N1 | 6.99 | 113.79 | 108.20 |
| 22 | AA | 1500 | A | N1-C6-N6 | -6.99 | 114.41 | 118.60 |
| 22 | AA | 1216 | A | C4-C5-C6 | -6.98 | 113.51 | 117.00 |
| 22 | AA | 1333 | A | C5-C6-N1 | 6.98 | 121.19 | 117.70 |
| 22 | AA | 737 | C | N3-C2-O2 | -6.98 | 117.01 | 121.90 |
| 57 | BA | 1029 | A | C5-C6-N1 | 6.98 | 121.19 | 117.70 |
| 57 | BA | 2090 | A | C4-C5-C6 | -6.98 | 113.51 | 117.00 |
| 22 | AA | 1138 | G | N3-C4-C5 | -6.98 | 125.11 | 128.60 |
| 22 | AA | 1312 | G | N1-C6-O6 | -6.98 | 115.71 | 119.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | AA | 649 | A | C4-C5-C6 | -6.98 | 113.51 | 117.00 |
| 22 | AA | 950 | U | O4'-C1'-N1 | 6.98 | 113.78 | 108.20 |
| 26 | BJ | 93 | ARG | NE-CZ-NH1 | 6.98 | 123.79 | 120.30 |
| 57 | BA | 692 | C | N1-C2-O2 | 6.98 | 123.08 | 118.90 |
| 57 | BA | 1775 | U | O4'-C1'-N1 | 6.98 | 113.78 | 108.20 |
| 57 | BA | 1785 | A | C5-C6-N1 | 6.98 | 121.19 | 117.70 |
| 22 | AA | 221 | C | O4'-C1'-N1 | 6.97 | 113.78 | 108.20 |
| 29 | BO | 31 | ARG | NE-CZ-NH1 | 6.97 | 123.79 | 120.30 |
| 57 | BA | 2013 | A | C5-C6-N1 | 6.97 | 121.19 | 117.70 |
| 57 | BA | 722 | A | C5-C6-N1 | 6.97 | 121.19 | 117.70 |
| 57 | BA | 983 | A | N1-C6-N6 | -6.97 | 114.42 | 118.60 |
| 22 | AA | 797 | C | N3-C2-O2 | -6.97 | 117.02 | 121.90 |
| 57 | BA | 2332 | C | N3-C2-O2 | -6.97 | 117.02 | 121.90 |
| 22 | AA | 1288 | A | C4-C5-C6 | -6.97 | 113.52 | 117.00 |
| 57 | BA | 218 | A | N1-C6-N6 | -6.97 | 114.42 | 118.60 |
| 57 | BA | 391 | A | N1-C6-N6 | -6.97 | 114.42 | 118.60 |
| 22 | AA | 924 | C | N3-C2-O2 | -6.96 | 117.02 | 121.90 |
| 57 | BA | 249 | C | O4'-C1'-N1 | 6.96 | 113.77 | 108.20 |
| 57 | BA | 1077 | A | C4-C5-C6 | -6.96 | 113.52 | 117.00 |
| 57 | BA | 1385 | A | C5-C6-N1 | 6.96 | 121.18 | 117.70 |
| 58 | Ba | 88 | C | N1-C2-O2 | 6.96 | 123.08 | 118.90 |
| 22 | AA | 984 | C | N3-C2-O2 | -6.96 | 117.03 | 121.90 |
| 57 | BA | 1207 | C | N3-C2-O2 | -6.96 | 117.03 | 121.90 |
| 57 | BA | 1498 | C | N3-C2-O2 | -6.96 | 117.03 | 121.90 |
| 57 | BA | 1772 | A | C4-C5-C6 | -6.96 | 113.52 | 117.00 |
| 22 | AA | 238 | A | C4-C5-C6 | -6.96 | 113.52 | 117.00 |
| 57 | BA | 2199 | A | C4-C5-C6 | -6.96 | 113.52 | 117.00 |
| 22 | AA | 389 | A | C4-C5-C6 | -6.96 | 113.52 | 117.00 |
| 22 | AA | 1098 | C | N3-C2-O2 | -6.96 | 117.03 | 121.90 |
| 57 | BA | 1477 | A | C4-C5-C6 | -6.96 | 113.52 | 117.00 |
| 57 | BA | 2434 | A | C4-C5-C6 | -6.96 | 113.52 | 117.00 |
| 22 | AA | 1308 | U | O4'-C1'-N1 | 6.96 | 113.77 | 108.20 |
| 57 | BA | 739 | A | C4-C5-C6 | -6.96 | 113.52 | 117.00 |
| 57 | BA | 2725 | A | C5-C6-N1 | 6.96 | 121.18 | 117.70 |
| 57 | BA | 2745 | C | N3-C2-O2 | -6.96 | 117.03 | 121.90 |
| 58 | Ba | 73 | A | C5-C6-N1 | 6.96 | 121.18 | 117.70 |
| 2 | AK | 52 | ARG | NE-CZ-NH1 | 6.96 | 123.78 | 120.30 |
| 41 | BZ | 9 | ARG | NE-CZ-NH1 | 6.96 | 123.78 | 120.30 |
| 57 | BA | 2430 | A | O4'-C1'-N9 | 6.96 | 113.76 | 108.20 |
| 22 | AA | 81 | A | C4-C5-C6 | -6.95 | 113.52 | 117.00 |
| 22 | AA | 1246 | A | C4-C5-C6 | -6.95 | 113.52 | 117.00 |
| 57 | BA | 47 | C | N3-C2-O2 | -6.95 | 117.03 | 121.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 439 | A | C5-C6-N1 | 6.95 | 121.18 | 117.70 |
| 57 | BA | 1304 | A | C5-C6-N1 | 6.95 | 121.18 | 117.70 |
| 57 | BA | 2728 | U | O4'-C1'-N1 | 6.95 | 113.76 | 108.20 |
| 57 | BA | 979 | A | C4-C5-C6 | -6.95 | 113.52 | 117.00 |
| 24 | A3 | 39 | A | C4-C5-C6 | -6.95 | 113.52 | 117.00 |
| 57 | BA | 447 | A | C5-C6-N1 | 6.95 | 121.17 | 117.70 |
| 22 | AA | 47 | C | O4'-C1'-N1 | 6.95 | 113.76 | 108.20 |
| 22 | AA | 525 | C | N3-C2-O2 | -6.95 | 117.03 | 121.90 |
| 57 | BA | 631 | A | C4-C5-C6 | -6.95 | 113.53 | 117.00 |
| 57 | BA | 946 | C | N3-C2-O2 | -6.95 | 117.04 | 121.90 |
| 57 | BA | 1634 | A | C5-C6-N1 | 6.95 | 121.17 | 117.70 |
| 57 | BA | 2198 | A | C4-C5-C6 | -6.95 | 113.53 | 117.00 |
| 22 | AA | 58 | C | N1-C2-O2 | 6.95 | 123.07 | 118.90 |
| 22 | AA | 913 | A | C4-C5-C6 | -6.95 | 113.53 | 117.00 |
| 32 | BR | 4 | ARG | NE-CZ-NH2 | -6.95 | 116.83 | 120.30 |
| 22 | AA | 757 | U | O4'-C1'-N1 | 6.95 | 113.76 | 108.20 |
| 22 | AA | 1410 | A | C4-C5-C6 | -6.95 | 113.53 | 117.00 |
| 57 | BA | 2108 | A | C4-C5-C6 | -6.95 | 113.53 | 117.00 |
| 57 | BA | 970 | U | O4'-C1'-N1 | 6.94 | 113.75 | 108.20 |
| 57 | BA | 1876 | A | C4-C5-C6 | -6.94 | 113.53 | 117.00 |
| 57 | BA | 1049 | C | N3-C2-O2 | -6.94 | 117.04 | 121.90 |
| 57 | BA | 1786 | A | C4-C5-C6 | -6.94 | 113.53 | 117.00 |
| 57 | BA | 1885 | A | C5-C6-N1 | 6.94 | 121.17 | 117.70 |
| 57 | BA | 2560 | A | C4-C5-C6 | -6.94 | 113.53 | 117.00 |
| 22 | AA | 162 | A | C5-C6-N1 | 6.94 | 121.17 | 117.70 |
| 57 | BA | 442 | G | O4'-C1'-N9 | 6.94 | 113.75 | 108.20 |
| 57 | BA | 1557 | C | N3-C2-O2 | -6.94 | 117.04 | 121.90 |
| 57 | BA | 2285 | C | N3-C2-O2 | -6.94 | 117.04 | 121.90 |
| 57 | BA | 851 | C | N3-C2-O2 | -6.94 | 117.04 | 121.90 |
| 57 | BA | 2000 | C | N3-C2-O2 | -6.94 | 117.04 | 121.90 |
| 22 | AA | 262 | A | C4-C5-C6 | -6.93 | 113.53 | 117.00 |
| 22 | AA | 872 | A | C4-C5-C6 | -6.93 | 113.53 | 117.00 |
| 57 | BA | 1405 | U | O4'-C1'-N1 | 6.93 | 113.75 | 108.20 |
| 57 | BA | 1745 | A | C4-C5-C6 | -6.93 | 113.53 | 117.00 |
| 57 | BA | 1928 | A | C4-C5-C6 | -6.93 | 113.53 | 117.00 |
| 3 | AL | 55 | ARG | NE-CZ-NH1 | 6.93 | 123.77 | 120.30 |
| 22 | AA | 16 | A | C4-C5-C6 | -6.93 | 113.53 | 117.00 |
| 57 | BA | 53 | A | C4-C5-C6 | -6.93 | 113.53 | 117.00 |
| 57 | BA | 309 | A | C4-C5-C6 | -6.93 | 113.53 | 117.00 |
| 57 | BA | 560 | C | N3-C2-O2 | -6.93 | 117.05 | 121.90 |
| 57 | BA | 637 | A | C4-C5-C6 | -6.93 | 113.53 | 117.00 |
| 57 | BA | 721 | A | C5-C6-N1 | 6.93 | 121.17 | 117.70 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 941 | A | C4-C5-C6 | -6.93 | 113.53 | 117.00 |
| 57 | BA | 165 | A | C5-C6-N1 | 6.93 | 121.17 | 117.70 |
| 57 | BA | 439 | A | C4-C5-C6 | -6.93 | 113.53 | 117.00 |
| 22 | AA | 229 | U | O4'-C1'-N1 | 6.93 | 113.74 | 108.20 |
| 22 | AA | 780 | A | N1-C6-N6 | -6.93 | 114.44 | 118.60 |
| 22 | AA | 1021 | A | C4-C5-C6 | -6.93 | 113.54 | 117.00 |
| 57 | BA | 33 | C | N3-C2-O2 | -6.93 | 117.05 | 121.90 |
| 57 | BA | 1858 | A | C5-C6-N1 | 6.93 | 121.17 | 117.70 |
| 22 | AA | 1536 | C | N3-C2-O2 | -6.93 | 117.05 | 121.90 |
| 32 | BR | 103 | ARG | NE-CZ-NH1 | 6.93 | 123.76 | 120.30 |
| 57 | BA | 89 | A | C5-C6-N1 | 6.93 | 121.16 | 117.70 |
| 57 | BA | 2021 | C | N3-C2-O2 | -6.93 | 117.05 | 121.90 |
| 57 | BA | 2889 | C | N3-C2-O2 | -6.93 | 117.05 | 121.90 |
| 22 | AA | 121 | U | N3-C2-O2 | -6.93 | 117.35 | 122.20 |
| 22 | AA | 1419 | G | O4'-C1'-N9 | 6.93 | 113.74 | 108.20 |
| 24 | A3 | 29 | C | N3-C2-O2 | -6.93 | 117.05 | 121.90 |
| 57 | BA | 817 | C | O4'-C1'-N1 | 6.93 | 113.74 | 108.20 |
| 57 | BA | 2274 | A | C4-C5-C6 | -6.93 | 113.54 | 117.00 |
| 57 | BA | 2884 | U | N3-C2-O2 | -6.93 | 117.35 | 122.20 |
| 22 | AA | 143 | A | C4-C5-C6 | -6.92 | 113.54 | 117.00 |
| 57 | BA | 83 | A | C4-C5-C6 | -6.92 | 113.54 | 117.00 |
| 57 | BA | 352 | A | C4-C5-C6 | -6.92 | 113.54 | 117.00 |
| 57 | BA | 743 | A | C4-C5-C6 | -6.92 | 113.54 | 117.00 |
| 57 | BA | 2824 | C | N3-C2-O2 | -6.92 | 117.05 | 121.90 |
| 22 | AA | 996 | A | C4-C5-C6 | -6.92 | 113.54 | 117.00 |
| 9 | AR | 62 | ARG | NE-CZ-NH1 | 6.92 | 123.76 | 120.30 |
| 57 | BA | 330 | A | N1-C6-N6 | -6.92 | 114.45 | 118.60 |
| 57 | BA | 480 | A | C4-C5-C6 | -6.92 | 113.54 | 117.00 |
| 57 | BA | 980 | A | C4-C5-C6 | -6.92 | 113.54 | 117.00 |
| 57 | BA | 1040 | A | C4-C5-C6 | -6.92 | 113.54 | 117.00 |
| 57 | BA | 1433 | A | N1-C6-N6 | -6.92 | 114.45 | 118.60 |
| 57 | BA | 2681 | C | N3-C2-O2 | -6.92 | 117.06 | 121.90 |
| 58 | Ba | 92 | C | N3-C2-O2 | -6.92 | 117.06 | 121.90 |
| 22 | AA | 128 | G | O4'-C1'-N9 | 6.92 | 113.74 | 108.20 |
| 22 | AA | 246 | A | C5-C6-N1 | 6.92 | 121.16 | 117.70 |
| 57 | BA | 935 | C | N3-C2-O2 | -6.92 | 117.06 | 121.90 |
| 57 | BA | 609 | A | C5-C6-N1 | 6.92 | 121.16 | 117.70 |
| 57 | BA | 634 | C | O4'-C1'-N1 | 6.92 | 113.73 | 108.20 |
| 57 | BA | 833 | A | C4-C5-C6 | -6.92 | 113.54 | 117.00 |
| 57 | BA | 1102 | C | O4'-C1'-N1 | 6.92 | 113.73 | 108.20 |
| 57 | BA | 2298 | A | C5-C6-N1 | 6.92 | 121.16 | 117.70 |
| 57 | BA | 2530 | A | C5-C6-N1 | 6.92 | 121.16 | 117.70 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 2577 | A | C5-C6-N1 | 6.92 | 121.16 | 117.70 |
| 22 | AA | 1227 | A | C4-C5-C6 | -6.92 | 113.54 | 117.00 |
| 57 | BA | 2095 | A | C4-C5-C6 | -6.92 | 113.54 | 117.00 |
| 22 | AA | 607 | A | N1-C6-N6 | -6.92 | 114.45 | 118.60 |
| 22 | AA | 1097 | C | N3-C2-O2 | -6.92 | 117.06 | 121.90 |
| 57 | BA | 1054 | A | C4-C5-C6 | -6.92 | 113.54 | 117.00 |
| 57 | BA | 2090 | A | C5-C6-N1 | 6.92 | 121.16 | 117.70 |
| 57 | BA | 2205 | A | N1-C6-N6 | -6.92 | 114.45 | 118.60 |
| 22 | AA | 841 | C | N1-C2-O2 | 6.91 | 123.05 | 118.90 |
| 22 | AA | 1408 | A | C4-C5-C6 | -6.91 | 113.54 | 117.00 |
| 57 | BA | 1635 | A | C4-C5-C6 | -6.91 | 113.54 | 117.00 |
| 57 | BA | 1691 | C | N3-C2-O2 | -6.91 | 117.06 | 121.90 |
| 57 | BA | 2589 | A | C4-C5-C6 | -6.91 | 113.54 | 117.00 |
| 58 | Ba | 35 | C | N3-C2-O2 | -6.91 | 117.06 | 121.90 |
| 39 | BX | 12 | ARG | NE-CZ-NH1 | 6.91 | 123.76 | 120.30 |
| 22 | AA | 496 | A | C5-C6-N1 | 6.91 | 121.16 | 117.70 |
| 57 | BA | 234 | U | O4'-C1'-N1 | 6.91 | 113.73 | 108.20 |
| 57 | BA | 1665 | A | C4-C5-C6 | -6.91 | 113.55 | 117.00 |
| 58 | Ba | 38 | C | N3-C2-O2 | -6.91 | 117.06 | 121.90 |
| 57 | BA | 104 | A | C4-C5-C6 | -6.91 | 113.55 | 117.00 |
| 57 | BA | 218 | A | C5-C6-N1 | 6.91 | 121.15 | 117.70 |
| 57 | BA | 643 | A | C5-C6-N1 | 6.91 | 121.15 | 117.70 |
| 57 | BA | 1914 | C | N3-C2-O2 | -6.91 | 117.06 | 121.90 |
| 57 | BA | 2369 | A | C4-C5-C6 | -6.91 | 113.55 | 117.00 |
| 57 | BA | 57 | C | N3-C2-O2 | -6.91 | 117.06 | 121.90 |
| 22 | AA | 197 | A | C4-C5-C6 | -6.91 | 113.55 | 117.00 |
| 22 | AA | 565 | U | O4'-C1'-N1 | 6.91 | 113.72 | 108.20 |
| 22 | AA | 1149 | C | N3-C2-O2 | -6.90 | 117.07 | 121.90 |
| 22 | AA | 510 | A | C4-C5-C6 | -6.90 | 113.55 | 117.00 |
| 22 | AA | 1447 | A | C4-C5-C6 | -6.90 | 113.55 | 117.00 |
| 22 | AA | 1105 | A | C4-C5-C6 | -6.90 | 113.55 | 117.00 |
| 57 | BA | 69 | C | N3-C2-O2 | -6.90 | 117.07 | 121.90 |
| 57 | BA | 267 | C | N3-C2-O2 | -6.90 | 117.07 | 121.90 |
| 22 | AA | 504 | C | N3-C2-O2 | -6.90 | 117.07 | 121.90 |
| 57 | BA | 666 | A | C4-C5-C6 | -6.90 | 113.55 | 117.00 |
| 57 | BA | 986 | C | N1-C2-O2 | 6.90 | 123.04 | 118.90 |
| 57 | BA | 1373 | A | N1-C6-N6 | -6.90 | 114.46 | 118.60 |
| 57 | BA | 1385 | A | C4-C5-C6 | -6.90 | 113.55 | 117.00 |
| 57 | BA | 1960 | A | C4-C5-C6 | -6.90 | 113.55 | 117.00 |
| 22 | AA | 352 | C | N3-C2-O2 | -6.90 | 117.07 | 121.90 |
| 22 | AA | 1208 | C | N3-C2-O2 | -6.90 | 117.07 | 121.90 |
| 22 | AA | 790 | A | C4-C5-C6 | -6.90 | 113.55 | 117.00 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 2679 | A | C4-C5-C6 | -6.90 | 113.55 | 117.00 |
| 22 | AA | 235 | C | N3-C2-O2 | -6.89 | 117.07 | 121.90 |
| 22 | AA | 482 | A | C5-C6-N1 | 6.89 | 121.15 | 117.70 |
| 23 | A2 | 51 | C | N3-C2-O2 | -6.89 | 117.07 | 121.90 |
| 57 | BA | 198 | C | N3-C2-O2 | -6.89 | 117.07 | 121.90 |
| 58 | Ba | 105 | G | O4'-C1'-N9 | 6.89 | 113.72 | 108.20 |
| 22 | AA | 432 | A | C4-C5-C6 | -6.89 | 113.55 | 117.00 |
| 22 | AA | 733 | G | N1-C6-O6 | -6.89 | 115.77 | 119.90 |
| 57 | BA | 1570 | A | N1-C6-N6 | -6.89 | 114.46 | 118.60 |
| 57 | BA | 1759 | A | C4-C5-C6 | -6.89 | 113.55 | 117.00 |
| 22 | AA | 460 | A | C5-C6-N1 | 6.89 | 121.15 | 117.70 |
| 57 | BA | 1306 | C | O4'-C1'-N1 | 6.89 | 113.71 | 108.20 |
| 22 | AA | 1319 | A | C5-C6-N1 | 6.89 | 121.14 | 117.70 |
| 43 | B1 | 56 | ARG | NE-CZ-NH2 | 6.89 | 123.74 | 120.30 |
| 57 | BA | 565 | C | N3-C2-O2 | -6.89 | 117.08 | 121.90 |
| 22 | AA | 1533 | C | N3-C2-O2 | -6.89 | 117.08 | 121.90 |
| 57 | BA | 413 | C | N3-C2-O2 | -6.89 | 117.08 | 121.90 |
| 57 | BA | 819 | A | C5-C6-N1 | 6.89 | 121.14 | 117.70 |
| 57 | BA | 948 | C | N3-C2-O2 | -6.89 | 117.08 | 121.90 |
| 22 | AA | 393 | A | C5-C6-N1 | 6.89 | 121.14 | 117.70 |
| 57 | BA | 927 | A | C4-C5-C6 | -6.89 | 113.56 | 117.00 |
| 57 | BA | 2554 | U | O4'-C1'-N1 | 6.89 | 113.71 | 108.20 |
| 57 | BA | 417 | C | N3-C2-O2 | -6.88 | 117.08 | 121.90 |
| 57 | BA | 866 | A | C4-C5-C6 | -6.88 | 113.56 | 117.00 |
| 57 | BA | 1615 | C | N3-C2-O2 | -6.88 | 117.08 | 121.90 |
| 57 | BA | 1883 | U | O4'-C1'-N1 | 6.88 | 113.71 | 108.20 |
| 57 | BA | 2589 | A | C5-C6-N1 | 6.88 | 121.14 | 117.70 |
| 22 | AA | 139 | A | C4-C5-C6 | -6.88 | 113.56 | 117.00 |
| 57 | BA | 1127 | A | C4-C5-C6 | -6.88 | 113.56 | 117.00 |
| 57 | BA | 1320 | C | N3-C2-O2 | -6.88 | 117.08 | 121.90 |
| 57 | BA | 1672 | A | C4-C5-C6 | -6.88 | 113.56 | 117.00 |
| 57 | BA | 2073 | C | N3-C2-O2 | -6.88 | 117.08 | 121.90 |
| 57 | BA | 272 | A | N1-C6-N6 | -6.88 | 114.47 | 118.60 |
| 57 | BA | 698 | C | N3-C2-O2 | -6.88 | 117.08 | 121.90 |
| 57 | BA | 2411 | A | C4-C5-C6 | -6.88 | 113.56 | 117.00 |
| 22 | AA | 32 | A | N1-C6-N6 | -6.88 | 114.47 | 118.60 |
| 22 | AA | 547 | A | C4-C5-C6 | -6.88 | 113.56 | 117.00 |
| 57 | BA | 2023 | C | O4'-C1'-N1 | 6.88 | 113.70 | 108.20 |
| 57 | BA | 2814 | A | C4-C5-C6 | -6.88 | 113.56 | 117.00 |
| 56 | BL | 68 | ARG | NE-CZ-NH1 | 6.88 | 123.74 | 120.30 |
| 57 | BA | 1208 | C | N3-C2-O2 | -6.88 | 117.09 | 121.90 |
| 57 | BA | 1230 | A | C4-C5-C6 | -6.88 | 113.56 | 117.00 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 2058 | A | C4-C5-C6 | -6.88 | 113.56 | 117.00 |
| 22 | AA | 1509 | C | N3-C2-O2 | -6.88 | 117.09 | 121.90 |
| 50 | B7 | 3 | ARG | NE-CZ-NH2 | 6.88 | 123.74 | 120.30 |
| 57 | BA | 226 | A | C4-C5-C6 | -6.87 | 113.56 | 117.00 |
| 22 | AA | 375 | U | O4'-C1'-N1 | 6.87 | 113.70 | 108.20 |
| 57 | BA | 311 | A | N1-C6-N6 | -6.87 | 114.48 | 118.60 |
| 57 | BA | 757 | G | O4'-C1'-N9 | 6.87 | 113.70 | 108.20 |
| 57 | BA | 1616 | A | C4-C5-C6 | -6.87 | 113.56 | 117.00 |
| 57 | BA | 2287 | A | C4-C5-C6 | -6.87 | 113.56 | 117.00 |
| 58 | Ba | 97 | C | N3-C2-O2 | -6.87 | 117.09 | 121.90 |
| 17 | AF | 109 | ARG | NE-CZ-NH1 | 6.87 | 123.73 | 120.30 |
| 19 | AH | 79 | ARG | NE-CZ-NH1 | 6.87 | 123.73 | 120.30 |
| 57 | BA | 28 | A | N1-C6-N6 | -6.87 | 114.48 | 118.60 |
| 22 | AA | 193 | C | N3-C2-O2 | -6.87 | 117.09 | 121.90 |
| 57 | BA | 582 | A | C4-C5-C6 | -6.87 | 113.57 | 117.00 |
| 57 | BA | 1076 | C | N3-C2-O2 | -6.87 | 117.09 | 121.90 |
| 57 | BA | 1746 | A | C4-C5-C6 | -6.87 | 113.57 | 117.00 |
| 58 | Ba | 50 | A | C4-C5-C6 | -6.87 | 113.57 | 117.00 |
| 22 | AA | 1151 | A | C5-C6-N1 | 6.87 | 121.13 | 117.70 |
| 57 | BA | 823 | C | N3-C2-O2 | -6.87 | 117.09 | 121.90 |
| 57 | BA | 1953 | A | C4-C5-C6 | -6.87 | 113.57 | 117.00 |
| 22 | AA | 222 | C | N3-C2-O2 | -6.87 | 117.09 | 121.90 |
| 22 | AA | 336 | A | C5-C6-N1 | 6.87 | 121.13 | 117.70 |
| 22 | AA | 1000 | A | C4-C5-C6 | -6.87 | 113.57 | 117.00 |
| 22 | AA | 1248 | A | C4-C5-C6 | -6.87 | 113.57 | 117.00 |
| 57 | BA | 401 | A | C5-C6-N1 | 6.87 | 121.13 | 117.70 |
| 57 | BA | 1175 | A | C4-C5-C6 | -6.87 | 113.57 | 117.00 |
| 57 | BA | 1414 | C | O4'-C1'-N1 | 6.87 | 113.69 | 108.20 |
| 57 | BA | 703 | U | O4'-C1'-N1 | 6.86 | 113.69 | 108.20 |
| 57 | BA | 750 | A | C4-C5-C6 | -6.86 | 113.57 | 117.00 |
| 57 | BA | 1998 | A | C4-C5-C6 | -6.86 | 113.57 | 117.00 |
| 57 | BA | 2170 | A | O4'-C1'-N9 | 6.86 | 113.69 | 108.20 |
| 57 | BA | 1151 | A | C4-C5-C6 | -6.86 | 113.57 | 117.00 |
| 57 | BA | 1656 | C | N3-C2-O2 | -6.86 | 117.10 | 121.90 |
| 57 | BA | 2441 | U | N3-C2-O2 | -6.86 | 117.40 | 122.20 |
| 12 | AT | 9 | ARG | NE-CZ-NH1 | 6.86 | 123.73 | 120.30 |
| 22 | AA | 744 | C | N3-C2-O2 | -6.86 | 117.10 | 121.90 |
| 57 | BA | 637 | A | C5-C6-N1 | 6.86 | 121.13 | 117.70 |
| 57 | BA | 2394 | C | N3-C2-O2 | -6.86 | 117.10 | 121.90 |
| 57 | BA | 2590 | A | C5-C6-N1 | 6.86 | 121.13 | 117.70 |
| 57 | BA | 1349 | C | N3-C2-O2 | -6.86 | 117.10 | 121.90 |
| 22 | AA | 719 | C | N3-C2-O2 | -6.86 | 117.10 | 121.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 79 | C | N3-C2-O2 | -6.86 | 117.10 | 121.90 |
| 57 | BA | 421 | C | N3-C2-O2 | -6.86 | 117.10 | 121.90 |
| 22 | AA | 440 | C | N3-C2-O2 | -6.86 | 117.10 | 121.90 |
| 22 | AA | 764 | C | N3-C2-O2 | -6.86 | 117.10 | 121.90 |
| 57 | BA | 550 | C | N3-C2-O2 | -6.86 | 117.10 | 121.90 |
| 57 | BA | 1437 | C | O4'-C1'-N1 | 6.86 | 113.68 | 108.20 |
| 57 | BA | 1362 | C | N3-C2-O2 | -6.85 | 117.10 | 121.90 |
| 22 | AA | 1229 | A | C4-C5-C6 | -6.85 | 113.57 | 117.00 |
| 57 | BA | 1664 | A | C4-C5-C6 | -6.85 | 113.57 | 117.00 |
| 21 | A1 | 206 | ARG | NE-CZ-NH1 | 6.85 | 123.72 | 120.30 |
| 22 | AA | 311 | C | N1-C2-O2 | 6.85 | 123.01 | 118.90 |
| 22 | AA | 363 | A | C4-C5-C6 | -6.85 | 113.58 | 117.00 |
| 57 | BA | 1043 | C | N3-C2-O2 | -6.85 | 117.11 | 121.90 |
| 57 | BA | 1626 | A | C5-C6-N1 | 6.85 | 121.12 | 117.70 |
| 22 | AA | 1352 | C | N3-C2-O2 | -6.85 | 117.11 | 121.90 |
| 44 | B2 | 48 | ARG | NE-CZ-NH1 | 6.85 | 123.72 | 120.30 |
| 57 | BA | 44 | A | C5-C6-N1 | 6.85 | 121.12 | 117.70 |
| 57 | BA | 1264 | A | C4-C5-C6 | -6.85 | 113.58 | 117.00 |
| 57 | BA | 2778 | A | C4-C5-C6 | -6.85 | 113.58 | 117.00 |
| 57 | BA | 502 | A | C4-C5-C6 | -6.85 | 113.58 | 117.00 |
| 22 | AA | 279 | A | C4-C5-C6 | -6.84 | 113.58 | 117.00 |
| 22 | AA | 1259 | C | N3-C2-O2 | -6.84 | 117.11 | 121.90 |
| 57 | BA | 2616 | C | N3-C2-O2 | -6.84 | 117.11 | 121.90 |
| 22 | AA | 635 | A | C4-C5-C6 | -6.84 | 113.58 | 117.00 |
| 22 | AA | 934 | C | N1-C2-O2 | 6.84 | 123.01 | 118.90 |
| 57 | BA | 1816 | C | N3-C2-O2 | -6.84 | 117.11 | 121.90 |
| 57 | BA | 2194 | U | O4'-C1'-N1 | 6.84 | 113.67 | 108.20 |
| 22 | AA | 1225 | A | N1-C6-N6 | -6.84 | 114.50 | 118.60 |
| 57 | BA | 1795 | C | N3-C2-O2 | -6.84 | 117.11 | 121.90 |
| 22 | AA | 994 | A | C4-C5-C6 | -6.84 | 113.58 | 117.00 |
| 36 | BU | 29 | ARG | NE-CZ-NH1 | 6.84 | 123.72 | 120.30 |
| 57 | BA | 125 | A | C4-C5-C6 | -6.84 | 113.58 | 117.00 |
| 57 | BA | 1272 | A | C4-C5-C6 | -6.84 | 113.58 | 117.00 |
| 57 | BA | 1526 | C | O4'-C1'-N1 | 6.84 | 113.67 | 108.20 |
| 57 | BA | 1582 | C | N3-C2-O2 | -6.84 | 117.11 | 121.90 |
| 57 | BA | 2163 | A | C4-C5-C6 | -6.84 | 113.58 | 117.00 |
| 57 | BA | 2651 | C | N3-C2-O2 | -6.84 | 117.11 | 121.90 |
| 28 | BN | 35 | ARG | NE-CZ-NH1 | 6.84 | 123.72 | 120.30 |
| 57 | BA | 155 | A | C4-C5-C6 | -6.84 | 113.58 | 117.00 |
| 57 | BA | 586 | A | C5-C6-N1 | 6.84 | 121.12 | 117.70 |
| 57 | BA | 715 | A | C4-C5-C6 | -6.84 | 113.58 | 117.00 |
| 57 | BA | 114 | U | O4'-C1'-N1 | 6.83 | 113.67 | 108.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 1604 | C | N3-C2-O2 | -6.83 | 117.12 | 121.90 |
| 22 | AA | 487 | A | C5-C6-N1 | 6.83 | 121.12 | 117.70 |
| 34 | BT | 71 | ARG | NE-CZ-NH1 | 6.83 | 123.72 | 120.30 |
| 57 | BA | 111 | A | C4-C5-C6 | -6.83 | 113.58 | 117.00 |
| 57 | BA | 295 | G | O4'-C1'-N9 | 6.83 | 113.67 | 108.20 |
| 57 | BA | 1373 | A | C5-C6-N1 | 6.83 | 121.12 | 117.70 |
| 22 | AA | 679 | C | N3-C2-O2 | -6.83 | 117.12 | 121.90 |
| 57 | BA | 1932 | A | C4-C5-C6 | -6.83 | 113.58 | 117.00 |
| 22 | AA | 126 | G | O4'-C1'-N9 | 6.83 | 113.66 | 108.20 |
| 57 | BA | 222 | A | C4-C5-C6 | -6.83 | 113.59 | 117.00 |
| 57 | BA | 614 | A | C4-C5-C6 | -6.83 | 113.59 | 117.00 |
| 57 | BA | 764 | A | C5-C6-N1 | 6.83 | 121.11 | 117.70 |
| 57 | BA | 2788 | C | N3-C2-O2 | -6.83 | 117.12 | 121.90 |
| 22 | AA | 770 | C | N3-C2-O2 | -6.83 | 117.12 | 121.90 |
| 22 | AA | 936 | C | O4'-C1'-N1 | 6.83 | 113.66 | 108.20 |
| 22 | AA | 1081 | A | C4-C5-C6 | -6.83 | 113.59 | 117.00 |
| 56 | BL | 116 | ARG | NE-CZ-NH1 | 6.83 | 123.71 | 120.30 |
| 57 | BA | 483 | A | C5-C6-N1 | 6.83 | 121.11 | 117.70 |
| 57 | BA | 911 | A | C4-C5-C6 | -6.83 | 113.59 | 117.00 |
| 57 | BA | 1344 | U | O4'-C1'-N1 | 6.83 | 113.66 | 108.20 |
| 57 | BA | 2183 | A | C5-C6-N1 | 6.83 | 121.11 | 117.70 |
| 57 | BA | 788 | A | C4-C5-C6 | -6.82 | 113.59 | 117.00 |
| 57 | BA | 1428 | C | N3-C2-O2 | -6.82 | 117.12 | 121.90 |
| 57 | BA | 2423 | U | O4'-C1'-N1 | 6.82 | 113.66 | 108.20 |
| 57 | BA | 837 | C | N3-C2-O2 | -6.82 | 117.12 | 121.90 |
| 57 | BA | 2440 | C | C6-N1-C2 | -6.82 | 117.57 | 120.30 |
| 22 | AA | 13 | U | O4'-C1'-N1 | 6.82 | 113.66 | 108.20 |
| 57 | BA | 2468 | A | C4-C5-C6 | -6.82 | 113.59 | 117.00 |
| 57 | BA | 378 | C | N1-C2-O2 | 6.82 | 122.99 | 118.90 |
| 57 | BA | 1285 | A | C4-C5-C6 | -6.82 | 113.59 | 117.00 |
| 57 | BA | 1977 | A | C4-C5-C6 | -6.82 | 113.59 | 117.00 |
| 22 | AA | 559 | A | O4'-C1'-N9 | 6.82 | 113.65 | 108.20 |
| 22 | AA | 1073 | U | O4'-C1'-N1 | 6.82 | 113.65 | 108.20 |
| 57 | BA | 548 | G | O4'-C1'-N9 | 6.82 | 113.65 | 108.20 |
| 22 | AA | 18 | C | N3-C2-O2 | -6.81 | 117.13 | 121.90 |
| 57 | BA | 599 | A | C4-C5-C6 | -6.81 | 113.59 | 117.00 |
| 22 | AA | 291 | U | O4'-C1'-N1 | 6.81 | 113.65 | 108.20 |
| 57 | BA | 2600 | A | C4-C5-C6 | -6.81 | 113.59 | 117.00 |
| 22 | AA | 50 | A | C4-C5-C6 | -6.81 | 113.59 | 117.00 |
| 22 | AA | 1069 | C | O4'-C1'-N1 | 6.81 | 113.65 | 108.20 |
| 22 | AA | 1394 | A | C4-C5-C6 | -6.81 | 113.59 | 117.00 |
| 57 | BA | 1470 | A | C5-C6-N1 | 6.81 | 121.11 | 117.70 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 430 | A | C4-C5-C6 | -6.81 | 113.59 | 117.00 |
| 57 | BA | 909 | A | C4-C5-C6 | -6.81 | 113.60 | 117.00 |
| 57 | BA | 933 | A | O4'-C1'-N9 | 6.81 | 113.65 | 108.20 |
| 58 | Ba | 12 | C | N3-C2-O2 | -6.81 | 117.13 | 121.90 |
| 22 | AA | 435 | A | C5-C6-N1 | 6.81 | 121.10 | 117.70 |
| 22 | AA | 1070 | U | O4'-C1'-N1 | 6.81 | 113.64 | 108.20 |
| 57 | BA | 2358 | A | C4-C5-C6 | -6.81 | 113.60 | 117.00 |
| 57 | BA | 2757 | A | N1-C6-N6 | -6.81 | 114.52 | 118.60 |
| 22 | AA | 781 | A | C4-C5-C6 | -6.80 | 113.60 | 117.00 |
| 57 | BA | 2411 | A | N1-C6-N6 | -6.80 | 114.52 | 118.60 |
| 22 | AA | 80 | A | C4-C5-C6 | -6.80 | 113.60 | 117.00 |
| 22 | AA | 576 | C | N3-C2-O2 | -6.80 | 117.14 | 121.90 |
| 40 | BY | 93 | ARG | NE-CZ-NH1 | 6.80 | 123.70 | 120.30 |
| 46 | B3 | 15 | ARG | NE-CZ-NH1 | 6.80 | 123.70 | 120.30 |
| 57 | BA | 793 | A | C4-C5-C6 | -6.80 | 113.60 | 117.00 |
| 57 | BA | 1590 | A | C4-C5-C6 | -6.80 | 113.60 | 117.00 |
| 22 | AA | 371 | A | C4-C5-C6 | -6.80 | 113.60 | 117.00 |
| 22 | AA | 866 | C | N3-C2-O2 | -6.80 | 117.14 | 121.90 |
| 57 | BA | 412 | A | C4-C5-C6 | -6.80 | 113.60 | 117.00 |
| 57 | BA | 2314 | A | C4-C5-C6 | -6.80 | 113.60 | 117.00 |
| 22 | AA | 753 | A | C5-C6-N1 | 6.80 | 121.10 | 117.70 |
| 57 | BA | 911 | A | N1-C6-N6 | -6.80 | 114.52 | 118.60 |
| 22 | AA | 10 | A | C4-C5-C6 | -6.80 | 113.60 | 117.00 |
| 22 | AA | 1016 | A | C4-C5-C6 | -6.80 | 113.60 | 117.00 |
| 57 | BA | 550 | C | O4'-C1'-N1 | 6.80 | 113.64 | 108.20 |
| 58 | Ba | 91 | C | N3-C2-O2 | -6.80 | 117.14 | 121.90 |
| 57 | BA | 2070 | A | C4-C5-C6 | -6.79 | 113.60 | 117.00 |
| 22 | AA | 1340 | A | C5-C6-N1 | 6.79 | 121.10 | 117.70 |
| 24 | A3 | 11 | A | C4-C5-C6 | -6.79 | 113.60 | 117.00 |
| 22 | AA | 660 | C | N3-C2-O2 | -6.79 | 117.15 | 121.90 |
| 22 | AA | 306 | A | C5-C6-N1 | 6.79 | 121.09 | 117.70 |
| 22 | AA | 1465 | A | C4-C5-C6 | -6.79 | 113.61 | 117.00 |
| 57 | BA | 1762 | A | C5-C6-N1 | 6.79 | 121.09 | 117.70 |
| 57 | BA | 1952 | A | C4-C5-C6 | -6.79 | 113.61 | 117.00 |
| 31 | BQ | 50 | ARG | NE-CZ-NH2 | 6.79 | 123.69 | 120.30 |
| 57 | BA | 208 | C | N3-C2-O2 | -6.79 | 117.15 | 121.90 |
| 57 | BA | 1302 | A | C4-C5-C6 | -6.79 | 113.61 | 117.00 |
| 57 | BA | 2675 | A | C4-C5-C6 | -6.79 | 113.61 | 117.00 |
| 57 | BA | 556 | A | C5-C6-N1 | 6.79 | 121.09 | 117.70 |
| 57 | BA | 1046 | A | C4-C5-C6 | -6.79 | 113.61 | 117.00 |
| 57 | BA | 1803 | A | N1-C6-N6 | -6.79 | 114.53 | 118.60 |
| 22 | AA | 554 | A | C4-C5-C6 | -6.78 | 113.61 | 117.00 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 475 | C | N3-C2-O2 | -6.78 | 117.15 | 121.90 |
| 57 | BA | 838 | C | N1-C2-O2 | 6.78 | 122.97 | 118.90 |
| 57 | BA | 2683 | C | N3-C2-O2 | -6.78 | 117.15 | 121.90 |
| 22 | AA | 995 | C | O4'-C1'-N1 | 6.78 | 113.63 | 108.20 |
| 57 | BA | 1119 | U | O4'-C1'-N1 | 6.78 | 113.62 | 108.20 |
| 22 | AA | 303 | A | C4-C5-C6 | -6.78 | 113.61 | 117.00 |
| 22 | AA | 1035 | A | C4-C5-C6 | -6.78 | 113.61 | 117.00 |
| 22 | AA | 1155 | A | C4-C5-C6 | -6.78 | 113.61 | 117.00 |
| 22 | AA | 1453 | G | O4'-C1'-N9 | 6.78 | 113.62 | 108.20 |
| 57 | BA | 902 | C | N3-C2-O2 | -6.78 | 117.15 | 121.90 |
| 57 | BA | 1080 | A | C4-C5-C6 | -6.78 | 113.61 | 117.00 |
| 57 | BA | 2851 | A | C4-C5-C6 | -6.78 | 113.61 | 117.00 |
| 14 | AC | 171 | ARG | NE-CZ-NH1 | 6.78 | 123.69 | 120.30 |
| 22 | AA | 236 | A | C4-C5-C6 | -6.78 | 113.61 | 117.00 |
| 57 | BA | 184 | C | N3-C2-O2 | -6.78 | 117.16 | 121.90 |
| 57 | BA | 1901 | A | C4-C5-C6 | -6.78 | 113.61 | 117.00 |
| 57 | BA | 2665 | A | C5-C6-N1 | 6.78 | 121.09 | 117.70 |
| 54 | BG | 147 | ARG | NE-CZ-NH1 | 6.78 | 123.69 | 120.30 |
| 57 | BA | 538 | A | C4-C5-C6 | -6.78 | 113.61 | 117.00 |
| 57 | BA | 994 | C | N3-C2-O2 | -6.78 | 117.16 | 121.90 |
| 57 | BA | 1525 | A | C4-C5-C6 | -6.78 | 113.61 | 117.00 |
| 57 | BA | 1801 | A | C4-C5-C6 | -6.77 | 113.61 | 117.00 |
| 22 | AA | 1152 | A | C4-C5-C6 | -6.77 | 113.61 | 117.00 |
| 23 | A2 | 47 | C | N3-C2-O2 | -6.77 | 117.16 | 121.90 |
| 57 | BA | 661 | A | N1-C6-N6 | -6.77 | 114.54 | 118.60 |
| 57 | BA | 1073 | A | C4-C5-C6 | -6.77 | 113.61 | 117.00 |
| 57 | BA | 2001 | C | O4'-C1'-N1 | 6.77 | 113.62 | 108.20 |
| 57 | BA | 2170 | A | C4-C5-C6 | -6.77 | 113.61 | 117.00 |
| 57 | BA | 2425 | A | C4-C5-C6 | -6.77 | 113.61 | 117.00 |
| 22 | AA | 355 | C | N3-C4-C5 | 6.77 | 124.61 | 121.90 |
| 22 | AA | 1493 | A | O4'-C1'-N9 | 6.77 | 113.62 | 108.20 |
| 57 | BA | 2887 | A | C5-C6-N1 | 6.77 | 121.08 | 117.70 |
| 24 | A3 | 43 | G | O4'-C1'-N9 | 6.77 | 113.61 | 108.20 |
| 57 | BA | 627 | A | C4-C5-C6 | -6.77 | 113.62 | 117.00 |
| 57 | BA | 627 | A | C5-C6-N1 | 6.77 | 121.08 | 117.70 |
| 57 | BA | 942 | G | N7-C8-N9 | 6.77 | 116.48 | 113.10 |
| 57 | BA | 2094 | A | C4-C5-C6 | -6.77 | 113.62 | 117.00 |
| 57 | BA | 2346 | A | C4-C5-C6 | -6.77 | 113.62 | 117.00 |
| 57 | BA | 2823 | A | N1-C6-N6 | -6.77 | 114.54 | 118.60 |
| 19 | AH | 12 | ARG | NE-CZ-NH1 | 6.76 | 123.68 | 120.30 |
| 22 | AA | 1209 | C | N3-C2-O2 | -6.76 | 117.17 | 121.90 |
| 42 | B0 | 13 | ARG | NE-CZ-NH2 | 6.76 | 123.68 | 120.30 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | A3 | 37 | U | O4'-C1'-N1 | 6.76 | 113.61 | 108.20 |
| 57 | BA | 2810 | A | C4-C5-C6 | -6.76 | 113.62 | 117.00 |
| 57 | BA | 2878 | U | O4'-C1'-N1 | 6.76 | 113.61 | 108.20 |
| 22 | AA | 1145 | A | N1-C6-N6 | -6.76 | 114.54 | 118.60 |
| 58 | Ba | 34 | A | C4-C5-C6 | -6.76 | 113.62 | 117.00 |
| 22 | AA | 1397 | C | N1-C2-O2 | 6.76 | 122.96 | 118.90 |
| 57 | BA | 984 | A | C4-C5-C6 | -6.76 | 113.62 | 117.00 |
| 57 | BA | 1111 | A | C5-C6-N1 | 6.76 | 121.08 | 117.70 |
| 57 | BA | 1969 | A | C4-C5-C6 | -6.76 | 113.62 | 117.00 |
| 57 | BA | 482 | A | C4-C5-C6 | -6.76 | 113.62 | 117.00 |
| 22 | AA | 1130 | A | C4-C5-C6 | -6.76 | 113.62 | 117.00 |
| 22 | AA | 1484 | C | O4'-C1'-N1 | 6.76 | 113.61 | 108.20 |
| 36 | BU | 63 | ARG | NE-CZ-NH1 | 6.76 | 123.68 | 120.30 |
| 57 | BA | 502 | A | C5-C6-N1 | 6.76 | 121.08 | 117.70 |
| 57 | BA | 305 | C | N1-C2-O2 | 6.75 | 122.95 | 118.90 |
| 57 | BA | 2748 | A | C5-C6-N1 | 6.75 | 121.08 | 117.70 |
| 22 | AA | 507 | C | N3-C2-O2 | -6.75 | 117.17 | 121.90 |
| 22 | AA | 1157 | A | N1-C6-N6 | -6.75 | 114.55 | 118.60 |
| 22 | AA | 1430 | A | C4-C5-C6 | -6.75 | 113.62 | 117.00 |
| 57 | BA | 5 | A | C4-C5-C6 | -6.75 | 113.62 | 117.00 |
| 22 | AA | 831 | A | C4-C5-C6 | -6.75 | 113.62 | 117.00 |
| 22 | AA | 412 | A | C1'-O4'-C4' | -6.75 | 104.50 | 109.90 |
| 29 | BO | 18 | ARG | NE-CZ-NH1 | 6.75 | 123.67 | 120.30 |
| 33 | BS | 33 | ARG | NE-CZ-NH1 | 6.75 | 123.67 | 120.30 |
| 57 | BA | 165 | A | C4-C5-C6 | -6.75 | 113.63 | 117.00 |
| 57 | BA | 765 | C | N1-C2-O2 | 6.75 | 122.95 | 118.90 |
| 22 | AA | 253 | A | N1-C6-N6 | -6.75 | 114.55 | 118.60 |
| 22 | AA | 609 | A | C4-C5-C6 | -6.75 | 113.63 | 117.00 |
| 37 | BV | 13 | ARG | NE-CZ-NH1 | 6.75 | 123.67 | 120.30 |
| 57 | BA | 21 | A | C4-C5-C6 | -6.75 | 113.63 | 117.00 |
| 57 | BA | 1183 | U | O4'-C1'-N1 | 6.75 | 113.60 | 108.20 |
| 57 | BA | 1641 | A | C5-C6-N1 | 6.75 | 121.07 | 117.70 |
| 57 | BA | 1765 | U | O4'-C1'-N1 | 6.75 | 113.60 | 108.20 |
| 57 | BA | 2883 | A | C4-C5-C6 | -6.75 | 113.63 | 117.00 |
| 31 | BQ | 16 | ARG | NE-CZ-NH1 | 6.75 | 123.67 | 120.30 |
| 57 | BA | 541 | A | C4-C5-C6 | -6.75 | 113.63 | 117.00 |
| 57 | BA | 1953 | A | C5-C6-N1 | 6.75 | 121.07 | 117.70 |
| 57 | BA | 103 | A | C4-C5-C6 | -6.74 | 113.63 | 117.00 |
| 57 | BA | 146 | A | C4-C5-C6 | -6.74 | 113.63 | 117.00 |
| 22 | AA | 1350 | A | N1-C6-N6 | -6.74 | 114.56 | 118.60 |
| 22 | AA | 1377 | A | C4-C5-C6 | -6.74 | 113.63 | 117.00 |
| 22 | AA | 1406 | U | O4'-C1'-N1 | 6.74 | 113.59 | 108.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 557 | C | N3-C2-O2 | -6.74 | 117.18 | 121.90 |
| 57 | BA | 2019 | A | C4-C5-C6 | -6.74 | 113.63 | 117.00 |
| 22 | AA | 212 | G | O4'-C1'-N9 | 6.74 | 113.59 | 108.20 |
| 4 | AM | 108 | ARG | NE-CZ-NH1 | 6.74 | 123.67 | 120.30 |
| 57 | BA | 1650 | A | C4-C5-C6 | -6.74 | 113.63 | 117.00 |
| 22 | AA | 1066 | C | N3-C2-O2 | -6.73 | 117.19 | 121.90 |
| 57 | BA | 1774 | C | N3-C2-O2 | -6.73 | 117.19 | 121.90 |
| 58 | Ba | 39 | A | C4-C5-C6 | -6.73 | 113.63 | 117.00 |
| 57 | BA | 3 | U | O4'-C1'-N1 | 6.73 | 113.58 | 108.20 |
| 57 | BA | 1502 | A | C4-C5-C6 | -6.73 | 113.64 | 117.00 |
| 26 | BJ | 124 | ARG | NE-CZ-NH1 | 6.73 | 123.67 | 120.30 |
| 57 | BA | 2173 | A | C5-C6-N1 | 6.73 | 121.06 | 117.70 |
| 22 | AA | 181 | A | C4-C5-C6 | -6.73 | 113.64 | 117.00 |
| 22 | AA | 1133 | G | O4'-C1'-N9 | 6.73 | 113.58 | 108.20 |
| 35 | BD | 257 | ARG | NE-CZ-NH1 | 6.73 | 123.66 | 120.30 |
| 51 | B8 | 12 | ARG | NE-CZ-NH2 | 6.73 | 123.66 | 120.30 |
| 57 | BA | 1630 | A | C4-C5-C6 | -6.73 | 113.64 | 117.00 |
| 57 | BA | 1802 | A | N1-C6-N6 | -6.73 | 114.56 | 118.60 |
| 57 | BA | 1085 | A | C4-C5-C6 | -6.73 | 113.64 | 117.00 |
| 57 | BA | 1035 | U | O4'-C1'-N1 | 6.72 | 113.58 | 108.20 |
| 57 | BA | 1576 | U | O4'-C1'-N1 | 6.72 | 113.58 | 108.20 |
| 22 | AA | 382 | A | C4-C5-C6 | -6.72 | 113.64 | 117.00 |
| 22 | AA | 1188 | A | C4-C5-C6 | -6.72 | 113.64 | 117.00 |
| 22 | AA | 1479 | C | O4'-C1'-N1 | 6.72 | 113.58 | 108.20 |
| 57 | BA | 384 | A | C4-C5-C6 | -6.72 | 113.64 | 117.00 |
| 57 | BA | 749 | A | C4-C5-C6 | -6.72 | 113.64 | 117.00 |
| 57 | BA | 1805 | A | C4-C5-C6 | -6.72 | 113.64 | 117.00 |
| 22 | AA | 747 | A | C4-C5-C6 | -6.72 | 113.64 | 117.00 |
| 57 | BA | 408 | G | N1-C6-O6 | -6.72 | 115.87 | 119.90 |
| 57 | BA | 1088 | A | N1-C6-N6 | -6.72 | 114.57 | 118.60 |
| 57 | BA | 1213 | A | C4-C5-C6 | -6.72 | 113.64 | 117.00 |
| 57 | BA | 574 | A | C4-C5-C6 | -6.72 | 113.64 | 117.00 |
| 57 | BA | 1313 | U | N3-C2-O2 | -6.72 | 117.50 | 122.20 |
| 57 | BA | 507 | A | C5-C6-N1 | 6.72 | 121.06 | 117.70 |
| 57 | BA | 1566 | A | C4-C5-C6 | -6.72 | 113.64 | 117.00 |
| 57 | BA | 2541 | A | C4-C5-C6 | -6.72 | 113.64 | 117.00 |
| 15 | AD | 43 | ARG | NE-CZ-NH1 | 6.72 | 123.66 | 120.30 |
| 57 | BA | 2009 | A | C5-C6-N1 | 6.72 | 121.06 | 117.70 |
| 57 | BA | 2179 | C | N3-C2-O2 | -6.72 | 117.20 | 121.90 |
| 57 | BA | 2736 | A | C4-C5-C6 | -6.72 | 113.64 | 117.00 |
| 3 | AL | 49 | ARG | NE-CZ-NH1 | 6.71 | 123.66 | 120.30 |
| 22 | AA | 779 | C | O4'-C1'-N1 | 6.71 | 113.57 | 108.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 239 | C | O4'-C1'-N1 | 6.71 | 113.57 | 108.20 |
| 57 | BA | 453 | A | C4-C5-C6 | -6.71 | 113.64 | 117.00 |
| 57 | BA | 1000 | A | C4-C5-C6 | -6.71 | 113.64 | 117.00 |
| 22 | AA | 288 | A | N1-C6-N6 | -6.71 | 114.57 | 118.60 |
| 22 | AA | 131 | A | C4-C5-C6 | -6.71 | 113.64 | 117.00 |
| 35 | BD | 12 | ARG | NE-CZ-NH1 | 6.71 | 123.66 | 120.30 |
| 57 | BA | 2077 | A | N1-C6-N6 | -6.71 | 114.57 | 118.60 |
| 46 | B3 | 30 | ARG | NE-CZ-NH1 | 6.71 | 123.65 | 120.30 |
| 57 | BA | 1058 | U | O4'-C1'-N1 | 6.71 | 113.57 | 108.20 |
| 57 | BA | 1306 | C | N3-C4-N4 | -6.71 | 113.30 | 118.00 |
| 57 | BA | 1353 | A | C4-C5-C6 | -6.71 | 113.65 | 117.00 |
| 57 | BA | 2461 | A | C4-C5-C6 | -6.71 | 113.65 | 117.00 |
| 22 | AA | 483 | C | N3-C2-O2 | -6.71 | 117.21 | 121.90 |
| 23 | A2 | 33 | A | C5-C6-N1 | 6.71 | 121.05 | 117.70 |
| 57 | BA | 2118 | U | O4'-C1'-N1 | 6.71 | 113.56 | 108.20 |
| 17 | AF | 79 | ARG | NE-CZ-NH1 | 6.70 | 123.65 | 120.30 |
| 57 | BA | 335 | C | N3-C2-O2 | -6.70 | 117.21 | 121.90 |
| 57 | BA | 1413 | A | C4-C5-C6 | -6.70 | 113.65 | 117.00 |
| 57 | BA | 1889 | A | C4-C5-C6 | -6.70 | 113.65 | 117.00 |
| 16 | AE | 92 | ARG | NE-CZ-NH1 | 6.70 | 123.65 | 120.30 |
| 22 | AA | 1419 | G | N1-C6-O6 | -6.70 | 115.88 | 119.90 |
| 57 | BA | 94 | A | C4-C5-C6 | -6.70 | 113.65 | 117.00 |
| 57 | BA | 1706 | C | O4'-C1'-N1 | 6.70 | 113.56 | 108.20 |
| 57 | BA | 2565 | A | C4-C5-C6 | -6.70 | 113.65 | 117.00 |
| 57 | BA | 1075 | C | N3-C2-O2 | -6.70 | 117.21 | 121.90 |
| 57 | BA | 1905 | C | N3-C2-O2 | -6.70 | 117.21 | 121.90 |
| 57 | BA | 2200 | C | O4'-C1'-N1 | 6.70 | 113.56 | 108.20 |
| 7 | AP | 5 | ARG | NE-CZ-NH1 | 6.70 | 123.65 | 120.30 |
| 57 | BA | 454 | A | C4-C5-C6 | -6.70 | 113.65 | 117.00 |
| 57 | BA | 1109 | C | N3-C2-O2 | -6.70 | 117.21 | 121.90 |
| 57 | BA | 1341 | G | O4'-C1'-N9 | 6.70 | 113.56 | 108.20 |
| 57 | BA | 1548 | A | C4-C5-C6 | -6.70 | 113.65 | 117.00 |
| 57 | BA | 2281 | A | C5-C6-N1 | 6.70 | 121.05 | 117.70 |
| 57 | BA | 334 | C | N3-C2-O2 | -6.70 | 117.21 | 121.90 |
| 57 | BA | 654 | A | O4'-C1'-N9 | 6.70 | 113.56 | 108.20 |
| 22 | AA | 728 | A | O4'-C1'-N9 | 6.70 | 113.56 | 108.20 |
| 57 | BA | 11 | C | N3-C2-O2 | -6.70 | 117.21 | 121.90 |
| 57 | BA | 477 | A | C5-C6-N1 | 6.70 | 121.05 | 117.70 |
| 57 | BA | 1515 | A | C4-C5-C6 | -6.70 | 113.65 | 117.00 |
| 57 | BA | 1877 | A | C4-C5-C6 | -6.70 | 113.65 | 117.00 |
| 22 | AA | 1446 | A | C4-C5-C6 | -6.69 | 113.65 | 117.00 |
| 22 | AA | 214 | C | N3-C2-O2 | -6.69 | 117.22 | 121.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 1496 | A | C4-C5-C6 | -6.69 | 113.65 | 117.00 |
| 57 | BA | 2071 | A | N1-C6-N6 | -6.69 | 114.58 | 118.60 |
| 57 | BA | 2223 | G | O4'-C1'-N9 | 6.69 | 113.55 | 108.20 |
| 22 | AA | 1507 | A | N1-C6-N6 | -6.69 | 114.59 | 118.60 |
| 57 | BA | 197 | A | C4-C5-C6 | -6.69 | 113.66 | 117.00 |
| 57 | BA | 158 | U | O4'-C1'-N1 | 6.69 | 113.55 | 108.20 |
| 57 | BA | 770 | G | O4'-C1'-N9 | 6.69 | 113.55 | 108.20 |
| 22 | AA | 155 | A | C4-C5-C6 | -6.69 | 113.66 | 117.00 |
| 22 | AA | 959 | A | C5-C6-N1 | 6.69 | 121.04 | 117.70 |
| 57 | BA | 441 | U | O4'-C1'-N1 | 6.69 | 113.55 | 108.20 |
| 57 | BA | 504 | A | C4-C5-C6 | -6.69 | 113.66 | 117.00 |
| 57 | BA | 1490 | A | C4-C5-C6 | -6.69 | 113.66 | 117.00 |
| 57 | BA | 1586 | A | C4-C5-C6 | -6.69 | 113.66 | 117.00 |
| 57 | BA | 2726 | A | C5-C6-N1 | 6.69 | 121.04 | 117.70 |
| 22 | AA | 767 | A | C4-C5-C6 | -6.69 | 113.66 | 117.00 |
| 22 | AA | 179 | A | C4-C5-C6 | -6.68 | 113.66 | 117.00 |
| 22 | AA | 1534 | A | C5-C6-N1 | 6.68 | 121.04 | 117.70 |
| 57 | BA | 19 | A | C4-C5-C6 | -6.68 | 113.66 | 117.00 |
| 57 | BA | 219 | A | C4-C5-C6 | -6.68 | 113.66 | 117.00 |
| 57 | BA | 1729 | U | O4'-C1'-N1 | 6.68 | 113.55 | 108.20 |
| 57 | BA | 2129 | C | N1-C2-O2 | 6.68 | 122.91 | 118.90 |
| 58 | Ba | 60 | C | N1-C2-O2 | 6.68 | 122.91 | 118.90 |
| 22 | AA | 583 | A | C4-C5-C6 | -6.68 | 113.66 | 117.00 |
| 57 | BA | 1822 | C | N3-C2-O2 | -6.68 | 117.22 | 121.90 |
| 57 | BA | 2078 | C | N1-C2-O2 | 6.68 | 122.91 | 118.90 |
| 57 | BA | 2309 | A | C4-C5-C6 | -6.68 | 113.66 | 117.00 |
| 57 | BA | 2227 | A | N1-C6-N6 | -6.68 | 114.59 | 118.60 |
| 22 | AA | 192 | A | N1-C6-N6 | -6.68 | 114.59 | 118.60 |
| 22 | AA | 322 | C | N3-C2-O2 | -6.68 | 117.22 | 121.90 |
| 57 | BA | 962 | G | N1-C6-O6 | -6.68 | 115.89 | 119.90 |
| 57 | BA | 2761 | A | C4-C5-C6 | -6.68 | 113.66 | 117.00 |
| 57 | BA | 347 | A | C4-C5-C6 | -6.68 | 113.66 | 117.00 |
| 57 | BA | 2247 | A | O4'-C1'-N9 | 6.68 | 113.54 | 108.20 |
| 57 | BA | 2619 | C | N3-C2-O2 | -6.68 | 117.23 | 121.90 |
| 57 | BA | 2085 | U | O4'-C1'-N1 | 6.68 | 113.54 | 108.20 |
| 57 | BA | 2573 | C | N3-C2-O2 | -6.68 | 117.23 | 121.90 |
| 57 | BA | 1815 | A | C4-C5-C6 | -6.67 | 113.66 | 117.00 |
| 57 | BA | 2195 | U | O4'-C1'-N1 | 6.67 | 113.54 | 108.20 |
| 57 | BA | 2199 | A | C5'-C4'-C3' | -6.67 | 105.32 | 116.00 |
| 57 | BA | 2205 | A | C5-C6-N1 | 6.67 | 121.04 | 117.70 |
| 57 | BA | 1786 | A | O4'-C1'-N9 | 6.67 | 113.54 | 108.20 |
| 22 | AA | 741 | G | O4'-C1'-N9 | 6.67 | 113.54 | 108.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 2211 | A | O4'-C1'-N9 | 6.67 | 113.54 | 108.20 |
| 22 | AA | 1110 | A | C5-C6-N1 | 6.67 | 121.03 | 117.70 |
| 57 | BA | 207 | A | N1-C6-N6 | -6.67 | 114.60 | 118.60 |
| 57 | BA | 2900 | A | C4-C5-C6 | -6.67 | 113.67 | 117.00 |
| 57 | BA | 1713 | A | C4-C5-C6 | -6.67 | 113.67 | 117.00 |
| 22 | AA | 640 | A | C4-C5-C6 | -6.67 | 113.67 | 117.00 |
| 57 | BA | 1354 | A | C4-C5-C6 | -6.67 | 113.67 | 117.00 |
| 58 | Ba | 70 | C | N3-C2-O2 | -6.67 | 117.23 | 121.90 |
| 22 | AA | 814 | A | C4-C5-C6 | -6.66 | 113.67 | 117.00 |
| 22 | AA | 1147 | C | O4'-C1'-N1 | 6.66 | 113.53 | 108.20 |
| 22 | AA | 1162 | C | N3-C2-O2 | -6.66 | 117.23 | 121.90 |
| 22 | AA | 1288 | A | C5-C6-N1 | 6.66 | 121.03 | 117.70 |
| 57 | BA | 1937 | A | C4-C5-C6 | -6.66 | 113.67 | 117.00 |
| 22 | AA | 1100 | C | N3-C2-O2 | -6.66 | 117.24 | 121.90 |
| 57 | BA | 1287 | A | C4-C5-C6 | -6.66 | 113.67 | 117.00 |
| 7 | AP | 35 | ARG | NE-CZ-NH1 | 6.66 | 123.63 | 120.30 |
| 22 | AA | 313 | A | C4-C5-C6 | -6.66 | 113.67 | 117.00 |
| 22 | AA | 1017 | U | O4'-C1'-N1 | 6.66 | 113.53 | 108.20 |
| 57 | BA | 2476 | A | C5-C6-N1 | 6.66 | 121.03 | 117.70 |
| 57 | BA | 2887 | A | C4-C5-C6 | -6.66 | 113.67 | 117.00 |
| 9 | AR | 72 | ARG | NE-CZ-NH1 | 6.66 | 123.63 | 120.30 |
| 22 | AA | 1501 | C | O4'-C1'-N1 | 6.66 | 113.53 | 108.20 |
| 57 | BA | 1504 | A | C5-C6-N1 | 6.66 | 121.03 | 117.70 |
| 57 | BA | 1612 | C | O4'-C1'-N1 | 6.66 | 113.53 | 108.20 |
| 57 | BA | 1790 | C | O4'-C1'-N1 | 6.66 | 113.53 | 108.20 |
| 57 | BA | 2805 | C | O4'-C1'-N1 | 6.66 | 113.53 | 108.20 |
| 57 | BA | 63 | A | C4-C5-C6 | -6.66 | 113.67 | 117.00 |
| 57 | BA | 1640 | A | C4-C5-C6 | -6.66 | 113.67 | 117.00 |
| 57 | BA | 2288 | A | C4-C5-C6 | -6.66 | 113.67 | 117.00 |
| 57 | BA | 2378 | A | C4-C5-C6 | -6.66 | 113.67 | 117.00 |
| 22 | AA | 1429 | A | C4-C5-C6 | -6.65 | 113.67 | 117.00 |
| 22 | AA | 48 | C | N3-C2-O2 | -6.65 | 117.24 | 121.90 |
| 22 | AA | 1103 | C | O4'-C1'-N1 | 6.65 | 113.52 | 108.20 |
| 55 | BH | 148 | ARG | NE-CZ-NH1 | 6.65 | 123.63 | 120.30 |
| 57 | BA | 972 | A | C4-C5-C6 | -6.65 | 113.67 | 117.00 |
| 57 | BA | 1790 | C | N3-C2-O2 | -6.65 | 117.24 | 121.90 |
| 22 | AA | 642 | A | N1-C6-N6 | -6.65 | 114.61 | 118.60 |
| 57 | BA | 888 | C | N3-C2-O2 | -6.65 | 117.25 | 121.90 |
| 57 | BA | 1010 | A | C4-C5-C6 | -6.65 | 113.67 | 117.00 |
| 57 | BA | 2386 | A | C5-C6-N1 | 6.65 | 121.03 | 117.70 |
| 57 | BA | 2145 | C | N3-C2-O2 | -6.65 | 117.25 | 121.90 |
| 20 | AI | 84 | ARG | NE-CZ-NH1 | 6.65 | 123.62 | 120.30 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 849 | A | C4-C5-C6 | -6.65 | 113.68 | 117.00 |
| 57 | BA | 1084 | A | C4-C5-C6 | -6.65 | 113.68 | 117.00 |
| 22 | AA | 1051 | C | N3-C2-O2 | -6.65 | 117.25 | 121.90 |
| 57 | BA | 182 | A | C5-C6-N1 | 6.65 | 121.02 | 117.70 |
| 57 | BA | 1453 | A | C4-C5-C6 | -6.65 | 113.68 | 117.00 |
| 57 | BA | 2497 | A | C4-C5-C6 | -6.65 | 113.68 | 117.00 |
| 22 | AA | 58 | C | O4'-C1'-N1 | 6.64 | 113.52 | 108.20 |
| 57 | BA | 1690 | A | C5-C6-N1 | 6.64 | 121.02 | 117.70 |
| 57 | BA | 1837 | C | N3-C2-O2 | -6.64 | 117.25 | 121.90 |
| 57 | BA | 2451 | A | O4'-C1'-N9 | 6.64 | 113.52 | 108.20 |
| 22 | AA | 120 | A | C4-C5-C6 | -6.64 | 113.68 | 117.00 |
| 22 | AA | 545 | C | O4'-C1'-N1 | 6.64 | 113.51 | 108.20 |
| 22 | AA | 1019 | A | C4-C5-C6 | -6.64 | 113.68 | 117.00 |
| 57 | BA | 223 | A | C4-C5-C6 | -6.64 | 113.68 | 117.00 |
| 57 | BA | 454 | A | C5-C6-N1 | 6.64 | 121.02 | 117.70 |
| 57 | BA | 1393 | A | C4-C5-C6 | -6.64 | 113.68 | 117.00 |
| 57 | BA | 2407 | A | C4-C5-C6 | -6.64 | 113.68 | 117.00 |
| 57 | BA | 2426 | A | C4-C5-C6 | -6.64 | 113.68 | 117.00 |
| 57 | BA | 804 | A | C4-C5-C6 | -6.64 | 113.68 | 117.00 |
| 57 | BA | 905 | A | C4-C5-C6 | -6.64 | 113.68 | 117.00 |
| 22 | AA | 228 | A | C4-C5-C6 | -6.64 | 113.68 | 117.00 |
| 57 | BA | 2453 | A | C5-C6-N1 | 6.64 | 121.02 | 117.70 |
| 57 | BA | 2813 | A | C4-C5-C6 | -6.64 | 113.68 | 117.00 |
| 24 | A3 | 74 | A | C4-C5-C6 | -6.64 | 113.68 | 117.00 |
| 57 | BA | 1423 | G | O4'-C1'-N9 | 6.64 | 113.51 | 108.20 |
| 57 | BA | 1689 | A | C5-C6-N1 | 6.64 | 121.02 | 117.70 |
| 57 | BA | 91 | A | C4-C5-C6 | -6.64 | 113.68 | 117.00 |
| 57 | BA | 501 | A | N1-C6-N6 | -6.64 | 114.62 | 118.60 |
| 57 | BA | 602 | A | C4-C5-C6 | -6.64 | 113.68 | 117.00 |
| 57 | BA | 1735 | A | C4-C5-C6 | -6.64 | 113.68 | 117.00 |
| 22 | AA | 496 | A | O4'-C1'-N9 | 6.63 | 113.51 | 108.20 |
| 22 | AA | 1375 | A | N1-C6-N6 | -6.63 | 114.62 | 118.60 |
| 57 | BA | 1564 | C | N1-C2-O2 | 6.63 | 122.88 | 118.90 |
| 57 | BA | 1757 | A | C4-C5-C6 | -6.63 | 113.68 | 117.00 |
| 57 | BA | 1830 | C | N3-C2-O2 | -6.63 | 117.26 | 121.90 |
| 57 | BA | 2730 | C | O4'-C1'-N1 | 6.63 | 113.51 | 108.20 |
| 57 | BA | 1269 | A | C4-C5-C6 | -6.63 | 113.68 | 117.00 |
| 57 | BA | 402 | A | C5-C6-N1 | 6.63 | 121.02 | 117.70 |
| 57 | BA | 825 | A | C4-C5-C6 | -6.63 | 113.69 | 117.00 |
| 57 | BA | 1809 | A | N1-C6-N6 | -6.63 | 114.62 | 118.60 |
| 22 | AA | 560 | A | C4-C5-C6 | -6.63 | 113.69 | 117.00 |
| 57 | BA | 14 | A | C4-C5-C6 | -6.63 | 113.69 | 117.00 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 1263 | U | O4'-C1'-N1 | 6.63 | 113.50 | 108.20 |
| 57 | BA | 1321 | A | C4-C5-C6 | -6.63 | 113.69 | 117.00 |
| 57 | BA | 1754 | A | C4-C5-C6 | -6.63 | 113.69 | 117.00 |
| 57 | BA | 1783 | A | C4-C5-C6 | -6.63 | 113.69 | 117.00 |
| 57 | BA | 2385 | C | N3-C2-O2 | -6.63 | 117.26 | 121.90 |
| 57 | BA | 2743 | U | O4'-C1'-N1 | 6.63 | 113.50 | 108.20 |
| 22 | AA | 495 | A | C4-C5-C6 | -6.62 | 113.69 | 117.00 |
| 57 | BA | 177 | G | O4'-C1'-N9 | 6.62 | 113.50 | 108.20 |
| 22 | AA | 107 | G | N1-C6-O6 | -6.62 | 115.92 | 119.90 |
| 46 | B3 | 10 | ARG | NE-CZ-NH1 | -6.62 | 116.99 | 120.30 |
| 57 | BA | 892 | A | C4-C5-C6 | -6.62 | 113.69 | 117.00 |
| 57 | BA | 142 | A | C4-C5-C6 | -6.62 | 113.69 | 117.00 |
| 57 | BA | 2310 | C | N3-C2-O2 | -6.62 | 117.27 | 121.90 |
| 57 | BA | 2333 | A | C4-C5-C6 | -6.62 | 113.69 | 117.00 |
| 57 | BA | 478 | A | C5-C6-N1 | 6.62 | 121.01 | 117.70 |
| 57 | BA | 210 | C | O4'-C1'-N1 | 6.62 | 113.49 | 108.20 |
| 57 | BA | 928 | A | C4-C5-C6 | -6.62 | 113.69 | 117.00 |
| 57 | BA | 1568 | G | N1-C6-O6 | -6.62 | 115.93 | 119.90 |
| 19 | AH | 87 | ARG | NE-CZ-NH1 | 6.61 | 123.61 | 120.30 |
| 57 | BA | 761 | A | C4-C5-C6 | -6.61 | 113.69 | 117.00 |
| 57 | BA | 1892 | C | N3-C2-O2 | -6.61 | 117.27 | 121.90 |
| 22 | AA | 564 | C | O4'-C1'-N1 | 6.61 | 113.49 | 108.20 |
| 22 | AA | 718 | A | C4-C5-C6 | -6.61 | 113.69 | 117.00 |
| 57 | BA | 1938 | A | C4-C5-C6 | -6.61 | 113.69 | 117.00 |
| 22 | AA | 946 | A | C4-C5-C6 | -6.61 | 113.69 | 117.00 |
| 57 | BA | 2634 | A | C4-C5-C6 | -6.61 | 113.70 | 117.00 |
| 22 | AA | 1145 | A | C5-C6-N1 | 6.61 | 121.00 | 117.70 |
| 36 | BU | 2 | ARG | NE-CZ-NH2 | 6.61 | 123.60 | 120.30 |
| 57 | BA | 2340 | A | C4-C5-C6 | -6.61 | 113.70 | 117.00 |
| 22 | AA | 720 | C | N3-C2-O2 | -6.61 | 117.28 | 121.90 |
| 57 | BA | 59 | U | O4'-C1'-N1 | 6.61 | 113.48 | 108.20 |
| 57 | BA | 1705 | A | C4-C5-C6 | -6.61 | 113.70 | 117.00 |
| 22 | AA | 121 | U | C3'-C2'-C1' | 6.60 | 106.78 | 101.50 |
| 32 | BR | 45 | ARG | NE-CZ-NH1 | 6.60 | 123.60 | 120.30 |
| 57 | BA | 2347 | C | N1-C2-O2 | 6.60 | 122.86 | 118.90 |
| 22 | AA | 801 | U | O4'-C1'-N1 | 6.60 | 113.48 | 108.20 |
| 22 | AA | 1539 | C | N3-C2-O2 | -6.60 | 117.28 | 121.90 |
| 57 | BA | 1190 | G | O4'-C1'-N9 | 6.60 | 113.48 | 108.20 |
| 57 | BA | 1941 | C | N3-C2-O2 | -6.60 | 117.28 | 121.90 |
| 57 | BA | 203 | A | C4-C5-C6 | -6.60 | 113.70 | 117.00 |
| 57 | BA | 213 | A | C4-C5-C6 | -6.60 | 113.70 | 117.00 |
| 57 | BA | 1591 | A | C4-C5-C6 | -6.60 | 113.70 | 117.00 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 2101 | A | C4-C5-C6 | -6.60 | 113.70 | 117.00 |
| 22 | AA | 564 | C | N3-C2-O2 | -6.60 | 117.28 | 121.90 |
| 22 | AA | 1171 | A | O4'-C1'-N9 | 6.60 | 113.48 | 108.20 |
| 57 | BA | 2781 | A | C4-C5-C6 | -6.60 | 113.70 | 117.00 |
| 57 | BA | 821 | A | C4-C5-C6 | -6.60 | 113.70 | 117.00 |
| 57 | BA | 2494 | G | N1-C6-O6 | -6.60 | 115.94 | 119.90 |
| 24 | A3 | 40 | C | N1-C2-O2 | 6.59 | 122.86 | 118.90 |
| 36 | BU | 52 | ARG | NE-CZ-NH2 | -6.59 | 117.00 | 120.30 |
| 57 | BA | 2055 | C | N3-C2-O2 | -6.59 | 117.28 | 121.90 |
| 57 | BA | 2198 | A | O4'-C1'-N9 | 6.59 | 113.47 | 108.20 |
| 58 | Ba | 14 | U | O4'-C1'-N1 | 6.59 | 113.48 | 108.20 |
| 22 | AA | 715 | A | C5-C6-N1 | 6.59 | 121.00 | 117.70 |
| 57 | BA | 527 | C | N1-C2-O2 | 6.59 | 122.86 | 118.90 |
| 57 | BA | 2866 | U | O4'-C1'-N1 | 6.59 | 113.47 | 108.20 |
| 22 | AA | 1252 | A | C4-C5-C6 | -6.59 | 113.71 | 117.00 |
| 57 | BA | 1646 | C | N3-C2-O2 | -6.59 | 117.29 | 121.90 |
| 57 | BA | 2667 | C | N3-C2-O2 | -6.59 | 117.29 | 121.90 |
| 22 | AA | 1492 | A | C4-C5-C6 | -6.59 | 113.71 | 117.00 |
| 57 | BA | 1493 | C | N3-C2-O2 | -6.59 | 117.29 | 121.90 |
| 22 | AA | 1269 | A | C4-C5-C6 | -6.58 | 113.71 | 117.00 |
| 22 | AA | 1463 | U | O4'-C1'-N1 | 6.58 | 113.47 | 108.20 |
| 57 | BA | 1143 | A | C4-C5-C6 | -6.58 | 113.71 | 117.00 |
| 57 | BA | 2273 | A | C4-C5-C6 | -6.58 | 113.71 | 117.00 |
| 57 | BA | 2602 | A | O4'-C1'-N9 | 6.58 | 113.47 | 108.20 |
| 58 | Ba | 11 | C | N3-C2-O2 | -6.58 | 117.29 | 121.90 |
| 58 | Ba | 27 | C | O4'-C1'-N1 | 6.58 | 113.47 | 108.20 |
| 22 | AA | 1236 | A | C4-C5-C6 | -6.58 | 113.71 | 117.00 |
| 57 | BA | 948 | C | O4'-C1'-N1 | 6.58 | 113.47 | 108.20 |
| 57 | BA | 1167 | C | N1-C2-O2 | 6.58 | 122.85 | 118.90 |
| 57 | BA | 2179 | C | O4'-C1'-N1 | 6.58 | 113.47 | 108.20 |
| 57 | BA | 1301 | A | C4-C5-C6 | -6.58 | 113.71 | 117.00 |
| 11 | AB | 94 | ARG | NE-CZ-NH1 | 6.58 | 123.59 | 120.30 |
| 57 | BA | 1987 | A | C4-C5-C6 | -6.58 | 113.71 | 117.00 |
| 22 | AA | 338 | A | N1-C6-N6 | -6.58 | 114.65 | 118.60 |
| 22 | AA | 468 | A | C4-C5-C6 | -6.58 | 113.71 | 117.00 |
| 57 | BA | 2435 | A | C4-C5-C6 | -6.58 | 113.71 | 117.00 |
| 57 | BA | 16 | C | O4'-C1'-N1 | 6.58 | 113.46 | 108.20 |
| 57 | BA | 1352 | U | O4'-C1'-N1 | 6.58 | 113.46 | 108.20 |
| 22 | AA | 1513 | A | O4'-C1'-N9 | 6.57 | 113.46 | 108.20 |
| 35 | BD | 101 | ARG | NE-CZ-NH1 | 6.57 | 123.59 | 120.30 |
| 57 | BA | 471 | A | C5-C6-N1 | 6.57 | 120.99 | 117.70 |
| 22 | AA | 1170 | A | C4-C5-C6 | -6.57 | 113.71 | 117.00 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 925 | A | C4-C5-C6 | -6.57 | 113.72 | 117.00 |
| 57 | BA | 1069 | A | C4-C5-C6 | -6.57 | 113.72 | 117.00 |
| 57 | BA | 1654 | A | N1-C6-N6 | -6.57 | 114.66 | 118.60 |
| 22 | AA | 1226 | C | N3-C2-O2 | -6.57 | 117.30 | 121.90 |
| 22 | AA | 1342 | C | O4'-C1'-N1 | 6.57 | 113.45 | 108.20 |
| 42 | B0 | 13 | ARG | NH1-CZ-NH2 | -6.57 | 112.18 | 119.40 |
| 57 | BA | 447 | A | C4-C5-C6 | -6.57 | 113.72 | 117.00 |
| 57 | BA | 1165 | A | C4-C5-C6 | -6.57 | 113.72 | 117.00 |
| 57 | BA | 1276 | A | C4-C5-C6 | -6.57 | 113.72 | 117.00 |
| 57 | BA | 1438 | U | O4'-C1'-N1 | 6.57 | 113.45 | 108.20 |
| 22 | AA | 848 | C | O4'-C1'-N1 | 6.57 | 113.45 | 108.20 |
| 57 | BA | 354 | A | C4-C5-C6 | -6.57 | 113.72 | 117.00 |
| 57 | BA | 1323 | C | N1-C2-O2 | 6.57 | 122.84 | 118.90 |
| 57 | BA | 1583 | A | C4-C5-C6 | -6.57 | 113.72 | 117.00 |
| 57 | BA | 2276 | G | O4'-C1'-N9 | 6.57 | 113.45 | 108.20 |
| 57 | BA | 2366 | A | C4-C5-C6 | -6.57 | 113.72 | 117.00 |
| 22 | AA | 288 | A | C4-C5-C6 | -6.56 | 113.72 | 117.00 |
| 57 | BA | 508 | A | C4-C5-C6 | -6.56 | 113.72 | 117.00 |
| 57 | BA | 525 | U | O4'-C1'-N1 | 6.56 | 113.45 | 108.20 |
| 57 | BA | 2875 | C | O4'-C1'-N1 | 6.56 | 113.45 | 108.20 |
| 58 | Ba | 119 | A | C4-C5-C6 | -6.56 | 113.72 | 117.00 |
| 57 | BA | 722 | A | C4-C5-C6 | -6.56 | 113.72 | 117.00 |
| 57 | BA | 1440 | U | O4'-C1'-N1 | 6.56 | 113.45 | 108.20 |
| 57 | BA | 166 | U | O4'-C1'-N1 | 6.56 | 113.45 | 108.20 |
| 57 | BA | 575 | A | C5-C6-N1 | 6.56 | 120.98 | 117.70 |
| 57 | BA | 1679 | A | C4-C5-C6 | -6.56 | 113.72 | 117.00 |
| 57 | BA | 2394 | C | O4'-C1'-N1 | 6.56 | 113.45 | 108.20 |
| 57 | BA | 2478 | A | C4-C5-C6 | -6.56 | 113.72 | 117.00 |
| 22 | AA | 470 | C | N3-C2-O2 | -6.56 | 117.31 | 121.90 |
| 57 | BA | 599 | A | N1-C6-N6 | -6.56 | 114.67 | 118.60 |
| 57 | BA | 2837 | A | C4-C5-C6 | -6.56 | 113.72 | 117.00 |
| 38 | BW | 84 | ARG | NE-CZ-NH2 | 6.56 | 123.58 | 120.30 |
| 22 | AA | 400 | C | N1-C2-O2 | 6.55 | 122.83 | 118.90 |
| 22 | AA | 518 | C | N3-C2-O2 | -6.55 | 117.31 | 121.90 |
| 22 | AA | 630 | A | C4-C5-C6 | -6.55 | 113.72 | 117.00 |
| 57 | BA | 721 | A | N1-C6-N6 | -6.55 | 114.67 | 118.60 |
| 57 | BA | 1152 | C | O4'-C1'-N1 | 6.55 | 113.44 | 108.20 |
| 22 | AA | 1520 | C | O4'-C1'-N1 | 6.55 | 113.44 | 108.20 |
| 24 | A3 | 25 | U | O4'-C1'-N1 | 6.55 | 113.44 | 108.20 |
| 58 | Ba | 108 | A | N1-C6-N6 | -6.55 | 114.67 | 118.60 |
| 22 | AA | 19 | A | C4-C5-C6 | -6.55 | 113.72 | 117.00 |
| 22 | AA | 72 | A | N1-C6-N6 | -6.55 | 114.67 | 118.60 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|---|---|---|---|---|---|---|---|
| 22 | AA | 430 | A | C4-C5-C6 | -6.55 | 113.72 | 117.00 |
| 57 | BA | 233 | A | N1-C6-N6 | -6.55 | 114.67 | 118.60 |
| 57 | BA | 2097 | A | C4-C5-C6 | -6.55 | 113.72 | 117.00 |
| 57 | BA | 2176 | A | C4-C5-C6 | -6.55 | 113.72 | 117.00 |
| 57 | BA | 2577 | A | C4-C5-C6 | -6.55 | 113.72 | 117.00 |
| 22 | AA | 270 | A | C4-C5-C6 | -6.55 | 113.72 | 117.00 |
| 22 | AA | 1468 | A | C5-C6-N1 | 6.55 | 120.97 | 117.70 |
| 57 | BA | 1070 | A | O4'-C1'-N9 | 6.55 | 113.44 | 108.20 |
| 57 | BA | 992 | C | N3-C2-O2 | -6.55 | 117.32 | 121.90 |
| 57 | BA | 1754 | A | N1-C6-N6 | -6.55 | 114.67 | 118.60 |
| 22 | AA | 349 | A | C4-C5-C6 | -6.55 | 113.73 | 117.00 |
| 22 | AA | 535 | A | C4-C5-C6 | -6.55 | 113.73 | 117.00 |
| 22 | AA | 872 | A | C1'-O4'-C4' | -6.55 | 104.66 | 109.90 |
| 22 | AA | 1005 | A | C4-C5-C6 | -6.55 | 113.73 | 117.00 |
| 22 | AA | 1171 | A | C4-C5-C6 | -6.55 | 113.73 | 117.00 |
| 57 | BA | 2284 | A | C4-C5-C6 | -6.55 | 113.73 | 117.00 |
| 57 | BA | 528 | A | C4-C5-C6 | -6.54 | 113.73 | 117.00 |
| 51 | B8 | 41 | ARG | NE-CZ-NH2 | 6.54 | 123.57 | 120.30 |
| 57 | BA | 86 | G | O4'-C1'-N9 | 6.54 | 113.44 | 108.20 |
| 22 | AA | 43 | C | N3-C2-O2 | -6.54 | 117.32 | 121.90 |
| 22 | AA | 1036 | A | C4-C5-C6 | -6.54 | 113.73 | 117.00 |
| 22 | AA | 1261 | A | C4-C5-C6 | -6.54 | 113.73 | 117.00 |
| 22 | AA | 1437 | A | C4-C5-C6 | -6.54 | 113.73 | 117.00 |
| 57 | BA | 844 | A | C4-C5-C6 | -6.54 | 113.73 | 117.00 |
| 22 | AA | 969 | A | C4-C5-C6 | -6.54 | 113.73 | 117.00 |
| 57 | BA | 779 | U | O4'-C1'-N1 | 6.54 | 113.43 | 108.20 |
| 57 | BA | 1887 | C | N3-C2-O2 | -6.54 | 117.32 | 121.90 |
| 22 | AA | 563 | A | C5-C6-N1 | 6.54 | 120.97 | 117.70 |
| 57 | BA | 1297 | C | N3-C2-O2 | -6.54 | 117.32 | 121.90 |
| 22 | AA | 676 | A | C4-C5-C6 | -6.54 | 113.73 | 117.00 |
| 22 | AA | 702 | A | C4-C5-C6 | -6.54 | 113.73 | 117.00 |
| 57 | BA | 416 | U | O4'-C1'-N1 | 6.54 | 113.43 | 108.20 |
| 57 | BA | 497 | A | C4-C5-C6 | -6.54 | 113.73 | 117.00 |
| 57 | BA | 1090 | A | C4-C5-C6 | -6.54 | 113.73 | 117.00 |
| 57 | BA | 2063 | C | N3-C4-C5 | 6.54 | 124.51 | 121.90 |
| 14 | AC | 58 | ARG | NE-CZ-NH1 | 6.53 | 123.57 | 120.30 |
| 57 | BA | 249 | C | N1-C2-O2 | 6.53 | 122.82 | 118.90 |
| 57 | BA | 257 | C | N3-C2-O2 | -6.53 | 117.33 | 121.90 |
| 57 | BA | 890 | C | N3-C2-O2 | -6.53 | 117.33 | 121.90 |
| 57 | BA | 1866 | A | C5-C6-N1 | 6.53 | 120.97 | 117.70 |
| 22 | AA | 1413 | A | C4-C5-C6 | -6.53 | 113.73 | 117.00 |
| 22 | AA | 906 | A | C4-C5-C6 | -6.53 | 113.73 | 117.00 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 2247 | A | C4-C5-C6 | -6.53 | 113.73 | 117.00 |
| 57 | BA | 484 | C | N3-C2-O2 | -6.53 | 117.33 | 121.90 |
| 57 | BA | 829 | A | C4-C5-C6 | -6.53 | 113.74 | 117.00 |
| 22 | AA | 754 | C | N1-C2-O2 | 6.53 | 122.82 | 118.90 |
| 22 | AA | 819 | A | C4-C5-C6 | -6.53 | 113.74 | 117.00 |
| 22 | AA | 1483 | A | C5-C6-N1 | 6.53 | 120.96 | 117.70 |
| 57 | BA | 2183 | A | C4-C5-C6 | -6.53 | 113.74 | 117.00 |
| 14 | AC | 228 | ARG | NE-CZ-NH1 | 6.53 | 123.56 | 120.30 |
| 22 | AA | 949 | A | C5-C6-N1 | 6.53 | 120.96 | 117.70 |
| 22 | AA | 1042 | A | C4-C5-C6 | -6.53 | 113.74 | 117.00 |
| 57 | BA | 2059 | A | C4-C5-C6 | -6.53 | 113.74 | 117.00 |
| 22 | AA | 54 | C | N3-C2-O2 | -6.52 | 117.33 | 121.90 |
| 57 | BA | 1599 | U | O4'-C1'-N1 | 6.52 | 113.42 | 108.20 |
| 57 | BA | 2432 | A | C4-C5-C6 | -6.52 | 113.74 | 117.00 |
| 57 | BA | 152 | A | C4-C5-C6 | -6.52 | 113.74 | 117.00 |
| 57 | BA | 987 | C | O4'-C1'-N1 | 6.52 | 113.42 | 108.20 |
| 57 | BA | 1749 | A | C4-C5-C6 | -6.52 | 113.74 | 117.00 |
| 58 | Ba | 110 | C | O4'-C1'-N1 | 6.52 | 113.42 | 108.20 |
| 13 | AU | 46 | ARG | NE-CZ-NH1 | 6.52 | 123.56 | 120.30 |
| 22 | AA | 1185 | G | N1-C6-O6 | -6.52 | 115.99 | 119.90 |
| 22 | AA | 1497 | G | O4'-C1'-N9 | 6.52 | 113.42 | 108.20 |
| 57 | BA | 655 | A | N1-C6-N6 | -6.52 | 114.69 | 118.60 |
| 57 | BA | 878 | A | C4-C5-C6 | -6.52 | 113.74 | 117.00 |
| 57 | BA | 1098 | A | C5-C6-N1 | 6.52 | 120.96 | 117.70 |
| 57 | BA | 1257 | C | N3-C2-O2 | -6.52 | 117.34 | 121.90 |
| 57 | BA | 1431 | A | N1-C6-N6 | -6.52 | 114.69 | 118.60 |
| 58 | Ba | 70 | C | O4'-C1'-N1 | 6.52 | 113.42 | 108.20 |
| 9 | AR | 52 | ARG | NE-CZ-NH1 | 6.52 | 123.56 | 120.30 |
| 22 | AA | 65 | A | C4-C5-C6 | -6.52 | 113.74 | 117.00 |
| 22 | AA | 533 | A | C4-C5-C6 | -6.52 | 113.74 | 117.00 |
| 57 | BA | 522 | A | C4-C5-C6 | -6.52 | 113.74 | 117.00 |
| 57 | BA | 1512 | C | O4'-C1'-N1 | 6.52 | 113.41 | 108.20 |
| 31 | BQ | 55 | ARG | NE-CZ-NH2 | 6.52 | 123.56 | 120.30 |
| 57 | BA | 348 | A | C4-C5-C6 | -6.52 | 113.74 | 117.00 |
| 57 | BA | 71 | A | C4-C5-C6 | -6.51 | 113.74 | 117.00 |
| 57 | BA | 237 | C | N1-C2-O2 | 6.51 | 122.81 | 118.90 |
| 57 | BA | 501 | A | C4-C5-C6 | -6.51 | 113.74 | 117.00 |
| 57 | BA | 2336 | A | C4-C5-C6 | -6.51 | 113.74 | 117.00 |
| 22 | AA | 1431 | A | C4-C5-C6 | -6.51 | 113.74 | 117.00 |
| 22 | AA | 675 | A | C4-C5-C6 | -6.51 | 113.74 | 117.00 |
| 22 | AA | 1238 | A | C4-C5-C6 | -6.51 | 113.74 | 117.00 |
| 22 | AA | 281 | G | O4'-C1'-N9 | 6.51 | 113.41 | 108.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | A3 | 17 | C | N3-C2-O2 | -6.51 | 117.34 | 121.90 |
| 57 | BA | 1535 | A | C4-C5-C6 | -6.51 | 113.75 | 117.00 |
| 57 | BA | 1124 | G | O4'-C1'-N9 | 6.51 | 113.41 | 108.20 |
| 57 | BA | 2563 | U | O4'-C1'-N1 | 6.51 | 113.41 | 108.20 |
| 22 | AA | 837 | U | O4'-C1'-N1 | 6.51 | 113.41 | 108.20 |
| 57 | BA | 1609 | A | C4-C5-C6 | -6.51 | 113.75 | 117.00 |
| 57 | BA | 2076 | U | N3-C2-O2 | -6.51 | 117.65 | 122.20 |
| 22 | AA | 300 | A | C4-C5-C6 | -6.50 | 113.75 | 117.00 |
| 57 | BA | 74 | A | C4-C5-C6 | -6.50 | 113.75 | 117.00 |
| 57 | BA | 456 | C | N3-C2-O2 | -6.50 | 117.35 | 121.90 |
| 57 | BA | 1611 | C | N1-C2-O2 | 6.50 | 122.80 | 118.90 |
| 57 | BA | 2239 | G | N1-C6-O6 | -6.50 | 116.00 | 119.90 |
| 57 | BA | 2797 | U | N3-C2-O2 | -6.50 | 117.65 | 122.20 |
| 22 | AA | 519 | C | C5'-C4'-C3' | -6.50 | 105.60 | 116.00 |
| 22 | AA | 689 | C | O4'-C1'-N1 | 6.50 | 113.40 | 108.20 |
| 22 | AA | 1145 | A | C4-C5-C6 | -6.50 | 113.75 | 117.00 |
| 57 | BA | 429 | A | C5-C6-N1 | 6.50 | 120.95 | 117.70 |
| 57 | BA | 613 | A | C4-C5-C6 | -6.50 | 113.75 | 117.00 |
| 57 | BA | 672 | C | N1-C2-O2 | 6.50 | 122.80 | 118.90 |
| 57 | BA | 1654 | A | C4-C5-C6 | -6.50 | 113.75 | 117.00 |
| 57 | BA | 2842 | G | O4'-C1'-N9 | 6.50 | 113.40 | 108.20 |
| 22 | AA | 176 | C | N1-C2-O2 | 6.50 | 122.80 | 118.90 |
| 22 | AA | 546 | A | C4-C5-C6 | -6.50 | 113.75 | 117.00 |
| 22 | AA | 796 | C | O4'-C1'-N1 | 6.50 | 113.40 | 108.20 |
| 57 | BA | 299 | A | C4-C5-C6 | -6.50 | 113.75 | 117.00 |
| 22 | AA | 1213 | A | C5-C6-N1 | 6.50 | 120.95 | 117.70 |
| 35 | BD | 268 | ARG | NE-CZ-NH1 | 6.50 | 123.55 | 120.30 |
| 57 | BA | 881 | G | N1-C6-O6 | -6.50 | 116.00 | 119.90 |
| 57 | BA | 1204 | A | O4'-C1'-N9 | 6.50 | 113.40 | 108.20 |
| 57 | BA | 2429 | G | O4'-C1'-N9 | 6.50 | 113.40 | 108.20 |
| 22 | AA | 77 | A | C4-C5-C6 | -6.50 | 113.75 | 117.00 |
| 22 | AA | 335 | C | N3-C2-O2 | -6.50 | 117.35 | 121.90 |
| 22 | AA | 501 | C | N1-C2-O2 | 6.50 | 122.80 | 118.90 |
| 22 | AA | 825 | A | C4-C5-C6 | -6.50 | 113.75 | 117.00 |
| 57 | BA | 344 | A | C4-C5-C6 | -6.50 | 113.75 | 117.00 |
| 57 | BA | 908 | C | O4'-C1'-N1 | 6.50 | 113.40 | 108.20 |
| 57 | BA | 444 | C | O4'-C1'-N1 | 6.50 | 113.40 | 108.20 |
| 22 | AA | 7 | A | C4-C5-C6 | -6.49 | 113.75 | 117.00 |
| 22 | AA | 48 | C | O4'-C1'-N1 | 6.49 | 113.39 | 108.20 |
| 22 | AA | 964 | A | C4-C5-C6 | -6.49 | 113.75 | 117.00 |
| 24 | A3 | 47 | A | C4-C5-C6 | -6.49 | 113.75 | 117.00 |
| 57 | BA | 262 | A | C4-C5-C6 | -6.49 | 113.75 | 117.00 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 732 | C | O4'-C1'-N1 | 6.49 | 113.39 | 108.20 |
| 57 | BA | 1978 | A | C4-C5-C6 | -6.49 | 113.75 | 117.00 |
| 57 | BA | 2755 | C | O4'-C1'-N1 | 6.49 | 113.39 | 108.20 |
| 22 | AA | 613 | C | N3-C2-O2 | -6.49 | 117.36 | 121.90 |
| 57 | BA | 2513 | A | C4-C5-C6 | -6.49 | 113.75 | 117.00 |
| 22 | AA | 1096 | C | N1-C2-O2 | 6.49 | 122.79 | 118.90 |
| 22 | AA | 1117 | A | C4-C5-C6 | -6.49 | 113.75 | 117.00 |
| 57 | BA | 201 | C | O4'-C1'-N1 | 6.49 | 113.39 | 108.20 |
| 57 | BA | 716 | A | C4-C5-C6 | -6.49 | 113.75 | 117.00 |
| 22 | AA | 312 | C | N1-C2-O2 | 6.49 | 122.79 | 118.90 |
| 22 | AA | 673 | A | C4-C5-C6 | -6.49 | 113.76 | 117.00 |
| 22 | AA | 985 | C | N3-C2-O2 | -6.49 | 117.36 | 121.90 |
| 22 | AA | 1493 | A | C4-C5-C6 | -6.49 | 113.76 | 117.00 |
| 57 | BA | 131 | A | C4-C5-C6 | -6.49 | 113.76 | 117.00 |
| 57 | BA | 2598 | A | C4-C5-C6 | -6.49 | 113.75 | 117.00 |
| 24 | A3 | 59 | A | C4-C5-C6 | -6.49 | 113.76 | 117.00 |
| 28 | BN | 116 | ARG | NE-CZ-NH1 | 6.49 | 123.54 | 120.30 |
| 22 | AA | 381 | C | N1-C2-O2 | 6.49 | 122.79 | 118.90 |
| 38 | BW | 88 | ARG | NE-CZ-NH1 | -6.49 | 117.06 | 120.30 |
| 57 | BA | 1603 | A | C4-C5-C6 | -6.49 | 113.76 | 117.00 |
| 37 | BV | 79 | ARG | NE-CZ-NH2 | 6.48 | 123.54 | 120.30 |
| 57 | BA | 99 | U | N3-C2-O2 | -6.48 | 117.66 | 122.20 |
| 22 | AA | 520 | A | C5-C6-N1 | 6.48 | 120.94 | 117.70 |
| 28 | BN | 96 | ARG | NE-CZ-NH2 | 6.48 | 123.54 | 120.30 |
| 39 | BX | 69 | ARG | NE-CZ-NH1 | 6.48 | 123.54 | 120.30 |
| 57 | BA | 391 | A | C4-C5-C6 | -6.48 | 113.76 | 117.00 |
| 22 | AA | 522 | C | N1-C2-O2 | 6.48 | 122.79 | 118.90 |
| 22 | AA | 784 | A | C4-C5-C6 | -6.48 | 113.76 | 117.00 |
| 57 | BA | 415 | A | C4-C5-C6 | -6.48 | 113.76 | 117.00 |
| 57 | BA | 1189 | A | C4-C5-C6 | -6.48 | 113.76 | 117.00 |
| 57 | BA | 1802 | A | C5-C6-N1 | 6.48 | 120.94 | 117.70 |
| 57 | BA | 2205 | A | C4-C5-C6 | -6.48 | 113.76 | 117.00 |
| 13 | AU | 34 | ARG | NH1-CZ-NH2 | -6.48 | 112.27 | 119.40 |
| 57 | BA | 1870 | C | N3-C2-O2 | -6.48 | 117.36 | 121.90 |
| 22 | AA | 223 | A | C4-C5-C6 | -6.48 | 113.76 | 117.00 |
| 22 | AA | 314 | C | N3-C2-O2 | -6.48 | 117.37 | 121.90 |
| 51 | B8 | 29 | ARG | NE-CZ-NH2 | 6.48 | 123.54 | 120.30 |
| 57 | BA | 426 | C | N1-C2-O2 | 6.48 | 122.79 | 118.90 |
| 57 | BA | 1495 | A | C4-C5-C6 | -6.48 | 113.76 | 117.00 |
| 57 | BA | 1997 | C | N1-C2-O2 | 6.48 | 122.79 | 118.90 |
| 57 | BA | 2499 | C | N3-C2-O2 | -6.48 | 117.37 | 121.90 |
| 53 | BF | 114 | ARG | NE-CZ-NH1 | 6.48 | 123.54 | 120.30 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 38 | A | C4-C5-C6 | -6.48 | 113.76 | 117.00 |
| 57 | BA | 2666 | C | O4'-C1'-N1 | 6.48 | 113.38 | 108.20 |
| 22 | AA | 234 | C | O4'-C1'-N1 | 6.47 | 113.38 | 108.20 |
| 23 | A2 | 46 | C | N3-C2-O2 | -6.47 | 117.37 | 121.90 |
| 57 | BA | 1677 | A | C4-C5-C6 | -6.47 | 113.76 | 117.00 |
| 57 | BA | 2261 | C | N3-C2-O2 | -6.47 | 117.37 | 121.90 |
| 57 | BA | 2672 | U | O4'-C1'-N1 | 6.47 | 113.38 | 108.20 |
| 22 | AA | 296 | U | O4'-C1'-N1 | 6.47 | 113.38 | 108.20 |
| 22 | AA | 862 | C | N1-C2-O2 | 6.47 | 122.78 | 118.90 |
| 57 | BA | 37 | C | O4'-C1'-N1 | 6.47 | 113.38 | 108.20 |
| 57 | BA | 975 | A | C4-C5-C6 | -6.47 | 113.76 | 117.00 |
| 22 | AA | 195 | A | C4-C5-C6 | -6.47 | 113.77 | 117.00 |
| 22 | AA | 53 | A | C4-C5-C6 | -6.47 | 113.77 | 117.00 |
| 22 | AA | 1196 | A | C4-C5-C6 | -6.47 | 113.77 | 117.00 |
| 57 | BA | 1219 | U | O4'-C1'-N1 | 6.47 | 113.38 | 108.20 |
| 57 | BA | 2133 | G | N3-C4-C5 | -6.47 | 125.36 | 128.60 |
| 57 | BA | 118 | A | C4-C5-C6 | -6.47 | 113.77 | 117.00 |
| 57 | BA | 206 | U | O4'-C1'-N1 | 6.47 | 113.37 | 108.20 |
| 57 | BA | 320 | A | C4-C5-C6 | -6.47 | 113.77 | 117.00 |
| 57 | BA | 56 | A | C4-C5-C6 | -6.47 | 113.77 | 117.00 |
| 57 | BA | 127 | A | C4-C5-C6 | -6.47 | 113.77 | 117.00 |
| 57 | BA | 657 | U | O4'-C1'-N1 | 6.47 | 113.37 | 108.20 |
| 57 | BA | 1919 | A | C4-C5-C6 | -6.46 | 113.77 | 117.00 |
| 57 | BA | 2465 | C | O4'-C1'-N1 | 6.46 | 113.37 | 108.20 |
| 22 | AA | 648 | A | C4-C5-C6 | -6.46 | 113.77 | 117.00 |
| 22 | AA | 340 | U | O4'-C1'-N1 | 6.46 | 113.37 | 108.20 |
| 22 | AA | 1508 | A | N1-C6-N6 | -6.46 | 114.72 | 118.60 |
| 58 | Ba | 57 | A | C5-C6-N1 | 6.46 | 120.93 | 117.70 |
| 22 | AA | 1004 | A | C4-C5-C6 | -6.46 | 113.77 | 117.00 |
| 57 | BA | 646 | U | O4'-C1'-N1 | 6.46 | 113.37 | 108.20 |
| 57 | BA | 1571 | A | C5-C6-N1 | 6.46 | 120.93 | 117.70 |
| 20 | AI | 122 | ARG | NE-CZ-NH2 | -6.46 | 117.07 | 120.30 |
| 22 | AA | 98 | A | C4-C5-C6 | -6.46 | 113.77 | 117.00 |
| 57 | BA | 639 | U | O4'-C1'-N1 | 6.46 | 113.37 | 108.20 |
| 57 | BA | 1525 | A | C5-C6-N1 | 6.46 | 120.93 | 117.70 |
| 22 | AA | 655 | A | C4-C5-C6 | -6.46 | 113.77 | 117.00 |
| 22 | AA | 1357 | A | N1-C6-N6 | -6.46 | 114.73 | 118.60 |
| 51 | B8 | 1 | PRO | CA-N-CD | -6.46 | 102.46 | 111.50 |
| 57 | BA | 82 | U | O4'-C1'-N1 | 6.46 | 113.37 | 108.20 |
| 57 | BA | 2462 | C | N3-C2-O2 | -6.46 | 117.38 | 121.90 |
| 22 | AA | 496 | A | C1'-O4'-C4' | -6.46 | 104.74 | 109.90 |
| 57 | BA | 2175 | C | O4'-C1'-N1 | 6.45 | 113.36 | 108.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 2459 | A | N1-C6-N6 | -6.45 | 114.73 | 118.60 |
| 57 | BA | 2487 | G | O4'-C1'-N9 | 6.45 | 113.36 | 108.20 |
| 22 | AA | 959 | A | C4-C5-C6 | -6.45 | 113.78 | 117.00 |
| 22 | AA | 1074 | G | N1-C6-O6 | -6.45 | 116.03 | 119.90 |
| 57 | BA | 233 | A | C4-C5-C6 | -6.45 | 113.77 | 117.00 |
| 57 | BA | 1295 | C | N3-C2-O2 | -6.45 | 117.38 | 121.90 |
| 57 | BA | 1700 | A | C4-C5-C6 | -6.45 | 113.77 | 117.00 |
| 57 | BA | 2283 | C | O4'-C1'-N1 | 6.45 | 113.36 | 108.20 |
| 57 | BA | 2359 | C | N3-C2-O2 | -6.45 | 117.39 | 121.90 |
| 22 | AA | 459 | A | C5-C6-N1 | 6.45 | 120.92 | 117.70 |
| 22 | AA | 1262 | C | N3-C2-O2 | -6.45 | 117.39 | 121.90 |
| 22 | AA | 1500 | A | C4-C5-C6 | -6.45 | 113.78 | 117.00 |
| 57 | BA | 347 | A | C5-C6-N1 | 6.45 | 120.92 | 117.70 |
| 57 | BA | 2104 | C | N3-C2-O2 | -6.45 | 117.39 | 121.90 |
| 35 | BD | 270 | ARG | NE-CZ-NH1 | 6.45 | 123.52 | 120.30 |
| 57 | BA | 176 | A | C4-C5-C6 | -6.45 | 113.78 | 117.00 |
| 57 | BA | 2007 | U | O4'-C1'-N1 | 6.45 | 113.36 | 108.20 |
| 57 | BA | 2386 | A | C4-C5-C6 | -6.45 | 113.78 | 117.00 |
| 57 | BA | 172 | A | C4-C5-C6 | -6.44 | 113.78 | 117.00 |
| 57 | BA | 920 | A | C4-C5-C6 | -6.44 | 113.78 | 117.00 |
| 57 | BA | 1009 | A | C4-C5-C6 | -6.44 | 113.78 | 117.00 |
| 57 | BA | 1433 | A | C4-C5-C6 | -6.44 | 113.78 | 117.00 |
| 57 | BA | 2196 | C | N1-C2-O2 | 6.44 | 122.77 | 118.90 |
| 57 | BA | 2601 | C | N3-C2-O2 | -6.44 | 117.39 | 121.90 |
| 57 | BA | 116 | C | O4'-C1'-N1 | 6.44 | 113.35 | 108.20 |
| 57 | BA | 1221 | C | O4'-C1'-N1 | 6.44 | 113.35 | 108.20 |
| 57 | BA | 2031 | A | C4-C5-C6 | -6.44 | 113.78 | 117.00 |
| 22 | AA | 882 | C | O4'-C1'-N1 | 6.44 | 113.35 | 108.20 |
| 57 | BA | 163 | C | N3-C2-O2 | -6.44 | 117.39 | 121.90 |
| 57 | BA | 240 | C | N3-C2-O2 | -6.44 | 117.39 | 121.90 |
| 57 | BA | 311 | A | C4-C5-C6 | -6.44 | 113.78 | 117.00 |
| 57 | BA | 889 | C | N3-C2-O2 | -6.44 | 117.39 | 121.90 |
| 57 | BA | 1558 | C | N3-C2-O2 | -6.44 | 117.39 | 121.90 |
| 57 | BA | 1890 | A | C4-C5-C6 | -6.44 | 113.78 | 117.00 |
| 57 | BA | 2773 | C | O4'-C1'-N1 | 6.44 | 113.35 | 108.20 |
| 57 | BA | 754 | U | O4'-C1'-N1 | 6.43 | 113.35 | 108.20 |
| 57 | BA | 1810 | A | C4-C5-C6 | -6.43 | 113.78 | 117.00 |
| 3 | AL | 11 | ARG | NE-CZ-NH1 | 6.43 | 123.52 | 120.30 |
| 57 | BA | 444 | C | N3-C2-O2 | -6.43 | 117.40 | 121.90 |
| 57 | BA | 1275 | A | C4-C5-C6 | -6.43 | 113.78 | 117.00 |
| 57 | BA | 1803 | A | C4-C5-C6 | -6.43 | 113.78 | 117.00 |
| 57 | BA | 2047 | C | N3-C2-O2 | -6.43 | 117.40 | 121.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 1342 | A | C4-C5-C6 | -6.43 | 113.78 | 117.00 |
| 22 | AA | 263 | A | C4-C5-C6 | -6.43 | 113.78 | 117.00 |
| 22 | AA | 703 | G | O4'-C1'-N9 | 6.43 | 113.34 | 108.20 |
| 22 | AA | 893 | C | N3-C2-O2 | -6.43 | 117.40 | 121.90 |
| 22 | AA | 1542 | A | C4-C5-C6 | -6.43 | 113.78 | 117.00 |
| 57 | BA | 1375 | U | O4'-C1'-N1 | 6.43 | 113.34 | 108.20 |
| 57 | BA | 2028 | U | O4'-C1'-N1 | 6.43 | 113.34 | 108.20 |
| 45 | BE | 77 | ARG | NE-CZ-NH2 | 6.43 | 123.51 | 120.30 |
| 57 | BA | 1597 | A | C4-C5-C6 | -6.43 | 113.79 | 117.00 |
| 57 | BA | 1772 | A | C4'-C3'-C2' | -6.43 | 96.17 | 102.60 |
| 22 | AA | 344 | A | C4-C5-C6 | -6.43 | 113.79 | 117.00 |
| 22 | AA | 687 | A | C5-C6-N1 | 6.43 | 120.91 | 117.70 |
| 22 | AA | 1101 | A | N1-C6-N6 | -6.43 | 114.74 | 118.60 |
| 22 | AA | 1480 | A | C4-C5-C6 | -6.43 | 113.79 | 117.00 |
| 22 | AA | 119 | A | C4-C5-C6 | -6.42 | 113.79 | 117.00 |
| 22 | AA | 1382 | C | N3-C4-C5 | 6.42 | 124.47 | 121.90 |
| 22 | AA | 1451 | U | O4'-C1'-N1 | 6.42 | 113.34 | 108.20 |
| 45 | BE | 128 | ARG | NH1-CZ-NH2 | -6.42 | 112.33 | 119.40 |
| 57 | BA | 1047 | G | O4'-C1'-N9 | 6.42 | 113.34 | 108.20 |
| 57 | BA | 1632 | A | C4-C5-C6 | -6.42 | 113.79 | 117.00 |
| 57 | BA | 2342 | C | N1-C2-O2 | 6.42 | 122.75 | 118.90 |
| 57 | BA | 832 | U | O4'-C1'-N1 | 6.42 | 113.34 | 108.20 |
| 57 | BA | 2564 | A | C4-C5-C6 | -6.42 | 113.79 | 117.00 |
| 22 | AA | 110 | C | N3-C2-O2 | -6.42 | 117.41 | 121.90 |
| 57 | BA | 1308 | A | C4-C5-C6 | -6.42 | 113.79 | 117.00 |
| 57 | BA | 1028 | A | C4-C5-C6 | -6.42 | 113.79 | 117.00 |
| 57 | BA | 717 | C | N3-C2-O2 | -6.42 | 117.41 | 121.90 |
| 57 | BA | 1610 | A | C4-C5-C6 | -6.42 | 113.79 | 117.00 |
| 57 | BA | 1644 | C | N3-C2-O2 | -6.42 | 117.41 | 121.90 |
| 57 | BA | 2114 | A | C4-C5-C6 | -6.42 | 113.79 | 117.00 |
| 22 | AA | 787 | A | C4-C5-C6 | -6.42 | 113.79 | 117.00 |
| 22 | AA | 999 | C | N3-C2-O2 | -6.42 | 117.41 | 121.90 |
| 22 | AA | 1403 | C | N3-C2-O2 | -6.42 | 117.41 | 121.90 |
| 57 | BA | 590 | A | C4-C5-C6 | -6.42 | 113.79 | 117.00 |
| 57 | BA | 1565 | C | N3-C2-O2 | -6.42 | 117.41 | 121.90 |
| 22 | AA | 307 | C | N3-C2-O2 | -6.41 | 117.41 | 121.90 |
| 24 | A3 | 58 | A | C4-C5-C6 | -6.41 | 113.79 | 117.00 |
| 57 | BA | 440 | C | N1-C2-O2 | 6.41 | 122.75 | 118.90 |
| 57 | BA | 742 | A | C4-C5-C6 | -6.41 | 113.79 | 117.00 |
| 35 | BD | 62 | ARG | NE-CZ-NH1 | 6.41 | 123.50 | 120.30 |
| 57 | BA | 300 | A | C4-C5-C6 | -6.41 | 113.79 | 117.00 |
| 57 | BA | 1760 | C | N3-C2-O2 | -6.41 | 117.41 | 121.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 2119 | A | C4-C5-C6 | -6.41 | 113.80 | 117.00 |
| 57 | BA | 2424 | C | C1'-O4'-C4' | -6.41 | 104.77 | 109.90 |
| 57 | BA | 2511 | U | O4'-C1'-N1 | 6.41 | 113.33 | 108.20 |
| 13 | AU | 20 | ARG | NE-CZ-NH1 | 6.41 | 123.50 | 120.30 |
| 22 | AA | 1219 | A | C4-C5-C6 | -6.41 | 113.80 | 117.00 |
| 24 | A3 | 73 | A | C4-C5-C6 | -6.41 | 113.80 | 117.00 |
| 57 | BA | 608 | A | C4-C5-C6 | -6.41 | 113.80 | 117.00 |
| 57 | BA | 1638 | C | N1-C2-O2 | 6.41 | 122.75 | 118.90 |
| 23 | A2 | 41 | A | C4-C5-C6 | -6.41 | 113.80 | 117.00 |
| 57 | BA | 2658 | C | N3-C2-O2 | -6.41 | 117.42 | 121.90 |
| 22 | AA | 559 | A | C4-C5-C6 | -6.41 | 113.80 | 117.00 |
| 22 | AA | 1176 | A | C4-C5-C6 | -6.41 | 113.80 | 117.00 |
| 22 | AA | 1360 | A | C4-C5-C6 | -6.41 | 113.80 | 117.00 |
| 24 | A3 | 1 | C | N1-C2-O2 | 6.41 | 122.74 | 118.90 |
| 57 | BA | 1265 | A | C4-C5-C6 | -6.41 | 113.80 | 117.00 |
| 57 | BA | 1882 | U | O4'-C1'-N1 | 6.40 | 113.32 | 108.20 |
| 23 | A2 | 14 | G | O4'-C1'-N9 | 6.40 | 113.32 | 108.20 |
| 46 | B3 | 15 | ARG | NH1-CZ-NH2 | -6.40 | 112.36 | 119.40 |
| 57 | BA | 432 | A | C4-C5-C6 | -6.40 | 113.80 | 117.00 |
| 57 | BA | 1742 | U | O4'-C1'-N1 | 6.40 | 113.32 | 108.20 |
| 58 | Ba | 55 | U | O4'-C1'-N1 | 6.40 | 113.32 | 108.20 |
| 22 | AA | 189 | A | C4-C5-C6 | -6.40 | 113.80 | 117.00 |
| 22 | AA | 749 | A | C4-C5-C6 | -6.40 | 113.80 | 117.00 |
| 22 | AA | 948 | C | O4'-C1'-N1 | 6.40 | 113.32 | 108.20 |
| 57 | BA | 1261 | C | O4'-C1'-N1 | 6.40 | 113.32 | 108.20 |
| 57 | BA | 1900 | A | C4-C5-C6 | -6.40 | 113.80 | 117.00 |
| 57 | BA | 2115 | G | O4'-C1'-N9 | 6.40 | 113.32 | 108.20 |
| 57 | BA | 2188 | U | O4'-C1'-N1 | 6.40 | 113.32 | 108.20 |
| 22 | AA | 599 | C | N3-C2-O2 | -6.40 | 117.42 | 121.90 |
| 57 | BA | 650 | C | O4'-C1'-N1 | 6.40 | 113.32 | 108.20 |
| 57 | BA | 1020 | A | C4-C5-C6 | -6.40 | 113.80 | 117.00 |
| 21 | A1 | 278 | ARG | NE-CZ-NH1 | 6.40 | 123.50 | 120.30 |
| 22 | AA | 169 | C | O4'-C1'-N1 | 6.40 | 113.32 | 108.20 |
| 22 | AA | 845 | A | C4-C5-C6 | -6.40 | 113.80 | 117.00 |
| 33 | BS | 13 | ARG | NE-CZ-NH1 | 6.40 | 123.50 | 120.30 |
| 57 | BA | 563 | A | C4-C5-C6 | -6.40 | 113.80 | 117.00 |
| 57 | BA | 1685 | C | O4'-C1'-N1 | 6.40 | 113.32 | 108.20 |
| 57 | BA | 1942 | C | N3-C2-O2 | -6.40 | 117.42 | 121.90 |
| 22 | AA | 320 | A | C4-C5-C6 | -6.40 | 113.80 | 117.00 |
| 22 | AA | 498 | A | C4-C5-C6 | -6.39 | 113.80 | 117.00 |
| 22 | AA | 614 | C | N1-C2-O2 | 6.39 | 122.74 | 118.90 |
| 57 | BA | 264 | C | N3-C2-O2 | -6.39 | 117.42 | 121.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 899 | A | C4-C5-C6 | -6.39 | 113.80 | 117.00 |
| 22 | AA | 135 | C | N3-C2-O2 | -6.39 | 117.42 | 121.90 |
| 22 | AA | 234 | C | N1-C2-O2 | 6.39 | 122.74 | 118.90 |
| 22 | AA | 1362 | A | C4-C5-C6 | -6.39 | 113.80 | 117.00 |
| 57 | BA | 1067 | A | C4-C5-C6 | -6.39 | 113.80 | 117.00 |
| 22 | AA | 1210 | C | N1-C2-O2 | 6.39 | 122.73 | 118.90 |
| 57 | BA | 626 | A | C4-C5-C6 | -6.39 | 113.80 | 117.00 |
| 57 | BA | 1211 | C | N3-C2-O2 | -6.39 | 117.43 | 121.90 |
| 22 | AA | 978 | A | C5-C6-N1 | 6.39 | 120.89 | 117.70 |
| 57 | BA | 1996 | C | O4'-C1'-N1 | 6.39 | 113.31 | 108.20 |
| 58 | Ba | 59 | A | C4-C5-C6 | -6.39 | 113.81 | 117.00 |
| 22 | AA | 1169 | A | C4-C5-C6 | -6.39 | 113.81 | 117.00 |
| 22 | AA | 1534 | A | C4-C5-C6 | -6.39 | 113.81 | 117.00 |
| 57 | BA | 2142 | A | N1-C6-N6 | -6.39 | 114.77 | 118.60 |
| 57 | BA | 2479 | U | O4'-C1'-N1 | 6.39 | 113.31 | 108.20 |
| 22 | AA | 290 | C | N1-C2-O2 | 6.38 | 122.73 | 118.90 |
| 57 | BA | 2135 | A | C4-C5-C6 | -6.38 | 113.81 | 117.00 |
| 57 | BA | 2637 | U | O4'-C1'-N1 | 6.38 | 113.31 | 108.20 |
| 58 | Ba | 43 | C | N3-C2-O2 | -6.38 | 117.43 | 121.90 |
| 22 | AA | 478 | A | C4-C5-C6 | -6.38 | 113.81 | 117.00 |
| 22 | AA | 479 | U | O4'-C1'-N1 | 6.38 | 113.31 | 108.20 |
| 22 | AA | 553 | A | C4-C5-C6 | -6.38 | 113.81 | 117.00 |
| 57 | BA | 1002 | G | O4'-C1'-N9 | 6.38 | 113.31 | 108.20 |
| 22 | AA | 768 | A | C4-C5-C6 | -6.38 | 113.81 | 117.00 |
| 57 | BA | 164 | C | N3-C2-O2 | -6.38 | 117.43 | 121.90 |
| 57 | BA | 598 | U | O4'-C1'-N1 | 6.38 | 113.30 | 108.20 |
| 22 | AA | 207 | C | O4'-C1'-N1 | 6.38 | 113.30 | 108.20 |
| 22 | AA | 493 | A | C4-C5-C6 | -6.38 | 113.81 | 117.00 |
| 57 | BA | 786 | C | N1-C2-O2 | 6.38 | 122.73 | 118.90 |
| 57 | BA | 1312 | U | O4'-C1'-N1 | 6.38 | 113.30 | 108.20 |
| 57 | BA | 2704 | C | N1-C2-O2 | 6.38 | 122.73 | 118.90 |
| 22 | AA | 873 | A | C4-C5-C6 | -6.38 | 113.81 | 117.00 |
| 57 | BA | 867 | C | O4'-C1'-N1 | 6.38 | 113.30 | 108.20 |
| 57 | BA | 1251 | C | C1'-O4'-C4' | -6.38 | 104.80 | 109.90 |
| 57 | BA | 1257 | C | O4'-C1'-N1 | 6.38 | 113.30 | 108.20 |
| 57 | BA | 1322 | A | C4-C5-C6 | -6.38 | 113.81 | 117.00 |
| 57 | BA | 1641 | A | C4-C5-C6 | -6.38 | 113.81 | 117.00 |
| 57 | BA | 2226 | C | N3-C2-O2 | -6.38 | 117.44 | 121.90 |
| 57 | BA | 2829 | A | C4-C5-C6 | -6.38 | 113.81 | 117.00 |
| 57 | BA | 2734 | A | C4-C5-C6 | -6.38 | 113.81 | 117.00 |
| 57 | BA | 478 | A | C4-C5-C6 | -6.37 | 113.81 | 117.00 |
| 57 | BA | 1446 | C | N1-C2-O2 | 6.37 | 122.72 | 118.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 1681 | G | O4'-C1'-N9 | 6.37 | 113.30 | 108.20 |
| 57 | BA | 2305 | U | O4'-C1'-N1 | 6.37 | 113.30 | 108.20 |
| 22 | AA | 923 | A | C4-C5-C6 | -6.37 | 113.81 | 117.00 |
| 57 | BA | 10 | A | C4-C5-C6 | -6.37 | 113.81 | 117.00 |
| 57 | BA | 1469 | A | C4-C5-C6 | -6.37 | 113.81 | 117.00 |
| 57 | BA | 2088 | A | C4-C5-C6 | -6.37 | 113.81 | 117.00 |
| 57 | BA | 2160 | C | N1-C2-O2 | 6.37 | 122.72 | 118.90 |
| 57 | BA | 2207 | C | N1-C2-O2 | 6.37 | 122.72 | 118.90 |
| 57 | BA | 816 | C | N1-C2-O2 | 6.37 | 122.72 | 118.90 |
| 22 | AA | 732 | C | N1-C2-O2 | 6.37 | 122.72 | 118.90 |
| 57 | BA | 459 | U | O4'-C1'-N1 | 6.37 | 113.29 | 108.20 |
| 57 | BA | 633 | A | C4-C5-C6 | -6.37 | 113.82 | 117.00 |
| 57 | BA | 1246 | A | C4-C5-C6 | -6.37 | 113.82 | 117.00 |
| 57 | BA | 2037 | A | C4-C5-C6 | -6.37 | 113.82 | 117.00 |
| 58 | Ba | 95 | U | O4'-C1'-N1 | 6.37 | 113.30 | 108.20 |
| 22 | AA | 597 | G | N1-C6-O6 | -6.37 | 116.08 | 119.90 |
| 50 | B7 | 34 | ARG | CD-NE-CZ | 6.37 | 132.51 | 123.60 |
| 22 | AA | 215 | C | O4'-C1'-N1 | 6.37 | 113.29 | 108.20 |
| 22 | AA | 342 | C | N1-C2-O2 | 6.37 | 122.72 | 118.90 |
| 22 | AA | 812 | G | O4'-C1'-N9 | 6.37 | 113.29 | 108.20 |
| 22 | AA | 1258 | G | N1-C6-O6 | -6.37 | 116.08 | 119.90 |
| 57 | BA | 466 | A | C4-C5-C6 | -6.37 | 113.82 | 117.00 |
| 57 | BA | 2473 | U | O4'-C1'-N1 | 6.37 | 113.29 | 108.20 |
| 57 | BA | 2706 | A | C4-C5-C6 | -6.37 | 113.82 | 117.00 |
| 22 | AA | 1277 | C | N3-C2-O2 | -6.36 | 117.45 | 121.90 |
| 28 | BN | 95 | ARG | NE-CZ-NH1 | 6.36 | 123.48 | 120.30 |
| 57 | BA | 2364 | C | O4'-C1'-N1 | 6.36 | 113.29 | 108.20 |
| 57 | BA | 2516 | A | C4-C5-C6 | -6.36 | 113.82 | 117.00 |
| 57 | BA | 2612 | C | N3-C2-O2 | -6.36 | 117.45 | 121.90 |
| 22 | AA | 1054 | C | N3-C2-O2 | -6.36 | 117.45 | 121.90 |
| 57 | BA | 2406 | A | C4-C5-C6 | -6.36 | 113.82 | 117.00 |
| 57 | BA | 1379 | U | O4'-C1'-N1 | 6.36 | 113.29 | 108.20 |
| 57 | BA | 1655 | A | N1-C6-N6 | -6.36 | 114.78 | 118.60 |
| 57 | BA | 2352 | A | C5-C6-N1 | 6.36 | 120.88 | 117.70 |
| 29 | BO | 78 | ARG | NE-CZ-NH1 | 6.36 | 123.48 | 120.30 |
| 57 | BA | 1894 | C | N3-C2-O2 | -6.36 | 117.45 | 121.90 |
| 57 | BA | 1417 | C | O4'-C1'-N1 | 6.36 | 113.29 | 108.20 |
| 22 | AA | 1507 | A | C4-C5-C6 | -6.36 | 113.82 | 117.00 |
| 41 | BZ | 93 | ARG | NE-CZ-NH1 | 6.36 | 123.48 | 120.30 |
| 57 | BA | 275 | C | N3-C2-O2 | -6.36 | 117.45 | 121.90 |
| 57 | BA | 2706 | A | C5-C6-N1 | 6.36 | 120.88 | 117.70 |
| 22 | AA | 130 | A | C4-C5-C6 | -6.35 | 113.82 | 117.00 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 296 | U | O4'-C1'-N1 | 6.35 | 113.28 | 108.20 |
| 57 | BA | 1544 | A | C4-C5-C6 | -6.35 | 113.82 | 117.00 |
| 24 | A3 | 48 | U | O4'-C1'-N1 | 6.35 | 113.28 | 108.20 |
| 24 | A3 | 77 | A | C4-C5-C6 | -6.35 | 113.82 | 117.00 |
| 57 | BA | 2602 | A | C4-C5-C6 | -6.35 | 113.82 | 117.00 |
| 57 | BA | 457 | A | C4-C5-C6 | -6.35 | 113.82 | 117.00 |
| 57 | BA | 1286 | A | C4-C5-C6 | -6.35 | 113.82 | 117.00 |
| 22 | AA | 864 | A | C4-C5-C6 | -6.35 | 113.83 | 117.00 |
| 24 | A3 | 46 | G | O4'-C1'-N9 | 6.35 | 113.28 | 108.20 |
| 29 | BO | 64 | ARG | NE-CZ-NH1 | 6.35 | 123.47 | 120.30 |
| 57 | BA | 157 | C | O4'-C1'-N1 | 6.35 | 113.28 | 108.20 |
| 57 | BA | 547 | A | C4-C5-C6 | -6.35 | 113.83 | 117.00 |
| 57 | BA | 2823 | A | C4-C5-C6 | -6.35 | 113.83 | 117.00 |
| 22 | AA | 364 | A | C4-C5-C6 | -6.35 | 113.83 | 117.00 |
| 57 | BA | 1347 | A | C4-C5-C6 | -6.35 | 113.83 | 117.00 |
| 22 | AA | 1274 | A | C4-C5-C6 | -6.35 | 113.83 | 117.00 |
| 57 | BA | 195 | A | N1-C6-N6 | -6.35 | 114.79 | 118.60 |
| 18 | AG | 78 | ARG | NE-CZ-NH1 | 6.34 | 123.47 | 120.30 |
| 22 | AA | 338 | A | C4-C5-C6 | -6.34 | 113.83 | 117.00 |
| 35 | BD | 51 | ARG | NE-CZ-NH2 | -6.34 | 117.13 | 120.30 |
| 57 | BA | 1474 | U | O4'-C1'-N1 | 6.34 | 113.27 | 108.20 |
| 57 | BA | 2568 | U | O4'-C1'-N1 | 6.34 | 113.27 | 108.20 |
| 22 | AA | 151 | A | O4'-C1'-N9 | 6.34 | 113.27 | 108.20 |
| 57 | BA | 1791 | A | C4-C5-C6 | -6.34 | 113.83 | 117.00 |
| 57 | BA | 2542 | A | C4-C5-C6 | -6.34 | 113.83 | 117.00 |
| 57 | BA | 1596 | A | C4-C5-C6 | -6.34 | 113.83 | 117.00 |
| 57 | BA | 1676 | A | C4-C5-C6 | -6.34 | 113.83 | 117.00 |
| 22 | AA | 457 | G | O4'-C1'-N9 | 6.34 | 113.27 | 108.20 |
| 57 | BA | 251 | A | C5-C6-N1 | 6.34 | 120.87 | 117.70 |
| 22 | AA | 188 | C | N3-C2-O2 | -6.33 | 117.47 | 121.90 |
| 22 | AA | 306 | A | C4-C5-C6 | -6.33 | 113.83 | 117.00 |
| 22 | AA | 1012 | A | C4-C5-C6 | -6.33 | 113.83 | 117.00 |
| 57 | BA | 1172 | C | N1-C2-O2 | 6.33 | 122.70 | 118.90 |
| 57 | BA | 1285 | A | C5-C6-N1 | 6.33 | 120.87 | 117.70 |
| 24 | A3 | 44 | A | C4-C5-C6 | -6.33 | 113.83 | 117.00 |
| 57 | BA | 1913 | A | C4-C5-C6 | -6.33 | 113.83 | 117.00 |
| 57 | BA | 845 | A | C5-C6-N1 | 6.33 | 120.87 | 117.70 |
| 57 | BA | 1156 | A | C4-C5-C6 | -6.33 | 113.83 | 117.00 |
| 57 | BA | 1226 | A | C4-C5-C6 | -6.33 | 113.83 | 117.00 |
| 57 | BA | 2268 | A | C5-C6-N1 | 6.33 | 120.87 | 117.70 |
| 57 | BA | 2412 | A | C4-C5-C6 | -6.33 | 113.83 | 117.00 |
| 22 | AA | 731 | G | O4'-C1'-N9 | 6.33 | 113.26 | 108.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 1593 | A | C4-C5-C6 | -6.33 | 113.83 | 117.00 |
| 22 | AA | 853 | C | O4'-C1'-N1 | 6.33 | 113.26 | 108.20 |
| 22 | AA | 1267 | C | N3-C2-O2 | -6.33 | 117.47 | 121.90 |
| 57 | BA | 645 | C | N3-C2-O2 | -6.33 | 117.47 | 121.90 |
| 57 | BA | 1261 | C | N1-C2-O2 | 6.33 | 122.70 | 118.90 |
| 57 | BA | 1614 | A | C4-C5-C6 | -6.33 | 113.84 | 117.00 |
| 6 | AO | 88 | ARG | NE-CZ-NH1 | 6.33 | 123.46 | 120.30 |
| 22 | AA | 264 | C | O4'-C1'-N1 | 6.33 | 113.26 | 108.20 |
| 57 | BA | 1096 | A | C4-C5-C6 | -6.33 | 113.84 | 117.00 |
| 57 | BA | 1395 | A | C4-C5-C6 | -6.33 | 113.84 | 117.00 |
| 57 | BA | 2184 | A | C4-C5-C6 | -6.33 | 113.84 | 117.00 |
| 22 | AA | 562 | U | O4'-C1'-N1 | 6.32 | 113.26 | 108.20 |
| 57 | BA | 109 | C | O4'-C1'-N1 | 6.32 | 113.26 | 108.20 |
| 57 | BA | 194 | G | N1-C6-O6 | -6.32 | 116.11 | 119.90 |
| 57 | BA | 379 | G | N1-C6-O6 | -6.32 | 116.11 | 119.90 |
| 57 | BA | 961 | C | N3-C2-O2 | -6.32 | 117.47 | 121.90 |
| 57 | BA | 1570 | A | C4-C5-C6 | -6.32 | 113.84 | 117.00 |
| 57 | BA | 2688 | G | O4'-C1'-N9 | 6.32 | 113.26 | 108.20 |
| 57 | BA | 228 | C | N3-C2-O2 | -6.32 | 117.47 | 121.90 |
| 57 | BA | 820 | A | C4-C5-C6 | -6.32 | 113.84 | 117.00 |
| 22 | AA | 1194 | U | O4'-C1'-N1 | 6.32 | 113.26 | 108.20 |
| 52 | B9 | 24 | ARG | NE-CZ-NH2 | 6.32 | 123.46 | 120.30 |
| 57 | BA | 1336 | A | C4-C5-C6 | -6.32 | 113.84 | 117.00 |
| 57 | BA | 1739 | A | C4-C5-C6 | -6.32 | 113.84 | 117.00 |
| 57 | BA | 2463 | C | N1-C2-O2 | 6.32 | 122.69 | 118.90 |
| 57 | BA | 2388 | A | C4-C5-C6 | -6.32 | 113.84 | 117.00 |
| 57 | BA | 383 | C | N3-C2-O2 | -6.32 | 117.48 | 121.90 |
| 57 | BA | 324 | A | C4-C5-C6 | -6.31 | 113.84 | 117.00 |
| 57 | BA | 736 | C | N3-C2-O2 | -6.31 | 117.48 | 121.90 |
| 22 | AA | 403 | C | N1-C2-O2 | 6.31 | 122.69 | 118.90 |
| 57 | BA | 710 | U | O4'-C1'-N1 | 6.31 | 113.25 | 108.20 |
| 22 | AA | 365 | U | N3-C2-O2 | -6.31 | 117.78 | 122.20 |
| 57 | BA | 164 | C | O4'-C1'-N1 | 6.31 | 113.25 | 108.20 |
| 57 | BA | 1159 | U | O4'-C1'-N1 | 6.31 | 113.25 | 108.20 |
| 57 | BA | 2809 | A | N1-C6-N6 | -6.31 | 114.81 | 118.60 |
| 57 | BA | 342 | A | C4-C5-C6 | -6.31 | 113.84 | 117.00 |
| 57 | BA | 1111 | A | C4-C5-C6 | -6.31 | 113.84 | 117.00 |
| 57 | BA | 2799 | A | C4-C5-C6 | -6.31 | 113.85 | 117.00 |
| 57 | BA | 1241 | A | C4-C5-C6 | -6.31 | 113.85 | 117.00 |
| 57 | BA | 2150 | C | O4'-C1'-N1 | 6.31 | 113.25 | 108.20 |
| 57 | BA | 1829 | A | C4-C5-C6 | -6.31 | 113.85 | 117.00 |
| 22 | AA | 620 | C | O4'-C1'-N1 | 6.30 | 113.24 | 108.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | AA | 1476 | A | C4-C5-C6 | -6.30 | 113.85 | 117.00 |
| 57 | BA | 624 | C | N1-C2-O2 | 6.30 | 122.68 | 118.90 |
| 57 | BA | 1551 | A | C4-C5-C6 | -6.30 | 113.85 | 117.00 |
| 57 | BA | 1800 | C | N1-C2-O2 | 6.30 | 122.68 | 118.90 |
| 57 | BA | 2106 | U | O4'-C1'-N1 | 6.30 | 113.24 | 108.20 |
| 57 | BA | 2322 | A | C4-C5-C6 | -6.30 | 113.85 | 117.00 |
| 57 | BA | 2587 | A | N1-C6-N6 | -6.30 | 114.82 | 118.60 |
| 22 | AA | 975 | A | C4-C5-C6 | -6.30 | 113.85 | 117.00 |
| 58 | Ba | 42 | C | N3-C2-O2 | -6.30 | 117.49 | 121.90 |
| 22 | AA | 663 | A | C4-C5-C6 | -6.30 | 113.85 | 117.00 |
| 57 | BA | 566 | U | O4'-C1'-N1 | 6.30 | 113.24 | 108.20 |
| 57 | BA | 1420 | A | C4-C5-C6 | -6.30 | 113.85 | 117.00 |
| 57 | BA | 2809 | A | C4-C5-C6 | -6.30 | 113.85 | 117.00 |
| 57 | BA | 217 | A | C4-C5-C6 | -6.30 | 113.85 | 117.00 |
| 57 | BA | 2155 | U | O4'-C1'-N1 | 6.30 | 113.24 | 108.20 |
| 57 | BA | 2328 | A | C4-C5-C6 | -6.30 | 113.85 | 117.00 |
| 57 | BA | 2062 | A | C4-C5-C6 | -6.30 | 113.85 | 117.00 |
| 57 | BA | 635 | C | N1-C2-O2 | 6.30 | 122.68 | 118.90 |
| 57 | BA | 640 | C | N1-C2-O2 | 6.29 | 122.68 | 118.90 |
| 22 | AA | 509 | A | C4-C5-C6 | -6.29 | 113.85 | 117.00 |
| 57 | BA | 14 | A | O4'-C1'-N9 | 6.29 | 113.23 | 108.20 |
| 57 | BA | 2885 | G | O4'-C1'-N9 | 6.29 | 113.24 | 108.20 |
| 57 | BA | 277 | G | O4'-C1'-N9 | 6.29 | 113.23 | 108.20 |
| 22 | AA | 412 | A | C4-C5-C6 | -6.29 | 113.86 | 117.00 |
| 22 | AA | 1510 | C | C5'-C4'-O4' | 6.29 | 116.65 | 109.10 |
| 57 | BA | 120 | U | O4'-C1'-N1 | 6.29 | 113.23 | 108.20 |
| 57 | BA | 1013 | C | O4'-C1'-N1 | 6.29 | 113.23 | 108.20 |
| 57 | BA | 1169 | A | C4-C5-C6 | -6.29 | 113.86 | 117.00 |
| 15 | AD | 55 | ARG | NE-CZ-NH1 | 6.29 | 123.44 | 120.30 |
| 15 | AD | 110 | ARG | NE-CZ-NH1 | 6.29 | 123.44 | 120.30 |
| 22 | AA | 545 | C | N1-C2-O2 | 6.29 | 122.67 | 118.90 |
| 57 | BA | 362 | A | C4-C5-C6 | -6.29 | 113.86 | 117.00 |
| 57 | BA | 1092 | C | O4'-C1'-N1 | 6.29 | 113.23 | 108.20 |
| 22 | AA | 106 | C | N1-C2-O2 | 6.28 | 122.67 | 118.90 |
| 22 | AA | 1132 | C | O4'-C1'-N1 | 6.28 | 113.23 | 108.20 |
| 22 | AA | 1150 | A | C4-C5-C6 | -6.28 | 113.86 | 117.00 |
| 57 | BA | 604 | G | C5'-C4'-O4' | 6.28 | 116.64 | 109.10 |
| 58 | Ba | 53 | A | C4-C5-C6 | -6.28 | 113.86 | 117.00 |
| 57 | BA | 2178 | C | O4'-C1'-N1 | 6.28 | 113.23 | 108.20 |
| 57 | BA | 2227 | A | C4-C5-C6 | -6.28 | 113.86 | 117.00 |
| 18 | AG | 1 | PRO | CA-N-CD | -6.28 | 102.71 | 111.50 |
| 22 | AA | 1271 | A | C4-C5-C6 | -6.28 | 113.86 | 117.00 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 55 | BH | 169 | ARG | NE-CZ-NH2 | 6.28 | 123.44 | 120.30 |
| 57 | BA | 1236 | G | O4'-C1'-N9 | 6.28 | 113.22 | 108.20 |
| 57 | BA | 1777 | U | N3-C2-O2 | -6.28 | 117.80 | 122.20 |
| 57 | BA | 2452 | C | N3-C2-O2 | -6.28 | 117.50 | 121.90 |
| 57 | BA | 2539 | C | N3-C2-O2 | -6.28 | 117.50 | 121.90 |
| 22 | AA | 284 | C | O4'-C1'-N1 | 6.28 | 113.22 | 108.20 |
| 22 | AA | 1504 | G | O4'-C1'-N9 | 6.28 | 113.22 | 108.20 |
| 57 | BA | 451 | U | O4'-C1'-N1 | 6.28 | 113.22 | 108.20 |
| 22 | AA | 624 | C | O4'-C1'-N1 | 6.28 | 113.22 | 108.20 |
| 31 | BQ | 114 | ARG | NE-CZ-NH2 | 6.28 | 123.44 | 120.30 |
| 57 | BA | 545 | U | O4'-C1'-N1 | 6.28 | 113.22 | 108.20 |
| 57 | BA | 688 | U | O4'-C1'-N1 | 6.28 | 113.22 | 108.20 |
| 57 | BA | 2374 | C | N1-C2-O2 | 6.28 | 122.67 | 118.90 |
| 22 | AA | 802 | A | C4-C5-C6 | -6.28 | 113.86 | 117.00 |
| 22 | AA | 865 | A | C4-C5-C6 | -6.28 | 113.86 | 117.00 |
| 22 | AA | 1456 | A | C4-C5-C6 | -6.28 | 113.86 | 117.00 |
| 57 | BA | 2456 | C | N1-C2-O2 | 6.28 | 122.67 | 118.90 |
| 57 | BA | 2774 | C | O4'-C1'-N1 | 6.28 | 113.22 | 108.20 |
| 57 | BA | 1994 | C | N3-C2-O2 | -6.27 | 117.51 | 121.90 |
| 22 | AA | 182 | A | C4-C5-C6 | -6.27 | 113.86 | 117.00 |
| 22 | AA | 1472 | U | O4'-C1'-N1 | 6.27 | 113.22 | 108.20 |
| 57 | BA | 1398 | C | N1-C2-O2 | 6.27 | 122.66 | 118.90 |
| 22 | AA | 1201 | A | C4-C5-C6 | -6.27 | 113.86 | 117.00 |
| 57 | BA | 1675 | C | N3-C2-O2 | -6.27 | 117.51 | 121.90 |
| 57 | BA | 2422 | C | N3-C2-O2 | -6.27 | 117.51 | 121.90 |
| 22 | AA | 71 | A | C4-C5-C6 | -6.27 | 113.87 | 117.00 |
| 44 | B2 | 7 | ARG | NH1-CZ-NH2 | -6.27 | 112.51 | 119.40 |
| 57 | BA | 675 | A | C4-C5-C6 | -6.27 | 113.87 | 117.00 |
| 57 | BA | 2061 | G | C4'-C3'-C2' | -6.27 | 96.33 | 102.60 |
| 57 | BA | 1319 | C | N1-C2-O2 | 6.26 | 122.66 | 118.90 |
| 57 | BA | 2247 | A | C5-C6-N1 | 6.26 | 120.83 | 117.70 |
| 57 | BA | 2762 | C | O4'-C1'-N1 | 6.26 | 113.21 | 108.20 |
| 22 | AA | 473 | U | O4'-C1'-N1 | 6.26 | 113.21 | 108.20 |
| 23 | A2 | 48 | C | N3-C2-O2 | -6.26 | 117.52 | 121.90 |
| 58 | Ba | 47 | C | N3-C2-O2 | -6.26 | 117.52 | 121.90 |
| 47 | B4 | 63 | ARG | NE-CZ-NH1 | 6.26 | 123.43 | 120.30 |
| 57 | BA | 910 | A | C4-C5-C6 | -6.26 | 113.87 | 117.00 |
| 57 | BA | 1462 | C | O4'-C1'-N1 | 6.26 | 113.21 | 108.20 |
| 57 | BA | 1652 | A | C4-C5-C6 | -6.26 | 113.87 | 117.00 |
| 57 | BA | 1791 | A | N1-C6-N6 | -6.26 | 114.84 | 118.60 |
| 22 | AA | 721 | G | O4'-C1'-N9 | 6.26 | 113.21 | 108.20 |
| 28 | BN | 37 | ARG | NE-CZ-NH2 | 6.26 | 123.43 | 120.30 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 196 | A | C4-C5-C6 | -6.26 | 113.87 | 117.00 |
| 22 | AA | 8 | A | C4-C5-C6 | -6.26 | 113.87 | 117.00 |
| 22 | AA | 796 | C | N1-C2-O2 | 6.26 | 122.66 | 118.90 |
| 24 | A3 | 45 | A | C4-C5-C6 | -6.26 | 113.87 | 117.00 |
| 22 | AA | 1538 | C | N3-C2-O2 | -6.26 | 117.52 | 121.90 |
| 57 | BA | 31 | C | O4'-C1'-N1 | 6.26 | 113.21 | 108.20 |
| 57 | BA | 1553 | A | C4-C5-C6 | -6.26 | 113.87 | 117.00 |
| 57 | BA | 2005 | A | C4-C5-C6 | -6.26 | 113.87 | 117.00 |
| 57 | BA | 2899 | A | C4-C5-C6 | -6.26 | 113.87 | 117.00 |
| 57 | BA | 29 | U | O4'-C1'-N1 | 6.25 | 113.20 | 108.20 |
| 57 | BA | 752 | A | C4-C5-C6 | -6.25 | 113.87 | 117.00 |
| 22 | AA | 1092 | A | C4-C5-C6 | -6.25 | 113.87 | 117.00 |
| 24 | A3 | 72 | C | O4'-C1'-N1 | 6.25 | 113.20 | 108.20 |
| 57 | BA | 2708 | G | O4'-C1'-N9 | 6.25 | 113.20 | 108.20 |
| 22 | AA | 1112 | C | N3-C2-O2 | -6.25 | 117.52 | 121.90 |
| 22 | AA | 1161 | C | N1-C2-O2 | 6.25 | 122.65 | 118.90 |
| 22 | AA | 1287 | A | C4-C5-C6 | -6.25 | 113.87 | 117.00 |
| 57 | BA | 437 | U | O4'-C1'-N1 | 6.25 | 113.20 | 108.20 |
| 57 | BA | 2417 | C | O4'-C1'-N1 | 6.25 | 113.20 | 108.20 |
| 22 | AA | 333 | U | O4'-C1'-N1 | 6.25 | 113.20 | 108.20 |
| 22 | AA | 480 | U | O4'-C1'-N1 | 6.25 | 113.20 | 108.20 |
| 22 | AA | 1023 | U | O4'-C1'-N1 | 6.25 | 113.20 | 108.20 |
| 22 | AA | 1254 | A | C4-C5-C6 | -6.25 | 113.88 | 117.00 |
| 46 | B3 | 37 | ARG | NE-CZ-NH1 | 6.25 | 123.42 | 120.30 |
| 57 | BA | 727 | A | C4-C5-C6 | -6.25 | 113.88 | 117.00 |
| 57 | BA | 2015 | A | C4-C5-C6 | -6.25 | 113.88 | 117.00 |
| 57 | BA | 2610 | C | N3-C4-C5 | 6.25 | 124.40 | 121.90 |
| 57 | BA | 2758 | A | C4-C5-C6 | -6.25 | 113.88 | 117.00 |
| 57 | BA | 2766 | A | C4-C5-C6 | -6.25 | 113.88 | 117.00 |
| 58 | Ba | 28 | C | N1-C2-O2 | 6.25 | 122.65 | 118.90 |
| 58 | Ba | 45 | A | C4-C5-C6 | -6.25 | 113.88 | 117.00 |
| 22 | AA | 419 | C | N1-C2-O2 | 6.25 | 122.65 | 118.90 |
| 22 | AA | 953 | G | N1-C6-O6 | -6.25 | 116.15 | 119.90 |
| 22 | AA | 977 | A | C4-C5-C6 | -6.25 | 113.88 | 117.00 |
| 57 | BA | 823 | C | N1-C2-O2 | 6.25 | 122.65 | 118.90 |
| 57 | BA | 2236 | U | O4'-C1'-N1 | 6.25 | 113.20 | 108.20 |
| 57 | BA | 1549 | A | C4-C5-C6 | -6.25 | 113.88 | 117.00 |
| 32 | BR | 96 | ARG | NE-CZ-NH1 | 6.24 | 123.42 | 120.30 |
| 57 | BA | 143 | C | O4'-C1'-N1 | 6.24 | 113.19 | 108.20 |
| 57 | BA | 1839 | G | O4'-C1'-N9 | 6.24 | 113.19 | 108.20 |
| 22 | AA | 73 | C | O4'-C1'-N1 | 6.24 | 113.19 | 108.20 |
| 57 | BA | 2436 | G | N1-C6-O6 | -6.24 | 116.16 | 119.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | AA | 287 | U | O4'-C1'-N1 | 6.24 | 113.19 | 108.20 |
| 22 | AA | 659 | U | O4'-C1'-N1 | 6.24 | 113.19 | 108.20 |
| 22 | AA | 1428 | A | C4-C5-C6 | -6.24 | 113.88 | 117.00 |
| 57 | BA | 794 | A | C4-C5-C6 | -6.24 | 113.88 | 117.00 |
| 57 | BA | 1221 | C | N1-C2-O2 | 6.24 | 122.64 | 118.90 |
| 57 | BA | 1754 | A | C5-C6-N1 | 6.24 | 120.82 | 117.70 |
| 57 | BA | 1762 | A | C4-C5-C6 | -6.24 | 113.88 | 117.00 |
| 57 | BA | 418 | C | N1-C2-O2 | 6.24 | 122.64 | 118.90 |
| 57 | BA | 569 | U | O4'-C1'-N1 | 6.24 | 113.19 | 108.20 |
| 57 | BA | 740 | C | O4'-C1'-N1 | 6.24 | 113.19 | 108.20 |
| 57 | BA | 1144 | A | C4-C5-C6 | -6.24 | 113.88 | 117.00 |
| 57 | BA | 1227 | G | N1-C6-O6 | -6.24 | 116.16 | 119.90 |
| 57 | BA | 2279 | G | N1-C6-O6 | -6.24 | 116.16 | 119.90 |
| 22 | AA | 741 | G | N1-C6-O6 | -6.24 | 116.16 | 119.90 |
| 57 | BA | 936 | A | C4-C5-C6 | -6.24 | 113.88 | 117.00 |
| 58 | Ba | 115 | A | C4-C5-C6 | -6.24 | 113.88 | 117.00 |
| 57 | BA | 1217 | U | O4'-C1'-N1 | 6.23 | 113.19 | 108.20 |
| 57 | BA | 2635 | A | C4-C5-C6 | -6.23 | 113.88 | 117.00 |
| 57 | BA | 1270 | C | O4'-C1'-N1 | 6.23 | 113.19 | 108.20 |
| 57 | BA | 2860 | A | C4-C5-C6 | -6.23 | 113.88 | 117.00 |
| 3 | AL | 53 | ARG | NE-CZ-NH1 | 6.23 | 123.42 | 120.30 |
| 22 | AA | 689 | C | N1-C2-O2 | 6.23 | 122.64 | 118.90 |
| 22 | AA | 876 | C | N3-C2-O2 | -6.23 | 117.54 | 121.90 |
| 23 | A2 | 18 | A | C4-C5-C6 | -6.23 | 113.89 | 117.00 |
| 38 | BW | 110 | ARG | NE-CZ-NH2 | 6.23 | 123.42 | 120.30 |
| 57 | BA | 330 | A | O4'-C1'-N9 | 6.23 | 113.18 | 108.20 |
| 57 | BA | 982 | C | N3-C2-O2 | -6.23 | 117.54 | 121.90 |
| 57 | BA | 944 | C | N3-C4-N4 | -6.23 | 113.64 | 118.00 |
| 57 | BA | 2173 | A | C4-C5-C6 | -6.23 | 113.89 | 117.00 |
| 22 | AA | 108 | G | N3-C4-C5 | -6.23 | 125.49 | 128.60 |
| 22 | AA | 192 | A | C4-C5-C6 | -6.23 | 113.89 | 117.00 |
| 22 | AA | 1132 | C | N1-C2-O2 | 6.23 | 122.64 | 118.90 |
| 22 | AA | 1425 | U | O4'-C1'-N1 | 6.23 | 113.18 | 108.20 |
| 35 | BD | 42 | ARG | NE-CZ-NH1 | 6.23 | 123.41 | 120.30 |
| 57 | BA | 383 | C | O4'-C1'-N1 | 6.23 | 113.18 | 108.20 |
| 57 | BA | 1936 | A | C4-C5-C6 | -6.23 | 113.89 | 117.00 |
| 57 | BA | 1561 | C | N1-C2-O2 | 6.23 | 122.64 | 118.90 |
| 16 | AE | 53 | ARG | NE-CZ-NH1 | 6.22 | 123.41 | 120.30 |
| 55 | BH | 68 | ARG | NE-CZ-NH1 | 6.22 | 123.41 | 120.30 |
| 8 | AQ | 61 | ARG | NE-CZ-NH1 | 6.22 | 123.41 | 120.30 |
| 14 | AC | 126 | ARG | NE-CZ-NH1 | 6.22 | 123.41 | 120.30 |
| 57 | BA | 282 | A | C4-C5-C6 | -6.22 | 113.89 | 117.00 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 998 | C | N1-C2-O2 | 6.22 | 122.63 | 118.90 |
| 57 | BA | 2566 | A | C4-C5-C6 | -6.22 | 113.89 | 117.00 |
| 22 | AA | 376 | G | N1-C6-O6 | -6.22 | 116.17 | 119.90 |
| 57 | BA | 2169 | A | C4-C5-C6 | -6.22 | 113.89 | 117.00 |
| 5 | AN | 64 | ARG | NE-CZ-NH1 | 6.22 | 123.41 | 120.30 |
| 22 | AA | 621 | A | C4-C5-C6 | -6.22 | 113.89 | 117.00 |
| 27 | BK | 126 | ARG | NE-CZ-NH1 | 6.22 | 123.41 | 120.30 |
| 32 | BR | 30 | ARG | NE-CZ-NH1 | 6.22 | 123.41 | 120.30 |
| 57 | BA | 1392 | A | C4-C5-C6 | -6.22 | 113.89 | 117.00 |
| 57 | BA | 2424 | C | N3-C2-O2 | -6.22 | 117.55 | 121.90 |
| 57 | BA | 1933 | G | O4'-C1'-N9 | 6.22 | 113.17 | 108.20 |
| 22 | AA | 623 | C | O4'-C1'-N1 | 6.22 | 113.17 | 108.20 |
| 22 | AA | 1358 | U | N3-C2-O2 | -6.22 | 117.85 | 122.20 |
| 57 | BA | 6 | A | C4-C5-C6 | -6.22 | 113.89 | 117.00 |
| 57 | BA | 116 | C | N1-C2-O2 | 6.22 | 122.63 | 118.90 |
| 57 | BA | 1008 | A | C4-C5-C6 | -6.22 | 113.89 | 117.00 |
| 57 | BA | 1520 | U | O4'-C1'-N1 | 6.22 | 113.17 | 108.20 |
| 57 | BA | 2332 | C | O4'-C1'-N1 | 6.22 | 113.17 | 108.20 |
| 16 | AE | 44 | ARG | NE-CZ-NH1 | 6.21 | 123.41 | 120.30 |
| 22 | AA | 385 | C | N1-C2-O2 | 6.21 | 122.63 | 118.90 |
| 22 | AA | 779 | C | N1-C2-O2 | 6.21 | 122.63 | 118.90 |
| 57 | BA | 1045 | C | N3-C2-O2 | -6.21 | 117.55 | 121.90 |
| 57 | BA | 2142 | A | C4-C5-C6 | -6.21 | 113.89 | 117.00 |
| 58 | Ba | 101 | A | C4-C5-C6 | -6.21 | 113.89 | 117.00 |
| 22 | AA | 33 | A | N1-C6-N6 | -6.21 | 114.87 | 118.60 |
| 22 | AA | 816 | A | C4-C5-C6 | -6.21 | 113.89 | 117.00 |
| 57 | BA | 1439 | A | C4-C5-C6 | -6.21 | 113.89 | 117.00 |
| 57 | BA | 2443 | C | N1-C2-O2 | 6.21 | 122.63 | 118.90 |
| 13 | AU | 44 | ARG | NE-CZ-NH1 | 6.21 | 123.41 | 120.30 |
| 22 | AA | 782 | A | C4-C5-C6 | -6.21 | 113.89 | 117.00 |
| 22 | AA | 998 | C | N1-C2-O2 | 6.21 | 122.63 | 118.90 |
| 57 | BA | 1022 | G | N1-C6-O6 | -6.21 | 116.17 | 119.90 |
| 57 | BA | 1585 | C | N3-C2-O2 | -6.21 | 117.55 | 121.90 |
| 57 | BA | 689 | A | C4-C5-C6 | -6.21 | 113.89 | 117.00 |
| 57 | BA | 1698 | A | N1-C6-N6 | -6.21 | 114.88 | 118.60 |
| 57 | BA | 1761 | C | N3-C2-O2 | -6.21 | 117.55 | 121.90 |
| 57 | BA | 2815 | C | O4'-C1'-N1 | 6.21 | 113.17 | 108.20 |
| 22 | AA | 441 | A | C4-C5-C6 | -6.21 | 113.90 | 117.00 |
| 22 | AA | 1314 | C | N1-C2-O2 | 6.21 | 122.62 | 118.90 |
| 22 | AA | 28 | A | C4-C5-C6 | -6.20 | 113.90 | 117.00 |
| 22 | AA | 431 | A | C4-C5-C6 | -6.20 | 113.90 | 117.00 |
| 57 | BA | 357 | C | O4'-C1'-N1 | 6.20 | 113.16 | 108.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 1135 | C | N3-C2-O2 | -6.20 | 117.56 | 121.90 |
| 57 | BA | 2126 | A | C4-C5-C6 | -6.20 | 113.90 | 117.00 |
| 57 | BA | 2610 | C | N3-C2-O2 | -6.20 | 117.56 | 121.90 |
| 57 | BA | 2617 | U | O4'-C1'-N1 | 6.20 | 113.16 | 108.20 |
| 57 | BA | 2700 | A | C5-C6-N1 | 6.20 | 120.80 | 117.70 |
| 57 | BA | 2710 | C | N1-C2-O2 | 6.20 | 122.62 | 118.90 |
| 22 | AA | 215 | C | N1-C2-O2 | 6.20 | 122.62 | 118.90 |
| 57 | BA | 80 | G | N1-C6-O6 | -6.20 | 116.18 | 119.90 |
| 57 | BA | 2824 | C | O4'-C1'-N1 | 6.20 | 113.16 | 108.20 |
| 22 | AA | 232 | G | N3-C2-N2 | -6.20 | 115.56 | 119.90 |
| 22 | AA | 919 | A | C4-C5-C6 | -6.20 | 113.90 | 117.00 |
| 57 | BA | 241 | A | N1-C6-N6 | -6.20 | 114.88 | 118.60 |
| 57 | BA | 683 | U | O4'-C1'-N1 | 6.20 | 113.16 | 108.20 |
| 22 | AA | 490 | C | O4'-C1'-N1 | 6.20 | 113.16 | 108.20 |
| 22 | AA | 569 | C | N3-C2-O2 | -6.20 | 117.56 | 121.90 |
| 57 | BA | 1173 | U | O4'-C1'-N1 | 6.20 | 113.16 | 108.20 |
| 57 | BA | 1406 | U | O4'-C1'-N1 | 6.20 | 113.16 | 108.20 |
| 57 | BA | 2759 | G | N1-C6-O6 | -6.20 | 116.18 | 119.90 |
| 22 | AA | 1467 | C | N3-C2-O2 | -6.20 | 117.56 | 121.90 |
| 57 | BA | 1253 | A | C4-C5-C6 | -6.20 | 113.90 | 117.00 |
| 57 | BA | 2850 | A | C4-C5-C6 | -6.20 | 113.90 | 117.00 |
| 57 | BA | 1655 | A | C5-C6-N1 | 6.19 | 120.80 | 117.70 |
| 57 | BA | 2752 | C | N3-C2-O2 | -6.19 | 117.56 | 121.90 |
| 57 | BA | 734 | A | C4-C5-C6 | -6.19 | 113.90 | 117.00 |
| 57 | BA | 2178 | C | N3-C2-O2 | -6.19 | 117.57 | 121.90 |
| 22 | AA | 539 | A | C4-C5-C6 | -6.19 | 113.91 | 117.00 |
| 22 | AA | 25 | C | N1-C2-O2 | 6.19 | 122.61 | 118.90 |
| 27 | BK | 102 | ARG | NE-CZ-NH1 | 6.19 | 123.39 | 120.30 |
| 22 | AA | 298 | A | C4-C5-C6 | -6.19 | 113.91 | 117.00 |
| 22 | AA | 1359 | C | N3-C2-O2 | -6.19 | 117.57 | 121.90 |
| 57 | BA | 817 | C | N1-C2-O2 | 6.19 | 122.61 | 118.90 |
| 57 | BA | 1064 | C | C4'-C3'-C2' | -6.19 | 96.41 | 102.60 |
| 57 | BA | 1176 | U | O4'-C1'-N1 | 6.19 | 113.15 | 108.20 |
| 57 | BA | 1326 | U | O4'-C1'-N1 | 6.19 | 113.15 | 108.20 |
| 57 | BA | 1541 | C | O4'-C1'-N1 | 6.19 | 113.15 | 108.20 |
| 57 | BA | 1758 | U | N3-C2-O2 | -6.19 | 117.87 | 122.20 |
| 57 | BA | 1925 | C | N3-C2-O2 | -6.19 | 117.57 | 121.90 |
| 57 | BA | 581 | C | O4'-C1'-N1 | 6.19 | 113.15 | 108.20 |
| 57 | BA | 2649 | C | O4'-C1'-N1 | 6.19 | 113.15 | 108.20 |
| 7 | AP | 28 | ARG | NE-CZ-NH1 | 6.18 | 123.39 | 120.30 |
| 22 | AA | 582 | C | N3-C2-O2 | -6.18 | 117.57 | 121.90 |
| 57 | BA | 1178 | C | N1-C2-O2 | 6.18 | 122.61 | 118.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 1881 | C | O4'-C1'-N1 | 6.18 | 113.15 | 108.20 |
| 22 | AA | 226 | G | N1-C6-O6 | -6.18 | 116.19 | 119.90 |
| 45 | BE | 124 | ARG | NE-CZ-NH1 | 6.18 | 123.39 | 120.30 |
| 57 | BA | 2329 | U | O4'-C1'-N1 | 6.18 | 113.15 | 108.20 |
| 22 | AA | 1117 | A | O4'-C1'-N9 | 6.18 | 113.14 | 108.20 |
| 57 | BA | 737 | C | O4'-C1'-N1 | 6.18 | 113.14 | 108.20 |
| 57 | BA | 2079 | U | O4'-C1'-N1 | 6.18 | 113.14 | 108.20 |
| 57 | BA | 676 | A | C4-C5-C6 | -6.18 | 113.91 | 117.00 |
| 57 | BA | 919 | U | O4'-C1'-N1 | 6.18 | 113.14 | 108.20 |
| 57 | BA | 1180 | U | O4'-C1'-N1 | 6.18 | 113.14 | 108.20 |
| 57 | BA | 1306 | C | N1-C2-O2 | 6.18 | 122.61 | 118.90 |
| 58 | Ba | 90 | C | N3-C4-N4 | -6.18 | 113.67 | 118.00 |
| 4 | AM | 106 | ARG | NE-CZ-NH1 | 6.18 | 123.39 | 120.30 |
| 15 | AD | 13 | ARG | NE-CZ-NH1 | 6.18 | 123.39 | 120.30 |
| 57 | BA | 129 | C | O4'-C1'-N1 | 6.18 | 113.14 | 108.20 |
| 57 | BA | 182 | A | C4-C5-C6 | -6.18 | 113.91 | 117.00 |
| 9 | AR | 60 | ARG | NE-CZ-NH1 | 6.18 | 123.39 | 120.30 |
| 22 | AA | 1121 | U | O4'-C1'-N1 | 6.18 | 113.14 | 108.20 |
| 22 | AA | 1208 | C | N1-C2-O2 | 6.18 | 122.61 | 118.90 |
| 57 | BA | 1080 | A | O4'-C1'-N9 | 6.18 | 113.14 | 108.20 |
| 57 | BA | 1365 | A | C4-C5-C6 | -6.18 | 113.91 | 117.00 |
| 57 | BA | 1457 | U | O4'-C1'-N1 | 6.18 | 113.14 | 108.20 |
| 57 | BA | 1528 | A | C4-C5-C6 | -6.18 | 113.91 | 117.00 |
| 57 | BA | 2055 | C | C3'-C2'-C1' | -6.18 | 96.56 | 101.50 |
| 26 | BJ | 52 | ARG | NE-CZ-NH1 | 6.17 | 123.39 | 120.30 |
| 57 | BA | 512 | G | O4'-C1'-N9 | 6.17 | 113.14 | 108.20 |
| 57 | BA | 1006 | C | N3-C2-O2 | -6.17 | 117.58 | 121.90 |
| 13 | AU | 6 | ARG | NE-CZ-NH1 | 6.17 | 123.39 | 120.30 |
| 22 | AA | 398 | U | C1'-O4'-C4' | -6.17 | 104.96 | 109.90 |
| 22 | AA | 880 | C | O4'-C1'-N1 | 6.17 | 113.14 | 108.20 |
| 22 | AA | 1140 | C | N1-C2-O2 | 6.17 | 122.60 | 118.90 |
| 57 | BA | 310 | A | C4-C5-C6 | -6.17 | 113.92 | 117.00 |
| 19 | AH | 14 | ARG | NE-CZ-NH1 | 6.17 | 123.39 | 120.30 |
| 57 | BA | 377 | G | N1-C6-O6 | -6.17 | 116.20 | 119.90 |
| 57 | BA | 2146 | C | N1-C2-O2 | 6.17 | 122.60 | 118.90 |
| 22 | AA | 275 | G | C5'-C4'-C3' | -6.17 | 106.13 | 116.00 |
| 22 | AA | 979 | C | O4'-C1'-N1 | 6.17 | 113.14 | 108.20 |
| 22 | AA | 1531 | A | C4-C5-C6 | -6.17 | 113.92 | 117.00 |
| 57 | BA | 368 | A | C4-C5-C6 | -6.17 | 113.92 | 117.00 |
| 57 | BA | 1637 | A | C4-C5-C6 | -6.17 | 113.92 | 117.00 |
| 57 | BA | 239 | C | N1-C2-O2 | 6.17 | 122.60 | 118.90 |
| 57 | BA | 693 | A | C4-C5-C6 | -6.17 | 113.92 | 117.00 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 867 | C | N3-C2-O2 | -6.17 | 117.58 | 121.90 |
| 57 | BA | 1666 | G | N1-C6-O6 | -6.17 | 116.20 | 119.90 |
| 57 | BA | 1924 | C | N1-C2-O2 | 6.17 | 122.60 | 118.90 |
| 57 | BA | 2042 | A | C4-C5-C6 | -6.17 | 113.92 | 117.00 |
| 57 | BA | 2472 | G | C4'-C3'-C2' | -6.17 | 96.43 | 102.60 |
| 57 | BA | 2657 | A | C4-C5-C6 | -6.17 | 113.92 | 117.00 |
| 22 | AA | 493 | A | C3'-C2'-C1' | 6.17 | 106.43 | 101.50 |
| 36 | BU | 50 | ARG | NE-CZ-NH1 | 6.17 | 123.38 | 120.30 |
| 57 | BA | 101 | A | C4-C5-C6 | -6.16 | 113.92 | 117.00 |
| 57 | BA | 944 | C | N1-C2-O2 | 6.16 | 122.60 | 118.90 |
| 57 | BA | 1731 | G | N3-C4-C5 | -6.16 | 125.52 | 128.60 |
| 22 | AA | 327 | A | C4-C5-C6 | -6.16 | 113.92 | 117.00 |
| 57 | BA | 181 | A | C4-C5-C6 | -6.16 | 113.92 | 117.00 |
| 57 | BA | 421 | C | N1-C2-O2 | 6.16 | 122.60 | 118.90 |
| 22 | AA | 1157 | A | C4-C5-C6 | -6.16 | 113.92 | 117.00 |
| 57 | BA | 1785 | A | C4-C5-C6 | -6.16 | 113.92 | 117.00 |
| 57 | BA | 2723 | C | N1-C2-O2 | 6.16 | 122.60 | 118.90 |
| 58 | Ba | 10 | G | C5'-C4'-C3' | -6.16 | 106.14 | 116.00 |
| 11 | AB | 20 | ARG | NE-CZ-NH2 | -6.16 | 117.22 | 120.30 |
| 22 | AA | 1384 | C | N1-C2-O2 | 6.16 | 122.59 | 118.90 |
| 57 | BA | 791 | C | N3-C2-O2 | -6.16 | 117.59 | 121.90 |
| 11 | AB | 138 | ARG | NE-CZ-NH1 | 6.16 | 123.38 | 120.30 |
| 57 | BA | 670 | A | C4-C5-C6 | -6.16 | 113.92 | 117.00 |
| 57 | BA | 2800 | A | C4-C5-C6 | -6.16 | 113.92 | 117.00 |
| 31 | BQ | 16 | ARG | NE-CZ-NH2 | -6.16 | 117.22 | 120.30 |
| 57 | BA | 1854 | A | C4-C5-C6 | -6.16 | 113.92 | 117.00 |
| 22 | AA | 388 | G | N3-C4-C5 | -6.15 | 125.52 | 128.60 |
| 22 | AA | 1424 | U | O4'-C1'-N1 | 6.15 | 113.12 | 108.20 |
| 55 | BH | 152 | ARG | NE-CZ-NH2 | 6.15 | 123.38 | 120.30 |
| 57 | BA | 2190 | G | O4'-C1'-N9 | 6.15 | 113.12 | 108.20 |
| 57 | BA | 385 | C | N1-C2-O2 | 6.15 | 122.59 | 118.90 |
| 57 | BA | 1126 | A | C4-C5-C6 | -6.15 | 113.92 | 117.00 |
| 57 | BA | 2264 | C | N3-C4-N4 | -6.15 | 113.69 | 118.00 |
| 22 | AA | 878 | A | C4-C5-C6 | -6.15 | 113.92 | 117.00 |
| 22 | AA | 1282 | C | N1-C2-O2 | 6.15 | 122.59 | 118.90 |
| 24 | A3 | 49 | C | N1-C2-O2 | 6.15 | 122.59 | 118.90 |
| 57 | BA | 1350 | C | N1-C2-O2 | 6.15 | 122.59 | 118.90 |
| 57 | BA | 1362 | C | O4'-C1'-N1 | 6.15 | 113.12 | 108.20 |
| 23 | A2 | 45 | G | C3'-C2'-C1' | 6.15 | 106.42 | 101.50 |
| 45 | BE | 179 | ARG | NE-CZ-NH1 | 6.15 | 123.37 | 120.30 |
| 22 | AA | 140 | U | O4'-C1'-N1 | 6.15 | 113.12 | 108.20 |
| 22 | AA | 429 | U | C5-C6-N1 | -6.15 | 119.63 | 122.70 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | AA | 1141 | C | O4'-C1'-N1 | 6.15 | 113.12 | 108.20 |
| 22 | AA | 1191 | A | C4-C5-C6 | -6.15 | 113.93 | 117.00 |
| 22 | AA | 1503 | A | C4-C5-C6 | -6.15 | 113.93 | 117.00 |
| 57 | BA | 20 | C | O4'-C1'-N1 | 6.15 | 113.12 | 108.20 |
| 57 | BA | 751 | A | C4-C5-C6 | -6.15 | 113.93 | 117.00 |
| 57 | BA | 2354 | C | O4'-C1'-N1 | 6.15 | 113.12 | 108.20 |
| 22 | AA | 280 | C | N1-C2-O2 | 6.14 | 122.59 | 118.90 |
| 54 | BG | 79 | ARG | NE-CZ-NH2 | 6.14 | 123.37 | 120.30 |
| 57 | BA | 2294 | G | O4'-C1'-N9 | 6.14 | 113.12 | 108.20 |
| 22 | AA | 736 | C | O4'-C1'-N1 | 6.14 | 113.11 | 108.20 |
| 25 | BC | 9 | ARG | NE-CZ-NH1 | 6.14 | 123.37 | 120.30 |
| 57 | BA | 1234 | U | O4'-C1'-N1 | 6.14 | 113.11 | 108.20 |
| 57 | BA | 1958 | C | N1-C2-O2 | 6.14 | 122.58 | 118.90 |
| 22 | AA | 1205 | U | O4'-C1'-N1 | 6.14 | 113.11 | 108.20 |
| 22 | AA | 1499 | A | C4-C5-C6 | -6.14 | 113.93 | 117.00 |
| 57 | BA | 472 | A | C4-C5-C6 | -6.14 | 113.93 | 117.00 |
| 57 | BA | 552 | U | O4'-C1'-N1 | 6.14 | 113.11 | 108.20 |
| 57 | BA | 2628 | C | N3-C2-O2 | -6.14 | 117.60 | 121.90 |
| 57 | BA | 1606 | C | O4'-C1'-N1 | 6.14 | 113.11 | 108.20 |
| 22 | AA | 330 | C | N3-C2-O2 | -6.14 | 117.60 | 121.90 |
| 22 | AA | 502 | A | C4-C5-C6 | -6.14 | 113.93 | 117.00 |
| 57 | BA | 74 | A | C2-N3-C4 | 6.14 | 113.67 | 110.60 |
| 57 | BA | 2740 | A | C4-C5-C6 | -6.13 | 113.93 | 117.00 |
| 57 | BA | 2154 | A | C4-C5-C6 | -6.13 | 113.93 | 117.00 |
| 57 | BA | 2537 | U | O4'-C1'-N1 | 6.13 | 113.11 | 108.20 |
| 22 | AA | 18 | C | O4'-C1'-N1 | 6.13 | 113.11 | 108.20 |
| 22 | AA | 416 | G | N1-C6-O6 | -6.13 | 116.22 | 119.90 |
| 57 | BA | 2510 | C | N1-C2-O2 | 6.13 | 122.58 | 118.90 |
| 20 | AI | 79 | ARG | NE-CZ-NH1 | 6.13 | 123.36 | 120.30 |
| 22 | AA | 44 | A | C4-C5-C6 | -6.13 | 113.94 | 117.00 |
| 43 | B1 | 71 | ARG | NE-CZ-NH1 | 6.13 | 123.36 | 120.30 |
| 57 | BA | 270 | A | C4-C5-C6 | -6.13 | 113.94 | 117.00 |
| 57 | BA | 957 | C | N3-C2-O2 | -6.13 | 117.61 | 121.90 |
| 57 | BA | 1367 | A | C4-C5-C6 | -6.13 | 113.94 | 117.00 |
| 57 | BA | 2071 | A | C4-C5-C6 | -6.13 | 113.94 | 117.00 |
| 15 | AD | 2 | ARG | NE-CZ-NH1 | 6.13 | 123.36 | 120.30 |
| 57 | BA | 1499 | C | O4'-C1'-N1 | 6.13 | 113.10 | 108.20 |
| 22 | AA | 127 | G | O4'-C1'-N9 | 6.12 | 113.10 | 108.20 |
| 22 | AA | 824 | G | O4'-C1'-N9 | 6.12 | 113.10 | 108.20 |
| 57 | BA | 659 | G | N1-C6-O6 | -6.12 | 116.23 | 119.90 |
| 57 | BA | 1348 | C | N3-C2-O2 | -6.12 | 117.61 | 121.90 |
| 57 | BA | 1736 | U | O4'-C1'-N1 | 6.12 | 113.10 | 108.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 2901 | C | O4'-C1'-N1 | 6.12 | 113.10 | 108.20 |
| 57 | BA | 526 | A | C4-C5-C6 | -6.12 | 113.94 | 117.00 |
| 22 | AA | 1535 | C | N3-C2-O2 | -6.12 | 117.62 | 121.90 |
| 57 | BA | 1065 | U | N3-C2-O2 | -6.12 | 117.92 | 122.20 |
| 57 | BA | 2667 | C | O4'-C1'-N1 | 6.12 | 113.09 | 108.20 |
| 22 | AA | 1082 | A | C4-C5-C6 | -6.12 | 113.94 | 117.00 |
| 57 | BA | 399 | U | O4'-C1'-N1 | 6.12 | 113.09 | 108.20 |
| 57 | BA | 1730 | C | N3-C2-O2 | -6.12 | 117.62 | 121.90 |
| 22 | AA | 328 | C | P-O3'-C3' | 6.12 | 127.04 | 119.70 |
| 22 | AA | 1014 | A | C4-C5-C6 | -6.12 | 113.94 | 117.00 |
| 57 | BA | 968 | C | N1-C2-O2 | 6.12 | 122.57 | 118.90 |
| 24 | A3 | 52 | C | N1-C2-O2 | 6.11 | 122.57 | 118.90 |
| 56 | BL | 50 | ARG | NE-CZ-NH1 | 6.11 | 123.36 | 120.30 |
| 57 | BA | 987 | C | N1-C2-O2 | 6.11 | 122.57 | 118.90 |
| 22 | AA | 366 | A | C4-C5-C6 | -6.11 | 113.94 | 117.00 |
| 22 | AA | 788 | U | O4'-C1'-N1 | 6.11 | 113.09 | 108.20 |
| 57 | BA | 1607 | C | N3-C2-O2 | -6.11 | 117.62 | 121.90 |
| 22 | AA | 1324 | A | C4-C5-C6 | -6.11 | 113.94 | 117.00 |
| 57 | BA | 792 | A | C4-C5-C6 | -6.11 | 113.94 | 117.00 |
| 57 | BA | 954 | G | N1-C6-O6 | -6.11 | 116.23 | 119.90 |
| 22 | AA | 171 | A | C4-C5-C6 | -6.11 | 113.95 | 117.00 |
| 22 | AA | 285 | C | O4'-C1'-N1 | 6.11 | 113.09 | 108.20 |
| 22 | AA | 618 | C | N3-C2-O2 | -6.11 | 117.62 | 121.90 |
| 22 | AA | 230 | G | N1-C6-O6 | -6.11 | 116.24 | 119.90 |
| 22 | AA | 860 | A | C4-C5-C6 | -6.11 | 113.95 | 117.00 |
| 57 | BA | 2873 | A | C4-C5-C6 | -6.11 | 113.95 | 117.00 |
| 21 | A1 | 627 | ARG | NE-CZ-NH1 | 6.11 | 123.35 | 120.30 |
| 22 | AA | 900 | A | C4-C5-C6 | -6.11 | 113.95 | 117.00 |
| 45 | BE | 13 | ARG | NE-CZ-NH2 | 6.11 | 123.35 | 120.30 |
| 57 | BA | 229 | C | N3-C2-O2 | -6.11 | 117.63 | 121.90 |
| 57 | BA | 418 | C | O4'-C1'-N1 | 6.11 | 113.08 | 108.20 |
| 57 | BA | 1450 | G | N1-C6-O6 | -6.11 | 116.24 | 119.90 |
| 22 | AA | 190 | A | C4-C5-C6 | -6.10 | 113.95 | 117.00 |
| 57 | BA | 195 | A | C4-C5-C6 | -6.10 | 113.95 | 117.00 |
| 57 | BA | 1049 | C | N1-C2-O2 | 6.10 | 122.56 | 118.90 |
| 1 | AJ | 62 | ARG | NE-CZ-NH1 | 6.10 | 123.35 | 120.30 |
| 22 | AA | 879 | C | N1-C2-O2 | 6.10 | 122.56 | 118.90 |
| 22 | AA | 1390 | U | O4'-C1'-N1 | 6.10 | 113.08 | 108.20 |
| 22 | AA | 1458 | G | O4'-C1'-N9 | 6.10 | 113.08 | 108.20 |
| 57 | BA | 144 | A | C4-C5-C6 | -6.10 | 113.95 | 117.00 |
| 57 | BA | 1929 | G | N3-C4-C5 | -6.10 | 125.55 | 128.60 |
| 14 | AC | 64 | ARG | NE-CZ-NH1 | 6.10 | 123.35 | 120.30 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | AA | 614 | C | O4'-C1'-N1 | 6.10 | 113.08 | 108.20 |
| 38 | BW | 8 | ARG | NE-CZ-NH1 | 6.10 | 123.35 | 120.30 |
| 22 | AA | 631 | C | N3-C2-O2 | -6.10 | 117.63 | 121.90 |
| 22 | AA | 1281 | C | N3-C2-O2 | -6.10 | 117.63 | 121.90 |
| 57 | BA | 435 | C | N3-C2-O2 | -6.10 | 117.63 | 121.90 |
| 57 | BA | 1867 | G | O4'-C1'-N9 | 6.10 | 113.08 | 108.20 |
| 22 | AA | 1285 | A | C4-C5-C6 | -6.10 | 113.95 | 117.00 |
| 22 | AA | 1336 | C | N3-C2-O2 | -6.10 | 117.63 | 121.90 |
| 57 | BA | 607 | U | O4'-C1'-N1 | 6.10 | 113.08 | 108.20 |
| 57 | BA | 1463 | C | O4'-C1'-N1 | 6.10 | 113.08 | 108.20 |
| 57 | BA | 1771 | C | N1-C2-O2 | 6.10 | 122.56 | 118.90 |
| 57 | BA | 2060 | A | C4-C5-C6 | -6.10 | 113.95 | 117.00 |
| 57 | BA | 2254 | C | N3-C2-O2 | -6.10 | 117.63 | 121.90 |
| 57 | BA | 2712 | C | N3-C2-O2 | -6.10 | 117.63 | 121.90 |
| 57 | BA | 1871 | A | C4-C5-C6 | -6.10 | 113.95 | 117.00 |
| 57 | BA | 2222 | C | O4'-C1'-N1 | 6.10 | 113.08 | 108.20 |
| 22 | AA | 817 | C | N3-C2-O2 | -6.09 | 117.63 | 121.90 |
| 57 | BA | 40 | U | O4'-C1'-N1 | 6.09 | 113.08 | 108.20 |
| 57 | BA | 606 | U | O4'-C1'-N1 | 6.09 | 113.08 | 108.20 |
| 57 | BA | 983 | A | C4-C5-C6 | -6.09 | 113.95 | 117.00 |
| 57 | BA | 943 | A | C4-C5-C6 | -6.09 | 113.95 | 117.00 |
| 57 | BA | 1542 | U | O4'-C1'-N1 | 6.09 | 113.07 | 108.20 |
| 57 | BA | 2313 | C | N1-C2-O2 | 6.09 | 122.56 | 118.90 |
| 22 | AA | 308 | C | O4'-C1'-N1 | 6.09 | 113.07 | 108.20 |
| 57 | BA | 1722 | A | C4-C5-C6 | -6.09 | 113.95 | 117.00 |
| 57 | BA | 1899 | A | C4-C5-C6 | -6.09 | 113.95 | 117.00 |
| 57 | BA | 2776 | A | C4-C5-C6 | -6.09 | 113.95 | 117.00 |
| 22 | AA | 823 | C | N3-C2-O2 | -6.09 | 117.64 | 121.90 |
| 57 | BA | 1981 | A | C4-C5-C6 | -6.09 | 113.96 | 117.00 |
| 57 | BA | 2660 | A | C3'-C2'-C1' | 6.09 | 106.37 | 101.50 |
| 57 | BA | 2786 | U | O4'-C1'-N1 | 6.09 | 113.07 | 108.20 |
| 57 | BA | 2820 | A | C4-C5-C6 | -6.09 | 113.96 | 117.00 |
| 57 | BA | 2117 | A | C4-C5-C6 | -6.08 | 113.96 | 117.00 |
| 22 | AA | 408 | A | C4-C5-C6 | -6.08 | 113.96 | 117.00 |
| 22 | AA | 571 | U | O4'-C1'-N1 | 6.08 | 113.07 | 108.20 |
| 22 | AA | 576 | C | O4'-C1'-N1 | 6.08 | 113.07 | 108.20 |
| 57 | BA | 332 | A | C4-C5-C6 | -6.08 | 113.96 | 117.00 |
| 57 | BA | 1083 | U | C1'-O4'-C4' | -6.08 | 105.03 | 109.90 |
| 57 | BA | 1859 | U | O4'-C1'-N1 | 6.08 | 113.07 | 108.20 |
| 57 | BA | 2576 | G | N3-C4-C5 | -6.08 | 125.56 | 128.60 |
| 50 | B7 | 28 | ARG | NE-CZ-NH1 | 6.08 | 123.34 | 120.30 |
| 57 | BA | 318 | C | O4'-C1'-N1 | 6.08 | 113.06 | 108.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 373 | U | O4'-C1'-N1 | 6.08 | 113.06 | 108.20 |
| 57 | BA | 394 | C | N1-C2-O2 | 6.08 | 122.55 | 118.90 |
| 22 | AA | 425 | G | N1-C6-O6 | -6.08 | 116.25 | 119.90 |
| 22 | AA | 1457 | G | O4'-C1'-N9 | 6.08 | 113.06 | 108.20 |
| 57 | BA | 28 | A | O4'-C1'-N9 | 6.08 | 113.06 | 108.20 |
| 57 | BA | 2013 | A | N1-C6-N6 | -6.08 | 114.95 | 118.60 |
| 57 | BA | 2015 | A | O4'-C1'-N9 | 6.08 | 113.06 | 108.20 |
| 22 | AA | 59 | A | C4-C5-C6 | -6.08 | 113.96 | 117.00 |
| 22 | AA | 471 | U | O4'-C1'-N1 | 6.08 | 113.06 | 108.20 |
| 22 | AA | 907 | A | C4-C5-C6 | -6.08 | 113.96 | 117.00 |
| 26 | BJ | 41 | ARG | NE-CZ-NH1 | 6.08 | 123.34 | 120.30 |
| 57 | BA | 55 | G | N1-C6-O6 | -6.08 | 116.25 | 119.90 |
| 57 | BA | 2159 | G | O4'-C1'-N9 | 6.08 | 113.06 | 108.20 |
| 21 | A1 | 336 | ARG | NE-CZ-NH1 | 6.07 | 123.34 | 120.30 |
| 22 | AA | 563 | A | C4-C5-C6 | -6.07 | 113.96 | 117.00 |
| 22 | AA | 870 | U | O4'-C1'-N1 | 6.07 | 113.06 | 108.20 |
| 22 | AA | 1101 | A | C4-C5-C6 | -6.07 | 113.96 | 117.00 |
| 57 | BA | 156 | A | C4-C5-C6 | -6.07 | 113.96 | 117.00 |
| 57 | BA | 1507 | C | N1-C2-O2 | 6.07 | 122.55 | 118.90 |
| 57 | BA | 1603 | A | C5-C6-N1 | 6.07 | 120.74 | 117.70 |
| 9 | AR | 69 | TYR | CB-CG-CD1 | -6.07 | 117.36 | 121.00 |
| 12 | AT | 59 | ARG | NE-CZ-NH1 | 6.07 | 123.33 | 120.30 |
| 22 | AA | 852 | G | N1-C6-O6 | -6.07 | 116.26 | 119.90 |
| 22 | AA | 955 | U | O4'-C1'-N1 | 6.07 | 113.06 | 108.20 |
| 22 | AA | 969 | A | C1'-O4'-C4' | -6.07 | 105.04 | 109.90 |
| 57 | BA | 130 | C | N1-C2-O2 | 6.07 | 122.54 | 118.90 |
| 57 | BA | 2587 | A | C4-C5-C6 | -6.07 | 113.97 | 117.00 |
| 22 | AA | 1521 | C | N1-C2-O2 | 6.07 | 122.54 | 118.90 |
| 57 | BA | 621 | A | C4-C5-C6 | -6.07 | 113.97 | 117.00 |
| 57 | BA | 661 | A | C4-C5-C6 | -6.07 | 113.97 | 117.00 |
| 57 | BA | 900 | A | C4-C5-C6 | -6.07 | 113.97 | 117.00 |
| 57 | BA | 998 | C | O4'-C1'-N1 | 6.07 | 113.06 | 108.20 |
| 57 | BA | 2281 | A | O4'-C1'-N9 | 6.07 | 113.06 | 108.20 |
| 22 | AA | 242 | G | N1-C6-O6 | -6.07 | 116.26 | 119.90 |
| 22 | AA | 1512 | U | O4'-C1'-N1 | 6.07 | 113.05 | 108.20 |
| 57 | BA | 461 | C | N3-C2-O2 | -6.07 | 117.65 | 121.90 |
| 57 | BA | 673 | C | N3-C2-O2 | -6.07 | 117.65 | 121.90 |
| 57 | BA | 1083 | U | O4'-C1'-N1 | 6.07 | 113.05 | 108.20 |
| 57 | BA | 66 | C | N1-C2-O2 | 6.07 | 122.54 | 118.90 |
| 57 | BA | 2392 | A | C4-C5-C6 | -6.07 | 113.97 | 117.00 |
| 57 | BA | 2667 | C | N3-C4-C5 | 6.07 | 124.33 | 121.90 |
| 57 | BA | 2189 | U | O4'-C1'-N1 | 6.06 | 113.05 | 108.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | AA | 267 | C | N1-C2-O2 | 6.06 | 122.54 | 118.90 |
| 57 | BA | 802 | A | C4-C5-C6 | -6.06 | 113.97 | 117.00 |
| 22 | AA | 832 | G | N1-C6-O6 | -6.06 | 116.27 | 119.90 |
| 57 | BA | 942 | G | N3-C4-C5 | -6.06 | 125.57 | 128.60 |
| 24 | A3 | 7 | G | O4'-C1'-N9 | 6.06 | 113.05 | 108.20 |
| 57 | BA | 1694 | C | N3-C2-O2 | -6.06 | 117.66 | 121.90 |
| 57 | BA | 2676 | C | O4'-C1'-N1 | 6.06 | 113.05 | 108.20 |
| 22 | AA | 672 | U | O4'-C1'-N1 | 6.05 | 113.04 | 108.20 |
| 22 | AA | 1414 | U | O4'-C1'-N1 | 6.05 | 113.04 | 108.20 |
| 22 | AA | 1460 | C | O4'-C1'-N1 | 6.05 | 113.04 | 108.20 |
| 57 | BA | 896 | A | C4-C5-C6 | -6.05 | 113.97 | 117.00 |
| 57 | BA | 1625 | C | N1-C2-O2 | 6.05 | 122.53 | 118.90 |
| 57 | BA | 288 | U | O4'-C1'-N1 | 6.05 | 113.04 | 108.20 |
| 18 | AG | 159 | ARG | NE-CZ-NH1 | 6.05 | 123.33 | 120.30 |
| 22 | AA | 595 | A | C4-C5-C6 | -6.05 | 113.97 | 117.00 |
| 22 | AA | 687 | A | C4-C5-C6 | -6.05 | 113.97 | 117.00 |
| 22 | AA | 896 | C | O4'-C1'-N1 | 6.05 | 113.04 | 108.20 |
| 22 | AA | 968 | A | C4-C5-C6 | -6.05 | 113.97 | 117.00 |
| 35 | BD | 220 | ARG | NH1-CZ-NH2 | -6.05 | 112.74 | 119.40 |
| 36 | BU | 91 | ARG | NE-CZ-NH1 | 6.05 | 123.33 | 120.30 |
| 57 | BA | 664 | G | N1-C6-O6 | -6.05 | 116.27 | 119.90 |
| 57 | BA | 1773 | A | C4-C5-C6 | -6.05 | 113.97 | 117.00 |
| 57 | BA | 2603 | G | N1-C6-O6 | -6.05 | 116.27 | 119.90 |
| 58 | Ba | 109 | A | C4-C5-C6 | -6.05 | 113.97 | 117.00 |
| 22 | AA | 51 | A | C1'-O4'-C4' | -6.05 | 105.06 | 109.90 |
| 22 | AA | 483 | C | N1-C2-O2 | 6.05 | 122.53 | 118.90 |
| 33 | BS | 81 | ARG | NE-CZ-NH1 | 6.05 | 123.33 | 120.30 |
| 57 | BA | 1758 | U | O4'-C1'-N1 | 6.05 | 113.04 | 108.20 |
| 57 | BA | 2352 | A | N1-C6-N6 | -6.05 | 114.97 | 118.60 |
| 22 | AA | 52 | C | N1-C2-O2 | 6.05 | 122.53 | 118.90 |
| 57 | BA | 940 | G | N9-C1'-C2' | -6.05 | 105.35 | 112.00 |
| 22 | AA | 1195 | C | N1-C2-O2 | 6.05 | 122.53 | 118.90 |
| 22 | AA | 1223 | C | N3-C4-N4 | -6.05 | 113.77 | 118.00 |
| 22 | AA | 1251 | A | C4-C5-C6 | -6.05 | 113.98 | 117.00 |
| 57 | BA | 1266 | G | O4'-C1'-N9 | 6.05 | 113.04 | 108.20 |
| 57 | BA | 1443 | U | O4'-C1'-N1 | 6.05 | 113.04 | 108.20 |
| 57 | BA | 1462 | C | N1-C2-O2 | 6.05 | 122.53 | 118.90 |
| 57 | BA | 2882 | A | C6-C5-N7 | 6.05 | 136.53 | 132.30 |
| 58 | Ba | 94 | A | C4-C5-C6 | -6.05 | 113.98 | 117.00 |
| 57 | BA | 2253 | G | C1'-O4'-C4' | -6.04 | 105.06 | 109.90 |
| 22 | AA | 117 | G | N1-C6-O6 | -6.04 | 116.27 | 119.90 |
| 23 | A2 | 13 | A | C4-C5-C6 | -6.04 | 113.98 | 117.00 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 218 | A | C4-C5-C6 | -6.04 | 113.98 | 117.00 |
| 57 | BA | 784 | G | N3-C4-C5 | -6.04 | 125.58 | 128.60 |
| 57 | BA | 791 | C | N3-C4-C5 | 6.04 | 124.32 | 121.90 |
| 57 | BA | 1089 | A | C4-C5-C6 | -6.04 | 113.98 | 117.00 |
| 22 | AA | 1277 | C | O4'-C1'-N1 | 6.04 | 113.03 | 108.20 |
| 57 | BA | 157 | C | N1-C2-O2 | 6.04 | 122.53 | 118.90 |
| 57 | BA | 1320 | C | N1-C2-O2 | 6.04 | 122.53 | 118.90 |
| 57 | BA | 2164 | C | N3-C2-O2 | -6.04 | 117.67 | 121.90 |
| 57 | BA | 2886 | A | C4-C5-C6 | -6.04 | 113.98 | 117.00 |
| 22 | AA | 482 | A | C4-C5-C6 | -6.04 | 113.98 | 117.00 |
| 22 | AA | 1471 | U | O4'-C1'-N1 | 6.04 | 113.03 | 108.20 |
| 57 | BA | 336 | C | O4'-C1'-N1 | 6.04 | 113.03 | 108.20 |
| 23 | A2 | 24 | A | C4-C5-C6 | -6.04 | 113.98 | 117.00 |
| 29 | BO | 70 | ARG | NE-CZ-NH1 | 6.04 | 123.32 | 120.30 |
| 22 | AA | 504 | C | N1-C2-O2 | 6.04 | 122.52 | 118.90 |
| 22 | AA | 1478 | U | O4'-C1'-N1 | 6.04 | 113.03 | 108.20 |
| 22 | AA | 1529 | G | O4'-C1'-N9 | 6.04 | 113.03 | 108.20 |
| 57 | BA | 721 | A | C4-C5-C6 | -6.04 | 113.98 | 117.00 |
| 5 | AN | 62 | ARG | NE-CZ-NH2 | 6.03 | 123.32 | 120.30 |
| 22 | AA | 151 | A | C6-C5-N7 | 6.03 | 136.52 | 132.30 |
| 22 | AA | 1224 | U | O4'-C1'-N1 | 6.03 | 113.03 | 108.20 |
| 22 | AA | 1228 | C | N1-C2-O2 | 6.03 | 122.52 | 118.90 |
| 57 | BA | 1575 | C | O4'-C1'-N1 | 6.03 | 113.03 | 108.20 |
| 57 | BA | 2368 | C | O4'-C1'-N1 | 6.03 | 113.03 | 108.20 |
| 57 | BA | 366 | C | O4'-C1'-N1 | 6.03 | 113.03 | 108.20 |
| 57 | BA | 601 | C | N1-C2-O2 | 6.03 | 122.52 | 118.90 |
| 57 | BA | 1124 | G | N1-C6-O6 | -6.03 | 116.28 | 119.90 |
| 57 | BA | 1670 | C | N3-C2-O2 | -6.03 | 117.68 | 121.90 |
| 23 | A2 | 23 | C | N3-C2-O2 | -6.03 | 117.68 | 121.90 |
| 22 | AA | 993 | G | N3-C4-C5 | -6.03 | 125.59 | 128.60 |
| 47 | B4 | 25 | ARG | NE-CZ-NH1 | 6.03 | 123.31 | 120.30 |
| 57 | BA | 207 | A | C4-C5-C6 | -6.03 | 113.99 | 117.00 |
| 57 | BA | 286 | U | O4'-C1'-N1 | 6.03 | 113.02 | 108.20 |
| 57 | BA | 529 | A | C4-C5-C6 | -6.03 | 113.99 | 117.00 |
| 57 | BA | 789 | A | N1-C6-N6 | -6.03 | 114.98 | 118.60 |
| 57 | BA | 1039 | A | C4-C5-C6 | -6.03 | 113.99 | 117.00 |
| 57 | BA | 1489 | C | O4'-C1'-N1 | 6.03 | 113.02 | 108.20 |
| 57 | BA | 1678 | A | C4-C5-C6 | -6.03 | 113.99 | 117.00 |
| 57 | BA | 2427 | C | N1-C2-O2 | 6.03 | 122.52 | 118.90 |
| 57 | BA | 2717 | C | N1-C2-O2 | 6.03 | 122.52 | 118.90 |
| 57 | BA | 2806 | C | N1-C2-O2 | 6.03 | 122.52 | 118.90 |
| 57 | BA | 130 | C | O4'-C1'-N1 | 6.03 | 113.02 | 108.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 865 | C | N3-C2-O2 | -6.03 | 117.68 | 121.90 |
| 22 | AA | 726 | C | N1-C2-O2 | 6.02 | 122.52 | 118.90 |
| 57 | BA | 1990 | C | O4'-C1'-N1 | 6.02 | 113.02 | 108.20 |
| 57 | BA | 2295 | C | O4'-C1'-N1 | 6.02 | 113.02 | 108.20 |
| 57 | BA | 947 | A | C4-C5-C6 | -6.02 | 113.99 | 117.00 |
| 57 | BA | 1150 | C | O4'-C1'-N1 | 6.02 | 113.02 | 108.20 |
| 57 | BA | 2868 | A | C4-C5-C6 | -6.02 | 113.99 | 117.00 |
| 22 | AA | 1044 | A | C4-C5-C6 | -6.02 | 113.99 | 117.00 |
| 57 | BA | 901 | C | N3-C2-O2 | -6.02 | 117.69 | 121.90 |
| 22 | AA | 3 | A | C4-C5-C6 | -6.02 | 113.99 | 117.00 |
| 22 | AA | 1389 | C | O4'-C1'-N1 | 6.02 | 113.02 | 108.20 |
| 57 | BA | 753 | A | C4-C5-C6 | -6.02 | 113.99 | 117.00 |
| 57 | BA | 2044 | C | N1-C2-O2 | 6.02 | 122.51 | 118.90 |
| 22 | AA | 1056 | U | O4'-C1'-N1 | 6.02 | 113.01 | 108.20 |
| 22 | AA | 1332 | A | N1-C6-N6 | -6.02 | 114.99 | 118.60 |
| 24 | A3 | 57 | C | N1-C2-O2 | 6.02 | 122.51 | 118.90 |
| 57 | BA | 1019 | U | O4'-C1'-N1 | 6.02 | 113.01 | 108.20 |
| 57 | BA | 1856 | U | O4'-C1'-N1 | 6.02 | 113.01 | 108.20 |
| 58 | Ba | 120 | U | N3-C2-O2 | -6.02 | 117.99 | 122.20 |
| 57 | BA | 2469 | A | C4-C5-C6 | -6.02 | 113.99 | 117.00 |
| 22 | AA | 436 | C | O4'-C1'-N1 | 6.01 | 113.01 | 108.20 |
| 57 | BA | 1872 | A | C4-C5-C6 | -6.01 | 113.99 | 117.00 |
| 57 | BA | 1892 | C | O4'-C1'-N1 | 6.01 | 113.01 | 108.20 |
| 57 | BA | 2811 | G | O4'-C1'-N9 | 6.01 | 113.01 | 108.20 |
| 22 | AA | 895 | G | N1-C6-O6 | -6.01 | 116.29 | 119.90 |
| 22 | AA | 1477 | U | O4'-C1'-N1 | 6.01 | 113.01 | 108.20 |
| 57 | BA | 392 | U | O4'-C1'-N1 | 6.01 | 113.01 | 108.20 |
| 57 | BA | 1573 | G | O4'-C1'-N9 | 6.01 | 113.01 | 108.20 |
| 57 | BA | 1789 | A | C4-C5-C6 | -6.01 | 113.99 | 117.00 |
| 57 | BA | 253 | C | N1-C2-O2 | 6.01 | 122.51 | 118.90 |
| 57 | BA | 1481 | U | O4'-C1'-N1 | 6.01 | 113.01 | 108.20 |
| 57 | BA | 2841 | C | N1-C2-O2 | 6.01 | 122.51 | 118.90 |
| 10 | AS | 77 | ARG | NH1-CZ-NH2 | -6.01 | 112.79 | 119.40 |
| 57 | BA | 2611 | C | N1-C2-O2 | 6.01 | 122.50 | 118.90 |
| 57 | BA | 1595 | C | N1-C2-O2 | 6.01 | 122.50 | 118.90 |
| 57 | BA | 1642 | G | O4'-C1'-N9 | 6.01 | 113.00 | 108.20 |
| 57 | BA | 1904 | G | O4'-C1'-N9 | 6.01 | 113.01 | 108.20 |
| 57 | BA | 2661 | G | N1-C6-O6 | -6.01 | 116.30 | 119.90 |
| 57 | BA | 2793 | C | O4'-C1'-N1 | 6.01 | 113.00 | 108.20 |
| 58 | Ba | 71 | C | O4'-C1'-N1 | 6.01 | 113.00 | 108.20 |
| 22 | AA | 521 | G | N1-C6-O6 | -6.00 | 116.30 | 119.90 |
| 22 | AA | 1427 | C | N1-C2-O2 | 6.00 | 122.50 | 118.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 2196 | C | N3-C4-N4 | -6.00 | 113.80 | 118.00 |
| 22 | AA | 205 | A | C4-C5-C6 | -6.00 | 114.00 | 117.00 |
| 24 | A3 | 66 | C | N1-C2-O2 | 6.00 | 122.50 | 118.90 |
| 57 | BA | 443 | A | C4-C5-C6 | -6.00 | 114.00 | 117.00 |
| 57 | BA | 730 | A | C4-C5-C6 | -6.00 | 114.00 | 117.00 |
| 57 | BA | 962 | G | C5'-C4'-O4' | 6.00 | 116.31 | 109.10 |
| 57 | BA | 1254 | A | C4-C5-C6 | -6.00 | 114.00 | 117.00 |
| 17 | AF | 38 | ARG | NE-CZ-NH2 | -6.00 | 117.30 | 120.30 |
| 22 | AA | 350 | G | N1-C6-O6 | -6.00 | 116.30 | 119.90 |
| 22 | AA | 948 | C | N1-C2-O2 | 6.00 | 122.50 | 118.90 |
| 22 | AA | 1104 | G | N1-C6-O6 | -6.00 | 116.30 | 119.90 |
| 22 | AA | 1319 | A | N1-C6-N6 | -6.00 | 115.00 | 118.60 |
| 22 | AA | 130 | A | O4'-C1'-N9 | 6.00 | 113.00 | 108.20 |
| 22 | AA | 1383 | C | O4'-C1'-N1 | 6.00 | 113.00 | 108.20 |
| 22 | AA | 1462 | C | O4'-C1'-N1 | 6.00 | 113.00 | 108.20 |
| 35 | BD | 47 | ARG | NE-CZ-NH1 | 6.00 | 123.30 | 120.30 |
| 57 | BA | 1416 | G | O4'-C1'-N9 | 6.00 | 113.00 | 108.20 |
| 57 | BA | 2258 | C | N1-C2-O2 | 6.00 | 122.50 | 118.90 |
| 57 | BA | 2356 | U | O4'-C1'-N1 | 6.00 | 113.00 | 108.20 |
| 57 | BA | 2662 | A | C4-C5-C6 | -6.00 | 114.00 | 117.00 |
| 22 | AA | 1400 | C | N3-C2-O2 | -6.00 | 117.70 | 121.90 |
| 57 | BA | 2001 | C | N1-C2-O2 | 6.00 | 122.50 | 118.90 |
| 22 | AA | 528 | C | O4'-C1'-N1 | 6.00 | 113.00 | 108.20 |
| 22 | AA | 1281 | C | N3-C4-C5 | 6.00 | 124.30 | 121.90 |
| 57 | BA | 2282 | G | N1-C6-O6 | -6.00 | 116.30 | 119.90 |
| 57 | BA | 1179 | G | N1-C6-O6 | -6.00 | 116.30 | 119.90 |
| 34 | BT | 100 | ARG | NE-CZ-NH2 | 5.99 | 123.30 | 120.30 |
| 57 | BA | 4 | U | O4'-C1'-N1 | 5.99 | 113.00 | 108.20 |
| 57 | BA | 440 | C | O4'-C1'-N1 | 5.99 | 113.00 | 108.20 |
| 22 | AA | 611 | C | N3-C2-O2 | -5.99 | 117.70 | 121.90 |
| 22 | AA | 765 | G | C1'-O4'-C4' | -5.99 | 105.11 | 109.90 |
| 57 | BA | 1245 | G | N1-C6-O6 | -5.99 | 116.31 | 119.90 |
| 22 | AA | 578 | C | O4'-C1'-N1 | 5.99 | 112.99 | 108.20 |
| 22 | AA | 638 | U | O4'-C1'-N1 | 5.99 | 112.99 | 108.20 |
| 22 | AA | 983 | A | C6-C5-N7 | 5.99 | 136.49 | 132.30 |
| 22 | AA | 1484 | C | N1-C2-O2 | 5.99 | 122.50 | 118.90 |
| 57 | BA | 301 | G | N3-C4-C5 | -5.99 | 125.61 | 128.60 |
| 22 | AA | 520 | A | C4-C5-C6 | -5.99 | 114.01 | 117.00 |
| 57 | BA | 1164 | C | O4'-C1'-N1 | 5.99 | 112.99 | 108.20 |
| 22 | AA | 578 | C | N1-C2-O2 | 5.99 | 122.49 | 118.90 |
| 22 | AA | 777 | A | C4-C5-C6 | -5.99 | 114.01 | 117.00 |
| 22 | AA | 475 | C | N1-C2-O2 | 5.99 | 122.49 | 118.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | AA | 1103 | C | N1-C2-O2 | 5.99 | 122.49 | 118.90 |
| 22 | AA | 1524 | C | N3-C4-C5 | 5.99 | 124.30 | 121.90 |
| 57 | BA | 171 | U | O4'-C1'-N1 | 5.99 | 112.99 | 108.20 |
| 57 | BA | 712 | G | O4'-C1'-N9 | 5.99 | 112.99 | 108.20 |
| 57 | BA | 1262 | A | C4-C5-C6 | -5.99 | 114.01 | 117.00 |
| 57 | BA | 2191 | A | C4-C5-C6 | -5.99 | 114.01 | 117.00 |
| 58 | Ba | 29 | A | C4-C5-C6 | -5.99 | 114.01 | 117.00 |
| 57 | BA | 1370 | C | N1-C2-O2 | 5.98 | 122.49 | 118.90 |
| 57 | BA | 1670 | C | O4'-C1'-N1 | 5.98 | 112.99 | 108.20 |
| 20 | AI | 48 | ARG | NE-CZ-NH1 | 5.98 | 123.29 | 120.30 |
| 22 | AA | 72 | A | C4-C5-C6 | -5.98 | 114.01 | 117.00 |
| 57 | BA | 140 | C | N3-C2-O2 | -5.98 | 117.71 | 121.90 |
| 57 | BA | 1927 | A | C4-C5-C6 | -5.98 | 114.01 | 117.00 |
| 4 | AM | 97 | ARG | NE-CZ-NH2 | -5.98 | 117.31 | 120.30 |
| 18 | AG | 2 | ARG | NH1-CZ-NH2 | -5.98 | 112.82 | 119.40 |
| 22 | AA | 1275 | A | C4-C5-C6 | -5.98 | 114.01 | 117.00 |
| 22 | AA | 1344 | C | O4'-C1'-N1 | 5.98 | 112.98 | 108.20 |
| 57 | BA | 173 | A | C4-C5-C6 | -5.98 | 114.01 | 117.00 |
| 57 | BA | 1072 | C | N1-C2-O2 | 5.98 | 122.49 | 118.90 |
| 57 | BA | 1166 | G | O4'-C1'-N9 | 5.98 | 112.98 | 108.20 |
| 57 | BA | 1966 | A | C4-C5-C6 | -5.98 | 114.01 | 117.00 |
| 22 | AA | 45 | G | O4'-C1'-N9 | 5.98 | 112.98 | 108.20 |
| 22 | AA | 753 | A | C4-C5-C6 | -5.98 | 114.01 | 117.00 |
| 57 | BA | 402 | A | N1-C6-N6 | -5.98 | 115.01 | 118.60 |
| 57 | BA | 2551 | C | N1-C2-O2 | 5.98 | 122.49 | 118.90 |
| 58 | Ba | 120 | U | O4'-C1'-N1 | 5.98 | 112.98 | 108.20 |
| 24 | A3 | 42 | C | N1-C2-O2 | 5.98 | 122.49 | 118.90 |
| 57 | BA | 618 | G | N1-C6-O6 | -5.98 | 116.31 | 119.90 |
| 22 | AA | 17 | U | O4'-C1'-N1 | 5.98 | 112.98 | 108.20 |
| 22 | AA | 556 | C | N1-C2-O2 | 5.98 | 122.48 | 118.90 |
| 22 | AA | 60 | A | C4-C5-C6 | -5.97 | 114.01 | 117.00 |
| 22 | AA | 348 | G | O4'-C1'-N9 | 5.97 | 112.98 | 108.20 |
| 22 | AA | 403 | C | O4'-C1'-N1 | 5.97 | 112.98 | 108.20 |
| 22 | AA | 797 | C | O4'-C1'-N1 | 5.97 | 112.98 | 108.20 |
| 22 | AA | 824 | G | N1-C6-O6 | -5.97 | 116.31 | 119.90 |
| 57 | BA | 160 | A | C4-C5-C6 | -5.97 | 114.01 | 117.00 |
| 57 | BA | 935 | C | O4'-C1'-N1 | 5.97 | 112.98 | 108.20 |
| 57 | BA | 1626 | A | C4-C5-C6 | -5.97 | 114.01 | 117.00 |
| 57 | BA | 1737 | G | N3-C2-N2 | -5.97 | 115.72 | 119.90 |
| 57 | BA | 1912 | A | C4-C5-C6 | -5.97 | 114.01 | 117.00 |
| 24 | A3 | 51 | U | O4'-C1'-N1 | 5.97 | 112.98 | 108.20 |
| 57 | BA | 507 | A | C4-C5-C6 | -5.97 | 114.01 | 117.00 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 1920 | C | N1-C2-O2 | 5.97 | 122.48 | 118.90 |
| 57 | BA | 2214 | C | N1-C2-O2 | 5.97 | 122.48 | 118.90 |
| 57 | BA | 2575 | C | N3-C4-C5 | -5.97 | 119.51 | 121.90 |
| 57 | BA | 2380 | C | N1-C2-O2 | 5.97 | 122.48 | 118.90 |
| 8 | AQ | 5 | ARG | NE-CZ-NH1 | 5.97 | 123.28 | 120.30 |
| 22 | AA | 612 | C | N1-C2-O2 | 5.97 | 122.48 | 118.90 |
| 22 | AA | 1328 | C | N1-C2-O2 | 5.97 | 122.48 | 118.90 |
| 57 | BA | 265 | A | C4-C5-C6 | -5.97 | 114.02 | 117.00 |
| 57 | BA | 2635 | A | O4'-C1'-N9 | 5.97 | 112.98 | 108.20 |
| 22 | AA | 1235 | U | O4'-C1'-N1 | 5.97 | 112.97 | 108.20 |
| 57 | BA | 1686 | C | O4'-C1'-N1 | 5.97 | 112.97 | 108.20 |
| 57 | BA | 2083 | G | N1-C6-O6 | -5.97 | 116.32 | 119.90 |
| 22 | AA | 196 | A | C4-C5-C6 | -5.97 | 114.02 | 117.00 |
| 22 | AA | 706 | A | C4-C5-C6 | -5.97 | 114.02 | 117.00 |
| 22 | AA | 1443 | C | O4'-C1'-N1 | 5.97 | 112.97 | 108.20 |
| 57 | BA | 873 | C | N1-C2-O2 | 5.97 | 122.48 | 118.90 |
| 57 | BA | 1847 | A | C4-C5-C6 | -5.97 | 114.02 | 117.00 |
| 57 | BA | 2283 | C | N1-C2-O2 | 5.97 | 122.48 | 118.90 |
| 22 | AA | 1510 | C | N1-C2-O2 | 5.96 | 122.48 | 118.90 |
| 57 | BA | 272 | A | C4-C5-C6 | -5.96 | 114.02 | 117.00 |
| 57 | BA | 1086 | A | C4-C5-C6 | -5.96 | 114.02 | 117.00 |
| 57 | BA | 28 | A | C4-C5-C6 | -5.96 | 114.02 | 117.00 |
| 58 | Ba | 15 | A | C4-C5-C6 | -5.96 | 114.02 | 117.00 |
| 22 | AA | 1226 | C | N1-C2-O2 | 5.96 | 122.48 | 118.90 |
| 57 | BA | 221 | A | C4-C5-C6 | -5.96 | 114.02 | 117.00 |
| 57 | BA | 705 | A | C4-C5-C6 | -5.96 | 114.02 | 117.00 |
| 57 | BA | 728 | G | O4'-C1'-N9 | 5.96 | 112.97 | 108.20 |
| 57 | BA | 1313 | U | C3'-C2'-C1' | 5.96 | 106.27 | 101.50 |
| 57 | BA | 1404 | C | N1-C2-O2 | 5.96 | 122.48 | 118.90 |
| 57 | BA | 2169 | A | O4'-C1'-N9 | 5.96 | 112.97 | 108.20 |
| 57 | BA | 2177 | C | N1-C2-O2 | 5.96 | 122.48 | 118.90 |
| 22 | AA | 246 | A | C4-C5-C6 | -5.96 | 114.02 | 117.00 |
| 22 | AA | 810 | C | N1-C2-O2 | 5.96 | 122.48 | 118.90 |
| 22 | AA | 507 | C | O4'-C1'-N1 | 5.96 | 112.97 | 108.20 |
| 22 | AA | 839 | C | N1-C2-O2 | 5.96 | 122.47 | 118.90 |
| 57 | BA | 652 | U | O4'-C1'-N1 | 5.96 | 112.97 | 108.20 |
| 57 | BA | 1070 | A | C4-C5-C6 | -5.96 | 114.02 | 117.00 |
| 57 | BA | 1651 | G | N1-C6-O6 | -5.96 | 116.33 | 119.90 |
| 22 | AA | 387 | U | O4'-C1'-N1 | 5.96 | 112.97 | 108.20 |
| 57 | BA | 1552 | A | N1-C6-N6 | -5.96 | 115.03 | 118.60 |
| 16 | AE | 19 | ARG | NE-CZ-NH1 | 5.96 | 123.28 | 120.30 |
| 22 | AA | 217 | C | N1-C2-O2 | 5.96 | 122.47 | 118.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 1643 | G | O4'-C1'-N9 | 5.96 | 112.96 | 108.20 |
| 32 | BR | 8 | ARG | NE-CZ-NH1 | 5.95 | 123.28 | 120.30 |
| 57 | BA | 2832 | U | O4'-C1'-N1 | 5.95 | 112.96 | 108.20 |
| 57 | BA | 1617 | C | N3-C2-O2 | -5.95 | 117.73 | 121.90 |
| 22 | AA | 163 | C | N1-C2-O2 | 5.95 | 122.47 | 118.90 |
| 22 | AA | 433 | G | N1-C6-O6 | -5.95 | 116.33 | 119.90 |
| 22 | AA | 1137 | C | N3-C2-O2 | -5.95 | 117.73 | 121.90 |
| 28 | BN | 69 | ARG | NE-CZ-NH1 | 5.95 | 123.28 | 120.30 |
| 57 | BA | 1200 | C | O4'-C1'-N1 | 5.95 | 112.96 | 108.20 |
| 57 | BA | 1862 | G | N1-C6-O6 | -5.95 | 116.33 | 119.90 |
| 57 | BA | 1934 | C | N1-C2-O2 | 5.95 | 122.47 | 118.90 |
| 57 | BA | 2066 | C | N1-C2-O2 | 5.95 | 122.47 | 118.90 |
| 57 | BA | 2727 | A | C4-C5-C6 | -5.95 | 114.02 | 117.00 |
| 24 | A3 | 28 | U | O4'-C1'-N1 | 5.95 | 112.96 | 108.20 |
| 57 | BA | 2547 | A | C4-C5-C6 | -5.95 | 114.03 | 117.00 |
| 22 | AA | 1444 | U | O4'-C1'-N1 | 5.95 | 112.96 | 108.20 |
| 22 | AA | 397 | A | C4-C5-C6 | -5.95 | 114.03 | 117.00 |
| 22 | AA | 759 | A | C4-C5-C6 | -5.95 | 114.03 | 117.00 |
| 23 | A2 | 45 | G | N3-C4-C5 | -5.95 | 125.63 | 128.60 |
| 57 | BA | 1293 | C | N3-C2-O2 | -5.95 | 117.74 | 121.90 |
| 57 | BA | 2505 | G | O4'-C1'-N9 | 5.95 | 112.96 | 108.20 |
| 22 | AA | 111 | G | N3-C2-N2 | -5.94 | 115.74 | 119.90 |
| 44 | B2 | 23 | ARG | NE-CZ-NH1 | 5.94 | 123.27 | 120.30 |
| 57 | BA | 1007 | C | N1-C2-O2 | 5.94 | 122.47 | 118.90 |
| 22 | AA | 695 | A | C4-C5-C6 | -5.94 | 114.03 | 117.00 |
| 22 | AA | 1508 | A | C4-C5-C6 | -5.94 | 114.03 | 117.00 |
| 57 | BA | 349 | U | O4'-C1'-N1 | 5.94 | 112.95 | 108.20 |
| 18 | AG | 9 | ARG | NE-CZ-NH1 | 5.94 | 123.27 | 120.30 |
| 22 | AA | 603 | U | O4'-C1'-N1 | 5.94 | 112.95 | 108.20 |
| 22 | AA | 1255 | G | N1-C6-O6 | -5.94 | 116.33 | 119.90 |
| 22 | AA | 1458 | G | N1-C6-O6 | -5.94 | 116.34 | 119.90 |
| 57 | BA | 723 | C | N1-C2-O2 | 5.94 | 122.47 | 118.90 |
| 57 | BA | 985 | C | N1-C2-O2 | 5.94 | 122.46 | 118.90 |
| 57 | BA | 1879 | C | N1-C2-O2 | 5.94 | 122.46 | 118.90 |
| 57 | BA | 1986 | C | N1-C2-O2 | 5.94 | 122.46 | 118.90 |
| 22 | AA | 1334 | G | N1-C6-O6 | -5.94 | 116.34 | 119.90 |
| 57 | BA | 886 | A | C4-C5-C6 | -5.94 | 114.03 | 117.00 |
| 22 | AA | 69 | G | N1-C6-O6 | -5.94 | 116.34 | 119.90 |
| 22 | AA | 1259 | C | N1-C2-O2 | 5.94 | 122.46 | 118.90 |
| 22 | AA | 1502 | A | C4-C5-C6 | -5.94 | 114.03 | 117.00 |
| 57 | BA | 345 | A | C4-C5-C6 | -5.94 | 114.03 | 117.00 |
| 57 | BA | 836 | G | N1-C6-O6 | -5.94 | 116.34 | 119.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 2530 | A | C4-C5-C6 | -5.94 | 114.03 | 117.00 |
| 4 | AM | 92 | ARG | NE-CZ-NH1 | 5.94 | 123.27 | 120.30 |
| 22 | AA | 489 | C | O4'-C1'-N1 | 5.94 | 112.95 | 108.20 |
| 57 | BA | 1490 | A | O4'-C1'-N9 | 5.94 | 112.95 | 108.20 |
| 57 | BA | 1747 | U | O4'-C1'-N1 | 5.94 | 112.95 | 108.20 |
| 10 | AS | 2 | ARG | NH1-CZ-NH2 | -5.93 | 112.87 | 119.40 |
| 22 | AA | 35 | G | N1-C6-O6 | -5.93 | 116.34 | 119.90 |
| 22 | AA | 309 | A | O4'-C1'-N9 | 5.93 | 112.95 | 108.20 |
| 22 | AA | 840 | C | N1-C2-O2 | 5.93 | 122.46 | 118.90 |
| 22 | AA | 1204 | A | C6-C5-N7 | 5.93 | 136.45 | 132.30 |
| 22 | AA | 1208 | C | O4'-C1'-N1 | 5.93 | 112.95 | 108.20 |
| 22 | AA | 1230 | C | O4'-C1'-N1 | 5.93 | 112.94 | 108.20 |
| 22 | AA | 1234 | C | O4'-C1'-N1 | 5.93 | 112.95 | 108.20 |
| 22 | AA | 1256 | A | C1'-O4'-C4' | -5.93 | 105.15 | 109.90 |
| 57 | BA | 474 | G | N1-C6-O6 | -5.93 | 116.34 | 119.90 |
| 57 | BA | 2401 | U | O4'-C1'-N1 | 5.93 | 112.95 | 108.20 |
| 57 | BA | 2687 | U | O4'-C1'-N1 | 5.93 | 112.95 | 108.20 |
| 57 | BA | 1121 | C | N1-C2-O2 | 5.93 | 122.46 | 118.90 |
| 57 | BA | 2714 | G | N3-C4-C5 | -5.93 | 125.64 | 128.60 |
| 22 | AA | 194 | C | N3-C2-O2 | -5.93 | 117.75 | 121.90 |
| 57 | BA | 1033 | U | N3-C2-O2 | -5.93 | 118.05 | 122.20 |
| 57 | BA | 1201 | U | O4'-C1'-N1 | 5.93 | 112.94 | 108.20 |
| 57 | BA | 2104 | C | O4'-C1'-N1 | 5.93 | 112.94 | 108.20 |
| 57 | BA | 2301 | C | O4'-C1'-N1 | 5.93 | 112.94 | 108.20 |
| 57 | BA | 2864 | G | N1-C6-O6 | -5.93 | 116.34 | 119.90 |
| 22 | AA | 856 | C | O4'-C1'-N1 | 5.93 | 112.94 | 108.20 |
| 22 | AA | 1382 | C | N3-C2-O2 | -5.93 | 117.75 | 121.90 |
| 23 | A2 | 27 | A | C4-C5-C6 | -5.93 | 114.04 | 117.00 |
| 57 | BA | 2397 | G | N1-C6-O6 | -5.93 | 116.34 | 119.90 |
| 13 | AU | 1 | PRO | CA-N-CD | -5.93 | 103.20 | 111.50 |
| 42 | B0 | 19 | ARG | NE-CZ-NH1 | 5.93 | 123.26 | 120.30 |
| 57 | BA | 739 | A | O4'-C1'-N9 | 5.93 | 112.94 | 108.20 |
| 57 | BA | 1214 | A | C4-C5-C6 | -5.93 | 114.04 | 117.00 |
| 22 | AA | 751 | U | O4'-C1'-N1 | 5.92 | 112.94 | 108.20 |
| 57 | BA | 104 | A | O4'-C1'-N9 | 5.92 | 112.94 | 108.20 |
| 57 | BA | 1387 | A | C4-C5-C6 | -5.92 | 114.04 | 117.00 |
| 57 | BA | 1832 | C | O4'-C1'-N1 | 5.92 | 112.94 | 108.20 |
| 57 | BA | 2052 | A | C4-C5-C6 | -5.92 | 114.04 | 117.00 |
| 57 | BA | 2065 | C | O4'-C1'-N1 | 5.92 | 112.94 | 108.20 |
| 22 | AA | 466 | A | C4-C5-C6 | -5.92 | 114.04 | 117.00 |
| 22 | AA | 866 | C | O4'-C1'-N1 | 5.92 | 112.94 | 108.20 |
| 22 | AA | 892 | A | C4-C5-C6 | -5.92 | 114.04 | 117.00 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | AA | 1008 | U | O4'-C1'-N1 | 5.92 | 112.94 | 108.20 |
| 22 | AA | 1330 | U | O4'-C1'-N1 | 5.92 | 112.94 | 108.20 |
| 33 | BS | 102 | ARG | NE-CZ-NH2 | -5.92 | 117.34 | 120.30 |
| 57 | BA | 595 | C | N1-C2-O2 | 5.92 | 122.45 | 118.90 |
| 57 | BA | 387 | U | O4'-C1'-N1 | 5.92 | 112.94 | 108.20 |
| 57 | BA | 1833 | C | N1-C2-O2 | 5.92 | 122.45 | 118.90 |
| 57 | BA | 2715 | C | N1-C2-O2 | 5.92 | 122.45 | 118.90 |
| 57 | BA | 2818 | U | O4'-C1'-N1 | 5.92 | 112.94 | 108.20 |
| 58 | Ba | 108 | A | C4-C5-C6 | -5.92 | 114.04 | 117.00 |
| 22 | AA | 251 | G | N3-C4-C5 | -5.92 | 125.64 | 128.60 |
| 57 | BA | 2089 | C | N1-C2-O2 | 5.92 | 122.45 | 118.90 |
| 57 | BA | 2765 | A | C4-C5-C6 | -5.92 | 114.04 | 117.00 |
| 22 | AA | 169 | C | N3-C2-O2 | -5.92 | 117.76 | 121.90 |
| 22 | AA | 811 | C | N3-C2-O2 | -5.92 | 117.76 | 121.90 |
| 22 | AA | 901 | A | C4-C5-C6 | -5.92 | 114.04 | 117.00 |
| 57 | BA | 610 | C | O4'-C1'-N1 | 5.92 | 112.93 | 108.20 |
| 57 | BA | 2359 | C | O4'-C1'-N1 | 5.92 | 112.93 | 108.20 |
| 57 | BA | 2402 | U | O4'-C1'-N1 | 5.92 | 112.93 | 108.20 |
| 57 | BA | 304 | U | O4'-C1'-N1 | 5.92 | 112.93 | 108.20 |
| 57 | BA | 876 | C | N3-C2-O2 | -5.92 | 117.76 | 121.90 |
| 22 | AA | 485 | U | O4'-C1'-N1 | 5.91 | 112.93 | 108.20 |
| 22 | AA | 843 | U | N3-C2-O2 | -5.91 | 118.06 | 122.20 |
| 57 | BA | 506 | G | N1-C6-O6 | -5.91 | 116.35 | 119.90 |
| 57 | BA | 1227 | G | O4'-C1'-N9 | 5.91 | 112.93 | 108.20 |
| 57 | BA | 1242 | U | O4'-C1'-N1 | 5.91 | 112.93 | 108.20 |
| 57 | BA | 1451 | C | N3-C4-C5 | 5.91 | 124.27 | 121.90 |
| 22 | AA | 1037 | C | O4'-C1'-N1 | 5.91 | 112.93 | 108.20 |
| 57 | BA | 196 | A | O4'-C1'-N9 | 5.91 | 112.93 | 108.20 |
| 57 | BA | 211 | C | O4'-C1'-N1 | 5.91 | 112.93 | 108.20 |
| 57 | BA | 1386 | C | N1-C2-O2 | 5.91 | 122.45 | 118.90 |
| 22 | AA | 826 | C | N1-C2-O2 | 5.91 | 122.45 | 118.90 |
| 22 | AA | 1396 | A | O4'-C1'-N9 | 5.91 | 112.93 | 108.20 |
| 23 | A2 | 17 | U | N3-C2-O2 | -5.91 | 118.06 | 122.20 |
| 57 | BA | 359 | G | N1-C6-O6 | -5.91 | 116.35 | 119.90 |
| 57 | BA | 1908 | C | N1-C2-O2 | 5.91 | 122.45 | 118.90 |
| 57 | BA | 2403 | C | O4'-C1'-N1 | 5.91 | 112.93 | 108.20 |
| 22 | AA | 137 | U | O4'-C1'-N1 | 5.91 | 112.93 | 108.20 |
| 22 | AA | 857 | C | O4'-C1'-N1 | 5.91 | 112.93 | 108.20 |
| 57 | BA | 96 | C | N1-C2-O2 | 5.91 | 122.44 | 118.90 |
| 57 | BA | 699 | A | C4-C5-C6 | -5.91 | 114.05 | 117.00 |
| 57 | BA | 718 | A | C4-C5-C6 | -5.91 | 114.05 | 117.00 |
| 57 | BA | 854 | C | N1-C2-O2 | 5.91 | 122.44 | 118.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 1382 | G | N3-C4-C5 | -5.91 | 125.65 | 128.60 |
| 57 | BA | 2705 | A | C4-C5-C6 | -5.91 | 114.05 | 117.00 |
| 57 | BA | 2741 | A | C4-C5-C6 | -5.91 | 114.05 | 117.00 |
| 58 | Ba | 106 | G | N1-C6-O6 | -5.91 | 116.36 | 119.90 |
| 34 | BT | 92 | ARG | NE-CZ-NH1 | 5.91 | 123.25 | 120.30 |
| 22 | AA | 210 | C | N3-C2-O2 | -5.91 | 117.77 | 121.90 |
| 22 | AA | 746 | A | C4-C5-C6 | -5.91 | 114.05 | 117.00 |
| 57 | BA | 2606 | C | N1-C2-O2 | 5.91 | 122.44 | 118.90 |
| 57 | BA | 1068 | G | O4'-C1'-N9 | 5.90 | 112.92 | 108.20 |
| 57 | BA | 1451 | C | N3-C2-O2 | -5.90 | 117.77 | 121.90 |
| 57 | BA | 1550 | C | N1-C2-O2 | 5.90 | 122.44 | 118.90 |
| 22 | AA | 1232 | U | O4'-C1'-N1 | 5.90 | 112.92 | 108.20 |
| 57 | BA | 2621 | G | N1-C6-O6 | -5.90 | 116.36 | 119.90 |
| 22 | AA | 596 | A | C4-C5-C6 | -5.90 | 114.05 | 117.00 |
| 22 | AA | 1485 | U | O4'-C1'-N1 | 5.90 | 112.92 | 108.20 |
| 57 | BA | 2801 | G | O4'-C1'-N9 | 5.90 | 112.92 | 108.20 |
| 22 | AA | 615 | G | N1-C6-O6 | -5.90 | 116.36 | 119.90 |
| 57 | BA | 1258 | U | O4'-C1'-N1 | 5.90 | 112.92 | 108.20 |
| 57 | BA | 2364 | C | N1-C2-O2 | 5.90 | 122.44 | 118.90 |
| 11 | AB | 221 | ARG | NE-CZ-NH1 | 5.90 | 123.25 | 120.30 |
| 24 | A3 | 60 | A | C4-C5-C6 | -5.90 | 114.05 | 117.00 |
| 57 | BA | 933 | A | C4-C5-C6 | -5.90 | 114.05 | 117.00 |
| 57 | BA | 2144 | G | O4'-C1'-N9 | 5.90 | 112.92 | 108.20 |
| 57 | BA | 2791 | G | O4'-C1'-N9 | 5.90 | 112.92 | 108.20 |
| 57 | BA | 2335 | A | C4-C5-C6 | -5.90 | 114.05 | 117.00 |
| 57 | BA | 2789 | C | N3-C2-O2 | -5.90 | 117.77 | 121.90 |
| 22 | AA | 36 | C | N1-C2-O2 | 5.89 | 122.44 | 118.90 |
| 22 | AA | 95 | C | N1-C2-O2 | 5.89 | 122.44 | 118.90 |
| 22 | AA | 629 | A | C4-C5-C6 | -5.89 | 114.05 | 117.00 |
| 22 | AA | 909 | A | C4-C5-C6 | -5.89 | 114.05 | 117.00 |
| 57 | BA | 457 | A | O4'-C1'-N9 | 5.89 | 112.92 | 108.20 |
| 57 | BA | 1050 | A | C4-C5-C6 | -5.89 | 114.05 | 117.00 |
| 57 | BA | 1170 | C | N1-C2-O2 | 5.89 | 122.44 | 118.90 |
| 57 | BA | 2608 | G | O4'-C1'-N9 | 5.89 | 112.92 | 108.20 |
| 22 | AA | 477 | C | N1-C2-O2 | 5.89 | 122.44 | 118.90 |
| 22 | AA | 1481 | U | O4'-C1'-N1 | 5.89 | 112.91 | 108.20 |
| 57 | BA | 643 | A | C4-C5-C6 | -5.89 | 114.05 | 117.00 |
| 57 | BA | 1397 | U | O4'-C1'-N1 | 5.89 | 112.91 | 108.20 |
| 57 | BA | 1434 | A | C4-C5-C6 | -5.89 | 114.05 | 117.00 |
| 22 | AA | 149 | A | C4-C5-C6 | -5.89 | 114.06 | 117.00 |
| 22 | AA | 272 | C | N1-C2-O2 | 5.89 | 122.43 | 118.90 |
| 22 | AA | 795 | C | N3-C2-O2 | -5.89 | 117.78 | 121.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|---|---|---|---|---|---|---|---|
| 22 | AA | 1032 | G | N3-C4-C5 | -5.89 | 125.66 | 128.60 |
| 23 | A2 | 33 | A | C4-C5-C6 | -5.89 | 114.06 | 117.00 |
| 57 | BA | 869 | G | N1-C6-O6 | -5.89 | 116.37 | 119.90 |
| 57 | BA | 2626 | C | O4'-C1'-N1 | 5.89 | 112.91 | 108.20 |
| 58 | Ba | 36 | C | N3-C2-O2 | -5.89 | 117.78 | 121.90 |
| 23 | A2 | 16 | A | C4-C5-C6 | -5.89 | 114.06 | 117.00 |
| 57 | BA | 2572 | A | O4'-C1'-N9 | 5.89 | 112.91 | 108.20 |
| 22 | AA | 180 | U | O4'-C1'-N1 | 5.88 | 112.91 | 108.20 |
| 57 | BA | 2013 | A | C4-C5-C6 | -5.88 | 114.06 | 117.00 |
| 57 | BA | 2682 | A | C4-C5-C6 | -5.88 | 114.06 | 117.00 |
| 57 | BA | 2826 | A | C4-C5-C6 | -5.88 | 114.06 | 117.00 |
| 22 | AA | 1186 | G | N1-C6-O6 | -5.88 | 116.37 | 119.90 |
| 57 | BA | 2197 | U | O4'-C1'-N1 | 5.88 | 112.91 | 108.20 |
| 22 | AA | 114 | U | O4'-C1'-N1 | 5.88 | 112.91 | 108.20 |
| 22 | AA | 865 | A | O4'-C1'-N9 | 5.88 | 112.91 | 108.20 |
| 57 | BA | 687 | C | N3-C2-O2 | -5.88 | 117.78 | 121.90 |
| 57 | BA | 706 | A | O4'-C1'-N9 | 5.88 | 112.91 | 108.20 |
| 57 | BA | 1508 | A | C4-C5-C6 | -5.88 | 114.06 | 117.00 |
| 57 | BA | 2570 | G | N1-C6-O6 | -5.88 | 116.37 | 119.90 |
| 22 | AA | 436 | C | N1-C2-O2 | 5.88 | 122.43 | 118.90 |
| 57 | BA | 1018 | U | O4'-C1'-N1 | 5.88 | 112.90 | 108.20 |
| 30 | BP | 2 | ARG | NH1-CZ-NH2 | -5.88 | 112.93 | 119.40 |
| 57 | BA | 1752 | C | N1-C2-O2 | 5.88 | 122.43 | 118.90 |
| 57 | BA | 2151 | U | O4'-C1'-N1 | 5.88 | 112.90 | 108.20 |
| 57 | BA | 2805 | C | N1-C2-O2 | 5.88 | 122.43 | 118.90 |
| 57 | BA | 471 | A | N1-C6-N6 | -5.88 | 115.07 | 118.60 |
| 57 | BA | 1305 | C | N3-C4-N4 | -5.88 | 113.89 | 118.00 |
| 22 | AA | 1223 | C | N3-C4-C5 | 5.88 | 124.25 | 121.90 |
| 57 | BA | 653 | U | P-O3'-C3' | 5.88 | 126.75 | 119.70 |
| 57 | BA | 1842 | G | N1-C6-O6 | -5.88 | 116.38 | 119.90 |
| 57 | BA | 2496 | C | N1-C2-O2 | 5.88 | 122.42 | 118.90 |
| 57 | BA | 2556 | C | N3-C2-O2 | -5.88 | 117.79 | 121.90 |
| 22 | AA | 1045 | C | N1-C2-O2 | 5.87 | 122.42 | 118.90 |
| 22 | AA | 1398 | A | C4-C5-C6 | -5.87 | 114.06 | 117.00 |
| 57 | BA | 241 | A | C4-C5-C6 | -5.87 | 114.06 | 117.00 |
| 57 | BA | 679 | C | N1-C2-O2 | 5.87 | 122.42 | 118.90 |
| 57 | BA | 2518 | A | C4-C5-C6 | -5.87 | 114.06 | 117.00 |
| 22 | AA | 519 | C | N3-C2-O2 | -5.87 | 117.79 | 121.90 |
| 57 | BA | 915 | C | N1-C2-O2 | 5.87 | 122.42 | 118.90 |
| 22 | AA | 341 | C | N1-C2-O2 | 5.87 | 122.42 | 118.90 |
| 36 | BU | 12 | ARG | NE-CZ-NH2 | 5.87 | 123.23 | 120.30 |
| 57 | BA | 331 | C | O4'-C1'-N1 | 5.87 | 112.90 | 108.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 17 | AF | 2 | ARG | NH1-CZ-NH2 | -5.87 | 112.94 | 119.40 |
| 22 | AA | 930 | C | O4'-C1'-N1 | 5.87 | 112.89 | 108.20 |
| 57 | BA | 1788 | C | N1-C2-O2 | 5.87 | 122.42 | 118.90 |
| 57 | BA | 1809 | A | C4-C5-C6 | -5.87 | 114.07 | 117.00 |
| 57 | BA | 281 | C | O4'-C1'-N1 | 5.87 | 112.89 | 108.20 |
| 57 | BA | 1166 | G | N3-C2-N2 | -5.87 | 115.79 | 119.90 |
| 22 | AA | 88 | U | O4'-C1'-N1 | 5.87 | 112.89 | 108.20 |
| 57 | BA | 190 | A | C4-C5-C6 | -5.87 | 114.07 | 117.00 |
| 57 | BA | 609 | A | C4-C5-C6 | -5.87 | 114.07 | 117.00 |
| 58 | Ba | 44 | G | N1-C6-O6 | -5.87 | 116.38 | 119.90 |
| 58 | Ba | 113 | C | N1-C2-O2 | 5.87 | 122.42 | 118.90 |
| 22 | AA | 446 | G | O4'-C1'-N9 | 5.86 | 112.89 | 108.20 |
| 22 | AA | 646 | G | N1-C6-O6 | -5.86 | 116.38 | 119.90 |
| 57 | BA | 764 | A | C4-C5-C6 | -5.86 | 114.07 | 117.00 |
| 57 | BA | 1153 | C | N1-C2-O2 | 5.86 | 122.42 | 118.90 |
| 57 | BA | 1666 | G | O4'-C1'-N9 | 5.86 | 112.89 | 108.20 |
| 57 | BA | 1874 | C | O4'-C1'-N1 | 5.86 | 112.89 | 108.20 |
| 57 | BA | 2051 | A | C4-C5-C6 | -5.86 | 114.07 | 117.00 |
| 57 | BA | 2153 | C | N1-C2-O2 | 5.86 | 122.42 | 118.90 |
| 57 | BA | 2221 | G | N1-C6-O6 | -5.86 | 116.38 | 119.90 |
| 22 | AA | 705 | G | N3-C2-N2 | -5.86 | 115.80 | 119.90 |
| 57 | BA | 616 | A | N1-C6-N6 | -5.86 | 115.08 | 118.60 |
| 57 | BA | 2715 | C | O4'-C1'-N1 | 5.86 | 112.89 | 108.20 |
| 22 | AA | 593 | U | O4'-C1'-N1 | 5.86 | 112.89 | 108.20 |
| 22 | AA | 995 | C | N3-C2-O2 | -5.86 | 117.80 | 121.90 |
| 22 | AA | 1350 | A | C4-C5-C6 | -5.86 | 114.07 | 117.00 |
| 57 | BA | 322 | A | C4-C5-C6 | -5.86 | 114.07 | 117.00 |
| 57 | BA | 811 | U | O4'-C1'-N1 | 5.86 | 112.89 | 108.20 |
| 57 | BA | 1488 | C | O4'-C1'-N1 | 5.86 | 112.89 | 108.20 |
| 57 | BA | 1691 | C | O4'-C1'-N1 | 5.86 | 112.89 | 108.20 |
| 57 | BA | 2377 | A | C4-C5-C6 | -5.86 | 114.07 | 117.00 |
| 22 | AA | 897 | C | N1-C2-O2 | 5.86 | 122.42 | 118.90 |
| 57 | BA | 2768 | U | O4'-C1'-N1 | 5.86 | 112.89 | 108.20 |
| 57 | BA | 2771 | C | N1-C2-O2 | 5.86 | 122.42 | 118.90 |
| 22 | AA | 1257 | A | C4-C5-C6 | -5.86 | 114.07 | 117.00 |
| 22 | AA | 1372 | U | O4'-C1'-N1 | 5.86 | 112.89 | 108.20 |
| 57 | BA | 934 | U | O4'-C1'-N1 | 5.86 | 112.89 | 108.20 |
| 57 | BA | 957 | C | N3-C4-C5 | 5.86 | 124.24 | 121.90 |
| 57 | BA | 1415 | U | O4'-C1'-N1 | 5.86 | 112.89 | 108.20 |
| 57 | BA | 1442 | U | O4'-C1'-N1 | 5.86 | 112.89 | 108.20 |
| 57 | BA | 1986 | C | O4'-C1'-N1 | 5.86 | 112.89 | 108.20 |
| 24 | A3 | 26 | C | N1-C2-O2 | 5.86 | 122.41 | 118.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 1278 | C | N1-C2-O2 | 5.86 | 122.41 | 118.90 |
| 57 | BA | 1408 | G | N1-C6-O6 | -5.86 | 116.39 | 119.90 |
| 57 | BA | 1470 | A | N1-C6-N6 | -5.86 | 115.09 | 118.60 |
| 57 | BA | 2170 | A | C3'-C2'-C1' | 5.86 | 106.19 | 101.50 |
| 58 | Ba | 4 | C | N1-C2-O2 | 5.86 | 122.41 | 118.90 |
| 57 | BA | 170 | U | O4'-C1'-N1 | 5.85 | 112.88 | 108.20 |
| 22 | AA | 356 | A | C4'-C3'-C2' | -5.85 | 96.75 | 102.60 |
| 22 | AA | 696 | A | C4-C5-C6 | -5.85 | 114.07 | 117.00 |
| 22 | AA | 960 | U | N3-C2-O2 | -5.85 | 118.10 | 122.20 |
| 57 | BA | 1536 | C | N3-C2-O2 | -5.85 | 117.80 | 121.90 |
| 57 | BA | 1961 | C | N1-C2-O2 | 5.85 | 122.41 | 118.90 |
| 57 | BA | 1383 | A | O4'-C1'-N9 | 5.85 | 112.88 | 108.20 |
| 57 | BA | 1572 | A | C4-C5-C6 | -5.85 | 114.08 | 117.00 |
| 57 | BA | 2549 | G | N1-C6-O6 | -5.85 | 116.39 | 119.90 |
| 22 | AA | 357 | G | N1-C6-O6 | -5.85 | 116.39 | 119.90 |
| 22 | AA | 1303 | C | N1-C2-O2 | 5.85 | 122.41 | 118.90 |
| 57 | BA | 331 | C | N1-C2-O2 | 5.85 | 122.41 | 118.90 |
| 57 | BA | 1662 | U | O4'-C1'-N1 | 5.85 | 112.88 | 108.20 |
| 57 | BA | 540 | C | N1-C2-O2 | 5.85 | 122.41 | 118.90 |
| 14 | AC | 171 | ARG | NE-CZ-NH2 | -5.85 | 117.38 | 120.30 |
| 57 | BA | 2748 | A | C4-C5-C6 | -5.85 | 114.08 | 117.00 |
| 22 | AA | 1197 | A | C4-C5-C6 | -5.84 | 114.08 | 117.00 |
| 57 | BA | 251 | A | C4-C5-C6 | -5.84 | 114.08 | 117.00 |
| 57 | BA | 2221 | G | O4'-C1'-N9 | 5.84 | 112.88 | 108.20 |
| 57 | BA | 2893 | A | C4-C5-C6 | -5.84 | 114.08 | 117.00 |
| 22 | AA | 388 | G | O4'-C1'-N9 | 5.84 | 112.87 | 108.20 |
| 22 | AA | 5 | U | N3-C2-O2 | -5.84 | 118.11 | 122.20 |
| 22 | AA | 492 | C | N1-C2-O2 | 5.84 | 122.41 | 118.90 |
| 22 | AA | 742 | G | N1-C6-O6 | -5.84 | 116.39 | 119.90 |
| 22 | AA | 1250 | A | C4-C5-C6 | -5.84 | 114.08 | 117.00 |
| 57 | BA | 771 | G | C5'-C4'-C3' | -5.84 | 106.65 | 116.00 |
| 57 | BA | 2147 | A | C4-C5-C6 | -5.84 | 114.08 | 117.00 |
| 6 | AO | 57 | ARG | NE-CZ-NH1 | 5.84 | 123.22 | 120.30 |
| 22 | AA | 116 | A | C4-C5-C6 | -5.84 | 114.08 | 117.00 |
| 57 | BA | 1965 | C | N3-C2-O2 | -5.84 | 117.81 | 121.90 |
| 57 | BA | 2852 | G | N1-C6-O6 | -5.84 | 116.40 | 119.90 |
| 57 | BA | 97 | C | O4'-C1'-N1 | 5.84 | 112.87 | 108.20 |
| 57 | BA | 112 | U | O4'-C1'-N1 | 5.84 | 112.87 | 108.20 |
| 57 | BA | 1331 | G | C5'-C4'-O4' | 5.84 | 116.11 | 109.10 |
| 57 | BA | 1819 | A | C4-C5-C6 | -5.84 | 114.08 | 117.00 |
| 22 | AA | 770 | C | O4'-C1'-N1 | 5.84 | 112.87 | 108.20 |
| 22 | AA | 968 | A | O4'-C1'-N9 | 5.84 | 112.87 | 108.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | AA | 1147 | C | N3-C2-O2 | -5.84 | 117.81 | 121.90 |
| 57 | BA | 53 | A | O4'-C1'-N9 | 5.84 | 112.87 | 108.20 |
| 57 | BA | 1193 | G | N1-C6-O6 | -5.84 | 116.40 | 119.90 |
| 57 | BA | 2066 | C | O4'-C1'-N1 | 5.84 | 112.87 | 108.20 |
| 57 | BA | 2453 | A | C4-C5-C6 | -5.84 | 114.08 | 117.00 |
| 57 | BA | 2806 | C | O4'-C1'-N1 | 5.84 | 112.87 | 108.20 |
| 22 | AA | 963 | G | N1-C6-O6 | -5.83 | 116.40 | 119.90 |
| 57 | BA | 1813 | G | O4'-C1'-N9 | 5.83 | 112.87 | 108.20 |
| 22 | AA | 1438 | G | N1-C6-O6 | -5.83 | 116.40 | 119.90 |
| 57 | BA | 587 | C | N3-C2-O2 | -5.83 | 117.82 | 121.90 |
| 57 | BA | 835 | C | N1-C2-O2 | 5.83 | 122.40 | 118.90 |
| 57 | BA | 1526 | C | N1-C2-O2 | 5.83 | 122.40 | 118.90 |
| 57 | BA | 1999 | C | N1-C2-O2 | 5.83 | 122.40 | 118.90 |
| 57 | BA | 2320 | U | O4'-C1'-N1 | 5.83 | 112.87 | 108.20 |
| 58 | Ba | 26 | C | C5'-C4'-C3' | -5.83 | 106.67 | 116.00 |
| 57 | BA | 1134 | A | O4'-C1'-N9 | 5.83 | 112.86 | 108.20 |
| 57 | BA | 1634 | A | C4-C5-C6 | -5.83 | 114.08 | 117.00 |
| 57 | BA | 1880 | U | O4'-C1'-N1 | 5.83 | 112.86 | 108.20 |
| 57 | BA | 863 | A | N1-C6-N6 | -5.83 | 115.10 | 118.60 |
| 22 | AA | 286 | C | N1-C2-O2 | 5.83 | 122.40 | 118.90 |
| 22 | AA | 794 | A | C4-C5-C6 | -5.83 | 114.09 | 117.00 |
| 22 | AA | 1242 | G | N1-C6-O6 | -5.83 | 116.40 | 119.90 |
| 57 | BA | 914 | G | C4'-C3'-C2' | -5.83 | 96.77 | 102.60 |
| 57 | BA | 1027 | A | C4-C5-C6 | -5.83 | 114.09 | 117.00 |
| 22 | AA | 1110 | A | C4-C5-C6 | -5.83 | 114.09 | 117.00 |
| 57 | BA | 41 | C | O4'-C1'-N1 | 5.83 | 112.86 | 108.20 |
| 57 | BA | 235 | U | O4'-C1'-N1 | 5.83 | 112.86 | 108.20 |
| 57 | BA | 583 | G | O4'-C1'-N9 | 5.83 | 112.86 | 108.20 |
| 57 | BA | 1787 | A | C4-C5-C6 | -5.83 | 114.09 | 117.00 |
| 22 | AA | 277 | C | O4'-C1'-N1 | 5.82 | 112.86 | 108.20 |
| 22 | AA | 384 | G | O4'-C1'-N9 | 5.82 | 112.86 | 108.20 |
| 23 | A2 | 55 | A | C4-C5-C6 | -5.82 | 114.09 | 117.00 |
| 57 | BA | 177 | G | N3-C4-C5 | -5.82 | 125.69 | 128.60 |
| 57 | BA | 2032 | G | N1-C6-O6 | -5.82 | 116.41 | 119.90 |
| 22 | AA | 85 | U | N3-C2-O2 | -5.82 | 118.12 | 122.20 |
| 22 | AA | 156 | C | O4'-C1'-N1 | 5.82 | 112.86 | 108.20 |
| 22 | AA | 201 | G | N1-C6-O6 | -5.82 | 116.41 | 119.90 |
| 57 | BA | 434 | U | O4'-C1'-N1 | 5.82 | 112.86 | 108.20 |
| 57 | BA | 694 | U | O4'-C1'-N1 | 5.82 | 112.86 | 108.20 |
| 58 | Ba | 111 | U | O4'-C1'-N1 | 5.82 | 112.86 | 108.20 |
| 22 | AA | 1318 | A | C4-C5-C6 | -5.82 | 114.09 | 117.00 |
| 48 | B5 | 12 | ARG | NE-CZ-NH2 | 5.82 | 123.21 | 120.30 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 316 | C | O4'-C1'-N1 | 5.82 | 112.86 | 108.20 |
| 57 | BA | 2368 | C | N3-C4-C5 | 5.82 | 124.23 | 121.90 |
| 57 | BA | 2660 | A | C4-C5-C6 | -5.82 | 114.09 | 117.00 |
| 22 | AA | 124 | C | O4'-C1'-N1 | 5.82 | 112.85 | 108.20 |
| 22 | AA | 1107 | C | O4'-C1'-N1 | 5.82 | 112.86 | 108.20 |
| 22 | AA | 1299 | A | C4-C5-C6 | -5.82 | 114.09 | 117.00 |
| 57 | BA | 327 | G | N3-C2-N2 | -5.82 | 115.83 | 119.90 |
| 57 | BA | 1073 | A | C5-C6-N6 | 5.82 | 128.35 | 123.70 |
| 57 | BA | 2788 | C | N1-C2-O2 | 5.82 | 122.39 | 118.90 |
| 22 | AA | 1411 | C | N1-C2-O2 | 5.82 | 122.39 | 118.90 |
| 31 | BQ | 51 | ARG | NE-CZ-NH2 | 5.82 | 123.21 | 120.30 |
| 57 | BA | 2182 | U | O4'-C1'-N1 | 5.82 | 112.85 | 108.20 |
| 57 | BA | 2749 | A | C4-C5-C6 | -5.82 | 114.09 | 117.00 |
| 57 | BA | 821 | A | O4'-C1'-N9 | 5.81 | 112.85 | 108.20 |
| 57 | BA | 2152 | G | N1-C6-O6 | -5.81 | 116.41 | 119.90 |
| 22 | AA | 373 | A | C4-C5-C6 | -5.81 | 114.09 | 117.00 |
| 57 | BA | 387 | U | N3-C2-O2 | -5.81 | 118.13 | 122.20 |
| 57 | BA | 2175 | C | N1-C2-O2 | 5.81 | 122.39 | 118.90 |
| 57 | BA | 2181 | U | O4'-C1'-N1 | 5.81 | 112.85 | 108.20 |
| 22 | AA | 156 | C | N1-C2-O2 | 5.81 | 122.39 | 118.90 |
| 22 | AA | 760 | G | O4'-C1'-N9 | 5.81 | 112.85 | 108.20 |
| 22 | AA | 372 | C | N3-C2-O2 | -5.81 | 117.83 | 121.90 |
| 22 | AA | 1038 | C | N1-C2-O2 | 5.81 | 122.39 | 118.90 |
| 22 | AA | 1509 | C | O4'-C1'-N1 | 5.81 | 112.85 | 108.20 |
| 57 | BA | 828 | U | N3-C2-O2 | -5.81 | 118.13 | 122.20 |
| 57 | BA | 355 | U | O4'-C1'-N1 | 5.81 | 112.84 | 108.20 |
| 57 | BA | 1424 | G | N1-C6-O6 | -5.81 | 116.42 | 119.90 |
| 24 | A3 | 54 | G | N1-C6-O6 | -5.81 | 116.42 | 119.90 |
| 55 | BH | 151 | ARG | NE-CZ-NH1 | 5.81 | 123.20 | 120.30 |
| 57 | BA | 506 | G | O4'-C1'-N9 | 5.81 | 112.84 | 108.20 |
| 57 | BA | 2450 | A | C6-C5-N7 | 5.81 | 136.36 | 132.30 |
| 22 | AA | 177 | G | N3-C4-C5 | -5.80 | 125.70 | 128.60 |
| 57 | BA | 594 | U | O4'-C1'-N1 | 5.80 | 112.84 | 108.20 |
| 57 | BA | 680 | C | N1-C2-O2 | 5.80 | 122.38 | 118.90 |
| 57 | BA | 2219 | U | O4'-C1'-N1 | 5.80 | 112.84 | 108.20 |
| 57 | BA | 2527 | C | N1-C2-O2 | 5.80 | 122.38 | 118.90 |
| 57 | BA | 1052 | C | N1-C2-O2 | 5.80 | 122.38 | 118.90 |
| 57 | BA | 1079 | C | O4'-C1'-N1 | 5.80 | 112.84 | 108.20 |
| 57 | BA | 1513 | U | O4'-C1'-N1 | 5.80 | 112.84 | 108.20 |
| 57 | BA | 1695 | G | O4'-C1'-N9 | 5.80 | 112.84 | 108.20 |
| 57 | BA | 2277 | G | N1-C6-O6 | -5.80 | 116.42 | 119.90 |
| 22 | AA | 427 | U | N3-C2-O2 | -5.80 | 118.14 | 122.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | AA | 835 | U | O4'-C1'-N1 | 5.80 | 112.84 | 108.20 |
| 22 | AA | 1033 | G | O4'-C1'-N9 | 5.80 | 112.84 | 108.20 |
| 22 | AA | 1303 | C | O4'-C1'-N1 | 5.80 | 112.84 | 108.20 |
| 57 | BA | 47 | C | O4'-C1'-N1 | 5.80 | 112.84 | 108.20 |
| 57 | BA | 2753 | A | C4-C5-C6 | -5.80 | 114.10 | 117.00 |
| 57 | BA | 960 | A | C4-C5-C6 | -5.80 | 114.10 | 117.00 |
| 57 | BA | 1658 | C | N1-C2-O2 | 5.80 | 122.38 | 118.90 |
| 22 | AA | 773 | G | O4'-C1'-N9 | 5.80 | 112.84 | 108.20 |
| 33 | BS | 16 | ARG | NH1-CZ-NH2 | -5.80 | 113.02 | 119.40 |
| 57 | BA | 842 | U | O4'-C1'-N1 | 5.80 | 112.84 | 108.20 |
| 57 | BA | 988 | A | C4-C5-C6 | -5.80 | 114.10 | 117.00 |
| 57 | BA | 2014 | A | C4-C5-C6 | -5.80 | 114.10 | 117.00 |
| 57 | BA | 2338 | C | O4'-C1'-N1 | 5.80 | 112.84 | 108.20 |
| 57 | BA | 2896 | C | N1-C2-O2 | 5.80 | 122.38 | 118.90 |
| 58 | Ba | 13 | G | N1-C6-O6 | -5.80 | 116.42 | 119.90 |
| 22 | AA | 927 | G | N1-C6-O6 | -5.79 | 116.42 | 119.90 |
| 22 | AA | 52 | C | O4'-C1'-N1 | 5.79 | 112.83 | 108.20 |
| 22 | AA | 109 | A | C4-C5-C6 | -5.79 | 114.10 | 117.00 |
| 57 | BA | 1192 | G | N1-C6-O6 | -5.79 | 116.42 | 119.90 |
| 57 | BA | 1471 | G | N1-C6-O6 | -5.79 | 116.42 | 119.90 |
| 22 | AA | 166 | U | O4'-C1'-N1 | 5.79 | 112.83 | 108.20 |
| 22 | AA | 1105 | A | O4'-C1'-N9 | 5.79 | 112.83 | 108.20 |
| 22 | AA | 1504 | G | N1-C6-O6 | -5.79 | 116.42 | 119.90 |
| 57 | BA | 1970 | A | C4-C5-C6 | -5.79 | 114.10 | 117.00 |
| 58 | Ba | 16 | G | O4'-C1'-N9 | 5.79 | 112.83 | 108.20 |
| 30 | BP | 59 | ARG | NH1-CZ-NH2 | -5.79 | 113.03 | 119.40 |
| 57 | BA | 1780 | A | C4-C5-C6 | -5.79 | 114.11 | 117.00 |
| 22 | AA | 162 | A | C4-C5-C6 | -5.79 | 114.11 | 117.00 |
| 22 | AA | 988 | G | O4'-C1'-N9 | 5.79 | 112.83 | 108.20 |
| 22 | AA | 1031 | C | N3-C2-O2 | -5.79 | 117.85 | 121.90 |
| 22 | AA | 1050 | G | C4'-C3'-C2' | -5.79 | 96.81 | 102.60 |
| 24 | A3 | 53 | G | O4'-C1'-N9 | 5.79 | 112.83 | 108.20 |
| 57 | BA | 1487 | U | O4'-C1'-N1 | 5.79 | 112.83 | 108.20 |
| 57 | BA | 2531 | A | C4-C5-C6 | -5.79 | 114.11 | 117.00 |
| 22 | AA | 172 | A | C4-C5-C6 | -5.79 | 114.11 | 117.00 |
| 22 | AA | 395 | C | N1-C2-O2 | 5.79 | 122.37 | 118.90 |
| 57 | BA | 789 | A | C4-C5-C6 | -5.79 | 114.11 | 117.00 |
| 57 | BA | 1644 | C | O4'-C1'-N1 | 5.79 | 112.83 | 108.20 |
| 57 | BA | 2008 | C | N1-C2-O2 | 5.79 | 122.37 | 118.90 |
| 22 | AA | 136 | C | N1-C2-O2 | 5.79 | 122.37 | 118.90 |
| 22 | AA | 200 | G | O4'-C1'-N9 | 5.79 | 112.83 | 108.20 |
| 22 | AA | 253 | A | C4-C5-C6 | -5.79 | 114.11 | 117.00 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 210 | C | N1-C2-O2 | 5.79 | 122.37 | 118.90 |
| 57 | BA | 1074 | G | N1-C6-O6 | -5.78 | 116.43 | 119.90 |
| 57 | BA | 2646 | C | C5'-C4'-O4' | 5.78 | 116.04 | 109.10 |
| 22 | AA | 651 | C | N1-C2-O2 | 5.78 | 122.37 | 118.90 |
| 22 | AA | 935 | A | C4-C5-C6 | -5.78 | 114.11 | 117.00 |
| 57 | BA | 558 | U | O4'-C1'-N1 | 5.78 | 112.82 | 108.20 |
| 57 | BA | 1600 | C | O4'-C1'-N1 | 5.78 | 112.82 | 108.20 |
| 57 | BA | 1748 | C | N1-C2-O2 | 5.78 | 122.37 | 118.90 |
| 57 | BA | 1988 | G | N1-C6-O6 | -5.78 | 116.43 | 119.90 |
| 57 | BA | 2361 | G | O4'-C1'-N9 | 5.78 | 112.83 | 108.20 |
| 57 | BA | 2460 | U | O4'-C1'-N1 | 5.78 | 112.83 | 108.20 |
| 57 | BA | 1678 | A | O4'-C1'-N9 | 5.78 | 112.82 | 108.20 |
| 21 | A1 | 142 | ARG | NE-CZ-NH1 | 5.78 | 123.19 | 120.30 |
| 22 | AA | 623 | C | N1-C2-O2 | 5.78 | 122.37 | 118.90 |
| 22 | AA | 912 | C | N1-C2-O2 | 5.78 | 122.37 | 118.90 |
| 22 | AA | 1503 | A | O4'-C1'-N9 | 5.78 | 112.82 | 108.20 |
| 53 | BF | 21 | ARG | NE-CZ-NH2 | 5.78 | 123.19 | 120.30 |
| 57 | BA | 557 | C | O4'-C1'-N1 | 5.78 | 112.82 | 108.20 |
| 57 | BA | 671 | C | N1-C2-O2 | 5.78 | 122.37 | 118.90 |
| 57 | BA | 991 | C | N1-C2-O2 | 5.78 | 122.37 | 118.90 |
| 57 | BA | 1266 | G | C3'-C2'-C1' | -5.78 | 96.88 | 101.50 |
| 57 | BA | 2017 | U | N1-C2-N3 | 5.78 | 118.37 | 114.90 |
| 22 | AA | 13 | U | C1'-O4'-C4' | -5.78 | 105.28 | 109.90 |
| 22 | AA | 745 | G | N1-C6-O6 | -5.78 | 116.43 | 119.90 |
| 35 | BD | 166 | ARG | NE-CZ-NH1 | 5.78 | 123.19 | 120.30 |
| 57 | BA | 1431 | A | C4-C5-C6 | -5.78 | 114.11 | 117.00 |
| 57 | BA | 1993 | U | O4'-C1'-N1 | 5.78 | 112.82 | 108.20 |
| 57 | BA | 2639 | A | C4-C5-C6 | -5.78 | 114.11 | 117.00 |
| 22 | AA | 437 | U | O4'-C1'-N1 | 5.77 | 112.82 | 108.20 |
| 22 | AA | 463 | U | O4'-C4'-C3' | 5.77 | 110.72 | 106.10 |
| 22 | AA | 717 | U | O4'-C1'-N1 | 5.77 | 112.82 | 108.20 |
| 57 | BA | 611 | C | N1-C2-O2 | 5.77 | 122.36 | 118.90 |
| 57 | BA | 1832 | C | N1-C2-O2 | 5.77 | 122.36 | 118.90 |
| 22 | AA | 308 | C | N1-C2-O2 | 5.77 | 122.36 | 118.90 |
| 22 | AA | 738 | C | N1-C2-O2 | 5.77 | 122.36 | 118.90 |
| 22 | AA | 1306 | A | C4-C5-C6 | -5.77 | 114.11 | 117.00 |
| 57 | BA | 8 | C | O4'-C1'-N1 | 5.77 | 112.82 | 108.20 |
| 57 | BA | 464 | U | O4'-C1'-N1 | 5.77 | 112.82 | 108.20 |
| 57 | BA | 509 | C | N1-C2-O2 | 5.77 | 122.36 | 118.90 |
| 57 | BA | 812 | C | N3-C2-O2 | -5.77 | 117.86 | 121.90 |
| 22 | AA | 259 | G | N1-C6-O6 | -5.77 | 116.44 | 119.90 |
| 22 | AA | 735 | C | N1-C2-O2 | 5.77 | 122.36 | 118.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 654 | A | C4-C5-C6 | -5.77 | 114.11 | 117.00 |
| 22 | AA | 513 | C | N1-C2-O2 | 5.77 | 122.36 | 118.90 |
| 57 | BA | 988 | A | O4'-C1'-N9 | 5.77 | 112.82 | 108.20 |
| 57 | BA | 1022 | G | O4'-C1'-N9 | 5.77 | 112.82 | 108.20 |
| 57 | BA | 1541 | C | N1-C2-O2 | 5.77 | 122.36 | 118.90 |
| 57 | BA | 2561 | U | O4'-C1'-N1 | 5.77 | 112.82 | 108.20 |
| 22 | AA | 402 | G | N1-C6-O6 | -5.77 | 116.44 | 119.90 |
| 57 | BA | 193 | U | O4'-C1'-N1 | 5.77 | 112.81 | 108.20 |
| 57 | BA | 879 | G | O4'-C1'-N9 | 5.77 | 112.81 | 108.20 |
| 22 | AA | 1069 | C | N1-C2-O2 | 5.77 | 122.36 | 118.90 |
| 22 | AA | 1114 | C | N1-C2-O2 | 5.76 | 122.36 | 118.90 |
| 57 | BA | 1452 | G | C5-C6-N1 | 5.76 | 114.38 | 111.50 |
| 57 | BA | 1768 | C | N1-C2-O2 | 5.76 | 122.36 | 118.90 |
| 57 | BA | 2204 | G | C5'-C4'-C3' | -5.76 | 106.78 | 116.00 |
| 57 | BA | 2423 | U | N3-C2-O2 | -5.76 | 118.16 | 122.20 |
| 57 | BA | 2556 | C | O4'-C1'-N1 | 5.76 | 112.81 | 108.20 |
| 57 | BA | 2589 | A | O4'-C1'-N9 | 5.76 | 112.81 | 108.20 |
| 3 | AL | 120 | ARG | NE-CZ-NH1 | 5.76 | 123.18 | 120.30 |
| 22 | AA | 1090 | U | O4'-C1'-N1 | 5.76 | 112.81 | 108.20 |
| 57 | BA | 279 | A | C4-C5-C6 | -5.76 | 114.12 | 117.00 |
| 57 | BA | 2050 | C | N1-C2-O2 | 5.76 | 122.36 | 118.90 |
| 22 | AA | 62 | U | O4'-C1'-N1 | 5.76 | 112.81 | 108.20 |
| 22 | AA | 438 | U | O4'-C1'-N1 | 5.76 | 112.81 | 108.20 |
| 22 | AA | 857 | C | N1-C2-O2 | 5.76 | 122.36 | 118.90 |
| 22 | AA | 561 | U | O4'-C1'-N1 | 5.76 | 112.81 | 108.20 |
| 22 | AA | 683 | G | N1-C6-O6 | -5.76 | 116.44 | 119.90 |
| 22 | AA | 1374 | A | C4-C5-C6 | -5.76 | 114.12 | 117.00 |
| 57 | BA | 105 | C | N1-C2-O2 | 5.76 | 122.36 | 118.90 |
| 57 | BA | 149 | A | C4-C5-C6 | -5.76 | 114.12 | 117.00 |
| 57 | BA | 1036 | G | N1-C6-O6 | -5.76 | 116.44 | 119.90 |
| 57 | BA | 2092 | U | N3-C2-O2 | -5.76 | 118.17 | 122.20 |
| 57 | BA | 371 | A | C4-C5-C6 | -5.76 | 114.12 | 117.00 |
| 57 | BA | 1461 | C | N3-C2-O2 | -5.76 | 117.87 | 121.90 |
| 22 | AA | 658 | C | O4'-C1'-N1 | 5.75 | 112.80 | 108.20 |
| 57 | BA | 135 | U | O4'-C1'-N1 | 5.75 | 112.80 | 108.20 |
| 57 | BA | 535 | G | N1-C6-O6 | -5.75 | 116.45 | 119.90 |
| 57 | BA | 872 | U | O4'-C1'-N1 | 5.75 | 112.80 | 108.20 |
| 57 | BA | 1310 | G | O4'-C1'-N9 | 5.75 | 112.80 | 108.20 |
| 57 | BA | 2643 | G | N1-C6-O6 | -5.75 | 116.45 | 119.90 |
| 58 | Ba | 99 | A | C4-C5-C6 | -5.75 | 114.12 | 117.00 |
| 22 | AA | 943 | U | O4'-C1'-N1 | 5.75 | 112.80 | 108.20 |
| 22 | AA | 965 | U | N3-C2-O2 | -5.75 | 118.17 | 122.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 36 | G | N3-C2-N2 | -5.75 | 115.87 | 119.90 |
| 57 | BA | 421 | C | O4'-C1'-N1 | 5.75 | 112.80 | 108.20 |
| 57 | BA | 1274 | A | C4-C5-C6 | -5.75 | 114.12 | 117.00 |
| 57 | BA | 1959 | G | N1-C6-O6 | -5.75 | 116.45 | 119.90 |
| 57 | BA | 2512 | C | O4'-C1'-N1 | 5.75 | 112.80 | 108.20 |
| 22 | AA | 370 | C | O4'-C1'-N1 | 5.75 | 112.80 | 108.20 |
| 22 | AA | 469 | C | N3-C2-O2 | -5.75 | 117.88 | 121.90 |
| 1 | AJ | 7 | ARG | NE-CZ-NH1 | 5.75 | 123.17 | 120.30 |
| 57 | BA | 1215 | G | N1-C6-O6 | -5.75 | 116.45 | 119.90 |
| 57 | BA | 1216 | G | N1-C6-O6 | -5.75 | 116.45 | 119.90 |
| 57 | BA | 1288 | G | N3-C4-C5 | -5.75 | 125.72 | 128.60 |
| 57 | BA | 2192 | U | O4'-C1'-N1 | 5.75 | 112.80 | 108.20 |
| 22 | AA | 1153 | G | N1-C6-O6 | -5.75 | 116.45 | 119.90 |
| 22 | AA | 1389 | C | N1-C2-O2 | 5.75 | 122.35 | 118.90 |
| 57 | BA | 863 | A | C4-C5-C6 | -5.75 | 114.13 | 117.00 |
| 57 | BA | 1329 | U | N3-C2-O2 | -5.75 | 118.18 | 122.20 |
| 22 | AA | 199 | A | C4-C5-C6 | -5.75 | 114.13 | 117.00 |
| 24 | A3 | 70 | C | O4'-C1'-N1 | 5.75 | 112.80 | 108.20 |
| 22 | AA | 608 | A | C4-C5-C6 | -5.74 | 114.13 | 117.00 |
| 57 | BA | 267 | C | O4'-C1'-N1 | 5.74 | 112.80 | 108.20 |
| 57 | BA | 1292 | G | N1-C6-O6 | -5.74 | 116.45 | 119.90 |
| 23 | A2 | 36 | U | O4'-C1'-N1 | 5.74 | 112.79 | 108.20 |
| 57 | BA | 952 | G | N1-C6-O6 | -5.74 | 116.45 | 119.90 |
| 22 | AA | 1504 | G | C1'-O4'-C4' | -5.74 | 105.31 | 109.90 |
| 57 | BA | 838 | C | O4'-C1'-N1 | 5.74 | 112.79 | 108.20 |
| 57 | BA | 885 | C | N1-C2-O2 | 5.74 | 122.34 | 118.90 |
| 57 | BA | 1624 | U | O4'-C1'-N1 | 5.74 | 112.79 | 108.20 |
| 22 | AA | 843 | U | C3'-C2'-C1' | 5.74 | 106.09 | 101.50 |
| 57 | BA | 87 | U | N3-C2-O2 | -5.74 | 118.18 | 122.20 |
| 57 | BA | 2493 | U | O4'-C1'-N1 | 5.74 | 112.79 | 108.20 |
| 22 | AA | 67 | C | O4'-C1'-N1 | 5.74 | 112.79 | 108.20 |
| 22 | AA | 1284 | C | N1-C2-O2 | 5.74 | 122.34 | 118.90 |
| 57 | BA | 199 | A | C4-C5-C6 | -5.74 | 114.13 | 117.00 |
| 57 | BA | 506 | G | N3-C4-C5 | -5.74 | 125.73 | 128.60 |
| 57 | BA | 576 | U | O4'-C1'-N1 | 5.74 | 112.79 | 108.20 |
| 57 | BA | 1231 | U | O4'-C1'-N1 | 5.74 | 112.79 | 108.20 |
| 57 | BA | 1719 | G | N1-C6-O6 | -5.74 | 116.46 | 119.90 |
| 57 | BA | 2614 | A | O4'-C1'-N9 | 5.74 | 112.79 | 108.20 |
| 22 | AA | 250 | A | C4-C5-C6 | -5.73 | 114.13 | 117.00 |
| 22 | AA | 1466 | C | N1-C2-O2 | 5.73 | 122.34 | 118.90 |
| 22 | AA | 1449 | C | N1-C2-O2 | 5.73 | 122.34 | 118.90 |
| 35 | BD | 174 | ARG | NE-CZ-NH1 | 5.73 | 123.17 | 120.30 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 514 | A | C4-C5-C6 | -5.73 | 114.13 | 117.00 |
| 57 | BA | 1422 | G | N1-C6-O6 | -5.73 | 116.46 | 119.90 |
| 57 | BA | 2041 | U | O4'-C1'-N1 | 5.73 | 112.79 | 108.20 |
| 57 | BA | 2737 | G | N1-C6-O6 | -5.73 | 116.46 | 119.90 |
| 57 | BA | 2821 | A | C4-C5-C6 | -5.73 | 114.13 | 117.00 |
| 22 | AA | 1452 | C | N3-C2-O2 | -5.73 | 117.89 | 121.90 |
| 57 | BA | 364 | C | N1-C2-O2 | 5.73 | 122.34 | 118.90 |
| 58 | Ba | 62 | C | N1-C2-O2 | 5.73 | 122.34 | 118.90 |
| 22 | AA | 204 | G | N1-C6-O6 | -5.73 | 116.46 | 119.90 |
| 22 | AA | 1217 | C | N1-C2-O2 | 5.73 | 122.34 | 118.90 |
| 30 | BP | 69 | ARG | NE-CZ-NH1 | 5.73 | 123.16 | 120.30 |
| 57 | BA | 353 | C | O4'-C1'-N1 | 5.73 | 112.78 | 108.20 |
| 57 | BA | 2646 | C | N1-C2-O2 | 5.73 | 122.34 | 118.90 |
| 57 | BA | 42 | A | O4'-C1'-N9 | 5.73 | 112.78 | 108.20 |
| 57 | BA | 1024 | G | O4'-C1'-N9 | 5.73 | 112.78 | 108.20 |
| 57 | BA | 1409 | U | O4'-C1'-N1 | 5.73 | 112.78 | 108.20 |
| 22 | AA | 189 | A | O4'-C1'-N9 | 5.72 | 112.78 | 108.20 |
| 22 | AA | 405 | U | O4'-C1'-N1 | 5.72 | 112.78 | 108.20 |
| 22 | AA | 1520 | C | N1-C2-O2 | 5.72 | 122.33 | 118.90 |
| 57 | BA | 650 | C | N1-C2-O2 | 5.72 | 122.33 | 118.90 |
| 57 | BA | 1489 | C | N1-C2-O2 | 5.72 | 122.33 | 118.90 |
| 57 | BA | 2301 | C | N1-C2-O2 | 5.72 | 122.33 | 118.90 |
| 57 | BA | 2735 | G | N1-C6-O6 | -5.72 | 116.47 | 119.90 |
| 22 | AA | 426 | U | O4'-C1'-N1 | 5.72 | 112.78 | 108.20 |
| 22 | AA | 914 | A | C5'-C4'-O4' | 5.72 | 115.97 | 109.10 |
| 57 | BA | 2730 | C | N1-C2-O2 | 5.72 | 122.33 | 118.90 |
| 22 | AA | 888 | G | O4'-C1'-N9 | 5.72 | 112.78 | 108.20 |
| 57 | BA | 576 | U | C3'-C2'-C1' | 5.72 | 106.08 | 101.50 |
| 57 | BA | 1094 | U | O4'-C1'-N1 | 5.72 | 112.78 | 108.20 |
| 57 | BA | 1100 | C | O4'-C1'-N1 | 5.72 | 112.78 | 108.20 |
| 57 | BA | 2438 | U | C5-C6-N1 | -5.72 | 119.84 | 122.70 |
| 21 | A1 | 263 | ARG | NE-CZ-NH1 | 5.72 | 123.16 | 120.30 |
| 22 | AA | 295 | C | N1-C2-O2 | 5.72 | 122.33 | 118.90 |
| 22 | AA | 339 | C | N1-C2-O2 | 5.72 | 122.33 | 118.90 |
| 22 | AA | 404 | G | C5-C6-N1 | 5.72 | 114.36 | 111.50 |
| 22 | AA | 795 | C | O4'-C1'-N1 | 5.72 | 112.78 | 108.20 |
| 57 | BA | 783 | A | C4-C5-C6 | -5.72 | 114.14 | 117.00 |
| 57 | BA | 1317 | G | N1-C6-O6 | -5.72 | 116.47 | 119.90 |
| 57 | BA | 2016 | U | O4'-C1'-N1 | 5.72 | 112.78 | 108.20 |
| 57 | BA | 2215 | C | N1-C2-O2 | 5.72 | 122.33 | 118.90 |
| 57 | BA | 635 | C | O4'-C1'-N1 | 5.72 | 112.77 | 108.20 |
| 57 | BA | 1118 | C | N1-C2-O2 | 5.72 | 122.33 | 118.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 2023 | C | N1-C2-O2 | 5.72 | 122.33 | 118.90 |
| 22 | AA | 1075 | U | O4'-C1'-N1 | 5.72 | 112.77 | 108.20 |
| 22 | AA | 1483 | A | C4-C5-C6 | -5.72 | 114.14 | 117.00 |
| 57 | BA | 2187 | U | O4'-C1'-N1 | 5.72 | 112.77 | 108.20 |
| 22 | AA | 1037 | C | N1-C2-O2 | 5.71 | 122.33 | 118.90 |
| 22 | AA | 1366 | C | N1-C2-O2 | 5.71 | 122.33 | 118.90 |
| 57 | BA | 1755 | A | C6-C5-N7 | 5.71 | 136.30 | 132.30 |
| 57 | BA | 2416 | C | N1-C2-O2 | 5.71 | 122.33 | 118.90 |
| 22 | AA | 894 | G | N1-C6-O6 | -5.71 | 116.47 | 119.90 |
| 22 | AA | 1011 | C | N1-C2-O2 | 5.71 | 122.33 | 118.90 |
| 22 | AA | 164 | G | N1-C6-O6 | -5.71 | 116.47 | 119.90 |
| 22 | AA | 552 | U | N3-C2-O2 | -5.71 | 118.20 | 122.20 |
| 57 | BA | 2076 | U | P-O3'-C3' | 5.71 | 126.55 | 119.70 |
| 22 | AA | 91 | U | O4'-C1'-N1 | 5.71 | 112.77 | 108.20 |
| 22 | AA | 677 | U | O4'-C1'-N1 | 5.71 | 112.77 | 108.20 |
| 22 | AA | 1270 | G | N1-C6-O6 | -5.71 | 116.47 | 119.90 |
| 57 | BA | 2295 | C | N1-C2-O2 | 5.71 | 122.33 | 118.90 |
| 57 | BA | 764 | A | O4'-C1'-N9 | 5.71 | 112.77 | 108.20 |
| 57 | BA | 1095 | A | C4-C5-C6 | -5.71 | 114.15 | 117.00 |
| 22 | AA | 419 | C | O4'-C1'-N1 | 5.71 | 112.77 | 108.20 |
| 57 | BA | 2572 | A | C4-C5-C6 | -5.71 | 114.15 | 117.00 |
| 22 | AA | 1046 | A | O4'-C1'-N9 | 5.71 | 112.76 | 108.20 |
| 57 | BA | 893 | C | N1-C2-O2 | 5.71 | 122.32 | 118.90 |
| 23 | A2 | 24 | A | O3'-P-O5' | -5.70 | 93.16 | 104.00 |
| 57 | BA | 836 | G | C5-C6-N1 | 5.70 | 114.35 | 111.50 |
| 58 | Ba | 26 | C | N1-C2-O2 | 5.70 | 122.32 | 118.90 |
| 57 | BA | 691 | C | N1-C2-O2 | 5.70 | 122.32 | 118.90 |
| 11 | AB | 136 | ARG | NE-CZ-NH1 | 5.70 | 123.15 | 120.30 |
| 22 | AA | 1302 | C | N1-C2-O2 | 5.70 | 122.32 | 118.90 |
| 57 | BA | 133 | U | O4'-C1'-N1 | 5.70 | 112.76 | 108.20 |
| 57 | BA | 496 | G | N1-C6-O6 | -5.70 | 116.48 | 119.90 |
| 57 | BA | 1120 | G | N1-C6-O6 | -5.70 | 116.48 | 119.90 |
| 57 | BA | 1498 | C | N1-C2-O2 | 5.70 | 122.32 | 118.90 |
| 57 | BA | 1686 | C | N1-C2-O2 | 5.70 | 122.32 | 118.90 |
| 58 | Ba | 9 | G | N1-C6-O6 | -5.70 | 116.48 | 119.90 |
| 22 | AA | 877 | G | N1-C6-O6 | -5.70 | 116.48 | 119.90 |
| 22 | AA | 1294 | G | N1-C6-O6 | -5.70 | 116.48 | 119.90 |
| 57 | BA | 1653 | G | P-O3'-C3' | 5.70 | 126.54 | 119.70 |
| 57 | BA | 2240 | U | O4'-C1'-N1 | 5.70 | 112.76 | 108.20 |
| 22 | AA | 580 | C | N1-C2-O2 | 5.70 | 122.32 | 118.90 |
| 22 | AA | 1143 | G | N1-C6-O6 | -5.70 | 116.48 | 119.90 |
| 57 | BA | 951 | 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($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 1602 | U | N3-C2-O2 | -5.70 | 118.21 | 122.20 |
| 57 | BA | 1617 | C | O4'-C1'-N1 | 5.70 | 112.76 | 108.20 |
| 57 | BA | 1663 | G | N3-C4-C5 | -5.70 | 125.75 | 128.60 |
| 57 | BA | 1777 | U | O4'-C1'-N1 | 5.70 | 112.76 | 108.20 |
| 58 | Ba | 93 | C | N1-C2-O2 | 5.70 | 122.32 | 118.90 |
| 23 | A2 | 59 | A | C4-C5-C6 | -5.69 | 114.15 | 117.00 |
| 57 | BA | 2429 | G | C3'-C2'-C1' | 5.69 | 106.06 | 101.50 |
| 22 | AA | 1276 | G | N1-C6-O6 | -5.69 | 116.48 | 119.90 |
| 57 | BA | 36 | G | N1-C6-O6 | -5.69 | 116.48 | 119.90 |
| 57 | BA | 2158 | A | C4-C5-C6 | -5.69 | 114.15 | 117.00 |
| 57 | BA | 2285 | C | N1-C2-O2 | 5.69 | 122.31 | 118.90 |
| 57 | BA | 2842 | G | N1-C6-O6 | -5.69 | 116.48 | 119.90 |
| 57 | BA | 2853 | C | O4'-C1'-N1 | 5.69 | 112.75 | 108.20 |
| 24 | A3 | 26 | C | O4'-C1'-N1 | 5.69 | 112.75 | 108.20 |
| 29 | BO | 105 | ARG | NE-CZ-NH1 | 5.69 | 123.15 | 120.30 |
| 31 | BQ | 38 | ARG | NE-CZ-NH1 | 5.69 | 123.14 | 120.30 |
| 57 | BA | 2601 | C | O4'-C1'-N1 | 5.69 | 112.75 | 108.20 |
| 22 | AA | 86 | G | O4'-C1'-N9 | 5.69 | 112.75 | 108.20 |
| 22 | AA | 514 | C | N1-C2-O2 | 5.69 | 122.31 | 118.90 |
| 22 | AA | 739 | C | N1-C2-O2 | 5.69 | 122.31 | 118.90 |
| 57 | BA | 1594 | U | O4'-C1'-N1 | 5.69 | 112.75 | 108.20 |
| 22 | AA | 709 | U | O4'-C1'-N1 | 5.69 | 112.75 | 108.20 |
| 57 | BA | 1330 | C | N1-C2-O2 | 5.69 | 122.31 | 118.90 |
| 57 | BA | 2508 | G | C4'-C3'-C2' | -5.69 | 96.91 | 102.60 |
| 57 | BA | 2652 | C | O4'-C1'-N1 | 5.69 | 112.75 | 108.20 |
| 57 | BA | 2902 | C | N1-C2-O2 | 5.69 | 122.31 | 118.90 |
| 22 | AA | 496 | A | C4-C5-C6 | -5.69 | 114.16 | 117.00 |
| 22 | AA | 871 | U | O4'-C1'-N1 | 5.69 | 112.75 | 108.20 |
| 57 | BA | 803 | U | O4'-C1'-N1 | 5.69 | 112.75 | 108.20 |
| 57 | BA | 1128 | G | N1-C6-O6 | -5.69 | 116.49 | 119.90 |
| 57 | BA | 1480 | C | O4'-C1'-N1 | 5.69 | 112.75 | 108.20 |
| 22 | AA | 162 | A | O4'-C1'-N9 | 5.68 | 112.75 | 108.20 |
| 22 | AA | 1383 | C | N3-C2-O2 | -5.68 | 117.92 | 121.90 |
| 57 | BA | 29 | U | N1-C2-N3 | 5.68 | 118.31 | 114.90 |
| 57 | BA | 343 | C | N1-C2-O2 | 5.68 | 122.31 | 118.90 |
| 14 | AC | 130 | ARG | NE-CZ-NH1 | 5.68 | 123.14 | 120.30 |
| 22 | AA | 936 | C | C4'-C3'-C2' | -5.68 | 96.92 | 102.60 |
| 22 | AA | 1059 | C | N1-C2-O2 | 5.68 | 122.31 | 118.90 |
| 24 | A3 | 24 | C | N1-C2-O2 | 5.68 | 122.31 | 118.90 |
| 57 | BA | 487 | C | N1-C2-O2 | 5.68 | 122.31 | 118.90 |
| 57 | BA | 990 | A | C3'-C2'-C1' | 5.68 | 106.05 | 101.50 |
| 57 | BA | 1334 | G | N1-C6-O6 | -5.68 | 116.49 | 119.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 15 | AD | 164 | ARG | NE-CZ-NH1 | 5.68 | 123.14 | 120.30 |
| 57 | BA | 2430 | A | C1'-O4'-C4' | -5.68 | 105.36 | 109.90 |
| 22 | AA | 908 | A | C4-C5-C6 | -5.68 | 114.16 | 117.00 |
| 57 | BA | 41 | C | N1-C2-O2 | 5.68 | 122.31 | 118.90 |
| 57 | BA | 597 | G | N1-C6-O6 | -5.68 | 116.49 | 119.90 |
| 57 | BA | 793 | A | O4'-C1'-N9 | 5.68 | 112.74 | 108.20 |
| 57 | BA | 1229 | C | O4'-C1'-N1 | 5.68 | 112.74 | 108.20 |
| 57 | BA | 1967 | C | O4'-C1'-N1 | 5.68 | 112.74 | 108.20 |
| 57 | BA | 2232 | C | O4'-C1'-N1 | 5.68 | 112.74 | 108.20 |
| 57 | BA | 2699 | C | O4'-C1'-N1 | 5.68 | 112.74 | 108.20 |
| 22 | AA | 65 | A | O4'-C1'-N9 | 5.68 | 112.74 | 108.20 |
| 22 | AA | 624 | C | N1-C2-O2 | 5.68 | 122.31 | 118.90 |
| 57 | BA | 644 | A | C4-C5-C6 | -5.68 | 114.16 | 117.00 |
| 57 | BA | 2548 | U | O4'-C1'-N1 | 5.68 | 112.74 | 108.20 |
| 22 | AA | 883 | C | N1-C2-O2 | 5.68 | 122.31 | 118.90 |
| 57 | BA | 143 | C | N1-C2-O2 | 5.68 | 122.31 | 118.90 |
| 57 | BA | 517 | C | O4'-C1'-N1 | 5.68 | 112.74 | 108.20 |
| 57 | BA | 2110 | G | O4'-C1'-N9 | 5.68 | 112.74 | 108.20 |
| 22 | AA | 1114 | C | O4'-C1'-N1 | 5.67 | 112.74 | 108.20 |
| 22 | AA | 1314 | C | N3-C4-C5 | 5.67 | 124.17 | 121.90 |
| 57 | BA | 1013 | C | N1-C2-O2 | 5.67 | 122.31 | 118.90 |
| 57 | BA | 1185 | G | C3'-C2'-C1' | 5.67 | 106.04 | 101.50 |
| 57 | BA | 1238 | G | N1-C6-O6 | -5.67 | 116.50 | 119.90 |
| 57 | BA | 2438 | U | O4'-C1'-N1 | 5.67 | 112.74 | 108.20 |
| 22 | AA | 165 | G | N1-C6-O6 | -5.67 | 116.50 | 119.90 |
| 22 | AA | 1187 | G | N1-C6-O6 | -5.67 | 116.50 | 119.90 |
| 57 | BA | 1314 | C | N1-C2-O2 | 5.67 | 122.30 | 118.90 |
| 57 | BA | 2584 | U | O4'-C1'-N1 | 5.67 | 112.74 | 108.20 |
| 58 | Ba | 66 | A | C4-C5-C6 | -5.67 | 114.16 | 117.00 |
| 22 | AA | 1192 | C | N3-C2-O2 | -5.67 | 117.93 | 121.90 |
| 57 | BA | 623 | C | N1-C2-O2 | 5.67 | 122.30 | 118.90 |
| 57 | BA | 1140 | C | N1-C2-O2 | 5.67 | 122.30 | 118.90 |
| 57 | BA | 1346 | G | N1-C6-O6 | -5.67 | 116.50 | 119.90 |
| 7 | AP | 14 | ARG | NE-CZ-NH1 | 5.67 | 123.13 | 120.30 |
| 22 | AA | 87 | C | N1-C2-O2 | 5.67 | 122.30 | 118.90 |
| 22 | AA | 216 | U | O4'-C1'-N1 | 5.67 | 112.73 | 108.20 |
| 57 | BA | 719 | C | N1-C2-O2 | 5.67 | 122.30 | 118.90 |
| 57 | BA | 1228 | G | O4'-C1'-N9 | 5.67 | 112.73 | 108.20 |
| 57 | BA | 2222 | C | N1-C2-O2 | 5.67 | 122.30 | 118.90 |
| 22 | AA | 1341 | U | O4'-C1'-N1 | 5.67 | 112.73 | 108.20 |
| 57 | BA | 142 | A | O4'-C1'-N9 | 5.67 | 112.73 | 108.20 |
| 57 | BA | 1203 | U | O4'-C1'-N1 | 5.67 | 112.73 | 108.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 1728 | C | O4'-C1'-N1 | 5.67 | 112.73 | 108.20 |
| 57 | BA | 2699 | C | N1-C2-O2 | 5.67 | 122.30 | 118.90 |
| 22 | AA | 766 | A | C4-C5-C6 | -5.66 | 114.17 | 117.00 |
| 57 | BA | 291 | G | N1-C6-O6 | -5.66 | 116.50 | 119.90 |
| 57 | BA | 2306 | C | N3-C2-O2 | -5.66 | 117.94 | 121.90 |
| 57 | BA | 2855 | C | N1-C2-O2 | 5.66 | 122.30 | 118.90 |
| 57 | BA | 486 | C | N1-C2-O2 | 5.66 | 122.30 | 118.90 |
| 57 | BA | 903 | C | N1-C2-O2 | 5.66 | 122.30 | 118.90 |
| 57 | BA | 1402 | U | O4'-C1'-N1 | 5.66 | 112.73 | 108.20 |
| 22 | AA | 392 | C | O4'-C1'-N1 | 5.66 | 112.73 | 108.20 |
| 29 | BO | 49 | ARG | NE-CZ-NH1 | 5.66 | 123.13 | 120.30 |
| 57 | BA | 283 | G | N1-C6-O6 | -5.66 | 116.50 | 119.90 |
| 57 | BA | 914 | G | C3'-C2'-C1' | -5.66 | 96.97 | 101.50 |
| 57 | BA | 1575 | C | N1-C2-O2 | 5.66 | 122.30 | 118.90 |
| 4 | AM | 89 | ARG | NH1-CZ-NH2 | -5.66 | 113.17 | 119.40 |
| 22 | AA | 1213 | A | P-O3'-C3' | 5.66 | 126.49 | 119.70 |
| 57 | BA | 831 | G | N1-C6-O6 | -5.66 | 116.50 | 119.90 |
| 57 | BA | 1270 | C | N1-C2-O2 | 5.66 | 122.29 | 118.90 |
| 57 | BA | 1974 | C | N1-C2-O2 | 5.66 | 122.29 | 118.90 |
| 22 | AA | 32 | A | C4-C5-C6 | -5.66 | 114.17 | 117.00 |
| 57 | BA | 1138 | G | O4'-C1'-N9 | 5.66 | 112.72 | 108.20 |
| 57 | BA | 2676 | C | N1-C2-O2 | 5.66 | 122.29 | 118.90 |
| 22 | AA | 1342 | C | N1-C2-O2 | 5.65 | 122.29 | 118.90 |
| 57 | BA | 2579 | C | N1-C2-O2 | 5.65 | 122.29 | 118.90 |
| 22 | AA | 758 | C | N3-C2-O2 | -5.65 | 117.94 | 121.90 |
| 35 | BD | 61 | TYR | CB-CG-CD1 | -5.65 | 117.61 | 121.00 |
| 38 | BW | 11 | ARG | NH1-CZ-NH2 | -5.65 | 113.18 | 119.40 |
| 57 | BA | 996 | A | C4-C5-C6 | -5.65 | 114.17 | 117.00 |
| 57 | BA | 1646 | C | C3'-C2'-C1' | 5.65 | 106.02 | 101.50 |
| 57 | BA | 2773 | C | N1-C2-O2 | 5.65 | 122.29 | 118.90 |
| 57 | BA | 2858 | C | N3-C2-O2 | -5.65 | 117.94 | 121.90 |
| 22 | AA | 1072 | G | N1-C6-O6 | -5.65 | 116.51 | 119.90 |
| 22 | AA | 1234 | C | N1-C2-O2 | 5.65 | 122.29 | 118.90 |
| 7 | AP | 8 | ARG | NE-CZ-NH1 | 5.65 | 123.12 | 120.30 |
| 57 | BA | 297 | G | O4'-C1'-N9 | 5.65 | 112.72 | 108.20 |
| 57 | BA | 1383 | A | C4-C5-C6 | -5.65 | 114.17 | 117.00 |
| 57 | BA | 1585 | C | O4'-C1'-N1 | 5.65 | 112.72 | 108.20 |
| 57 | BA | 1727 | C | N1-C2-O2 | 5.65 | 122.29 | 118.90 |
| 57 | BA | 2507 | C | N1-C2-O2 | 5.65 | 122.29 | 118.90 |
| 22 | AA | 153 | C | N1-C2-O2 | 5.65 | 122.29 | 118.90 |
| 22 | AA | 194 | C | O4'-C1'-N1 | 5.65 | 112.72 | 108.20 |
| 22 | AA | 952 | U | O4'-C1'-N1 | 5.65 | 112.72 | 108.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 326 | G | N1-C6-O6 | -5.65 | 116.51 | 119.90 |
| 57 | BA | 531 | C | N1-C2-O2 | 5.65 | 122.29 | 118.90 |
| 58 | Ba | 68 | C | O4'-C1'-N1 | 5.65 | 112.72 | 108.20 |
| 22 | AA | 761 | G | N1-C6-O6 | -5.65 | 116.51 | 119.90 |
| 57 | BA | 2211 | A | C4-C5-C6 | -5.65 | 114.18 | 117.00 |
| 22 | AA | 258 | G | N1-C6-O6 | -5.64 | 116.51 | 119.90 |
| 57 | BA | 2006 | C | O4'-C1'-N1 | 5.64 | 112.72 | 108.20 |
| 57 | BA | 2174 | C | N3-C2-O2 | -5.64 | 117.95 | 121.90 |
| 12 | AT | 59 | ARG | NE-CZ-NH2 | 5.64 | 123.12 | 120.30 |
| 57 | BA | 268 | C | N1-C2-O2 | 5.64 | 122.28 | 118.90 |
| 57 | BA | 738 | G | N1-C6-O6 | -5.64 | 116.52 | 119.90 |
| 57 | BA | 814 | C | N1-C2-O2 | 5.64 | 122.28 | 118.90 |
| 57 | BA | 903 | C | O4'-C1'-N1 | 5.64 | 112.71 | 108.20 |
| 57 | BA | 1522 | A | C4-C5-C6 | -5.64 | 114.18 | 117.00 |
| 57 | BA | 2300 | C | O4'-C1'-N1 | 5.64 | 112.71 | 108.20 |
| 57 | BA | 2447 | G | N3-C4-C5 | -5.64 | 125.78 | 128.60 |
| 57 | BA | 2889 | C | O4'-C1'-N1 | 5.64 | 112.71 | 108.20 |
| 22 | AA | 68 | G | N3-C2-N2 | -5.64 | 115.95 | 119.90 |
| 57 | BA | 1160 | G | N1-C6-O6 | -5.64 | 116.52 | 119.90 |
| 57 | BA | 2103 | C | O4'-C1'-N1 | 5.64 | 112.71 | 108.20 |
| 22 | AA | 90 | C | O4'-C1'-N1 | 5.64 | 112.71 | 108.20 |
| 22 | AA | 1218 | C | N1-C2-O2 | 5.64 | 122.28 | 118.90 |
| 22 | AA | 1399 | C | O4'-C1'-N1 | 5.64 | 112.71 | 108.20 |
| 57 | BA | 76 | C | N1-C2-O2 | 5.64 | 122.28 | 118.90 |
| 57 | BA | 1073 | A | C6-C5-N7 | 5.64 | 136.25 | 132.30 |
| 57 | BA | 2555 | U | O4'-C1'-N1 | 5.64 | 112.71 | 108.20 |
| 52 | B9 | 12 | ARG | NE-CZ-NH1 | 5.64 | 123.12 | 120.30 |
| 57 | BA | 36 | G | N9-C4-C5 | 5.64 | 107.66 | 105.40 |
| 57 | BA | 1706 | C | N1-C2-O2 | 5.64 | 122.28 | 118.90 |
| 57 | BA | 1849 | G | N1-C6-O6 | -5.64 | 116.52 | 119.90 |
| 24 | A3 | 68 | C | O4'-C1'-N1 | 5.64 | 112.71 | 108.20 |
| 57 | BA | 604 | G | C5'-C4'-C3' | -5.64 | 106.98 | 116.00 |
| 57 | BA | 740 | C | N1-C2-O2 | 5.64 | 122.28 | 118.90 |
| 57 | BA | 970 | U | N3-C2-O2 | -5.64 | 118.25 | 122.20 |
| 57 | BA | 1260 | A | C4-C5-C6 | -5.64 | 114.18 | 117.00 |
| 57 | BA | 2300 | C | N1-C2-O2 | 5.64 | 122.28 | 118.90 |
| 22 | AA | 33 | A | C4-C5-C6 | -5.63 | 114.18 | 117.00 |
| 22 | AA | 590 | U | O4'-C1'-N1 | 5.63 | 112.71 | 108.20 |
| 22 | AA | 1272 | G | N1-C6-O6 | -5.63 | 116.52 | 119.90 |
| 57 | BA | 969 | G | O4'-C1'-N9 | 5.63 | 112.71 | 108.20 |
| 57 | BA | 2208 | C | N1-C2-O2 | 5.63 | 122.28 | 118.90 |
| 57 | BA | 2326 | C | N1-C2-O2 | 5.63 | 122.28 | 118.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 2439 | A | C4-C5-C6 | -5.63 | 114.18 | 117.00 |
| 57 | BA | 2665 | A | C4-C5-C6 | -5.63 | 114.18 | 117.00 |
| 22 | AA | 956 | U | O4'-C1'-N1 | 5.63 | 112.70 | 108.20 |
| 57 | BA | 13 | A | C6-C5-N7 | 5.63 | 136.24 | 132.30 |
| 57 | BA | 1123 | C | O4'-C1'-N1 | 5.63 | 112.70 | 108.20 |
| 57 | BA | 1311 | G | O4'-C1'-N9 | 5.63 | 112.70 | 108.20 |
| 57 | BA | 2483 | C | N1-C2-O2 | 5.63 | 122.28 | 118.90 |
| 57 | BA | 2835 | A | C4-C5-C6 | -5.63 | 114.19 | 117.00 |
| 22 | AA | 386 | C | O4'-C1'-N1 | 5.63 | 112.70 | 108.20 |
| 57 | BA | 22 | C | N1-C2-O2 | 5.63 | 122.28 | 118.90 |
| 57 | BA | 959 | A | C4-C5-C6 | -5.63 | 114.19 | 117.00 |
| 22 | AA | 886 | G | N1-C6-O6 | -5.63 | 116.52 | 119.90 |
| 57 | BA | 1843 | C | N1-C2-O2 | 5.63 | 122.28 | 118.90 |
| 57 | BA | 2212 | A | C4-C5-C6 | -5.63 | 114.19 | 117.00 |
| 57 | BA | 2223 | G | N1-C6-O6 | -5.63 | 116.52 | 119.90 |
| 57 | BA | 2785 | C | N1-C2-O2 | 5.63 | 122.28 | 118.90 |
| 22 | AA | 1320 | C | N3-C2-O2 | -5.62 | 117.96 | 121.90 |
| 57 | BA | 1233 | C | N1-C2-O2 | 5.62 | 122.28 | 118.90 |
| 57 | BA | 2631 | G | N1-C6-O6 | -5.62 | 116.53 | 119.90 |
| 2 | AK | 105 | ARG | NE-CZ-NH1 | 5.62 | 123.11 | 120.30 |
| 22 | AA | 183 | C | C1'-O4'-C4' | -5.62 | 105.40 | 109.90 |
| 22 | AA | 1113 | C | N1-C2-O2 | 5.62 | 122.27 | 118.90 |
| 57 | BA | 912 | C | N1-C2-O2 | 5.62 | 122.27 | 118.90 |
| 57 | BA | 1744 | A | C4-C5-C6 | -5.62 | 114.19 | 117.00 |
| 22 | AA | 932 | C | N1-C2-O2 | 5.62 | 122.27 | 118.90 |
| 57 | BA | 705 | A | N1-C6-N6 | -5.62 | 115.23 | 118.60 |
| 57 | BA | 2190 | G | N1-C6-O6 | -5.62 | 116.53 | 119.90 |
| 57 | BA | 2542 | A | O4'-C1'-N9 | 5.62 | 112.70 | 108.20 |
| 6 | AO | 71 | ARG | NE-CZ-NH1 | 5.62 | 123.11 | 120.30 |
| 22 | AA | 225 | C | N1-C2-O2 | 5.62 | 122.27 | 118.90 |
| 22 | AA | 230 | G | O4'-C1'-N9 | 5.62 | 112.70 | 108.20 |
| 57 | BA | 678 | C | N1-C2-O2 | 5.62 | 122.27 | 118.90 |
| 58 | Ba | 3 | C | N1-C2-O2 | 5.62 | 122.27 | 118.90 |
| 22 | AA | 580 | C | O4'-C1'-N1 | 5.62 | 112.69 | 108.20 |
| 57 | BA | 1263 | U | N3-C2-O2 | -5.62 | 118.27 | 122.20 |
| 57 | BA | 1352 | U | C5-C6-N1 | -5.62 | 119.89 | 122.70 |
| 57 | BA | 2545 | G | N1-C6-O6 | -5.62 | 116.53 | 119.90 |
| 22 | AA | 1348 | U | N3-C2-O2 | -5.62 | 118.27 | 122.20 |
| 57 | BA | 2533 | U | O4'-C1'-N1 | 5.62 | 112.69 | 108.20 |
| 57 | BA | 2562 | U | O4'-C1'-N1 | 5.62 | 112.69 | 108.20 |
| 22 | AA | 1094 | G | N1-C6-O6 | -5.62 | 116.53 | 119.90 |
| 57 | BA | 238 | C | N1-C2-O2 | 5.62 | 122.27 | 118.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 1185 | G | N1-C6-O6 | -5.62 | 116.53 | 119.90 |
| 57 | BA | 1577 | C | N1-C2-O2 | 5.62 | 122.27 | 118.90 |
| 57 | BA | 2063 | C | N3-C4-N4 | -5.62 | 114.07 | 118.00 |
| 22 | AA | 225 | C | O4'-C1'-N1 | 5.61 | 112.69 | 108.20 |
| 22 | AA | 316 | C | N1-C2-O2 | 5.61 | 122.27 | 118.90 |
| 22 | AA | 409 | U | O4'-C1'-N1 | 5.61 | 112.69 | 108.20 |
| 22 | AA | 457 | G | N1-C6-O6 | -5.61 | 116.53 | 119.90 |
| 22 | AA | 634 | C | N1-C2-O2 | 5.61 | 122.27 | 118.90 |
| 22 | AA | 1130 | A | O4'-C1'-N9 | 5.61 | 112.69 | 108.20 |
| 22 | AA | 1443 | C | N1-C2-O2 | 5.61 | 122.27 | 118.90 |
| 57 | BA | 105 | C | O4'-C1'-N1 | 5.61 | 112.69 | 108.20 |
| 57 | BA | 1451 | C | O4'-C1'-N1 | 5.61 | 112.69 | 108.20 |
| 57 | BA | 2063 | C | N1-C2-O2 | 5.61 | 122.27 | 118.90 |
| 22 | AA | 990 | C | N1-C2-O2 | 5.61 | 122.27 | 118.90 |
| 57 | BA | 285 | G | N1-C6-O6 | -5.61 | 116.53 | 119.90 |
| 57 | BA | 787 | C | N1-C2-O2 | 5.61 | 122.27 | 118.90 |
| 23 | A2 | 49 | U | O4'-C1'-N1 | 5.61 | 112.69 | 108.20 |
| 57 | BA | 301 | G | N1-C6-O6 | -5.61 | 116.53 | 119.90 |
| 57 | BA | 584 | C | O4'-C1'-N1 | 5.61 | 112.69 | 108.20 |
| 57 | BA | 1185 | G | O4'-C1'-N9 | 5.61 | 112.69 | 108.20 |
| 57 | BA | 1316 | U | O4'-C1'-N1 | 5.61 | 112.69 | 108.20 |
| 57 | BA | 1448 | G | N1-C6-O6 | -5.61 | 116.53 | 119.90 |
| 57 | BA | 1956 | U | N3-C2-O2 | -5.61 | 118.27 | 122.20 |
| 57 | BA | 1996 | C | N1-C2-O2 | 5.61 | 122.27 | 118.90 |
| 57 | BA | 2361 | G | N1-C6-O6 | -5.61 | 116.53 | 119.90 |
| 22 | AA | 275 | G | N1-C6-O6 | -5.61 | 116.54 | 119.90 |
| 22 | AA | 1296 | C | N1-C2-O2 | 5.61 | 122.27 | 118.90 |
| 57 | BA | 256 | A | C4-C5-C6 | -5.61 | 114.20 | 117.00 |
| 57 | BA | 1045 | C | C3'-C2'-C1' | 5.61 | 105.99 | 101.50 |
| 22 | AA | 1448 | C | N1-C2-O2 | 5.61 | 122.26 | 118.90 |
| 57 | BA | 2870 | C | N1-C2-O2 | 5.61 | 122.26 | 118.90 |
| 22 | AA | 351 | G | O4'-C1'-N9 | 5.60 | 112.68 | 108.20 |
| 57 | BA | 134 | G | N1-C6-O6 | -5.60 | 116.54 | 119.90 |
| 57 | BA | 521 | U | O4'-C1'-N1 | 5.60 | 112.68 | 108.20 |
| 57 | BA | 565 | C | N3-C4-C5 | 5.60 | 124.14 | 121.90 |
| 57 | BA | 1996 | C | N3-C4-C5 | 5.60 | 124.14 | 121.90 |
| 57 | BA | 2831 | G | N1-C6-O6 | -5.60 | 116.54 | 119.90 |
| 57 | BA | 711 | G | N1-C6-O6 | -5.60 | 116.54 | 119.90 |
| 57 | BA | 1134 | A | C4-C5-C6 | -5.60 | 114.20 | 117.00 |
| 22 | AA | 772 | U | O4'-C1'-N1 | 5.60 | 112.68 | 108.20 |
| 22 | AA | 1198 | G | N1-C6-O6 | -5.60 | 116.54 | 119.90 |
| 22 | AA | 202 | G | N3-C4-C5 | -5.60 | 125.80 | 128.60 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 53 | BF | 117 | ARG | NE-CZ-NH1 | 5.60 | 123.10 | 120.30 |
| 57 | BA | 468 | G | O4'-C1'-N9 | 5.60 | 112.68 | 108.20 |
| 57 | BA | 551 | G | O4'-C1'-N9 | 5.60 | 112.68 | 108.20 |
| 57 | BA | 2098 | U | O4'-C1'-N1 | 5.60 | 112.68 | 108.20 |
| 57 | BA | 2779 | U | O4'-C1'-N1 | 5.60 | 112.68 | 108.20 |
| 22 | AA | 1218 | C | O4'-C1'-N1 | 5.59 | 112.68 | 108.20 |
| 22 | AA | 1243 | C | N1-C2-O2 | 5.59 | 122.26 | 118.90 |
| 57 | BA | 580 | U | N3-C2-O2 | -5.59 | 118.28 | 122.20 |
| 57 | BA | 2398 | U | O4'-C1'-N1 | 5.59 | 112.68 | 108.20 |
| 22 | AA | 420 | U | C5'-C4'-O4' | 5.59 | 115.81 | 109.10 |
| 57 | BA | 509 | C | N3-C4-C5 | 5.59 | 124.14 | 121.90 |
| 57 | BA | 1340 | U | N3-C2-O2 | -5.59 | 118.28 | 122.20 |
| 57 | BA | 2784 | U | O4'-C1'-N1 | 5.59 | 112.67 | 108.20 |
| 22 | AA | 243 | A | O4'-C1'-N9 | 5.59 | 112.67 | 108.20 |
| 22 | AA | 931 | C | N1-C2-O2 | 5.59 | 122.25 | 118.90 |
| 22 | AA | 1469 | C | N3-C2-O2 | -5.59 | 117.99 | 121.90 |
| 31 | BQ | 18 | ARG | NE-CZ-NH2 | 5.59 | 123.10 | 120.30 |
| 57 | BA | 211 | C | N1-C2-O2 | 5.59 | 122.25 | 118.90 |
| 57 | BA | 252 | G | O4'-C1'-N9 | 5.59 | 112.67 | 108.20 |
| 57 | BA | 2446 | G | N1-C6-O6 | -5.59 | 116.55 | 119.90 |
| 57 | BA | 2795 | C | N1-C2-O2 | 5.59 | 122.25 | 118.90 |
| 57 | BA | 565 | C | O4'-C1'-N1 | 5.59 | 112.67 | 108.20 |
| 22 | AA | 283 | U | O4'-C1'-N1 | 5.59 | 112.67 | 108.20 |
| 22 | AA | 1019 | A | O4'-C1'-N9 | 5.59 | 112.67 | 108.20 |
| 22 | AA | 1369 | C | N1-C2-O2 | 5.59 | 122.25 | 118.90 |
| 22 | AA | 1509 | C | N1-C2-O2 | 5.59 | 122.25 | 118.90 |
| 57 | BA | 467 | G | O4'-C1'-N9 | 5.59 | 112.67 | 108.20 |
| 57 | BA | 1844 | C | N1-C2-O2 | 5.59 | 122.25 | 118.90 |
| 20 | AI | 44 | ARG | NE-CZ-NH1 | 5.59 | 123.09 | 120.30 |
| 22 | AA | 532 | A | C2-N3-C4 | 5.59 | 113.39 | 110.60 |
| 22 | AA | 849 | G | N1-C6-O6 | -5.59 | 116.55 | 119.90 |
| 22 | AA | 932 | C | O4'-C1'-N1 | 5.59 | 112.67 | 108.20 |
| 57 | BA | 1868 | C | N1-C2-O2 | 5.59 | 122.25 | 118.90 |
| 58 | Ba | 20 | G | N1-C6-O6 | -5.59 | 116.55 | 119.90 |
| 58 | Ba | 57 | A | C4-C5-C6 | -5.59 | 114.21 | 117.00 |
| 57 | BA | 302 | C | O4'-C1'-N1 | 5.58 | 112.67 | 108.20 |
| 57 | BA | 1191 | G | O4'-C1'-N9 | 5.58 | 112.67 | 108.20 |
| 57 | BA | 2084 | C | O4'-C1'-N1 | 5.58 | 112.67 | 108.20 |
| 22 | AA | 41 | G | N1-C6-O6 | -5.58 | 116.55 | 119.90 |
| 22 | AA | 202 | G | N1-C6-O6 | -5.58 | 116.55 | 119.90 |
| 57 | BA | 581 | C | N1-C2-O2 | 5.58 | 122.25 | 118.90 |
| 57 | BA | 1114 | C | N1-C2-O2 | 5.58 | 122.25 | 118.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|---|---|---|---|---|---|---|---|
| 58 | Ba | 27 | C | N1-C2-O2 | 5.58 | 122.25 | 118.90 |
| 22 | AA | 868 | C | N1-C2-O2 | 5.58 | 122.25 | 118.90 |
| 22 | AA | 1165 | U | O4'-C1'-N1 | 5.58 | 112.67 | 108.20 |
| 22 | AA | 1256 | A | C4-C5-C6 | -5.58 | 114.21 | 117.00 |
| 57 | BA | 74 | A | C5'-C4'-C3' | -5.58 | 107.07 | 116.00 |
| 57 | BA | 556 | A | C4-C5-C6 | -5.58 | 114.21 | 117.00 |
| 57 | BA | 1022 | G | C5-C6-N1 | 5.58 | 114.29 | 111.50 |
| 57 | BA | 1993 | U | N3-C2-O2 | -5.58 | 118.29 | 122.20 |
| 57 | BA | 2061 | G | C2'-C3'-O3' | 5.58 | 122.63 | 113.70 |
| 57 | BA | 2102 | G | N1-C6-O6 | -5.58 | 116.55 | 119.90 |
| 22 | AA | 284 | C | N1-C2-O2 | 5.58 | 122.25 | 118.90 |
| 22 | AA | 637 | C | N1-C2-O2 | 5.58 | 122.25 | 118.90 |
| 22 | AA | 828 | U | O4'-C1'-N1 | 5.58 | 112.66 | 108.20 |
| 57 | BA | 1860 | G | N1-C6-O6 | -5.58 | 116.55 | 119.90 |
| 22 | AA | 132 | C | N1-C2-O2 | 5.58 | 122.25 | 118.90 |
| 22 | AA | 221 | C | N1-C2-O2 | 5.58 | 122.25 | 118.90 |
| 22 | AA | 334 | C | N1-C2-O2 | 5.58 | 122.25 | 118.90 |
| 22 | AA | 1282 | C | N3-C4-C5 | 5.58 | 124.13 | 121.90 |
| 24 | A3 | 14 | A | C4-C5-C6 | -5.58 | 114.21 | 117.00 |
| 57 | BA | 908 | C | N1-C2-O2 | 5.58 | 122.25 | 118.90 |
| 57 | BA | 2307 | G | N1-C6-O6 | -5.58 | 116.55 | 119.90 |
| 57 | BA | 2769 | U | O4'-C1'-N1 | 5.58 | 112.66 | 108.20 |
| 57 | BA | 2061 | G | O4'-C1'-N9 | 5.58 | 112.66 | 108.20 |
| 57 | BA | 2470 | G | N1-C6-O6 | -5.58 | 116.55 | 119.90 |
| 22 | AA | 54 | C | O4'-C1'-N1 | 5.58 | 112.66 | 108.20 |
| 22 | AA | 111 | G | N1-C6-O6 | -5.58 | 116.56 | 119.90 |
| 57 | BA | 149 | A | N1-C6-N6 | -5.58 | 115.25 | 118.60 |
| 57 | BA | 183 | C | N1-C2-O2 | 5.58 | 122.25 | 118.90 |
| 57 | BA | 523 | C | N1-C2-O2 | 5.58 | 122.25 | 118.90 |
| 57 | BA | 2235 | G | N1-C6-O6 | -5.58 | 116.55 | 119.90 |
| 57 | BA | 2416 | C | O4'-C1'-N1 | 5.58 | 112.66 | 108.20 |
| 58 | Ba | 88 | C | C1'-O4'-C4' | -5.58 | 105.44 | 109.90 |
| 22 | AA | 1470 | U | O4'-C1'-N1 | 5.57 | 112.66 | 108.20 |
| 57 | BA | 1153 | C | O4'-C1'-N1 | 5.57 | 112.66 | 108.20 |
| 57 | BA | 1841 | U | O4'-C1'-N1 | 5.57 | 112.66 | 108.20 |
| 57 | BA | 1846 | G | N1-C6-O6 | -5.57 | 116.56 | 119.90 |
| 57 | BA | 1985 | C | O4'-C1'-N1 | 5.57 | 112.66 | 108.20 |
| 24 | A3 | 75 | C | N1-C2-O2 | 5.57 | 122.24 | 118.90 |
| 57 | BA | 1916 | A | C4-C5-C6 | -5.57 | 114.21 | 117.00 |
| 57 | BA | 2248 | C | N1-C2-O2 | 5.57 | 122.24 | 118.90 |
| 57 | BA | 795 | C | N1-C2-O2 | 5.57 | 122.24 | 118.90 |
| 57 | BA | 848 | C | N1-C2-O2 | 5.57 | 122.24 | 118.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 2793 | C | N1-C2-O2 | 5.57 | 122.24 | 118.90 |
| 22 | AA | 1231 | G | N1-C6-O6 | -5.57 | 116.56 | 119.90 |
| 35 | BD | 176 | ARG | NE-CZ-NH1 | 5.57 | 123.08 | 120.30 |
| 57 | BA | 1772 | A | O4'-C1'-N9 | 5.57 | 112.65 | 108.20 |
| 57 | BA | 2350 | C | O4'-C1'-N1 | 5.57 | 112.65 | 108.20 |
| 57 | BA | 2517 | C | N3-C2-O2 | -5.57 | 118.00 | 121.90 |
| 22 | AA | 736 | C | N1-C2-O2 | 5.57 | 122.24 | 118.90 |
| 57 | BA | 445 | C | N3-C4-C5 | 5.57 | 124.13 | 121.90 |
| 57 | BA | 1064 | C | N1-C2-O2 | 5.57 | 122.24 | 118.90 |
| 57 | BA | 1330 | C | O4'-C1'-N1 | 5.57 | 112.65 | 108.20 |
| 57 | BA | 1701 | A | C4-C5-C6 | -5.57 | 114.22 | 117.00 |
| 57 | BA | 1881 | C | N1-C2-O2 | 5.57 | 122.24 | 118.90 |
| 57 | BA | 2854 | G | N1-C6-O6 | -5.57 | 116.56 | 119.90 |
| 57 | BA | 2901 | C | N1-C2-O2 | 5.57 | 122.24 | 118.90 |
| 22 | AA | 346 | G | N3-C4-C5 | -5.56 | 125.82 | 128.60 |
| 57 | BA | 1764 | C | O4'-C1'-N1 | 5.56 | 112.65 | 108.20 |
| 57 | BA | 1905 | C | N1-C2-O2 | 5.56 | 122.24 | 118.90 |
| 57 | BA | 2615 | U | O4'-C1'-N1 | 5.56 | 112.65 | 108.20 |
| 58 | Ba | 3 | C | O4'-C1'-N1 | 5.56 | 112.65 | 108.20 |
| 22 | AA | 3 | A | C3'-C2'-C1' | 5.56 | 105.95 | 101.50 |
| 22 | AA | 23 | C | N1-C2-O2 | 5.56 | 122.24 | 118.90 |
| 22 | AA | 232 | G | O4'-C1'-N9 | 5.56 | 112.65 | 108.20 |
| 22 | AA | 717 | U | P-O3'-C3' | 5.56 | 126.38 | 119.70 |
| 22 | AA | 785 | G | N1-C6-O6 | -5.56 | 116.56 | 119.90 |
| 22 | AA | 1423 | G | N1-C6-O6 | -5.56 | 116.56 | 119.90 |
| 57 | BA | 97 | C | N1-C2-O2 | 5.56 | 122.24 | 118.90 |
| 57 | BA | 1465 | G | N1-C6-O6 | -5.56 | 116.56 | 119.90 |
| 57 | BA | 1750 | G | N1-C6-O6 | -5.56 | 116.56 | 119.90 |
| 57 | BA | 2141 | G | O4'-C1'-N9 | 5.56 | 112.65 | 108.20 |
| 57 | BA | 706 | A | C4-C5-C6 | -5.56 | 114.22 | 117.00 |
| 57 | BA | 1519 | G | N1-C6-O6 | -5.56 | 116.56 | 119.90 |
| 22 | AA | 1147 | C | N3-C4-C5 | 5.56 | 124.12 | 121.90 |
| 22 | AA | 1540 | U | O4'-C1'-N1 | 5.56 | 112.65 | 108.20 |
| 57 | BA | 414 | C | C4'-C3'-C2' | -5.56 | 97.04 | 102.60 |
| 57 | BA | 685 | A | C4-C5-C6 | -5.56 | 114.22 | 117.00 |
| 57 | BA | 1990 | C | N1-C2-O2 | 5.56 | 122.24 | 118.90 |
| 57 | BA | 2129 | C | C1'-O4'-C4' | -5.56 | 105.45 | 109.90 |
| 57 | BA | 2593 | U | O4'-C1'-N1 | 5.56 | 112.65 | 108.20 |
| 22 | AA | 108 | G | N1-C6-O6 | -5.56 | 116.56 | 119.90 |
| 57 | BA | 43 | G | N1-C6-O6 | -5.56 | 116.57 | 119.90 |
| 57 | BA | 928 | A | O4'-C1'-N9 | 5.56 | 112.65 | 108.20 |
| 57 | BA | 1130 | U | O4'-C1'-N1 | 5.56 | 112.65 | 108.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | AA | 99 | C | O4'-C1'-N1 | 5.56 | 112.64 | 108.20 |
| 57 | BA | 60 | G | O3'-P-O5' | -5.56 | 93.44 | 104.00 |
| 24 | A3 | 67 | C | N1-C2-O2 | 5.55 | 122.23 | 118.90 |
| 57 | BA | 806 | C | N1-C2-O2 | 5.55 | 122.23 | 118.90 |
| 57 | BA | 840 | C | O4'-C1'-N1 | 5.55 | 112.64 | 108.20 |
| 57 | BA | 1414 | C | N1-C2-O2 | 5.55 | 122.23 | 118.90 |
| 57 | BA | 1690 | A | N1-C6-N6 | -5.55 | 115.27 | 118.60 |
| 57 | BA | 2017 | U | O4'-C1'-N1 | 5.55 | 112.64 | 108.20 |
| 58 | Ba | 110 | C | N1-C2-O2 | 5.55 | 122.23 | 118.90 |
| 57 | BA | 816 | C | O4'-C1'-N1 | 5.55 | 112.64 | 108.20 |
| 57 | BA | 2843 | G | O4'-C1'-N9 | 5.55 | 112.64 | 108.20 |
| 15 | AD | 187 | ARG | NE-CZ-NH1 | 5.55 | 123.08 | 120.30 |
| 22 | AA | 245 | U | N3-C2-O2 | -5.55 | 118.31 | 122.20 |
| 22 | AA | 470 | C | O4'-C1'-N1 | 5.55 | 112.64 | 108.20 |
| 43 | B1 | 26 | ARG | NH1-CZ-NH2 | -5.55 | 113.29 | 119.40 |
| 57 | BA | 58 | G | O4'-C1'-N9 | 5.55 | 112.64 | 108.20 |
| 57 | BA | 2355 | G | N1-C6-O6 | -5.55 | 116.57 | 119.90 |
| 22 | AA | 135 | C | O4'-C1'-N1 | 5.55 | 112.64 | 108.20 |
| 57 | BA | 367 | G | O4'-C1'-N9 | 5.55 | 112.64 | 108.20 |
| 57 | BA | 496 | G | O4'-C1'-N9 | 5.55 | 112.64 | 108.20 |
| 57 | BA | 861 | A | C4-C5-C6 | -5.55 | 114.22 | 117.00 |
| 57 | BA | 2354 | C | N1-C2-O2 | 5.55 | 122.23 | 118.90 |
| 22 | AA | 855 | U | O4'-C1'-N1 | 5.55 | 112.64 | 108.20 |
| 54 | BG | 70 | ARG | NE-CZ-NH2 | 5.55 | 123.07 | 120.30 |
| 57 | BA | 141 | G | N3-C4-C5 | -5.55 | 125.83 | 128.60 |
| 22 | AA | 386 | C | N1-C2-O2 | 5.55 | 122.23 | 118.90 |
| 22 | AA | 1020 | G | N1-C6-O6 | -5.55 | 116.57 | 119.90 |
| 22 | AA | 1302 | C | N3-C4-C5 | 5.55 | 124.12 | 121.90 |
| 57 | BA | 575 | A | C1'-O4'-C4' | -5.55 | 105.46 | 109.90 |
| 57 | BA | 1121 | C | O4'-C1'-N1 | 5.55 | 112.64 | 108.20 |
| 57 | BA | 1888 | G | O4'-C1'-N9 | 5.55 | 112.64 | 108.20 |
| 57 | BA | 2816 | G | N1-C6-O6 | -5.55 | 116.57 | 119.90 |
| 27 | BK | 64 | ARG | NE-CZ-NH1 | 5.54 | 123.07 | 120.30 |
| 57 | BA | 153 | U | O4'-C1'-N1 | 5.54 | 112.64 | 108.20 |
| 57 | BA | 2045 | C | N1-C2-O2 | 5.54 | 122.23 | 118.90 |
| 57 | BA | 2839 | G | N1-C6-O6 | -5.54 | 116.57 | 119.90 |
| 21 | A1 | 623 | ARG | NE-CZ-NH1 | 5.54 | 123.07 | 120.30 |
| 22 | AA | 443 | C | N1-C2-O2 | 5.54 | 122.23 | 118.90 |
| 22 | AA | 708 | C | N1-C2-O2 | 5.54 | 122.23 | 118.90 |
| 22 | AA | 845 | A | C1'-O4'-C4' | -5.54 | 105.47 | 109.90 |
| 22 | AA | 1071 | C | O4'-C1'-N1 | 5.54 | 112.64 | 108.20 |
| 22 | AA | 1332 | A | C4-C5-C6 | -5.54 | 114.23 | 117.00 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 23 | A2 | 29 | G | N3-C4-C5 | -5.54 | 125.83 | 128.60 |
| 57 | BA | 475 | C | O4'-C1'-N1 | 5.54 | 112.63 | 108.20 |
| 57 | BA | 1480 | C | N1-C2-O2 | 5.54 | 122.23 | 118.90 |
| 58 | Ba | 112 | G | N1-C6-O6 | -5.54 | 116.57 | 119.90 |
| 22 | AA | 66 | A | C4-C5-C6 | -5.54 | 114.23 | 117.00 |
| 22 | AA | 444 | G | N1-C6-O6 | -5.54 | 116.58 | 119.90 |
| 22 | AA | 980 | C | N3-C2-O2 | -5.54 | 118.02 | 121.90 |
| 22 | AA | 1384 | C | O4'-C1'-N1 | 5.54 | 112.63 | 108.20 |
| 57 | BA | 188 | G | N1-C6-O6 | -5.54 | 116.58 | 119.90 |
| 57 | BA | 351 | C | N1-C2-O2 | 5.54 | 122.22 | 118.90 |
| 57 | BA | 1129 | A | C5'-C4'-O4' | 5.54 | 115.75 | 109.10 |
| 57 | BA | 1332 | G | P-O3'-C3' | 5.54 | 126.35 | 119.70 |
| 57 | BA | 2064 | C | N1-C2-O2 | 5.54 | 122.22 | 118.90 |
| 58 | Ba | 31 | C | N1-C2-O2 | 5.54 | 122.22 | 118.90 |
| 22 | AA | 756 | C | N1-C2-O2 | 5.54 | 122.22 | 118.90 |
| 57 | BA | 268 | C | O4'-C1'-N1 | 5.54 | 112.63 | 108.20 |
| 57 | BA | 462 | C | N1-C2-O2 | 5.54 | 122.22 | 118.90 |
| 57 | BA | 882 | G | N1-C6-O6 | -5.54 | 116.58 | 119.90 |
| 57 | BA | 2535 | G | N3-C2-N2 | -5.54 | 116.02 | 119.90 |
| 57 | BA | 2616 | C | O4'-C1'-N1 | 5.54 | 112.63 | 108.20 |
| 58 | Ba | 37 | C | N3-C2-O2 | -5.54 | 118.02 | 121.90 |
| 22 | AA | 87 | C | O4'-C1'-N1 | 5.54 | 112.63 | 108.20 |
| 57 | BA | 1621 | U | O4'-C1'-N1 | 5.54 | 112.63 | 108.20 |
| 12 | AT | 24 | ARG | NH1-CZ-NH2 | -5.54 | 113.31 | 119.40 |
| 22 | AA | 815 | A | C6-C5-N7 | 5.54 | 136.17 | 132.30 |
| 22 | AA | 1039 | G | N1-C6-O6 | -5.54 | 116.58 | 119.90 |
| 24 | A3 | 72 | C | N1-C2-O2 | 5.54 | 122.22 | 118.90 |
| 57 | BA | 246 | C | O4'-C1'-N1 | 5.54 | 112.63 | 108.20 |
| 57 | BA | 714 | U | O4'-C1'-N1 | 5.54 | 112.63 | 108.20 |
| 57 | BA | 924 | G | N1-C6-O6 | -5.54 | 116.58 | 119.90 |
| 57 | BA | 2739 | U | C5-C6-N1 | -5.54 | 119.93 | 122.70 |
| 57 | BA | 2843 | G | N1-C6-O6 | -5.54 | 116.58 | 119.90 |
| 24 | A3 | 43 | G | N1-C6-O6 | -5.53 | 116.58 | 119.90 |
| 57 | BA | 1908 | C | O4'-C1'-N1 | 5.53 | 112.63 | 108.20 |
| 57 | BA | 2403 | C | N1-C2-O2 | 5.53 | 122.22 | 118.90 |
| 57 | BA | 2646 | C | O4'-C1'-N1 | 5.53 | 112.63 | 108.20 |
| 22 | AA | 714 | G | O4'-C1'-N9 | 5.53 | 112.63 | 108.20 |
| 57 | BA | 1607 | C | O4'-C1'-N1 | 5.53 | 112.63 | 108.20 |
| 57 | BA | 2653 | U | N3-C2-O2 | -5.53 | 118.33 | 122.20 |
| 57 | BA | 2000 | C | O4'-C1'-N1 | 5.53 | 112.62 | 108.20 |
| 22 | AA | 841 | C | O4'-C1'-N1 | 5.53 | 112.62 | 108.20 |
| 22 | AA | 1047 | G | N3-C4-C5 | -5.53 | 125.83 | 128.60 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | AA | 1526 | G | N1-C6-O6 | -5.53 | 116.58 | 119.90 |
| 57 | BA | 1533 | C | N1-C2-O2 | 5.53 | 122.22 | 118.90 |
| 22 | AA | 74 | A | C6-C5-N7 | 5.53 | 136.17 | 132.30 |
| 22 | AA | 764 | C | O4'-C1'-N1 | 5.53 | 112.62 | 108.20 |
| 22 | AA | 973 | G | N1-C6-O6 | -5.53 | 116.58 | 119.90 |
| 22 | AA | 1364 | U | O4'-C1'-N1 | 5.53 | 112.62 | 108.20 |
| 57 | BA | 393 | C | N1-C2-O2 | 5.53 | 122.22 | 118.90 |
| 57 | BA | 636 | G | N1-C6-O6 | -5.53 | 116.58 | 119.90 |
| 57 | BA | 832 | U | N3-C2-O2 | -5.53 | 118.33 | 122.20 |
| 57 | BA | 1585 | C | N3-C4-C5 | 5.53 | 124.11 | 121.90 |
| 57 | BA | 1768 | C | O4'-C1'-N1 | 5.53 | 112.62 | 108.20 |
| 22 | AA | 573 | A | C6-C5-N7 | 5.53 | 136.17 | 132.30 |
| 22 | AA | 1253 | G | C5'-C4'-C3' | -5.53 | 107.16 | 116.00 |
| 57 | BA | 1926 | U | N3-C2-O2 | -5.53 | 118.33 | 122.20 |
| 57 | BA | 2143 | C | O4'-C1'-N1 | 5.53 | 112.62 | 108.20 |
| 57 | BA | 2458 | G | N3-C4-C5 | -5.53 | 125.84 | 128.60 |
| 57 | BA | 1388 | G | O4'-C1'-N9 | 5.52 | 112.62 | 108.20 |
| 22 | AA | 558 | G | O4'-C1'-N9 | 5.52 | 112.62 | 108.20 |
| 22 | AA | 1040 | U | O4'-C1'-N1 | 5.52 | 112.62 | 108.20 |
| 22 | AA | 1501 | C | N1-C2-O2 | 5.52 | 122.21 | 118.90 |
| 57 | BA | 1718 | G | N1-C6-O6 | -5.52 | 116.59 | 119.90 |
| 22 | AA | 161 | A | C8-N9-C4 | -5.52 | 103.59 | 105.80 |
| 22 | AA | 218 | U | O4'-C1'-N1 | 5.52 | 112.62 | 108.20 |
| 22 | AA | 1292 | G | N1-C6-O6 | -5.52 | 116.59 | 119.90 |
| 22 | AA | 1307 | U | O4'-C1'-N1 | 5.52 | 112.62 | 108.20 |
| 57 | BA | 665 | U | O4'-C1'-N1 | 5.52 | 112.62 | 108.20 |
| 57 | BA | 1076 | C | N1-C2-O2 | 5.52 | 122.21 | 118.90 |
| 57 | BA | 1569 | A | C6-C5-N7 | 5.52 | 136.16 | 132.30 |
| 57 | BA | 2082 | A | N1-C6-N6 | -5.52 | 115.29 | 118.60 |
| 57 | BA | 2422 | C | C1'-O4'-C4' | -5.52 | 105.48 | 109.90 |
| 57 | BA | 2476 | A | C6-C5-N7 | 5.52 | 136.16 | 132.30 |
| 57 | BA | 2771 | C | O4'-C1'-N1 | 5.52 | 112.61 | 108.20 |
| 58 | Ba | 93 | C | O4'-C1'-N1 | 5.52 | 112.61 | 108.20 |
| 57 | BA | 580 | U | O4'-C1'-N1 | 5.52 | 112.61 | 108.20 |
| 57 | BA | 1793 | C | N1-C2-O2 | 5.52 | 122.21 | 118.90 |
| 57 | BA | 2161 | C | N3-C2-O2 | -5.52 | 118.04 | 121.90 |
| 22 | AA | 536 | C | N1-C2-O2 | 5.51 | 122.21 | 118.90 |
| 57 | BA | 100 | U | N3-C2-O2 | -5.51 | 118.34 | 122.20 |
| 57 | BA | 256 | A | N1-C6-N6 | -5.51 | 115.29 | 118.60 |
| 57 | BA | 315 | G | N1-C6-O6 | -5.51 | 116.59 | 119.90 |
| 57 | BA | 1615 | C | C2-N3-C4 | -5.51 | 117.14 | 119.90 |
| 20 | AI | 129 | ARG | NH1-CZ-NH2 | -5.51 | 113.34 | 119.40 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | AA | 1496 | C | N1-C2-O2 | 5.51 | 122.21 | 118.90 |
| 57 | BA | 542 | C | O4'-C1'-N1 | 5.51 | 112.61 | 108.20 |
| 20 | AI | 48 | ARG | NE-CZ-NH2 | -5.51 | 117.55 | 120.30 |
| 22 | AA | 203 | G | N1-C6-O6 | -5.51 | 116.59 | 119.90 |
| 24 | A3 | 9 | G | N3-C4-C5 | -5.51 | 125.84 | 128.60 |
| 57 | BA | 49 | A | C4-C5-C6 | -5.51 | 114.24 | 117.00 |
| 57 | BA | 1499 | C | N1-C2-O2 | 5.51 | 122.21 | 118.90 |
| 57 | BA | 2691 | C | N1-C2-O2 | 5.51 | 122.21 | 118.90 |
| 57 | BA | 2785 | C | O4'-C1'-N1 | 5.51 | 112.61 | 108.20 |
| 22 | AA | 129 | A | C6-C5-N7 | 5.51 | 136.16 | 132.30 |
| 22 | AA | 1144 | G | N1-C6-O6 | -5.51 | 116.59 | 119.90 |
| 57 | BA | 645 | C | O4'-C1'-N1 | 5.51 | 112.61 | 108.20 |
| 57 | BA | 709 | U | O4'-C1'-N1 | 5.51 | 112.61 | 108.20 |
| 22 | AA | 383 | A | C4-C5-C6 | -5.51 | 114.25 | 117.00 |
| 57 | BA | 560 | C | N1-C2-O2 | 5.51 | 122.20 | 118.90 |
| 57 | BA | 1021 | A | C4-C5-C6 | -5.51 | 114.25 | 117.00 |
| 57 | BA | 2099 | U | O4'-C1'-N1 | 5.51 | 112.61 | 108.20 |
| 57 | BA | 2206 | C | N1-C2-O2 | 5.51 | 122.20 | 118.90 |
| 57 | BA | 2558 | C | N1-C2-O2 | 5.51 | 122.20 | 118.90 |
| 22 | AA | 1109 | C | O4'-C1'-N1 | 5.51 | 112.61 | 108.20 |
| 22 | AA | 1228 | C | O4'-C1'-N1 | 5.51 | 112.61 | 108.20 |
| 22 | AA | 1474 | U | O4'-C1'-N1 | 5.51 | 112.61 | 108.20 |
| 49 | B6 | 5 | ARG | NE-CZ-NH1 | 5.51 | 123.05 | 120.30 |
| 53 | BF | 79 | ARG | NE-CZ-NH1 | 5.51 | 123.05 | 120.30 |
| 57 | BA | 647 | G | N1-C6-O6 | -5.51 | 116.60 | 119.90 |
| 57 | BA | 1091 | G | N1-C6-O6 | -5.51 | 116.60 | 119.90 |
| 57 | BA | 1162 | G | N1-C6-O6 | -5.51 | 116.60 | 119.90 |
| 57 | BA | 2368 | C | N1-C2-O2 | 5.51 | 122.20 | 118.90 |
| 57 | BA | 2815 | C | N1-C2-O2 | 5.51 | 122.20 | 118.90 |
| 57 | BA | 2840 | C | N1-C2-O2 | 5.51 | 122.20 | 118.90 |
| 40 | BY | 81 | ARG | NE-CZ-NH1 | 5.50 | 123.05 | 120.30 |
| 57 | BA | 1130 | U | C3'-C2'-C1' | -5.50 | 97.10 | 101.50 |
| 57 | BA | 1931 | U | N3-C2-O2 | -5.50 | 118.35 | 122.20 |
| 57 | BA | 2671 | G | N1-C6-O6 | -5.50 | 116.60 | 119.90 |
| 57 | BA | 2704 | C | N3-C4-C5 | 5.50 | 124.10 | 121.90 |
| 51 | B8 | 39 | ARG | NE-CZ-NH2 | 5.50 | 123.05 | 120.30 |
| 57 | BA | 984 | A | O4'-C1'-N9 | 5.50 | 112.60 | 108.20 |
| 58 | Ba | 1 | U | O4'-C1'-N1 | 5.50 | 112.60 | 108.20 |
| 22 | AA | 665 | A | C6-C5-N7 | 5.50 | 136.15 | 132.30 |
| 22 | AA | 793 | U | C4'-C3'-C2' | -5.50 | 97.10 | 102.60 |
| 57 | BA | 782 | A | C4-C5-C6 | -5.50 | 114.25 | 117.00 |
| 57 | BA | 2036 | C | N1-C2-O2 | 5.50 | 122.20 | 118.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 2141 | G | N1-C6-O6 | -5.50 | 116.60 | 119.90 |
| 12 | AT | 9 | ARG | NH1-CZ-NH2 | -5.50 | 113.35 | 119.40 |
| 57 | BA | 2622 | U | O4'-C1'-N1 | 5.50 | 112.60 | 108.20 |
| 22 | AA | 914 | A | C4-C5-C6 | -5.50 | 114.25 | 117.00 |
| 57 | BA | 2532 | G | N3-C2-N2 | -5.50 | 116.05 | 119.90 |
| 22 | AA | 1203 | C | N1-C2-O2 | 5.50 | 122.20 | 118.90 |
| 57 | BA | 516 | C | N1-C2-O2 | 5.50 | 122.20 | 118.90 |
| 57 | BA | 551 | G | N1-C6-O6 | -5.50 | 116.60 | 119.90 |
| 57 | BA | 1131 | G | N1-C6-O6 | -5.50 | 116.60 | 119.90 |
| 57 | BA | 2107 | G | N1-C6-O6 | -5.50 | 116.60 | 119.90 |
| 57 | BA | 2772 | C | N1-C2-O2 | 5.50 | 122.20 | 118.90 |
| 58 | Ba | 71 | C | N1-C2-O2 | 5.50 | 122.20 | 118.90 |
| 22 | AA | 264 | C | N3-C2-O2 | -5.50 | 118.05 | 121.90 |
| 22 | AA | 639 | G | N1-C6-O6 | -5.50 | 116.60 | 119.90 |
| 22 | AA | 999 | C | O4'-C1'-N1 | 5.50 | 112.60 | 108.20 |
| 57 | BA | 1101 | U | O4'-C1'-N1 | 5.50 | 112.60 | 108.20 |
| 57 | BA | 1204 | A | C2-N3-C4 | 5.50 | 113.35 | 110.60 |
| 57 | BA | 2339 | C | N1-C2-O2 | 5.50 | 122.20 | 118.90 |
| 22 | AA | 993 | G | O4'-C1'-N9 | 5.49 | 112.59 | 108.20 |
| 40 | BY | 85 | ARG | NE-CZ-NH1 | 5.49 | 123.05 | 120.30 |
| 57 | BA | 314 | C | N1-C2-O2 | 5.49 | 122.20 | 118.90 |
| 57 | BA | 1137 | G | O4'-C1'-N9 | 5.49 | 112.59 | 108.20 |
| 57 | BA | 1363 | C | O4'-C1'-N1 | 5.49 | 112.59 | 108.20 |
| 57 | BA | 1830 | C | N3-C4-N4 | -5.49 | 114.16 | 118.00 |
| 57 | BA | 2678 | C | N1-C2-O2 | 5.49 | 122.20 | 118.90 |
| 57 | BA | 2789 | C | O4'-C1'-N1 | 5.49 | 112.59 | 108.20 |
| 57 | BA | 620 | G | N1-C6-O6 | -5.49 | 116.61 | 119.90 |
| 57 | BA | 1941 | C | N3-C4-C5 | 5.49 | 124.10 | 121.90 |
| 57 | BA | 2180 | U | O4'-C1'-N1 | 5.49 | 112.59 | 108.20 |
| 22 | AA | 329 | A | C4-C5-C6 | -5.49 | 114.25 | 117.00 |
| 22 | AA | 971 | G | O4'-C1'-N9 | 5.49 | 112.59 | 108.20 |
| 23 | A2 | 19 | A | C4-C5-C6 | -5.49 | 114.25 | 117.00 |
| 23 | A2 | 23 | C | N3-C4-C5 | 5.49 | 124.10 | 121.90 |
| 57 | BA | 255 | A | C4-C5-C6 | -5.49 | 114.25 | 117.00 |
| 57 | BA | 772 | C | N1-C2-O2 | 5.49 | 122.19 | 118.90 |
| 57 | BA | 2442 | C | N1-C2-O2 | 5.49 | 122.19 | 118.90 |
| 22 | AA | 193 | C | N1-C2-O2 | 5.49 | 122.19 | 118.90 |
| 22 | AA | 307 | C | O4'-C1'-N1 | 5.49 | 112.59 | 108.20 |
| 22 | AA | 1521 | C | O4'-C1'-N1 | 5.49 | 112.59 | 108.20 |
| 57 | BA | 897 | C | N3-C2-O2 | -5.49 | 118.06 | 121.90 |
| 57 | BA | 1059 | G | N1-C6-O6 | -5.49 | 116.61 | 119.90 |
| 57 | BA | 1135 | C | O4'-C1'-N1 | 5.49 | 112.59 | 108.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 2200 | C | C2-N3-C4 | -5.49 | 117.16 | 119.90 |
| 57 | BA | 2540 | C | N1-C2-O2 | 5.49 | 122.19 | 118.90 |
| 22 | AA | 620 | C | N3-C2-O2 | -5.49 | 118.06 | 121.90 |
| 22 | AA | 1214 | C | N3-C4-C5 | 5.49 | 124.09 | 121.90 |
| 57 | BA | 1257 | C | N1-C2-O2 | 5.49 | 122.19 | 118.90 |
| 57 | BA | 2238 | G | N3-C4-C5 | -5.49 | 125.86 | 128.60 |
| 57 | BA | 519 | U | O4'-C1'-N1 | 5.48 | 112.59 | 108.20 |
| 57 | BA | 2757 | A | C5'-C4'-O4' | 5.48 | 115.68 | 109.10 |
| 22 | AA | 622 | A | C6-C5-N7 | 5.48 | 136.14 | 132.30 |
| 57 | BA | 353 | C | N1-C2-O2 | 5.48 | 122.19 | 118.90 |
| 57 | BA | 699 | A | O4'-C1'-N9 | 5.48 | 112.59 | 108.20 |
| 57 | BA | 1310 | G | N1-C6-O6 | -5.48 | 116.61 | 119.90 |
| 57 | BA | 2033 | A | C6-C5-N7 | 5.48 | 136.14 | 132.30 |
| 57 | BA | 2760 | C | N3-C2-O2 | -5.48 | 118.06 | 121.90 |
| 22 | AA | 304 | U | O4'-C1'-N1 | 5.48 | 112.58 | 108.20 |
| 22 | AA | 429 | U | C3'-C2'-C1' | -5.48 | 97.12 | 101.50 |
| 22 | AA | 542 | G | N1-C6-O6 | -5.48 | 116.61 | 119.90 |
| 22 | AA | 856 | C | N1-C2-O2 | 5.48 | 122.19 | 118.90 |
| 22 | AA | 1109 | C | N1-C2-O2 | 5.48 | 122.19 | 118.90 |
| 57 | BA | 398 | C | N1-C2-O2 | 5.48 | 122.19 | 118.90 |
| 57 | BA | 1668 | A | C4-C5-C6 | -5.48 | 114.26 | 117.00 |
| 57 | BA | 2103 | C | N1-C2-O2 | 5.48 | 122.19 | 118.90 |
| 22 | AA | 592 | G | N1-C6-O6 | -5.48 | 116.61 | 119.90 |
| 57 | BA | 209 | C | O4'-C1'-N1 | 5.48 | 112.58 | 108.20 |
| 57 | BA | 921 | C | N1-C2-O2 | 5.48 | 122.19 | 118.90 |
| 22 | AA | 434 | U | O4'-C1'-N1 | 5.48 | 112.58 | 108.20 |
| 22 | AA | 517 | G | O4'-C1'-N9 | 5.48 | 112.58 | 108.20 |
| 57 | BA | 1725 | U | O4'-C1'-N1 | 5.48 | 112.58 | 108.20 |
| 22 | AA | 1183 | U | N3-C2-O2 | -5.47 | 118.37 | 122.20 |
| 22 | AA | 1367 | C | N1-C2-O2 | 5.47 | 122.19 | 118.90 |
| 57 | BA | 1015 | U | O4'-C1'-N1 | 5.47 | 112.58 | 108.20 |
| 57 | BA | 2636 | C | N1-C2-O2 | 5.47 | 122.19 | 118.90 |
| 58 | Ba | 89 | U | O4'-C1'-N1 | 5.47 | 112.58 | 108.20 |
| 22 | AA | 743 | A | C4-C5-C6 | -5.47 | 114.26 | 117.00 |
| 57 | BA | 1258 | U | N3-C2-O2 | -5.47 | 118.37 | 122.20 |
| 57 | BA | 1531 | C | N1-C2-O2 | 5.47 | 122.18 | 118.90 |
| 57 | BA | 2313 | C | N3-C4-N4 | -5.47 | 114.17 | 118.00 |
| 57 | BA | 2393 | U | O4'-C1'-N1 | 5.47 | 112.58 | 108.20 |
| 57 | BA | 2629 | U | N3-C2-O2 | -5.47 | 118.37 | 122.20 |
| 57 | BA | 2825 | G | N3-C4-C5 | -5.47 | 125.86 | 128.60 |
| 22 | AA | 942 | G | N1-C6-O6 | -5.47 | 116.62 | 119.90 |
| 28 | BN | 27 | ARG | NE-CZ-NH1 | 5.47 | 123.04 | 120.30 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 914 | G | N1-C6-O6 | -5.47 | 116.62 | 119.90 |
| 57 | BA | 1963 | U | N3-C2-O2 | -5.47 | 118.37 | 122.20 |
| 22 | AA | 586 | C | N1-C2-O2 | 5.47 | 122.18 | 118.90 |
| 22 | AA | 868 | C | O4'-C1'-N1 | 5.47 | 112.58 | 108.20 |
| 57 | BA | 1615 | C | N3-C4-C5 | 5.47 | 124.09 | 121.90 |
| 57 | BA | 2459 | A | C4-C5-C6 | -5.47 | 114.27 | 117.00 |
| 22 | AA | 128 | G | N1-C6-O6 | -5.47 | 116.62 | 119.90 |
| 23 | A2 | 24 | A | C5'-C4'-C3' | -5.47 | 107.25 | 116.00 |
| 57 | BA | 532 | A | C4-C5-C6 | -5.47 | 114.27 | 117.00 |
| 57 | BA | 1769 | U | O4'-C1'-N1 | 5.47 | 112.57 | 108.20 |
| 22 | AA | 215 | C | N3-C4-N4 | -5.47 | 114.17 | 118.00 |
| 22 | AA | 986 | U | O4'-C1'-N1 | 5.47 | 112.57 | 108.20 |
| 22 | AA | 1225 | A | C4-C5-C6 | -5.47 | 114.27 | 117.00 |
| 57 | BA | 191 | A | C4-C5-C6 | -5.47 | 114.27 | 117.00 |
| 57 | BA | 877 | A | C6-C5-N7 | 5.47 | 136.13 | 132.30 |
| 57 | BA | 971 | G | O4'-C1'-N9 | 5.47 | 112.57 | 108.20 |
| 57 | BA | 2752 | C | C2-N3-C4 | -5.47 | 117.17 | 119.90 |
| 22 | AA | 1281 | C | O4'-C1'-N1 | 5.46 | 112.57 | 108.20 |
| 22 | AA | 1388 | C | N1-C2-O2 | 5.46 | 122.18 | 118.90 |
| 34 | BT | 52 | ARG | NE-CZ-NH2 | -5.46 | 117.57 | 120.30 |
| 36 | BU | 69 | ARG | NE-CZ-NH2 | 5.46 | 123.03 | 120.30 |
| 57 | BA | 147 | C | N1-C2-O2 | 5.46 | 122.18 | 118.90 |
| 57 | BA | 735 | A | C4-C5-C6 | -5.46 | 114.27 | 117.00 |
| 57 | BA | 809 | G | N1-C6-O6 | -5.46 | 116.62 | 119.90 |
| 57 | BA | 1667 | G | O4'-C1'-N9 | 5.46 | 112.57 | 108.20 |
| 22 | AA | 512 | U | O4'-C1'-N1 | 5.46 | 112.57 | 108.20 |
| 57 | BA | 1378 | A | C6-C5-N7 | 5.46 | 136.12 | 132.30 |
| 57 | BA | 1512 | C | N1-C2-O2 | 5.46 | 122.18 | 118.90 |
| 57 | BA | 1592 | C | O4'-C1'-N1 | 5.46 | 112.57 | 108.20 |
| 57 | BA | 2430 | A | N1-C6-N6 | -5.46 | 115.32 | 118.60 |
| 58 | Ba | 48 | U | O4'-C1'-N1 | 5.46 | 112.57 | 108.20 |
| 22 | AA | 1491 | G | N1-C6-O6 | -5.46 | 116.62 | 119.90 |
| 57 | BA | 1472 | C | N1-C2-O2 | 5.46 | 122.18 | 118.90 |
| 57 | BA | 2096 | C | O4'-C1'-N1 | 5.46 | 112.57 | 108.20 |
| 57 | BA | 1110 | G | O4'-C1'-N9 | 5.46 | 112.57 | 108.20 |
| 22 | AA | 526 | C | N1-C2-O2 | 5.46 | 122.18 | 118.90 |
| 22 | AA | 971 | G | N1-C6-O6 | -5.46 | 116.62 | 119.90 |
| 57 | BA | 1092 | C | N1-C2-O2 | 5.46 | 122.17 | 118.90 |
| 57 | BA | 1812 | U | O4'-C1'-N1 | 5.46 | 112.57 | 108.20 |
| 58 | Ba | 40 | U | O4'-C1'-N1 | 5.46 | 112.57 | 108.20 |
| 22 | AA | 39 | G | N3-C4-C5 | -5.46 | 125.87 | 128.60 |
| 22 | AA | 750 | C | N1-C2-O2 | 5.46 | 122.17 | 118.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | AA | 1129 | C | N1-C2-O2 | 5.46 | 122.17 | 118.90 |
| 57 | BA | 2879 | A | C4-C5-C6 | -5.46 | 114.27 | 117.00 |
| 15 | AD | 61 | ARG | NE-CZ-NH1 | 5.46 | 123.03 | 120.30 |
| 57 | BA | 1909 | C | N1-C2-O2 | 5.46 | 122.17 | 118.90 |
| 57 | BA | 2620 | C | N1-C2-O2 | 5.46 | 122.17 | 118.90 |
| 23 | A2 | 58 | C | N1-C2-O2 | 5.45 | 122.17 | 118.90 |
| 57 | BA | 2238 | G | N1-C6-O6 | -5.45 | 116.63 | 119.90 |
| 22 | AA | 47 | C | N3-C4-N4 | -5.45 | 114.18 | 118.00 |
| 57 | BA | 1037 | G | N1-C6-O6 | -5.45 | 116.63 | 119.90 |
| 58 | Ba | 26 | C | C5'-C4'-O4' | 5.45 | 115.64 | 109.10 |
| 22 | AA | 1369 | C | O4'-C1'-N1 | 5.45 | 112.56 | 108.20 |
| 57 | BA | 215 | G | N1-C6-O6 | -5.45 | 116.63 | 119.90 |
| 57 | BA | 937 | C | N1-C2-O2 | 5.45 | 122.17 | 118.90 |
| 22 | AA | 465 | A | C4-C5-C6 | -5.45 | 114.28 | 117.00 |
| 22 | AA | 526 | C | O4'-C1'-N1 | 5.45 | 112.56 | 108.20 |
| 22 | AA | 900 | A | O4'-C1'-N9 | 5.45 | 112.56 | 108.20 |
| 57 | BA | 808 | G | O4'-C1'-N9 | 5.45 | 112.56 | 108.20 |
| 57 | BA | 872 | U | N3-C2-O2 | -5.45 | 118.39 | 122.20 |
| 57 | BA | 2254 | C | O4'-C1'-N1 | 5.45 | 112.56 | 108.20 |
| 22 | AA | 833 | G | N1-C6-O6 | -5.45 | 116.63 | 119.90 |
| 57 | BA | 1760 | C | O4'-C1'-N1 | 5.45 | 112.56 | 108.20 |
| 22 | AA | 209 | U | O4'-C1'-N1 | 5.45 | 112.56 | 108.20 |
| 57 | BA | 1115 | G | O4'-C1'-N9 | 5.45 | 112.56 | 108.20 |
| 57 | BA | 1243 | C | O4'-C1'-N1 | 5.45 | 112.56 | 108.20 |
| 57 | BA | 1547 | C | O4'-C1'-N1 | 5.45 | 112.56 | 108.20 |
| 22 | AA | 1344 | C | N1-C2-O2 | 5.44 | 122.17 | 118.90 |
| 57 | BA | 1117 | C | N1-C2-O2 | 5.44 | 122.17 | 118.90 |
| 57 | BA | 2641 | G | N1-C6-O6 | -5.44 | 116.63 | 119.90 |
| 22 | AA | 931 | C | O4'-C1'-N1 | 5.44 | 112.55 | 108.20 |
| 57 | BA | 765 | C | O4'-C1'-N1 | 5.44 | 112.55 | 108.20 |
| 57 | BA | 965 | C | O4'-C1'-N1 | 5.44 | 112.55 | 108.20 |
| 57 | BA | 1207 | C | N1-C2-O2 | 5.44 | 122.17 | 118.90 |
| 57 | BA | 1795 | C | N1-C2-O2 | 5.44 | 122.17 | 118.90 |
| 57 | BA | 2650 | U | O4'-C1'-N1 | 5.44 | 112.55 | 108.20 |
| 22 | AA | 1258 | G | N9-C4-C5 | 5.44 | 107.58 | 105.40 |
| 57 | BA | 2621 | G | O4'-C1'-N9 | 5.44 | 112.55 | 108.20 |
| 22 | AA | 331 | G | N1-C6-O6 | -5.44 | 116.64 | 119.90 |
| 24 | A3 | 53 | G | N1-C6-O6 | -5.44 | 116.64 | 119.90 |
| 12 | AT | 28 | ARG | NE-CZ-NH1 | 5.44 | 123.02 | 120.30 |
| 22 | AA | 13 | U | N3-C2-O2 | -5.44 | 118.39 | 122.20 |
| 22 | AA | 522 | C | N3-C4-N4 | -5.44 | 114.19 | 118.00 |
| 57 | BA | 277 | G | N1-C6-O6 | -5.44 | 116.64 | 119.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 874 | G | N1-C6-O6 | -5.44 | 116.64 | 119.90 |
| 57 | BA | 999 | U | C5-C6-N1 | -5.44 | 119.98 | 122.70 |
| 57 | BA | 1281 | G | N1-C6-O6 | -5.44 | 116.64 | 119.90 |
| 58 | Ba | 17 | C | O4'-C1'-N1 | 5.44 | 112.55 | 108.20 |
| 22 | AA | 591 | U | O4'-C1'-N1 | 5.44 | 112.55 | 108.20 |
| 22 | AA | 1164 | G | N1-C6-O6 | -5.44 | 116.64 | 119.90 |
| 22 | AA | 1453 | G | N3-C4-C5 | -5.44 | 125.88 | 128.60 |
| 58 | Ba | 19 | C | N1-C2-O2 | 5.44 | 122.16 | 118.90 |
| 57 | BA | 225 | C | N3-C4-N4 | -5.43 | 114.19 | 118.00 |
| 57 | BA | 1844 | C | O4'-C1'-N1 | 5.43 | 112.55 | 108.20 |
| 57 | BA | 2892 | G | C5'-C4'-C3' | -5.43 | 107.30 | 116.00 |
| 22 | AA | 1089 | G | N1-C6-O6 | -5.43 | 116.64 | 119.90 |
| 23 | A2 | 28 | U | O4'-C1'-N1 | 5.43 | 112.55 | 108.20 |
| 24 | A3 | 5 | G | O4'-C1'-N9 | 5.43 | 112.55 | 108.20 |
| 24 | A3 | 52 | C | O4'-C1'-N1 | 5.43 | 112.55 | 108.20 |
| 57 | BA | 29 | U | N3-C2-O2 | -5.43 | 118.40 | 122.20 |
| 57 | BA | 225 | C | N1-C2-O2 | 5.43 | 122.16 | 118.90 |
| 57 | BA | 246 | C | N1-C2-O2 | 5.43 | 122.16 | 118.90 |
| 57 | BA | 310 | A | O4'-C1'-N9 | 5.43 | 112.55 | 108.20 |
| 57 | BA | 904 | G | N1-C6-O6 | -5.43 | 116.64 | 119.90 |
| 57 | BA | 1188 | U | O4'-C1'-N1 | 5.43 | 112.55 | 108.20 |
| 57 | BA | 2710 | C | O4'-C1'-N1 | 5.43 | 112.55 | 108.20 |
| 58 | Ba | 81 | G | N1-C6-O6 | -5.43 | 116.64 | 119.90 |
| 22 | AA | 507 | C | N1-C2-O2 | 5.43 | 122.16 | 118.90 |
| 57 | BA | 470 | A | C4-C5-C6 | -5.43 | 114.28 | 117.00 |
| 57 | BA | 2026 | U | O4'-C1'-N1 | 5.43 | 112.55 | 108.20 |
| 57 | BA | 2655 | G | N3-C4-C5 | -5.43 | 125.88 | 128.60 |
| 22 | AA | 423 | G | N3-C4-C5 | -5.43 | 125.89 | 128.60 |
| 22 | AA | 1047 | G | C5-C6-N1 | 5.43 | 114.22 | 111.50 |
| 22 | AA | 1286 | U | C1'-O4'-C4' | -5.43 | 105.56 | 109.90 |
| 57 | BA | 453 | A | O4'-C1'-N9 | 5.43 | 112.54 | 108.20 |
| 57 | BA | 575 | A | O4'-C1'-N9 | 5.43 | 112.54 | 108.20 |
| 57 | BA | 1537 | G | N3-C4-C5 | -5.43 | 125.89 | 128.60 |
| 57 | BA | 1684 | G | N1-C6-O6 | -5.43 | 116.64 | 119.90 |
| 57 | BA | 2807 | U | O4'-C1'-N1 | 5.43 | 112.54 | 108.20 |
| 22 | AA | 1475 | G | N1-C6-O6 | -5.43 | 116.64 | 119.90 |
| 57 | BA | 1005 | C | N1-C2-O2 | 5.43 | 122.16 | 118.90 |
| 22 | AA | 43 | C | O4'-C1'-N1 | 5.43 | 112.54 | 108.20 |
| 22 | AA | 124 | C | N1-C2-O2 | 5.43 | 122.16 | 118.90 |
| 22 | AA | 1194 | U | N3-C2-O2 | -5.43 | 118.40 | 122.20 |
| 22 | AA | 1409 | C | N1-C2-O2 | 5.43 | 122.16 | 118.90 |
| 57 | BA | 573 | U | C5'-C4'-C3' | -5.43 | 107.32 | 116.00 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 2136 | G | N1-C6-O6 | -5.43 | 116.64 | 119.90 |
| 57 | BA | 2413 | G | N1-C6-O6 | -5.43 | 116.64 | 119.90 |
| 57 | BA | 2588 | G | O4'-C1'-N9 | 5.43 | 112.54 | 108.20 |
| 57 | BA | 2796 | U | N3-C2-O2 | -5.43 | 118.40 | 122.20 |
| 22 | AA | 722 | G | N1-C6-O6 | -5.42 | 116.64 | 119.90 |
| 57 | BA | 1351 | C | N1-C2-O2 | 5.42 | 122.16 | 118.90 |
| 57 | BA | 2904 | U | O4'-C1'-N1 | 5.42 | 112.54 | 108.20 |
| 32 | BR | 46 | ARG | NE-CZ-NH1 | 5.42 | 123.01 | 120.30 |
| 57 | BA | 441 | U | N3-C2-O2 | -5.42 | 118.40 | 122.20 |
| 57 | BA | 2450 | A | C1'-O4'-C4' | -5.42 | 105.56 | 109.90 |
| 22 | AA | 513 | C | O4'-C1'-N1 | 5.42 | 112.54 | 108.20 |
| 22 | AA | 799 | G | N1-C6-O6 | -5.42 | 116.65 | 119.90 |
| 24 | A3 | 70 | C | N1-C2-O2 | 5.42 | 122.15 | 118.90 |
| 57 | BA | 210 | C | N3-C4-N4 | -5.42 | 114.20 | 118.00 |
| 57 | BA | 871 | U | N3-C2-O2 | -5.42 | 118.41 | 122.20 |
| 57 | BA | 901 | C | O4'-C1'-N1 | 5.42 | 112.54 | 108.20 |
| 58 | Ba | 33 | G | N1-C6-O6 | -5.42 | 116.65 | 119.90 |
| 57 | BA | 1680 | U | O4'-C1'-N1 | 5.42 | 112.54 | 108.20 |
| 57 | BA | 1726 | C | N1-C2-O2 | 5.42 | 122.15 | 118.90 |
| 57 | BA | 2299 | U | O4'-C1'-N1 | 5.42 | 112.54 | 108.20 |
| 22 | AA | 267 | C | O4'-C1'-N1 | 5.42 | 112.53 | 108.20 |
| 57 | BA | 2484 | G | N1-C6-O6 | -5.42 | 116.65 | 119.90 |
| 58 | Ba | 96 | G | N1-C6-O6 | -5.42 | 116.65 | 119.90 |
| 22 | AA | 339 | C | O4'-C1'-N1 | 5.42 | 112.53 | 108.20 |
| 57 | BA | 269 | C | N1-C2-O2 | 5.42 | 122.15 | 118.90 |
| 57 | BA | 737 | C | N1-C2-O2 | 5.42 | 122.15 | 118.90 |
| 57 | BA | 1427 | A | C6-C5-N7 | 5.42 | 136.09 | 132.30 |
| 22 | AA | 949 | A | C4-C5-C6 | -5.42 | 114.29 | 117.00 |
| 57 | BA | 1808 | A | O4'-C1'-N9 | 5.42 | 112.53 | 108.20 |
| 57 | BA | 2121 | G | N1-C6-O6 | -5.42 | 116.65 | 119.90 |
| 57 | BA | 2417 | C | N1-C2-O2 | 5.42 | 122.15 | 118.90 |
| 57 | BA | 2877 | G | O4'-C1'-N9 | 5.42 | 112.53 | 108.20 |
| 58 | Ba | 27 | C | N3-C4-C5 | 5.42 | 124.07 | 121.90 |
| 3 | AL | 13 | ARG | NE-CZ-NH1 | 5.41 | 123.01 | 120.30 |
| 22 | AA | 268 | U | C5-C6-N1 | -5.41 | 119.99 | 122.70 |
| 22 | AA | 1190 | G | N3-C2-N2 | -5.41 | 116.11 | 119.90 |
| 57 | BA | 61 | C | N1-C2-O2 | 5.41 | 122.15 | 118.90 |
| 57 | BA | 404 | A | O4'-C1'-N9 | 5.41 | 112.53 | 108.20 |
| 57 | BA | 1399 | C | N3-C4-N4 | -5.41 | 114.21 | 118.00 |
| 57 | BA | 1689 | A | C4-C5-C6 | -5.41 | 114.29 | 117.00 |
| 45 | BE | 128 | ARG | NE-CZ-NH2 | 5.41 | 123.01 | 120.30 |
| 57 | BA | 528 | A | O4'-C1'-N9 | 5.41 | 112.53 | 108.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 1724 | G | N1-C6-O6 | -5.41 | 116.65 | 119.90 |
| 22 | AA | 106 | C | O4'-C1'-N1 | 5.41 | 112.53 | 108.20 |
| 22 | AA | 887 | G | N1-C6-O6 | -5.41 | 116.65 | 119.90 |
| 22 | AA | 1487 | G | O4'-C1'-N9 | 5.41 | 112.53 | 108.20 |
| 37 | BV | 68 | ARG | NH1-CZ-NH2 | -5.41 | 113.45 | 119.40 |
| 43 | B1 | 36 | ARG | NH1-CZ-NH2 | -5.41 | 113.45 | 119.40 |
| 57 | BA | 1357 | C | N1-C2-O2 | 5.41 | 122.15 | 118.90 |
| 57 | BA | 2666 | C | N3-C4-C5 | 5.41 | 124.06 | 121.90 |
| 22 | AA | 808 | C | N1-C2-O2 | 5.41 | 122.14 | 118.90 |
| 22 | AA | 1524 | C | N1-C2-O2 | 5.41 | 122.14 | 118.90 |
| 57 | BA | 573 | U | O4'-C1'-N1 | 5.41 | 112.53 | 108.20 |
| 57 | BA | 1017 | G | N1-C6-O6 | -5.41 | 116.65 | 119.90 |
| 57 | BA | 1370 | C | O4'-C1'-N1 | 5.41 | 112.53 | 108.20 |
| 57 | BA | 1533 | C | O4'-C1'-N1 | 5.41 | 112.53 | 108.20 |
| 57 | BA | 1914 | C | N1-C2-O2 | 5.41 | 122.14 | 118.90 |
| 58 | Ba | 11 | C | N1-C2-O2 | 5.41 | 122.14 | 118.90 |
| 22 | AA | 1120 | C | O4'-C1'-N1 | 5.41 | 112.53 | 108.20 |
| 57 | BA | 114 | U | N3-C2-O2 | -5.41 | 118.42 | 122.20 |
| 57 | BA | 731 | C | O4'-C1'-N1 | 5.41 | 112.53 | 108.20 |
| 22 | AA | 691 | G | N3-C2-N2 | -5.41 | 116.12 | 119.90 |
| 22 | AA | 699 | C | N1-C2-O2 | 5.41 | 122.14 | 118.90 |
| 22 | AA | 1523 | G | N3-C2-N2 | -5.41 | 116.12 | 119.90 |
| 24 | A3 | 75 | C | O4'-C1'-N1 | 5.41 | 112.52 | 108.20 |
| 57 | BA | 280 | U | O4'-C1'-N1 | 5.41 | 112.53 | 108.20 |
| 57 | BA | 413 | C | O4'-C1'-N1 | 5.41 | 112.52 | 108.20 |
| 57 | BA | 1146 | C | N1-C2-O2 | 5.41 | 122.14 | 118.90 |
| 57 | BA | 1298 | C | N1-C2-O2 | 5.41 | 122.14 | 118.90 |
| 57 | BA | 1931 | U | O4'-C1'-N1 | 5.41 | 112.53 | 108.20 |
| 57 | BA | 2673 | G | N1-C6-O6 | -5.41 | 116.66 | 119.90 |
| 11 | AB | 136 | ARG | NE-CZ-NH2 | -5.40 | 117.60 | 120.30 |
| 11 | AB | 207 | ARG | NE-CZ-NH1 | 5.40 | 123.00 | 120.30 |
| 22 | AA | 1388 | C | O4'-C1'-N1 | 5.40 | 112.52 | 108.20 |
| 57 | BA | 15 | G | O4'-C1'-N9 | 5.40 | 112.52 | 108.20 |
| 22 | AA | 472 | U | O4'-C1'-N1 | 5.40 | 112.52 | 108.20 |
| 57 | BA | 510 | C | N1-C2-O2 | 5.40 | 122.14 | 118.90 |
| 57 | BA | 1518 | C | N1-C2-O2 | 5.40 | 122.14 | 118.90 |
| 58 | Ba | 18 | G | N1-C6-O6 | -5.40 | 116.66 | 119.90 |
| 58 | Ba | 77 | U | O4'-C1'-N1 | 5.40 | 112.52 | 108.20 |
| 22 | AA | 737 | C | N1-C2-O2 | 5.40 | 122.14 | 118.90 |
| 22 | AA | 1313 | U | O4'-C1'-N1 | 5.40 | 112.52 | 108.20 |
| 24 | A3 | 40 | C | C6-N1-C2 | -5.40 | 118.14 | 120.30 |
| 57 | BA | 116 | C | N3-C4-N4 | -5.40 | 114.22 | 118.00 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 273 | G | N1-C6-O6 | -5.40 | 116.66 | 119.90 |
| 57 | BA | 660 | C | N1-C2-O2 | 5.40 | 122.14 | 118.90 |
| 57 | BA | 1161 | C | N1-C2-O2 | 5.40 | 122.14 | 118.90 |
| 58 | Ba | 58 | A | C6-C5-N7 | 5.40 | 136.08 | 132.30 |
| 22 | AA | 160 | A | O4'-C1'-N9 | 5.40 | 112.52 | 108.20 |
| 22 | AA | 345 | C | N3-C2-O2 | -5.40 | 118.12 | 121.90 |
| 38 | BW | 99 | ARG | NE-CZ-NH1 | 5.40 | 123.00 | 120.30 |
| 57 | BA | 902 | C | N1-C2-O2 | 5.40 | 122.14 | 118.90 |
| 57 | BA | 1291 | C | N1-C2-O2 | 5.40 | 122.14 | 118.90 |
| 22 | AA | 126 | G | N1-C6-O6 | -5.40 | 116.66 | 119.90 |
| 22 | AA | 1106 | G | N1-C6-O6 | -5.40 | 116.66 | 119.90 |
| 24 | A3 | 69 | C | N1-C2-O2 | 5.40 | 122.14 | 118.90 |
| 57 | BA | 1985 | C | N1-C2-O2 | 5.40 | 122.14 | 118.90 |
| 57 | BA | 2658 | C | N3-C4-C5 | 5.40 | 124.06 | 121.90 |
| 22 | AA | 1 | A | C4-C5-C6 | -5.39 | 114.30 | 117.00 |
| 22 | AA | 601 | G | N1-C6-O6 | -5.39 | 116.66 | 119.90 |
| 22 | AA | 1119 | C | O4'-C1'-N1 | 5.39 | 112.52 | 108.20 |
| 57 | BA | 200 | U | O4'-C1'-N1 | 5.39 | 112.52 | 108.20 |
| 57 | BA | 303 | G | N1-C6-O6 | -5.39 | 116.66 | 119.90 |
| 57 | BA | 351 | C | O4'-C1'-N1 | 5.39 | 112.52 | 108.20 |
| 57 | BA | 445 | C | N1-C2-O2 | 5.39 | 122.14 | 118.90 |
| 57 | BA | 1663 | G | C5-C6-N1 | 5.39 | 114.20 | 111.50 |
| 57 | BA | 2774 | C | N1-C2-O2 | 5.39 | 122.14 | 118.90 |
| 57 | BA | 2865 | U | N3-C2-O2 | -5.39 | 118.42 | 122.20 |
| 58 | Ba | 54 | G | N1-C6-O6 | -5.39 | 116.66 | 119.90 |
| 22 | AA | 1399 | C | N1-C2-O2 | 5.39 | 122.14 | 118.90 |
| 31 | BQ | 66 | ARG | NE-CZ-NH1 | 5.39 | 123.00 | 120.30 |
| 57 | BA | 823 | C | N3-C4-C5 | 5.39 | 124.06 | 121.90 |
| 57 | BA | 1332 | G | N3-C4-C5 | -5.39 | 125.90 | 128.60 |
| 57 | BA | 2193 | G | N1-C6-O6 | -5.39 | 116.67 | 119.90 |
| 22 | AA | 341 | C | O4'-C1'-N1 | 5.39 | 112.51 | 108.20 |
| 26 | BJ | 55 | ARG | NH1-CZ-NH2 | -5.39 | 113.47 | 119.40 |
| 57 | BA | 840 | C | N1-C2-O2 | 5.39 | 122.14 | 118.90 |
| 57 | BA | 1720 | U | O4'-C1'-N1 | 5.39 | 112.51 | 108.20 |
| 14 | AC | 178 | ARG | NE-CZ-NH1 | 5.39 | 122.99 | 120.30 |
| 22 | AA | 63 | C | N1-C2-O2 | 5.39 | 122.13 | 118.90 |
| 22 | AA | 474 | G | N1-C6-O6 | -5.39 | 116.67 | 119.90 |
| 22 | AA | 817 | C | N3-C4-C5 | 5.39 | 124.06 | 121.90 |
| 22 | AA | 930 | C | N1-C2-O2 | 5.39 | 122.13 | 118.90 |
| 57 | BA | 151 | C | N1-C2-O2 | 5.39 | 122.13 | 118.90 |
| 57 | BA | 433 | C | O4'-C1'-N1 | 5.39 | 112.51 | 108.20 |
| 22 | AA | 139 | A | C6-C5-N7 | 5.39 | 136.07 | 132.30 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 1038 | G | N1-C6-O6 | -5.39 | 116.67 | 119.90 |
| 57 | BA | 2817 | U | N3-C2-O2 | -5.39 | 118.43 | 122.20 |
| 45 | BE | 46 | ARG | NE-CZ-NH1 | 5.39 | 122.99 | 120.30 |
| 57 | BA | 289 | G | N1-C6-O6 | -5.39 | 116.67 | 119.90 |
| 57 | BA | 820 | A | N1-C6-N6 | -5.39 | 115.37 | 118.60 |
| 57 | BA | 1376 | C | N1-C2-O2 | 5.39 | 122.13 | 118.90 |
| 57 | BA | 2064 | C | N3-C4-N4 | -5.39 | 114.23 | 118.00 |
| 22 | AA | 183 | C | N1-C2-O2 | 5.38 | 122.13 | 118.90 |
| 22 | AA | 245 | U | N1-C2-N3 | 5.38 | 118.13 | 114.90 |
| 22 | AA | 719 | C | C3'-C2'-C1' | 5.38 | 105.81 | 101.50 |
| 57 | BA | 248 | G | N1-C6-O6 | -5.38 | 116.67 | 119.90 |
| 57 | BA | 788 | A | O4'-C1'-N9 | 5.38 | 112.51 | 108.20 |
| 57 | BA | 2510 | C | O4'-C1'-N1 | 5.38 | 112.51 | 108.20 |
| 57 | BA | 2692 | G | C4'-C3'-C2' | -5.38 | 97.22 | 102.60 |
| 22 | AA | 780 | A | C4-C5-C6 | -5.38 | 114.31 | 117.00 |
| 22 | AA | 1054 | C | O4'-C1'-N1 | 5.38 | 112.51 | 108.20 |
| 57 | BA | 851 | C | N1-C2-O2 | 5.38 | 122.13 | 118.90 |
| 22 | AA | 848 | C | N1-C2-O2 | 5.38 | 122.13 | 118.90 |
| 22 | AA | 1105 | A | C6-C5-N7 | 5.38 | 136.07 | 132.30 |
| 24 | A3 | 57 | C | O4'-C1'-N1 | 5.38 | 112.50 | 108.20 |
| 57 | BA | 370 | G | N1-C6-O6 | -5.38 | 116.67 | 119.90 |
| 57 | BA | 1300 | G | O4'-C1'-N9 | 5.38 | 112.50 | 108.20 |
| 57 | BA | 2043 | C | N1-C2-O2 | 5.38 | 122.13 | 118.90 |
| 57 | BA | 2458 | G | N1-C6-O6 | -5.38 | 116.67 | 119.90 |
| 57 | BA | 2606 | C | N3-C4-C5 | 5.38 | 124.05 | 121.90 |
| 57 | BA | 1660 | G | N1-C6-O6 | -5.38 | 116.67 | 119.90 |
| 57 | BA | 1898 | U | O4'-C1'-N1 | 5.38 | 112.50 | 108.20 |
| 57 | BA | 2812 | G | N1-C6-O6 | -5.38 | 116.67 | 119.90 |
| 24 | A3 | 68 | C | N1-C2-O2 | 5.38 | 122.13 | 118.90 |
| 57 | BA | 31 | C | N1-C2-O2 | 5.38 | 122.13 | 118.90 |
| 57 | BA | 42 | A | C6-C5-N7 | 5.38 | 136.06 | 132.30 |
| 57 | BA | 196 | A | C1'-O4'-C4' | -5.38 | 105.60 | 109.90 |
| 57 | BA | 1335 | C | N1-C2-O2 | 5.38 | 122.13 | 118.90 |
| 57 | BA | 1565 | C | O4'-C1'-N1 | 5.38 | 112.50 | 108.20 |
| 57 | BA | 1601 | G | N1-C6-O6 | -5.38 | 116.67 | 119.90 |
| 57 | BA | 2515 | C | N1-C2-O2 | 5.38 | 122.13 | 118.90 |
| 22 | AA | 458 | U | O4'-C1'-N1 | 5.38 | 112.50 | 108.20 |
| 22 | AA | 1086 | U | N3-C2-O2 | -5.38 | 118.44 | 122.20 |
| 57 | BA | 1356 | G | N1-C6-O6 | -5.38 | 116.67 | 119.90 |
| 58 | Ba | 12 | C | N1-C2-O2 | 5.38 | 122.13 | 118.90 |
| 22 | AA | 396 | C | N1-C2-O2 | 5.38 | 122.12 | 118.90 |
| 22 | AA | 774 | G | N1-C6-O6 | -5.38 | 116.67 | 119.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | AA | 778 | G | N1-C6-O6 | -5.38 | 116.67 | 119.90 |
| 22 | AA | 896 | C | N1-C2-O2 | 5.38 | 122.12 | 118.90 |
| 22 | AA | 1479 | C | N1-C2-O2 | 5.38 | 122.12 | 118.90 |
| 24 | A3 | 20 | G | N1-C6-O6 | -5.38 | 116.67 | 119.90 |
| 57 | BA | 209 | C | N1-C2-O2 | 5.38 | 122.12 | 118.90 |
| 57 | BA | 252 | G | N1-C6-O6 | -5.38 | 116.67 | 119.90 |
| 57 | BA | 2794 | C | N1-C2-O2 | 5.38 | 122.12 | 118.90 |
| 22 | AA | 70 | U | N3-C2-O2 | -5.37 | 118.44 | 122.20 |
| 22 | AA | 763 | G | N7-C8-N9 | 5.37 | 115.79 | 113.10 |
| 22 | AA | 818 | G | O4'-C1'-N9 | 5.37 | 112.50 | 108.20 |
| 22 | AA | 1081 | A | C5'-C4'-O4' | 5.37 | 115.55 | 109.10 |
| 22 | AA | 1264 | U | O4'-C1'-N1 | 5.37 | 112.50 | 108.20 |
| 34 | BT | 20 | ARG | NE-CZ-NH2 | 5.37 | 122.99 | 120.30 |
| 57 | BA | 145 | C | N1-C2-O2 | 5.37 | 122.12 | 118.90 |
| 57 | BA | 1741 | C | N1-C2-O2 | 5.37 | 122.12 | 118.90 |
| 57 | BA | 2057 | G | N1-C6-O6 | -5.37 | 116.68 | 119.90 |
| 57 | BA | 2347 | C | O4'-C1'-N1 | 5.37 | 112.50 | 108.20 |
| 57 | BA | 2571 | U | N3-C2-O2 | -5.37 | 118.44 | 122.20 |
| 22 | AA | 487 | A | C4-C5-C6 | -5.37 | 114.31 | 117.00 |
| 22 | AA | 1412 | C | N1-C2-O2 | 5.37 | 122.12 | 118.90 |
| 22 | AA | 353 | A | C4-C5-C6 | -5.37 | 114.31 | 117.00 |
| 22 | AA | 1355 | G | N1-C6-O6 | -5.37 | 116.68 | 119.90 |
| 57 | BA | 2056 | G | O4'-C1'-N9 | 5.37 | 112.50 | 108.20 |
| 22 | AA | 773 | G | N1-C6-O6 | -5.37 | 116.68 | 119.90 |
| 57 | BA | 963 | U | O4'-C1'-N1 | 5.37 | 112.50 | 108.20 |
| 22 | AA | 1279 | G | N1-C6-O6 | -5.37 | 116.68 | 119.90 |
| 6 | AO | 83 | ARG | NE-CZ-NH1 | 5.37 | 122.98 | 120.30 |
| 22 | AA | 8 | A | O4'-C1'-N9 | 5.37 | 112.49 | 108.20 |
| 22 | AA | 1064 | G | O4'-C1'-N9 | 5.37 | 112.49 | 108.20 |
| 57 | BA | 284 | U | O4'-C1'-N1 | 5.37 | 112.49 | 108.20 |
| 57 | BA | 596 | U | O4'-C1'-N1 | 5.37 | 112.49 | 108.20 |
| 57 | BA | 796 | C | N1-C2-O2 | 5.37 | 122.12 | 118.90 |
| 57 | BA | 1417 | C | N1-C2-O2 | 5.37 | 122.12 | 118.90 |
| 57 | BA | 1702 | G | N1-C6-O6 | -5.37 | 116.68 | 119.90 |
| 57 | BA | 1808 | A | C4-C5-C6 | -5.37 | 114.32 | 117.00 |
| 57 | BA | 1885 | A | C4-C5-C6 | -5.37 | 114.32 | 117.00 |
| 57 | BA | 2331 | G | N1-C6-O6 | -5.37 | 116.68 | 119.90 |
| 57 | BA | 2895 | G | N1-C6-O6 | -5.37 | 116.68 | 119.90 |
| 22 | AA | 1273 | C | N1-C2-O2 | 5.36 | 122.12 | 118.90 |
| 57 | BA | 1140 | C | O4'-C1'-N1 | 5.36 | 112.49 | 108.20 |
| 57 | BA | 1612 | C | N1-C2-O2 | 5.36 | 122.12 | 118.90 |
| 57 | BA | 2150 | C | N1-C2-O2 | 5.36 | 122.12 | 118.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 2243 | U | N3-C2-O2 | -5.36 | 118.44 | 122.20 |
| 57 | BA | 2889 | C | N1-C2-O2 | 5.36 | 122.12 | 118.90 |
| 58 | Ba | 92 | C | O4'-C1'-N1 | 5.36 | 112.49 | 108.20 |
| 22 | AA | 489 | C | N1-C2-O2 | 5.36 | 122.12 | 118.90 |
| 22 | AA | 1490 | U | O4'-C1'-N1 | 5.36 | 112.49 | 108.20 |
| 57 | BA | 524 | G | N1-C6-O6 | -5.36 | 116.68 | 119.90 |
| 57 | BA | 592 | A | C6-C5-N7 | 5.36 | 136.05 | 132.30 |
| 57 | BA | 871 | U | O4'-C1'-N1 | 5.36 | 112.49 | 108.20 |
| 57 | BA | 1830 | C | N1-C2-O2 | 5.36 | 122.12 | 118.90 |
| 58 | Ba | 13 | G | C3'-C2'-C1' | 5.36 | 105.79 | 101.50 |
| 22 | AA | 1 | A | O4'-C1'-N9 | 5.36 | 112.49 | 108.20 |
| 22 | AA | 1420 | U | O4'-C1'-N1 | 5.36 | 112.49 | 108.20 |
| 41 | BZ | 19 | ARG | NH1-CZ-NH2 | -5.36 | 113.50 | 119.40 |
| 57 | BA | 1267 | U | N3-C2-O2 | -5.36 | 118.45 | 122.20 |
| 57 | BA | 1447 | C | N1-C2-O2 | 5.36 | 122.12 | 118.90 |
| 57 | BA | 1798 | U | O4'-C1'-N1 | 5.36 | 112.49 | 108.20 |
| 57 | BA | 1858 | A | N1-C6-N6 | -5.36 | 115.38 | 118.60 |
| 57 | BA | 2145 | C | O4'-C1'-N1 | 5.36 | 112.49 | 108.20 |
| 57 | BA | 2311 | A | O4'-C1'-N9 | 5.36 | 112.49 | 108.20 |
| 58 | Ba | 4 | C | O4'-C1'-N1 | 5.36 | 112.49 | 108.20 |
| 22 | AA | 285 | C | N1-C2-O2 | 5.36 | 122.11 | 118.90 |
| 22 | AA | 729 | A | C4'-C3'-C2' | -5.36 | 97.24 | 102.60 |
| 22 | AA | 1223 | C | N1-C2-O2 | 5.36 | 122.11 | 118.90 |
| 22 | AA | 1337 | G | N1-C6-O6 | -5.36 | 116.69 | 119.90 |
| 57 | BA | 2131 | U | N3-C2-O2 | -5.36 | 118.45 | 122.20 |
| 57 | BA | 2657 | A | O4'-C1'-N9 | 5.36 | 112.49 | 108.20 |
| 22 | AA | 854 | U | O4'-C1'-N1 | 5.36 | 112.49 | 108.20 |
| 57 | BA | 1598 | A | C4-C5-C6 | -5.36 | 114.32 | 117.00 |
| 57 | BA | 1961 | C | O4'-C1'-N1 | 5.36 | 112.49 | 108.20 |
| 22 | AA | 428 | G | C5-C6-N1 | 5.36 | 114.18 | 111.50 |
| 22 | AA | 732 | C | O4'-C1'-N1 | 5.36 | 112.48 | 108.20 |
| 57 | BA | 455 | C | N1-C2-O2 | 5.36 | 122.11 | 118.90 |
| 57 | BA | 1164 | C | N1-C2-O2 | 5.36 | 122.11 | 118.90 |
| 57 | BA | 1277 | G | N1-C6-O6 | -5.36 | 116.69 | 119.90 |
| 57 | BA | 1488 | C | N1-C2-O2 | 5.36 | 122.11 | 118.90 |
| 57 | BA | 2081 | U | O4'-C1'-N1 | 5.36 | 112.48 | 108.20 |
| 57 | BA | 2538 | C | N3-C2-O2 | -5.36 | 118.15 | 121.90 |
| 22 | AA | 564 | C | N3-C4-C5 | 5.35 | 124.04 | 121.90 |
| 57 | BA | 2780 | G | O4'-C1'-N9 | 5.35 | 112.48 | 108.20 |
| 57 | BA | 268 | C | N3-C4-N4 | -5.35 | 114.25 | 118.00 |
| 57 | BA | 1199 | U | O4'-C1'-N1 | 5.35 | 112.48 | 108.20 |
| 57 | BA | 1290 | C | O4'-C1'-N1 | 5.35 | 112.48 | 108.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 2742 | G | N1-C6-O6 | -5.35 | 116.69 | 119.90 |
| 23 | A2 | 19 | A | C2-N3-C4 | 5.35 | 113.28 | 110.60 |
| 2 | AK | 6 | ARG | NE-CZ-NH1 | 5.35 | 122.97 | 120.30 |
| 22 | AA | 693 | G | C3'-C2'-C1' | 5.35 | 105.78 | 101.50 |
| 57 | BA | 1944 | U | N3-C2-O2 | -5.35 | 118.45 | 122.20 |
| 22 | AA | 695 | A | N1-C6-N6 | -5.35 | 115.39 | 118.60 |
| 22 | AA | 726 | C | O4'-C1'-N1 | 5.35 | 112.48 | 108.20 |
| 57 | BA | 561 | G | P-O3'-C3' | 5.35 | 126.12 | 119.70 |
| 57 | BA | 1044 | C | N1-C2-O2 | 5.35 | 122.11 | 118.90 |
| 57 | BA | 1303 | G | N3-C4-C5 | -5.35 | 125.93 | 128.60 |
| 57 | BA | 2362 | C | O4'-C1'-N1 | 5.35 | 112.48 | 108.20 |
| 22 | AA | 6 | G | N1-C6-O6 | -5.35 | 116.69 | 119.90 |
| 57 | BA | 2828 | G | N1-C6-O6 | -5.35 | 116.69 | 119.90 |
| 58 | Ba | 75 | G | N1-C6-O6 | -5.35 | 116.69 | 119.90 |
| 22 | AA | 157 | U | O4'-C1'-N1 | 5.34 | 112.48 | 108.20 |
| 22 | AA | 1409 | C | O4'-C1'-N1 | 5.34 | 112.48 | 108.20 |
| 50 | B7 | 14 | ARG | NE-CZ-NH2 | 5.34 | 122.97 | 120.30 |
| 57 | BA | 819 | A | C4-C5-C6 | -5.34 | 114.33 | 117.00 |
| 57 | BA | 922 | C | N1-C2-O2 | 5.34 | 122.11 | 118.90 |
| 57 | BA | 1368 | G | O4'-C1'-N9 | 5.34 | 112.47 | 108.20 |
| 57 | BA | 2303 | G | N1-C6-O6 | -5.34 | 116.69 | 119.90 |
| 57 | BA | 1662 | U | N3-C2-O2 | -5.34 | 118.46 | 122.20 |
| 57 | BA | 2232 | C | N1-C2-O2 | 5.34 | 122.11 | 118.90 |
| 22 | AA | 1115 | U | N1-C2-N3 | 5.34 | 118.10 | 114.90 |
| 22 | AA | 1262 | C | O4'-C1'-N1 | 5.34 | 112.47 | 108.20 |
| 57 | BA | 785 | G | N1-C6-O6 | -5.34 | 116.69 | 119.90 |
| 57 | BA | 878 | A | O4'-C1'-N9 | 5.34 | 112.47 | 108.20 |
| 57 | BA | 1866 | A | C4-C5-C6 | -5.34 | 114.33 | 117.00 |
| 57 | BA | 1918 | A | C6-C5-N7 | 5.34 | 136.04 | 132.30 |
| 57 | BA | 2595 | G | N1-C6-O6 | -5.34 | 116.69 | 119.90 |
| 57 | BA | 2788 | C | N3-C4-C5 | 5.34 | 124.04 | 121.90 |
| 22 | AA | 355 | C | N1-C2-O2 | 5.34 | 122.10 | 118.90 |
| 22 | AA | 369 | G | N1-C6-O6 | -5.34 | 116.70 | 119.90 |
| 24 | A3 | 66 | C | O4'-C1'-N1 | 5.34 | 112.47 | 108.20 |
| 38 | BW | 95 | ARG | NH1-CZ-NH2 | -5.34 | 113.53 | 119.40 |
| 57 | BA | 366 | C | N1-C2-O2 | 5.34 | 122.10 | 118.90 |
| 57 | BA | 2134 | A | C4-C5-C6 | -5.34 | 114.33 | 117.00 |
| 12 | AT | 59 | ARG | NH1-CZ-NH2 | -5.34 | 113.53 | 119.40 |
| 22 | AA | 644 | U | O4'-C1'-N1 | 5.34 | 112.47 | 108.20 |
| 22 | AA | 1086 | U | O4'-C1'-N1 | 5.34 | 112.47 | 108.20 |
| 22 | AA | 1154 | G | N1-C6-O6 | -5.34 | 116.70 | 119.90 |
| 22 | AA | 1539 | C | N1-C2-O2 | 5.34 | 122.10 | 118.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 813 | U | O4'-C1'-N1 | 5.34 | 112.47 | 108.20 |
| 57 | BA | 2077 | A | C4-C5-C6 | -5.34 | 114.33 | 117.00 |
| 57 | BA | 312 | G | N3-C4-C5 | -5.34 | 125.93 | 128.60 |
| 57 | BA | 776 | G | O4'-C1'-N9 | 5.34 | 112.47 | 108.20 |
| 57 | BA | 1106 | G | N1-C6-O6 | -5.34 | 116.70 | 119.90 |
| 57 | BA | 2206 | C | O4'-C1'-N1 | 5.34 | 112.47 | 108.20 |
| 57 | BA | 2554 | U | N3-C2-O2 | -5.34 | 118.47 | 122.20 |
| 57 | BA | 2629 | U | C3'-C2'-C1' | 5.34 | 105.77 | 101.50 |
| 6 | AO | 76 | ARG | NE-CZ-NH1 | 5.33 | 122.97 | 120.30 |
| 57 | BA | 164 | C | N3-C4-C5 | 5.33 | 124.03 | 121.90 |
| 57 | BA | 1123 | C | N1-C2-O2 | 5.33 | 122.10 | 118.90 |
| 22 | AA | 142 | G | N1-C6-O6 | -5.33 | 116.70 | 119.90 |
| 22 | AA | 1028 | C | N1-C2-O2 | 5.33 | 122.10 | 118.90 |
| 57 | BA | 295 | G | N1-C6-O6 | -5.33 | 116.70 | 119.90 |
| 57 | BA | 868 | U | O4'-C1'-N1 | 5.33 | 112.47 | 108.20 |
| 57 | BA | 1290 | C | N1-C2-O2 | 5.33 | 122.10 | 118.90 |
| 57 | BA | 2149 | U | O4'-C1'-N1 | 5.33 | 112.47 | 108.20 |
| 14 | AC | 231 | ARG | NH1-CZ-NH2 | -5.33 | 113.53 | 119.40 |
| 22 | AA | 175 | C | N1-C2-O2 | 5.33 | 122.10 | 118.90 |
| 22 | AA | 203 | G | N3-C2-N2 | -5.33 | 116.17 | 119.90 |
| 22 | AA | 680 | C | N1-C2-O2 | 5.33 | 122.10 | 118.90 |
| 22 | AA | 1136 | C | N1-C2-O2 | 5.33 | 122.10 | 118.90 |
| 22 | AA | 1260 | G | N1-C6-O6 | -5.33 | 116.70 | 119.90 |
| 22 | AA | 1488 | G | N1-C6-O6 | -5.33 | 116.70 | 119.90 |
| 57 | BA | 95 | A | O4'-C1'-N9 | 5.33 | 112.47 | 108.20 |
| 57 | BA | 593 | U | O4'-C1'-N1 | 5.33 | 112.47 | 108.20 |
| 57 | BA | 1399 | C | N1-C2-O2 | 5.33 | 122.10 | 118.90 |
| 57 | BA | 1823 | G | N1-C6-O6 | -5.33 | 116.70 | 119.90 |
| 57 | BA | 1838 | C | N3-C4-C5 | 5.33 | 124.03 | 121.90 |
| 57 | BA | 2263 | C | N1-C2-O2 | 5.33 | 122.10 | 118.90 |
| 22 | AA | 269 | C | N1-C2-O2 | 5.33 | 122.10 | 118.90 |
| 22 | AA | 1174 | G | N1-C6-O6 | -5.33 | 116.70 | 119.90 |
| 22 | AA | 1249 | C | N3-C2-O2 | -5.33 | 118.17 | 121.90 |
| 22 | AA | 18 | C | N1-C2-O2 | 5.33 | 122.10 | 118.90 |
| 22 | AA | 488 | C | O4'-C1'-N1 | 5.33 | 112.46 | 108.20 |
| 22 | AA | 884 | U | N3-C2-O2 | -5.33 | 118.47 | 122.20 |
| 57 | BA | 2084 | C | N1-C2-O2 | 5.33 | 122.10 | 118.90 |
| 22 | AA | 713 | G | O4'-C1'-N9 | 5.33 | 112.46 | 108.20 |
| 57 | BA | 1703 | G | N1-C6-O6 | -5.33 | 116.70 | 119.90 |
| 57 | BA | 2863 | C | O4'-C1'-N1 | 5.33 | 112.46 | 108.20 |
| 22 | AA | 697 | U | O4'-C1'-N1 | 5.33 | 112.46 | 108.20 |
| 22 | AA | 1009 | U | O4'-C1'-N1 | 5.33 | 112.46 | 108.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 84 | A | O4'-C1'-N9 | 5.33 | 112.46 | 108.20 |
| 57 | BA | 707 | G | N1-C6-O6 | -5.33 | 116.70 | 119.90 |
| 57 | BA | 1029 | A | C4-C5-C6 | -5.33 | 114.34 | 117.00 |
| 57 | BA | 1051 | G | N1-C6-O6 | -5.33 | 116.70 | 119.90 |
| 57 | BA | 1802 | A | C4-C5-C6 | -5.33 | 114.34 | 117.00 |
| 57 | BA | 2207 | C | O4'-C1'-N1 | 5.33 | 112.46 | 108.20 |
| 57 | BA | 2888 | C | N1-C2-O2 | 5.33 | 122.10 | 118.90 |
| 23 | A2 | 57 | C | N1-C2-O2 | 5.32 | 122.09 | 118.90 |
| 57 | BA | 264 | C | O4'-C1'-N1 | 5.32 | 112.46 | 108.20 |
| 57 | BA | 856 | G | N1-C6-O6 | -5.32 | 116.70 | 119.90 |
| 57 | BA | 969 | G | N3-C2-N2 | -5.32 | 116.17 | 119.90 |
| 57 | BA | 1122 | G | N1-C6-O6 | -5.32 | 116.71 | 119.90 |
| 57 | BA | 1694 | C | N1-C2-O2 | 5.32 | 122.09 | 118.90 |
| 57 | BA | 1704 | C | N1-C2-O2 | 5.32 | 122.09 | 118.90 |
| 57 | BA | 2305 | U | N3-C2-O2 | -5.32 | 118.47 | 122.20 |
| 35 | BD | 68 | ARG | NE-CZ-NH1 | 5.32 | 122.96 | 120.30 |
| 57 | BA | 451 | U | C1'-O4'-C4' | -5.32 | 105.64 | 109.90 |
| 57 | BA | 570 | G | N3-C4-C5 | -5.32 | 125.94 | 128.60 |
| 57 | BA | 718 | A | C2-N3-C4 | 5.32 | 113.26 | 110.60 |
| 57 | BA | 1988 | G | O4'-C1'-N9 | 5.32 | 112.46 | 108.20 |
| 22 | AA | 534 | U | O4'-C1'-N1 | 5.32 | 112.45 | 108.20 |
| 22 | AA | 711 | G | N1-C6-O6 | -5.32 | 116.71 | 119.90 |
| 57 | BA | 423 | A | C6-C5-N7 | 5.32 | 136.02 | 132.30 |
| 22 | AA | 1172 | C | N1-C2-O2 | 5.32 | 122.09 | 118.90 |
| 57 | BA | 1195 | G | N1-C6-O6 | -5.32 | 116.71 | 119.90 |
| 57 | BA | 1222 | U | O4'-C1'-N1 | 5.32 | 112.45 | 108.20 |
| 57 | BA | 2658 | C | C1'-O4'-C4' | -5.32 | 105.65 | 109.90 |
| 22 | AA | 625 | U | O4'-C1'-N1 | 5.32 | 112.45 | 108.20 |
| 23 | A2 | 29 | G | N1-C6-O6 | -5.32 | 116.71 | 119.90 |
| 57 | BA | 529 | A | O4'-C1'-N9 | 5.32 | 112.45 | 108.20 |
| 57 | BA | 1194 | A | O4'-C1'-N9 | 5.32 | 112.45 | 108.20 |
| 57 | BA | 1568 | G | N3-C2-N2 | -5.32 | 116.18 | 119.90 |
| 57 | BA | 433 | C | N1-C2-O2 | 5.31 | 122.09 | 118.90 |
| 57 | BA | 1266 | G | N1-C6-O6 | -5.31 | 116.71 | 119.90 |
| 57 | BA | 1374 | G | N1-C6-O6 | -5.31 | 116.71 | 119.90 |
| 57 | BA | 2006 | C | N1-C2-O2 | 5.31 | 122.09 | 118.90 |
| 57 | BA | 2280 | G | N1-C6-O6 | -5.31 | 116.71 | 119.90 |
| 57 | BA | 2425 | A | O4'-C1'-N9 | 5.31 | 112.45 | 108.20 |
| 22 | AA | 1133 | G | N1-C6-O6 | -5.31 | 116.71 | 119.90 |
| 22 | AA | 1286 | U | N3-C2-O2 | -5.31 | 118.48 | 122.20 |
| 57 | BA | 413 | C | N1-C2-O2 | 5.31 | 122.09 | 118.90 |
| 57 | BA | 1838 | C | N1-C2-O2 | 5.31 | 122.09 | 118.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 2502 | G | C3'-C2'-C1' | 5.31 | 105.75 | 101.50 |
| 57 | BA | 2661 | G | C2'-C3'-O3' | 5.31 | 122.20 | 113.70 |
| 22 | AA | 74 | A | O4'-C1'-N9 | 5.31 | 112.45 | 108.20 |
| 57 | BA | 337 | C | N1-C2-O2 | 5.31 | 122.09 | 118.90 |
| 57 | BA | 625 | G | C5'-C4'-O4' | 5.31 | 115.47 | 109.10 |
| 57 | BA | 873 | C | O4'-C1'-N1 | 5.31 | 112.45 | 108.20 |
| 57 | BA | 2827 | C | N1-C2-O2 | 5.31 | 122.09 | 118.90 |
| 22 | AA | 995 | C | N3-C4-C5 | 5.31 | 124.02 | 121.90 |
| 22 | AA | 1421 | G | N1-C6-O6 | -5.31 | 116.72 | 119.90 |
| 57 | BA | 732 | C | N3-C4-N4 | -5.31 | 114.28 | 118.00 |
| 57 | BA | 1427 | A | C3'-C2'-C1' | -5.31 | 97.25 | 101.50 |
| 57 | BA | 1653 | G | N1-C6-O6 | -5.31 | 116.72 | 119.90 |
| 57 | BA | 2065 | C | N1-C2-O2 | 5.31 | 122.08 | 118.90 |
| 57 | BA | 2161 | C | O4'-C1'-N1 | 5.31 | 112.45 | 108.20 |
| 57 | BA | 2891 | U | O4'-C1'-N1 | 5.31 | 112.45 | 108.20 |
| 22 | AA | 661 | G | N1-C6-O6 | -5.31 | 116.72 | 119.90 |
| 22 | AA | 1317 | C | C2-N3-C4 | -5.31 | 117.25 | 119.90 |
| 57 | BA | 357 | C | N1-C2-O2 | 5.31 | 122.08 | 118.90 |
| 58 | Ba | 38 | C | N1-C2-O2 | 5.31 | 122.08 | 118.90 |
| 58 | Ba | 118 | C | N1-C2-O2 | 5.31 | 122.08 | 118.90 |
| 2 | AK | 97 | ARG | NE-CZ-NH1 | 5.30 | 122.95 | 120.30 |
| 22 | AA | 1449 | C | O4'-C1'-N1 | 5.30 | 112.44 | 108.20 |
| 57 | BA | 23 | G | N1-C6-O6 | -5.30 | 116.72 | 119.90 |
| 57 | BA | 75 | G | C1'-O4'-C4' | -5.30 | 105.66 | 109.90 |
| 57 | BA | 493 | G | O4'-C1'-N9 | 5.30 | 112.44 | 108.20 |
| 57 | BA | 2080 | A | C6-C5-N7 | 5.30 | 136.01 | 132.30 |
| 57 | BA | 2160 | C | O4'-C1'-N1 | 5.30 | 112.44 | 108.20 |
| 57 | BA | 2072 | C | N1-C2-O2 | 5.30 | 122.08 | 118.90 |
| 57 | BA | 2312 | U | C3'-C2'-C1' | 5.30 | 105.74 | 101.50 |
| 35 | BD | 100 | ARG | NE-CZ-NH1 | 5.30 | 122.95 | 120.30 |
| 57 | BA | 395 | U | N3-C2-O2 | -5.30 | 118.49 | 122.20 |
| 57 | BA | 1587 | G | N1-C6-O6 | -5.30 | 116.72 | 119.90 |
| 57 | BA | 1629 | U | N3-C2-O2 | -5.30 | 118.49 | 122.20 |
| 57 | BA | 2452 | C | O4'-C1'-N1 | 5.30 | 112.44 | 108.20 |
| 22 | AA | 534 | U | N3-C2-O2 | -5.30 | 118.49 | 122.20 |
| 22 | AA | 853 | C | N1-C2-O2 | 5.30 | 122.08 | 118.90 |
| 22 | AA | 1525 | G | N1-C6-O6 | -5.30 | 116.72 | 119.90 |
| 57 | BA | 2599 | G | N1-C6-O6 | -5.30 | 116.72 | 119.90 |
| 57 | BA | 150 | U | O4'-C1'-N1 | 5.30 | 112.44 | 108.20 |
| 57 | BA | 330 | A | C4-C5-C6 | -5.30 | 114.35 | 117.00 |
| 22 | AA | 575 | G | N1-C6-O6 | -5.30 | 116.72 | 119.90 |
| 22 | AA | 737 | C | O4'-C1'-N1 | 5.30 | 112.44 | 108.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 1732 | C | N1-C2-O2 | 5.30 | 122.08 | 118.90 |
| 57 | BA | 2573 | C | N3-C4-C5 | 5.30 | 124.02 | 121.90 |
| 57 | BA | 2845 | U | O4'-C1'-N1 | 5.30 | 112.44 | 108.20 |
| 22 | AA | 972 | C | N1-C2-O2 | 5.29 | 122.08 | 118.90 |
| 30 | BP | 132 | ARG | NE-CZ-NH2 | -5.29 | 117.65 | 120.30 |
| 57 | BA | 2038 | G | N1-C6-O6 | -5.29 | 116.72 | 119.90 |
| 57 | BA | 2666 | C | C2-N3-C4 | -5.29 | 117.25 | 119.90 |
| 57 | BA | 459 | U | N3-C2-O2 | -5.29 | 118.49 | 122.20 |
| 57 | BA | 462 | C | O4'-C1'-N1 | 5.29 | 112.44 | 108.20 |
| 57 | BA | 1351 | C | O4'-C1'-N1 | 5.29 | 112.43 | 108.20 |
| 57 | BA | 1693 | U | N3-C2-O2 | -5.29 | 118.50 | 122.20 |
| 57 | BA | 2367 | G | N1-C6-O6 | -5.29 | 116.72 | 119.90 |
| 22 | AA | 255 | G | N1-C6-O6 | -5.29 | 116.72 | 119.90 |
| 22 | AA | 832 | G | O4'-C1'-N9 | 5.29 | 112.43 | 108.20 |
| 22 | AA | 936 | C | N3-C4-N4 | -5.29 | 114.30 | 118.00 |
| 57 | BA | 228 | C | N1-C2-O2 | 5.29 | 122.08 | 118.90 |
| 57 | BA | 2023 | C | C5'-C4'-C3' | -5.29 | 107.53 | 116.00 |
| 57 | BA | 2096 | C | N1-C2-O2 | 5.29 | 122.08 | 118.90 |
| 57 | BA | 2145 | C | N1-C2-O2 | 5.29 | 122.08 | 118.90 |
| 57 | BA | 2225 | A | O4'-C1'-N9 | 5.29 | 112.43 | 108.20 |
| 57 | BA | 239 | C | N3-C4-N4 | -5.29 | 114.30 | 118.00 |
| 57 | BA | 2512 | C | N1-C2-O2 | 5.29 | 122.07 | 118.90 |
| 22 | AA | 47 | C | N1-C2-O2 | 5.29 | 122.07 | 118.90 |
| 22 | AA | 1115 | U | O4'-C1'-N1 | 5.29 | 112.43 | 108.20 |
| 57 | BA | 1571 | A | C4-C5-C6 | -5.29 | 114.36 | 117.00 |
| 57 | BA | 1995 | U | N3-C2-O2 | -5.29 | 118.50 | 122.20 |
| 58 | Ba | 17 | C | N1-C2-O2 | 5.29 | 122.07 | 118.90 |
| 57 | BA | 837 | C | O4'-C1'-N1 | 5.29 | 112.43 | 108.20 |
| 22 | AA | 616 | G | N1-C6-O6 | -5.29 | 116.73 | 119.90 |
| 22 | AA | 882 | C | N1-C2-O2 | 5.29 | 122.07 | 118.90 |
| 57 | BA | 20 | C | N1-C2-O2 | 5.29 | 122.07 | 118.90 |
| 57 | BA | 2678 | C | O4'-C1'-N1 | 5.29 | 112.43 | 108.20 |
| 22 | AA | 198 | G | N1-C6-O6 | -5.28 | 116.73 | 119.90 |
| 22 | AA | 485 | U | N3-C2-O2 | -5.28 | 118.50 | 122.20 |
| 22 | AA | 1184 | G | N3-C2-N2 | -5.28 | 116.20 | 119.90 |
| 22 | AA | 1513 | A | C6-C5-N7 | 5.28 | 136.00 | 132.30 |
| 57 | BA | 917 | A | C5'-C4'-C3' | -5.28 | 107.55 | 116.00 |
| 57 | BA | 1363 | C | N1-C2-O2 | 5.28 | 122.07 | 118.90 |
| 57 | BA | 1897 | G | N1-C6-O6 | -5.28 | 116.73 | 119.90 |
| 57 | BA | 2443 | C | N3-C4-C5 | 5.28 | 124.01 | 121.90 |
| 58 | Ba | 89 | U | N3-C2-O2 | -5.28 | 118.50 | 122.20 |
| 22 | AA | 20 | U | O4'-C1'-N1 | 5.28 | 112.42 | 108.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | AA | 970 | C | O4'-C1'-N1 | 5.28 | 112.43 | 108.20 |
| 13 | AU | 66 | ARG | NE-CZ-NH1 | 5.28 | 122.94 | 120.30 |
| 57 | BA | 994 | C | O4'-C1'-N1 | 5.28 | 112.42 | 108.20 |
| 57 | BA | 2652 | C | N1-C2-O2 | 5.28 | 122.07 | 118.90 |
| 35 | BD | 211 | ARG | NH1-CZ-NH2 | -5.28 | 113.59 | 119.40 |
| 57 | BA | 658 | U | O4'-C1'-N1 | 5.28 | 112.42 | 108.20 |
| 57 | BA | 2601 | C | N1-C2-O2 | 5.28 | 122.07 | 118.90 |
| 22 | AA | 962 | C | N1-C2-O2 | 5.28 | 122.07 | 118.90 |
| 22 | AA | 1375 | A | C4-C5-C6 | -5.28 | 114.36 | 117.00 |
| 22 | AA | 1504 | G | N3-C2-N2 | -5.28 | 116.21 | 119.90 |
| 24 | A3 | 77 | A | C1'-O4'-C4' | -5.28 | 105.68 | 109.90 |
| 57 | BA | 622 | G | N1-C6-O6 | -5.28 | 116.73 | 119.90 |
| 57 | BA | 1032 | A | C4-C5-C6 | -5.28 | 114.36 | 117.00 |
| 57 | BA | 1202 | G | N1-C6-O6 | -5.28 | 116.73 | 119.90 |
| 57 | BA | 1576 | U | C5-C6-N1 | -5.28 | 120.06 | 122.70 |
| 57 | BA | 2506 | U | N3-C2-O2 | -5.28 | 118.50 | 122.20 |
| 22 | AA | 1194 | U | N1-C2-N3 | 5.28 | 118.06 | 114.90 |
| 22 | AA | 1279 | G | C1'-O4'-C4' | -5.28 | 105.68 | 109.90 |
| 57 | BA | 838 | C | N3-C4-C5 | 5.28 | 124.01 | 121.90 |
| 57 | BA | 1098 | A | C5'-C4'-O4' | 5.28 | 115.43 | 109.10 |
| 57 | BA | 1423 | G | N1-C6-O6 | -5.28 | 116.73 | 119.90 |
| 22 | AA | 433 | G | O4'-C1'-N9 | 5.27 | 112.42 | 108.20 |
| 22 | AA | 499 | A | C1'-O4'-C4' | -5.27 | 105.68 | 109.90 |
| 57 | BA | 1895 | C | N1-C2-O2 | 5.27 | 122.06 | 118.90 |
| 22 | AA | 866 | C | N1-C2-O2 | 5.27 | 122.06 | 118.90 |
| 22 | AA | 1464 | U | O4'-C1'-N1 | 5.27 | 112.42 | 108.20 |
| 57 | BA | 700 | G | O4'-C1'-N9 | 5.27 | 112.42 | 108.20 |
| 57 | BA | 1043 | C | N1-C2-O2 | 5.27 | 122.06 | 118.90 |
| 57 | BA | 1608 | A | C4-C5-C6 | -5.27 | 114.36 | 117.00 |
| 57 | BA | 187 | G | N1-C6-O6 | -5.27 | 116.74 | 119.90 |
| 57 | BA | 1969 | A | O4'-C1'-N9 | 5.27 | 112.42 | 108.20 |
| 22 | AA | 314 | C | N3-C4-C5 | 5.27 | 124.01 | 121.90 |
| 22 | AA | 315 | A | C6-C5-N7 | 5.27 | 135.99 | 132.30 |
| 57 | BA | 37 | C | C4'-C3'-C2' | -5.27 | 97.33 | 102.60 |
| 57 | BA | 1081 | U | O4'-C1'-N1 | 5.27 | 112.42 | 108.20 |
| 57 | BA | 1168 | G | N1-C6-O6 | -5.27 | 116.74 | 119.90 |
| 57 | BA | 1275 | A | C5'-C4'-O4' | 5.27 | 115.42 | 109.10 |
| 57 | BA | 2209 | G | N1-C6-O6 | -5.27 | 116.74 | 119.90 |
| 57 | BA | 2279 | G | O4'-C1'-N9 | 5.27 | 112.42 | 108.20 |
| 58 | Ba | 26 | C | N3-C4-C5 | 5.27 | 124.01 | 121.90 |
| 5 | AN | 52 | ARG | NH1-CZ-NH2 | -5.27 | 113.61 | 119.40 |
| 22 | AA | 167 | A | C6-C5-N7 | 5.27 | 135.99 | 132.30 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 23 | A2 | 15 | G | N3-C4-C5 | -5.27 | 125.97 | 128.60 |
| 57 | BA | 906 | U | N1-C2-N3 | 5.27 | 118.06 | 114.90 |
| 57 | BA | 2133 | G | N1-C6-O6 | -5.27 | 116.74 | 119.90 |
| 57 | BA | 2165 | C | N3-C2-O2 | -5.27 | 118.21 | 121.90 |
| 57 | BA | 2594 | C | N1-C2-O2 | 5.27 | 122.06 | 118.90 |
| 58 | Ba | 83 | G | N1-C6-O6 | -5.27 | 116.74 | 119.90 |
| 22 | AA | 518 | C | N3-C4-C5 | 5.27 | 124.01 | 121.90 |
| 22 | AA | 822 | U | N3-C2-O2 | -5.27 | 118.51 | 122.20 |
| 53 | BF | 67 | ARG | NE-CZ-NH1 | 5.27 | 122.93 | 120.30 |
| 6 | AO | 16 | ARG | NE-CZ-NH1 | 5.26 | 122.93 | 120.30 |
| 22 | AA | 904 | U | O4'-C1'-N1 | 5.26 | 112.41 | 108.20 |
| 22 | AA | 1186 | G | O4'-C1'-N9 | 5.26 | 112.41 | 108.20 |
| 22 | AA | 1280 | A | C6-C5-N7 | 5.26 | 135.99 | 132.30 |
| 57 | BA | 680 | C | O4'-C1'-N1 | 5.26 | 112.41 | 108.20 |
| 57 | BA | 2045 | C | O4'-C1'-N1 | 5.26 | 112.41 | 108.20 |
| 57 | BA | 2395 | C | O4'-C1'-N1 | 5.26 | 112.41 | 108.20 |
| 58 | Ba | 97 | C | O4'-C1'-N1 | 5.26 | 112.41 | 108.20 |
| 57 | BA | 973 | A | C4-C5-C6 | -5.26 | 114.37 | 117.00 |
| 5 | AN | 8 | ARG | NE-CZ-NH1 | 5.26 | 122.93 | 120.30 |
| 22 | AA | 177 | G | N3-C2-N2 | -5.26 | 116.22 | 119.90 |
| 22 | AA | 597 | G | O4'-C1'-N9 | 5.26 | 112.41 | 108.20 |
| 22 | AA | 846 | G | N1-C6-O6 | -5.26 | 116.74 | 119.90 |
| 57 | BA | 205 | G | N1-C6-O6 | -5.26 | 116.74 | 119.90 |
| 57 | BA | 567 | U | O4'-C1'-N1 | 5.26 | 112.41 | 108.20 |
| 57 | BA | 1019 | U | N3-C2-O2 | -5.26 | 118.52 | 122.20 |
| 57 | BA | 1194 | A | C6-C5-N7 | 5.26 | 135.98 | 132.30 |
| 57 | BA | 1475 | G | O4'-C1'-N9 | 5.26 | 112.41 | 108.20 |
| 57 | BA | 2409 | G | N1-C6-O6 | -5.26 | 116.74 | 119.90 |
| 58 | Ba | 91 | C | N1-C2-O2 | 5.26 | 122.06 | 118.90 |
| 22 | AA | 985 | C | O4'-C1'-N1 | 5.26 | 112.41 | 108.20 |
| 22 | AA | 1241 | G | N1-C6-O6 | -5.26 | 116.74 | 119.90 |
| 57 | BA | 758 | C | O4'-C1'-N1 | 5.26 | 112.41 | 108.20 |
| 57 | BA | 1109 | C | N1-C2-O2 | 5.26 | 122.06 | 118.90 |
| 57 | BA | 2577 | A | C3'-C2'-C1' | 5.26 | 105.71 | 101.50 |
| 57 | BA | 2661 | G | C5'-C4'-O4' | 5.26 | 115.41 | 109.10 |
| 22 | AA | 227 | G | N1-C6-O6 | -5.26 | 116.75 | 119.90 |
| 22 | AA | 544 | G | O4'-C1'-N9 | 5.26 | 112.41 | 108.20 |
| 22 | AA | 642 | A | C4-C5-C6 | -5.26 | 114.37 | 117.00 |
| 22 | AA | 1395 | C | N1-C2-O2 | 5.26 | 122.06 | 118.90 |
| 32 | BR | 4 | ARG | CD-NE-CZ | 5.26 | 130.96 | 123.60 |
| 57 | BA | 112 | U | C4'-C3'-C2' | -5.26 | 97.34 | 102.60 |
| 57 | BA | 2138 | G | N1-C6-O6 | -5.26 | 116.75 | 119.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 2768 | U | N3-C2-O2 | -5.26 | 118.52 | 122.20 |
| 22 | AA | 206 | C | N1-C2-O2 | 5.26 | 122.05 | 118.90 |
| 22 | AA | 385 | C | O4'-C1'-N1 | 5.26 | 112.41 | 108.20 |
| 22 | AA | 444 | G | O4'-C1'-N9 | 5.26 | 112.41 | 108.20 |
| 22 | AA | 1352 | C | O4'-C1'-N1 | 5.26 | 112.41 | 108.20 |
| 57 | BA | 712 | G | C4'-C3'-C2' | -5.26 | 97.34 | 102.60 |
| 57 | BA | 990 | A | O4'-C1'-N9 | 5.26 | 112.41 | 108.20 |
| 57 | BA | 1104 | C | N1-C2-O2 | 5.26 | 122.05 | 118.90 |
| 57 | BA | 2640 | G | N1-C6-O6 | -5.26 | 116.75 | 119.90 |
| 22 | AA | 1007 | U | O4'-C1'-N1 | 5.25 | 112.40 | 108.20 |
| 57 | BA | 784 | G | C5-C6-N1 | 5.25 | 114.13 | 111.50 |
| 57 | BA | 907 | G | N1-C6-O6 | -5.25 | 116.75 | 119.90 |
| 57 | BA | 1337 | G | N1-C6-O6 | -5.25 | 116.75 | 119.90 |
| 22 | AA | 34 | C | N1-C2-O2 | 5.25 | 122.05 | 118.90 |
| 22 | AA | 37 | U | C5-C6-N1 | -5.25 | 120.07 | 122.70 |
| 22 | AA | 756 | C | O4'-C1'-N1 | 5.25 | 112.40 | 108.20 |
| 22 | AA | 1001 | C | N1-C2-O2 | 5.25 | 122.05 | 118.90 |
| 57 | BA | 536 | G | N1-C6-O6 | -5.25 | 116.75 | 119.90 |
| 57 | BA | 588 | U | O4'-C1'-N1 | 5.25 | 112.40 | 108.20 |
| 57 | BA | 2855 | C | O4'-C1'-N1 | 5.25 | 112.40 | 108.20 |
| 22 | AA | 94 | G | C5-C6-N1 | 5.25 | 114.13 | 111.50 |
| 22 | AA | 271 | C | N1-C2-O2 | 5.25 | 122.05 | 118.90 |
| 57 | BA | 79 | C | N1-C2-O2 | 5.25 | 122.05 | 118.90 |
| 57 | BA | 401 | A | C6-C5-N7 | 5.25 | 135.98 | 132.30 |
| 57 | BA | 1476 | U | O4'-C1'-N1 | 5.25 | 112.40 | 108.20 |
| 57 | BA | 1478 | G | N1-C6-O6 | -5.25 | 116.75 | 119.90 |
| 57 | BA | 2421 | G | N1-C6-O6 | -5.25 | 116.75 | 119.90 |
| 58 | Ba | 92 | C | N1-C2-O2 | 5.25 | 122.05 | 118.90 |
| 2 | AK | 121 | ARG | NE-CZ-NH2 | -5.25 | 117.67 | 120.30 |
| 22 | AA | 1457 | G | N1-C6-O6 | -5.25 | 116.75 | 119.90 |
| 26 | BJ | 60 | ARG | NE-CZ-NH1 | 5.25 | 122.92 | 120.30 |
| 57 | BA | 1972 | G | N1-C6-O6 | -5.25 | 116.75 | 119.90 |
| 8 | AQ | 10 | ARG | NH1-CZ-NH2 | -5.25 | 113.63 | 119.40 |
| 22 | AA | 483 | C | N3-C4-N4 | -5.25 | 114.33 | 118.00 |
| 22 | AA | 1119 | C | N1-C2-O2 | 5.25 | 122.05 | 118.90 |
| 22 | AA | 1491 | G | O4'-C1'-N9 | 5.25 | 112.40 | 108.20 |
| 57 | BA | 1325 | U | N3-C2-O2 | -5.25 | 118.53 | 122.20 |
| 57 | BA | 1867 | G | N1-C6-O6 | -5.25 | 116.75 | 119.90 |
| 57 | BA | 2757 | A | C4-C5-C6 | -5.25 | 114.38 | 117.00 |
| 9 | AR | 11 | ARG | NE-CZ-NH1 | -5.25 | 117.68 | 120.30 |
| 22 | AA | 207 | C | N1-C2-O2 | 5.25 | 122.05 | 118.90 |
| 22 | AA | 1063 | C | N1-C2-O2 | 5.25 | 122.05 | 118.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 36 | BU | 49 | ARG | NE-CZ-NH1 | 5.25 | 122.92 | 120.30 |
| 51 | B8 | 7 | ARG | NH1-CZ-NH2 | -5.25 | 113.63 | 119.40 |
| 57 | BA | 872 | U | N1-C2-N3 | 5.25 | 118.05 | 114.90 |
| 57 | BA | 917 | A | C4-C5-C6 | -5.25 | 114.38 | 117.00 |
| 57 | BA | 2329 | U | N3-C2-O2 | -5.25 | 118.53 | 122.20 |
| 57 | BA | 2540 | C | N3-C4-C5 | 5.25 | 124.00 | 121.90 |
| 22 | AA | 40 | C | N1-C2-O2 | 5.25 | 122.05 | 118.90 |
| 22 | AA | 112 | G | N1-C6-O6 | -5.25 | 116.75 | 119.90 |
| 22 | AA | 197 | A | C1'-O4'-C4' | -5.25 | 105.70 | 109.90 |
| 22 | AA | 662 | U | C5-C6-N1 | -5.24 | 120.08 | 122.70 |
| 22 | AA | 1011 | C | O4'-C1'-N1 | 5.24 | 112.39 | 108.20 |
| 57 | BA | 167 | A | C4-C5-C6 | -5.24 | 114.38 | 117.00 |
| 57 | BA | 227 | A | O4'-C1'-N9 | 5.24 | 112.39 | 108.20 |
| 57 | BA | 673 | C | N3-C4-C5 | 5.24 | 124.00 | 121.90 |
| 57 | BA | 673 | C | O4'-C1'-N1 | 5.24 | 112.39 | 108.20 |
| 58 | Ba | 37 | C | O4'-C1'-N1 | 5.24 | 112.39 | 108.20 |
| 57 | BA | 54 | G | O4'-C1'-N9 | 5.24 | 112.39 | 108.20 |
| 57 | BA | 1145 | C | O4'-C1'-N1 | 5.24 | 112.39 | 108.20 |
| 57 | BA | 2482 | A | C4-C5-C6 | -5.24 | 114.38 | 117.00 |
| 22 | AA | 810 | C | N3-C4-C5 | 5.24 | 124.00 | 121.90 |
| 57 | BA | 499 | U | N3-C2-O2 | -5.24 | 118.53 | 122.20 |
| 57 | BA | 666 | A | C6-C5-N7 | 5.24 | 135.97 | 132.30 |
| 57 | BA | 1284 | A | C6-C5-N7 | 5.24 | 135.97 | 132.30 |
| 57 | BA | 1790 | C | N3-C4-C5 | 5.24 | 124.00 | 121.90 |
| 58 | Ba | 8 | C | N1-C2-O2 | 5.24 | 122.04 | 118.90 |
| 22 | AA | 997 | U | O4'-C1'-N1 | 5.24 | 112.39 | 108.20 |
| 57 | BA | 409 | G | O4'-C1'-N9 | 5.24 | 112.39 | 108.20 |
| 57 | BA | 1965 | C | N1-C2-O2 | 5.24 | 122.04 | 118.90 |
| 57 | BA | 2081 | U | C5-C6-N1 | -5.24 | 120.08 | 122.70 |
| 57 | BA | 2374 | C | C5'-C4'-O4' | 5.24 | 115.39 | 109.10 |
| 57 | BA | 2414 | G | N1-C6-O6 | -5.24 | 116.76 | 119.90 |
| 20 | AI | 10 | ARG | NE-CZ-NH1 | 5.24 | 122.92 | 120.30 |
| 57 | BA | 1218 | G | N1-C6-O6 | -5.24 | 116.76 | 119.90 |
| 22 | AA | 293 | G | N1-C6-O6 | -5.24 | 116.76 | 119.90 |
| 22 | AA | 922 | G | N1-C6-O6 | -5.24 | 116.76 | 119.90 |
| 22 | AA | 979 | C | N1-C2-O2 | 5.24 | 122.04 | 118.90 |
| 23 | A2 | 51 | C | N1-C2-O2 | 5.24 | 122.04 | 118.90 |
| 24 | A3 | 31 | G | N1-C6-O6 | -5.24 | 116.76 | 119.90 |
| 57 | BA | 96 | C | O4'-C1'-N1 | 5.24 | 112.39 | 108.20 |
| 57 | BA | 382 | A | O4'-C1'-N9 | 5.24 | 112.39 | 108.20 |
| 57 | BA | 2055 | C | N1-C2-O2 | 5.24 | 122.04 | 118.90 |
| 57 | BA | 514 | A | C5'-C4'-O4' | 5.23 | 115.38 | 109.10 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 1486 | U | O4'-C1'-N1 | 5.23 | 112.39 | 108.20 |
| 57 | BA | 2801 | G | N1-C6-O6 | -5.23 | 116.76 | 119.90 |
| 16 | AE | 67 | ARG | NE-CZ-NH1 | 5.23 | 122.92 | 120.30 |
| 53 | BF | 102 | ARG | CD-NE-CZ | 5.23 | 130.93 | 123.60 |
| 57 | BA | 360 | U | N3-C2-O2 | -5.23 | 118.54 | 122.20 |
| 57 | BA | 524 | G | O4'-C1'-N9 | 5.23 | 112.39 | 108.20 |
| 57 | BA | 1397 | U | C5-C6-N1 | -5.23 | 120.08 | 122.70 |
| 57 | BA | 1465 | G | N3-C4-C5 | -5.23 | 125.98 | 128.60 |
| 57 | BA | 1529 | G | N1-C6-O6 | -5.23 | 116.76 | 119.90 |
| 57 | BA | 1698 | A | C4-C5-C6 | -5.23 | 114.38 | 117.00 |
| 14 | AC | 163 | ARG | NE-CZ-NH1 | 5.23 | 122.92 | 120.30 |
| 22 | AA | 585 | G | N1-C6-O6 | -5.23 | 116.76 | 119.90 |
| 22 | AA | 1290 | G | N1-C6-O6 | -5.23 | 116.76 | 119.90 |
| 22 | AA | 1416 | G | N1-C6-O6 | -5.23 | 116.76 | 119.90 |
| 23 | A2 | 47 | C | N1-C2-O2 | 5.23 | 122.04 | 118.90 |
| 57 | BA | 1329 | U | C5-C6-N1 | -5.23 | 120.08 | 122.70 |
| 57 | BA | 1858 | A | C4-C5-C6 | -5.23 | 114.39 | 117.00 |
| 18 | AG | 77 | ARG | NE-CZ-NH1 | 5.23 | 122.92 | 120.30 |
| 22 | AA | 90 | C | N1-C2-O2 | 5.23 | 122.04 | 118.90 |
| 22 | AA | 322 | C | N1-C2-O2 | 5.23 | 122.04 | 118.90 |
| 22 | AA | 893 | C | N3-C4-C5 | 5.23 | 123.99 | 121.90 |
| 22 | AA | 1460 | C | N1-C2-O2 | 5.23 | 122.04 | 118.90 |
| 57 | BA | 219 | A | C6-C5-N7 | 5.23 | 135.96 | 132.30 |
| 57 | BA | 570 | G | C3'-C2'-C1' | 5.23 | 105.68 | 101.50 |
| 57 | BA | 2332 | C | N1-C2-O2 | 5.23 | 122.04 | 118.90 |
| 22 | AA | 70 | U | O4'-C1'-N1 | 5.23 | 112.38 | 108.20 |
| 22 | AA | 936 | C | N1-C2-O2 | 5.23 | 122.04 | 118.90 |
| 53 | BF | 44 | ARG | NE-CZ-NH2 | 5.23 | 122.91 | 120.30 |
| 57 | BA | 645 | C | N1-C2-O2 | 5.23 | 122.04 | 118.90 |
| 57 | BA | 2214 | C | N3-C4-C5 | 5.23 | 123.99 | 121.90 |
| 12 | AT | 9 | ARG | NE-CZ-NH2 | 5.23 | 122.91 | 120.30 |
| 14 | AC | 155 | ARG | NE-CZ-NH1 | 5.23 | 122.91 | 120.30 |
| 57 | BA | 632 | A | C4-C5-C6 | -5.23 | 114.39 | 117.00 |
| 57 | BA | 2710 | C | C3'-C2'-C1' | 5.23 | 105.68 | 101.50 |
| 22 | AA | 213 | G | O4'-C1'-N9 | 5.22 | 112.38 | 108.20 |
| 22 | AA | 1378 | C | N1-C2-O2 | 5.22 | 122.03 | 118.90 |
| 57 | BA | 468 | G | N3-C2-N2 | -5.22 | 116.24 | 119.90 |
| 57 | BA | 2020 | A | C1'-O4'-C4' | -5.22 | 105.72 | 109.90 |
| 57 | BA | 2228 | G | N1-C6-O6 | -5.22 | 116.77 | 119.90 |
| 57 | BA | 2502 | G | O4'-C4'-C3' | 5.22 | 110.28 | 106.10 |
| 57 | BA | 2728 | U | C5-C6-N1 | -5.22 | 120.09 | 122.70 |
| 22 | AA | 505 | G | N1-C6-O6 | -5.22 | 116.77 | 119.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | AA | 710 | G | N1-C6-O6 | -5.22 | 116.77 | 119.90 |
| 22 | AA | 1376 | U | O4'-C1'-N1 | 5.22 | 112.38 | 108.20 |
| 22 | AA | 1487 | G | N1-C6-O6 | -5.22 | 116.77 | 119.90 |
| 57 | BA | 382 | A | C6-C5-N7 | 5.22 | 135.96 | 132.30 |
| 57 | BA | 638 | G | C5'-C4'-O4' | 5.22 | 115.37 | 109.10 |
| 57 | BA | 281 | C | N1-C2-O2 | 5.22 | 122.03 | 118.90 |
| 57 | BA | 1233 | C | O4'-C1'-N1 | 5.22 | 112.38 | 108.20 |
| 57 | BA | 1778 | U | O4'-C1'-N1 | 5.22 | 112.38 | 108.20 |
| 57 | BA | 2100 | G | N1-C6-O6 | -5.22 | 116.77 | 119.90 |
| 12 | AT | 73 | ARG | NH1-CZ-NH2 | -5.22 | 113.66 | 119.40 |
| 13 | AU | 17 | ARG | NE-CZ-NH1 | 5.22 | 122.91 | 120.30 |
| 22 | AA | 73 | C | N3-C4-N4 | -5.22 | 114.35 | 118.00 |
| 22 | AA | 178 | C | O4'-C1'-N1 | 5.22 | 112.38 | 108.20 |
| 22 | AA | 219 | U | O4'-C1'-N1 | 5.22 | 112.38 | 108.20 |
| 22 | AA | 1060 | U | N3-C2-O2 | -5.22 | 118.55 | 122.20 |
| 57 | BA | 69 | C | O4'-C1'-N1 | 5.22 | 112.38 | 108.20 |
| 57 | BA | 214 | G | N1-C6-O6 | -5.22 | 116.77 | 119.90 |
| 57 | BA | 1016 | G | N1-C6-O6 | -5.22 | 116.77 | 119.90 |
| 57 | BA | 1374 | G | O4'-C1'-N9 | 5.22 | 112.38 | 108.20 |
| 57 | BA | 1547 | C | N1-C2-O2 | 5.22 | 122.03 | 118.90 |
| 57 | BA | 1902 | C | N3-C4-N4 | -5.22 | 114.35 | 118.00 |
| 57 | BA | 2395 | C | N1-C2-O2 | 5.22 | 122.03 | 118.90 |
| 57 | BA | 2754 | U | N3-C2-O2 | -5.22 | 118.55 | 122.20 |
| 22 | AA | 456 | A | C6-C5-N7 | 5.22 | 135.95 | 132.30 |
| 22 | AA | 694 | A | C4-C5-C6 | -5.22 | 114.39 | 117.00 |
| 22 | AA | 829 | G | N1-C6-O6 | -5.22 | 116.77 | 119.90 |
| 22 | AA | 934 | C | N3-C4-N4 | -5.22 | 114.35 | 118.00 |
| 57 | BA | 1441 | G | N1-C6-O6 | -5.22 | 116.77 | 119.90 |
| 57 | BA | 1804 | C | O4'-C1'-N1 | 5.22 | 112.37 | 108.20 |
| 57 | BA | 2241 | A | C6-C5-N7 | 5.22 | 135.95 | 132.30 |
| 57 | BA | 2558 | C | O4'-C1'-N1 | 5.22 | 112.37 | 108.20 |
| 57 | BA | 2563 | U | C5-C6-N1 | -5.22 | 120.09 | 122.70 |
| 57 | BA | 2642 | G | N1-C6-O6 | -5.22 | 116.77 | 119.90 |
| 22 | AA | 235 | C | N1-C2-O2 | 5.21 | 122.03 | 118.90 |
| 22 | AA | 523 | A | C6-C5-N7 | 5.21 | 135.95 | 132.30 |
| 25 | BC | 134 | ARG | NE-CZ-NH1 | 5.21 | 122.91 | 120.30 |
| 51 | B8 | 29 | ARG | NH1-CZ-NH2 | -5.21 | 113.66 | 119.40 |
| 57 | BA | 294 | A | C1'-O4'-C4' | -5.21 | 105.73 | 109.90 |
| 58 | Ba | 14 | U | N3-C2-O2 | -5.21 | 118.55 | 122.20 |
| 22 | AA | 1124 | G | N1-C6-O6 | -5.21 | 116.77 | 119.90 |
| 57 | BA | 962 | G | C1'-O4'-C4' | -5.21 | 105.73 | 109.90 |
| 22 | AA | 920 | U | O4'-C1'-N1 | 5.21 | 112.37 | 108.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 493 | G | N1-C6-O6 | -5.21 | 116.77 | 119.90 |
| 57 | BA | 1182 | G | N1-C6-O6 | -5.21 | 116.77 | 119.90 |
| 57 | BA | 2261 | C | C5'-C4'-C3' | -5.21 | 107.66 | 116.00 |
| 24 | A3 | 67 | C | O4'-C1'-N1 | 5.21 | 112.37 | 108.20 |
| 57 | BA | 1116 | G | O4'-C1'-N9 | 5.21 | 112.37 | 108.20 |
| 57 | BA | 1310 | G | N3-C2-N2 | -5.21 | 116.25 | 119.90 |
| 57 | BA | 1784 | A | C5'-C4'-O4' | 5.21 | 115.35 | 109.10 |
| 57 | BA | 2298 | A | C4-C5-C6 | -5.21 | 114.39 | 117.00 |
| 22 | AA | 353 | A | C3'-C2'-C1' | 5.21 | 105.67 | 101.50 |
| 22 | AA | 448 | A | C6-C5-N7 | 5.21 | 135.94 | 132.30 |
| 22 | AA | 961 | U | O4'-C1'-N1 | 5.21 | 112.37 | 108.20 |
| 57 | BA | 26 | G | N3-C2-N2 | -5.21 | 116.25 | 119.90 |
| 57 | BA | 1203 | U | C5-C6-N1 | -5.21 | 120.10 | 122.70 |
| 57 | BA | 1254 | A | O4'-C4'-C3' | 5.21 | 110.27 | 106.10 |
| 57 | BA | 1437 | C | N1-C2-O2 | 5.21 | 122.03 | 118.90 |
| 57 | BA | 1659 | G | N1-C6-O6 | -5.21 | 116.78 | 119.90 |
| 57 | BA | 2215 | C | O4'-C1'-N1 | 5.21 | 112.37 | 108.20 |
| 22 | AA | 43 | C | N1-C2-O2 | 5.21 | 122.02 | 118.90 |
| 22 | AA | 645 | G | N1-C6-O6 | -5.21 | 116.78 | 119.90 |
| 22 | AA | 729 | A | C4-C5-C6 | -5.21 | 114.40 | 117.00 |
| 22 | AA | 771 | G | N1-C6-O6 | -5.21 | 116.78 | 119.90 |
| 22 | AA | 903 | G | N1-C6-O6 | -5.21 | 116.78 | 119.90 |
| 22 | AA | 989 | U | C5-C6-N1 | -5.21 | 120.10 | 122.70 |
| 22 | AA | 1027 | C | N1-C2-O2 | 5.21 | 122.02 | 118.90 |
| 57 | BA | 175 | G | N1-C6-O6 | -5.21 | 116.78 | 119.90 |
| 57 | BA | 2462 | C | O4'-C1'-N1 | 5.21 | 112.37 | 108.20 |
| 57 | BA | 2712 | C | N3-C4-C5 | 5.21 | 123.98 | 121.90 |
| 58 | Ba | 20 | G | O4'-C1'-N9 | 5.21 | 112.37 | 108.20 |
| 33 | BS | 13 | ARG | NH1-CZ-NH2 | -5.21 | 113.67 | 119.40 |
| 57 | BA | 2311 | A | C1'-O4'-C4' | -5.21 | 105.74 | 109.90 |
| 22 | AA | 239 | U | O4'-C1'-N1 | 5.20 | 112.36 | 108.20 |
| 22 | AA | 464 | U | C5'-C4'-O4' | 5.20 | 115.34 | 109.10 |
| 22 | AA | 897 | C | N3-C4-C5 | 5.20 | 123.98 | 121.90 |
| 28 | BN | 13 | ARG | NE-CZ-NH2 | 5.20 | 122.90 | 120.30 |
| 57 | BA | 1997 | C | N3-C4-C5 | 5.20 | 123.98 | 121.90 |
| 57 | BA | 2010 | G | N1-C6-O6 | -5.20 | 116.78 | 119.90 |
| 57 | BA | 2027 | G | N1-C6-O6 | -5.20 | 116.78 | 119.90 |
| 57 | BA | 2846 | G | N1-C6-O6 | -5.20 | 116.78 | 119.90 |
| 24 | A3 | 3 | C | O4'-C1'-N1 | 5.20 | 112.36 | 108.20 |
| 57 | BA | 395 | U | O4'-C1'-N1 | 5.20 | 112.36 | 108.20 |
| 57 | BA | 590 | A | O4'-C1'-N9 | 5.20 | 112.36 | 108.20 |
| 7 | AP | 25 | ARG | NE-CZ-NH2 | -5.20 | 117.70 | 120.30 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 14 | AC | 135 | ARG | NE-CZ-NH1 | 5.20 | 122.90 | 120.30 |
| 22 | AA | 113 | G | N1-C6-O6 | -5.20 | 116.78 | 119.90 |
| 22 | AA | 953 | G | C5-C6-N1 | 5.20 | 114.10 | 111.50 |
| 22 | AA | 1221 | G | N1-C6-O6 | -5.20 | 116.78 | 119.90 |
| 22 | AA | 1321 | U | N3-C2-O2 | -5.20 | 118.56 | 122.20 |
| 28 | BN | 99 | ARG | NE-CZ-NH1 | 5.20 | 122.90 | 120.30 |
| 57 | BA | 23 | G | O4'-C1'-N9 | 5.20 | 112.36 | 108.20 |
| 57 | BA | 132 | G | N1-C6-O6 | -5.20 | 116.78 | 119.90 |
| 57 | BA | 257 | C | N3-C4-C5 | 5.20 | 123.98 | 121.90 |
| 57 | BA | 2053 | G | N1-C6-O6 | -5.20 | 116.78 | 119.90 |
| 22 | AA | 1230 | C | N1-C2-O2 | 5.20 | 122.02 | 118.90 |
| 23 | A2 | 29 | G | C5-C6-N1 | 5.20 | 114.10 | 111.50 |
| 57 | BA | 769 | U | N3-C2-O2 | -5.20 | 118.56 | 122.20 |
| 57 | BA | 1624 | U | C5'-C4'-C3' | -5.20 | 107.68 | 116.00 |
| 57 | BA | 2139 | U | N1-C2-N3 | 5.20 | 118.02 | 114.90 |
| 22 | AA | 1508 | A | O4'-C1'-N9 | 5.20 | 112.36 | 108.20 |
| 57 | BA | 57 | C | N1-C2-O2 | 5.20 | 122.02 | 118.90 |
| 57 | BA | 427 | U | O4'-C1'-N1 | 5.20 | 112.36 | 108.20 |
| 57 | BA | 1716 | U | N3-C2-O2 | -5.20 | 118.56 | 122.20 |
| 57 | BA | 2225 | A | C6-C5-N7 | 5.20 | 135.94 | 132.30 |
| 57 | BA | 2243 | U | N1-C2-N3 | 5.20 | 118.02 | 114.90 |
| 57 | BA | 2465 | C | N1-C2-O2 | 5.20 | 122.02 | 118.90 |
| 57 | BA | 2848 | G | O4'-C1'-N9 | 5.20 | 112.36 | 108.20 |
| 22 | AA | 633 | G | O4'-C1'-N9 | 5.20 | 112.36 | 108.20 |
| 22 | AA | 925 | G | N1-C6-O6 | -5.20 | 116.78 | 119.90 |
| 22 | AA | 1273 | C | N3-C4-C5 | 5.20 | 123.98 | 121.90 |
| 36 | BU | 27 | ARG | NE-CZ-NH1 | 5.20 | 122.90 | 120.30 |
| 53 | BF | 49 | ARG | NH1-CZ-NH2 | -5.20 | 113.69 | 119.40 |
| 57 | BA | 460 | A | C4-C5-C6 | -5.20 | 114.40 | 117.00 |
| 57 | BA | 2615 | U | N3-C2-O2 | -5.20 | 118.56 | 122.20 |
| 22 | AA | 73 | C | N1-C2-O2 | 5.19 | 122.02 | 118.90 |
| 57 | BA | 1663 | G | N1-C6-O6 | -5.19 | 116.78 | 119.90 |
| 57 | BA | 1863 | G | N1-C6-O6 | -5.19 | 116.78 | 119.90 |
| 58 | Ba | 65 | U | O4'-C1'-N1 | 5.19 | 112.36 | 108.20 |
| 21 | A1 | 42 | ARG | NE-CZ-NH1 | 5.19 | 122.90 | 120.30 |
| 22 | AA | 392 | C | N1-C2-O2 | 5.19 | 122.02 | 118.90 |
| 24 | A3 | 17 | C | N1-C2-O2 | 5.19 | 122.02 | 118.90 |
| 57 | BA | 51 | G | O4'-C1'-N9 | 5.19 | 112.35 | 108.20 |
| 57 | BA | 123 | G | N1-C6-O6 | -5.19 | 116.78 | 119.90 |
| 57 | BA | 2011 | U | O4'-C1'-N1 | 5.19 | 112.35 | 108.20 |
| 57 | BA | 2171 | A | C6-C5-N7 | 5.19 | 135.93 | 132.30 |
| 57 | BA | 2499 | C | N1-C2-O2 | 5.19 | 122.02 | 118.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | AA | 1220 | G | C4'-C3'-C2' | -5.19 | 97.41 | 102.60 |
| 57 | BA | 151 | C | O4'-C1'-N1 | 5.19 | 112.35 | 108.20 |
| 57 | BA | 1068 | G | N1-C6-O6 | -5.19 | 116.79 | 119.90 |
| 57 | BA | 1393 | A | C5'-C4'-O4' | 5.19 | 115.33 | 109.10 |
| 57 | BA | 2703 | C | N1-C2-O2 | 5.19 | 122.02 | 118.90 |
| 57 | BA | 2802 | G | N1-C6-O6 | -5.19 | 116.79 | 119.90 |
| 22 | AA | 378 | G | N1-C6-O6 | -5.19 | 116.79 | 119.90 |
| 22 | AA | 712 | A | C6-C5-N7 | 5.19 | 135.93 | 132.30 |
| 1 | AJ | 89 | ARG | NE-CZ-NH1 | 5.19 | 122.89 | 120.30 |
| 22 | AA | 497 | G | P-O3'-C3' | 5.19 | 125.92 | 119.70 |
| 22 | AA | 716 | A | C6-C5-N7 | 5.19 | 135.93 | 132.30 |
| 22 | AA | 879 | C | N3-C4-C5 | 5.19 | 123.97 | 121.90 |
| 22 | AA | 1138 | G | C8-N9-C4 | -5.19 | 104.33 | 106.40 |
| 22 | AA | 1317 | C | N1-C2-O2 | 5.19 | 122.01 | 118.90 |
| 38 | BW | 11 | ARG | NE-CZ-NH2 | 5.19 | 122.89 | 120.30 |
| 57 | BA | 814 | C | O4'-C1'-N1 | 5.19 | 112.35 | 108.20 |
| 57 | BA | 1458 | U | O4'-C1'-N1 | 5.19 | 112.35 | 108.20 |
| 57 | BA | 1770 | G | N1-C6-O6 | -5.19 | 116.79 | 119.90 |
| 57 | BA | 1837 | C | N1-C2-O2 | 5.19 | 122.01 | 118.90 |
| 57 | BA | 2349 | G | C5-C6-N1 | 5.19 | 114.09 | 111.50 |
| 22 | AA | 40 | C | O4'-C1'-N1 | 5.19 | 112.35 | 108.20 |
| 22 | AA | 740 | U | O4'-C1'-N1 | 5.19 | 112.35 | 108.20 |
| 24 | A3 | 13 | C | N1-C2-O2 | 5.19 | 122.01 | 118.90 |
| 24 | A3 | 15 | G | N3-C2-N2 | -5.19 | 116.27 | 119.90 |
| 57 | BA | 446 | G | O4'-C1'-N9 | 5.19 | 112.35 | 108.20 |
| 57 | BA | 1133 | A | O4'-C1'-N9 | 5.19 | 112.35 | 108.20 |
| 57 | BA | 1293 | C | O4'-C1'-N1 | 5.19 | 112.35 | 108.20 |
| 57 | BA | 2290 | G | N3-C4-C5 | -5.19 | 126.01 | 128.60 |
| 22 | AA | 67 | C | N1-C2-O2 | 5.18 | 122.01 | 118.90 |
| 22 | AA | 627 | G | N1-C6-O6 | -5.18 | 116.79 | 119.90 |
| 22 | AA | 1333 | A | C4-C5-C6 | -5.18 | 114.41 | 117.00 |
| 57 | BA | 423 | A | C5-C6-N6 | 5.18 | 127.85 | 123.70 |
| 57 | BA | 436 | C | O4'-C1'-N1 | 5.18 | 112.35 | 108.20 |
| 57 | BA | 956 | G | N1-C6-O6 | -5.18 | 116.79 | 119.90 |
| 57 | BA | 1493 | C | N1-C2-O2 | 5.18 | 122.01 | 118.90 |
| 57 | BA | 1556 | C | N1-C2-O2 | 5.18 | 122.01 | 118.90 |
| 57 | BA | 2384 | U | O4'-C1'-N1 | 5.18 | 112.35 | 108.20 |
| 57 | BA | 2585 | U | N3-C2-O2 | -5.18 | 118.57 | 122.20 |
| 57 | BA | 2600 | A | C6-C5-N7 | 5.18 | 135.93 | 132.30 |
| 57 | BA | 2663 | G | C5'-C4'-O4' | 5.18 | 115.32 | 109.10 |
| 57 | BA | 2669 | G | N1-C6-O6 | -5.18 | 116.79 | 119.90 |
| 57 | BA | 2674 | G | N1-C6-O6 | -5.18 | 116.79 | 119.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | AA | 191 | G | O4'-C1'-N9 | 5.18 | 112.35 | 108.20 |
| 57 | BA | 2277 | G | C5'-C4'-O4' | 5.18 | 115.32 | 109.10 |
| 22 | AA | 629 | A | O4'-C1'-N9 | 5.18 | 112.34 | 108.20 |
| 22 | AA | 939 | G | N1-C6-O6 | -5.18 | 116.79 | 119.90 |
| 57 | BA | 1726 | C | O4'-C1'-N1 | 5.18 | 112.34 | 108.20 |
| 57 | BA | 2576 | G | N9-C1'-C2' | -5.18 | 106.30 | 112.00 |
| 57 | BA | 2811 | G | N1-C6-O6 | -5.18 | 116.79 | 119.90 |
| 22 | AA | 92 | U | O4'-C1'-N1 | 5.18 | 112.34 | 108.20 |
| 22 | AA | 563 | A | C1'-O4'-C4' | -5.18 | 105.76 | 109.90 |
| 57 | BA | 426 | C | O4'-C1'-N1 | 5.18 | 112.34 | 108.20 |
| 57 | BA | 1003 | G | N1-C6-O6 | -5.18 | 116.79 | 119.90 |
| 57 | BA | 1166 | G | C8-N9-C4 | -5.18 | 104.33 | 106.40 |
| 57 | BA | 1843 | C | O4'-C1'-N1 | 5.18 | 112.34 | 108.20 |
| 57 | BA | 2880 | C | N1-C2-O2 | 5.18 | 122.01 | 118.90 |
| 58 | Ba | 76 | G | O4'-C1'-N9 | 5.18 | 112.34 | 108.20 |
| 22 | AA | 305 | G | O4'-C4'-C3' | 5.18 | 110.24 | 106.10 |
| 57 | BA | 485 | C | N1-C2-O2 | 5.18 | 122.01 | 118.90 |
| 22 | AA | 5 | U | N1-C2-N3 | 5.18 | 118.01 | 114.90 |
| 22 | AA | 974 | A | C6-C5-N7 | 5.18 | 135.92 | 132.30 |
| 22 | AA | 987 | G | N1-C6-O6 | -5.18 | 116.79 | 119.90 |
| 57 | BA | 302 | C | N1-C2-O2 | 5.18 | 122.01 | 118.90 |
| 57 | BA | 898 | C | N1-C2-O2 | 5.18 | 122.01 | 118.90 |
| 57 | BA | 2140 | G | N1-C6-O6 | -5.18 | 116.79 | 119.90 |
| 57 | BA | 2474 | U | O4'-C1'-N1 | 5.18 | 112.34 | 108.20 |
| 22 | AA | 958 | A | C6-C5-N7 | 5.17 | 135.92 | 132.30 |
| 57 | BA | 274 | C | N1-C2-O2 | 5.17 | 122.00 | 118.90 |
| 57 | BA | 560 | C | O4'-C1'-N1 | 5.17 | 112.34 | 108.20 |
| 57 | BA | 579 | G | N3-C4-C5 | -5.17 | 126.01 | 128.60 |
| 57 | BA | 582 | A | O4'-C1'-N9 | 5.17 | 112.34 | 108.20 |
| 57 | BA | 1203 | U | N3-C2-O2 | -5.17 | 118.58 | 122.20 |
| 57 | BA | 1259 | G | N1-C6-O6 | -5.17 | 116.80 | 119.90 |
| 57 | BA | 2693 | G | N1-C6-O6 | -5.17 | 116.80 | 119.90 |
| 13 | AU | 20 | ARG | NH1-CZ-NH2 | -5.17 | 113.71 | 119.40 |
| 22 | AA | 417 | G | N1-C6-O6 | -5.17 | 116.80 | 119.90 |
| 22 | AA | 830 | G | N1-C6-O6 | -5.17 | 116.80 | 119.90 |
| 22 | AA | 1351 | U | O4'-C1'-N1 | 5.17 | 112.34 | 108.20 |
| 57 | BA | 1369 | G | N1-C6-O6 | -5.17 | 116.80 | 119.90 |
| 57 | BA | 2078 | C | N3-C4-C5 | 5.17 | 123.97 | 121.90 |
| 57 | BA | 2582 | G | N3-C4-C5 | -5.17 | 126.02 | 128.60 |
| 57 | BA | 2782 | G | N1-C6-O6 | -5.17 | 116.80 | 119.90 |
| 22 | AA | 398 | U | C5'-C4'-O4' | 5.17 | 115.30 | 109.10 |
| 22 | AA | 722 | G | N3-C4-C5 | -5.17 | 126.02 | 128.60 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | AA | 1131 | G | N1-C6-O6 | -5.17 | 116.80 | 119.90 |
| 57 | BA | 33 | C | N3-C4-C5 | 5.17 | 123.97 | 121.90 |
| 57 | BA | 154 | U | O4'-C1'-N1 | 5.17 | 112.33 | 108.20 |
| 57 | BA | 179 | C | N1-C2-O2 | 5.17 | 122.00 | 118.90 |
| 57 | BA | 963 | U | N1-C2-N3 | 5.17 | 118.00 | 114.90 |
| 57 | BA | 971 | G | N1-C6-O6 | -5.17 | 116.80 | 119.90 |
| 57 | BA | 1606 | C | C4'-C3'-C2' | -5.17 | 97.43 | 102.60 |
| 57 | BA | 1879 | C | O4'-C1'-N1 | 5.17 | 112.33 | 108.20 |
| 58 | Ba | 25 | U | N3-C2-O2 | -5.17 | 118.58 | 122.20 |
| 16 | AE | 68 | ARG | NE-CZ-NH1 | 5.17 | 122.88 | 120.30 |
| 22 | AA | 469 | C | N3-C4-C5 | 5.17 | 123.97 | 121.90 |
| 22 | AA | 1128 | C | N1-C2-O2 | 5.17 | 122.00 | 118.90 |
| 22 | AA | 1380 | U | N3-C2-O2 | -5.17 | 118.58 | 122.20 |
| 23 | A2 | 26 | U | N3-C2-O2 | -5.17 | 118.58 | 122.20 |
| 57 | BA | 334 | C | O4'-C1'-N1 | 5.17 | 112.33 | 108.20 |
| 57 | BA | 728 | G | N1-C6-O6 | -5.17 | 116.80 | 119.90 |
| 57 | BA | 1145 | C | N1-C2-O2 | 5.17 | 122.00 | 118.90 |
| 57 | BA | 1305 | C | N1-C2-O2 | 5.17 | 122.00 | 118.90 |
| 57 | BA | 1448 | G | O4'-C1'-N9 | 5.17 | 112.33 | 108.20 |
| 57 | BA | 1649 | G | N1-C6-O6 | -5.17 | 116.80 | 119.90 |
| 57 | BA | 1894 | C | O4'-C1'-N1 | 5.17 | 112.33 | 108.20 |
| 22 | AA | 289 | G | N3-C4-C5 | -5.17 | 126.02 | 128.60 |
| 22 | AA | 748 | G | N1-C6-O6 | -5.17 | 116.80 | 119.90 |
| 57 | BA | 2486 | C | N1-C2-O2 | 5.17 | 122.00 | 118.90 |
| 57 | BA | 2881 | U | O4'-C1'-N1 | 5.17 | 112.33 | 108.20 |
| 22 | AA | 16 | A | C6-C5-N7 | 5.16 | 135.91 | 132.30 |
| 22 | AA | 511 | C | N1-C2-O2 | 5.16 | 122.00 | 118.90 |
| 57 | BA | 1007 | C | N3-C4-C5 | 5.16 | 123.97 | 121.90 |
| 57 | BA | 1401 | G | N1-C6-O6 | -5.16 | 116.80 | 119.90 |
| 57 | BA | 1494 | A | C6-C5-N7 | 5.16 | 135.91 | 132.30 |
| 57 | BA | 1993 | U | N1-C2-N3 | 5.16 | 118.00 | 114.90 |
| 22 | AA | 152 | A | C6-C5-N7 | 5.16 | 135.91 | 132.30 |
| 57 | BA | 854 | C | O4'-C1'-N1 | 5.16 | 112.33 | 108.20 |
| 57 | BA | 894 | U | C5-C6-N1 | -5.16 | 120.12 | 122.70 |
| 57 | BA | 1753 | G | N3-C2-N2 | -5.16 | 116.29 | 119.90 |
| 7 | AP | 56 | ARG | NE-CZ-NH1 | 5.16 | 122.88 | 120.30 |
| 22 | AA | 384 | G | N1-C6-O6 | -5.16 | 116.80 | 119.90 |
| 22 | AA | 464 | U | O4'-C1'-N1 | 5.16 | 112.33 | 108.20 |
| 24 | A3 | 17 | C | O4'-C1'-N1 | 5.16 | 112.33 | 108.20 |
| 57 | BA | 407 | G | N1-C6-O6 | -5.16 | 116.80 | 119.90 |
| 57 | BA | 1484 | U | O4'-C1'-N1 | 5.16 | 112.33 | 108.20 |
| 57 | BA | 2102 | G | O4'-C1'-N9 | 5.16 | 112.33 | 108.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 2420 | C | O4'-C1'-N1 | 5.16 | 112.33 | 108.20 |
| 57 | BA | 2620 | C | O4'-C1'-N1 | 5.16 | 112.33 | 108.20 |
| 22 | AA | 459 | A | C6-C5-N7 | 5.16 | 135.91 | 132.30 |
| 22 | AA | 792 | A | O4'-C1'-N9 | 5.16 | 112.33 | 108.20 |
| 22 | AA | 1293 | C | N1-C2-O2 | 5.16 | 122.00 | 118.90 |
| 22 | AA | 1511 | G | C5-C6-N1 | 5.16 | 114.08 | 111.50 |
| 57 | BA | 1192 | G | O4'-C1'-N9 | 5.16 | 112.33 | 108.20 |
| 57 | BA | 1896 | G | N1-C6-O6 | -5.16 | 116.81 | 119.90 |
| 22 | AA | 12 | U | O4'-C1'-N1 | 5.16 | 112.33 | 108.20 |
| 22 | AA | 483 | C | C3'-C2'-C1' | 5.16 | 105.62 | 101.50 |
| 22 | AA | 1244 | G | N1-C6-O6 | -5.16 | 116.81 | 119.90 |
| 35 | BD | 188 | ARG | NE-CZ-NH1 | 5.16 | 122.88 | 120.30 |
| 57 | BA | 966 | G | N1-C6-O6 | -5.16 | 116.81 | 119.90 |
| 57 | BA | 2488 | G | N1-C6-O6 | -5.16 | 116.81 | 119.90 |
| 22 | AA | 134 | G | N1-C6-O6 | -5.16 | 116.81 | 119.90 |
| 22 | AA | 427 | U | O4'-C1'-N1 | 5.16 | 112.32 | 108.20 |
| 57 | BA | 1063 | G | N1-C6-O6 | -5.16 | 116.81 | 119.90 |
| 22 | AA | 664 | G | N3-C4-C5 | -5.15 | 126.02 | 128.60 |
| 57 | BA | 629 | G | N1-C6-O6 | -5.15 | 116.81 | 119.90 |
| 57 | BA | 738 | G | O4'-C1'-N9 | 5.15 | 112.32 | 108.20 |
| 57 | BA | 2902 | C | O4'-C1'-N1 | 5.15 | 112.32 | 108.20 |
| 58 | Ba | 30 | C | N1-C2-O2 | 5.15 | 121.99 | 118.90 |
| 7 | AP | 14 | ARG | NE-CZ-NH2 | 5.15 | 122.88 | 120.30 |
| 22 | AA | 637 | C | O4'-C1'-N1 | 5.15 | 112.32 | 108.20 |
| 22 | AA | 717 | U | N3-C2-O2 | -5.15 | 118.59 | 122.20 |
| 22 | AA | 787 | A | O4'-C1'-N9 | 5.15 | 112.32 | 108.20 |
| 57 | BA | 449 | A | C4-C5-C6 | -5.15 | 114.42 | 117.00 |
| 57 | BA | 456 | C | N1-C2-O2 | 5.15 | 121.99 | 118.90 |
| 57 | BA | 702 | U | N3-C2-O2 | -5.15 | 118.59 | 122.20 |
| 57 | BA | 2467 | C | O4'-C1'-N1 | 5.15 | 112.32 | 108.20 |
| 57 | BA | 2475 | C | N1-C2-O2 | 5.15 | 121.99 | 118.90 |
| 57 | BA | 2836 | U | C5-C6-N1 | -5.15 | 120.12 | 122.70 |
| 22 | AA | 1055 | A | O4'-C1'-N9 | 5.15 | 112.32 | 108.20 |
| 22 | AA | 1291 | U | O4'-C1'-N1 | 5.15 | 112.32 | 108.20 |
| 22 | AA | 1524 | C | C2-N3-C4 | -5.15 | 117.33 | 119.90 |
| 23 | A2 | 46 | C | N1-C2-O2 | 5.15 | 121.99 | 118.90 |
| 57 | BA | 236 | C | O4'-C1'-N1 | 5.15 | 112.32 | 108.20 |
| 57 | BA | 923 | G | N1-C6-O6 | -5.15 | 116.81 | 119.90 |
| 57 | BA | 1202 | G | O4'-C1'-N9 | 5.15 | 112.32 | 108.20 |
| 57 | BA | 2585 | U | O4'-C1'-N1 | 5.15 | 112.32 | 108.20 |
| 57 | BA | 2762 | C | N1-C2-O2 | 5.15 | 121.99 | 118.90 |
| 58 | Ba | 23 | 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($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | AA | 44 | A | O4'-C1'-N9 | 5.15 | 112.32 | 108.20 |
| 57 | BA | 383 | C | N3-C4-N4 | -5.15 | 114.39 | 118.00 |
| 4 | AM | 91 | ARG | NH1-CZ-NH2 | -5.15 | 113.74 | 119.40 |
| 22 | AA | 314 | C | N1-C2-O2 | 5.15 | 121.99 | 118.90 |
| 22 | AA | 1439 | G | N1-C6-O6 | -5.15 | 116.81 | 119.90 |
| 57 | BA | 108 | G | O4'-C1'-N9 | 5.15 | 112.32 | 108.20 |
| 57 | BA | 254 | G | C5'-C4'-O4' | 5.15 | 115.28 | 109.10 |
| 57 | BA | 356 | G | N1-C6-O6 | -5.15 | 116.81 | 119.90 |
| 57 | BA | 674 | G | N1-C6-O6 | -5.15 | 116.81 | 119.90 |
| 57 | BA | 841 | G | N1-C6-O6 | -5.15 | 116.81 | 119.90 |
| 57 | BA | 853 | C | N1-C2-O2 | 5.15 | 121.99 | 118.90 |
| 57 | BA | 1153 | C | N3-C4-C5 | 5.15 | 123.96 | 121.90 |
| 57 | BA | 1853 | A | C6-C5-N7 | 5.15 | 135.90 | 132.30 |
| 57 | BA | 77 | G | N1-C6-O6 | -5.15 | 116.81 | 119.90 |
| 57 | BA | 744 | U | N3-C2-O2 | -5.15 | 118.60 | 122.20 |
| 57 | BA | 1100 | C | N1-C2-O2 | 5.15 | 121.99 | 118.90 |
| 57 | BA | 2677 | G | N1-C6-O6 | -5.15 | 116.81 | 119.90 |
| 57 | BA | 2822 | G | N1-C6-O6 | -5.15 | 116.81 | 119.90 |
| 22 | AA | 48 | C | N1-C2-O2 | 5.14 | 121.99 | 118.90 |
| 22 | AA | 243 | A | C1'-O4'-C4' | -5.14 | 105.78 | 109.90 |
| 22 | AA | 799 | G | O4'-C1'-N9 | 5.14 | 112.32 | 108.20 |
| 57 | BA | 188 | G | O4'-C1'-N9 | 5.14 | 112.31 | 108.20 |
| 57 | BA | 600 | G | N1-C6-O6 | -5.14 | 116.81 | 119.90 |
| 57 | BA | 1198 | U | N3-C2-O2 | -5.14 | 118.60 | 122.20 |
| 57 | BA | 1361 | G | N1-C6-O6 | -5.14 | 116.81 | 119.90 |
| 57 | BA | 2755 | C | N1-C2-O2 | 5.14 | 121.99 | 118.90 |
| 22 | AA | 274 | A | C6-C5-N7 | 5.14 | 135.90 | 132.30 |
| 57 | BA | 1206 | G | N1-C6-O6 | -5.14 | 116.81 | 119.90 |
| 57 | BA | 1335 | C | O4'-C1'-N1 | 5.14 | 112.31 | 108.20 |
| 57 | BA | 1782 | U | O4'-C1'-N1 | 5.14 | 112.31 | 108.20 |
| 57 | BA | 2176 | A | C6-C5-N7 | 5.14 | 135.90 | 132.30 |
| 57 | BA | 2431 | U | O4'-C1'-N1 | 5.14 | 112.31 | 108.20 |
| 22 | AA | 921 | U | O4'-C1'-N1 | 5.14 | 112.31 | 108.20 |
| 24 | A3 | 29 | C | O4'-C1'-N1 | 5.14 | 112.31 | 108.20 |
| 57 | BA | 1847 | A | C2-N3-C4 | 5.14 | 113.17 | 110.60 |
| 57 | BA | 2858 | C | N3-C4-C5 | 5.14 | 123.96 | 121.90 |
| 58 | Ba | 82 | U | O4'-C1'-N1 | 5.14 | 112.31 | 108.20 |
| 6 | AO | 79 | ARG | NE-CZ-NH1 | 5.14 | 122.87 | 120.30 |
| 22 | AA | 269 | C | O4'-C1'-N1 | 5.14 | 112.31 | 108.20 |
| 57 | BA | 81 | G | N1-C6-O6 | -5.14 | 116.82 | 119.90 |
| 57 | BA | 901 | C | N3-C4-C5 | 5.14 | 123.95 | 121.90 |
| 57 | BA | 1309 | G | N1-C6-O6 | -5.14 | 116.82 | 119.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 1352 | U | N1-C2-N3 | 5.14 | 117.98 | 114.90 |
| 57 | BA | 1597 | A | O4'-C1'-N9 | 5.14 | 112.31 | 108.20 |
| 58 | Ba | 73 | A | C4-C5-C6 | -5.14 | 114.43 | 117.00 |
| 22 | AA | 811 | C | N3-C4-C5 | 5.14 | 123.95 | 121.90 |
| 22 | AA | 1245 | C | N1-C2-O2 | 5.14 | 121.98 | 118.90 |
| 45 | BE | 124 | ARG | NH1-CZ-NH2 | -5.14 | 113.75 | 119.40 |
| 45 | BE | 184 | ARG | NE-CZ-NH2 | 5.14 | 122.87 | 120.30 |
| 57 | BA | 1314 | C | C5'-C4'-O4' | 5.14 | 115.26 | 109.10 |
| 57 | BA | 1349 | C | O4'-C1'-N1 | 5.14 | 112.31 | 108.20 |
| 57 | BA | 2517 | C | C1'-O4'-C4' | -5.14 | 105.79 | 109.90 |
| 57 | BA | 2853 | C | N1-C2-O2 | 5.14 | 121.98 | 118.90 |
| 22 | AA | 37 | U | O4'-C1'-N1 | 5.13 | 112.31 | 108.20 |
| 22 | AA | 286 | C | O4'-C1'-N1 | 5.13 | 112.31 | 108.20 |
| 22 | AA | 1278 | G | N1-C6-O6 | -5.13 | 116.82 | 119.90 |
| 22 | AA | 1293 | C | O4'-C1'-N1 | 5.13 | 112.31 | 108.20 |
| 22 | AA | 1370 | G | N1-C6-O6 | -5.13 | 116.82 | 119.90 |
| 57 | BA | 208 | C | N1-C2-O2 | 5.13 | 121.98 | 118.90 |
| 57 | BA | 337 | C | O4'-C1'-N1 | 5.13 | 112.31 | 108.20 |
| 57 | BA | 374 | A | C4-C5-C6 | -5.13 | 114.43 | 117.00 |
| 57 | BA | 1146 | C | O4'-C1'-N1 | 5.13 | 112.31 | 108.20 |
| 57 | BA | 1957 | C | N1-C2-O2 | 5.13 | 121.98 | 118.90 |
| 57 | BA | 905 | A | C6-C5-N7 | 5.13 | 135.89 | 132.30 |
| 9 | AR | 11 | ARG | NE-CZ-NH2 | 5.13 | 122.87 | 120.30 |
| 16 | AE | 137 | ARG | NE-CZ-NH1 | 5.13 | 122.87 | 120.30 |
| 22 | AA | 155 | A | C6-C5-N7 | 5.13 | 135.89 | 132.30 |
| 22 | AA | 266 | G | N3-C4-C5 | -5.13 | 126.03 | 128.60 |
| 48 | B5 | 9 | ARG | NH1-CZ-NH2 | -5.13 | 113.76 | 119.40 |
| 57 | BA | 236 | C | N1-C2-O2 | 5.13 | 121.98 | 118.90 |
| 57 | BA | 2342 | C | C6-N1-C2 | -5.13 | 118.25 | 120.30 |
| 57 | BA | 2049 | G | N1-C6-O6 | -5.13 | 116.82 | 119.90 |
| 20 | AI | 17 | ARG | NH1-CZ-NH2 | -5.13 | 113.76 | 119.40 |
| 22 | AA | 834 | U | O4'-C1'-N1 | 5.13 | 112.30 | 108.20 |
| 22 | AA | 846 | G | O4'-C1'-N9 | 5.13 | 112.30 | 108.20 |
| 57 | BA | 381 | G | N1-C6-O6 | -5.13 | 116.82 | 119.90 |
| 57 | BA | 641 | U | N3-C2-O2 | -5.13 | 118.61 | 122.20 |
| 57 | BA | 2526 | G | N1-C6-O6 | -5.13 | 116.82 | 119.90 |
| 57 | BA | 2711 | A | C6-C5-N7 | 5.13 | 135.89 | 132.30 |
| 22 | AA | 488 | C | N1-C2-O2 | 5.13 | 121.98 | 118.90 |
| 22 | AA | 678 | U | O4'-C1'-N1 | 5.13 | 112.30 | 108.20 |
| 22 | AA | 816 | A | C5'-C4'-O4' | 5.13 | 115.25 | 109.10 |
| 22 | AA | 991 | U | N3-C2-O2 | -5.13 | 118.61 | 122.20 |
| 22 | AA | 1279 | G | C5-C6-N1 | 5.13 | 114.06 | 111.50 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 44 | B2 | 47 | ARG | NE-CZ-NH2 | 5.13 | 122.86 | 120.30 |
| 57 | BA | 208 | C | O4'-C1'-N1 | 5.13 | 112.30 | 108.20 |
| 57 | BA | 378 | C | N3-C4-C5 | 5.13 | 123.95 | 121.90 |
| 57 | BA | 475 | C | N1-C2-O2 | 5.13 | 121.98 | 118.90 |
| 57 | BA | 523 | C | C4'-C3'-C2' | -5.13 | 97.47 | 102.60 |
| 57 | BA | 546 | U | O4'-C1'-N1 | 5.13 | 112.30 | 108.20 |
| 57 | BA | 843 | G | N1-C6-O6 | -5.13 | 116.82 | 119.90 |
| 57 | BA | 1028 | A | O4'-C1'-N9 | 5.13 | 112.30 | 108.20 |
| 57 | BA | 1865 | U | O4'-C1'-N1 | 5.13 | 112.30 | 108.20 |
| 38 | BW | 92 | ARG | NE-CZ-NH1 | 5.12 | 122.86 | 120.30 |
| 57 | BA | 313 | G | N1-C6-O6 | -5.12 | 116.83 | 119.90 |
| 22 | AA | 371 | A | C5'-C4'-O4' | 5.12 | 115.25 | 109.10 |
| 22 | AA | 671 | G | O4'-C1'-N9 | 5.12 | 112.30 | 108.20 |
| 57 | BA | 1312 | U | C5-C6-N1 | -5.12 | 120.14 | 122.70 |
| 57 | BA | 1410 | G | N1-C6-O6 | -5.12 | 116.83 | 119.90 |
| 57 | BA | 1800 | C | N3-C4-C5 | 5.12 | 123.95 | 121.90 |
| 57 | BA | 1904 | G | N1-C6-O6 | -5.12 | 116.83 | 119.90 |
| 22 | AA | 647 | C | N1-C2-O2 | 5.12 | 121.97 | 118.90 |
| 22 | AA | 1018 | G | N1-C6-O6 | -5.12 | 116.83 | 119.90 |
| 57 | BA | 1028 | A | N1-C6-N6 | -5.12 | 115.53 | 118.60 |
| 22 | AA | 1021 | A | C6-C5-N7 | 5.12 | 135.88 | 132.30 |
| 57 | BA | 2808 | G | N3-C2-N2 | -5.12 | 116.32 | 119.90 |
| 14 | AC | 10 | ARG | NE-CZ-NH1 | 5.12 | 122.86 | 120.30 |
| 17 | AF | 24 | ARG | NE-CZ-NH1 | 5.12 | 122.86 | 120.30 |
| 22 | AA | 335 | C | N1-C2-O2 | 5.12 | 121.97 | 118.90 |
| 22 | AA | 442 | G | N1-C6-O6 | -5.12 | 116.83 | 119.90 |
| 22 | AA | 514 | C | O4'-C1'-N1 | 5.12 | 112.30 | 108.20 |
| 22 | AA | 1329 | A | C6-C5-N7 | 5.12 | 135.88 | 132.30 |
| 23 | A2 | 22 | G | N3-C4-C5 | -5.12 | 126.04 | 128.60 |
| 57 | BA | 1529 | G | O4'-C1'-N9 | 5.12 | 112.29 | 108.20 |
| 57 | BA | 2245 | U | N1-C2-N3 | 5.12 | 117.97 | 114.90 |
| 22 | AA | 724 | G | C5-C6-N1 | 5.12 | 114.06 | 111.50 |
| 23 | A2 | 45 | G | N1-C6-O6 | -5.12 | 116.83 | 119.90 |
| 22 | AA | 163 | C | O4'-C1'-N1 | 5.12 | 112.29 | 108.20 |
| 22 | AA | 319 | G | N1-C6-O6 | -5.12 | 116.83 | 119.90 |
| 22 | AA | 1006 | G | N1-C6-O6 | -5.12 | 116.83 | 119.90 |
| 45 | BE | 124 | ARG | NE-CZ-NH2 | 5.12 | 122.86 | 120.30 |
| 48 | B5 | 16 | ARG | NE-CZ-NH1 | 5.12 | 122.86 | 120.30 |
| 57 | BA | 698 | C | N1-C2-O2 | 5.12 | 121.97 | 118.90 |
| 57 | BA | 731 | C | N1-C2-O2 | 5.12 | 121.97 | 118.90 |
| 57 | BA | 1141 | U | N3-C2-O2 | -5.12 | 118.62 | 122.20 |
| 57 | BA | 2714 | G | C5'-C4'-O4' | 5.12 | 115.24 | 109.10 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | AA | 1025 | U | O4'-C1'-N1 | 5.11 | 112.29 | 108.20 |
| 48 | B5 | 12 | ARG | NE-CZ-NH1 | 5.11 | 122.86 | 120.30 |
| 57 | BA | 568 | U | N3-C2-O2 | -5.11 | 118.62 | 122.20 |
| 22 | AA | 245 | U | O4'-C1'-N1 | 5.11 | 112.29 | 108.20 |
| 57 | BA | 882 | G | N3-C4-C5 | -5.11 | 126.04 | 128.60 |
| 57 | BA | 964 | C | N3-C4-N4 | -5.11 | 114.42 | 118.00 |
| 22 | AA | 1327 | C | N1-C2-O2 | 5.11 | 121.97 | 118.90 |
| 22 | AA | 1328 | C | O4'-C1'-N1 | 5.11 | 112.29 | 108.20 |
| 57 | BA | 327 | G | N1-C6-O6 | -5.11 | 116.83 | 119.90 |
| 57 | BA | 815 | C | N1-C2-O2 | 5.11 | 121.97 | 118.90 |
| 57 | BA | 1379 | U | N3-C2-O2 | -5.11 | 118.62 | 122.20 |
| 57 | BA | 2649 | C | N1-C2-O2 | 5.11 | 121.97 | 118.90 |
| 57 | BA | 2695 | U | O4'-C1'-N1 | 5.11 | 112.29 | 108.20 |
| 57 | BA | 2897 | U | O4'-C1'-N1 | 5.11 | 112.29 | 108.20 |
| 22 | AA | 144 | G | N1-C6-O6 | -5.11 | 116.83 | 119.90 |
| 22 | AA | 1346 | A | C6-C5-N7 | 5.11 | 135.88 | 132.30 |
| 47 | B4 | 59 | ARG | NE-CZ-NH1 | 5.11 | 122.85 | 120.30 |
| 57 | BA | 1119 | U | C5-C6-N1 | -5.11 | 120.15 | 122.70 |
| 21 | A1 | 87 | ARG | NH1-CZ-NH2 | -5.11 | 113.78 | 119.40 |
| 22 | AA | 969 | A | C5'-C4'-O4' | 5.11 | 115.23 | 109.10 |
| 22 | AA | 1206 | G | C5-C6-N1 | 5.11 | 114.05 | 111.50 |
| 22 | AA | 1221 | G | C4'-C3'-C2' | -5.11 | 97.49 | 102.60 |
| 22 | AA | 1326 | U | O4'-C1'-N1 | 5.11 | 112.29 | 108.20 |
| 57 | BA | 129 | C | N1-C2-O2 | 5.11 | 121.96 | 118.90 |
| 57 | BA | 847 | U | C3'-C2'-C1' | 5.11 | 105.59 | 101.50 |
| 57 | BA | 1098 | A | C4-C5-C6 | -5.11 | 114.45 | 117.00 |
| 57 | BA | 1295 | C | O4'-C1'-N1 | 5.11 | 112.29 | 108.20 |
| 57 | BA | 1639 | C | N1-C2-O2 | 5.11 | 121.96 | 118.90 |
| 57 | BA | 2517 | C | N3-C4-C5 | 5.11 | 123.94 | 121.90 |
| 58 | Ba | 49 | C | N1-C2-O2 | 5.11 | 121.96 | 118.90 |
| 22 | AA | 498 | A | C6-C5-N7 | 5.11 | 135.87 | 132.30 |
| 22 | AA | 782 | A | O4'-C1'-N9 | 5.11 | 112.28 | 108.20 |
| 22 | AA | 895 | G | O4'-C1'-N9 | 5.11 | 112.28 | 108.20 |
| 22 | AA | 1210 | C | N3-C4-C5 | 5.11 | 123.94 | 121.90 |
| 22 | AA | 1248 | A | C6-C5-N7 | 5.11 | 135.87 | 132.30 |
| 22 | AA | 1263 | C | N1-C2-O2 | 5.11 | 121.96 | 118.90 |
| 22 | AA | 1405 | G | O4'-C1'-N9 | 5.11 | 112.28 | 108.20 |
| 57 | BA | 7 | G | N1-C6-O6 | -5.11 | 116.84 | 119.90 |
| 57 | BA | 16 | C | N1-C2-O2 | 5.11 | 121.96 | 118.90 |
| 57 | BA | 121 | G | N3-C4-C5 | -5.11 | 126.05 | 128.60 |
| 57 | BA | 234 | U | N3-C2-O2 | -5.11 | 118.62 | 122.20 |
| 57 | BA | 1513 | U | N3-C2-O2 | -5.11 | 118.63 | 122.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 1568 | G | N9-C4-C5 | 5.11 | 107.44 | 105.40 |
| 57 | BA | 1830 | C | N3-C4-C5 | 5.11 | 123.94 | 121.90 |
| 57 | BA | 1887 | C | N1-C2-O2 | 5.11 | 121.96 | 118.90 |
| 57 | BA | 249 | C | N3-C4-C5 | 5.10 | 123.94 | 121.90 |
| 57 | BA | 448 | U | N3-C2-O2 | -5.10 | 118.63 | 122.20 |
| 57 | BA | 2312 | U | O4'-C4'-C3' | 5.10 | 110.18 | 106.10 |
| 57 | BA | 2651 | C | O4'-C1'-N1 | 5.10 | 112.28 | 108.20 |
| 22 | AA | 1265 | C | N1-C2-O2 | 5.10 | 121.96 | 118.90 |
| 57 | BA | 1388 | G | N1-C6-O6 | -5.10 | 116.84 | 119.90 |
| 57 | BA | 1403 | A | C6-C5-N7 | 5.10 | 135.87 | 132.30 |
| 57 | BA | 1888 | G | N3-C4-C5 | -5.10 | 126.05 | 128.60 |
| 57 | BA | 2400 | G | N1-C6-O6 | -5.10 | 116.84 | 119.90 |
| 57 | BA | 2452 | C | N1-C2-O2 | 5.10 | 121.96 | 118.90 |
| 22 | AA | 1098 | C | N1-C2-O2 | 5.10 | 121.96 | 118.90 |
| 47 | B4 | 56 | ARG | NE-CZ-NH1 | 5.10 | 122.85 | 120.30 |
| 57 | BA | 389 | G | N1-C6-O6 | -5.10 | 116.84 | 119.90 |
| 57 | BA | 2294 | G | N1-C6-O6 | -5.10 | 116.84 | 119.90 |
| 58 | Ba | 21 | G | O4'-C1'-N9 | 5.10 | 112.28 | 108.20 |
| 22 | AA | 105 | G | N1-C6-O6 | -5.10 | 116.84 | 119.90 |
| 22 | AA | 1090 | U | N3-C2-O2 | -5.10 | 118.63 | 122.20 |
| 22 | AA | 1535 | C | N1-C2-O2 | 5.10 | 121.96 | 118.90 |
| 22 | AA | 1538 | C | N1-C2-O2 | 5.10 | 121.96 | 118.90 |
| 57 | BA | 825 | A | C6-C5-N7 | 5.10 | 135.87 | 132.30 |
| 57 | BA | 1107 | G | O4'-C1'-N9 | 5.10 | 112.28 | 108.20 |
| 57 | BA | 1552 | A | C4-C5-C6 | -5.10 | 114.45 | 117.00 |
| 57 | BA | 2706 | A | O4'-C1'-N9 | 5.10 | 112.28 | 108.20 |
| 58 | Ba | 114 | C | N1-C2-O2 | 5.10 | 121.96 | 118.90 |
| 22 | AA | 211 | G | N3-C4-C5 | -5.10 | 126.05 | 128.60 |
| 22 | AA | 1118 | U | N1-C2-N3 | 5.10 | 117.96 | 114.90 |
| 24 | A3 | 6 | G | N1-C6-O6 | -5.10 | 116.84 | 119.90 |
| 57 | BA | 407 | G | O4'-C1'-N9 | 5.10 | 112.28 | 108.20 |
| 57 | BA | 2117 | A | O4'-C1'-N9 | 5.10 | 112.28 | 108.20 |
| 57 | BA | 2186 | G | N1-C6-O6 | -5.10 | 116.84 | 119.90 |
| 57 | BA | 2874 | C | N1-C2-O2 | 5.10 | 121.96 | 118.90 |
| 58 | Ba | 35 | C | N1-C2-O2 | 5.10 | 121.96 | 118.90 |
| 5 | AN | 60 | ARG | NE-CZ-NH1 | 5.10 | 122.85 | 120.30 |
| 10 | AS | 54 | ARG | NH1-CZ-NH2 | -5.10 | 113.80 | 119.40 |
| 22 | AA | 936 | C | C2-N3-C4 | -5.10 | 117.35 | 119.90 |
| 57 | BA | 1779 | U | N3-C2-O2 | -5.10 | 118.63 | 122.20 |
| 57 | BA | 2245 | U | N3-C2-O2 | -5.10 | 118.63 | 122.20 |
| 57 | BA | 2310 | C | N1-C2-O2 | 5.10 | 121.96 | 118.90 |
| 22 | AA | 370 | C | N1-C2-O2 | 5.09 | 121.96 | 118.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | AA | 576 | C | N1-C2-O2 | 5.09 | 121.96 | 118.90 |
| 22 | AA | 862 | C | N3-C4-C5 | 5.09 | 123.94 | 121.90 |
| 22 | AA | 1385 | G | N1-C6-O6 | -5.09 | 116.84 | 119.90 |
| 57 | BA | 703 | U | N3-C2-O2 | -5.09 | 118.63 | 122.20 |
| 57 | BA | 962 | G | O4'-C1'-N9 | 5.09 | 112.28 | 108.20 |
| 57 | BA | 1115 | G | N1-C6-O6 | -5.09 | 116.84 | 119.90 |
| 57 | BA | 1188 | U | N3-C2-O2 | -5.09 | 118.63 | 122.20 |
| 57 | BA | 2271 | G | O4'-C1'-N9 | 5.09 | 112.28 | 108.20 |
| 57 | BA | 2581 | G | N3-C4-C5 | -5.09 | 126.05 | 128.60 |
| 57 | BA | 536 | G | O4'-C1'-N9 | 5.09 | 112.27 | 108.20 |
| 57 | BA | 1075 | C | O4'-C1'-N1 | 5.09 | 112.28 | 108.20 |
| 57 | BA | 1271 | G | N1-C6-O6 | -5.09 | 116.84 | 119.90 |
| 57 | BA | 2584 | U | N3-C2-O2 | -5.09 | 118.64 | 122.20 |
| 58 | Ba | 19 | C | O4'-C1'-N1 | 5.09 | 112.27 | 108.20 |
| 58 | Ba | 105 | G | N1-C6-O6 | -5.09 | 116.84 | 119.90 |
| 4 | AM | 112 | ARG | NE-CZ-NH2 | -5.09 | 117.75 | 120.30 |
| 22 | AA | 325 | A | C6-C5-N7 | 5.09 | 135.86 | 132.30 |
| 57 | BA | 334 | C | N1-C2-O2 | 5.09 | 121.95 | 118.90 |
| 57 | BA | 1105 | U | O4'-C1'-N1 | 5.09 | 112.27 | 108.20 |
| 57 | BA | 1176 | U | N3-C2-O2 | -5.09 | 118.64 | 122.20 |
| 57 | BA | 1271 | G | N3-C4-C5 | -5.09 | 126.05 | 128.60 |
| 57 | BA | 1275 | A | C2-N3-C4 | 5.09 | 113.14 | 110.60 |
| 57 | BA | 1958 | C | O4'-C1'-N1 | 5.09 | 112.27 | 108.20 |
| 57 | BA | 2108 | A | C6-C5-N7 | 5.09 | 135.86 | 132.30 |
| 22 | AA | 13 | U | N1-C2-N3 | 5.09 | 117.95 | 114.90 |
| 22 | AA | 501 | C | C5'-C4'-O4' | 5.09 | 115.21 | 109.10 |
| 22 | AA | 976 | G | N1-C6-O6 | -5.09 | 116.85 | 119.90 |
| 22 | AA | 1507 | A | O4'-C1'-N9 | 5.09 | 112.27 | 108.20 |
| 22 | AA | 1522 | U | N3-C2-O2 | -5.09 | 118.64 | 122.20 |
| 57 | BA | 623 | C | O4'-C1'-N1 | 5.09 | 112.27 | 108.20 |
| 57 | BA | 1023 | U | C5-C6-N1 | -5.09 | 120.16 | 122.70 |
| 57 | BA | 1920 | C | O4'-C1'-N1 | 5.09 | 112.27 | 108.20 |
| 57 | BA | 2234 | G | N7-C8-N9 | 5.09 | 115.64 | 113.10 |
| 57 | BA | 2308 | G | N1-C6-O6 | -5.09 | 116.85 | 119.90 |
| 57 | BA | 2323 | G | N1-C6-O6 | -5.09 | 116.85 | 119.90 |
| 57 | BA | 2349 | G | N1-C6-O6 | -5.09 | 116.85 | 119.90 |
| 57 | BA | 2637 | U | N3-C2-O2 | -5.09 | 118.64 | 122.20 |
| 58 | Ba | 46 | A | C6-C5-N7 | 5.09 | 135.86 | 132.30 |
| 20 | AI | 122 | ARG | NE-CZ-NH1 | 5.09 | 122.84 | 120.30 |
| 22 | AA | 378 | G | C5'-C4'-O4' | 5.09 | 115.21 | 109.10 |
| 57 | BA | 897 | C | N3-C4-N4 | -5.09 | 114.44 | 118.00 |
| 57 | BA | 1655 | A | C4-C5-C6 | -5.09 | 114.46 | 117.00 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 2591 | C | N3-C4-C5 | 5.09 | 123.94 | 121.90 |
| 22 | AA | 783 | C | O4'-C1'-N1 | 5.09 | 112.27 | 108.20 |
| 22 | AA | 807 | A | C6-C5-N7 | 5.09 | 135.86 | 132.30 |
| 22 | AA | 1118 | U | C5'-C4'-O4' | 5.09 | 115.20 | 109.10 |
| 57 | BA | 59 | U | N3-C2-O2 | -5.09 | 118.64 | 122.20 |
| 57 | BA | 112 | U | N3-C2-O2 | -5.09 | 118.64 | 122.20 |
| 57 | BA | 306 | U | O4'-C1'-N1 | 5.09 | 112.27 | 108.20 |
| 57 | BA | 1417 | C | N3-C4-N4 | -5.09 | 114.44 | 118.00 |
| 57 | BA | 1646 | C | N1-C2-O2 | 5.09 | 121.95 | 118.90 |
| 57 | BA | 1886 | U | O4'-C1'-N1 | 5.09 | 112.27 | 108.20 |
| 57 | BA | 1967 | C | N1-C2-O2 | 5.09 | 121.95 | 118.90 |
| 57 | BA | 2591 | C | O4'-C1'-N1 | 5.09 | 112.27 | 108.20 |
| 22 | AA | 318 | G | N1-C6-O6 | -5.08 | 116.85 | 119.90 |
| 57 | BA | 1199 | U | C5-C6-N1 | -5.08 | 120.16 | 122.70 |
| 57 | BA | 2201 | G | N1-C6-O6 | -5.08 | 116.85 | 119.90 |
| 57 | BA | 2875 | C | N1-C2-O2 | 5.08 | 121.95 | 118.90 |
| 57 | BA | 199 | A | O3'-P-O5' | -5.08 | 94.34 | 104.00 |
| 57 | BA | 1157 | G | N3-C4-C5 | -5.08 | 126.06 | 128.60 |
| 57 | BA | 1729 | U | N3-C2-O2 | -5.08 | 118.64 | 122.20 |
| 57 | BA | 2509 | G | N1-C6-O6 | -5.08 | 116.85 | 119.90 |
| 57 | BA | 58 | G | N1-C6-O6 | -5.08 | 116.85 | 119.90 |
| 57 | BA | 1005 | C | C5'-C4'-O4' | 5.08 | 115.20 | 109.10 |
| 58 | Ba | 56 | G | N1-C6-O6 | -5.08 | 116.85 | 119.90 |
| 23 | A2 | 52 | U | N3-C2-O2 | -5.08 | 118.64 | 122.20 |
| 57 | BA | 445 | C | N3-C4-N4 | -5.08 | 114.44 | 118.00 |
| 57 | BA | 2143 | C | N1-C2-O2 | 5.08 | 121.95 | 118.90 |
| 22 | AA | 276 | G | N1-C6-O6 | -5.08 | 116.85 | 119.90 |
| 24 | A3 | 3 | C | N1-C2-O2 | 5.08 | 121.95 | 118.90 |
| 33 | BS | 94 | ARG | NH1-CZ-NH2 | -5.08 | 113.81 | 119.40 |
| 57 | BA | 1107 | G | N1-C6-O6 | -5.08 | 116.85 | 119.90 |
| 57 | BA | 1344 | U | N3-C2-O2 | -5.08 | 118.64 | 122.20 |
| 57 | BA | 1581 | G | N1-C6-O6 | -5.08 | 116.85 | 119.90 |
| 57 | BA | 1582 | C | N1-C2-O2 | 5.08 | 121.95 | 118.90 |
| 57 | BA | 1648 | U | C5'-C4'-C3' | -5.08 | 107.87 | 116.00 |
| 57 | BA | 2892 | G | O4'-C1'-N9 | 5.08 | 112.26 | 108.20 |
| 57 | BA | 24 | G | N1-C6-O6 | -5.08 | 116.85 | 119.90 |
| 57 | BA | 109 | C | N1-C2-O2 | 5.08 | 121.95 | 118.90 |
| 57 | BA | 317 | G | N1-C6-O6 | -5.08 | 116.85 | 119.90 |
| 57 | BA | 2880 | C | C5'-C4'-O4' | 5.08 | 115.19 | 109.10 |
| 2 | AK | 126 | ARG | CD-NE-CZ | 5.08 | 130.71 | 123.60 |
| 22 | AA | 564 | C | N1-C2-O2 | 5.08 | 121.94 | 118.90 |
| 57 | BA | 122 | G | N1-C6-O6 | -5.08 | 116.85 | 119.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 505 | A | O4'-C1'-N9 | 5.08 | 112.26 | 108.20 |
| 57 | BA | 1532 | A | C6-C5-N7 | 5.08 | 135.85 | 132.30 |
| 57 | BA | 2001 | C | N3-C4-C5 | 5.08 | 123.93 | 121.90 |
| 57 | BA | 2467 | C | N3-C4-C5 | 5.08 | 123.93 | 121.90 |
| 15 | AD | 80 | ARG | NH1-CZ-NH2 | -5.07 | 113.82 | 119.40 |
| 22 | AA | 150 | U | O4'-C1'-N1 | 5.07 | 112.26 | 108.20 |
| 22 | AA | 805 | C | C5'-C4'-O4' | 5.07 | 115.19 | 109.10 |
| 22 | AA | 839 | C | C3'-C2'-C1' | -5.07 | 97.44 | 101.50 |
| 57 | BA | 192 | C | N3-C2-O2 | -5.07 | 118.35 | 121.90 |
| 57 | BA | 1244 | A | C6-C5-N7 | 5.07 | 135.85 | 132.30 |
| 57 | BA | 2000 | C | N1-C2-O2 | 5.07 | 121.94 | 118.90 |
| 57 | BA | 2249 | U | O4'-C4'-C3' | 5.07 | 110.16 | 106.10 |
| 57 | BA | 2266 | A | C6-C5-N7 | 5.07 | 135.85 | 132.30 |
| 58 | Ba | 43 | C | N1-C2-O2 | 5.07 | 121.94 | 118.90 |
| 22 | AA | 521 | G | O4'-C1'-N9 | 5.07 | 112.26 | 108.20 |
| 57 | BA | 2496 | C | N3-C4-C5 | 5.07 | 123.93 | 121.90 |
| 58 | Ba | 16 | G | N1-C6-O6 | -5.07 | 116.86 | 119.90 |
| 22 | AA | 25 | C | N3-C4-C5 | 5.07 | 123.93 | 121.90 |
| 22 | AA | 377 | G | N1-C6-O6 | -5.07 | 116.86 | 119.90 |
| 22 | AA | 474 | G | O4'-C1'-N9 | 5.07 | 112.26 | 108.20 |
| 22 | AA | 764 | C | N1-C2-O2 | 5.07 | 121.94 | 118.90 |
| 22 | AA | 1343 | G | N1-C6-O6 | -5.07 | 116.86 | 119.90 |
| 22 | AA | 1494 | G | N1-C6-O6 | -5.07 | 116.86 | 119.90 |
| 57 | BA | 999 | U | N1-C2-N3 | 5.07 | 117.94 | 114.90 |
| 57 | BA | 1013 | C | C5'-C4'-C3' | -5.07 | 107.89 | 116.00 |
| 57 | BA | 1304 | A | C6-C5-N7 | 5.07 | 135.85 | 132.30 |
| 57 | BA | 1370 | C | N3-C4-C5 | 5.07 | 123.93 | 121.90 |
| 57 | BA | 1779 | U | O4'-C1'-N1 | 5.07 | 112.26 | 108.20 |
| 57 | BA | 2725 | A | C4-C5-C6 | -5.07 | 114.46 | 117.00 |
| 57 | BA | 2728 | U | N3-C2-O2 | -5.07 | 118.65 | 122.20 |
| 22 | AA | 194 | C | N3-C4-C5 | 5.07 | 123.93 | 121.90 |
| 57 | BA | 100 | U | O4'-C1'-N1 | 5.07 | 112.25 | 108.20 |
| 10 | AS | 31 | ARG | NE-CZ-NH1 | 5.07 | 122.83 | 120.30 |
| 57 | BA | 2394 | C | N1-C2-O2 | 5.07 | 121.94 | 118.90 |
| 57 | BA | 2731 | G | N1-C6-O6 | -5.07 | 116.86 | 119.90 |
| 21 | A1 | 206 | ARG | NE-CZ-NH2 | -5.07 | 117.77 | 120.30 |
| 22 | AA | 662 | U | N3-C2-O2 | -5.07 | 118.65 | 122.20 |
| 22 | AA | 980 | C | N3-C4-C5 | 5.07 | 123.93 | 121.90 |
| 56 | BL | 123 | ARG | NE-CZ-NH2 | -5.07 | 117.77 | 120.30 |
| 57 | BA | 261 | G | N1-C6-O6 | -5.07 | 116.86 | 119.90 |
| 57 | BA | 940 | G | O4'-C1'-N9 | 5.07 | 112.25 | 108.20 |
| 57 | BA | 1058 | U | N3-C2-O2 | -5.07 | 118.65 | 122.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 1752 | C | O4'-C1'-N1 | 5.07 | 112.25 | 108.20 |
| 57 | BA | 2016 | U | N3-C2-O2 | -5.07 | 118.65 | 122.20 |
| 57 | BA | 2373 | G | N1-C6-O6 | -5.07 | 116.86 | 119.90 |
| 24 | A3 | 41 | C | O4'-C1'-N1 | 5.06 | 112.25 | 108.20 |
| 57 | BA | 1437 | C | C3'-C2'-C1' | 5.06 | 105.55 | 101.50 |
| 57 | BA | 1592 | C | N1-C2-O2 | 5.06 | 121.94 | 118.90 |
| 57 | BA | 2613 | U | N3-C2-O2 | -5.06 | 118.66 | 122.20 |
| 22 | AA | 202 | G | C5-C6-N1 | 5.06 | 114.03 | 111.50 |
| 22 | AA | 731 | G | C4'-C3'-C2' | -5.06 | 97.54 | 102.60 |
| 22 | AA | 875 | U | O4'-C1'-N1 | 5.06 | 112.25 | 108.20 |
| 57 | BA | 85 | G | N1-C6-O6 | -5.06 | 116.86 | 119.90 |
| 57 | BA | 325 | G | N1-C6-O6 | -5.06 | 116.86 | 119.90 |
| 57 | BA | 669 | G | N1-C6-O6 | -5.06 | 116.86 | 119.90 |
| 57 | BA | 2199 | A | C5'-C4'-O4' | 5.06 | 115.17 | 109.10 |
| 57 | BA | 2766 | A | C2-N3-C4 | 5.06 | 113.13 | 110.60 |
| 22 | AA | 96 | U | C5-C6-N1 | -5.06 | 120.17 | 122.70 |
| 22 | AA | 722 | G | C5-C6-N1 | 5.06 | 114.03 | 111.50 |
| 22 | AA | 1112 | C | N1-C2-O2 | 5.06 | 121.94 | 118.90 |
| 57 | BA | 190 | A | C4'-C3'-C2' | -5.06 | 97.54 | 102.60 |
| 57 | BA | 1133 | A | C6-C5-N7 | 5.06 | 135.84 | 132.30 |
| 22 | AA | 56 | U | O4'-C1'-N1 | 5.06 | 112.25 | 108.20 |
| 22 | AA | 409 | U | N3-C2-O2 | -5.06 | 118.66 | 122.20 |
| 22 | AA | 443 | C | O4'-C1'-N1 | 5.06 | 112.25 | 108.20 |
| 22 | AA | 1086 | U | N1-C2-N3 | 5.06 | 117.94 | 114.90 |
| 22 | AA | 1319 | A | C4-C5-C6 | -5.06 | 114.47 | 117.00 |
| 57 | BA | 87 | U | O4'-C1'-N1 | 5.06 | 112.25 | 108.20 |
| 57 | BA | 565 | C | N1-C2-O2 | 5.06 | 121.94 | 118.90 |
| 57 | BA | 827 | U | O4'-C1'-N1 | 5.06 | 112.25 | 108.20 |
| 22 | AA | 401 | C | N1-C2-O2 | 5.06 | 121.93 | 118.90 |
| 22 | AA | 911 | U | O4'-C1'-N1 | 5.06 | 112.25 | 108.20 |
| 22 | AA | 1051 | C | N1-C2-O2 | 5.06 | 121.93 | 118.90 |
| 22 | AA | 1434 | A | O4'-C1'-N9 | 5.06 | 112.25 | 108.20 |
| 23 | A2 | 27 | A | C4'-C3'-C2' | -5.06 | 97.54 | 102.60 |
| 49 | B6 | 27 | ARG | NE-CZ-NH1 | 5.06 | 122.83 | 120.30 |
| 57 | BA | 206 | U | N3-C2-O2 | -5.06 | 118.66 | 122.20 |
| 57 | BA | 510 | C | O4'-C1'-N1 | 5.06 | 112.25 | 108.20 |
| 57 | BA | 1209 | U | N3-C2-O2 | -5.06 | 118.66 | 122.20 |
| 57 | BA | 1315 | C | N1-C2-O2 | 5.06 | 121.94 | 118.90 |
| 57 | BA | 1701 | A | O4'-C1'-N9 | 5.06 | 112.25 | 108.20 |
| 57 | BA | 1822 | C | N1-C2-O2 | 5.06 | 121.93 | 118.90 |
| 57 | BA | 2733 | A | C6-C5-N7 | 5.06 | 135.84 | 132.30 |
| 57 | BA | 2792 | A | O4'-C1'-N9 | 5.06 | 112.25 | 108.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|---|---|---|---|---|---|---|---|
| 4 | AM | 56 | ARG | NE-CZ-NH1 | 5.06 | 122.83 | 120.30 |
| 22 | AA | 394 | G | N3-C2-N2 | -5.06 | 116.36 | 119.90 |
| 29 | BO | 71 | ARG | NE-CZ-NH1 | 5.06 | 122.83 | 120.30 |
| 57 | BA | 993 | G | N1-C6-O6 | -5.06 | 116.87 | 119.90 |
| 57 | BA | 2489 | U | C3'-C2'-C1' | 5.06 | 105.55 | 101.50 |
| 22 | AA | 1533 | C | N1-C2-O2 | 5.05 | 121.93 | 118.90 |
| 35 | BD | 12 | ARG | NE-CZ-NH2 | -5.05 | 117.77 | 120.30 |
| 56 | BL | 51 | ARG | NE-CZ-NH1 | 5.05 | 122.83 | 120.30 |
| 57 | BA | 93 | G | N1-C6-O6 | -5.05 | 116.87 | 119.90 |
| 57 | BA | 229 | C | N1-C2-O2 | 5.05 | 121.93 | 118.90 |
| 57 | BA | 318 | C | N1-C2-O2 | 5.05 | 121.93 | 118.90 |
| 57 | BA | 451 | U | N3-C2-O2 | -5.05 | 118.66 | 122.20 |
| 57 | BA | 601 | C | O4'-C1'-N1 | 5.05 | 112.24 | 108.20 |
| 57 | BA | 1489 | C | N3-C4-C5 | 5.05 | 123.92 | 121.90 |
| 57 | BA | 1697 | G | N9-C1'-C2' | -5.05 | 106.44 | 112.00 |
| 57 | BA | 1784 | A | C4-C5-C6 | -5.05 | 114.47 | 117.00 |
| 8 | AQ | 76 | ARG | NE-CZ-NH1 | 5.05 | 122.83 | 120.30 |
| 22 | AA | 107 | G | C5'-C4'-O4' | 5.05 | 115.16 | 109.10 |
| 22 | AA | 1415 | G | N1-C6-O6 | -5.05 | 116.87 | 119.90 |
| 57 | BA | 678 | C | O4'-C1'-N1 | 5.05 | 112.24 | 108.20 |
| 57 | BA | 1887 | C | O4'-C1'-N1 | 5.05 | 112.24 | 108.20 |
| 22 | AA | 205 | A | C3'-C2'-C1' | 5.05 | 105.54 | 101.50 |
| 22 | AA | 445 | G | N1-C6-O6 | -5.05 | 116.87 | 119.90 |
| 22 | AA | 666 | G | N3-C2-N2 | -5.05 | 116.36 | 119.90 |
| 22 | AA | 1118 | U | N3-C2-O2 | -5.05 | 118.66 | 122.20 |
| 22 | AA | 1336 | C | N1-C2-O2 | 5.05 | 121.93 | 118.90 |
| 24 | A3 | 69 | C | O4'-C1'-N1 | 5.05 | 112.24 | 108.20 |
| 57 | BA | 559 | G | C5-C6-N1 | 5.05 | 114.03 | 111.50 |
| 57 | BA | 688 | U | C5-C6-N1 | -5.05 | 120.17 | 122.70 |
| 57 | BA | 2275 | C | N1-C2-O2 | 5.05 | 121.93 | 118.90 |
| 57 | BA | 2603 | G | N9-C4-C5 | 5.05 | 107.42 | 105.40 |
| 57 | BA | 2696 | U | N3-C2-O2 | -5.05 | 118.66 | 122.20 |
| 57 | BA | 2874 | C | C3'-C2'-C1' | 5.05 | 105.54 | 101.50 |
| 58 | Ba | 47 | C | O4'-C1'-N1 | 5.05 | 112.24 | 108.20 |
| 22 | AA | 671 | G | N1-C6-O6 | -5.05 | 116.87 | 119.90 |
| 22 | AA | 941 | G | N1-C6-O6 | -5.05 | 116.87 | 119.90 |
| 22 | AA | 1028 | C | O4'-C1'-N1 | 5.05 | 112.24 | 108.20 |
| 22 | AA | 1468 | A | C4-C5-C6 | -5.05 | 114.47 | 117.00 |
| 57 | BA | 87 | U | C3'-C2'-C1' | 5.05 | 105.54 | 101.50 |
| 57 | BA | 119 | A | C6-C5-N7 | 5.05 | 135.83 | 132.30 |
| 57 | BA | 719 | C | O4'-C1'-N1 | 5.05 | 112.24 | 108.20 |
| 57 | BA | 1087 | G | N1-C6-O6 | -5.05 | 116.87 | 119.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 2089 | C | N3-C4-C5 | 5.05 | 123.92 | 121.90 |
| 22 | AA | 445 | G | O4'-C1'-N9 | 5.05 | 112.24 | 108.20 |
| 22 | AA | 924 | C | N1-C2-O2 | 5.05 | 121.93 | 118.90 |
| 22 | AA | 940 | C | O4'-C1'-N1 | 5.05 | 112.24 | 108.20 |
| 22 | AA | 1300 | G | O4'-C1'-N9 | 5.05 | 112.24 | 108.20 |
| 57 | BA | 409 | G | C4'-C3'-C2' | -5.05 | 97.55 | 102.60 |
| 57 | BA | 1691 | C | N1-C2-O2 | 5.05 | 121.93 | 118.90 |
| 57 | BA | 2667 | C | N1-C2-O2 | 5.05 | 121.93 | 118.90 |
| 22 | AA | 117 | G | C5-C6-N1 | 5.05 | 114.02 | 111.50 |
| 22 | AA | 248 | C | N1-C2-O2 | 5.05 | 121.93 | 118.90 |
| 22 | AA | 358 | U | N3-C2-O2 | -5.05 | 118.67 | 122.20 |
| 22 | AA | 670 | G | N1-C6-O6 | -5.05 | 116.87 | 119.90 |
| 22 | AA | 731 | G | N1-C6-O6 | -5.05 | 116.87 | 119.90 |
| 22 | AA | 952 | U | C5'-C4'-O4' | 5.05 | 115.16 | 109.10 |
| 22 | AA | 1447 | A | O4'-C1'-N9 | 5.05 | 112.24 | 108.20 |
| 22 | AA | 1527 | U | O4'-C1'-N1 | 5.05 | 112.24 | 108.20 |
| 37 | BV | 21 | ARG | NE-CZ-NH2 | 5.05 | 122.82 | 120.30 |
| 57 | BA | 301 | G | C4'-C3'-C2' | -5.05 | 97.55 | 102.60 |
| 57 | BA | 772 | C | O4'-C1'-N1 | 5.05 | 112.24 | 108.20 |
| 57 | BA | 1728 | C | N1-C2-O2 | 5.05 | 121.93 | 118.90 |
| 57 | BA | 1893 | C | N1-C2-O2 | 5.05 | 121.93 | 118.90 |
| 57 | BA | 2283 | C | N3-C4-N4 | -5.05 | 114.47 | 118.00 |
| 57 | BA | 2375 | G | N1-C6-O6 | -5.05 | 116.87 | 119.90 |
| 22 | AA | 186 | C | N1-C2-O2 | 5.04 | 121.93 | 118.90 |
| 22 | AA | 985 | C | N1-C2-O2 | 5.04 | 121.93 | 118.90 |
| 57 | BA | 1099 | G | N1-C6-O6 | -5.04 | 116.87 | 119.90 |
| 57 | BA | 1102 | C | N1-C2-O2 | 5.04 | 121.93 | 118.90 |
| 22 | AA | 186 | C | O4'-C1'-N1 | 5.04 | 112.23 | 108.20 |
| 22 | AA | 277 | C | N1-C2-O2 | 5.04 | 121.93 | 118.90 |
| 22 | AA | 1071 | C | N1-C2-O2 | 5.04 | 121.93 | 118.90 |
| 22 | AA | 1330 | U | N3-C2-O2 | -5.04 | 118.67 | 122.20 |
| 57 | BA | 147 | C | O4'-C1'-N1 | 5.04 | 112.23 | 108.20 |
| 57 | BA | 611 | C | O4'-C1'-N1 | 5.04 | 112.23 | 108.20 |
| 57 | BA | 1841 | U | N3-C2-O2 | -5.04 | 118.67 | 122.20 |
| 57 | BA | 1851 | U | N3-C2-O2 | -5.04 | 118.67 | 122.20 |
| 57 | BA | 2750 | A | C6-C5-N7 | 5.04 | 135.83 | 132.30 |
| 22 | AA | 15 | G | N1-C6-O6 | -5.04 | 116.88 | 119.90 |
| 22 | AA | 233 | C | N1-C2-O2 | 5.04 | 121.92 | 118.90 |
| 57 | BA | 243 | U | O4'-C1'-N1 | 5.04 | 112.23 | 108.20 |
| 57 | BA | 287 | G | N1-C6-O6 | -5.04 | 116.88 | 119.90 |
| 57 | BA | 347 | A | O4'-C1'-N9 | 5.04 | 112.23 | 108.20 |
| 57 | BA | 1589 | U | O4'-C1'-N1 | 5.04 | 112.23 | 108.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 1965 | C | N3-C4-C5 | 5.04 | 123.92 | 121.90 |
| 57 | BA | 2439 | A | C2-N3-C4 | 5.04 | 113.12 | 110.60 |
| 57 | BA | 2703 | C | O4'-C1'-N1 | 5.04 | 112.23 | 108.20 |
| 57 | BA | 1531 | C | O4'-C1'-N1 | 5.04 | 112.23 | 108.20 |
| 57 | BA | 2491 | U | O4'-C1'-N1 | 5.04 | 112.23 | 108.20 |
| 57 | BA | 2731 | G | C5'-C4'-C3' | -5.04 | 107.94 | 116.00 |
| 58 | Ba | 10 | G | O4'-C4'-C3' | 5.04 | 110.13 | 106.10 |
| 58 | Ba | 31 | C | O4'-C1'-N1 | 5.04 | 112.23 | 108.20 |
| 17 | AF | 110 | ARG | NE-CZ-NH1 | 5.04 | 122.82 | 120.30 |
| 22 | AA | 271 | C | O4'-C1'-N1 | 5.04 | 112.23 | 108.20 |
| 57 | BA | 339 | U | O4'-C1'-N1 | 5.04 | 112.23 | 108.20 |
| 57 | BA | 816 | C | C5'-C4'-C3' | -5.04 | 107.94 | 116.00 |
| 57 | BA | 2480 | C | N3-C4-N4 | -5.04 | 114.47 | 118.00 |
| 57 | BA | 2736 | A | C6-C5-N7 | 5.04 | 135.83 | 132.30 |
| 58 | Ba | 28 | C | O4'-C1'-N1 | 5.04 | 112.23 | 108.20 |
| 22 | AA | 768 | A | O4'-C1'-N9 | 5.04 | 112.23 | 108.20 |
| 57 | BA | 2270 | A | C6-C5-N7 | 5.04 | 135.83 | 132.30 |
| 57 | BA | 2675 | A | C6-C5-N7 | 5.04 | 135.83 | 132.30 |
| 22 | AA | 406 | G | N3-C4-C5 | -5.04 | 126.08 | 128.60 |
| 22 | AA | 460 | A | C6-C5-N7 | 5.04 | 135.83 | 132.30 |
| 22 | AA | 544 | G | N1-C6-O6 | -5.04 | 116.88 | 119.90 |
| 22 | AA | 550 | G | N1-C6-O6 | -5.04 | 116.88 | 119.90 |
| 22 | AA | 1273 | C | O4'-C1'-N1 | 5.04 | 112.23 | 108.20 |
| 57 | BA | 241 | A | O4'-C1'-N9 | 5.04 | 112.23 | 108.20 |
| 57 | BA | 997 | G | N1-C6-O6 | -5.04 | 116.88 | 119.90 |
| 57 | BA | 1195 | G | O4'-C1'-N9 | 5.04 | 112.23 | 108.20 |
| 57 | BA | 2824 | C | N3-C4-C5 | 5.04 | 123.91 | 121.90 |
| 58 | Ba | 64 | G | N1-C6-O6 | -5.04 | 116.88 | 119.90 |
| 22 | AA | 224 | U | O4'-C1'-N1 | 5.03 | 112.23 | 108.20 |
| 22 | AA | 1067 | A | C6-C5-N7 | 5.03 | 135.82 | 132.30 |
| 22 | AA | 1102 | A | C4-C5-C6 | -5.03 | 114.48 | 117.00 |
| 57 | BA | 588 | U | N3-C2-O2 | -5.03 | 118.68 | 122.20 |
| 57 | BA | 1277 | G | O4'-C1'-N9 | 5.03 | 112.23 | 108.20 |
| 57 | BA | 1971 | U | O4'-C1'-N1 | 5.03 | 112.23 | 108.20 |
| 22 | AA | 1038 | C | O4'-C1'-N1 | 5.03 | 112.23 | 108.20 |
| 22 | AA | 1481 | U | N1-C2-N3 | 5.03 | 117.92 | 114.90 |
| 57 | BA | 66 | C | N3-C4-N4 | -5.03 | 114.48 | 118.00 |
| 57 | BA | 767 | U | O4'-C1'-N1 | 5.03 | 112.22 | 108.20 |
| 57 | BA | 1566 | A | C6-C5-N7 | 5.03 | 135.82 | 132.30 |
| 57 | BA | 2007 | U | N3-C2-O2 | -5.03 | 118.68 | 122.20 |
| 57 | BA | 916 | G | N7-C8-N9 | 5.03 | 115.61 | 113.10 |
| 57 | BA | 926 | G | N1-C6-O6 | -5.03 | 116.88 | 119.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 1578 | U | N1-C2-N3 | 5.03 | 117.92 | 114.90 |
| 57 | BA | 1818 | U | C5-C6-N1 | -5.03 | 120.19 | 122.70 |
| 57 | BA | 2717 | C | N3-C4-C5 | 5.03 | 123.91 | 121.90 |
| 22 | AA | 290 | C | O4'-C1'-N1 | 5.03 | 112.22 | 108.20 |
| 57 | BA | 1159 | U | N3-C2-O2 | -5.03 | 118.68 | 122.20 |
| 57 | BA | 1822 | C | O4'-C1'-N1 | 5.03 | 112.22 | 108.20 |
| 57 | BA | 1974 | C | O4'-C1'-N1 | 5.03 | 112.22 | 108.20 |
| 22 | AA | 496 | A | C5'-C4'-O4' | 5.03 | 115.13 | 109.10 |
| 25 | BC | 122 | ARG | NE-CZ-NH1 | 5.03 | 122.81 | 120.30 |
| 56 | BL | 116 | ARG | NE-CZ-NH2 | -5.03 | 117.79 | 120.30 |
| 57 | BA | 310 | A | C5'-C4'-C3' | -5.03 | 107.95 | 116.00 |
| 57 | BA | 376 | G | N1-C6-O6 | -5.03 | 116.88 | 119.90 |
| 57 | BA | 396 | G | N3-C4-C5 | -5.03 | 126.09 | 128.60 |
| 57 | BA | 897 | C | N3-C4-C5 | 5.03 | 123.91 | 121.90 |
| 57 | BA | 1774 | C | N1-C2-O2 | 5.03 | 121.92 | 118.90 |
| 22 | AA | 79 | G | N1-C6-O6 | -5.03 | 116.89 | 119.90 |
| 22 | AA | 518 | C | N1-C2-O2 | 5.03 | 121.92 | 118.90 |
| 22 | AA | 1211 | U | N3-C2-O2 | -5.03 | 118.68 | 122.20 |
| 22 | AA | 1312 | G | N9-C4-C5 | 5.03 | 107.41 | 105.40 |
| 57 | BA | 156 | A | O4'-C1'-N9 | 5.03 | 112.22 | 108.20 |
| 57 | BA | 1473 | G | N1-C6-O6 | -5.03 | 116.88 | 119.90 |
| 57 | BA | 1645 | G | O4'-C1'-N9 | 5.03 | 112.22 | 108.20 |
| 57 | BA | 1650 | A | C6-C5-N7 | 5.03 | 135.82 | 132.30 |
| 57 | BA | 2856 | A | C6-C5-N7 | 5.03 | 135.82 | 132.30 |
| 58 | Ba | 10 | G | N1-C6-O6 | -5.03 | 116.89 | 119.90 |
| 22 | AA | 359 | G | N1-C6-O6 | -5.02 | 116.89 | 119.90 |
| 22 | AA | 811 | C | O4'-C1'-N1 | 5.02 | 112.22 | 108.20 |
| 22 | AA | 836 | G | N1-C6-O6 | -5.02 | 116.89 | 119.90 |
| 57 | BA | 1243 | C | N1-C2-O2 | 5.02 | 121.92 | 118.90 |
| 57 | BA | 1313 | U | O4'-C1'-N1 | 5.02 | 112.22 | 108.20 |
| 57 | BA | 1607 | C | N1-C2-O2 | 5.02 | 121.92 | 118.90 |
| 22 | AA | 792 | A | C1'-O4'-C4' | -5.02 | 105.88 | 109.90 |
| 22 | AA | 1053 | G | O4'-C1'-N9 | 5.02 | 112.22 | 108.20 |
| 22 | AA | 1074 | G | C5'-C4'-C3' | -5.02 | 107.97 | 116.00 |
| 29 | BO | 78 | ARG | NE-CZ-NH2 | -5.02 | 117.79 | 120.30 |
| 35 | BD | 132 | ARG | NE-CZ-NH1 | 5.02 | 122.81 | 120.30 |
| 57 | BA | 52 | A | C4-C5-C6 | -5.02 | 114.49 | 117.00 |
| 57 | BA | 631 | A | C6-C5-N7 | 5.02 | 135.81 | 132.30 |
| 57 | BA | 1244 | A | O4'-C1'-N9 | 5.02 | 112.22 | 108.20 |
| 57 | BA | 1251 | C | N1-C2-O2 | 5.02 | 121.91 | 118.90 |
| 57 | BA | 1508 | A | C1'-O4'-C4' | -5.02 | 105.88 | 109.90 |
| 57 | BA | 2216 | G | N1-C6-O6 | -5.02 | 116.89 | 119.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 2644 | G | N1-C6-O6 | -5.02 | 116.89 | 119.90 |
| 22 | AA | 1107 | C | N1-C2-O2 | 5.02 | 121.91 | 118.90 |
| 57 | BA | 1669 | A | C4-C5-C6 | -5.02 | 114.49 | 117.00 |
| 57 | BA | 2233 | U | N3-C2-O2 | -5.02 | 118.69 | 122.20 |
| 22 | AA | 56 | U | N1-C2-N3 | 5.02 | 117.91 | 114.90 |
| 22 | AA | 455 | G | N1-C6-O6 | -5.02 | 116.89 | 119.90 |
| 22 | AA | 945 | G | C5-C6-N1 | 5.02 | 114.01 | 111.50 |
| 57 | BA | 480 | A | C5'-C4'-O4' | 5.02 | 115.12 | 109.10 |
| 57 | BA | 888 | C | N1-C2-O2 | 5.02 | 121.91 | 118.90 |
| 57 | BA | 1901 | A | C6-C5-N7 | 5.02 | 135.81 | 132.30 |
| 57 | BA | 2061 | G | N3-C4-C5 | -5.02 | 126.09 | 128.60 |
| 57 | BA | 2471 | A | C6-C5-N7 | 5.02 | 135.81 | 132.30 |
| 57 | BA | 2681 | C | N1-C2-O2 | 5.02 | 121.91 | 118.90 |
| 57 | BA | 2880 | C | C6-N1-C2 | -5.02 | 118.29 | 120.30 |
| 3 | AL | 11 | ARG | NE-CZ-NH2 | -5.02 | 117.79 | 120.30 |
| 22 | AA | 191 | G | N1-C6-O6 | -5.02 | 116.89 | 119.90 |
| 22 | AA | 1384 | C | N3-C4-C5 | 5.02 | 123.91 | 121.90 |
| 57 | BA | 294 | A | C6-C5-N7 | 5.02 | 135.81 | 132.30 |
| 57 | BA | 544 | C | N3-C4-C5 | 5.02 | 123.91 | 121.90 |
| 57 | BA | 1021 | A | C5'-C4'-C3' | -5.02 | 107.97 | 116.00 |
| 57 | BA | 1435 | G | N1-C6-O6 | -5.02 | 116.89 | 119.90 |
| 57 | BA | 1824 | G | N1-C6-O6 | -5.02 | 116.89 | 119.90 |
| 14 | AC | 142 | ARG | NE-CZ-NH1 | 5.02 | 122.81 | 120.30 |
| 22 | AA | 257 | G | N1-C6-O6 | -5.02 | 116.89 | 119.90 |
| 22 | AA | 414 | A | C6-C5-N7 | 5.02 | 135.81 | 132.30 |
| 57 | BA | 2562 | U | N3-C2-O2 | -5.02 | 118.69 | 122.20 |
| 4 | AM | 78 | ARG | NH1-CZ-NH2 | -5.01 | 113.88 | 119.40 |
| 22 | AA | 64 | G | N1-C6-O6 | -5.01 | 116.89 | 119.90 |
| 22 | AA | 641 | U | O4'-C4'-C3' | 5.01 | 110.11 | 106.10 |
| 28 | BN | 34 | ARG | NE-CZ-NH1 | 5.01 | 122.81 | 120.30 |
| 57 | BA | 855 | G | O4'-C1'-N9 | 5.01 | 112.21 | 108.20 |
| 57 | BA | 1055 | G | N1-C6-O6 | -5.01 | 116.89 | 119.90 |
| 57 | BA | 1078 | U | O4'-C4'-C3' | 5.01 | 110.11 | 106.10 |
| 57 | BA | 1363 | C | N3-C4-C5 | 5.01 | 123.91 | 121.90 |
| 57 | BA | 1808 | A | C3'-C2'-C1' | 5.01 | 105.51 | 101.50 |
| 57 | BA | 1826 | G | N1-C6-O6 | -5.01 | 116.89 | 119.90 |
| 57 | BA | 1836 | C | N1-C2-O2 | 5.01 | 121.91 | 118.90 |
| 57 | BA | 2025 | C | O4'-C1'-N1 | 5.01 | 112.21 | 108.20 |
| 57 | BA | 2087 | G | N1-C6-O6 | -5.01 | 116.89 | 119.90 |
| 57 | BA | 2188 | U | N3-C2-O2 | -5.01 | 118.69 | 122.20 |
| 57 | BA | 2792 | A | C6-C5-N7 | 5.01 | 135.81 | 132.30 |
| 22 | AA | 490 | C | N1-C2-O2 | 5.01 | 121.91 | 118.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | AA | 812 | G | N1-C6-O6 | -5.01 | 116.89 | 119.90 |
| 30 | BP | 59 | ARG | NE-CZ-NH2 | 5.01 | 122.81 | 120.30 |
| 57 | BA | 858 | G | C1'-O4'-C4' | -5.01 | 105.89 | 109.90 |
| 57 | BA | 1567 | G | N1-C6-O6 | -5.01 | 116.89 | 119.90 |
| 22 | AA | 309 | A | N9-C1'-C2' | -5.01 | 106.49 | 112.00 |
| 22 | AA | 311 | C | N3-C4-C5 | 5.01 | 123.90 | 121.90 |
| 22 | AA | 805 | C | N1-C2-O2 | 5.01 | 121.91 | 118.90 |
| 22 | AA | 1297 | G | O4'-C1'-N9 | 5.01 | 112.21 | 108.20 |
| 22 | AA | 1459 | G | N1-C6-O6 | -5.01 | 116.89 | 119.90 |
| 24 | A3 | 19 | G | N1-C6-O6 | -5.01 | 116.89 | 119.90 |
| 33 | BS | 13 | ARG | NE-CZ-NH2 | 5.01 | 122.81 | 120.30 |
| 57 | BA | 38 | A | O4'-C1'-N9 | 5.01 | 112.21 | 108.20 |
| 57 | BA | 1463 | C | N1-C2-O2 | 5.01 | 121.91 | 118.90 |
| 57 | BA | 2264 | C | O4'-C1'-N1 | 5.01 | 112.21 | 108.20 |
| 57 | BA | 2653 | U | N1-C2-N3 | 5.01 | 117.91 | 114.90 |
| 57 | BA | 2761 | A | O4'-C1'-N9 | 5.01 | 112.21 | 108.20 |
| 22 | AA | 102 | G | N1-C6-O6 | -5.01 | 116.89 | 119.90 |
| 22 | AA | 352 | C | N3-C4-C5 | 5.01 | 123.90 | 121.90 |
| 57 | BA | 1711 | A | C6-C5-N7 | 5.01 | 135.81 | 132.30 |
| 57 | BA | 2304 | G | N1-C6-O6 | -5.01 | 116.89 | 119.90 |
| 57 | BA | 2765 | A | C1'-O4'-C4' | -5.01 | 105.89 | 109.90 |
| 22 | AA | 110 | C | N3-C4-C5 | 5.01 | 123.90 | 121.90 |
| 22 | AA | 1441 | A | C6-C5-N7 | 5.01 | 135.81 | 132.30 |
| 57 | BA | 754 | U | C5'-C4'-O4' | 5.01 | 115.11 | 109.10 |
| 57 | BA | 964 | C | O4'-C1'-N1 | 5.01 | 112.20 | 108.20 |
| 57 | BA | 1411 | U | O4'-C1'-N1 | 5.01 | 112.21 | 108.20 |
| 57 | BA | 1610 | A | O4'-C1'-N9 | 5.01 | 112.21 | 108.20 |
| 57 | BA | 1685 | C | N1-C2-O2 | 5.01 | 121.90 | 118.90 |
| 57 | BA | 1786 | A | C1'-O4'-C4' | -5.01 | 105.89 | 109.90 |
| 57 | BA | 1811 | G | N1-C6-O6 | -5.01 | 116.90 | 119.90 |
| 4 | AM | 100 | ARG | NH1-CZ-NH2 | -5.00 | 113.89 | 119.40 |
| 22 | AA | 532 | A | C4-C5-C6 | -5.00 | 114.50 | 117.00 |
| 57 | BA | 2035 | G | N1-C6-O6 | -5.00 | 116.90 | 119.90 |
| 58 | Ba | 79 | G | N1-C6-O6 | -5.00 | 116.90 | 119.90 |
| 22 | AA | 1353 | G | O4'-C1'-N9 | 5.00 | 112.20 | 108.20 |
| 57 | BA | 341 | C | O4'-C1'-N1 | 5.00 | 112.20 | 108.20 |
| 57 | BA | 346 | A | C1'-O4'-C4' | -5.00 | 105.90 | 109.90 |
| 57 | BA | 554 | U | N3-C2-O2 | -5.00 | 118.70 | 122.20 |
| 57 | BA | 605 | G | C5'-C4'-O4' | 5.00 | 115.10 | 109.10 |
| 57 | BA | 1118 | C | O4'-C1'-N1 | 5.00 | 112.20 | 108.20 |
| 57 | BA | 1136 | G | C5'-C4'-O4' | 5.00 | 115.10 | 109.10 |
| 58 | Ba | 100 | G | N1-C6-O6 | -5.00 | 116.90 | 119.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | AA | 368 | U | N1-C2-N3 | 5.00 | 117.90 | 114.90 |
| 22 | AA | 380 | G | O4'-C1'-N9 | 5.00 | 112.20 | 108.20 |
| 22 | AA | 429 | U | N3-C2-O2 | -5.00 | 118.70 | 122.20 |
| 22 | AA | 500 | G | C5'-C4'-O4' | 5.00 | 115.10 | 109.10 |
| 22 | AA | 859 | G | N1-C6-O6 | -5.00 | 116.90 | 119.90 |
| 22 | AA | 1401 | G | N3-C4-C5 | -5.00 | 126.10 | 128.60 |
| 23 | A2 | 40 | G | N1-C6-O6 | -5.00 | 116.90 | 119.90 |
| 57 | BA | 442 | G | N1-C6-O6 | -5.00 | 116.90 | 119.90 |
| 57 | BA | 1623 | G | N1-C6-O6 | -5.00 | 116.90 | 119.90 |
| 57 | BA | 2352 | A | C4-C5-C6 | -5.00 | 114.50 | 117.00 |
| 57 | BA | 2683 | C | N3-C4-C5 | 5.00 | 123.90 | 121.90 |

There are no chirality outliers.

All (1070) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 21 | A1 | 289 | ILE | Peptide |
| 21 | A1 | 374 | LEU | Peptide |
| 23 | A2 | 23 | C | Sidechain |
| 23 | A2 | 34 | U | Sidechain |
| 23 | A2 | 39 | U | Sidechain |
| 23 | A2 | 44 | U | Sidechain |
| 23 | A2 | 45 | G | Sidechain |
| 24 | A3 | 1 | C | Sidechain |
| 24 | A3 | 14 | A | Sidechain |
| 24 | A3 | 15 | G | Sidechain |
| 24 | A3 | 20 | G | Sidechain |
| 24 | A3 | 23 | G | Sidechain |
| 24 | A3 | 28 | U | Sidechain |
| 24 | A3 | 30 | G | Sidechain |
| 24 | A3 | 40 | C | Sidechain |
| 24 | A3 | 46 | G | Sidechain |
| 24 | A3 | 47 | A | Sidechain |
| 24 | A3 | 60 | A | Sidechain |
| 24 | A3 | 64 | G | Sidechain |
| 24 | A3 | 65 | G | Sidechain |
| 24 | A3 | 69 | C | Sidechain |
| 24 | A3 | 7 | G | Sidechain |
| 22 | AA | 100 | G | Sidechain |
| 22 | AA | 1008 | U | Sidechain |
| 22 | AA | 1010 | U | Sidechain |
| 22 | AA | 1013 | G | Sidechain |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 22 | AA | 1016 | A | Sidechain |
| 22 | AA | 1026 | G | Sidechain |
| 22 | AA | 1027 | C | Sidechain |
| 22 | AA | 1028 | C | Sidechain |
| 22 | AA | 1030 | U | Sidechain |
| 22 | AA | 1032 | G | Sidechain |
| 22 | AA | 1051 | C | Sidechain |
| 22 | AA | 1054 | C | Sidechain |
| 22 | AA | 1067 | A | Sidechain |
| 22 | AA | 1071 | C | Sidechain |
| 22 | AA | 1072 | G | Sidechain |
| 22 | AA | 1077 | G | Sidechain |
| 22 | AA | 1080 | A | Sidechain |
| 22 | AA | 1082 | A | Sidechain |
| 22 | AA | 1084 | G | Sidechain |
| 22 | AA | 1087 | G | Sidechain |
| 22 | AA | 1093 | A | Sidechain |
| 22 | AA | 1094 | G | Sidechain |
| 22 | AA | 1095 | U | Sidechain |
| 22 | AA | 1099 | G | Sidechain |
| 22 | AA | 110 | C | Sidechain |
| 22 | AA | 1100 | C | Sidechain |
| 22 | AA | 1101 | A | Sidechain |
| 22 | AA | 1109 | C | Sidechain |
| 22 | AA | 1111 | A | Sidechain |
| 22 | AA | 1112 | C | Sidechain |
| 22 | AA | 1114 | C | Sidechain |
| 22 | AA | 1115 | U | Sidechain |
| 22 | AA | 1117 | A | Sidechain |
| 22 | AA | 1118 | U | Sidechain |
| 22 | AA | 1120 | C | Sidechain |
| 22 | AA | 1122 | U | Sidechain |
| 22 | AA | 1131 | G | Sidechain |
| 22 | AA | 1139 | G | Sidechain |
| 22 | AA | 1142 | G | Sidechain |
| 22 | AA | 1148 | U | Sidechain |
| 22 | AA | 1149 | C | Sidechain |
| 22 | AA | 1153 | G | Sidechain |
| 22 | AA | 1155 | A | Sidechain |
| 22 | AA | 1157 | A | Sidechain |
| 22 | AA | 1160 | G | Sidechain |
| 22 | AA | 1169 | A | Sidechain |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 22 | AA | 117 | G | Sidechain |
| 22 | AA | 1170 | A | Sidechain |
| 22 | AA | 1176 | A | Sidechain |
| 22 | AA | 1178 | G | Sidechain |
| 22 | AA | 1179 | A | Sidechain |
| 22 | AA | 119 | A | Sidechain |
| 22 | AA | 1191 | A | Sidechain |
| 22 | AA | 1195 | C | Sidechain |
| 22 | AA | 1209 | C | Sidechain |
| 22 | AA | 121 | U | Sidechain |
| 22 | AA | 1213 | A | Sidechain |
| 22 | AA | 1225 | A | Sidechain |
| 22 | AA | 1226 | C | Sidechain |
| 22 | AA | 1233 | G | Sidechain |
| 22 | AA | 1234 | C | Sidechain |
| 22 | AA | 1240 | U | Sidechain |
| 22 | AA | 1250 | A | Sidechain |
| 22 | AA | 1251 | A | Sidechain |
| 22 | AA | 1264 | U | Sidechain |
| 22 | AA | 1266 | G | Sidechain |
| 22 | AA | 1267 | C | Sidechain |
| 22 | AA | 1269 | A | Sidechain |
| 22 | AA | 1278 | G | Sidechain |
| 22 | AA | 128 | G | Sidechain |
| 22 | AA | 1282 | C | Sidechain |
| 22 | AA | 1287 | A | Sidechain |
| 22 | AA | 1289 | A | Sidechain |
| 22 | AA | 1296 | C | Sidechain |
| 22 | AA | 1297 | G | Sidechain |
| 22 | AA | 1298 | U | Sidechain |
| 22 | AA | 1299 | A | Sidechain |
| 22 | AA | 130 | A | Sidechain |
| 22 | AA | 1300 | G | Sidechain |
| 22 | AA | 1303 | C | Sidechain |
| 22 | AA | 1304 | G | Sidechain |
| 22 | AA | 1305 | G | Sidechain |
| 22 | AA | 1306 | A | Sidechain |
| 22 | AA | 1308 | U | Sidechain |
| 22 | AA | 1316 | G | Sidechain |
| 22 | AA | 1317 | C | Sidechain |
| 22 | AA | 1319 | A | Sidechain |
| 22 | AA | 1326 | U | Sidechain |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 22 | AA | 1330 | U | Sidechain |
| 22 | AA | 1343 | G | Sidechain |
| 22 | AA | 1345 | U | Sidechain |
| 22 | AA | 1349 | A | Sidechain |
| 22 | AA | 1357 | A | Sidechain |
| 22 | AA | 1358 | U | Sidechain |
| 22 | AA | 1360 | A | Sidechain |
| 22 | AA | 1361 | G | Sidechain |
| 22 | AA | 1362 | A | Sidechain |
| 22 | AA | 1363 | A | Sidechain |
| 22 | AA | 1366 | C | Sidechain |
| 22 | AA | 1373 | G | Sidechain |
| 22 | AA | 1374 | A | Sidechain |
| 22 | AA | 1380 | U | Sidechain |
| 22 | AA | 1382 | C | Sidechain |
| 22 | AA | 1392 | G | Sidechain |
| 22 | AA | 1394 | A | Sidechain |
| 22 | AA | 1396 | A | Sidechain |
| 22 | AA | 1400 | C | Sidechain |
| 22 | AA | 1401 | G | Sidechain |
| 22 | AA | 1411 | C | Sidechain |
| 22 | AA | 1419 | G | Sidechain |
| 22 | AA | 1426 | G | Sidechain |
| 22 | AA | 143 | A | Sidechain |
| 22 | AA | 1430 | A | Sidechain |
| 22 | AA | 1432 | G | Sidechain |
| 22 | AA | 1433 | A | Sidechain |
| 22 | AA | 1447 | A | Sidechain |
| 22 | AA | 1448 | C | Sidechain |
| 22 | AA | 1449 | C | Sidechain |
| 22 | AA | 1451 | U | Sidechain |
| 22 | AA | 1453 | G | Sidechain |
| 22 | AA | 1468 | A | Sidechain |
| 22 | AA | 1477 | U | Sidechain |
| 22 | AA | 1489 | G | Sidechain |
| 22 | AA | 149 | A | Sidechain |
| 22 | AA | 1490 | U | Sidechain |
| 22 | AA | 1502 | A | Sidechain |
| 22 | AA | 1503 | A | Sidechain |
| 22 | AA | 1506 | U | Sidechain |
| 22 | AA | 1512 | U | Sidechain |
| 22 | AA | 1513 | A | Sidechain |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 22 | AA | 1517 | G | Sidechain |
| 22 | AA | 1528 | U | Sidechain |
| 22 | AA | 153 | C | Sidechain |
| 22 | AA | 1535 | C | Sidechain |
| 22 | AA | 1537 | U | Sidechain |
| 22 | AA | 1542 | A | Sidechain |
| 22 | AA | 158 | G | Sidechain |
| 22 | AA | 159 | G | Sidechain |
| 22 | AA | 161 | A | Sidechain |
| 22 | AA | 173 | U | Sidechain |
| 22 | AA | 179 | A | Sidechain |
| 22 | AA | 182 | A | Sidechain |
| 22 | AA | 184 | G | Sidechain |
| 22 | AA | 187 | G | Sidechain |
| 22 | AA | 188 | C | Sidechain |
| 22 | AA | 2 | A | Sidechain |
| 22 | AA | 201 | G | Sidechain |
| 22 | AA | 202 | G | Sidechain |
| 22 | AA | 205 | A | Sidechain |
| 22 | AA | 209 | U | Sidechain |
| 22 | AA | 21 | G | Sidechain |
| 22 | AA | 212 | G | Sidechain |
| 22 | AA | 214 | C | Sidechain |
| 22 | AA | 215 | C | Sidechain |
| 22 | AA | 217 | C | Sidechain |
| 22 | AA | 222 | C | Sidechain |
| 22 | AA | 223 | A | Sidechain |
| 22 | AA | 234 | C | Sidechain |
| 22 | AA | 236 | A | Sidechain |
| 22 | AA | 244 | U | Sidechain |
| 22 | AA | 245 | U | Sidechain |
| 22 | AA | 246 | A | Sidechain |
| 22 | AA | 249 | U | Sidechain |
| 22 | AA | 252 | U | Sidechain |
| 22 | AA | 262 | A | Sidechain |
| 22 | AA | 264 | C | Sidechain |
| 22 | AA | 268 | U | Sidechain |
| 22 | AA | 269 | C | Sidechain |
| 22 | AA | 270 | A | Sidechain |
| 22 | AA | 272 | C | Sidechain |
| 22 | AA | 278 | G | Sidechain |
| 22 | AA | 279 | A | Sidechain |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 22 | AA | 281 | G | Sidechain |
| 22 | AA | 282 | A | Sidechain |
| 22 | AA | 285 | C | Sidechain |
| 22 | AA | 286 | C | Sidechain |
| 22 | AA | 293 | G | Sidechain |
| 22 | AA | 3 | A | Sidechain |
| 22 | AA | 304 | U | Sidechain |
| 22 | AA | 306 | A | Sidechain |
| 22 | AA | 308 | C | Sidechain |
| 22 | AA | 313 | A | Sidechain |
| 22 | AA | 314 | C | Sidechain |
| 22 | AA | 316 | C | Sidechain |
| 22 | AA | 324 | G | Sidechain |
| 22 | AA | 325 | A | Sidechain |
| 22 | AA | 33 | A | Sidechain |
| 22 | AA | 330 | C | Sidechain |
| 22 | AA | 332 | G | Sidechain |
| 22 | AA | 333 | U | Sidechain |
| 22 | AA | 336 | A | Sidechain |
| 22 | AA | 345 | C | Sidechain |
| 22 | AA | 346 | G | Sidechain |
| 22 | AA | 354 | G | Sidechain |
| 22 | AA | 36 | C | Sidechain |
| 22 | AA | 362 | G | Sidechain |
| 22 | AA | 368 | U | Sidechain |
| 22 | AA | 371 | A | Sidechain |
| 22 | AA | 376 | G | Sidechain |
| 22 | AA | 380 | G | Sidechain |
| 22 | AA | 383 | A | Sidechain |
| 22 | AA | 387 | U | Sidechain |
| 22 | AA | 390 | U | Sidechain |
| 22 | AA | 391 | G | Sidechain |
| 22 | AA | 392 | C | Sidechain |
| 22 | AA | 394 | G | Sidechain |
| 22 | AA | 395 | C | Sidechain |
| 22 | AA | 404 | G | Sidechain |
| 22 | AA | 410 | G | Sidechain |
| 22 | AA | 42 | G | Sidechain |
| 22 | AA | 423 | G | Sidechain |
| 22 | AA | 426 | U | Sidechain |
| 22 | AA | 428 | G | Sidechain |
| 22 | AA | 429 | U | Sidechain |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 22 | AA | 442 | G | Sidechain |
| 22 | AA | 448 | A | Sidechain |
| 22 | AA | 455 | G | Sidechain |
| 22 | AA | 457 | G | Sidechain |
| 22 | AA | 459 | A | Sidechain |
| 22 | AA | 46 | G | Sidechain |
| 22 | AA | 460 | A | Sidechain |
| 22 | AA | 463 | U | Sidechain |
| 22 | AA | 469 | C | Sidechain |
| 22 | AA | 472 | U | Sidechain |
| 22 | AA | 48 | C | Sidechain |
| 22 | AA | 481 | G | Sidechain |
| 22 | AA | 488 | C | Sidechain |
| 22 | AA | 490 | C | Sidechain |
| 22 | AA | 491 | G | Sidechain |
| 22 | AA | 493 | A | Sidechain |
| 22 | AA | 506 | G | Sidechain |
| 22 | AA | 51 | A | Sidechain |
| 22 | AA | 517 | G | Sidechain |
| 22 | AA | 518 | C | Sidechain |
| 22 | AA | 521 | G | Sidechain |
| 22 | AA | 522 | C | Sidechain |
| 22 | AA | 529 | G | Sidechain |
| 22 | AA | 530 | G | Sidechain |
| 22 | AA | 534 | U | Sidechain |
| 22 | AA | 535 | A | Sidechain |
| 22 | AA | 540 | G | Sidechain |
| 22 | AA | 551 | U | Sidechain |
| 22 | AA | 554 | A | Sidechain |
| 22 | AA | 558 | G | Sidechain |
| 22 | AA | 56 | U | Sidechain |
| 22 | AA | 560 | A | Sidechain |
| 22 | AA | 562 | U | Sidechain |
| 22 | AA | 563 | A | Sidechain |
| 22 | AA | 566 | G | Sidechain |
| 22 | AA | 568 | G | Sidechain |
| 22 | AA | 572 | A | Sidechain |
| 22 | AA | 590 | U | Sidechain |
| 22 | AA | 592 | G | Sidechain |
| 22 | AA | 594 | U | Sidechain |
| 22 | AA | 595 | A | Sidechain |
| 22 | AA | 597 | G | Sidechain |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 22 | AA | 60 | A | Sidechain |
| 22 | AA | 600 | A | Sidechain |
| 22 | AA | 608 | A | Sidechain |
| 22 | AA | 612 | C | Sidechain |
| 22 | AA | 618 | C | Sidechain |
| 22 | AA | 620 | C | Sidechain |
| 22 | AA | 623 | C | Sidechain |
| 22 | AA | 631 | C | Sidechain |
| 22 | AA | 639 | G | Sidechain |
| 22 | AA | 640 | A | Sidechain |
| 22 | AA | 641 | U | Sidechain |
| 22 | AA | 642 | A | Sidechain |
| 22 | AA | 654 | G | Sidechain |
| 22 | AA | 664 | G | Sidechain |
| 22 | AA | 665 | A | Sidechain |
| 22 | AA | 666 | G | Sidechain |
| 22 | AA | 67 | C | Sidechain |
| 22 | AA | 676 | A | Sidechain |
| 22 | AA | 679 | C | Sidechain |
| 22 | AA | 686 | U | Sidechain |
| 22 | AA | 690 | G | Sidechain |
| 22 | AA | 691 | G | Sidechain |
| 22 | AA | 692 | U | Sidechain |
| 22 | AA | 695 | A | Sidechain |
| 22 | AA | 697 | U | Sidechain |
| 22 | AA | 70 | U | Sidechain |
| 22 | AA | 703 | G | Sidechain |
| 22 | AA | 71 | A | Sidechain |
| 22 | AA | 722 | G | Sidechain |
| 22 | AA | 725 | G | Sidechain |
| 22 | AA | 728 | A | Sidechain |
| 22 | AA | 737 | C | Sidechain |
| 22 | AA | 745 | G | Sidechain |
| 22 | AA | 752 | G | Sidechain |
| 22 | AA | 754 | C | Sidechain |
| 22 | AA | 761 | G | Sidechain |
| 22 | AA | 771 | G | Sidechain |
| 22 | AA | 775 | G | Sidechain |
| 22 | AA | 778 | G | Sidechain |
| 22 | AA | 779 | C | Sidechain |
| 22 | AA | 781 | A | Sidechain |
| 22 | AA | 788 | U | Sidechain |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 22 | AA | 790 | A | Sidechain |
| 22 | AA | 791 | G | Sidechain |
| 22 | AA | 793 | U | Sidechain |
| 22 | AA | 795 | C | Sidechain |
| 22 | AA | 8 | A | Sidechain |
| 22 | AA | 80 | A | Sidechain |
| 22 | AA | 802 | A | Sidechain |
| 22 | AA | 805 | C | Sidechain |
| 22 | AA | 811 | C | Sidechain |
| 22 | AA | 816 | A | Sidechain |
| 22 | AA | 824 | G | Sidechain |
| 22 | AA | 826 | C | Sidechain |
| 22 | AA | 828 | U | Sidechain |
| 22 | AA | 838 | G | Sidechain |
| 22 | AA | 842 | U | Sidechain |
| 22 | AA | 843 | U | Sidechain |
| 22 | AA | 855 | U | Sidechain |
| 22 | AA | 859 | G | Sidechain |
| 22 | AA | 860 | A | Sidechain |
| 22 | AA | 863 | U | Sidechain |
| 22 | AA | 864 | A | Sidechain |
| 22 | AA | 87 | C | Sidechain |
| 22 | AA | 872 | A | Sidechain |
| 22 | AA | 874 | G | Sidechain |
| 22 | AA | 883 | C | Sidechain |
| 22 | AA | 892 | A | Sidechain |
| 22 | AA | 898 | G | Sidechain |
| 22 | AA | 900 | A | Sidechain |
| 22 | AA | 906 | A | Sidechain |
| 22 | AA | 91 | U | Sidechain |
| 22 | AA | 912 | C | Sidechain |
| 22 | AA | 914 | A | Sidechain |
| 22 | AA | 937 | A | Sidechain |
| 22 | AA | 938 | A | Sidechain |
| 22 | AA | 939 | G | Sidechain |
| 22 | AA | 94 | G | Sidechain |
| 22 | AA | 942 | G | Sidechain |
| 22 | AA | 946 | A | Sidechain |
| 22 | AA | 949 | A | Sidechain |
| 22 | AA | 95 | C | Sidechain |
| 22 | AA | 951 | G | Sidechain |
| 22 | AA | 958 | A | Sidechain |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 22 | AA | 960 | U | Sidechain |
| 22 | AA | 961 | U | Sidechain |
| 22 | AA | 962 | C | Sidechain |
| 22 | AA | 971 | G | Sidechain |
| 22 | AA | 972 | C | Sidechain |
| 22 | AA | 979 | C | Sidechain |
| 22 | AA | 985 | C | Sidechain |
| 22 | AA | 99 | C | Sidechain |
| 22 | AA | 991 | U | Sidechain |
| 22 | AA | 997 | U | Sidechain |
| 15 | AD | 61 | ARG | Sidechain |
| 18 | AG | 101 | ARG | Sidechain |
| 18 | AG | 118 | ARG | Sidechain |
| 3 | AL | 109 | ARG | Sidechain |
| 6 | AO | 88 | ARG | Sidechain |
| 7 | AP | 25 | ARG | Sidechain |
| 9 | AR | 2 | ARG | Sidechain |
| 10 | AS | 79 | TYR | Sidechain |
| 42 | B0 | 54 | ARG | Sidechain |
| 51 | B8 | 12 | ARG | Sidechain |
| 57 | BA | 100 | U | Sidechain |
| 57 | BA | 1004 | U | Sidechain |
| 57 | BA | 1012 | U | Sidechain |
| 57 | BA | 1013 | C | Sidechain |
| 57 | BA | 1014 | A | Sidechain |
| 57 | BA | 1017 | G | Sidechain |
| 57 | BA | 102 | U | Sidechain |
| 57 | BA | 1025 | G | Sidechain |
| 57 | BA | 1026 | G | Sidechain |
| 57 | BA | 1027 | A | Sidechain |
| 57 | BA | 1028 | A | Sidechain |
| 57 | BA | 103 | A | Sidechain |
| 57 | BA | 104 | A | Sidechain |
| 57 | BA | 1045 | C | Sidechain |
| 57 | BA | 1046 | A | Sidechain |
| 57 | BA | 1047 | G | Sidechain |
| 57 | BA | 1048 | A | Sidechain |
| 57 | BA | 1050 | A | Sidechain |
| 57 | BA | 1057 | A | Sidechain |
| 57 | BA | 106 | C | Sidechain |
| 57 | BA | 1063 | G | Sidechain |
| 57 | BA | 1066 | U | Sidechain |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 57 | BA | 1069 | A | Sidechain |
| 57 | BA | 107 | G | Sidechain |
| 57 | BA | 1071 | G | Sidechain |
| 57 | BA | 1072 | C | Sidechain |
| 57 | BA | 1075 | C | Sidechain |
| 57 | BA | 1081 | U | Sidechain |
| 57 | BA | 1082 | U | Sidechain |
| 57 | BA | 1083 | U | Sidechain |
| 57 | BA | 1085 | A | Sidechain |
| 57 | BA | 1088 | A | Sidechain |
| 57 | BA | 109 | C | Sidechain |
| 57 | BA | 1095 | A | Sidechain |
| 57 | BA | 1097 | U | Sidechain |
| 57 | BA | 1099 | G | Sidechain |
| 57 | BA | 1104 | C | Sidechain |
| 57 | BA | 1108 | U | Sidechain |
| 57 | BA | 1111 | A | Sidechain |
| 57 | BA | 1119 | U | Sidechain |
| 57 | BA | 1130 | U | Sidechain |
| 57 | BA | 1132 | U | Sidechain |
| 57 | BA | 1133 | A | Sidechain |
| 57 | BA | 1134 | A | Sidechain |
| 57 | BA | 1135 | C | Sidechain |
| 57 | BA | 1138 | G | Sidechain |
| 57 | BA | 1142 | A | Sidechain |
| 57 | BA | 1148 | U | Sidechain |
| 57 | BA | 1158 | C | Sidechain |
| 57 | BA | 1165 | A | Sidechain |
| 57 | BA | 1167 | C | Sidechain |
| 57 | BA | 1168 | G | Sidechain |
| 57 | BA | 1169 | A | Sidechain |
| 57 | BA | 1171 | G | Sidechain |
| 57 | BA | 1174 | U | Sidechain |
| 57 | BA | 1177 | G | Sidechain |
| 57 | BA | 1178 | C | Sidechain |
| 57 | BA | 1179 | G | Sidechain |
| 57 | BA | 1182 | G | Sidechain |
| 57 | BA | 1187 | G | Sidechain |
| 57 | BA | 1188 | U | Sidechain |
| 57 | BA | 1189 | A | Sidechain |
| 57 | BA | 1198 | U | Sidechain |
| 57 | BA | 12 | U | Sidechain |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 57 | BA | 1200 | C | Sidechain |
| 57 | BA | 1202 | G | Sidechain |
| 57 | BA | 1205 | A | Sidechain |
| 57 | BA | 1206 | G | Sidechain |
| 57 | BA | 1209 | U | Sidechain |
| 57 | BA | 1210 | G | Sidechain |
| 57 | BA | 1223 | G | Sidechain |
| 57 | BA | 1225 | G | Sidechain |
| 57 | BA | 1226 | A | Sidechain |
| 57 | BA | 1227 | G | Sidechain |
| 57 | BA | 1230 | A | Sidechain |
| 57 | BA | 1232 | G | Sidechain |
| 57 | BA | 1236 | G | Sidechain |
| 57 | BA | 1238 | G | Sidechain |
| 57 | BA | 124 | G | Sidechain |
| 57 | BA | 1245 | G | Sidechain |
| 57 | BA | 1251 | C | Sidechain |
| 57 | BA | 1252 | G | Sidechain |
| 57 | BA | 1254 | A | Sidechain |
| 57 | BA | 1255 | U | Sidechain |
| 57 | BA | 1263 | U | Sidechain |
| 57 | BA | 1267 | U | Sidechain |
| 57 | BA | 1268 | A | Sidechain |
| 57 | BA | 1271 | G | Sidechain |
| 57 | BA | 1273 | U | Sidechain |
| 57 | BA | 1281 | G | Sidechain |
| 57 | BA | 1283 | G | Sidechain |
| 57 | BA | 1288 | G | Sidechain |
| 57 | BA | 1291 | C | Sidechain |
| 57 | BA | 1299 | G | Sidechain |
| 57 | BA | 1302 | A | Sidechain |
| 57 | BA | 1310 | G | Sidechain |
| 57 | BA | 1311 | G | Sidechain |
| 57 | BA | 1315 | C | Sidechain |
| 57 | BA | 1324 | G | Sidechain |
| 57 | BA | 1329 | U | Sidechain |
| 57 | BA | 1343 | G | Sidechain |
| 57 | BA | 1353 | A | Sidechain |
| 57 | BA | 1356 | G | Sidechain |
| 57 | BA | 1364 | G | Sidechain |
| 57 | BA | 1370 | C | Sidechain |
| 57 | BA | 1376 | C | Sidechain |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 57 | BA | 1377 | G | Sidechain |
| 57 | BA | 1378 | A | Sidechain |
| 57 | BA | 138 | U | Sidechain |
| 57 | BA | 1398 | C | Sidechain |
| 57 | BA | 1402 | U | Sidechain |
| 57 | BA | 1405 | U | Sidechain |
| 57 | BA | 1406 | U | Sidechain |
| 57 | BA | 1410 | G | Sidechain |
| 57 | BA | 1425 | G | Sidechain |
| 57 | BA | 1427 | A | Sidechain |
| 57 | BA | 1431 | A | Sidechain |
| 57 | BA | 144 | A | Sidechain |
| 57 | BA | 1450 | G | Sidechain |
| 57 | BA | 146 | A | Sidechain |
| 57 | BA | 1464 | G | Sidechain |
| 57 | BA | 1465 | G | Sidechain |
| 57 | BA | 1467 | U | Sidechain |
| 57 | BA | 1469 | A | Sidechain |
| 57 | BA | 1473 | G | Sidechain |
| 57 | BA | 1474 | U | Sidechain |
| 57 | BA | 1482 | G | Sidechain |
| 57 | BA | 1483 | G | Sidechain |
| 57 | BA | 1492 | G | Sidechain |
| 57 | BA | 1494 | A | Sidechain |
| 57 | BA | 1495 | A | Sidechain |
| 57 | BA | 1508 | A | Sidechain |
| 57 | BA | 1517 | G | Sidechain |
| 57 | BA | 152 | A | Sidechain |
| 57 | BA | 1532 | A | Sidechain |
| 57 | BA | 1535 | A | Sidechain |
| 57 | BA | 1537 | G | Sidechain |
| 57 | BA | 1544 | A | Sidechain |
| 57 | BA | 1546 | G | Sidechain |
| 57 | BA | 1548 | A | Sidechain |
| 57 | BA | 1549 | A | Sidechain |
| 57 | BA | 1551 | A | Sidechain |
| 57 | BA | 1554 | U | Sidechain |
| 57 | BA | 1555 | G | Sidechain |
| 57 | BA | 1560 | G | Sidechain |
| 57 | BA | 1561 | C | Sidechain |
| 57 | BA | 1564 | C | Sidechain |
| 57 | BA | 1569 | A | Sidechain |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 57 | BA | 1570 | A | Sidechain |
| 57 | BA | 1573 | G | Sidechain |
| 57 | BA | 1575 | C | Sidechain |
| 57 | BA | 1583 | A | Sidechain |
| 57 | BA | 1596 | A | Sidechain |
| 57 | BA | 1599 | U | Sidechain |
| 57 | BA | 160 | A | Sidechain |
| 57 | BA | 1601 | G | Sidechain |
| 57 | BA | 1602 | U | Sidechain |
| 57 | BA | 1606 | C | Sidechain |
| 57 | BA | 1610 | A | Sidechain |
| 57 | BA | 1616 | A | Sidechain |
| 57 | BA | 1627 | G | Sidechain |
| 57 | BA | 1630 | A | Sidechain |
| 57 | BA | 1631 | G | Sidechain |
| 57 | BA | 1632 | A | Sidechain |
| 57 | BA | 1639 | C | Sidechain |
| 57 | BA | 1641 | A | Sidechain |
| 57 | BA | 1643 | G | Sidechain |
| 57 | BA | 1645 | G | Sidechain |
| 57 | BA | 1650 | A | Sidechain |
| 57 | BA | 1651 | G | Sidechain |
| 57 | BA | 1652 | A | Sidechain |
| 57 | BA | 1653 | G | Sidechain |
| 57 | BA | 1656 | C | Sidechain |
| 57 | BA | 1663 | G | Sidechain |
| 57 | BA | 1667 | G | Sidechain |
| 57 | BA | 1671 | U | Sidechain |
| 57 | BA | 1672 | A | Sidechain |
| 57 | BA | 1680 | U | Sidechain |
| 57 | BA | 1681 | G | Sidechain |
| 57 | BA | 1682 | G | Sidechain |
| 57 | BA | 1687 | G | Sidechain |
| 57 | BA | 169 | G | Sidechain |
| 57 | BA | 1695 | G | Sidechain |
| 57 | BA | 1698 | A | Sidechain |
| 57 | BA | 17 | G | Sidechain |
| 57 | BA | 1701 | A | Sidechain |
| 57 | BA | 1704 | C | Sidechain |
| 57 | BA | 1705 | A | Sidechain |
| 57 | BA | 1706 | C | Sidechain |
| 57 | BA | 1708 | C | Sidechain |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 57 | BA | 1710 | G | Sidechain |
| 57 | BA | 1713 | A | Sidechain |
| 57 | BA | 1721 | G | Sidechain |
| 57 | BA | 1726 | C | Sidechain |
| 57 | BA | 1736 | U | Sidechain |
| 57 | BA | 1739 | A | Sidechain |
| 57 | BA | 1744 | A | Sidechain |
| 57 | BA | 1745 | A | Sidechain |
| 57 | BA | 1749 | A | Sidechain |
| 57 | BA | 1750 | G | Sidechain |
| 57 | BA | 1761 | C | Sidechain |
| 57 | BA | 1762 | A | Sidechain |
| 57 | BA | 177 | G | Sidechain |
| 57 | BA | 1773 | A | Sidechain |
| 57 | BA | 1786 | A | Sidechain |
| 57 | BA | 179 | C | Sidechain |
| 57 | BA | 1797 | G | Sidechain |
| 57 | BA | 1798 | U | Sidechain |
| 57 | BA | 1799 | G | Sidechain |
| 57 | BA | 1802 | A | Sidechain |
| 57 | BA | 1805 | A | Sidechain |
| 57 | BA | 1807 | G | Sidechain |
| 57 | BA | 181 | A | Sidechain |
| 57 | BA | 1818 | U | Sidechain |
| 57 | BA | 182 | A | Sidechain |
| 57 | BA | 1821 | A | Sidechain |
| 57 | BA | 1830 | C | Sidechain |
| 57 | BA | 1831 | G | Sidechain |
| 57 | BA | 1842 | G | Sidechain |
| 57 | BA | 1848 | A | Sidechain |
| 57 | BA | 1851 | U | Sidechain |
| 57 | BA | 1857 | G | Sidechain |
| 57 | BA | 1865 | U | Sidechain |
| 57 | BA | 1866 | A | Sidechain |
| 57 | BA | 1869 | G | Sidechain |
| 57 | BA | 1870 | C | Sidechain |
| 57 | BA | 1881 | C | Sidechain |
| 57 | BA | 1883 | U | Sidechain |
| 57 | BA | 1885 | A | Sidechain |
| 57 | BA | 1900 | A | Sidechain |
| 57 | BA | 191 | A | Sidechain |
| 57 | BA | 1918 | A | Sidechain |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 57 | BA | 1922 | G | Sidechain |
| 57 | BA | 1926 | U | Sidechain |
| 57 | BA | 1927 | A | Sidechain |
| 57 | BA | 1938 | A | Sidechain |
| 57 | BA | 194 | G | Sidechain |
| 57 | BA | 1941 | C | Sidechain |
| 57 | BA | 1945 | G | Sidechain |
| 57 | BA | 1948 | G | Sidechain |
| 57 | BA | 1952 | A | Sidechain |
| 57 | BA | 1953 | A | Sidechain |
| 57 | BA | 1970 | A | Sidechain |
| 57 | BA | 1972 | G | Sidechain |
| 57 | BA | 1973 | G | Sidechain |
| 57 | BA | 1976 | U | Sidechain |
| 57 | BA | 1982 | U | Sidechain |
| 57 | BA | 199 | A | Sidechain |
| 57 | BA | 1996 | C | Sidechain |
| 57 | BA | 1997 | C | Sidechain |
| 57 | BA | 2 | G | Sidechain |
| 57 | BA | 2002 | G | Sidechain |
| 57 | BA | 2007 | U | Sidechain |
| 57 | BA | 2011 | U | Sidechain |
| 57 | BA | 2012 | G | Sidechain |
| 57 | BA | 2019 | A | Sidechain |
| 57 | BA | 203 | A | Sidechain |
| 57 | BA | 2033 | A | Sidechain |
| 57 | BA | 2035 | G | Sidechain |
| 57 | BA | 2050 | C | Sidechain |
| 57 | BA | 2051 | A | Sidechain |
| 57 | BA | 2053 | G | Sidechain |
| 57 | BA | 2057 | G | Sidechain |
| 57 | BA | 2059 | A | Sidechain |
| 57 | BA | 2063 | C | Sidechain |
| 57 | BA | 2065 | C | Sidechain |
| 57 | BA | 2068 | U | Sidechain |
| 57 | BA | 207 | A | Sidechain |
| 57 | BA | 2074 | U | Sidechain |
| 57 | BA | 2077 | A | Sidechain |
| 57 | BA | 208 | C | Sidechain |
| 57 | BA | 2080 | A | Sidechain |
| 57 | BA | 2090 | A | Sidechain |
| 57 | BA | 2091 | C | Sidechain |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 57 | BA | 2097 | A | Sidechain |
| 57 | BA | 21 | A | Sidechain |
| 57 | BA | 2102 | G | Sidechain |
| 57 | BA | 2111 | U | Sidechain |
| 57 | BA | 2112 | G | Sidechain |
| 57 | BA | 2113 | U | Sidechain |
| 57 | BA | 2114 | A | Sidechain |
| 57 | BA | 2120 | G | Sidechain |
| 57 | BA | 2133 | G | Sidechain |
| 57 | BA | 2138 | G | Sidechain |
| 57 | BA | 2152 | G | Sidechain |
| 57 | BA | 2153 | C | Sidechain |
| 57 | BA | 2154 | A | Sidechain |
| 57 | BA | 2167 | U | Sidechain |
| 57 | BA | 2168 | G | Sidechain |
| 57 | BA | 217 | A | Sidechain |
| 57 | BA | 218 | A | Sidechain |
| 57 | BA | 2182 | U | Sidechain |
| 57 | BA | 2188 | U | Sidechain |
| 57 | BA | 219 | A | Sidechain |
| 57 | BA | 2197 | U | Sidechain |
| 57 | BA | 2204 | G | Sidechain |
| 57 | BA | 2205 | A | Sidechain |
| 57 | BA | 2206 | C | Sidechain |
| 57 | BA | 2210 | U | Sidechain |
| 57 | BA | 2226 | C | Sidechain |
| 57 | BA | 2227 | A | Sidechain |
| 57 | BA | 2228 | G | Sidechain |
| 57 | BA | 223 | A | Sidechain |
| 57 | BA | 2230 | G | Sidechain |
| 57 | BA | 2236 | U | Sidechain |
| 57 | BA | 2246 | G | Sidechain |
| 57 | BA | 2252 | G | Sidechain |
| 57 | BA | 2253 | G | Sidechain |
| 57 | BA | 2254 | C | Sidechain |
| 57 | BA | 2258 | C | Sidechain |
| 57 | BA | 226 | A | Sidechain |
| 57 | BA | 2266 | A | Sidechain |
| 57 | BA | 2268 | A | Sidechain |
| 57 | BA | 227 | A | Sidechain |
| 57 | BA | 2273 | A | Sidechain |
| 57 | BA | 2282 | G | Sidechain |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 57 | BA | 2286 | G | Sidechain |
| 57 | BA | 229 | C | Sidechain |
| 57 | BA | 2295 | C | Sidechain |
| 57 | BA | 2300 | C | Sidechain |
| 57 | BA | 2301 | C | Sidechain |
| 57 | BA | 2304 | G | Sidechain |
| 57 | BA | 2305 | U | Sidechain |
| 57 | BA | 2307 | G | Sidechain |
| 57 | BA | 2308 | G | Sidechain |
| 57 | BA | 231 | A | Sidechain |
| 57 | BA | 2324 | U | Sidechain |
| 57 | BA | 2325 | G | Sidechain |
| 57 | BA | 2327 | A | Sidechain |
| 57 | BA | 2333 | A | Sidechain |
| 57 | BA | 2337 | G | Sidechain |
| 57 | BA | 2341 | G | Sidechain |
| 57 | BA | 2357 | G | Sidechain |
| 57 | BA | 2358 | A | Sidechain |
| 57 | BA | 2365 | G | Sidechain |
| 57 | BA | 2369 | A | Sidechain |
| 57 | BA | 2375 | G | Sidechain |
| 57 | BA | 2376 | A | Sidechain |
| 57 | BA | 2382 | G | Sidechain |
| 57 | BA | 2384 | U | Sidechain |
| 57 | BA | 2391 | G | Sidechain |
| 57 | BA | 2392 | A | Sidechain |
| 57 | BA | 2399 | G | Sidechain |
| 57 | BA | 2400 | G | Sidechain |
| 57 | BA | 2405 | G | Sidechain |
| 57 | BA | 2408 | U | Sidechain |
| 57 | BA | 2411 | A | Sidechain |
| 57 | BA | 2420 | C | Sidechain |
| 57 | BA | 2422 | C | Sidechain |
| 57 | BA | 2424 | C | Sidechain |
| 57 | BA | 243 | U | Sidechain |
| 57 | BA | 2431 | U | Sidechain |
| 57 | BA | 2433 | A | Sidechain |
| 57 | BA | 2437 | G | Sidechain |
| 57 | BA | 2438 | U | Sidechain |
| 57 | BA | 2441 | U | Sidechain |
| 57 | BA | 2442 | C | Sidechain |
| 57 | BA | 2447 | G | Sidechain |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 57 | BA | 2451 | A | Sidechain |
| 57 | BA | 2453 | A | Sidechain |
| 57 | BA | 2458 | G | Sidechain |
| 57 | BA | 2461 | A | Sidechain |
| 57 | BA | 2468 | A | Sidechain |
| 57 | BA | 2471 | A | Sidechain |
| 57 | BA | 2472 | G | Sidechain |
| 57 | BA | 2475 | C | Sidechain |
| 57 | BA | 2476 | A | Sidechain |
| 57 | BA | 248 | G | Sidechain |
| 57 | BA | 2488 | G | Sidechain |
| 57 | BA | 249 | C | Sidechain |
| 57 | BA | 25 | U | Sidechain |
| 57 | BA | 250 | G | Sidechain |
| 57 | BA | 2507 | C | Sidechain |
| 57 | BA | 2508 | G | Sidechain |
| 57 | BA | 2516 | A | Sidechain |
| 57 | BA | 2517 | C | Sidechain |
| 57 | BA | 2518 | A | Sidechain |
| 57 | BA | 2520 | C | Sidechain |
| 57 | BA | 2521 | C | Sidechain |
| 57 | BA | 2522 | U | Sidechain |
| 57 | BA | 2530 | A | Sidechain |
| 57 | BA | 2531 | A | Sidechain |
| 57 | BA | 2532 | G | Sidechain |
| 57 | BA | 2536 | G | Sidechain |
| 57 | BA | 2542 | A | Sidechain |
| 57 | BA | 2550 | G | Sidechain |
| 57 | BA | 2555 | U | Sidechain |
| 57 | BA | 2557 | G | Sidechain |
| 57 | BA | 2560 | A | Sidechain |
| 57 | BA | 2562 | U | Sidechain |
| 57 | BA | 2565 | A | Sidechain |
| 57 | BA | 2566 | A | Sidechain |
| 57 | BA | 2573 | C | Sidechain |
| 57 | BA | 2575 | C | Sidechain |
| 57 | BA | 2576 | G | Sidechain |
| 57 | BA | 2583 | G | Sidechain |
| 57 | BA | 2588 | G | Sidechain |
| 57 | BA | 2591 | C | Sidechain |
| 57 | BA | 2601 | C | Sidechain |
| 57 | BA | 2608 | G | Sidechain |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 57 | BA | 2611 | C | Sidechain |
| 57 | BA | 2613 | U | Sidechain |
| 57 | BA | 2624 | G | Sidechain |
| 57 | BA | 2625 | G | Sidechain |
| 57 | BA | 263 | G | Sidechain |
| 57 | BA | 2637 | U | Sidechain |
| 57 | BA | 2638 | G | Sidechain |
| 57 | BA | 264 | C | Sidechain |
| 57 | BA | 2645 | G | Sidechain |
| 57 | BA | 265 | A | Sidechain |
| 57 | BA | 2650 | U | Sidechain |
| 57 | BA | 2659 | G | Sidechain |
| 57 | BA | 2663 | G | Sidechain |
| 57 | BA | 2664 | G | Sidechain |
| 57 | BA | 2679 | A | Sidechain |
| 57 | BA | 2680 | U | Sidechain |
| 57 | BA | 2682 | A | Sidechain |
| 57 | BA | 2700 | A | Sidechain |
| 57 | BA | 2708 | G | Sidechain |
| 57 | BA | 2718 | G | Sidechain |
| 57 | BA | 272 | A | Sidechain |
| 57 | BA | 2721 | A | Sidechain |
| 57 | BA | 2723 | C | Sidechain |
| 57 | BA | 2726 | A | Sidechain |
| 57 | BA | 2727 | A | Sidechain |
| 57 | BA | 2732 | G | Sidechain |
| 57 | BA | 2734 | A | Sidechain |
| 57 | BA | 2737 | G | Sidechain |
| 57 | BA | 2739 | U | Sidechain |
| 57 | BA | 2740 | A | Sidechain |
| 57 | BA | 275 | C | Sidechain |
| 57 | BA | 2751 | G | Sidechain |
| 57 | BA | 2753 | A | Sidechain |
| 57 | BA | 2756 | U | Sidechain |
| 57 | BA | 276 | U | Sidechain |
| 57 | BA | 2768 | U | Sidechain |
| 57 | BA | 277 | G | Sidechain |
| 57 | BA | 2772 | C | Sidechain |
| 57 | BA | 2776 | A | Sidechain |
| 57 | BA | 278 | A | Sidechain |
| 57 | BA | 2780 | G | Sidechain |
| 57 | BA | 2786 | U | Sidechain |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 57 | BA | 2787 | C | Sidechain |
| 57 | BA | 279 | A | Sidechain |
| 57 | BA | 2796 | U | Sidechain |
| 57 | BA | 2797 | U | Sidechain |
| 57 | BA | 28 | A | Sidechain |
| 57 | BA | 2807 | U | Sidechain |
| 57 | BA | 2809 | A | Sidechain |
| 57 | BA | 2810 | A | Sidechain |
| 57 | BA | 2816 | G | Sidechain |
| 57 | BA | 2824 | C | Sidechain |
| 57 | BA | 2831 | G | Sidechain |
| 57 | BA | 2832 | U | Sidechain |
| 57 | BA | 2836 | U | Sidechain |
| 57 | BA | 2839 | G | Sidechain |
| 57 | BA | 2840 | C | Sidechain |
| 57 | BA | 2848 | G | Sidechain |
| 57 | BA | 2851 | A | Sidechain |
| 57 | BA | 2856 | A | Sidechain |
| 57 | BA | 2857 | G | Sidechain |
| 57 | BA | 2866 | U | Sidechain |
| 57 | BA | 2868 | A | Sidechain |
| 57 | BA | 2869 | G | Sidechain |
| 57 | BA | 2874 | C | Sidechain |
| 57 | BA | 2879 | A | Sidechain |
| 57 | BA | 2881 | U | Sidechain |
| 57 | BA | 2885 | G | Sidechain |
| 57 | BA | 2888 | C | Sidechain |
| 57 | BA | 2889 | C | Sidechain |
| 57 | BA | 2892 | G | Sidechain |
| 57 | BA | 2895 | G | Sidechain |
| 57 | BA | 2899 | A | Sidechain |
| 57 | BA | 293 | U | Sidechain |
| 57 | BA | 297 | G | Sidechain |
| 57 | BA | 301 | G | Sidechain |
| 57 | BA | 303 | G | Sidechain |
| 57 | BA | 307 | G | Sidechain |
| 57 | BA | 308 | G | Sidechain |
| 57 | BA | 313 | G | Sidechain |
| 57 | BA | 33 | C | Sidechain |
| 57 | BA | 333 | G | Sidechain |
| 57 | BA | 343 | C | Sidechain |
| 57 | BA | 346 | A | Sidechain |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 57 | BA | 347 | A | Sidechain |
| 57 | BA | 352 | A | Sidechain |
| 57 | BA | 354 | A | Sidechain |
| 57 | BA | 361 | G | Sidechain |
| 57 | BA | 363 | G | Sidechain |
| 57 | BA | 367 | G | Sidechain |
| 57 | BA | 374 | A | Sidechain |
| 57 | BA | 377 | G | Sidechain |
| 57 | BA | 380 | G | Sidechain |
| 57 | BA | 385 | C | Sidechain |
| 57 | BA | 39 | G | Sidechain |
| 57 | BA | 390 | U | Sidechain |
| 57 | BA | 392 | U | Sidechain |
| 57 | BA | 394 | C | Sidechain |
| 57 | BA | 395 | U | Sidechain |
| 57 | BA | 403 | U | Sidechain |
| 57 | BA | 415 | A | Sidechain |
| 57 | BA | 416 | U | Sidechain |
| 57 | BA | 418 | C | Sidechain |
| 57 | BA | 420 | C | Sidechain |
| 57 | BA | 422 | A | Sidechain |
| 57 | BA | 43 | G | Sidechain |
| 57 | BA | 442 | G | Sidechain |
| 57 | BA | 446 | G | Sidechain |
| 57 | BA | 447 | A | Sidechain |
| 57 | BA | 449 | A | Sidechain |
| 57 | BA | 45 | G | Sidechain |
| 57 | BA | 450 | G | Sidechain |
| 57 | BA | 455 | C | Sidechain |
| 57 | BA | 457 | A | Sidechain |
| 57 | BA | 459 | U | Sidechain |
| 57 | BA | 460 | A | Sidechain |
| 57 | BA | 461 | C | Sidechain |
| 57 | BA | 463 | G | Sidechain |
| 57 | BA | 464 | U | Sidechain |
| 57 | BA | 474 | G | Sidechain |
| 57 | BA | 477 | A | Sidechain |
| 57 | BA | 478 | A | Sidechain |
| 57 | BA | 48 | G | Sidechain |
| 57 | BA | 480 | A | Sidechain |
| 57 | BA | 481 | G | Sidechain |
| 57 | BA | 486 | C | Sidechain |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 57 | BA | 492 | A | Sidechain |
| 57 | BA | 493 | G | Sidechain |
| 57 | BA | 498 | G | Sidechain |
| 57 | BA | 500 | G | Sidechain |
| 57 | BA | 501 | A | Sidechain |
| 57 | BA | 507 | A | Sidechain |
| 57 | BA | 510 | C | Sidechain |
| 57 | BA | 52 | A | Sidechain |
| 57 | BA | 528 | A | Sidechain |
| 57 | BA | 53 | A | Sidechain |
| 57 | BA | 544 | C | Sidechain |
| 57 | BA | 568 | U | Sidechain |
| 57 | BA | 573 | U | Sidechain |
| 57 | BA | 575 | A | Sidechain |
| 57 | BA | 576 | U | Sidechain |
| 57 | BA | 577 | G | Sidechain |
| 57 | BA | 58 | G | Sidechain |
| 57 | BA | 581 | C | Sidechain |
| 57 | BA | 583 | G | Sidechain |
| 57 | BA | 587 | C | Sidechain |
| 57 | BA | 59 | U | Sidechain |
| 57 | BA | 592 | A | Sidechain |
| 57 | BA | 594 | U | Sidechain |
| 57 | BA | 60 | G | Sidechain |
| 57 | BA | 603 | A | Sidechain |
| 57 | BA | 607 | U | Sidechain |
| 57 | BA | 608 | A | Sidechain |
| 57 | BA | 611 | C | Sidechain |
| 57 | BA | 617 | G | Sidechain |
| 57 | BA | 622 | G | Sidechain |
| 57 | BA | 623 | C | Sidechain |
| 57 | BA | 626 | A | Sidechain |
| 57 | BA | 63 | A | Sidechain |
| 57 | BA | 630 | G | Sidechain |
| 57 | BA | 632 | A | Sidechain |
| 57 | BA | 636 | G | Sidechain |
| 57 | BA | 637 | A | Sidechain |
| 57 | BA | 642 | U | Sidechain |
| 57 | BA | 666 | A | Sidechain |
| 57 | BA | 671 | C | Sidechain |
| 57 | BA | 672 | C | Sidechain |
| 57 | BA | 676 | A | Sidechain |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 57 | BA | 685 | A | Sidechain |
| 57 | BA | 687 | C | Sidechain |
| 57 | BA | 688 | U | Sidechain |
| 57 | BA | 692 | C | Sidechain |
| 57 | BA | 693 | A | Sidechain |
| 57 | BA | 697 | G | Sidechain |
| 57 | BA | 700 | G | Sidechain |
| 57 | BA | 708 | G | Sidechain |
| 57 | BA | 71 | A | Sidechain |
| 57 | BA | 715 | A | Sidechain |
| 57 | BA | 717 | C | Sidechain |
| 57 | BA | 718 | A | Sidechain |
| 57 | BA | 72 | U | Sidechain |
| 57 | BA | 721 | A | Sidechain |
| 57 | BA | 726 | G | Sidechain |
| 57 | BA | 728 | G | Sidechain |
| 57 | BA | 729 | G | Sidechain |
| 57 | BA | 73 | A | Sidechain |
| 57 | BA | 735 | A | Sidechain |
| 57 | BA | 736 | C | Sidechain |
| 57 | BA | 738 | G | Sidechain |
| 57 | BA | 74 | A | Sidechain |
| 57 | BA | 75 | G | Sidechain |
| 57 | BA | 751 | A | Sidechain |
| 57 | BA | 757 | G | Sidechain |
| 57 | BA | 764 | A | Sidechain |
| 57 | BA | 772 | C | Sidechain |
| 57 | BA | 776 | G | Sidechain |
| 57 | BA | 78 | U | Sidechain |
| 57 | BA | 782 | A | Sidechain |
| 57 | BA | 783 | A | Sidechain |
| 57 | BA | 786 | C | Sidechain |
| 57 | BA | 789 | A | Sidechain |
| 57 | BA | 791 | C | Sidechain |
| 57 | BA | 794 | A | Sidechain |
| 57 | BA | 795 | C | Sidechain |
| 57 | BA | 800 | A | Sidechain |
| 57 | BA | 801 | G | Sidechain |
| 57 | BA | 802 | A | Sidechain |
| 57 | BA | 804 | A | Sidechain |
| 57 | BA | 810 | U | Sidechain |
| 57 | BA | 813 | U | Sidechain |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 57 | BA | 819 | A | Sidechain |
| 57 | BA | 820 | A | Sidechain |
| 57 | BA | 828 | U | Sidechain |
| 57 | BA | 834 | G | Sidechain |
| 57 | BA | 837 | C | Sidechain |
| 57 | BA | 838 | C | Sidechain |
| 57 | BA | 841 | G | Sidechain |
| 57 | BA | 845 | A | Sidechain |
| 57 | BA | 858 | G | Sidechain |
| 57 | BA | 86 | G | Sidechain |
| 57 | BA | 861 | A | Sidechain |
| 57 | BA | 867 | C | Sidechain |
| 57 | BA | 87 | U | Sidechain |
| 57 | BA | 871 | U | Sidechain |
| 57 | BA | 876 | C | Sidechain |
| 57 | BA | 881 | G | Sidechain |
| 57 | BA | 883 | G | Sidechain |
| 57 | BA | 89 | A | Sidechain |
| 57 | BA | 894 | U | Sidechain |
| 57 | BA | 902 | C | Sidechain |
| 57 | BA | 905 | A | Sidechain |
| 57 | BA | 909 | A | Sidechain |
| 57 | BA | 910 | A | Sidechain |
| 57 | BA | 912 | C | Sidechain |
| 57 | BA | 914 | G | Sidechain |
| 57 | BA | 915 | C | Sidechain |
| 57 | BA | 916 | G | Sidechain |
| 57 | BA | 923 | G | Sidechain |
| 57 | BA | 927 | A | Sidechain |
| 57 | BA | 931 | U | Sidechain |
| 57 | BA | 934 | U | Sidechain |
| 57 | BA | 936 | A | Sidechain |
| 57 | BA | 940 | G | Sidechain |
| 57 | BA | 945 | A | Sidechain |
| 57 | BA | 950 | G | Sidechain |
| 57 | BA | 956 | G | Sidechain |
| 57 | BA | 957 | C | Sidechain |
| 57 | BA | 959 | A | Sidechain |
| 57 | BA | 962 | G | Sidechain |
| 57 | BA | 963 | U | Sidechain |
| 57 | BA | 966 | G | Sidechain |
| 57 | BA | 968 | C | Sidechain |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 57 | BA | 969 | G | Sidechain |
| 57 | BA | 970 | U | Sidechain |
| 57 | BA | 971 | G | Sidechain |
| 57 | BA | 983 | A | Sidechain |
| 57 | BA | 984 | A | Sidechain |
| 57 | BA | 989 | G | Sidechain |
| 57 | BA | 99 | U | Sidechain |
| 57 | BA | 990 | A | Sidechain |
| 35 | BD | 155 | ARG | Sidechain |
| 55 | BH | 175 | LYS | Peptide |
| 55 | BH | 57 | TYR | Sidechain |
| 26 | BJ | 137 | ARG | Sidechain |
| 28 | BN | 116 | ARG | Sidechain |
| 28 | BN | 52 | ASP | Peptide |
| 29 | BO | 31 | ARG | Sidechain |
| 32 | BR | 8 | ARG | Sidechain |
| 34 | BT | 71 | ARG | Sidechain |
| 36 | BU | 50 | ARG | Sidechain |
| 36 | BU | 54 | ARG | Sidechain |
| 38 | BW | 25 | ARG | Sidechain |
| 40 | BY | 6 | ARG | Sidechain |
| 58 | Ba | 105 | G | Sidechain |
| 58 | Ba | 11 | C | Sidechain |
| 58 | Ba | 117 | G | Sidechain |
| 58 | Ba | 15 | A | Sidechain |
| 58 | Ba | 21 | G | Sidechain |
| 58 | Ba | 35 | C | Sidechain |
| 58 | Ba | 40 | U | Sidechain |
| 58 | Ba | 41 | G | Sidechain |
| 58 | Ba | 50 | A | Sidechain |
| 58 | Ba | 51 | G | Sidechain |
| 58 | Ba | 57 | A | Sidechain |
| 58 | Ba | 64 | G | Sidechain |
| 58 | Ba | 73 | A | Sidechain |
| 58 | Ba | 90 | C | Sidechain |
| 58 | Ba | 92 | C | 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 | AJ | 794 | 0 | 803 | 0 | 0 |
| 2 | AK | 923 | 0 | 912 | 0 | 0 |
| 3 | AL | 923 | 0 | 954 | 0 | 0 |
| 4 | AM | 876 | 0 | 910 | 0 | 0 |
| 5 | AN | 771 | 0 | 777 | 0 | 0 |
| 6 | AO | 690 | 0 | 691 | 0 | 0 |
| 7 | AP | 620 | 0 | 611 | 0 | 0 |
| 8 | AQ | 657 | 0 | 687 | 0 | 0 |
| 9 | AR | 603 | 0 | 602 | 0 | 0 |
| 10 | AS | 708 | 0 | 732 | 0 | 0 |
| 11 | AB | 1805 | 0 | 1750 | 0 | 0 |
| 12 | AT | 636 | 0 | 652 | 0 | 0 |
| 13 | AU | 564 | 0 | 579 | 0 | 0 |
| 14 | AC | 1761 | 0 | 1793 | 0 | 0 |
| 15 | AD | 1587 | 0 | 1596 | 0 | 0 |
| 16 | AE | 1182 | 0 | 1185 | 0 | 0 |
| 17 | AF | 1061 | 0 | 971 | 0 | 0 |
| 18 | AG | 1347 | 0 | 1347 | 0 | 0 |
| 19 | AH | 948 | 0 | 975 | 0 | 0 |
| 20 | AI | 1000 | 0 | 1011 | 0 | 0 |
| 21 | A1 | 4989 | 0 | 4915 | 0 | 0 |
| 22 | AA | 33089 | 0 | 16668 | 0 | 0 |
| 23 | A2 | 993 | 0 | 501 | 0 | 0 |
| 24 | A3 | 1640 | 0 | 845 | 0 | 0 |
| 25 | BC | 1733 | 0 | 1824 | 0 | 0 |
| 26 | BJ | 1233 | 0 | 1283 | 0 | 0 |
| 27 | BK | 1032 | 0 | 1088 | 0 | 0 |
| 28 | BN | 1129 | 0 | 1162 | 0 | 0 |
| 29 | BO | 947 | 0 | 1023 | 0 | 0 |
| 30 | BP | 1053 | 0 | 1129 | 0 | 0 |
| 31 | BQ | 1074 | 0 | 1157 | 0 | 0 |
| 32 | BR | 1008 | 0 | 1045 | 0 | 0 |
| 33 | BS | 900 | 0 | 935 | 0 | 0 |
| 34 | BT | 917 | 0 | 965 | 0 | 0 |
| 35 | BD | 2092 | 0 | 2170 | 0 | 0 |
| 36 | BU | 947 | 0 | 1022 | 0 | 0 |
| 37 | BV | 816 | 0 | 839 | 0 | 0 |
| 38 | BW | 857 | 0 | 922 | 0 | 0 |
| 39 | BX | 787 | 0 | 846 | 0 | 0 |
| 40 | BY | 789 | 0 | 847 | 0 | 0 |
| 41 | BZ | 753 | 0 | 780 | 0 | 0 |
| 42 | B0 | 634 | 0 | 656 | 0 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 43 | B1 | 625 | 0 | 655 | 0 | 0 |
| 44 | B2 | 509 | 0 | 543 | 0 | 0 |
| 45 | BE | 1565 | 0 | 1616 | 0 | 0 |
| 46 | B3 | 449 | 0 | 491 | 0 | 0 |
| 47 | B4 | 549 | 0 | 552 | 0 | 0 |
| 48 | B5 | 444 | 0 | 461 | 0 | 0 |
| 49 | B6 | 441 | 0 | 485 | 0 | 0 |
| 50 | B7 | 377 | 0 | 418 | 0 | 0 |
| 51 | B8 | 504 | 0 | 574 | 0 | 0 |
| 52 | B9 | 302 | 0 | 343 | 0 | 0 |
| 53 | BF | 1552 | 0 | 1619 | 0 | 0 |
| 54 | BG | 1420 | 0 | 1460 | 0 | 0 |
| 55 | BH | 1323 | 0 | 1374 | 0 | 0 |
| 56 | BL | 1111 | 0 | 1148 | 0 | 0 |
| 57 | BA | 62351 | 0 | 31378 | 0 | 0 |
| 58 | Ba | 2566 | 0 | 1302 | 0 | 0 |
| All | All | 154956 | 0 | 106579 | 0 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

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 | AJ | 44/103 (43%) | 40 (91%) | 1 (2%) | 3 (7%) | 1 15 |
| 2 | AK | 57/128 (44%) | 52 (91%) | 5 (9%) | 0 | 100 100 |
| 3 | AL | 64/123 (52%) | 54 (84%) | 8 (12%) | 2 (3%) | 4 27 |
| 4 | AM | 56/117 (48%) | 51 (91%) | 4 (7%) | 1 (2%) | 8 40 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 5 | AN | 41/100 (41%) | 37 (90%) | 3 (7%) | 1 (2%) | 6 | 33 |
| 6 | AO | 44/88 (50%) | 43 (98%) | 1 (2%) | 0 | 100 | 100 |
| 7 | AP | 34/82 (42%) | 31 (91%) | 3 (9%) | 0 | 100 | 100 |
| 8 | AQ | 52/83 (63%) | 48 (92%) | 4 (8%) | 0 | 100 | 100 |
| 9 | AR | 36/74 (49%) | 34 (94%) | 2 (6%) | 0 | 100 | 100 |
| 10 | AS | 54/91 (59%) | 53 (98%) | 1 (2%) | 0 | 100 | 100 |
| 11 | AB | 123/240 (51%) | 114 (93%) | 7 (6%) | 2 (2%) | 9 | 44 |
| 12 | AT | 32/86 (37%) | 30 (94%) | 2 (6%) | 0 | 100 | 100 |
| 13 | AU | 24/70 (34%) | 18 (75%) | 3 (12%) | 3 (12%) | 0 | 5 |
| 14 | AC | 126/232 (54%) | 122 (97%) | 4 (3%) | 0 | 100 | 100 |
| 15 | AD | 107/205 (52%) | 102 (95%) | 5 (5%) | 0 | 100 | 100 |
| 16 | AE | 89/166 (54%) | 84 (94%) | 4 (4%) | 1 (1%) | 14 | 52 |
| 17 | AF | 65/135 (48%) | 61 (94%) | 4 (6%) | 0 | 100 | 100 |
| 18 | AG | 84/178 (47%) | 79 (94%) | 5 (6%) | 0 | 100 | 100 |
| 19 | AH | 77/129 (60%) | 70 (91%) | 7 (9%) | 0 | 100 | 100 |
| 20 | AI | 69/129 (54%) | 63 (91%) | 6 (9%) | 0 | 100 | 100 |
| 21 | A1 | 434/639 (68%) | 390 (90%) | 38 (9%) | 6 (1%) | 11 | 46 |
| 25 | BC | 232/234 (99%) | 213 (92%) | 18 (8%) | 1 (0%) | 34 | 72 |
| 26 | BJ | 162/164 (99%) | 158 (98%) | 3 (2%) | 1 (1%) | 25 | 66 |
| 27 | BK | 139/141 (99%) | 133 (96%) | 6 (4%) | 0 | 100 | 100 |
| 28 | BN | 140/142 (99%) | 131 (94%) | 9 (6%) | 0 | 100 | 100 |
| 29 | BO | 121/123 (98%) | 107 (88%) | 11 (9%) | 3 (2%) | 5 | 32 |
| 30 | BP | 142/144 (99%) | 127 (89%) | 13 (9%) | 2 (1%) | 11 | 46 |
| 31 | BQ | 134/136 (98%) | 126 (94%) | 6 (4%) | 2 (2%) | 10 | 46 |
| 32 | BR | 125/127 (98%) | 112 (90%) | 11 (9%) | 2 (2%) | 9 | 44 |
| 33 | BS | 115/117 (98%) | 115 (100%) | 0 | 0 | 100 | 100 |
| 34 | BT | 112/114 (98%) | 107 (96%) | 3 (3%) | 2 (2%) | 8 | 40 |
| 35 | BD | 270/272 (99%) | 252 (93%) | 15 (6%) | 3 (1%) | 14 | 52 |
| 36 | BU | 115/117 (98%) | 108 (94%) | 5 (4%) | 2 (2%) | 9 | 42 |
| 37 | BV | 101/103 (98%) | 94 (93%) | 4 (4%) | 3 (3%) | 4 | 28 |
| 38 | BW | 108/110 (98%) | 103 (95%) | 4 (4%) | 1 (1%) | 17 | 57 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 39 | BX | 98/100 (98%) | 83 (85%) | 12 (12%) | 3 (3%) | 4 | 27 |
| 40 | BY | 101/103 (98%) | 97 (96%) | 4 (4%) | 0 | 100 | 100 |
| 41 | BZ | 92/94 (98%) | 90 (98%) | 2 (2%) | 0 | 100 | 100 |
| 42 | B0 | 82/84 (98%) | 72 (88%) | 6 (7%) | 4 (5%) | 2 | 20 |
| 43 | B1 | 75/77 (97%) | 69 (92%) | 5 (7%) | 1 (1%) | 12 | 48 |
| 44 | B2 | 61/63 (97%) | 54 (88%) | 7 (12%) | 0 | 100 | 100 |
| 45 | BE | 207/209 (99%) | 181 (87%) | 20 (10%) | 6 (3%) | 4 | 29 |
| 46 | B3 | 56/58 (97%) | 53 (95%) | 3 (5%) | 0 | 100 | 100 |
| 47 | B4 | 68/70 (97%) | 62 (91%) | 6 (9%) | 0 | 100 | 100 |
| 48 | B5 | 54/56 (96%) | 50 (93%) | 3 (6%) | 1 (2%) | 8 | 38 |
| 49 | B6 | 52/54 (96%) | 51 (98%) | 1 (2%) | 0 | 100 | 100 |
| 50 | B7 | 44/46 (96%) | 42 (96%) | 2 (4%) | 0 | 100 | 100 |
| 51 | B8 | 62/64 (97%) | 61 (98%) | 1 (2%) | 0 | 100 | 100 |
| 52 | B9 | 36/38 (95%) | 31 (86%) | 3 (8%) | 2 (6%) | 2 | 19 |
| 53 | BF | 199/201 (99%) | 186 (94%) | 7 (4%) | 6 (3%) | 4 | 28 |
| 54 | BG | 176/178 (99%) | 155 (88%) | 15 (8%) | 6 (3%) | 3 | 26 |
| 55 | BH | 174/176 (99%) | 157 (90%) | 14 (8%) | 3 (2%) | 9 | 42 |
| 56 | BL | 147/149 (99%) | 133 (90%) | 13 (9%) | 1 (1%) | 22 | 63 |
| All | All | 5512/7062 (78%) | 5089 (92%) | 349 (6%) | 74 (1%) | 16 | 48 |

All (74) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 21 | A1 | 242 | THR |
| 21 | A1 | 493 | LYS |
| 32 | BR | 13 | ASN |
| 35 | BD | 140 | VAL |
| 42 | B0 | 40 | ARG |
| 45 | BE | 122 | VAL |
| 56 | BL | 35 | LYS |
| 1 | AJ | 57 | VAL |
| 13 | AU | 3 | ILE |
| 13 | AU | 19 | LYS |
| 21 | A1 | 174 | GLN |
| 30 | BP | 53 | GLY |
| 34 | BT | 5 | LYS |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 35 | BD | 77 | VAL |
| 42 | B0 | 36 | ILE |
| 43 | B1 | 27 | ARG |
| 45 | BE | 37 | VAL |
| 53 | BF | 62 | GLN |
| 53 | BF | 79 | ARG |
| 53 | BF | 96 | VAL |
| 54 | BG | 132 | ARG |
| 55 | BH | 29 | ASN |
| 55 | BH | 46 | ASP |
| 4 | AM | 22 | TYR |
| 11 | AB | 18 | GLN |
| 16 | AE | 23 | THR |
| 21 | A1 | 249 | LEU |
| 21 | A1 | 284 | SER |
| 21 | A1 | 566 | VAL |
| 30 | BP | 36 | LYS |
| 31 | BQ | 43 | ALA |
| 36 | BU | 5 | ARG |
| 38 | BW | 28 | LYS |
| 39 | BX | 51 | PHE |
| 53 | BF | 6 | LYS |
| 53 | BF | 46 | GLN |
| 54 | BG | 80 | GLN |
| 3 | AL | 75 | GLU |
| 31 | BQ | 58 | LYS |
| 35 | BD | 162 | GLN |
| 36 | BU | 102 | LYS |
| 37 | BV | 91 | GLN |
| 39 | BX | 69 | ARG |
| 42 | B0 | 23 | LYS |
| 52 | B9 | 16 | ILE |
| 1 | AJ | 42 | LEU |
| 3 | AL | 43 | LYS |
| 11 | AB | 17 | HIS |
| 25 | BC | 166 | ASP |
| 26 | BJ | 70 | CYS |
| 37 | BV | 53 | PHE |
| 42 | B0 | 68 | PHE |
| 45 | BE | 119 | ALA |
| 45 | BE | 167 | ASN |
| 54 | BG | 81 | GLY |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 54 | BG | 88 | VAL |
| 54 | BG | 103 | ILE |
| 55 | BH | 94 | ARG |
| 29 | BO | 5 | GLN |
| 32 | BR | 80 | PHE |
| 37 | BV | 101 | ILE |
| 39 | BX | 74 | ILE |
| 45 | BE | 113 | SER |
| 48 | B5 | 54 | ILE |
| 53 | BF | 183 | PHE |
| 54 | BG | 35 | LEU |
| 1 | AJ | 74 | VAL |
| 34 | BT | 32 | VAL |
| 45 | BE | 117 | GLY |
| 52 | B9 | 7 | VAL |
| 29 | BO | 93 | GLN |
| 29 | BO | 122 | VAL |
| 5 | AN | 71 | GLY |
| 13 | AU | 2 | 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 | AJ | 90/90 (100%) | 88 (98%) | 2 (2%) | 52 | 71 |
| 2 | AK | 98/98 (100%) | 97 (99%) | 1 (1%) | 76 | 86 |
| 3 | AL | 103/103 (100%) | 102 (99%) | 1 (1%) | 76 | 86 |
| 4 | AM | 95/95 (100%) | 95 (100%) | 0 | 100 | 100 |
| 5 | AN | 83/83 (100%) | 82 (99%) | 1 (1%) | 71 | 83 |
| 6 | AO | 76/76 (100%) | 74 (97%) | 2 (3%) | 46 | 66 |
| 7 | AP | 65/65 (100%) | 64 (98%) | 1 (2%) | 65 | 80 |
| 8 | AQ | 77/77 (100%) | 75 (97%) | 2 (3%) | 46 | 66 |
| 9 | AR | 64/64 (100%) | 62 (97%) | 2 (3%) | 40 | 62 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 10 | AS | 78/78 (100%) | 74 (95%) | 4 (5%) | 24 | 48 |
| 11 | AB | 198/198 (100%) | 196 (99%) | 2 (1%) | 76 | 86 |
| 12 | AT | 65/65 (100%) | 65 (100%) | 0 | 100 | 100 |
| 13 | AU | 60/60 (100%) | 58 (97%) | 2 (3%) | 38 | 61 |
| 14 | AC | 189/189 (100%) | 181 (96%) | 8 (4%) | 30 | 54 |
| 15 | AD | 172/172 (100%) | 168 (98%) | 4 (2%) | 50 | 70 |
| 16 | AE | 125/125 (100%) | 119 (95%) | 6 (5%) | 25 | 51 |
| 17 | AF | 116/116 (100%) | 111 (96%) | 5 (4%) | 29 | 53 |
| 18 | AG | 146/146 (100%) | 143 (98%) | 3 (2%) | 53 | 72 |
| 19 | AH | 104/104 (100%) | 101 (97%) | 3 (3%) | 42 | 64 |
| 20 | AI | 106/106 (100%) | 102 (96%) | 4 (4%) | 33 | 57 |
| 21 | A1 | 568/568 (100%) | 559 (98%) | 9 (2%) | 62 | 79 |
| 25 | BC | 181/181 (100%) | 174 (96%) | 7 (4%) | 32 | 56 |
| 26 | BJ | 122/122 (100%) | 120 (98%) | 2 (2%) | 62 | 79 |
| 27 | BK | 109/109 (100%) | 106 (97%) | 3 (3%) | 43 | 65 |
| 28 | BN | 116/116 (100%) | 110 (95%) | 6 (5%) | 23 | 48 |
| 29 | BO | 104/104 (100%) | 95 (91%) | 9 (9%) | 10 | 31 |
| 30 | BP | 103/103 (100%) | 96 (93%) | 7 (7%) | 16 | 41 |
| 31 | BQ | 109/109 (100%) | 105 (96%) | 4 (4%) | 34 | 58 |
| 32 | BR | 103/103 (100%) | 100 (97%) | 3 (3%) | 42 | 64 |
| 33 | BS | 87/87 (100%) | 86 (99%) | 1 (1%) | 73 | 84 |
| 34 | BT | 99/99 (100%) | 97 (98%) | 2 (2%) | 55 | 74 |
| 35 | BD | 217/217 (100%) | 212 (98%) | 5 (2%) | 50 | 70 |
| 36 | BU | 89/89 (100%) | 86 (97%) | 3 (3%) | 37 | 60 |
| 37 | BV | 84/84 (100%) | 83 (99%) | 1 (1%) | 71 | 83 |
| 38 | BW | 93/93 (100%) | 90 (97%) | 3 (3%) | 39 | 61 |
| 39 | BX | 84/84 (100%) | 83 (99%) | 1 (1%) | 71 | 83 |
| 40 | BY | 84/84 (100%) | 82 (98%) | 2 (2%) | 49 | 69 |
| 41 | BZ | 78/78 (100%) | 77 (99%) | 1 (1%) | 69 | 81 |
| 42 | B0 | 62/62 (100%) | 56 (90%) | 6 (10%) | 8 | 27 |
| 43 | B1 | 67/67 (100%) | 66 (98%) | 1 (2%) | 65 | 80 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 44 | B2 | 55/55 (100%) | 54 (98%) | 1 (2%) | 59 | 77 |
| 45 | BE | 164/164 (100%) | 163 (99%) | 1 (1%) | 86 | 92 |
| 46 | B3 | 48/48 (100%) | 48 (100%) | 0 | 100 | 100 |
| 47 | B4 | 62/62 (100%) | 61 (98%) | 1 (2%) | 62 | 79 |
| 48 | B5 | 47/47 (100%) | 45 (96%) | 2 (4%) | 29 | 53 |
| 49 | B6 | 48/48 (100%) | 48 (100%) | 0 | 100 | 100 |
| 50 | B7 | 38/38 (100%) | 37 (97%) | 1 (3%) | 46 | 66 |
| 51 | B8 | 51/51 (100%) | 51 (100%) | 0 | 100 | 100 |
| 52 | B9 | 34/34 (100%) | 34 (100%) | 0 | 100 | 100 |
| 53 | BF | 165/165 (100%) | 161 (98%) | 4 (2%) | 49 | 69 |
| 54 | BG | 149/149 (100%) | 141 (95%) | 8 (5%) | 22 | 47 |
| 55 | BH | 137/137 (100%) | 132 (96%) | 5 (4%) | 35 | 59 |
| 56 | BL | 114/114 (100%) | 114 (100%) | 0 | 100 | 100 |
| All | All | 5781/5781 (100%) | 5629 (97%) | 152 (3%) | 49 | 66 |

All (152) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | AJ | 37 | ARG |
| 1 | AJ | 58 | ASN |
| 2 | AK | 55 | ARG |
| 3 | AL | 49 | ARG |
| 5 | AN | 95 | LEU |
| 6 | AO | 57 | ARG |
| 6 | AO | 88 | ARG |
| 7 | AP | 47 | GLU |
| 8 | AQ | 64 | ARG |
| 8 | AQ | 68 | LYS |
| 9 | AR | 15 | GLU |
| 9 | AR | 65 | SER |
| 10 | AS | 6 | LYS |
| 10 | AS | 82 | HIS |
| 10 | AS | 86 | LYS |
| 10 | AS | 91 | LYS |
| 11 | AB | 14 | HIS |
| 11 | AB | 183 | PHE |
| 13 | AU | 19 | LYS |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 13 | AU | 68 | ARG |
| 14 | AC | 3 | LYS |
| 14 | AC | 28 | PHE |
| 14 | AC | 35 | ASP |
| 14 | AC | 48 | LYS |
| 14 | AC | 57 | GLU |
| 14 | AC | 187 | GLU |
| 14 | AC | 227 | GLN |
| 14 | AC | 231 | ARG |
| 15 | AD | 71 | PHE |
| 15 | AD | 72 | ARG |
| 15 | AD | 131 | ILE |
| 15 | AD | 187 | ARG |
| 16 | AE | 12 | GLU |
| 16 | AE | 22 | LYS |
| 16 | AE | 49 | TYR |
| 16 | AE | 92 | ARG |
| 16 | AE | 121 | ASN |
| 16 | AE | 122 | VAL |
| 17 | AF | 6 | ILE |
| 17 | AF | 69 | GLU |
| 17 | AF | 98 | GLU |
| 17 | AF | 112 | ARG |
| 17 | AF | 118 | ASN |
| 18 | AG | 143 | MET |
| 18 | AG | 150 | PHE |
| 18 | AG | 153 | TYR |
| 19 | AH | 26 | MET |
| 19 | AH | 65 | PHE |
| 19 | AH | 76 | ARG |
| 20 | AI | 26 | LYS |
| 20 | AI | 79 | ARG |
| 20 | AI | 80 | HIS |
| 20 | AI | 122 | ARG |
| 21 | A1 | 228 | ARG |
| 21 | A1 | 256 | ILE |
| 21 | A1 | 322 | GLN |
| 21 | A1 | 370 | ASP |
| 21 | A1 | 421 | MET |
| 21 | A1 | 468 | TYR |
| 21 | A1 | 490 | TYR |
| 21 | A1 | 526 | GLN |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 21 | A1 | 561 | TYR |
| 25 | BC | 39 | VAL |
| 25 | BC | 105 | LYS |
| 25 | BC | 162 | ARG |
| 25 | BC | 172 | HIS |
| 25 | BC | 186 | LYS |
| 25 | BC | 208 | TYR |
| 25 | BC | 234 | ASN |
| 26 | BJ | 55 | ARG |
| 26 | BJ | 94 | LEU |
| 27 | BK | 4 | VAL |
| 27 | BK | 45 | THR |
| 27 | BK | 87 | SER |
| 28 | BN | 2 | LYS |
| 28 | BN | 44 | TYR |
| 28 | BN | 47 | HIS |
| 28 | BN | 49 | ASP |
| 28 | BN | 61 | LYS |
| 28 | BN | 98 | GLU |
| 29 | BO | 23 | LYS |
| 29 | BO | 31 | ARG |
| 29 | BO | 47 | ILE |
| 29 | BO | 64 | ARG |
| 29 | BO | 70 | ARG |
| 29 | BO | 80 | ASP |
| 29 | BO | 107 | LEU |
| 29 | BO | 113 | MET |
| 29 | BO | 122 | VAL |
| 30 | BP | 4 | ASN |
| 30 | BP | 21 | ARG |
| 30 | BP | 33 | ARG |
| 30 | BP | 39 | LYS |
| 30 | BP | 47 | ARG |
| 30 | BP | 111 | ILE |
| 30 | BP | 126 | ARG |
| 31 | BQ | 12 | MET |
| 31 | BQ | 63 | ILE |
| 31 | BQ | 93 | VAL |
| 31 | BQ | 97 | GLN |
| 32 | BR | 1 | MET |
| 32 | BR | 16 | HIS |
| 32 | BR | 99 | LYS |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 33 | BS | 18 | LEU |
| 34 | BT | 50 | ARG |
| 34 | BT | 109 | ILE |
| 35 | BD | 200 | MET |
| 35 | BD | 211 | ARG |
| 35 | BD | 212 | TRP |
| 35 | BD | 217 | PRO |
| 35 | BD | 269 | ARG |
| 36 | BU | 4 | LYS |
| 36 | BU | 88 | GLU |
| 36 | BU | 96 | ASP |
| 37 | BV | 86 | GLN |
| 38 | BW | 60 | HIS |
| 38 | BW | 95 | ARG |
| 38 | BW | 110 | ARG |
| 39 | BX | 76 | ARG |
| 40 | BY | 46 | LYS |
| 40 | BY | 65 | GLN |
| 41 | BZ | 42 | LEU |
| 42 | B0 | 19 | ARG |
| 42 | B0 | 22 | VAL |
| 42 | B0 | 23 | LYS |
| 42 | B0 | 35 | ILE |
| 42 | B0 | 40 | ARG |
| 42 | B0 | 49 | ASN |
| 43 | B1 | 26 | ARG |
| 44 | B2 | 47 | ARG |
| 45 | BE | 128 | ARG |
| 47 | B4 | 63 | ARG |
| 48 | B5 | 6 | LYS |
| 48 | B5 | 32 | THR |
| 50 | B7 | 1 | MET |
| 53 | BF | 60 | TRP |
| 53 | BF | 67 | ARG |
| 53 | BF | 88 | ARG |
| 53 | BF | 152 | GLU |
| 54 | BG | 34 | THR |
| 54 | BG | 65 | LEU |
| 54 | BG | 91 | ARG |
| 54 | BG | 94 | ARG |
| 54 | BG | 103 | ILE |
| 54 | BG | 111 | ARG |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 54 | BG | 119 | LYS |
| 54 | BG | 134 | GLN |
| 55 | BH | 2 | ARG |
| 55 | BH | 68 | ARG |
| 55 | BH | 104 | LEU |
| 55 | BH | 154 | GLU |
| 55 | BH | 166 | GLU |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA (i)

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 22 | AA | 1538/1542 (99%) | 194 (12%) | 57 (3%) |
| 23 | A2 | 46/47 (97%) | 13 (28%) | 1 (2%) |
| 24 | A3 | 75/77 (97%) | 12 (16%) | 2 (2%) |
| 57 | BA | 2899/2904 (99%) | 404 (13%) | 115 (3%) |
| 58 | Ba | 119/120 (99%) | 11 (9%) | 0 |
| All | All | 4677/4690 (99%) | 634 (13%) | 175 (3%) |

All (634) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 22 | AA | 2 | A |
| 22 | AA | 3 | A |
| 22 | AA | 5 | U |
| 22 | AA | 6 | G |
| 22 | AA | 7 | A |
| 22 | AA | 8 | A |
| 22 | AA | 9 | G |
| 22 | AA | 32 | A |
| 22 | AA | 39 | G |
| 22 | AA | 48 | C |
| 22 | AA | 49 | U |
| 22 | AA | 50 | A |
| 22 | AA | 52 | C |
| 22 | AA | 55 | A |
| 22 | AA | 56 | U |
| 22 | AA | 60 | A |
| 22 | AA | 84 | U |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 22 | AA | 108 | G |
| 22 | AA | 109 | A |
| 22 | AA | 120 | A |
| 22 | AA | 131 | A |
| 22 | AA | 144 | G |
| 22 | AA | 149 | A |
| 22 | AA | 153 | C |
| 22 | AA | 163 | C |
| 22 | AA | 184 | G |
| 22 | AA | 204 | G |
| 22 | AA | 214 | C |
| 22 | AA | 243 | A |
| 22 | AA | 244 | U |
| 22 | AA | 247 | G |
| 22 | AA | 250 | A |
| 22 | AA | 251 | G |
| 22 | AA | 262 | A |
| 22 | AA | 263 | A |
| 22 | AA | 266 | G |
| 22 | AA | 267 | C |
| 22 | AA | 280 | C |
| 22 | AA | 289 | G |
| 22 | AA | 298 | A |
| 22 | AA | 328 | C |
| 22 | AA | 329 | A |
| 22 | AA | 330 | C |
| 22 | AA | 332 | G |
| 22 | AA | 347 | G |
| 22 | AA | 352 | C |
| 22 | AA | 353 | A |
| 22 | AA | 354 | G |
| 22 | AA | 367 | U |
| 22 | AA | 368 | U |
| 22 | AA | 372 | C |
| 22 | AA | 373 | A |
| 22 | AA | 381 | C |
| 22 | AA | 390 | U |
| 22 | AA | 398 | U |
| 22 | AA | 406 | G |
| 22 | AA | 412 | A |
| 22 | AA | 413 | G |
| 22 | AA | 422 | C |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 22 | AA | 429 | U |
| 22 | AA | 451 | A |
| 22 | AA | 464 | U |
| 22 | AA | 465 | A |
| 22 | AA | 466 | A |
| 22 | AA | 468 | A |
| 22 | AA | 481 | G |
| 22 | AA | 482 | A |
| 22 | AA | 484 | G |
| 22 | AA | 486 | U |
| 22 | AA | 487 | A |
| 22 | AA | 494 | G |
| 22 | AA | 496 | A |
| 22 | AA | 498 | A |
| 22 | AA | 505 | G |
| 22 | AA | 508 | U |
| 22 | AA | 511 | C |
| 22 | AA | 512 | U |
| 22 | AA | 518 | C |
| 22 | AA | 519 | C |
| 22 | AA | 520 | A |
| 22 | AA | 524 | G |
| 22 | AA | 527 | 7MG |
| 22 | AA | 531 | U |
| 22 | AA | 532 | A |
| 22 | AA | 547 | A |
| 22 | AA | 559 | A |
| 22 | AA | 564 | C |
| 22 | AA | 566 | G |
| 22 | AA | 572 | A |
| 22 | AA | 573 | A |
| 22 | AA | 576 | C |
| 22 | AA | 631 | C |
| 22 | AA | 633 | G |
| 22 | AA | 665 | A |
| 22 | AA | 688 | G |
| 22 | AA | 695 | A |
| 22 | AA | 718 | A |
| 22 | AA | 719 | C |
| 22 | AA | 720 | C |
| 22 | AA | 721 | G |
| 22 | AA | 723 | U |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 22 | AA | 755 | G |
| 22 | AA | 766 | A |
| 22 | AA | 812 | G |
| 22 | AA | 817 | C |
| 22 | AA | 821 | G |
| 22 | AA | 828 | U |
| 22 | AA | 840 | C |
| 22 | AA | 841 | C |
| 22 | AA | 843 | U |
| 22 | AA | 846 | G |
| 22 | AA | 874 | G |
| 22 | AA | 885 | G |
| 22 | AA | 889 | A |
| 22 | AA | 890 | G |
| 22 | AA | 914 | A |
| 22 | AA | 927 | G |
| 22 | AA | 934 | C |
| 22 | AA | 935 | A |
| 22 | AA | 938 | A |
| 22 | AA | 960 | U |
| 22 | AA | 962 | C |
| 22 | AA | 966 | 2MG |
| 22 | AA | 968 | A |
| 22 | AA | 969 | A |
| 22 | AA | 975 | A |
| 22 | AA | 977 | A |
| 22 | AA | 981 | U |
| 22 | AA | 993 | G |
| 22 | AA | 1004 | A |
| 22 | AA | 1026 | G |
| 22 | AA | 1044 | A |
| 22 | AA | 1050 | G |
| 22 | AA | 1051 | C |
| 22 | AA | 1064 | G |
| 22 | AA | 1065 | U |
| 22 | AA | 1094 | G |
| 22 | AA | 1101 | A |
| 22 | AA | 1102 | A |
| 22 | AA | 1110 | A |
| 22 | AA | 1136 | C |
| 22 | AA | 1138 | G |
| 22 | AA | 1139 | G |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 22 | AA | 1140 | C |
| 22 | AA | 1152 | A |
| 22 | AA | 1159 | U |
| 22 | AA | 1168 | U |
| 22 | AA | 1169 | A |
| 22 | AA | 1183 | U |
| 22 | AA | 1184 | G |
| 22 | AA | 1191 | A |
| 22 | AA | 1196 | A |
| 22 | AA | 1212 | U |
| 22 | AA | 1214 | C |
| 22 | AA | 1215 | G |
| 22 | AA | 1228 | C |
| 22 | AA | 1238 | A |
| 22 | AA | 1241 | G |
| 22 | AA | 1256 | A |
| 22 | AA | 1257 | A |
| 22 | AA | 1258 | G |
| 22 | AA | 1279 | G |
| 22 | AA | 1280 | A |
| 22 | AA | 1281 | C |
| 22 | AA | 1285 | A |
| 22 | AA | 1297 | G |
| 22 | AA | 1302 | C |
| 22 | AA | 1303 | C |
| 22 | AA | 1305 | G |
| 22 | AA | 1306 | A |
| 22 | AA | 1319 | A |
| 22 | AA | 1320 | C |
| 22 | AA | 1322 | C |
| 22 | AA | 1340 | A |
| 22 | AA | 1346 | A |
| 22 | AA | 1359 | C |
| 22 | AA | 1360 | A |
| 22 | AA | 1398 | A |
| 22 | AA | 1401 | G |
| 22 | AA | 1447 | A |
| 22 | AA | 1491 | G |
| 22 | AA | 1492 | A |
| 22 | AA | 1493 | A |
| 22 | AA | 1502 | A |
| 22 | AA | 1503 | A |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 22 | AA | 1506 | U |
| 22 | AA | 1507 | A |
| 22 | AA | 1529 | G |
| 22 | AA | 1530 | G |
| 22 | AA | 1535 | C |
| 22 | AA | 1537 | U |
| 22 | AA | 1539 | C |
| 22 | AA | 1540 | U |
| 22 | AA | 1542 | A |
| 23 | A2 | 14 | G |
| 23 | A2 | 16 | A |
| 23 | A2 | 19 | A |
| 23 | A2 | 21 | U |
| 23 | A2 | 25 | U |
| 23 | A2 | 26 | U |
| 23 | A2 | 27 | A |
| 23 | A2 | 29 | G |
| 23 | A2 | 30 | U |
| 23 | A2 | 34 | U |
| 23 | A2 | 46 | C |
| 23 | A2 | 47 | C |
| 23 | A2 | 56 | G |
| 24 | A3 | 2 | G |
| 24 | A3 | 9 | G |
| 24 | A3 | 10 | G |
| 24 | A3 | 16 | C |
| 24 | A3 | 17 | C |
| 24 | A3 | 21 | H2U |
| 24 | A3 | 39 | A |
| 24 | A3 | 49 | C |
| 24 | A3 | 74 | A |
| 24 | A3 | 75 | C |
| 24 | A3 | 76 | C |
| 24 | A3 | 77 | A |
| 57 | BA | 13 | A |
| 57 | BA | 35 | G |
| 57 | BA | 61 | C |
| 57 | BA | 62 | U |
| 57 | BA | 71 | A |
| 57 | BA | 74 | A |
| 57 | BA | 75 | G |
| 57 | BA | 91 | A |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 57 | BA | 98 | G |
| 57 | BA | 100 | U |
| 57 | BA | 119 | A |
| 57 | BA | 120 | U |
| 57 | BA | 139 | U |
| 57 | BA | 140 | C |
| 57 | BA | 149 | A |
| 57 | BA | 163 | C |
| 57 | BA | 180 | G |
| 57 | BA | 196 | A |
| 57 | BA | 197 | A |
| 57 | BA | 199 | A |
| 57 | BA | 204 | A |
| 57 | BA | 205 | G |
| 57 | BA | 216 | A |
| 57 | BA | 222 | A |
| 57 | BA | 230 | G |
| 57 | BA | 242 | G |
| 57 | BA | 243 | U |
| 57 | BA | 248 | G |
| 57 | BA | 250 | G |
| 57 | BA | 265 | A |
| 57 | BA | 266 | G |
| 57 | BA | 271 | G |
| 57 | BA | 272 | A |
| 57 | BA | 277 | G |
| 57 | BA | 299 | A |
| 57 | BA | 311 | A |
| 57 | BA | 324 | A |
| 57 | BA | 330 | A |
| 57 | BA | 332 | A |
| 57 | BA | 333 | G |
| 57 | BA | 338 | G |
| 57 | BA | 360 | U |
| 57 | BA | 361 | G |
| 57 | BA | 368 | A |
| 57 | BA | 372 | G |
| 57 | BA | 386 | G |
| 57 | BA | 387 | U |
| 57 | BA | 388 | G |
| 57 | BA | 394 | C |
| 57 | BA | 395 | U |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 57 | BA | 396 | G |
| 57 | BA | 406 | G |
| 57 | BA | 411 | G |
| 57 | BA | 424 | G |
| 57 | BA | 435 | C |
| 57 | BA | 451 | U |
| 57 | BA | 454 | A |
| 57 | BA | 458 | G |
| 57 | BA | 480 | A |
| 57 | BA | 481 | G |
| 57 | BA | 482 | A |
| 57 | BA | 489 | G |
| 57 | BA | 490 | C |
| 57 | BA | 491 | G |
| 57 | BA | 504 | A |
| 57 | BA | 505 | A |
| 57 | BA | 531 | C |
| 57 | BA | 532 | A |
| 57 | BA | 533 | G |
| 57 | BA | 544 | C |
| 57 | BA | 545 | U |
| 57 | BA | 546 | U |
| 57 | BA | 550 | C |
| 57 | BA | 562 | U |
| 57 | BA | 573 | U |
| 57 | BA | 575 | A |
| 57 | BA | 588 | U |
| 57 | BA | 603 | A |
| 57 | BA | 604 | G |
| 57 | BA | 613 | A |
| 57 | BA | 615 | U |
| 57 | BA | 637 | A |
| 57 | BA | 638 | G |
| 57 | BA | 652 | U |
| 57 | BA | 654 | A |
| 57 | BA | 671 | C |
| 57 | BA | 686 | U |
| 57 | BA | 718 | A |
| 57 | BA | 719 | C |
| 57 | BA | 730 | A |
| 57 | BA | 747 | 5MU |
| 57 | BA | 752 | A |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 57 | BA | 764 | A |
| 57 | BA | 776 | G |
| 57 | BA | 781 | A |
| 57 | BA | 782 | A |
| 57 | BA | 783 | A |
| 57 | BA | 784 | G |
| 57 | BA | 789 | A |
| 57 | BA | 790 | U |
| 57 | BA | 791 | C |
| 57 | BA | 792 | A |
| 57 | BA | 805 | G |
| 57 | BA | 812 | C |
| 57 | BA | 846 | U |
| 57 | BA | 850 | U |
| 57 | BA | 851 | C |
| 57 | BA | 859 | G |
| 57 | BA | 866 | A |
| 57 | BA | 887 | U |
| 57 | BA | 890 | C |
| 57 | BA | 896 | A |
| 57 | BA | 901 | C |
| 57 | BA | 910 | A |
| 57 | BA | 914 | G |
| 57 | BA | 915 | C |
| 57 | BA | 920 | A |
| 57 | BA | 945 | A |
| 57 | BA | 946 | C |
| 57 | BA | 961 | C |
| 57 | BA | 974 | G |
| 57 | BA | 995 | C |
| 57 | BA | 996 | A |
| 57 | BA | 1009 | A |
| 57 | BA | 1012 | U |
| 57 | BA | 1019 | U |
| 57 | BA | 1020 | A |
| 57 | BA | 1022 | G |
| 57 | BA | 1025 | G |
| 57 | BA | 1033 | U |
| 57 | BA | 1046 | A |
| 57 | BA | 1047 | G |
| 57 | BA | 1048 | A |
| 57 | BA | 1057 | A |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 57 | BA | 1062 | G |
| 57 | BA | 1065 | U |
| 57 | BA | 1066 | U |
| 57 | BA | 1068 | G |
| 57 | BA | 1069 | A |
| 57 | BA | 1070 | A |
| 57 | BA | 1071 | G |
| 57 | BA | 1073 | A |
| 57 | BA | 1078 | U |
| 57 | BA | 1079 | C |
| 57 | BA | 1087 | G |
| 57 | BA | 1088 | A |
| 57 | BA | 1095 | A |
| 57 | BA | 1096 | A |
| 57 | BA | 1098 | A |
| 57 | BA | 1112 | G |
| 57 | BA | 1128 | G |
| 57 | BA | 1129 | A |
| 57 | BA | 1130 | U |
| 57 | BA | 1132 | U |
| 57 | BA | 1133 | A |
| 57 | BA | 1135 | C |
| 57 | BA | 1143 | A |
| 57 | BA | 1155 | A |
| 57 | BA | 1175 | A |
| 57 | BA | 1176 | U |
| 57 | BA | 1177 | G |
| 57 | BA | 1212 | G |
| 57 | BA | 1225 | G |
| 57 | BA | 1238 | G |
| 57 | BA | 1241 | A |
| 57 | BA | 1248 | G |
| 57 | BA | 1254 | A |
| 57 | BA | 1255 | U |
| 57 | BA | 1256 | G |
| 57 | BA | 1257 | C |
| 57 | BA | 1266 | G |
| 57 | BA | 1271 | G |
| 57 | BA | 1272 | A |
| 57 | BA | 1273 | U |
| 57 | BA | 1287 | A |
| 57 | BA | 1300 | G |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 57 | BA | 1301 | A |
| 57 | BA | 1302 | A |
| 57 | BA | 1303 | G |
| 57 | BA | 1314 | C |
| 57 | BA | 1324 | G |
| 57 | BA | 1329 | U |
| 57 | BA | 1332 | G |
| 57 | BA | 1333 | G |
| 57 | BA | 1341 | G |
| 57 | BA | 1348 | C |
| 57 | BA | 1349 | C |
| 57 | BA | 1350 | C |
| 57 | BA | 1365 | A |
| 57 | BA | 1366 | A |
| 57 | BA | 1379 | U |
| 57 | BA | 1383 | A |
| 57 | BA | 1384 | A |
| 57 | BA | 1386 | C |
| 57 | BA | 1394 | U |
| 57 | BA | 1396 | U |
| 57 | BA | 1416 | G |
| 57 | BA | 1417 | C |
| 57 | BA | 1451 | C |
| 57 | BA | 1452 | G |
| 57 | BA | 1455 | G |
| 57 | BA | 1458 | U |
| 57 | BA | 1459 | G |
| 57 | BA | 1475 | G |
| 57 | BA | 1482 | G |
| 57 | BA | 1493 | C |
| 57 | BA | 1508 | A |
| 57 | BA | 1509 | A |
| 57 | BA | 1524 | G |
| 57 | BA | 1552 | A |
| 57 | BA | 1568 | G |
| 57 | BA | 1569 | A |
| 57 | BA | 1598 | A |
| 57 | BA | 1607 | C |
| 57 | BA | 1608 | A |
| 57 | BA | 1610 | A |
| 57 | BA | 1611 | C |
| 57 | BA | 1619 | G |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 57 | BA | 1646 | C |
| 57 | BA | 1647 | U |
| 57 | BA | 1648 | U |
| 57 | BA | 1654 | A |
| 57 | BA | 1669 | A |
| 57 | BA | 1674 | G |
| 57 | BA | 1700 | A |
| 57 | BA | 1713 | A |
| 57 | BA | 1729 | U |
| 57 | BA | 1730 | C |
| 57 | BA | 1732 | C |
| 57 | BA | 1733 | G |
| 57 | BA | 1758 | U |
| 57 | BA | 1762 | A |
| 57 | BA | 1764 | C |
| 57 | BA | 1773 | A |
| 57 | BA | 1791 | A |
| 57 | BA | 1800 | C |
| 57 | BA | 1816 | C |
| 57 | BA | 1839 | G |
| 57 | BA | 1900 | A |
| 57 | BA | 1901 | A |
| 57 | BA | 1906 | G |
| 57 | BA | 1912 | A |
| 57 | BA | 1914 | C |
| 57 | BA | 1916 | A |
| 57 | BA | 1919 | A |
| 57 | BA | 1928 | A |
| 57 | BA | 1930 | G |
| 57 | BA | 1937 | A |
| 57 | BA | 1941 | C |
| 57 | BA | 1942 | C |
| 57 | BA | 1955 | U |
| 57 | BA | 1964 | G |
| 57 | BA | 1965 | C |
| 57 | BA | 1966 | A |
| 57 | BA | 1970 | A |
| 57 | BA | 1971 | U |
| 57 | BA | 1972 | G |
| 57 | BA | 1982 | U |
| 57 | BA | 1992 | G |
| 57 | BA | 1993 | U |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 57 | BA | 1998 | A |
| 57 | BA | 2023 | C |
| 57 | BA | 2031 | A |
| 57 | BA | 2032 | G |
| 57 | BA | 2056 | G |
| 57 | BA | 2061 | G |
| 57 | BA | 2062 | A |
| 57 | BA | 2068 | U |
| 57 | BA | 2069 | 7MG |
| 57 | BA | 2076 | U |
| 57 | BA | 2077 | A |
| 57 | BA | 2092 | U |
| 57 | BA | 2111 | U |
| 57 | BA | 2112 | G |
| 57 | BA | 2113 | U |
| 57 | BA | 2116 | G |
| 57 | BA | 2117 | A |
| 57 | BA | 2118 | U |
| 57 | BA | 2119 | A |
| 57 | BA | 2126 | A |
| 57 | BA | 2127 | G |
| 57 | BA | 2130 | U |
| 57 | BA | 2131 | U |
| 57 | BA | 2132 | U |
| 57 | BA | 2133 | G |
| 57 | BA | 2134 | A |
| 57 | BA | 2146 | C |
| 57 | BA | 2147 | A |
| 57 | BA | 2148 | G |
| 57 | BA | 2154 | A |
| 57 | BA | 2158 | A |
| 57 | BA | 2164 | C |
| 57 | BA | 2165 | C |
| 57 | BA | 2170 | A |
| 57 | BA | 2198 | A |
| 57 | BA | 2203 | U |
| 57 | BA | 2212 | A |
| 57 | BA | 2213 | U |
| 57 | BA | 2239 | G |
| 57 | BA | 2249 | U |
| 57 | BA | 2250 | G |
| 57 | BA | 2251 | OMG |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 57 | BA | 2253 | G |
| 57 | BA | 2254 | C |
| 57 | BA | 2266 | A |
| 57 | BA | 2276 | G |
| 57 | BA | 2282 | G |
| 57 | BA | 2283 | C |
| 57 | BA | 2287 | A |
| 57 | BA | 2288 | A |
| 57 | BA | 2289 | G |
| 57 | BA | 2306 | C |
| 57 | BA | 2307 | G |
| 57 | BA | 2308 | G |
| 57 | BA | 2309 | A |
| 57 | BA | 2312 | U |
| 57 | BA | 2321 | U |
| 57 | BA | 2325 | G |
| 57 | BA | 2327 | A |
| 57 | BA | 2333 | A |
| 57 | BA | 2334 | U |
| 57 | BA | 2335 | A |
| 57 | BA | 2336 | A |
| 57 | BA | 2337 | G |
| 57 | BA | 2345 | G |
| 57 | BA | 2346 | A |
| 57 | BA | 2347 | C |
| 57 | BA | 2382 | G |
| 57 | BA | 2383 | G |
| 57 | BA | 2385 | C |
| 57 | BA | 2390 | U |
| 57 | BA | 2402 | U |
| 57 | BA | 2403 | C |
| 57 | BA | 2423 | U |
| 57 | BA | 2424 | C |
| 57 | BA | 2425 | A |
| 57 | BA | 2426 | A |
| 57 | BA | 2428 | G |
| 57 | BA | 2429 | G |
| 57 | BA | 2431 | U |
| 57 | BA | 2433 | A |
| 57 | BA | 2435 | A |
| 57 | BA | 2439 | A |
| 57 | BA | 2441 | U |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 57 | BA | 2447 | G |
| 57 | BA | 2448 | A |
| 57 | BA | 2449 | H2U |
| 57 | BA | 2452 | C |
| 57 | BA | 2472 | G |
| 57 | BA | 2476 | A |
| 57 | BA | 2478 | A |
| 57 | BA | 2489 | U |
| 57 | BA | 2490 | G |
| 57 | BA | 2491 | U |
| 57 | BA | 2492 | U |
| 57 | BA | 2493 | U |
| 57 | BA | 2501 | C |
| 57 | BA | 2502 | G |
| 57 | BA | 2504 | PSU |
| 57 | BA | 2505 | G |
| 57 | BA | 2507 | C |
| 57 | BA | 2513 | A |
| 57 | BA | 2518 | A |
| 57 | BA | 2519 | U |
| 57 | BA | 2529 | G |
| 57 | BA | 2534 | A |
| 57 | BA | 2555 | U |
| 57 | BA | 2565 | A |
| 57 | BA | 2566 | A |
| 57 | BA | 2572 | A |
| 57 | BA | 2573 | C |
| 57 | BA | 2574 | G |
| 57 | BA | 2577 | A |
| 57 | BA | 2585 | U |
| 57 | BA | 2599 | G |
| 57 | BA | 2602 | A |
| 57 | BA | 2613 | U |
| 57 | BA | 2629 | U |
| 57 | BA | 2654 | A |
| 57 | BA | 2658 | C |
| 57 | BA | 2659 | G |
| 57 | BA | 2661 | G |
| 57 | BA | 2663 | G |
| 57 | BA | 2685 | G |
| 57 | BA | 2689 | U |
| 57 | BA | 2690 | U |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 57 | BA | 2714 | G |
| 57 | BA | 2733 | A |
| 57 | BA | 2757 | A |
| 57 | BA | 2778 | A |
| 57 | BA | 2791 | G |
| 57 | BA | 2792 | A |
| 57 | BA | 2797 | U |
| 57 | BA | 2799 | A |
| 57 | BA | 2800 | A |
| 57 | BA | 2820 | A |
| 57 | BA | 2823 | A |
| 57 | BA | 2834 | G |
| 57 | BA | 2850 | A |
| 57 | BA | 2886 | A |
| 57 | BA | 2894 | G |
| 57 | BA | 2895 | G |
| 57 | BA | 2903 | U |
| 57 | BA | 2904 | U |
| 58 | Ba | 12 | C |
| 58 | Ba | 13 | G |
| 58 | Ba | 14 | U |
| 58 | Ba | 15 | A |
| 58 | Ba | 25 | U |
| 58 | Ba | 41 | G |
| 58 | Ba | 42 | C |
| 58 | Ba | 90 | C |
| 58 | Ba | 99 | A |
| 58 | Ba | 109 | A |
| 58 | Ba | 120 | U |

All (175) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 22 | AA | 2 | A |
| 22 | AA | 3 | A |
| 22 | AA | 5 | U |
| 22 | AA | 6 | G |
| 22 | AA | 13 | U |
| 22 | AA | 48 | C |
| 22 | AA | 49 | U |
| 22 | AA | 51 | A |
| 22 | AA | 71 | A |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 22 | AA | 121 | U |
| 22 | AA | 161 | A |
| 22 | AA | 197 | A |
| 22 | AA | 205 | A |
| 22 | AA | 243 | A |
| 22 | AA | 262 | A |
| 22 | AA | 279 | A |
| 22 | AA | 297 | G |
| 22 | AA | 305 | G |
| 22 | AA | 328 | C |
| 22 | AA | 329 | A |
| 22 | AA | 331 | G |
| 22 | AA | 367 | U |
| 22 | AA | 372 | C |
| 22 | AA | 412 | A |
| 22 | AA | 451 | A |
| 22 | AA | 464 | U |
| 22 | AA | 465 | A |
| 22 | AA | 497 | G |
| 22 | AA | 531 | U |
| 22 | AA | 575 | G |
| 22 | AA | 619 | U |
| 22 | AA | 700 | G |
| 22 | AA | 717 | U |
| 22 | AA | 719 | C |
| 22 | AA | 765 | G |
| 22 | AA | 812 | G |
| 22 | AA | 840 | C |
| 22 | AA | 845 | A |
| 22 | AA | 934 | C |
| 22 | AA | 974 | A |
| 22 | AA | 1101 | A |
| 22 | AA | 1183 | U |
| 22 | AA | 1213 | A |
| 22 | AA | 1214 | C |
| 22 | AA | 1225 | A |
| 22 | AA | 1238 | A |
| 22 | AA | 1256 | A |
| 22 | AA | 1281 | C |
| 22 | AA | 1302 | C |
| 22 | AA | 1305 | G |
| 22 | AA | 1319 | A |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 22 | AA | 1380 | U |
| 22 | AA | 1397 | C |
| 22 | AA | 1491 | G |
| 22 | AA | 1529 | G |
| 22 | AA | 1537 | U |
| 22 | AA | 1539 | C |
| 23 | A2 | 33 | A |
| 24 | A3 | 9 | G |
| 24 | A3 | 10 | G |
| 57 | BA | 13 | A |
| 57 | BA | 48 | G |
| 57 | BA | 61 | C |
| 57 | BA | 119 | A |
| 57 | BA | 121 | G |
| 57 | BA | 140 | C |
| 57 | BA | 190 | A |
| 57 | BA | 196 | A |
| 57 | BA | 242 | G |
| 57 | BA | 249 | C |
| 57 | BA | 301 | G |
| 57 | BA | 311 | A |
| 57 | BA | 332 | A |
| 57 | BA | 387 | U |
| 57 | BA | 394 | C |
| 57 | BA | 395 | U |
| 57 | BA | 479 | A |
| 57 | BA | 489 | G |
| 57 | BA | 529 | A |
| 57 | BA | 544 | C |
| 57 | BA | 545 | U |
| 57 | BA | 561 | G |
| 57 | BA | 587 | C |
| 57 | BA | 603 | A |
| 57 | BA | 620 | G |
| 57 | BA | 637 | A |
| 57 | BA | 651 | G |
| 57 | BA | 653 | U |
| 57 | BA | 718 | A |
| 57 | BA | 752 | A |
| 57 | BA | 782 | A |
| 57 | BA | 804 | A |
| 57 | BA | 850 | U |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 57 | BA | 859 | G |
| 57 | BA | 866 | A |
| 57 | BA | 896 | A |
| 57 | BA | 920 | A |
| 57 | BA | 958 | U |
| 57 | BA | 960 | A |
| 57 | BA | 995 | C |
| 57 | BA | 1019 | U |
| 57 | BA | 1033 | U |
| 57 | BA | 1061 | U |
| 57 | BA | 1078 | U |
| 57 | BA | 1088 | A |
| 57 | BA | 1095 | A |
| 57 | BA | 1128 | G |
| 57 | BA | 1133 | A |
| 57 | BA | 1142 | A |
| 57 | BA | 1254 | A |
| 57 | BA | 1256 | G |
| 57 | BA | 1286 | A |
| 57 | BA | 1301 | A |
| 57 | BA | 1313 | U |
| 57 | BA | 1324 | G |
| 57 | BA | 1325 | U |
| 57 | BA | 1332 | G |
| 57 | BA | 1349 | C |
| 57 | BA | 1365 | A |
| 57 | BA | 1393 | A |
| 57 | BA | 1451 | C |
| 57 | BA | 1458 | U |
| 57 | BA | 1474 | U |
| 57 | BA | 1508 | A |
| 57 | BA | 1568 | G |
| 57 | BA | 1607 | C |
| 57 | BA | 1610 | A |
| 57 | BA | 1614 | A |
| 57 | BA | 1646 | C |
| 57 | BA | 1647 | U |
| 57 | BA | 1653 | G |
| 57 | BA | 1668 | A |
| 57 | BA | 1674 | G |
| 57 | BA | 1729 | U |
| 57 | BA | 1758 | U |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 57 | BA | 1786 | A |
| 57 | BA | 1929 | G |
| 57 | BA | 1937 | A |
| 57 | BA | 1939 | 5MU |
| 57 | BA | 1941 | C |
| 57 | BA | 2042 | A |
| 57 | BA | 2060 | A |
| 57 | BA | 2061 | G |
| 57 | BA | 2062 | A |
| 57 | BA | 2068 | U |
| 57 | BA | 2076 | U |
| 57 | BA | 2092 | U |
| 57 | BA | 2117 | A |
| 57 | BA | 2131 | U |
| 57 | BA | 2133 | G |
| 57 | BA | 2248 | C |
| 57 | BA | 2251 | OMG |
| 57 | BA | 2253 | G |
| 57 | BA | 2308 | G |
| 57 | BA | 2336 | A |
| 57 | BA | 2345 | G |
| 57 | BA | 2402 | U |
| 57 | BA | 2422 | C |
| 57 | BA | 2423 | U |
| 57 | BA | 2430 | A |
| 57 | BA | 2440 | C |
| 57 | BA | 2447 | G |
| 57 | BA | 2489 | U |
| 57 | BA | 2529 | G |
| 57 | BA | 2564 | A |
| 57 | BA | 2571 | U |
| 57 | BA | 2615 | U |
| 57 | BA | 2629 | U |
| 57 | BA | 2655 | G |
| 57 | BA | 2660 | A |
| 57 | BA | 2755 | C |
| 57 | BA | 2756 | U |
| 57 | BA | 2790 | U |
| 57 | BA | 2885 | G |
| 57 | BA | 2894 | G |

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

39 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 | $\#\|Z\| > 2$ |
| 22 | UR3 | AA | 1498 | 22 | 19,22,23 | 0.71 | 0 | 26,32,35 | 1.01 | 2 (7%) |
| 24 | PSU | A3 | 56 | 24 | 18,21,22 | 0.84 | 0 | 22,30,33 | 1.12 | 2 (9%) |
| 24 | 4SU | A3 | 8 | 24 | 18,21,22 | 1.39 | 1 (5%) | 26,30,33 | 1.16 | 2 (7%) |
| 57 | 5MU | BA | 1939 | 57 | 19,22,23 | 0.72 | 0 | 28,32,35 | 1.31 | 3 (10%) |
| 57 | PSU | BA | 2504 | 57 | 18,21,22 | 0.78 | 0 | 22,30,33 | 1.15 | 2 (9%) |
| 24 | OMC | A3 | 33 | 24 | 19,22,23 | 0.70 | 0 | 26,31,34 | 1.09 | 1 (3%) |
| 57 | 6MZ | BA | 2030 | 57 | 18,25,26 | 0.92 | 1 (5%) | 16,36,39 | 1.41 | 2 (12%) |
| 57 | PSU | BA | 955 | 57 | 18,21,22 | 0.80 | 0 | 22,30,33 | 1.08 | 2 (9%) |
| 57 | 6MZ | BA | 1618 | 57 | 18,25,26 | 0.93 | 0 | 16,36,39 | 1.47 | 2 (12%) |
| 57 | PSU | BA | 1911 | 57 | 18,21,22 | 0.83 | 0 | 22,30,33 | 1.03 | 2 (9%) |
| 57 | 2MA | BA | 2503 | 57 | 17,25,26 | 1.21 | 3 (17%) | 17,37,40 | 1.60 | 3 (17%) |
| 57 | 7MG | BA | 2069 | 57 | 22,26,27 | 4.62 | 2 (9%) | 29,39,42 | 1.41 | 1 (3%) |
| 57 | PSU | BA | 2605 | 57 | 18,21,22 | 0.87 | 0 | 22,30,33 | 1.27 | 3 (13%) |
| 22 | 2MG | AA | 1207 | 22 | 18,26,27 | 1.01 | 2 (11%) | 16,38,41 | 1.11 | 2 (12%) |
| 57 | 2MG | BA | 2445 | 57 | 18,26,27 | 0.96 | 2 (11%) | 16,38,41 | 1.31 | 2 (12%) |
| 57 | H2U | BA | 2449 | 57 | 18,21,22 | 1.14 | 2 (11%) | 21,30,33 | 1.07 | 0 |
| 22 | 5MC | AA | 1407 | 22 | 18,22,23 | 0.59 | 0 | 26,32,35 | 1.38 | 4 (15%) |
| 57 | 5MC | BA | 1962 | 57 | 18,22,23 | 0.57 | 0 | 26,32,35 | 1.51 | 5 (19%) |
| 24 | 5MU | A3 | 55 | 24 | 19,22,23 | 0.67 | 0 | 28,32,35 | 1.33 | 4 (14%) |
| 57 | 3TD | BA | 1915 | 57 | 18,22,23 | 0.83 | 0 | 22,32,35 | 1.42 | 3 (13%) |
| 57 | OMG | BA | 2251 | 57 | 18,26,27 | 1.01 | 1 (5%) | 19,38,41 | 1.32 | 3 (15%) |
| 24 | H2U | A3 | 21 | 24 | 18,21,22 | 1.04 | 2 (11%) | 21,30,33 | 0.83 | 0 |
| 57 | OMU | BA | 2552 | 57 | 19,22,23 | 0.60 | 0 | 26,31,34 | 0.91 | 1 (3%) |
| 22 | PSU | AA | 516 | 22 | 18,21,22 | 0.81 | 0 | 22,30,33 | 1.24 | 2 (9%) |
| 57 | 1MG | BA | 745 | 57 | 18,26,27 | 1.08 | 2 (11%) | 19,39,42 | 1.10 | 1 (5%) |
| 22 | 5MC | AA | 967 | 22 | 18,22,23 | 0.61 | 0 | 26,32,35 | 1.44 | 4 (15%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 57 | PSU | BA | 2457 | 57 | 18,21,22 | 0.79 | 0 | 22,30,33 | 1.14 | 2 (9%) |
| 22 | 2MG | AA | 1516 | 22 | 18,26,27 | 0.93 | 1 (5%) | 16,38,41 | 1.14 | 2 (12%) |
| 57 | 5MU | BA | 747 | 57 | 19,22,23 | 0.72 | 0 | 28,32,35 | 1.34 | 3 (10%) |
| 57 | PSU | BA | 746 | 57 | 18,21,22 | 0.80 | 0 | 22,30,33 | 1.22 | 3 (13%) |
| 22 | MA6 | AA | 1519 | 22 | 19,26,27 | 0.95 | 2 (10%) | 18,38,41 | 0.93 | 0 |
| 57 | PSU | BA | 2580 | 57 | 18,21,22 | 0.82 | 0 | 22,30,33 | 1.50 | 4 (18%) |
| 22 | 7MG | AA | 527 | 22 | 22,26,27 | 4.55 | 2 (9%) | 29,39,42 | 1.47 | 2 (6%) |
| 57 | 2MG | BA | 1835 | 57 | 18,26,27 | 0.98 | 1 (5%) | 16,38,41 | 1.15 | 2 (12%) |
| 22 | MA6 | AA | 1518 | 22 | 19,26,27 | 0.94 | 1 (5%) | 18,38,41 | 0.89 | 0 |
| 22 | 2MG | AA | 966 | 22 | 18,26,27 | 1.00 | 2 (11%) | 16,38,41 | 1.28 | 2 (12%) |
| 22 | 4OC | AA | 1402 | 22 | 20,23,24 | 0.65 | 0 | 26,32,35 | 1.22 | 2 (7%) |
| 57 | PSU | BA | 1917 | 57 | 18,21,22 | 0.78 | 0 | 22,30,33 | 1.13 | 2 (9%) |
| 57 | OMC | BA | 2498 | 57 | 19,22,23 | 0.76 | 0 | 26,31,34 | 1.25 | 1 (3%) |

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 |
|---|---|---|---|---|---|---|---|
| 22 | UR3 | AA | 1498 | 22 | - | 0/7/25/26 | 0/2/2/2 |
| 24 | PSU | A3 | 56 | 24 | - | 2/7/25/26 | 0/2/2/2 |
| 24 | 4SU | A3 | 8 | 24 | - | 0/7/25/26 | 0/2/2/2 |
| 57 | 5MU | BA | 1939 | 57 | - | 0/7/25/26 | 0/2/2/2 |
| 57 | PSU | BA | 2504 | 57 | - | 2/7/25/26 | 0/2/2/2 |
| 24 | OMC | A3 | 33 | 24 | - | 0/9/27/28 | 0/2/2/2 |
| 57 | 6MZ | BA | 2030 | 57 | - | 1/5/27/28 | 0/3/3/3 |
| 57 | PSU | BA | 955 | 57 | - | 0/7/25/26 | 0/2/2/2 |
| 57 | 6MZ | BA | 1618 | 57 | - | 0/5/27/28 | 0/3/3/3 |
| 57 | PSU | BA | 1911 | 57 | - | 0/7/25/26 | 0/2/2/2 |
| 57 | 2MA | BA | 2503 | 57 | - | 1/3/25/26 | 0/3/3/3 |
| 57 | 7MG | BA | 2069 | 57 | - | 0/7/37/38 | 0/3/3/3 |
| 57 | PSU | BA | 2605 | 57 | - | 0/7/25/26 | 0/2/2/2 |
| 22 | 2MG | AA | 1207 | 22 | - | 0/5/27/28 | 0/3/3/3 |
| 57 | 2MG | BA | 2445 | 57 | - | 0/5/27/28 | 0/3/3/3 |
| 57 | H2U | BA | 2449 | 57 | - | 0/7/38/39 | 0/2/2/2 |
| 22 | 5MC | AA | 1407 | 22 | - | 0/7/25/26 | 0/2/2/2 |
| 57 | 5MC | BA | 1962 | 57 | - | 0/7/25/26 | 0/2/2/2 |
| 24 | 5MU | A3 | 55 | 24 | - | 0/7/25/26 | 0/2/2/2 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 57 | 3TD | BA | 1915 | 57 | - | 1/7/25/26 | 0/2/2/2 |
| 57 | OMG | BA | 2251 | 57 | - | 0/5/27/28 | 0/3/3/3 |
| 24 | H2U | A3 | 21 | 24 | - | 1/7/38/39 | 0/2/2/2 |
| 57 | OMU | BA | 2552 | 57 | - | 0/9/27/28 | 0/2/2/2 |
| 22 | PSU | AA | 516 | 22 | - | 0/7/25/26 | 0/2/2/2 |
| 57 | 1MG | BA | 745 | 57 | - | 0/3/25/26 | 0/3/3/3 |
| 22 | 5MC | AA | 967 | 22 | - | 0/7/25/26 | 0/2/2/2 |
| 57 | PSU | BA | 2457 | 57 | - | 0/7/25/26 | 0/2/2/2 |
| 22 | 2MG | AA | 1516 | 22 | - | 0/5/27/28 | 0/3/3/3 |
| 57 | 5MU | BA | 747 | 57 | - | 0/7/25/26 | 0/2/2/2 |
| 57 | PSU | BA | 746 | 57 | - | 0/7/25/26 | 0/2/2/2 |
| 22 | MA6 | AA | 1519 | 22 | - | 0/7/29/30 | 0/3/3/3 |
| 57 | PSU | BA | 2580 | 57 | - | 0/7/25/26 | 0/2/2/2 |
| 22 | 7MG | AA | 527 | 22 | - | 1/7/37/38 | 0/3/3/3 |
| 57 | 2MG | BA | 1835 | 57 | - | 0/5/27/28 | 0/3/3/3 |
| 22 | MA6 | AA | 1518 | 22 | - | 0/7/29/30 | 0/3/3/3 |
| 22 | 2MG | AA | 966 | 22 | - | 0/5/27/28 | 0/3/3/3 |
| 22 | 4OC | AA | 1402 | 22 | - | 0/9/29/30 | 0/2/2/2 |
| 57 | PSU | BA | 1917 | 57 | - | 0/7/25/26 | 0/2/2/2 |
| 57 | OMC | BA | 2498 | 57 | - | 1/9/27/28 | 0/2/2/2 |

All (27) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 2069 | 7MG | C8-N9 | -21.38 | 1.34 | 1.46 |
| 22 | AA | 527 | 7MG | C8-N9 | -21.04 | 1.34 | 1.46 |
| 24 | A3 | 8 | 4SU | C5-C4 | -4.96 | 1.36 | 1.42 |
| 57 | BA | 2449 | H2U | C4-N3 | -3.07 | 1.32 | 1.37 |
| 57 | BA | 2449 | H2U | C2-N3 | -2.94 | 1.32 | 1.38 |
| 24 | A3 | 21 | H2U | C4-N3 | -2.73 | 1.33 | 1.37 |
| 24 | A3 | 21 | H2U | C2-N3 | -2.57 | 1.33 | 1.38 |
| 57 | BA | 745 | 1MG | C8-N7 | -2.47 | 1.30 | 1.35 |
| 57 | BA | 2503 | 2MA | C8-N7 | -2.46 | 1.30 | 1.35 |
| 22 | AA | 1207 | 2MG | C8-N7 | -2.39 | 1.31 | 1.35 |
| 57 | BA | 2503 | 2MA | C6-N1 | -2.32 | 1.32 | 1.38 |
| 57 | BA | 1835 | 2MG | C8-N7 | -2.31 | 1.31 | 1.35 |
| 22 | AA | 1518 | MA6 | C8-N7 | -2.25 | 1.30 | 1.34 |
| 57 | BA | 2445 | 2MG | C8-N7 | -2.24 | 1.31 | 1.35 |
| 22 | AA | 527 | 7MG | C5-N7 | 2.24 | 1.38 | 1.35 |
| 22 | AA | 966 | 2MG | C8-N7 | -2.24 | 1.31 | 1.35 |
| 22 | AA | 1519 | MA6 | C8-N7 | -2.20 | 1.30 | 1.34 |
| 22 | AA | 1516 | 2MG | C8-N7 | -2.20 | 1.31 | 1.35 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 22 | AA | 1519 | MA6 | C6-N1 | 2.15 | 1.36 | 1.33 |
| 57 | BA | 2251 | OMG | C8-N7 | -2.14 | 1.31 | 1.35 |
| 57 | BA | 2069 | 7MG | C5-N7 | 2.12 | 1.38 | 1.35 |
| 57 | BA | 2503 | 2MA | C5-C4 | -2.09 | 1.37 | 1.43 |
| 57 | BA | 2030 | 6MZ | C8-N7 | -2.08 | 1.31 | 1.34 |
| 57 | BA | 745 | 1MG | C5-C4 | -2.08 | 1.37 | 1.43 |
| 22 | AA | 966 | 2MG | C5-C4 | -2.05 | 1.37 | 1.43 |
| 57 | BA | 2445 | 2MG | C5-C4 | -2.05 | 1.37 | 1.43 |
| 22 | AA | 1207 | 2MG | C5-C4 | -2.04 | 1.37 | 1.43 |

All (83) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 2069 | 7MG | N9-C8-N7 | 6.06 | 112.04 | 103.38 |
| 22 | AA | 527 | 7MG | N9-C8-N7 | 5.81 | 111.68 | 103.38 |
| 57 | BA | 2503 | 2MA | C5-C6-N1 | 4.24 | 121.33 | 114.02 |
| 57 | BA | 1618 | 6MZ | C9-N6-C6 | 4.04 | 126.35 | 122.87 |
| 57 | BA | 1915 | 3TD | C6-C5-C4 | 3.86 | 120.89 | 118.22 |
| 57 | BA | 2580 | PSU | C6-C5-C4 | 3.79 | 120.85 | 118.20 |
| 57 | BA | 2605 | PSU | C6-C5-C4 | 3.76 | 120.82 | 118.20 |
| 57 | BA | 2498 | OMC | O2-C2-N3 | -3.68 | 116.35 | 122.33 |
| 57 | BA | 2030 | 6MZ | C9-N6-C6 | 3.64 | 126.01 | 122.87 |
| 57 | BA | 2504 | PSU | C6-C5-C4 | 3.57 | 120.69 | 118.20 |
| 57 | BA | 2445 | 2MG | O6-C6-N1 | -3.49 | 116.52 | 120.65 |
| 22 | AA | 516 | PSU | C6-C5-C4 | 3.33 | 120.53 | 118.20 |
| 57 | BA | 1917 | PSU | C6-C5-C4 | 3.33 | 120.53 | 118.20 |
| 24 | A3 | 8 | 4SU | C5-C4-N3 | 3.33 | 117.78 | 114.69 |
| 57 | BA | 2503 | 2MA | N1-C2-N3 | 3.30 | 128.53 | 123.06 |
| 57 | BA | 1962 | 5MC | N4-C4-N3 | -3.30 | 112.46 | 118.48 |
| 57 | BA | 747 | 5MU | C6-C5-C4 | 3.29 | 120.78 | 118.03 |
| 24 | A3 | 55 | 5MU | C5M-C5-C6 | -3.27 | 118.48 | 122.85 |
| 22 | AA | 966 | 2MG | O6-C6-N1 | -3.20 | 116.87 | 120.65 |
| 57 | BA | 955 | PSU | C6-C5-C4 | 3.18 | 120.42 | 118.20 |
| 57 | BA | 1962 | 5MC | C5-C6-N1 | -3.12 | 120.13 | 123.34 |
| 22 | AA | 1407 | 5MC | O2-C2-N3 | -3.11 | 117.28 | 122.33 |
| 24 | A3 | 33 | OMC | O2-C2-N3 | -3.10 | 117.29 | 122.33 |
| 57 | BA | 1939 | 5MU | C6-C5-C4 | 3.09 | 120.61 | 118.03 |
| 22 | AA | 1207 | 2MG | O6-C6-N1 | -3.07 | 117.03 | 120.65 |
| 57 | BA | 1618 | 6MZ | C2-N1-C6 | 3.02 | 119.18 | 116.59 |
| 57 | BA | 2251 | OMG | O6-C6-N1 | -3.02 | 117.09 | 120.65 |
| 22 | AA | 1516 | 2MG | O6-C6-N1 | -3.01 | 117.10 | 120.65 |
| 57 | BA | 745 | 1MG | C2-N1-C6 | 2.98 | 123.37 | 120.95 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | A3 | 56 | PSU | C6-C5-C4 | 2.98 | 120.28 | 118.20 |
| 57 | BA | 1835 | 2MG | O6-C6-N1 | -2.98 | 117.13 | 120.65 |
| 57 | BA | 746 | PSU | C6-C5-C4 | 2.97 | 120.28 | 118.20 |
| 24 | A3 | 55 | 5MU | C6-C5-C4 | 2.94 | 120.49 | 118.03 |
| 57 | BA | 1939 | 5MU | C5M-C5-C6 | -2.94 | 118.92 | 122.85 |
| 57 | BA | 1962 | 5MC | CM5-C5-C6 | -2.93 | 118.94 | 122.85 |
| 57 | BA | 747 | 5MU | C5M-C5-C6 | -2.92 | 118.94 | 122.85 |
| 57 | BA | 2030 | 6MZ | C2-N1-C6 | 2.87 | 119.05 | 116.59 |
| 24 | A3 | 8 | 4SU | C4-N3-C2 | -2.85 | 124.58 | 127.34 |
| 22 | AA | 967 | 5MC | C5-C6-N1 | -2.83 | 120.42 | 123.34 |
| 57 | BA | 2457 | PSU | C6-C5-C4 | 2.80 | 120.16 | 118.20 |
| 57 | BA | 2580 | PSU | C3'-C2'-C1' | 2.74 | 104.83 | 101.64 |
| 57 | BA | 1911 | PSU | C6-C5-C4 | 2.74 | 120.11 | 118.20 |
| 22 | AA | 1407 | 5MC | C5-C6-N1 | -2.73 | 120.53 | 123.34 |
| 57 | BA | 1939 | 5MU | C5-C6-N1 | -2.73 | 120.53 | 123.34 |
| 22 | AA | 967 | 5MC | O2-C2-N3 | -2.70 | 117.94 | 122.33 |
| 22 | AA | 1407 | 5MC | CM5-C5-C6 | -2.68 | 119.27 | 122.85 |
| 57 | BA | 2445 | 2MG | O6-C6-C5 | 2.65 | 129.56 | 124.37 |
| 57 | BA | 1962 | 5MC | O2-C2-N3 | -2.63 | 118.05 | 122.33 |
| 57 | BA | 2251 | OMG | O6-C6-C5 | 2.63 | 129.51 | 124.37 |
| 22 | AA | 1402 | 4OC | O2-C2-N3 | -2.57 | 118.14 | 122.33 |
| 22 | AA | 967 | 5MC | N4-C4-N3 | -2.53 | 113.86 | 118.48 |
| 22 | AA | 967 | 5MC | CM5-C5-C6 | -2.50 | 119.51 | 122.85 |
| 22 | AA | 516 | PSU | C5-C6-N1 | -2.50 | 118.36 | 122.11 |
| 22 | AA | 1516 | 2MG | O6-C6-C5 | 2.49 | 129.24 | 124.37 |
| 57 | BA | 747 | 5MU | C5-C6-N1 | -2.46 | 120.81 | 123.34 |
| 22 | AA | 1207 | 2MG | O6-C6-C5 | 2.46 | 129.18 | 124.37 |
| 57 | BA | 2605 | PSU | C5-C6-N1 | -2.46 | 118.42 | 122.11 |
| 22 | AA | 527 | 7MG | O4'-C1'-N9 | 2.42 | 112.59 | 109.30 |
| 57 | BA | 1915 | 3TD | C5-C6-N1 | -2.40 | 118.51 | 122.11 |
| 57 | BA | 955 | PSU | C5-C6-N1 | -2.40 | 118.51 | 122.11 |
| 22 | AA | 966 | 2MG | O6-C6-C5 | 2.40 | 129.05 | 124.37 |
| 57 | BA | 2504 | PSU | C5-C6-N1 | -2.38 | 118.55 | 122.11 |
| 57 | BA | 2580 | PSU | O4'-C1'-C2' | 2.34 | 108.44 | 105.14 |
| 24 | A3 | 55 | 5MU | C5-C6-N1 | -2.33 | 120.95 | 123.34 |
| 57 | BA | 2580 | PSU | C5-C6-N1 | -2.32 | 118.63 | 122.11 |
| 24 | A3 | 56 | PSU | C5-C6-N1 | -2.31 | 118.65 | 122.11 |
| 57 | BA | 1962 | 5MC | C5-C4-N3 | 2.31 | 124.16 | 121.67 |
| 57 | BA | 1835 | 2MG | O6-C6-C5 | 2.30 | 128.86 | 124.37 |
| 57 | BA | 2605 | PSU | O4'-C1'-C2' | 2.28 | 108.36 | 105.14 |
| 22 | AA | 1407 | 5MC | N4-C4-N3 | -2.25 | 114.38 | 118.48 |
| 57 | BA | 1915 | 3TD | C4-N3-C2 | -2.21 | 122.21 | 124.61 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | BA | 1917 | PSU | C5-C6-N1 | -2.21 | 118.80 | 122.11 |
| 57 | BA | 746 | PSU | C3'-C2'-C1' | 2.15 | 104.14 | 101.64 |
| 57 | BA | 2503 | 2MA | C2'-C3'-C4' | -2.12 | 98.52 | 102.64 |
| 57 | BA | 1911 | PSU | C5-C6-N1 | -2.11 | 118.94 | 122.11 |
| 57 | BA | 746 | PSU | C5-C6-N1 | -2.09 | 118.98 | 122.11 |
| 22 | AA | 1498 | UR3 | O4-C4-N3 | 2.07 | 122.53 | 119.66 |
| 22 | AA | 1498 | UR3 | O4'-C4'-C3' | 2.07 | 109.21 | 105.11 |
| 57 | BA | 2251 | OMG | O3'-C3'-C2' | 2.07 | 117.03 | 111.17 |
| 24 | A3 | 55 | 5MU | C5M-C5-C4 | 2.05 | 121.02 | 118.77 |
| 57 | BA | 2552 | OMU | N3-C2-N1 | 2.05 | 117.61 | 114.89 |
| 22 | AA | 1402 | 4OC | O4'-C1'-N1 | 2.04 | 113.03 | 108.36 |
| 57 | BA | 2457 | PSU | C5-C6-N1 | -2.03 | 119.07 | 122.11 |

There are no chirality outliers.

All (10) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 24 | A3 | 56 | PSU | O4'-C1'-C5-C4 |
| 57 | BA | 2504 | PSU | O4'-C1'-C5-C4 |
| 57 | BA | 2504 | PSU | O4'-C4'-C5'-O5' |
| 24 | A3 | 56 | PSU | O4'-C1'-C5-C6 |
| 57 | BA | 1915 | 3TD | O4'-C1'-C5-C6 |
| 24 | A3 | 21 | H2U | O4'-C4'-C5'-O5' |
| 57 | BA | 2498 | OMC | O4'-C4'-C5'-O5' |
| 57 | BA | 2503 | 2MA | O4'-C4'-C5'-O5' |
| 22 | AA | 527 | 7MG | O4'-C4'-C5'-O5' |
| 57 | BA | 2030 | 6MZ | O4'-C4'-C5'-O5' |

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)

There are no ligands in this entry.

## 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.

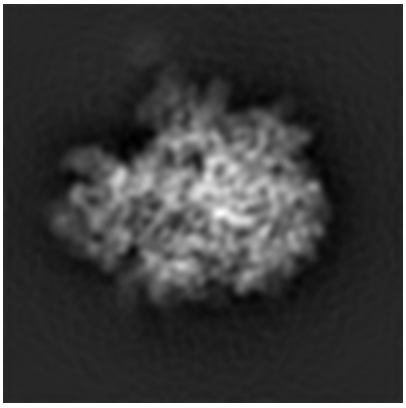
# 6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-5562. These allow visual inspection of the internal detail of the map and identification of artifacts.

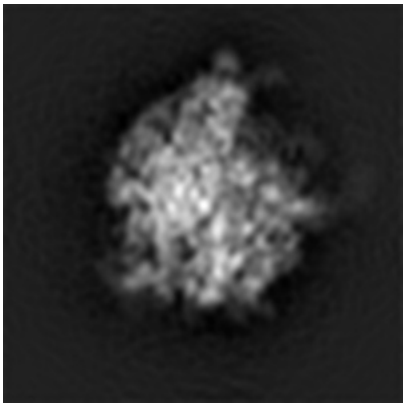
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

## 6.1 Orthogonal projections (i)

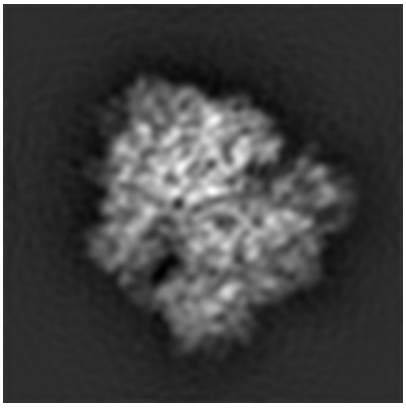
### 6.1.1 Primary map



X



Y

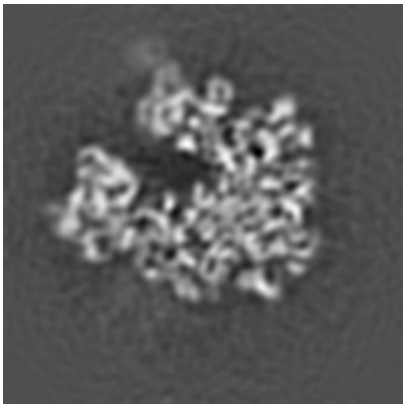


Z

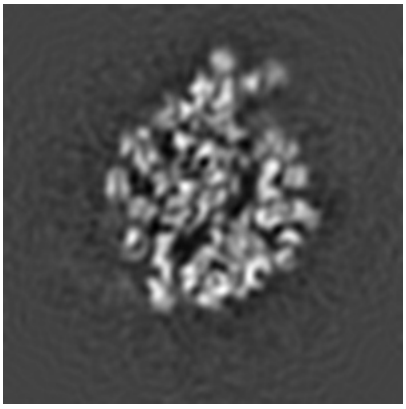
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

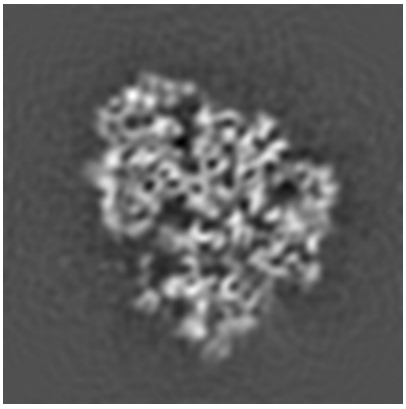
### 6.2.1 Primary map



X Index: 67



Y Index: 67

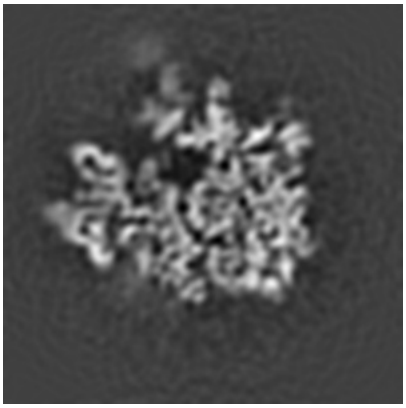


Z Index: 67

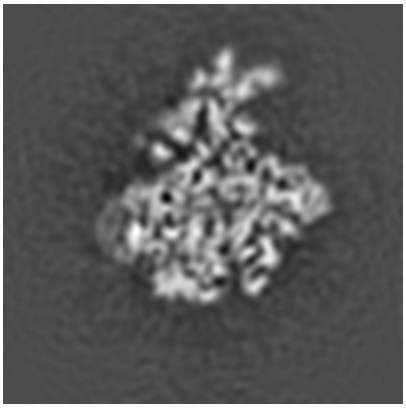
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

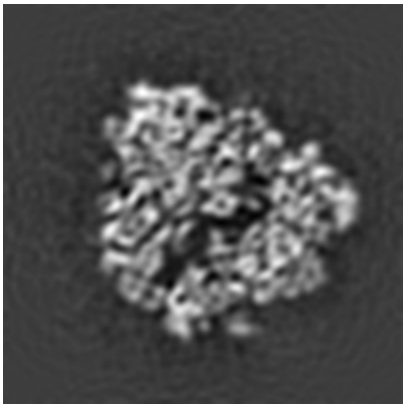
### 6.3.1 Primary map



X Index: 70



Y Index: 71

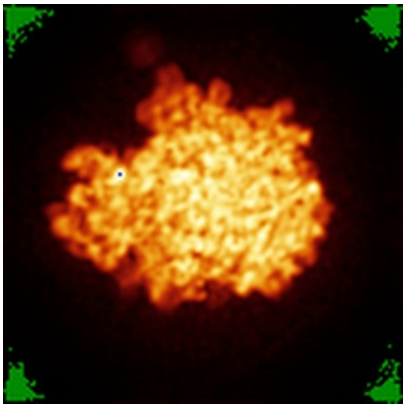


Z Index: 73

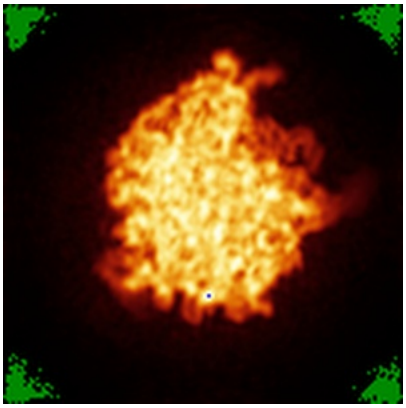
The images above show the largest variance slices of the map in three orthogonal directions.

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

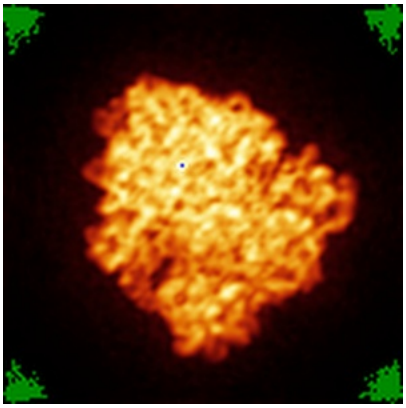
### 6.4.1 Primary map



X



Y

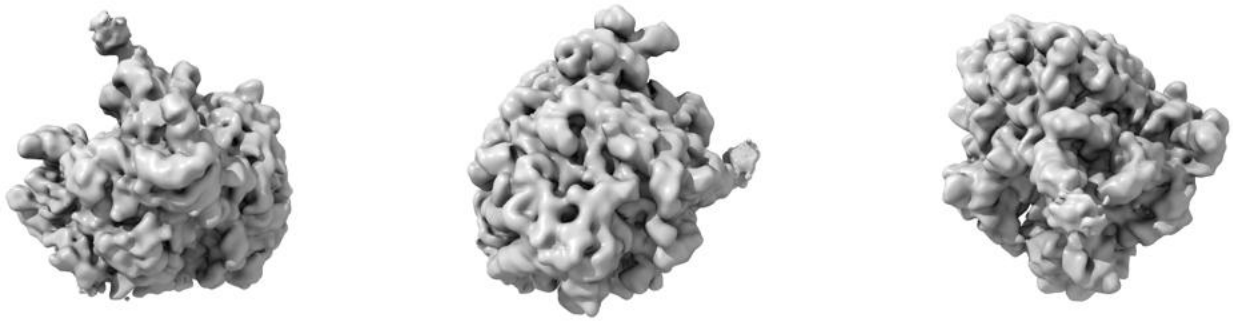


Z

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

## 6.5 Orthogonal surface views (i)

### 6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 22.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

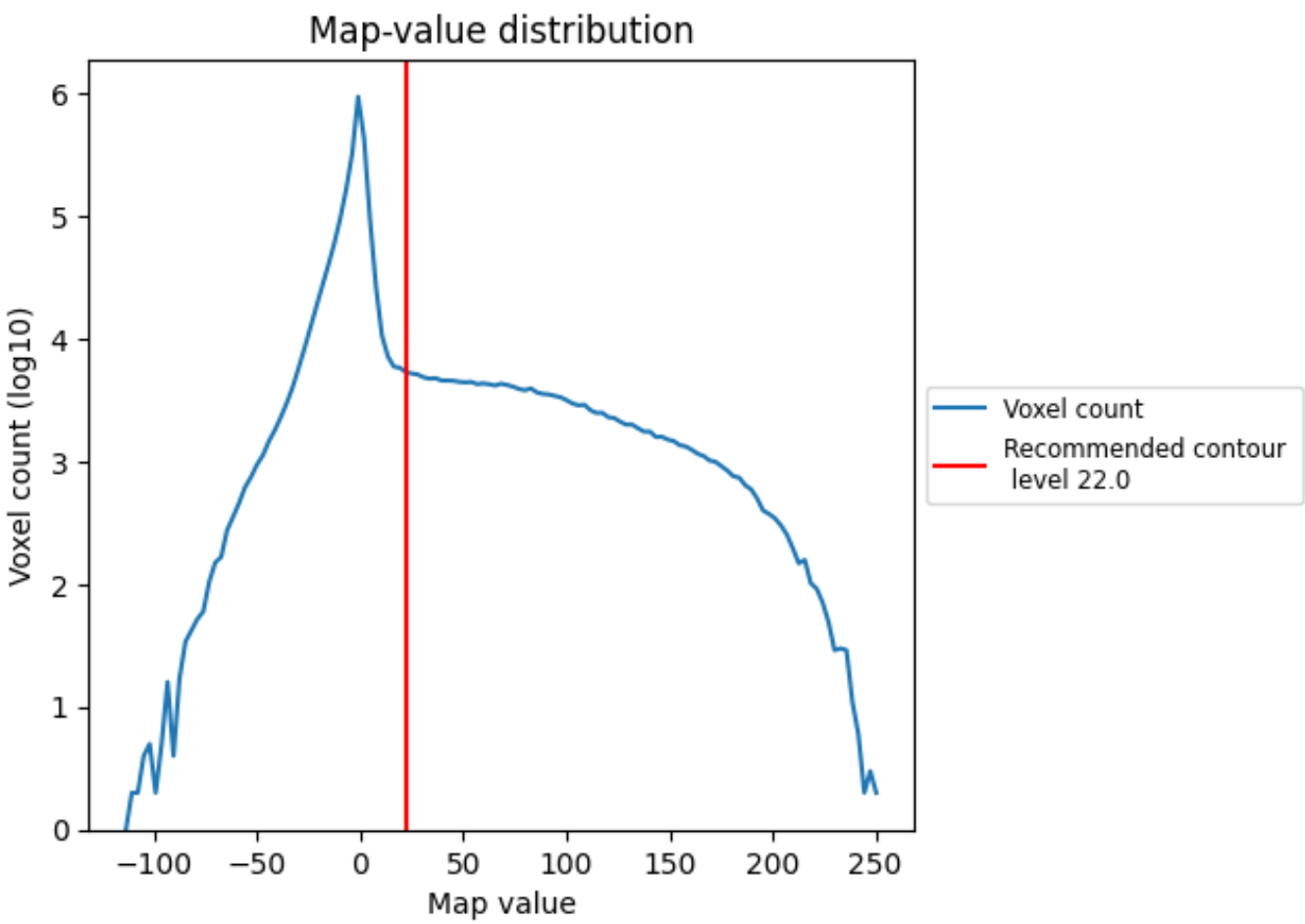
## 6.6 Mask visualisation (i)

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

# 7 Map analysis (i)

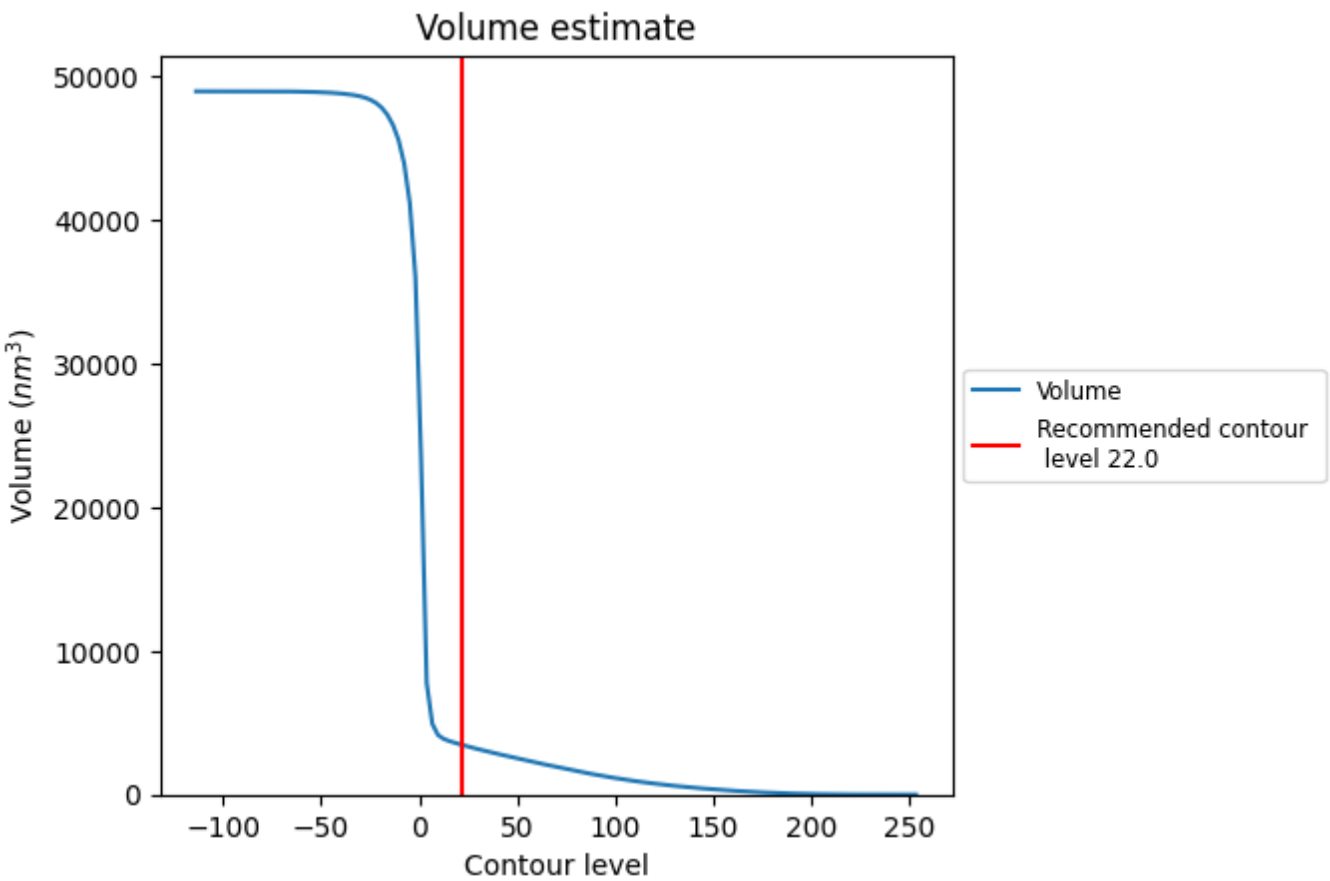
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution (i)




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

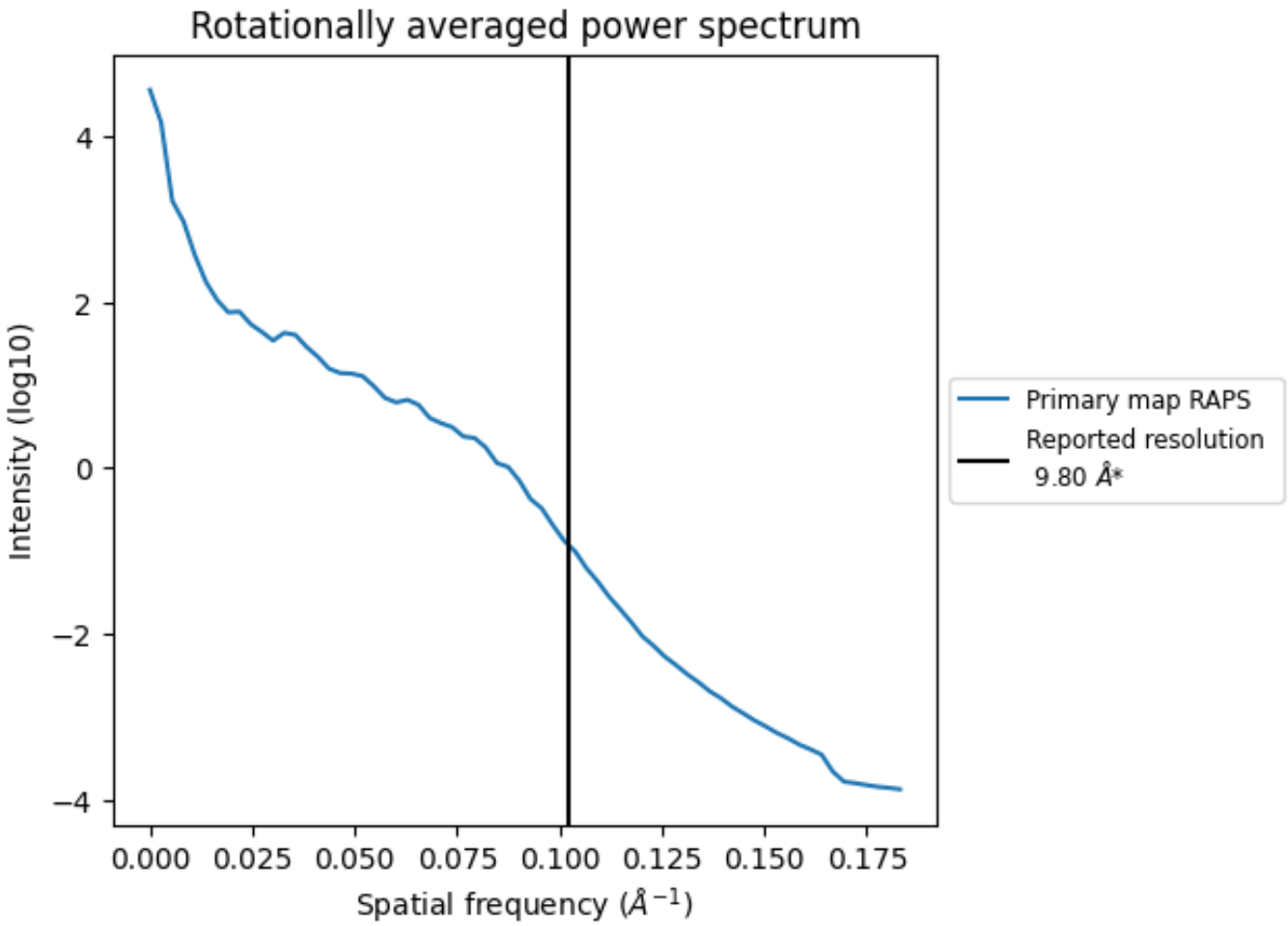
## 7.2 Volume estimate (i)




The volume at the recommended contour level is 3450 $nm^3$; this corresponds to an approximate mass of 3116 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 0.102 Å$^{-1}$

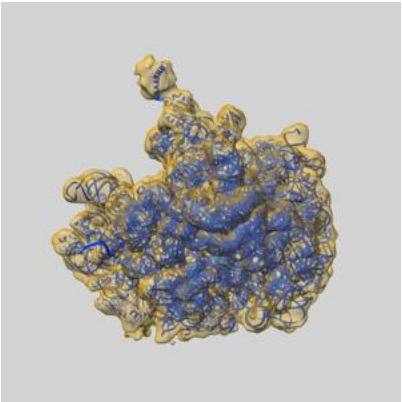
# 8 Fourier-Shell correlation (i)

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

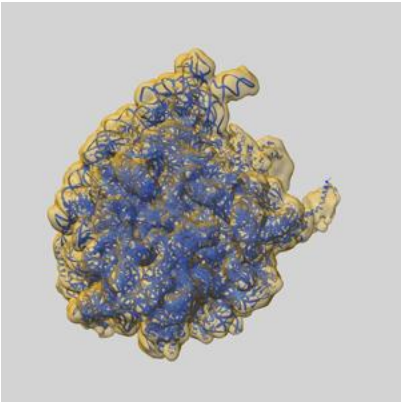
# 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-5562 and PDB model 4V6V. Per-residue inclusion information can be found in section 3 on page 14.

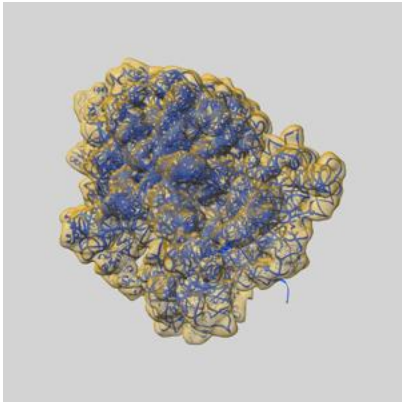
## 9.1 Map-model overlay (i)



X



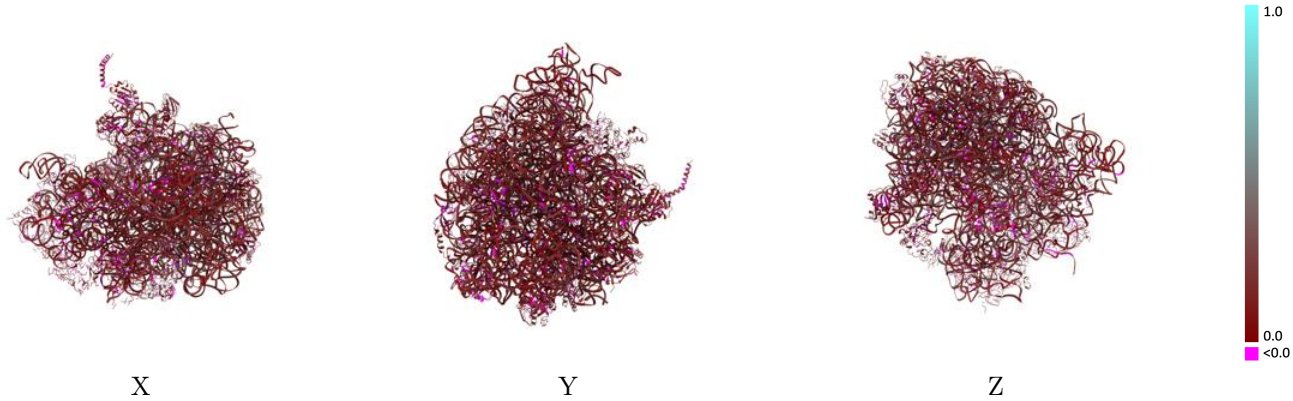
Y



Z

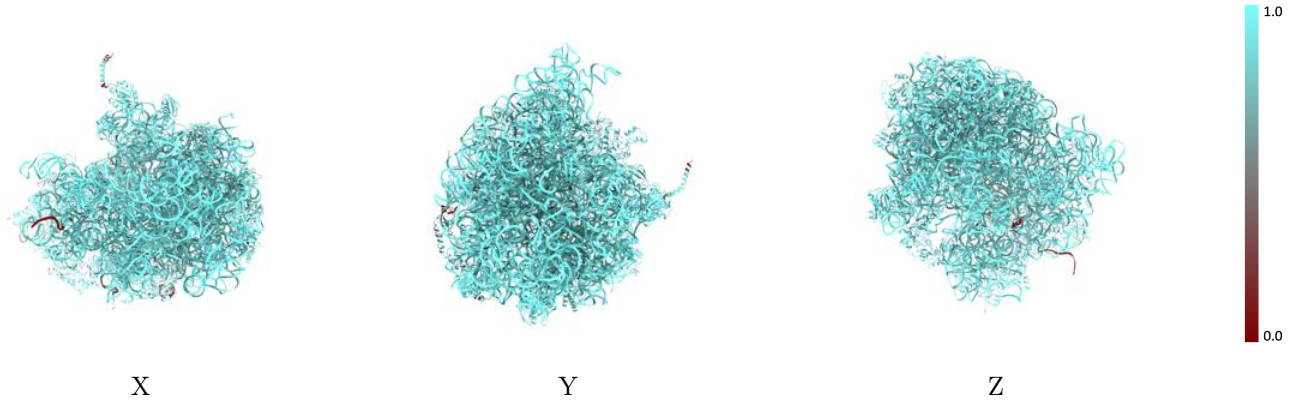
The images above show the 3D surface view of the map at the recommended contour level 22.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



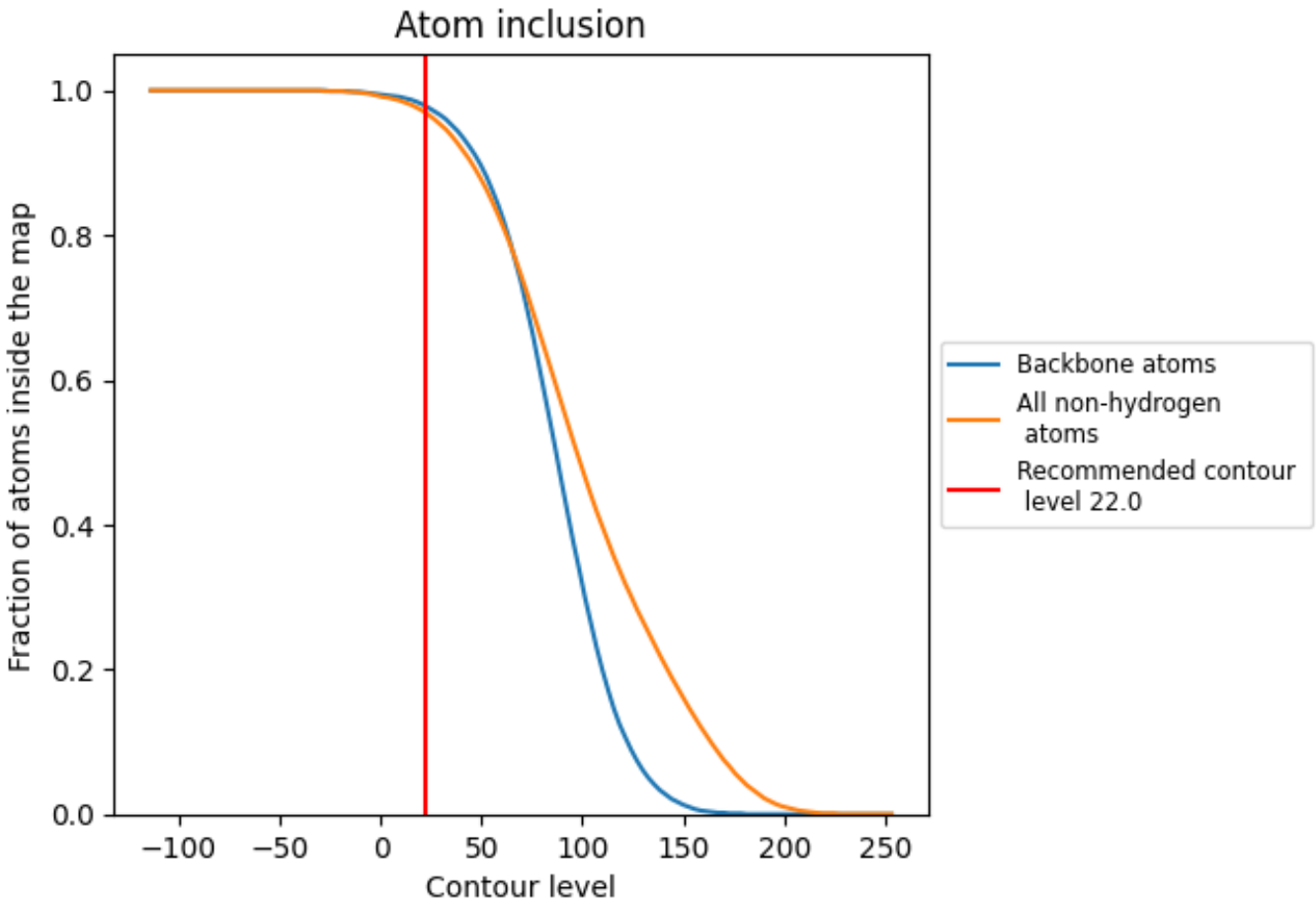

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (22.0).

## 9.4 Atom inclusion (i)




At the recommended contour level, 98% of all backbone atoms, 97% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (22.0) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.9700 | 0.1260 |
| A1 | 0.9130 | 0.1120 |
| A2 | 0.4660 | 0.0110 |
| A3 | 0.9840 | 0.1530 |
| AA | 0.9950 | 0.1430 |
| AB | 0.9200 | 0.1050 |
| AC | 0.9110 | 0.0970 |
| AD | 0.9760 | 0.0960 |
| AE | 0.8840 | 0.0850 |
| AF | 0.8220 | 0.0930 |
| AG | 0.9590 | 0.1070 |
| AH | 0.9560 | 0.1020 |
| AI | 0.9750 | 0.0840 |
| AJ | 0.9580 | 0.0780 |
| AK | 0.8950 | 0.0910 |
| AL | 0.9260 | 0.0940 |
| AM | 0.9720 | 0.1100 |
| AN | 0.9470 | 0.0640 |
| AO | 0.9800 | 0.1040 |
| AP | 0.9730 | 0.0620 |
| AQ | 0.9630 | 0.1070 |
| AR | 0.9090 | 0.0770 |
| AS | 0.9540 | 0.0810 |
| AT | 0.9610 | 0.1110 |
| AU | 0.8750 | 0.0990 |
| B0 | 0.9000 | 0.0370 |
| B1 | 0.9550 | 0.0880 |
| B2 | 0.9660 | 0.1380 |
| B3 | 0.9660 | 0.1170 |
| B4 | 0.8850 | 0.0850 |
| B5 | 0.9300 | 0.0630 |
| B6 | 0.9540 | 0.0900 |
| B7 | 0.9270 | 0.0670 |
| B8 | 0.9430 | 0.0620 |
| B9 | 0.9520 | 0.0520 |

*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion | Q-score |
|---|---|---|
| BA | 0.9930 | 0.1450 |
| BC | 0.8760 | 0.0490 |
| BD | 0.9380 | 0.0750 |
| BE | 0.9420 | 0.0870 |
| BF | 0.9720 | 0.0950 |
| BG | 0.9730 | 0.0890 |
| BH | 0.9810 | 0.1240 |
| BJ | 0.8870 | 0.0810 |
| BK | 0.9790 | 0.0960 |
| BL | 0.7430 | 0.1000 |
| BN | 0.9590 | 0.0980 |
| BO | 0.9100 | 0.0960 |
| BP | 0.9510 | 0.0750 |
| BQ | 0.9500 | 0.0920 |
| BR | 0.9520 | 0.0900 |
| BS | 0.9760 | 0.0940 |
| BT | 0.9350 | 0.1020 |
| BU | 0.9660 | 0.0980 |
| BV | 0.9400 | 0.0990 |
| BW | 0.9250 | 0.0900 |
| BX | 0.9600 | 0.0890 |
| BY | 0.9600 | 0.1060 |
| BZ | 0.9730 | 0.1180 |
| Ba | 0.9960 | 0.1520 |