# Full wwPDB EM Validation Report (i)

Feb 22, 2024 – 05:58 PM EST

| | | |
|---|---|---|
| PDB ID | : | 4V6I |
| EMDB ID | : | EMD-1669 |
| Title | : | Localization of the small subunit ribosomal proteins into a 6.1 A cryo-EM map of Saccharomyces cerevisiae translating 80S ribosome |
| Authors | : | Armache, J.-P.; Jarasch, A.; Anger, A.M.; Villa, E.; Becker, T.; Bhushan, S.; Jossinet, F.; Habeck, M.; Dindar, G.; Franckenberg, S.; Marquez, V.; Mielke, T.; Thomm, M.; Berninghausen, O.; Beatrix, B.; Soeding, J.; Westhof, E.; Wilson, D.N.; Beckmann, R. |
| Deposited on | : | 2010-10-12 |
| Resolution | : | 8.80 Å(reported) |

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

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

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

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

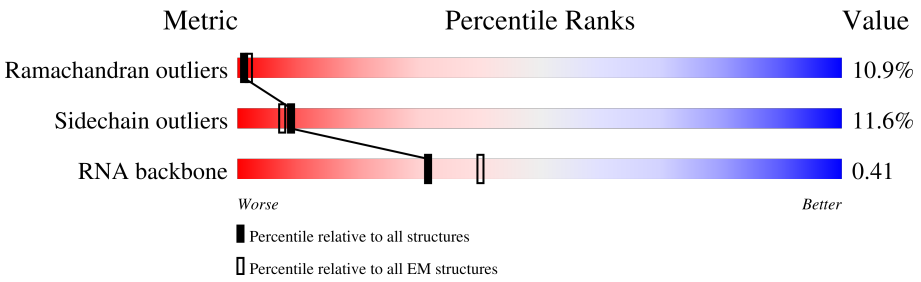
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev70 |
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | 1.9.13 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | 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 8.80 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 | Aa | 319 | 47%; 72%, 19%, 8%, • |
| 2 | AA | 252 | 27%; 65%, 25%, 6%, 5% |
| 3 | AB | 240 | 41%; 49%, 23%, 10%, •, 15% |
| 4 | AD | 261 | 24%; 43%, 21%, 11%, •, 23% |
| 5 | AC | 197 | 35%; 49%, 31%, 14%, 6% |
| 6 | AE | 254 | 33%; 64%, 19%, 13%, • |
| 7 | AG | 144 | 31%; 78%, 21%, • |
| 8 | AF | 225 | 38%; 61%, 19%, 7%, •, 12% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 9 | AH | 130 | 38% 61% 24% 10% 5% |
| 10 | AI | 143 | 32% 50% 21% 15% • 12% |
| 11 | AJ | 121 | 38% 62% 21% 9% • 7% |
| 12 | AK | 137 | 30% 48% 28% 7% • 13% |
| 13 | AL | 145 | 31% 57% 32% 6% 5% |
| 14 | AM | 146 | 66% 53% 32% 10% • • |
| 15 | AN | 56 | 50% 36% 23% 25% • 14% |
| 16 | AO | 151 | 38% 48% 19% 11% • 20% |
| 17 | AQ | 136 | 67% 51% 31% 12% 6% |
| 18 | AP | 156 | 30% 31% 12% 9% • 46% |
| 19 | AR | 142 | 39% 37% 17% 8% 38% |
| 20 | AS | 144 | 42% 55% 32% 8% 6% |
| 21 | AT | 87 | 55% 62% 18% 16% • |
| 22 | AV | 108 | 44% 44% 24% 6% • 21% |
| 23 | AW | 93 | 23% 78% 20% • |
| 24 | AX | 82 | 28% 32% 23% • • 39% |
| 25 | AY | 67 | 58% 58% 27% • 10% |
| 26 | AZ | 63 | 43% 51% 21% 17% 11% |
| 27 | Ab | 37 | 5% 89% 8% • |
| 28 | Ac | 26 | 35% 92% • • |
| 29 | AU | 135 | 30% 38% 18% 14% • 29% |
| 30 | BA | 217 | 73% 76% 20% • |
| 31 | BB | 254 | 47% 67% 17% 13% • |
| 32 | BC | 388 | 30% 56% 28% 12% • |
| 33 | BD | 362 | 30% 55% 23% 7% 6% 9% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 34 | BE | 174 | 33% 60% 20% 11% 6% |
| 35 | BG | 176 | 28% 36% 28% 22% 14% |
| 36 | BF | 191 | 37% 79% 16% |
| 37 | BH | 256 | 21% 46% 19% 7% 23% |
| 38 | Bs | 312 | 57% 60% 16% 5% 18% |
| 39 | BJ | 165 | 48% 53% 17% 5% 23% |
| 40 | BK | 199 | 33% 63% 21% 13% |
| 41 | BN | 138 | 27% 55% 33% 11% |
| 42 | BM | 137 | 67% 60% 26% 9% |
| 43 | BP | 204 | 30% 50% 25% 16% 5% |
| 44 | BO | 149 | 42% 54% 26% 15% 5% |
| 45 | BR | 186 | 30% 49% 20% 12% 5% 13% |
| 46 | BT | 189 | 42% 67% 23% 8% |
| 47 | BU | 160 | 25% 64% 27% 6% |
| 48 | BW | 121 | 31% 50% 24% 10% 13% |
| 49 | BV | 170 | 40% 71% 16% 11% |
| 50 | BX | 142 | 34% 53% 23% 9% 14% |
| 51 | BZ | 155 | 25% 25% 11% 7% 53% |
| 52 | BY | 123 | 15% 67% 25% 5% |
| 53 | Ba | 136 | 30% 32% 18% 14% 6% 30% |
| 54 | Bd | 59 | 12% 25% 10% 63% |
| 55 | Bc | 120 | 8% 62% 21% 10% 6% |
| 56 | Bf | 105 | 40% 76% 17% 6% |
| 57 | Be | 244 | 29% 70% 19% 7% |
| 58 | Bg | 113 | 35% 62% 20% 12% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 59 | Bh | 130 | 43% 65% 24% 7% • |
| 60 | Bi | 118 | 49% 53% 25% 14% 8% |
| 61 | Bj | 107 | 46% 46% 27% 15% 6% 7% |
| 62 | Bk | 100 | 12% 46% 15% 13% • 23% |
| 63 | Bm | 92 | 51% 72% 22% • • |
| 64 | Bl | 88 | 28% 64% 20% 14% • |
| 65 | Bn | 78 | 33% 59% 21% 12% 9% |
| 66 | Bo | 51 | 43% 45% 29% 18% 8% |
| 67 | Bp | 52 | 38% 46% 17% 12% • 23% |
| 68 | Bq | 25 | 48% 44% 40% 16% |
| 69 | Br | 106 | 46% 53% 25% 14% 8% |
| 70 | Bx | 21 | 19% 76% 19% 5% |
| 70 | By | 21 | 5% 95% 5% |
| 71 | Bz | 15 | 33% 87% 7% 7% |
| 72 | Bt | 106 | 33% 43% 9% •• 45% |
| 72 | Bu | 106 | 55% 41% 12% •• 45% |
| 73 | Bv | 106 | 40% 49% 5% • 45% |
| 73 | Bw | 106 | 52% 49% 5% • 45% |
| 74 | BQ | 297 | 16% 60% 21% 13% 6% |
| 75 | BL | 170 | 19% 96% • • |
| 76 | BS | 167 | 41% 43% 31% 14% 13% |
| 77 | BI | 221 | 20% 57% 15% 7% • 18% |
| 78 | CA | 1800 | 11% 11% 52% 32% • • |
| 79 | CB | 75 | 95% • 56% 41% |
| 80 | CC | 11 | 91% 9% 27% 64% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 81 | DA | 3396 | 10% 7% 49% 43% |
| 82 | DB | 158 | 9% 9% 42% 49% |
| 83 | DC | 118 | 44% 56% |

# 2 Entry composition (i)

There are 83 unique types of molecules in this entry. The entry contains 191627 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 40S ribosomal protein RACK1 (RACK1).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 1 | Aa | 319 | 2442 | 1544 | 420 | 469 | 9 | 0 | 0 |

- Molecule 2 is a protein called 40S ribosomal protein rpS0 (S2p).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 2 | AA | 252 | 1922 | 1204 | 336 | 380 | 2 | 0 | 0 |

- Molecule 3 is a protein called 40S ribosomal protein rpS3 (S3p).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 3 | AB | 204 | 1511 | 945 | 282 | 278 | 6 | 0 | 0 |

- Molecule 4 is a protein called 40S ribosomal protein rpS4 (S4e).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 4 | AD | 200 | 1591 | 1018 | 288 | 283 | 2 | 0 | 0 |

- Molecule 5 is a protein called 40S ribosomal protein rpS9 (S4p).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 5 | AC | 197 | 1521 | 951 | 298 | 270 | 2 | 0 | 0 |

- Molecule 6 is a protein called 40S ribosomal protein rpS2 (S5p).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 6 | AE | 254 | 1936 | 1224 | 360 | 349 | 3 | 0 | 0 |

- Molecule 7 is a protein called 40S ribosomal protein rpS7 (S7e).

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 7 | AG | 143 | 716 | 429 | 143 | 144 | 0 | 0 |

- Molecule 8 is a protein called 40S ribosomal protein rpS5 (S7p).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 8 | AF | 199 | 1543 | 958 | 293 | 289 | 3 | 0 | 0 |

- Molecule 9 is a protein called 40S ribosomal protein rpS22 (S8p).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 9 | AH | 130 | 1030 | 655 | 189 | 182 | 4 | 0 | 0 |

- Molecule 10 is a protein called 40S ribosomal protein rpS16 (S9p).

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 10 | AI | 126 | 998 | 639 | 184 | 175 | 0 | 0 |

- Molecule 11 is a protein called 40S ribosomal protein rpS20 (S10p).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 11 | AJ | 113 | 849 | 528 | 158 | 162 | 1 | 0 | 0 |

- Molecule 12 is a protein called 40S ribosomal protein rpS14 (S11p).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 12 | AK | 119 | 833 | 508 | 157 | 165 | 3 | 0 | 0 |

- Molecule 13 is a protein called 40S ribosomal protein rpS23 (S12p).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 13 | AL | 145 | 978 | 588 | 203 | 184 | 3 | 0 | 0 |

- Molecule 14 is a protein called 40S ribosomal protein rpS18 (S13p).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 14 | AM | 140 | 1156 | 719 | 231 | 204 | 2 | 0 | 0 |

- Molecule 15 is a protein called 40S ribosomal protein rpS29 (S14p).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 15 | AN | 48 | 353 | 209 | 79 | 61 | 4 | 0 | 0 |

- Molecule 16 is a protein called 40S ribosomal protein rpS13 (S15p).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 16 | AO | 121 | 978 | 624 | 183 | 170 | 1 | 0 | 0 |

- Molecule 17 is a protein called 40S ribosomal protein rpS17 (S17e).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 17 | AQ | 136 | 1098 | 682 | 213 | 201 | 2 | 0 | 0 |

- Molecule 18 is a protein called 40S ribosomal protein rpS11 (S17p).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 18 | AP | 85 | 631 | 402 | 124 | 104 | 1 | 0 | 0 |

- Molecule 19 is a protein called 40S ribosomal protein rpS15 (S19p).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 19 | AR | 88 | 676 | 429 | 123 | 118 | 6 | 0 | 0 |

- Molecule 20 is a protein called 40S ribosomal protein rpS19 (S19e).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 20 | AS | 144 | 1120 | 699 | 209 | 209 | 3 | 0 | 0 |

- Molecule 21 is a protein called 40S ribosomal protein rpS21 (S21e).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 21 | AT | 87 | 685 | 420 | 125 | 138 | 2 | 0 | 0 |

- Molecule 22 is a protein called 40S ribosomal protein rpS25 (S25e).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 22 | AV | 85 | 688 | 437 | 128 | 122 | 1 | 0 | 0 |

- Molecule 23 is a protein called 40S ribosomal protein rpS26 (S26e).

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 23 | AW | 92 | 461 | 276 | 92 | 93 | 0 | 0 |

- Molecule 24 is a protein called 40S ribosomal protein rpS27 (S27e).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 24 | AX | 50 | 366 | 229 | 60 | 72 | 5 | 0 | 0 |

- Molecule 25 is a protein called 40S ribosomal protein rpS28 (S28e).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 25 | AY | 60 | 445 | 276 | 80 | 87 | 2 | 0 | 0 |

- Molecule 26 is a protein called 40S ribosomal protein rpS30 (S30e).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 26 | AZ | 63 | 492 | 307 | 102 | 81 | 2 | 0 | 0 |

- Molecule 27 is a protein called Unknown 40S ribosomal protein XS1.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 27 | Ab | 36 | 181 | 108 | 36 | 37 | 0 | 0 |

- Molecule 28 is a protein called Unknown 40S ribosomal protein XS2.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 28 | Ac | 25 | 126 | 75 | 25 | 26 | 0 | 0 |

- Molecule 29 is a protein called 40S ribosomal protein S24.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 29 | AU | 96 | 714 | 450 | 134 | 129 | 1 | 0 | 0 |

- Molecule 30 is a protein called 60S ribosomal protein rpL1 (L1p).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 30 | BA | 217 | 1718 | 1097 | 299 | 312 | 10 | 0 | 0 |

- Molecule 31 is a protein called 60S ribosomal protein rpL2 (L2p).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 31 | BB | 254 | 1904 | 1183 | 385 | 334 | 2 | 0 | 0 |

- Molecule 32 is a protein called 60S ribosomal protein rpL3 (L3p).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 32 | BC | 388 | 3055 | 1933 | 579 | 534 | 9 | 0 | 0 |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| BC | 388 | GLY | - | expression tag | UNP P14126 |

- Molecule 33 is a protein called 60S ribosomal protein rpL4 (L4p).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 33 | BD | 329 | 2486 | 1564 | 480 | 438 | 4 | 0 | 0 |

- Molecule 34 is a protein called 60S ribosomal protein rpL11 (L5p).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 34 | BE | 168 | 1341 | 839 | 252 | 245 | 5 | 0 | 0 |

- Molecule 35 is a protein called 60S ribosomal protein rpL6 (L6e).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 35 | BG | 176 | 1409 | 907 | 252 | 248 | 2 | 0 | 0 |

- Molecule 36 is a protein called 60S ribosomal protein rpL9 (L6p).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 36 | BF | 191 | 1516 | 961 | 274 | 277 | 4 | 0 | 0 |

- Molecule 37 is a protein called 60S ribosomal protein rpL8 (L7ae).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 37 | BH | 197 | 1505 | 959 | 269 | 274 | 3 | 0 | 0 |

- Molecule 38 is a protein called 60S acidic ribosomal protein rpP0 (L10P).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 38 | Bs | 257 | 1976 | 1269 | 334 | 368 | 5 | 0 | 0 |

- Molecule 39 is a protein called 60S ribosomal protein rpL12 (L11p).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 39 | BJ | 127 | 954 | 601 | 174 | 178 | 1 | 0 | 0 |

- Molecule 40 is a protein called 60S ribosomal protein rpL16 (L13p).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 40 | BK | 199 | 1570 | 1011 | 291 | 266 | 2 | 0 | 0 |

- Molecule 41 is a protein called 60S ribosomal protein rpL14 (L14e).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 41 | BN | 138 | 1068 | 683 | 201 | 181 | 3 | 0 | 0 |

- Molecule 42 is a protein called 60S ribosomal protein rpL23 (L14p).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 42 | BM | 131 | 972 | 611 | 182 | 172 | 7 | 0 | 0 |

- Molecule 43 is a protein called 60S ribosomal protein rpL15 (L15e).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 43 | BP | 193 | 1625 | 1016 | 341 | 266 | 2 | 0 | 0 |

- Molecule 44 is a protein called 60S ribosomal protein rpL28 (L15p).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 44 | BO | 149 | 1182 | 754 | 232 | 192 | 4 | 0 | 0 |

- Molecule 45 is a protein called 60S ribosomal protein rpL18 (L18e).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 45 | BR | 161 | 1243 | 786 | 242 | 212 | 3 | 0 | 0 |

- Molecule 46 is a protein called 60S ribosomal protein rpL19 (L19e).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 46 | BT | 189 | 1530 | 940 | 327 | 262 | 1 | 0 | 0 |

- Molecule 47 is a protein called 60S ribosomal protein rpL21 (L21e).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 47 | BU | 160 | 1261 | 793 | 242 | 222 | 4 | 0 | 0 |

- Molecule 48 is a protein called 60S ribosomal protein rpL22 (L22e).

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 48 | BW | 105 | 830 | 535 | 140 | 155 | 0 | 0 |

- Molecule 49 is a protein called 60S ribosomal protein rpL17 (L22p).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 49 | BV | 170 | 1312 | 814 | 254 | 243 | 1 | 0 | 0 |

- Molecule 50 is a protein called 60S ribosomal protein rpL25 (L23p).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 50 | BX | 122 | 978 | 629 | 172 | 175 | 2 | 0 | 0 |

- Molecule 51 is a protein called 60S ribosomal protein rpL24 (L24e).

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 51 | BZ | 73 | 579 | 366 | 115 | 98 | 0 | 0 |

- Molecule 52 is a protein called 60S ribosomal protein rpL26 (L24p).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 52 | BY | 123 | 972 | 611 | 188 | 172 | 1 | 0 | 0 |

- Molecule 53 is a protein called 60S ribosomal protein rpL27 (L27e).

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 53 | Ba | 95 | 708 | 455 | 134 | 119 | 0 | 0 |

- Molecule 54 is a protein called 60S ribosomal protein rpL29 (L29e).

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 54 | Bd | 22 | 174 | 109 | 40 | 25 | 0 | 0 |

- Molecule 55 is a protein called 60S ribosomal protein rpL35 (L29p).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 55 | Bc | 118 | 965 | 612 | 185 | 167 | 1 | 0 | 0 |

- Molecule 56 is a protein called 60S ribosomal protein rpL30 (L30e).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 56 | Bf | 105 | 785 | 501 | 133 | 150 | 1 | 0 | 0 |

- Molecule 57 is a protein called 60S ribosomal protein rpL7 (L30p).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 57 | Be | 239 | 1919 | 1235 | 348 | 335 | 1 | 0 | 0 |

- Molecule 58 is a protein called 60S ribosomal protein rpL31 (L31e).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 58 | Bg | 110 | 873 | 552 | 169 | 150 | 2 | 0 | 0 |

- Molecule 59 is a protein called 60S ribosomal protein pL32 (L32e).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 59 | Bh | 130 | 1043 | 660 | 208 | 173 | 2 | 0 | 0 |

- Molecule 60 is a protein called 60S ribosomal protein rpL34 (L34e).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 60 | Bi | 118 | 926 | 572 | 188 | 161 | 5 | 0 | 0 |

- Molecule 61 is a protein called 60S ribosomal protein rpL33 (L35ae).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 61 | Bj | 100 | 738 | 461 | 147 | 128 | 2 | 0 | 0 |

- Molecule 62 is a protein called 60S ribosomal protein rpL36 (L36e).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 62 | Bk | 77 | 619 | 384 | 129 | 105 | 1 | 0 | 0 |

- Molecule 63 is a protein called 60S ribosomal protein rpL43 (L37ae).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 63 | Bm | 92 | 703 | 434 | 139 | 123 | 7 | 0 | 0 |

- Molecule 64 is a protein called 60S ribosomal protein rpL37 (L37e).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 64 | Bl | 88 | 678 | 410 | 148 | 114 | 6 | 0 | 0 |

- Molecule 65 is a protein called 60S ribosomal protein rpL38 (L38e).

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 65 | Bn | 78 | 604 | 385 | 113 | 106 | 0 | 0 |

- Molecule 66 is a protein called 60S ribosomal protein rpL39 (L39e).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 66 | Bo | 51 | 445 | 277 | 98 | 67 | 3 | 0 | 0 |

- Molecule 67 is a protein called 60S ribosomal protein rpL40 (L40e).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 67 | Bp | 40 | 330 | 201 | 72 | 52 | 5 | 0 | 0 |

- Molecule 68 is a protein called 60S ribosomal protein rpL41 (L41e).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 68 | Bq | 25 | 234 | 142 | 63 | 28 | 1 | 0 | 0 |

- Molecule 69 is a protein called 60S ribosomal protein rpL42 (L44e).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 69 | Br | 106 | 834 | 521 | 169 | 138 | 6 | 0 | 0 |

- Molecule 70 is a protein called Unknown protein.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 70 | Bx | 20 | 100 | 60 | 20 | 20 | 0 | 0 |
| 70 | By | 20 | 100 | 60 | 20 | 20 | 0 | 0 |

- Molecule 71 is a protein called Unknown protein.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 71 | Bz | 14 | 70 | 42 | 14 | 14 | 0 | 0 |

- Molecule 72 is a protein called 60S acidic ribosomal protein rpP11 (P1).

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 72 | Bt | 58 | 440 | 281 | 68 | 91 | 0 | 0 |
| 72 | Bu | 58 | 440 | 281 | 68 | 91 | 0 | 0 |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| Bt | 37 | ASP | VAL | conflict | UNP P05318 |
| Bu | 37 | ASP | VAL | conflict | UNP P05318 |

- Molecule 73 is a protein called 60S acidic ribosomal protein (P2).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 73 | Bv | 58 | 429 | 271 | 66 | 91 | 1 | 0 | 0 |
| 73 | Bw | 58 | 429 | 271 | 66 | 91 | 1 | 0 | 0 |

- Molecule 74 is a protein called 60S ribosomal protein rpL5 (L18p).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 74 | BQ | 297 | 2356 | 1485 | 414 | 454 | 3 | 0 | 0 |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| BQ | 112 | ARG | LYS | conflict | UNP P26321 |

- Molecule 75 is a protein called 60S ribosomal protein rpL13 (L13e).

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 75 | BL | 169 | 845 | 507 | 169 | 169 | 0 | 0 |

- Molecule 76 is a protein called 60S ribosomal protein rpL20 (L18ae).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 76 | BS | 167 | 1420 | 916 | 263 | 234 | 7 | 0 | 0 |

- Molecule 77 is a protein called 60S ribosomal protein rpL10 (L10e).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 77 | BI | 181 | 1444 | 907 | 281 | 248 | 8 | 0 | 0 |

- Molecule 78 is a RNA chain called 18S rRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 78 | CA | 1721 | 33643 | 14904 | 5670 | 11348 | 1721 | 0 | 10 |

- Molecule 79 is a RNA chain called P-SITE TRNA ASP.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 79 | CB | 75 | 1599 | 712 | 280 | 532 | 75 | 0 | 0 |

- Molecule 80 is a RNA chain called MRNA, RNA (5'-R(P*AP*AP*AP*AP*GP*AP*CP*UP*UP*CP*A)-3').

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 80 | CC | 11 | 236 | 106 | 45 | 74 | 11 | 0 | 0 |

- Molecule 81 is a RNA chain called 25S rRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 81 | DA | 3354 | 68830 | 30640 | 12220 | 22616 | 3354 | 0 | 75 |

- Molecule 82 is a RNA chain called 5.8S rRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 82 | DB | 157 | 3129 | 1391 | 523 | 1058 | 157 | 0 | 0 |

- Molecule 83 is a RNA chain called 5S rRNA.

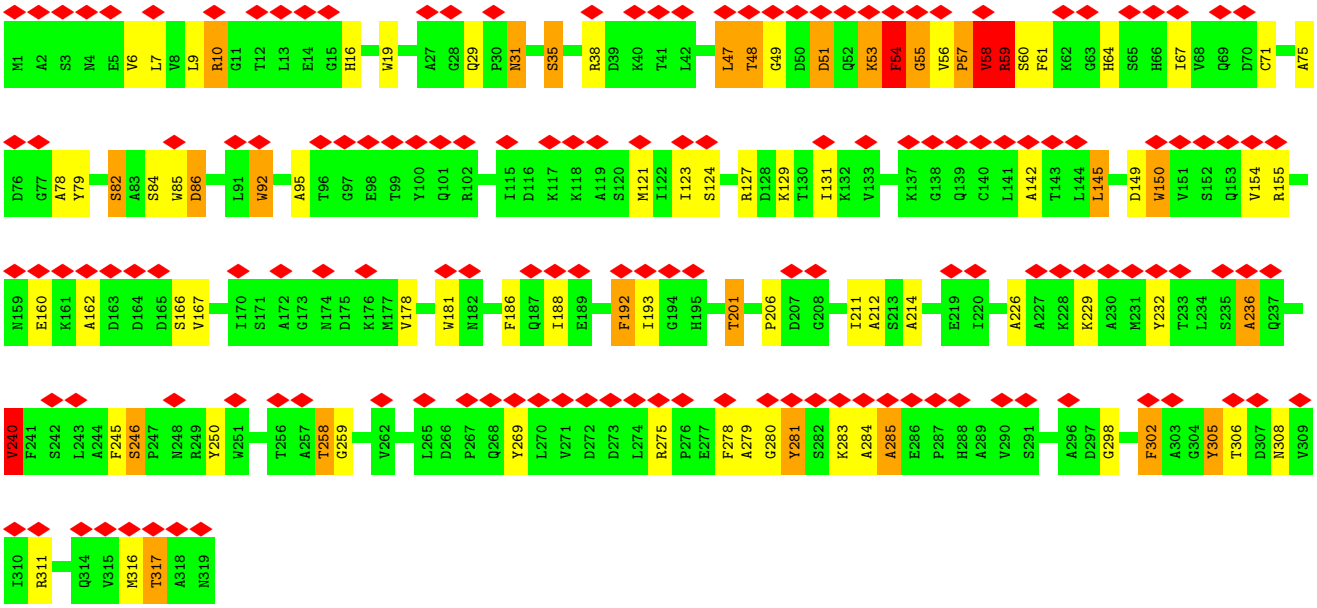
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 83 | DC | 118 | 2513 | 1122 | 446 | 827 | 118 | 0 | 0 |

# 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.

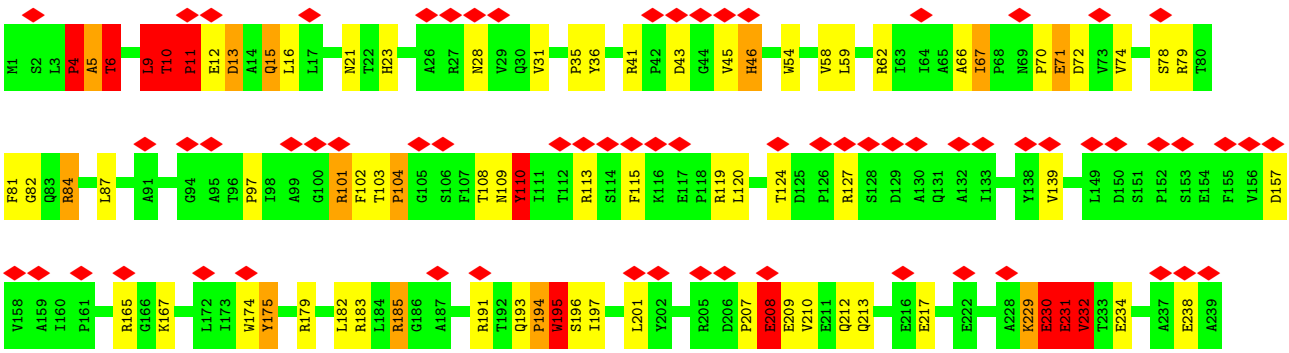
- Molecule 1: 40S ribosomal protein RACK1 (RACK1)

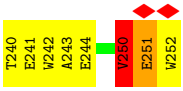
Chain Aa: 47% 72% 19% 8%




- Molecule 2: 40S ribosomal protein rpS0 (S2p)

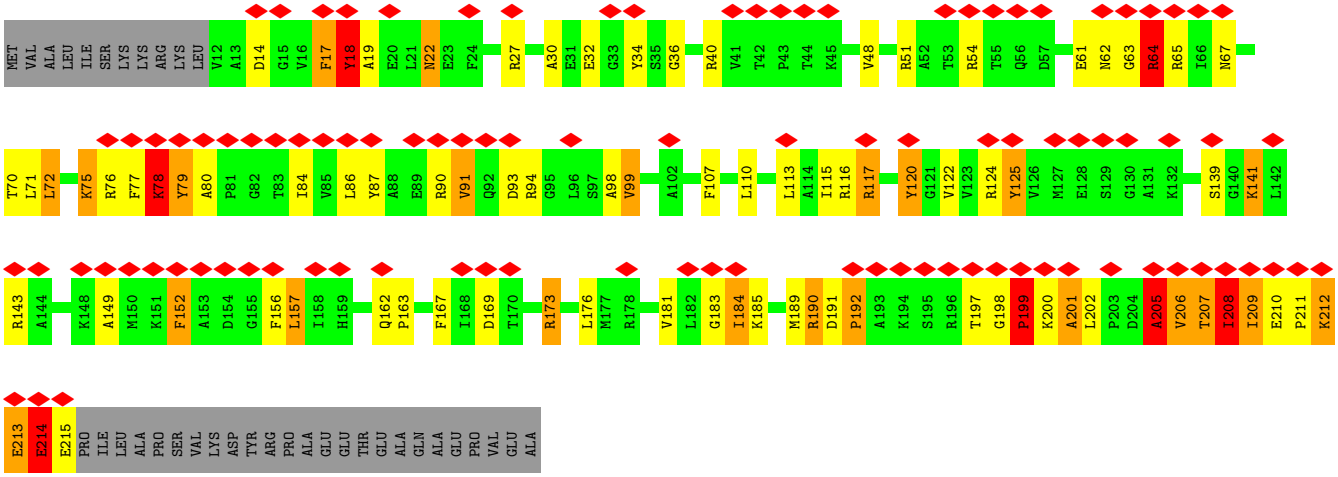
Chain AA: 27% 65% 25% 6% 5%





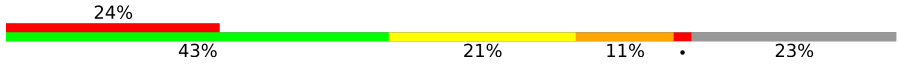

- Molecule 3: 40S ribosomal protein rpS3 (S3p)

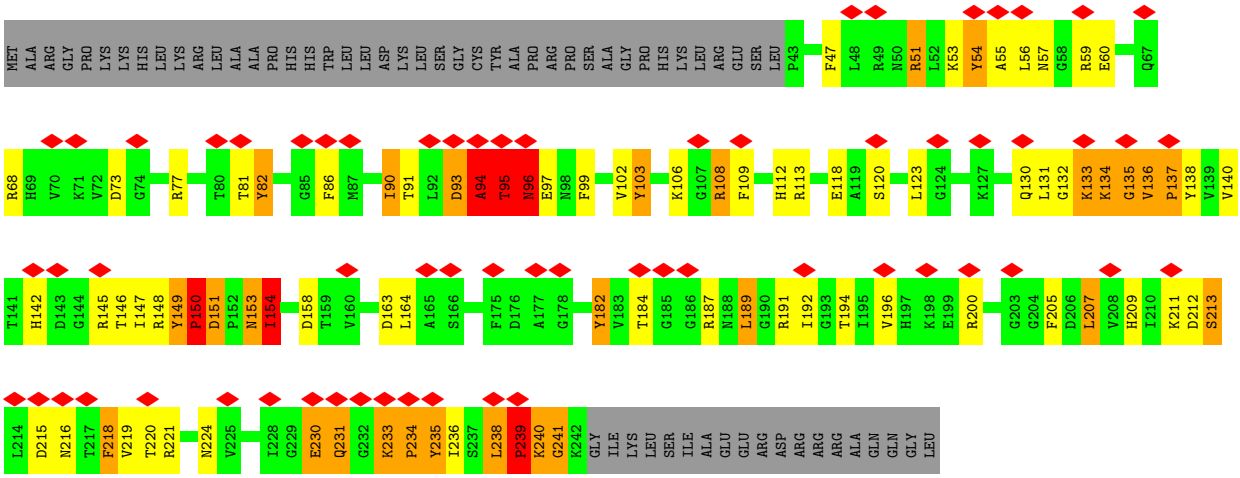
Chain AB:




- Molecule 4: 40S ribosomal protein rpS4 (S4e)

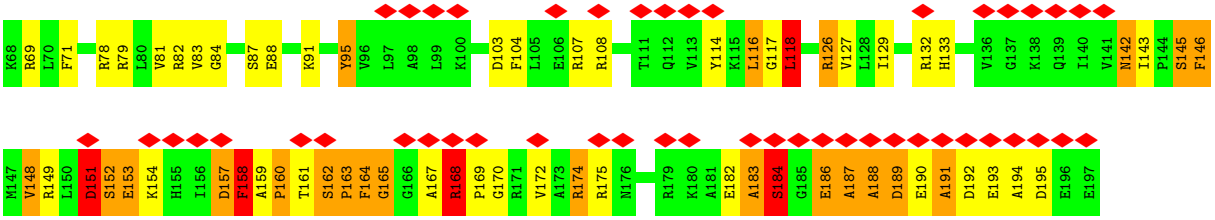
Chain AD:



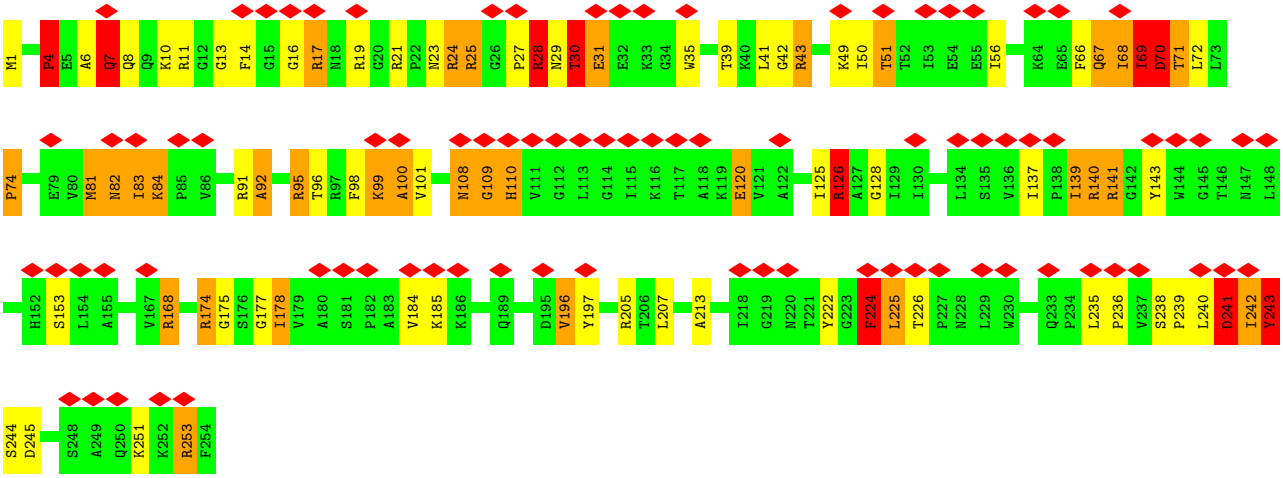

- Molecule 5: 40S ribosomal protein rpS9 (S4p)

Chain AC:



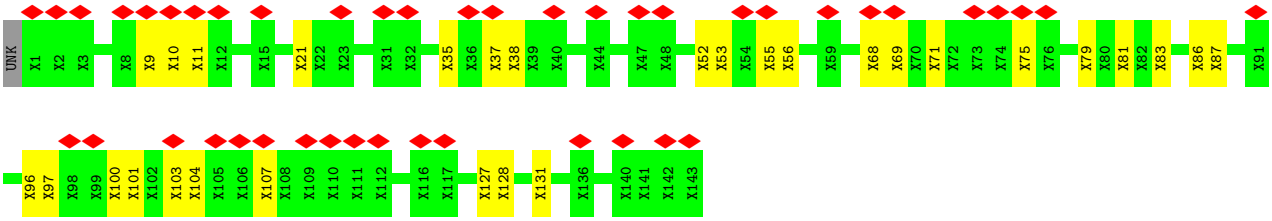

• Molecule 6: 40S ribosomal protein rpS2 (S5p)

Chain AE:



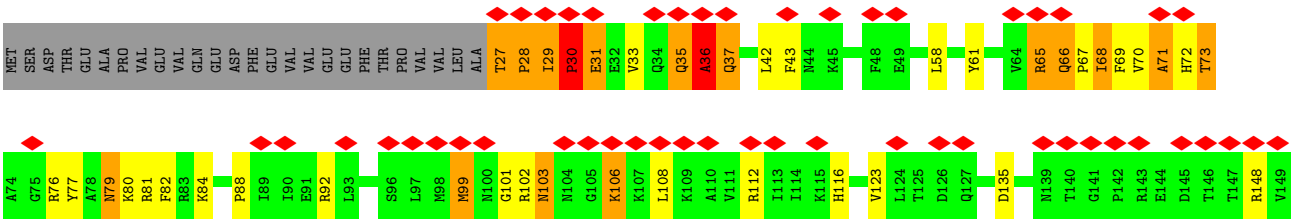

• Molecule 7: 40S ribosomal protein rpS7 (S7e)

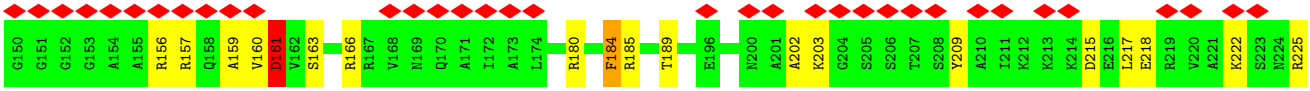
Chain AG:




• Molecule 8: 40S ribosomal protein rpS5 (S7p)

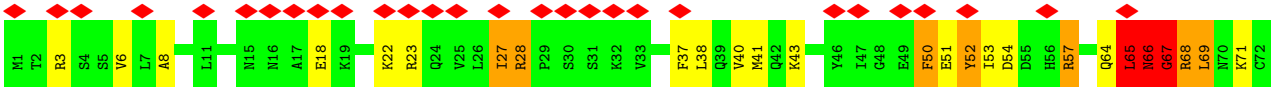
Chain AF:

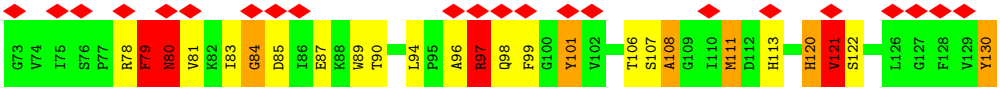





• Molecule 9: 40S ribosomal protein rpS22 (S8p)

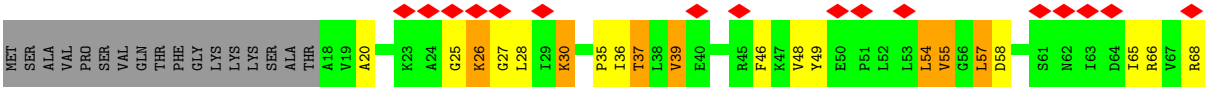
Chain AH:

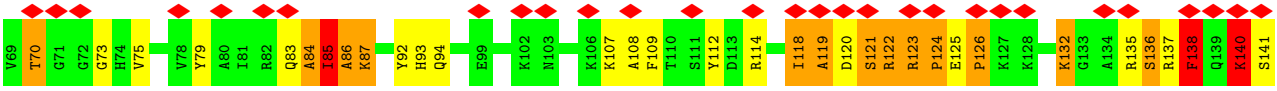



• Molecule 10: 40S ribosomal protein rpS16 (S9p)

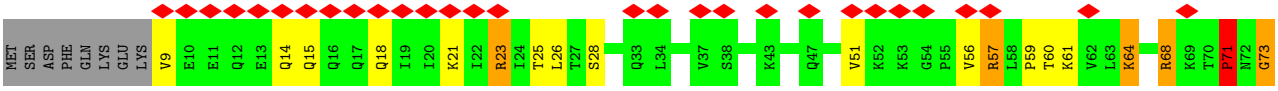
Chain AI:

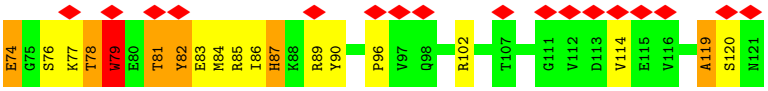


• Molecule 11: 40S ribosomal protein rpS20 (S10p)

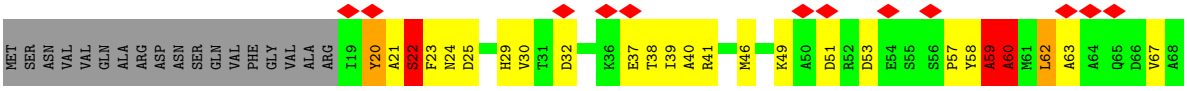
Chain AJ:

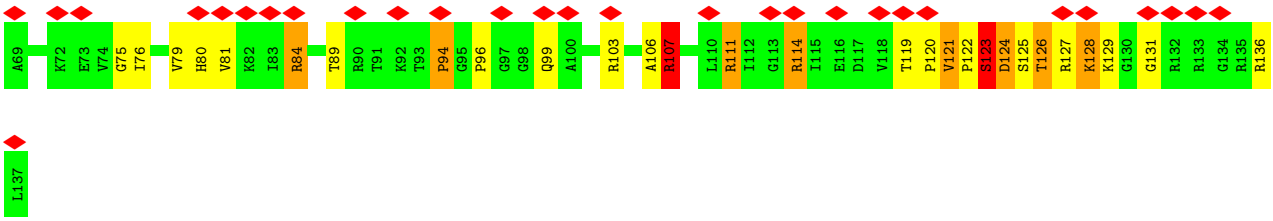



• Molecule 12: 40S ribosomal protein rpS14 (S11p)

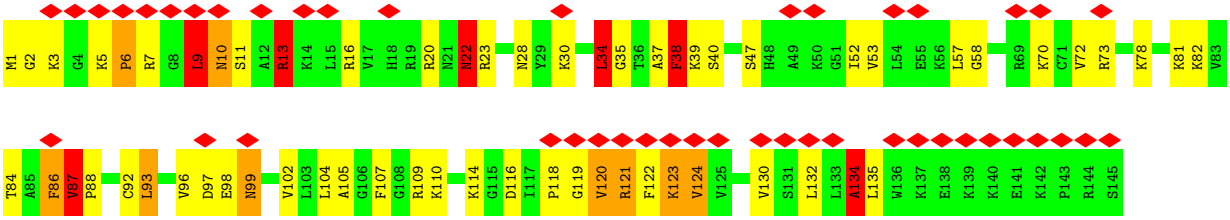
Chain AK:





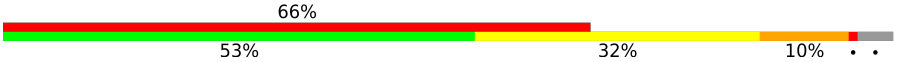

• Molecule 13: 40S ribosomal protein rpS23 (S12p)

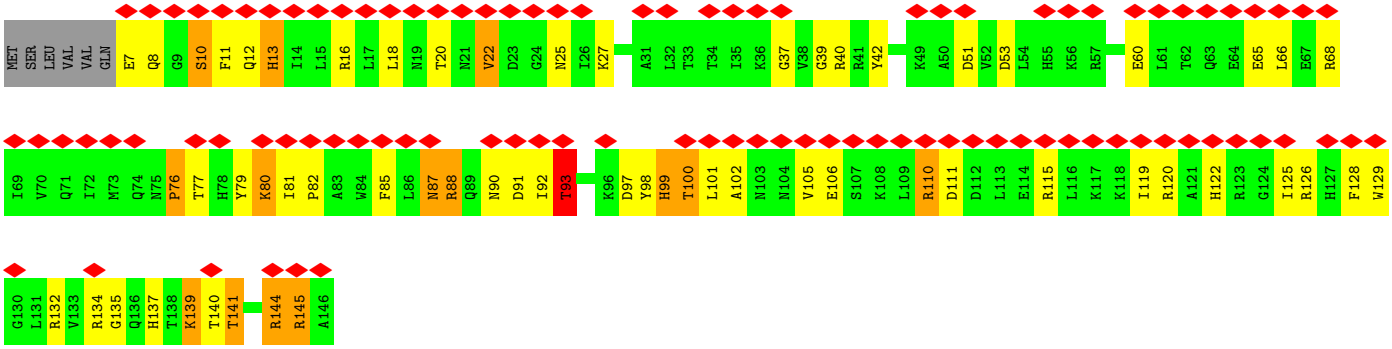
Chain AL:




• Molecule 14: 40S ribosomal protein rpS18 (S13p)

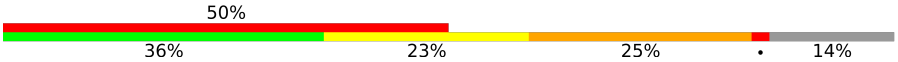
Chain AM:

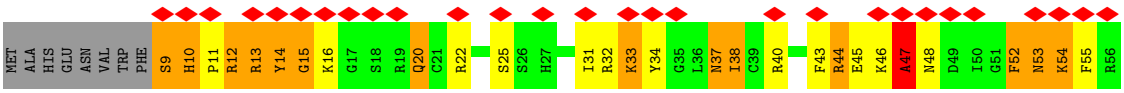



• Molecule 15: 40S ribosomal protein rpS29 (S14p)

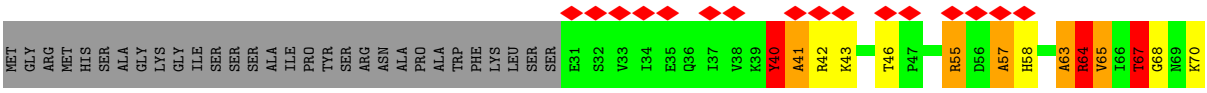
Chain AN:

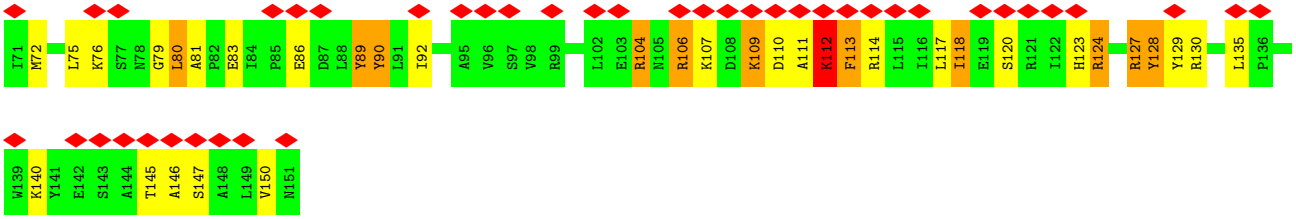



• Molecule 16: 40S ribosomal protein rpS13 (S15p)

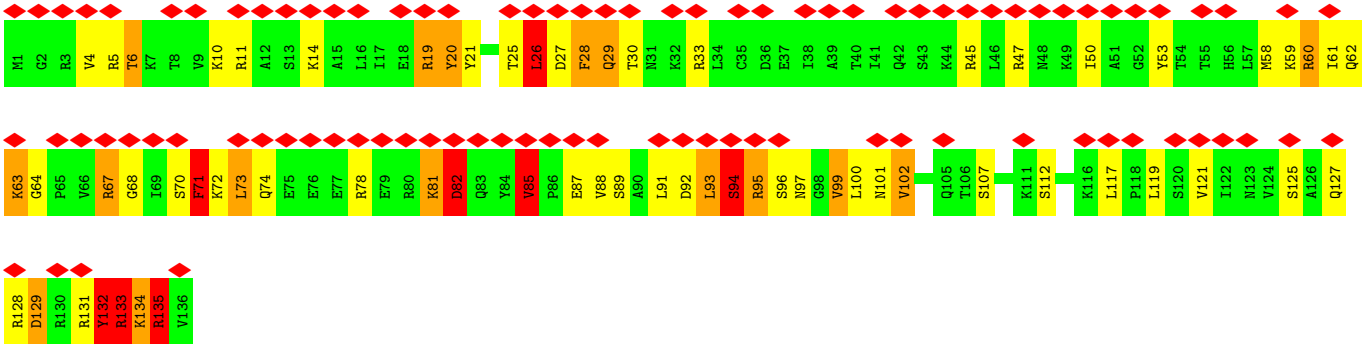
Chain AO:





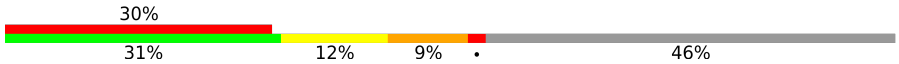

- Molecule 17: 40S ribosomal protein rpS17 (S17e)

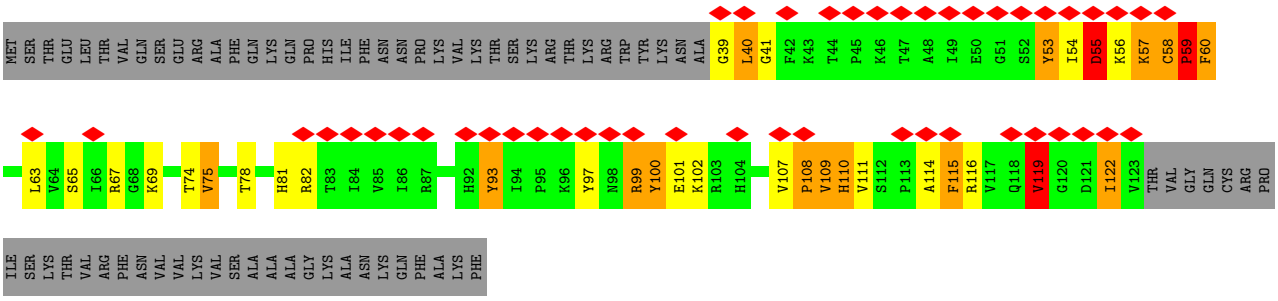
Chain AQ:




- Molecule 18: 40S ribosomal protein rpS11 (S17p)

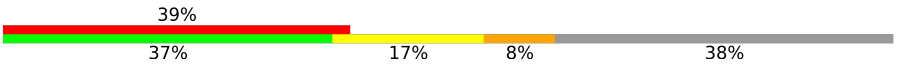
Chain AP:

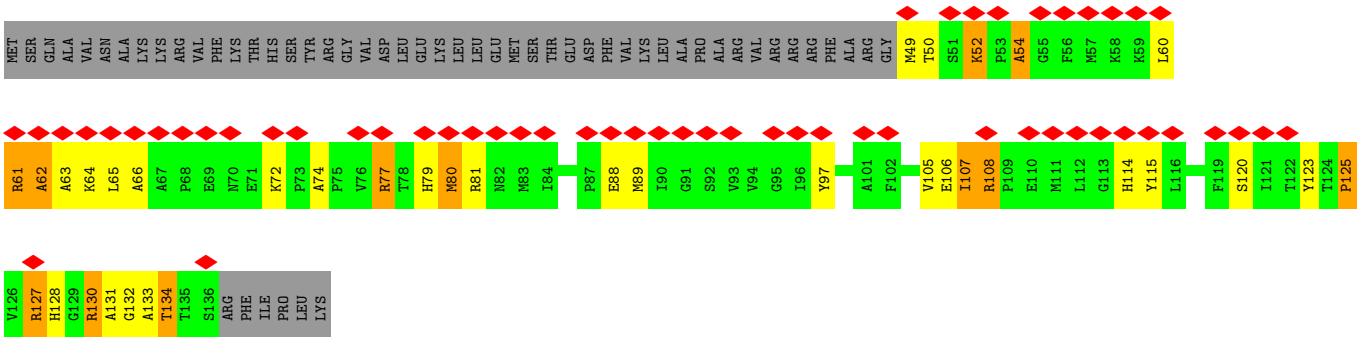



- Molecule 19: 40S ribosomal protein rpS15 (S19p)

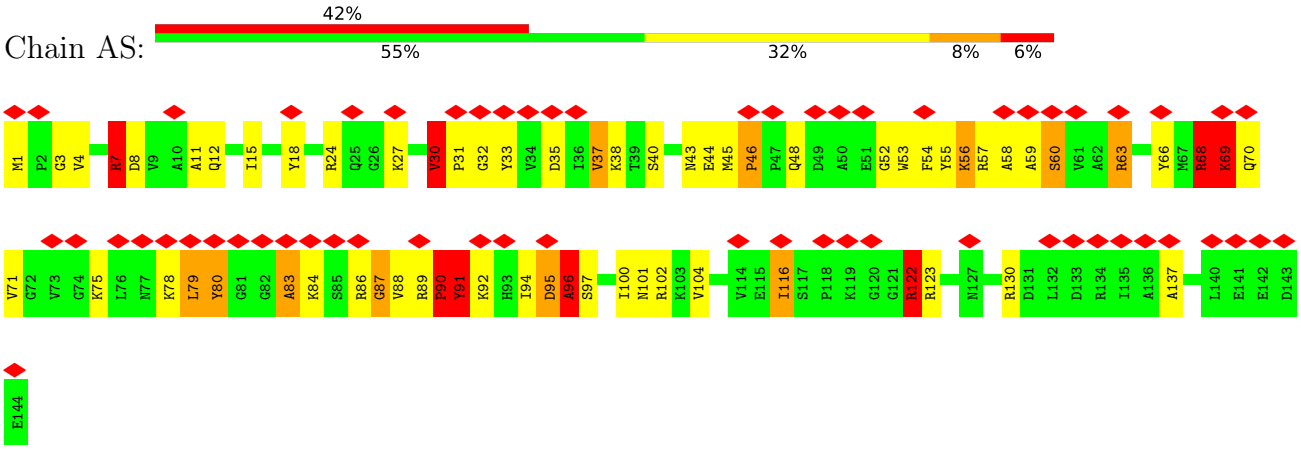
Chain AR:



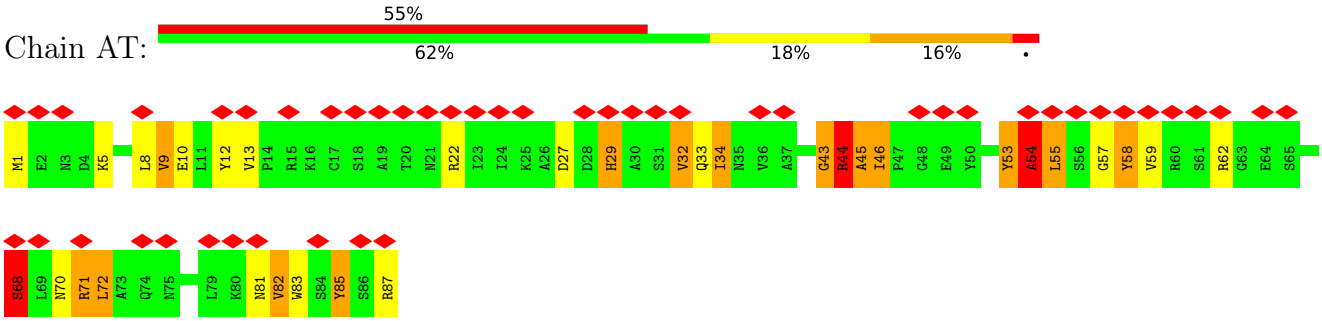
• Molecule 20: 40S ribosomal protein rpS19 (S19e)

Chain AS:



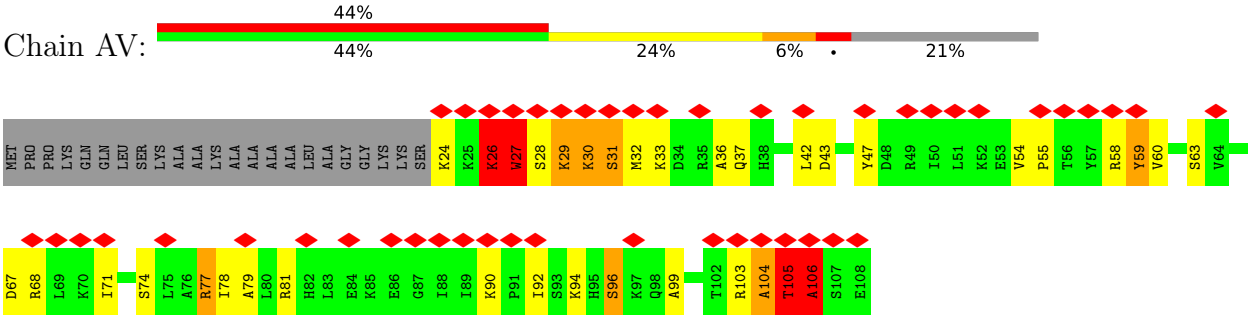

• Molecule 21: 40S ribosomal protein rpS21 (S21e)

Chain AT:



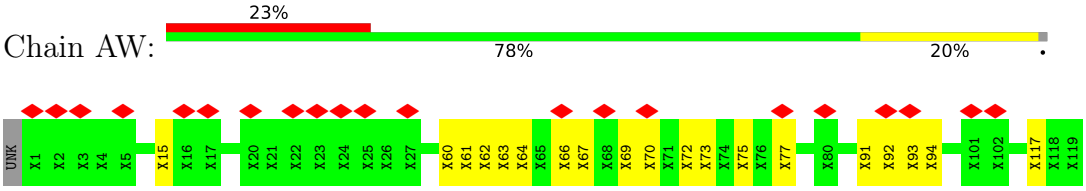

• Molecule 22: 40S ribosomal protein rpS25 (S25e)

Chain AV:



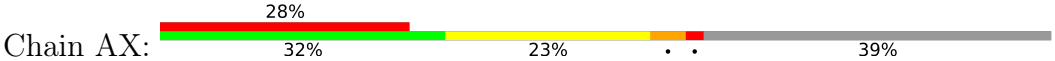

• Molecule 23: 40S ribosomal protein rpS26 (S26e)

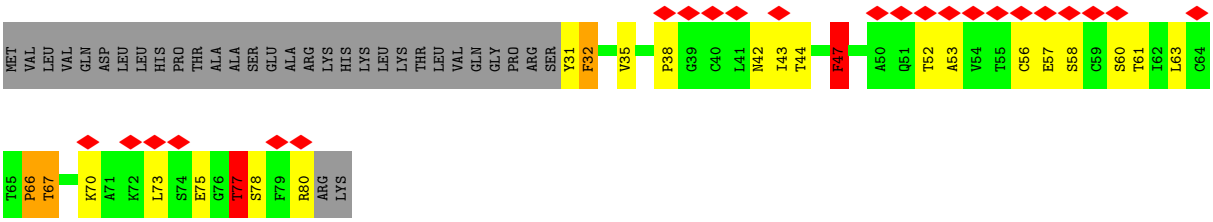
Chain AW:




• Molecule 24: 40S ribosomal protein rpS27 (S27e)

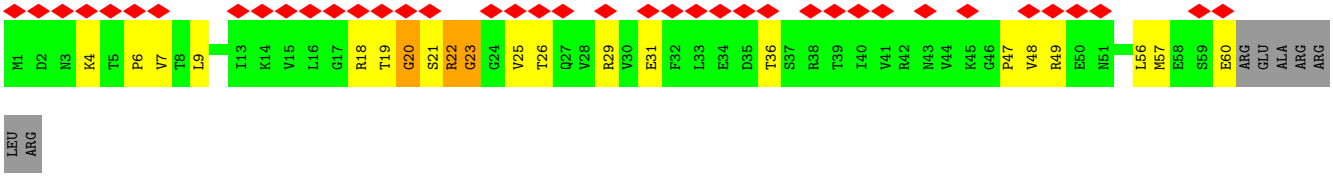
Chain AX:





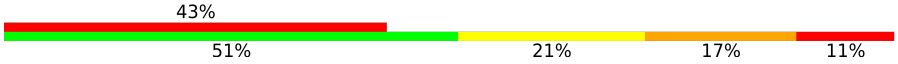

• Molecule 25: 40S ribosomal protein rpS28 (S28e)

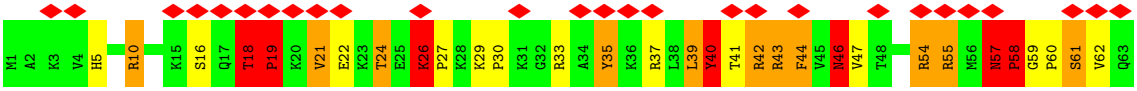
Chain AY:




• Molecule 26: 40S ribosomal protein rpS30 (S30e)

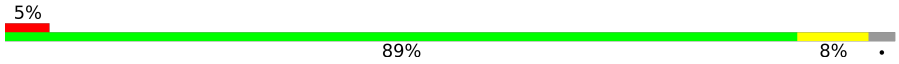
Chain AZ:

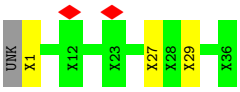



• Molecule 27: Unknown 40S ribosomal protein XS1

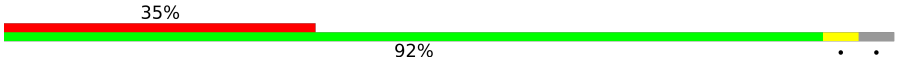
Chain Ab:

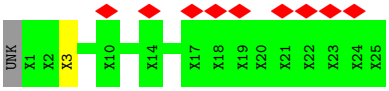



• Molecule 28: Unknown 40S ribosomal protein XS2

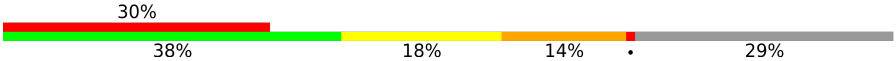
Chain Ac:

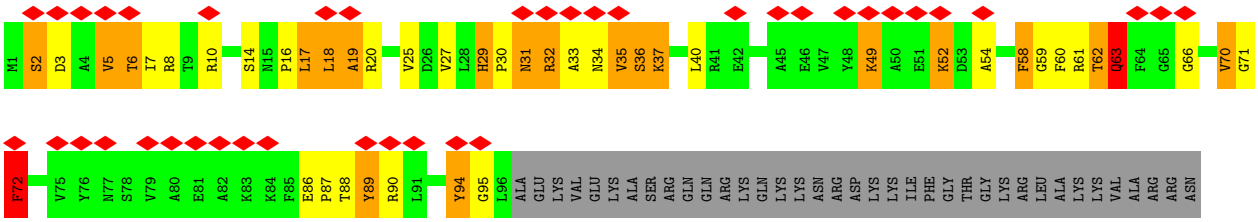



• Molecule 29: 40S ribosomal protein S24

Chain AU:

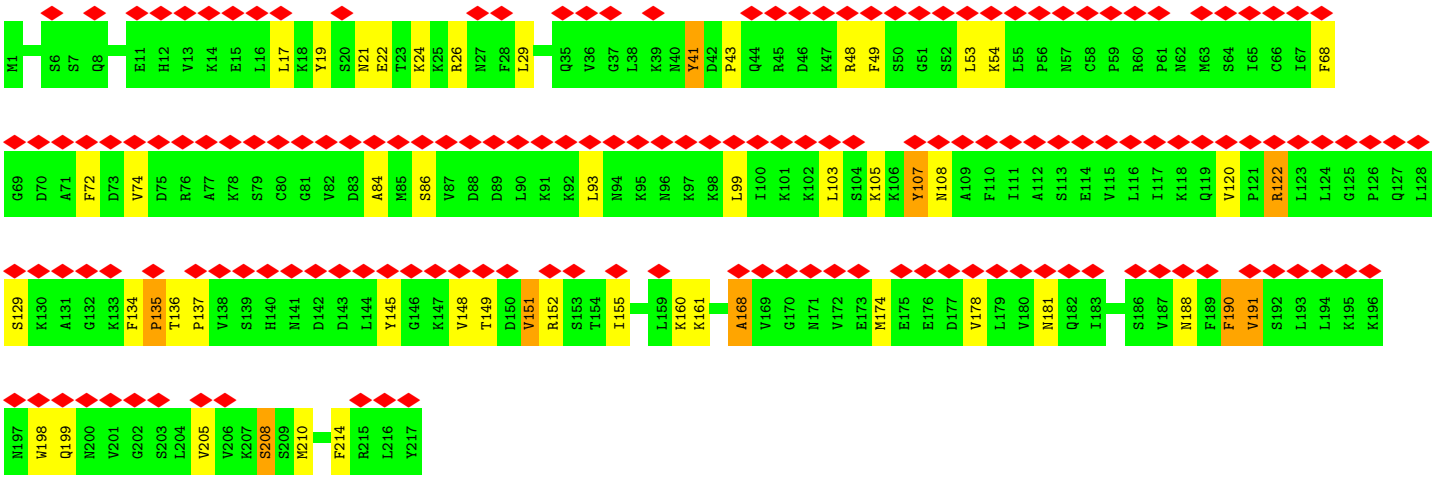


ALA
ASP

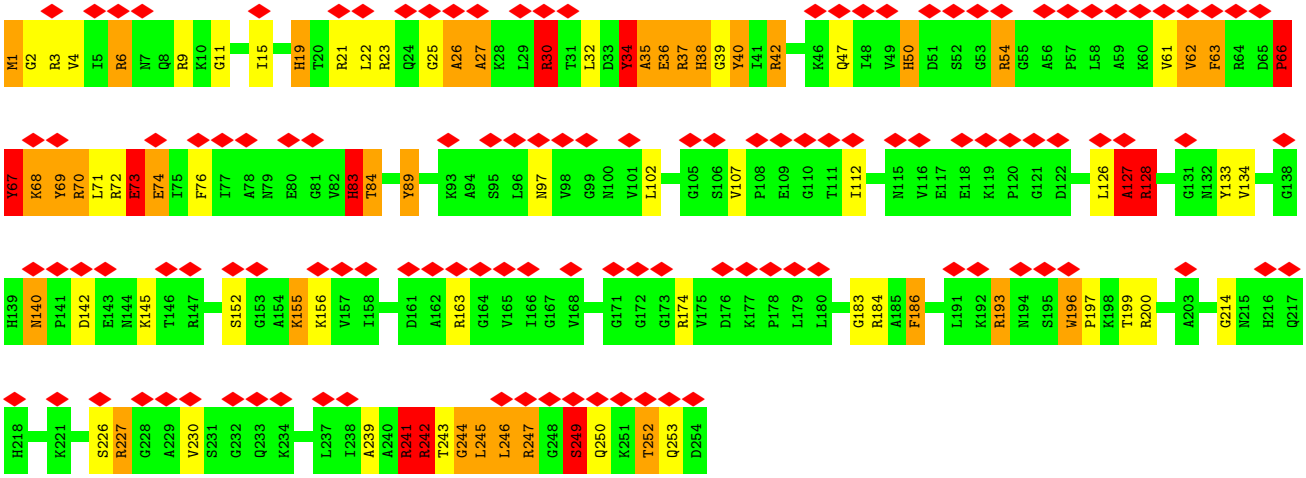
- Molecule 30: 60S ribosomal protein rpL1 (L1p)

Chain BA:



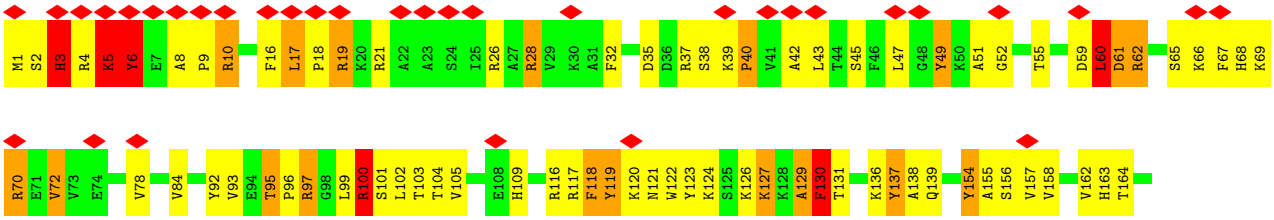

- Molecule 31: 60S ribosomal protein rpL2 (L2p)

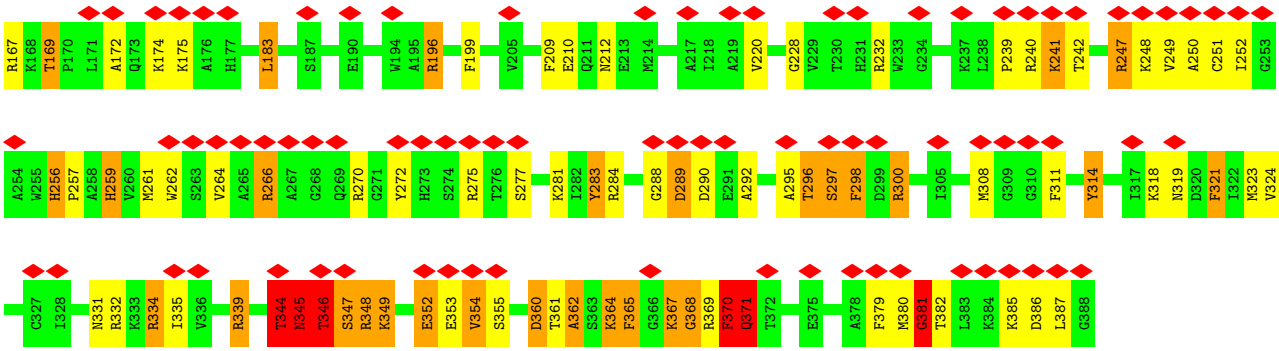
Chain BB:




- Molecule 32: 60S ribosomal protein rpL3 (L3p)

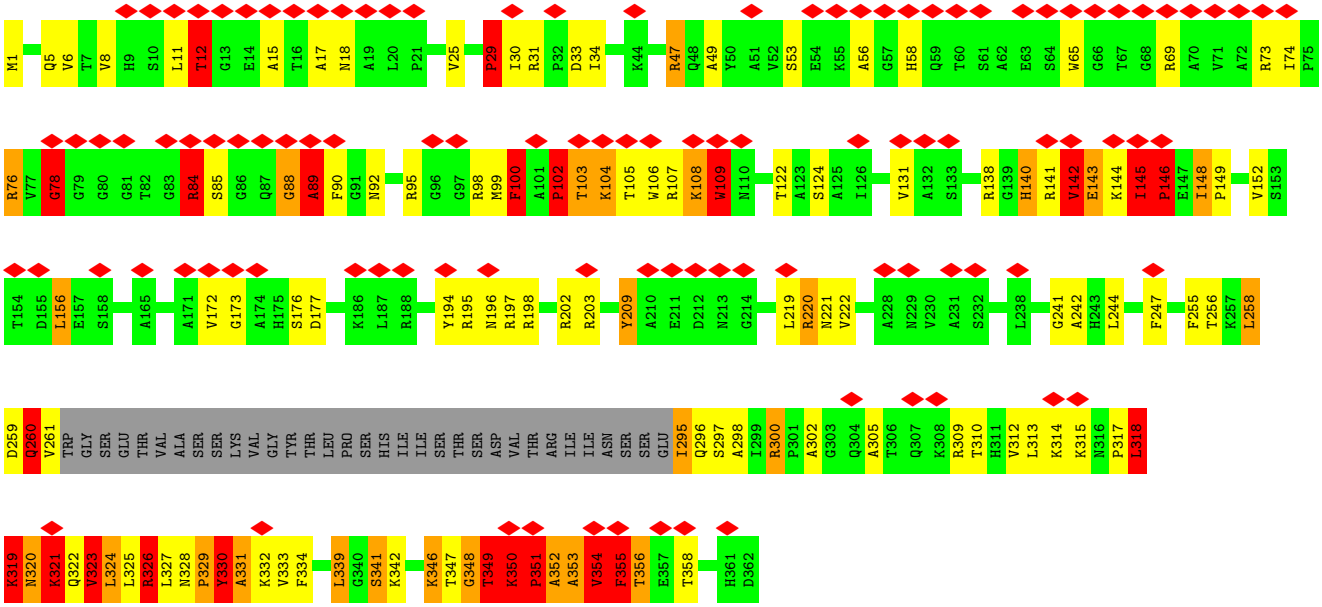
Chain BC:





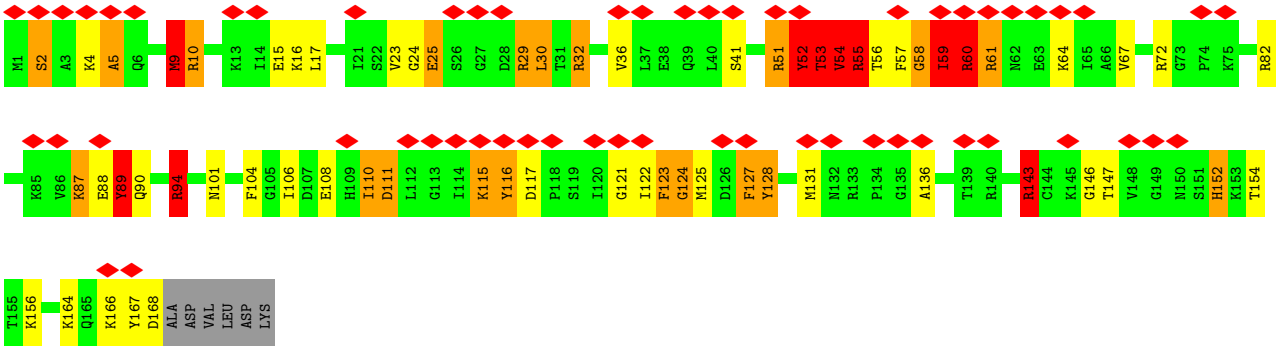

• Molecule 33: 60S ribosomal protein rpL4 (L4p)

Chain BD:




• Molecule 34: 60S ribosomal protein rpL11 (L5p)

Chain BE:




• Molecule 35: 60S ribosomal protein rpL6 (L6e)

Chain BG: 28% 36% 28% 22% 14%

M1 S2 A3 Q4 K5 A6 P7 K8 W9 Y10 P11 S12 E13 D14 V15 A16 A17 L18 K19 K20 T21 R22 K23 A24 A25 R26 P27 Q28 K29 L30 R31 L34 V35 P36 G37 T38 L42 L43 A44 G45 R46 F47 R48 G49 K50 R51 V52 V53 Y54 L55 K56 H57 L58 E59 D60 N61 T62 L63

L64 I65 S66 G67 P68 F69 K70 V71 N72 G73 V74 P75 L76 R77 R78 V79 N80 A81 R82 Y83 V84 I85 S88 T89 S92 V93 E94 G95 V96 N97 V98 E99 K100 F101 N102 V103 E104 Y105 F106 L111 T112 K113 K114 K117 E118 A119 E124 Q125 Q126 N127 K128 E129 I130 K131 A132

E133 R134 K139 V140 V141 D142 K143 A144 L145 I146 A147 E148 I149 K150 K151 T152 P153 L154 L155 K156 Q157 Y158 L159 S160 F163 S164 L165 K166 N167 G168 D169 K170 P171 H172 F176

- Molecule 36: 60S ribosomal protein rpL9 (L6p)

Chain BF: 37% 79% 16%

M1 K2 Y3 I4 Q5 T6 E7 I10 E11 V12 P13 E14 G15 V18 S19 R23 P30 R31 G32 T33 L34 T35 K36 N37 L38 K39 H40 I41 D42 V43 T44 F45 T46 K47 V48 N49 N50 Q51 L52 I53 K54 V55 A56 G60 G61 R62 K63 H64 V65 R69 K72 S73

T83 Y86 K87 Y88 R91 Y92 H96 F97 N100 I103 V104 E105 K106 D107 G108 A109 R115 N116 F117 K121 K122 I123 R124 R129 D130 T133 I134 T138 N139 V140 K141 D142 S147 G148 N149 S150 V151 A158 A159 D160 L161 R168 R173 K174 F175 L176

D177 G178 I179 K184 G185 F186 E189 D190 L191

- Molecule 37: 60S ribosomal protein rpL8 (L7ae)

Chain BH: 21% 46% 19% 7% 23%

MET ALA PRO GLY LYS LYS VAL ALA PRO ALA PRO PHE GLY ALA LYS SER THR LYS SER ASN LYS THR ARG ASN PRO LEU THR HIS SER THR PRO LYS ASN PHE GLY ILE GLY GLN ALA VAL GLN PRO LYS ARG ASN LEU SER ARG TYR VAL LYS TRP PRO GLU TYR VAL ARG VAL GLN R60

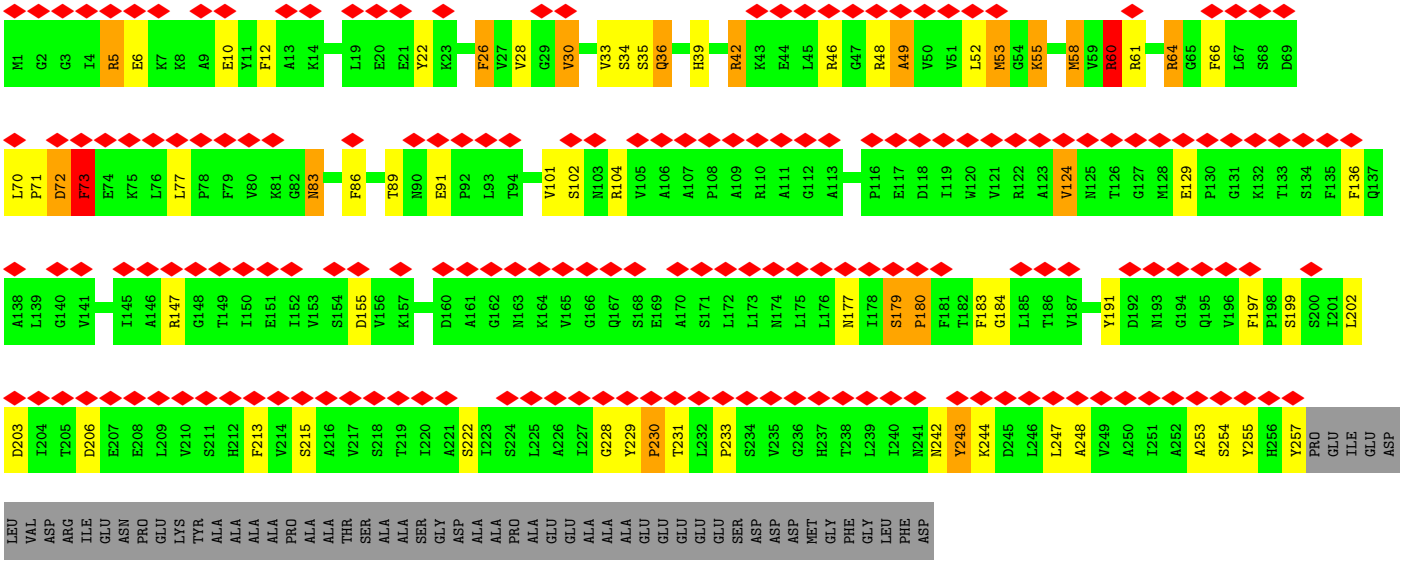
Q61 K62 K63 I64 L65 S66 I67 R68 L69 K70 P73 T74 I75 A76 Q77 F78 Q79 Y80 R84 A88 E89 T90 F91 K92 K96 Y97 R98 A103 E104 R108 L109 T110 K111 E112 A115 V116 A117 E118 G119 K120 S121 K122 Q123 D124 A125 S126 P127 K128 P129 Y130 A131 Y134

G135 L136 N137 H138 V139 V140 L150 V151 L152 V157 D158 P159 I160 E161 L162 V163 V164 F165 M173 Y177 A178 K181 R185 T188 L189 V190 K193 T194 V197 A198 A199 L200 T201 E202 V203 R204 D207 A210 S216 T217 I218 D219 A220 N221 F222 A223 D224 K225

Y226 D227 E228 V229 K230 K231 H232 W233 G234 G235 G236 I237 L238 M246 D247 K248 R249 A250 K251 N252 S253 D254 S255 A256

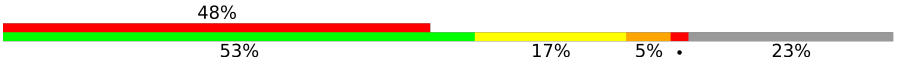
- Molecule 38: 60S acidic ribosomal protein rpP0 (L10P)

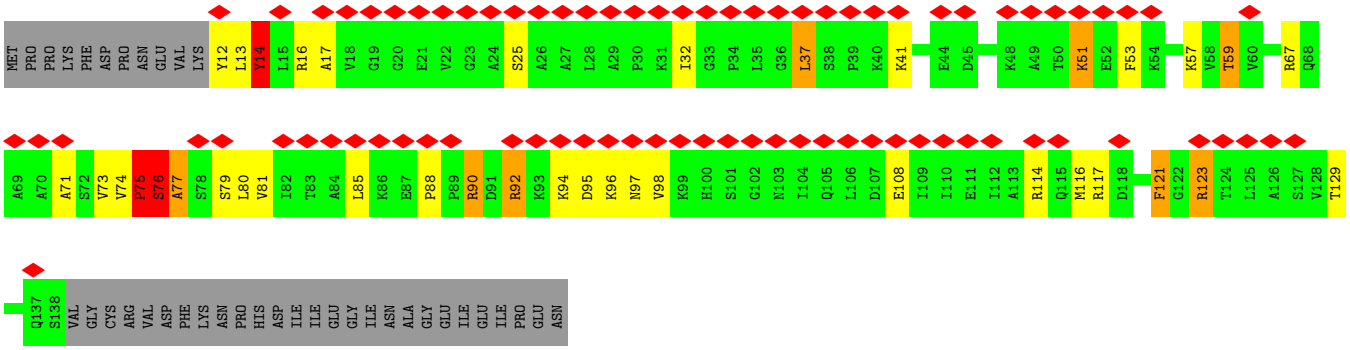
Chain Bs: 57% 60% 16% 5% 18%




- Molecule 39: 60S ribosomal protein rpL12 (L11p)

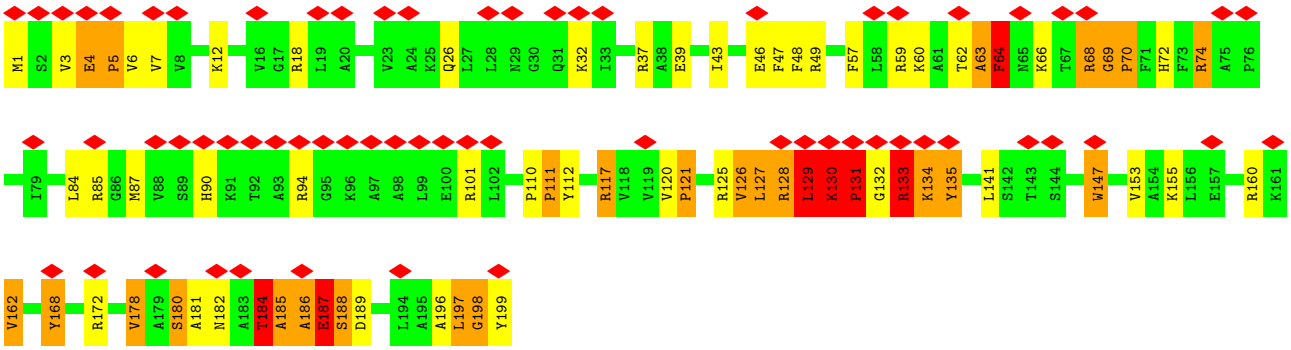
Chain BJ:



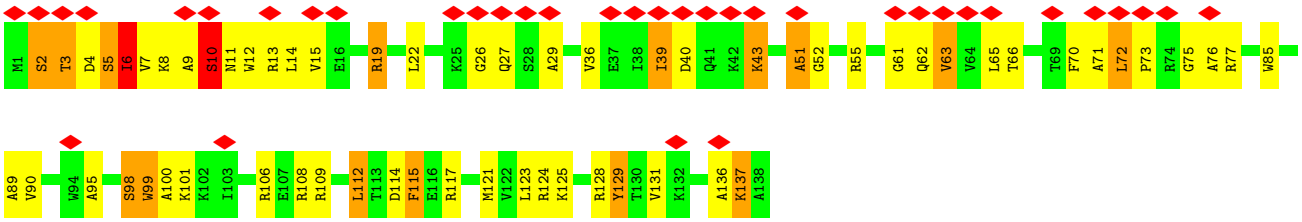

- Molecule 40: 60S ribosomal protein rpL16 (L13p)

Chain BK:



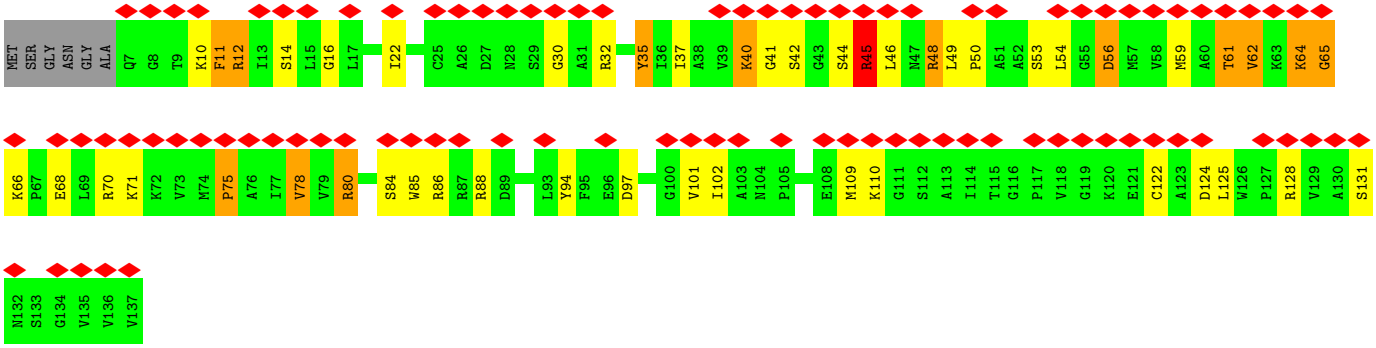

- Molecule 41: 60S ribosomal protein rpL14 (L14e)

Chain BN:



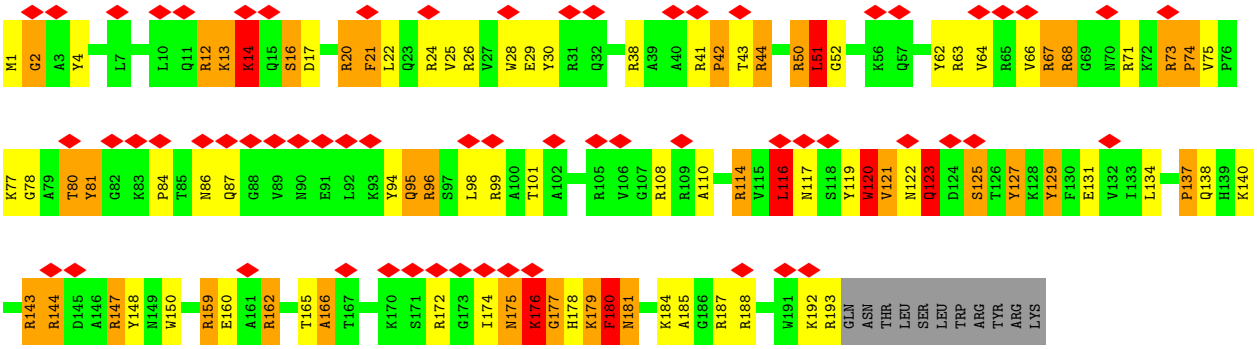

• Molecule 42: 60S ribosomal protein rpL23 (L14p)

Chain BM:



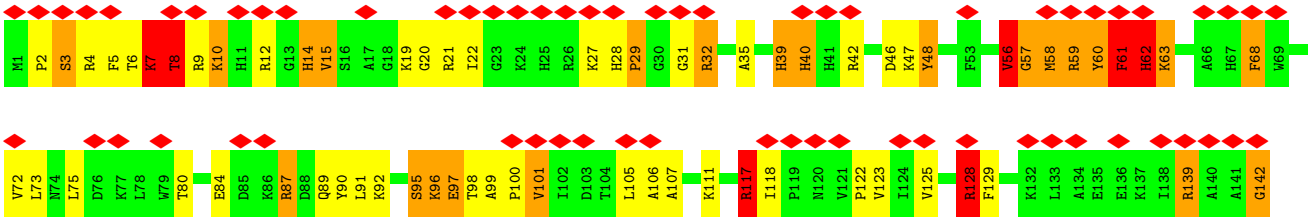

• Molecule 43: 60S ribosomal protein rpL15 (L15e)

Chain BP:



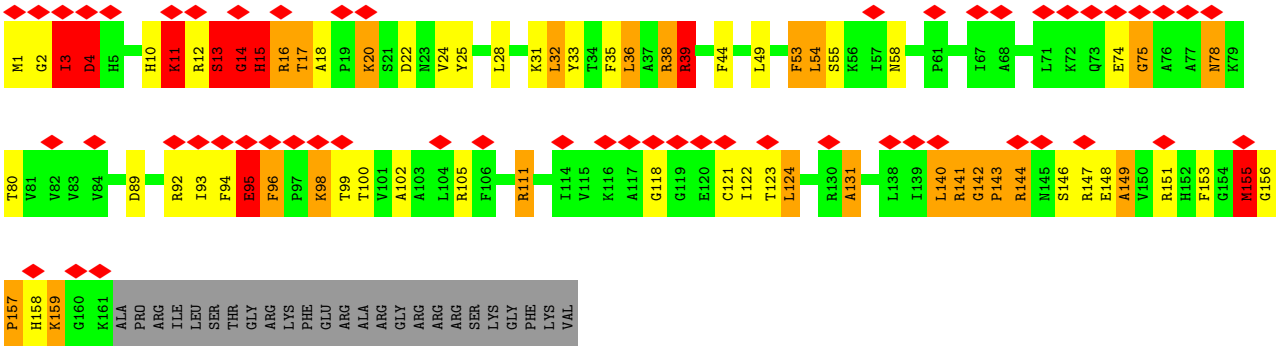

• Molecule 44: 60S ribosomal protein rpL28 (L15p)

Chain BO:



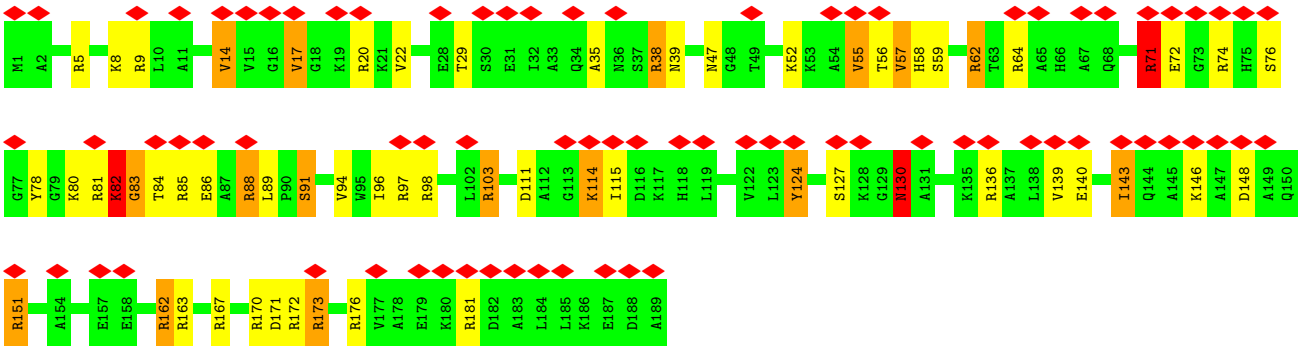
• Molecule 45: 60S ribosomal protein rpL18 (L18e)

Chain BR:



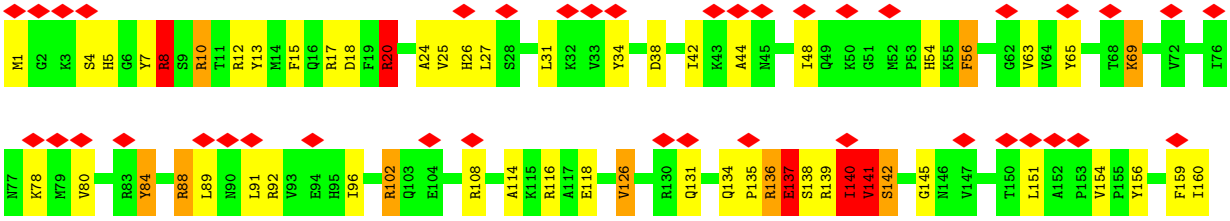

• Molecule 46: 60S ribosomal protein rpL19 (L19e)

Chain BT:



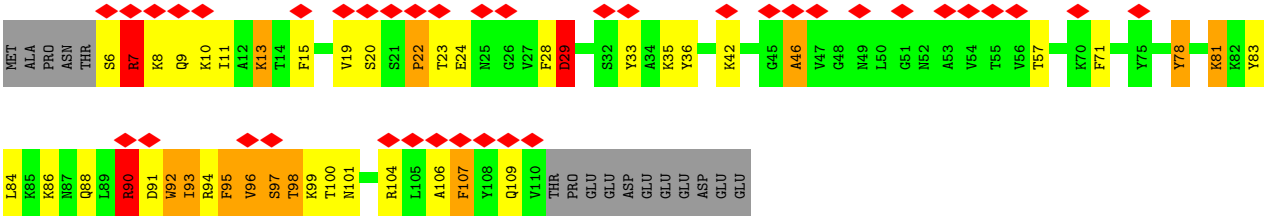

• Molecule 47: 60S ribosomal protein rpL21 (L21e)

Chain BU:



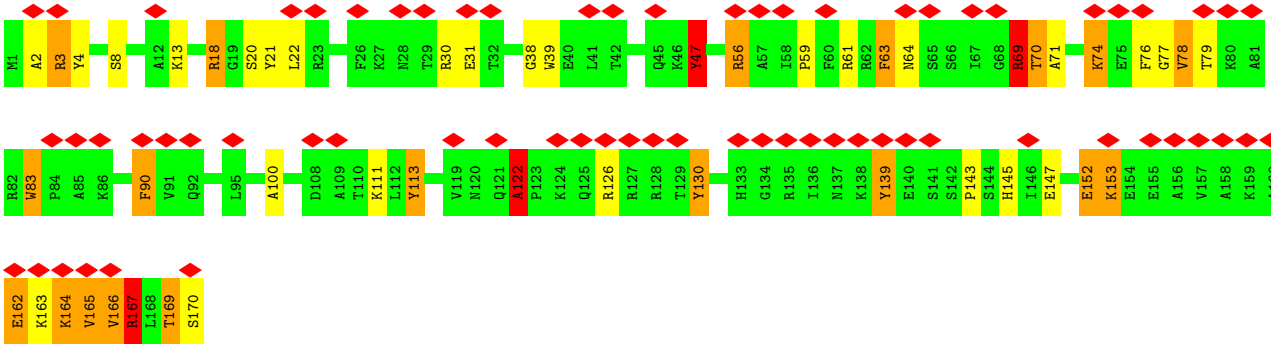

• Molecule 48: 60S ribosomal protein rpL22 (L22e)

Chain BW:



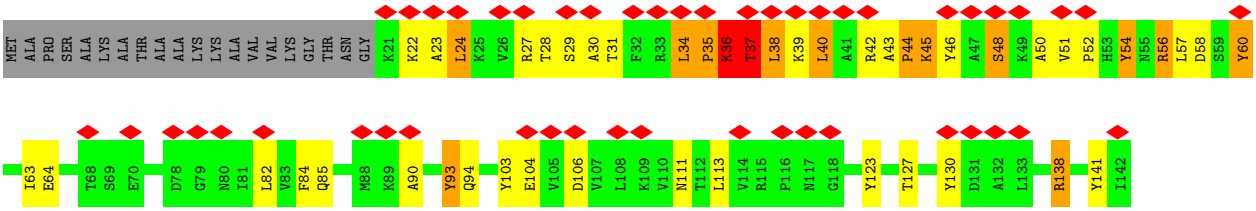

• Molecule 49: 60S ribosomal protein rpL17 (L22p)

Chain BV:



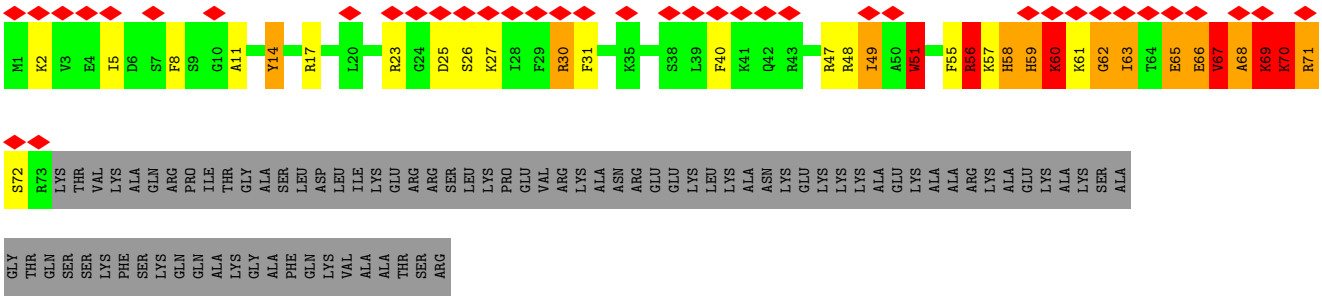

• Molecule 50: 60S ribosomal protein rpL25 (L23p)

Chain BX:



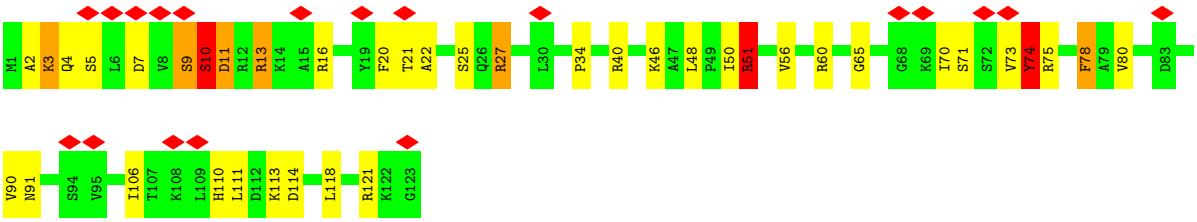

• Molecule 51: 60S ribosomal protein rpL24 (L24e)

Chain BZ:



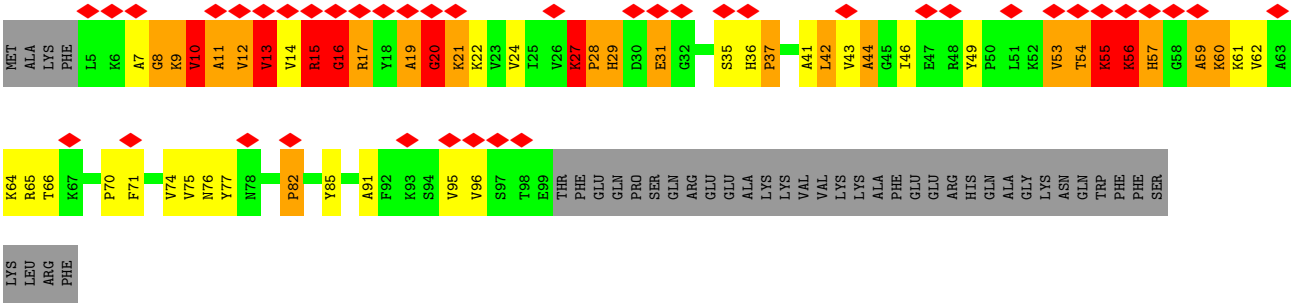

• Molecule 52: 60S ribosomal protein rpL26 (L24p)

Chain BY:



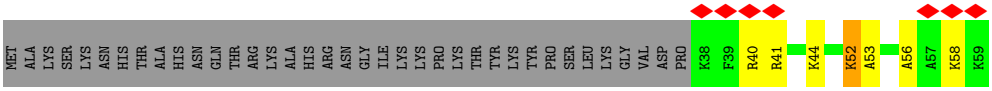

• Molecule 53: 60S ribosomal protein rpL27 (L27e)

Chain Ba:




• Molecule 54: 60S ribosomal protein rpL29 (L29e)

Chain Bd:

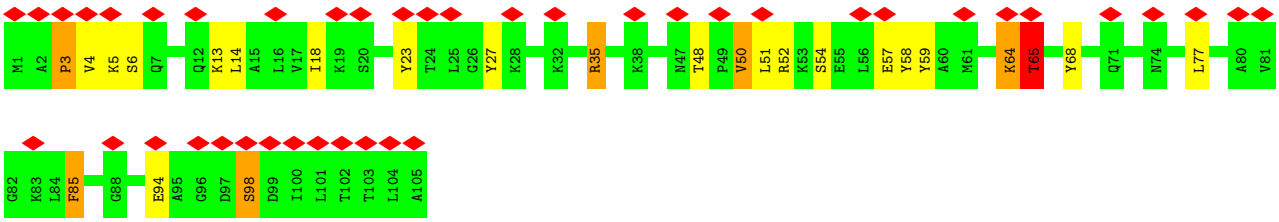



• Molecule 55: 60S ribosomal protein rpL35 (L29p)

Chain Bc:

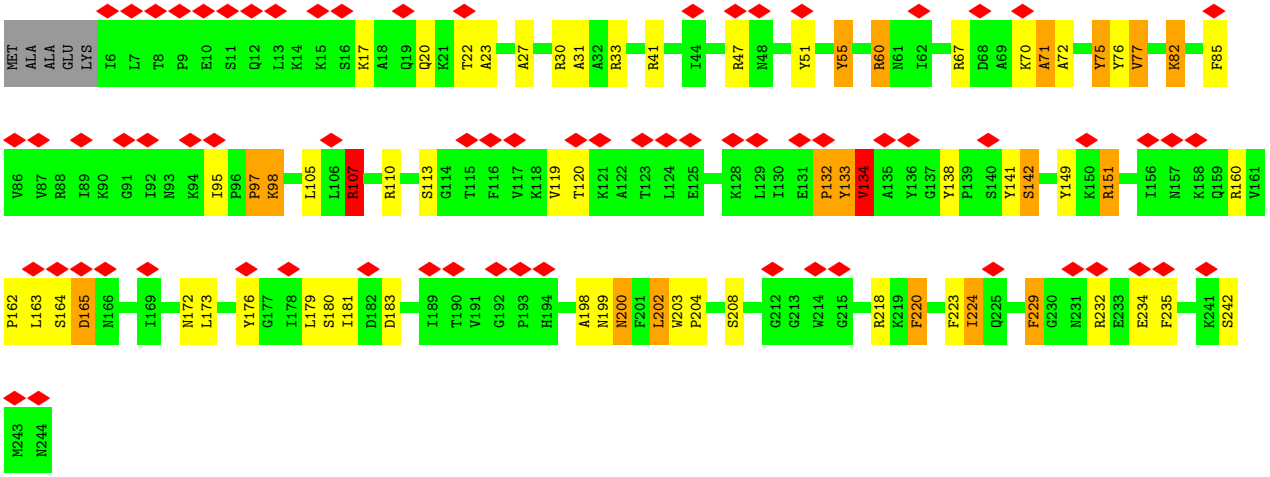
• Molecule 56: 60S ribosomal protein rpL30 (L30e)

Chain Bf:



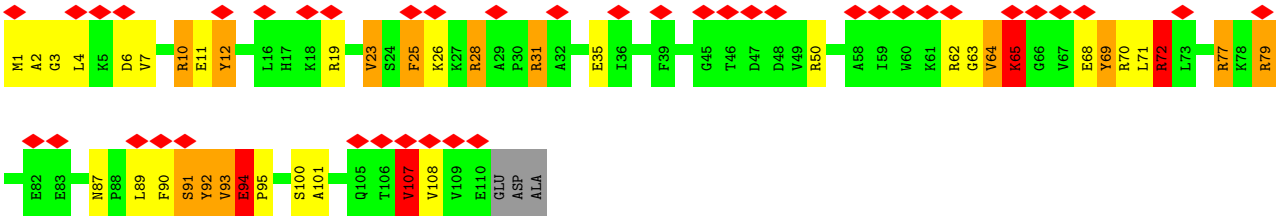
• Molecule 57: 60S ribosomal protein rpL7 (L30p)

Chain Be:



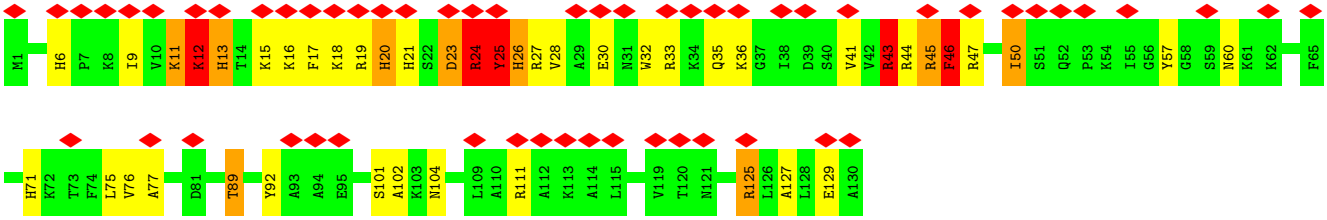

• Molecule 58: 60S ribosomal protein rpL31 (L31e)

Chain Bg:



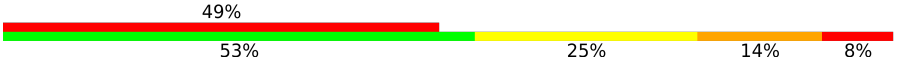

• Molecule 59: 60S ribosomal protein pL32 (L32e)

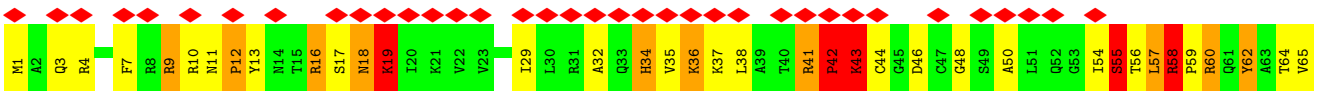
Chain Bh:

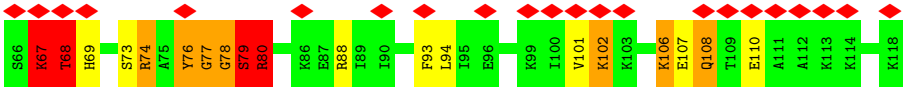



• Molecule 60: 60S ribosomal protein rpL34 (L34e)

Chain Bi:

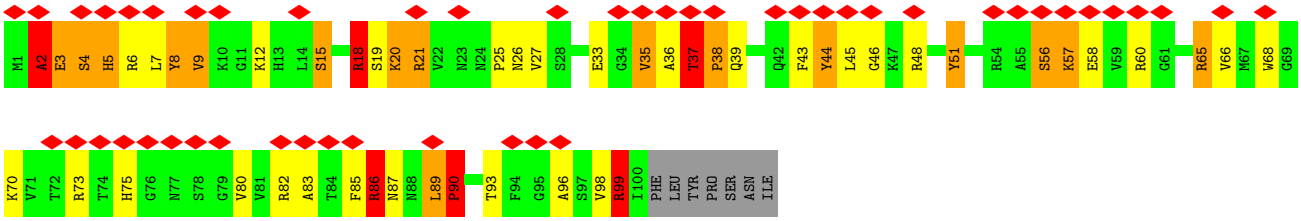




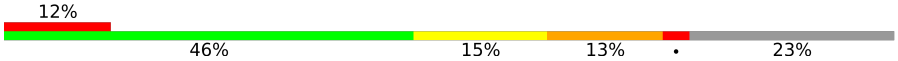

- Molecule 61: 60S ribosomal protein rpL33 (L35ae)

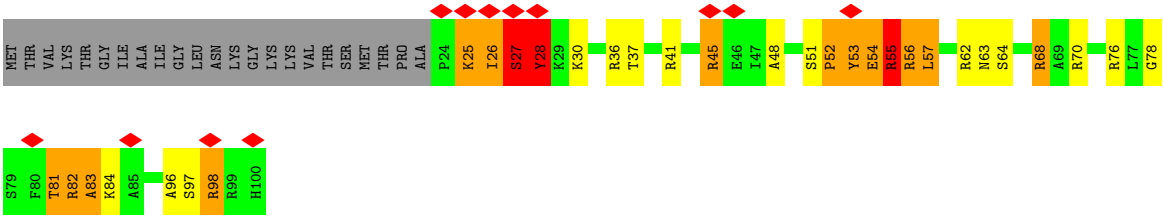
Chain Bj:




- Molecule 62: 60S ribosomal protein rpL36 (L36e)

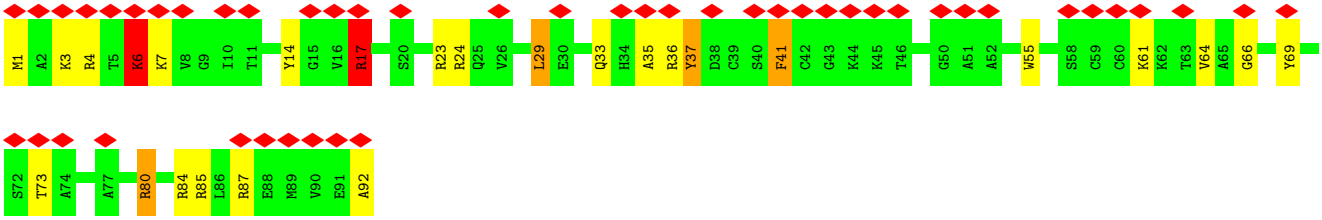
Chain Bk:



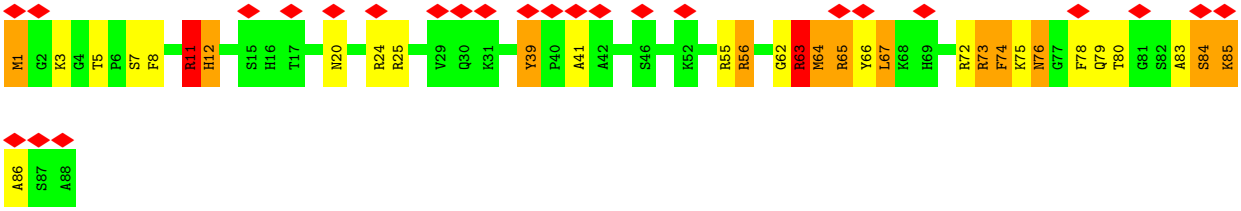

- Molecule 63: 60S ribosomal protein rpL43 (L37ae)

Chain Bm:



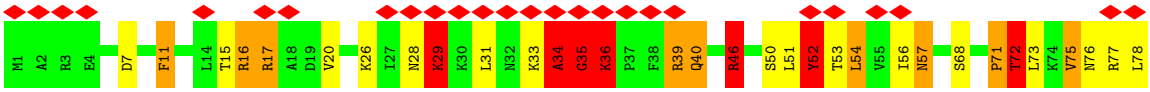

- Molecule 64: 60S ribosomal protein rpL37 (L37e)

Chain Bl:



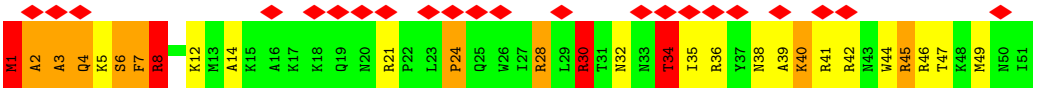

- Molecule 65: 60S ribosomal protein rpL38 (L38e)

Chain Bn:



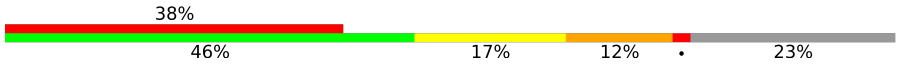

- Molecule 66: 60S ribosomal protein rpL39 (L39e)

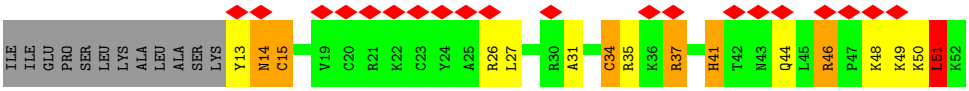
Chain Bo:




- Molecule 67: 60S ribosomal protein rpL40 (L40e)

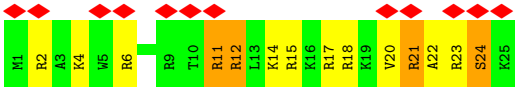
Chain Bp:



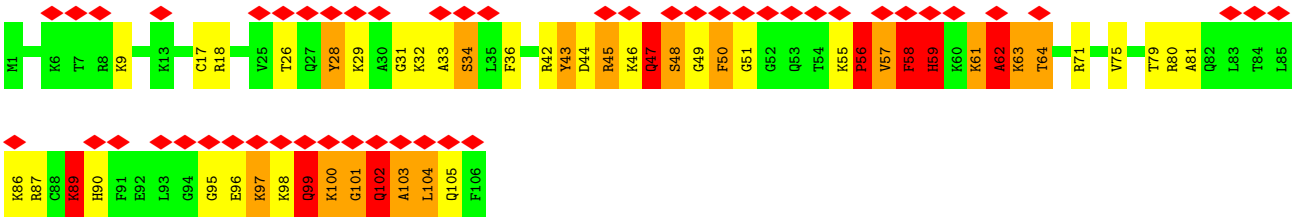

- Molecule 68: 60S ribosomal protein rpL41 (L41e)

Chain Bq:



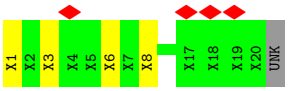

- Molecule 69: 60S ribosomal protein rpL42 (L44e)

Chain Br:




- Molecule 70: Unknown protein

Chain Bx:

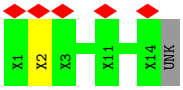



- Molecule 70: Unknown protein

Chain By: 5% 95% 5%

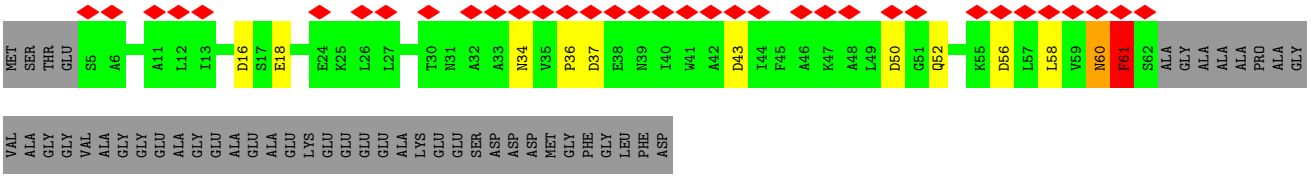
• Molecule 71: Unknown protein

Chain Bz: 33% 87% 7% 7%



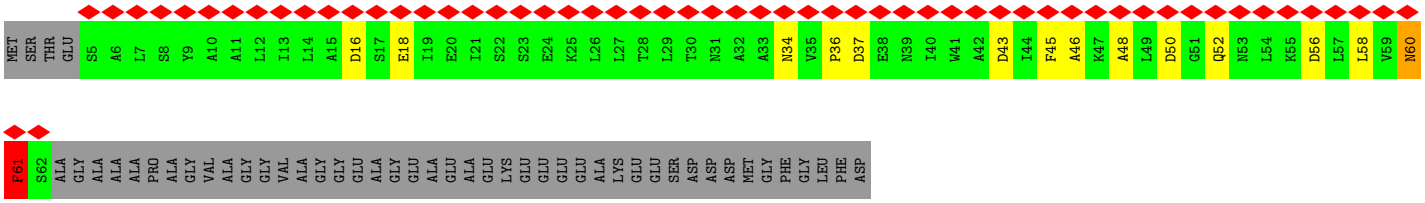

• Molecule 72: 60S acidic ribosomal protein rpP11 (P1)

Chain Bt: 33% 43% 9% 45%



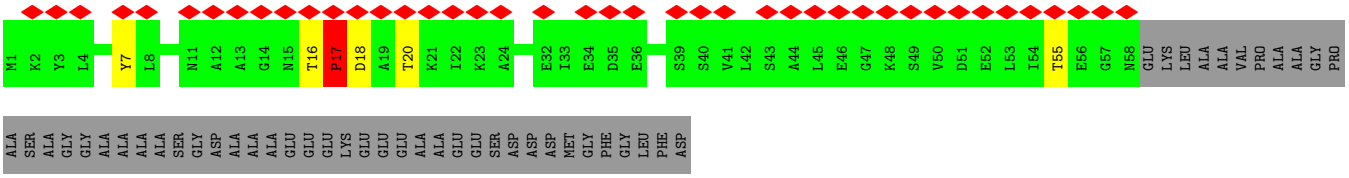

• Molecule 72: 60S acidic ribosomal protein rpP11 (P1)

Chain Bu: 55% 41% 12% 45%



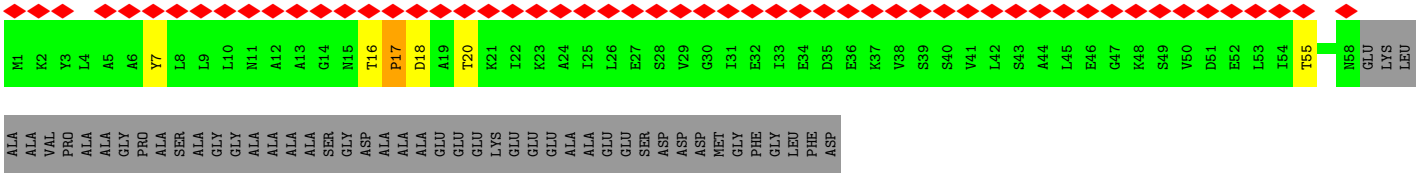

• Molecule 73: 60S acidic ribosomal protein (P2)

Chain Bv: 40% 49% 5% 45%



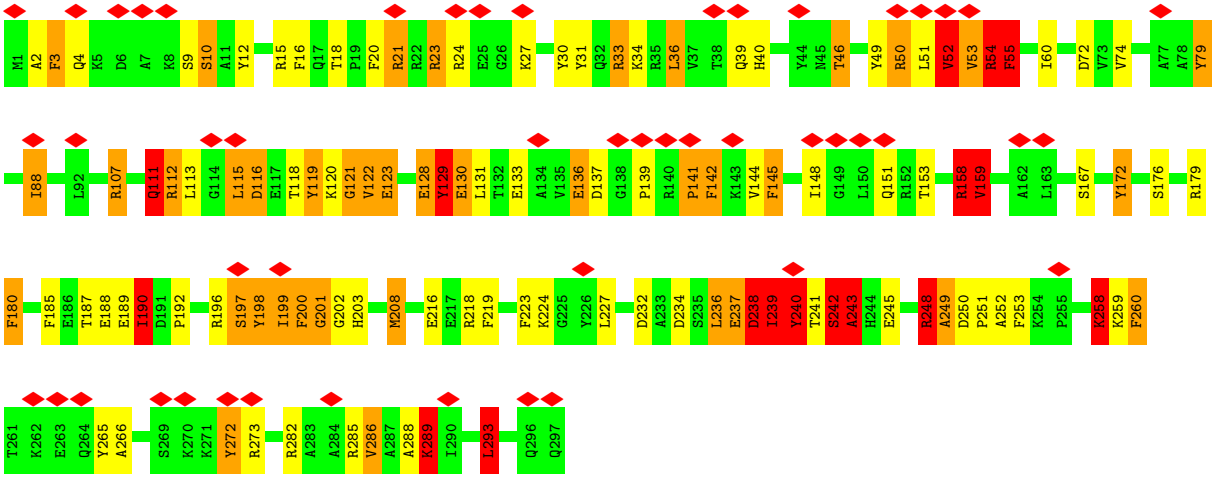

• Molecule 73: 60S acidic ribosomal protein (P2)

Chain Bw: 52% 49% 5% 45%



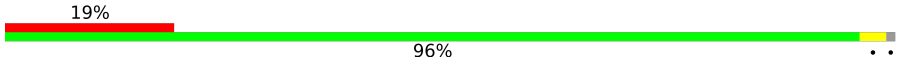

- Molecule 74: 60S ribosomal protein rpL5 (L18p)

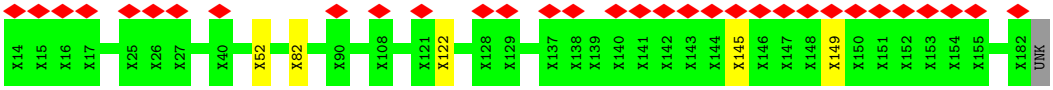
Chain BQ:




- Molecule 75: 60S ribosomal protein rpL13 (L13e)

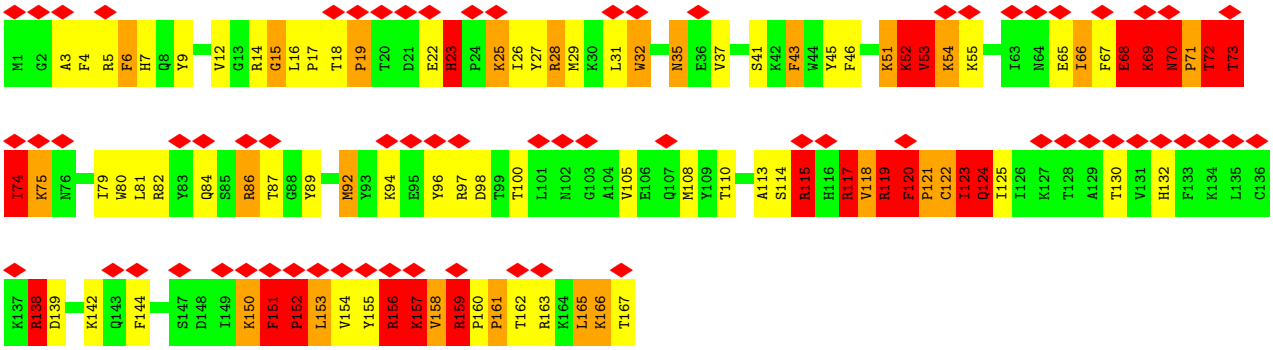
Chain BL:



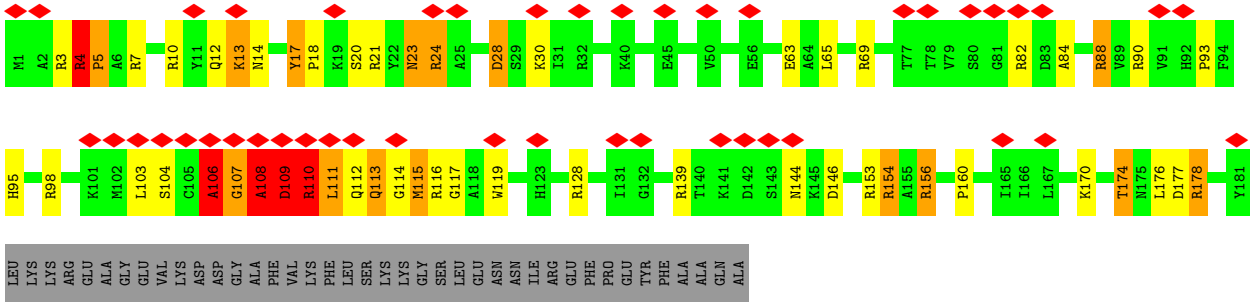

- Molecule 76: 60S ribosomal protein rpL20 (L18ae)

Chain BS:



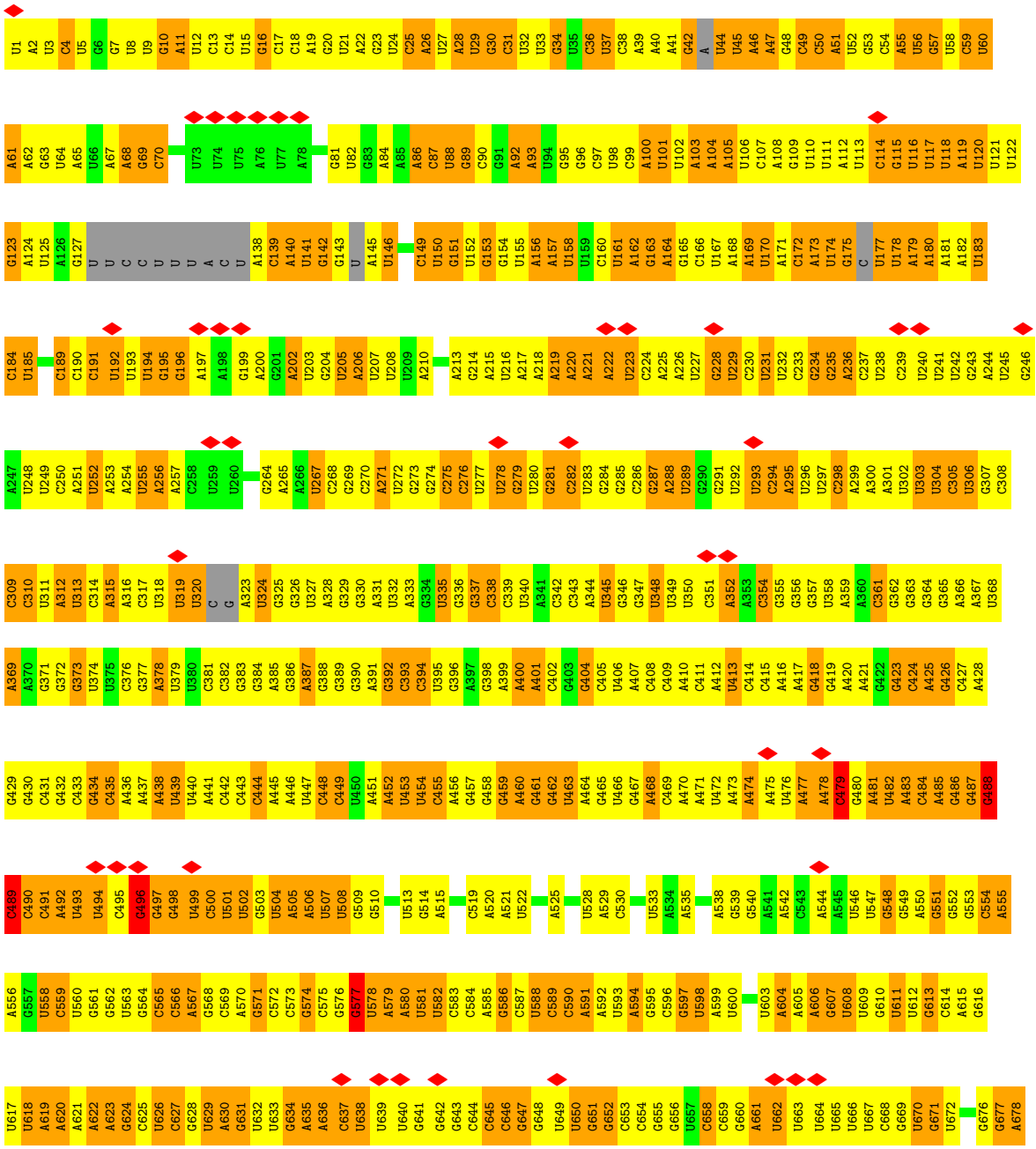

- Molecule 77: 60S ribosomal protein rpL10 (L10e)

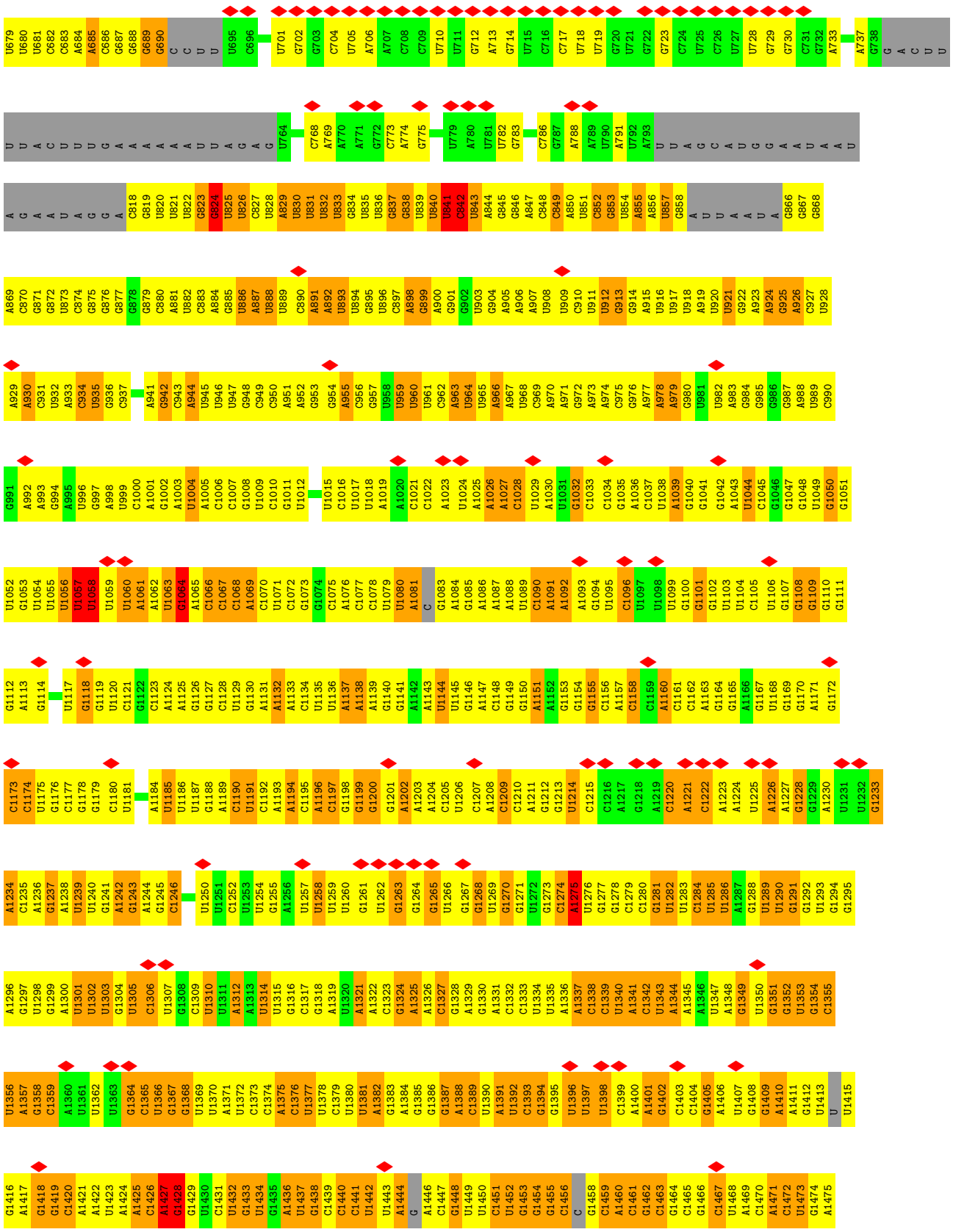
Chain BI:

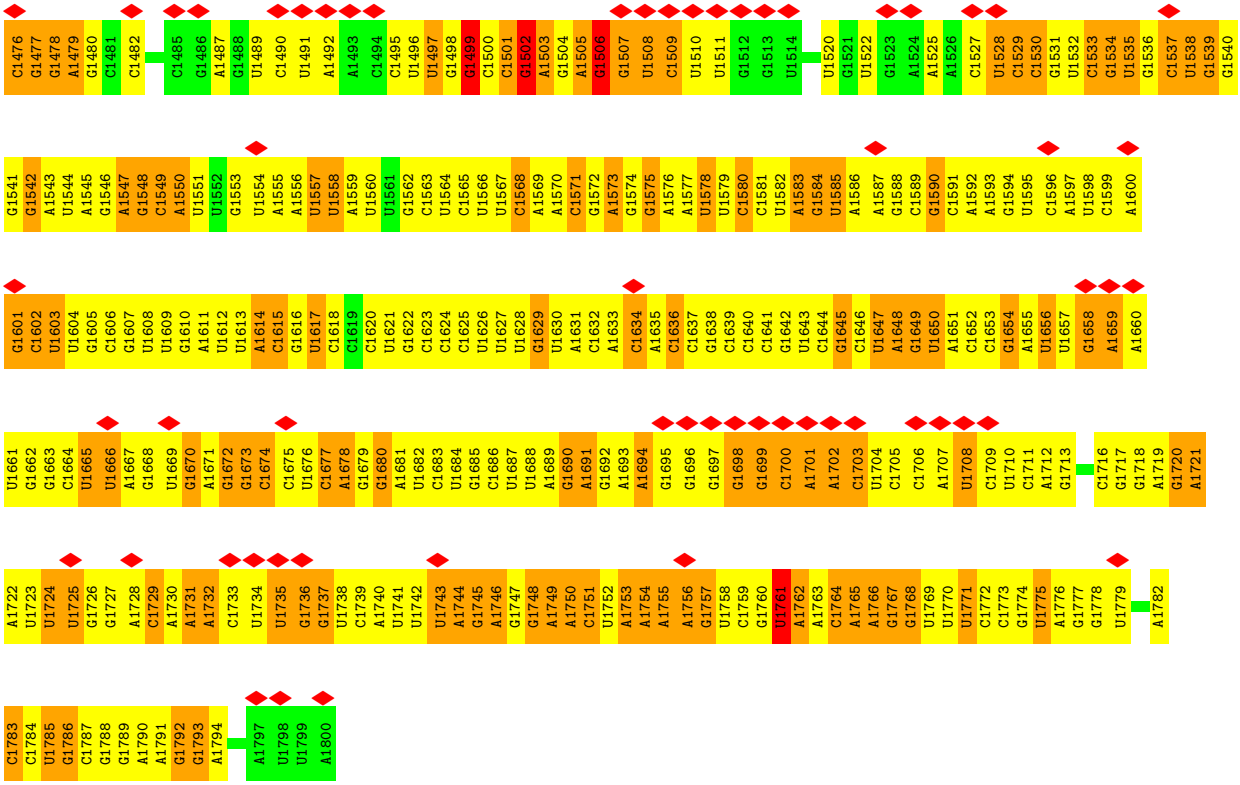



- Molecule 78: 18S rRNA

Chain CA:

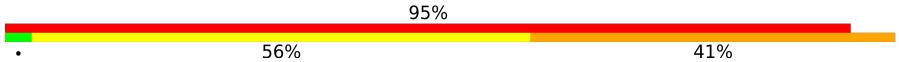


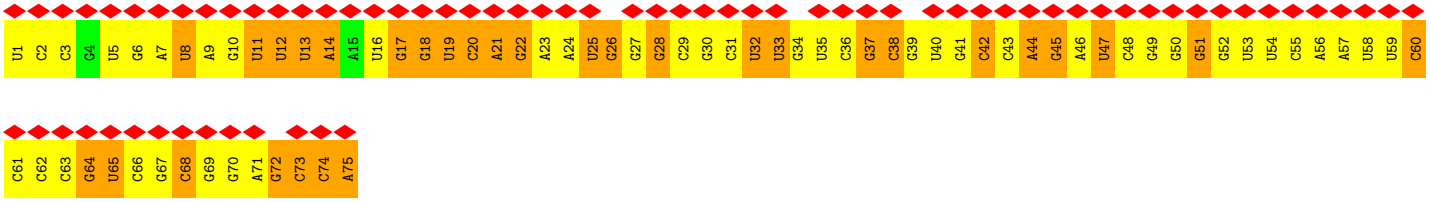

U679 U680 U681 C682 C683 A684 A685 C686 G687 G688 G689 G690 C C U U U695 G696 U701 G702 G703 C704 U705 A706 A707 C708 C709 U710 U711 G712 A713 G714 U715 C716 C717 U718 U719 G720 U721 G722 G723 C724 U725 C726 U727 U728 G729 G730 C731 G732 A733 A737 G738 G A C U U
U U A C U U U G A A A A A U U A G A G U764 C768 A769 A770 A771 G772 C773 A774 G775 U779 A780 U781 U782 G783 C786 G787 A788 A789 U790 A791 U792 A793 U U A G C A U G G A A U A A U
A G A A U A G G A C818 G819 U820 U821 U822 G823 G824 U825 U826 C827 U828 A829 U830 U831 U832 U833 G834 U835 U836 G837 G838 U839 U840 U841 C842 U843 A844 G845 G846 A847 C848 C849 A850 U851 C852 G853 U854 A855 A856 U857 G858 A U U A A U A G866 G867 G868
A869 C870 G871 G872 U873 C874 G875 G876 G877 G878 G879 C880 A881 U882 C883 A884 G885 U886 A887 U888 U889 C890 A891 A892 U893 U894 G895 U896 C897 A898 G899 A900 G901 G902 U903 G904 A905 A906 A907 U908 U909 C910 U911 U912 G913 G914 A915 U916 U917 U918 A919 U920 U921 G922 A923 A924 G925 A926 C927 U928
A929 A930 C931 U932 A933 C934 U935 G936 C937 A941 G942 C943 A944 U945 U946 U947 G948 C949 C950 A951 A952 G953 G954 A955 C956 G957 U958 U959 U960 U961 C962 A963 U964 U965 A966 A967 U968 C969 A970 A971 G972 A973 A974 C975 G976 A977 A978 A979 G980 U981 U982 A983 G984 G985 G986 G987 A988 U989 C990
G991 A992 A993 G994 A995 U996 G997 A998 U999 C1000 A1001 G1002 A1003 U1004 A1005 C1006 C1007 G1008 U1009 C1010 G1011 U1012 U1015 C1016 U1017 U1018 A1019 A1020 C1021 C1022 A1023 U1024 A1025 A1026 A1027 C1028 U1029 A1030 U1031 G1032 C1033 C1034 G1035 A1036 C1037 U1038 A1039 G1040 G1041 G1042 A1043 U1044 C1045 G1046 G1047 G1048 U1049 G1050 G1051
U1052 G1053 U1054 U1055 U1056 U1057 U1058 U1059 U1060 A1061 A1062 U1063 G1064 A1065 C1066 C1067 C1068 A1069 C1070 U1071 C1072 G1073 G1074 C1075 A1076 C1077 C1078 U1079 U1080 A1081 C G1083 A1084 G1085 A1086 A1087 A1088 U1089 C1090 A1091 A1092 A1093 G1094 U1095 C1096 U1097 U1098 U1099 G1100 G1101 G1102 U1103 U1104 C1105 U1106 G1107 G1108 G1109 G1110 G1111
G1112 A1113 G1114 U1117 G1118 G1119 U1120 C1121 G1122 C1123 A1124 A1125 G1126 G1127 C1128 U1129 G1130 A1131 A1132 A1133 C1134 U1135 U1136 A1137 A1138 A1139 G1140 G1141 A1142 A1143 U1144 U1145 G1146 A1147 C1148 G1149 G1150 A1151 A1152 G1153 G1154 G1155 C1156 A1157 C1158 C1159 A1160 C1161 C1162 A1163 G1164 G1165 A1166 G1167 U1168 G1169 G1170 A1171 G1172
C1173 C1174 U1175 G1176 C1177 G1178 G1179 C1180 U1181 A1184 U1185 U1186 U1187 G1188 A1189 C1190 U1191 C1192 A1193 A1194 C1195 A1196 C1197 G1198 G1199 G1200 G1201 A1202 A1203 A1204 C1205 U1206 C1207 A1208 C1209 C1210 A1211 G1212 G1213 U1214 C1215 C1216 A1217 G1218 A1219 C1220 A1221 C1222 A1223 A1224 U1225 A1226 A1227 G1228 G1229 A1230 U1231 U1232 G1233
A1234 C1235 A1236 G1237 A1238 U1239 U1240 G1241 A1242 G1243 A1244 G1245 C1246 U1250 U1251 C1252 U1253 U1254 G1255 A1256 U1257 U1258 C1259 G1260 G1261 U1262 G1263 G1264 G1265 U1266 G1267 G1268 U1269 G1270 C1271 U1272 G1273 C1274 A1275 U1276 G1277 G1278 C1279 C1280 G1281 U1282 U1283 C1284 U1285 U1286 A1287 G1288 U1289 U1290 G1291 G1292 U1293 G1294 G1295
A1296 G1297 U1298 G1299 A1300 U1301 U1302 U1303 G1304 U1305 C1306 U1307 G1308 C1309 U1310 U1311 A1312 A1313 U1314 U1315 G1316 C1317 G1318 A1319 U1320 A1321 A1322 C1323 G1324 A1325 A1326 C1327 G1328 A1329 G1330 A1331 C1332 C1333 U1334 U1335 A1336 A1337 C1338 C1339 U1340 A1341 C1342 U1343 A1344 A1345 A1346 U1347 A1348 G1349 U1350 G1351 G1352 U1353 G1354 C1355
U1356 A1357 G1358 C1359 A1360 U1361 U1362 U1363 G1364 C1365 U1366 G1367 G1368 U1369 U1370 A1371 U1372 C1373 C1374 A1375 C1376 U1377 U1378 C1379 C1380 U1381 U1382 G1383 A1384 G1385 G1386 G1387 A1388 G1389 U1390 A1391 U1392 C1393 G1394 G1395 U1396 U1397 U1398 C1399 A1400 A1401 G1402 C1403 C1404 G1405 A1406 U1407 G1408 G1409 A1410 A1411 G1412 U1413 U U1415
G1416 A1417 G1418 G1419 C1420 A1421 A1422 U1423 A1424 A1425 C1426 A1427 G1428 G1429 U1430 C1431 A1432 G1433 U1434 G1435 A1436 U1437 G1438 C1439 C1440 A1441 U1442 U1443 A1444 G A1446 C1447 G1448 A1449 U1450 C1451 U1452 G1453 G1454 G1455 C1456 C G1458 C1459 A1460 C1461 G1462 C1463 G1464 C1465 G1466 C1467 U1468 A1469 C1470 A1471 C1472 U1473 G1474 A1475




- Molecule 79: P-SITE TRNA ASP

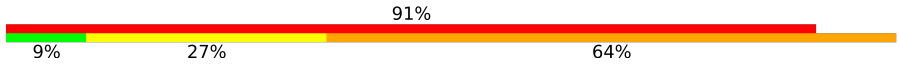
Chain CB:

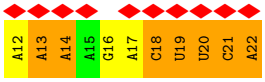



- Molecule 80: MRNA, RNA (5'-R(P*AP*AP*AP*AP*GP*AP*CP*UP*UP*CP*A)-3')

Chain CC:




- Molecule 81: 25S rRNA

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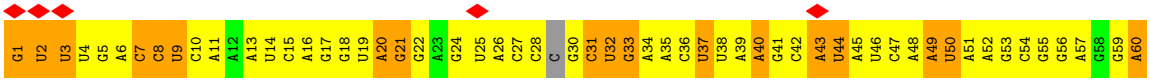

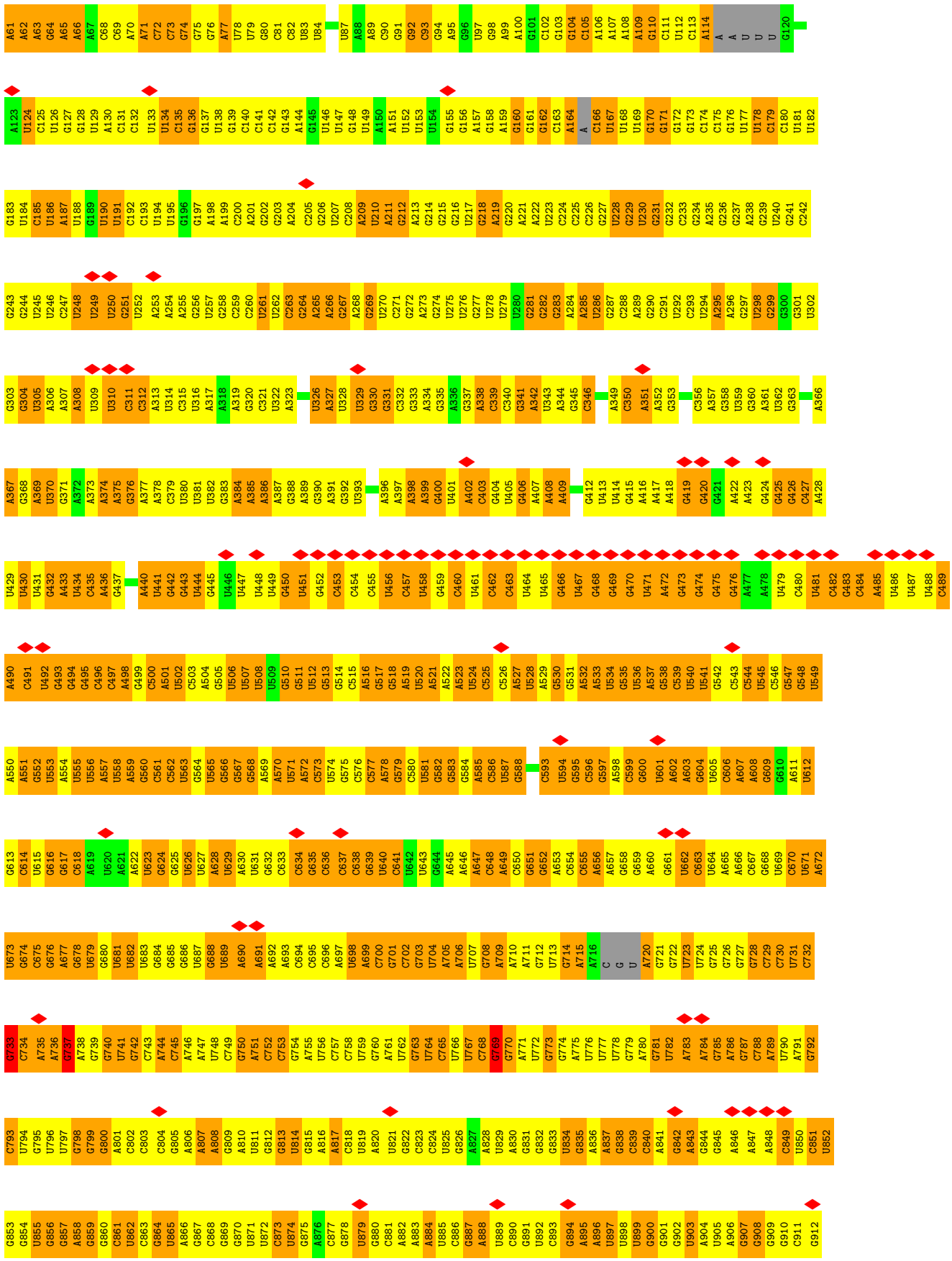
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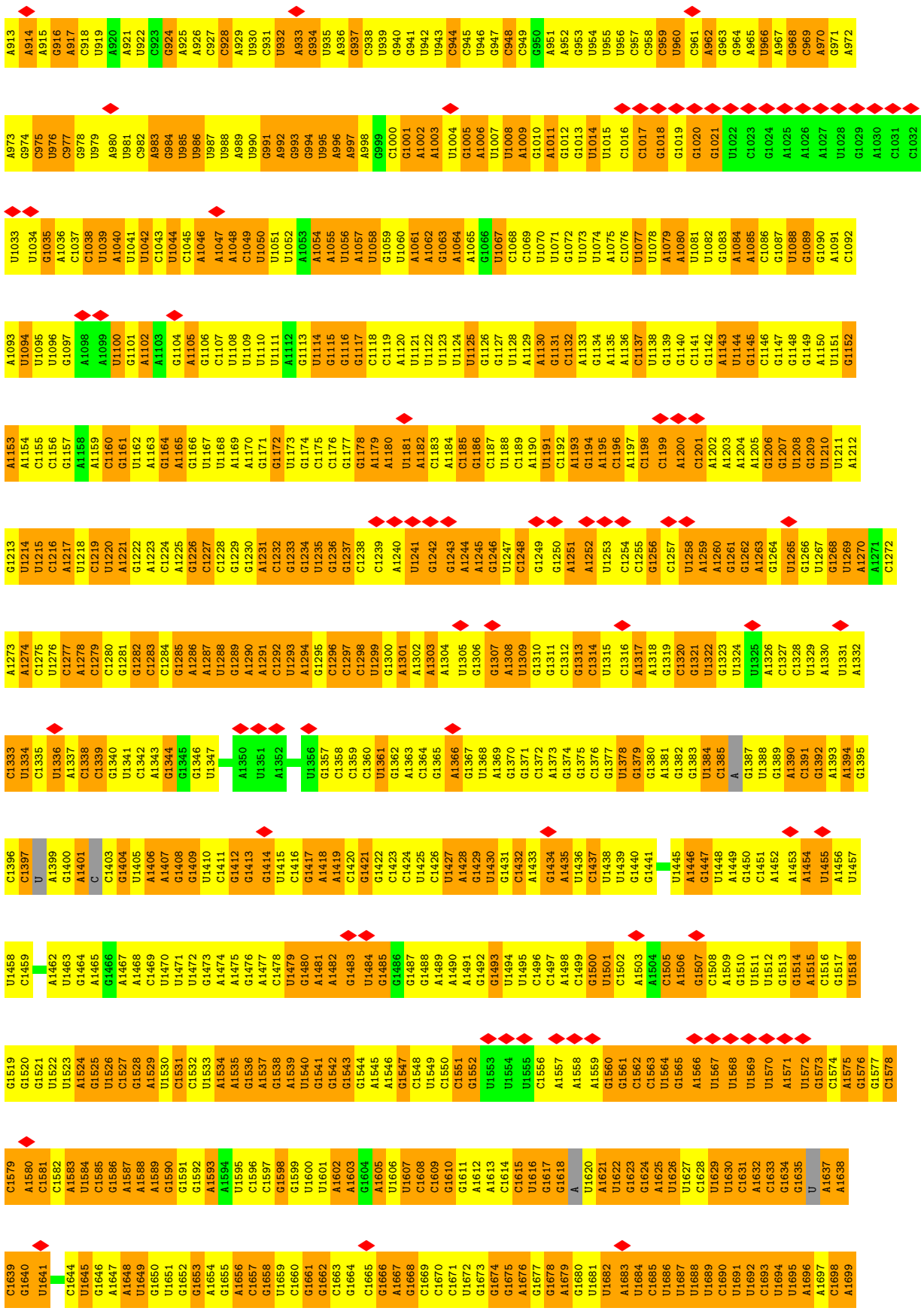
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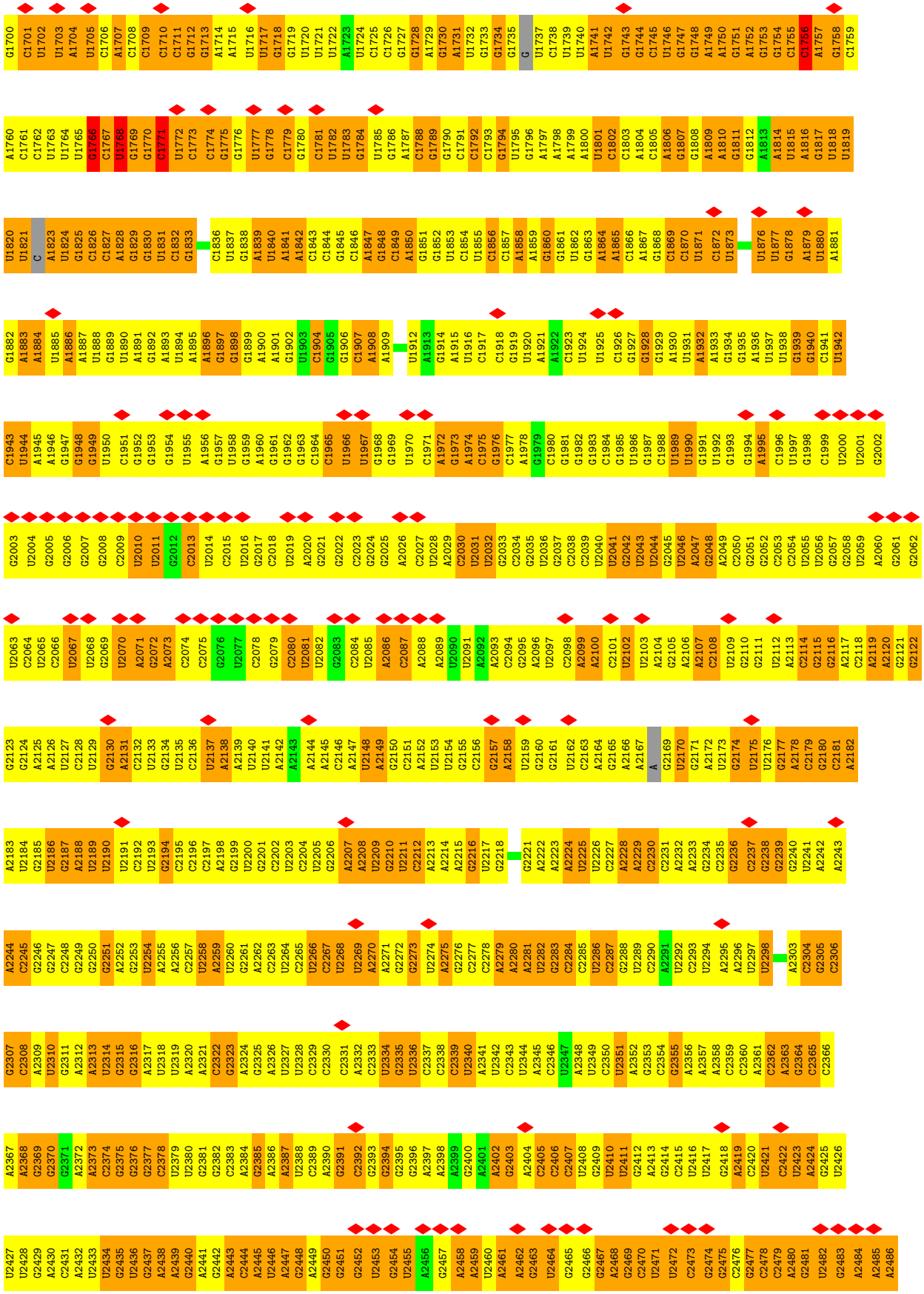
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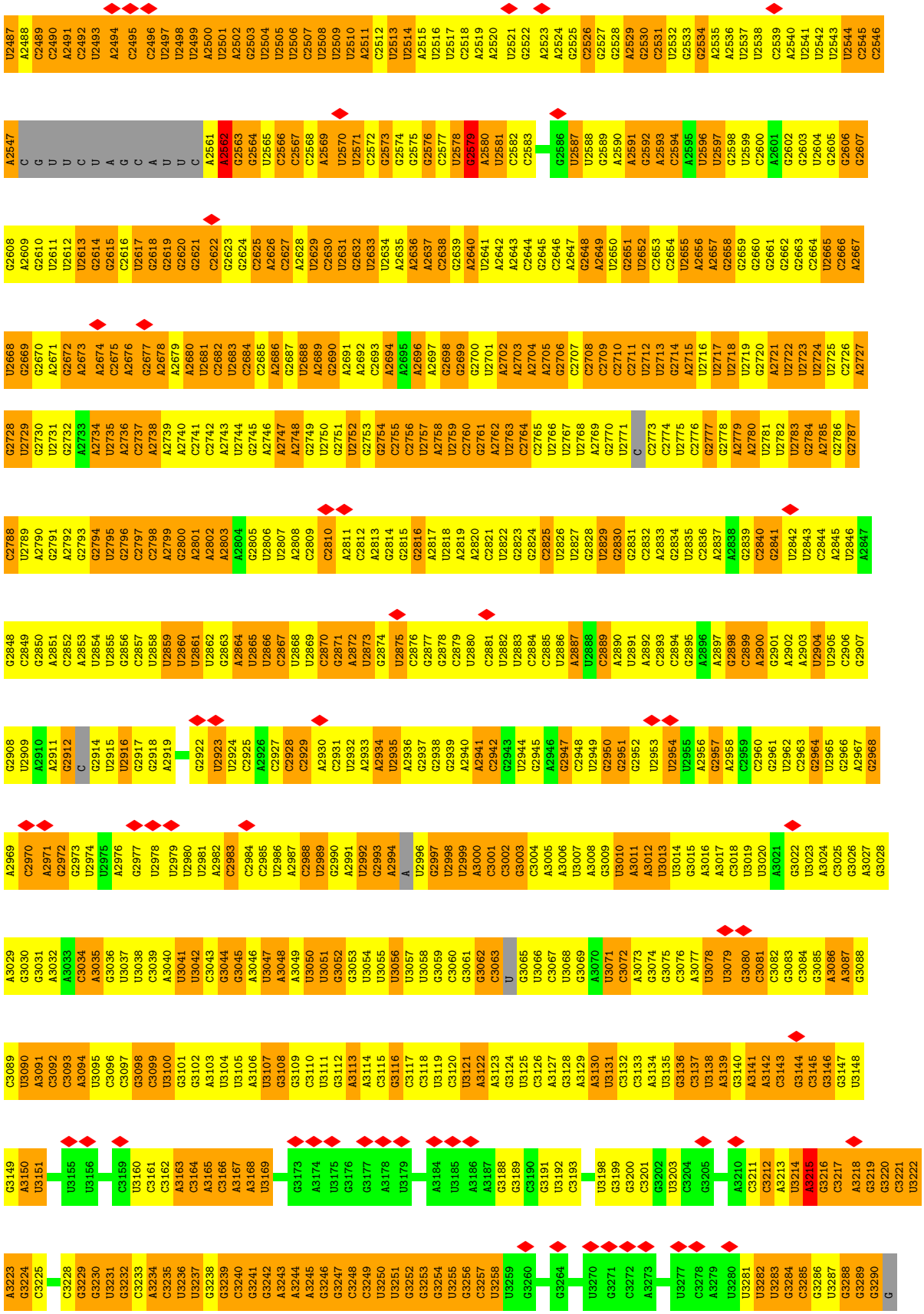
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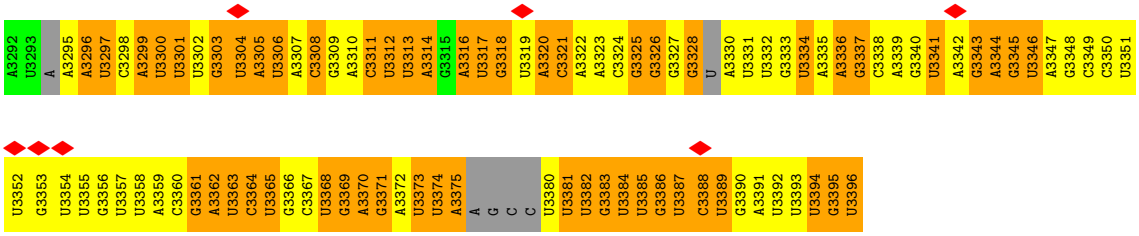
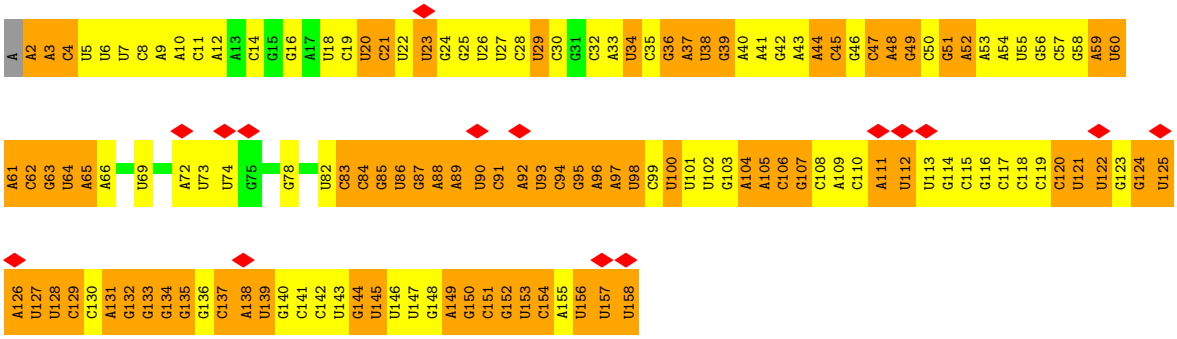
G2848 G2849 G2850 A2851 C2852 A2853 U2854 U2855 G2856 C2857 U2858 U2859 U2860 U2861 U2862 G2863 A2864 U2865 U2866 C2867 U2868 U2869 C2870 G2871 A2872 U2873 G2874 U2875 C2876 G2877 G2878 G2879 U2880 C2881 U2882 U2883 C2884 C2885 U2886 A2887 U2888 C2889 A2890 U2891 A2892 C2893 C2894 G2895 A2896 A2897 G2898 C2899 A2900 G2901 A2902 A2903 U2904 U2905 C2906 G2907
G2908 U2909 A2910 A2911 G2912 C G2914 U2915 U2916 G2917 G2918 A2919 G2922 U2923 U2924 C2925 A2926 C2927 C2928 C2929 A2930 C2931 U2932 A2933 A2934 U2935 A2936 G2937 G2938 G2939 A2940 A2941 C2942 G2943 U2944 G2945 A2946 G2947 C2948 U2949 G2950 G2951 G2952 U2953 U2954 U2955 A2956 G2957 A2958 C2959 C2960 G2961 U2962 C2963 G2964 U2965 G2966 A2967 G2968
A2969 C2970 A2971 G2972 C2973 U2974 U2975 A2976 G2977 U2978 U2979 U2980 U2981 A2982 C2983 C2984 C2985 U2986 A2987 C2988 U2989 C2990 A2991 U2992 G2993 A2994 A U2996 G2997 U2998 U2999 A3000 C3001 C3002 G3003 C3004 A3005 A3006 U3007 A3008 G3009 U3010 A3011 A3012 U3013 U3014 G3015 A3016 A3017 C3018 U3019 U3020 A3021 G3022 U3023 A3024 C3025 G3026 A3027 G3028
A3029 G3030 G3031 A3032 A3033 C3034 A3035 G3036 U3037 U3038 C3039 A3040 U3041 U3042 C3043 G3044 G3045 A3046 U3047 A3048 A3049 U3050 U3051 G3052 G3053 U3054 U3055 U3056 U3057 U3058 G3059 C3060 G3061 G3062 C3063 U G3065 U3066 C3067 U3068 G3069 A3070 U3071 C3072 A3073 G3074 G3075 C3076 A3077 U3078 U3079 G3080 C3081 C3082 G3083 C3084 G3085 A3086 A3087 G3088
C3089 U3090 A3091 C3092 C3093 A3094 U3095 C3096 C3097 G3098 C3099 U3100 G3101 G3102 A3103 U3104 U3105 A3106 U3107 G3108 G3109 C3110 U3111 G3112 A3113 A3114 C3115 G3116 C3117 C3118 U3119 C3120 U3121 A3122 A3123 G3124 U3125 C3126 A3127 G3128 A3129 A3130 U3131 C3132 C3133 A3134 U3135 G3136 C3137 U3138 A3139 G3140 A3141 A3142 C3143 G3144 C3145 G3146 U3147 U3148
G3149 A3150 U3151 U3155 U3156 C3159 U3160 C3161 C3162 A3163 C3164 A3165 C3166 A3167 A3168 U3169 G3173 A3174 U3175 G3176 G3177 A3178 U3179 A3184 U3185 A3186 A3187 G3188 G3189 C3190 G3191 U3192 C3193 U3198 G3199 G3200 C3201 G3202 U3203 C3204 G3205 A3210 C3211 C3212 A3213 U3214 A3215 G3216 C3217 A3218 G3219 G3220 C3221 U3222
A3223 G3224 C3225 C3228 G3229 G3230 U3231 G3232 C3233 A3234 C3235 U3236 U3237 G3238 G3239 C3240 G3241 G3242 A3243 A3244 A3245 G3246 G3247 C3248 C3249 U3250 U3251 U3252 G3253 G3254 U3255 G3256 C3257 U3258 U3259 G3260 G3264 U3270 G3271 C3272 A3273 U3277 C3278 A3279 U3280 U3281 U3282 U3283 G3284 C3285 U3286 U3287 G3288 G3289 G3290 G



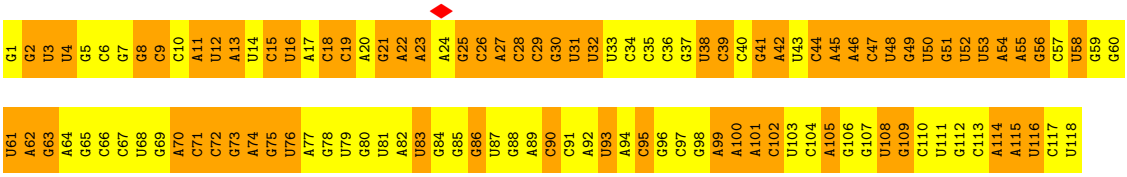

- Molecule 82: 5.8S rRNA

Chain DB:




- Molecule 83: 5S rRNA

Chain DC:



# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of particles used | 20400 | Depositor |
| Resolution determination method | Not provided | |
| CTF correction method | Not provided | |
| Microscope | FEI POLARA 300 | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 25 | Depositor |
| Minimum defocus (nm) | 1200 | Depositor |
| Maximum defocus (nm) | 4500 | Depositor |
| Magnification | 39000 | Depositor |
| Image detector | KODAK SO-163 FILM | Depositor |
| Maximum map value | 7.747 | Depositor |
| Minimum map value | -3.672 | Depositor |
| Average map value | 0.049 | Depositor |
| Map value standard deviation | 0.609 | Depositor |
| Recommended contour level | 1.75 | Depositor |
| Map size (Å) | 455.4, 455.4, 455.4 | wwPDB |
| Map dimensions | 368, 368, 368 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.2375, 1.2375, 1.2375 | Depositor |

# 5 Model quality (i)

## 5.1 Standard geometry (i)

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 | Aa | 1.65 | 23/2495 (0.9%) | 2.01 | 81/3391 (2.4%) |
| 2 | AA | 1.99 | 33/1962 (1.7%) | 2.62 | 83/2674 (3.1%) |
| 3 | AB | 1.87 | 20/1530 (1.3%) | 2.48 | 72/2049 (3.5%) |
| 4 | AD | 1.95 | 29/1620 (1.8%) | 2.88 | 94/2182 (4.3%) |
| 5 | AC | 2.12 | 34/1544 (2.2%) | 3.02 | 112/2059 (5.4%) |
| 6 | AE | 1.82 | 21/1971 (1.1%) | 2.46 | 79/2664 (3.0%) |
| 8 | AF | 1.70 | 13/1561 (0.8%) | 1.94 | 47/2103 (2.2%) |
| 9 | AH | 1.85 | 10/1047 (1.0%) | 2.39 | 47/1405 (3.3%) |
| 10 | AI | 1.94 | 15/1016 (1.5%) | 2.50 | 48/1362 (3.5%) |
| 11 | AJ | 1.93 | 13/857 (1.5%) | 2.90 | 38/1148 (3.3%) |
| 12 | AK | 1.98 | 14/843 (1.7%) | 2.28 | 38/1134 (3.4%) |
| 13 | AL | 2.41 | 23/990 (2.3%) | 3.21 | 80/1304 (6.1%) |
| 14 | AM | 1.85 | 23/1175 (2.0%) | 2.38 | 47/1577 (3.0%) |
| 15 | AN | 1.78 | 5/358 (1.4%) | 2.77 | 29/469 (6.2%) |
| 16 | AO | 1.85 | 10/994 (1.0%) | 2.70 | 58/1339 (4.3%) |
| 17 | AQ | 2.16 | 24/1109 (2.2%) | 3.08 | 59/1483 (4.0%) |
| 18 | AP | 2.29 | 17/646 (2.6%) | 3.39 | 49/867 (5.7%) |
| 19 | AR | 1.65 | 5/691 (0.7%) | 2.07 | 20/931 (2.1%) |
| 20 | AS | 1.83 | 17/1138 (1.5%) | 2.73 | 74/1527 (4.8%) |
| 21 | AT | 2.06 | 13/694 (1.9%) | 2.67 | 32/935 (3.4%) |
| 22 | AV | 1.91 | 14/698 (2.0%) | 2.68 | 44/932 (4.7%) |
| 24 | AX | 1.77 | 5/372 (1.3%) | 2.15 | 13/504 (2.6%) |
| 25 | AY | 1.80 | 3/447 (0.7%) | 2.08 | 19/601 (3.2%) |
| 26 | AZ | 2.63 | 17/499 (3.4%) | 3.77 | 31/660 (4.7%) |
| 29 | AU | 1.93 | 8/725 (1.1%) | 2.49 | 45/969 (4.6%) |
| 30 | BA | 1.42 | 4/1745 (0.2%) | 1.78 | 32/2342 (1.4%) |
| 31 | BB | 2.07 | 31/1938 (1.6%) | 2.90 | 100/2600 (3.8%) |
| 32 | BC | 2.25 | 65/3124 (2.1%) | 3.27 | 171/4196 (4.1%) |
| 33 | BD | 2.15 | 53/2531 (2.1%) | 2.93 | 146/3414 (4.3%) |
| 34 | BE | 2.08 | 25/1362 (1.8%) | 3.17 | 79/1824 (4.3%) |
| 35 | BG | 2.50 | 42/1433 (2.9%) | 3.60 | 142/1922 (7.4%) |
| 36 | BF | 1.65 | 9/1537 (0.6%) | 2.05 | 27/2068 (1.3%) |
| 37 | BH | 2.09 | 26/1527 (1.7%) | 2.60 | 82/2052 (4.0%) |
| 38 | Bs | 1.71 | 18/2013 (0.9%) | 2.32 | 75/2731 (2.7%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 39 | BJ | 1.89 | 16/964 (1.7%) | 2.63 | 44/1295 (3.4%) |
| 40 | BK | 1.93 | 21/1600 (1.3%) | 2.78 | 76/2146 (3.5%) |
| 41 | BN | 1.88 | 15/1083 (1.4%) | 2.30 | 56/1456 (3.8%) |
| 42 | BM | 1.73 | 12/987 (1.2%) | 2.20 | 45/1326 (3.4%) |
| 43 | BP | 2.03 | 23/1659 (1.4%) | 2.68 | 113/2221 (5.1%) |
| 44 | BO | 2.47 | 29/1213 (2.4%) | 3.20 | 74/1623 (4.6%) |
| 45 | BR | 2.41 | 29/1264 (2.3%) | 3.18 | 68/1701 (4.0%) |
| 46 | BT | 1.82 | 26/1547 (1.7%) | 2.27 | 54/2060 (2.6%) |
| 47 | BU | 1.78 | 21/1285 (1.6%) | 2.44 | 54/1720 (3.1%) |
| 48 | BW | 2.02 | 13/846 (1.5%) | 2.75 | 47/1142 (4.1%) |
| 49 | BV | 1.71 | 14/1335 (1.0%) | 2.03 | 40/1794 (2.2%) |
| 50 | BX | 1.58 | 5/993 (0.5%) | 2.19 | 41/1336 (3.1%) |
| 51 | BZ | 2.29 | 14/590 (2.4%) | 2.74 | 40/783 (5.1%) |
| 52 | BY | 1.61 | 10/983 (1.0%) | 1.95 | 25/1312 (1.9%) |
| 53 | Ba | 2.24 | 20/722 (2.8%) | 3.30 | 75/967 (7.8%) |
| 54 | Bd | 1.63 | 2/177 (1.1%) | 1.91 | 5/231 (2.2%) |
| 55 | Bc | 2.06 | 14/974 (1.4%) | 2.76 | 53/1294 (4.1%) |
| 56 | Bf | 1.59 | 7/793 (0.9%) | 1.92 | 17/1062 (1.6%) |
| 57 | Be | 1.85 | 25/1957 (1.3%) | 2.29 | 69/2631 (2.6%) |
| 58 | Bg | 1.83 | 16/887 (1.8%) | 2.38 | 32/1185 (2.7%) |
| 59 | Bh | 1.80 | 11/1064 (1.0%) | 2.30 | 47/1423 (3.3%) |
| 60 | Bi | 2.51 | 24/935 (2.6%) | 3.64 | 59/1242 (4.8%) |
| 61 | Bj | 2.79 | 19/751 (2.5%) | 3.05 | 68/1004 (6.8%) |
| 62 | Bk | 2.48 | 19/625 (3.0%) | 3.48 | 45/826 (5.4%) |
| 63 | Bm | 1.73 | 9/710 (1.3%) | 2.09 | 24/944 (2.5%) |
| 64 | Bl | 2.03 | 9/693 (1.3%) | 2.42 | 34/915 (3.7%) |
| 65 | Bn | 2.32 | 13/610 (2.1%) | 3.37 | 37/813 (4.6%) |
| 66 | Bo | 1.80 | 4/452 (0.9%) | 2.23 | 17/598 (2.8%) |
| 67 | Bp | 1.57 | 2/335 (0.6%) | 2.25 | 18/442 (4.1%) |
| 68 | Bq | 1.98 | 3/235 (1.3%) | 2.32 | 14/300 (4.7%) |
| 69 | Br | 2.01 | 14/846 (1.7%) | 2.74 | 44/1113 (4.0%) |
| 72 | Bt | 0.69 | 1/445 (0.2%) | 1.49 | 16/606 (2.6%) |
| 72 | Bu | 0.92 | 1/445 (0.2%) | 1.63 | 18/606 (3.0%) |
| 73 | Bv | 0.97 | 0/431 | 1.29 | 4/582 (0.7%) |
| 73 | Bw | 0.96 | 0/431 | 1.28 | 4/582 (0.7%) |
| 74 | BQ | 2.23 | 50/2404 (2.1%) | 3.27 | 146/3236 (4.5%) |
| 76 | BS | 1.92 | 23/1458 (1.6%) | 2.70 | 109/1957 (5.6%) |
| 77 | BI | 0.95 | 1/1473 (0.1%) | 1.60 | 29/1976 (1.5%) |
| 78 | CA | 2.64 | 1783/37406 (4.8%) | 2.65 | 3176/57948 (5.5%) |
| 79 | CB | 2.75 | 77/1785 (4.3%) | 2.58 | 142/2779 (5.1%) |
| 80 | CC | 3.40 | 11/264 (4.2%) | 3.22 | 29/407 (7.1%) |
| 81 | DA | 2.74 | 3996/76832 (5.2%) | 2.77 | 7042/119578 (5.9%) |
| 82 | DB | 2.68 | 166/3480 (4.8%) | 2.64 | 305/5395 (5.7%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 83 | DC | 2.90 | 156/2808 (5.6%) | 3.09 | 331/4372 (7.6%) |
| All | All | 2.44 | 7406/202969 (3.6%) | 2.70 | 14979/298347 (5.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 1 | Aa | 0 | 18 |
| 2 | AA | 1 | 30 |
| 3 | AB | 0 | 29 |
| 4 | AD | 0 | 36 |
| 5 | AC | 2 | 40 |
| 6 | AE | 3 | 29 |
| 7 | AG | 0 | 52 |
| 8 | AF | 0 | 14 |
| 9 | AH | 0 | 15 |
| 10 | AI | 0 | 14 |
| 11 | AJ | 0 | 17 |
| 12 | AK | 1 | 15 |
| 13 | AL | 0 | 14 |
| 14 | AM | 0 | 12 |
| 15 | AN | 0 | 12 |
| 16 | AO | 2 | 15 |
| 17 | AQ | 0 | 29 |
| 18 | AP | 0 | 15 |
| 19 | AR | 0 | 8 |
| 20 | AS | 0 | 19 |
| 21 | AT | 0 | 15 |
| 22 | AV | 0 | 12 |
| 23 | AW | 0 | 20 |
| 24 | AX | 0 | 2 |
| 25 | AY | 0 | 4 |
| 26 | AZ | 0 | 25 |
| 27 | Ab | 0 | 3 |
| 28 | Ac | 0 | 1 |
| 29 | AU | 2 | 12 |
| 30 | BA | 0 | 8 |
| 31 | BB | 2 | 45 |
| 32 | BC | 2 | 56 |
| 33 | BD | 2 | 53 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 34 | BE | 2 | 25 |
| 35 | BG | 2 | 57 |
| 36 | BF | 0 | 10 |
| 37 | BH | 0 | 36 |
| 38 | Bs | 0 | 18 |
| 39 | BJ | 1 | 10 |
| 40 | BK | 0 | 29 |
| 41 | BN | 1 | 13 |
| 42 | BM | 0 | 11 |
| 43 | BP | 4 | 44 |
| 44 | BO | 1 | 28 |
| 45 | BR | 0 | 31 |
| 46 | BT | 0 | 17 |
| 47 | BU | 1 | 16 |
| 48 | BW | 0 | 12 |
| 49 | BV | 0 | 20 |
| 50 | BX | 0 | 13 |
| 51 | BZ | 0 | 18 |
| 52 | BY | 0 | 8 |
| 53 | Ba | 0 | 25 |
| 54 | Bd | 0 | 1 |
| 55 | Bc | 0 | 16 |
| 56 | Bf | 0 | 6 |
| 57 | Be | 1 | 14 |
| 58 | Bg | 0 | 13 |
| 59 | Bh | 0 | 14 |
| 60 | Bi | 0 | 25 |
| 61 | Bj | 1 | 26 |
| 62 | Bk | 1 | 15 |
| 63 | Bm | 1 | 5 |
| 64 | Bl | 0 | 13 |
| 65 | Bn | 0 | 15 |
| 66 | Bo | 0 | 15 |
| 67 | Bp | 0 | 8 |
| 68 | Bq | 0 | 4 |
| 69 | Br | 0 | 23 |
| 70 | Bx | 0 | 7 |
| 71 | Bz | 0 | 1 |
| 72 | Bt | 0 | 3 |
| 72 | Bu | 0 | 3 |
| 73 | Bv | 0 | 1 |
| 73 | Bw | 0 | 1 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 74 | BQ | 0 | 48 |
| 75 | BL | 0 | 5 |
| 76 | BS | 1 | 41 |
| 77 | BI | 2 | 24 |
| 78 | CA | 10 | 22 |
| 79 | CB | 1 | 0 |
| 80 | CC | 1 | 0 |
| 81 | DA | 32 | 15 |
| 82 | DB | 5 | 0 |
| All | All | 85 | 1514 |

All (7406) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1261 | G | C2'-C1' | 59.16 | 2.18 | 1.53 |
| 79 | CB | 55 | C | C2'-C1' | -55.11 | 0.92 | 1.53 |
| 78 | CA | 636 | A | C2'-C1' | 54.35 | 2.13 | 1.53 |
| 81 | DA | 3215 | A | C2'-C1' | -49.15 | 0.99 | 1.53 |
| 78 | CA | 1190 | C | O5'-C5' | -48.72 | 0.65 | 1.42 |
| 81 | DA | 2989 | U | O4'-C1' | 48.03 | 2.04 | 1.41 |
| 81 | DA | 1209 | G | C2'-C1' | 42.87 | 2.00 | 1.53 |
| 81 | DA | 3215 | A | O4'-C1' | 42.29 | 1.96 | 1.41 |
| 78 | CA | 1190 | C | C5'-C4' | 40.55 | 2.00 | 1.51 |
| 81 | DA | 1207 | G | O4'-C1' | 39.11 | 1.92 | 1.41 |
| 81 | DA | 3221 | C | O4'-C1' | 38.99 | 1.92 | 1.41 |
| 80 | CC | 18 | C | O3'-P | 38.63 | 2.07 | 1.61 |
| 81 | DA | 2934 | A | C2'-C1' | 36.86 | 1.93 | 1.53 |
| 81 | DA | 2648 | G | C2'-C1' | 35.51 | 1.92 | 1.53 |
| 81 | DA | 636 | C | O4'-C1' | 35.16 | 1.87 | 1.41 |
| 78 | CA | 45 | U | C2'-C1' | 32.91 | 1.89 | 1.53 |
| 78 | CA | 123 | G | O4'-C1' | 32.61 | 1.84 | 1.41 |
| 81 | DA | 1314 | C | C2'-C1' | -32.07 | 1.18 | 1.53 |
| 44 | BO | 20 | GLY | C-N | -31.71 | 0.61 | 1.34 |
| 81 | DA | 2174 | G | C2'-C1' | -31.58 | 1.18 | 1.53 |
| 61 | Bj | 33 | GLU | CG-CD | 31.56 | 1.99 | 1.51 |
| 81 | DA | 2607 | G | C2'-C1' | -31.35 | 1.18 | 1.53 |
| 78 | CA | 1583 | A | C2'-C1' | -30.62 | 1.19 | 1.53 |
| 81 | DA | 1401 | A | C2'-C1' | 30.07 | 1.86 | 1.53 |
| 81 | DA | 1298 | C | C2'-C1' | -29.58 | 1.20 | 1.53 |
| 78 | CA | 1393 | C | C2'-C1' | 29.58 | 1.85 | 1.53 |
| 78 | CA | 1546 | G | C2'-C1' | -29.57 | 1.20 | 1.53 |
| 83 | DC | 26 | C | C2'-C1' | -29.50 | 1.21 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1221 | A | O4'-C1' | -28.54 | 1.04 | 1.41 |
| 81 | DA | 677 | A | C2'-C1' | 28.39 | 1.84 | 1.53 |
| 81 | DA | 2440 | G | C2'-C1' | -28.23 | 1.22 | 1.53 |
| 83 | DC | 46 | A | C2'-C1' | 28.20 | 1.84 | 1.53 |
| 78 | CA | 295 | A | O4'-C1' | -28.09 | 1.05 | 1.41 |
| 78 | CA | 306 | U | C2'-C1' | 28.02 | 1.84 | 1.53 |
| 78 | CA | 46 | A | O4'-C1' | -27.93 | 1.05 | 1.41 |
| 78 | CA | 1255 | G | O3'-P | 27.90 | 1.94 | 1.61 |
| 81 | DA | 2166 | A | O4'-C1' | 27.90 | 1.77 | 1.41 |
| 81 | DA | 3304 | U | C4'-C3' | 27.83 | 1.83 | 1.53 |
| 81 | DA | 1802 | C | O4'-C1' | 27.82 | 1.77 | 1.41 |
| 81 | DA | 2880 | U | C2'-C1' | -27.80 | 1.22 | 1.53 |
| 78 | CA | 1583 | A | O4'-C1' | 27.66 | 1.77 | 1.41 |
| 35 | BG | 69 | PHE | CD1-CE1 | 27.57 | 1.94 | 1.39 |
| 78 | CA | 631 | G | C2'-C1' | 27.41 | 1.83 | 1.53 |
| 78 | CA | 196 | G | C2'-C1' | -27.33 | 1.23 | 1.53 |
| 61 | Bj | 33 | GLU | CD-OE2 | -27.19 | 0.95 | 1.25 |
| 81 | DA | 636 | C | C2'-C1' | -27.04 | 1.23 | 1.53 |
| 81 | DA | 71 | A | C2'-C1' | -26.95 | 1.23 | 1.53 |
| 78 | CA | 591 | A | O4'-C1' | 26.77 | 1.76 | 1.41 |
| 32 | BC | 381 | GLY | C-O | -26.66 | 0.81 | 1.23 |
| 81 | DA | 173 | G | C2'-C1' | -26.59 | 1.24 | 1.53 |
| 78 | CA | 1602 | C | O4'-C1' | 26.56 | 1.76 | 1.41 |
| 81 | DA | 3092 | C | O4'-C1' | 26.53 | 1.76 | 1.41 |
| 81 | DA | 1055 | A | C2'-C1' | 26.48 | 1.82 | 1.53 |
| 78 | CA | 1190 | C | P-OP1 | -26.48 | 1.03 | 1.49 |
| 81 | DA | 3212 | C | O4'-C1' | 26.47 | 1.76 | 1.41 |
| 78 | CA | 990 | C | C2'-C1' | -26.40 | 1.24 | 1.53 |
| 81 | DA | 2187 | G | C2'-C1' | 26.36 | 1.82 | 1.53 |
| 78 | CA | 1541 | G | C2'-C1' | -26.27 | 1.24 | 1.53 |
| 33 | BD | 78 | GLY | C-O | -26.26 | 0.81 | 1.23 |
| 62 | Bk | 25 | LYS | C-O | -26.21 | 0.73 | 1.23 |
| 65 | Bn | 35 | GLY | C-O | -26.15 | 0.81 | 1.23 |
| 78 | CA | 172 | C | O4'-C1' | 26.09 | 1.75 | 1.41 |
| 81 | DA | 672 | A | P-O5' | -26.01 | 1.33 | 1.59 |
| 81 | DA | 3142 | A | C2'-C1' | 25.80 | 1.81 | 1.53 |
| 81 | DA | 242 | C | C2'-C1' | -25.78 | 1.25 | 1.53 |
| 81 | DA | 3034 | C | O4'-C1' | 25.77 | 1.75 | 1.41 |
| 78 | CA | 46 | A | C2'-C1' | 25.76 | 1.81 | 1.53 |
| 78 | CA | 305 | C | O4'-C1' | 25.73 | 1.75 | 1.41 |
| 81 | DA | 2788 | C | O4'-C1' | 25.65 | 1.75 | 1.41 |
| 78 | CA | 900 | A | C4'-O4' | -25.64 | 1.12 | 1.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2757 | U | O4'-C1' | 25.57 | 1.74 | 1.41 |
| 64 | Bl | 39 | TYR | C-O | -25.54 | 0.74 | 1.23 |
| 40 | BK | 184 | THR | C-O | -25.49 | 0.74 | 1.23 |
| 81 | DA | 1429 | G | C2'-C1' | -25.47 | 1.25 | 1.53 |
| 81 | DA | 745 | C | C2'-C1' | -25.46 | 1.25 | 1.53 |
| 81 | DA | 3131 | U | O4'-C1' | 25.34 | 1.74 | 1.41 |
| 81 | DA | 427 | C | C2'-C1' | -25.30 | 1.25 | 1.53 |
| 81 | DA | 3241 | G | O4'-C1' | 25.15 | 1.74 | 1.41 |
| 78 | CA | 1690 | G | O4'-C1' | 25.04 | 1.74 | 1.41 |
| 40 | BK | 69 | GLY | C-O | -25.00 | 0.83 | 1.23 |
| 83 | DC | 102 | C | O4'-C1' | 24.73 | 1.73 | 1.41 |
| 78 | CA | 228 | G | C2'-C1' | 24.71 | 1.80 | 1.53 |
| 81 | DA | 671 | U | O4'-C1' | -24.68 | 1.09 | 1.41 |
| 78 | CA | 140 | A | C2'-C1' | 24.68 | 1.80 | 1.53 |
| 32 | BC | 368 | GLY | C-O | -24.65 | 0.84 | 1.23 |
| 74 | BQ | 39 | GLN | C-N | 24.54 | 1.90 | 1.34 |
| 57 | Be | 202 | LEU | C-O | -24.53 | 0.76 | 1.23 |
| 32 | BC | 17 | LEU | C-O | -24.45 | 0.76 | 1.23 |
| 78 | CA | 1081 | A | C2'-C1' | 24.42 | 1.80 | 1.53 |
| 81 | DA | 1820 | U | O4'-C1' | 24.30 | 1.73 | 1.41 |
| 81 | DA | 2440 | G | O4'-C1' | 24.30 | 1.73 | 1.41 |
| 81 | DA | 1298 | C | O4'-C1' | 24.28 | 1.73 | 1.41 |
| 81 | DA | 1316 | C | C2'-C1' | -24.16 | 1.26 | 1.53 |
| 81 | DA | 1285 | G | C2'-C1' | 24.15 | 1.79 | 1.53 |
| 81 | DA | 147 | U | P-O5' | -24.14 | 1.35 | 1.59 |
| 32 | BC | 289 | ASP | C-O | -24.13 | 0.77 | 1.23 |
| 78 | CA | 469 | C | O4'-C1' | 24.11 | 1.73 | 1.41 |
| 82 | DB | 154 | C | O4'-C1' | 24.11 | 1.73 | 1.41 |
| 82 | DB | 105 | A | C2'-C1' | -24.02 | 1.26 | 1.53 |
| 78 | CA | 295 | A | C2'-C1' | 24.02 | 1.79 | 1.53 |
| 81 | DA | 1975 | C | O4'-C1' | 24.01 | 1.72 | 1.41 |
| 74 | BQ | 201 | GLY | C-O | -24.00 | 0.85 | 1.23 |
| 78 | CA | 856 | A | C2'-C1' | 23.98 | 1.79 | 1.53 |
| 81 | DA | 1623 | G | C2'-C1' | -23.96 | 1.26 | 1.53 |
| 26 | AZ | 44 | PHE | C-O | -23.95 | 0.77 | 1.23 |
| 81 | DA | 1314 | C | O4'-C1' | 23.90 | 1.72 | 1.41 |
| 81 | DA | 71 | A | O4'-C1' | 23.83 | 1.72 | 1.41 |
| 60 | Bi | 77 | GLY | C-O | -23.77 | 0.85 | 1.23 |
| 78 | CA | 1348 | A | C2'-C1' | -23.69 | 1.27 | 1.53 |
| 78 | CA | 874 | C | O4'-C1' | 23.62 | 1.72 | 1.41 |
| 45 | BR | 140 | LEU | C-O | -23.61 | 0.78 | 1.23 |
| 34 | BE | 123 | PHE | C-O | -23.59 | 0.78 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 331 | G | C2'-C1' | 23.53 | 1.79 | 1.53 |
| 81 | DA | 638 | C | O4'-C1' | 23.50 | 1.72 | 1.41 |
| 81 | DA | 3147 | G | C2'-C1' | -23.22 | 1.27 | 1.53 |
| 9 | AH | 66 | ASN | C-O | -23.14 | 0.79 | 1.23 |
| 78 | CA | 1141 | G | C2'-C1' | -23.11 | 1.27 | 1.53 |
| 81 | DA | 2869 | U | C2'-C1' | 22.98 | 1.78 | 1.53 |
| 81 | DA | 1821 | U | O4'-C1' | 22.96 | 1.71 | 1.41 |
| 13 | AL | 7 | ARG | CZ-NH1 | -22.96 | 1.03 | 1.33 |
| 33 | BD | 84 | ARG | C-O | -22.95 | 0.79 | 1.23 |
| 74 | BQ | 237 | GLU | C-O | -22.95 | 0.79 | 1.23 |
| 81 | DA | 2175 | U | P-O5' | -22.94 | 1.36 | 1.59 |
| 81 | DA | 1688 | U | O4'-C1' | 22.94 | 1.71 | 1.41 |
| 81 | DA | 1076 | C | C2'-C1' | -22.87 | 1.28 | 1.53 |
| 81 | DA | 3004 | C | C2'-C1' | -22.86 | 1.28 | 1.53 |
| 78 | CA | 1394 | G | O4'-C1' | -22.84 | 1.11 | 1.41 |
| 79 | CB | 55 | C | O4'-C1' | 22.80 | 1.71 | 1.41 |
| 13 | AL | 22 | ASN | C-O | -22.78 | 0.80 | 1.23 |
| 74 | BQ | 123 | GLU | C-O | -22.77 | 0.80 | 1.23 |
| 32 | BC | 297 | SER | C-O | -22.75 | 0.80 | 1.23 |
| 78 | CA | 609 | U | O4'-C1' | 22.72 | 1.71 | 1.41 |
| 81 | DA | 702 | C | O4'-C1' | 22.68 | 1.71 | 1.41 |
| 81 | DA | 2770 | G | O4'-C1' | 22.68 | 1.71 | 1.41 |
| 81 | DA | 2770 | G | C2'-C1' | -22.66 | 1.28 | 1.53 |
| 78 | CA | 374 | U | C2'-C1' | -22.65 | 1.28 | 1.53 |
| 81 | DA | 1620 | U | C2'-C1' | -22.61 | 1.28 | 1.53 |
| 31 | BB | 196 | TRP | C-O | -22.61 | 0.80 | 1.23 |
| 32 | BC | 256 | HIS | C-O | -22.59 | 0.80 | 1.23 |
| 81 | DA | 1054 | A | C2'-C1' | 22.59 | 1.78 | 1.53 |
| 81 | DA | 3253 | G | C2'-C1' | -22.46 | 1.28 | 1.53 |
| 3 | AB | 78 | LYS | C-O | -22.44 | 0.80 | 1.23 |
| 81 | DA | 1866 | C | O4'-C1' | 22.40 | 1.70 | 1.41 |
| 78 | CA | 1201 | G | C2'-C1' | -22.39 | 1.28 | 1.53 |
| 81 | DA | 2625 | C | O4'-C1' | 22.37 | 1.70 | 1.41 |
| 81 | DA | 3239 | G | C2'-C1' | -22.31 | 1.28 | 1.53 |
| 81 | DA | 597 | G | C2'-C1' | -22.28 | 1.28 | 1.53 |
| 55 | Bc | 104 | GLN | C-O | -22.25 | 0.81 | 1.23 |
| 81 | DA | 3306 | U | C2'-C1' | -22.24 | 1.28 | 1.53 |
| 81 | DA | 1871 | U | C5'-C4' | -22.22 | 1.24 | 1.51 |
| 18 | AP | 122 | ILE | C-O | -22.22 | 0.81 | 1.23 |
| 81 | DA | 338 | A | O4'-C1' | 22.18 | 1.70 | 1.41 |
| 35 | BG | 152 | THR | C-O | -22.16 | 0.81 | 1.23 |
| 82 | DB | 3 | A | C2'-C1' | -22.16 | 1.28 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 51 | BZ | 70 | LYS | C-O | -22.11 | 0.81 | 1.23 |
| 81 | DA | 1971 | C | O4'-C1' | 22.06 | 1.70 | 1.41 |
| 81 | DA | 1685 | C | O4'-C1' | 22.05 | 1.70 | 1.41 |
| 81 | DA | 70 | A | C2'-C1' | -22.01 | 1.29 | 1.53 |
| 60 | Bi | 108 | GLN | C-O | -22.01 | 0.81 | 1.23 |
| 81 | DA | 427 | C | O4'-C1' | 21.99 | 1.70 | 1.41 |
| 81 | DA | 7 | C | O4'-C1' | 21.93 | 1.70 | 1.41 |
| 81 | DA | 1379 | G | C2'-C1' | -21.90 | 1.29 | 1.53 |
| 78 | CA | 1200 | G | O4'-C1' | 21.90 | 1.70 | 1.41 |
| 78 | CA | 294 | C | O4'-C1' | 21.87 | 1.70 | 1.41 |
| 81 | DA | 3217 | C | C2'-C1' | 21.82 | 1.77 | 1.53 |
| 79 | CB | 41 | G | C2'-C1' | -21.76 | 1.29 | 1.53 |
| 81 | DA | 1207 | G | C2'-C1' | -21.76 | 1.29 | 1.53 |
| 60 | Bi | 78 | GLY | C-O | -21.76 | 0.88 | 1.23 |
| 81 | DA | 209 | A | C2'-C1' | 21.75 | 1.77 | 1.53 |
| 81 | DA | 2634 | U | C2'-C1' | -21.70 | 1.29 | 1.53 |
| 37 | BH | 236 | GLY | C-O | -21.69 | 0.89 | 1.23 |
| 83 | DC | 17 | A | O4'-C1' | 21.64 | 1.69 | 1.41 |
| 81 | DA | 1859 | A | C2'-C1' | 21.61 | 1.77 | 1.53 |
| 53 | Ba | 8 | GLY | C-O | -21.59 | 0.89 | 1.23 |
| 81 | DA | 2157 | G | O4'-C1' | 21.58 | 1.69 | 1.41 |
| 6 | AE | 7 | GLN | C-O | -21.56 | 0.82 | 1.23 |
| 36 | BF | 2 | LYS | C-O | -21.55 | 0.82 | 1.23 |
| 81 | DA | 2363 | A | C2'-C1' | 21.55 | 1.77 | 1.53 |
| 81 | DA | 124 | U | O4'-C1' | 21.52 | 1.69 | 1.41 |
| 33 | BD | 148 | ILE | C-O | -21.52 | 0.82 | 1.23 |
| 81 | DA | 3245 | A | C2'-C1' | -21.51 | 1.29 | 1.53 |
| 81 | DA | 169 | U | C2'-C1' | 21.48 | 1.76 | 1.53 |
| 81 | DA | 1682 | U | C2'-C1' | 21.47 | 1.76 | 1.53 |
| 81 | DA | 3304 | U | C3'-C2' | 21.43 | 1.76 | 1.52 |
| 35 | BG | 148 | GLU | C-O | -21.43 | 0.82 | 1.23 |
| 35 | BG | 2 | SER | C-O | -21.41 | 0.82 | 1.23 |
| 78 | CA | 1201 | G | O4'-C1' | 21.37 | 1.69 | 1.41 |
| 81 | DA | 2899 | C | O4'-C1' | 21.33 | 1.69 | 1.41 |
| 78 | CA | 1091 | A | C2'-C1' | 21.30 | 1.76 | 1.53 |
| 81 | DA | 2721 | A | O4'-C1' | 21.30 | 1.69 | 1.41 |
| 45 | BR | 142 | GLY | C-O | -21.25 | 0.89 | 1.23 |
| 44 | BO | 73 | LEU | C-O | 21.22 | 1.63 | 1.23 |
| 81 | DA | 2630 | C | O4'-C1' | 21.22 | 1.69 | 1.41 |
| 78 | CA | 853 | G | C2'-C1' | 21.17 | 1.76 | 1.53 |
| 78 | CA | 1702 | A | C2'-C1' | 21.16 | 1.76 | 1.53 |
| 81 | DA | 1014 | U | C2'-C1' | -21.15 | 1.30 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 44 | BO | 21 | ARG | C-N | 21.15 | 1.82 | 1.34 |
| 81 | DA | 2760 | C | C2'-C1' | -21.12 | 1.30 | 1.53 |
| 78 | CA | 610 | G | O4'-C1' | -21.09 | 1.14 | 1.41 |
| 82 | DB | 46 | G | C2'-C1' | -21.08 | 1.30 | 1.53 |
| 11 | AJ | 81 | THR | C-O | -21.05 | 0.83 | 1.23 |
| 81 | DA | 1747 | G | C2'-C1' | -21.03 | 1.30 | 1.53 |
| 78 | CA | 1436 | A | C2'-C1' | -21.03 | 1.30 | 1.53 |
| 21 | AT | 9 | VAL | C-O | -21.02 | 0.83 | 1.23 |
| 10 | AI | 140 | LYS | C-O | -20.98 | 0.83 | 1.23 |
| 81 | DA | 1866 | C | C2'-C1' | -20.94 | 1.30 | 1.53 |
| 81 | DA | 672 | A | C2'-C1' | -20.94 | 1.30 | 1.53 |
| 48 | BW | 93 | ILE | C-O | -20.94 | 0.83 | 1.23 |
| 81 | DA | 2685 | C | C2'-C1' | -20.92 | 1.30 | 1.53 |
| 81 | DA | 2001 | U | C2'-C1' | 20.89 | 1.76 | 1.53 |
| 81 | DA | 1808 | G | C2'-C1' | -20.89 | 1.30 | 1.53 |
| 81 | DA | 2362 | C | C2'-C1' | 20.87 | 1.76 | 1.53 |
| 48 | BW | 90 | ARG | C-O | -20.84 | 0.83 | 1.23 |
| 62 | Bk | 83 | ALA | C-O | -20.84 | 0.83 | 1.23 |
| 81 | DA | 1316 | C | O4'-C1' | 20.83 | 1.68 | 1.41 |
| 81 | DA | 1572 | U | O4'-C1' | 20.83 | 1.68 | 1.41 |
| 81 | DA | 9 | U | C2'-C1' | -20.83 | 1.30 | 1.53 |
| 81 | DA | 3006 | A | C2'-C1' | -20.83 | 1.30 | 1.53 |
| 81 | DA | 1561 | G | C2'-C1' | -20.83 | 1.30 | 1.53 |
| 81 | DA | 1821 | U | C2'-C1' | -20.82 | 1.30 | 1.53 |
| 78 | CA | 573 | C | C2'-O2' | -20.82 | 1.14 | 1.41 |
| 13 | AL | 87 | VAL | C-O | -20.82 | 0.83 | 1.23 |
| 17 | AQ | 26 | LEU | C-O | -20.81 | 0.83 | 1.23 |
| 78 | CA | 897 | C | O4'-C1' | 20.75 | 1.68 | 1.41 |
| 81 | DA | 798 | G | O4'-C1' | -20.72 | 1.14 | 1.41 |
| 2 | AA | 229 | LYS | C-O | -20.71 | 0.84 | 1.23 |
| 81 | DA | 1579 | C | O4'-C1' | 20.70 | 1.68 | 1.41 |
| 44 | BO | 142 | GLY | C-O | -20.69 | 0.90 | 1.23 |
| 81 | DA | 3224 | G | O4'-C1' | -20.67 | 1.14 | 1.41 |
| 83 | DC | 118 | U | C2'-C1' | -20.64 | 1.30 | 1.53 |
| 78 | CA | 1615 | C | O4'-C1' | 20.64 | 1.68 | 1.41 |
| 81 | DA | 2948 | C | O4'-C1' | 20.64 | 1.68 | 1.41 |
| 81 | DA | 3249 | C | C2'-C1' | -20.63 | 1.30 | 1.53 |
| 62 | Bk | 81 | THR | C-O | -20.62 | 0.84 | 1.23 |
| 81 | DA | 2637 | A | C2'-C1' | 20.62 | 1.76 | 1.53 |
| 37 | BH | 158 | ASP | C-O | -20.62 | 0.84 | 1.23 |
| 38 | Bs | 5 | ARG | C-O | -20.61 | 0.84 | 1.23 |
| 45 | BR | 157 | PRO | C-O | -20.59 | 0.82 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2699 | G | C2'-C1' | -20.57 | 1.30 | 1.53 |
| 74 | BQ | 238 | ASP | C-O | -20.56 | 0.84 | 1.23 |
| 78 | CA | 368 | U | C2'-C1' | -20.54 | 1.30 | 1.53 |
| 81 | DA | 2689 | A | C2'-C1' | -20.53 | 1.30 | 1.53 |
| 81 | DA | 656 | A | C2'-C1' | -20.52 | 1.30 | 1.53 |
| 81 | DA | 1947 | G | O4'-C1' | -20.52 | 1.15 | 1.41 |
| 81 | DA | 2619 | G | C2'-C1' | -20.52 | 1.30 | 1.53 |
| 78 | CA | 1386 | G | O4'-C1' | -20.50 | 1.15 | 1.41 |
| 43 | BP | 74 | PRO | C-O | -20.48 | 0.82 | 1.23 |
| 81 | DA | 647 | A | C2'-C1' | -20.45 | 1.30 | 1.53 |
| 81 | DA | 1688 | U | C2'-C1' | -20.45 | 1.30 | 1.53 |
| 34 | BE | 89 | TYR | C-O | -20.45 | 0.84 | 1.23 |
| 81 | DA | 2623 | G | C2'-C1' | 20.44 | 1.75 | 1.53 |
| 37 | BH | 73 | PRO | C-O | -20.44 | 0.82 | 1.23 |
| 2 | AA | 11 | PRO | C-O | -20.43 | 0.82 | 1.23 |
| 81 | DA | 422 | A | C2'-C1' | 20.42 | 1.75 | 1.53 |
| 35 | BG | 5 | LYS | C-O | -20.39 | 0.84 | 1.23 |
| 81 | DA | 2674 | A | C2'-C1' | -20.38 | 1.30 | 1.53 |
| 81 | DA | 3003 | G | O4'-C1' | -20.37 | 1.15 | 1.41 |
| 78 | CA | 960 | U | C2'-C1' | 20.35 | 1.75 | 1.53 |
| 81 | DA | 2756 | C | C2'-C1' | -20.32 | 1.30 | 1.53 |
| 82 | DB | 62 | C | C2'-C1' | -20.32 | 1.30 | 1.53 |
| 32 | BC | 362 | ALA | C-O | -20.31 | 0.84 | 1.23 |
| 81 | DA | 1174 | G | C2'-C1' | -20.26 | 1.31 | 1.53 |
| 78 | CA | 990 | C | O4'-C1' | 20.22 | 1.68 | 1.41 |
| 65 | Bn | 34 | ALA | C-O | -20.19 | 0.84 | 1.23 |
| 78 | CA | 955 | A | C2'-C1' | 20.16 | 1.75 | 1.53 |
| 78 | CA | 591 | A | C2'-C1' | -20.12 | 1.31 | 1.53 |
| 74 | BQ | 197 | SER | C-O | -20.11 | 0.85 | 1.23 |
| 35 | BG | 15 | VAL | C-O | -20.10 | 0.85 | 1.23 |
| 81 | DA | 1059 | G | C2'-C1' | -20.10 | 1.31 | 1.53 |
| 78 | CA | 635 | A | O4'-C1' | 20.10 | 1.67 | 1.41 |
| 81 | DA | 3330 | A | C2'-C1' | -20.06 | 1.31 | 1.53 |
| 81 | DA | 2966 | G | C2'-C1' | -20.04 | 1.31 | 1.53 |
| 57 | Be | 98 | LYS | N-CA | -20.03 | 1.06 | 1.46 |
| 78 | CA | 948 | G | C2'-C1' | -20.02 | 1.31 | 1.53 |
| 81 | DA | 2264 | U | O4'-C1' | 20.01 | 1.67 | 1.41 |
| 45 | BR | 95 | GLU | C-O | -20.00 | 0.85 | 1.23 |
| 78 | CA | 296 | U | O4'-C1' | 19.97 | 1.67 | 1.41 |
| 81 | DA | 2496 | C | C2'-C1' | -19.95 | 1.31 | 1.53 |
| 81 | DA | 2339 | C | C2'-C1' | 19.94 | 1.75 | 1.53 |
| 81 | DA | 993 | G | C2'-C1' | -19.92 | 1.31 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 59 | Bh | 12 | LYS | C-O | -19.90 | 0.85 | 1.23 |
| 81 | DA | 1396 | C | O4'-C1' | 19.87 | 1.67 | 1.41 |
| 81 | DA | 2899 | C | C2'-C1' | -19.87 | 1.31 | 1.53 |
| 6 | AE | 92 | ALA | C-O | -19.86 | 0.85 | 1.23 |
| 3 | AB | 205 | ALA | C-O | -19.85 | 0.85 | 1.23 |
| 55 | Bc | 102 | GLU | C-O | -19.85 | 0.85 | 1.23 |
| 78 | CA | 652 | G | C2'-C1' | -19.83 | 1.31 | 1.53 |
| 78 | CA | 1580 | C | O4'-C1' | 19.83 | 1.67 | 1.41 |
| 81 | DA | 2720 | G | O4'-C1' | 19.79 | 1.67 | 1.41 |
| 81 | DA | 1115 | G | O4'-C1' | 19.79 | 1.67 | 1.41 |
| 81 | DA | 3243 | A | C2'-C1' | -19.78 | 1.31 | 1.53 |
| 81 | DA | 2173 | U | C2'-C1' | -19.77 | 1.31 | 1.53 |
| 37 | BH | 228 | GLU | C-O | -19.77 | 0.85 | 1.23 |
| 40 | BK | 63 | ALA | C-O | -19.75 | 0.85 | 1.23 |
| 6 | AE | 4 | PRO | C-O | -19.75 | 0.83 | 1.23 |
| 46 | BT | 82 | LYS | C-O | -19.75 | 0.85 | 1.23 |
| 81 | DA | 907 | G | C2'-C1' | -19.71 | 1.31 | 1.53 |
| 81 | DA | 1884 | A | C2'-C1' | -19.71 | 1.31 | 1.53 |
| 35 | BG | 8 | LYS | C-O | -19.70 | 0.85 | 1.23 |
| 81 | DA | 70 | A | O4'-C1' | 19.70 | 1.67 | 1.41 |
| 82 | DB | 35 | C | O4'-C1' | 19.69 | 1.67 | 1.41 |
| 81 | DA | 2316 | G | C2'-C1' | -19.68 | 1.31 | 1.53 |
| 1 | Aa | 53 | LYS | C-O | -19.67 | 0.85 | 1.23 |
| 81 | DA | 2630 | C | C2'-C1' | -19.64 | 1.31 | 1.53 |
| 82 | DB | 32 | C | C2'-C1' | -19.64 | 1.31 | 1.53 |
| 81 | DA | 1333 | C | O4'-C1' | 19.61 | 1.67 | 1.41 |
| 81 | DA | 3149 | G | C2'-C1' | 19.60 | 1.75 | 1.53 |
| 81 | DA | 675 | C | O4'-C1' | 19.58 | 1.67 | 1.41 |
| 31 | BB | 249 | SER | C-O | -19.57 | 0.86 | 1.23 |
| 78 | CA | 847 | A | C2'-C1' | -19.57 | 1.31 | 1.53 |
| 82 | DB | 45 | C | O4'-C1' | 19.56 | 1.67 | 1.41 |
| 5 | AC | 162 | SER | C-O | -19.52 | 0.86 | 1.23 |
| 81 | DA | 2439 | A | O4'-C1' | 19.51 | 1.67 | 1.41 |
| 81 | DA | 3244 | A | C2'-C1' | -19.49 | 1.31 | 1.53 |
| 81 | DA | 251 | G | C2'-C1' | -19.49 | 1.31 | 1.53 |
| 81 | DA | 1582 | C | O4'-C1' | 19.48 | 1.67 | 1.41 |
| 81 | DA | 2638 | C | O4'-C1' | 19.46 | 1.67 | 1.41 |
| 26 | AZ | 40 | TYR | C-O | -19.40 | 0.86 | 1.23 |
| 81 | DA | 147 | U | C4'-C3' | -19.38 | 1.31 | 1.53 |
| 78 | CA | 1452 | U | C2'-C1' | -19.38 | 1.32 | 1.53 |
| 81 | DA | 1747 | G | O4'-C1' | 19.37 | 1.66 | 1.41 |
| 83 | DC | 53 | U | O4'-C1' | 19.36 | 1.66 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 174 | U | O4'-C1' | 19.35 | 1.66 | 1.41 |
| 81 | DA | 2487 | U | C2'-C1' | 19.35 | 1.74 | 1.53 |
| 44 | BO | 40 | HIS | C-O | -19.34 | 0.86 | 1.23 |
| 81 | DA | 2880 | U | O4'-C1' | 19.32 | 1.66 | 1.41 |
| 13 | AL | 34 | LEU | C-O | -19.30 | 0.86 | 1.23 |
| 81 | DA | 665 | A | C2'-C1' | -19.29 | 1.32 | 1.53 |
| 81 | DA | 1128 | U | C2'-C1' | -19.28 | 1.32 | 1.53 |
| 81 | DA | 2509 | U | C2'-C1' | -19.27 | 1.32 | 1.53 |
| 81 | DA | 2948 | C | C2'-C1' | -19.27 | 1.32 | 1.53 |
| 18 | AP | 57 | LYS | C-O | -19.25 | 0.86 | 1.23 |
| 81 | DA | 2788 | C | C2'-C1' | -19.25 | 1.32 | 1.53 |
| 81 | DA | 1295 | G | C2'-C1' | -19.24 | 1.32 | 1.53 |
| 82 | DB | 50 | C | C2'-C1' | 19.24 | 1.74 | 1.53 |
| 45 | BR | 143 | PRO | C-O | -19.22 | 0.84 | 1.23 |
| 78 | CA | 174 | U | C2'-C1' | -19.21 | 1.32 | 1.53 |
| 31 | BB | 73 | GLU | C-O | -19.21 | 0.86 | 1.23 |
| 22 | AV | 26 | LYS | C-O | -19.17 | 0.86 | 1.23 |
| 81 | DA | 201 | A | C2'-C1' | -19.17 | 1.32 | 1.53 |
| 17 | AQ | 81 | LYS | C-O | -19.16 | 0.86 | 1.23 |
| 81 | DA | 1713 | G | C2'-C1' | -19.16 | 1.32 | 1.53 |
| 61 | Bj | 33 | GLU | CB-CG | -19.15 | 1.15 | 1.52 |
| 81 | DA | 2816 | G | C2'-C1' | -19.14 | 1.32 | 1.53 |
| 81 | DA | 2231 | C | C2'-C1' | -19.14 | 1.32 | 1.53 |
| 74 | BQ | 121 | GLY | C-O | -19.11 | 0.93 | 1.23 |
| 81 | DA | 517 | G | C2'-C1' | -19.10 | 1.32 | 1.53 |
| 81 | DA | 3052 | G | C2'-C1' | -19.10 | 1.32 | 1.53 |
| 81 | DA | 203 | G | C2'-C1' | -19.10 | 1.32 | 1.53 |
| 69 | Br | 58 | PHE | C-O | -19.09 | 0.87 | 1.23 |
| 81 | DA | 3298 | C | O4'-C1' | 19.08 | 1.66 | 1.41 |
| 43 | BP | 80 | THR | C-O | -19.07 | 0.87 | 1.23 |
| 60 | Bi | 79 | SER | C-O | -19.05 | 0.87 | 1.23 |
| 78 | CA | 393 | C | O4'-C1' | 19.03 | 1.66 | 1.41 |
| 78 | CA | 1755 | A | O4'-C1' | -19.01 | 1.17 | 1.41 |
| 81 | DA | 3236 | U | C2'-C1' | -18.99 | 1.32 | 1.53 |
| 81 | DA | 671 | U | C2'-C1' | 18.98 | 1.74 | 1.53 |
| 81 | DA | 924 | G | C2'-C1' | -18.98 | 1.32 | 1.53 |
| 81 | DA | 1789 | G | C2'-C1' | -18.98 | 1.32 | 1.53 |
| 2 | AA | 10 | THR | C-O | -18.97 | 0.87 | 1.23 |
| 82 | DB | 32 | C | O4'-C1' | 18.93 | 1.66 | 1.41 |
| 81 | DA | 514 | G | C2'-C1' | -18.91 | 1.32 | 1.53 |
| 81 | DA | 608 | A | O4'-C1' | 18.91 | 1.66 | 1.41 |
| 78 | CA | 1112 | G | C2'-C1' | -18.90 | 1.32 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2755 | C | C2'-C1' | -18.90 | 1.32 | 1.53 |
| 81 | DA | 2160 | G | C2'-C1' | -18.90 | 1.32 | 1.53 |
| 81 | DA | 518 | G | O4'-C1' | 18.88 | 1.66 | 1.41 |
| 18 | AP | 40 | LEU | C-O | -18.85 | 0.87 | 1.23 |
| 78 | CA | 1565 | C | O4'-C1' | 18.84 | 1.66 | 1.41 |
| 83 | DC | 31 | U | C2'-C1' | 18.82 | 1.74 | 1.53 |
| 31 | BB | 252 | THR | C-O | -18.82 | 0.87 | 1.23 |
| 44 | BO | 3 | SER | C-O | -18.82 | 0.87 | 1.23 |
| 78 | CA | 1546 | G | C3'-O3' | -18.81 | 1.15 | 1.42 |
| 81 | DA | 1160 | C | C2'-C1' | -18.81 | 1.32 | 1.53 |
| 82 | DB | 154 | C | C2'-C1' | -18.79 | 1.32 | 1.53 |
| 81 | DA | 1177 | G | C2'-C1' | -18.73 | 1.32 | 1.53 |
| 81 | DA | 1203 | A | C2'-C1' | -18.73 | 1.32 | 1.53 |
| 81 | DA | 3241 | G | C2'-C1' | -18.72 | 1.32 | 1.53 |
| 51 | BZ | 51 | TRP | C-O | -18.72 | 0.87 | 1.23 |
| 78 | CA | 1793 | G | C2'-C1' | -18.69 | 1.32 | 1.53 |
| 81 | DA | 1802 | C | C2'-C1' | -18.68 | 1.32 | 1.53 |
| 81 | DA | 1551 | C | O4'-C1' | 18.68 | 1.66 | 1.41 |
| 81 | DA | 1585 | C | O4'-C1' | 18.65 | 1.65 | 1.41 |
| 17 | AQ | 63 | LYS | C-O | -18.64 | 0.88 | 1.23 |
| 81 | DA | 2438 | A | O4'-C1' | 18.61 | 1.65 | 1.41 |
| 78 | CA | 1096 | C | O4'-C1' | 18.60 | 1.65 | 1.41 |
| 81 | DA | 1743 | G | C2'-C1' | -18.60 | 1.32 | 1.53 |
| 81 | DA | 1297 | C | O4'-C1' | 18.56 | 1.65 | 1.41 |
| 81 | DA | 560 | G | C2'-C1' | 18.56 | 1.73 | 1.53 |
| 81 | DA | 3115 | C | O4'-C1' | 18.56 | 1.65 | 1.41 |
| 81 | DA | 2231 | C | O4'-C1' | 18.56 | 1.65 | 1.41 |
| 31 | BB | 127 | ALA | C-O | -18.55 | 0.88 | 1.23 |
| 81 | DA | 594 | U | O4'-C1' | 18.54 | 1.65 | 1.41 |
| 81 | DA | 1319 | G | C2'-C1' | -18.49 | 1.33 | 1.53 |
| 61 | Bj | 33 | GLU | CD-OE1 | 18.48 | 1.46 | 1.25 |
| 33 | BD | 89 | ALA | C-O | -18.46 | 0.88 | 1.23 |
| 14 | AM | 99 | HIS | C-O | -18.45 | 0.88 | 1.23 |
| 60 | Bi | 16 | ARG | C-O | -18.44 | 0.88 | 1.23 |
| 81 | DA | 2746 | A | C2'-C1' | -18.44 | 1.33 | 1.53 |
| 81 | DA | 242 | C | O4'-C1' | 18.43 | 1.65 | 1.41 |
| 81 | DA | 1263 | A | C2'-C1' | -18.41 | 1.33 | 1.53 |
| 78 | CA | 280 | U | O4'-C1' | 18.39 | 1.65 | 1.41 |
| 81 | DA | 665 | A | O4'-C1' | 18.39 | 1.65 | 1.41 |
| 78 | CA | 874 | C | C2'-C1' | -18.38 | 1.33 | 1.53 |
| 4 | AD | 90 | ILE | C-O | -18.37 | 0.88 | 1.23 |
| 81 | DA | 3000 | A | C2'-C1' | -18.37 | 1.33 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 1086 | A | C2'-C1' | -18.37 | 1.33 | 1.53 |
| 81 | DA | 415 | G | C2'-C1' | -18.37 | 1.33 | 1.53 |
| 81 | DA | 777 | U | C2'-C1' | -18.35 | 1.33 | 1.53 |
| 81 | DA | 1095 | U | C4'-C3' | 18.35 | 1.73 | 1.53 |
| 78 | CA | 1254 | U | O3'-P | 18.31 | 1.83 | 1.61 |
| 78 | CA | 1392 | U | C2'-C1' | 18.29 | 1.73 | 1.53 |
| 81 | DA | 699 | A | O4'-C1' | 18.27 | 1.65 | 1.41 |
| 81 | DA | 855 | U | C2'-C1' | -18.26 | 1.33 | 1.53 |
| 81 | DA | 2829 | U | C2'-C1' | -18.26 | 1.33 | 1.53 |
| 81 | DA | 185 | C | C2'-C1' | -18.23 | 1.33 | 1.53 |
| 81 | DA | 2916 | U | C2'-C1' | -18.23 | 1.33 | 1.53 |
| 81 | DA | 1701 | C | C2'-C1' | -18.21 | 1.33 | 1.53 |
| 80 | CC | 18 | C | O4'-C1' | 18.21 | 1.65 | 1.41 |
| 81 | DA | 1591 | G | C2'-C1' | -18.20 | 1.33 | 1.53 |
| 20 | AS | 90 | PRO | C-O | -18.19 | 0.86 | 1.23 |
| 81 | DA | 2628 | A | C2'-C1' | -18.19 | 1.33 | 1.53 |
| 81 | DA | 1552 | G | C2'-C1' | -18.19 | 1.33 | 1.53 |
| 76 | BS | 15 | GLY | C-O | -18.18 | 0.94 | 1.23 |
| 32 | BC | 5 | LYS | C-O | -18.18 | 0.88 | 1.23 |
| 78 | CA | 630 | A | C2'-C1' | 18.17 | 1.73 | 1.53 |
| 12 | AK | 123 | SER | C-O | -18.15 | 0.88 | 1.23 |
| 81 | DA | 531 | G | C2'-C1' | -18.15 | 1.33 | 1.53 |
| 83 | DC | 42 | A | O4'-C1' | 18.12 | 1.65 | 1.41 |
| 81 | DA | 2916 | U | O4'-C1' | 18.12 | 1.65 | 1.41 |
| 81 | DA | 2756 | C | O4'-C1' | 18.09 | 1.65 | 1.41 |
| 53 | Ba | 13 | VAL | C-O | -18.08 | 0.89 | 1.23 |
| 81 | DA | 3333 | G | C2'-C1' | -18.07 | 1.33 | 1.53 |
| 33 | BD | 331 | ALA | C-O | -18.06 | 0.89 | 1.23 |
| 78 | CA | 203 | U | C2'-C1' | -18.04 | 1.33 | 1.53 |
| 81 | DA | 751 | A | C2'-C1' | -18.04 | 1.33 | 1.53 |
| 32 | BC | 3 | HIS | C-O | -18.01 | 0.89 | 1.23 |
| 81 | DA | 910 | G | C2'-C1' | -17.99 | 1.33 | 1.53 |
| 81 | DA | 3002 | C | O4'-C1' | 17.99 | 1.65 | 1.41 |
| 78 | CA | 589 | C | O4'-C1' | 17.98 | 1.65 | 1.41 |
| 81 | DA | 1260 | A | C2'-C1' | 17.94 | 1.73 | 1.53 |
| 81 | DA | 2887 | A | C2'-C1' | -17.93 | 1.33 | 1.53 |
| 78 | CA | 169 | A | C2'-C1' | 17.91 | 1.73 | 1.53 |
| 81 | DA | 317 | A | C2'-C1' | -17.90 | 1.33 | 1.53 |
| 81 | DA | 80 | G | C2'-C1' | -17.89 | 1.33 | 1.53 |
| 83 | DC | 49 | G | O4'-C1' | 17.89 | 1.65 | 1.41 |
| 81 | DA | 1871 | U | C4'-O4' | -17.89 | 1.22 | 1.45 |
| 81 | DA | 2108 | C | O4'-C1' | 17.88 | 1.64 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 1674 | C | O4'-C1' | 17.88 | 1.64 | 1.41 |
| 81 | DA | 3220 | G | C2'-C1' | -17.87 | 1.33 | 1.53 |
| 45 | BR | 98 | LYS | C-O | -17.86 | 0.89 | 1.23 |
| 74 | BQ | 128 | GLU | C-O | -17.86 | 0.89 | 1.23 |
| 81 | DA | 3382 | U | C2'-C1' | -17.85 | 1.33 | 1.53 |
| 78 | CA | 668 | C | O4'-C1' | 17.84 | 1.64 | 1.41 |
| 83 | DC | 54 | A | O4'-C1' | 17.84 | 1.64 | 1.41 |
| 81 | DA | 576 | C | C2'-C1' | -17.84 | 1.33 | 1.53 |
| 81 | DA | 1432 | C | C2'-C1' | 17.84 | 1.73 | 1.53 |
| 43 | BP | 16 | SER | C-O | -17.83 | 0.89 | 1.23 |
| 81 | DA | 1260 | A | O4'-C1' | -17.82 | 1.18 | 1.41 |
| 81 | DA | 1637 | A | C2'-C1' | -17.81 | 1.33 | 1.53 |
| 82 | DB | 103 | G | C2'-C1' | -17.81 | 1.33 | 1.53 |
| 78 | CA | 1200 | G | C2'-C1' | -17.81 | 1.33 | 1.53 |
| 81 | DA | 1678 | G | O4'-C1' | -17.81 | 1.18 | 1.41 |
| 78 | CA | 1086 | A | O4'-C1' | 17.80 | 1.64 | 1.41 |
| 78 | CA | 280 | U | C2'-C1' | -17.80 | 1.33 | 1.53 |
| 32 | BC | 360 | ASP | C-O | -17.79 | 0.89 | 1.23 |
| 78 | CA | 1520 | U | C5'-C4' | -17.77 | 1.30 | 1.51 |
| 81 | DA | 1256 | G | C2'-C1' | -17.77 | 1.33 | 1.53 |
| 78 | CA | 219 | A | C2'-C1' | 17.76 | 1.72 | 1.53 |
| 81 | DA | 2408 | U | C2'-C1' | -17.74 | 1.33 | 1.53 |
| 81 | DA | 386 | A | O4'-C1' | 17.73 | 1.64 | 1.41 |
| 81 | DA | 3249 | C | O4'-C1' | 17.73 | 1.64 | 1.41 |
| 81 | DA | 2407 | C | O4'-C1' | 17.72 | 1.64 | 1.41 |
| 81 | DA | 607 | A | O4'-C1' | -17.70 | 1.18 | 1.41 |
| 81 | DA | 745 | C | O4'-C1' | 17.70 | 1.64 | 1.41 |
| 26 | AZ | 39 | LEU | C-O | -17.69 | 0.89 | 1.23 |
| 81 | DA | 1397 | C | O4'-C1' | 17.69 | 1.64 | 1.41 |
| 81 | DA | 2182 | A | C2'-C1' | -17.68 | 1.33 | 1.53 |
| 81 | DA | 2606 | G | O4'-C1' | -17.65 | 1.18 | 1.41 |
| 81 | DA | 1513 | G | C2'-C1' | -17.62 | 1.33 | 1.53 |
| 78 | CA | 651 | G | C2'-C1' | -17.62 | 1.33 | 1.53 |
| 78 | CA | 1602 | C | C2'-C1' | -17.62 | 1.33 | 1.53 |
| 78 | CA | 1791 | A | O4'-C1' | 17.61 | 1.64 | 1.41 |
| 81 | DA | 1889 | G | C2'-C1' | -17.61 | 1.33 | 1.53 |
| 60 | Bi | 68 | THR | C-O | -17.60 | 0.90 | 1.23 |
| 81 | DA | 2403 | G | C2'-C1' | 17.59 | 1.72 | 1.53 |
| 81 | DA | 3240 | C | C2'-C1' | -17.59 | 1.34 | 1.53 |
| 81 | DA | 774 | G | C2'-C1' | -17.58 | 1.34 | 1.53 |
| 78 | CA | 672 | U | O4'-C1' | 17.57 | 1.64 | 1.41 |
| 81 | DA | 2844 | C | C2'-C1' | -17.57 | 1.34 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 577 | C | O4'-C1' | 17.57 | 1.64 | 1.41 |
| 78 | CA | 1180 | C | O4'-C1' | 17.57 | 1.64 | 1.41 |
| 81 | DA | 1506 | A | C2'-C1' | 17.56 | 1.72 | 1.53 |
| 8 | AF | 35 | GLN | C-O | -17.56 | 0.90 | 1.23 |
| 81 | DA | 2623 | G | O4'-C1' | -17.54 | 1.18 | 1.41 |
| 5 | AC | 157 | ASP | C-O | -17.52 | 0.90 | 1.23 |
| 81 | DA | 3081 | C | C2'-C1' | -17.51 | 1.34 | 1.53 |
| 74 | BQ | 115 | LEU | C-O | -17.51 | 0.90 | 1.23 |
| 78 | CA | 1161 | C | O4'-C1' | 17.49 | 1.64 | 1.41 |
| 83 | DC | 27 | A | O4'-C1' | 17.48 | 1.64 | 1.41 |
| 81 | DA | 1265 | U | C2'-C1' | -17.48 | 1.34 | 1.53 |
| 81 | DA | 1947 | G | C2'-C1' | 17.44 | 1.72 | 1.53 |
| 78 | CA | 1570 | A | O4'-C1' | 17.43 | 1.64 | 1.41 |
| 81 | DA | 3094 | A | O4'-C1' | 17.41 | 1.64 | 1.41 |
| 81 | DA | 752 | C | O4'-C1' | 17.39 | 1.64 | 1.41 |
| 4 | AD | 93 | ASP | C-O | -17.39 | 0.90 | 1.23 |
| 81 | DA | 1939 | G | C2'-C1' | -17.37 | 1.34 | 1.53 |
| 11 | AJ | 119 | ALA | C-O | -17.35 | 0.90 | 1.23 |
| 65 | Bn | 71 | PRO | C-O | -17.34 | 0.88 | 1.23 |
| 78 | CA | 172 | C | C2'-C1' | -17.32 | 1.34 | 1.53 |
| 78 | CA | 206 | A | O4'-C1' | 17.32 | 1.64 | 1.41 |
| 78 | CA | 471 | A | O4'-C1' | 17.30 | 1.64 | 1.41 |
| 29 | AU | 36 | SER | C-O | -17.29 | 0.90 | 1.23 |
| 81 | DA | 1633 | C | O4'-C1' | 17.29 | 1.64 | 1.41 |
| 78 | CA | 1149 | G | C2'-C1' | -17.29 | 1.34 | 1.53 |
| 81 | DA | 2100 | A | C2'-C1' | -17.28 | 1.34 | 1.53 |
| 2 | AA | 195 | TRP | C-O | -17.27 | 0.90 | 1.23 |
| 81 | DA | 573 | C | O4'-C1' | 17.25 | 1.64 | 1.41 |
| 78 | CA | 354 | C | O4'-C1' | 17.23 | 1.64 | 1.41 |
| 83 | DC | 45 | A | O4'-C1' | 17.23 | 1.64 | 1.41 |
| 32 | BC | 298 | PHE | C-O | -17.23 | 0.90 | 1.23 |
| 81 | DA | 2617 | U | C2'-C1' | 17.21 | 1.72 | 1.53 |
| 81 | DA | 1535 | A | C2'-C1' | 17.21 | 1.72 | 1.53 |
| 45 | BR | 13 | SER | C-O | 17.20 | 1.56 | 1.23 |
| 1 | Aa | 54 | PHE | C-O | -17.19 | 0.90 | 1.23 |
| 81 | DA | 2632 | G | C2'-C1' | -17.19 | 1.34 | 1.53 |
| 31 | BB | 62 | VAL | C-O | -17.17 | 0.90 | 1.23 |
| 78 | CA | 369 | A | C2'-C1' | 17.17 | 1.72 | 1.53 |
| 81 | DA | 1811 | G | C2'-C1' | 17.16 | 1.72 | 1.53 |
| 78 | CA | 1336 | A | O4'-C1' | 17.16 | 1.64 | 1.41 |
| 81 | DA | 2653 | C | O4'-C1' | 17.16 | 1.64 | 1.41 |
| 81 | DA | 1552 | G | O4'-C1' | 17.16 | 1.64 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 229 | G | C2'-C1' | -17.15 | 1.34 | 1.53 |
| 81 | DA | 233 | C | C2'-C1' | 17.13 | 1.72 | 1.53 |
| 81 | DA | 2438 | A | C2'-C1' | -17.12 | 1.34 | 1.53 |
| 78 | CA | 686 | C | O4'-C1' | 17.11 | 1.63 | 1.41 |
| 81 | DA | 3350 | C | O4'-C1' | 17.11 | 1.63 | 1.41 |
| 81 | DA | 2971 | A | C2'-C1' | 17.10 | 1.72 | 1.53 |
| 16 | AO | 67 | THR | C-O | -17.10 | 0.90 | 1.23 |
| 81 | DA | 1085 | A | O4'-C1' | 17.10 | 1.63 | 1.41 |
| 81 | DA | 247 | C | O4'-C1' | 17.08 | 1.63 | 1.41 |
| 78 | CA | 123 | G | C2'-C1' | -17.06 | 1.34 | 1.53 |
| 43 | BP | 116 | LEU | C-O | -17.05 | 0.91 | 1.23 |
| 78 | CA | 218 | A | C2'-C1' | -17.05 | 1.34 | 1.53 |
| 45 | BR | 3 | ILE | C-O | -17.03 | 0.91 | 1.23 |
| 58 | Bg | 107 | VAL | C-O | -17.01 | 0.91 | 1.23 |
| 81 | DA | 3031 | G | C2'-C1' | -17.01 | 1.34 | 1.53 |
| 81 | DA | 3103 | A | O4'-C1' | 16.99 | 1.63 | 1.41 |
| 81 | DA | 576 | C | O4'-C1' | 16.98 | 1.63 | 1.41 |
| 81 | DA | 2827 | U | C2'-C1' | 16.98 | 1.72 | 1.53 |
| 81 | DA | 2724 | U | C2'-C1' | -16.95 | 1.34 | 1.53 |
| 81 | DA | 114 | A | C2'-C1' | 16.95 | 1.72 | 1.53 |
| 81 | DA | 110 | G | C2'-C1' | -16.94 | 1.34 | 1.53 |
| 78 | CA | 1562 | G | C2'-C1' | 16.94 | 1.72 | 1.53 |
| 81 | DA | 1687 | U | C2'-C1' | -16.94 | 1.34 | 1.53 |
| 82 | DB | 98 | U | C2'-C1' | -16.93 | 1.34 | 1.53 |
| 81 | DA | 722 | G | C2'-C1' | -16.90 | 1.34 | 1.53 |
| 78 | CA | 1405 | G | C2'-C1' | 16.90 | 1.72 | 1.53 |
| 37 | BH | 89 | GLU | C-O | -16.89 | 0.91 | 1.23 |
| 83 | DC | 60 | G | C2'-C1' | -16.87 | 1.34 | 1.53 |
| 81 | DA | 3110 | C | C2'-C1' | -16.87 | 1.34 | 1.53 |
| 61 | Bj | 66 | VAL | CA-CB | -16.86 | 1.19 | 1.54 |
| 78 | CA | 1614 | A | O4'-C1' | 16.86 | 1.63 | 1.41 |
| 55 | Bc | 94 | LYS | C-O | -16.86 | 0.91 | 1.23 |
| 78 | CA | 1613 | U | C2'-C1' | 16.86 | 1.71 | 1.53 |
| 78 | CA | 433 | C | O4'-C1' | 16.85 | 1.63 | 1.41 |
| 81 | DA | 498 | A | O4'-C1' | 16.84 | 1.63 | 1.41 |
| 2 | AA | 251 | GLU | C-O | -16.84 | 0.91 | 1.23 |
| 81 | DA | 1871 | U | C3'-C2' | -16.82 | 1.34 | 1.52 |
| 78 | CA | 650 | U | C2'-C1' | 16.82 | 1.71 | 1.53 |
| 78 | CA | 1189 | A | O3'-P | 16.82 | 1.81 | 1.61 |
| 10 | AI | 119 | ALA | C-O | -16.82 | 0.91 | 1.23 |
| 83 | DC | 2 | G | C2'-C1' | 16.81 | 1.71 | 1.53 |
| 78 | CA | 298 | C | O4'-C1' | 16.80 | 1.63 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 841 | A | C2'-C1' | -16.79 | 1.34 | 1.53 |
| 81 | DA | 1618 | G | C2'-C1' | -16.79 | 1.34 | 1.53 |
| 81 | DA | 3094 | A | C2'-C1' | -16.79 | 1.34 | 1.53 |
| 81 | DA | 2942 | C | O4'-C1' | 16.78 | 1.63 | 1.41 |
| 81 | DA | 2059 | U | C2'-C1' | -16.77 | 1.34 | 1.53 |
| 78 | CA | 1238 | A | C2'-C1' | 16.75 | 1.71 | 1.53 |
| 81 | DA | 1783 | U | C2'-C1' | -16.75 | 1.34 | 1.53 |
| 81 | DA | 1842 | A | O4'-C1' | 16.74 | 1.63 | 1.41 |
| 78 | CA | 942 | G | C2'-C1' | -16.74 | 1.34 | 1.53 |
| 81 | DA | 238 | A | O4'-C1' | 16.74 | 1.63 | 1.41 |
| 83 | DC | 25 | G | O4'-C1' | -16.74 | 1.19 | 1.41 |
| 78 | CA | 894 | U | O4'-C1' | 16.73 | 1.63 | 1.41 |
| 81 | DA | 2514 | U | C2'-C1' | 16.73 | 1.71 | 1.53 |
| 81 | DA | 638 | C | C2'-C1' | -16.71 | 1.34 | 1.53 |
| 81 | DA | 2308 | C | C2'-C1' | -16.70 | 1.34 | 1.53 |
| 83 | DC | 48 | U | C2'-C1' | -16.70 | 1.34 | 1.53 |
| 78 | CA | 1179 | G | C2'-C1' | -16.69 | 1.34 | 1.53 |
| 78 | CA | 154 | G | O4'-C1' | 16.66 | 1.63 | 1.41 |
| 4 | AD | 94 | ALA | C-O | -16.65 | 0.91 | 1.23 |
| 78 | CA | 1185 | U | C2'-C1' | -16.64 | 1.35 | 1.53 |
| 81 | DA | 3361 | G | O4'-C1' | 16.63 | 1.63 | 1.41 |
| 81 | DA | 3350 | C | C2'-C1' | -16.61 | 1.35 | 1.53 |
| 81 | DA | 2251 | G | C2'-C1' | -16.60 | 1.35 | 1.53 |
| 81 | DA | 2628 | A | O4'-C1' | 16.59 | 1.63 | 1.41 |
| 81 | DA | 2172 | A | C2'-C1' | -16.59 | 1.35 | 1.53 |
| 83 | DC | 37 | G | O4'-C1' | 16.59 | 1.63 | 1.41 |
| 81 | DA | 3255 | U | C2'-C1' | -16.58 | 1.35 | 1.53 |
| 78 | CA | 850 | A | C2'-C1' | -16.58 | 1.35 | 1.53 |
| 82 | DB | 44 | A | C2'-C1' | -16.58 | 1.35 | 1.53 |
| 81 | DA | 2697 | A | O4'-C1' | 16.57 | 1.63 | 1.41 |
| 81 | DA | 1585 | C | C2'-C1' | -16.56 | 1.35 | 1.53 |
| 81 | DA | 2873 | U | C2'-C1' | -16.56 | 1.35 | 1.53 |
| 81 | DA | 2392 | C | O4'-C1' | 16.55 | 1.63 | 1.41 |
| 81 | DA | 3131 | U | C2'-C1' | -16.55 | 1.35 | 1.53 |
| 81 | DA | 1277 | C | C2'-C1' | -16.55 | 1.35 | 1.53 |
| 5 | AC | 164 | PHE | C-O | -16.51 | 0.92 | 1.23 |
| 81 | DA | 3306 | U | O4'-C1' | 16.51 | 1.63 | 1.41 |
| 81 | DA | 599 | C | O4'-C1' | 16.49 | 1.63 | 1.41 |
| 78 | CA | 1607 | G | C2'-C1' | -16.48 | 1.35 | 1.53 |
| 81 | DA | 1515 | A | C2'-C1' | -16.47 | 1.35 | 1.53 |
| 26 | AZ | 18 | THR | C-O | -16.47 | 0.92 | 1.23 |
| 81 | DA | 1007 | U | C2'-C1' | -16.47 | 1.35 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1786 | G | O4'-C1' | -16.46 | 1.20 | 1.41 |
| 81 | DA | 1694 | U | C2'-C1' | 16.46 | 1.71 | 1.53 |
| 81 | DA | 1908 | A | C2'-C1' | -16.44 | 1.35 | 1.53 |
| 81 | DA | 2508 | U | O4'-C1' | 16.43 | 1.63 | 1.41 |
| 78 | CA | 1420 | C | O4'-C1' | 16.41 | 1.62 | 1.41 |
| 81 | DA | 1432 | C | O4'-C1' | -16.41 | 1.20 | 1.41 |
| 78 | CA | 386 | G | C2'-C1' | -16.41 | 1.35 | 1.53 |
| 81 | DA | 727 | G | O4'-C1' | 16.40 | 1.62 | 1.41 |
| 81 | DA | 3030 | G | C2'-C1' | -16.39 | 1.35 | 1.53 |
| 81 | DA | 2735 | U | C2'-C1' | -16.39 | 1.35 | 1.53 |
| 78 | CA | 989 | U | C2'-C1' | -16.39 | 1.35 | 1.53 |
| 81 | DA | 2131 | A | C2'-C1' | -16.38 | 1.35 | 1.53 |
| 78 | CA | 120 | U | C3'-C2' | 16.37 | 1.71 | 1.52 |
| 78 | CA | 338 | C | C2'-C1' | -16.36 | 1.35 | 1.53 |
| 81 | DA | 2277 | C | C2'-C1' | -16.36 | 1.35 | 1.53 |
| 81 | DA | 384 | A | C2'-C1' | -16.35 | 1.35 | 1.53 |
| 81 | DA | 2376 | G | O4'-C1' | 16.35 | 1.62 | 1.41 |
| 81 | DA | 2741 | C | O4'-C1' | 16.31 | 1.62 | 1.41 |
| 81 | DA | 2308 | C | O4'-C1' | 16.31 | 1.62 | 1.41 |
| 81 | DA | 109 | A | C2'-C1' | -16.29 | 1.35 | 1.53 |
| 78 | CA | 1652 | C | O4'-C1' | 16.29 | 1.62 | 1.41 |
| 81 | DA | 2172 | A | O3'-P | -16.29 | 1.41 | 1.61 |
| 78 | CA | 204 | G | C2'-C1' | -16.28 | 1.35 | 1.53 |
| 61 | Bj | 8 | TYR | C-O | -16.28 | 0.92 | 1.23 |
| 78 | CA | 668 | C | C2'-C1' | -16.27 | 1.35 | 1.53 |
| 82 | DB | 40 | A | C2'-C1' | -16.27 | 1.35 | 1.53 |
| 78 | CA | 888 | U | C2'-C1' | -16.27 | 1.35 | 1.53 |
| 78 | CA | 1282 | U | C2'-C1' | -16.26 | 1.35 | 1.53 |
| 83 | DC | 26 | C | O4'-C1' | 16.26 | 1.62 | 1.41 |
| 83 | DC | 30 | G | C2'-C1' | -16.25 | 1.35 | 1.53 |
| 78 | CA | 29 | U | O4'-C1' | 16.24 | 1.62 | 1.41 |
| 81 | DA | 2233 | A | C2'-C1' | 16.23 | 1.71 | 1.53 |
| 81 | DA | 3382 | U | O4'-C1' | 16.23 | 1.62 | 1.41 |
| 81 | DA | 180 | C | O4'-C1' | 16.21 | 1.62 | 1.41 |
| 78 | CA | 1564 | U | O4'-C1' | 16.20 | 1.62 | 1.41 |
| 81 | DA | 2101 | C | C2'-C1' | -16.20 | 1.35 | 1.53 |
| 81 | DA | 742 | G | C2'-C1' | 16.18 | 1.71 | 1.53 |
| 81 | DA | 2254 | U | C2'-C1' | 16.17 | 1.71 | 1.53 |
| 81 | DA | 2721 | A | C2'-C1' | -16.16 | 1.35 | 1.53 |
| 83 | DC | 3 | U | C2'-C1' | 16.15 | 1.71 | 1.53 |
| 78 | CA | 1111 | G | C2'-C1' | -16.14 | 1.35 | 1.53 |
| 81 | DA | 1896 | A | C2'-C1' | -16.13 | 1.35 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 46 | BT | 71 | ARG | C-O | -16.13 | 0.92 | 1.23 |
| 39 | BJ | 76 | SER | C-O | -16.13 | 0.92 | 1.23 |
| 74 | BQ | 190 | ILE | C-O | -16.13 | 0.92 | 1.23 |
| 81 | DA | 1895 | A | C2'-C1' | 16.12 | 1.71 | 1.53 |
| 81 | DA | 2297 | U | C2'-C1' | -16.12 | 1.35 | 1.53 |
| 81 | DA | 1199 | C | O4'-C1' | 16.11 | 1.62 | 1.41 |
| 78 | CA | 1375 | A | O4'-C1' | 16.10 | 1.62 | 1.41 |
| 78 | CA | 1022 | C | O4'-C1' | 16.09 | 1.62 | 1.41 |
| 81 | DA | 220 | G | C2'-C1' | 16.09 | 1.71 | 1.53 |
| 81 | DA | 2074 | C | O4'-C1' | 16.09 | 1.62 | 1.41 |
| 78 | CA | 1209 | C | O4'-C1' | 16.08 | 1.62 | 1.41 |
| 81 | DA | 1978 | A | O4'-C1' | 16.07 | 1.62 | 1.41 |
| 78 | CA | 1386 | G | C2'-C1' | 16.05 | 1.71 | 1.53 |
| 81 | DA | 1711 | C | C2'-C1' | -16.05 | 1.35 | 1.53 |
| 78 | CA | 312 | A | O4'-C1' | 16.04 | 1.62 | 1.41 |
| 78 | CA | 1192 | C | O4'-C1' | 16.04 | 1.62 | 1.41 |
| 81 | DA | 2506 | U | O4'-C1' | 16.04 | 1.62 | 1.41 |
| 35 | BG | 99 | GLU | CA-CB | 16.02 | 1.89 | 1.53 |
| 81 | DA | 531 | G | O4'-C1' | 16.02 | 1.62 | 1.41 |
| 81 | DA | 3001 | C | O4'-C1' | 16.01 | 1.62 | 1.41 |
| 78 | CA | 427 | C | O4'-C1' | 16.00 | 1.62 | 1.41 |
| 81 | DA | 2760 | C | O4'-C1' | 15.97 | 1.62 | 1.41 |
| 81 | DA | 27 | C | O4'-C1' | 15.97 | 1.62 | 1.41 |
| 81 | DA | 1160 | C | O4'-C1' | 15.95 | 1.62 | 1.41 |
| 81 | DA | 1329 | U | O4'-C1' | 15.95 | 1.62 | 1.41 |
| 76 | BS | 123 | ILE | C-O | -15.92 | 0.93 | 1.23 |
| 78 | CA | 105 | A | C2'-C1' | -15.91 | 1.35 | 1.53 |
| 12 | AK | 22 | SER | C-O | -15.91 | 0.93 | 1.23 |
| 81 | DA | 2394 | G | C2'-C1' | -15.91 | 1.35 | 1.53 |
| 81 | DA | 2952 | G | C2'-C1' | -15.91 | 1.35 | 1.53 |
| 78 | CA | 1541 | G | O4'-C1' | 15.91 | 1.62 | 1.41 |
| 81 | DA | 2957 | G | C2'-C1' | -15.91 | 1.35 | 1.53 |
| 81 | DA | 2491 | A | C2'-C1' | -15.89 | 1.35 | 1.53 |
| 60 | Bi | 55 | SER | C-O | -15.87 | 0.93 | 1.23 |
| 83 | DC | 71 | C | O4'-C1' | 15.86 | 1.62 | 1.41 |
| 35 | BG | 38 | THR | C-O | -15.86 | 0.93 | 1.23 |
| 78 | CA | 1007 | C | O4'-C1' | 15.86 | 1.62 | 1.41 |
| 78 | CA | 1108 | G | O4'-C1' | -15.85 | 1.21 | 1.41 |
| 78 | CA | 1458 | G | C2'-C1' | -15.85 | 1.35 | 1.53 |
| 81 | DA | 3099 | C | C2'-C1' | -15.85 | 1.35 | 1.53 |
| 69 | Br | 47 | GLN | C-O | -15.85 | 0.93 | 1.23 |
| 78 | CA | 1666 | U | C2'-C1' | 15.85 | 1.70 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1943 | C | C2'-C1' | -15.85 | 1.35 | 1.53 |
| 78 | CA | 1580 | C | C2'-C1' | -15.85 | 1.35 | 1.53 |
| 79 | CB | 22 | G | C2'-C1' | -15.84 | 1.35 | 1.53 |
| 81 | DA | 1076 | C | O4'-C1' | 15.84 | 1.62 | 1.41 |
| 81 | DA | 172 | G | C2'-C1' | -15.84 | 1.35 | 1.53 |
| 81 | DA | 3285 | C | O4'-C1' | 15.84 | 1.62 | 1.41 |
| 81 | DA | 2476 | C | O4'-C1' | 15.81 | 1.62 | 1.41 |
| 81 | DA | 160 | G | C2'-C1' | -15.80 | 1.35 | 1.53 |
| 81 | DA | 873 | C | O4'-C1' | 15.79 | 1.62 | 1.41 |
| 78 | CA | 1586 | A | C2'-C1' | -15.79 | 1.35 | 1.53 |
| 35 | BG | 3 | ALA | C-O | -15.77 | 0.93 | 1.23 |
| 78 | CA | 1300 | A | C2'-C1' | 15.77 | 1.70 | 1.53 |
| 81 | DA | 3223 | A | O4'-C1' | 15.76 | 1.62 | 1.41 |
| 81 | DA | 2677 | G | C2'-C1' | 15.76 | 1.70 | 1.53 |
| 81 | DA | 3018 | C | O4'-C1' | 15.76 | 1.62 | 1.41 |
| 78 | CA | 1752 | U | C2'-C1' | -15.75 | 1.36 | 1.53 |
| 81 | DA | 2685 | C | O4'-C1' | 15.75 | 1.62 | 1.41 |
| 81 | DA | 1301 | A | C2'-C1' | -15.75 | 1.36 | 1.53 |
| 78 | CA | 93 | A | C2'-C1' | -15.74 | 1.36 | 1.53 |
| 82 | DB | 45 | C | C2'-C1' | -15.73 | 1.36 | 1.53 |
| 81 | DA | 1366 | A | C2'-C1' | -15.72 | 1.36 | 1.53 |
| 81 | DA | 2744 | U | C2'-C1' | -15.72 | 1.36 | 1.53 |
| 33 | BD | 12 | THR | C-O | -15.72 | 0.93 | 1.23 |
| 81 | DA | 962 | A | O4'-C1' | -15.71 | 1.21 | 1.41 |
| 81 | DA | 1563 | C | O4'-C1' | 15.71 | 1.62 | 1.41 |
| 81 | DA | 3002 | C | C2'-C1' | -15.71 | 1.36 | 1.53 |
| 32 | BC | 130 | PHE | C-O | -15.70 | 0.93 | 1.23 |
| 38 | Bs | 72 | ASP | C-O | -15.70 | 0.93 | 1.23 |
| 78 | CA | 444 | C | O4'-C1' | 15.69 | 1.62 | 1.41 |
| 81 | DA | 608 | A | C2'-C1' | -15.68 | 1.36 | 1.53 |
| 81 | DA | 2922 | G | C2'-C1' | -15.68 | 1.36 | 1.53 |
| 81 | DA | 1879 | A | O4'-C1' | 15.68 | 1.62 | 1.41 |
| 81 | DA | 928 | C | C2'-C1' | -15.66 | 1.36 | 1.53 |
| 81 | DA | 2197 | C | O4'-C1' | 15.66 | 1.62 | 1.41 |
| 81 | DA | 2749 | G | C2'-C1' | -15.65 | 1.36 | 1.53 |
| 33 | BD | 145 | ILE | C-O | -15.65 | 0.93 | 1.23 |
| 81 | DA | 2885 | C | C2'-C1' | -15.65 | 1.36 | 1.53 |
| 81 | DA | 179 | C | O4'-C1' | 15.64 | 1.61 | 1.41 |
| 78 | CA | 1772 | C | C2'-C1' | -15.62 | 1.36 | 1.53 |
| 81 | DA | 1871 | U | P-O5' | -15.61 | 1.44 | 1.59 |
| 81 | DA | 848 | A | C2'-C1' | -15.60 | 1.36 | 1.53 |
| 81 | DA | 406 | G | C2'-C1' | 15.60 | 1.70 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 1586 | A | O3'-P | -15.60 | 1.42 | 1.61 |
| 44 | BO | 7 | LYS | C-O | -15.59 | 0.93 | 1.23 |
| 81 | DA | 1685 | C | C2'-C1' | -15.59 | 1.36 | 1.53 |
| 81 | DA | 2662 | G | C2'-C1' | -15.58 | 1.36 | 1.53 |
| 81 | DA | 3004 | C | O4'-C1' | 15.57 | 1.61 | 1.41 |
| 78 | CA | 1585 | U | C2'-C1' | 15.57 | 1.70 | 1.53 |
| 81 | DA | 182 | U | C2'-C1' | 15.56 | 1.70 | 1.53 |
| 41 | BN | 77 | ARG | N-CA | -15.55 | 1.15 | 1.46 |
| 81 | DA | 1704 | A | O4'-C1' | -15.55 | 1.21 | 1.41 |
| 78 | CA | 87 | C | O4'-C1' | 15.54 | 1.61 | 1.41 |
| 81 | DA | 295 | A | O4'-C1' | 15.54 | 1.61 | 1.41 |
| 81 | DA | 1014 | U | O4'-C1' | 15.54 | 1.61 | 1.41 |
| 4 | AD | 153 | ASN | C-O | -15.54 | 0.93 | 1.23 |
| 78 | CA | 287 | G | C2'-C1' | -15.53 | 1.36 | 1.53 |
| 69 | Br | 89 | LYS | C-O | -15.52 | 0.93 | 1.23 |
| 81 | DA | 3234 | A | C2'-C1' | 15.51 | 1.70 | 1.53 |
| 78 | CA | 1475 | A | O4'-C1' | 15.51 | 1.61 | 1.41 |
| 35 | BG | 27 | PRO | C-O | -15.50 | 0.92 | 1.23 |
| 78 | CA | 310 | C | O4'-C1' | 15.50 | 1.61 | 1.41 |
| 81 | DA | 2507 | C | O4'-C1' | 15.49 | 1.61 | 1.41 |
| 2 | AA | 250 | VAL | C-O | -15.49 | 0.94 | 1.23 |
| 81 | DA | 2624 | G | C2'-C1' | -15.49 | 1.36 | 1.53 |
| 81 | DA | 386 | A | C2'-C1' | -15.49 | 1.36 | 1.53 |
| 78 | CA | 1473 | U | C2'-C1' | 15.47 | 1.70 | 1.53 |
| 78 | CA | 658 | C | C3'-C2' | -15.47 | 1.35 | 1.52 |
| 81 | DA | 2431 | C | O4'-C1' | 15.47 | 1.61 | 1.41 |
| 81 | DA | 2507 | C | C2'-C1' | -15.45 | 1.36 | 1.53 |
| 81 | DA | 2180 | G | C2'-C1' | -15.44 | 1.36 | 1.53 |
| 78 | CA | 1616 | G | C2'-C1' | -15.44 | 1.36 | 1.53 |
| 81 | DA | 3245 | A | O4'-C1' | 15.43 | 1.61 | 1.41 |
| 78 | CA | 1793 | G | O4'-C1' | 15.42 | 1.61 | 1.41 |
| 81 | DA | 2420 | C | O4'-C1' | 15.41 | 1.61 | 1.41 |
| 81 | DA | 2063 | U | O4'-C1' | 15.40 | 1.61 | 1.41 |
| 78 | CA | 571 | G | O4'-C1' | 15.39 | 1.61 | 1.41 |
| 81 | DA | 1366 | A | O4'-C1' | 15.39 | 1.61 | 1.41 |
| 81 | DA | 1625 | A | O4'-C1' | 15.38 | 1.61 | 1.41 |
| 47 | BU | 126 | VAL | C-O | -15.37 | 0.94 | 1.23 |
| 78 | CA | 1536 | G | C2'-C1' | -15.37 | 1.36 | 1.53 |
| 81 | DA | 2248 | C | O4'-C1' | 15.37 | 1.61 | 1.41 |
| 78 | CA | 1678 | A | C2'-C1' | -15.36 | 1.36 | 1.53 |
| 81 | DA | 2465 | G | C2'-C1' | -15.36 | 1.36 | 1.53 |
| 78 | CA | 1771 | U | C2'-C1' | -15.35 | 1.36 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1261 | G | O4'-C1' | -15.34 | 1.21 | 1.41 |
| 81 | DA | 2074 | C | C2'-C1' | -15.33 | 1.36 | 1.53 |
| 78 | CA | 1156 | C | O4'-C1' | 15.33 | 1.61 | 1.41 |
| 78 | CA | 415 | C | C2'-C1' | 15.32 | 1.70 | 1.53 |
| 78 | CA | 1123 | C | O4'-C1' | 15.32 | 1.61 | 1.41 |
| 81 | DA | 306 | A | C2'-C1' | 15.31 | 1.70 | 1.53 |
| 53 | Ba | 60 | LYS | C-O | -15.30 | 0.94 | 1.23 |
| 78 | CA | 1209 | C | C2'-C1' | -15.28 | 1.36 | 1.53 |
| 79 | CB | 25 | U | C2'-C1' | -15.28 | 1.36 | 1.53 |
| 81 | DA | 877 | C | C2'-C1' | -15.27 | 1.36 | 1.53 |
| 81 | DA | 1825 | G | C2'-C1' | -15.26 | 1.36 | 1.53 |
| 81 | DA | 462 | C | O4'-C1' | 15.25 | 1.61 | 1.41 |
| 81 | DA | 881 | C | C2'-C1' | -15.24 | 1.36 | 1.53 |
| 82 | DB | 115 | C | O4'-C1' | 15.24 | 1.61 | 1.41 |
| 81 | DA | 959 | C | O4'-C1' | 15.23 | 1.61 | 1.41 |
| 78 | CA | 589 | C | C2'-C1' | -15.23 | 1.36 | 1.53 |
| 81 | DA | 1128 | U | O4'-C1' | 15.23 | 1.61 | 1.41 |
| 81 | DA | 1711 | C | O4'-C1' | 15.22 | 1.61 | 1.41 |
| 81 | DA | 1831 | U | C2'-C1' | 15.22 | 1.70 | 1.53 |
| 81 | DA | 9 | U | O4'-C1' | 15.22 | 1.61 | 1.41 |
| 78 | CA | 1384 | A | O4'-C1' | 15.21 | 1.61 | 1.41 |
| 78 | CA | 1158 | C | O4'-C1' | 15.21 | 1.61 | 1.41 |
| 33 | BD | 323 | VAL | C-O | -15.20 | 0.94 | 1.23 |
| 81 | DA | 2316 | G | O4'-C1' | 15.20 | 1.61 | 1.41 |
| 81 | DA | 634 | C | C2'-C1' | -15.18 | 1.36 | 1.53 |
| 81 | DA | 2353 | G | C2'-C1' | -15.18 | 1.36 | 1.53 |
| 81 | DA | 2042 | G | O4'-C1' | 15.17 | 1.61 | 1.41 |
| 81 | DA | 517 | G | O4'-C1' | 15.17 | 1.61 | 1.41 |
| 81 | DA | 1943 | C | O4'-C1' | 15.16 | 1.61 | 1.41 |
| 78 | CA | 1476 | C | O3'-P | -15.15 | 1.43 | 1.61 |
| 81 | DA | 2844 | C | O4'-C1' | 15.15 | 1.61 | 1.41 |
| 81 | DA | 409 | A | O4'-C1' | 15.14 | 1.61 | 1.41 |
| 81 | DA | 694 | C | O4'-C1' | 15.14 | 1.61 | 1.41 |
| 33 | BD | 321 | LYS | C-O | -15.13 | 0.94 | 1.23 |
| 82 | DB | 61 | A | C2'-C1' | -15.13 | 1.36 | 1.53 |
| 81 | DA | 1728 | G | C2'-C1' | -15.12 | 1.36 | 1.53 |
| 81 | DA | 491 | C | O4'-C1' | 15.11 | 1.61 | 1.41 |
| 81 | DA | 1682 | U | O4'-C1' | 15.11 | 1.61 | 1.41 |
| 78 | CA | 1107 | G | O4'-C1' | 15.11 | 1.61 | 1.41 |
| 81 | DA | 2637 | A | O4'-C1' | -15.11 | 1.22 | 1.41 |
| 81 | DA | 2709 | C | O4'-C1' | 15.08 | 1.61 | 1.41 |
| 81 | DA | 412 | G | C2'-C1' | -15.08 | 1.36 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1653 | G | C2'-C1' | -15.07 | 1.36 | 1.53 |
| 78 | CA | 1192 | C | C2'-C1' | -15.07 | 1.36 | 1.53 |
| 81 | DA | 2646 | C | O4'-C1' | 15.06 | 1.61 | 1.41 |
| 81 | DA | 2758 | A | O4'-C1' | -15.05 | 1.22 | 1.41 |
| 81 | DA | 1455 | U | C2'-C1' | 15.05 | 1.70 | 1.53 |
| 78 | CA | 1624 | C | O4'-C1' | 15.04 | 1.61 | 1.41 |
| 81 | DA | 2165 | G | O4'-C1' | -15.02 | 1.22 | 1.41 |
| 81 | DA | 374 | A | O4'-C1' | -15.01 | 1.22 | 1.41 |
| 78 | CA | 943 | C | C2'-C1' | -15.01 | 1.36 | 1.53 |
| 81 | DA | 1571 | A | C2'-C1' | 14.99 | 1.69 | 1.53 |
| 81 | DA | 352 | A | C2'-C1' | 14.99 | 1.69 | 1.53 |
| 81 | DA | 2840 | C | C2'-C1' | 14.99 | 1.69 | 1.53 |
| 81 | DA | 1665 | C | O4'-C1' | 14.97 | 1.61 | 1.41 |
| 83 | DC | 35 | C | O4'-C1' | 14.97 | 1.61 | 1.41 |
| 81 | DA | 1257 | C | C2'-C1' | -14.96 | 1.36 | 1.53 |
| 81 | DA | 2303 | A | C2'-C1' | 14.95 | 1.69 | 1.53 |
| 81 | DA | 560 | G | O4'-C1' | -14.94 | 1.22 | 1.41 |
| 78 | CA | 1281 | G | C2'-C1' | -14.93 | 1.36 | 1.53 |
| 81 | DA | 1429 | G | O4'-C1' | 14.91 | 1.61 | 1.41 |
| 78 | CA | 1477 | G | C2'-C1' | -14.91 | 1.36 | 1.53 |
| 78 | CA | 1162 | C | O4'-C1' | 14.87 | 1.60 | 1.41 |
| 78 | CA | 831 | U | C2'-C1' | 14.87 | 1.69 | 1.53 |
| 81 | DA | 3313 | U | O3'-P | -14.85 | 1.43 | 1.61 |
| 81 | DA | 2776 | C | O4'-C1' | 14.85 | 1.60 | 1.41 |
| 32 | BC | 266 | ARG | CD-NE | 14.84 | 1.71 | 1.46 |
| 81 | DA | 55 | G | C2'-C1' | -14.84 | 1.37 | 1.53 |
| 81 | DA | 1665 | C | C2'-C1' | -14.84 | 1.37 | 1.53 |
| 82 | DB | 28 | C | O4'-C1' | 14.83 | 1.60 | 1.41 |
| 81 | DA | 3304 | U | C4'-O4' | 14.82 | 1.64 | 1.45 |
| 81 | DA | 2785 | A | O4'-C1' | 14.82 | 1.60 | 1.41 |
| 78 | CA | 943 | C | O4'-C1' | 14.80 | 1.60 | 1.41 |
| 81 | DA | 2606 | G | C2'-C1' | 14.80 | 1.69 | 1.53 |
| 78 | CA | 120 | U | O3'-P | 14.80 | 1.78 | 1.61 |
| 78 | CA | 1336 | A | C2'-C1' | -14.80 | 1.37 | 1.53 |
| 78 | CA | 1332 | C | O4'-C1' | 14.79 | 1.60 | 1.41 |
| 81 | DA | 846 | A | O4'-C1' | 14.79 | 1.60 | 1.41 |
| 81 | DA | 1627 | U | C2'-C1' | 14.78 | 1.69 | 1.53 |
| 78 | CA | 1679 | G | C2'-C1' | -14.78 | 1.37 | 1.53 |
| 78 | CA | 151 | G | C2'-C1' | -14.77 | 1.37 | 1.53 |
| 81 | DA | 2682 | C | O4'-C1' | 14.76 | 1.60 | 1.41 |
| 81 | DA | 1640 | G | C2'-C1' | -14.76 | 1.37 | 1.53 |
| 78 | CA | 256 | A | O4'-C1' | 14.75 | 1.60 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 76 | BS | 15 | GLY | N-CA | -14.74 | 1.24 | 1.46 |
| 78 | CA | 658 | C | C4'-O4' | -14.74 | 1.26 | 1.45 |
| 81 | DA | 1295 | G | O4'-C1' | 14.74 | 1.60 | 1.41 |
| 81 | DA | 2108 | C | C2'-C1' | -14.74 | 1.37 | 1.53 |
| 81 | DA | 1663 | C | C2'-C1' | -14.74 | 1.37 | 1.53 |
| 78 | CA | 583 | C | C2'-C1' | -14.72 | 1.37 | 1.53 |
| 81 | DA | 871 | U | C2'-C1' | -14.71 | 1.37 | 1.53 |
| 81 | DA | 1424 | C | O4'-C1' | 14.71 | 1.60 | 1.41 |
| 81 | DA | 2798 | C | C2'-C1' | -14.71 | 1.37 | 1.53 |
| 78 | CA | 323 | A | C2'-C1' | 14.70 | 1.69 | 1.53 |
| 78 | CA | 1375 | A | C2'-C1' | -14.68 | 1.37 | 1.53 |
| 81 | DA | 2149 | A | C2'-C1' | 14.68 | 1.69 | 1.53 |
| 78 | CA | 1548 | G | O4'-C1' | -14.67 | 1.22 | 1.41 |
| 81 | DA | 3041 | U | C2'-C1' | -14.67 | 1.37 | 1.53 |
| 78 | CA | 404 | G | C2'-C1' | -14.66 | 1.37 | 1.53 |
| 81 | DA | 2422 | C | C2'-C1' | -14.66 | 1.37 | 1.53 |
| 78 | CA | 1762 | A | O4'-C1' | 14.66 | 1.60 | 1.41 |
| 78 | CA | 1310 | U | C3'-C2' | -14.66 | 1.36 | 1.52 |
| 81 | DA | 972 | A | C2'-C1' | -14.66 | 1.37 | 1.53 |
| 81 | DA | 2837 | A | C2'-C1' | 14.65 | 1.69 | 1.53 |
| 81 | DA | 202 | G | C2'-C1' | -14.63 | 1.37 | 1.53 |
| 83 | DC | 47 | C | P-O5' | -14.62 | 1.45 | 1.59 |
| 81 | DA | 788 | C | O4'-C1' | 14.62 | 1.60 | 1.41 |
| 81 | DA | 193 | C | O4'-C1' | 14.61 | 1.60 | 1.41 |
| 78 | CA | 39 | A | C2'-C1' | -14.61 | 1.37 | 1.53 |
| 81 | DA | 836 | A | O4'-C1' | 14.61 | 1.60 | 1.41 |
| 81 | DA | 877 | C | O4'-C1' | 14.61 | 1.60 | 1.41 |
| 81 | DA | 2489 | C | O4'-C1' | 14.61 | 1.60 | 1.41 |
| 78 | CA | 832 | U | C2'-C1' | -14.60 | 1.37 | 1.53 |
| 81 | DA | 1422 | G | C2'-C1' | -14.60 | 1.37 | 1.53 |
| 81 | DA | 3050 | U | O4'-C1' | 14.60 | 1.60 | 1.41 |
| 78 | CA | 1528 | U | C2'-C1' | 14.58 | 1.69 | 1.53 |
| 82 | DB | 108 | C | O4'-C1' | 14.57 | 1.60 | 1.41 |
| 81 | DA | 3296 | A | O4'-C1' | 14.57 | 1.60 | 1.41 |
| 81 | DA | 2013 | C | O4'-C1' | 14.56 | 1.60 | 1.41 |
| 81 | DA | 2332 | A | C2'-C1' | -14.56 | 1.37 | 1.53 |
| 81 | DA | 1725 | C | O4'-C1' | 14.56 | 1.60 | 1.41 |
| 81 | DA | 562 | C | O4'-C1' | 14.55 | 1.60 | 1.41 |
| 81 | DA | 1673 | G | C2'-C1' | -14.55 | 1.37 | 1.53 |
| 81 | DA | 104 | G | O4'-C1' | -14.54 | 1.22 | 1.41 |
| 81 | DA | 725 | G | C2'-C1' | -14.53 | 1.37 | 1.53 |
| 81 | DA | 2187 | G | O4'-C1' | -14.53 | 1.22 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 988 | A | O4'-C1' | 14.51 | 1.60 | 1.41 |
| 81 | DA | 3334 | U | C2'-C1' | 14.51 | 1.69 | 1.53 |
| 82 | DB | 21 | C | O4'-C1' | 14.51 | 1.60 | 1.41 |
| 78 | CA | 1228 | G | C2'-C1' | -14.50 | 1.37 | 1.53 |
| 78 | CA | 1783 | C | O4'-C1' | 14.49 | 1.60 | 1.41 |
| 78 | CA | 554 | C | O4'-C1' | 14.49 | 1.60 | 1.41 |
| 81 | DA | 2684 | C | O4'-C1' | 14.47 | 1.60 | 1.41 |
| 81 | DA | 2893 | C | C2'-C1' | -14.47 | 1.37 | 1.53 |
| 81 | DA | 3258 | U | C2'-C1' | 14.47 | 1.69 | 1.53 |
| 81 | DA | 1396 | C | C2'-C1' | -14.47 | 1.37 | 1.53 |
| 78 | CA | 1751 | C | O4'-C1' | 14.46 | 1.60 | 1.41 |
| 78 | CA | 571 | G | C2'-C1' | -14.45 | 1.37 | 1.53 |
| 81 | DA | 3099 | C | O4'-C1' | 14.44 | 1.60 | 1.41 |
| 81 | DA | 1531 | C | O4'-C1' | 14.44 | 1.60 | 1.41 |
| 78 | CA | 1028 | C | O4'-C1' | 14.43 | 1.60 | 1.41 |
| 82 | DB | 56 | G | C2'-C1' | -14.43 | 1.37 | 1.53 |
| 81 | DA | 33 | G | C2'-C1' | -14.43 | 1.37 | 1.53 |
| 78 | CA | 826 | U | C2'-C1' | -14.42 | 1.37 | 1.53 |
| 81 | DA | 3162 | C | C2'-C1' | -14.42 | 1.37 | 1.53 |
| 81 | DA | 2100 | A | O4'-C1' | 14.41 | 1.60 | 1.41 |
| 78 | CA | 890 | C | O4'-C1' | 14.40 | 1.60 | 1.41 |
| 79 | CB | 36 | C | O4'-C1' | 14.39 | 1.60 | 1.41 |
| 81 | DA | 3089 | C | O4'-C1' | 14.39 | 1.60 | 1.41 |
| 81 | DA | 111 | C | C2'-C1' | -14.39 | 1.37 | 1.53 |
| 78 | CA | 1341 | A | C2'-C1' | 14.38 | 1.69 | 1.53 |
| 81 | DA | 2857 | C | C2'-C1' | -14.38 | 1.37 | 1.53 |
| 82 | DB | 91 | C | C2'-C1' | 14.38 | 1.69 | 1.53 |
| 78 | CA | 572 | C | O4'-C1' | 14.37 | 1.60 | 1.41 |
| 81 | DA | 658 | G | C2'-C1' | -14.37 | 1.37 | 1.53 |
| 78 | CA | 297 | U | O4'-C1' | 14.37 | 1.60 | 1.41 |
| 81 | DA | 2963 | C | C2'-C1' | -14.34 | 1.37 | 1.53 |
| 45 | BR | 14 | GLY | N-CA | -14.33 | 1.24 | 1.46 |
| 81 | DA | 74 | G | C2'-C1' | -14.32 | 1.37 | 1.53 |
| 81 | DA | 3005 | A | C2'-C1' | 14.32 | 1.69 | 1.53 |
| 78 | CA | 849 | C | O4'-C1' | 14.32 | 1.60 | 1.41 |
| 81 | DA | 924 | G | O4'-C1' | 14.31 | 1.60 | 1.41 |
| 78 | CA | 1674 | C | C2'-C1' | -14.30 | 1.37 | 1.53 |
| 44 | BO | 8 | THR | C-O | -14.30 | 0.96 | 1.23 |
| 83 | DC | 14 | U | O4'-C1' | 14.30 | 1.60 | 1.41 |
| 81 | DA | 1000 | C | O4'-C1' | 14.30 | 1.60 | 1.41 |
| 83 | DC | 107 | G | C2'-C1' | 14.29 | 1.69 | 1.53 |
| 81 | DA | 2099 | A | O3'-P | -14.28 | 1.44 | 1.61 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 750 | G | C2'-C1' | -14.27 | 1.37 | 1.53 |
| 78 | CA | 1355 | C | O4'-C1' | 14.27 | 1.60 | 1.41 |
| 81 | DA | 1674 | G | C2'-C1' | -14.27 | 1.37 | 1.53 |
| 2 | AA | 11 | PRO | N-CD | 14.26 | 1.67 | 1.47 |
| 10 | AI | 54 | LEU | C-O | -14.26 | 0.96 | 1.23 |
| 82 | DB | 52 | A | O4'-C1' | 14.26 | 1.60 | 1.41 |
| 81 | DA | 656 | A | O4'-C1' | 14.25 | 1.60 | 1.41 |
| 81 | DA | 3165 | A | O4'-C1' | 14.25 | 1.60 | 1.41 |
| 81 | DA | 1142 | G | C2'-C1' | -14.21 | 1.37 | 1.53 |
| 81 | DA | 2073 | A | O4'-C1' | 14.21 | 1.60 | 1.41 |
| 81 | DA | 2235 | C | O4'-C1' | 14.20 | 1.60 | 1.41 |
| 81 | DA | 1397 | C | C2'-C1' | -14.19 | 1.37 | 1.53 |
| 81 | DA | 3254 | G | O4'-C1' | 14.19 | 1.60 | 1.41 |
| 81 | DA | 2385 | G | C2'-C1' | -14.18 | 1.37 | 1.53 |
| 78 | CA | 1607 | G | O4'-C1' | 14.18 | 1.60 | 1.41 |
| 81 | DA | 1896 | A | O4'-C1' | 14.18 | 1.60 | 1.41 |
| 81 | DA | 1162 | U | O4'-C1' | 14.17 | 1.60 | 1.41 |
| 81 | DA | 2177 | G | C2'-C1' | -14.17 | 1.37 | 1.53 |
| 78 | CA | 314 | C | O4'-C1' | 14.17 | 1.60 | 1.41 |
| 78 | CA | 268 | C | C2'-C1' | -14.16 | 1.37 | 1.53 |
| 81 | DA | 598 | A | C2'-C1' | -14.15 | 1.37 | 1.53 |
| 81 | DA | 1742 | U | O4'-C1' | 14.15 | 1.60 | 1.41 |
| 81 | DA | 521 | A | O4'-C1' | -14.14 | 1.23 | 1.41 |
| 81 | DA | 1639 | C | O4'-C1' | 14.13 | 1.60 | 1.41 |
| 81 | DA | 3384 | U | C2'-C1' | -14.13 | 1.37 | 1.53 |
| 81 | DA | 2363 | A | O4'-C1' | -14.12 | 1.23 | 1.41 |
| 82 | DB | 107 | G | C2'-C1' | -14.12 | 1.37 | 1.53 |
| 81 | DA | 1292 | C | O4'-C1' | 14.12 | 1.60 | 1.41 |
| 81 | DA | 2728 | G | C2'-C1' | -14.12 | 1.37 | 1.53 |
| 81 | DA | 2345 | A | C2'-C1' | -14.10 | 1.37 | 1.53 |
| 78 | CA | 297 | U | C2'-C1' | -14.10 | 1.37 | 1.53 |
| 81 | DA | 2644 | C | C2'-C1' | 14.10 | 1.68 | 1.53 |
| 81 | DA | 2724 | U | O4'-C1' | 14.10 | 1.59 | 1.41 |
| 81 | DA | 2042 | G | C2'-C1' | -14.09 | 1.37 | 1.53 |
| 81 | DA | 1879 | A | C2'-C1' | -14.09 | 1.37 | 1.53 |
| 78 | CA | 621 | A | C2'-C1' | 14.09 | 1.68 | 1.53 |
| 81 | DA | 2141 | U | O4'-C1' | 14.09 | 1.59 | 1.41 |
| 81 | DA | 678 | G | C2'-C1' | -14.09 | 1.37 | 1.53 |
| 83 | DC | 104 | C | C2'-C1' | -14.09 | 1.37 | 1.53 |
| 81 | DA | 3282 | U | O4'-C1' | 14.07 | 1.59 | 1.41 |
| 81 | DA | 2634 | U | O4'-C1' | 14.06 | 1.59 | 1.41 |
| 81 | DA | 2693 | C | O4'-C1' | 14.06 | 1.59 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2730 | G | C2'-C1' | -14.06 | 1.37 | 1.53 |
| 78 | CA | 252 | U | C2'-C1' | 14.05 | 1.68 | 1.53 |
| 78 | CA | 1384 | A | C2'-C1' | -14.04 | 1.38 | 1.53 |
| 79 | CB | 72 | G | O4'-C1' | -14.04 | 1.23 | 1.41 |
| 81 | DA | 3305 | A | O3'-P | -14.04 | 1.44 | 1.61 |
| 81 | DA | 198 | A | O4'-C1' | 14.04 | 1.59 | 1.41 |
| 81 | DA | 299 | G | C2'-C1' | -14.04 | 1.38 | 1.53 |
| 78 | CA | 1406 | A | C2'-C1' | -14.02 | 1.38 | 1.53 |
| 81 | DA | 637 | C | C2'-C1' | -14.02 | 1.38 | 1.53 |
| 45 | BR | 13 | SER | CA-CB | 14.01 | 1.74 | 1.52 |
| 81 | DA | 332 | C | O4'-C1' | 14.01 | 1.59 | 1.41 |
| 78 | CA | 235 | G | C2'-C1' | -14.01 | 1.38 | 1.53 |
| 81 | DA | 436 | A | O4'-C1' | 14.00 | 1.59 | 1.41 |
| 81 | DA | 2737 | C | O4'-C1' | 13.99 | 1.59 | 1.41 |
| 81 | DA | 1055 | A | O4'-C1' | 13.97 | 1.59 | 1.41 |
| 78 | CA | 615 | A | O4'-C1' | 13.97 | 1.59 | 1.41 |
| 81 | DA | 3013 | U | C2'-C1' | -13.97 | 1.38 | 1.53 |
| 79 | CB | 28 | G | C2'-C1' | -13.97 | 1.38 | 1.53 |
| 81 | DA | 774 | G | O4'-C1' | 13.96 | 1.59 | 1.41 |
| 78 | CA | 1764 | C | O4'-C1' | 13.95 | 1.59 | 1.41 |
| 81 | DA | 3240 | C | O4'-C1' | 13.95 | 1.59 | 1.41 |
| 81 | DA | 3000 | A | O4'-C1' | 13.94 | 1.59 | 1.41 |
| 82 | DB | 39 | G | C2'-C1' | 13.93 | 1.68 | 1.53 |
| 81 | DA | 1169 | A | C2'-C1' | -13.92 | 1.38 | 1.53 |
| 81 | DA | 3072 | C | C2'-C1' | -13.92 | 1.38 | 1.53 |
| 81 | DA | 3311 | C | C2'-C1' | -13.92 | 1.38 | 1.53 |
| 79 | CB | 45 | G | C2'-C1' | -13.91 | 1.38 | 1.53 |
| 81 | DA | 2378 | C | O4'-C1' | 13.91 | 1.59 | 1.41 |
| 78 | CA | 346 | G | O4'-C1' | 13.91 | 1.59 | 1.41 |
| 81 | DA | 2873 | U | O4'-C1' | 13.91 | 1.59 | 1.41 |
| 78 | CA | 1441 | C | O4'-C1' | 13.90 | 1.59 | 1.41 |
| 81 | DA | 3036 | G | O4'-C1' | 13.90 | 1.59 | 1.41 |
| 81 | DA | 49 | A | C2'-C1' | 13.90 | 1.68 | 1.53 |
| 81 | DA | 2876 | C | C2'-C1' | -13.90 | 1.38 | 1.53 |
| 81 | DA | 3352 | U | C2'-C1' | -13.90 | 1.38 | 1.53 |
| 81 | DA | 1977 | C | O4'-C1' | 13.89 | 1.59 | 1.41 |
| 81 | DA | 2372 | A | O4'-C1' | 13.88 | 1.59 | 1.41 |
| 78 | CA | 1090 | C | O4'-C1' | 13.88 | 1.59 | 1.41 |
| 78 | CA | 314 | C | C2'-C1' | -13.87 | 1.38 | 1.53 |
| 81 | DA | 3036 | G | C2'-C1' | -13.87 | 1.38 | 1.53 |
| 81 | DA | 720 | A | C2'-C1' | 13.87 | 1.68 | 1.53 |
| 81 | DA | 989 | A | C2'-C1' | 13.87 | 1.68 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 3365 | U | O4'-C1' | 13.87 | 1.59 | 1.41 |
| 78 | CA | 1417 | A | O4'-C1' | 13.85 | 1.59 | 1.41 |
| 81 | DA | 1420 | C | O4'-C1' | 13.85 | 1.59 | 1.41 |
| 81 | DA | 2279 | A | C2'-C1' | -13.84 | 1.38 | 1.53 |
| 81 | DA | 2863 | G | C2'-C1' | -13.84 | 1.38 | 1.53 |
| 81 | DA | 2511 | A | C2'-C1' | -13.84 | 1.38 | 1.53 |
| 78 | CA | 394 | C | O4'-C1' | 13.82 | 1.59 | 1.41 |
| 81 | DA | 3312 | U | C2'-C1' | -13.82 | 1.38 | 1.53 |
| 78 | CA | 1188 | G | C2'-C1' | -13.82 | 1.38 | 1.53 |
| 81 | DA | 1919 | G | C2'-C1' | -13.82 | 1.38 | 1.53 |
| 81 | DA | 1251 | A | C2'-C1' | -13.81 | 1.38 | 1.53 |
| 81 | DA | 183 | G | C2'-C1' | -13.81 | 1.38 | 1.53 |
| 78 | CA | 1210 | C | O4'-C1' | 13.80 | 1.59 | 1.41 |
| 17 | AQ | 82 | ASP | C-O | -13.79 | 0.97 | 1.23 |
| 78 | CA | 435 | C | O4'-C1' | 13.79 | 1.59 | 1.41 |
| 81 | DA | 1483 | G | C2'-C1' | 13.79 | 1.68 | 1.53 |
| 74 | BQ | 129 | TYR | C-O | -13.79 | 0.97 | 1.23 |
| 81 | DA | 671 | U | C4'-C3' | 13.77 | 1.68 | 1.53 |
| 43 | BP | 13 | LYS | C-O | -13.77 | 0.97 | 1.23 |
| 78 | CA | 233 | C | O4'-C1' | 13.76 | 1.59 | 1.41 |
| 5 | AC | 18 | PRO | C-O | -13.76 | 0.95 | 1.23 |
| 81 | DA | 874 | U | C2'-C1' | -13.76 | 1.38 | 1.53 |
| 81 | DA | 2131 | A | O4'-C1' | 13.76 | 1.59 | 1.41 |
| 81 | DA | 548 | G | C2'-C1' | -13.76 | 1.38 | 1.53 |
| 81 | DA | 702 | C | C2'-C1' | -13.75 | 1.38 | 1.53 |
| 81 | DA | 1060 | U | O4'-C1' | 13.75 | 1.59 | 1.41 |
| 81 | DA | 761 | A | O4'-C1' | 13.74 | 1.59 | 1.41 |
| 81 | DA | 2708 | C | C2'-C1' | -13.74 | 1.38 | 1.53 |
| 81 | DA | 1508 | C | O4'-C1' | 13.73 | 1.59 | 1.41 |
| 82 | DB | 148 | G | C2'-C1' | -13.73 | 1.38 | 1.53 |
| 81 | DA | 109 | A | O4'-C1' | 13.73 | 1.59 | 1.41 |
| 78 | CA | 1391 | A | C2'-C1' | -13.73 | 1.38 | 1.53 |
| 81 | DA | 54 | C | C2'-C1' | -13.71 | 1.38 | 1.53 |
| 81 | DA | 2416 | U | C2'-C1' | -13.70 | 1.38 | 1.53 |
| 82 | DB | 106 | C | O4'-C1' | 13.71 | 1.59 | 1.41 |
| 81 | DA | 103 | G | O4'-C1' | 13.70 | 1.59 | 1.41 |
| 5 | AC | 23 | ARG | CZ-NH2 | -13.70 | 1.15 | 1.33 |
| 78 | CA | 1746 | A | O4'-C1' | 13.70 | 1.59 | 1.41 |
| 78 | CA | 1705 | C | O4'-C1' | 13.70 | 1.59 | 1.41 |
| 81 | DA | 1916 | U | C2'-C1' | -13.69 | 1.38 | 1.53 |
| 81 | DA | 1633 | C | C2'-C1' | -13.69 | 1.38 | 1.53 |
| 78 | CA | 269 | G | C2'-C1' | -13.69 | 1.38 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 3022 | G | C2'-C1' | -13.68 | 1.38 | 1.53 |
| 78 | CA | 681 | U | C2'-C1' | 13.68 | 1.68 | 1.53 |
| 78 | CA | 1733 | C | O4'-C1' | 13.67 | 1.59 | 1.41 |
| 78 | CA | 1452 | U | O4'-C1' | 13.67 | 1.59 | 1.41 |
| 81 | DA | 1679 | A | O4'-C1' | 13.67 | 1.59 | 1.41 |
| 78 | CA | 175 | G | C2'-C1' | -13.66 | 1.38 | 1.53 |
| 81 | DA | 274 | G | C2'-C1' | -13.66 | 1.38 | 1.53 |
| 81 | DA | 251 | G | O4'-C1' | 13.66 | 1.59 | 1.41 |
| 81 | DA | 862 | U | C2'-C1' | -13.66 | 1.38 | 1.53 |
| 81 | DA | 624 | G | C2'-C1' | -13.66 | 1.38 | 1.53 |
| 79 | CB | 36 | C | C2'-C1' | -13.66 | 1.38 | 1.53 |
| 81 | DA | 1227 | C | C2'-C1' | -13.65 | 1.38 | 1.53 |
| 82 | DB | 94 | C | O4'-C1' | 13.65 | 1.59 | 1.41 |
| 82 | DB | 102 | U | C2'-C1' | -13.64 | 1.38 | 1.53 |
| 81 | DA | 3244 | A | O4'-C1' | 13.64 | 1.59 | 1.41 |
| 81 | DA | 2657 | A | O4'-C1' | 13.63 | 1.59 | 1.41 |
| 81 | DA | 2710 | C | O4'-C1' | 13.63 | 1.59 | 1.41 |
| 78 | CA | 160 | C | O4'-C1' | 13.62 | 1.59 | 1.41 |
| 78 | CA | 1237 | G | O4'-C1' | 13.62 | 1.59 | 1.41 |
| 81 | DA | 2209 | U | C2'-C1' | -13.62 | 1.38 | 1.53 |
| 78 | CA | 1563 | C | C2'-C1' | -13.61 | 1.38 | 1.53 |
| 81 | DA | 3072 | C | O4'-C1' | 13.61 | 1.59 | 1.41 |
| 74 | BQ | 129 | TYR | N-CA | 13.60 | 1.73 | 1.46 |
| 81 | DA | 1145 | G | C2'-C1' | -13.60 | 1.38 | 1.53 |
| 78 | CA | 1643 | U | C2'-C1' | 13.60 | 1.68 | 1.53 |
| 81 | DA | 1978 | A | C2'-C1' | -13.60 | 1.38 | 1.53 |
| 81 | DA | 580 | C | O4'-C1' | 13.60 | 1.59 | 1.41 |
| 81 | DA | 2711 | C | O4'-C1' | 13.58 | 1.59 | 1.41 |
| 81 | DA | 2665 | U | C2'-C1' | 13.58 | 1.68 | 1.53 |
| 81 | DA | 3391 | A | O4'-C1' | 13.57 | 1.59 | 1.41 |
| 59 | Bh | 20 | HIS | C-O | -13.56 | 0.97 | 1.23 |
| 78 | CA | 1589 | C | O4'-C1' | 13.56 | 1.59 | 1.41 |
| 81 | DA | 2774 | C | C2'-C1' | -13.56 | 1.38 | 1.53 |
| 78 | CA | 1267 | G | C2'-C1' | -13.56 | 1.38 | 1.53 |
| 78 | CA | 68 | A | C2'-C1' | -13.55 | 1.38 | 1.53 |
| 78 | CA | 690 | G | C2'-C1' | -13.55 | 1.38 | 1.53 |
| 81 | DA | 2904 | U | O4'-C1' | 13.54 | 1.59 | 1.41 |
| 78 | CA | 818 | C | O4'-C1' | 13.54 | 1.59 | 1.41 |
| 81 | DA | 2050 | C | O4'-C1' | 13.54 | 1.59 | 1.41 |
| 78 | CA | 662 | U | O4'-C1' | 13.53 | 1.59 | 1.41 |
| 81 | DA | 3146 | G | C2'-C1' | -13.53 | 1.38 | 1.53 |
| 78 | CA | 679 | U | C2'-C1' | 13.52 | 1.68 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 948 | C | O4'-C1' | 13.52 | 1.59 | 1.41 |
| 81 | DA | 1403 | C | O4'-C1' | 13.52 | 1.59 | 1.41 |
| 83 | DC | 113 | C | O4'-C1' | 13.52 | 1.59 | 1.41 |
| 78 | CA | 1625 | C | O4'-C1' | 13.51 | 1.59 | 1.41 |
| 81 | DA | 2475 | G | O4'-C1' | 13.51 | 1.59 | 1.41 |
| 81 | DA | 3299 | A | O4'-C1' | -13.51 | 1.24 | 1.41 |
| 78 | CA | 1569 | A | C2'-C1' | -13.50 | 1.38 | 1.53 |
| 78 | CA | 1478 | G | O4'-C1' | -13.49 | 1.24 | 1.41 |
| 81 | DA | 2118 | C | O4'-C1' | 13.49 | 1.59 | 1.41 |
| 81 | DA | 957 | C | O4'-C1' | 13.49 | 1.59 | 1.41 |
| 81 | DA | 290 | G | C2'-C1' | -13.48 | 1.38 | 1.53 |
| 81 | DA | 1208 | U | C2'-C1' | 13.48 | 1.68 | 1.53 |
| 44 | BO | 73 | LEU | C-N | -13.48 | 1.03 | 1.34 |
| 78 | CA | 597 | G | C2'-C1' | -13.47 | 1.38 | 1.53 |
| 81 | DA | 2520 | A | C2'-C1' | 13.47 | 1.68 | 1.53 |
| 81 | DA | 752 | C | C2'-C1' | -13.47 | 1.38 | 1.53 |
| 81 | DA | 259 | C | O4'-C1' | 13.46 | 1.59 | 1.41 |
| 81 | DA | 1690 | C | C2'-C1' | -13.46 | 1.38 | 1.53 |
| 81 | DA | 2901 | G | C2'-C1' | -13.46 | 1.38 | 1.53 |
| 81 | DA | 2809 | C | C2'-C1' | -13.45 | 1.38 | 1.53 |
| 78 | CA | 1379 | C | O4'-C1' | 13.45 | 1.59 | 1.41 |
| 81 | DA | 2491 | A | O4'-C1' | 13.45 | 1.59 | 1.41 |
| 78 | CA | 434 | G | C2'-C1' | 13.44 | 1.68 | 1.53 |
| 81 | DA | 1040 | A | O4'-C1' | 13.44 | 1.59 | 1.41 |
| 49 | BV | 152 | GLU | C-O | -13.43 | 0.97 | 1.23 |
| 78 | CA | 1120 | U | O4'-C1' | 13.43 | 1.59 | 1.41 |
| 81 | DA | 2646 | C | C2'-C1' | -13.43 | 1.38 | 1.53 |
| 81 | DA | 2462 | A | O4'-C1' | 13.43 | 1.59 | 1.41 |
| 81 | DA | 1869 | C | O4'-C1' | 13.42 | 1.59 | 1.41 |
| 78 | CA | 1007 | C | C2'-C1' | -13.42 | 1.38 | 1.53 |
| 81 | DA | 1332 | A | C2'-C1' | -13.42 | 1.38 | 1.53 |
| 81 | DA | 1496 | C | O4'-C1' | 13.42 | 1.59 | 1.41 |
| 81 | DA | 2295 | A | C2'-C1' | -13.42 | 1.38 | 1.53 |
| 81 | DA | 2700 | G | C2'-C1' | -13.41 | 1.38 | 1.53 |
| 78 | CA | 346 | G | C2'-C1' | -13.41 | 1.38 | 1.53 |
| 78 | CA | 1280 | C | O4'-C1' | 13.40 | 1.59 | 1.41 |
| 81 | DA | 3337 | G | C2'-C1' | -13.40 | 1.38 | 1.53 |
| 81 | DA | 2462 | A | C2'-C1' | -13.40 | 1.38 | 1.53 |
| 78 | CA | 1623 | C | O4'-C1' | 13.39 | 1.59 | 1.41 |
| 81 | DA | 1660 | C | O4'-C1' | 13.39 | 1.59 | 1.41 |
| 81 | DA | 1660 | C | C2'-C1' | -13.39 | 1.38 | 1.53 |
| 81 | DA | 3082 | C | O4'-C1' | 13.39 | 1.59 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1358 | C | O4'-C1' | 13.39 | 1.59 | 1.41 |
| 81 | DA | 1426 | C | O3'-P | -13.38 | 1.45 | 1.61 |
| 81 | DA | 3298 | C | C2'-C1' | -13.38 | 1.38 | 1.53 |
| 81 | DA | 1664 | G | C2'-C1' | -13.38 | 1.38 | 1.53 |
| 33 | BD | 296 | GLN | N-CA | 13.37 | 1.73 | 1.46 |
| 81 | DA | 3285 | C | C2'-C1' | -13.37 | 1.38 | 1.53 |
| 81 | DA | 2146 | C | O4'-C1' | 13.37 | 1.59 | 1.41 |
| 81 | DA | 3256 | G | C2'-C1' | -13.36 | 1.38 | 1.53 |
| 81 | DA | 2874 | G | C2'-C1' | -13.36 | 1.38 | 1.53 |
| 81 | DA | 1551 | C | C2'-C1' | -13.36 | 1.38 | 1.53 |
| 78 | CA | 1677 | C | O4'-C1' | 13.36 | 1.59 | 1.41 |
| 81 | DA | 1624 | G | O4'-C1' | 13.35 | 1.59 | 1.41 |
| 81 | DA | 454 | C | O4'-C1' | 13.35 | 1.59 | 1.41 |
| 81 | DA | 1015 | U | C2'-C1' | 13.35 | 1.68 | 1.53 |
| 78 | CA | 1374 | C | O4'-C1' | 13.35 | 1.58 | 1.41 |
| 78 | CA | 32 | U | C2'-C1' | 13.34 | 1.68 | 1.53 |
| 78 | CA | 164 | A | C2'-C1' | -13.34 | 1.38 | 1.53 |
| 78 | CA | 617 | U | O4'-C1' | 13.33 | 1.58 | 1.41 |
| 81 | DA | 405 | U | C2'-C1' | -13.33 | 1.38 | 1.53 |
| 81 | DA | 2755 | C | O4'-C1' | 13.33 | 1.58 | 1.41 |
| 81 | DA | 2881 | C | O4'-C1' | 13.32 | 1.58 | 1.41 |
| 81 | DA | 360 | G | C2'-C1' | -13.32 | 1.38 | 1.53 |
| 81 | DA | 1916 | U | O4'-C1' | 13.32 | 1.58 | 1.41 |
| 81 | DA | 1085 | A | C2'-C1' | -13.32 | 1.38 | 1.53 |
| 81 | DA | 175 | C | O4'-C1' | 13.32 | 1.58 | 1.41 |
| 81 | DA | 3018 | C | C2'-C1' | -13.31 | 1.38 | 1.53 |
| 78 | CA | 1436 | A | O4'-C1' | 13.31 | 1.58 | 1.41 |
| 80 | CC | 17 | A | O4'-C1' | 13.31 | 1.58 | 1.41 |
| 81 | DA | 2763 | U | C2'-C1' | 13.31 | 1.68 | 1.53 |
| 81 | DA | 1221 | A | C2'-C1' | 13.30 | 1.68 | 1.53 |
| 81 | DA | 1689 | U | O4'-C1' | -13.30 | 1.24 | 1.41 |
| 81 | DA | 3371 | G | C2'-C1' | -13.30 | 1.38 | 1.53 |
| 78 | CA | 1610 | G | C2'-C1' | -13.28 | 1.38 | 1.53 |
| 81 | DA | 1139 | G | C2'-C1' | -13.28 | 1.38 | 1.53 |
| 78 | CA | 1702 | A | O4'-C1' | -13.27 | 1.24 | 1.41 |
| 81 | DA | 1525 | G | O4'-C1' | 13.27 | 1.58 | 1.41 |
| 81 | DA | 15 | C | O4'-C1' | 13.26 | 1.58 | 1.41 |
| 81 | DA | 566 | G | C2'-C1' | -13.26 | 1.38 | 1.53 |
| 78 | CA | 181 | A | O4'-C1' | 13.25 | 1.58 | 1.41 |
| 78 | CA | 1564 | U | C2'-C1' | -13.25 | 1.38 | 1.53 |
| 78 | CA | 338 | C | O4'-C1' | 13.25 | 1.58 | 1.41 |
| 79 | CB | 64 | G | C2'-C1' | -13.24 | 1.38 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 361 | C | O4'-C1' | 13.24 | 1.58 | 1.41 |
| 81 | DA | 556 | U | C2'-C1' | -13.24 | 1.38 | 1.53 |
| 81 | DA | 973 | A | C2'-C1' | -13.24 | 1.38 | 1.53 |
| 81 | DA | 1847 | A | C2'-C1' | 13.24 | 1.68 | 1.53 |
| 78 | CA | 138 | A | O4'-C1' | -13.23 | 1.24 | 1.41 |
| 81 | DA | 863 | C | O4'-C1' | 13.22 | 1.58 | 1.41 |
| 82 | DB | 118 | C | O4'-C1' | 13.21 | 1.58 | 1.41 |
| 78 | CA | 1478 | G | P-O5' | -13.21 | 1.46 | 1.59 |
| 33 | BD | 349 | THR | C-O | -13.20 | 0.98 | 1.23 |
| 81 | DA | 1870 | C | C3'-O3' | 13.20 | 1.60 | 1.42 |
| 81 | DA | 2337 | C | O4'-C1' | 13.20 | 1.58 | 1.41 |
| 78 | CA | 830 | U | O4'-C1' | 13.19 | 1.58 | 1.41 |
| 82 | DB | 59 | A | C2'-C1' | -13.19 | 1.38 | 1.53 |
| 81 | DA | 1199 | C | C2'-C1' | -13.19 | 1.38 | 1.53 |
| 34 | BE | 89 | TYR | CA-CB | 13.19 | 1.82 | 1.53 |
| 78 | CA | 1627 | U | O4'-C1' | 13.18 | 1.58 | 1.41 |
| 81 | DA | 513 | G | C2'-C1' | -13.18 | 1.38 | 1.53 |
| 81 | DA | 2798 | C | O4'-C1' | 13.18 | 1.58 | 1.41 |
| 78 | CA | 606 | A | C2'-C1' | -13.18 | 1.38 | 1.53 |
| 81 | DA | 419 | G | O4'-C1' | -13.18 | 1.24 | 1.41 |
| 81 | DA | 3236 | U | O4'-C1' | 13.18 | 1.58 | 1.41 |
| 81 | DA | 2031 | U | C2'-C1' | -13.18 | 1.38 | 1.53 |
| 81 | DA | 2821 | C | O4'-C1' | 13.18 | 1.58 | 1.41 |
| 83 | DC | 67 | C | O4'-C1' | 13.17 | 1.58 | 1.41 |
| 78 | CA | 632 | U | O4'-C1' | 13.16 | 1.58 | 1.41 |
| 78 | CA | 1721 | A | O4'-C1' | 13.16 | 1.58 | 1.41 |
| 81 | DA | 1572 | U | C2'-C1' | -13.16 | 1.38 | 1.53 |
| 81 | DA | 968 | G | C2'-C1' | -13.16 | 1.38 | 1.53 |
| 81 | DA | 1679 | A | C2'-C1' | -13.16 | 1.38 | 1.53 |
| 81 | DA | 1917 | C | O4'-C1' | 13.16 | 1.58 | 1.41 |
| 81 | DA | 2616 | C | O4'-C1' | 13.15 | 1.58 | 1.41 |
| 78 | CA | 623 | A | C2'-C1' | 13.14 | 1.67 | 1.53 |
| 78 | CA | 1348 | A | O4'-C1' | 13.13 | 1.58 | 1.41 |
| 81 | DA | 2638 | C | C2'-C1' | -13.13 | 1.39 | 1.53 |
| 81 | DA | 526 | C | C2'-C1' | -13.11 | 1.39 | 1.53 |
| 78 | CA | 956 | C | O4'-C1' | 13.11 | 1.58 | 1.41 |
| 74 | BQ | 111 | GLN | C-O | -13.11 | 0.98 | 1.23 |
| 79 | CB | 43 | C | C2'-C1' | -13.11 | 1.39 | 1.53 |
| 81 | DA | 180 | C | C2'-C1' | -13.11 | 1.39 | 1.53 |
| 81 | DA | 260 | C | O4'-C1' | 13.11 | 1.58 | 1.41 |
| 82 | DB | 113 | U | C2'-C1' | -13.10 | 1.39 | 1.53 |
| 81 | DA | 2008 | G | C2'-C1' | -13.10 | 1.39 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 317 | A | O4'-C1' | 13.09 | 1.58 | 1.41 |
| 81 | DA | 881 | C | O4'-C1' | 13.09 | 1.58 | 1.41 |
| 81 | DA | 2439 | A | C2'-C1' | -13.09 | 1.39 | 1.53 |
| 81 | DA | 3295 | A | C2'-C1' | -13.09 | 1.39 | 1.53 |
| 82 | DB | 98 | U | P-O5' | -13.09 | 1.46 | 1.59 |
| 81 | DA | 2130 | G | C2'-C1' | 13.08 | 1.67 | 1.53 |
| 81 | DA | 1976 | G | O4'-C1' | -13.08 | 1.24 | 1.41 |
| 81 | DA | 3393 | U | C2'-C1' | -13.07 | 1.39 | 1.53 |
| 81 | DA | 113 | C | O4'-C1' | 13.06 | 1.58 | 1.41 |
| 82 | DB | 56 | G | O4'-C1' | 13.06 | 1.58 | 1.41 |
| 81 | DA | 2136 | C | O4'-C1' | 13.05 | 1.58 | 1.41 |
| 81 | DA | 2864 | A | C2'-C1' | -13.05 | 1.39 | 1.53 |
| 81 | DA | 726 | G | C2'-C1' | -13.05 | 1.39 | 1.53 |
| 81 | DA | 962 | A | C2'-C1' | 13.04 | 1.67 | 1.53 |
| 81 | DA | 419 | G | C2'-C1' | 13.04 | 1.67 | 1.53 |
| 78 | CA | 291 | G | C2'-C1' | -13.04 | 1.39 | 1.53 |
| 81 | DA | 2801 | A | O4'-C1' | -13.04 | 1.24 | 1.41 |
| 81 | DA | 1192 | C | O4'-C1' | 13.03 | 1.58 | 1.41 |
| 81 | DA | 1649 | U | C2'-C1' | 13.03 | 1.67 | 1.53 |
| 81 | DA | 775 | A | C2'-C1' | -13.03 | 1.39 | 1.53 |
| 78 | CA | 583 | C | O4'-C1' | 13.02 | 1.58 | 1.41 |
| 81 | DA | 3303 | G | C2'-C1' | -13.01 | 1.39 | 1.53 |
| 82 | DB | 38 | U | O4'-C1' | 13.01 | 1.58 | 1.41 |
| 81 | DA | 571 | U | C2'-C1' | -13.01 | 1.39 | 1.53 |
| 81 | DA | 2857 | C | O4'-C1' | 13.01 | 1.58 | 1.41 |
| 81 | DA | 3312 | U | O4'-C1' | 13.01 | 1.58 | 1.41 |
| 78 | CA | 276 | C | O4'-C1' | 13.00 | 1.58 | 1.41 |
| 81 | DA | 1069 | C | O4'-C1' | 13.00 | 1.58 | 1.41 |
| 6 | AE | 92 | ALA | CA-CB | 12.99 | 1.79 | 1.52 |
| 34 | BE | 52 | TYR | CB-CG | 12.99 | 1.71 | 1.51 |
| 81 | DA | 1078 | U | C2'-C1' | 12.99 | 1.67 | 1.53 |
| 81 | DA | 2072 | G | O4'-C1' | -12.97 | 1.24 | 1.41 |
| 81 | DA | 2608 | G | C2'-C1' | -12.97 | 1.39 | 1.53 |
| 81 | DA | 1991 | G | O4'-C1' | -12.97 | 1.24 | 1.41 |
| 81 | DA | 93 | C | O4'-C1' | 12.97 | 1.58 | 1.41 |
| 81 | DA | 2594 | C | C2'-C1' | -12.96 | 1.39 | 1.53 |
| 78 | CA | 51 | A | O4'-C1' | 12.95 | 1.58 | 1.41 |
| 81 | DA | 949 | C | O4'-C1' | 12.95 | 1.58 | 1.41 |
| 78 | CA | 143 | G | C2'-C1' | -12.95 | 1.39 | 1.53 |
| 81 | DA | 261 | U | C2'-C1' | -12.95 | 1.39 | 1.53 |
| 81 | DA | 1940 | G | O4'-C1' | 12.95 | 1.58 | 1.41 |
| 78 | CA | 61 | A | O4'-C1' | 12.94 | 1.58 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 326 | G | C4'-C3' | -12.94 | 1.39 | 1.53 |
| 81 | DA | 2236 | G | C2'-C1' | -12.94 | 1.39 | 1.53 |
| 78 | CA | 922 | G | C2'-C1' | -12.94 | 1.39 | 1.53 |
| 78 | CA | 980 | G | C2'-C1' | -12.93 | 1.39 | 1.53 |
| 81 | DA | 2035 | G | C2'-C1' | -12.93 | 1.39 | 1.53 |
| 82 | DB | 9 | A | C2'-C1' | -12.92 | 1.39 | 1.53 |
| 78 | CA | 1606 | C | O4'-C1' | 12.92 | 1.58 | 1.41 |
| 81 | DA | 220 | G | O4'-C1' | -12.91 | 1.24 | 1.41 |
| 82 | DB | 117 | C | O4'-C1' | 12.91 | 1.58 | 1.41 |
| 81 | DA | 808 | A | C2'-C1' | -12.91 | 1.39 | 1.53 |
| 78 | CA | 99 | C | O4'-C1' | 12.90 | 1.58 | 1.41 |
| 81 | DA | 2496 | C | O4'-C1' | 12.90 | 1.58 | 1.41 |
| 82 | DB | 95 | G | O4'-C1' | 12.90 | 1.58 | 1.41 |
| 78 | CA | 826 | U | O4'-C1' | 12.90 | 1.58 | 1.41 |
| 81 | DA | 3326 | G | O4'-C1' | 12.89 | 1.58 | 1.41 |
| 81 | DA | 2272 | G | O4'-C1' | -12.88 | 1.25 | 1.41 |
| 81 | DA | 1191 | U | O4'-C1' | 12.88 | 1.58 | 1.41 |
| 83 | DC | 103 | U | O4'-C1' | 12.87 | 1.58 | 1.41 |
| 81 | DA | 435 | C | O4'-C1' | 12.87 | 1.58 | 1.41 |
| 81 | DA | 3063 | C | C2'-C1' | -12.87 | 1.39 | 1.53 |
| 78 | CA | 268 | C | O4'-C1' | 12.86 | 1.58 | 1.41 |
| 81 | DA | 2858 | U | C2'-C1' | -12.86 | 1.39 | 1.53 |
| 78 | CA | 1048 | G | C2'-C1' | -12.86 | 1.39 | 1.53 |
| 81 | DA | 1839 | A | C2'-C1' | -12.85 | 1.39 | 1.53 |
| 78 | CA | 890 | C | C2'-C1' | -12.85 | 1.39 | 1.53 |
| 81 | DA | 2417 | U | C2'-C1' | -12.85 | 1.39 | 1.53 |
| 81 | DA | 3096 | C | O4'-C1' | 12.85 | 1.58 | 1.41 |
| 81 | DA | 3229 | G | C2'-C1' | -12.84 | 1.39 | 1.53 |
| 78 | CA | 1282 | U | O4'-C1' | 12.84 | 1.58 | 1.41 |
| 81 | DA | 1827 | C | O4'-C1' | 12.84 | 1.58 | 1.41 |
| 78 | CA | 1632 | C | O4'-C1' | 12.83 | 1.58 | 1.41 |
| 78 | CA | 196 | G | O4'-C1' | 12.83 | 1.58 | 1.41 |
| 81 | DA | 648 | C | O4'-C1' | 12.83 | 1.58 | 1.41 |
| 81 | DA | 845 | G | O4'-C1' | -12.83 | 1.25 | 1.41 |
| 81 | DA | 3223 | A | C2'-C1' | -12.82 | 1.39 | 1.53 |
| 81 | DA | 2825 | C | O4'-C1' | 12.82 | 1.58 | 1.41 |
| 81 | DA | 558 | U | C2'-C1' | -12.81 | 1.39 | 1.53 |
| 81 | DA | 2720 | G | C2'-C1' | -12.80 | 1.39 | 1.53 |
| 78 | CA | 1549 | C | O4'-C1' | 12.80 | 1.58 | 1.41 |
| 81 | DA | 1701 | C | O4'-C1' | 12.80 | 1.58 | 1.41 |
| 81 | DA | 2893 | C | O4'-C1' | 12.80 | 1.58 | 1.41 |
| 78 | CA | 179 | A | C2'-C1' | 12.79 | 1.67 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 851 | C | O4'-C1' | 12.79 | 1.58 | 1.41 |
| 81 | DA | 1414 | G | C2'-C1' | 12.79 | 1.67 | 1.53 |
| 78 | CA | 1787 | C | O4'-C1' | 12.79 | 1.58 | 1.41 |
| 79 | CB | 23 | A | C2'-C1' | -12.79 | 1.39 | 1.53 |
| 61 | Bj | 66 | VAL | CB-CG2 | 12.78 | 1.79 | 1.52 |
| 81 | DA | 799 | G | C2'-C1' | -12.78 | 1.39 | 1.53 |
| 81 | DA | 1340 | G | C2'-C1' | -12.78 | 1.39 | 1.53 |
| 81 | DA | 1832 | C | C2'-C1' | -12.78 | 1.39 | 1.53 |
| 81 | DA | 1897 | G | C2'-C1' | -12.78 | 1.39 | 1.53 |
| 78 | CA | 449 | C | O4'-C1' | 12.78 | 1.58 | 1.41 |
| 81 | DA | 2681 | U | O4'-C1' | 12.77 | 1.58 | 1.41 |
| 78 | CA | 1034 | C | O4'-C1' | 12.77 | 1.58 | 1.41 |
| 81 | DA | 3148 | U | O4'-C1' | 12.77 | 1.58 | 1.41 |
| 81 | DA | 1592 | G | C2'-C1' | -12.77 | 1.39 | 1.53 |
| 81 | DA | 3052 | G | O4'-C1' | 12.77 | 1.58 | 1.41 |
| 81 | DA | 2118 | C | C2'-C1' | -12.77 | 1.39 | 1.53 |
| 51 | BZ | 60 | LYS | C-O | -12.76 | 0.99 | 1.23 |
| 78 | CA | 190 | C | O4'-C1' | 12.75 | 1.58 | 1.41 |
| 78 | CA | 877 | G | C2'-C1' | -12.73 | 1.39 | 1.53 |
| 79 | CB | 75 | A | C2'-C1' | 12.73 | 1.67 | 1.53 |
| 37 | BH | 129 | PRO | N-CD | 12.73 | 1.65 | 1.47 |
| 81 | DA | 535 | G | C2'-C1' | -12.73 | 1.39 | 1.53 |
| 81 | DA | 2059 | U | O4'-C1' | 12.73 | 1.58 | 1.41 |
| 81 | DA | 887 | G | C2'-C1' | -12.72 | 1.39 | 1.53 |
| 83 | DC | 117 | C | O4'-C1' | 12.72 | 1.58 | 1.41 |
| 81 | DA | 2466 | G | C2'-C1' | -12.72 | 1.39 | 1.53 |
| 81 | DA | 847 | A | C2'-C1' | -12.72 | 1.39 | 1.53 |
| 81 | DA | 1049 | C | O4'-C1' | 12.72 | 1.58 | 1.41 |
| 78 | CA | 110 | U | O4'-C1' | 12.71 | 1.58 | 1.41 |
| 81 | DA | 900 | G | C2'-C1' | -12.71 | 1.39 | 1.53 |
| 81 | DA | 1791 | C | C2'-C1' | -12.71 | 1.39 | 1.53 |
| 81 | DA | 959 | C | C2'-C1' | -12.69 | 1.39 | 1.53 |
| 29 | AU | 70 | VAL | CB-CG1 | 12.69 | 1.79 | 1.52 |
| 81 | DA | 1059 | G | O4'-C1' | 12.69 | 1.58 | 1.41 |
| 81 | DA | 1086 | C | O4'-C1' | 12.69 | 1.58 | 1.41 |
| 78 | CA | 1148 | C | O4'-C1' | 12.69 | 1.58 | 1.41 |
| 81 | DA | 1870 | C | C3'-C2' | -12.68 | 1.38 | 1.52 |
| 81 | DA | 2648 | G | O4'-C1' | -12.68 | 1.25 | 1.41 |
| 78 | CA | 457 | G | C2'-C1' | -12.68 | 1.39 | 1.53 |
| 82 | DB | 119 | C | O4'-C1' | 12.68 | 1.58 | 1.41 |
| 81 | DA | 1017 | C | O4'-C1' | 12.68 | 1.58 | 1.41 |
| 81 | DA | 2277 | C | O4'-C1' | 12.68 | 1.58 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2726 | C | O4'-C1' | 12.67 | 1.58 | 1.41 |
| 81 | DA | 1650 | G | C2'-C1' | -12.66 | 1.39 | 1.53 |
| 81 | DA | 1209 | G | O4'-C1' | -12.65 | 1.25 | 1.41 |
| 81 | DA | 2032 | U | C2'-C1' | -12.65 | 1.39 | 1.53 |
| 78 | CA | 872 | G | C2'-C1' | -12.65 | 1.39 | 1.53 |
| 81 | DA | 3048 | A | O4'-C1' | 12.65 | 1.58 | 1.41 |
| 83 | DC | 114 | A | C2'-C1' | -12.65 | 1.39 | 1.53 |
| 78 | CA | 1149 | G | O4'-C1' | 12.64 | 1.58 | 1.41 |
| 81 | DA | 496 | C | O4'-C1' | 12.64 | 1.58 | 1.41 |
| 81 | DA | 751 | A | O4'-C1' | 12.64 | 1.58 | 1.41 |
| 78 | CA | 1164 | G | O4'-C1' | -12.64 | 1.25 | 1.41 |
| 81 | DA | 1827 | C | C2'-C1' | -12.63 | 1.39 | 1.53 |
| 79 | CB | 61 | C | O4'-C1' | 12.62 | 1.58 | 1.41 |
| 78 | CA | 368 | U | O4'-C1' | 12.61 | 1.58 | 1.41 |
| 78 | CA | 913 | G | C2'-C1' | -12.61 | 1.39 | 1.53 |
| 79 | CB | 41 | G | O4'-C1' | 12.61 | 1.58 | 1.41 |
| 81 | DA | 1201 | C | O4'-C1' | 12.61 | 1.58 | 1.41 |
| 78 | CA | 834 | G | O4'-C1' | 12.60 | 1.58 | 1.41 |
| 83 | DC | 54 | A | C2'-C1' | -12.60 | 1.39 | 1.53 |
| 82 | DB | 130 | C | O4'-C1' | 12.60 | 1.58 | 1.41 |
| 81 | DA | 63 | A | O4'-C1' | -12.58 | 1.25 | 1.41 |
| 79 | CB | 43 | C | O4'-C1' | 12.58 | 1.58 | 1.41 |
| 81 | DA | 482 | C | O4'-C1' | 12.58 | 1.57 | 1.41 |
| 81 | DA | 2296 | A | C2'-C1' | 12.57 | 1.67 | 1.53 |
| 81 | DA | 580 | C | C2'-C1' | -12.57 | 1.39 | 1.53 |
| 81 | DA | 3089 | C | C2'-C1' | -12.57 | 1.39 | 1.53 |
| 39 | BJ | 75 | PRO | C-O | -12.56 | 0.98 | 1.23 |
| 81 | DA | 2972 | G | C2'-C1' | -12.56 | 1.39 | 1.53 |
| 81 | DA | 1335 | C | O4'-C1' | 12.56 | 1.57 | 1.41 |
| 81 | DA | 457 | C | O4'-C1' | 12.54 | 1.57 | 1.41 |
| 34 | BE | 9 | MET | C-O | -12.54 | 0.99 | 1.23 |
| 81 | DA | 634 | C | O4'-C1' | 12.54 | 1.57 | 1.41 |
| 78 | CA | 308 | C | O4'-C1' | 12.54 | 1.57 | 1.41 |
| 81 | DA | 1334 | U | O4'-C1' | 12.54 | 1.57 | 1.41 |
| 81 | DA | 3108 | G | C2'-C1' | -12.54 | 1.39 | 1.53 |
| 81 | DA | 684 | G | O4'-C1' | 12.53 | 1.57 | 1.41 |
| 78 | CA | 443 | C | O4'-C1' | 12.53 | 1.57 | 1.41 |
| 81 | DA | 3335 | A | C2'-C1' | -12.52 | 1.39 | 1.53 |
| 83 | DC | 46 | A | O3'-P | -12.52 | 1.46 | 1.61 |
| 81 | DA | 808 | A | O4'-C1' | 12.52 | 1.57 | 1.41 |
| 81 | DA | 21 | G | O4'-C1' | -12.52 | 1.25 | 1.41 |
| 81 | DA | 2918 | G | C2'-C1' | -12.51 | 1.39 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2018 | C | O4'-C1' | 12.51 | 1.57 | 1.41 |
| 81 | DA | 3347 | A | O4'-C1' | 12.50 | 1.57 | 1.41 |
| 82 | DB | 100 | U | C2'-C1' | -12.50 | 1.39 | 1.53 |
| 81 | DA | 1140 | G | C2'-C1' | -12.50 | 1.39 | 1.53 |
| 81 | DA | 436 | A | C2'-C1' | -12.50 | 1.39 | 1.53 |
| 81 | DA | 1328 | C | C2'-C1' | -12.49 | 1.39 | 1.53 |
| 81 | DA | 1038 | C | O4'-C1' | 12.49 | 1.57 | 1.41 |
| 78 | CA | 979 | A | O4'-C1' | 12.48 | 1.57 | 1.41 |
| 81 | DA | 2459 | A | C2'-C1' | -12.48 | 1.39 | 1.53 |
| 78 | CA | 549 | G | C2'-C1' | -12.48 | 1.39 | 1.53 |
| 81 | DA | 2876 | C | O4'-C1' | 12.48 | 1.57 | 1.41 |
| 83 | DC | 102 | C | C2'-C1' | -12.48 | 1.39 | 1.53 |
| 81 | DA | 1405 | U | C2'-C1' | -12.47 | 1.39 | 1.53 |
| 78 | CA | 1571 | C | C2'-C1' | -12.47 | 1.39 | 1.53 |
| 81 | DA | 699 | A | C2'-C1' | 12.47 | 1.67 | 1.53 |
| 81 | DA | 337 | G | C2'-C1' | 12.47 | 1.67 | 1.53 |
| 81 | DA | 1681 | U | O4'-C1' | 12.47 | 1.57 | 1.41 |
| 78 | CA | 317 | C | O4'-C1' | 12.46 | 1.57 | 1.41 |
| 81 | DA | 2257 | C | O4'-C1' | -12.46 | 1.25 | 1.41 |
| 81 | DA | 406 | G | O4'-C1' | -12.46 | 1.25 | 1.41 |
| 81 | DA | 1203 | A | O4'-C1' | 12.46 | 1.57 | 1.41 |
| 81 | DA | 2506 | U | C2'-C1' | -12.46 | 1.39 | 1.53 |
| 83 | DC | 20 | A | C2'-C1' | -12.46 | 1.39 | 1.53 |
| 81 | DA | 2067 | U | C2'-C1' | 12.46 | 1.67 | 1.53 |
| 81 | DA | 3028 | G | C2'-C1' | -12.46 | 1.39 | 1.53 |
| 83 | DC | 47 | C | O3'-P | -12.45 | 1.46 | 1.61 |
| 78 | CA | 406 | U | C2'-C1' | -12.45 | 1.39 | 1.53 |
| 81 | DA | 512 | U | C2'-C1' | -12.45 | 1.39 | 1.53 |
| 78 | CA | 851 | U | C2'-C1' | -12.45 | 1.39 | 1.53 |
| 81 | DA | 283 | G | C2'-C1' | -12.43 | 1.39 | 1.53 |
| 81 | DA | 1336 | U | C2'-C1' | -12.43 | 1.39 | 1.53 |
| 81 | DA | 3242 | G | C2'-C1' | 12.43 | 1.67 | 1.53 |
| 81 | DA | 3257 | C | O4'-C1' | 12.42 | 1.57 | 1.41 |
| 82 | DB | 105 | A | O4'-C1' | 12.42 | 1.57 | 1.41 |
| 60 | Bi | 79 | SER | N-CA | 12.42 | 1.71 | 1.46 |
| 81 | DA | 1306 | G | O4'-C1' | 12.42 | 1.57 | 1.41 |
| 81 | DA | 1667 | A | O4'-C1' | 12.41 | 1.57 | 1.41 |
| 78 | CA | 107 | C | O4'-C1' | 12.41 | 1.57 | 1.41 |
| 81 | DA | 2139 | A | C2'-C1' | -12.40 | 1.39 | 1.53 |
| 81 | DA | 1204 | A | C2'-C1' | -12.40 | 1.39 | 1.53 |
| 83 | DC | 11 | A | C2'-C1' | -12.40 | 1.39 | 1.53 |
| 81 | DA | 350 | C | O4'-C1' | 12.40 | 1.57 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1446 | A | C2'-C1' | 12.40 | 1.67 | 1.53 |
| 81 | DA | 360 | G | O4'-C1' | 12.39 | 1.57 | 1.41 |
| 78 | CA | 1476 | C | O4'-C1' | 12.38 | 1.57 | 1.41 |
| 83 | DC | 13 | A | O4'-C1' | 12.38 | 1.57 | 1.41 |
| 74 | BQ | 158 | ARG | NE-CZ | 12.38 | 1.49 | 1.33 |
| 78 | CA | 386 | G | O4'-C1' | 12.38 | 1.57 | 1.41 |
| 78 | CA | 1455 | G | C2'-C1' | -12.38 | 1.39 | 1.53 |
| 81 | DA | 3084 | C | O4'-C1' | 12.37 | 1.57 | 1.41 |
| 81 | DA | 1653 | G | O4'-C1' | 12.37 | 1.57 | 1.41 |
| 81 | DA | 756 | U | O4'-C1' | 12.36 | 1.57 | 1.41 |
| 81 | DA | 2594 | C | O4'-C1' | 12.36 | 1.57 | 1.41 |
| 32 | BC | 381 | GLY | N-CA | 12.35 | 1.64 | 1.46 |
| 81 | DA | 1364 | C | O4'-C1' | 12.35 | 1.57 | 1.41 |
| 81 | DA | 2519 | A | C2'-C1' | -12.35 | 1.39 | 1.53 |
| 78 | CA | 430 | G | C2'-C1' | -12.35 | 1.39 | 1.53 |
| 81 | DA | 1712 | G | C2'-C1' | -12.35 | 1.39 | 1.53 |
| 81 | DA | 2486 | A | C2'-C1' | -12.33 | 1.39 | 1.53 |
| 83 | DC | 43 | U | C2'-C1' | -12.33 | 1.39 | 1.53 |
| 78 | CA | 1180 | C | C2'-C1' | -12.32 | 1.39 | 1.53 |
| 81 | DA | 1077 | U | O4'-C1' | 12.32 | 1.57 | 1.41 |
| 78 | CA | 230 | C | O4'-C1' | 12.32 | 1.57 | 1.41 |
| 78 | CA | 1759 | C | C2'-C1' | -12.32 | 1.39 | 1.53 |
| 81 | DA | 384 | A | O4'-C1' | 12.32 | 1.57 | 1.41 |
| 81 | DA | 2582 | C | O4'-C1' | 12.32 | 1.57 | 1.41 |
| 81 | DA | 3162 | C | O4'-C1' | 12.32 | 1.57 | 1.41 |
| 81 | DA | 1478 | C | C2'-C1' | -12.31 | 1.39 | 1.53 |
| 78 | CA | 849 | C | C2'-C1' | -12.31 | 1.39 | 1.53 |
| 81 | DA | 3388 | C | O4'-C1' | 12.31 | 1.57 | 1.41 |
| 78 | CA | 97 | C | O4'-C1' | 12.30 | 1.57 | 1.41 |
| 78 | CA | 1573 | A | C2'-C1' | 12.30 | 1.66 | 1.53 |
| 81 | DA | 1951 | C | O4'-C1' | 12.30 | 1.57 | 1.41 |
| 81 | DA | 2445 | A | O4'-C1' | 12.30 | 1.57 | 1.41 |
| 15 | AN | 54 | LYS | N-CA | 12.29 | 1.71 | 1.46 |
| 81 | DA | 286 | U | O4'-C1' | 12.30 | 1.57 | 1.41 |
| 81 | DA | 105 | C | O4'-C1' | 12.29 | 1.57 | 1.41 |
| 81 | DA | 863 | C | C2'-C1' | -12.29 | 1.39 | 1.53 |
| 81 | DA | 3076 | C | O4'-C1' | 12.29 | 1.57 | 1.41 |
| 78 | CA | 1340 | U | C2'-C1' | 12.28 | 1.66 | 1.53 |
| 81 | DA | 878 | G | C2'-C1' | -12.28 | 1.39 | 1.53 |
| 81 | DA | 724 | U | O4'-C1' | 12.27 | 1.57 | 1.41 |
| 81 | DA | 3248 | C | O4'-C1' | 12.27 | 1.57 | 1.41 |
| 81 | DA | 2420 | C | C2'-C1' | -12.26 | 1.39 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2656 | A | C2'-C1' | -12.26 | 1.39 | 1.53 |
| 82 | DB | 128 | U | O4'-C1' | 12.26 | 1.57 | 1.41 |
| 81 | DA | 2217 | U | C2'-C1' | -12.26 | 1.39 | 1.53 |
| 81 | DA | 2764 | C | O4'-C1' | 12.25 | 1.57 | 1.41 |
| 82 | DB | 41 | A | C2'-C1' | -12.25 | 1.39 | 1.53 |
| 81 | DA | 1455 | U | O4'-C1' | -12.24 | 1.25 | 1.41 |
| 81 | DA | 1117 | G | C2'-C1' | -12.23 | 1.39 | 1.53 |
| 81 | DA | 3093 | C | O4'-C1' | 12.23 | 1.57 | 1.41 |
| 81 | DA | 1433 | A | O4'-C1' | 12.23 | 1.57 | 1.41 |
| 4 | AD | 96 | ASN | C-O | -12.22 | 1.00 | 1.23 |
| 78 | CA | 1586 | A | C3'-C2' | -12.22 | 1.39 | 1.52 |
| 81 | DA | 1623 | G | O4'-C1' | 12.22 | 1.57 | 1.41 |
| 81 | DA | 1196 | C | O4'-C1' | 12.21 | 1.57 | 1.41 |
| 78 | CA | 872 | G | O4'-C1' | 12.21 | 1.57 | 1.41 |
| 81 | DA | 2204 | C | O4'-C1' | 12.21 | 1.57 | 1.41 |
| 81 | DA | 1423 | C | O4'-C1' | 12.21 | 1.57 | 1.41 |
| 81 | DA | 2242 | A | O4'-C1' | 12.20 | 1.57 | 1.41 |
| 81 | DA | 1251 | A | O4'-C1' | 12.20 | 1.57 | 1.41 |
| 81 | DA | 2626 | A | C2'-C1' | -12.20 | 1.40 | 1.53 |
| 81 | DA | 3111 | U | C2'-C1' | 12.20 | 1.66 | 1.53 |
| 13 | AL | 135 | LEU | N-CA | 12.19 | 1.70 | 1.46 |
| 81 | DA | 2708 | C | O4'-C1' | 12.19 | 1.57 | 1.41 |
| 81 | DA | 2774 | C | O4'-C1' | 12.18 | 1.57 | 1.41 |
| 81 | DA | 760 | G | C2'-C1' | -12.18 | 1.40 | 1.53 |
| 78 | CA | 573 | C | O4'-C1' | 12.18 | 1.57 | 1.41 |
| 78 | CA | 326 | G | C2'-C1' | -12.16 | 1.40 | 1.53 |
| 81 | DA | 2437 | G | C2'-C1' | 12.16 | 1.66 | 1.53 |
| 78 | CA | 146 | U | C2'-C1' | -12.15 | 1.40 | 1.53 |
| 57 | Be | 132 | PRO | C-O | -12.14 | 0.98 | 1.23 |
| 78 | CA | 162 | A | O4'-C1' | 12.14 | 1.57 | 1.41 |
| 81 | DA | 562 | C | C2'-C1' | -12.14 | 1.40 | 1.53 |
| 81 | DA | 2619 | G | O4'-C1' | 12.13 | 1.57 | 1.41 |
| 81 | DA | 1193 | A | C2'-C1' | 12.12 | 1.66 | 1.53 |
| 81 | DA | 333 | G | C2'-C1' | -12.12 | 1.40 | 1.53 |
| 78 | CA | 651 | G | O4'-C1' | 12.12 | 1.57 | 1.41 |
| 41 | BN | 108 | ARG | CD-NE | 12.12 | 1.67 | 1.46 |
| 81 | DA | 1 | G | C2'-C1' | 12.11 | 1.66 | 1.53 |
| 81 | DA | 912 | G | C2'-C1' | -12.11 | 1.40 | 1.53 |
| 81 | DA | 2094 | C | O4'-C1' | 12.11 | 1.57 | 1.41 |
| 82 | DB | 37 | A | C2'-C1' | 12.11 | 1.66 | 1.53 |
| 81 | DA | 961 | C | O4'-C1' | 12.10 | 1.57 | 1.41 |
| 81 | DA | 1696 | A | C2'-C1' | -12.10 | 1.40 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2501 | U | C2'-C1' | -12.10 | 1.40 | 1.53 |
| 81 | DA | 3090 | U | O4'-C1' | 12.09 | 1.57 | 1.41 |
| 81 | DA | 2049 | A | O4'-C1' | 12.09 | 1.57 | 1.41 |
| 81 | DA | 641 | C | O4'-C1' | 12.09 | 1.57 | 1.41 |
| 81 | DA | 2048 | G | O4'-C1' | 12.09 | 1.57 | 1.41 |
| 44 | BO | 7 | LYS | N-CA | -12.08 | 1.22 | 1.46 |
| 78 | CA | 1 | U | OP3-P | -12.08 | 1.46 | 1.61 |
| 81 | DA | 202 | G | O4'-C1' | 12.08 | 1.57 | 1.41 |
| 78 | CA | 146 | U | O4'-C1' | 12.08 | 1.57 | 1.41 |
| 82 | DB | 89 | A | C2'-C1' | -12.08 | 1.40 | 1.53 |
| 78 | CA | 164 | A | C4'-C3' | -12.07 | 1.39 | 1.53 |
| 33 | BD | 89 | ALA | CA-CB | 12.06 | 1.77 | 1.52 |
| 78 | CA | 1291 | G | C2'-C1' | -12.06 | 1.40 | 1.53 |
| 81 | DA | 646 | A | C2'-C1' | -12.06 | 1.40 | 1.53 |
| 78 | CA | 1474 | G | C2'-C1' | -12.06 | 1.40 | 1.53 |
| 78 | CA | 949 | C | O4'-C1' | 12.06 | 1.57 | 1.41 |
| 81 | DA | 2746 | A | O4'-C1' | 12.05 | 1.57 | 1.41 |
| 33 | BD | 323 | VAL | N-CA | 12.05 | 1.70 | 1.46 |
| 81 | DA | 1904 | C | O4'-C1' | 12.04 | 1.57 | 1.41 |
| 78 | CA | 672 | U | C2'-C1' | -12.04 | 1.40 | 1.53 |
| 81 | DA | 208 | C | O4'-C1' | 12.04 | 1.57 | 1.41 |
| 81 | DA | 47 | C | O4'-C1' | 12.04 | 1.57 | 1.41 |
| 81 | DA | 226 | C | O4'-C1' | 12.04 | 1.57 | 1.41 |
| 78 | CA | 267 | U | C2'-C1' | 12.04 | 1.66 | 1.53 |
| 78 | CA | 1539 | G | C2'-C1' | 12.03 | 1.66 | 1.53 |
| 81 | DA | 2885 | C | O4'-C1' | 12.02 | 1.57 | 1.41 |
| 81 | DA | 1646 | G | C2'-C1' | -12.02 | 1.40 | 1.53 |
| 81 | DA | 701 | G | C2'-C1' | -12.02 | 1.40 | 1.53 |
| 81 | DA | 2244 | A | O4'-C1' | -12.01 | 1.26 | 1.41 |
| 81 | DA | 1289 | G | C2'-C1' | -12.01 | 1.40 | 1.53 |
| 81 | DA | 2998 | U | C2'-C1' | 12.01 | 1.66 | 1.53 |
| 81 | DA | 132 | C | O4'-C1' | 12.00 | 1.57 | 1.41 |
| 81 | DA | 515 | C | O4'-C1' | 12.00 | 1.57 | 1.41 |
| 78 | CA | 885 | G | O4'-C1' | 11.98 | 1.57 | 1.41 |
| 81 | DA | 2895 | G | C2'-C1' | -11.97 | 1.40 | 1.53 |
| 57 | Be | 220 | PHE | CB-CG | -11.97 | 1.31 | 1.51 |
| 78 | CA | 1226 | A | O4'-C1' | 11.97 | 1.57 | 1.41 |
| 81 | DA | 2204 | C | C2'-C1' | -11.97 | 1.40 | 1.53 |
| 81 | DA | 2884 | C | O4'-C1' | 11.97 | 1.57 | 1.41 |
| 82 | DB | 96 | A | C2'-C1' | 11.97 | 1.66 | 1.53 |
| 81 | DA | 131 | C | O4'-C1' | 11.96 | 1.57 | 1.41 |
| 78 | CA | 1299 | G | C2'-C1' | -11.96 | 1.40 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 83 | DC | 37 | G | C2'-C1' | -11.96 | 1.40 | 1.53 |
| 78 | CA | 424 | C | C2'-C1' | -11.95 | 1.40 | 1.53 |
| 81 | DA | 928 | C | O4'-C1' | 11.94 | 1.57 | 1.41 |
| 81 | DA | 1227 | C | O4'-C1' | 11.94 | 1.57 | 1.41 |
| 81 | DA | 1808 | G | O4'-C1' | 11.94 | 1.57 | 1.41 |
| 81 | DA | 787 | G | C2'-C1' | -11.94 | 1.40 | 1.53 |
| 81 | DA | 2038 | C | O4'-C1' | 11.94 | 1.57 | 1.41 |
| 78 | CA | 105 | A | O4'-C1' | 11.93 | 1.57 | 1.41 |
| 78 | CA | 235 | G | O4'-C1' | 11.93 | 1.57 | 1.41 |
| 81 | DA | 901 | G | C2'-C1' | -11.93 | 1.40 | 1.53 |
| 81 | DA | 838 | G | O4'-C1' | -11.92 | 1.26 | 1.41 |
| 81 | DA | 2589 | G | C2'-C1' | -11.92 | 1.40 | 1.53 |
| 81 | DA | 2892 | A | O4'-C1' | 11.92 | 1.57 | 1.41 |
| 78 | CA | 1144 | U | O4'-C1' | 11.91 | 1.57 | 1.41 |
| 83 | DC | 98 | G | C2'-C1' | -11.91 | 1.40 | 1.53 |
| 81 | DA | 526 | C | O4'-C1' | 11.91 | 1.57 | 1.41 |
| 81 | DA | 606 | C | O4'-C1' | 11.91 | 1.57 | 1.41 |
| 81 | DA | 2173 | U | O4'-C1' | 11.91 | 1.57 | 1.41 |
| 74 | BQ | 201 | GLY | N-CA | -11.90 | 1.28 | 1.46 |
| 82 | DB | 38 | U | C2'-C1' | -11.90 | 1.40 | 1.53 |
| 81 | DA | 964 | G | C2'-C1' | -11.90 | 1.40 | 1.53 |
| 81 | DA | 1509 | A | C2'-C1' | -11.90 | 1.40 | 1.53 |
| 81 | DA | 15 | C | C2'-C1' | -11.89 | 1.40 | 1.53 |
| 81 | DA | 281 | G | C2'-C1' | -11.89 | 1.40 | 1.53 |
| 81 | DA | 1811 | G | O4'-C1' | -11.89 | 1.26 | 1.41 |
| 81 | DA | 3063 | C | O4'-C1' | 11.89 | 1.57 | 1.41 |
| 32 | BC | 297 | SER | CA-CB | 11.89 | 1.70 | 1.52 |
| 79 | CB | 2 | C | O4'-C1' | 11.89 | 1.57 | 1.41 |
| 81 | DA | 2267 | C | O4'-C1' | 11.89 | 1.57 | 1.41 |
| 81 | DA | 3120 | C | O4'-C1' | 11.89 | 1.57 | 1.41 |
| 81 | DA | 2377 | G | C2'-C1' | -11.88 | 1.40 | 1.53 |
| 81 | DA | 2008 | G | O4'-C1' | 11.88 | 1.57 | 1.41 |
| 78 | CA | 554 | C | C2'-C1' | -11.88 | 1.40 | 1.53 |
| 81 | DA | 2346 | C | O4'-C1' | 11.87 | 1.57 | 1.41 |
| 81 | DA | 1713 | G | O4'-C1' | 11.87 | 1.57 | 1.41 |
| 81 | DA | 2436 | U | C2'-C1' | -11.85 | 1.40 | 1.53 |
| 81 | DA | 2495 | C | O4'-C1' | 11.85 | 1.57 | 1.41 |
| 82 | DB | 10 | A | C2'-C1' | -11.85 | 1.40 | 1.53 |
| 81 | DA | 385 | A | O4'-C1' | 11.85 | 1.57 | 1.41 |
| 78 | CA | 1146 | G | C2'-C1' | -11.85 | 1.40 | 1.53 |
| 78 | CA | 858 | G | C2'-C1' | 11.84 | 1.66 | 1.53 |
| 81 | DA | 2023 | C | O4'-C1' | 11.84 | 1.57 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 484 | C | O4'-C1' | 11.84 | 1.57 | 1.41 |
| 81 | DA | 1363 | A | C2'-C1' | -11.83 | 1.40 | 1.53 |
| 78 | CA | 393 | C | C2'-C1' | -11.82 | 1.40 | 1.53 |
| 81 | DA | 1478 | C | O4'-C1' | 11.82 | 1.57 | 1.41 |
| 81 | DA | 68 | C | C2'-C1' | -11.82 | 1.40 | 1.53 |
| 81 | DA | 2769 | A | C2'-C1' | -11.82 | 1.40 | 1.53 |
| 79 | CB | 48 | C | O4'-C1' | 11.81 | 1.57 | 1.41 |
| 81 | DA | 415 | G | O4'-C1' | 11.81 | 1.57 | 1.41 |
| 81 | DA | 529 | A | O4'-C1' | 11.80 | 1.56 | 1.41 |
| 81 | DA | 909 | G | O4'-C1' | 11.80 | 1.56 | 1.41 |
| 81 | DA | 1287 | A | O4'-C1' | 11.80 | 1.56 | 1.41 |
| 78 | CA | 1078 | C | O4'-C1' | 11.80 | 1.56 | 1.41 |
| 81 | DA | 2136 | C | C2'-C1' | -11.80 | 1.40 | 1.53 |
| 78 | CA | 950 | C | O4'-C1' | 11.79 | 1.56 | 1.41 |
| 78 | CA | 442 | C | O4'-C1' | 11.79 | 1.56 | 1.41 |
| 78 | CA | 1531 | G | O4'-C1' | 11.79 | 1.56 | 1.41 |
| 81 | DA | 2490 | C | O4'-C1' | 11.78 | 1.56 | 1.41 |
| 81 | DA | 515 | C | C2'-C1' | -11.78 | 1.40 | 1.53 |
| 81 | DA | 765 | C | C2'-C1' | -11.77 | 1.40 | 1.53 |
| 81 | DA | 2155 | G | C2'-C1' | -11.77 | 1.40 | 1.53 |
| 3 | AB | 199 | PRO | C-O | -11.76 | 0.99 | 1.23 |
| 81 | DA | 559 | A | C2'-C1' | -11.76 | 1.40 | 1.53 |
| 81 | DA | 1526 | U | C2'-C1' | -11.76 | 1.40 | 1.53 |
| 78 | CA | 1470 | C | O4'-C1' | 11.76 | 1.56 | 1.41 |
| 81 | DA | 1621 | A | C2'-C1' | -11.76 | 1.40 | 1.53 |
| 74 | BQ | 197 | SER | CA-CB | -11.75 | 1.35 | 1.52 |
| 78 | CA | 1337 | A | C2'-C1' | 11.75 | 1.66 | 1.53 |
| 78 | CA | 1584 | G | O4'-C1' | -11.75 | 1.26 | 1.41 |
| 81 | DA | 2247 | G | C2'-C1' | -11.75 | 1.40 | 1.53 |
| 81 | DA | 2989 | U | C2'-C1' | 11.74 | 1.66 | 1.53 |
| 81 | DA | 1564 | U | C2'-C1' | -11.73 | 1.40 | 1.53 |
| 81 | DA | 996 | A | C2'-C1' | 11.73 | 1.66 | 1.53 |
| 81 | DA | 1004 | U | O4'-C1' | 11.73 | 1.56 | 1.41 |
| 81 | DA | 2478 | C | O4'-C1' | 11.73 | 1.56 | 1.41 |
| 78 | CA | 1288 | G | C2'-C1' | -11.73 | 1.40 | 1.53 |
| 83 | DC | 29 | C | C2'-C1' | -11.72 | 1.40 | 1.53 |
| 78 | CA | 36 | C | O4'-C1' | 11.72 | 1.56 | 1.41 |
| 81 | DA | 1332 | A | O4'-C1' | 11.72 | 1.56 | 1.41 |
| 81 | DA | 3331 | U | C2'-C1' | 11.72 | 1.66 | 1.53 |
| 82 | DB | 142 | C | O4'-C1' | 11.71 | 1.56 | 1.41 |
| 78 | CA | 1531 | G | C2'-C1' | -11.71 | 1.40 | 1.53 |
| 78 | CA | 1214 | U | C2'-C1' | 11.71 | 1.66 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2366 | C | O4'-C1' | 11.71 | 1.56 | 1.41 |
| 78 | CA | 1215 | C | O4'-C1' | 11.70 | 1.56 | 1.41 |
| 81 | DA | 2230 | C | O4'-C1' | 11.70 | 1.56 | 1.41 |
| 83 | DC | 40 | C | O4'-C1' | 11.70 | 1.56 | 1.41 |
| 83 | DC | 97 | C | O4'-C1' | 11.70 | 1.56 | 1.41 |
| 81 | DA | 1222 | G | C2'-C1' | 11.69 | 1.66 | 1.53 |
| 81 | DA | 1738 | C | O4'-C1' | 11.69 | 1.56 | 1.41 |
| 81 | DA | 192 | C | O4'-C1' | 11.69 | 1.56 | 1.41 |
| 81 | DA | 2966 | G | O4'-C1' | 11.67 | 1.56 | 1.41 |
| 81 | DA | 2942 | C | C2'-C1' | -11.67 | 1.40 | 1.53 |
| 78 | CA | 1205 | C | O4'-C1' | 11.67 | 1.56 | 1.41 |
| 81 | DA | 2445 | A | C2'-C1' | -11.67 | 1.40 | 1.53 |
| 81 | DA | 1562 | C | O4'-C1' | 11.66 | 1.56 | 1.41 |
| 78 | CA | 1169 | G | C2'-C1' | -11.66 | 1.40 | 1.53 |
| 78 | CA | 1735 | U | O4'-C1' | 11.66 | 1.56 | 1.41 |
| 81 | DA | 1904 | C | C2'-C1' | -11.66 | 1.40 | 1.53 |
| 81 | DA | 743 | C | C2'-C1' | -11.65 | 1.40 | 1.53 |
| 81 | DA | 1413 | G | O4'-C1' | 11.65 | 1.56 | 1.41 |
| 81 | DA | 3110 | C | O4'-C1' | 11.65 | 1.56 | 1.41 |
| 78 | CA | 1664 | C | O4'-C1' | 11.65 | 1.56 | 1.41 |
| 81 | DA | 2650 | U | O4'-C1' | 11.65 | 1.56 | 1.41 |
| 81 | DA | 323 | A | C2'-C1' | -11.64 | 1.40 | 1.53 |
| 81 | DA | 1597 | C | O4'-C1' | 11.63 | 1.56 | 1.41 |
| 81 | DA | 2528 | G | O4'-C1' | -11.63 | 1.26 | 1.41 |
| 78 | CA | 402 | C | O4'-C1' | 11.62 | 1.56 | 1.41 |
| 79 | CB | 26 | G | C2'-C1' | -11.62 | 1.40 | 1.53 |
| 81 | DA | 1984 | C | O4'-C1' | 11.62 | 1.56 | 1.41 |
| 81 | DA | 1333 | C | C2'-C1' | -11.62 | 1.40 | 1.53 |
| 81 | DA | 3121 | U | O4'-C1' | 11.62 | 1.56 | 1.41 |
| 81 | DA | 2744 | U | O4'-C1' | 11.61 | 1.56 | 1.41 |
| 78 | CA | 1705 | C | C2'-C1' | -11.61 | 1.40 | 1.53 |
| 81 | DA | 265 | A | O4'-C1' | -11.60 | 1.26 | 1.41 |
| 81 | DA | 2355 | G | C2'-C1' | -11.59 | 1.40 | 1.53 |
| 79 | CB | 2 | C | C2'-C1' | -11.58 | 1.40 | 1.53 |
| 78 | CA | 969 | C | O4'-C1' | 11.58 | 1.56 | 1.41 |
| 78 | CA | 1467 | C | O4'-C1' | 11.58 | 1.56 | 1.41 |
| 81 | DA | 2965 | U | O4'-C1' | 11.57 | 1.56 | 1.41 |
| 78 | CA | 1709 | C | O4'-C1' | 11.57 | 1.56 | 1.41 |
| 81 | DA | 1663 | C | O4'-C1' | 11.57 | 1.56 | 1.41 |
| 78 | CA | 641 | G | C2'-C1' | -11.56 | 1.40 | 1.53 |
| 81 | DA | 31 | C | O4'-C1' | 11.56 | 1.56 | 1.41 |
| 78 | CA | 846 | G | C2'-C1' | -11.56 | 1.40 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1037 | C | O4'-C1' | 11.56 | 1.56 | 1.41 |
| 81 | DA | 1211 | U | C2'-C1' | -11.56 | 1.40 | 1.53 |
| 81 | DA | 1225 | A | O4'-C1' | 11.56 | 1.56 | 1.41 |
| 81 | DA | 2684 | C | C2'-C1' | -11.56 | 1.40 | 1.53 |
| 62 | Bk | 82 | ARG | C-O | -11.56 | 1.01 | 1.23 |
| 78 | CA | 1543 | A | C2'-C1' | -11.55 | 1.40 | 1.53 |
| 78 | CA | 81 | G | C2'-C1' | -11.55 | 1.40 | 1.53 |
| 78 | CA | 184 | C | O4'-C1' | 11.54 | 1.56 | 1.41 |
| 81 | DA | 1848 | G | O4'-C1' | 11.55 | 1.56 | 1.41 |
| 82 | DB | 35 | C | C2'-C1' | -11.54 | 1.40 | 1.53 |
| 81 | DA | 1385 | C | O4'-C1' | 11.54 | 1.56 | 1.41 |
| 81 | DA | 1718 | G | C2'-C1' | -11.54 | 1.40 | 1.53 |
| 81 | DA | 2421 | U | O4'-C1' | 11.54 | 1.56 | 1.41 |
| 78 | CA | 1576 | A | C2'-C1' | 11.54 | 1.66 | 1.53 |
| 78 | CA | 1088 | A | C2'-C1' | 11.53 | 1.66 | 1.53 |
| 81 | DA | 1790 | G | P-O5' | -11.54 | 1.48 | 1.59 |
| 78 | CA | 320 | U | O4'-C1' | 11.53 | 1.56 | 1.41 |
| 78 | CA | 1786 | G | O4'-C1' | 11.53 | 1.56 | 1.41 |
| 81 | DA | 1632 | A | C2'-C1' | -11.53 | 1.40 | 1.53 |
| 81 | DA | 536 | U | O4'-C1' | 11.53 | 1.56 | 1.41 |
| 78 | CA | 254 | A | C2'-C1' | 11.52 | 1.66 | 1.53 |
| 81 | DA | 2726 | C | C2'-C1' | -11.52 | 1.40 | 1.53 |
| 81 | DA | 2041 | U | C2'-C1' | 11.52 | 1.66 | 1.53 |
| 81 | DA | 2950 | G | C2'-C1' | 11.52 | 1.66 | 1.53 |
| 78 | CA | 1472 | C | O4'-C1' | 11.52 | 1.56 | 1.41 |
| 61 | Bj | 20 | LYS | C-O | -11.52 | 1.01 | 1.23 |
| 78 | CA | 1137 | A | O4'-C1' | 11.51 | 1.56 | 1.41 |
| 81 | DA | 682 | U | O4'-C1' | 11.51 | 1.56 | 1.41 |
| 78 | CA | 1339 | C | C2'-C1' | -11.51 | 1.40 | 1.53 |
| 78 | CA | 333 | A | C2'-C1' | -11.50 | 1.40 | 1.53 |
| 78 | CA | 1752 | U | O4'-C1' | 11.50 | 1.56 | 1.41 |
| 81 | DA | 2778 | G | O4'-C1' | 11.50 | 1.56 | 1.41 |
| 81 | DA | 2886 | U | C2'-C1' | 11.50 | 1.66 | 1.53 |
| 81 | DA | 2998 | U | O4'-C1' | -11.50 | 1.26 | 1.41 |
| 81 | DA | 2489 | C | C2'-C1' | -11.50 | 1.40 | 1.53 |
| 78 | CA | 1120 | U | C2'-C1' | -11.49 | 1.40 | 1.53 |
| 81 | DA | 908 | G | O4'-C1' | 11.49 | 1.56 | 1.41 |
| 81 | DA | 776 | U | C2'-C1' | -11.49 | 1.40 | 1.53 |
| 78 | CA | 1546 | G | O3'-P | -11.48 | 1.47 | 1.61 |
| 81 | DA | 2275 | A | C2'-C1' | -11.48 | 1.40 | 1.53 |
| 83 | DC | 28 | C | C2'-C1' | -11.48 | 1.40 | 1.53 |
| 83 | DC | 17 | A | C2'-C1' | -11.48 | 1.40 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 158 | U | O4'-C1' | 11.48 | 1.56 | 1.41 |
| 78 | CA | 669 | G | C2'-C1' | -11.47 | 1.40 | 1.53 |
| 80 | CC | 17 | A | C2'-C1' | -11.47 | 1.40 | 1.53 |
| 81 | DA | 1187 | C | C2'-C1' | -11.47 | 1.40 | 1.53 |
| 81 | DA | 1581 | C | O4'-C1' | 11.46 | 1.56 | 1.41 |
| 79 | CB | 65 | U | C2'-C1' | -11.46 | 1.40 | 1.53 |
| 81 | DA | 1306 | G | C2'-C1' | -11.46 | 1.40 | 1.53 |
| 81 | DA | 673 | U | P-O5' | -11.46 | 1.48 | 1.59 |
| 81 | DA | 1376 | C | C2'-C1' | -11.46 | 1.40 | 1.53 |
| 81 | DA | 1479 | U | C2'-C1' | -11.46 | 1.40 | 1.53 |
| 35 | BG | 153 | PRO | N-CD | -11.46 | 1.31 | 1.47 |
| 78 | CA | 1447 | C | O4'-C1' | 11.46 | 1.56 | 1.41 |
| 81 | DA | 1574 | C | O4'-C1' | 11.46 | 1.56 | 1.41 |
| 81 | DA | 2682 | C | C2'-C1' | -11.46 | 1.40 | 1.53 |
| 81 | DA | 2830 | G | C2'-C1' | -11.46 | 1.40 | 1.53 |
| 81 | DA | 3365 | U | C2'-C1' | -11.45 | 1.40 | 1.53 |
| 1 | Aa | 55 | GLY | N-CA | -11.45 | 1.28 | 1.46 |
| 81 | DA | 747 | A | C2'-C1' | -11.45 | 1.40 | 1.53 |
| 78 | CA | 383 | G | C2'-C1' | -11.45 | 1.40 | 1.53 |
| 81 | DA | 1365 | G | C2'-C1' | -11.44 | 1.40 | 1.53 |
| 81 | DA | 2963 | C | O4'-C1' | 11.44 | 1.56 | 1.41 |
| 81 | DA | 727 | G | C2'-C1' | -11.44 | 1.40 | 1.53 |
| 81 | DA | 339 | C | O4'-C1' | 11.44 | 1.56 | 1.41 |
| 81 | DA | 2414 | G | C2'-C1' | -11.44 | 1.40 | 1.53 |
| 81 | DA | 2675 | C | O4'-C1' | 11.43 | 1.56 | 1.41 |
| 81 | DA | 2163 | C | O4'-C1' | 11.43 | 1.56 | 1.41 |
| 78 | CA | 888 | U | O4'-C1' | 11.43 | 1.56 | 1.41 |
| 81 | DA | 2605 | G | C2'-C1' | -11.43 | 1.40 | 1.53 |
| 81 | DA | 1132 | C | C2'-C1' | -11.42 | 1.40 | 1.53 |
| 81 | DA | 3117 | C | O4'-C1' | 11.42 | 1.56 | 1.41 |
| 78 | CA | 1370 | U | C2'-C1' | -11.42 | 1.40 | 1.53 |
| 81 | DA | 679 | U | C2'-C1' | -11.41 | 1.40 | 1.53 |
| 81 | DA | 2988 | C | O4'-C1' | 11.41 | 1.56 | 1.41 |
| 83 | DC | 22 | A | O4'-C1' | -11.41 | 1.26 | 1.41 |
| 78 | CA | 1210 | C | C2'-C1' | -11.41 | 1.40 | 1.53 |
| 81 | DA | 2167 | A | C2'-C1' | -11.40 | 1.40 | 1.53 |
| 81 | DA | 1089 | G | C2'-C1' | -11.40 | 1.40 | 1.53 |
| 81 | DA | 3117 | C | C2'-C1' | -11.40 | 1.40 | 1.53 |
| 81 | DA | 265 | A | C2'-C1' | 11.40 | 1.65 | 1.53 |
| 81 | DA | 514 | G | O4'-C1' | 11.40 | 1.56 | 1.41 |
| 81 | DA | 558 | U | O4'-C1' | 11.40 | 1.56 | 1.41 |
| 78 | CA | 682 | C | O4'-C1' | 11.39 | 1.56 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2971 | A | O4'-C1' | -11.39 | 1.26 | 1.41 |
| 81 | DA | 781 | G | C2'-C1' | -11.39 | 1.40 | 1.53 |
| 14 | AM | 13 | HIS | N-CA | -11.39 | 1.23 | 1.46 |
| 81 | DA | 2841 | G | C2'-C1' | -11.39 | 1.40 | 1.53 |
| 78 | CA | 615 | A | C2'-C1' | -11.38 | 1.40 | 1.53 |
| 81 | DA | 3224 | G | C2'-C1' | 11.39 | 1.65 | 1.53 |
| 65 | Bn | 71 | PRO | CA-CB | -11.38 | 1.30 | 1.53 |
| 78 | CA | 1675 | C | O4'-C1' | 11.38 | 1.56 | 1.41 |
| 81 | DA | 1416 | C | O4'-C1' | 11.37 | 1.56 | 1.41 |
| 81 | DA | 1578 | C | O4'-C1' | 11.37 | 1.56 | 1.41 |
| 81 | DA | 2961 | G | C2'-C1' | -11.37 | 1.40 | 1.53 |
| 81 | DA | 812 | G | C2'-C1' | -11.37 | 1.40 | 1.53 |
| 81 | DA | 3138 | U | C2'-C1' | -11.37 | 1.40 | 1.53 |
| 78 | CA | 294 | C | C2'-C1' | -11.36 | 1.40 | 1.53 |
| 81 | DA | 1017 | C | C2'-C1' | -11.36 | 1.40 | 1.53 |
| 78 | CA | 249 | U | C5'-C4' | 11.36 | 1.65 | 1.51 |
| 81 | DA | 3113 | A | O4'-C1' | 11.36 | 1.56 | 1.41 |
| 83 | DC | 5 | G | C2'-C1' | -11.36 | 1.40 | 1.53 |
| 81 | DA | 1560 | G | C2'-C1' | -11.35 | 1.40 | 1.53 |
| 81 | DA | 2818 | U | C2'-C1' | 11.35 | 1.65 | 1.53 |
| 81 | DA | 1424 | C | C2'-C1' | -11.35 | 1.40 | 1.53 |
| 78 | CA | 203 | U | O4'-C1' | 11.35 | 1.56 | 1.41 |
| 81 | DA | 237 | G | O4'-C1' | 11.34 | 1.56 | 1.41 |
| 81 | DA | 3149 | G | O4'-C1' | -11.34 | 1.26 | 1.41 |
| 81 | DA | 578 | A | O4'-C1' | 11.34 | 1.56 | 1.41 |
| 81 | DA | 2225 | U | O4'-C1' | 11.34 | 1.56 | 1.41 |
| 81 | DA | 2754 | G | O4'-C1' | -11.34 | 1.26 | 1.41 |
| 81 | DA | 753 | C | O4'-C1' | 11.33 | 1.56 | 1.41 |
| 81 | DA | 1912 | U | C2'-C1' | -11.33 | 1.40 | 1.53 |
| 81 | DA | 2452 | G | C2'-C1' | 11.33 | 1.65 | 1.53 |
| 81 | DA | 3126 | C | C2'-C1' | -11.33 | 1.40 | 1.53 |
| 78 | CA | 448 | C | C2'-C1' | -11.32 | 1.40 | 1.53 |
| 78 | CA | 1407 | U | O4'-C1' | 11.32 | 1.56 | 1.41 |
| 81 | DA | 506 | U | O4'-C1' | 11.32 | 1.56 | 1.41 |
| 81 | DA | 2492 | C | C2'-C1' | -11.32 | 1.41 | 1.53 |
| 81 | DA | 1510 | G | C2'-C1' | -11.31 | 1.41 | 1.53 |
| 81 | DA | 1927 | G | O4'-C1' | -11.31 | 1.26 | 1.41 |
| 81 | DA | 20 | A | C2'-C1' | -11.31 | 1.41 | 1.53 |
| 81 | DA | 1101 | G | C2'-C1' | -11.31 | 1.41 | 1.53 |
| 81 | DA | 1790 | G | C2'-C1' | -11.31 | 1.41 | 1.53 |
| 78 | CA | 1135 | U | C2'-C1' | -11.30 | 1.41 | 1.53 |
| 81 | DA | 1210 | U | O4'-C1' | 11.30 | 1.56 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1401 | A | O4'-C1' | -11.30 | 1.26 | 1.41 |
| 21 | AT | 10 | GLU | N-CA | 11.30 | 1.69 | 1.46 |
| 74 | BQ | 128 | GLU | CA-CB | 11.30 | 1.78 | 1.53 |
| 81 | DA | 1104 | G | O4'-C1' | -11.30 | 1.26 | 1.41 |
| 83 | DC | 43 | U | O4'-C1' | 11.29 | 1.56 | 1.41 |
| 81 | DA | 291 | C | O4'-C1' | 11.29 | 1.56 | 1.41 |
| 81 | DA | 956 | U | C2'-C1' | -11.29 | 1.41 | 1.53 |
| 78 | CA | 1181 | U | C2'-C1' | -11.29 | 1.41 | 1.53 |
| 81 | DA | 2705 | A | O4'-C1' | -11.29 | 1.26 | 1.41 |
| 81 | DA | 3239 | G | O4'-C1' | 11.29 | 1.56 | 1.41 |
| 81 | DA | 2348 | A | O4'-C1' | 11.28 | 1.56 | 1.41 |
| 81 | DA | 2128 | C | O4'-C1' | 11.28 | 1.56 | 1.41 |
| 81 | DA | 2455 | U | O4'-C1' | 11.28 | 1.56 | 1.41 |
| 78 | CA | 1203 | A | C2'-C1' | -11.28 | 1.41 | 1.53 |
| 82 | DB | 65 | A | C2'-C1' | -11.28 | 1.41 | 1.53 |
| 44 | BO | 63 | LYS | N-CA | -11.27 | 1.23 | 1.46 |
| 81 | DA | 3143 | C | O4'-C1' | 11.27 | 1.56 | 1.41 |
| 78 | CA | 431 | C | O4'-C1' | 11.27 | 1.56 | 1.41 |
| 81 | DA | 3025 | C | O4'-C1' | 11.26 | 1.56 | 1.41 |
| 81 | DA | 3118 | C | O4'-C1' | 11.26 | 1.56 | 1.41 |
| 81 | DA | 3355 | U | C2'-C1' | 11.26 | 1.65 | 1.53 |
| 82 | DB | 11 | C | O4'-C1' | 11.26 | 1.56 | 1.41 |
| 81 | DA | 2531 | C | P-O5' | -11.25 | 1.48 | 1.59 |
| 81 | DA | 46 | U | C2'-C1' | -11.25 | 1.41 | 1.53 |
| 65 | Bn | 34 | ALA | N-CA | -11.25 | 1.23 | 1.46 |
| 78 | CA | 931 | C | O4'-C1' | 11.25 | 1.56 | 1.41 |
| 81 | DA | 2858 | U | O4'-C1' | 11.25 | 1.56 | 1.41 |
| 81 | DA | 1608 | C | C2'-C1' | -11.24 | 1.41 | 1.53 |
| 81 | DA | 1907 | C | O4'-C1' | 11.24 | 1.56 | 1.41 |
| 81 | DA | 1539 | A | O4'-C1' | 11.24 | 1.56 | 1.41 |
| 81 | DA | 216 | G | C2'-C1' | -11.23 | 1.41 | 1.53 |
| 81 | DA | 2407 | C | C2'-C1' | -11.23 | 1.41 | 1.53 |
| 81 | DA | 1646 | G | O4'-C1' | 11.23 | 1.56 | 1.41 |
| 81 | DA | 407 | A | C2'-C1' | -11.23 | 1.41 | 1.53 |
| 81 | DA | 244 | G | C2'-C1' | -11.22 | 1.41 | 1.53 |
| 81 | DA | 861 | C | O4'-C1' | 11.22 | 1.56 | 1.41 |
| 81 | DA | 2856 | G | C2'-C1' | -11.22 | 1.41 | 1.53 |
| 78 | CA | 1412 | G | O4'-C1' | 11.22 | 1.56 | 1.41 |
| 81 | DA | 2714 | G | C2'-C1' | -11.22 | 1.41 | 1.53 |
| 82 | DB | 86 | U | C2'-C1' | 11.22 | 1.65 | 1.53 |
| 81 | DA | 3096 | C | C2'-C1' | -11.22 | 1.41 | 1.53 |
| 78 | CA | 443 | C | C2'-C1' | -11.21 | 1.41 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1264 | G | C2'-C1' | -11.21 | 1.41 | 1.53 |
| 81 | DA | 2960 | C | O4'-C1' | 11.21 | 1.56 | 1.41 |
| 81 | DA | 1525 | G | C2'-C1' | -11.21 | 1.41 | 1.53 |
| 81 | DA | 1225 | A | C2'-C1' | -11.21 | 1.41 | 1.53 |
| 81 | DA | 3056 | U | O4'-C1' | 11.21 | 1.56 | 1.41 |
| 78 | CA | 889 | U | O4'-C1' | 11.21 | 1.56 | 1.41 |
| 81 | DA | 452 | G | O4'-C1' | 11.21 | 1.56 | 1.41 |
| 81 | DA | 2284 | C | O4'-C1' | 11.21 | 1.56 | 1.41 |
| 78 | CA | 1772 | C | O4'-C1' | 11.20 | 1.56 | 1.41 |
| 79 | CB | 71 | A | O4'-C1' | 11.20 | 1.56 | 1.41 |
| 81 | DA | 2305 | G | C2'-C1' | -11.19 | 1.41 | 1.53 |
| 81 | DA | 2383 | C | C2'-C1' | -11.19 | 1.41 | 1.53 |
| 81 | DA | 2984 | C | O4'-C1' | 11.19 | 1.56 | 1.41 |
| 81 | DA | 1638 | A | C2'-C1' | -11.19 | 1.41 | 1.53 |
| 78 | CA | 1668 | G | C2'-C1' | -11.19 | 1.41 | 1.53 |
| 81 | DA | 2206 | G | C2'-C1' | 11.19 | 1.65 | 1.53 |
| 78 | CA | 1649 | G | C2'-C1' | 11.18 | 1.65 | 1.53 |
| 53 | Ba | 57 | HIS | CB-CG | -11.18 | 1.29 | 1.50 |
| 81 | DA | 945 | C | O4'-C1' | 11.18 | 1.56 | 1.41 |
| 78 | CA | 310 | C | C2'-C1' | -11.18 | 1.41 | 1.53 |
| 81 | DA | 105 | C | C2'-C1' | -11.18 | 1.41 | 1.53 |
| 78 | CA | 851 | U | O4'-C1' | 11.17 | 1.56 | 1.41 |
| 81 | DA | 2252 | A | O4'-C1' | 11.17 | 1.56 | 1.41 |
| 82 | DB | 118 | C | C2'-C1' | -11.17 | 1.41 | 1.53 |
| 81 | DA | 1944 | U | O4'-C1' | 11.17 | 1.56 | 1.41 |
| 81 | DA | 2115 | G | C2'-C1' | -11.17 | 1.41 | 1.53 |
| 82 | DB | 142 | C | C2'-C1' | -11.17 | 1.41 | 1.53 |
| 81 | DA | 512 | U | O4'-C1' | 11.16 | 1.56 | 1.41 |
| 41 | BN | 76 | ALA | C-N | 11.16 | 1.59 | 1.34 |
| 81 | DA | 982 | C | O4'-C1' | 11.16 | 1.56 | 1.41 |
| 78 | CA | 447 | U | C2'-C1' | -11.16 | 1.41 | 1.53 |
| 78 | CA | 374 | U | O4'-C1' | 11.16 | 1.56 | 1.41 |
| 81 | DA | 2743 | A | O4'-C1' | 11.16 | 1.56 | 1.41 |
| 81 | DA | 1496 | C | C2'-C1' | -11.15 | 1.41 | 1.53 |
| 78 | CA | 16 | G | C2'-C1' | 11.15 | 1.65 | 1.53 |
| 81 | DA | 142 | C | O4'-C1' | 11.15 | 1.56 | 1.41 |
| 78 | CA | 1648 | A | C2'-C1' | -11.14 | 1.41 | 1.53 |
| 81 | DA | 3233 | C | O4'-C1' | 11.14 | 1.56 | 1.41 |
| 81 | DA | 1706 | C | O4'-C1' | 11.13 | 1.56 | 1.41 |
| 78 | CA | 637 | C | C2'-C1' | 11.13 | 1.65 | 1.53 |
| 78 | CA | 1364 | G | O4'-C1' | 11.13 | 1.56 | 1.41 |
| 81 | DA | 1420 | C | C2'-C1' | -11.13 | 1.41 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2670 | G | C2'-C1' | -11.13 | 1.41 | 1.53 |
| 78 | CA | 191 | C | O4'-C1' | 11.13 | 1.56 | 1.41 |
| 78 | CA | 394 | C | C2'-C1' | -11.13 | 1.41 | 1.53 |
| 81 | DA | 1677 | G | O4'-C1' | -11.13 | 1.27 | 1.41 |
| 83 | DC | 35 | C | C2'-C1' | -11.13 | 1.41 | 1.53 |
| 78 | CA | 202 | A | C2'-C1' | -11.12 | 1.41 | 1.53 |
| 81 | DA | 1238 | C | O4'-C1' | 11.12 | 1.56 | 1.41 |
| 83 | DC | 15 | C | O4'-C1' | 11.12 | 1.56 | 1.41 |
| 81 | DA | 1054 | A | O4'-C1' | -11.12 | 1.27 | 1.41 |
| 78 | CA | 38 | C | C2'-C1' | -11.10 | 1.41 | 1.53 |
| 81 | DA | 2331 | C | O4'-C1' | 11.10 | 1.56 | 1.41 |
| 78 | CA | 287 | G | O4'-C1' | 11.10 | 1.56 | 1.41 |
| 78 | CA | 1215 | C | C2'-C1' | -11.10 | 1.41 | 1.53 |
| 81 | DA | 81 | C | C2'-C1' | -11.10 | 1.41 | 1.53 |
| 81 | DA | 829 | U | O4'-C1' | 11.10 | 1.56 | 1.41 |
| 78 | CA | 1463 | C | O4'-C1' | 11.09 | 1.56 | 1.41 |
| 81 | DA | 2884 | C | C2'-C1' | -11.09 | 1.41 | 1.53 |
| 78 | CA | 1207 | C | O4'-C1' | 11.09 | 1.56 | 1.41 |
| 3 | AB | 205 | ALA | N-CA | 11.09 | 1.68 | 1.46 |
| 81 | DA | 50 | U | O4'-C1' | 11.09 | 1.56 | 1.41 |
| 81 | DA | 2796 | G | C2'-C1' | 11.09 | 1.65 | 1.53 |
| 78 | CA | 1659 | A | O4'-C1' | 11.08 | 1.56 | 1.41 |
| 81 | DA | 2676 | A | O4'-C1' | 11.08 | 1.56 | 1.41 |
| 81 | DA | 1178 | G | O4'-C1' | 11.07 | 1.56 | 1.41 |
| 3 | AB | 200 | LYS | N-CA | -11.07 | 1.24 | 1.46 |
| 78 | CA | 1314 | U | C2'-C1' | -11.07 | 1.41 | 1.53 |
| 78 | CA | 1380 | U | C2'-C1' | -11.07 | 1.41 | 1.53 |
| 78 | CA | 1571 | C | O4'-C1' | 11.06 | 1.56 | 1.41 |
| 81 | DA | 327 | A | O4'-C1' | 11.06 | 1.56 | 1.41 |
| 81 | DA | 1654 | A | C2'-C1' | -11.06 | 1.41 | 1.53 |
| 81 | DA | 2009 | C | O4'-C1' | 11.06 | 1.56 | 1.41 |
| 81 | DA | 1933 | A | C2'-C1' | 11.05 | 1.65 | 1.53 |
| 81 | DA | 2239 | G | C2'-C1' | -11.05 | 1.41 | 1.53 |
| 81 | DA | 1615 | C | C2'-C1' | -11.05 | 1.41 | 1.53 |
| 78 | CA | 1108 | G | C2'-C1' | 11.04 | 1.65 | 1.53 |
| 81 | DA | 3091 | A | O4'-C1' | 11.04 | 1.56 | 1.41 |
| 45 | BR | 55 | SER | CB-OG | -11.04 | 1.27 | 1.42 |
| 78 | CA | 1326 | A | O4'-C1' | 11.04 | 1.55 | 1.41 |
| 81 | DA | 454 | C | C2'-C1' | -11.03 | 1.41 | 1.53 |
| 81 | DA | 237 | G | C2'-C1' | -11.03 | 1.41 | 1.53 |
| 81 | DA | 2745 | G | C2'-C1' | 11.03 | 1.65 | 1.53 |
| 78 | CA | 1162 | C | C2'-C1' | -11.03 | 1.41 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 600 | G | O4'-C1' | 11.03 | 1.55 | 1.41 |
| 81 | DA | 2618 | G | C2'-C1' | 11.03 | 1.65 | 1.53 |
| 78 | CA | 1238 | A | O4'-C1' | -11.03 | 1.27 | 1.41 |
| 81 | DA | 298 | U | O4'-C1' | 11.01 | 1.55 | 1.41 |
| 81 | DA | 692 | A | O4'-C1' | 11.01 | 1.55 | 1.41 |
| 81 | DA | 1882 | G | C2'-C1' | -11.01 | 1.41 | 1.53 |
| 82 | DB | 63 | G | O4'-C1' | 11.01 | 1.55 | 1.41 |
| 81 | DA | 2722 | U | O3'-P | -11.01 | 1.48 | 1.61 |
| 81 | DA | 744 | A | O4'-C1' | 11.00 | 1.55 | 1.41 |
| 78 | CA | 10 | G | C2'-C1' | -11.00 | 1.41 | 1.53 |
| 81 | DA | 135 | C | C2'-C1' | 11.00 | 1.65 | 1.53 |
| 81 | DA | 627 | U | C2'-C1' | -11.00 | 1.41 | 1.53 |
| 81 | DA | 2678 | A | C2'-C1' | -10.99 | 1.41 | 1.53 |
| 78 | CA | 342 | C | O4'-C1' | 10.99 | 1.55 | 1.41 |
| 5 | AC | 142 | ASN | CG-OD1 | 10.99 | 1.48 | 1.24 |
| 81 | DA | 1820 | U | C2'-C1' | -10.98 | 1.41 | 1.53 |
| 81 | DA | 321 | C | C2'-C1' | -10.98 | 1.41 | 1.53 |
| 79 | CB | 71 | A | C2'-C1' | -10.97 | 1.41 | 1.53 |
| 81 | DA | 2699 | G | O4'-C1' | 10.97 | 1.55 | 1.41 |
| 81 | DA | 2841 | G | O4'-C1' | 10.97 | 1.55 | 1.41 |
| 81 | DA | 3330 | A | O4'-C1' | 10.97 | 1.55 | 1.41 |
| 81 | DA | 1516 | C | C2'-C1' | -10.97 | 1.41 | 1.53 |
| 81 | DA | 2785 | A | C2'-C1' | -10.96 | 1.41 | 1.53 |
| 78 | CA | 596 | C | O4'-C1' | 10.96 | 1.55 | 1.41 |
| 78 | CA | 980 | G | O4'-C1' | 10.96 | 1.55 | 1.41 |
| 81 | DA | 1645 | U | C2'-C1' | -10.96 | 1.41 | 1.53 |
| 81 | DA | 2110 | G | C2'-C1' | -10.95 | 1.41 | 1.53 |
| 81 | DA | 3304 | U | C5'-C4' | 10.95 | 1.64 | 1.51 |
| 78 | CA | 1412 | G | C2'-C1' | -10.95 | 1.41 | 1.53 |
| 78 | CA | 1433 | G | O4'-C1' | 10.95 | 1.55 | 1.41 |
| 78 | CA | 560 | U | O4'-C1' | 10.95 | 1.55 | 1.41 |
| 81 | DA | 466 | G | C2'-C1' | -10.94 | 1.41 | 1.53 |
| 81 | DA | 1515 | A | O4'-C1' | 10.94 | 1.55 | 1.41 |
| 81 | DA | 2393 | G | O4'-C1' | -10.94 | 1.27 | 1.41 |
| 81 | DA | 3296 | A | C2'-C1' | -10.94 | 1.41 | 1.53 |
| 81 | DA | 1704 | A | C2'-C1' | 10.93 | 1.65 | 1.53 |
| 83 | DC | 113 | C | C2'-C1' | -10.93 | 1.41 | 1.53 |
| 79 | CB | 37 | G | C2'-C1' | -10.93 | 1.41 | 1.53 |
| 81 | DA | 1927 | G | C2'-C1' | 10.93 | 1.65 | 1.53 |
| 16 | AO | 68 | GLY | N-CA | 10.92 | 1.62 | 1.46 |
| 81 | DA | 637 | C | O4'-C1' | 10.91 | 1.55 | 1.41 |
| 81 | DA | 867 | G | C2'-C1' | -10.91 | 1.41 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 1765 | A | O4'-C1' | 10.91 | 1.55 | 1.41 |
| 43 | BP | 74 | PRO | CA-CB | 10.90 | 1.75 | 1.53 |
| 79 | CB | 72 | G | C2'-C1' | 10.90 | 1.65 | 1.53 |
| 81 | DA | 200 | C | O4'-C1' | 10.90 | 1.55 | 1.41 |
| 81 | DA | 2852 | C | O4'-C1' | 10.90 | 1.55 | 1.41 |
| 78 | CA | 48 | G | C2'-C1' | -10.89 | 1.41 | 1.53 |
| 78 | CA | 614 | C | O4'-C1' | 10.89 | 1.55 | 1.41 |
| 78 | CA | 1148 | C | C2'-C1' | -10.89 | 1.41 | 1.53 |
| 81 | DA | 241 | G | C2'-C1' | -10.89 | 1.41 | 1.53 |
| 81 | DA | 2416 | U | O3'-P | -10.89 | 1.48 | 1.61 |
| 17 | AQ | 82 | ASP | CA-CB | 10.88 | 1.77 | 1.53 |
| 81 | DA | 428 | A | C2'-C1' | -10.88 | 1.41 | 1.53 |
| 12 | AK | 125 | SER | CA-CB | -10.88 | 1.36 | 1.52 |
| 78 | CA | 1178 | G | O4'-C1' | 10.88 | 1.55 | 1.41 |
| 81 | DA | 2590 | A | C2'-C1' | -10.88 | 1.41 | 1.53 |
| 81 | DA | 1233 | G | O4'-C1' | -10.88 | 1.27 | 1.41 |
| 81 | DA | 1686 | U | O4'-C1' | 10.88 | 1.55 | 1.41 |
| 81 | DA | 8 | C | C2'-C1' | -10.87 | 1.41 | 1.53 |
| 81 | DA | 2832 | C | O4'-C1' | 10.87 | 1.55 | 1.41 |
| 82 | DB | 54 | A | O4'-C1' | 10.87 | 1.55 | 1.41 |
| 81 | DA | 2707 | C | C2'-C1' | -10.87 | 1.41 | 1.53 |
| 81 | DA | 3140 | G | C2'-C1' | 10.86 | 1.65 | 1.53 |
| 81 | DA | 489 | C | O4'-C1' | 10.86 | 1.55 | 1.41 |
| 81 | DA | 713 | U | C2'-C1' | -10.86 | 1.41 | 1.53 |
| 78 | CA | 1545 | A | C4'-O4' | -10.86 | 1.31 | 1.45 |
| 81 | DA | 2531 | C | O4'-C1' | -10.86 | 1.27 | 1.41 |
| 31 | BB | 62 | VAL | CA-CB | 10.85 | 1.77 | 1.54 |
| 81 | DA | 1250 | G | C2'-C1' | 10.85 | 1.65 | 1.53 |
| 81 | DA | 226 | C | C2'-C1' | -10.85 | 1.41 | 1.53 |
| 81 | DA | 3132 | C | O4'-C1' | 10.85 | 1.55 | 1.41 |
| 81 | DA | 2312 | A | C2'-C1' | -10.85 | 1.41 | 1.53 |
| 81 | DA | 49 | A | O4'-C1' | -10.84 | 1.27 | 1.41 |
| 81 | DA | 2245 | C | O4'-C1' | 10.84 | 1.55 | 1.41 |
| 81 | DA | 2295 | A | O4'-C1' | 10.84 | 1.55 | 1.41 |
| 78 | CA | 1765 | A | C2'-C1' | -10.83 | 1.41 | 1.53 |
| 81 | DA | 1395 | G | C2'-C1' | -10.83 | 1.41 | 1.53 |
| 81 | DA | 833 | G | C2'-C1' | -10.83 | 1.41 | 1.53 |
| 78 | CA | 299 | A | C2'-C1' | 10.83 | 1.65 | 1.53 |
| 81 | DA | 2212 | C | O4'-C1' | 10.82 | 1.55 | 1.41 |
| 78 | CA | 15 | U | C2'-C1' | -10.82 | 1.41 | 1.53 |
| 78 | CA | 1178 | G | C2'-C1' | -10.82 | 1.41 | 1.53 |
| 81 | DA | 2653 | C | C2'-C1' | -10.82 | 1.41 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 3313 | U | C2'-C1' | -10.82 | 1.41 | 1.53 |
| 81 | DA | 654 | C | C2'-C1' | -10.82 | 1.41 | 1.53 |
| 81 | DA | 2288 | G | C2'-C1' | -10.82 | 1.41 | 1.53 |
| 78 | CA | 31 | C | O4'-C1' | 10.82 | 1.55 | 1.41 |
| 78 | CA | 448 | C | O4'-C1' | 10.82 | 1.55 | 1.41 |
| 81 | DA | 1626 | U | C2'-C1' | -10.81 | 1.41 | 1.53 |
| 81 | DA | 1376 | C | O4'-C1' | 10.81 | 1.55 | 1.41 |
| 81 | DA | 255 | A | C2'-C1' | 10.79 | 1.65 | 1.53 |
| 81 | DA | 1021 | G | C2'-C1' | -10.79 | 1.41 | 1.53 |
| 78 | CA | 965 | U | O4'-C1' | 10.79 | 1.55 | 1.41 |
| 78 | CA | 312 | A | C2'-C1' | -10.79 | 1.41 | 1.53 |
| 78 | CA | 949 | C | C2'-C1' | -10.79 | 1.41 | 1.53 |
| 78 | CA | 15 | U | O4'-C1' | 10.78 | 1.55 | 1.41 |
| 83 | DC | 3 | U | O4'-C1' | 10.78 | 1.55 | 1.41 |
| 21 | AT | 9 | VAL | CA-CB | -10.78 | 1.32 | 1.54 |
| 80 | CC | 18 | C | C2'-C1' | -10.78 | 1.41 | 1.53 |
| 81 | DA | 824 | C | C2'-C1' | -10.78 | 1.41 | 1.53 |
| 81 | DA | 2417 | U | O4'-C1' | 10.77 | 1.55 | 1.41 |
| 78 | CA | 1203 | A | O4'-C1' | 10.77 | 1.55 | 1.41 |
| 81 | DA | 2434 | U | O4'-C1' | 10.77 | 1.55 | 1.41 |
| 81 | DA | 2149 | A | O4'-C1' | -10.77 | 1.27 | 1.41 |
| 81 | DA | 1863 | G | C2'-C1' | -10.76 | 1.41 | 1.53 |
| 81 | DA | 2499 | U | O4'-C1' | 10.76 | 1.55 | 1.41 |
| 81 | DA | 2673 | A | P-O5' | -10.76 | 1.49 | 1.59 |
| 81 | DA | 111 | C | O4'-C1' | 10.76 | 1.55 | 1.41 |
| 81 | DA | 1809 | A | O4'-C1' | 10.76 | 1.55 | 1.41 |
| 81 | DA | 2832 | C | C2'-C1' | -10.76 | 1.41 | 1.53 |
| 81 | DA | 1264 | G | O4'-C1' | 10.76 | 1.55 | 1.41 |
| 82 | DB | 112 | U | C2'-C1' | 10.76 | 1.65 | 1.53 |
| 79 | CB | 66 | C | O4'-C1' | 10.75 | 1.55 | 1.41 |
| 82 | DB | 6 | U | O4'-C1' | 10.75 | 1.55 | 1.41 |
| 81 | DA | 125 | C | O4'-C1' | 10.75 | 1.55 | 1.41 |
| 81 | DA | 2679 | A | C2'-C1' | -10.75 | 1.41 | 1.53 |
| 81 | DA | 882 | A | O4'-C1' | 10.75 | 1.55 | 1.41 |
| 81 | DA | 2207 | A | O4'-C1' | -10.74 | 1.27 | 1.41 |
| 5 | AC | 157 | ASP | CA-CB | 10.74 | 1.77 | 1.53 |
| 81 | DA | 1616 | U | C2'-C1' | -10.74 | 1.41 | 1.53 |
| 81 | DA | 2515 | A | O4'-C1' | 10.74 | 1.55 | 1.41 |
| 81 | DA | 1277 | C | O4'-C1' | 10.73 | 1.55 | 1.41 |
| 38 | Bs | 242 | ASN | CB-CG | -10.73 | 1.26 | 1.51 |
| 78 | CA | 1739 | C | O4'-C1' | 10.73 | 1.55 | 1.41 |
| 81 | DA | 1574 | C | C2'-C1' | -10.72 | 1.41 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 108 | A | C2'-C1' | -10.72 | 1.41 | 1.53 |
| 81 | DA | 1721 | U | C2'-C1' | -10.71 | 1.41 | 1.53 |
| 81 | DA | 1141 | C | C2'-C1' | -10.71 | 1.41 | 1.53 |
| 83 | DC | 15 | C | C2'-C1' | -10.71 | 1.41 | 1.53 |
| 81 | DA | 2182 | A | O4'-C1' | 10.71 | 1.55 | 1.41 |
| 78 | CA | 1332 | C | C2'-C1' | -10.71 | 1.41 | 1.53 |
| 83 | DC | 1 | G | OP3-P | -10.70 | 1.48 | 1.61 |
| 81 | DA | 1190 | A | C2'-C1' | -10.70 | 1.41 | 1.53 |
| 81 | DA | 2179 | C | O4'-C1' | 10.70 | 1.55 | 1.41 |
| 81 | DA | 1146 | C | O4'-C1' | 10.70 | 1.55 | 1.41 |
| 81 | DA | 2970 | C | O4'-C1' | 10.70 | 1.55 | 1.41 |
| 81 | DA | 1917 | C | C2'-C1' | -10.69 | 1.41 | 1.53 |
| 32 | BC | 3 | HIS | CA-CB | 10.69 | 1.77 | 1.53 |
| 81 | DA | 2402 | A | C2'-C1' | 10.68 | 1.65 | 1.53 |
| 80 | CC | 12 | A | O4'-C1' | -10.68 | 1.27 | 1.41 |
| 78 | CA | 202 | A | O4'-C1' | 10.68 | 1.55 | 1.41 |
| 81 | DA | 520 | U | O4'-C1' | 10.68 | 1.55 | 1.41 |
| 81 | DA | 2469 | G | O4'-C1' | 10.68 | 1.55 | 1.41 |
| 81 | DA | 2444 | C | O4'-C1' | 10.68 | 1.55 | 1.41 |
| 81 | DA | 2664 | C | O4'-C1' | 10.68 | 1.55 | 1.41 |
| 78 | CA | 469 | C | C2'-C1' | 10.67 | 1.65 | 1.53 |
| 81 | DA | 2669 | G | O4'-C1' | -10.67 | 1.27 | 1.41 |
| 81 | DA | 13 | A | O4'-C1' | 10.66 | 1.55 | 1.41 |
| 81 | DA | 2224 | A | C2'-C1' | -10.66 | 1.41 | 1.53 |
| 82 | DB | 4 | C | C2'-C1' | -10.66 | 1.41 | 1.53 |
| 81 | DA | 3077 | A | O4'-C1' | 10.66 | 1.55 | 1.41 |
| 78 | CA | 1147 | A | O4'-C1' | 10.65 | 1.55 | 1.41 |
| 81 | DA | 2348 | A | C2'-C1' | -10.65 | 1.41 | 1.53 |
| 81 | DA | 2828 | G | C2'-C1' | -10.65 | 1.41 | 1.53 |
| 81 | DA | 1068 | C | O4'-C1' | 10.65 | 1.55 | 1.41 |
| 81 | DA | 615 | U | C2'-C1' | -10.64 | 1.41 | 1.53 |
| 81 | DA | 650 | C | O4'-C1' | 10.64 | 1.55 | 1.41 |
| 81 | DA | 433 | A | O4'-C1' | 10.63 | 1.55 | 1.41 |
| 81 | DA | 633 | C | O4'-C1' | 10.63 | 1.55 | 1.41 |
| 81 | DA | 1119 | C | O4'-C1' | 10.63 | 1.55 | 1.41 |
| 81 | DA | 3255 | U | O4'-C1' | 10.63 | 1.55 | 1.41 |
| 81 | DA | 1691 | U | O4'-C1' | 10.63 | 1.55 | 1.41 |
| 78 | CA | 1461 | C | O4'-C1' | 10.63 | 1.55 | 1.41 |
| 81 | DA | 2917 | G | C2'-C1' | -10.63 | 1.41 | 1.53 |
| 78 | CA | 989 | U | O4'-C1' | 10.62 | 1.55 | 1.41 |
| 78 | CA | 1199 | G | C2'-C1' | 10.62 | 1.65 | 1.53 |
| 81 | DA | 2723 | U | O4'-C1' | 10.62 | 1.55 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 3042 | U | O4'-C1' | 10.62 | 1.55 | 1.41 |
| 37 | BH | 89 | GLU | N-CA | 10.62 | 1.67 | 1.46 |
| 81 | DA | 2191 | U | C2'-C1' | -10.62 | 1.41 | 1.53 |
| 81 | DA | 518 | G | C2'-C1' | -10.61 | 1.41 | 1.53 |
| 81 | DA | 379 | C | O4'-C1' | 10.61 | 1.55 | 1.41 |
| 83 | DC | 53 | U | C2'-C1' | -10.60 | 1.41 | 1.53 |
| 81 | DA | 1 | G | OP3-P | -10.60 | 1.48 | 1.61 |
| 79 | CB | 18 | G | C2'-C1' | -10.59 | 1.41 | 1.53 |
| 81 | DA | 1560 | G | O4'-C1' | 10.59 | 1.55 | 1.41 |
| 81 | DA | 2293 | C | O4'-C1' | 10.59 | 1.55 | 1.41 |
| 78 | CA | 401 | A | O4'-C1' | 10.59 | 1.55 | 1.41 |
| 81 | DA | 2805 | G | C2'-C1' | -10.59 | 1.41 | 1.53 |
| 78 | CA | 1128 | C | O4'-C1' | 10.59 | 1.55 | 1.41 |
| 81 | DA | 2046 | U | O3'-P | -10.58 | 1.48 | 1.61 |
| 81 | DA | 2607 | G | O4'-C1' | 10.58 | 1.55 | 1.41 |
| 81 | DA | 2039 | C | O4'-C1' | 10.58 | 1.55 | 1.41 |
| 81 | DA | 2450 | G | O4'-C1' | -10.58 | 1.27 | 1.41 |
| 81 | DA | 824 | C | O4'-C1' | 10.58 | 1.55 | 1.41 |
| 81 | DA | 1658 | G | C2'-C1' | -10.58 | 1.41 | 1.53 |
| 81 | DA | 2835 | U | C2'-C1' | -10.58 | 1.41 | 1.53 |
| 78 | CA | 1581 | C | C2'-C1' | -10.58 | 1.41 | 1.53 |
| 81 | DA | 654 | C | O4'-C1' | 10.57 | 1.55 | 1.41 |
| 81 | DA | 1341 | U | C2'-C1' | -10.57 | 1.41 | 1.53 |
| 78 | CA | 169 | A | O4'-C1' | -10.57 | 1.27 | 1.41 |
| 81 | DA | 272 | G | C2'-C1' | -10.57 | 1.41 | 1.53 |
| 79 | CB | 1 | U | OP3-P | -10.56 | 1.48 | 1.61 |
| 81 | DA | 2360 | C | C2'-C1' | -10.56 | 1.41 | 1.53 |
| 34 | BE | 115 | LYS | CA-CB | -10.56 | 1.30 | 1.53 |
| 80 | CC | 12 | A | OP3-P | -10.56 | 1.48 | 1.61 |
| 81 | DA | 1259 | A | C2'-C1' | 10.56 | 1.65 | 1.53 |
| 78 | CA | 1456 | C | O4'-C1' | 10.55 | 1.55 | 1.41 |
| 59 | Bh | 20 | HIS | CA-CB | 10.55 | 1.77 | 1.53 |
| 81 | DA | 840 | C | O4'-C1' | 10.55 | 1.55 | 1.41 |
| 81 | DA | 2863 | G | O4'-C1' | 10.55 | 1.55 | 1.41 |
| 78 | CA | 1656 | U | O4'-C1' | 10.54 | 1.55 | 1.41 |
| 81 | DA | 1669 | C | O4'-C1' | 10.54 | 1.55 | 1.41 |
| 81 | DA | 2672 | G | C2'-C1' | -10.54 | 1.41 | 1.53 |
| 81 | DA | 2950 | G | O4'-C1' | -10.54 | 1.27 | 1.41 |
| 78 | CA | 852 | C | O4'-C1' | 10.54 | 1.55 | 1.41 |
| 81 | DA | 2778 | G | C2'-C1' | -10.54 | 1.41 | 1.53 |
| 81 | DA | 704 | U | O3'-P | -10.54 | 1.48 | 1.61 |
| 81 | DA | 2775 | U | C2'-C1' | 10.54 | 1.65 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2175 | U | C4'-C3' | -10.53 | 1.41 | 1.53 |
| 81 | DA | 2944 | U | O4'-C1' | 10.53 | 1.55 | 1.41 |
| 81 | DA | 1092 | C | O4'-C1' | 10.52 | 1.55 | 1.41 |
| 81 | DA | 8 | C | O4'-C1' | 10.52 | 1.55 | 1.41 |
| 81 | DA | 3039 | C | O4'-C1' | 10.52 | 1.55 | 1.41 |
| 81 | DA | 992 | A | C2'-C1' | 10.52 | 1.65 | 1.53 |
| 78 | CA | 899 | G | C2'-C1' | -10.51 | 1.41 | 1.53 |
| 81 | DA | 815 | G | C2'-C1' | -10.51 | 1.41 | 1.53 |
| 78 | CA | 1408 | G | C2'-C1' | 10.51 | 1.65 | 1.53 |
| 81 | DA | 2266 | U | C2'-C1' | -10.51 | 1.41 | 1.53 |
| 81 | DA | 1480 | G | O4'-C1' | -10.51 | 1.27 | 1.41 |
| 78 | CA | 1 | U | P-O5' | -10.50 | 1.49 | 1.59 |
| 81 | DA | 84 | U | C2'-C1' | -10.50 | 1.41 | 1.53 |
| 81 | DA | 766 | U | C4'-C3' | 10.50 | 1.64 | 1.53 |
| 78 | CA | 142 | G | O4'-C1' | 10.49 | 1.55 | 1.41 |
| 81 | DA | 435 | C | C2'-C1' | -10.49 | 1.41 | 1.53 |
| 81 | DA | 1362 | G | C2'-C1' | -10.49 | 1.41 | 1.53 |
| 81 | DA | 606 | C | C2'-C1' | -10.49 | 1.41 | 1.53 |
| 81 | DA | 2651 | G | C2'-C1' | -10.48 | 1.41 | 1.53 |
| 83 | DC | 115 | A | O4'-C1' | -10.48 | 1.28 | 1.41 |
| 12 | AK | 125 | SER | CB-OG | -10.48 | 1.28 | 1.42 |
| 78 | CA | 1629 | G | C2'-C1' | -10.48 | 1.41 | 1.53 |
| 81 | DA | 816 | A | O4'-C1' | 10.48 | 1.55 | 1.41 |
| 78 | CA | 548 | G | O4'-C1' | 10.47 | 1.55 | 1.41 |
| 81 | DA | 868 | C | O4'-C1' | 10.47 | 1.55 | 1.41 |
| 81 | DA | 2202 | C | C2'-C1' | -10.47 | 1.41 | 1.53 |
| 78 | CA | 273 | G | O4'-C1' | 10.46 | 1.55 | 1.41 |
| 81 | DA | 1036 | A | C2'-C1' | 10.46 | 1.64 | 1.53 |
| 79 | CB | 45 | G | O4'-C1' | 10.46 | 1.55 | 1.41 |
| 81 | DA | 2208 | A | C2'-C1' | 10.46 | 1.64 | 1.53 |
| 81 | DA | 1531 | C | C2'-C1' | -10.46 | 1.41 | 1.53 |
| 81 | DA | 344 | A | O4'-C1' | 10.46 | 1.55 | 1.41 |
| 81 | DA | 1084 | A | C2'-C1' | -10.46 | 1.41 | 1.53 |
| 81 | DA | 2662 | G | O4'-C1' | 10.46 | 1.55 | 1.41 |
| 78 | CA | 1279 | C | O4'-C1' | 10.45 | 1.55 | 1.41 |
| 81 | DA | 3375 | A | O4'-C1' | 10.45 | 1.55 | 1.41 |
| 81 | DA | 3308 | C | O4'-C1' | 10.45 | 1.55 | 1.41 |
| 81 | DA | 1499 | C | O4'-C1' | 10.44 | 1.55 | 1.41 |
| 81 | DA | 2750 | U | C2'-C1' | -10.44 | 1.41 | 1.53 |
| 81 | DA | 263 | C | O4'-C1' | 10.43 | 1.55 | 1.41 |
| 81 | DA | 2174 | G | C4'-C3' | -10.43 | 1.41 | 1.53 |
| 81 | DA | 3340 | G | C2'-C1' | -10.43 | 1.41 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 1233 | G | C2'-C1' | 10.43 | 1.64 | 1.53 |
| 81 | DA | 584 | G | C2'-C1' | -10.43 | 1.41 | 1.53 |
| 81 | DA | 2819 | A | C2'-C1' | -10.42 | 1.41 | 1.53 |
| 81 | DA | 3253 | G | O4'-C1' | 10.42 | 1.55 | 1.41 |
| 81 | DA | 1873 | U | C2'-C1' | -10.42 | 1.41 | 1.53 |
| 78 | CA | 1228 | G | O4'-C1' | 10.42 | 1.55 | 1.41 |
| 78 | CA | 28 | A | C2'-C1' | -10.42 | 1.41 | 1.53 |
| 81 | DA | 3006 | A | O4'-C1' | 10.41 | 1.55 | 1.41 |
| 81 | DA | 786 | A | C2'-C1' | 10.41 | 1.64 | 1.53 |
| 81 | DA | 2020 | A | O4'-C1' | 10.41 | 1.55 | 1.41 |
| 81 | DA | 1258 | U | P-O5' | -10.40 | 1.49 | 1.59 |
| 81 | DA | 2390 | A | C2'-C1' | -10.40 | 1.42 | 1.53 |
| 78 | CA | 1547 | A | P-O5' | 10.40 | 1.70 | 1.59 |
| 81 | DA | 2364 | G | C2'-C1' | -10.40 | 1.42 | 1.53 |
| 81 | DA | 1586 | G | C2'-C1' | -10.40 | 1.42 | 1.53 |
| 81 | DA | 1796 | G | C2'-C1' | -10.40 | 1.42 | 1.53 |
| 78 | CA | 38 | C | O4'-C1' | 10.39 | 1.55 | 1.41 |
| 81 | DA | 586 | C | O4'-C1' | 10.39 | 1.55 | 1.41 |
| 81 | DA | 424 | G | O4'-C1' | 10.39 | 1.55 | 1.41 |
| 81 | DA | 2671 | A | O4'-C1' | 10.39 | 1.55 | 1.41 |
| 81 | DA | 547 | G | C2'-C1' | -10.39 | 1.42 | 1.53 |
| 81 | DA | 793 | C | O4'-C1' | 10.39 | 1.55 | 1.41 |
| 37 | BH | 129 | PRO | N-CA | -10.39 | 1.29 | 1.47 |
| 81 | DA | 2627 | C | O4'-C1' | 10.38 | 1.55 | 1.41 |
| 78 | CA | 1599 | C | O4'-C1' | 10.38 | 1.55 | 1.41 |
| 82 | DB | 106 | C | C2'-C1' | -10.38 | 1.42 | 1.53 |
| 78 | CA | 1134 | C | O4'-C1' | 10.37 | 1.55 | 1.41 |
| 81 | DA | 393 | U | C2'-C1' | -10.37 | 1.42 | 1.53 |
| 78 | CA | 39 | A | O4'-C1' | 10.37 | 1.55 | 1.41 |
| 81 | DA | 977 | C | O4'-C1' | 10.37 | 1.55 | 1.41 |
| 78 | CA | 1376 | C | O4'-C1' | 10.37 | 1.55 | 1.41 |
| 81 | DA | 1846 | C | O4'-C1' | 10.37 | 1.55 | 1.41 |
| 81 | DA | 1141 | C | O4'-C1' | 10.37 | 1.55 | 1.41 |
| 81 | DA | 193 | C | C2'-C1' | -10.36 | 1.42 | 1.53 |
| 81 | DA | 208 | C | C2'-C1' | -10.36 | 1.42 | 1.53 |
| 81 | DA | 254 | A | O4'-C1' | 10.36 | 1.55 | 1.41 |
| 4 | AD | 93 | ASP | CA-CB | 10.36 | 1.76 | 1.53 |
| 78 | CA | 330 | G | C2'-C1' | -10.36 | 1.42 | 1.53 |
| 81 | DA | 2886 | U | O4'-C1' | -10.36 | 1.28 | 1.41 |
| 81 | DA | 1671 | C | O4'-C1' | 10.36 | 1.55 | 1.41 |
| 78 | CA | 1365 | C | O4'-C1' | 10.35 | 1.55 | 1.41 |
| 78 | CA | 1195 | C | O4'-C1' | 10.35 | 1.55 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 408 | A | C2'-C1' | -10.35 | 1.42 | 1.53 |
| 78 | CA | 1202 | A | O4'-C1' | -10.34 | 1.28 | 1.41 |
| 81 | DA | 1745 | C | O4'-C1' | 10.34 | 1.55 | 1.41 |
| 81 | DA | 2750 | U | O4'-C1' | 10.34 | 1.55 | 1.41 |
| 78 | CA | 1327 | C | O4'-C1' | 10.34 | 1.55 | 1.41 |
| 81 | DA | 73 | C | C2'-C1' | 10.34 | 1.64 | 1.53 |
| 81 | DA | 849 | C | O4'-C1' | 10.34 | 1.55 | 1.41 |
| 81 | DA | 2800 | G | C2'-C1' | 10.34 | 1.64 | 1.53 |
| 81 | DA | 141 | C | C2'-C1' | -10.33 | 1.42 | 1.53 |
| 78 | CA | 1090 | C | C2'-C1' | -10.33 | 1.42 | 1.53 |
| 78 | CA | 1794 | A | C2'-C1' | 10.33 | 1.64 | 1.53 |
| 81 | DA | 82 | C | O4'-C1' | 10.33 | 1.55 | 1.41 |
| 81 | DA | 413 | U | O4'-C1' | 10.33 | 1.55 | 1.41 |
| 81 | DA | 2051 | G | O4'-C1' | 10.33 | 1.55 | 1.41 |
| 81 | DA | 1224 | C | O4'-C1' | 10.33 | 1.55 | 1.41 |
| 81 | DA | 1383 | G | C2'-C1' | -10.33 | 1.42 | 1.53 |
| 81 | DA | 1814 | A | C2'-C1' | 10.33 | 1.64 | 1.53 |
| 81 | DA | 2174 | G | C5'-C4' | 10.32 | 1.63 | 1.51 |
| 81 | DA | 460 | C | O4'-C1' | 10.32 | 1.55 | 1.41 |
| 81 | DA | 1118 | C | O4'-C1' | 10.32 | 1.55 | 1.41 |
| 83 | DC | 9 | C | O4'-C1' | 10.32 | 1.55 | 1.41 |
| 81 | DA | 1547 | G | O4'-C1' | 10.31 | 1.55 | 1.41 |
| 81 | DA | 2738 | A | C2'-C1' | -10.31 | 1.42 | 1.53 |
| 78 | CA | 553 | G | C2'-C1' | -10.31 | 1.42 | 1.53 |
| 81 | DA | 2452 | G | O4'-C1' | 10.31 | 1.55 | 1.41 |
| 81 | DA | 3001 | C | C2'-C1' | -10.31 | 1.42 | 1.53 |
| 4 | AD | 153 | ASN | CA-CB | 10.30 | 1.79 | 1.53 |
| 81 | DA | 2794 | G | C2'-C1' | -10.30 | 1.42 | 1.53 |
| 81 | DA | 171 | G | C2'-C1' | -10.30 | 1.42 | 1.53 |
| 81 | DA | 2207 | A | C2'-C1' | 10.29 | 1.64 | 1.53 |
| 81 | DA | 3031 | G | O4'-C1' | 10.29 | 1.55 | 1.41 |
| 78 | CA | 1373 | C | O4'-C1' | 10.29 | 1.55 | 1.41 |
| 81 | DA | 1086 | C | C2'-C1' | -10.29 | 1.42 | 1.53 |
| 81 | DA | 1423 | C | C2'-C1' | -10.29 | 1.42 | 1.53 |
| 81 | DA | 2104 | A | O4'-C1' | 10.29 | 1.55 | 1.41 |
| 78 | CA | 282 | C | O4'-C1' | 10.28 | 1.55 | 1.41 |
| 81 | DA | 1016 | C | O4'-C1' | 10.28 | 1.55 | 1.41 |
| 81 | DA | 2816 | G | O4'-C1' | 10.28 | 1.55 | 1.41 |
| 78 | CA | 1593 | A | O4'-C1' | 10.28 | 1.55 | 1.41 |
| 78 | CA | 847 | A | O4'-C1' | 10.28 | 1.55 | 1.41 |
| 78 | CA | 1758 | U | C2'-C1' | -10.28 | 1.42 | 1.53 |
| 81 | DA | 3060 | C | O4'-C1' | 10.28 | 1.55 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1548 | C | O4'-C1' | 10.28 | 1.55 | 1.41 |
| 78 | CA | 1199 | G | O4'-C1' | -10.27 | 1.28 | 1.41 |
| 81 | DA | 3321 | C | O4'-C1' | 10.27 | 1.55 | 1.41 |
| 81 | DA | 3032 | A | O4'-C1' | 10.27 | 1.55 | 1.41 |
| 78 | CA | 573 | C | C2'-C1' | -10.27 | 1.42 | 1.53 |
| 78 | CA | 616 | G | C2'-C1' | -10.27 | 1.42 | 1.53 |
| 82 | DB | 100 | U | O4'-C1' | 10.26 | 1.54 | 1.41 |
| 78 | CA | 1439 | C | C2'-C1' | -10.26 | 1.42 | 1.53 |
| 81 | DA | 882 | A | C2'-C1' | -10.26 | 1.42 | 1.53 |
| 81 | DA | 2331 | C | C2'-C1' | -10.26 | 1.42 | 1.53 |
| 81 | DA | 2442 | G | O4'-C1' | 10.26 | 1.54 | 1.41 |
| 81 | DA | 3061 | G | C2'-C1' | -10.26 | 1.42 | 1.53 |
| 78 | CA | 300 | A | O4'-C1' | 10.26 | 1.54 | 1.41 |
| 81 | DA | 712 | G | C2'-C1' | -10.26 | 1.42 | 1.53 |
| 81 | DA | 3384 | U | O4'-C1' | 10.26 | 1.54 | 1.41 |
| 81 | DA | 1265 | U | O4'-C1' | 10.25 | 1.54 | 1.41 |
| 81 | DA | 321 | C | O4'-C1' | 10.25 | 1.54 | 1.41 |
| 81 | DA | 1341 | U | O4'-C1' | 10.25 | 1.54 | 1.41 |
| 81 | DA | 2861 | U | C2'-C1' | -10.25 | 1.42 | 1.53 |
| 82 | DB | 98 | U | C5'-C4' | 10.25 | 1.63 | 1.51 |
| 81 | DA | 582 | G | C2'-C1' | -10.24 | 1.42 | 1.53 |
| 34 | BE | 124 | GLY | CA-C | -10.23 | 1.35 | 1.51 |
| 81 | DA | 1894 | U | O4'-C1' | 10.23 | 1.54 | 1.41 |
| 81 | DA | 3076 | C | C2'-C1' | -10.22 | 1.42 | 1.53 |
| 83 | DC | 110 | C | O4'-C1' | 10.22 | 1.54 | 1.41 |
| 81 | DA | 1452 | A | O4'-C1' | 10.22 | 1.54 | 1.41 |
| 78 | CA | 1529 | C | C2'-C1' | -10.21 | 1.42 | 1.53 |
| 81 | DA | 1437 | C | O4'-C1' | 10.21 | 1.54 | 1.41 |
| 83 | DC | 27 | A | C2'-C1' | -10.21 | 1.42 | 1.53 |
| 81 | DA | 2475 | G | C2'-C1' | 10.21 | 1.64 | 1.53 |
| 61 | Bj | 8 | TYR | N-CA | 10.21 | 1.66 | 1.46 |
| 78 | CA | 109 | G | C2'-C1' | -10.21 | 1.42 | 1.53 |
| 78 | CA | 1440 | C | O4'-C1' | 10.21 | 1.54 | 1.41 |
| 83 | DC | 32 | U | C2'-C1' | -10.20 | 1.42 | 1.53 |
| 81 | DA | 1503 | A | C2'-C1' | -10.20 | 1.42 | 1.53 |
| 78 | CA | 1371 | A | O4'-C1' | 10.20 | 1.54 | 1.41 |
| 81 | DA | 3339 | A | C2'-C1' | -10.20 | 1.42 | 1.53 |
| 81 | DA | 1778 | G | O4'-C1' | 10.20 | 1.54 | 1.41 |
| 78 | CA | 855 | A | C2'-C1' | -10.19 | 1.42 | 1.53 |
| 82 | DB | 119 | C | C2'-C1' | -10.19 | 1.42 | 1.53 |
| 81 | DA | 319 | A | C2'-C1' | -10.19 | 1.42 | 1.53 |
| 81 | DA | 1541 | G | O4'-C1' | 10.19 | 1.54 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 3102 | G | C2'-C1' | -10.19 | 1.42 | 1.53 |
| 83 | DC | 25 | G | C2'-C1' | 10.18 | 1.64 | 1.53 |
| 81 | DA | 652 | G | C2'-C1' | -10.18 | 1.42 | 1.53 |
| 81 | DA | 2834 | G | C2'-C1' | -10.18 | 1.42 | 1.53 |
| 81 | DA | 27 | C | C2'-C1' | -10.18 | 1.42 | 1.53 |
| 37 | BH | 229 | VAL | N-CA | -10.17 | 1.26 | 1.46 |
| 78 | CA | 587 | C | C2'-C1' | -10.17 | 1.42 | 1.53 |
| 78 | CA | 1367 | G | C2'-C1' | -10.17 | 1.42 | 1.53 |
| 81 | DA | 1980 | C | O4'-C1' | 10.17 | 1.54 | 1.41 |
| 81 | DA | 2809 | C | O4'-C1' | 10.16 | 1.54 | 1.41 |
| 78 | CA | 1683 | C | O4'-C1' | 10.16 | 1.54 | 1.41 |
| 78 | CA | 418 | G | C2'-C1' | -10.16 | 1.42 | 1.53 |
| 81 | DA | 3314 | A | C2'-C1' | -10.16 | 1.42 | 1.53 |
| 81 | DA | 539 | C | O4'-C1' | 10.15 | 1.54 | 1.41 |
| 81 | DA | 802 | C | C2'-C1' | -10.15 | 1.42 | 1.53 |
| 81 | DA | 1951 | C | C2'-C1' | -10.15 | 1.42 | 1.53 |
| 81 | DA | 2422 | C | O4'-C1' | 10.15 | 1.54 | 1.41 |
| 81 | DA | 1483 | G | O4'-C1' | -10.15 | 1.28 | 1.41 |
| 81 | DA | 2898 | G | O4'-C1' | 10.15 | 1.54 | 1.41 |
| 81 | DA | 2929 | C | O4'-C1' | 10.15 | 1.54 | 1.41 |
| 81 | DA | 3341 | U | C2'-C1' | -10.15 | 1.42 | 1.53 |
| 82 | DB | 10 | A | O4'-C1' | 10.14 | 1.54 | 1.41 |
| 78 | CA | 444 | C | C2'-C1' | -10.14 | 1.42 | 1.53 |
| 81 | DA | 2153 | U | C2'-C1' | -10.14 | 1.42 | 1.53 |
| 79 | CB | 29 | C | O4'-C1' | 10.14 | 1.54 | 1.41 |
| 81 | DA | 2278 | C | O4'-C1' | 10.14 | 1.54 | 1.41 |
| 81 | DA | 2025 | G | O4'-C1' | -10.13 | 1.28 | 1.41 |
| 78 | CA | 195 | G | O4'-C1' | 10.13 | 1.54 | 1.41 |
| 81 | DA | 1239 | C | C2'-C1' | -10.13 | 1.42 | 1.53 |
| 81 | DA | 890 | C | O4'-C1' | 10.13 | 1.54 | 1.41 |
| 81 | DA | 3301 | U | O4'-C1' | 10.13 | 1.54 | 1.41 |
| 78 | CA | 1418 | G | C2'-C1' | -10.12 | 1.42 | 1.53 |
| 81 | DA | 1589 | A | C2'-C1' | -10.12 | 1.42 | 1.53 |
| 81 | DA | 2829 | U | O4'-C1' | 10.12 | 1.54 | 1.41 |
| 78 | CA | 880 | C | O4'-C1' | 10.12 | 1.54 | 1.41 |
| 78 | CA | 1439 | C | O4'-C1' | 10.12 | 1.54 | 1.41 |
| 81 | DA | 3015 | G | C2'-C1' | -10.12 | 1.42 | 1.53 |
| 78 | CA | 1679 | G | O4'-C1' | 10.12 | 1.54 | 1.41 |
| 81 | DA | 2015 | C | O4'-C1' | 10.11 | 1.54 | 1.41 |
| 81 | DA | 3082 | C | C2'-C1' | -10.11 | 1.42 | 1.53 |
| 81 | DA | 2698 | G | C2'-C1' | -10.11 | 1.42 | 1.53 |
| 78 | CA | 889 | U | C2'-C1' | -10.10 | 1.42 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 1299 | G | O4'-C1' | 10.10 | 1.54 | 1.41 |
| 78 | CA | 1636 | C | O4'-C1' | 10.10 | 1.54 | 1.41 |
| 81 | DA | 75 | G | C2'-C1' | -10.10 | 1.42 | 1.53 |
| 83 | DC | 51 | G | O4'-C1' | -10.10 | 1.28 | 1.41 |
| 78 | CA | 1686 | C | O4'-C1' | 10.10 | 1.54 | 1.41 |
| 81 | DA | 2561 | A | P-OP2 | 10.10 | 1.66 | 1.49 |
| 81 | DA | 250 | U | C5'-C4' | 10.10 | 1.63 | 1.51 |
| 81 | DA | 1000 | C | C2'-C1' | -10.10 | 1.42 | 1.53 |
| 81 | DA | 2047 | A | O4'-C1' | 10.10 | 1.54 | 1.41 |
| 81 | DA | 2230 | C | C2'-C1' | -10.10 | 1.42 | 1.53 |
| 81 | DA | 2306 | C | C2'-C1' | -10.10 | 1.42 | 1.53 |
| 78 | CA | 151 | G | O4'-C1' | 10.09 | 1.54 | 1.41 |
| 81 | DA | 458 | U | C2'-C1' | -10.09 | 1.42 | 1.53 |
| 81 | DA | 1867 | A | C2'-C1' | 10.09 | 1.64 | 1.53 |
| 81 | DA | 1996 | C | O4'-C1' | 10.09 | 1.54 | 1.41 |
| 81 | DA | 2218 | G | C2'-C1' | -10.09 | 1.42 | 1.53 |
| 81 | DA | 3101 | G | C2'-C1' | -10.08 | 1.42 | 1.53 |
| 81 | DA | 613 | G | C2'-C1' | -10.08 | 1.42 | 1.53 |
| 81 | DA | 2917 | G | O4'-C1' | -10.08 | 1.28 | 1.41 |
| 81 | DA | 2179 | C | C2'-C1' | -10.07 | 1.42 | 1.53 |
| 58 | Bg | 108 | VAL | N-CA | 10.07 | 1.66 | 1.46 |
| 78 | CA | 685 | A | C2'-C1' | -10.07 | 1.42 | 1.53 |
| 81 | DA | 1695 | U | C2'-C1' | 10.07 | 1.64 | 1.53 |
| 78 | CA | 1197 | C | O4'-C1' | 10.07 | 1.54 | 1.41 |
| 78 | CA | 833 | U | O4'-C1' | -10.07 | 1.28 | 1.41 |
| 78 | CA | 1653 | C | O4'-C1' | 10.07 | 1.54 | 1.41 |
| 78 | CA | 1644 | C | O4'-C1' | 10.06 | 1.54 | 1.41 |
| 81 | DA | 2696 | A | C2'-C1' | -10.06 | 1.42 | 1.53 |
| 81 | DA | 2927 | C | O4'-C1' | 10.06 | 1.54 | 1.41 |
| 5 | AC | 163 | PRO | N-CD | -10.06 | 1.33 | 1.47 |
| 78 | CA | 1575 | G | C2'-C1' | -10.06 | 1.42 | 1.53 |
| 81 | DA | 2735 | U | O4'-C1' | 10.06 | 1.54 | 1.41 |
| 78 | CA | 119 | A | O4'-C1' | 10.06 | 1.54 | 1.41 |
| 78 | CA | 411 | C | C2'-C1' | 10.05 | 1.64 | 1.53 |
| 81 | DA | 2051 | G | C2'-C1' | -10.05 | 1.42 | 1.53 |
| 81 | DA | 3039 | C | C2'-C1' | -10.06 | 1.42 | 1.53 |
| 78 | CA | 1470 | C | C2'-C1' | -10.05 | 1.42 | 1.53 |
| 82 | DB | 145 | U | O4'-C1' | 10.05 | 1.54 | 1.41 |
| 78 | CA | 839 | U | C2'-C1' | 10.04 | 1.64 | 1.53 |
| 81 | DA | 2210 | G | C2'-C1' | -10.04 | 1.42 | 1.53 |
| 78 | CA | 47 | A | P-O5' | -10.04 | 1.49 | 1.59 |
| 81 | DA | 3145 | C | P-O5' | -10.04 | 1.49 | 1.59 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 33 | BD | 78 | GLY | N-CA | 10.04 | 1.61 | 1.46 |
| 81 | DA | 201 | A | O4'-C1' | 10.04 | 1.54 | 1.41 |
| 60 | Bi | 78 | GLY | N-CA | -10.03 | 1.31 | 1.46 |
| 81 | DA | 159 | A | C2'-C1' | 10.03 | 1.64 | 1.53 |
| 81 | DA | 312 | C | C2'-C1' | -10.03 | 1.42 | 1.53 |
| 81 | DA | 81 | C | O4'-C1' | 10.03 | 1.54 | 1.41 |
| 78 | CA | 1719 | A | C2'-C1' | -10.03 | 1.42 | 1.53 |
| 13 | AL | 35 | GLY | CA-C | -10.03 | 1.35 | 1.51 |
| 82 | DB | 18 | U | O4'-C1' | 10.02 | 1.54 | 1.41 |
| 82 | DB | 54 | A | C2'-C1' | -10.02 | 1.42 | 1.53 |
| 78 | CA | 834 | G | C2'-C1' | -10.02 | 1.42 | 1.53 |
| 81 | DA | 2934 | A | O4'-C1' | -10.02 | 1.28 | 1.41 |
| 78 | CA | 1241 | G | C2'-C1' | 10.01 | 1.64 | 1.53 |
| 81 | DA | 1645 | U | O4'-C1' | 10.01 | 1.54 | 1.41 |
| 81 | DA | 3053 | G | C2'-C1' | -10.01 | 1.42 | 1.53 |
| 48 | BW | 90 | ARG | CA-CB | 10.01 | 1.75 | 1.53 |
| 78 | CA | 1174 | C | C2'-C1' | -10.00 | 1.42 | 1.53 |
| 81 | DA | 3005 | A | O4'-C1' | -10.00 | 1.28 | 1.41 |
| 34 | BE | 116 | TYR | CE1-CZ | -9.99 | 1.25 | 1.38 |
| 81 | DA | 244 | G | O4'-C1' | 9.99 | 1.54 | 1.41 |
| 81 | DA | 918 | C | O4'-C1' | 9.99 | 1.54 | 1.41 |
| 81 | DA | 1270 | A | O4'-C1' | -9.99 | 1.28 | 1.41 |
| 81 | DA | 3081 | C | O4'-C1' | 9.99 | 1.54 | 1.41 |
| 81 | DA | 1155 | C | O4'-C1' | 9.99 | 1.54 | 1.41 |
| 26 | AZ | 44 | PHE | CA-CB | -9.98 | 1.31 | 1.53 |
| 81 | DA | 2812 | C | O4'-C1' | 9.98 | 1.54 | 1.41 |
| 81 | DA | 759 | U | C2'-C1' | -9.98 | 1.42 | 1.53 |
| 81 | DA | 2228 | A | C2'-C1' | 9.98 | 1.64 | 1.53 |
| 81 | DA | 2376 | G | C2'-C1' | -9.97 | 1.42 | 1.53 |
| 79 | CB | 62 | C | O4'-C1' | 9.97 | 1.54 | 1.41 |
| 81 | DA | 320 | G | C2'-C1' | -9.97 | 1.42 | 1.53 |
| 78 | CA | 663 | U | O4'-C1' | 9.97 | 1.54 | 1.41 |
| 81 | DA | 302 | U | C2'-C1' | -9.96 | 1.42 | 1.53 |
| 81 | DA | 1431 | G | C2'-C1' | -9.96 | 1.42 | 1.53 |
| 78 | CA | 977 | A | O4'-C1' | 9.96 | 1.54 | 1.41 |
| 81 | DA | 976 | U | C2'-C1' | 9.96 | 1.64 | 1.53 |
| 78 | CA | 1124 | A | C2'-C1' | 9.96 | 1.64 | 1.53 |
| 78 | CA | 1478 | G | C2'-C1' | -9.96 | 1.42 | 1.53 |
| 81 | DA | 640 | U | O4'-C1' | 9.96 | 1.54 | 1.41 |
| 81 | DA | 507 | U | O4'-C1' | 9.95 | 1.54 | 1.41 |
| 81 | DA | 2310 | U | O4'-C1' | 9.95 | 1.54 | 1.41 |
| 81 | DA | 643 | U | C2'-C1' | -9.94 | 1.42 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1699 | A | C2'-C1' | 9.94 | 1.64 | 1.53 |
| 82 | DB | 8 | C | O4'-C1' | 9.94 | 1.54 | 1.41 |
| 82 | DB | 53 | A | C2'-C1' | -9.94 | 1.42 | 1.53 |
| 81 | DA | 1590 | G | C2'-C1' | -9.94 | 1.42 | 1.53 |
| 78 | CA | 112 | A | O4'-C1' | 9.93 | 1.54 | 1.41 |
| 81 | DA | 2317 | A | O4'-C1' | 9.93 | 1.54 | 1.41 |
| 25 | AY | 57 | MET | N-CA | -9.93 | 1.26 | 1.46 |
| 78 | CA | 220 | A | O4'-C1' | 9.93 | 1.54 | 1.41 |
| 78 | CA | 392 | G | C2'-C1' | -9.93 | 1.42 | 1.53 |
| 78 | CA | 1370 | U | O4'-C1' | 9.93 | 1.54 | 1.41 |
| 81 | DA | 2515 | A | C2'-C1' | -9.93 | 1.42 | 1.53 |
| 81 | DA | 847 | A | O4'-C1' | 9.93 | 1.54 | 1.41 |
| 81 | DA | 1237 | G | C2'-C1' | -9.93 | 1.42 | 1.53 |
| 81 | DA | 1779 | C | O4'-C1' | 9.93 | 1.54 | 1.41 |
| 81 | DA | 2830 | G | O4'-C1' | 9.92 | 1.54 | 1.41 |
| 78 | CA | 305 | C | C2'-C1' | -9.92 | 1.42 | 1.53 |
| 81 | DA | 543 | C | O4'-C1' | 9.92 | 1.54 | 1.41 |
| 81 | DA | 614 | C | C2'-C1' | -9.92 | 1.42 | 1.53 |
| 81 | DA | 1162 | U | C2'-C1' | -9.92 | 1.42 | 1.53 |
| 81 | DA | 1791 | C | O4'-C1' | 9.92 | 1.54 | 1.41 |
| 78 | CA | 1788 | G | C2'-C1' | -9.92 | 1.42 | 1.53 |
| 81 | DA | 3025 | C | C2'-C1' | -9.91 | 1.42 | 1.53 |
| 81 | DA | 650 | C | C2'-C1' | -9.91 | 1.42 | 1.53 |
| 81 | DA | 2748 | A | C2'-C1' | 9.90 | 1.64 | 1.53 |
| 81 | DA | 1850 | A | C2'-C1' | 9.90 | 1.64 | 1.53 |
| 81 | DA | 1610 | G | C2'-C1' | -9.90 | 1.42 | 1.53 |
| 81 | DA | 3343 | G | C2'-C1' | -9.90 | 1.42 | 1.53 |
| 82 | DB | 103 | G | O4'-C1' | 9.89 | 1.54 | 1.41 |
| 81 | DA | 2652 | U | C2'-C1' | -9.89 | 1.42 | 1.53 |
| 81 | DA | 2739 | A | C2'-C1' | -9.89 | 1.42 | 1.53 |
| 81 | DA | 178 | U | O4'-C1' | 9.89 | 1.54 | 1.41 |
| 81 | DA | 179 | C | C2'-C1' | -9.89 | 1.42 | 1.53 |
| 81 | DA | 2400 | G | C2'-C1' | -9.89 | 1.42 | 1.53 |
| 79 | CB | 69 | G | C2'-C1' | -9.88 | 1.42 | 1.53 |
| 78 | CA | 950 | C | C2'-C1' | -9.88 | 1.42 | 1.53 |
| 81 | DA | 872 | U | O4'-C1' | 9.88 | 1.54 | 1.41 |
| 78 | CA | 271 | A | C2'-C1' | -9.88 | 1.42 | 1.53 |
| 81 | DA | 2476 | C | C2'-C1' | -9.88 | 1.42 | 1.53 |
| 2 | AA | 10 | THR | N-CA | -9.88 | 1.26 | 1.46 |
| 81 | DA | 1445 | U | O4'-C1' | 9.87 | 1.54 | 1.41 |
| 81 | DA | 2311 | G | O4'-C1' | 9.88 | 1.54 | 1.41 |
| 81 | DA | 2982 | A | C2'-C1' | -9.87 | 1.42 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 74 | BQ | 158 | ARG | CZ-NH2 | 9.87 | 1.45 | 1.33 |
| 78 | CA | 623 | A | O4'-C1' | -9.87 | 1.28 | 1.41 |
| 81 | DA | 2306 | C | O4'-C1' | 9.87 | 1.54 | 1.41 |
| 81 | DA | 1095 | U | O3'-P | -9.87 | 1.49 | 1.61 |
| 81 | DA | 2390 | A | O4'-C1' | 9.87 | 1.54 | 1.41 |
| 81 | DA | 1363 | A | O4'-C1' | 9.86 | 1.54 | 1.41 |
| 10 | AI | 141 | SER | N-CA | -9.86 | 1.26 | 1.46 |
| 78 | CA | 1579 | U | O4'-C1' | 9.86 | 1.54 | 1.41 |
| 81 | DA | 668 | G | C2'-C1' | -9.86 | 1.42 | 1.53 |
| 81 | DA | 1247 | U | C2'-C1' | 9.86 | 1.64 | 1.53 |
| 78 | CA | 435 | C | C2'-C1' | -9.86 | 1.42 | 1.53 |
| 81 | DA | 1977 | C | C2'-C1' | -9.86 | 1.42 | 1.53 |
| 81 | DA | 3352 | U | O4'-C1' | 9.86 | 1.54 | 1.41 |
| 44 | BO | 3 | SER | CA-CB | -9.85 | 1.38 | 1.52 |
| 81 | DA | 1735 | G | C2'-C1' | -9.85 | 1.42 | 1.53 |
| 17 | AQ | 82 | ASP | N-CA | -9.85 | 1.26 | 1.46 |
| 78 | CA | 1139 | A | C2'-C1' | -9.85 | 1.42 | 1.53 |
| 78 | CA | 1476 | C | C2'-C1' | 9.85 | 1.64 | 1.53 |
| 81 | DA | 3248 | C | C2'-C1' | -9.85 | 1.42 | 1.53 |
| 81 | DA | 1331 | U | O4'-C1' | 9.85 | 1.54 | 1.41 |
| 81 | DA | 2304 | C | C2'-C1' | -9.85 | 1.42 | 1.53 |
| 83 | DC | 39 | C | O4'-C1' | 9.85 | 1.54 | 1.41 |
| 81 | DA | 2673 | A | O4'-C1' | 9.85 | 1.54 | 1.41 |
| 81 | DA | 2144 | A | C2'-C1' | -9.84 | 1.42 | 1.53 |
| 81 | DA | 714 | G | C2'-C1' | -9.84 | 1.42 | 1.53 |
| 81 | DA | 1105 | A | C2'-C1' | 9.84 | 1.64 | 1.53 |
| 79 | CB | 73 | C | O4'-C1' | 9.83 | 1.54 | 1.41 |
| 81 | DA | 3147 | G | O4'-C1' | 9.83 | 1.54 | 1.41 |
| 78 | CA | 1624 | C | C2'-C1' | -9.83 | 1.42 | 1.53 |
| 78 | CA | 271 | A | O4'-C1' | 9.83 | 1.54 | 1.41 |
| 81 | DA | 535 | G | O4'-C1' | 9.83 | 1.54 | 1.41 |
| 81 | DA | 1201 | C | C2'-C1' | -9.83 | 1.42 | 1.53 |
| 81 | DA | 1336 | U | O4'-C1' | 9.82 | 1.54 | 1.41 |
| 78 | CA | 609 | U | C2'-C1' | -9.82 | 1.42 | 1.53 |
| 81 | DA | 2609 | A | O4'-C1' | 9.82 | 1.54 | 1.41 |
| 11 | AJ | 85 | ARG | CD-NE | 9.82 | 1.63 | 1.46 |
| 78 | CA | 178 | U | O3'-P | -9.82 | 1.49 | 1.61 |
| 78 | CA | 628 | G | C2'-C1' | -9.82 | 1.42 | 1.53 |
| 81 | DA | 3151 | U | C2'-C1' | 9.82 | 1.64 | 1.53 |
| 81 | DA | 2264 | U | C2'-C1' | -9.81 | 1.42 | 1.53 |
| 81 | DA | 2370 | G | C2'-C1' | -9.81 | 1.42 | 1.53 |
| 78 | CA | 337 | G | O4'-C1' | -9.81 | 1.28 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 743 | C | O4'-C1' | 9.81 | 1.54 | 1.41 |
| 81 | DA | 2813 | A | O4'-C1' | 9.81 | 1.54 | 1.41 |
| 83 | DC | 59 | G | C2'-C1' | -9.81 | 1.42 | 1.53 |
| 83 | DC | 87 | U | C2'-C1' | -9.81 | 1.42 | 1.53 |
| 78 | CA | 1726 | G | C2'-C1' | -9.81 | 1.42 | 1.53 |
| 26 | AZ | 40 | TYR | N-CA | 9.80 | 1.66 | 1.46 |
| 81 | DA | 2583 | C | O4'-C1' | 9.80 | 1.54 | 1.41 |
| 81 | DA | 1132 | C | O4'-C1' | 9.80 | 1.54 | 1.41 |
| 81 | DA | 2676 | A | C2'-C1' | -9.79 | 1.42 | 1.53 |
| 81 | DA | 788 | C | C2'-C1' | -9.79 | 1.42 | 1.53 |
| 81 | DA | 2329 | C | O4'-C1' | 9.79 | 1.54 | 1.41 |
| 78 | CA | 1584 | G | C2'-C1' | -9.79 | 1.42 | 1.53 |
| 78 | CA | 1353 | U | O4'-C1' | 9.79 | 1.54 | 1.41 |
| 78 | CA | 1692 | G | C2'-C1' | -9.78 | 1.42 | 1.53 |
| 5 | AC | 162 | SER | CA-CB | 9.78 | 1.67 | 1.52 |
| 5 | AC | 165 | GLY | N-CA | -9.78 | 1.31 | 1.46 |
| 78 | CA | 1774 | G | C2'-C1' | -9.78 | 1.42 | 1.53 |
| 81 | DA | 2717 | U | O4'-C1' | 9.78 | 1.54 | 1.41 |
| 78 | CA | 223 | U | C2'-C1' | 9.77 | 1.64 | 1.53 |
| 81 | DA | 1406 | A | O4'-C1' | 9.77 | 1.54 | 1.41 |
| 78 | CA | 868 | G | C2'-C1' | -9.77 | 1.42 | 1.53 |
| 78 | CA | 584 | C | C2'-C1' | -9.77 | 1.42 | 1.53 |
| 81 | DA | 693 | A | C2'-C1' | 9.76 | 1.64 | 1.53 |
| 81 | DA | 1392 | G | C2'-C1' | -9.76 | 1.42 | 1.53 |
| 81 | DA | 1545 | A | C2'-C1' | -9.76 | 1.42 | 1.53 |
| 78 | CA | 120 | U | C5'-C4' | 9.76 | 1.63 | 1.51 |
| 81 | DA | 550 | A | C2'-C1' | 9.76 | 1.64 | 1.53 |
| 81 | DA | 1983 | G | C2'-C1' | -9.76 | 1.42 | 1.53 |
| 81 | DA | 1867 | A | O4'-C1' | -9.76 | 1.28 | 1.41 |
| 81 | DA | 3055 | U | C2'-C1' | 9.76 | 1.64 | 1.53 |
| 32 | BC | 298 | PHE | CA-CB | 9.75 | 1.75 | 1.53 |
| 8 | AF | 35 | GLN | N-CA | -9.75 | 1.26 | 1.46 |
| 81 | DA | 2330 | C | O4'-C1' | 9.75 | 1.54 | 1.41 |
| 81 | DA | 1279 | C | O4'-C1' | 9.74 | 1.54 | 1.41 |
| 81 | DA | 1863 | G | O4'-C1' | 9.74 | 1.54 | 1.41 |
| 78 | CA | 1358 | G | C2'-C1' | -9.74 | 1.42 | 1.53 |
| 81 | DA | 1312 | C | O4'-C1' | 9.74 | 1.54 | 1.41 |
| 81 | DA | 3322 | A | C2'-C1' | -9.73 | 1.42 | 1.53 |
| 78 | CA | 1476 | C | C3'-O3' | -9.73 | 1.28 | 1.42 |
| 81 | DA | 1631 | C | O4'-C1' | 9.73 | 1.54 | 1.41 |
| 81 | DA | 1650 | G | O4'-C1' | 9.73 | 1.54 | 1.41 |
| 81 | DA | 1246 | G | C2'-C1' | -9.73 | 1.42 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1445 | U | C2'-C1' | -9.73 | 1.42 | 1.53 |
| 81 | DA | 798 | G | C4'-C3' | -9.72 | 1.42 | 1.53 |
| 81 | DA | 1179 | A | C2'-C1' | 9.72 | 1.64 | 1.53 |
| 81 | DA | 1476 | G | C2'-C1' | -9.72 | 1.42 | 1.53 |
| 81 | DA | 1381 | A | C2'-C1' | -9.71 | 1.42 | 1.53 |
| 81 | DA | 1618 | G | O4'-C1' | 9.72 | 1.54 | 1.41 |
| 81 | DA | 2031 | U | O4'-C1' | 9.72 | 1.54 | 1.41 |
| 26 | AZ | 39 | LEU | N-CA | -9.71 | 1.26 | 1.46 |
| 81 | DA | 1690 | C | O4'-C1' | 9.71 | 1.54 | 1.41 |
| 81 | DA | 2711 | C | C2'-C1' | -9.71 | 1.42 | 1.53 |
| 81 | DA | 63 | A | C2'-C1' | 9.71 | 1.64 | 1.53 |
| 81 | DA | 1154 | A | C2'-C1' | 9.71 | 1.64 | 1.53 |
| 81 | DA | 1259 | A | O4'-C1' | -9.71 | 1.29 | 1.41 |
| 78 | CA | 197 | A | O4'-C1' | 9.70 | 1.54 | 1.41 |
| 81 | DA | 2989 | U | C5'-C4' | 9.70 | 1.62 | 1.51 |
| 78 | CA | 1309 | C | O4'-C1' | 9.70 | 1.54 | 1.41 |
| 78 | CA | 1556 | A | P-O5' | -9.69 | 1.50 | 1.59 |
| 81 | DA | 1693 | C | C2'-C1' | -9.69 | 1.42 | 1.53 |
| 81 | DA | 2449 | A | O4'-C1' | 9.69 | 1.54 | 1.41 |
| 78 | CA | 92 | A | C4'-C3' | -9.69 | 1.42 | 1.53 |
| 60 | Bi | 55 | SER | CA-CB | -9.68 | 1.38 | 1.52 |
| 81 | DA | 1575 | A | C2'-C1' | 9.68 | 1.64 | 1.53 |
| 81 | DA | 2217 | U | O4'-C1' | 9.68 | 1.54 | 1.41 |
| 81 | DA | 814 | U | C2'-C1' | -9.67 | 1.42 | 1.53 |
| 60 | Bi | 108 | GLN | CA-CB | 9.67 | 1.75 | 1.53 |
| 78 | CA | 42 | G | C2'-C1' | -9.66 | 1.42 | 1.53 |
| 83 | DC | 57 | C | O4'-C1' | 9.66 | 1.54 | 1.41 |
| 13 | AL | 34 | LEU | N-CA | 9.66 | 1.65 | 1.46 |
| 31 | BB | 37 | ARG | C-O | -9.66 | 1.05 | 1.23 |
| 78 | CA | 1405 | G | O4'-C1' | -9.66 | 1.29 | 1.41 |
| 43 | BP | 16 | SER | CA-CB | 9.65 | 1.67 | 1.52 |
| 78 | CA | 30 | G | C2'-C1' | -9.65 | 1.42 | 1.53 |
| 81 | DA | 249 | U | O4'-C1' | 9.65 | 1.54 | 1.41 |
| 81 | DA | 520 | U | C2'-C1' | -9.64 | 1.42 | 1.53 |
| 78 | CA | 408 | C | O4'-C1' | 9.64 | 1.54 | 1.41 |
| 81 | DA | 192 | C | C2'-C1' | -9.64 | 1.42 | 1.53 |
| 83 | DC | 46 | A | O4'-C1' | -9.64 | 1.29 | 1.41 |
| 81 | DA | 1072 | G | C2'-C1' | -9.63 | 1.42 | 1.53 |
| 78 | CA | 267 | U | O4'-C1' | 9.63 | 1.54 | 1.41 |
| 78 | CA | 856 | A | O4'-C1' | -9.63 | 1.29 | 1.41 |
| 81 | DA | 3067 | C | O4'-C1' | 9.63 | 1.54 | 1.41 |
| 78 | CA | 1174 | C | O4'-C1' | 9.63 | 1.54 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 3344 | A | C2'-C1' | 9.62 | 1.64 | 1.53 |
| 81 | DA | 3146 | G | O4'-C1' | 9.62 | 1.54 | 1.41 |
| 78 | CA | 1080 | U | O3'-P | -9.62 | 1.49 | 1.61 |
| 81 | DA | 1787 | A | O4'-C1' | 9.62 | 1.54 | 1.41 |
| 81 | DA | 2478 | C | C2'-C1' | -9.61 | 1.42 | 1.53 |
| 81 | DA | 2592 | G | O4'-C1' | 9.61 | 1.54 | 1.41 |
| 78 | CA | 181 | A | C2'-C1' | -9.60 | 1.42 | 1.53 |
| 81 | DA | 2368 | A | C2'-C1' | -9.60 | 1.42 | 1.53 |
| 79 | CB | 63 | C | O4'-C1' | 9.60 | 1.54 | 1.41 |
| 81 | DA | 2228 | A | O4'-C1' | -9.60 | 1.29 | 1.41 |
| 82 | DB | 122 | U | C2'-C1' | 9.60 | 1.64 | 1.53 |
| 78 | CA | 1716 | C | O4'-C1' | 9.59 | 1.54 | 1.41 |
| 81 | DA | 1048 | A | O4'-C1' | 9.59 | 1.54 | 1.41 |
| 81 | DA | 1990 | U | O4'-C1' | 9.59 | 1.54 | 1.41 |
| 81 | DA | 3091 | A | C5'-C4' | 9.59 | 1.62 | 1.51 |
| 83 | DC | 99 | A | O4'-C1' | 9.59 | 1.54 | 1.41 |
| 33 | BD | 12 | THR | N-CA | 9.59 | 1.65 | 1.46 |
| 78 | CA | 840 | U | C2'-C1' | 9.59 | 1.63 | 1.53 |
| 78 | CA | 1480 | G | C2'-C1' | 9.59 | 1.63 | 1.53 |
| 78 | CA | 1378 | U | O4'-C1' | 9.59 | 1.54 | 1.41 |
| 81 | DA | 1730 | G | C2'-C1' | 9.59 | 1.63 | 1.53 |
| 32 | BC | 17 | LEU | CA-CB | -9.58 | 1.31 | 1.53 |
| 35 | BG | 152 | THR | N-CA | 9.58 | 1.65 | 1.46 |
| 81 | DA | 927 | C | O4'-C1' | 9.58 | 1.54 | 1.41 |
| 81 | DA | 1394 | A | C2'-C1' | -9.58 | 1.42 | 1.53 |
| 82 | DB | 108 | C | C2'-C1' | -9.58 | 1.42 | 1.53 |
| 81 | DA | 2044 | U | O4'-C1' | 9.58 | 1.54 | 1.41 |
| 81 | DA | 1948 | G | C2'-C1' | -9.57 | 1.42 | 1.53 |
| 31 | BB | 196 | TRP | CA-CB | 9.57 | 1.75 | 1.53 |
| 81 | DA | 2908 | G | C2'-C1' | -9.57 | 1.42 | 1.53 |
| 34 | BE | 115 | LYS | CB-CG | 9.57 | 1.78 | 1.52 |
| 78 | CA | 667 | U | C2'-C1' | 9.57 | 1.63 | 1.53 |
| 81 | DA | 2447 | A | C2'-C1' | -9.57 | 1.42 | 1.53 |
| 78 | CA | 1545 | A | C2'-C1' | 9.57 | 1.63 | 1.53 |
| 81 | DA | 1805 | C | O4'-C1' | 9.56 | 1.54 | 1.41 |
| 32 | BC | 360 | ASP | N-CA | -9.56 | 1.27 | 1.46 |
| 81 | DA | 2561 | A | C5'-C4' | 9.56 | 1.62 | 1.51 |
| 81 | DA | 1517 | G | C2'-C1' | -9.56 | 1.42 | 1.53 |
| 81 | DA | 2297 | U | O4'-C1' | 9.56 | 1.54 | 1.41 |
| 81 | DA | 2298 | U | C2'-C1' | -9.56 | 1.42 | 1.53 |
| 78 | CA | 1441 | C | C2'-C1' | -9.56 | 1.42 | 1.53 |
| 81 | DA | 1454 | A | C2'-C1' | -9.55 | 1.42 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 1749 | A | C2'-C1' | 9.55 | 1.63 | 1.53 |
| 81 | DA | 102 | C | O4'-C1' | 9.55 | 1.54 | 1.41 |
| 81 | DA | 232 | G | C2'-C1' | -9.55 | 1.42 | 1.53 |
| 81 | DA | 1500 | G | C2'-C1' | -9.55 | 1.42 | 1.53 |
| 81 | DA | 1175 | C | O4'-C1' | 9.55 | 1.54 | 1.41 |
| 78 | CA | 1177 | C | O4'-C1' | 9.54 | 1.54 | 1.41 |
| 45 | BR | 140 | LEU | N-CA | -9.54 | 1.27 | 1.46 |
| 81 | DA | 1047 | A | C2'-C1' | 9.54 | 1.63 | 1.53 |
| 81 | DA | 1609 | C | O4'-C1' | 9.54 | 1.54 | 1.41 |
| 81 | DA | 1828 | A | C2'-C1' | -9.54 | 1.42 | 1.53 |
| 81 | DA | 2366 | C | C2'-C1' | -9.54 | 1.42 | 1.53 |
| 33 | BD | 149 | PRO | N-CD | -9.54 | 1.34 | 1.47 |
| 78 | CA | 956 | C | C2'-C1' | -9.54 | 1.42 | 1.53 |
| 78 | CA | 1286 | U | O4'-C1' | 9.54 | 1.54 | 1.41 |
| 78 | CA | 1678 | A | O4'-C1' | 9.54 | 1.54 | 1.41 |
| 81 | DA | 184 | U | O4'-C1' | 9.54 | 1.54 | 1.41 |
| 81 | DA | 1119 | C | C2'-C1' | -9.54 | 1.42 | 1.53 |
| 81 | DA | 2443 | A | C2'-C1' | -9.54 | 1.42 | 1.53 |
| 81 | DA | 2482 | U | C2'-C1' | -9.54 | 1.42 | 1.53 |
| 78 | CA | 303 | U | O4'-C1' | 9.53 | 1.54 | 1.41 |
| 81 | DA | 3354 | U | C2'-C1' | 9.53 | 1.63 | 1.53 |
| 81 | DA | 288 | C | C2'-C1' | -9.53 | 1.42 | 1.53 |
| 81 | DA | 1844 | C | C2'-C1' | -9.53 | 1.42 | 1.53 |
| 81 | DA | 926 | A | C2'-C1' | -9.53 | 1.42 | 1.53 |
| 78 | CA | 382 | C | O4'-C1' | 9.52 | 1.54 | 1.41 |
| 81 | DA | 2087 | C | O3'-P | 9.52 | 1.72 | 1.61 |
| 81 | DA | 2839 | G | C2'-C1' | -9.52 | 1.42 | 1.53 |
| 81 | DA | 3141 | A | P-O5' | -9.52 | 1.50 | 1.59 |
| 82 | DB | 147 | U | O4'-C1' | 9.51 | 1.54 | 1.41 |
| 81 | DA | 43 | A | O4'-C1' | -9.51 | 1.29 | 1.41 |
| 81 | DA | 866 | A | O4'-C1' | 9.51 | 1.54 | 1.41 |
| 81 | DA | 5 | G | C2'-C1' | -9.51 | 1.42 | 1.53 |
| 81 | DA | 2172 | A | C3'-O3' | -9.50 | 1.28 | 1.42 |
| 81 | DA | 1297 | C | C2'-C1' | -9.50 | 1.43 | 1.53 |
| 78 | CA | 1651 | A | O4'-C1' | 9.50 | 1.53 | 1.41 |
| 81 | DA | 3019 | U | O4'-C1' | 9.49 | 1.53 | 1.41 |
| 78 | CA | 638 | U | C2'-C1' | -9.49 | 1.43 | 1.53 |
| 81 | DA | 302 | U | O4'-C1' | 9.48 | 1.53 | 1.41 |
| 81 | DA | 270 | U | C2'-C1' | 9.48 | 1.63 | 1.53 |
| 81 | DA | 841 | A | O4'-C1' | 9.48 | 1.53 | 1.41 |
| 81 | DA | 2294 | U | C2'-C1' | 9.48 | 1.63 | 1.53 |
| 83 | DC | 118 | U | O4'-C1' | 9.48 | 1.53 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2383 | C | O4'-C1' | 9.48 | 1.53 | 1.41 |
| 78 | CA | 666 | U | O4'-C1' | 9.47 | 1.53 | 1.41 |
| 78 | CA | 208 | U | C4'-C3' | 9.47 | 1.63 | 1.53 |
| 78 | CA | 222 | A | P-O5' | 9.47 | 1.69 | 1.59 |
| 78 | CA | 273 | G | C2'-C1' | -9.47 | 1.43 | 1.53 |
| 78 | CA | 1198 | G | C2'-C1' | -9.47 | 1.43 | 1.53 |
| 81 | DA | 2398 | A | O4'-C1' | 9.47 | 1.53 | 1.41 |
| 81 | DA | 1272 | C | O4'-C1' | 9.47 | 1.53 | 1.41 |
| 78 | CA | 1119 | G | C2'-C1' | -9.47 | 1.43 | 1.53 |
| 78 | CA | 1393 | C | O4'-C1' | 9.47 | 1.53 | 1.41 |
| 81 | DA | 927 | C | C2'-C1' | -9.47 | 1.43 | 1.53 |
| 81 | DA | 2097 | U | O4'-C1' | 9.47 | 1.53 | 1.41 |
| 81 | DA | 790 | U | C2'-C1' | -9.46 | 1.43 | 1.53 |
| 81 | DA | 510 | G | C2'-C1' | -9.46 | 1.43 | 1.53 |
| 78 | CA | 1645 | G | C2'-C1' | -9.46 | 1.43 | 1.53 |
| 81 | DA | 38 | U | C2'-C1' | -9.46 | 1.43 | 1.53 |
| 81 | DA | 1034 | U | O4'-C1' | 9.46 | 1.53 | 1.41 |
| 81 | DA | 1614 | C | O4'-C1' | 9.46 | 1.53 | 1.41 |
| 81 | DA | 1872 | C | O4'-C1' | 9.46 | 1.53 | 1.41 |
| 78 | CA | 286 | C | O4'-C1' | 9.46 | 1.53 | 1.41 |
| 81 | DA | 3395 | G | O4'-C1' | 9.46 | 1.53 | 1.41 |
| 60 | Bi | 68 | THR | CA-CB | 9.45 | 1.77 | 1.53 |
| 81 | DA | 426 | G | O4'-C1' | 9.45 | 1.53 | 1.41 |
| 78 | CA | 1125 | A | O4'-C1' | 9.45 | 1.53 | 1.41 |
| 81 | DA | 1784 | G | C2'-C1' | -9.45 | 1.43 | 1.53 |
| 81 | DA | 2861 | U | O4'-C1' | 9.45 | 1.53 | 1.41 |
| 81 | DA | 2867 | C | O4'-C1' | 9.45 | 1.53 | 1.41 |
| 82 | DB | 110 | C | O4'-C1' | 9.45 | 1.53 | 1.41 |
| 81 | DA | 1409 | G | C2'-C1' | -9.44 | 1.43 | 1.53 |
| 81 | DA | 3105 | U | O4'-C1' | 9.44 | 1.53 | 1.41 |
| 81 | DA | 2053 | C | O4'-C1' | 9.44 | 1.53 | 1.41 |
| 81 | DA | 664 | U | C2'-C1' | -9.44 | 1.43 | 1.53 |
| 81 | DA | 3387 | U | C2'-C1' | 9.44 | 1.63 | 1.53 |
| 81 | DA | 794 | U | O4'-C1' | 9.44 | 1.53 | 1.41 |
| 78 | CA | 648 | G | C2'-C1' | -9.43 | 1.43 | 1.53 |
| 81 | DA | 1608 | C | O4'-C1' | 9.43 | 1.53 | 1.41 |
| 76 | BS | 123 | ILE | N-CA | 9.43 | 1.65 | 1.46 |
| 81 | DA | 1361 | U | C2'-C1' | 9.43 | 1.63 | 1.53 |
| 81 | DA | 2968 | G | C2'-C1' | 9.43 | 1.63 | 1.53 |
| 81 | DA | 3250 | U | C2'-C1' | -9.43 | 1.43 | 1.53 |
| 81 | DA | 1796 | G | O4'-C1' | 9.43 | 1.53 | 1.41 |
| 81 | DA | 224 | C | C2'-C1' | -9.43 | 1.43 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1148 | G | C2'-C1' | -9.43 | 1.43 | 1.53 |
| 10 | AI | 120 | ASP | N-CA | -9.42 | 1.27 | 1.46 |
| 78 | CA | 1773 | C | O4'-C1' | 9.42 | 1.53 | 1.41 |
| 81 | DA | 2205 | U | O4'-C1' | 9.42 | 1.53 | 1.41 |
| 81 | DA | 2343 | C | O4'-C1' | 9.42 | 1.53 | 1.41 |
| 81 | DA | 2736 | A | C2'-C1' | 9.42 | 1.63 | 1.53 |
| 13 | AL | 6 | PRO | N-CD | -9.41 | 1.34 | 1.47 |
| 78 | CA | 357 | G | C2'-C1' | -9.41 | 1.43 | 1.53 |
| 78 | CA | 1598 | U | O4'-C1' | 9.41 | 1.53 | 1.41 |
| 81 | DA | 1254 | C | O4'-C1' | 9.41 | 1.53 | 1.41 |
| 78 | CA | 240 | U | C5'-C4' | 9.41 | 1.62 | 1.51 |
| 81 | DA | 264 | G | O4'-C1' | 9.41 | 1.53 | 1.41 |
| 81 | DA | 1521 | G | C2'-C1' | -9.40 | 1.43 | 1.53 |
| 33 | BD | 321 | LYS | CA-CB | 9.40 | 1.74 | 1.53 |
| 78 | CA | 1371 | A | C2'-C1' | -9.40 | 1.43 | 1.53 |
| 81 | DA | 403 | C | O4'-C1' | 9.40 | 1.53 | 1.41 |
| 81 | DA | 804 | C | O4'-C1' | 9.40 | 1.53 | 1.41 |
| 81 | DA | 2200 | U | C2'-C1' | -9.40 | 1.43 | 1.53 |
| 81 | DA | 2415 | C | C2'-C1' | -9.39 | 1.43 | 1.53 |
| 81 | DA | 1805 | C | C2'-C1' | -9.39 | 1.43 | 1.53 |
| 81 | DA | 3338 | C | C2'-C1' | -9.39 | 1.43 | 1.53 |
| 81 | DA | 1415 | U | C2'-C1' | -9.39 | 1.43 | 1.53 |
| 37 | BH | 158 | ASP | CA-CB | 9.39 | 1.74 | 1.53 |
| 81 | DA | 195 | U | C2'-C1' | -9.39 | 1.43 | 1.53 |
| 81 | DA | 2602 | G | C2'-C1' | -9.39 | 1.43 | 1.53 |
| 74 | BQ | 121 | GLY | N-CA | -9.38 | 1.31 | 1.46 |
| 78 | CA | 671 | G | C2'-C1' | -9.38 | 1.43 | 1.53 |
| 81 | DA | 340 | C | O4'-C1' | 9.38 | 1.53 | 1.41 |
| 81 | DA | 458 | U | O4'-C1' | 9.38 | 1.53 | 1.41 |
| 82 | DB | 83 | C | O4'-C1' | -9.38 | 1.29 | 1.41 |
| 1 | Aa | 53 | LYS | CA-CB | 9.38 | 1.74 | 1.53 |
| 81 | DA | 1381 | A | O4'-C1' | 9.38 | 1.53 | 1.41 |
| 81 | DA | 614 | C | O4'-C1' | 9.38 | 1.53 | 1.41 |
| 78 | CA | 1281 | G | O4'-C1' | 9.37 | 1.53 | 1.41 |
| 78 | CA | 954 | G | C2'-C1' | -9.37 | 1.43 | 1.53 |
| 81 | DA | 1202 | A | C2'-C1' | -9.37 | 1.43 | 1.53 |
| 60 | Bi | 16 | ARG | CA-CB | 9.36 | 1.74 | 1.53 |
| 81 | DA | 2791 | G | O4'-C1' | -9.36 | 1.29 | 1.41 |
| 83 | DC | 107 | G | O4'-C1' | -9.36 | 1.29 | 1.41 |
| 78 | CA | 868 | G | O4'-C1' | -9.36 | 1.29 | 1.41 |
| 78 | CA | 636 | A | O4'-C1' | -9.36 | 1.29 | 1.41 |
| 78 | CA | 1291 | G | O4'-C1' | 9.36 | 1.53 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 1742 | U | O4'-C1' | 9.36 | 1.53 | 1.41 |
| 69 | Br | 47 | GLN | CA-CB | 9.35 | 1.74 | 1.53 |
| 78 | CA | 14 | C | O4'-C1' | 9.35 | 1.53 | 1.41 |
| 12 | AK | 124 | ASP | N-CA | -9.35 | 1.27 | 1.46 |
| 79 | CB | 38 | C | O4'-C1' | 9.35 | 1.53 | 1.41 |
| 81 | DA | 745 | C | O3'-P | -9.35 | 1.50 | 1.61 |
| 81 | DA | 3088 | G | O4'-C1' | 9.35 | 1.53 | 1.41 |
| 82 | DB | 3 | A | O4'-C1' | 9.34 | 1.53 | 1.41 |
| 78 | CA | 1133 | A | C2'-C1' | -9.34 | 1.43 | 1.53 |
| 32 | BC | 362 | ALA | CA-CB | 9.34 | 1.72 | 1.52 |
| 32 | BC | 289 | ASP | CA-CB | 9.33 | 1.74 | 1.53 |
| 78 | CA | 1071 | U | C2'-C1' | -9.33 | 1.43 | 1.53 |
| 81 | DA | 185 | C | O4'-C1' | 9.33 | 1.53 | 1.41 |
| 78 | CA | 1399 | C | O4'-C1' | 9.33 | 1.53 | 1.41 |
| 78 | CA | 1454 | G | C2'-C1' | -9.33 | 1.43 | 1.53 |
| 78 | CA | 1212 | G | O4'-C1' | 9.33 | 1.53 | 1.41 |
| 81 | DA | 379 | C | C2'-C1' | -9.33 | 1.43 | 1.53 |
| 81 | DA | 914 | A | C2'-C1' | 9.32 | 1.63 | 1.53 |
| 81 | DA | 1318 | A | C2'-C1' | -9.32 | 1.43 | 1.53 |
| 81 | DA | 1836 | C | C2'-C1' | -9.32 | 1.43 | 1.53 |
| 81 | DA | 2658 | G | C2'-C1' | -9.32 | 1.43 | 1.53 |
| 82 | DB | 137 | C | O4'-C1' | 9.32 | 1.53 | 1.41 |
| 45 | BR | 157 | PRO | CA-CB | -9.32 | 1.34 | 1.53 |
| 78 | CA | 216 | U | O4'-C1' | 9.32 | 1.53 | 1.41 |
| 81 | DA | 240 | U | O4'-C1' | 9.32 | 1.53 | 1.41 |
| 17 | AQ | 63 | LYS | N-CA | -9.32 | 1.27 | 1.46 |
| 78 | CA | 1003 | A | C2'-C1' | 9.31 | 1.63 | 1.53 |
| 81 | DA | 2688 | U | O4'-C1' | 9.31 | 1.53 | 1.41 |
| 57 | Be | 98 | LYS | CA-C | 9.30 | 1.77 | 1.52 |
| 78 | CA | 1711 | C | O4'-C1' | 9.30 | 1.53 | 1.41 |
| 81 | DA | 546 | C | O4'-C1' | 9.30 | 1.53 | 1.41 |
| 81 | DA | 874 | U | O4'-C1' | 9.30 | 1.53 | 1.41 |
| 81 | DA | 1467 | A | O4'-C1' | 9.30 | 1.53 | 1.41 |
| 81 | DA | 1273 | A | O4'-C1' | 9.30 | 1.53 | 1.41 |
| 81 | DA | 1394 | A | O4'-C1' | 9.30 | 1.53 | 1.41 |
| 81 | DA | 1416 | C | C2'-C1' | -9.30 | 1.43 | 1.53 |
| 81 | DA | 162 | G | C2'-C1' | 9.29 | 1.63 | 1.53 |
| 81 | DA | 853 | G | C2'-C1' | -9.29 | 1.43 | 1.53 |
| 81 | DA | 2702 | A | C2'-C1' | -9.29 | 1.43 | 1.53 |
| 81 | DA | 3305 | A | O4'-C1' | 9.29 | 1.53 | 1.41 |
| 18 | AP | 40 | LEU | CA-CB | -9.29 | 1.32 | 1.53 |
| 41 | BN | 76 | ALA | C-O | -9.29 | 1.05 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1567 | U | O4'-C1' | 9.29 | 1.53 | 1.41 |
| 81 | DA | 3341 | U | O4'-C1' | 9.29 | 1.53 | 1.41 |
| 78 | CA | 1284 | C | O4'-C1' | 9.28 | 1.53 | 1.41 |
| 81 | DA | 2270 | A | O4'-C1' | 9.28 | 1.53 | 1.41 |
| 78 | CA | 427 | C | C2'-C1' | -9.28 | 1.43 | 1.53 |
| 81 | DA | 1949 | G | C2'-C1' | -9.28 | 1.43 | 1.53 |
| 81 | DA | 2831 | G | C2'-C1' | -9.28 | 1.43 | 1.53 |
| 81 | DA | 497 | C | O4'-C1' | 9.27 | 1.53 | 1.41 |
| 81 | DA | 1852 | G | C2'-C1' | -9.27 | 1.43 | 1.53 |
| 78 | CA | 361 | C | C2'-C1' | -9.27 | 1.43 | 1.53 |
| 78 | CA | 307 | G | C2'-C1' | -9.27 | 1.43 | 1.53 |
| 81 | DA | 3212 | C | C2'-C1' | -9.27 | 1.43 | 1.53 |
| 81 | DA | 785 | G | O4'-C1' | -9.26 | 1.29 | 1.41 |
| 78 | CA | 1035 | G | C2'-C1' | -9.26 | 1.43 | 1.53 |
| 78 | CA | 1380 | U | O4'-C1' | 9.26 | 1.53 | 1.41 |
| 78 | CA | 1127 | G | C2'-C1' | -9.26 | 1.43 | 1.53 |
| 34 | BE | 52 | TYR | CA-CB | 9.26 | 1.74 | 1.53 |
| 78 | CA | 157 | A | O4'-C1' | 9.26 | 1.53 | 1.41 |
| 78 | CA | 275 | C | O4'-C1' | 9.25 | 1.53 | 1.41 |
| 81 | DA | 295 | A | C2'-C1' | -9.25 | 1.43 | 1.53 |
| 81 | DA | 1707 | A | O4'-C1' | 9.25 | 1.53 | 1.41 |
| 78 | CA | 414 | C | O4'-C1' | 9.25 | 1.53 | 1.41 |
| 81 | DA | 127 | G | C2'-C1' | -9.25 | 1.43 | 1.53 |
| 81 | DA | 143 | G | C2'-C1' | -9.25 | 1.43 | 1.53 |
| 76 | BS | 124 | GLN | N-CA | -9.25 | 1.27 | 1.46 |
| 81 | DA | 2139 | A | O4'-C1' | 9.25 | 1.53 | 1.41 |
| 81 | DA | 3027 | A | C2'-C1' | -9.25 | 1.43 | 1.53 |
| 74 | BQ | 158 | ARG | CZ-NH1 | -9.24 | 1.21 | 1.33 |
| 81 | DA | 311 | C | C2'-C1' | -9.24 | 1.43 | 1.53 |
| 81 | DA | 861 | C | C2'-C1' | -9.24 | 1.43 | 1.53 |
| 82 | DB | 65 | A | O4'-C1' | 9.24 | 1.53 | 1.41 |
| 78 | CA | 29 | U | C2'-C1' | -9.24 | 1.43 | 1.53 |
| 81 | DA | 2034 | C | O4'-C1' | 9.24 | 1.53 | 1.41 |
| 81 | DA | 357 | A | C2'-C1' | -9.23 | 1.43 | 1.53 |
| 81 | DA | 998 | A | C2'-C1' | -9.23 | 1.43 | 1.53 |
| 81 | DA | 2424 | A | O4'-C1' | -9.23 | 1.29 | 1.41 |
| 81 | DA | 2781 | U | C2'-C1' | 9.23 | 1.63 | 1.53 |
| 81 | DA | 2983 | C | O4'-C1' | 9.23 | 1.53 | 1.41 |
| 81 | DA | 16 | A | C2'-C1' | -9.23 | 1.43 | 1.53 |
| 81 | DA | 500 | C | O4'-C1' | 9.23 | 1.53 | 1.41 |
| 81 | DA | 561 | C | O4'-C1' | 9.23 | 1.53 | 1.41 |
| 78 | CA | 560 | U | C2'-C1' | -9.22 | 1.43 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2075 | C | O4'-C1' | 9.22 | 1.53 | 1.41 |
| 78 | CA | 555 | A | C5'-C4' | -9.22 | 1.40 | 1.51 |
| 81 | DA | 894 | G | O4'-C1' | -9.22 | 1.29 | 1.41 |
| 81 | DA | 1283 | C | O4'-C1' | 9.21 | 1.53 | 1.41 |
| 83 | DC | 46 | A | C3'-C2' | -9.21 | 1.42 | 1.52 |
| 82 | DB | 57 | C | C2'-C1' | -9.21 | 1.43 | 1.53 |
| 81 | DA | 754 | G | O4'-C1' | 9.21 | 1.53 | 1.41 |
| 81 | DA | 1320 | C | O4'-C1' | 9.21 | 1.53 | 1.41 |
| 81 | DA | 1836 | C | O4'-C1' | 9.21 | 1.53 | 1.41 |
| 81 | DA | 1985 | G | C2'-C1' | -9.21 | 1.43 | 1.53 |
| 81 | DA | 2338 | C | C2'-C1' | -9.21 | 1.43 | 1.53 |
| 81 | DA | 3230 | G | C2'-C1' | -9.21 | 1.43 | 1.53 |
| 82 | DB | 151 | C | O4'-C1' | 9.21 | 1.53 | 1.41 |
| 78 | CA | 1334 | U | O4'-C1' | 9.21 | 1.53 | 1.41 |
| 81 | DA | 1282 | G | C2'-C1' | -9.21 | 1.43 | 1.53 |
| 81 | DA | 1999 | C | O4'-C1' | 9.20 | 1.53 | 1.41 |
| 78 | CA | 546 | U | O4'-C1' | 9.20 | 1.53 | 1.41 |
| 40 | BK | 63 | ALA | CA-CB | 9.20 | 1.71 | 1.52 |
| 81 | DA | 1678 | G | C2'-C1' | 9.19 | 1.63 | 1.53 |
| 81 | DA | 649 | A | C2'-C1' | -9.19 | 1.43 | 1.53 |
| 81 | DA | 1710 | C | C2'-C1' | 9.19 | 1.63 | 1.53 |
| 78 | CA | 819 | G | C2'-C1' | -9.19 | 1.43 | 1.53 |
| 78 | CA | 1006 | C | O4'-C1' | 9.19 | 1.53 | 1.41 |
| 81 | DA | 1697 | A | O4'-C1' | 9.19 | 1.53 | 1.41 |
| 81 | DA | 2871 | G | C2'-C1' | -9.19 | 1.43 | 1.53 |
| 81 | DA | 1973 | G | O4'-C1' | 9.19 | 1.53 | 1.41 |
| 31 | BB | 252 | THR | N-CA | 9.18 | 1.64 | 1.46 |
| 81 | DA | 3138 | U | O4'-C1' | 9.18 | 1.53 | 1.41 |
| 78 | CA | 1479 | A | O4'-C1' | -9.18 | 1.29 | 1.41 |
| 81 | DA | 309 | U | O4'-C1' | 9.18 | 1.53 | 1.41 |
| 78 | CA | 1453 | G | O4'-C1' | 9.18 | 1.53 | 1.41 |
| 81 | DA | 359 | U | C2'-C1' | -9.18 | 1.43 | 1.53 |
| 37 | BH | 237 | ILE | N-CA | -9.17 | 1.28 | 1.46 |
| 81 | DA | 596 | C | C2'-C1' | -9.17 | 1.43 | 1.53 |
| 78 | CA | 597 | G | O4'-C1' | 9.17 | 1.53 | 1.41 |
| 81 | DA | 633 | C | C2'-C1' | -9.17 | 1.43 | 1.53 |
| 78 | CA | 1739 | C | C2'-C1' | -9.17 | 1.43 | 1.53 |
| 78 | CA | 617 | U | C2'-C1' | -9.16 | 1.43 | 1.53 |
| 81 | DA | 2318 | U | O4'-C1' | 9.16 | 1.53 | 1.41 |
| 81 | DA | 2645 | G | O4'-C1' | -9.16 | 1.29 | 1.41 |
| 17 | AQ | 81 | LYS | N-CA | -9.16 | 1.28 | 1.46 |
| 81 | DA | 674 | G | O4'-C1' | 9.16 | 1.53 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1963 | G | O4'-C1' | -9.16 | 1.29 | 1.41 |
| 81 | DA | 904 | A | C2'-C1' | -9.16 | 1.43 | 1.53 |
| 78 | CA | 1735 | U | C5'-C4' | 9.15 | 1.62 | 1.51 |
| 81 | DA | 36 | C | O4'-C1' | 9.15 | 1.53 | 1.41 |
| 78 | CA | 1532 | U | O4'-C1' | 9.15 | 1.53 | 1.41 |
| 81 | DA | 1185 | C | O4'-C1' | 9.15 | 1.53 | 1.41 |
| 81 | DA | 1434 | G | C2'-C1' | -9.15 | 1.43 | 1.53 |
| 78 | CA | 154 | G | C2'-C1' | -9.15 | 1.43 | 1.53 |
| 78 | CA | 226 | A | C3'-C2' | -9.15 | 1.42 | 1.52 |
| 78 | CA | 1700 | C | O4'-C1' | 9.15 | 1.53 | 1.41 |
| 81 | DA | 1960 | A | O4'-C1' | 9.15 | 1.53 | 1.41 |
| 78 | CA | 1569 | A | O4'-C1' | 9.14 | 1.53 | 1.41 |
| 81 | DA | 1547 | G | C2'-C1' | -9.14 | 1.43 | 1.53 |
| 78 | CA | 1706 | C | O4'-C1' | 9.14 | 1.53 | 1.41 |
| 81 | DA | 778 | U | C2'-C1' | -9.13 | 1.43 | 1.53 |
| 81 | DA | 2323 | G | C2'-C1' | 9.14 | 1.63 | 1.53 |
| 78 | CA | 1646 | C | C2'-C1' | -9.13 | 1.43 | 1.53 |
| 81 | DA | 1599 | G | C2'-C1' | -9.13 | 1.43 | 1.53 |
| 81 | DA | 1783 | U | O4'-C1' | 9.12 | 1.53 | 1.41 |
| 26 | AZ | 18 | THR | N-CA | 9.11 | 1.64 | 1.46 |
| 81 | DA | 1612 | A | C2'-C1' | 9.12 | 1.63 | 1.53 |
| 81 | DA | 3029 | A | C2'-C1' | -9.12 | 1.43 | 1.53 |
| 78 | CA | 978 | A | C2'-C1' | -9.11 | 1.43 | 1.53 |
| 81 | DA | 3133 | C | O4'-C1' | 9.11 | 1.53 | 1.41 |
| 79 | CB | 68 | C | O4'-C1' | 9.11 | 1.53 | 1.41 |
| 81 | DA | 452 | G | C2'-C1' | -9.10 | 1.43 | 1.53 |
| 81 | DA | 998 | A | O4'-C1' | 9.10 | 1.53 | 1.41 |
| 81 | DA | 1854 | C | O4'-C1' | 9.10 | 1.53 | 1.41 |
| 81 | DA | 2484 | A | O4'-C1' | -9.10 | 1.29 | 1.41 |
| 78 | CA | 683 | C | O4'-C1' | 9.10 | 1.53 | 1.41 |
| 81 | DA | 2250 | G | O4'-C1' | 9.10 | 1.53 | 1.41 |
| 78 | CA | 426 | G | C2'-C1' | -9.10 | 1.43 | 1.53 |
| 78 | CA | 1620 | C | C2'-C1' | -9.10 | 1.43 | 1.53 |
| 81 | DA | 2666 | C | C2'-C1' | -9.10 | 1.43 | 1.53 |
| 81 | DA | 2940 | A | C2'-C1' | -9.10 | 1.43 | 1.53 |
| 78 | CA | 1550 | A | C2'-C1' | -9.09 | 1.43 | 1.53 |
| 81 | DA | 1268 | G | O4'-C1' | 9.09 | 1.53 | 1.41 |
| 81 | DA | 1538 | G | C2'-C1' | -9.09 | 1.43 | 1.53 |
| 81 | DA | 1709 | C | O4'-C1' | 9.09 | 1.53 | 1.41 |
| 81 | DA | 673 | U | O3'-P | -9.09 | 1.50 | 1.61 |
| 81 | DA | 2144 | A | O4'-C1' | -9.09 | 1.29 | 1.41 |
| 39 | BJ | 76 | SER | CA-CB | -9.08 | 1.39 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 1759 | C | O4'-C1' | 9.08 | 1.53 | 1.41 |
| 81 | DA | 623 | U | O4'-C1' | 9.08 | 1.53 | 1.41 |
| 78 | CA | 121 | U | P-O5' | 9.08 | 1.68 | 1.59 |
| 81 | DA | 839 | C | O4'-C1' | 9.08 | 1.53 | 1.41 |
| 81 | DA | 2278 | C | C2'-C1' | -9.08 | 1.43 | 1.53 |
| 2 | AA | 11 | PRO | N-CA | -9.08 | 1.31 | 1.47 |
| 81 | DA | 284 | A | C2'-C1' | -9.08 | 1.43 | 1.53 |
| 81 | DA | 1057 | A | C2'-C1' | 9.08 | 1.63 | 1.53 |
| 81 | DA | 1334 | U | C2'-C1' | -9.08 | 1.43 | 1.53 |
| 83 | DC | 88 | G | C2'-C1' | -9.08 | 1.43 | 1.53 |
| 81 | DA | 2510 | U | O4'-C1' | 9.07 | 1.53 | 1.41 |
| 13 | AL | 13 | ARG | CG-CD | -9.07 | 1.29 | 1.51 |
| 55 | Bc | 108 | GLN | C-O | -9.06 | 1.06 | 1.23 |
| 81 | DA | 779 | G | C2'-C1' | -9.06 | 1.43 | 1.53 |
| 81 | DA | 1001 | G | C2'-C1' | -9.06 | 1.43 | 1.53 |
| 81 | DA | 1234 | G | C2'-C1' | -9.06 | 1.43 | 1.53 |
| 81 | DA | 1296 | C | O4'-C1' | 9.06 | 1.53 | 1.41 |
| 81 | DA | 1582 | C | C2'-C1' | -9.06 | 1.43 | 1.53 |
| 78 | CA | 1101 | G | C2'-C1' | -9.06 | 1.43 | 1.53 |
| 83 | DC | 63 | G | C2'-C1' | -9.06 | 1.43 | 1.53 |
| 78 | CA | 923 | A | O4'-C1' | 9.05 | 1.53 | 1.41 |
| 78 | CA | 1234 | A | O4'-C1' | -9.05 | 1.29 | 1.41 |
| 78 | CA | 1471 | A | C2'-C1' | 9.05 | 1.63 | 1.53 |
| 81 | DA | 3304 | U | O3'-P | 9.05 | 1.72 | 1.61 |
| 2 | AA | 12 | GLU | N-CA | 9.05 | 1.64 | 1.46 |
| 81 | DA | 1512 | U | C2'-C1' | -9.05 | 1.43 | 1.53 |
| 81 | DA | 1832 | C | O4'-C1' | 9.05 | 1.53 | 1.41 |
| 81 | DA | 2386 | A | C2'-C1' | -9.05 | 1.43 | 1.53 |
| 81 | DA | 2437 | G | O4'-C1' | -9.05 | 1.29 | 1.41 |
| 78 | CA | 960 | U | O4'-C1' | 9.05 | 1.53 | 1.41 |
| 81 | DA | 1327 | C | C2'-C1' | -9.04 | 1.43 | 1.53 |
| 81 | DA | 3391 | A | C2'-C1' | -9.04 | 1.43 | 1.53 |
| 78 | CA | 1751 | C | C2'-C1' | -9.04 | 1.43 | 1.53 |
| 69 | Br | 89 | LYS | N-CA | 9.04 | 1.64 | 1.46 |
| 45 | BR | 4 | ASP | N-CA | -9.03 | 1.28 | 1.46 |
| 78 | CA | 447 | U | O4'-C1' | 9.03 | 1.53 | 1.41 |
| 78 | CA | 1301 | U | O4'-C1' | 9.03 | 1.53 | 1.41 |
| 81 | DA | 1914 | G | C2'-C1' | -9.03 | 1.43 | 1.53 |
| 81 | DA | 2332 | A | O4'-C1' | 9.03 | 1.53 | 1.41 |
| 81 | DA | 1169 | A | O4'-C1' | 9.03 | 1.53 | 1.41 |
| 78 | CA | 274 | G | C2'-C1' | -9.02 | 1.43 | 1.53 |
| 81 | DA | 2080 | C | O4'-C1' | 9.02 | 1.53 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 224 | C | O4'-C1' | 9.02 | 1.53 | 1.41 |
| 83 | DC | 6 | C | O4'-C1' | 9.02 | 1.53 | 1.41 |
| 78 | CA | 158 | U | C2'-C1' | -9.02 | 1.43 | 1.53 |
| 78 | CA | 1632 | C | C2'-C1' | -9.02 | 1.43 | 1.53 |
| 81 | DA | 618 | C | O4'-C1' | 9.02 | 1.53 | 1.41 |
| 81 | DA | 691 | A | C2'-C1' | 9.02 | 1.63 | 1.53 |
| 78 | CA | 645 | C | C2'-C1' | 9.01 | 1.63 | 1.53 |
| 81 | DA | 956 | U | O4'-C1' | 9.01 | 1.53 | 1.41 |
| 81 | DA | 887 | G | O4'-C1' | 9.01 | 1.53 | 1.41 |
| 83 | DC | 76 | U | O4'-C1' | 9.01 | 1.53 | 1.41 |
| 78 | CA | 1376 | C | C2'-C1' | -9.00 | 1.43 | 1.53 |
| 81 | DA | 3345 | G | C2'-C1' | 9.00 | 1.63 | 1.53 |
| 81 | DA | 2436 | U | O4'-C1' | 9.00 | 1.53 | 1.41 |
| 13 | AL | 93 | LEU | N-CA | -9.00 | 1.28 | 1.46 |
| 83 | DC | 94 | A | C2'-C1' | -9.00 | 1.43 | 1.53 |
| 81 | DA | 385 | A | C2'-C1' | -9.00 | 1.43 | 1.53 |
| 78 | CA | 1211 | A | C2'-C1' | -8.99 | 1.43 | 1.53 |
| 81 | DA | 297 | G | C2'-C1' | 8.99 | 1.63 | 1.53 |
| 81 | DA | 1730 | G | O4'-C1' | -8.99 | 1.29 | 1.41 |
| 81 | DA | 2181 | C | C2'-C1' | -8.99 | 1.43 | 1.53 |
| 81 | DA | 2965 | U | C2'-C1' | -8.99 | 1.43 | 1.53 |
| 81 | DA | 678 | G | O4'-C1' | -8.99 | 1.29 | 1.41 |
| 81 | DA | 1955 | U | C2'-C1' | 8.99 | 1.63 | 1.53 |
| 16 | AO | 67 | THR | N-CA | -8.99 | 1.28 | 1.46 |
| 78 | CA | 1455 | G | O4'-C1' | 8.99 | 1.53 | 1.41 |
| 81 | DA | 851 | C | C2'-C1' | -8.99 | 1.43 | 1.53 |
| 81 | DA | 840 | C | C2'-C1' | -8.98 | 1.43 | 1.53 |
| 81 | DA | 2882 | U | O4'-C1' | 8.98 | 1.53 | 1.41 |
| 79 | CB | 74 | C | O4'-C1' | 8.98 | 1.53 | 1.41 |
| 81 | DA | 77 | A | C2'-C1' | -8.98 | 1.43 | 1.53 |
| 81 | DA | 1708 | C | O4'-C1' | 8.98 | 1.53 | 1.41 |
| 78 | CA | 1562 | G | O4'-C1' | 8.97 | 1.53 | 1.41 |
| 78 | CA | 1467 | C | C2'-C1' | -8.97 | 1.43 | 1.53 |
| 81 | DA | 1367 | G | C2'-C1' | -8.97 | 1.43 | 1.53 |
| 81 | DA | 2395 | G | C2'-C1' | -8.97 | 1.43 | 1.53 |
| 81 | DA | 2808 | A | O4'-C1' | -8.96 | 1.30 | 1.41 |
| 33 | BD | 349 | THR | N-CA | 8.96 | 1.64 | 1.46 |
| 78 | CA | 1204 | A | O4'-C1' | 8.96 | 1.53 | 1.41 |
| 81 | DA | 1542 | G | C2'-C1' | -8.96 | 1.43 | 1.53 |
| 81 | DA | 2066 | C | O4'-C1' | 8.95 | 1.53 | 1.41 |
| 78 | CA | 25 | C | O4'-C1' | 8.95 | 1.53 | 1.41 |
| 81 | DA | 3301 | U | C2'-C1' | -8.95 | 1.43 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 412 | G | O4'-C1' | 8.95 | 1.53 | 1.41 |
| 78 | CA | 1774 | G | O4'-C1' | 8.94 | 1.53 | 1.41 |
| 81 | DA | 2764 | C | C2'-C1' | -8.94 | 1.43 | 1.53 |
| 74 | BQ | 40 | HIS | C-N | 8.94 | 1.54 | 1.34 |
| 78 | CA | 1003 | A | O4'-C1' | -8.94 | 1.30 | 1.41 |
| 17 | AQ | 81 | LYS | CA-CB | 8.94 | 1.73 | 1.53 |
| 81 | DA | 2391 | G | C2'-C1' | -8.94 | 1.43 | 1.53 |
| 81 | DA | 3034 | C | C2'-C1' | -8.94 | 1.43 | 1.53 |
| 81 | DA | 1614 | C | C2'-C1' | -8.94 | 1.43 | 1.53 |
| 81 | DA | 1431 | G | O4'-C1' | 8.93 | 1.53 | 1.41 |
| 81 | DA | 2145 | A | O4'-C1' | 8.93 | 1.53 | 1.41 |
| 82 | DB | 134 | G | C2'-C1' | 8.93 | 1.63 | 1.53 |
| 81 | DA | 529 | A | C2'-C1' | -8.93 | 1.43 | 1.53 |
| 78 | CA | 1100 | G | C5'-C4' | 8.93 | 1.62 | 1.51 |
| 81 | DA | 3085 | G | C2'-C1' | -8.93 | 1.43 | 1.53 |
| 67 | Bp | 34 | CYS | CB-SG | -8.93 | 1.67 | 1.82 |
| 69 | Br | 48 | SER | N-CA | -8.93 | 1.28 | 1.46 |
| 81 | DA | 1848 | G | C2'-C1' | -8.93 | 1.43 | 1.53 |
| 78 | CA | 1267 | G | O4'-C1' | 8.93 | 1.53 | 1.41 |
| 81 | DA | 1669 | C | C2'-C1' | -8.93 | 1.43 | 1.53 |
| 81 | DA | 2079 | G | O3'-P | -8.92 | 1.50 | 1.61 |
| 46 | BT | 82 | LYS | N-CA | 8.92 | 1.64 | 1.46 |
| 81 | DA | 32 | U | C2'-C1' | -8.92 | 1.43 | 1.53 |
| 81 | DA | 1900 | A | C2'-C1' | -8.92 | 1.43 | 1.53 |
| 81 | DA | 1615 | C | O4'-C1' | 8.92 | 1.53 | 1.41 |
| 80 | CC | 16 | G | C2'-C1' | 8.92 | 1.63 | 1.53 |
| 81 | DA | 2339 | C | O4'-C1' | 8.91 | 1.53 | 1.41 |
| 81 | DA | 2758 | A | C2'-C1' | 8.91 | 1.63 | 1.53 |
| 29 | AU | 37 | LYS | N-CA | -8.91 | 1.28 | 1.46 |
| 81 | DA | 1080 | A | O4'-C1' | -8.91 | 1.30 | 1.41 |
| 81 | DA | 455 | C | O4'-C1' | 8.90 | 1.53 | 1.41 |
| 81 | DA | 1147 | G | O4'-C1' | -8.90 | 1.30 | 1.41 |
| 81 | DA | 2354 | C | O4'-C1' | 8.90 | 1.53 | 1.41 |
| 81 | DA | 3297 | U | O4'-C1' | 8.90 | 1.53 | 1.41 |
| 78 | CA | 153 | G | C2'-C1' | -8.90 | 1.43 | 1.53 |
| 78 | CA | 994 | G | O4'-C1' | -8.90 | 1.30 | 1.41 |
| 78 | CA | 625 | C | O4'-C1' | 8.90 | 1.53 | 1.41 |
| 78 | CA | 1534 | G | P-O5' | -8.90 | 1.50 | 1.59 |
| 81 | DA | 902 | G | C2'-C1' | -8.90 | 1.43 | 1.53 |
| 81 | DA | 823 | C | C2'-C1' | -8.89 | 1.43 | 1.53 |
| 81 | DA | 947 | G | C2'-C1' | -8.89 | 1.43 | 1.53 |
| 78 | CA | 1736 | G | C2'-C1' | -8.89 | 1.43 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 235 | A | C4'-O4' | -8.89 | 1.33 | 1.45 |
| 82 | DB | 129 | C | O4'-C1' | 8.89 | 1.53 | 1.41 |
| 81 | DA | 2823 | G | C2'-C1' | -8.89 | 1.43 | 1.53 |
| 81 | DA | 11 | A | O4'-C1' | 8.88 | 1.53 | 1.41 |
| 81 | DA | 1995 | A | O4'-C1' | 8.88 | 1.53 | 1.41 |
| 78 | CA | 204 | G | O4'-C1' | 8.87 | 1.53 | 1.41 |
| 81 | DA | 2480 | A | O3'-P | -8.87 | 1.50 | 1.61 |
| 45 | BR | 98 | LYS | N-CA | 8.87 | 1.64 | 1.46 |
| 81 | DA | 2813 | A | C2'-C1' | -8.87 | 1.43 | 1.53 |
| 81 | DA | 61 | A | C2'-C1' | -8.87 | 1.43 | 1.53 |
| 81 | DA | 1616 | U | O4'-C1' | 8.87 | 1.53 | 1.41 |
| 81 | DA | 2781 | U | O4'-C1' | -8.87 | 1.30 | 1.41 |
| 83 | DC | 28 | C | O4'-C1' | 8.87 | 1.53 | 1.41 |
| 81 | DA | 2128 | C | C2'-C1' | -8.86 | 1.43 | 1.53 |
| 32 | BC | 130 | PHE | N-CA | 8.86 | 1.64 | 1.46 |
| 81 | DA | 1588 | A | O4'-C1' | -8.86 | 1.30 | 1.41 |
| 81 | DA | 1060 | U | C2'-C1' | -8.86 | 1.43 | 1.53 |
| 81 | DA | 2582 | C | C2'-C1' | -8.85 | 1.43 | 1.53 |
| 81 | DA | 1187 | C | O4'-C1' | 8.85 | 1.53 | 1.41 |
| 81 | DA | 2289 | U | O4'-C1' | 8.85 | 1.53 | 1.41 |
| 40 | BK | 70 | PRO | N-CA | 8.85 | 1.62 | 1.47 |
| 81 | DA | 1928 | G | C2'-C1' | -8.84 | 1.43 | 1.53 |
| 39 | BJ | 76 | SER | N-CA | 8.84 | 1.64 | 1.46 |
| 81 | DA | 312 | C | O4'-C1' | 8.84 | 1.53 | 1.41 |
| 37 | BH | 228 | GLU | CA-CB | 8.84 | 1.73 | 1.53 |
| 81 | DA | 3388 | C | C2'-C1' | -8.84 | 1.43 | 1.53 |
| 81 | DA | 2649 | A | C2'-C1' | -8.83 | 1.43 | 1.53 |
| 78 | CA | 1550 | A | O4'-C1' | 8.83 | 1.53 | 1.41 |
| 81 | DA | 64 | G | C2'-C1' | -8.83 | 1.43 | 1.53 |
| 81 | DA | 2071 | A | O3'-P | -8.83 | 1.50 | 1.61 |
| 81 | DA | 2668 | U | O4'-C1' | 8.83 | 1.53 | 1.41 |
| 78 | CA | 471 | A | C2'-C1' | -8.82 | 1.43 | 1.53 |
| 78 | CA | 1242 | A | O4'-C1' | 8.82 | 1.53 | 1.41 |
| 81 | DA | 724 | U | C2'-C1' | -8.82 | 1.43 | 1.53 |
| 81 | DA | 1243 | G | C2'-C1' | -8.82 | 1.43 | 1.53 |
| 42 | BM | 41 | GLY | N-CA | 8.82 | 1.59 | 1.46 |
| 78 | CA | 1558 | U | C5'-C4' | -8.82 | 1.40 | 1.51 |
| 81 | DA | 2365 | C | O4'-C1' | 8.81 | 1.53 | 1.41 |
| 81 | DA | 796 | U | O4'-C1' | 8.81 | 1.53 | 1.41 |
| 81 | DA | 2825 | C | C2'-C1' | -8.81 | 1.43 | 1.53 |
| 81 | DA | 1190 | A | O4'-C1' | 8.81 | 1.53 | 1.41 |
| 81 | DA | 2849 | C | C2'-C1' | -8.81 | 1.43 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 615 | U | O4'-C1' | 8.80 | 1.53 | 1.41 |
| 81 | DA | 791 | A | C2'-C1' | -8.80 | 1.43 | 1.53 |
| 78 | CA | 818 | C | C2'-C1' | -8.80 | 1.43 | 1.53 |
| 78 | CA | 430 | G | O4'-C1' | 8.80 | 1.53 | 1.41 |
| 78 | CA | 1685 | G | C2'-C1' | -8.80 | 1.43 | 1.53 |
| 81 | DA | 3143 | C | C2'-C1' | -8.79 | 1.43 | 1.53 |
| 81 | DA | 694 | C | C2'-C1' | -8.79 | 1.43 | 1.53 |
| 78 | CA | 1789 | G | C2'-C1' | -8.78 | 1.43 | 1.53 |
| 81 | DA | 1307 | G | C2'-C1' | -8.78 | 1.43 | 1.53 |
| 81 | DA | 993 | G | O4'-C1' | 8.77 | 1.53 | 1.41 |
| 81 | DA | 3091 | A | P-O5' | 8.77 | 1.68 | 1.59 |
| 78 | CA | 899 | G | O4'-C1' | -8.77 | 1.30 | 1.41 |
| 81 | DA | 3242 | G | P-O5' | -8.77 | 1.50 | 1.59 |
| 44 | BO | 40 | HIS | CA-CB | -8.77 | 1.34 | 1.53 |
| 78 | CA | 124 | A | O4'-C1' | 8.77 | 1.53 | 1.41 |
| 81 | DA | 1657 | C | C2'-C1' | 8.76 | 1.62 | 1.53 |
| 2 | AA | 11 | PRO | CA-CB | -8.76 | 1.36 | 1.53 |
| 81 | DA | 450 | G | C2'-C1' | -8.76 | 1.43 | 1.53 |
| 81 | DA | 2285 | C | O4'-C1' | 8.76 | 1.53 | 1.41 |
| 78 | CA | 45 | U | O4'-C1' | -8.76 | 1.30 | 1.41 |
| 81 | DA | 695 | C | O4'-C1' | 8.75 | 1.53 | 1.41 |
| 81 | DA | 2190 | U | O4'-C1' | 8.75 | 1.53 | 1.41 |
| 81 | DA | 2435 | G | C2'-C1' | 8.75 | 1.62 | 1.53 |
| 81 | DA | 3040 | A | C2'-C1' | -8.75 | 1.43 | 1.53 |
| 83 | DC | 115 | A | C2'-C1' | 8.75 | 1.62 | 1.53 |
| 81 | DA | 1549 | U | C2'-C1' | -8.75 | 1.43 | 1.53 |
| 81 | DA | 3137 | C | C2'-C1' | -8.75 | 1.43 | 1.53 |
| 78 | CA | 1734 | U | O4'-C1' | 8.75 | 1.53 | 1.41 |
| 81 | DA | 679 | U | O4'-C1' | 8.75 | 1.53 | 1.41 |
| 81 | DA | 3220 | G | C3'-C2' | 8.75 | 1.62 | 1.52 |
| 10 | AI | 54 | LEU | N-CA | -8.74 | 1.28 | 1.46 |
| 81 | DA | 146 | U | C5'-C4' | 8.74 | 1.61 | 1.51 |
| 78 | CA | 683 | C | C2'-C1' | 8.74 | 1.62 | 1.53 |
| 81 | DA | 407 | A | O4'-C1' | 8.74 | 1.53 | 1.41 |
| 81 | DA | 616 | G | C2'-C1' | -8.74 | 1.43 | 1.53 |
| 81 | DA | 2377 | G | P-O5' | -8.74 | 1.51 | 1.59 |
| 81 | DA | 146 | U | P-O5' | -8.74 | 1.51 | 1.59 |
| 81 | DA | 2859 | U | C2'-C1' | 8.73 | 1.62 | 1.53 |
| 81 | DA | 2177 | G | O4'-C1' | 8.73 | 1.52 | 1.41 |
| 81 | DA | 1371 | G | C2'-C1' | -8.73 | 1.43 | 1.53 |
| 82 | DB | 127 | U | O4'-C1' | 8.73 | 1.52 | 1.41 |
| 78 | CA | 1147 | A | C2'-C1' | -8.72 | 1.43 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1488 | G | C2'-C1' | -8.72 | 1.43 | 1.53 |
| 78 | CA | 1747 | G | P-O5' | -8.72 | 1.51 | 1.59 |
| 81 | DA | 1177 | G | O4'-C1' | 8.72 | 1.52 | 1.41 |
| 81 | DA | 1039 | U | O4'-C1' | 8.72 | 1.52 | 1.41 |
| 82 | DB | 29 | U | O4'-C1' | 8.72 | 1.52 | 1.41 |
| 33 | BD | 84 | ARG | NE-CZ | 8.72 | 1.44 | 1.33 |
| 78 | CA | 1465 | C | O4'-C1' | 8.72 | 1.52 | 1.41 |
| 78 | CA | 1540 | G | C2'-C1' | -8.72 | 1.43 | 1.53 |
| 81 | DA | 2367 | A | O4'-C1' | 8.71 | 1.52 | 1.41 |
| 81 | DA | 2713 | U | O4'-C1' | 8.71 | 1.52 | 1.41 |
| 81 | DA | 941 | G | C2'-C1' | -8.70 | 1.43 | 1.53 |
| 81 | DA | 2723 | U | C2'-C1' | -8.70 | 1.43 | 1.53 |
| 81 | DA | 673 | U | C2'-C1' | -8.70 | 1.43 | 1.53 |
| 78 | CA | 337 | G | C2'-C1' | 8.70 | 1.62 | 1.53 |
| 78 | CA | 163 | G | O3'-P | -8.69 | 1.50 | 1.61 |
| 81 | DA | 1738 | C | C2'-C1' | -8.69 | 1.43 | 1.53 |
| 81 | DA | 2642 | A | O4'-C1' | 8.69 | 1.52 | 1.41 |
| 81 | DA | 1421 | G | C2'-C1' | -8.69 | 1.43 | 1.53 |
| 81 | DA | 2265 | C | C2'-C1' | -8.69 | 1.43 | 1.53 |
| 81 | DA | 2335 | G | O4'-C1' | -8.69 | 1.30 | 1.41 |
| 81 | DA | 2486 | A | O4'-C1' | 8.69 | 1.52 | 1.41 |
| 81 | DA | 2716 | U | O4'-C1' | 8.69 | 1.52 | 1.41 |
| 82 | DB | 28 | C | C2'-C1' | -8.69 | 1.43 | 1.53 |
| 81 | DA | 1292 | C | C2'-C1' | -8.68 | 1.43 | 1.53 |
| 78 | CA | 1297 | G | O4'-C1' | -8.68 | 1.30 | 1.41 |
| 81 | DA | 2621 | G | C2'-C1' | -8.68 | 1.43 | 1.53 |
| 78 | CA | 288 | A | C2'-C1' | 8.68 | 1.62 | 1.53 |
| 78 | CA | 1543 | A | O4'-C1' | 8.68 | 1.52 | 1.41 |
| 83 | DC | 104 | C | O4'-C1' | 8.68 | 1.52 | 1.41 |
| 81 | DA | 176 | G | C2'-C1' | -8.67 | 1.43 | 1.53 |
| 26 | AZ | 39 | LEU | CA-CB | 8.67 | 1.73 | 1.53 |
| 81 | DA | 1291 | A | C2'-C1' | 8.67 | 1.62 | 1.53 |
| 2 | AA | 252 | TRP | CA-CB | 8.66 | 1.73 | 1.53 |
| 43 | BP | 80 | THR | CA-CB | 8.66 | 1.75 | 1.53 |
| 78 | CA | 324 | U | C2'-C1' | -8.66 | 1.43 | 1.53 |
| 78 | CA | 1087 | A | P-O5' | -8.66 | 1.51 | 1.59 |
| 78 | CA | 1648 | A | C5'-C4' | 8.66 | 1.61 | 1.51 |
| 47 | BU | 126 | VAL | N-CA | -8.66 | 1.29 | 1.46 |
| 78 | CA | 407 | A | C2'-C1' | 8.66 | 1.62 | 1.53 |
| 81 | DA | 604 | G | C2'-C1' | 8.66 | 1.62 | 1.53 |
| 81 | DA | 2156 | C | O4'-C1' | 8.65 | 1.52 | 1.41 |
| 60 | Bi | 56 | THR | N-CA | -8.65 | 1.29 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 856 | G | O4'-C1' | 8.65 | 1.52 | 1.41 |
| 78 | CA | 1423 | U | O4'-C1' | 8.65 | 1.52 | 1.41 |
| 81 | DA | 3322 | A | O4'-C1' | 8.65 | 1.52 | 1.41 |
| 5 | AC | 162 | SER | N-CA | -8.64 | 1.29 | 1.46 |
| 53 | Ba | 60 | LYS | N-CA | 8.64 | 1.63 | 1.46 |
| 79 | CB | 65 | U | O4'-C1' | 8.64 | 1.52 | 1.41 |
| 81 | DA | 2526 | C | O4'-C1' | 8.64 | 1.52 | 1.41 |
| 43 | BP | 17 | ASP | N-CA | -8.64 | 1.29 | 1.46 |
| 78 | CA | 333 | A | O4'-C1' | 8.64 | 1.52 | 1.41 |
| 78 | CA | 664 | U | C2'-C1' | -8.64 | 1.43 | 1.53 |
| 81 | DA | 801 | A | C3'-C2' | -8.64 | 1.43 | 1.52 |
| 31 | BB | 73 | GLU | CA-CB | 8.64 | 1.73 | 1.53 |
| 78 | CA | 621 | A | O4'-C1' | -8.64 | 1.30 | 1.41 |
| 81 | DA | 311 | C | O4'-C1' | 8.64 | 1.52 | 1.41 |
| 81 | DA | 425 | G | C2'-C1' | -8.64 | 1.43 | 1.53 |
| 81 | DA | 1262 | G | C2'-C1' | -8.63 | 1.43 | 1.53 |
| 81 | DA | 2159 | U | O4'-C1' | -8.63 | 1.30 | 1.41 |
| 81 | DA | 2257 | C | C2'-C1' | 8.63 | 1.62 | 1.53 |
| 78 | CA | 1379 | C | C2'-C1' | -8.63 | 1.43 | 1.53 |
| 78 | CA | 1767 | G | O4'-C1' | 8.63 | 1.52 | 1.41 |
| 81 | DA | 3220 | G | O4'-C1' | 8.63 | 1.52 | 1.41 |
| 44 | BO | 57 | GLY | C-O | -8.63 | 1.09 | 1.23 |
| 82 | DB | 19 | C | O4'-C1' | 8.63 | 1.52 | 1.41 |
| 78 | CA | 1748 | G | C2'-C1' | -8.63 | 1.43 | 1.53 |
| 81 | DA | 2154 | U | C2'-C1' | -8.63 | 1.43 | 1.53 |
| 81 | DA | 326 | U | O4'-C1' | 8.63 | 1.52 | 1.41 |
| 81 | DA | 1338 | C | C3'-C2' | 8.62 | 1.62 | 1.52 |
| 81 | DA | 1392 | G | O4'-C1' | 8.62 | 1.52 | 1.41 |
| 81 | DA | 2463 | G | O4'-C1' | -8.63 | 1.30 | 1.41 |
| 81 | DA | 541 | U | C2'-C1' | 8.62 | 1.62 | 1.53 |
| 81 | DA | 1428 | A | O4'-C1' | 8.62 | 1.52 | 1.41 |
| 81 | DA | 1864 | A | C2'-C1' | 8.62 | 1.62 | 1.53 |
| 81 | DA | 2994 | A | C2'-C1' | 8.62 | 1.62 | 1.53 |
| 81 | DA | 2430 | A | O4'-C1' | 8.62 | 1.52 | 1.41 |
| 51 | BZ | 51 | TRP | N-CA | 8.62 | 1.63 | 1.46 |
| 78 | CA | 222 | A | O4'-C1' | -8.62 | 1.30 | 1.41 |
| 78 | CA | 1364 | G | C2'-C1' | -8.62 | 1.43 | 1.53 |
| 81 | DA | 2151 | C | O4'-C1' | 8.62 | 1.52 | 1.41 |
| 81 | DA | 2391 | G | O4'-C1' | 8.61 | 1.52 | 1.41 |
| 78 | CA | 470 | A | O4'-C1' | 8.61 | 1.52 | 1.41 |
| 81 | DA | 990 | U | O3'-P | -8.61 | 1.50 | 1.61 |
| 81 | DA | 1726 | C | O4'-C1' | 8.61 | 1.52 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1880 | U | O4'-C1' | 8.61 | 1.52 | 1.41 |
| 49 | BV | 170 | SER | C-OXT | -8.60 | 1.07 | 1.23 |
| 81 | DA | 2 | U | C2'-C1' | 8.60 | 1.62 | 1.53 |
| 81 | DA | 1580 | A | C2'-C1' | -8.60 | 1.43 | 1.53 |
| 81 | DA | 1611 | G | C2'-C1' | -8.60 | 1.43 | 1.53 |
| 82 | DB | 92 | A | C2'-C1' | -8.60 | 1.43 | 1.53 |
| 81 | DA | 1675 | G | O4'-C1' | -8.60 | 1.30 | 1.41 |
| 81 | DA | 2512 | C | O4'-C1' | 8.60 | 1.52 | 1.41 |
| 81 | DA | 140 | C | O4'-C1' | 8.60 | 1.52 | 1.41 |
| 81 | DA | 1479 | U | O4'-C1' | 8.60 | 1.52 | 1.41 |
| 78 | CA | 1246 | C | C2'-C1' | -8.59 | 1.43 | 1.53 |
| 81 | DA | 627 | U | O4'-C1' | 8.59 | 1.52 | 1.41 |
| 79 | CB | 27 | G | C2'-C1' | -8.59 | 1.44 | 1.53 |
| 81 | DA | 3002 | C | O3'-P | -8.59 | 1.50 | 1.61 |
| 78 | CA | 833 | U | C2'-C1' | 8.59 | 1.62 | 1.53 |
| 78 | CA | 1306 | C | C3'-C2' | 8.59 | 1.62 | 1.52 |
| 81 | DA | 273 | A | C2'-C1' | -8.58 | 1.44 | 1.53 |
| 78 | CA | 166 | C | O4'-C1' | 8.58 | 1.52 | 1.41 |
| 78 | CA | 366 | A | O4'-C1' | 8.58 | 1.52 | 1.41 |
| 81 | DA | 1346 | G | O4'-C1' | -8.58 | 1.30 | 1.41 |
| 81 | DA | 1702 | U | O4'-C1' | -8.58 | 1.30 | 1.41 |
| 78 | CA | 626 | U | C2'-C1' | -8.58 | 1.44 | 1.53 |
| 78 | CA | 1134 | C | C2'-C1' | -8.57 | 1.44 | 1.53 |
| 81 | DA | 1050 | U | C2'-C1' | 8.57 | 1.62 | 1.53 |
| 81 | DA | 3069 | G | C2'-C1' | -8.57 | 1.44 | 1.53 |
| 78 | CA | 42 | G | O4'-C1' | 8.57 | 1.52 | 1.41 |
| 81 | DA | 783 | A | C2'-C1' | -8.57 | 1.44 | 1.53 |
| 81 | DA | 2199 | G | C2'-C1' | -8.56 | 1.44 | 1.53 |
| 81 | DA | 1195 | A | O4'-C1' | -8.56 | 1.30 | 1.41 |
| 13 | AL | 87 | VAL | N-CA | 8.56 | 1.63 | 1.46 |
| 78 | CA | 1682 | U | O4'-C1' | 8.56 | 1.52 | 1.41 |
| 81 | DA | 2618 | G | O4'-C1' | -8.56 | 1.30 | 1.41 |
| 1 | Aa | 58 | VAL | C-N | 8.55 | 1.53 | 1.34 |
| 81 | DA | 759 | U | C5'-C4' | 8.55 | 1.61 | 1.51 |
| 40 | BK | 184 | THR | N-CA | 8.55 | 1.63 | 1.46 |
| 81 | DA | 453 | C | O4'-C1' | 8.55 | 1.52 | 1.41 |
| 78 | CA | 1591 | C | O4'-C1' | 8.55 | 1.52 | 1.41 |
| 81 | DA | 2393 | G | P-O5' | -8.54 | 1.51 | 1.59 |
| 78 | CA | 1581 | C | O4'-C1' | 8.54 | 1.52 | 1.41 |
| 81 | DA | 472 | A | O4'-C1' | 8.54 | 1.52 | 1.41 |
| 78 | CA | 392 | G | O4'-C1' | 8.54 | 1.52 | 1.41 |
| 82 | DB | 93 | U | C2'-C1' | 8.54 | 1.62 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 108 | A | O4'-C1' | 8.54 | 1.52 | 1.41 |
| 81 | DA | 3008 | A | C2'-C1' | -8.54 | 1.44 | 1.53 |
| 78 | CA | 610 | G | C2'-C1' | 8.53 | 1.62 | 1.53 |
| 78 | CA | 424 | C | O4'-C1' | 8.53 | 1.52 | 1.41 |
| 81 | DA | 2737 | C | C2'-C1' | -8.53 | 1.44 | 1.53 |
| 82 | DB | 53 | A | O4'-C1' | 8.53 | 1.52 | 1.41 |
| 81 | DA | 554 | A | O4'-C1' | 8.53 | 1.52 | 1.41 |
| 83 | DC | 70 | A | O4'-C1' | 8.53 | 1.52 | 1.41 |
| 78 | CA | 1139 | A | O4'-C1' | 8.53 | 1.52 | 1.41 |
| 81 | DA | 2213 | A | O4'-C1' | 8.53 | 1.52 | 1.41 |
| 81 | DA | 995 | U | O4'-C1' | 8.52 | 1.52 | 1.41 |
| 81 | DA | 1178 | G | C2'-C1' | -8.52 | 1.44 | 1.53 |
| 78 | CA | 1560 | U | O4'-C1' | 8.52 | 1.52 | 1.41 |
| 81 | DA | 524 | U | C2'-C1' | 8.52 | 1.62 | 1.53 |
| 81 | DA | 498 | A | C2'-C1' | -8.52 | 1.44 | 1.53 |
| 81 | DA | 2343 | C | C2'-C1' | -8.52 | 1.44 | 1.53 |
| 81 | DA | 649 | A | O4'-C1' | 8.52 | 1.52 | 1.41 |
| 81 | DA | 346 | C | O4'-C1' | 8.51 | 1.52 | 1.41 |
| 81 | DA | 871 | U | O4'-C1' | 8.51 | 1.52 | 1.41 |
| 81 | DA | 982 | C | C2'-C1' | 8.51 | 1.62 | 1.53 |
| 81 | DA | 1806 | A | C2'-C1' | -8.51 | 1.44 | 1.53 |
| 81 | DA | 641 | C | C2'-C1' | -8.51 | 1.44 | 1.53 |
| 81 | DA | 893 | C | O4'-C1' | 8.51 | 1.52 | 1.41 |
| 81 | DA | 2517 | U | O4'-C1' | 8.51 | 1.52 | 1.41 |
| 81 | DA | 2800 | G | O4'-C1' | 8.51 | 1.52 | 1.41 |
| 78 | CA | 628 | G | O4'-C1' | 8.50 | 1.52 | 1.41 |
| 81 | DA | 162 | G | O4'-C1' | -8.50 | 1.30 | 1.41 |
| 81 | DA | 1961 | G | C2'-C1' | -8.50 | 1.44 | 1.53 |
| 74 | BQ | 190 | ILE | CA-CB | -8.49 | 1.35 | 1.54 |
| 81 | DA | 2680 | A | C2'-C1' | -8.49 | 1.44 | 1.53 |
| 81 | DA | 3137 | C | O4'-C1' | 8.49 | 1.52 | 1.41 |
| 78 | CA | 570 | A | O4'-C1' | -8.49 | 1.30 | 1.41 |
| 4 | AD | 191 | ARG | NE-CZ | 8.49 | 1.44 | 1.33 |
| 81 | DA | 985 | U | C5'-C4' | 8.49 | 1.61 | 1.51 |
| 81 | DA | 1652 | G | C2'-C1' | -8.49 | 1.44 | 1.53 |
| 4 | AD | 241 | GLY | CA-C | -8.48 | 1.38 | 1.51 |
| 81 | DA | 603 | A | O4'-C1' | 8.48 | 1.52 | 1.41 |
| 78 | CA | 1329 | A | O4'-C1' | 8.48 | 1.52 | 1.41 |
| 81 | DA | 951 | A | O4'-C1' | 8.48 | 1.52 | 1.41 |
| 81 | DA | 1301 | A | O4'-C1' | 8.48 | 1.52 | 1.41 |
| 81 | DA | 2359 | C | O4'-C1' | 8.48 | 1.52 | 1.41 |
| 81 | DA | 2238 | G | C2'-C1' | -8.47 | 1.44 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 652 | G | O4'-C1' | 8.47 | 1.52 | 1.41 |
| 81 | DA | 322 | U | O4'-C1' | 8.47 | 1.52 | 1.41 |
| 78 | CA | 425 | A | C2'-C1' | -8.47 | 1.44 | 1.53 |
| 78 | CA | 1323 | C | O4'-C1' | 8.47 | 1.52 | 1.41 |
| 81 | DA | 767 | U | C2'-C1' | -8.47 | 1.44 | 1.53 |
| 81 | DA | 1382 | G | C2'-C1' | -8.47 | 1.44 | 1.53 |
| 81 | DA | 3335 | A | O4'-C1' | 8.47 | 1.52 | 1.41 |
| 81 | DA | 938 | C | O4'-C1' | 8.46 | 1.52 | 1.41 |
| 32 | BC | 256 | HIS | CA-CB | -8.45 | 1.35 | 1.53 |
| 81 | DA | 823 | C | O4'-C1' | 8.45 | 1.52 | 1.41 |
| 81 | DA | 670 | C | O4'-C1' | 8.45 | 1.52 | 1.41 |
| 82 | DB | 89 | A | O4'-C1' | 8.45 | 1.52 | 1.41 |
| 78 | CA | 233 | C | C2'-C1' | -8.45 | 1.44 | 1.53 |
| 78 | CA | 356 | G | C2'-C1' | -8.45 | 1.44 | 1.53 |
| 81 | DA | 675 | C | C2'-C1' | 8.45 | 1.62 | 1.53 |
| 81 | DA | 1079 | A | C2'-C1' | 8.45 | 1.62 | 1.53 |
| 78 | CA | 30 | G | C4'-O4' | -8.45 | 1.34 | 1.45 |
| 81 | DA | 2743 | A | C2'-C1' | -8.45 | 1.44 | 1.53 |
| 81 | DA | 917 | A | C2'-C1' | -8.44 | 1.44 | 1.53 |
| 81 | DA | 45 | A | O4'-C1' | 8.44 | 1.52 | 1.41 |
| 82 | DB | 47 | C | O4'-C1' | 8.44 | 1.52 | 1.41 |
| 81 | DA | 667 | C | O4'-C1' | 8.43 | 1.52 | 1.41 |
| 78 | CA | 970 | A | C2'-C1' | 8.43 | 1.62 | 1.53 |
| 81 | DA | 2279 | A | O3'-P | -8.43 | 1.51 | 1.61 |
| 81 | DA | 1508 | C | C2'-C1' | -8.43 | 1.44 | 1.53 |
| 81 | DA | 2490 | C | C2'-C1' | -8.43 | 1.44 | 1.53 |
| 81 | DA | 2729 | U | O4'-C1' | 8.43 | 1.52 | 1.41 |
| 81 | DA | 3126 | C | O4'-C1' | 8.43 | 1.52 | 1.41 |
| 78 | CA | 529 | A | P-O5' | 8.43 | 1.68 | 1.59 |
| 81 | DA | 790 | U | C4'-C3' | -8.43 | 1.43 | 1.53 |
| 81 | DA | 1820 | U | C5'-C4' | 8.42 | 1.61 | 1.51 |
| 81 | DA | 1364 | C | C2'-C1' | -8.42 | 1.44 | 1.53 |
| 81 | DA | 2087 | C | O4'-C1' | 8.42 | 1.52 | 1.41 |
| 1 | Aa | 57 | PRO | CA-C | 8.41 | 1.69 | 1.52 |
| 78 | CA | 1279 | C | C2'-C1' | -8.41 | 1.44 | 1.53 |
| 78 | CA | 613 | G | C2'-C1' | 8.40 | 1.62 | 1.53 |
| 78 | CA | 1202 | A | C2'-C1' | 8.40 | 1.62 | 1.53 |
| 81 | DA | 3062 | G | O4'-C1' | -8.40 | 1.30 | 1.41 |
| 78 | CA | 585 | A | O4'-C1' | 8.40 | 1.52 | 1.41 |
| 81 | DA | 16 | A | O4'-C1' | 8.40 | 1.52 | 1.41 |
| 81 | DA | 381 | U | C2'-C1' | -8.40 | 1.44 | 1.53 |
| 78 | CA | 1754 | A | C2'-C1' | -8.39 | 1.44 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 172 | G | O4'-C1' | 8.39 | 1.52 | 1.41 |
| 81 | DA | 1211 | U | O4'-C1' | 8.39 | 1.52 | 1.41 |
| 81 | DA | 1812 | G | C2'-C1' | -8.38 | 1.44 | 1.53 |
| 81 | DA | 20 | A | O4'-C1' | 8.38 | 1.52 | 1.41 |
| 81 | DA | 1778 | G | C2'-C1' | -8.38 | 1.44 | 1.53 |
| 78 | CA | 114 | C | C2'-C1' | 8.38 | 1.62 | 1.53 |
| 78 | CA | 1536 | G | O4'-C1' | 8.38 | 1.52 | 1.41 |
| 4 | AD | 91 | THR | N-CA | -8.38 | 1.29 | 1.46 |
| 78 | CA | 1368 | G | C2'-C1' | -8.38 | 1.44 | 1.53 |
| 81 | DA | 843 | A | C2'-C1' | 8.38 | 1.62 | 1.53 |
| 81 | DA | 3243 | A | O4'-C1' | 8.38 | 1.52 | 1.41 |
| 81 | DA | 888 | A | O4'-C1' | 8.38 | 1.52 | 1.41 |
| 81 | DA | 2846 | U | O4'-C1' | 8.38 | 1.52 | 1.41 |
| 46 | BT | 82 | LYS | CA-CB | -8.37 | 1.35 | 1.53 |
| 78 | CA | 1243 | G | C5'-C4' | 8.37 | 1.61 | 1.51 |
| 81 | DA | 1268 | G | C2'-C1' | -8.37 | 1.44 | 1.53 |
| 35 | BG | 27 | PRO | N-CA | 8.37 | 1.61 | 1.47 |
| 81 | DA | 2315 | G | C2'-C1' | -8.37 | 1.44 | 1.53 |
| 2 | AA | 252 | TRP | CB-CG | 8.37 | 1.65 | 1.50 |
| 81 | DA | 2600 | C | O4'-C1' | 8.37 | 1.52 | 1.41 |
| 82 | DB | 104 | A | O4'-C1' | 8.37 | 1.52 | 1.41 |
| 82 | DB | 136 | G | C2'-C1' | -8.37 | 1.44 | 1.53 |
| 81 | DA | 2671 | A | C2'-C1' | -8.37 | 1.44 | 1.53 |
| 5 | AC | 18 | PRO | CA-CB | -8.36 | 1.36 | 1.53 |
| 78 | CA | 347 | G | C2'-C1' | -8.36 | 1.44 | 1.53 |
| 78 | CA | 1163 | A | C2'-C1' | -8.36 | 1.44 | 1.53 |
| 81 | DA | 1421 | G | O4'-C1' | 8.36 | 1.52 | 1.41 |
| 81 | DA | 2298 | U | O4'-C1' | 8.36 | 1.52 | 1.41 |
| 81 | DA | 2849 | C | O4'-C1' | 8.36 | 1.52 | 1.41 |
| 81 | DA | 2248 | C | C2'-C1' | -8.36 | 1.44 | 1.53 |
| 82 | DB | 94 | C | C2'-C1' | -8.36 | 1.44 | 1.53 |
| 78 | CA | 1037 | C | C2'-C1' | -8.35 | 1.44 | 1.53 |
| 81 | DA | 1752 | A | O4'-C1' | 8.35 | 1.52 | 1.41 |
| 78 | CA | 1592 | A | C2'-C1' | -8.35 | 1.44 | 1.53 |
| 83 | DC | 14 | U | C2'-C1' | -8.35 | 1.44 | 1.53 |
| 81 | DA | 2138 | A | C2'-C1' | 8.34 | 1.62 | 1.53 |
| 78 | CA | 1667 | A | O4'-C1' | 8.34 | 1.52 | 1.41 |
| 78 | CA | 1726 | G | O4'-C1' | 8.34 | 1.52 | 1.41 |
| 32 | BC | 360 | ASP | CA-CB | 8.34 | 1.72 | 1.53 |
| 78 | CA | 255 | U | C5'-C4' | 8.34 | 1.61 | 1.51 |
| 81 | DA | 776 | U | O4'-C1' | 8.34 | 1.52 | 1.41 |
| 78 | CA | 306 | U | O4'-C1' | 8.33 | 1.52 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 82 | U | O4'-C1' | 8.33 | 1.52 | 1.41 |
| 81 | DA | 2736 | A | O4'-C1' | -8.33 | 1.30 | 1.41 |
| 10 | AI | 140 | LYS | CA-CB | 8.33 | 1.72 | 1.53 |
| 81 | DA | 750 | G | O4'-C1' | 8.33 | 1.52 | 1.41 |
| 81 | DA | 1144 | U | O4'-C1' | 8.33 | 1.52 | 1.41 |
| 78 | CA | 117 | U | O4'-C1' | 8.32 | 1.52 | 1.41 |
| 81 | DA | 2027 | C | O4'-C1' | 8.32 | 1.52 | 1.41 |
| 81 | DA | 2907 | G | O4'-C1' | -8.32 | 1.30 | 1.41 |
| 81 | DA | 937 | G | C2'-C1' | -8.32 | 1.44 | 1.53 |
| 32 | BC | 371 | GLN | C-N | -8.32 | 1.15 | 1.34 |
| 81 | DA | 3132 | C | C2'-C1' | -8.32 | 1.44 | 1.53 |
| 81 | DA | 2871 | G | O4'-C1' | 8.31 | 1.52 | 1.41 |
| 13 | AL | 87 | VAL | CA-CB | -8.31 | 1.37 | 1.54 |
| 81 | DA | 938 | C | C2'-C1' | -8.31 | 1.44 | 1.53 |
| 81 | DA | 1824 | U | O4'-C1' | 8.31 | 1.52 | 1.41 |
| 81 | DA | 3097 | C | O4'-C1' | 8.31 | 1.52 | 1.41 |
| 78 | CA | 368 | U | O3'-P | -8.31 | 1.51 | 1.61 |
| 81 | DA | 1274 | A | O4'-C1' | 8.30 | 1.52 | 1.41 |
| 78 | CA | 993 | A | O4'-C1' | 8.30 | 1.52 | 1.41 |
| 81 | DA | 1133 | A | C2'-C1' | -8.30 | 1.44 | 1.53 |
| 81 | DA | 2038 | C | C2'-C1' | -8.30 | 1.44 | 1.53 |
| 81 | DA | 3058 | U | C2'-C1' | -8.30 | 1.44 | 1.53 |
| 81 | DA | 3289 | G | C2'-C1' | -8.30 | 1.44 | 1.53 |
| 81 | DA | 1034 | U | C2'-C1' | -8.30 | 1.44 | 1.53 |
| 78 | CA | 344 | A | O4'-C1' | 8.29 | 1.52 | 1.41 |
| 78 | CA | 967 | A | C2'-C1' | 8.29 | 1.62 | 1.53 |
| 78 | CA | 1105 | C | O4'-C1' | 8.29 | 1.52 | 1.41 |
| 81 | DA | 1151 | U | O4'-C1' | 8.29 | 1.52 | 1.41 |
| 78 | CA | 1128 | C | C2'-C1' | -8.29 | 1.44 | 1.53 |
| 78 | CA | 559 | C | O4'-C1' | 8.29 | 1.52 | 1.41 |
| 81 | DA | 2274 | U | O4'-C1' | 8.29 | 1.52 | 1.41 |
| 81 | DA | 166 | C | C2'-C1' | -8.29 | 1.44 | 1.53 |
| 81 | DA | 2064 | C | O3'-P | -8.29 | 1.51 | 1.61 |
| 81 | DA | 829 | U | C2'-C1' | -8.28 | 1.44 | 1.53 |
| 81 | DA | 2197 | C | C2'-C1' | 8.28 | 1.62 | 1.53 |
| 78 | CA | 1646 | C | O4'-C1' | 8.28 | 1.52 | 1.41 |
| 78 | CA | 1389 | C | O4'-C1' | -8.28 | 1.30 | 1.41 |
| 81 | DA | 910 | G | O3'-P | -8.27 | 1.51 | 1.61 |
| 81 | DA | 2101 | C | O4'-C1' | 8.27 | 1.52 | 1.41 |
| 8 | AF | 36 | ALA | N-CA | -8.27 | 1.29 | 1.46 |
| 81 | DA | 499 | G | C2'-C1' | -8.27 | 1.44 | 1.53 |
| 78 | CA | 1359 | C | O4'-C1' | 8.27 | 1.52 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 82 | DB | 21 | C | C2'-C1' | -8.27 | 1.44 | 1.53 |
| 81 | DA | 1587 | A | C2'-C1' | 8.27 | 1.62 | 1.53 |
| 34 | BE | 123 | PHE | N-CA | 8.27 | 1.62 | 1.46 |
| 81 | DA | 1426 | C | C4'-C3' | -8.27 | 1.44 | 1.53 |
| 81 | DA | 2712 | U | C2'-C1' | 8.27 | 1.62 | 1.53 |
| 78 | CA | 1047 | G | C2'-C1' | -8.26 | 1.44 | 1.53 |
| 81 | DA | 103 | G | C2'-C1' | 8.26 | 1.62 | 1.53 |
| 81 | DA | 3338 | C | O4'-C1' | 8.26 | 1.52 | 1.41 |
| 81 | DA | 911 | C | C2'-C1' | -8.26 | 1.44 | 1.53 |
| 81 | DA | 636 | C | P-O5' | -8.26 | 1.51 | 1.59 |
| 81 | DA | 1968 | G | C2'-C1' | -8.25 | 1.44 | 1.53 |
| 81 | DA | 2719 | U | O4'-C1' | 8.25 | 1.52 | 1.41 |
| 78 | CA | 1315 | U | C2'-C1' | -8.25 | 1.44 | 1.53 |
| 78 | CA | 409 | C | O4'-C1' | 8.25 | 1.52 | 1.41 |
| 81 | DA | 519 | A | O4'-C1' | -8.24 | 1.30 | 1.41 |
| 81 | DA | 1067 | U | O4'-C1' | 8.24 | 1.52 | 1.41 |
| 83 | DC | 69 | G | C2'-C1' | -8.24 | 1.44 | 1.53 |
| 81 | DA | 2527 | G | O4'-C1' | -8.23 | 1.30 | 1.41 |
| 78 | CA | 163 | G | C4'-C3' | -8.23 | 1.44 | 1.53 |
| 81 | DA | 450 | G | O4'-C1' | 8.23 | 1.52 | 1.41 |
| 81 | DA | 782 | U | C2'-C1' | 8.23 | 1.62 | 1.53 |
| 78 | CA | 916 | U | O4'-C1' | 8.22 | 1.52 | 1.41 |
| 78 | CA | 1733 | C | C2'-C1' | -8.22 | 1.44 | 1.53 |
| 81 | DA | 1695 | U | O4'-C1' | -8.22 | 1.30 | 1.41 |
| 81 | DA | 2590 | A | O4'-C1' | 8.22 | 1.52 | 1.41 |
| 81 | DA | 3370 | A | C2'-C1' | -8.22 | 1.44 | 1.53 |
| 83 | DC | 103 | U | C2'-C1' | -8.22 | 1.44 | 1.53 |
| 36 | BF | 46 | THR | CA-C | 8.22 | 1.74 | 1.52 |
| 78 | CA | 596 | C | C2'-C1' | -8.22 | 1.44 | 1.53 |
| 78 | CA | 818 | C | P-OP2 | 8.22 | 1.62 | 1.49 |
| 78 | CA | 1212 | G | C2'-C1' | -8.22 | 1.44 | 1.53 |
| 81 | DA | 858 | A | O3'-P | -8.22 | 1.51 | 1.61 |
| 81 | DA | 1293 | U | O4'-C1' | 8.22 | 1.52 | 1.41 |
| 81 | DA | 3118 | C | C2'-C1' | -8.22 | 1.44 | 1.53 |
| 81 | DA | 628 | A | C2'-C1' | 8.21 | 1.62 | 1.53 |
| 81 | DA | 2167 | A | O4'-C1' | 8.21 | 1.52 | 1.41 |
| 78 | CA | 1225 | U | O4'-C1' | 8.21 | 1.52 | 1.41 |
| 81 | DA | 1469 | C | C2'-C1' | -8.21 | 1.44 | 1.53 |
| 78 | CA | 1340 | U | P-O5' | -8.21 | 1.51 | 1.59 |
| 78 | CA | 177 | U | C2'-C1' | -8.21 | 1.44 | 1.53 |
| 81 | DA | 555 | U | C2'-C1' | 8.21 | 1.62 | 1.53 |
| 78 | CA | 1418 | G | O4'-C1' | 8.21 | 1.52 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 1647 | U | C2'-C1' | -8.21 | 1.44 | 1.53 |
| 81 | DA | 3133 | C | C2'-C1' | -8.21 | 1.44 | 1.53 |
| 81 | DA | 2811 | A | O4'-C1' | 8.20 | 1.52 | 1.41 |
| 81 | DA | 2954 | U | O4'-C1' | 8.20 | 1.52 | 1.41 |
| 57 | Be | 203 | TRP | N-CA | 8.20 | 1.62 | 1.46 |
| 81 | DA | 972 | A | O4'-C1' | 8.20 | 1.52 | 1.41 |
| 83 | DC | 97 | C | C2'-C1' | -8.20 | 1.44 | 1.53 |
| 83 | DC | 1 | G | O4'-C1' | 8.20 | 1.52 | 1.41 |
| 81 | DA | 2171 | G | C2'-C1' | -8.19 | 1.44 | 1.53 |
| 82 | DB | 30 | C | C2'-C1' | -8.19 | 1.44 | 1.53 |
| 81 | DA | 2757 | U | O3'-P | -8.19 | 1.51 | 1.61 |
| 78 | CA | 551 | G | C2'-C1' | -8.19 | 1.44 | 1.53 |
| 78 | CA | 1596 | C | O4'-C1' | 8.19 | 1.52 | 1.41 |
| 81 | DA | 3088 | G | C2'-C1' | -8.19 | 1.44 | 1.53 |
| 78 | CA | 1756 | A | C2'-C1' | 8.19 | 1.62 | 1.53 |
| 81 | DA | 2327 | U | O4'-C1' | 8.19 | 1.52 | 1.41 |
| 78 | CA | 387 | A | C2'-C1' | 8.18 | 1.62 | 1.53 |
| 78 | CA | 1339 | C | O4'-C1' | 8.18 | 1.52 | 1.41 |
| 81 | DA | 647 | A | O4'-C1' | 8.18 | 1.52 | 1.41 |
| 81 | DA | 3054 | U | C2'-C1' | -8.18 | 1.44 | 1.53 |
| 81 | DA | 791 | A | O3'-P | -8.18 | 1.51 | 1.61 |
| 81 | DA | 2833 | A | C2'-C1' | -8.18 | 1.44 | 1.53 |
| 81 | DA | 1528 | G | O4'-C1' | -8.18 | 1.31 | 1.41 |
| 81 | DA | 2006 | G | C2'-C1' | -8.18 | 1.44 | 1.53 |
| 81 | DA | 2443 | A | O4'-C1' | 8.18 | 1.52 | 1.41 |
| 81 | DA | 268 | A | C2'-C1' | 8.17 | 1.62 | 1.53 |
| 81 | DA | 975 | C | C2'-C1' | 8.17 | 1.62 | 1.53 |
| 81 | DA | 1447 | G | O4'-C1' | 8.17 | 1.52 | 1.41 |
| 81 | DA | 2317 | A | C2'-C1' | -8.17 | 1.44 | 1.53 |
| 81 | DA | 538 | G | C2'-C1' | -8.17 | 1.44 | 1.53 |
| 83 | DC | 65 | G | O4'-C1' | 8.17 | 1.52 | 1.41 |
| 78 | CA | 1545 | A | O4'-C1' | -8.17 | 1.31 | 1.41 |
| 78 | CA | 1021 | C | O4'-C1' | 8.17 | 1.52 | 1.41 |
| 22 | AV | 105 | THR | CA-CB | 8.16 | 1.74 | 1.53 |
| 78 | CA | 1419 | G | C2'-C1' | -8.16 | 1.44 | 1.53 |
| 81 | DA | 3257 | C | C2'-C1' | -8.16 | 1.44 | 1.53 |
| 81 | DA | 197 | G | C2'-C1' | -8.16 | 1.44 | 1.53 |
| 14 | AM | 99 | HIS | N-CA | 8.16 | 1.62 | 1.46 |
| 81 | DA | 869 | G | C2'-C1' | -8.16 | 1.44 | 1.53 |
| 81 | DA | 1956 | A | C2'-C1' | 8.16 | 1.62 | 1.53 |
| 81 | DA | 566 | G | O4'-C1' | 8.16 | 1.52 | 1.41 |
| 81 | DA | 463 | C | O4'-C1' | 8.15 | 1.52 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 83 | DC | 61 | U | C2'-C1' | 8.15 | 1.62 | 1.53 |
| 81 | DA | 3216 | G | O4'-C1' | -8.15 | 1.31 | 1.41 |
| 81 | DA | 375 | A | C2'-C1' | 8.15 | 1.62 | 1.53 |
| 81 | DA | 637 | C | C5'-C4' | -8.15 | 1.41 | 1.51 |
| 81 | DA | 159 | A | O4'-C1' | 8.15 | 1.52 | 1.41 |
| 81 | DA | 1075 | A | C2'-C1' | -8.15 | 1.44 | 1.53 |
| 45 | BR | 140 | LEU | CA-CB | 8.14 | 1.72 | 1.53 |
| 81 | DA | 1101 | G | O4'-C1' | 8.14 | 1.52 | 1.41 |
| 81 | DA | 2509 | U | O3'-P | -8.14 | 1.51 | 1.61 |
| 81 | DA | 1406 | A | C2'-C1' | -8.14 | 1.44 | 1.53 |
| 81 | DA | 3054 | U | O4'-C1' | 8.14 | 1.52 | 1.41 |
| 78 | CA | 389 | G | C2'-C1' | -8.14 | 1.44 | 1.53 |
| 81 | DA | 855 | U | O3'-P | -8.14 | 1.51 | 1.61 |
| 81 | DA | 1129 | A | C2'-C1' | -8.14 | 1.44 | 1.53 |
| 78 | CA | 339 | C | O4'-C1' | 8.14 | 1.52 | 1.41 |
| 81 | DA | 1327 | C | O4'-C1' | 8.13 | 1.52 | 1.41 |
| 81 | DA | 2827 | U | O4'-C1' | -8.13 | 1.31 | 1.41 |
| 81 | DA | 532 | A | C2'-C1' | -8.13 | 1.44 | 1.53 |
| 81 | DA | 556 | U | O4'-C1' | 8.13 | 1.52 | 1.41 |
| 81 | DA | 1183 | C | O4'-C1' | 8.13 | 1.52 | 1.41 |
| 81 | DA | 1814 | A | O4'-C1' | -8.13 | 1.31 | 1.41 |
| 81 | DA | 1984 | C | C2'-C1' | -8.13 | 1.44 | 1.53 |
| 81 | DA | 2797 | C | O4'-C1' | 8.13 | 1.52 | 1.41 |
| 78 | CA | 1125 | A | C2'-C1' | -8.13 | 1.44 | 1.53 |
| 81 | DA | 1503 | A | O4'-C1' | 8.13 | 1.52 | 1.41 |
| 81 | DA | 264 | G | C2'-C1' | -8.12 | 1.44 | 1.53 |
| 81 | DA | 2647 | A | O4'-C1' | -8.12 | 1.31 | 1.41 |
| 78 | CA | 416 | A | O4'-C1' | 8.12 | 1.52 | 1.41 |
| 81 | DA | 2646 | C | C3'-C2' | -8.12 | 1.43 | 1.52 |
| 78 | CA | 689 | G | C2'-C1' | -8.12 | 1.44 | 1.53 |
| 78 | CA | 1033 | C | O4'-C1' | 8.12 | 1.52 | 1.41 |
| 81 | DA | 288 | C | O4'-C1' | 8.12 | 1.52 | 1.41 |
| 81 | DA | 2337 | C | C2'-C1' | -8.12 | 1.44 | 1.53 |
| 81 | DA | 424 | G | C2'-C1' | -8.12 | 1.44 | 1.53 |
| 81 | DA | 186 | U | C2'-C1' | 8.12 | 1.62 | 1.53 |
| 81 | DA | 771 | A | O4'-C1' | 8.11 | 1.52 | 1.41 |
| 81 | DA | 3130 | A | O4'-C1' | -8.11 | 1.31 | 1.41 |
| 81 | DA | 2755 | C | O3'-P | -8.11 | 1.51 | 1.61 |
| 81 | DA | 3314 | A | O4'-C1' | 8.11 | 1.52 | 1.41 |
| 78 | CA | 288 | A | O3'-P | -8.11 | 1.51 | 1.61 |
| 81 | DA | 489 | C | C2'-C1' | -8.11 | 1.44 | 1.53 |
| 81 | DA | 1451 | C | O4'-C1' | 8.11 | 1.52 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1791 | C | O3'-P | -8.11 | 1.51 | 1.61 |
| 35 | BG | 38 | THR | CA-CB | 8.10 | 1.74 | 1.53 |
| 78 | CA | 1329 | A | C2'-C1' | -8.10 | 1.44 | 1.53 |
| 81 | DA | 1964 | C | O4'-C1' | 8.10 | 1.52 | 1.41 |
| 78 | CA | 688 | G | C2'-C1' | -8.10 | 1.44 | 1.53 |
| 78 | CA | 1141 | G | O4'-C1' | 8.10 | 1.52 | 1.41 |
| 78 | CA | 438 | A | O4'-C1' | 8.10 | 1.52 | 1.41 |
| 81 | DA | 755 | A | C2'-C1' | -8.10 | 1.44 | 1.53 |
| 78 | CA | 1032 | G | O4'-C1' | 8.09 | 1.52 | 1.41 |
| 81 | DA | 1164 | G | C2'-C1' | -8.09 | 1.44 | 1.53 |
| 81 | DA | 1229 | G | O4'-C1' | -8.09 | 1.31 | 1.41 |
| 1 | Aa | 59 | ARG | N-CA | 8.09 | 1.62 | 1.46 |
| 79 | CB | 67 | G | C2'-C1' | -8.09 | 1.44 | 1.53 |
| 81 | DA | 1907 | C | C2'-C1' | -8.09 | 1.44 | 1.53 |
| 78 | CA | 223 | U | C3'-C2' | -8.09 | 1.43 | 1.52 |
| 78 | CA | 1083 | G | P-OP2 | 8.09 | 1.62 | 1.49 |
| 81 | DA | 205 | C | O4'-C1' | 8.08 | 1.52 | 1.41 |
| 81 | DA | 432 | G | C2'-C1' | -8.08 | 1.44 | 1.53 |
| 81 | DA | 2614 | G | O4'-C1' | -8.08 | 1.31 | 1.41 |
| 78 | CA | 1356 | U | C2'-C1' | -8.08 | 1.44 | 1.53 |
| 78 | CA | 1028 | C | C2'-C1' | -8.08 | 1.44 | 1.53 |
| 81 | DA | 1120 | A | C2'-C1' | -8.07 | 1.44 | 1.53 |
| 81 | DA | 1175 | C | C2'-C1' | -8.07 | 1.44 | 1.53 |
| 81 | DA | 1596 | C | C2'-C1' | -8.07 | 1.44 | 1.53 |
| 81 | DA | 3222 | U | O3'-P | -8.07 | 1.51 | 1.61 |
| 81 | DA | 2263 | C | O4'-C1' | 8.06 | 1.52 | 1.41 |
| 5 | AC | 164 | PHE | N-CA | 8.06 | 1.62 | 1.46 |
| 63 | Bm | 37 | TYR | CE1-CZ | 8.06 | 1.49 | 1.38 |
| 78 | CA | 1342 | C | O4'-C1' | 8.06 | 1.52 | 1.41 |
| 41 | BN | 108 | ARG | NE-CZ | 8.06 | 1.43 | 1.33 |
| 78 | CA | 1551 | U | P-O5' | 8.06 | 1.67 | 1.59 |
| 81 | DA | 1328 | C | O4'-C1' | 8.05 | 1.52 | 1.41 |
| 81 | DA | 2625 | C | C2'-C1' | -8.05 | 1.44 | 1.53 |
| 78 | CA | 18 | C | O4'-C1' | 8.05 | 1.52 | 1.41 |
| 78 | CA | 635 | A | C2'-C1' | -8.05 | 1.44 | 1.53 |
| 81 | DA | 812 | G | O4'-C1' | 8.05 | 1.52 | 1.41 |
| 78 | CA | 234 | G | C2'-C1' | 8.04 | 1.62 | 1.53 |
| 81 | DA | 3304 | U | O4'-C1' | 8.04 | 1.52 | 1.41 |
| 81 | DA | 584 | G | O4'-C1' | 8.04 | 1.52 | 1.41 |
| 81 | DA | 2787 | G | C2'-C1' | -8.04 | 1.44 | 1.53 |
| 78 | CA | 70 | C | O4'-C1' | 8.04 | 1.52 | 1.41 |
| 81 | DA | 1413 | G | C2'-C1' | -8.04 | 1.44 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 14 | AM | 88 | ARG | CZ-NH1 | 8.04 | 1.43 | 1.33 |
| 81 | DA | 919 | U | O4'-C1' | 8.04 | 1.52 | 1.41 |
| 81 | DA | 2683 | U | O3'-P | -8.04 | 1.51 | 1.61 |
| 81 | DA | 256 | G | C2'-C1' | -8.04 | 1.44 | 1.53 |
| 78 | CA | 1585 | U | O4'-C1' | 8.03 | 1.52 | 1.41 |
| 81 | DA | 2987 | A | O4'-C1' | 8.03 | 1.52 | 1.41 |
| 81 | DA | 2464 | U | C2'-C1' | -8.03 | 1.44 | 1.53 |
| 81 | DA | 2742 | C | O4'-C1' | 8.03 | 1.52 | 1.41 |
| 57 | Be | 218 | ARG | CZ-NH1 | 8.03 | 1.43 | 1.33 |
| 83 | DC | 85 | G | O4'-C1' | -8.03 | 1.31 | 1.41 |
| 81 | DA | 2387 | A | O4'-C1' | 8.03 | 1.52 | 1.41 |
| 78 | CA | 1342 | C | C2'-C1' | -8.03 | 1.44 | 1.53 |
| 81 | DA | 1779 | C | C2'-C1' | 8.02 | 1.62 | 1.53 |
| 81 | DA | 2860 | U | O4'-C1' | 8.02 | 1.52 | 1.41 |
| 78 | CA | 1107 | G | C2'-C1' | -8.02 | 1.44 | 1.53 |
| 81 | DA | 1982 | G | C2'-C1' | -8.02 | 1.44 | 1.53 |
| 78 | CA | 145 | A | O4'-C1' | -8.02 | 1.31 | 1.41 |
| 81 | DA | 1783 | U | C4'-C3' | 8.02 | 1.61 | 1.53 |
| 81 | DA | 2742 | C | C2'-C1' | -8.02 | 1.44 | 1.53 |
| 78 | CA | 1453 | G | C2'-C1' | 8.01 | 1.62 | 1.53 |
| 81 | DA | 555 | U | O4'-C1' | -8.01 | 1.31 | 1.41 |
| 81 | DA | 2465 | G | O4'-C1' | 8.01 | 1.52 | 1.41 |
| 82 | DB | 44 | A | O3'-P | -8.01 | 1.51 | 1.61 |
| 33 | BD | 355 | PHE | CA-CB | 8.01 | 1.71 | 1.53 |
| 78 | CA | 837 | G | O3'-P | -8.01 | 1.51 | 1.61 |
| 81 | DA | 1462 | A | O4'-C1' | 8.01 | 1.52 | 1.41 |
| 81 | DA | 248 | U | P-O5' | -8.01 | 1.51 | 1.59 |
| 81 | DA | 2365 | C | C2'-C1' | -8.01 | 1.44 | 1.53 |
| 81 | DA | 3386 | G | C2'-C1' | -8.01 | 1.44 | 1.53 |
| 81 | DA | 3016 | A | C2'-C1' | -8.01 | 1.44 | 1.53 |
| 78 | CA | 1383 | G | C2'-C1' | -8.00 | 1.44 | 1.53 |
| 81 | DA | 90 | C | C2'-C1' | -8.00 | 1.44 | 1.53 |
| 81 | DA | 510 | G | O4'-C1' | 8.00 | 1.52 | 1.41 |
| 81 | DA | 99 | A | O4'-C1' | 8.00 | 1.52 | 1.41 |
| 81 | DA | 187 | A | O4'-C1' | 8.00 | 1.52 | 1.41 |
| 66 | Bo | 4 | GLN | N-CA | 8.00 | 1.62 | 1.46 |
| 81 | DA | 3369 | G | O4'-C1' | 8.00 | 1.52 | 1.41 |
| 74 | BQ | 237 | GLU | CA-CB | -8.00 | 1.36 | 1.53 |
| 81 | DA | 2923 | U | C2'-C1' | -8.00 | 1.44 | 1.53 |
| 81 | DA | 3037 | U | O4'-C1' | 8.00 | 1.52 | 1.41 |
| 81 | DA | 629 | U | O4'-C1' | 7.99 | 1.52 | 1.41 |
| 61 | Bj | 20 | LYS | N-CA | 7.99 | 1.62 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 274 | G | O4'-C1' | 7.99 | 1.52 | 1.41 |
| 81 | DA | 2162 | U | O3'-P | -7.99 | 1.51 | 1.61 |
| 78 | CA | 425 | A | O4'-C1' | 7.98 | 1.52 | 1.41 |
| 81 | DA | 1549 | U | O4'-C1' | 7.98 | 1.52 | 1.41 |
| 81 | DA | 2033 | G | C2'-C1' | -7.98 | 1.44 | 1.53 |
| 81 | DA | 1568 | U | O4'-C1' | 7.98 | 1.52 | 1.41 |
| 78 | CA | 1703 | C | O4'-C1' | 7.98 | 1.52 | 1.41 |
| 81 | DA | 2099 | A | O4'-C1' | 7.98 | 1.52 | 1.41 |
| 4 | AD | 96 | ASN | N-CA | 7.97 | 1.62 | 1.46 |
| 78 | CA | 1001 | A | O4'-C1' | 7.97 | 1.52 | 1.41 |
| 81 | DA | 1473 | G | C2'-C1' | -7.97 | 1.44 | 1.53 |
| 81 | DA | 3127 | A | C2'-C1' | -7.97 | 1.44 | 1.53 |
| 78 | CA | 184 | C | C2'-C1' | -7.97 | 1.44 | 1.53 |
| 78 | CA | 1188 | G | O4'-C1' | 7.97 | 1.52 | 1.41 |
| 81 | DA | 713 | U | O4'-C1' | 7.97 | 1.52 | 1.41 |
| 81 | DA | 68 | C | O4'-C1' | 7.96 | 1.52 | 1.41 |
| 81 | DA | 228 | U | O3'-P | -7.96 | 1.51 | 1.61 |
| 81 | DA | 1883 | A | C2'-C1' | 7.96 | 1.62 | 1.53 |
| 81 | DA | 148 | G | C4'-C3' | -7.96 | 1.44 | 1.53 |
| 81 | DA | 170 | G | C2'-C1' | 7.96 | 1.62 | 1.53 |
| 81 | DA | 1374 | G | C2'-C1' | -7.96 | 1.44 | 1.53 |
| 82 | DB | 141 | C | O4'-C1' | 7.96 | 1.51 | 1.41 |
| 2 | AA | 229 | LYS | CA-CB | 7.96 | 1.71 | 1.53 |
| 83 | DC | 65 | G | C2'-C1' | -7.96 | 1.44 | 1.53 |
| 81 | DA | 1248 | C | O4'-C1' | 7.95 | 1.51 | 1.41 |
| 33 | BD | 148 | ILE | CA-CB | -7.95 | 1.36 | 1.54 |
| 78 | CA | 977 | A | C2'-C1' | -7.95 | 1.44 | 1.53 |
| 82 | DB | 97 | A | O3'-P | -7.95 | 1.51 | 1.61 |
| 22 | AV | 26 | LYS | C-N | 7.95 | 1.52 | 1.34 |
| 81 | DA | 128 | G | C2'-C1' | -7.95 | 1.44 | 1.53 |
| 81 | DA | 1511 | U | O4'-C1' | 7.95 | 1.51 | 1.41 |
| 32 | BC | 5 | LYS | N-CA | 7.95 | 1.62 | 1.46 |
| 38 | Bs | 72 | ASP | N-CA | 7.95 | 1.62 | 1.46 |
| 78 | CA | 177 | U | O4'-C1' | 7.95 | 1.51 | 1.41 |
| 78 | CA | 344 | A | C2'-C1' | -7.95 | 1.44 | 1.53 |
| 78 | CA | 684 | A | C2'-C1' | -7.95 | 1.44 | 1.53 |
| 81 | DA | 420 | G | C2'-C1' | 7.95 | 1.62 | 1.53 |
| 81 | DA | 1790 | G | O4'-C1' | -7.94 | 1.31 | 1.41 |
| 24 | AX | 78 | SER | CA-CB | 7.94 | 1.64 | 1.52 |
| 81 | DA | 3364 | C | O4'-C1' | 7.94 | 1.51 | 1.41 |
| 2 | AA | 104 | PRO | CA-CB | -7.94 | 1.37 | 1.53 |
| 78 | CA | 1113 | A | O4'-C1' | -7.94 | 1.31 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 547 | U | O4'-C1' | 7.93 | 1.51 | 1.41 |
| 81 | DA | 248 | U | C2'-C1' | 7.93 | 1.62 | 1.53 |
| 81 | DA | 785 | G | C2'-C1' | 7.93 | 1.62 | 1.53 |
| 81 | DA | 1535 | A | O4'-C1' | -7.93 | 1.31 | 1.41 |
| 81 | DA | 2235 | C | C2'-C1' | -7.93 | 1.44 | 1.53 |
| 78 | CA | 1412 | G | C4'-O4' | -7.93 | 1.35 | 1.45 |
| 78 | CA | 1440 | C | C2'-C1' | -7.93 | 1.44 | 1.53 |
| 81 | DA | 78 | U | O4'-C1' | 7.93 | 1.51 | 1.41 |
| 81 | DA | 1634 | G | C2'-C1' | -7.93 | 1.44 | 1.53 |
| 53 | Ba | 14 | VAL | N-CA | 7.92 | 1.62 | 1.46 |
| 78 | CA | 48 | G | O4'-C1' | 7.92 | 1.51 | 1.41 |
| 81 | DA | 811 | U | O4'-C1' | 7.92 | 1.51 | 1.41 |
| 81 | DA | 3151 | U | O4'-C1' | -7.92 | 1.31 | 1.41 |
| 82 | DB | 83 | C | C2'-C1' | 7.92 | 1.62 | 1.53 |
| 78 | CA | 1615 | C | C4'-C3' | -7.92 | 1.44 | 1.53 |
| 81 | DA | 2253 | G | O4'-C1' | -7.92 | 1.31 | 1.41 |
| 81 | DA | 166 | C | O4'-C1' | 7.92 | 1.51 | 1.41 |
| 32 | BC | 26 | ARG | CD-NE | 7.92 | 1.59 | 1.46 |
| 81 | DA | 997 | A | C2'-C1' | 7.92 | 1.62 | 1.53 |
| 78 | CA | 1777 | G | C2'-C1' | -7.92 | 1.44 | 1.53 |
| 81 | DA | 3304 | U | C3'-O3' | 7.92 | 1.53 | 1.42 |
| 81 | DA | 1497 | C | O4'-C1' | 7.92 | 1.51 | 1.41 |
| 78 | CA | 125 | U | O4'-C1' | 7.91 | 1.51 | 1.41 |
| 81 | DA | 3161 | C | O4'-C1' | 7.91 | 1.51 | 1.41 |
| 78 | CA | 1717 | G | C2'-C1' | -7.91 | 1.44 | 1.53 |
| 31 | BB | 249 | SER | N-CA | -7.91 | 1.30 | 1.46 |
| 78 | CA | 1205 | C | C2'-C1' | -7.91 | 1.44 | 1.53 |
| 51 | BZ | 61 | LYS | N-CA | -7.91 | 1.30 | 1.46 |
| 78 | CA | 432 | G | C2'-C1' | -7.91 | 1.44 | 1.53 |
| 81 | DA | 599 | C | C2'-C1' | -7.91 | 1.44 | 1.53 |
| 81 | DA | 945 | C | C2'-C1' | -7.91 | 1.44 | 1.53 |
| 78 | CA | 1110 | G | C2'-C1' | -7.91 | 1.44 | 1.53 |
| 81 | DA | 83 | U | C2'-C1' | -7.90 | 1.44 | 1.53 |
| 81 | DA | 1918 | C | O4'-C1' | 7.90 | 1.51 | 1.41 |
| 78 | CA | 848 | C | O4'-C1' | 7.90 | 1.51 | 1.41 |
| 78 | CA | 1757 | G | C2'-C1' | -7.90 | 1.44 | 1.53 |
| 81 | DA | 1285 | G | C3'-C2' | -7.90 | 1.44 | 1.52 |
| 81 | DA | 767 | U | O4'-C1' | 7.89 | 1.51 | 1.41 |
| 81 | DA | 178 | U | P-O5' | -7.89 | 1.51 | 1.59 |
| 81 | DA | 293 | C | O4'-C1' | 7.89 | 1.51 | 1.41 |
| 81 | DA | 297 | G | O4'-C1' | -7.89 | 1.31 | 1.41 |
| 81 | DA | 2663 | G | O4'-C1' | -7.88 | 1.31 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2642 | A | C2'-C1' | -7.88 | 1.44 | 1.53 |
| 81 | DA | 335 | G | O4'-C1' | 7.88 | 1.51 | 1.41 |
| 22 | AV | 26 | LYS | CA-CB | -7.88 | 1.36 | 1.53 |
| 81 | DA | 1196 | C | C2'-C1' | -7.88 | 1.44 | 1.53 |
| 81 | DA | 2354 | C | C2'-C1' | -7.87 | 1.44 | 1.53 |
| 81 | DA | 2906 | C | O4'-C1' | 7.87 | 1.51 | 1.41 |
| 78 | CA | 1194 | A | O4'-C1' | 7.87 | 1.51 | 1.41 |
| 81 | DA | 3385 | U | C2'-C1' | -7.87 | 1.44 | 1.53 |
| 78 | CA | 588 | U | C5'-C4' | -7.87 | 1.42 | 1.51 |
| 78 | CA | 228 | G | P-O5' | 7.86 | 1.67 | 1.59 |
| 81 | DA | 866 | A | C2'-C1' | -7.86 | 1.44 | 1.53 |
| 31 | BB | 62 | VAL | N-CA | -7.86 | 1.30 | 1.46 |
| 81 | DA | 760 | G | O4'-C1' | 7.86 | 1.51 | 1.41 |
| 81 | DA | 1239 | C | O4'-C1' | 7.86 | 1.51 | 1.41 |
| 81 | DA | 2518 | C | O4'-C1' | 7.86 | 1.51 | 1.41 |
| 78 | CA | 1163 | A | O4'-C1' | 7.86 | 1.51 | 1.41 |
| 81 | DA | 547 | G | O4'-C1' | 7.86 | 1.51 | 1.41 |
| 78 | CA | 352 | A | C2'-C1' | 7.86 | 1.61 | 1.53 |
| 78 | CA | 1586 | A | O4'-C1' | 7.86 | 1.51 | 1.41 |
| 79 | CB | 68 | C | C2'-C1' | -7.86 | 1.44 | 1.53 |
| 81 | DA | 2811 | A | C2'-C1' | -7.86 | 1.44 | 1.53 |
| 81 | DA | 1078 | U | O4'-C1' | 7.86 | 1.51 | 1.41 |
| 78 | CA | 554 | C | O3'-P | -7.85 | 1.51 | 1.61 |
| 78 | CA | 1296 | A | O4'-C1' | 7.85 | 1.51 | 1.41 |
| 79 | CB | 75 | A | O4'-C1' | -7.85 | 1.31 | 1.41 |
| 78 | CA | 22 | A | O4'-C1' | 7.85 | 1.51 | 1.41 |
| 81 | DA | 672 | A | O3'-P | -7.85 | 1.51 | 1.61 |
| 81 | DA | 2730 | G | O4'-C1' | 7.85 | 1.51 | 1.41 |
| 78 | CA | 51 | A | C2'-C1' | -7.85 | 1.44 | 1.53 |
| 78 | CA | 1243 | G | O4'-C1' | 7.85 | 1.51 | 1.41 |
| 78 | CA | 106 | U | C2'-C1' | -7.85 | 1.44 | 1.53 |
| 83 | DC | 75 | G | C2'-C1' | -7.84 | 1.44 | 1.53 |
| 78 | CA | 1233 | G | O4'-C1' | -7.83 | 1.31 | 1.41 |
| 81 | DA | 1213 | G | C2'-C1' | -7.83 | 1.44 | 1.53 |
| 81 | DA | 2201 | G | C2'-C1' | -7.83 | 1.44 | 1.53 |
| 81 | DA | 3284 | G | C2'-C1' | -7.83 | 1.44 | 1.53 |
| 81 | DA | 1403 | C | C2'-C1' | -7.83 | 1.44 | 1.53 |
| 81 | DA | 3238 | G | C2'-C1' | -7.83 | 1.44 | 1.53 |
| 78 | CA | 1263 | G | O4'-C1' | -7.83 | 1.31 | 1.41 |
| 81 | DA | 2624 | G | O4'-C1' | 7.83 | 1.51 | 1.41 |
| 78 | CA | 1083 | G | O4'-C1' | 7.82 | 1.51 | 1.41 |
| 81 | DA | 2605 | G | O4'-C1' | 7.82 | 1.51 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 3246 | G | C2'-C1' | -7.82 | 1.44 | 1.53 |
| 81 | DA | 405 | U | O4'-C1' | 7.81 | 1.51 | 1.41 |
| 81 | DA | 3374 | U | C2'-C1' | -7.81 | 1.44 | 1.53 |
| 78 | CA | 55 | A | O4'-C1' | 7.81 | 1.51 | 1.41 |
| 81 | DA | 2654 | C | O4'-C1' | 7.81 | 1.51 | 1.41 |
| 81 | DA | 2479 | C | C2'-C1' | -7.81 | 1.44 | 1.53 |
| 78 | CA | 97 | C | C2'-C1' | -7.81 | 1.44 | 1.53 |
| 81 | DA | 2032 | U | O4'-C1' | 7.81 | 1.51 | 1.41 |
| 81 | DA | 1137 | C | O4'-C1' | 7.80 | 1.51 | 1.41 |
| 37 | BH | 158 | ASP | N-CA | -7.80 | 1.30 | 1.46 |
| 81 | DA | 997 | A | O4'-C1' | -7.80 | 1.31 | 1.41 |
| 81 | DA | 1451 | C | C2'-C1' | -7.80 | 1.44 | 1.53 |
| 78 | CA | 156 | A | C2'-C1' | 7.80 | 1.61 | 1.53 |
| 81 | DA | 822 | G | C2'-C1' | -7.80 | 1.44 | 1.53 |
| 78 | CA | 1146 | G | O4'-C1' | 7.79 | 1.51 | 1.41 |
| 83 | DC | 108 | U | O4'-C1' | 7.79 | 1.51 | 1.41 |
| 81 | DA | 3360 | C | O4'-C1' | 7.79 | 1.51 | 1.41 |
| 78 | CA | 442 | C | C2'-C1' | -7.79 | 1.44 | 1.53 |
| 81 | DA | 254 | A | C2'-C1' | -7.78 | 1.44 | 1.53 |
| 81 | DA | 1174 | G | O4'-C1' | 7.78 | 1.51 | 1.41 |
| 19 | AR | 108 | ARG | NE-CZ | 7.78 | 1.43 | 1.33 |
| 78 | CA | 127 | G | C3'-C2' | -7.78 | 1.44 | 1.52 |
| 78 | CA | 217 | A | C3'-C2' | 7.78 | 1.61 | 1.52 |
| 81 | DA | 1516 | C | O4'-C1' | 7.78 | 1.51 | 1.41 |
| 81 | DA | 1681 | U | C2'-C1' | -7.78 | 1.44 | 1.53 |
| 81 | DA | 3348 | G | O4'-C1' | -7.78 | 1.31 | 1.41 |
| 78 | CA | 459 | G | O4'-C1' | 7.77 | 1.51 | 1.41 |
| 81 | DA | 2604 | U | C2'-C1' | -7.77 | 1.44 | 1.53 |
| 57 | Be | 133 | TYR | N-CA | -7.77 | 1.30 | 1.46 |
| 78 | CA | 56 | U | C3'-O3' | 7.77 | 1.53 | 1.42 |
| 78 | CA | 900 | A | C3'-C2' | -7.76 | 1.44 | 1.52 |
| 81 | DA | 2362 | C | C3'-C2' | -7.76 | 1.44 | 1.52 |
| 81 | DA | 2940 | A | O4'-C1' | 7.76 | 1.51 | 1.41 |
| 81 | DA | 3027 | A | O4'-C1' | 7.76 | 1.51 | 1.41 |
| 48 | BW | 93 | ILE | CA-CB | 7.76 | 1.72 | 1.54 |
| 81 | DA | 430 | U | C2'-C1' | -7.76 | 1.44 | 1.53 |
| 81 | DA | 1689 | U | C5'-C4' | -7.76 | 1.42 | 1.51 |
| 41 | BN | 108 | ARG | CZ-NH1 | 7.76 | 1.43 | 1.33 |
| 78 | CA | 270 | C | C2'-C1' | -7.76 | 1.44 | 1.53 |
| 78 | CA | 178 | U | C2'-C1' | -7.76 | 1.44 | 1.53 |
| 81 | DA | 2446 | U | O4'-C1' | 7.76 | 1.51 | 1.41 |
| 81 | DA | 1121 | U | O4'-C1' | 7.75 | 1.51 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 1077 | C | C2'-C1' | -7.75 | 1.44 | 1.53 |
| 81 | DA | 161 | G | O3'-P | -7.75 | 1.51 | 1.61 |
| 78 | CA | 929 | A | C2'-C1' | -7.75 | 1.44 | 1.53 |
| 82 | DB | 7 | U | C2'-C1' | -7.75 | 1.44 | 1.53 |
| 81 | DA | 2765 | C | C2'-C1' | -7.75 | 1.44 | 1.53 |
| 81 | DA | 1181 | U | C2'-C1' | 7.75 | 1.61 | 1.53 |
| 81 | DA | 2135 | U | O4'-C1' | 7.75 | 1.51 | 1.41 |
| 81 | DA | 3034 | C | O3'-P | -7.75 | 1.51 | 1.61 |
| 76 | BS | 52 | LYS | CA-CB | 7.74 | 1.71 | 1.53 |
| 81 | DA | 1571 | A | O4'-C1' | -7.74 | 1.31 | 1.41 |
| 83 | DC | 10 | C | O4'-C1' | 7.74 | 1.51 | 1.41 |
| 13 | AL | 38 | PHE | CE1-CZ | 7.74 | 1.52 | 1.37 |
| 78 | CA | 1668 | G | O4'-C1' | 7.74 | 1.51 | 1.41 |
| 2 | AA | 195 | TRP | N-CA | 7.74 | 1.61 | 1.46 |
| 78 | CA | 1409 | G | C2'-C1' | 7.74 | 1.61 | 1.53 |
| 81 | DA | 178 | U | O3'-P | -7.74 | 1.51 | 1.61 |
| 81 | DA | 1743 | G | O4'-C1' | 7.74 | 1.51 | 1.41 |
| 83 | DC | 117 | C | C2'-C1' | -7.74 | 1.44 | 1.53 |
| 78 | CA | 1667 | A | C2'-C1' | -7.73 | 1.44 | 1.53 |
| 81 | DA | 2848 | G | C2'-C1' | -7.73 | 1.44 | 1.53 |
| 11 | AJ | 120 | SER | N-CA | 7.73 | 1.61 | 1.46 |
| 81 | DA | 2404 | A | O4'-C1' | 7.73 | 1.51 | 1.41 |
| 21 | AT | 57 | GLY | N-CA | -7.72 | 1.34 | 1.46 |
| 78 | CA | 120 | U | P-O5' | 7.72 | 1.67 | 1.59 |
| 81 | DA | 2773 | C | O4'-C1' | 7.72 | 1.51 | 1.41 |
| 11 | AJ | 14 | GLN | CD-OE1 | 7.72 | 1.41 | 1.24 |
| 81 | DA | 543 | C | C2'-C1' | -7.72 | 1.44 | 1.53 |
| 81 | DA | 3363 | U | C2'-C1' | 7.72 | 1.61 | 1.53 |
| 78 | CA | 219 | A | C5'-C4' | 7.72 | 1.60 | 1.51 |
| 78 | CA | 1010 | C | O4'-C1' | 7.72 | 1.51 | 1.41 |
| 81 | DA | 1914 | G | O4'-C1' | 7.72 | 1.51 | 1.41 |
| 81 | DA | 2471 | U | C2'-C1' | 7.72 | 1.61 | 1.53 |
| 78 | CA | 584 | C | O4'-C1' | 7.72 | 1.51 | 1.41 |
| 82 | DB | 151 | C | C5'-C4' | 7.72 | 1.60 | 1.51 |
| 78 | CA | 855 | A | C5'-C4' | 7.72 | 1.60 | 1.51 |
| 79 | CB | 29 | C | C2'-C1' | -7.72 | 1.44 | 1.53 |
| 81 | DA | 1042 | U | C2'-C1' | -7.71 | 1.44 | 1.53 |
| 78 | CA | 1169 | G | O4'-C1' | 7.71 | 1.51 | 1.41 |
| 82 | DB | 101 | U | O4'-C1' | 7.70 | 1.51 | 1.41 |
| 81 | DA | 1839 | A | O4'-C1' | 7.70 | 1.51 | 1.41 |
| 78 | CA | 1400 | A | O4'-C1' | 7.70 | 1.51 | 1.41 |
| 78 | CA | 326 | G | O4'-C1' | 7.70 | 1.51 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1908 | A | O4'-C1' | 7.70 | 1.51 | 1.41 |
| 81 | DA | 1953 | G | O3'-P | -7.70 | 1.51 | 1.61 |
| 81 | DA | 2352 | A | O4'-C1' | 7.70 | 1.51 | 1.41 |
| 81 | DA | 2887 | A | O4'-C1' | 7.69 | 1.51 | 1.41 |
| 81 | DA | 430 | U | O4'-C1' | 7.69 | 1.51 | 1.41 |
| 81 | DA | 953 | G | C2'-C1' | -7.69 | 1.44 | 1.53 |
| 78 | CA | 239 | C | C4'-C3' | 7.69 | 1.61 | 1.53 |
| 81 | DA | 1757 | A | N9-C4 | -7.69 | 1.33 | 1.37 |
| 81 | DA | 3331 | U | O4'-C1' | -7.69 | 1.31 | 1.41 |
| 74 | BQ | 137 | ASP | N-CA | -7.69 | 1.30 | 1.46 |
| 17 | AQ | 63 | LYS | C-N | 7.68 | 1.46 | 1.33 |
| 81 | DA | 1726 | C | C2'-C1' | -7.68 | 1.44 | 1.53 |
| 81 | DA | 3305 | A | C2'-C1' | -7.68 | 1.44 | 1.53 |
| 83 | DC | 76 | U | C2'-C1' | 7.68 | 1.61 | 1.53 |
| 81 | DA | 1165 | A | O4'-C1' | 7.68 | 1.51 | 1.41 |
| 78 | CA | 1566 | U | C2'-C1' | 7.68 | 1.61 | 1.53 |
| 81 | DA | 2271 | A | C2'-C1' | 7.68 | 1.61 | 1.53 |
| 78 | CA | 1438 | G | O4'-C1' | 7.66 | 1.51 | 1.41 |
| 79 | CB | 21 | A | O4'-C1' | 7.66 | 1.51 | 1.41 |
| 81 | DA | 848 | A | O4'-C1' | 7.66 | 1.51 | 1.41 |
| 81 | DA | 1465 | A | C2'-C1' | -7.66 | 1.45 | 1.53 |
| 78 | CA | 1480 | G | O4'-C1' | -7.66 | 1.31 | 1.41 |
| 81 | DA | 3086 | A | C2'-C1' | 7.66 | 1.61 | 1.53 |
| 81 | DA | 54 | C | O4'-C1' | 7.66 | 1.51 | 1.41 |
| 81 | DA | 2864 | A | O4'-C1' | 7.66 | 1.51 | 1.41 |
| 81 | DA | 2667 | A | C2'-C1' | -7.66 | 1.45 | 1.53 |
| 78 | CA | 1288 | G | O4'-C1' | 7.65 | 1.51 | 1.41 |
| 81 | DA | 2007 | G | C2'-C1' | -7.65 | 1.45 | 1.53 |
| 81 | DA | 95 | A | C2'-C1' | -7.65 | 1.45 | 1.53 |
| 81 | DA | 2795 | U | C2'-C1' | 7.65 | 1.61 | 1.53 |
| 81 | DA | 1389 | G | C2'-C1' | -7.65 | 1.45 | 1.53 |
| 78 | CA | 1542 | G | C2'-C1' | 7.65 | 1.61 | 1.53 |
| 81 | DA | 3392 | U | C2'-C1' | -7.65 | 1.45 | 1.53 |
| 46 | BT | 127 | SER | CA-CB | 7.63 | 1.64 | 1.52 |
| 78 | CA | 1075 | C | O4'-C1' | 7.63 | 1.51 | 1.41 |
| 78 | CA | 1173 | C | O4'-C1' | 7.63 | 1.51 | 1.41 |
| 81 | DA | 1082 | U | O4'-C1' | 7.63 | 1.51 | 1.41 |
| 81 | DA | 1173 | U | O4'-C1' | 7.63 | 1.51 | 1.41 |
| 81 | DA | 1972 | A | O4'-C1' | -7.63 | 1.31 | 1.41 |
| 78 | CA | 1323 | C | C2'-C1' | -7.63 | 1.45 | 1.53 |
| 81 | DA | 602 | A | O4'-C1' | 7.63 | 1.51 | 1.41 |
| 81 | DA | 1267 | U | C2'-C1' | 7.63 | 1.61 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 61 | Bj | 20 | LYS | C-N | 7.63 | 1.51 | 1.34 |
| 81 | DA | 757 | C | O4'-C1' | 7.62 | 1.51 | 1.41 |
| 81 | DA | 1018 | G | O4'-C1' | 7.62 | 1.51 | 1.41 |
| 40 | BK | 18 | ARG | CZ-NH1 | 7.62 | 1.43 | 1.33 |
| 81 | DA | 2933 | A | O4'-C1' | 7.62 | 1.51 | 1.41 |
| 81 | DA | 3247 | G | O4'-C1' | 7.62 | 1.51 | 1.41 |
| 78 | CA | 687 | G | O4'-C1' | 7.62 | 1.51 | 1.41 |
| 81 | DA | 544 | C | O4'-C1' | 7.62 | 1.51 | 1.41 |
| 78 | CA | 56 | U | O3'-P | 7.61 | 1.70 | 1.61 |
| 81 | DA | 1510 | G | O4'-C1' | 7.61 | 1.51 | 1.41 |
| 78 | CA | 1461 | C | C2'-C1' | -7.61 | 1.45 | 1.53 |
| 81 | DA | 1546 | A | C2'-C1' | -7.61 | 1.45 | 1.53 |
| 74 | BQ | 123 | GLU | CA-CB | 7.61 | 1.70 | 1.53 |
| 81 | DA | 1784 | G | O4'-C1' | 7.61 | 1.51 | 1.41 |
| 83 | DC | 66 | C | O4'-C1' | 7.61 | 1.51 | 1.41 |
| 81 | DA | 1114 | U | C2'-C1' | -7.60 | 1.45 | 1.53 |
| 81 | DA | 1362 | G | O4'-C1' | -7.60 | 1.31 | 1.41 |
| 24 | AX | 47 | PHE | CG-CD1 | 7.60 | 1.50 | 1.38 |
| 82 | DB | 24 | G | C2'-C1' | -7.60 | 1.45 | 1.53 |
| 81 | DA | 323 | A | O4'-C1' | 7.60 | 1.51 | 1.41 |
| 81 | DA | 1576 | G | O4'-C1' | 7.60 | 1.51 | 1.41 |
| 81 | DA | 2780 | A | C2'-C1' | -7.60 | 1.45 | 1.53 |
| 78 | CA | 412 | A | C2'-C1' | 7.59 | 1.61 | 1.53 |
| 78 | CA | 605 | A | C2'-C1' | -7.59 | 1.45 | 1.53 |
| 78 | CA | 1787 | C | C2'-C1' | -7.59 | 1.45 | 1.53 |
| 81 | DA | 45 | A | C2'-C1' | -7.59 | 1.45 | 1.53 |
| 78 | CA | 1126 | G | C2'-C1' | -7.59 | 1.45 | 1.53 |
| 81 | DA | 397 | A | C2'-C1' | 7.59 | 1.61 | 1.53 |
| 81 | DA | 2902 | A | C2'-C1' | -7.59 | 1.45 | 1.53 |
| 78 | CA | 1756 | A | O4'-C1' | -7.59 | 1.31 | 1.41 |
| 81 | DA | 1040 | A | C2'-C1' | -7.59 | 1.45 | 1.53 |
| 78 | CA | 171 | A | C2'-C1' | 7.58 | 1.61 | 1.53 |
| 20 | AS | 46 | PRO | N-CD | -7.58 | 1.37 | 1.47 |
| 78 | CA | 1240 | U | O4'-C1' | 7.58 | 1.51 | 1.41 |
| 78 | CA | 1627 | U | C2'-C1' | -7.58 | 1.45 | 1.53 |
| 78 | CA | 1712 | A | C2'-C1' | 7.58 | 1.61 | 1.53 |
| 79 | CB | 17 | G | O4'-C1' | 7.58 | 1.51 | 1.41 |
| 4 | AD | 112 | HIS | CB-CG | 7.58 | 1.63 | 1.50 |
| 45 | BR | 143 | PRO | CA-CB | 7.58 | 1.68 | 1.53 |
| 82 | DB | 138 | A | O4'-C1' | 7.58 | 1.51 | 1.41 |
| 81 | DA | 167 | U | O4'-C1' | -7.58 | 1.31 | 1.41 |
| 81 | DA | 256 | G | O4'-C1' | 7.58 | 1.51 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 885 | G | C4'-C3' | -7.57 | 1.44 | 1.53 |
| 81 | DA | 2154 | U | O4'-C1' | 7.57 | 1.51 | 1.41 |
| 34 | BE | 104 | PHE | CG-CD1 | 7.57 | 1.50 | 1.38 |
| 81 | DA | 2385 | G | O4'-C1' | 7.57 | 1.51 | 1.41 |
| 81 | DA | 3086 | A | O4'-C1' | 7.57 | 1.51 | 1.41 |
| 78 | CA | 964 | U | C2'-C1' | 7.57 | 1.61 | 1.53 |
| 81 | DA | 904 | A | O4'-C1' | 7.57 | 1.51 | 1.41 |
| 61 | Bj | 48 | ARG | CZ-NH2 | 7.57 | 1.42 | 1.33 |
| 78 | CA | 1554 | U | C2'-C1' | 7.57 | 1.61 | 1.53 |
| 81 | DA | 1637 | A | O4'-C1' | 7.57 | 1.51 | 1.41 |
| 81 | DA | 2156 | C | C2'-C1' | -7.57 | 1.45 | 1.53 |
| 81 | DA | 3306 | U | P-O5' | -7.57 | 1.52 | 1.59 |
| 78 | CA | 1080 | U | O4'-C1' | 7.56 | 1.51 | 1.41 |
| 81 | DA | 1687 | U | O4'-C1' | 7.56 | 1.51 | 1.41 |
| 78 | CA | 928 | U | C2'-C1' | 7.56 | 1.61 | 1.53 |
| 78 | CA | 1747 | G | C2'-C1' | -7.56 | 1.45 | 1.53 |
| 81 | DA | 227 | G | C2'-C1' | -7.56 | 1.45 | 1.53 |
| 81 | DA | 516 | A | O4'-C1' | 7.56 | 1.51 | 1.41 |
| 78 | CA | 404 | G | O4'-C1' | 7.56 | 1.51 | 1.41 |
| 81 | DA | 344 | A | C2'-C1' | -7.56 | 1.45 | 1.53 |
| 81 | DA | 983 | A | O4'-C1' | -7.56 | 1.31 | 1.41 |
| 61 | Bj | 66 | VAL | CB-CG1 | -7.55 | 1.36 | 1.52 |
| 81 | DA | 1165 | A | C2'-C1' | -7.55 | 1.45 | 1.53 |
| 81 | DA | 1996 | C | C2'-C1' | 7.55 | 1.61 | 1.53 |
| 78 | CA | 1466 | G | C2'-C1' | -7.55 | 1.45 | 1.53 |
| 81 | DA | 1453 | A | C2'-C1' | 7.55 | 1.61 | 1.53 |
| 81 | DA | 2706 | G | C2'-C1' | -7.55 | 1.45 | 1.53 |
| 74 | BQ | 239 | ILE | N-CA | 7.55 | 1.61 | 1.46 |
| 81 | DA | 316 | U | C2'-C1' | 7.55 | 1.61 | 1.53 |
| 81 | DA | 163 | C | O4'-C1' | 7.55 | 1.51 | 1.41 |
| 81 | DA | 418 | A | C2'-C1' | 7.55 | 1.61 | 1.53 |
| 81 | DA | 721 | G | C2'-C1' | 7.55 | 1.61 | 1.53 |
| 81 | DA | 2932 | U | P-O5' | -7.55 | 1.52 | 1.59 |
| 81 | DA | 3092 | C | C2'-C1' | 7.55 | 1.61 | 1.53 |
| 78 | CA | 193 | U | O4'-C1' | 7.54 | 1.51 | 1.41 |
| 81 | DA | 444 | U | O4'-C1' | 7.54 | 1.51 | 1.41 |
| 82 | DB | 18 | U | C2'-C1' | -7.54 | 1.45 | 1.53 |
| 32 | BC | 382 | THR | N-CA | 7.54 | 1.61 | 1.46 |
| 62 | Bk | 25 | LYS | C-N | 7.54 | 1.51 | 1.34 |
| 78 | CA | 301 | A | O4'-C1' | 7.54 | 1.51 | 1.41 |
| 78 | CA | 1016 | C | C2'-C1' | -7.54 | 1.45 | 1.53 |
| 81 | DA | 638 | C | C4'-C3' | -7.54 | 1.44 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1807 | G | C2'-C1' | -7.54 | 1.45 | 1.53 |
| 51 | BZ | 60 | LYS | N-CA | 7.54 | 1.61 | 1.46 |
| 81 | DA | 1567 | U | C2'-C1' | -7.54 | 1.45 | 1.53 |
| 78 | CA | 1179 | G | O4'-C1' | 7.54 | 1.51 | 1.41 |
| 81 | DA | 1502 | C | O4'-C1' | 7.54 | 1.51 | 1.41 |
| 78 | CA | 1421 | A | O4'-C1' | -7.53 | 1.31 | 1.41 |
| 81 | DA | 3349 | C | O4'-C1' | 7.53 | 1.51 | 1.41 |
| 81 | DA | 3211 | C | O4'-C1' | 7.53 | 1.51 | 1.41 |
| 78 | CA | 1234 | A | C4'-C3' | -7.53 | 1.44 | 1.53 |
| 81 | DA | 1180 | A | O4'-C1' | -7.52 | 1.31 | 1.41 |
| 81 | DA | 174 | C | O4'-C1' | 7.52 | 1.51 | 1.41 |
| 81 | DA | 3308 | C | C2'-C1' | -7.52 | 1.45 | 1.53 |
| 81 | DA | 1012 | G | O4'-C1' | 7.52 | 1.51 | 1.41 |
| 81 | DA | 1564 | U | O4'-C1' | 7.52 | 1.51 | 1.41 |
| 78 | CA | 1563 | C | O4'-C1' | 7.52 | 1.51 | 1.41 |
| 81 | DA | 1509 | A | O4'-C1' | 7.52 | 1.51 | 1.41 |
| 81 | DA | 2244 | A | C2'-C1' | 7.52 | 1.61 | 1.53 |
| 81 | DA | 2346 | C | C2'-C1' | -7.52 | 1.45 | 1.53 |
| 83 | DC | 60 | G | O3'-P | -7.52 | 1.52 | 1.61 |
| 81 | DA | 497 | C | C2'-C1' | -7.51 | 1.45 | 1.53 |
| 81 | DA | 855 | U | O4'-C1' | 7.51 | 1.51 | 1.41 |
| 34 | BE | 54 | VAL | C-N | -7.51 | 1.16 | 1.34 |
| 78 | CA | 1410 | A | O4'-C1' | 7.51 | 1.51 | 1.41 |
| 78 | CA | 4 | C | O4'-C1' | 7.51 | 1.51 | 1.41 |
| 78 | CA | 513 | U | O3'-P | -7.51 | 1.52 | 1.61 |
| 81 | DA | 2282 | U | O4'-C1' | 7.51 | 1.51 | 1.41 |
| 78 | CA | 1127 | G | O4'-C1' | 7.51 | 1.51 | 1.41 |
| 81 | DA | 1942 | U | O4'-C1' | 7.51 | 1.51 | 1.41 |
| 81 | DA | 398 | A | O4'-C1' | 7.50 | 1.51 | 1.41 |
| 81 | DA | 1254 | C | C2'-C1' | -7.50 | 1.45 | 1.53 |
| 81 | DA | 3375 | A | C2'-C1' | -7.50 | 1.45 | 1.53 |
| 81 | DA | 587 | U | O4'-C1' | 7.50 | 1.51 | 1.41 |
| 35 | BG | 99 | GLU | CB-CG | 7.50 | 1.66 | 1.52 |
| 81 | DA | 1958 | U | O4'-C1' | 7.50 | 1.51 | 1.41 |
| 81 | DA | 3079 | U | C2'-C1' | -7.50 | 1.45 | 1.53 |
| 78 | CA | 460 | A | C4'-C3' | -7.50 | 1.45 | 1.53 |
| 83 | DC | 93 | U | C2'-C1' | -7.50 | 1.45 | 1.53 |
| 78 | CA | 478 | A | C2'-C1' | 7.50 | 1.61 | 1.53 |
| 78 | CA | 918 | U | C4'-C3' | -7.50 | 1.45 | 1.53 |
| 81 | DA | 3100 | U | O4'-C1' | 7.50 | 1.51 | 1.41 |
| 78 | CA | 205 | U | C2'-C1' | -7.50 | 1.45 | 1.53 |
| 81 | DA | 891 | G | C2'-C1' | -7.50 | 1.45 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2685 | C | O3'-P | -7.49 | 1.52 | 1.61 |
| 82 | DB | 97 | A | C2'-C1' | -7.49 | 1.45 | 1.53 |
| 81 | DA | 794 | U | C2'-C1' | -7.49 | 1.45 | 1.53 |
| 81 | DA | 1143 | A | C2'-C1' | -7.49 | 1.45 | 1.53 |
| 78 | CA | 1234 | A | C2'-C1' | 7.49 | 1.61 | 1.53 |
| 81 | DA | 170 | G | O4'-C1' | 7.49 | 1.51 | 1.41 |
| 81 | DA | 803 | C | O4'-C1' | 7.49 | 1.51 | 1.41 |
| 81 | DA | 2109 | U | O4'-C1' | 7.49 | 1.51 | 1.41 |
| 78 | CA | 1306 | C | C2'-C1' | -7.48 | 1.45 | 1.53 |
| 81 | DA | 1197 | A | O4'-C1' | 7.48 | 1.51 | 1.41 |
| 81 | DA | 2196 | C | O4'-C1' | 7.48 | 1.51 | 1.41 |
| 78 | CA | 37 | U | C2'-C1' | 7.48 | 1.61 | 1.53 |
| 81 | DA | 327 | A | C2'-C1' | -7.48 | 1.45 | 1.53 |
| 78 | CA | 163 | G | C2'-C1' | -7.47 | 1.45 | 1.53 |
| 78 | CA | 1012 | U | O4'-C1' | 7.47 | 1.51 | 1.41 |
| 79 | CB | 42 | C | O4'-C1' | 7.47 | 1.51 | 1.41 |
| 81 | DA | 2289 | U | C2'-C1' | -7.47 | 1.45 | 1.53 |
| 79 | CB | 63 | C | C2'-C1' | -7.47 | 1.45 | 1.53 |
| 81 | DA | 62 | A | O4'-C1' | 7.47 | 1.51 | 1.41 |
| 81 | DA | 1318 | A | O4'-C1' | 7.47 | 1.51 | 1.41 |
| 78 | CA | 1176 | G | C2'-C1' | -7.47 | 1.45 | 1.53 |
| 81 | DA | 3107 | U | C2'-C1' | 7.47 | 1.61 | 1.53 |
| 78 | CA | 232 | U | C4'-O4' | -7.47 | 1.35 | 1.45 |
| 78 | CA | 634 | G | O4'-C1' | -7.47 | 1.31 | 1.41 |
| 81 | DA | 857 | G | C2'-C1' | -7.47 | 1.45 | 1.53 |
| 81 | DA | 2178 | A | C2'-C1' | -7.47 | 1.45 | 1.53 |
| 81 | DA | 2757 | U | P-O5' | -7.47 | 1.52 | 1.59 |
| 81 | DA | 2905 | U | O4'-C1' | 7.47 | 1.51 | 1.41 |
| 81 | DA | 3325 | G | O4'-C1' | -7.47 | 1.31 | 1.41 |
| 78 | CA | 1032 | G | C2'-C1' | -7.46 | 1.45 | 1.53 |
| 81 | DA | 922 | U | C2'-C1' | 7.46 | 1.61 | 1.53 |
| 81 | DA | 1016 | C | C2'-C1' | -7.46 | 1.45 | 1.53 |
| 81 | DA | 2142 | A | C2'-C1' | 7.46 | 1.61 | 1.53 |
| 81 | DA | 1058 | U | O4'-C1' | 7.46 | 1.51 | 1.41 |
| 81 | DA | 1404 | G | O3'-P | 7.46 | 1.70 | 1.61 |
| 81 | DA | 3148 | U | O3'-P | -7.46 | 1.52 | 1.61 |
| 78 | CA | 1367 | G | O4'-C1' | 7.46 | 1.51 | 1.41 |
| 81 | DA | 1167 | U | O4'-C1' | 7.46 | 1.51 | 1.41 |
| 81 | DA | 2396 | G | C2'-C1' | -7.46 | 1.45 | 1.53 |
| 81 | DA | 1671 | C | C2'-C1' | -7.46 | 1.45 | 1.53 |
| 42 | BM | 84 | SER | CA-CB | 7.45 | 1.64 | 1.52 |
| 2 | AA | 251 | GLU | N-CA | 7.45 | 1.61 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 5 | AC | 168 | ARG | CA-CB | 7.45 | 1.70 | 1.53 |
| 78 | CA | 1771 | U | O4'-C1' | 7.45 | 1.51 | 1.41 |
| 81 | DA | 2233 | A | O4'-C1' | -7.45 | 1.31 | 1.41 |
| 82 | DB | 6 | U | C2'-C1' | -7.45 | 1.45 | 1.53 |
| 78 | CA | 1710 | U | O4'-C1' | 7.45 | 1.51 | 1.41 |
| 78 | CA | 433 | C | C2'-C1' | -7.45 | 1.45 | 1.53 |
| 81 | DA | 868 | C | C2'-C1' | -7.45 | 1.45 | 1.53 |
| 81 | DA | 2915 | U | O3'-P | -7.45 | 1.52 | 1.61 |
| 81 | DA | 2927 | C | C2'-C1' | -7.45 | 1.45 | 1.53 |
| 81 | DA | 1950 | U | O4'-C1' | 7.44 | 1.51 | 1.41 |
| 81 | DA | 916 | G | C2'-C1' | 7.44 | 1.61 | 1.53 |
| 81 | DA | 870 | G | C2'-C1' | -7.44 | 1.45 | 1.53 |
| 81 | DA | 2087 | C | C2'-C1' | -7.44 | 1.45 | 1.53 |
| 81 | DA | 236 | G | P-O5' | -7.44 | 1.52 | 1.59 |
| 82 | DB | 113 | U | O4'-C1' | 7.44 | 1.51 | 1.41 |
| 81 | DA | 2319 | U | P-O5' | -7.43 | 1.52 | 1.59 |
| 81 | DA | 2175 | U | O5'-C5' | -7.43 | 1.30 | 1.42 |
| 78 | CA | 413 | U | O4'-C1' | 7.43 | 1.51 | 1.41 |
| 81 | DA | 2836 | C | O4'-C1' | 7.43 | 1.51 | 1.41 |
| 81 | DA | 2697 | A | C2'-C1' | -7.43 | 1.45 | 1.53 |
| 81 | DA | 3325 | G | C2'-C1' | 7.43 | 1.61 | 1.53 |
| 17 | AQ | 26 | LEU | CA-CB | -7.42 | 1.36 | 1.53 |
| 81 | DA | 1069 | C | C2'-C1' | -7.42 | 1.45 | 1.53 |
| 81 | DA | 2898 | G | C2'-C1' | -7.42 | 1.45 | 1.53 |
| 82 | DB | 2 | A | C2'-C1' | 7.42 | 1.61 | 1.53 |
| 78 | CA | 250 | C | O3'-P | -7.42 | 1.52 | 1.61 |
| 81 | DA | 1534 | A | C2'-C1' | 7.42 | 1.61 | 1.53 |
| 81 | DA | 554 | A | C2'-C1' | -7.42 | 1.45 | 1.53 |
| 78 | CA | 1390 | U | C2'-C1' | -7.42 | 1.45 | 1.53 |
| 82 | DB | 30 | C | O4'-C1' | 7.42 | 1.51 | 1.41 |
| 78 | CA | 36 | C | C2'-C1' | -7.42 | 1.45 | 1.53 |
| 78 | CA | 155 | U | C2'-C1' | 7.41 | 1.61 | 1.53 |
| 78 | CA | 283 | U | O4'-C1' | 7.41 | 1.51 | 1.41 |
| 81 | DA | 1121 | U | C2'-C1' | -7.41 | 1.45 | 1.53 |
| 81 | DA | 2469 | G | C2'-C1' | -7.41 | 1.45 | 1.53 |
| 78 | CA | 409 | C | C2'-C1' | -7.41 | 1.45 | 1.53 |
| 78 | CA | 1349 | G | C2'-C1' | -7.41 | 1.45 | 1.53 |
| 81 | DA | 141 | C | O4'-C1' | 7.41 | 1.51 | 1.41 |
| 81 | DA | 2142 | A | O4'-C1' | 7.41 | 1.51 | 1.41 |
| 78 | CA | 1528 | U | P-O5' | -7.41 | 1.52 | 1.59 |
| 81 | DA | 10 | C | O4'-C1' | 7.41 | 1.51 | 1.41 |
| 81 | DA | 759 | U | O4'-C1' | 7.41 | 1.51 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2272 | G | C2'-C1' | 7.41 | 1.61 | 1.53 |
| 81 | DA | 113 | C | C2'-C1' | -7.41 | 1.45 | 1.53 |
| 78 | CA | 1544 | U | C3'-O3' | -7.41 | 1.31 | 1.42 |
| 81 | DA | 653 | A | C2'-C1' | -7.41 | 1.45 | 1.53 |
| 81 | DA | 2209 | U | O4'-C1' | 7.41 | 1.51 | 1.41 |
| 81 | DA | 625 | G | C2'-C1' | -7.40 | 1.45 | 1.53 |
| 78 | CA | 1381 | U | O3'-P | -7.40 | 1.52 | 1.61 |
| 26 | AZ | 44 | PHE | C-N | 7.40 | 1.51 | 1.34 |
| 81 | DA | 368 | G | C2'-C1' | -7.40 | 1.45 | 1.53 |
| 81 | DA | 2518 | C | C2'-C1' | -7.40 | 1.45 | 1.53 |
| 31 | BB | 74 | GLU | N-CA | 7.40 | 1.61 | 1.46 |
| 78 | CA | 1239 | U | C2'-C1' | -7.40 | 1.45 | 1.53 |
| 78 | CA | 1475 | A | C2'-C1' | -7.40 | 1.45 | 1.53 |
| 78 | CA | 27 | U | C2'-C1' | 7.40 | 1.61 | 1.53 |
| 78 | CA | 1749 | A | O4'-C1' | 7.40 | 1.51 | 1.41 |
| 78 | CA | 1356 | U | O4'-C1' | 7.39 | 1.51 | 1.41 |
| 82 | DB | 109 | A | C2'-C1' | -7.39 | 1.45 | 1.53 |
| 81 | DA | 2171 | G | O4'-C1' | 7.39 | 1.51 | 1.41 |
| 35 | BG | 3 | ALA | CA-CB | 7.39 | 1.68 | 1.52 |
| 81 | DA | 559 | A | O4'-C1' | 7.39 | 1.51 | 1.41 |
| 81 | DA | 1628 | C | C2'-C1' | -7.39 | 1.45 | 1.53 |
| 35 | BG | 99 | GLU | N-CA | 7.38 | 1.61 | 1.46 |
| 44 | BO | 58 | MET | CA-CB | 7.38 | 1.70 | 1.53 |
| 81 | DA | 146 | U | C4'-C3' | 7.38 | 1.61 | 1.53 |
| 13 | AL | 34 | LEU | C-N | 7.38 | 1.46 | 1.33 |
| 78 | CA | 1544 | U | C2'-C1' | -7.38 | 1.45 | 1.53 |
| 81 | DA | 3043 | C | O4'-C1' | 7.38 | 1.51 | 1.41 |
| 55 | Bc | 104 | GLN | CA-CB | -7.38 | 1.37 | 1.53 |
| 81 | DA | 2202 | C | O4'-C1' | 7.38 | 1.51 | 1.41 |
| 78 | CA | 922 | G | O4'-C1' | 7.37 | 1.51 | 1.41 |
| 81 | DA | 238 | A | C2'-C1' | -7.37 | 1.45 | 1.53 |
| 81 | DA | 527 | A | C2'-C1' | 7.37 | 1.61 | 1.53 |
| 81 | DA | 906 | A | O4'-C1' | -7.37 | 1.32 | 1.41 |
| 10 | AI | 55 | VAL | N-CA | 7.37 | 1.61 | 1.46 |
| 44 | BO | 60 | TYR | CG-CD1 | 7.37 | 1.48 | 1.39 |
| 81 | DA | 1303 | A | O4'-C1' | -7.37 | 1.32 | 1.41 |
| 83 | DC | 17 | A | C5'-C4' | 7.37 | 1.60 | 1.51 |
| 81 | DA | 1437 | C | C2'-C1' | 7.36 | 1.61 | 1.53 |
| 81 | DA | 2526 | C | P-O5' | -7.36 | 1.52 | 1.59 |
| 81 | DA | 3099 | C | C5'-C4' | 7.36 | 1.60 | 1.51 |
| 78 | CA | 1546 | G | C3'-C2' | -7.36 | 1.44 | 1.52 |
| 81 | DA | 5 | G | O4'-C1' | 7.36 | 1.51 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 433 | A | C2'-C1' | -7.36 | 1.45 | 1.53 |
| 81 | DA | 1269 | U | O4'-C1' | 7.36 | 1.51 | 1.41 |
| 81 | DA | 700 | C | C4'-C3' | 7.36 | 1.61 | 1.53 |
| 81 | DA | 1228 | C | O4'-C1' | 7.36 | 1.51 | 1.41 |
| 45 | BR | 54 | LEU | CA-CB | -7.35 | 1.36 | 1.53 |
| 81 | DA | 2704 | A | C2'-C1' | 7.35 | 1.61 | 1.53 |
| 81 | DA | 1236 | G | O4'-C1' | -7.35 | 1.32 | 1.41 |
| 83 | DC | 80 | G | C2'-C1' | -7.34 | 1.45 | 1.53 |
| 35 | BG | 8 | LYS | N-CA | -7.34 | 1.31 | 1.46 |
| 78 | CA | 1690 | G | C2'-C1' | -7.34 | 1.45 | 1.53 |
| 78 | CA | 1207 | C | C2'-C1' | -7.33 | 1.45 | 1.53 |
| 81 | DA | 1440 | G | C2'-C1' | -7.33 | 1.45 | 1.53 |
| 81 | DA | 3386 | G | O4'-C1' | 7.33 | 1.51 | 1.41 |
| 83 | DC | 101 | A | P-O5' | -7.33 | 1.52 | 1.59 |
| 1 | Aa | 61 | PHE | N-CA | -7.33 | 1.31 | 1.46 |
| 81 | DA | 643 | U | O4'-C1' | 7.33 | 1.51 | 1.41 |
| 81 | DA | 700 | C | O4'-C1' | 7.33 | 1.51 | 1.41 |
| 81 | DA | 1250 | G | O4'-C1' | -7.33 | 1.32 | 1.41 |
| 78 | CA | 1398 | U | O4'-C1' | -7.33 | 1.32 | 1.41 |
| 81 | DA | 261 | U | O4'-C1' | 7.33 | 1.51 | 1.41 |
| 81 | DA | 1886 | A | O4'-C1' | 7.33 | 1.51 | 1.41 |
| 1 | Aa | 54 | PHE | CA-CB | -7.33 | 1.37 | 1.53 |
| 83 | DC | 98 | G | O4'-C1' | 7.33 | 1.51 | 1.41 |
| 78 | CA | 620 | A | C2'-C1' | 7.32 | 1.61 | 1.53 |
| 81 | DA | 2095 | G | C2'-C1' | -7.32 | 1.45 | 1.53 |
| 81 | DA | 2822 | U | O4'-C1' | 7.32 | 1.51 | 1.41 |
| 78 | CA | 438 | A | C2'-C1' | -7.32 | 1.45 | 1.53 |
| 83 | DC | 114 | A | O4'-C1' | -7.32 | 1.32 | 1.41 |
| 81 | DA | 2242 | A | C2'-C1' | -7.32 | 1.45 | 1.53 |
| 76 | BS | 159 | ARG | NE-CZ | 7.31 | 1.42 | 1.33 |
| 1 | Aa | 124 | SER | CA-CB | 7.31 | 1.64 | 1.52 |
| 81 | DA | 267 | G | O4'-C1' | 7.31 | 1.51 | 1.41 |
| 81 | DA | 2364 | G | O4'-C1' | 7.31 | 1.51 | 1.41 |
| 81 | DA | 772 | U | C2'-C1' | -7.31 | 1.45 | 1.53 |
| 81 | DA | 1937 | U | O4'-C1' | 7.31 | 1.51 | 1.41 |
| 78 | CA | 463 | U | C2'-C1' | -7.30 | 1.45 | 1.53 |
| 78 | CA | 1480 | G | P-O5' | -7.30 | 1.52 | 1.59 |
| 79 | CB | 40 | U | C2'-C1' | 7.30 | 1.61 | 1.53 |
| 81 | DA | 579 | G | O4'-C1' | -7.30 | 1.32 | 1.41 |
| 81 | DA | 2338 | C | O3'-P | -7.30 | 1.52 | 1.61 |
| 81 | DA | 3358 | U | O4'-C1' | 7.30 | 1.51 | 1.41 |
| 78 | CA | 1310 | U | C4'-O4' | -7.30 | 1.36 | 1.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2240 | G | C2'-C1' | -7.30 | 1.45 | 1.53 |
| 78 | CA | 659 | C | O4'-C1' | 7.30 | 1.51 | 1.41 |
| 81 | DA | 666 | A | O4'-C1' | -7.30 | 1.32 | 1.41 |
| 78 | CA | 183 | U | O4'-C1' | 7.29 | 1.51 | 1.41 |
| 79 | CB | 16 | U | O4'-C1' | 7.29 | 1.51 | 1.41 |
| 81 | DA | 245 | U | O4'-C1' | 7.29 | 1.51 | 1.41 |
| 81 | DA | 3008 | A | O4'-C1' | 7.29 | 1.51 | 1.41 |
| 78 | CA | 1631 | A | O4'-C1' | 7.29 | 1.51 | 1.41 |
| 81 | DA | 183 | G | O3'-P | -7.29 | 1.52 | 1.61 |
| 81 | DA | 2881 | C | C2'-C1' | -7.29 | 1.45 | 1.53 |
| 78 | CA | 323 | A | O4'-C1' | -7.29 | 1.32 | 1.41 |
| 78 | CA | 1135 | U | O4'-C1' | 7.29 | 1.51 | 1.41 |
| 81 | DA | 766 | U | C2'-C1' | 7.29 | 1.61 | 1.53 |
| 81 | DA | 2583 | C | C2'-C1' | -7.29 | 1.45 | 1.53 |
| 48 | BW | 93 | ILE | N-CA | -7.28 | 1.31 | 1.46 |
| 81 | DA | 503 | C | O4'-C1' | 7.28 | 1.51 | 1.41 |
| 59 | Bh | 12 | LYS | CA-CB | 7.28 | 1.70 | 1.53 |
| 72 | Bu | 61 | PHE | CA-CB | 7.28 | 1.70 | 1.53 |
| 78 | CA | 1547 | A | O4'-C1' | 7.28 | 1.51 | 1.41 |
| 81 | DA | 494 | G | C2'-C1' | -7.28 | 1.45 | 1.53 |
| 78 | CA | 892 | A | O4'-C1' | 7.27 | 1.51 | 1.41 |
| 81 | DA | 7 | C | C2'-C1' | -7.27 | 1.45 | 1.53 |
| 81 | DA | 909 | G | C2'-C1' | -7.27 | 1.45 | 1.53 |
| 81 | DA | 3395 | G | C2'-C1' | -7.27 | 1.45 | 1.53 |
| 81 | DA | 252 | U | C2'-C1' | -7.27 | 1.45 | 1.53 |
| 81 | DA | 2423 | U | O4'-C1' | 7.27 | 1.51 | 1.41 |
| 81 | DA | 2198 | A | O4'-C1' | 7.26 | 1.51 | 1.41 |
| 81 | DA | 2234 | G | C2'-C1' | -7.26 | 1.45 | 1.53 |
| 81 | DA | 1111 | U | O4'-C1' | 7.26 | 1.51 | 1.41 |
| 78 | CA | 406 | U | O4'-C1' | 7.26 | 1.51 | 1.41 |
| 78 | CA | 866 | G | P-OP2 | 7.26 | 1.61 | 1.49 |
| 17 | AQ | 63 | LYS | CA-CB | 7.26 | 1.70 | 1.53 |
| 78 | CA | 288 | A | O4'-C1' | 7.26 | 1.51 | 1.41 |
| 33 | BD | 332 | LYS | N-CA | 7.25 | 1.60 | 1.46 |
| 78 | CA | 1477 | G | C3'-C2' | -7.25 | 1.44 | 1.52 |
| 78 | CA | 548 | G | C2'-C1' | -7.25 | 1.45 | 1.53 |
| 81 | DA | 339 | C | C2'-C1' | -7.25 | 1.45 | 1.53 |
| 81 | DA | 3050 | U | O3'-P | -7.25 | 1.52 | 1.61 |
| 81 | DA | 1380 | G | C2'-C1' | -7.25 | 1.45 | 1.53 |
| 81 | DA | 1988 | C | O4'-C1' | 7.25 | 1.51 | 1.41 |
| 81 | DA | 2851 | A | O4'-C1' | 7.25 | 1.51 | 1.41 |
| 81 | DA | 1870 | C | C4'-C3' | -7.25 | 1.45 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 954 | U | O4'-C1' | 7.24 | 1.51 | 1.41 |
| 58 | Bg | 28 | ARG | CZ-NH1 | 7.24 | 1.42 | 1.33 |
| 81 | DA | 3305 | A | C3'-C2' | -7.24 | 1.44 | 1.52 |
| 74 | BQ | 115 | LEU | N-CA | -7.24 | 1.31 | 1.46 |
| 82 | DB | 7 | U | O4'-C1' | 7.24 | 1.51 | 1.41 |
| 81 | DA | 1004 | U | C2'-C1' | -7.24 | 1.45 | 1.53 |
| 81 | DA | 1056 | U | P-O5' | -7.24 | 1.52 | 1.59 |
| 81 | DA | 3012 | A | C2'-C1' | -7.24 | 1.45 | 1.53 |
| 82 | DB | 62 | C | O4'-C1' | 7.24 | 1.51 | 1.41 |
| 78 | CA | 331 | A | O4'-C1' | 7.23 | 1.51 | 1.41 |
| 81 | DA | 223 | U | C2'-C1' | -7.23 | 1.45 | 1.53 |
| 81 | DA | 1462 | A | C2'-C1' | -7.23 | 1.45 | 1.53 |
| 81 | DA | 1774 | C | O4'-C1' | 7.23 | 1.51 | 1.41 |
| 22 | AV | 81 | ARG | CD-NE | 7.23 | 1.58 | 1.46 |
| 78 | CA | 98 | U | C2'-C1' | -7.23 | 1.45 | 1.53 |
| 81 | DA | 90 | C | O4'-C1' | 7.23 | 1.51 | 1.41 |
| 81 | DA | 247 | C | C5'-C4' | 7.23 | 1.60 | 1.51 |
| 81 | DA | 500 | C | C2'-C1' | -7.23 | 1.45 | 1.53 |
| 81 | DA | 773 | G | C2'-C1' | -7.23 | 1.45 | 1.53 |
| 81 | DA | 3392 | U | O4'-C1' | 7.23 | 1.51 | 1.41 |
| 76 | BS | 45 | TYR | CG-CD2 | 7.23 | 1.48 | 1.39 |
| 53 | Ba | 13 | VAL | C-N | 7.23 | 1.50 | 1.34 |
| 34 | BE | 123 | PHE | C-N | 7.22 | 1.46 | 1.33 |
| 81 | DA | 1145 | G | O4'-C1' | 7.22 | 1.51 | 1.41 |
| 81 | DA | 3078 | U | C2'-C1' | -7.22 | 1.45 | 1.53 |
| 81 | DA | 1068 | C | C2'-C1' | -7.22 | 1.45 | 1.53 |
| 81 | DA | 1183 | C | C2'-C1' | -7.22 | 1.45 | 1.53 |
| 81 | DA | 2835 | U | O4'-C1' | 7.22 | 1.51 | 1.41 |
| 78 | CA | 563 | U | O4'-C1' | 7.22 | 1.51 | 1.41 |
| 81 | DA | 1626 | U | O4'-C1' | 7.22 | 1.51 | 1.41 |
| 78 | CA | 1776 | A | O4'-C1' | 7.22 | 1.51 | 1.41 |
| 81 | DA | 1837 | U | C2'-C1' | -7.22 | 1.45 | 1.53 |
| 81 | DA | 1043 | C | O4'-C1' | 7.21 | 1.51 | 1.41 |
| 81 | DA | 1797 | A | C2'-C1' | -7.21 | 1.45 | 1.53 |
| 76 | BS | 154 | VAL | CA-CB | -7.21 | 1.39 | 1.54 |
| 78 | CA | 62 | A | O4'-C1' | 7.21 | 1.51 | 1.41 |
| 81 | DA | 1602 | A | O4'-C1' | 7.21 | 1.51 | 1.41 |
| 81 | DA | 335 | G | C2'-C1' | -7.21 | 1.45 | 1.53 |
| 81 | DA | 416 | A | C2'-C1' | -7.21 | 1.45 | 1.53 |
| 81 | DA | 2457 | G | C2'-C1' | -7.21 | 1.45 | 1.53 |
| 78 | CA | 399 | A | O4'-C1' | -7.21 | 1.32 | 1.41 |
| 81 | DA | 1936 | A | C2'-C1' | -7.21 | 1.45 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 3328 | G | O4'-C1' | -7.21 | 1.32 | 1.41 |
| 78 | CA | 1547 | A | C2'-C1' | -7.21 | 1.45 | 1.53 |
| 82 | DB | 152 | G | C2'-C1' | 7.21 | 1.61 | 1.53 |
| 83 | DC | 16 | U | C2'-C1' | 7.21 | 1.61 | 1.53 |
| 81 | DA | 244 | G | P-O5' | 7.20 | 1.67 | 1.59 |
| 78 | CA | 1349 | G | O4'-C1' | 7.20 | 1.51 | 1.41 |
| 81 | DA | 184 | U | O3'-P | -7.20 | 1.52 | 1.61 |
| 81 | DA | 1674 | G | O4'-C1' | 7.20 | 1.51 | 1.41 |
| 78 | CA | 227 | U | P-O5' | -7.20 | 1.52 | 1.59 |
| 32 | BC | 297 | SER | N-CA | -7.19 | 1.31 | 1.46 |
| 43 | BP | 117 | ASN | N-CA | -7.19 | 1.31 | 1.46 |
| 78 | CA | 1043 | A | C2'-C1' | 7.19 | 1.61 | 1.53 |
| 78 | CA | 1601 | G | C2'-C1' | -7.19 | 1.45 | 1.53 |
| 81 | DA | 422 | A | O4'-C1' | -7.19 | 1.32 | 1.41 |
| 81 | DA | 960 | U | C2'-C1' | -7.19 | 1.45 | 1.53 |
| 60 | Bi | 60 | ARG | CZ-NH2 | 7.19 | 1.42 | 1.33 |
| 79 | CB | 61 | C | C2'-C1' | -7.19 | 1.45 | 1.53 |
| 81 | DA | 832 | G | O4'-C1' | -7.19 | 1.32 | 1.41 |
| 81 | DA | 3351 | U | C2'-C1' | 7.19 | 1.61 | 1.53 |
| 55 | Bc | 103 | LYS | N-CA | -7.19 | 1.31 | 1.46 |
| 81 | DA | 125 | C | C2'-C1' | -7.18 | 1.45 | 1.53 |
| 81 | DA | 326 | U | C2'-C1' | -7.18 | 1.45 | 1.53 |
| 2 | AA | 251 | GLU | C-N | 7.18 | 1.50 | 1.34 |
| 81 | DA | 981 | U | C5'-C4' | 7.18 | 1.59 | 1.51 |
| 81 | DA | 2431 | C | C2'-C1' | -7.18 | 1.45 | 1.53 |
| 81 | DA | 2282 | U | C2'-C1' | -7.18 | 1.45 | 1.53 |
| 33 | BD | 146 | PRO | N-CA | 7.18 | 1.59 | 1.47 |
| 81 | DA | 2680 | A | O4'-C1' | 7.18 | 1.50 | 1.41 |
| 78 | CA | 852 | C | P-O5' | 7.17 | 1.67 | 1.59 |
| 81 | DA | 162 | G | O3'-P | -7.17 | 1.52 | 1.61 |
| 81 | DA | 310 | U | O4'-C1' | 7.17 | 1.50 | 1.41 |
| 81 | DA | 2727 | A | C2'-C1' | -7.17 | 1.45 | 1.53 |
| 81 | DA | 2329 | C | C2'-C1' | -7.17 | 1.45 | 1.53 |
| 14 | AM | 12 | GLN | C-N | -7.17 | 1.17 | 1.34 |
| 81 | DA | 799 | G | C2'-O2' | -7.17 | 1.32 | 1.41 |
| 78 | CA | 1157 | A | O4'-C1' | 7.17 | 1.50 | 1.41 |
| 81 | DA | 3129 | A | C2'-C1' | -7.17 | 1.45 | 1.53 |
| 78 | CA | 671 | G | O4'-C1' | 7.17 | 1.50 | 1.41 |
| 81 | DA | 2728 | G | O4'-C1' | 7.16 | 1.50 | 1.41 |
| 81 | DA | 2099 | A | C2'-C1' | -7.16 | 1.45 | 1.53 |
| 83 | DC | 48 | U | O3'-P | -7.16 | 1.52 | 1.61 |
| 78 | CA | 951 | A | O4'-C1' | -7.16 | 1.32 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2792 | A | O4'-C1' | -7.16 | 1.32 | 1.41 |
| 78 | CA | 1165 | G | C2'-C1' | -7.16 | 1.45 | 1.53 |
| 78 | CA | 1606 | C | C2'-C1' | -7.16 | 1.45 | 1.53 |
| 81 | DA | 655 | C | O4'-C1' | 7.15 | 1.50 | 1.41 |
| 81 | DA | 2222 | A | C2'-C1' | -7.15 | 1.45 | 1.53 |
| 51 | BZ | 47 | ARG | CZ-NH1 | 7.15 | 1.42 | 1.33 |
| 78 | CA | 634 | G | C2'-C1' | 7.15 | 1.61 | 1.53 |
| 81 | DA | 2530 | G | P-O5' | -7.15 | 1.52 | 1.59 |
| 81 | DA | 1360 | C | O4'-C1' | 7.15 | 1.50 | 1.41 |
| 78 | CA | 1609 | U | O4'-C1' | 7.15 | 1.50 | 1.41 |
| 78 | CA | 1574 | G | O4'-C1' | 7.14 | 1.50 | 1.41 |
| 81 | DA | 2616 | C | C2'-C1' | -7.14 | 1.45 | 1.53 |
| 81 | DA | 536 | U | C2'-C1' | -7.14 | 1.45 | 1.53 |
| 48 | BW | 98 | THR | CA-C | -7.14 | 1.34 | 1.52 |
| 78 | CA | 837 | G | C5'-C4' | 7.14 | 1.59 | 1.51 |
| 45 | BR | 118 | GLY | CA-C | -7.14 | 1.40 | 1.51 |
| 78 | CA | 1698 | G | C2'-C1' | -7.14 | 1.45 | 1.53 |
| 81 | DA | 974 | G | C2'-C1' | -7.14 | 1.45 | 1.53 |
| 81 | DA | 2356 | A | C2'-C1' | -7.14 | 1.45 | 1.53 |
| 81 | DA | 2924 | U | C2'-C1' | -7.14 | 1.45 | 1.53 |
| 81 | DA | 3305 | A | C3'-O3' | -7.14 | 1.32 | 1.42 |
| 81 | DA | 171 | G | O4'-C1' | 7.13 | 1.50 | 1.41 |
| 78 | CA | 1072 | C | O4'-C1' | 7.13 | 1.50 | 1.41 |
| 81 | DA | 279 | U | C2'-C1' | -7.13 | 1.45 | 1.53 |
| 58 | Bg | 19 | ARG | CZ-NH2 | 7.13 | 1.42 | 1.33 |
| 78 | CA | 1769 | U | C2'-C1' | -7.13 | 1.45 | 1.53 |
| 81 | DA | 2054 | C | C2'-C1' | -7.13 | 1.45 | 1.53 |
| 38 | Bs | 5 | ARG | CA-CB | -7.13 | 1.38 | 1.53 |
| 81 | DA | 1075 | A | O4'-C1' | 7.13 | 1.50 | 1.41 |
| 81 | DA | 1782 | U | O4'-C1' | 7.13 | 1.50 | 1.41 |
| 81 | DA | 3367 | C | O4'-C1' | 7.13 | 1.50 | 1.41 |
| 78 | CA | 208 | U | P-O5' | -7.12 | 1.52 | 1.59 |
| 81 | DA | 894 | G | C2'-C1' | 7.12 | 1.61 | 1.53 |
| 81 | DA | 1241 | U | O4'-C1' | 7.12 | 1.50 | 1.41 |
| 81 | DA | 1372 | C | O4'-C1' | 7.12 | 1.50 | 1.41 |
| 81 | DA | 2599 | U | O4'-C1' | 7.12 | 1.50 | 1.41 |
| 78 | CA | 554 | C | C3'-C2' | -7.12 | 1.45 | 1.52 |
| 81 | DA | 701 | G | O3'-P | -7.12 | 1.52 | 1.61 |
| 81 | DA | 1337 | A | O4'-C1' | 7.12 | 1.50 | 1.41 |
| 82 | DB | 98 | U | O4'-C1' | 7.12 | 1.50 | 1.41 |
| 81 | DA | 1578 | C | C2'-C1' | -7.12 | 1.45 | 1.53 |
| 81 | DA | 801 | A | C3'-O3' | 7.12 | 1.52 | 1.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1405 | U | O4'-C1' | 7.12 | 1.50 | 1.41 |
| 81 | DA | 2812 | C | C2'-C1' | -7.12 | 1.45 | 1.53 |
| 45 | BR | 13 | SER | CA-C | 7.11 | 1.71 | 1.52 |
| 81 | DA | 2243 | A | C2'-C1' | 7.11 | 1.61 | 1.53 |
| 81 | DA | 3078 | U | O4'-C1' | 7.11 | 1.50 | 1.41 |
| 45 | BR | 95 | GLU | CA-CB | -7.11 | 1.38 | 1.53 |
| 81 | DA | 1633 | C | O3'-P | -7.11 | 1.52 | 1.61 |
| 78 | CA | 189 | C | O4'-C1' | 7.11 | 1.50 | 1.41 |
| 81 | DA | 2087 | C | C3'-C2' | 7.11 | 1.60 | 1.52 |
| 81 | DA | 1703 | U | O4'-C1' | 7.11 | 1.50 | 1.41 |
| 81 | DA | 1117 | G | O4'-C1' | 7.10 | 1.50 | 1.41 |
| 74 | BQ | 201 | GLY | C-N | 7.10 | 1.45 | 1.33 |
| 78 | CA | 947 | U | O4'-C1' | 7.10 | 1.50 | 1.41 |
| 81 | DA | 2985 | C | O4'-C1' | 7.10 | 1.50 | 1.41 |
| 81 | DA | 294 | U | C2'-C1' | -7.10 | 1.45 | 1.53 |
| 78 | CA | 1240 | U | C5'-C4' | 7.09 | 1.59 | 1.51 |
| 81 | DA | 38 | U | O4'-C1' | 7.09 | 1.50 | 1.41 |
| 81 | DA | 605 | U | O4'-C1' | 7.09 | 1.50 | 1.41 |
| 81 | DA | 258 | G | C5'-C4' | 7.09 | 1.59 | 1.51 |
| 81 | DA | 2030 | C | O4'-C1' | 7.09 | 1.50 | 1.41 |
| 81 | DA | 2821 | C | C2'-C1' | -7.09 | 1.45 | 1.53 |
| 81 | DA | 696 | C | O4'-C1' | 7.09 | 1.50 | 1.41 |
| 81 | DA | 1232 | C | O4'-C1' | 7.09 | 1.50 | 1.41 |
| 83 | DC | 86 | G | O4'-C1' | 7.09 | 1.50 | 1.41 |
| 20 | AS | 52 | GLY | C-N | 7.09 | 1.50 | 1.34 |
| 34 | BE | 55 | ARG | C-O | 7.09 | 1.36 | 1.23 |
| 78 | CA | 1553 | G | C2'-C1' | -7.08 | 1.45 | 1.53 |
| 2 | AA | 84 | ARG | NE-CZ | 7.08 | 1.42 | 1.33 |
| 55 | Bc | 104 | GLN | N-CA | 7.08 | 1.60 | 1.46 |
| 76 | BS | 70 | ASN | CA-CB | 7.08 | 1.71 | 1.53 |
| 81 | DA | 1589 | A | O4'-C1' | 7.08 | 1.50 | 1.41 |
| 78 | CA | 1648 | A | O4'-C1' | 7.08 | 1.50 | 1.41 |
| 41 | BN | 6 | ILE | N-CA | 7.08 | 1.60 | 1.46 |
| 78 | CA | 513 | U | C4'-C3' | -7.08 | 1.45 | 1.53 |
| 81 | DA | 722 | G | O4'-C1' | 7.08 | 1.50 | 1.41 |
| 81 | DA | 1754 | G | C5'-C4' | 7.08 | 1.59 | 1.51 |
| 59 | Bh | 21 | HIS | N-CA | -7.07 | 1.32 | 1.46 |
| 78 | CA | 1762 | A | C2'-C1' | -7.07 | 1.45 | 1.53 |
| 81 | DA | 969 | C | C2'-C1' | 7.07 | 1.61 | 1.53 |
| 12 | AK | 124 | ASP | CG-OD1 | -7.07 | 1.09 | 1.25 |
| 35 | BG | 5 | LYS | CA-CB | -7.07 | 1.38 | 1.53 |
| 78 | CA | 367 | A | O4'-C1' | -7.07 | 1.32 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 1482 | C | P-O5' | -7.07 | 1.52 | 1.59 |
| 33 | BD | 331 | ALA | N-CA | 7.07 | 1.60 | 1.46 |
| 82 | DB | 61 | A | O4'-C1' | 7.07 | 1.50 | 1.41 |
| 78 | CA | 17 | C | C2'-C1' | -7.07 | 1.45 | 1.53 |
| 81 | DA | 834 | U | O3'-P | -7.07 | 1.52 | 1.61 |
| 81 | DA | 416 | A | O4'-C1' | 7.06 | 1.50 | 1.41 |
| 81 | DA | 69 | C | C2'-C1' | -7.06 | 1.45 | 1.53 |
| 81 | DA | 2517 | U | C2'-C1' | -7.05 | 1.45 | 1.53 |
| 81 | DA | 2925 | C | C2'-C1' | -7.05 | 1.45 | 1.53 |
| 81 | DA | 1676 | A | O4'-C1' | 7.05 | 1.50 | 1.41 |
| 78 | CA | 1769 | U | O4'-C1' | 7.05 | 1.50 | 1.41 |
| 81 | DA | 2310 | U | C2'-C1' | -7.05 | 1.45 | 1.53 |
| 6 | AE | 4 | PRO | N-CA | 7.05 | 1.59 | 1.47 |
| 78 | CA | 351 | C | C2'-C1' | 7.05 | 1.61 | 1.53 |
| 81 | DA | 2600 | C | C2'-C1' | -7.05 | 1.45 | 1.53 |
| 69 | Br | 89 | LYS | CA-CB | -7.04 | 1.38 | 1.53 |
| 81 | DA | 834 | U | C2'-C1' | -7.04 | 1.45 | 1.53 |
| 81 | DA | 332 | C | C2'-C1' | -7.04 | 1.45 | 1.53 |
| 1 | Aa | 155 | ARG | CZ-NH1 | 7.04 | 1.42 | 1.33 |
| 78 | CA | 684 | A | O4'-C1' | 7.04 | 1.50 | 1.41 |
| 78 | CA | 1374 | C | C2'-C1' | -7.04 | 1.45 | 1.53 |
| 81 | DA | 1372 | C | C2'-C1' | -7.04 | 1.45 | 1.53 |
| 81 | DA | 2376 | G | P-O5' | -7.04 | 1.52 | 1.59 |
| 81 | DA | 1541 | G | C2'-C1' | -7.04 | 1.45 | 1.53 |
| 81 | DA | 2492 | C | O4'-C1' | 7.04 | 1.50 | 1.41 |
| 82 | DB | 26 | U | C2'-C1' | -7.03 | 1.45 | 1.53 |
| 78 | CA | 1185 | U | O4'-C1' | 7.03 | 1.50 | 1.41 |
| 16 | AO | 124 | ARG | CD-NE | 7.03 | 1.58 | 1.46 |
| 83 | DC | 46 | A | C3'-O3' | -7.02 | 1.32 | 1.42 |
| 78 | CA | 1556 | A | C3'-C2' | -7.02 | 1.45 | 1.52 |
| 78 | CA | 1104 | U | C2'-C1' | -7.02 | 1.45 | 1.53 |
| 78 | CA | 1112 | G | O4'-C1' | 7.02 | 1.50 | 1.41 |
| 81 | DA | 1136 | A | C2'-C1' | -7.02 | 1.45 | 1.53 |
| 81 | DA | 1741 | A | C2'-C1' | -7.02 | 1.45 | 1.53 |
| 78 | CA | 919 | A | O4'-C1' | 7.01 | 1.50 | 1.41 |
| 81 | DA | 1753 | G | O4'-C1' | 7.01 | 1.50 | 1.41 |
| 81 | DA | 3313 | U | P-O5' | -7.01 | 1.52 | 1.59 |
| 35 | BG | 3 | ALA | N-CA | -7.01 | 1.32 | 1.46 |
| 35 | BG | 5 | LYS | N-CA | 7.01 | 1.60 | 1.46 |
| 78 | CA | 223 | U | C5'-C4' | 7.01 | 1.59 | 1.51 |
| 81 | DA | 1296 | C | P-O5' | -7.01 | 1.52 | 1.59 |
| 81 | DA | 2223 | A | C2'-C1' | -7.01 | 1.45 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 82 | DB | 95 | G | C2'-C1' | -7.01 | 1.45 | 1.53 |
| 78 | CA | 23 | G | C2'-C1' | -7.01 | 1.45 | 1.53 |
| 81 | DA | 185 | C | O3'-P | -7.01 | 1.52 | 1.61 |
| 81 | DA | 2017 | G | C2'-C1' | -7.01 | 1.45 | 1.53 |
| 81 | DA | 780 | A | O4'-C1' | 7.00 | 1.50 | 1.41 |
| 83 | DC | 47 | C | O4'-C1' | 7.00 | 1.50 | 1.41 |
| 78 | CA | 614 | C | C2'-C1' | -7.00 | 1.45 | 1.53 |
| 81 | DA | 660 | A | C2'-C1' | -6.99 | 1.45 | 1.53 |
| 81 | DA | 2837 | A | O4'-C1' | -6.99 | 1.32 | 1.41 |
| 32 | BC | 10 | ARG | NE-CZ | 6.99 | 1.42 | 1.33 |
| 81 | DA | 2473 | C | C2'-C1' | 6.99 | 1.61 | 1.53 |
| 78 | CA | 318 | U | O4'-C1' | 6.99 | 1.50 | 1.41 |
| 81 | DA | 142 | C | C2'-C1' | -6.99 | 1.45 | 1.53 |
| 78 | CA | 974 | A | O4'-C1' | 6.99 | 1.50 | 1.41 |
| 81 | DA | 2957 | G | O4'-C1' | 6.99 | 1.50 | 1.41 |
| 78 | CA | 1009 | U | C2'-C1' | -6.99 | 1.45 | 1.53 |
| 81 | DA | 1150 | A | O4'-C1' | 6.99 | 1.50 | 1.41 |
| 81 | DA | 2099 | A | C4'-C3' | -6.99 | 1.45 | 1.53 |
| 78 | CA | 255 | U | C2'-C1' | -6.98 | 1.45 | 1.53 |
| 6 | AE | 7 | GLN | CA-CB | -6.98 | 1.38 | 1.53 |
| 40 | BK | 184 | THR | C-N | 6.98 | 1.50 | 1.34 |
| 78 | CA | 221 | A | C2'-C1' | 6.98 | 1.61 | 1.53 |
| 4 | AD | 94 | ALA | CA-CB | -6.98 | 1.37 | 1.52 |
| 81 | DA | 3090 | U | C4'-C3' | 6.98 | 1.60 | 1.53 |
| 78 | CA | 968 | U | O4'-C1' | 6.98 | 1.50 | 1.41 |
| 78 | CA | 1341 | A | O4'-C1' | -6.98 | 1.32 | 1.41 |
| 81 | DA | 13 | A | C2'-C1' | -6.98 | 1.45 | 1.53 |
| 81 | DA | 1395 | G | O4'-C1' | 6.97 | 1.50 | 1.41 |
| 81 | DA | 1587 | A | O4'-C1' | -6.97 | 1.32 | 1.41 |
| 81 | DA | 3107 | U | P-O5' | -6.97 | 1.52 | 1.59 |
| 81 | DA | 1492 | G | C2'-C1' | -6.97 | 1.45 | 1.53 |
| 82 | DB | 117 | C | C2'-C1' | -6.97 | 1.45 | 1.53 |
| 78 | CA | 1164 | G | C2'-C1' | 6.97 | 1.61 | 1.53 |
| 81 | DA | 1378 | U | O4'-C1' | 6.97 | 1.50 | 1.41 |
| 81 | DA | 1721 | U | O4'-C1' | 6.97 | 1.50 | 1.41 |
| 81 | DA | 2696 | A | O4'-C1' | 6.97 | 1.50 | 1.41 |
| 17 | AQ | 94 | SER | CA-CB | 6.97 | 1.63 | 1.52 |
| 78 | CA | 1092 | A | C3'-C2' | -6.97 | 1.45 | 1.52 |
| 81 | DA | 1346 | G | C2'-C1' | 6.97 | 1.61 | 1.53 |
| 81 | DA | 2175 | U | C3'-C2' | -6.97 | 1.45 | 1.52 |
| 81 | DA | 534 | U | C2'-C1' | 6.96 | 1.61 | 1.53 |
| 81 | DA | 1370 | G | C2'-C1' | -6.96 | 1.45 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1373 | A | C2'-C1' | -6.96 | 1.45 | 1.53 |
| 81 | DA | 2222 | A | O4'-C1' | 6.96 | 1.50 | 1.41 |
| 81 | DA | 3340 | G | O4'-C1' | 6.96 | 1.50 | 1.41 |
| 78 | CA | 1753 | A | C2'-C1' | -6.96 | 1.45 | 1.53 |
| 81 | DA | 1389 | G | O4'-C1' | 6.96 | 1.50 | 1.41 |
| 81 | DA | 2522 | G | C4'-C3' | 6.96 | 1.60 | 1.53 |
| 81 | DA | 2666 | C | O4'-C1' | 6.96 | 1.50 | 1.41 |
| 79 | CB | 31 | C | C2'-C1' | -6.96 | 1.45 | 1.53 |
| 5 | AC | 163 | PRO | N-CA | 6.96 | 1.59 | 1.47 |
| 81 | DA | 3353 | G | C2'-C1' | -6.95 | 1.45 | 1.53 |
| 81 | DA | 2659 | G | C2'-C1' | -6.95 | 1.45 | 1.53 |
| 81 | DA | 2422 | C | O3'-P | -6.95 | 1.52 | 1.61 |
| 81 | DA | 990 | U | C5'-C4' | 6.95 | 1.59 | 1.51 |
| 26 | AZ | 35 | TYR | CE2-CZ | 6.94 | 1.47 | 1.38 |
| 78 | CA | 381 | C | O4'-C1' | 6.94 | 1.50 | 1.41 |
| 78 | CA | 465 | G | O4'-C1' | -6.94 | 1.32 | 1.41 |
| 1 | Aa | 58 | VAL | CA-CB | -6.94 | 1.40 | 1.54 |
| 78 | CA | 1171 | A | C2'-C1' | -6.94 | 1.45 | 1.53 |
| 81 | DA | 1438 | U | O4'-C1' | 6.94 | 1.50 | 1.41 |
| 81 | DA | 2374 | C | O4'-C1' | 6.94 | 1.50 | 1.41 |
| 83 | DC | 13 | A | C2'-C1' | -6.94 | 1.45 | 1.53 |
| 81 | DA | 429 | U | C2'-C1' | 6.94 | 1.60 | 1.53 |
| 81 | DA | 2163 | C | C2'-C1' | 6.94 | 1.60 | 1.53 |
| 81 | DA | 2287 | C | O4'-C1' | 6.94 | 1.50 | 1.41 |
| 81 | DA | 185 | C | C4'-O4' | 6.94 | 1.54 | 1.45 |
| 81 | DA | 1021 | G | O4'-C1' | 6.94 | 1.50 | 1.41 |
| 81 | DA | 3141 | A | C2'-C1' | -6.94 | 1.45 | 1.53 |
| 78 | CA | 1334 | U | C2'-C1' | -6.94 | 1.45 | 1.53 |
| 78 | CA | 923 | A | C2'-C1' | -6.93 | 1.45 | 1.53 |
| 78 | CA | 1550 | A | C4'-C3' | -6.93 | 1.45 | 1.53 |
| 81 | DA | 984 | G | C2'-C1' | 6.93 | 1.60 | 1.53 |
| 81 | DA | 1011 | A | O4'-C1' | 6.93 | 1.50 | 1.41 |
| 81 | DA | 3047 | U | O4'-C1' | 6.93 | 1.50 | 1.41 |
| 81 | DA | 1184 | A | O4'-C1' | 6.93 | 1.50 | 1.41 |
| 78 | CA | 625 | C | C2'-C1' | -6.93 | 1.45 | 1.53 |
| 81 | DA | 36 | C | C2'-C1' | -6.93 | 1.45 | 1.53 |
| 81 | DA | 1575 | A | O4'-C1' | -6.93 | 1.32 | 1.41 |
| 35 | BG | 8 | LYS | CA-CB | 6.93 | 1.69 | 1.53 |
| 78 | CA | 141 | U | O3'-P | -6.93 | 1.52 | 1.61 |
| 81 | DA | 306 | A | O4'-C1' | -6.93 | 1.32 | 1.41 |
| 81 | DA | 709 | A | O4'-C1' | 6.93 | 1.50 | 1.41 |
| 78 | CA | 927 | C | C2'-C1' | -6.92 | 1.45 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 48 | BW | 94 | ARG | CA-C | -6.92 | 1.34 | 1.52 |
| 78 | CA | 2 | A | O4'-C1' | -6.92 | 1.32 | 1.41 |
| 81 | DA | 1793 | C | C3'-C2' | -6.92 | 1.45 | 1.52 |
| 81 | DA | 2617 | U | O4'-C1' | -6.92 | 1.32 | 1.41 |
| 32 | BC | 256 | HIS | N-CA | 6.92 | 1.60 | 1.46 |
| 81 | DA | 720 | A | P-OP2 | 6.92 | 1.60 | 1.49 |
| 81 | DA | 1801 | U | O4'-C1' | 6.92 | 1.50 | 1.41 |
| 41 | BN | 108 | ARG | CA-CB | 6.92 | 1.69 | 1.53 |
| 60 | Bi | 16 | ARG | N-CA | -6.92 | 1.32 | 1.46 |
| 81 | DA | 1441 | G | C2'-C1' | -6.92 | 1.45 | 1.53 |
| 5 | AC | 157 | ASP | C-N | 6.92 | 1.50 | 1.34 |
| 22 | AV | 106 | ALA | CA-CB | 6.91 | 1.67 | 1.52 |
| 78 | CA | 858 | G | C3'-C2' | -6.91 | 1.45 | 1.52 |
| 78 | CA | 1368 | G | O4'-C1' | 6.91 | 1.50 | 1.41 |
| 81 | DA | 2099 | A | C3'-C2' | -6.91 | 1.45 | 1.52 |
| 78 | CA | 164 | A | P-O5' | -6.91 | 1.52 | 1.59 |
| 78 | CA | 1546 | G | P-O5' | -6.91 | 1.52 | 1.59 |
| 74 | BQ | 79 | TYR | CG-CD2 | 6.91 | 1.48 | 1.39 |
| 81 | DA | 1690 | C | O3'-P | -6.91 | 1.52 | 1.61 |
| 81 | DA | 3332 | U | C2'-C1' | 6.91 | 1.60 | 1.53 |
| 32 | BC | 247 | ARG | CZ-NH1 | 6.91 | 1.42 | 1.33 |
| 78 | CA | 1773 | C | C2'-C1' | -6.91 | 1.45 | 1.53 |
| 78 | CA | 100 | A | C2'-C1' | 6.91 | 1.60 | 1.53 |
| 81 | DA | 2192 | C | C2'-C1' | -6.91 | 1.45 | 1.53 |
| 79 | CB | 70 | G | C2'-C1' | -6.91 | 1.45 | 1.53 |
| 81 | DA | 1485 | G | O4'-C1' | 6.91 | 1.50 | 1.41 |
| 81 | DA | 2351 | U | C2'-C1' | -6.90 | 1.45 | 1.53 |
| 81 | DA | 2954 | U | C2'-C1' | -6.90 | 1.45 | 1.53 |
| 81 | DA | 2164 | A | C2'-C1' | -6.90 | 1.45 | 1.53 |
| 81 | DA | 2421 | U | O3'-P | -6.90 | 1.52 | 1.61 |
| 81 | DA | 3011 | A | O4'-C1' | 6.90 | 1.50 | 1.41 |
| 81 | DA | 2058 | G | C2'-C1' | -6.90 | 1.45 | 1.53 |
| 78 | CA | 1550 | A | C3'-O3' | 6.90 | 1.51 | 1.42 |
| 81 | DA | 2252 | A | C2'-C1' | -6.90 | 1.45 | 1.53 |
| 81 | DA | 2505 | U | O3'-P | -6.90 | 1.52 | 1.61 |
| 58 | Bg | 77 | ARG | NE-CZ | 6.89 | 1.42 | 1.33 |
| 81 | DA | 659 | G | O4'-C1' | 6.89 | 1.50 | 1.41 |
| 81 | DA | 2430 | A | C2'-C1' | -6.89 | 1.45 | 1.53 |
| 55 | Bc | 94 | LYS | CA-CB | 6.89 | 1.69 | 1.53 |
| 78 | CA | 307 | G | C3'-C2' | -6.89 | 1.45 | 1.52 |
| 78 | CA | 1010 | C | C2'-C1' | -6.89 | 1.45 | 1.53 |
| 78 | CA | 1156 | C | C2'-C1' | -6.89 | 1.45 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1514 | G | C2'-C1' | -6.89 | 1.45 | 1.53 |
| 78 | CA | 1725 | U | O4'-C1' | 6.89 | 1.50 | 1.41 |
| 21 | AT | 87 | ARG | CD-NE | 6.89 | 1.58 | 1.46 |
| 78 | CA | 883 | C | C2'-C1' | -6.89 | 1.45 | 1.53 |
| 81 | DA | 1901 | A | C2'-C1' | -6.89 | 1.45 | 1.53 |
| 83 | DC | 77 | A | O4'-C1' | 6.89 | 1.50 | 1.41 |
| 33 | BD | 98 | ARG | NE-CZ | 6.89 | 1.42 | 1.33 |
| 78 | CA | 1226 | A | C2'-C1' | -6.89 | 1.45 | 1.53 |
| 78 | CA | 414 | C | C2'-C1' | -6.89 | 1.45 | 1.53 |
| 81 | DA | 2286 | U | C2'-C1' | -6.89 | 1.45 | 1.53 |
| 39 | BJ | 25 | SER | CA-CB | 6.88 | 1.63 | 1.52 |
| 81 | DA | 859 | G | O4'-C1' | 6.88 | 1.50 | 1.41 |
| 74 | BQ | 112 | ARG | N-CA | -6.88 | 1.32 | 1.46 |
| 81 | DA | 1498 | A | C2'-C1' | -6.88 | 1.45 | 1.53 |
| 81 | DA | 2979 | U | O4'-C1' | 6.88 | 1.50 | 1.41 |
| 78 | CA | 49 | C | O4'-C1' | 6.88 | 1.50 | 1.41 |
| 81 | DA | 2687 | G | C2'-C1' | -6.87 | 1.45 | 1.53 |
| 82 | DB | 20 | U | O4'-C1' | 6.87 | 1.50 | 1.41 |
| 81 | DA | 2985 | C | C2'-C1' | -6.87 | 1.45 | 1.53 |
| 78 | CA | 82 | U | C2'-C1' | -6.87 | 1.45 | 1.53 |
| 13 | AL | 13 | ARG | CZ-NH2 | -6.87 | 1.24 | 1.33 |
| 31 | BB | 42 | ARG | CD-NE | 6.87 | 1.58 | 1.46 |
| 83 | DC | 77 | A | C2'-C1' | 6.87 | 1.60 | 1.53 |
| 78 | CA | 1000 | C | C2'-C1' | 6.86 | 1.60 | 1.53 |
| 79 | CB | 49 | G | C2'-C1' | -6.86 | 1.45 | 1.53 |
| 12 | AK | 84 | ARG | CZ-NH1 | 6.86 | 1.42 | 1.33 |
| 20 | AS | 12 | GLN | CA-CB | -6.86 | 1.38 | 1.53 |
| 78 | CA | 230 | C | C4'-C3' | 6.86 | 1.60 | 1.53 |
| 78 | CA | 1785 | U | C2'-C1' | -6.86 | 1.45 | 1.53 |
| 81 | DA | 1342 | C | C2'-C1' | -6.86 | 1.45 | 1.53 |
| 81 | DA | 1898 | G | O3'-P | -6.86 | 1.52 | 1.61 |
| 53 | Ba | 70 | PRO | N-CD | -6.86 | 1.38 | 1.47 |
| 78 | CA | 40 | A | O4'-C1' | 6.86 | 1.50 | 1.41 |
| 81 | DA | 3085 | G | O4'-C1' | -6.86 | 1.32 | 1.41 |
| 80 | CC | 14 | A | O4'-C1' | 6.86 | 1.50 | 1.41 |
| 78 | CA | 1566 | U | O4'-C1' | -6.85 | 1.32 | 1.41 |
| 81 | DA | 3380 | U | P-OP2 | 6.85 | 1.60 | 1.49 |
| 47 | BU | 12 | ARG | NE-CZ | 6.85 | 1.42 | 1.33 |
| 81 | DA | 35 | A | C2'-C1' | -6.85 | 1.45 | 1.53 |
| 81 | DA | 932 | U | O4'-C1' | 6.85 | 1.50 | 1.41 |
| 81 | DA | 1832 | C | P-O5' | -6.85 | 1.52 | 1.59 |
| 78 | CA | 1656 | U | C2'-C1' | -6.85 | 1.45 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 381 | U | O4'-C1' | 6.85 | 1.50 | 1.41 |
| 81 | DA | 1819 | U | C2'-C1' | 6.85 | 1.60 | 1.53 |
| 78 | CA | 190 | C | C2'-C1' | -6.85 | 1.45 | 1.53 |
| 81 | DA | 1873 | U | O4'-C1' | 6.85 | 1.50 | 1.41 |
| 81 | DA | 1400 | G | O3'-P | -6.85 | 1.52 | 1.61 |
| 78 | CA | 1697 | G | C2'-C1' | -6.84 | 1.45 | 1.53 |
| 31 | BB | 127 | ALA | N-CA | 6.84 | 1.60 | 1.46 |
| 78 | CA | 1473 | U | O4'-C1' | -6.84 | 1.32 | 1.41 |
| 83 | DC | 67 | C | C2'-C1' | -6.84 | 1.45 | 1.53 |
| 78 | CA | 1263 | G | C2'-C1' | 6.84 | 1.60 | 1.53 |
| 18 | AP | 122 | ILE | C-N | 6.84 | 1.49 | 1.34 |
| 78 | CA | 1544 | U | O3'-P | -6.84 | 1.52 | 1.61 |
| 81 | DA | 1288 | U | O4'-C1' | 6.84 | 1.50 | 1.41 |
| 81 | DA | 1717 | U | O3'-P | -6.84 | 1.52 | 1.61 |
| 81 | DA | 2853 | A | C2'-C1' | -6.83 | 1.45 | 1.53 |
| 78 | CA | 428 | A | C2'-C1' | 6.83 | 1.60 | 1.53 |
| 78 | CA | 1339 | C | O3'-P | -6.83 | 1.52 | 1.61 |
| 78 | CA | 586 | G | C3'-C2' | -6.83 | 1.45 | 1.52 |
| 81 | DA | 1083 | G | O4'-C1' | -6.83 | 1.32 | 1.41 |
| 81 | DA | 680 | G | O4'-C1' | -6.83 | 1.32 | 1.41 |
| 81 | DA | 235 | A | O4'-C1' | 6.83 | 1.50 | 1.41 |
| 81 | DA | 629 | U | C2'-C1' | -6.83 | 1.45 | 1.53 |
| 81 | DA | 2389 | C | O4'-C1' | 6.83 | 1.50 | 1.41 |
| 78 | CA | 918 | U | O4'-C1' | 6.82 | 1.50 | 1.41 |
| 78 | CA | 1026 | A | O4'-C1' | 6.82 | 1.50 | 1.41 |
| 81 | DA | 1565 | G | C2'-C1' | -6.82 | 1.45 | 1.53 |
| 78 | CA | 1071 | U | O4'-C1' | 6.82 | 1.50 | 1.41 |
| 18 | AP | 107 | VAL | C-N | 6.82 | 1.47 | 1.34 |
| 46 | BT | 5 | ARG | NE-CZ | 6.82 | 1.42 | 1.33 |
| 81 | DA | 169 | U | C5'-C4' | 6.82 | 1.59 | 1.51 |
| 81 | DA | 1945 | A | C2'-C1' | -6.82 | 1.45 | 1.53 |
| 78 | CA | 1669 | U | O4'-C1' | 6.81 | 1.50 | 1.41 |
| 8 | AF | 184 | PHE | CG-CD1 | 6.81 | 1.49 | 1.38 |
| 79 | CB | 48 | C | C2'-C1' | -6.81 | 1.45 | 1.53 |
| 81 | DA | 1853 | U | C2'-C1' | 6.81 | 1.60 | 1.53 |
| 81 | DA | 2628 | A | O3'-P | -6.81 | 1.52 | 1.61 |
| 81 | DA | 3105 | U | C2'-C1' | -6.81 | 1.45 | 1.53 |
| 78 | CA | 965 | U | C2'-C1' | -6.81 | 1.45 | 1.53 |
| 78 | CA | 1081 | A | O4'-C1' | -6.81 | 1.32 | 1.41 |
| 81 | DA | 545 | U | C2'-C1' | 6.81 | 1.60 | 1.53 |
| 81 | DA | 1077 | U | C2'-C1' | -6.81 | 1.45 | 1.53 |
| 81 | DA | 349 | A | C2'-C1' | -6.80 | 1.45 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 686 | C | C2'-C1' | -6.80 | 1.45 | 1.53 |
| 81 | DA | 1856 | C | C2'-C1' | -6.80 | 1.45 | 1.53 |
| 81 | DA | 3324 | C | C2'-C1' | -6.80 | 1.45 | 1.53 |
| 81 | DA | 626 | U | O4'-C1' | 6.80 | 1.50 | 1.41 |
| 83 | DC | 19 | C | O4'-C1' | 6.80 | 1.50 | 1.41 |
| 81 | DA | 1108 | U | O4'-C1' | 6.80 | 1.50 | 1.41 |
| 81 | DA | 30 | G | P-OP2 | 6.79 | 1.60 | 1.49 |
| 81 | DA | 726 | G | C5'-C4' | 6.79 | 1.59 | 1.51 |
| 81 | DA | 1620 | U | P-OP2 | 6.79 | 1.60 | 1.49 |
| 81 | DA | 3303 | G | P-O5' | -6.79 | 1.52 | 1.59 |
| 83 | DC | 11 | A | O4'-C1' | 6.79 | 1.50 | 1.41 |
| 83 | DC | 36 | C | O4'-C1' | 6.79 | 1.50 | 1.41 |
| 4 | AD | 60 | GLU | CD-OE2 | 6.79 | 1.33 | 1.25 |
| 78 | CA | 1338 | C | C4'-C3' | -6.79 | 1.45 | 1.53 |
| 78 | CA | 1792 | G | O4'-C1' | -6.79 | 1.32 | 1.41 |
| 78 | CA | 1558 | U | C2'-C1' | 6.79 | 1.60 | 1.53 |
| 81 | DA | 931 | C | O4'-C1' | 6.79 | 1.50 | 1.41 |
| 29 | AU | 89 | TYR | CG-CD2 | 6.78 | 1.48 | 1.39 |
| 81 | DA | 1506 | A | O4'-C1' | -6.78 | 1.32 | 1.41 |
| 81 | DA | 2737 | C | O3'-P | -6.78 | 1.53 | 1.61 |
| 5 | AC | 78 | ARG | CZ-NH2 | 6.78 | 1.41 | 1.33 |
| 26 | AZ | 19 | PRO | N-CA | 6.78 | 1.58 | 1.47 |
| 81 | DA | 934 | G | O4'-C1' | 6.78 | 1.50 | 1.41 |
| 78 | CA | 1306 | C | P-O5' | 6.78 | 1.66 | 1.59 |
| 81 | DA | 1 | G | O4'-C1' | -6.78 | 1.32 | 1.41 |
| 81 | DA | 1042 | U | O4'-C1' | 6.78 | 1.50 | 1.41 |
| 83 | DC | 82 | A | O4'-C1' | 6.78 | 1.50 | 1.41 |
| 81 | DA | 2251 | G | O4'-C1' | 6.78 | 1.50 | 1.41 |
| 81 | DA | 1 | G | P-OP2 | 6.77 | 1.60 | 1.49 |
| 78 | CA | 670 | U | O4'-C1' | 6.77 | 1.50 | 1.41 |
| 81 | DA | 1512 | U | O4'-C1' | 6.77 | 1.50 | 1.41 |
| 81 | DA | 1752 | A | C2'-C1' | -6.77 | 1.46 | 1.53 |
| 81 | DA | 2415 | C | O4'-C1' | 6.77 | 1.50 | 1.41 |
| 81 | DA | 2603 | G | C2'-C1' | -6.77 | 1.46 | 1.53 |
| 35 | BG | 8 | LYS | C-N | 6.77 | 1.49 | 1.34 |
| 81 | DA | 1560 | G | O3'-P | -6.77 | 1.53 | 1.61 |
| 81 | DA | 2621 | G | O4'-C1' | 6.77 | 1.50 | 1.41 |
| 20 | AS | 63 | ARG | NE-CZ | 6.77 | 1.41 | 1.33 |
| 34 | BE | 9 | MET | CA-CB | 6.77 | 1.68 | 1.53 |
| 81 | DA | 1654 | A | O4'-C1' | 6.77 | 1.50 | 1.41 |
| 81 | DA | 2279 | A | O4'-C1' | -6.76 | 1.32 | 1.41 |
| 81 | DA | 561 | C | C2'-C1' | -6.76 | 1.46 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1322 | U | O4'-C1' | 6.76 | 1.50 | 1.41 |
| 81 | DA | 1750 | A | C2'-C1' | -6.76 | 1.46 | 1.53 |
| 81 | DA | 2631 | U | C2'-C1' | -6.76 | 1.46 | 1.53 |
| 43 | BP | 14 | LYS | N-CA | -6.76 | 1.32 | 1.46 |
| 62 | Bk | 83 | ALA | N-CA | -6.76 | 1.32 | 1.46 |
| 81 | DA | 563 | U | O4'-C1' | 6.76 | 1.50 | 1.41 |
| 13 | AL | 23 | ARG | N-CA | -6.76 | 1.32 | 1.46 |
| 38 | Bs | 55 | LYS | CA-CB | 6.75 | 1.68 | 1.53 |
| 81 | DA | 948 | C | C2'-C1' | -6.75 | 1.46 | 1.53 |
| 78 | CA | 1087 | A | O4'-C1' | 6.75 | 1.50 | 1.41 |
| 78 | CA | 1397 | U | P-O5' | -6.75 | 1.52 | 1.59 |
| 81 | DA | 724 | U | C4'-C3' | -6.75 | 1.45 | 1.53 |
| 81 | DA | 1252 | A | O4'-C1' | 6.75 | 1.50 | 1.41 |
| 81 | DA | 765 | C | O4'-C1' | 6.75 | 1.50 | 1.41 |
| 81 | DA | 1415 | U | O4'-C1' | 6.75 | 1.50 | 1.41 |
| 81 | DA | 2085 | U | O4'-C1' | 6.75 | 1.50 | 1.41 |
| 78 | CA | 139 | C | O4'-C1' | 6.75 | 1.50 | 1.41 |
| 81 | DA | 374 | A | C2'-C1' | 6.75 | 1.60 | 1.53 |
| 81 | DA | 790 | U | C5'-C4' | -6.75 | 1.43 | 1.51 |
| 9 | AH | 51 | GLU | CD-OE1 | 6.75 | 1.33 | 1.25 |
| 81 | DA | 104 | G | C2'-C1' | 6.75 | 1.60 | 1.53 |
| 64 | Bl | 39 | TYR | C-N | 6.74 | 1.47 | 1.34 |
| 78 | CA | 546 | U | C2'-C1' | -6.74 | 1.46 | 1.53 |
| 81 | DA | 279 | U | O4'-C1' | 6.74 | 1.50 | 1.41 |
| 81 | DA | 1810 | A | C2'-C1' | -6.74 | 1.46 | 1.53 |
| 81 | DA | 3318 | G | C2'-C1' | -6.74 | 1.46 | 1.53 |
| 35 | BG | 99 | GLU | CD-OE1 | 6.74 | 1.33 | 1.25 |
| 47 | BU | 140 | ILE | C-O | 6.74 | 1.36 | 1.23 |
| 81 | DA | 138 | U | O4'-C1' | 6.74 | 1.50 | 1.41 |
| 81 | DA | 766 | U | P-O5' | -6.74 | 1.53 | 1.59 |
| 78 | CA | 401 | A | C2'-C1' | -6.74 | 1.46 | 1.53 |
| 78 | CA | 978 | A | O4'-C1' | 6.74 | 1.50 | 1.41 |
| 81 | DA | 393 | U | O4'-C1' | 6.74 | 1.50 | 1.41 |
| 81 | DA | 2622 | C | O4'-C1' | 6.74 | 1.50 | 1.41 |
| 32 | BC | 62 | ARG | CD-NE | 6.73 | 1.57 | 1.46 |
| 81 | DA | 233 | C | O4'-C1' | 6.73 | 1.50 | 1.41 |
| 81 | DA | 640 | U | C2'-C1' | -6.73 | 1.46 | 1.53 |
| 81 | DA | 795 | G | C2'-C1' | -6.73 | 1.46 | 1.53 |
| 81 | DA | 1518 | U | O4'-C1' | 6.73 | 1.50 | 1.41 |
| 78 | CA | 1778 | G | C2'-C1' | -6.73 | 1.46 | 1.53 |
| 57 | Be | 142 | SER | CA-CB | -6.73 | 1.42 | 1.52 |
| 81 | DA | 1082 | U | C2'-C1' | 6.73 | 1.60 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 255 | U | C3'-C2' | 6.73 | 1.60 | 1.52 |
| 81 | DA | 792 | G | O4'-C1' | 6.73 | 1.50 | 1.41 |
| 81 | DA | 1206 | G | O4'-C1' | -6.73 | 1.32 | 1.41 |
| 81 | DA | 2194 | G | O4'-C1' | -6.72 | 1.32 | 1.41 |
| 78 | CA | 1623 | C | C2'-C1' | -6.72 | 1.46 | 1.53 |
| 81 | DA | 2922 | G | O4'-C1' | 6.72 | 1.50 | 1.41 |
| 81 | DA | 357 | A | O4'-C1' | 6.72 | 1.50 | 1.41 |
| 81 | DA | 3311 | C | O4'-C1' | 6.72 | 1.50 | 1.41 |
| 83 | DC | 55 | A | C2'-C1' | 6.72 | 1.60 | 1.53 |
| 81 | DA | 1009 | A | C5'-C4' | 6.72 | 1.59 | 1.51 |
| 78 | CA | 1446 | A | O4'-C1' | 6.71 | 1.50 | 1.41 |
| 45 | BR | 3 | ILE | CA-CB | 6.71 | 1.70 | 1.54 |
| 78 | CA | 160 | C | C2'-C1' | -6.71 | 1.46 | 1.53 |
| 81 | DA | 1989 | U | O3'-P | -6.71 | 1.53 | 1.61 |
| 8 | AF | 27 | THR | N-CA | -6.71 | 1.32 | 1.46 |
| 81 | DA | 2851 | A | C2'-C1' | -6.71 | 1.46 | 1.53 |
| 81 | DA | 2956 | A | O3'-P | -6.71 | 1.53 | 1.61 |
| 81 | DA | 2996 | U | P-OP2 | 6.71 | 1.60 | 1.49 |
| 78 | CA | 979 | A | C2'-C1' | -6.71 | 1.46 | 1.53 |
| 78 | CA | 1321 | A | C3'-C2' | -6.71 | 1.45 | 1.52 |
| 81 | DA | 2146 | C | C2'-C1' | -6.71 | 1.46 | 1.53 |
| 78 | CA | 643 | G | C2'-C1' | -6.71 | 1.46 | 1.53 |
| 81 | DA | 82 | C | C2'-C1' | -6.70 | 1.46 | 1.53 |
| 81 | DA | 2054 | C | O4'-C1' | 6.70 | 1.50 | 1.41 |
| 35 | BG | 148 | GLU | N-CA | -6.70 | 1.32 | 1.46 |
| 81 | DA | 276 | U | P-O5' | -6.70 | 1.53 | 1.59 |
| 81 | DA | 1625 | A | C2'-C1' | -6.70 | 1.46 | 1.53 |
| 81 | DA | 1670 | C | O4'-C1' | 6.70 | 1.50 | 1.41 |
| 81 | DA | 1893 | A | C2'-C1' | -6.70 | 1.46 | 1.53 |
| 44 | BO | 58 | MET | N-CA | 6.70 | 1.59 | 1.46 |
| 78 | CA | 29 | U | O3'-P | -6.70 | 1.53 | 1.61 |
| 81 | DA | 3250 | U | O4'-C1' | 6.70 | 1.50 | 1.41 |
| 81 | DA | 756 | U | C2'-C1' | -6.70 | 1.46 | 1.53 |
| 4 | AD | 241 | GLY | N-CA | 6.70 | 1.56 | 1.46 |
| 78 | CA | 1415 | U | C2'-C1' | -6.70 | 1.46 | 1.53 |
| 81 | DA | 2852 | C | C2'-C1' | -6.70 | 1.46 | 1.53 |
| 78 | CA | 1078 | C | C2'-C1' | -6.69 | 1.46 | 1.53 |
| 78 | CA | 1237 | G | C3'-C2' | -6.69 | 1.45 | 1.52 |
| 81 | DA | 271 | C | C2'-C1' | 6.69 | 1.60 | 1.53 |
| 81 | DA | 1620 | U | O4'-C1' | 6.69 | 1.50 | 1.41 |
| 81 | DA | 3029 | A | O4'-C1' | 6.69 | 1.50 | 1.41 |
| 81 | DA | 3240 | C | P-O5' | -6.69 | 1.53 | 1.59 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 83 | DC | 9 | C | O3'-P | -6.69 | 1.53 | 1.61 |
| 78 | CA | 937 | C | C2'-C1' | -6.69 | 1.46 | 1.53 |
| 81 | DA | 1696 | A | O4'-C1' | 6.69 | 1.50 | 1.41 |
| 81 | DA | 989 | A | P-O5' | 6.69 | 1.66 | 1.59 |
| 81 | DA | 1823 | A | P-OP2 | 6.69 | 1.60 | 1.49 |
| 78 | CA | 98 | U | O4'-C1' | 6.68 | 1.50 | 1.41 |
| 78 | CA | 974 | A | C2'-C1' | -6.68 | 1.46 | 1.53 |
| 81 | DA | 2529 | A | P-O5' | -6.68 | 1.53 | 1.59 |
| 78 | CA | 1708 | U | O4'-C1' | 6.68 | 1.50 | 1.41 |
| 78 | CA | 177 | U | P-OP2 | 6.68 | 1.60 | 1.49 |
| 78 | CA | 218 | A | O4'-C1' | 6.68 | 1.50 | 1.41 |
| 78 | CA | 1474 | G | O4'-C1' | 6.68 | 1.50 | 1.41 |
| 81 | DA | 1871 | U | O3'-P | 6.68 | 1.69 | 1.61 |
| 81 | DA | 1952 | G | C2'-C1' | -6.67 | 1.46 | 1.53 |
| 81 | DA | 2709 | C | C2'-C1' | -6.67 | 1.46 | 1.53 |
| 81 | DA | 3310 | A | C2'-C1' | -6.67 | 1.46 | 1.53 |
| 81 | DA | 2256 | A | C2'-C1' | 6.67 | 1.60 | 1.53 |
| 5 | AC | 62 | ARG | NE-CZ | 6.67 | 1.41 | 1.33 |
| 78 | CA | 139 | C | C2'-C1' | -6.67 | 1.46 | 1.53 |
| 81 | DA | 1780 | G | C2'-C1' | -6.67 | 1.46 | 1.53 |
| 78 | CA | 1543 | A | O3'-P | -6.67 | 1.53 | 1.61 |
| 22 | AV | 96 | SER | CA-CB | 6.67 | 1.62 | 1.52 |
| 78 | CA | 933 | A | C2'-C1' | -6.66 | 1.46 | 1.53 |
| 25 | AY | 23 | GLY | CA-C | -6.66 | 1.41 | 1.51 |
| 78 | CA | 1191 | U | O4'-C1' | -6.66 | 1.32 | 1.41 |
| 81 | DA | 33 | G | O4'-C1' | 6.66 | 1.50 | 1.41 |
| 81 | DA | 2636 | A | C2'-C1' | -6.66 | 1.46 | 1.53 |
| 81 | DA | 2865 | U | O3'-P | -6.66 | 1.53 | 1.61 |
| 81 | DA | 663 | C | P-O5' | -6.66 | 1.53 | 1.59 |
| 81 | DA | 1470 | U | C2'-C1' | -6.66 | 1.46 | 1.53 |
| 81 | DA | 3139 | A | C2'-C1' | -6.65 | 1.46 | 1.53 |
| 78 | CA | 900 | A | P-O5' | -6.65 | 1.53 | 1.59 |
| 81 | DA | 770 | G | C5'-C4' | 6.65 | 1.59 | 1.51 |
| 81 | DA | 47 | C | C2'-C1' | -6.65 | 1.46 | 1.53 |
| 81 | DA | 991 | G | O4'-C1' | 6.65 | 1.50 | 1.41 |
| 81 | DA | 2909 | U | O4'-C1' | 6.65 | 1.50 | 1.41 |
| 81 | DA | 3065 | G | C2'-C1' | -6.65 | 1.46 | 1.53 |
| 12 | AK | 41 | ARG | NE-CZ | 6.65 | 1.41 | 1.33 |
| 78 | CA | 1778 | G | O4'-C1' | 6.65 | 1.50 | 1.41 |
| 20 | AS | 53 | TRP | C-N | -6.65 | 1.18 | 1.34 |
| 33 | BD | 323 | VAL | CA-CB | -6.65 | 1.40 | 1.54 |
| 79 | CB | 64 | G | O4'-C1' | 6.65 | 1.50 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 791 | A | O4'-C1' | 6.65 | 1.50 | 1.41 |
| 78 | CA | 1448 | G | O4'-C1' | 6.65 | 1.50 | 1.41 |
| 81 | DA | 612 | U | C2'-C1' | -6.65 | 1.46 | 1.53 |
| 81 | DA | 2644 | C | O4'-C1' | -6.65 | 1.33 | 1.41 |
| 78 | CA | 47 | A | C4'-O4' | -6.64 | 1.36 | 1.45 |
| 78 | CA | 1469 | A | O4'-C1' | 6.64 | 1.50 | 1.41 |
| 81 | DA | 1661 | G | C2'-C1' | -6.64 | 1.46 | 1.53 |
| 78 | CA | 687 | G | C4'-O4' | -6.64 | 1.36 | 1.45 |
| 78 | CA | 853 | G | O4'-C1' | -6.64 | 1.33 | 1.41 |
| 81 | DA | 2174 | G | O4'-C1' | -6.64 | 1.33 | 1.41 |
| 81 | DA | 2732 | G | C2'-C1' | -6.64 | 1.46 | 1.53 |
| 78 | CA | 1612 | U | C2'-C1' | 6.64 | 1.60 | 1.53 |
| 20 | AS | 102 | ARG | CZ-NH2 | -6.64 | 1.24 | 1.33 |
| 81 | DA | 1257 | C | P-O5' | -6.64 | 1.53 | 1.59 |
| 13 | AL | 2 | GLY | N-CA | -6.63 | 1.36 | 1.46 |
| 57 | Be | 75 | TYR | CG-CD2 | 6.63 | 1.47 | 1.39 |
| 81 | DA | 2986 | U | C2'-C1' | -6.63 | 1.46 | 1.53 |
| 81 | DA | 1457 | U | O4'-C1' | 6.63 | 1.50 | 1.41 |
| 35 | BG | 153 | PRO | CA-C | -6.63 | 1.39 | 1.52 |
| 81 | DA | 769 | G | C2'-C1' | -6.63 | 1.46 | 1.53 |
| 81 | DA | 1930 | A | C2'-C1' | -6.63 | 1.46 | 1.53 |
| 82 | DB | 29 | U | C2'-C1' | -6.63 | 1.46 | 1.53 |
| 78 | CA | 1264 | G | O4'-C1' | 6.63 | 1.50 | 1.41 |
| 81 | DA | 2378 | C | C2'-C1' | -6.63 | 1.46 | 1.53 |
| 81 | DA | 2458 | A | O4'-C1' | 6.63 | 1.50 | 1.41 |
| 81 | DA | 970 | A | C2'-C1' | -6.62 | 1.46 | 1.53 |
| 81 | DA | 1407 | A | O4'-C1' | 6.62 | 1.50 | 1.41 |
| 81 | DA | 2120 | A | O4'-C1' | 6.62 | 1.50 | 1.41 |
| 78 | CA | 599 | A | O4'-C1' | 6.62 | 1.50 | 1.41 |
| 78 | CA | 619 | A | O3'-P | -6.62 | 1.53 | 1.61 |
| 81 | DA | 1092 | C | C2'-C1' | -6.62 | 1.46 | 1.53 |
| 81 | DA | 1216 | C | O4'-C1' | 6.62 | 1.50 | 1.41 |
| 81 | DA | 2451 | G | P-O5' | -6.62 | 1.53 | 1.59 |
| 81 | DA | 3035 | A | P-O5' | -6.62 | 1.53 | 1.59 |
| 81 | DA | 750 | G | P-O5' | -6.62 | 1.53 | 1.59 |
| 81 | DA | 1749 | A | C2'-C1' | -6.62 | 1.46 | 1.53 |
| 81 | DA | 2627 | C | P-O5' | -6.62 | 1.53 | 1.59 |
| 49 | BV | 39 | TRP | NE1-CE2 | 6.62 | 1.46 | 1.37 |
| 81 | DA | 3149 | G | C3'-C2' | -6.62 | 1.45 | 1.52 |
| 62 | Bk | 25 | LYS | CA-CB | -6.62 | 1.39 | 1.53 |
| 81 | DA | 1074 | U | O4'-C1' | 6.62 | 1.50 | 1.41 |
| 81 | DA | 3382 | U | O3'-P | -6.62 | 1.53 | 1.61 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 82 | DB | 132 | G | C2'-C1' | 6.62 | 1.60 | 1.53 |
| 81 | DA | 1124 | U | O4'-C1' | 6.62 | 1.50 | 1.41 |
| 81 | DA | 1716 | U | C2'-C1' | 6.62 | 1.60 | 1.53 |
| 78 | CA | 1347 | U | C2'-C1' | 6.62 | 1.60 | 1.53 |
| 81 | DA | 908 | G | C2'-C1' | -6.62 | 1.46 | 1.53 |
| 82 | DB | 2 | A | P-OP2 | 6.62 | 1.60 | 1.49 |
| 78 | CA | 997 | G | C2'-C1' | -6.61 | 1.46 | 1.53 |
| 78 | CA | 1206 | U | C2'-C1' | -6.61 | 1.46 | 1.53 |
| 78 | CA | 1655 | A | O4'-C1' | 6.61 | 1.50 | 1.41 |
| 81 | DA | 2911 | A | C2'-C1' | -6.61 | 1.46 | 1.53 |
| 72 | Bt | 61 | PHE | CA-CB | 6.61 | 1.68 | 1.53 |
| 81 | DA | 673 | U | O4'-C1' | 6.61 | 1.50 | 1.41 |
| 81 | DA | 1299 | U | C2'-C1' | -6.61 | 1.46 | 1.53 |
| 78 | CA | 1566 | U | C5'-C4' | 6.61 | 1.59 | 1.51 |
| 81 | DA | 2672 | G | O3'-P | -6.61 | 1.53 | 1.61 |
| 81 | DA | 284 | A | O4'-C1' | 6.61 | 1.50 | 1.41 |
| 81 | DA | 842 | G | C2'-C1' | -6.61 | 1.46 | 1.53 |
| 81 | DA | 1501 | U | C2'-C1' | -6.61 | 1.46 | 1.53 |
| 81 | DA | 3136 | G | O4'-C1' | -6.61 | 1.33 | 1.41 |
| 78 | CA | 57 | G | P-O5' | 6.61 | 1.66 | 1.59 |
| 81 | DA | 2766 | U | C2'-C1' | -6.61 | 1.46 | 1.53 |
| 78 | CA | 149 | C | O4'-C1' | 6.61 | 1.50 | 1.41 |
| 78 | CA | 1505 | A | C6-N6 | 6.61 | 1.39 | 1.33 |
| 81 | DA | 2664 | C | C2'-C1' | -6.61 | 1.46 | 1.53 |
| 81 | DA | 3366 | G | C2'-C1' | -6.61 | 1.46 | 1.53 |
| 33 | BD | 95 | ARG | CZ-NH1 | 6.60 | 1.41 | 1.33 |
| 81 | DA | 813 | G | C2'-C1' | -6.60 | 1.46 | 1.53 |
| 78 | CA | 257 | A | C4'-C3' | 6.60 | 1.60 | 1.53 |
| 81 | DA | 1168 | U | C2'-C1' | 6.60 | 1.60 | 1.53 |
| 81 | DA | 1197 | A | C2'-C1' | -6.60 | 1.46 | 1.53 |
| 81 | DA | 2209 | U | C5'-C4' | 6.60 | 1.59 | 1.51 |
| 14 | AM | 115 | ARG | NE-CZ | 6.59 | 1.41 | 1.33 |
| 31 | BB | 63 | PHE | N-CA | 6.59 | 1.59 | 1.46 |
| 78 | CA | 1535 | U | O4'-C1' | -6.59 | 1.33 | 1.41 |
| 81 | DA | 806 | A | C2'-C1' | 6.59 | 1.60 | 1.53 |
| 81 | DA | 2773 | C | P-OP2 | 6.59 | 1.60 | 1.49 |
| 81 | DA | 3061 | G | O4'-C1' | 6.59 | 1.50 | 1.41 |
| 81 | DA | 1550 | C | O4'-C1' | 6.59 | 1.50 | 1.41 |
| 78 | CA | 257 | A | C5'-C4' | 6.59 | 1.59 | 1.51 |
| 78 | CA | 441 | A | C2'-C1' | -6.59 | 1.46 | 1.53 |
| 81 | DA | 496 | C | C2'-C1' | -6.59 | 1.46 | 1.53 |
| 82 | DB | 43 | A | P-O5' | -6.59 | 1.53 | 1.59 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 52 | U | O4'-C1' | 6.59 | 1.50 | 1.41 |
| 81 | DA | 1245 | A | C2'-C1' | 6.58 | 1.60 | 1.53 |
| 33 | BD | 141 | ARG | NE-CZ | 6.58 | 1.41 | 1.33 |
| 81 | DA | 493 | G | C2'-C1' | -6.58 | 1.46 | 1.53 |
| 78 | CA | 618 | U | O4'-C1' | 6.58 | 1.50 | 1.41 |
| 78 | CA | 704 | C | C4'-C3' | -6.58 | 1.46 | 1.53 |
| 78 | CA | 998 | A | O4'-C1' | 6.58 | 1.50 | 1.41 |
| 81 | DA | 3035 | A | O4'-C1' | 6.58 | 1.50 | 1.41 |
| 78 | CA | 1776 | A | C2'-C1' | -6.58 | 1.46 | 1.53 |
| 78 | CA | 1 | U | C5'-C4' | -6.58 | 1.43 | 1.51 |
| 81 | DA | 637 | C | O3'-P | -6.58 | 1.53 | 1.61 |
| 81 | DA | 2314 | U | O4'-C1' | 6.58 | 1.50 | 1.41 |
| 78 | CA | 838 | G | O4'-C1' | 6.58 | 1.50 | 1.41 |
| 81 | DA | 3394 | U | O4'-C1' | 6.58 | 1.50 | 1.41 |
| 78 | CA | 852 | C | O3'-P | -6.57 | 1.53 | 1.61 |
| 81 | DA | 329 | U | O4'-C1' | -6.57 | 1.33 | 1.41 |
| 81 | DA | 2342 | U | O4'-C1' | 6.57 | 1.50 | 1.41 |
| 78 | CA | 869 | A | C2'-C1' | -6.57 | 1.46 | 1.53 |
| 80 | CC | 12 | A | P-OP2 | 6.57 | 1.60 | 1.49 |
| 81 | DA | 2989 | U | C3'-C2' | 6.57 | 1.60 | 1.52 |
| 81 | DA | 3313 | U | C3'-O3' | -6.57 | 1.32 | 1.42 |
| 5 | AC | 108 | ARG | NE-CZ | 6.57 | 1.41 | 1.33 |
| 78 | CA | 907 | A | C2'-C1' | -6.57 | 1.46 | 1.53 |
| 81 | DA | 3114 | A | O4'-C1' | 6.57 | 1.50 | 1.41 |
| 78 | CA | 1417 | A | C2'-C1' | -6.56 | 1.46 | 1.53 |
| 4 | AD | 97 | GLU | N-CA | -6.56 | 1.33 | 1.46 |
| 78 | CA | 117 | U | P-O5' | -6.56 | 1.53 | 1.59 |
| 78 | CA | 1330 | G | C2'-C1' | -6.56 | 1.46 | 1.53 |
| 81 | DA | 286 | U | C2'-C1' | -6.56 | 1.46 | 1.53 |
| 81 | DA | 1737 | U | P-OP2 | 6.56 | 1.60 | 1.49 |
| 81 | DA | 1870 | C | C2'-C1' | -6.56 | 1.46 | 1.53 |
| 81 | DA | 126 | U | C2'-C1' | 6.56 | 1.60 | 1.53 |
| 81 | DA | 672 | A | O5'-C5' | -6.56 | 1.32 | 1.42 |
| 81 | DA | 1481 | A | C2'-C1' | -6.56 | 1.46 | 1.53 |
| 81 | DA | 2290 | C | O4'-C1' | 6.56 | 1.50 | 1.41 |
| 81 | DA | 1772 | U | O4'-C1' | 6.56 | 1.50 | 1.41 |
| 81 | DA | 2184 | U | C2'-C1' | -6.56 | 1.46 | 1.53 |
| 81 | DA | 2797 | C | C2'-C1' | 6.56 | 1.60 | 1.53 |
| 81 | DA | 538 | G | O4'-C1' | 6.55 | 1.50 | 1.41 |
| 81 | DA | 2312 | A | O4'-C1' | 6.55 | 1.50 | 1.41 |
| 57 | Be | 120 | THR | CA-CB | -6.55 | 1.36 | 1.53 |
| 37 | BH | 89 | GLU | CD-OE1 | -6.55 | 1.18 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 1720 | G | O4'-C1' | -6.55 | 1.33 | 1.41 |
| 81 | DA | 744 | A | C2'-O2' | -6.55 | 1.33 | 1.41 |
| 78 | CA | 257 | A | C3'-C2' | -6.55 | 1.45 | 1.52 |
| 78 | CA | 323 | A | P-OP2 | 6.55 | 1.60 | 1.49 |
| 78 | CA | 1581 | C | P-O5' | -6.55 | 1.53 | 1.59 |
| 78 | CA | 1788 | G | O4'-C1' | 6.55 | 1.50 | 1.41 |
| 81 | DA | 25 | U | O4'-C1' | 6.55 | 1.50 | 1.41 |
| 81 | DA | 715 | A | C2'-C1' | -6.55 | 1.46 | 1.53 |
| 81 | DA | 1449 | A | O4'-C1' | 6.55 | 1.50 | 1.41 |
| 81 | DA | 1717 | U | C2'-C1' | -6.55 | 1.46 | 1.53 |
| 81 | DA | 2245 | C | C2'-C1' | -6.55 | 1.46 | 1.53 |
| 81 | DA | 1403 | C | P-OP2 | 6.54 | 1.60 | 1.49 |
| 81 | DA | 1679 | A | O3'-P | -6.54 | 1.53 | 1.61 |
| 83 | DC | 5 | G | O4'-C1' | 6.54 | 1.50 | 1.41 |
| 81 | DA | 2674 | A | O4'-C1' | 6.54 | 1.50 | 1.41 |
| 79 | CB | 42 | C | C2'-C1' | -6.54 | 1.46 | 1.53 |
| 81 | DA | 2194 | G | O3'-P | -6.54 | 1.53 | 1.61 |
| 14 | AM | 37 | GLY | CA-C | -6.54 | 1.41 | 1.51 |
| 81 | DA | 565 | U | O4'-C1' | 6.54 | 1.50 | 1.41 |
| 81 | DA | 697 | A | O4'-C1' | 6.54 | 1.50 | 1.41 |
| 78 | CA | 622 | A | C2'-C1' | 6.54 | 1.60 | 1.53 |
| 81 | DA | 846 | A | C2'-C1' | -6.54 | 1.46 | 1.53 |
| 81 | DA | 2227 | C | O4'-C1' | 6.54 | 1.50 | 1.41 |
| 81 | DA | 1538 | G | O3'-P | -6.54 | 1.53 | 1.61 |
| 81 | DA | 1115 | G | C2'-C1' | 6.54 | 1.60 | 1.53 |
| 81 | DA | 1369 | A | O4'-C1' | 6.54 | 1.50 | 1.41 |
| 78 | CA | 332 | U | C4'-C3' | -6.53 | 1.46 | 1.53 |
| 81 | DA | 1507 | G | O4'-C1' | -6.53 | 1.33 | 1.41 |
| 81 | DA | 1343 | A | O4'-C1' | -6.53 | 1.33 | 1.41 |
| 78 | CA | 1365 | C | C2'-C1' | -6.53 | 1.46 | 1.53 |
| 81 | DA | 30 | G | O4'-C1' | -6.53 | 1.33 | 1.41 |
| 81 | DA | 747 | A | C3'-C2' | -6.53 | 1.45 | 1.52 |
| 79 | CB | 1 | U | P-OP2 | 6.53 | 1.60 | 1.49 |
| 81 | DA | 724 | U | O3'-P | -6.53 | 1.53 | 1.61 |
| 81 | DA | 1593 | A | O4'-C1' | 6.53 | 1.50 | 1.41 |
| 78 | CA | 1654 | G | C2'-C1' | -6.53 | 1.46 | 1.53 |
| 81 | DA | 1469 | C | O4'-C1' | 6.53 | 1.50 | 1.41 |
| 81 | DA | 1621 | A | O4'-C1' | 6.53 | 1.50 | 1.41 |
| 65 | Bn | 72 | THR | N-CA | 6.52 | 1.59 | 1.46 |
| 78 | CA | 202 | A | C3'-O3' | 6.52 | 1.51 | 1.42 |
| 81 | DA | 1727 | G | O4'-C1' | 6.52 | 1.50 | 1.41 |
| 81 | DA | 289 | A | C2'-C1' | -6.52 | 1.46 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1912 | U | O4'-C1' | 6.52 | 1.50 | 1.41 |
| 78 | CA | 1730 | A | O4'-C1' | 6.52 | 1.50 | 1.41 |
| 78 | CA | 522 | U | C4'-C3' | -6.52 | 1.46 | 1.53 |
| 55 | Bc | 94 | LYS | N-CA | -6.51 | 1.33 | 1.46 |
| 81 | DA | 399 | A | O4'-C1' | 6.51 | 1.50 | 1.41 |
| 81 | DA | 87 | U | O4'-C1' | 6.51 | 1.50 | 1.41 |
| 81 | DA | 264 | G | C4'-C3' | -6.51 | 1.46 | 1.53 |
| 81 | DA | 1166 | G | C2'-C1' | 6.51 | 1.60 | 1.53 |
| 81 | DA | 1399 | A | P-OP2 | 6.51 | 1.60 | 1.49 |
| 81 | DA | 2408 | U | O4'-C1' | 6.51 | 1.50 | 1.41 |
| 78 | CA | 145 | A | C2'-C1' | 6.51 | 1.60 | 1.53 |
| 78 | CA | 983 | A | O4'-C1' | 6.51 | 1.50 | 1.41 |
| 37 | BH | 112 | GLU | CG-CD | 6.51 | 1.61 | 1.51 |
| 78 | CA | 165 | G | C3'-C2' | -6.51 | 1.45 | 1.52 |
| 78 | CA | 1242 | A | C5'-C4' | 6.51 | 1.59 | 1.51 |
| 81 | DA | 102 | C | C2'-C1' | -6.51 | 1.46 | 1.53 |
| 81 | DA | 737 | G | C2-N3 | 6.51 | 1.38 | 1.32 |
| 81 | DA | 2719 | U | O3'-P | -6.51 | 1.53 | 1.61 |
| 43 | BP | 16 | SER | N-CA | -6.50 | 1.33 | 1.46 |
| 81 | DA | 1051 | U | O4'-C1' | 6.50 | 1.50 | 1.41 |
| 49 | BV | 61 | ARG | CG-CD | 6.50 | 1.68 | 1.51 |
| 61 | Bj | 9 | VAL | N-CA | 6.50 | 1.59 | 1.46 |
| 81 | DA | 80 | G | O4'-C1' | 6.50 | 1.50 | 1.41 |
| 81 | DA | 1208 | U | O4'-C1' | -6.50 | 1.33 | 1.41 |
| 81 | DA | 1147 | G | C2'-C1' | 6.50 | 1.60 | 1.53 |
| 82 | DB | 114 | G | C2'-C1' | -6.50 | 1.46 | 1.53 |
| 78 | CA | 1048 | G | O4'-C1' | 6.50 | 1.50 | 1.41 |
| 81 | DA | 2138 | A | O4'-C1' | -6.50 | 1.33 | 1.41 |
| 82 | DB | 120 | C | O4'-C1' | 6.50 | 1.50 | 1.41 |
| 22 | AV | 27 | TRP | N-CA | 6.50 | 1.59 | 1.46 |
| 33 | BD | 346 | LYS | CA-CB | 6.50 | 1.68 | 1.53 |
| 55 | Bc | 94 | LYS | C-N | 6.50 | 1.49 | 1.34 |
| 81 | DA | 2341 | A | O4'-C1' | 6.50 | 1.50 | 1.41 |
| 78 | CA | 348 | U | O4'-C1' | 6.50 | 1.50 | 1.41 |
| 81 | DA | 2530 | G | O4'-C1' | 6.50 | 1.50 | 1.41 |
| 78 | CA | 1034 | C | C2'-C1' | -6.49 | 1.46 | 1.53 |
| 81 | DA | 1208 | U | O3'-P | -6.49 | 1.53 | 1.61 |
| 81 | DA | 1940 | G | C2'-C1' | -6.49 | 1.46 | 1.53 |
| 81 | DA | 3363 | U | O4'-C1' | 6.49 | 1.50 | 1.41 |
| 78 | CA | 106 | U | O4'-C1' | 6.49 | 1.50 | 1.41 |
| 32 | BC | 9 | PRO | CA-C | -6.49 | 1.39 | 1.52 |
| 81 | DA | 1135 | A | C2'-C1' | -6.49 | 1.46 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1640 | G | O3'-P | -6.49 | 1.53 | 1.61 |
| 78 | CA | 1204 | A | C2'-C1' | -6.49 | 1.46 | 1.53 |
| 81 | DA | 375 | A | O4'-C1' | 6.49 | 1.50 | 1.41 |
| 16 | AO | 67 | THR | C-N | 6.49 | 1.44 | 1.33 |
| 81 | DA | 2767 | U | C2'-C1' | -6.49 | 1.46 | 1.53 |
| 78 | CA | 434 | G | O4'-C1' | -6.48 | 1.33 | 1.41 |
| 62 | Bk | 81 | THR | CA-CB | 6.48 | 1.70 | 1.53 |
| 78 | CA | 1770 | U | C2'-C1' | 6.48 | 1.60 | 1.53 |
| 81 | DA | 2276 | G | C2'-C1' | -6.48 | 1.46 | 1.53 |
| 78 | CA | 1675 | C | C2'-C1' | -6.48 | 1.46 | 1.53 |
| 81 | DA | 213 | A | C2'-C1' | 6.48 | 1.60 | 1.53 |
| 81 | DA | 783 | A | O4'-C1' | -6.48 | 1.33 | 1.41 |
| 81 | DA | 1598 | G | O4'-C1' | -6.48 | 1.33 | 1.41 |
| 81 | DA | 484 | C | C2'-C1' | -6.48 | 1.46 | 1.53 |
| 81 | DA | 98 | G | C2'-C1' | -6.48 | 1.46 | 1.53 |
| 34 | BE | 123 | PHE | CA-CB | -6.48 | 1.39 | 1.53 |
| 78 | CA | 44 | U | P-OP2 | 6.47 | 1.59 | 1.49 |
| 81 | DA | 1756 | C | C3'-C2' | 6.47 | 1.60 | 1.52 |
| 81 | DA | 2914 | G | P-OP2 | 6.47 | 1.59 | 1.49 |
| 33 | BD | 84 | ARG | CA-CB | -6.47 | 1.39 | 1.53 |
| 78 | CA | 1738 | U | O4'-C1' | 6.47 | 1.50 | 1.41 |
| 81 | DA | 2037 | G | C2'-C1' | -6.47 | 1.46 | 1.53 |
| 78 | CA | 241 | U | C5'-C4' | 6.47 | 1.59 | 1.51 |
| 33 | BD | 78 | GLY | C-N | 6.47 | 1.44 | 1.33 |
| 36 | BF | 2 | LYS | CA-CB | 6.47 | 1.68 | 1.53 |
| 78 | CA | 225 | A | C5'-C4' | 6.47 | 1.59 | 1.51 |
| 78 | CA | 233 | C | C4'-C3' | 6.47 | 1.60 | 1.53 |
| 81 | DA | 26 | A | C2'-C1' | 6.47 | 1.60 | 1.53 |
| 81 | DA | 124 | U | C2'-C1' | 6.47 | 1.60 | 1.53 |
| 81 | DA | 218 | G | C2'-C1' | 6.47 | 1.60 | 1.53 |
| 81 | DA | 2997 | G | C2'-C1' | -6.46 | 1.46 | 1.53 |
| 78 | CA | 1261 | G | C2'-C1' | -6.46 | 1.46 | 1.53 |
| 78 | CA | 1446 | A | P-OP2 | 6.46 | 1.59 | 1.49 |
| 35 | BG | 100 | LYS | N-CA | -6.46 | 1.33 | 1.46 |
| 47 | BU | 156 | TYR | CG-CD1 | 6.46 | 1.47 | 1.39 |
| 78 | CA | 1415 | U | P-OP2 | 6.46 | 1.59 | 1.49 |
| 81 | DA | 52 | A | C2'-C1' | -6.46 | 1.46 | 1.53 |
| 81 | DA | 369 | A | C2'-C1' | 6.46 | 1.60 | 1.53 |
| 81 | DA | 1286 | A | O4'-C1' | 6.46 | 1.50 | 1.41 |
| 81 | DA | 2361 | A | O3'-P | -6.46 | 1.53 | 1.61 |
| 78 | CA | 1153 | G | C2'-C1' | -6.46 | 1.46 | 1.53 |
| 81 | DA | 144 | A | O4'-C1' | 6.46 | 1.50 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 90 | C | C2'-C1' | -6.45 | 1.46 | 1.53 |
| 81 | DA | 2770 | G | P-O5' | -6.45 | 1.53 | 1.59 |
| 78 | CA | 319 | U | O4'-C1' | 6.45 | 1.50 | 1.41 |
| 78 | CA | 646 | C | O3'-P | -6.45 | 1.53 | 1.61 |
| 46 | BT | 172 | ARG | NE-CZ | 6.45 | 1.41 | 1.33 |
| 81 | DA | 942 | U | O4'-C1' | 6.45 | 1.50 | 1.41 |
| 81 | DA | 1457 | U | C2'-C1' | -6.45 | 1.46 | 1.53 |
| 81 | DA | 797 | U | C2'-C1' | -6.45 | 1.46 | 1.53 |
| 8 | AF | 156 | ARG | CD-NE | 6.45 | 1.57 | 1.46 |
| 78 | CA | 706 | A | C4'-C3' | -6.45 | 1.46 | 1.53 |
| 81 | DA | 603 | A | C2'-C1' | -6.45 | 1.46 | 1.53 |
| 81 | DA | 575 | G | C2'-C1' | -6.44 | 1.46 | 1.53 |
| 81 | DA | 1180 | A | C2'-C1' | 6.44 | 1.60 | 1.53 |
| 78 | CA | 343 | C | O4'-C1' | 6.44 | 1.50 | 1.41 |
| 78 | CA | 1018 | U | C2'-C1' | -6.44 | 1.46 | 1.53 |
| 81 | DA | 2916 | U | C4'-C3' | -6.44 | 1.46 | 1.53 |
| 81 | DA | 2930 | A | C2'-C1' | -6.44 | 1.46 | 1.53 |
| 81 | DA | 3048 | A | P-O5' | 6.44 | 1.66 | 1.59 |
| 78 | CA | 1045 | C | O4'-C1' | 6.44 | 1.50 | 1.41 |
| 78 | CA | 689 | G | O3'-P | -6.44 | 1.53 | 1.61 |
| 81 | DA | 2622 | C | C2'-C1' | -6.44 | 1.46 | 1.53 |
| 60 | Bi | 77 | GLY | C-N | 6.44 | 1.44 | 1.33 |
| 81 | DA | 926 | A | O4'-C1' | 6.43 | 1.50 | 1.41 |
| 78 | CA | 1252 | C | C4'-C3' | -6.43 | 1.46 | 1.53 |
| 81 | DA | 187 | A | C2'-C1' | -6.43 | 1.46 | 1.53 |
| 81 | DA | 3299 | A | C2'-C1' | 6.43 | 1.60 | 1.53 |
| 78 | CA | 1758 | U | O4'-C1' | 6.43 | 1.50 | 1.41 |
| 81 | DA | 680 | G | C2'-C1' | 6.42 | 1.60 | 1.53 |
| 81 | DA | 1043 | C | C2'-C1' | -6.42 | 1.46 | 1.53 |
| 81 | DA | 2919 | A | O4'-C1' | 6.42 | 1.50 | 1.41 |
| 81 | DA | 1307 | G | O4'-C1' | 6.42 | 1.50 | 1.41 |
| 81 | DA | 968 | G | O4'-C1' | 6.42 | 1.50 | 1.41 |
| 81 | DA | 1689 | U | P-O5' | -6.42 | 1.53 | 1.59 |
| 81 | DA | 2906 | C | C2'-C1' | -6.42 | 1.46 | 1.53 |
| 78 | CA | 1791 | A | C2'-C1' | 6.42 | 1.60 | 1.53 |
| 81 | DA | 373 | A | O4'-C1' | 6.42 | 1.50 | 1.41 |
| 81 | DA | 1360 | C | C2'-C1' | -6.42 | 1.46 | 1.53 |
| 50 | BX | 93 | TYR | CG-CD1 | 6.41 | 1.47 | 1.39 |
| 78 | CA | 822 | U | C4'-O4' | 6.41 | 1.53 | 1.45 |
| 78 | CA | 687 | G | C3'-C2' | -6.41 | 1.45 | 1.52 |
| 81 | DA | 1837 | U | O4'-C1' | 6.41 | 1.50 | 1.41 |
| 81 | DA | 777 | U | C3'-O3' | 6.41 | 1.51 | 1.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1856 | C | O4'-C1' | 6.41 | 1.50 | 1.41 |
| 53 | Ba | 56 | LYS | N-CA | -6.41 | 1.33 | 1.46 |
| 83 | DC | 21 | G | C2'-C1' | -6.41 | 1.46 | 1.53 |
| 78 | CA | 120 | U | C3'-O3' | 6.41 | 1.51 | 1.42 |
| 81 | DA | 299 | G | O4'-C1' | -6.41 | 1.33 | 1.41 |
| 74 | BQ | 243 | ALA | CA-CB | 6.40 | 1.65 | 1.52 |
| 81 | DA | 2941 | A | C2'-C1' | 6.40 | 1.60 | 1.53 |
| 82 | DB | 135 | G | C2'-C1' | -6.40 | 1.46 | 1.53 |
| 45 | BR | 14 | GLY | CA-C | -6.40 | 1.41 | 1.51 |
| 78 | CA | 647 | G | P-O5' | -6.40 | 1.53 | 1.59 |
| 83 | DC | 36 | C | C2'-C1' | -6.40 | 1.46 | 1.53 |
| 46 | BT | 71 | ARG | N-CA | 6.40 | 1.59 | 1.46 |
| 49 | BV | 153 | LYS | N-CA | -6.40 | 1.33 | 1.46 |
| 78 | CA | 1383 | G | O4'-C1' | 6.40 | 1.50 | 1.41 |
| 78 | CA | 1398 | U | C2'-C1' | -6.40 | 1.46 | 1.53 |
| 81 | DA | 501 | A | C2'-C1' | -6.40 | 1.46 | 1.53 |
| 81 | DA | 1458 | U | O4'-C1' | 6.40 | 1.50 | 1.41 |
| 81 | DA | 2084 | C | O4'-C1' | 6.40 | 1.50 | 1.41 |
| 81 | DA | 2107 | A | C2'-C1' | -6.40 | 1.46 | 1.53 |
| 78 | CA | 47 | A | O5'-C5' | -6.40 | 1.32 | 1.42 |
| 81 | DA | 637 | C | C4'-O4' | 6.40 | 1.53 | 1.45 |
| 81 | DA | 1806 | A | O4'-C1' | 6.40 | 1.50 | 1.41 |
| 78 | CA | 17 | C | O4'-C1' | 6.39 | 1.50 | 1.41 |
| 81 | DA | 1161 | G | O4'-C1' | 6.39 | 1.50 | 1.41 |
| 81 | DA | 1953 | G | C4'-C3' | -6.39 | 1.46 | 1.53 |
| 9 | AH | 79 | PHE | CG-CD2 | 6.39 | 1.48 | 1.38 |
| 78 | CA | 145 | A | P-OP2 | 6.39 | 1.59 | 1.49 |
| 78 | CA | 1594 | G | C2'-C1' | -6.39 | 1.46 | 1.53 |
| 81 | DA | 161 | G | C4'-O4' | -6.39 | 1.37 | 1.45 |
| 81 | DA | 223 | U | O4'-C1' | 6.39 | 1.50 | 1.41 |
| 81 | DA | 537 | A | O4'-C1' | 6.39 | 1.50 | 1.41 |
| 81 | DA | 1809 | A | C2'-C1' | -6.39 | 1.46 | 1.53 |
| 82 | DB | 44 | A | O4'-C1' | 6.39 | 1.50 | 1.41 |
| 78 | CA | 1786 | G | C2'-C1' | -6.39 | 1.46 | 1.53 |
| 81 | DA | 770 | G | O4'-C1' | 6.39 | 1.50 | 1.41 |
| 81 | DA | 291 | C | C2'-C1' | -6.39 | 1.46 | 1.53 |
| 81 | DA | 974 | G | C3'-O3' | 6.39 | 1.51 | 1.42 |
| 81 | DA | 2707 | C | O4'-C1' | 6.39 | 1.50 | 1.41 |
| 47 | BU | 92 | ARG | CD-NE | 6.38 | 1.57 | 1.46 |
| 81 | DA | 818 | C | C4'-C3' | -6.38 | 1.46 | 1.53 |
| 81 | DA | 1988 | C | O3'-P | -6.38 | 1.53 | 1.61 |
| 78 | CA | 478 | A | O4'-C1' | -6.38 | 1.33 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 215 | A | O4'-C1' | 6.38 | 1.50 | 1.41 |
| 81 | DA | 776 | U | P-O5' | -6.38 | 1.53 | 1.59 |
| 81 | DA | 197 | G | O4'-C1' | 6.38 | 1.50 | 1.41 |
| 81 | DA | 1623 | G | C5'-C4' | 6.38 | 1.59 | 1.51 |
| 81 | DA | 2682 | C | O3'-P | -6.38 | 1.53 | 1.61 |
| 81 | DA | 2262 | A | O4'-C1' | 6.38 | 1.50 | 1.41 |
| 12 | AK | 94 | PRO | C-N | 6.37 | 1.44 | 1.33 |
| 81 | DA | 1131 | G | O4'-C1' | 6.37 | 1.50 | 1.41 |
| 81 | DA | 2292 | U | O4'-C1' | 6.37 | 1.50 | 1.41 |
| 49 | BV | 90 | PHE | CG-CD1 | 6.37 | 1.48 | 1.38 |
| 78 | CA | 999 | U | O4'-C1' | 6.37 | 1.50 | 1.41 |
| 81 | DA | 1113 | G | O4'-C1' | -6.37 | 1.33 | 1.41 |
| 81 | DA | 1990 | U | P-O5' | -6.36 | 1.53 | 1.59 |
| 76 | BS | 138 | ARG | CD-NE | 6.36 | 1.57 | 1.46 |
| 78 | CA | 963 | A | C2'-C1' | -6.36 | 1.46 | 1.53 |
| 81 | DA | 820 | A | O4'-C1' | 6.36 | 1.50 | 1.41 |
| 81 | DA | 1838 | G | O4'-C1' | 6.36 | 1.50 | 1.41 |
| 81 | DA | 1079 | A | O4'-C1' | 6.36 | 1.50 | 1.41 |
| 10 | AI | 135 | ARG | CZ-NH1 | 6.35 | 1.41 | 1.33 |
| 81 | DA | 243 | G | C2'-C1' | -6.35 | 1.46 | 1.53 |
| 81 | DA | 2043 | U | O4'-C1' | 6.35 | 1.50 | 1.41 |
| 9 | AH | 66 | ASN | CA-CB | -6.35 | 1.36 | 1.53 |
| 81 | DA | 1647 | A | C2'-C1' | 6.35 | 1.60 | 1.53 |
| 78 | CA | 572 | C | C2'-C1' | -6.35 | 1.46 | 1.53 |
| 81 | DA | 747 | A | C4'-C3' | -6.35 | 1.46 | 1.53 |
| 81 | DA | 939 | U | O4'-C1' | 6.35 | 1.49 | 1.41 |
| 81 | DA | 1126 | G | C2'-C1' | -6.35 | 1.46 | 1.53 |
| 81 | DA | 1468 | A | O4'-C1' | 6.35 | 1.49 | 1.41 |
| 81 | DA | 1454 | A | O4'-C1' | 6.34 | 1.49 | 1.41 |
| 81 | DA | 1768 | U | C2-N3 | 6.34 | 1.42 | 1.37 |
| 81 | DA | 2493 | U | P-O5' | -6.34 | 1.53 | 1.59 |
| 45 | BR | 121 | CYS | CB-SG | 6.34 | 1.93 | 1.82 |
| 81 | DA | 2161 | G | C2'-C1' | -6.34 | 1.46 | 1.53 |
| 81 | DA | 89 | A | O4'-C1' | 6.34 | 1.49 | 1.41 |
| 81 | DA | 2367 | A | C2'-C1' | -6.34 | 1.46 | 1.53 |
| 81 | DA | 3233 | C | C2'-C1' | -6.34 | 1.46 | 1.53 |
| 78 | CA | 1266 | U | O4'-C1' | 6.34 | 1.49 | 1.41 |
| 78 | CA | 1404 | C | C2'-C1' | -6.34 | 1.46 | 1.53 |
| 81 | DA | 114 | A | O4'-C1' | -6.34 | 1.33 | 1.41 |
| 78 | CA | 1130 | G | C4'-O4' | -6.33 | 1.37 | 1.45 |
| 74 | BQ | 238 | ASP | C-N | 6.33 | 1.48 | 1.34 |
| 78 | CA | 886 | U | O3'-P | 6.33 | 1.68 | 1.61 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 1528 | U | O4'-C1' | -6.33 | 1.33 | 1.41 |
| 81 | DA | 3042 | U | C2'-C1' | -6.33 | 1.46 | 1.53 |
| 81 | DA | 3150 | A | O4'-C1' | -6.33 | 1.33 | 1.41 |
| 33 | BD | 326 | ARG | NE-CZ | 6.33 | 1.41 | 1.33 |
| 78 | CA | 317 | C | C2'-C1' | -6.33 | 1.46 | 1.53 |
| 78 | CA | 562 | G | C2'-C1' | -6.33 | 1.46 | 1.53 |
| 78 | CA | 653 | C | O4'-C1' | 6.33 | 1.49 | 1.41 |
| 78 | CA | 558 | U | C2'-C1' | 6.33 | 1.60 | 1.53 |
| 78 | CA | 1087 | A | C2'-C1' | -6.33 | 1.46 | 1.53 |
| 81 | DA | 638 | C | C3'-C2' | -6.33 | 1.45 | 1.52 |
| 81 | DA | 1884 | A | O4'-C1' | 6.33 | 1.49 | 1.41 |
| 81 | DA | 2668 | U | O3'-P | -6.33 | 1.53 | 1.61 |
| 81 | DA | 2694 | A | O4'-C1' | 6.33 | 1.49 | 1.41 |
| 78 | CA | 1140 | G | C4'-C3' | -6.33 | 1.46 | 1.53 |
| 25 | AY | 29 | ARG | CZ-NH2 | 6.32 | 1.41 | 1.33 |
| 78 | CA | 1168 | U | O4'-C1' | 6.32 | 1.49 | 1.41 |
| 81 | DA | 434 | U | C3'-C2' | 6.32 | 1.59 | 1.52 |
| 81 | DA | 1944 | U | C2'-C1' | -6.32 | 1.46 | 1.53 |
| 78 | CA | 138 | A | P-OP2 | 6.32 | 1.59 | 1.49 |
| 78 | CA | 680 | U | C4'-C3' | -6.32 | 1.46 | 1.53 |
| 78 | CA | 1283 | U | C2'-C1' | 6.32 | 1.60 | 1.53 |
| 44 | BO | 56 | VAL | C-N | 6.32 | 1.44 | 1.33 |
| 55 | Bc | 104 | GLN | C-N | 6.32 | 1.48 | 1.34 |
| 78 | CA | 1235 | C | C2'-C1' | 6.32 | 1.60 | 1.53 |
| 81 | DA | 568 | G | C2'-C1' | -6.32 | 1.46 | 1.53 |
| 81 | DA | 1773 | C | C2'-C1' | 6.32 | 1.60 | 1.53 |
| 21 | AT | 5 | LYS | C-N | 6.32 | 1.44 | 1.33 |
| 81 | DA | 242 | C | C5'-C4' | 6.32 | 1.58 | 1.51 |
| 5 | AC | 19 | TYR | N-CA | -6.31 | 1.33 | 1.46 |
| 57 | Be | 47 | ARG | CZ-NH1 | 6.31 | 1.41 | 1.33 |
| 78 | CA | 791 | A | C4'-C3' | -6.31 | 1.46 | 1.53 |
| 81 | DA | 1358 | C | C2'-C1' | -6.31 | 1.46 | 1.53 |
| 81 | DA | 1447 | G | C2'-C1' | -6.31 | 1.46 | 1.53 |
| 1 | Aa | 82 | SER | CA-CB | 6.31 | 1.62 | 1.52 |
| 81 | DA | 1120 | A | O4'-C1' | 6.31 | 1.49 | 1.41 |
| 81 | DA | 1205 | A | O4'-C1' | 6.31 | 1.49 | 1.41 |
| 33 | BD | 76 | ARG | CZ-NH1 | 6.31 | 1.41 | 1.33 |
| 45 | BR | 74 | GLU | CG-CD | 6.31 | 1.61 | 1.51 |
| 57 | Be | 202 | LEU | C-N | 6.31 | 1.48 | 1.34 |
| 78 | CA | 1719 | A | O4'-C1' | 6.31 | 1.49 | 1.41 |
| 81 | DA | 2394 | G | O4'-C1' | 6.31 | 1.49 | 1.41 |
| 3 | AB | 78 | LYS | CA-CB | -6.30 | 1.40 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 12 | AK | 22 | SER | N-CA | 6.30 | 1.58 | 1.46 |
| 78 | CA | 1167 | G | C2'-C1' | 6.30 | 1.60 | 1.53 |
| 59 | Bh | 20 | HIS | N-CA | -6.30 | 1.33 | 1.46 |
| 81 | DA | 1288 | U | O3'-P | -6.30 | 1.53 | 1.61 |
| 81 | DA | 2501 | U | O4'-C1' | 6.30 | 1.49 | 1.41 |
| 81 | DA | 1637 | A | P-OP2 | 6.30 | 1.59 | 1.49 |
| 1 | Aa | 58 | VAL | CA-C | 6.30 | 1.69 | 1.52 |
| 81 | DA | 3256 | G | O4'-C1' | 6.30 | 1.49 | 1.41 |
| 78 | CA | 253 | A | O3'-P | -6.30 | 1.53 | 1.61 |
| 78 | CA | 837 | G | C4'-C3' | -6.30 | 1.46 | 1.53 |
| 81 | DA | 2363 | A | P-O5' | -6.29 | 1.53 | 1.59 |
| 81 | DA | 2423 | U | P-O5' | -6.29 | 1.53 | 1.59 |
| 81 | DA | 112 | U | C2'-C1' | -6.29 | 1.46 | 1.53 |
| 81 | DA | 1008 | U | C2'-C1' | 6.29 | 1.60 | 1.53 |
| 78 | CA | 1657 | U | O4'-C1' | 6.29 | 1.49 | 1.41 |
| 78 | CA | 238 | U | O3'-P | -6.29 | 1.53 | 1.61 |
| 81 | DA | 1339 | C | O4'-C1' | 6.29 | 1.49 | 1.41 |
| 81 | DA | 1991 | G | C4'-C3' | -6.29 | 1.46 | 1.53 |
| 81 | DA | 2237 | C | O4'-C1' | 6.29 | 1.49 | 1.41 |
| 81 | DA | 749 | C | O4'-C1' | 6.29 | 1.49 | 1.41 |
| 81 | DA | 2284 | C | C2'-C1' | -6.29 | 1.46 | 1.53 |
| 81 | DA | 2928 | C | O3'-P | -6.29 | 1.53 | 1.61 |
| 81 | DA | 503 | C | C2'-C1' | -6.29 | 1.46 | 1.53 |
| 81 | DA | 170 | G | C5'-C4' | 6.29 | 1.58 | 1.51 |
| 81 | DA | 1797 | A | O4'-C1' | 6.28 | 1.49 | 1.41 |
| 78 | CA | 616 | G | O4'-C1' | 6.28 | 1.49 | 1.41 |
| 78 | CA | 975 | C | C2'-C1' | -6.28 | 1.46 | 1.53 |
| 81 | DA | 1748 | G | O3'-P | -6.28 | 1.53 | 1.61 |
| 40 | BK | 172 | ARG | CZ-NH1 | 6.28 | 1.41 | 1.33 |
| 81 | DA | 79 | U | O4'-C1' | 6.28 | 1.49 | 1.41 |
| 81 | DA | 2427 | U | C2'-C1' | -6.28 | 1.46 | 1.53 |
| 81 | DA | 265 | A | P-O5' | -6.28 | 1.53 | 1.59 |
| 81 | DA | 2048 | G | C2'-C1' | -6.28 | 1.46 | 1.53 |
| 81 | DA | 2069 | G | C2'-C1' | -6.28 | 1.46 | 1.53 |
| 78 | CA | 1763 | A | O4'-C1' | 6.28 | 1.49 | 1.41 |
| 81 | DA | 2022 | G | C2'-C1' | -6.28 | 1.46 | 1.53 |
| 81 | DA | 1304 | A | C2'-C1' | 6.27 | 1.60 | 1.53 |
| 81 | DA | 440 | A | C2'-C1' | -6.27 | 1.46 | 1.53 |
| 81 | DA | 693 | A | O4'-C1' | 6.27 | 1.49 | 1.41 |
| 81 | DA | 3057 | U | C2'-C1' | -6.27 | 1.46 | 1.53 |
| 1 | Aa | 54 | PHE | C-N | 6.27 | 1.44 | 1.33 |
| 1 | Aa | 298 | GLY | N-CA | -6.27 | 1.36 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 57 | Be | 202 | LEU | N-CA | 6.27 | 1.58 | 1.46 |
| 78 | CA | 50 | C | O4'-C1' | 6.27 | 1.49 | 1.41 |
| 78 | CA | 276 | C | C2'-C1' | -6.27 | 1.46 | 1.53 |
| 81 | DA | 2145 | A | C2'-C1' | -6.27 | 1.46 | 1.53 |
| 78 | CA | 1642 | G | C2'-C1' | 6.27 | 1.60 | 1.53 |
| 83 | DC | 1 | G | P-OP2 | 6.27 | 1.59 | 1.49 |
| 78 | CA | 217 | A | C4'-C3' | 6.26 | 1.60 | 1.53 |
| 78 | CA | 1246 | C | C4'-C3' | -6.26 | 1.46 | 1.53 |
| 81 | DA | 341 | G | C2'-C1' | -6.26 | 1.46 | 1.53 |
| 34 | BE | 94 | ARG | CZ-NH1 | 6.26 | 1.41 | 1.33 |
| 83 | DC | 39 | C | C2'-C1' | -6.26 | 1.46 | 1.53 |
| 81 | DA | 800 | G | C2'-C1' | 6.26 | 1.60 | 1.53 |
| 81 | DA | 1267 | U | O4'-C1' | 6.26 | 1.49 | 1.41 |
| 81 | DA | 2162 | U | C2'-C1' | -6.26 | 1.46 | 1.53 |
| 43 | BP | 116 | LEU | N-CA | 6.26 | 1.58 | 1.46 |
| 81 | DA | 1656 | A | O4'-C1' | 6.26 | 1.49 | 1.41 |
| 81 | DA | 2405 | C | C2'-C1' | -6.26 | 1.46 | 1.53 |
| 81 | DA | 2152 | A | C2'-C1' | -6.25 | 1.46 | 1.53 |
| 78 | CA | 1750 | A | O4'-C1' | 6.25 | 1.49 | 1.41 |
| 81 | DA | 2434 | U | C2'-C1' | -6.25 | 1.46 | 1.53 |
| 81 | DA | 2905 | U | C2'-C1' | -6.25 | 1.46 | 1.53 |
| 81 | DA | 1379 | G | O4'-C1' | 6.25 | 1.49 | 1.41 |
| 81 | DA | 1182 | A | C2'-C1' | -6.25 | 1.46 | 1.53 |
| 81 | DA | 3074 | G | O4'-C1' | 6.25 | 1.49 | 1.41 |
| 81 | DA | 1107 | C | O4'-C1' | 6.25 | 1.49 | 1.41 |
| 81 | DA | 1870 | C | O3'-P | 6.25 | 1.68 | 1.61 |
| 81 | DA | 3065 | G | P-OP2 | 6.25 | 1.59 | 1.49 |
| 20 | AS | 52 | GLY | CA-C | -6.24 | 1.41 | 1.51 |
| 68 | Bq | 12 | ARG | CZ-NH1 | 6.24 | 1.41 | 1.33 |
| 81 | DA | 43 | A | P-O5' | -6.24 | 1.53 | 1.59 |
| 81 | DA | 1215 | U | O4'-C1' | 6.24 | 1.49 | 1.41 |
| 78 | CA | 1090 | C | O3'-P | -6.24 | 1.53 | 1.61 |
| 56 | Bf | 35 | ARG | CD-NE | 6.24 | 1.57 | 1.46 |
| 78 | CA | 1683 | C | C2'-C1' | -6.24 | 1.46 | 1.53 |
| 78 | CA | 1616 | G | C4'-C3' | -6.24 | 1.46 | 1.53 |
| 20 | AS | 24 | ARG | CZ-NH1 | 6.24 | 1.41 | 1.33 |
| 78 | CA | 1447 | C | C2'-C1' | 6.23 | 1.60 | 1.53 |
| 78 | CA | 1243 | G | O3'-P | -6.23 | 1.53 | 1.61 |
| 81 | DA | 2502 | A | C2'-C1' | 6.23 | 1.60 | 1.53 |
| 83 | DC | 49 | G | C2'-C1' | 6.23 | 1.60 | 1.53 |
| 81 | DA | 3336 | A | C2'-C1' | 6.23 | 1.60 | 1.53 |
| 31 | BB | 250 | GLN | N-CA | 6.23 | 1.58 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | BH | 89 | GLU | CA-CB | -6.23 | 1.40 | 1.53 |
| 65 | Bn | 35 | GLY | N-CA | -6.23 | 1.36 | 1.46 |
| 81 | DA | 1658 | G | O4'-C1' | 6.23 | 1.49 | 1.41 |
| 81 | DA | 2382 | G | C2'-C1' | -6.23 | 1.46 | 1.53 |
| 81 | DA | 3113 | A | C2'-C1' | -6.23 | 1.46 | 1.53 |
| 31 | BB | 246 | LEU | CA-CB | 6.22 | 1.68 | 1.53 |
| 78 | CA | 651 | G | C4'-O4' | -6.22 | 1.37 | 1.45 |
| 78 | CA | 959 | U | O4'-C1' | -6.22 | 1.33 | 1.41 |
| 81 | DA | 1974 | A | C4'-C3' | 6.22 | 1.59 | 1.53 |
| 81 | DA | 949 | C | C2'-C1' | -6.22 | 1.46 | 1.53 |
| 81 | DA | 2738 | A | O4'-C1' | 6.22 | 1.49 | 1.41 |
| 78 | CA | 1331 | A | O4'-C1' | 6.22 | 1.49 | 1.41 |
| 78 | CA | 1458 | G | P-OP2 | 6.22 | 1.59 | 1.49 |
| 81 | DA | 28 | C | O4'-C1' | 6.22 | 1.49 | 1.41 |
| 81 | DA | 1166 | G | O4'-C1' | 6.22 | 1.49 | 1.41 |
| 81 | DA | 3166 | C | O4'-C1' | 6.22 | 1.49 | 1.41 |
| 78 | CA | 947 | U | C2'-C1' | 6.21 | 1.60 | 1.53 |
| 78 | CA | 1709 | C | C2'-C1' | -6.21 | 1.46 | 1.53 |
| 81 | DA | 609 | G | O4'-C1' | -6.21 | 1.33 | 1.41 |
| 78 | CA | 885 | G | C2'-C1' | -6.21 | 1.46 | 1.53 |
| 81 | DA | 523 | A | C2'-C1' | 6.21 | 1.60 | 1.53 |
| 81 | DA | 2855 | U | C2'-C1' | -6.21 | 1.46 | 1.53 |
| 78 | CA | 1033 | C | C2'-C1' | -6.21 | 1.46 | 1.53 |
| 78 | CA | 1492 | A | P-O5' | -6.21 | 1.53 | 1.59 |
| 81 | DA | 957 | C | C2'-C1' | -6.21 | 1.46 | 1.53 |
| 81 | DA | 1235 | U | C2'-C1' | -6.21 | 1.46 | 1.53 |
| 81 | DA | 146 | U | O3'-P | 6.21 | 1.68 | 1.61 |
| 81 | DA | 672 | A | O4'-C1' | 6.21 | 1.49 | 1.41 |
| 81 | DA | 2976 | A | O4'-C1' | 6.21 | 1.49 | 1.41 |
| 78 | CA | 179 | A | P-O5' | -6.20 | 1.53 | 1.59 |
| 78 | CA | 1302 | U | O3'-P | -6.20 | 1.53 | 1.61 |
| 50 | BX | 93 | TYR | CZ-OH | 6.20 | 1.48 | 1.37 |
| 81 | DA | 161 | G | C2'-C1' | -6.20 | 1.46 | 1.53 |
| 81 | DA | 597 | G | P-O5' | -6.20 | 1.53 | 1.59 |
| 81 | DA | 972 | A | O3'-P | -6.20 | 1.53 | 1.61 |
| 2 | AA | 183 | ARG | NE-CZ | 6.20 | 1.41 | 1.33 |
| 81 | DA | 754 | G | O3'-P | -6.20 | 1.53 | 1.61 |
| 81 | DA | 2444 | C | C2'-C1' | -6.20 | 1.46 | 1.53 |
| 37 | BH | 134 | TYR | CB-CG | 6.20 | 1.60 | 1.51 |
| 78 | CA | 1540 | G | O4'-C1' | 6.20 | 1.49 | 1.41 |
| 81 | DA | 1751 | G | O4'-C1' | 6.20 | 1.49 | 1.41 |
| 83 | DC | 9 | C | P-O5' | -6.19 | 1.53 | 1.59 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 13 | AL | 39 | LYS | CB-CG | 6.19 | 1.69 | 1.52 |
| 78 | CA | 57 | G | C4'-O4' | -6.19 | 1.37 | 1.45 |
| 81 | DA | 1692 | U | O4'-C1' | -6.19 | 1.33 | 1.41 |
| 81 | DA | 3160 | U | O4'-C1' | 6.19 | 1.49 | 1.41 |
| 51 | BZ | 71 | ARG | N-CA | -6.19 | 1.33 | 1.46 |
| 78 | CA | 150 | U | O3'-P | -6.19 | 1.53 | 1.61 |
| 81 | DA | 2075 | C | C2'-C1' | -6.19 | 1.46 | 1.53 |
| 36 | BF | 2 | LYS | C-N | 6.19 | 1.48 | 1.34 |
| 78 | CA | 973 | A | O4'-C1' | 6.19 | 1.49 | 1.41 |
| 81 | DA | 2882 | U | C2'-C1' | -6.19 | 1.46 | 1.53 |
| 78 | CA | 1222 | C | P-O5' | -6.19 | 1.53 | 1.59 |
| 15 | AN | 13 | ARG | CZ-NH1 | 6.18 | 1.41 | 1.33 |
| 55 | Bc | 38 | ARG | CZ-NH1 | 6.18 | 1.41 | 1.33 |
| 81 | DA | 230 | U | C2'-C1' | 6.18 | 1.60 | 1.53 |
| 81 | DA | 2169 | G | P-OP2 | 6.18 | 1.59 | 1.49 |
| 81 | DA | 2330 | C | C2'-C1' | -6.18 | 1.46 | 1.53 |
| 81 | DA | 3054 | U | O3'-P | -6.18 | 1.53 | 1.61 |
| 81 | DA | 1387 | G | P-OP2 | 6.18 | 1.59 | 1.49 |
| 6 | AE | 4 | PRO | CA-CB | -6.18 | 1.41 | 1.53 |
| 78 | CA | 1321 | A | C2'-C1' | 6.18 | 1.60 | 1.53 |
| 81 | DA | 683 | U | O4'-C1' | 6.18 | 1.49 | 1.41 |
| 81 | DA | 1202 | A | O4'-C1' | 6.18 | 1.49 | 1.41 |
| 37 | BH | 216 | SER | CA-CB | 6.18 | 1.62 | 1.52 |
| 81 | DA | 1898 | G | C2'-C1' | -6.18 | 1.46 | 1.53 |
| 81 | DA | 285 | A | C2'-C1' | 6.17 | 1.60 | 1.53 |
| 81 | DA | 425 | G | O3'-P | -6.17 | 1.53 | 1.61 |
| 82 | DB | 110 | C | C2'-C1' | -6.17 | 1.46 | 1.53 |
| 14 | AM | 10 | SER | CA-CB | 6.17 | 1.62 | 1.52 |
| 78 | CA | 1021 | C | C2'-C1' | -6.17 | 1.46 | 1.53 |
| 81 | DA | 2109 | U | C2'-C1' | -6.17 | 1.46 | 1.53 |
| 81 | DA | 2423 | U | O3'-P | -6.17 | 1.53 | 1.61 |
| 57 | Be | 176 | TYR | CZ-OH | 6.17 | 1.48 | 1.37 |
| 63 | Bm | 85 | ARG | CZ-NH2 | 6.17 | 1.41 | 1.33 |
| 78 | CA | 658 | C | O4'-C1' | 6.17 | 1.49 | 1.41 |
| 81 | DA | 781 | G | O4'-C1' | 6.17 | 1.49 | 1.41 |
| 81 | DA | 1622 | U | O4'-C1' | 6.17 | 1.49 | 1.41 |
| 81 | DA | 2112 | U | O4'-C1' | 6.17 | 1.49 | 1.41 |
| 81 | DA | 2723 | U | C3'-C2' | -6.17 | 1.46 | 1.52 |
| 78 | CA | 612 | U | O4'-C1' | 6.17 | 1.49 | 1.41 |
| 78 | CA | 935 | U | O4'-C1' | 6.17 | 1.49 | 1.41 |
| 78 | CA | 1145 | U | O4'-C1' | 6.17 | 1.49 | 1.41 |
| 78 | CA | 853 | G | P-O5' | 6.16 | 1.66 | 1.59 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 1023 | A | C2'-C1' | 6.16 | 1.60 | 1.53 |
| 81 | DA | 211 | A | C2'-C1' | 6.16 | 1.60 | 1.53 |
| 78 | CA | 775 | G | C4'-C3' | -6.16 | 1.46 | 1.53 |
| 81 | DA | 2981 | U | O4'-C1' | 6.16 | 1.49 | 1.41 |
| 38 | Bs | 129 | GLU | CG-CD | 6.16 | 1.61 | 1.51 |
| 44 | BO | 142 | GLY | C-N | 6.16 | 1.44 | 1.33 |
| 81 | DA | 2710 | C | C2'-C1' | -6.16 | 1.46 | 1.53 |
| 82 | DB | 138 | A | C2'-C1' | -6.15 | 1.46 | 1.53 |
| 57 | Be | 113 | SER | CA-CB | 6.15 | 1.62 | 1.52 |
| 78 | CA | 169 | A | C4'-O4' | -6.15 | 1.37 | 1.45 |
| 81 | DA | 1400 | G | C3'-O3' | -6.15 | 1.33 | 1.42 |
| 78 | CA | 18 | C | C2'-C1' | -6.15 | 1.46 | 1.53 |
| 81 | DA | 257 | U | P-O5' | -6.15 | 1.53 | 1.59 |
| 81 | DA | 636 | C | O3'-P | -6.15 | 1.53 | 1.61 |
| 81 | DA | 681 | U | O4'-C1' | 6.15 | 1.49 | 1.41 |
| 81 | DA | 1474 | A | O4'-C1' | 6.15 | 1.49 | 1.41 |
| 78 | CA | 881 | A | C4'-C3' | -6.14 | 1.46 | 1.53 |
| 81 | DA | 55 | G | O4'-C1' | 6.14 | 1.49 | 1.41 |
| 81 | DA | 704 | U | C3'-O3' | -6.14 | 1.33 | 1.42 |
| 81 | DA | 2870 | C | C2'-C1' | 6.14 | 1.60 | 1.53 |
| 81 | DA | 2204 | C | O3'-P | -6.14 | 1.53 | 1.61 |
| 81 | DA | 2903 | A | C4'-C3' | -6.14 | 1.46 | 1.53 |
| 78 | CA | 1051 | G | C2-N3 | 6.14 | 1.37 | 1.32 |
| 81 | DA | 2406 | C | O4'-C1' | 6.14 | 1.49 | 1.41 |
| 81 | DA | 1390 | A | O4'-C1' | -6.14 | 1.33 | 1.41 |
| 81 | DA | 1142 | G | O4'-C1' | 6.14 | 1.49 | 1.41 |
| 81 | DA | 1189 | C | C2'-C1' | 6.14 | 1.60 | 1.53 |
| 81 | DA | 2201 | G | O4'-C1' | 6.14 | 1.49 | 1.41 |
| 81 | DA | 952 | A | C2'-C1' | -6.13 | 1.46 | 1.53 |
| 81 | DA | 2024 | G | C2'-C1' | -6.13 | 1.46 | 1.53 |
| 81 | DA | 1833 | G | C2'-C1' | -6.13 | 1.46 | 1.53 |
| 78 | CA | 1446 | A | C2'-C1' | 6.13 | 1.60 | 1.53 |
| 81 | DA | 1505 | C | C2'-C1' | -6.13 | 1.46 | 1.53 |
| 81 | DA | 1593 | A | C2'-C1' | -6.13 | 1.46 | 1.53 |
| 78 | CA | 119 | A | C4'-C3' | 6.13 | 1.59 | 1.53 |
| 81 | DA | 944 | C | O4'-C1' | 6.13 | 1.49 | 1.41 |
| 81 | DA | 1285 | G | O4'-C1' | 6.13 | 1.49 | 1.41 |
| 81 | DA | 2723 | U | O3'-P | 6.13 | 1.68 | 1.61 |
| 78 | CA | 11 | A | C2'-C1' | -6.13 | 1.46 | 1.53 |
| 78 | CA | 207 | U | P-O5' | -6.12 | 1.53 | 1.59 |
| 78 | CA | 1403 | C | O4'-C1' | 6.12 | 1.49 | 1.41 |
| 81 | DA | 2667 | A | O4'-C1' | 6.12 | 1.49 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 31 | BB | 183 | GLY | CA-C | -6.12 | 1.42 | 1.51 |
| 49 | BV | 31 | GLU | CB-CG | 6.12 | 1.63 | 1.52 |
| 78 | CA | 165 | G | C4'-C3' | -6.12 | 1.46 | 1.53 |
| 78 | CA | 910 | C | C2'-C1' | -6.12 | 1.46 | 1.53 |
| 81 | DA | 1133 | A | O4'-C1' | 6.12 | 1.49 | 1.41 |
| 64 | Bl | 73 | ARG | NE-CZ | 6.12 | 1.41 | 1.33 |
| 78 | CA | 1681 | A | C2'-C1' | -6.12 | 1.46 | 1.53 |
| 81 | DA | 784 | A | O4'-C1' | -6.12 | 1.33 | 1.41 |
| 81 | DA | 1408 | G | C2'-C1' | -6.12 | 1.46 | 1.53 |
| 81 | DA | 2174 | G | O3'-P | -6.12 | 1.53 | 1.61 |
| 81 | DA | 2099 | A | C4'-O4' | -6.12 | 1.37 | 1.45 |
| 78 | CA | 894 | U | C4'-C3' | -6.11 | 1.46 | 1.53 |
| 81 | DA | 777 | U | O4'-C1' | 6.11 | 1.49 | 1.41 |
| 78 | CA | 1690 | G | C5'-C4' | 6.11 | 1.58 | 1.51 |
| 74 | BQ | 79 | TYR | CE2-CZ | 6.11 | 1.46 | 1.38 |
| 81 | DA | 42 | C | C4'-C3' | -6.11 | 1.46 | 1.53 |
| 81 | DA | 366 | A | C4'-C3' | -6.11 | 1.46 | 1.53 |
| 81 | DA | 2273 | G | C2'-C1' | -6.11 | 1.46 | 1.53 |
| 78 | CA | 868 | G | C4'-C3' | -6.11 | 1.46 | 1.53 |
| 31 | BB | 174 | ARG | CZ-NH1 | 6.11 | 1.41 | 1.33 |
| 78 | CA | 189 | C | C2'-C1' | 6.11 | 1.60 | 1.53 |
| 78 | CA | 1092 | A | O4'-C1' | -6.11 | 1.33 | 1.41 |
| 79 | CB | 30 | G | C2'-C1' | -6.11 | 1.46 | 1.53 |
| 81 | DA | 3083 | G | C2'-C1' | -6.11 | 1.46 | 1.53 |
| 83 | DC | 87 | U | O4'-C1' | 6.11 | 1.49 | 1.41 |
| 35 | BG | 158 | TYR | CZ-OH | 6.11 | 1.48 | 1.37 |
| 81 | DA | 606 | C | O3'-P | -6.11 | 1.53 | 1.61 |
| 56 | Bf | 23 | TYR | CE2-CZ | 6.10 | 1.46 | 1.38 |
| 81 | DA | 856 | G | C2'-C1' | -6.10 | 1.46 | 1.53 |
| 78 | CA | 1763 | A | C2'-C1' | -6.10 | 1.46 | 1.53 |
| 81 | DA | 328 | U | O3'-P | -6.10 | 1.53 | 1.61 |
| 81 | DA | 2185 | G | O4'-C1' | -6.10 | 1.33 | 1.41 |
| 11 | AJ | 82 | TYR | N-CA | -6.10 | 1.34 | 1.46 |
| 32 | BC | 38 | SER | CA-CB | 6.10 | 1.62 | 1.52 |
| 78 | CA | 229 | U | C5'-C4' | 6.10 | 1.58 | 1.51 |
| 78 | CA | 348 | U | C2'-C1' | -6.10 | 1.46 | 1.53 |
| 78 | CA | 1766 | A | O4'-C1' | 6.10 | 1.49 | 1.41 |
| 81 | DA | 1200 | A | O4'-C1' | 6.10 | 1.49 | 1.41 |
| 81 | DA | 1849 | C | O4'-C1' | 6.10 | 1.49 | 1.41 |
| 83 | DC | 94 | A | O4'-C1' | 6.10 | 1.49 | 1.41 |
| 18 | AP | 57 | LYS | C-N | 6.10 | 1.48 | 1.34 |
| 81 | DA | 2379 | U | O4'-C1' | 6.10 | 1.49 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 1621 | U | C2'-C1' | -6.09 | 1.46 | 1.53 |
| 83 | DC | 41 | G | C2'-C1' | -6.09 | 1.46 | 1.53 |
| 81 | DA | 2319 | U | O4'-C1' | -6.09 | 1.33 | 1.41 |
| 42 | BM | 32 | ARG | NE-CZ | 6.09 | 1.41 | 1.33 |
| 51 | BZ | 14 | TYR | CE1-CZ | 6.09 | 1.46 | 1.38 |
| 58 | Bg | 94 | GLU | C-N | 6.09 | 1.45 | 1.34 |
| 81 | DA | 2626 | A | P-O5' | -6.09 | 1.53 | 1.59 |
| 78 | CA | 899 | G | C4'-O4' | -6.09 | 1.37 | 1.45 |
| 81 | DA | 651 | G | C2'-C1' | -6.09 | 1.46 | 1.53 |
| 42 | BM | 41 | GLY | CA-C | -6.09 | 1.42 | 1.51 |
| 78 | CA | 1307 | U | O4'-C1' | 6.09 | 1.49 | 1.41 |
| 78 | CA | 1547 | A | O5'-C5' | 6.09 | 1.54 | 1.44 |
| 81 | DA | 539 | C | C2'-C1' | -6.09 | 1.46 | 1.53 |
| 81 | DA | 769 | G | O3'-P | -6.09 | 1.53 | 1.61 |
| 81 | DA | 330 | G | O4'-C1' | 6.08 | 1.49 | 1.41 |
| 81 | DA | 1641 | U | P-O5' | -6.08 | 1.53 | 1.59 |
| 81 | DA | 1902 | G | O4'-C1' | -6.08 | 1.33 | 1.41 |
| 82 | DB | 34 | U | O4'-C1' | 6.08 | 1.49 | 1.41 |
| 46 | BT | 167 | ARG | NE-CZ | 6.08 | 1.41 | 1.33 |
| 81 | DA | 2009 | C | C2'-C1' | -6.08 | 1.46 | 1.53 |
| 81 | DA | 3134 | A | C2'-C1' | -6.08 | 1.46 | 1.53 |
| 78 | CA | 101 | U | O4'-C1' | 6.08 | 1.49 | 1.41 |
| 81 | DA | 3024 | A | C2'-C1' | -6.08 | 1.46 | 1.53 |
| 81 | DA | 2765 | C | O4'-C1' | 6.08 | 1.49 | 1.41 |
| 31 | BB | 155 | LYS | N-CA | -6.08 | 1.34 | 1.46 |
| 42 | BM | 131 | SER | CA-CB | 6.08 | 1.62 | 1.52 |
| 52 | BY | 74 | TYR | N-CA | -6.08 | 1.34 | 1.46 |
| 81 | DA | 3318 | G | O4'-C1' | 6.08 | 1.49 | 1.41 |
| 55 | Bc | 48 | ARG | NE-CZ | 6.07 | 1.41 | 1.33 |
| 78 | CA | 21 | U | O4'-C1' | 6.07 | 1.49 | 1.41 |
| 78 | CA | 245 | U | P-O5' | -6.07 | 1.53 | 1.59 |
| 81 | DA | 3114 | A | C2'-C1' | -6.07 | 1.46 | 1.53 |
| 78 | CA | 173 | A | P-O5' | -6.07 | 1.53 | 1.59 |
| 78 | CA | 331 | A | C2'-C1' | -6.07 | 1.46 | 1.53 |
| 78 | CA | 1296 | A | C2'-C1' | -6.07 | 1.46 | 1.53 |
| 81 | DA | 463 | C | C2'-C1' | -6.07 | 1.46 | 1.53 |
| 78 | CA | 173 | A | O4'-C1' | -6.07 | 1.33 | 1.41 |
| 78 | CA | 296 | U | C3'-C2' | -6.07 | 1.46 | 1.52 |
| 81 | DA | 2717 | U | C2'-C1' | -6.07 | 1.46 | 1.53 |
| 78 | CA | 661 | A | O3'-P | -6.07 | 1.53 | 1.61 |
| 81 | DA | 988 | U | C4'-C3' | 6.07 | 1.59 | 1.53 |
| 81 | DA | 1106 | G | C2'-C1' | 6.07 | 1.60 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1344 | G | C2'-C1' | -6.07 | 1.46 | 1.53 |
| 1 | Aa | 10 | ARG | CZ-NH2 | 6.06 | 1.41 | 1.33 |
| 81 | DA | 2734 | A | O3'-P | -6.06 | 1.53 | 1.61 |
| 82 | DB | 42 | G | O4'-C1' | -6.06 | 1.33 | 1.41 |
| 2 | AA | 10 | THR | CA-CB | 6.06 | 1.69 | 1.53 |
| 78 | CA | 886 | U | C2'-C1' | 6.06 | 1.60 | 1.53 |
| 81 | DA | 3144 | G | C2'-C1' | -6.06 | 1.46 | 1.53 |
| 33 | BD | 261 | VAL | N-CA | 6.06 | 1.58 | 1.46 |
| 78 | CA | 325 | G | C2'-C1' | -6.06 | 1.46 | 1.53 |
| 53 | Ba | 74 | VAL | CA-CB | -6.06 | 1.42 | 1.54 |
| 1 | Aa | 155 | ARG | CD-NE | 6.05 | 1.56 | 1.46 |
| 78 | CA | 1451 | C | C2'-C1' | -6.05 | 1.46 | 1.53 |
| 78 | CA | 1525 | A | C5'-C4' | 6.05 | 1.58 | 1.51 |
| 81 | DA | 3368 | U | O4'-C1' | 6.05 | 1.49 | 1.41 |
| 41 | BN | 75 | GLY | C-N | 6.05 | 1.48 | 1.34 |
| 78 | CA | 1170 | G | O4'-C1' | 6.05 | 1.49 | 1.41 |
| 78 | CA | 1090 | C | C4'-O4' | -6.05 | 1.37 | 1.45 |
| 81 | DA | 776 | U | O3'-P | -6.05 | 1.53 | 1.61 |
| 53 | Ba | 9 | LYS | N-CA | -6.05 | 1.34 | 1.46 |
| 81 | DA | 313 | A | O4'-C1' | -6.05 | 1.33 | 1.41 |
| 81 | DA | 931 | C | C2'-C1' | -6.05 | 1.46 | 1.53 |
| 81 | DA | 1631 | C | C2'-C1' | -6.05 | 1.46 | 1.53 |
| 81 | DA | 2779 | A | C2'-C1' | -6.05 | 1.46 | 1.53 |
| 81 | DA | 3383 | G | O4'-C1' | -6.05 | 1.33 | 1.41 |
| 68 | Bq | 15 | ARG | CZ-NH1 | 6.05 | 1.41 | 1.33 |
| 83 | DC | 8 | G | O3'-P | -6.05 | 1.53 | 1.61 |
| 78 | CA | 1731 | A | C2'-C1' | -6.04 | 1.46 | 1.53 |
| 81 | DA | 3295 | A | P-OP2 | 6.04 | 1.59 | 1.49 |
| 79 | CB | 38 | C | C2'-C1' | -6.04 | 1.46 | 1.53 |
| 81 | DA | 3246 | G | O3'-P | -6.04 | 1.53 | 1.61 |
| 78 | CA | 818 | C | C5'-C4' | 6.04 | 1.58 | 1.51 |
| 81 | DA | 2373 | A | O4'-C1' | 6.04 | 1.49 | 1.41 |
| 5 | AC | 168 | ARG | C-O | -6.04 | 1.11 | 1.23 |
| 78 | CA | 1016 | C | O4'-C1' | 6.04 | 1.49 | 1.41 |
| 81 | DA | 835 | G | C2'-C1' | -6.03 | 1.46 | 1.53 |
| 81 | DA | 2672 | G | O4'-C1' | 6.03 | 1.49 | 1.41 |
| 81 | DA | 2860 | U | C2'-C1' | 6.03 | 1.59 | 1.53 |
| 2 | AA | 78 | SER | CA-CB | 6.03 | 1.61 | 1.52 |
| 78 | CA | 925 | G | C2'-C1' | -6.03 | 1.46 | 1.53 |
| 10 | AI | 119 | ALA | N-CA | 6.03 | 1.58 | 1.46 |
| 81 | DA | 922 | U | O4'-C1' | 6.03 | 1.49 | 1.41 |
| 81 | DA | 1484 | U | O4'-C1' | 6.03 | 1.49 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1573 | G | O4'-C1' | 6.03 | 1.49 | 1.41 |
| 2 | AA | 101 | ARG | NE-CZ | 6.02 | 1.40 | 1.33 |
| 81 | DA | 1474 | A | C2'-C1' | -6.02 | 1.46 | 1.53 |
| 78 | CA | 1018 | U | O4'-C1' | 6.02 | 1.49 | 1.41 |
| 78 | CA | 1189 | A | O4'-C1' | 6.02 | 1.49 | 1.41 |
| 78 | CA | 1173 | C | C2'-C1' | -6.02 | 1.46 | 1.53 |
| 78 | CA | 1463 | C | C2'-C1' | -6.02 | 1.46 | 1.53 |
| 78 | CA | 1588 | G | C2'-C1' | -6.02 | 1.46 | 1.53 |
| 78 | CA | 1676 | U | O3'-P | -6.02 | 1.53 | 1.61 |
| 81 | DA | 260 | C | C2'-C1' | -6.02 | 1.46 | 1.53 |
| 81 | DA | 2267 | C | C2'-C1' | -6.02 | 1.46 | 1.53 |
| 81 | DA | 2706 | G | O4'-C1' | 6.02 | 1.49 | 1.41 |
| 74 | BQ | 133 | GLU | CD-OE1 | 6.01 | 1.32 | 1.25 |
| 78 | CA | 1094 | G | C2'-C1' | -6.01 | 1.46 | 1.53 |
| 81 | DA | 41 | G | C2'-C1' | 6.01 | 1.59 | 1.53 |
| 81 | DA | 2462 | A | O3'-P | -6.01 | 1.53 | 1.61 |
| 8 | AF | 112 | ARG | CD-NE | 6.01 | 1.56 | 1.46 |
| 76 | BS | 84 | GLN | C-N | -6.01 | 1.20 | 1.34 |
| 81 | DA | 181 | U | O4'-C1' | 6.01 | 1.49 | 1.41 |
| 81 | DA | 2419 | A | C2'-C1' | -6.01 | 1.46 | 1.53 |
| 81 | DA | 3282 | U | C2'-C1' | -6.01 | 1.46 | 1.53 |
| 33 | BD | 69 | ARG | CZ-NH2 | 6.01 | 1.40 | 1.33 |
| 78 | CA | 663 | U | C2'-C1' | -6.01 | 1.46 | 1.53 |
| 81 | DA | 34 | A | C2'-C1' | -6.01 | 1.46 | 1.53 |
| 78 | CA | 941 | A | O4'-C1' | 6.00 | 1.49 | 1.41 |
| 81 | DA | 271 | C | O4'-C1' | 6.00 | 1.49 | 1.41 |
| 81 | DA | 2104 | A | C2'-C1' | -6.00 | 1.46 | 1.53 |
| 81 | DA | 3041 | U | O3'-P | -6.00 | 1.53 | 1.61 |
| 78 | CA | 542 | A | O3'-P | -6.00 | 1.53 | 1.61 |
| 81 | DA | 298 | U | C2'-C1' | -6.00 | 1.46 | 1.53 |
| 81 | DA | 2679 | A | O3'-P | -6.00 | 1.53 | 1.61 |
| 81 | DA | 2961 | G | O4'-C1' | 6.00 | 1.49 | 1.41 |
| 78 | CA | 931 | C | C2'-C1' | -6.00 | 1.46 | 1.53 |
| 78 | CA | 1550 | A | C3'-C2' | 6.00 | 1.59 | 1.52 |
| 81 | DA | 253 | A | C2'-C1' | 5.99 | 1.59 | 1.53 |
| 81 | DA | 1584 | U | C2'-C1' | -5.99 | 1.46 | 1.53 |
| 82 | DB | 14 | C | O4'-C1' | 5.99 | 1.49 | 1.41 |
| 20 | AS | 86 | ARG | CZ-NH2 | 5.99 | 1.40 | 1.33 |
| 32 | BC | 116 | ARG | NE-CZ | 5.99 | 1.40 | 1.33 |
| 81 | DA | 1818 | U | C2'-C1' | -5.99 | 1.46 | 1.53 |
| 3 | AB | 64 | ARG | CZ-NH2 | 5.99 | 1.40 | 1.33 |
| 47 | BU | 20 | ARG | NE-CZ | 5.99 | 1.40 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 1377 | U | O4'-C1' | 5.99 | 1.49 | 1.41 |
| 81 | DA | 2947 | G | C2'-C1' | -5.99 | 1.46 | 1.53 |
| 58 | Bg | 62 | ARG | CZ-NH2 | 5.99 | 1.40 | 1.33 |
| 83 | DC | 29 | C | C3'-O3' | 5.99 | 1.50 | 1.42 |
| 81 | DA | 638 | C | P-O5' | -5.98 | 1.53 | 1.59 |
| 36 | BF | 186 | PHE | CG-CD2 | 5.98 | 1.47 | 1.38 |
| 78 | CA | 1244 | A | O4'-C1' | 5.98 | 1.49 | 1.41 |
| 81 | DA | 3247 | G | C2'-C1' | -5.98 | 1.46 | 1.53 |
| 2 | AA | 127 | ARG | CZ-NH1 | 5.98 | 1.40 | 1.33 |
| 40 | BK | 85 | ARG | CZ-NH2 | 5.98 | 1.40 | 1.33 |
| 78 | CA | 908 | U | C2'-C1' | -5.98 | 1.46 | 1.53 |
| 81 | DA | 890 | C | C2'-C1' | -5.98 | 1.46 | 1.53 |
| 78 | CA | 1024 | U | O4'-C1' | 5.97 | 1.49 | 1.41 |
| 79 | CB | 14 | A | O4'-C1' | 5.97 | 1.49 | 1.41 |
| 81 | DA | 1037 | C | C2'-C1' | -5.97 | 1.46 | 1.53 |
| 78 | CA | 910 | C | O4'-C1' | 5.97 | 1.49 | 1.41 |
| 78 | CA | 1664 | C | C2'-C1' | -5.97 | 1.46 | 1.53 |
| 81 | DA | 173 | G | P-O5' | -5.97 | 1.53 | 1.59 |
| 81 | DA | 1274 | A | C2'-C1' | -5.97 | 1.46 | 1.53 |
| 42 | BM | 65 | GLY | N-CA | 5.97 | 1.55 | 1.46 |
| 78 | CA | 1261 | G | C4'-C3' | -5.97 | 1.46 | 1.52 |
| 81 | DA | 2506 | U | C3'-C2' | 5.97 | 1.59 | 1.52 |
| 81 | DA | 219 | A | C2'-C1' | -5.97 | 1.46 | 1.53 |
| 81 | DA | 1404 | G | C4'-C3' | 5.97 | 1.59 | 1.53 |
| 78 | CA | 642 | G | C4'-O4' | -5.97 | 1.37 | 1.45 |
| 78 | CA | 832 | U | O4'-C1' | 5.97 | 1.49 | 1.41 |
| 81 | DA | 608 | A | C5'-C4' | 5.97 | 1.58 | 1.51 |
| 81 | DA | 802 | C | C4'-C3' | -5.97 | 1.46 | 1.52 |
| 81 | DA | 2655 | U | O4'-C1' | 5.97 | 1.49 | 1.41 |
| 81 | DA | 1296 | C | C2'-C1' | -5.96 | 1.46 | 1.53 |
| 9 | AH | 66 | ASN | C-N | 5.96 | 1.43 | 1.33 |
| 13 | AL | 7 | ARG | CG-CD | 5.96 | 1.66 | 1.51 |
| 13 | AL | 58 | GLY | N-CA | -5.96 | 1.37 | 1.46 |
| 82 | DB | 103 | G | O3'-P | -5.96 | 1.53 | 1.61 |
| 4 | AD | 90 | ILE | CA-CB | 5.96 | 1.68 | 1.54 |
| 62 | Bk | 53 | TYR | CE1-CZ | 5.96 | 1.46 | 1.38 |
| 78 | CA | 1143 | A | O4'-C1' | 5.96 | 1.49 | 1.41 |
| 81 | DA | 2322 | C | O4'-C1' | 5.96 | 1.49 | 1.41 |
| 38 | Bs | 102 | SER | CA-CB | 5.96 | 1.61 | 1.52 |
| 81 | DA | 2002 | G | C2'-C1' | -5.96 | 1.46 | 1.53 |
| 81 | DA | 875 | G | O4'-C1' | 5.96 | 1.49 | 1.41 |
| 81 | DA | 1256 | G | O3'-P | -5.96 | 1.54 | 1.61 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 11 | AJ | 89 | ARG | CD-NE | 5.95 | 1.56 | 1.46 |
| 61 | Bj | 15 | SER | CA-CB | 5.95 | 1.61 | 1.52 |
| 81 | DA | 2618 | G | P-O5' | -5.95 | 1.53 | 1.59 |
| 39 | BJ | 75 | PRO | CA-CB | -5.95 | 1.41 | 1.53 |
| 78 | CA | 1764 | C | C2'-C1' | -5.95 | 1.46 | 1.53 |
| 81 | DA | 46 | U | O4'-C1' | 5.95 | 1.49 | 1.41 |
| 81 | DA | 778 | U | C5'-C4' | 5.95 | 1.58 | 1.51 |
| 81 | DA | 1384 | U | O4'-C1' | -5.95 | 1.33 | 1.41 |
| 11 | AJ | 57 | ARG | NE-CZ | 5.95 | 1.40 | 1.33 |
| 48 | BW | 6 | SER | N-CA | 5.95 | 1.58 | 1.46 |
| 81 | DA | 257 | U | O4'-C1' | 5.95 | 1.49 | 1.41 |
| 81 | DA | 1298 | C | P-O5' | -5.95 | 1.53 | 1.59 |
| 81 | DA | 2437 | G | P-O5' | -5.95 | 1.53 | 1.59 |
| 30 | BA | 129 | SER | CA-CB | 5.95 | 1.61 | 1.52 |
| 31 | BB | 54 | ARG | CZ-NH1 | 5.94 | 1.40 | 1.33 |
| 81 | DA | 1966 | U | O4'-C1' | 5.94 | 1.49 | 1.41 |
| 81 | DA | 2620 | G | O4'-C1' | -5.94 | 1.33 | 1.41 |
| 81 | DA | 388 | G | C2'-C1' | -5.94 | 1.46 | 1.53 |
| 81 | DA | 722 | G | C4'-C3' | 5.94 | 1.59 | 1.53 |
| 81 | DA | 1847 | A | O4'-C1' | -5.94 | 1.33 | 1.41 |
| 78 | CA | 1616 | G | O4'-C1' | 5.94 | 1.49 | 1.41 |
| 81 | DA | 1716 | U | O4'-C1' | 5.94 | 1.49 | 1.41 |
| 81 | DA | 2989 | U | C4'-C3' | -5.94 | 1.46 | 1.52 |
| 16 | AO | 90 | TYR | CE2-CZ | 5.94 | 1.46 | 1.38 |
| 18 | AP | 57 | LYS | N-CA | 5.94 | 1.58 | 1.46 |
| 34 | BE | 128 | TYR | CG-CD1 | 5.94 | 1.46 | 1.39 |
| 78 | CA | 329 | G | O4'-C1' | 5.93 | 1.49 | 1.41 |
| 81 | DA | 1189 | C | O4'-C1' | 5.93 | 1.49 | 1.41 |
| 81 | DA | 2349 | U | O4'-C1' | 5.93 | 1.49 | 1.41 |
| 81 | DA | 2878 | G | C2'-C1' | -5.93 | 1.46 | 1.53 |
| 4 | AD | 93 | ASP | C-N | 5.93 | 1.47 | 1.34 |
| 78 | CA | 944 | A | O4'-C1' | -5.93 | 1.33 | 1.41 |
| 78 | CA | 1665 | U | C2'-C1' | -5.93 | 1.46 | 1.53 |
| 81 | DA | 45 | A | P-O5' | -5.93 | 1.53 | 1.59 |
| 47 | BU | 141 | VAL | N-CA | 5.92 | 1.58 | 1.46 |
| 52 | BY | 13 | ARG | CZ-NH1 | 5.92 | 1.40 | 1.33 |
| 81 | DA | 2117 | A | O4'-C1' | 5.92 | 1.49 | 1.41 |
| 2 | AA | 35 | PRO | CA-C | -5.92 | 1.41 | 1.52 |
| 39 | BJ | 77 | ALA | N-CA | 5.92 | 1.58 | 1.46 |
| 59 | Bh | 27 | ARG | CD-NE | 5.92 | 1.56 | 1.46 |
| 78 | CA | 586 | G | C2'-C1' | -5.92 | 1.46 | 1.53 |
| 78 | CA | 1090 | C | C4'-C3' | -5.92 | 1.46 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 1138 | A | C2'-C1' | -5.92 | 1.46 | 1.53 |
| 78 | CA | 1312 | A | C2'-C1' | 5.92 | 1.59 | 1.53 |
| 78 | CA | 1392 | U | C4'-C3' | -5.92 | 1.46 | 1.52 |
| 81 | DA | 69 | C | O4'-C1' | 5.92 | 1.49 | 1.41 |
| 81 | DA | 1485 | G | C2'-C1' | -5.92 | 1.46 | 1.53 |
| 81 | DA | 3090 | U | C5'-C4' | 5.92 | 1.58 | 1.51 |
| 20 | AS | 60 | SER | CA-CB | 5.92 | 1.61 | 1.52 |
| 81 | DA | 1198 | C | O4'-C1' | 5.92 | 1.49 | 1.41 |
| 81 | DA | 1920 | U | C2'-C1' | -5.92 | 1.46 | 1.53 |
| 81 | DA | 2409 | G | C2'-C1' | -5.92 | 1.46 | 1.53 |
| 81 | DA | 765 | C | C4'-C3' | -5.92 | 1.46 | 1.52 |
| 5 | AC | 69 | ARG | CD-NE | 5.92 | 1.56 | 1.46 |
| 76 | BS | 70 | ASN | N-CA | 5.91 | 1.58 | 1.46 |
| 81 | DA | 504 | A | O4'-C1' | 5.91 | 1.49 | 1.41 |
| 81 | DA | 1497 | C | C2'-C1' | -5.91 | 1.46 | 1.53 |
| 81 | DA | 31 | C | C2'-C1' | -5.91 | 1.46 | 1.53 |
| 81 | DA | 1232 | C | C2'-C1' | 5.91 | 1.59 | 1.53 |
| 81 | DA | 1935 | G | C2'-C1' | -5.91 | 1.46 | 1.53 |
| 78 | CA | 1075 | C | C2'-C1' | -5.91 | 1.46 | 1.53 |
| 12 | AK | 111 | ARG | CD-NE | 5.91 | 1.56 | 1.46 |
| 22 | AV | 68 | ARG | CD-NE | 5.91 | 1.56 | 1.46 |
| 78 | CA | 275 | C | C2'-C1' | 5.91 | 1.59 | 1.53 |
| 81 | DA | 2762 | A | C2'-C1' | -5.91 | 1.46 | 1.53 |
| 47 | BU | 118 | GLU | CD-OE1 | 5.91 | 1.32 | 1.25 |
| 81 | DA | 1481 | A | O4'-C1' | 5.91 | 1.49 | 1.41 |
| 81 | DA | 203 | G | O4'-C1' | 5.90 | 1.49 | 1.41 |
| 81 | DA | 2900 | A | C2'-C1' | -5.90 | 1.46 | 1.53 |
| 81 | DA | 3047 | U | C2'-C1' | -5.90 | 1.46 | 1.53 |
| 44 | BO | 139 | ARG | NE-CZ | 5.90 | 1.40 | 1.33 |
| 78 | CA | 1689 | A | O4'-C1' | 5.90 | 1.49 | 1.41 |
| 82 | DB | 141 | C | C2'-C1' | -5.90 | 1.46 | 1.53 |
| 14 | AM | 145 | ARG | CZ-NH2 | 5.90 | 1.40 | 1.33 |
| 49 | BV | 20 | SER | CB-OG | 5.90 | 1.50 | 1.42 |
| 78 | CA | 1237 | G | C2'-C1' | -5.90 | 1.46 | 1.53 |
| 78 | CA | 1306 | C | O3'-P | 5.90 | 1.68 | 1.61 |
| 78 | CA | 1369 | U | O4'-C1' | 5.90 | 1.49 | 1.41 |
| 81 | DA | 596 | C | O3'-P | -5.90 | 1.54 | 1.61 |
| 19 | AR | 61 | ARG | CZ-NH1 | 5.90 | 1.40 | 1.33 |
| 78 | CA | 4 | C | O3'-P | -5.90 | 1.54 | 1.61 |
| 81 | DA | 653 | A | O4'-C1' | 5.90 | 1.49 | 1.41 |
| 81 | DA | 988 | U | P-O5' | -5.90 | 1.53 | 1.59 |
| 20 | AS | 95 | ASP | C-O | -5.89 | 1.12 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 33 | BD | 84 | ARG | C-N | 5.89 | 1.47 | 1.34 |
| 44 | BO | 29 | PRO | N-CD | -5.89 | 1.39 | 1.47 |
| 78 | CA | 288 | A | C3'-C2' | -5.89 | 1.46 | 1.52 |
| 81 | DA | 936 | A | O4'-C1' | 5.89 | 1.49 | 1.41 |
| 81 | DA | 2400 | G | O4'-C1' | 5.89 | 1.49 | 1.41 |
| 81 | DA | 2652 | U | O4'-C1' | 5.89 | 1.49 | 1.41 |
| 81 | DA | 3359 | A | C2'-C1' | -5.89 | 1.46 | 1.53 |
| 81 | DA | 700 | C | C5'-C4' | 5.89 | 1.58 | 1.51 |
| 81 | DA | 502 | U | C2'-C1' | 5.89 | 1.59 | 1.53 |
| 78 | CA | 326 | G | C5'-C4' | 5.89 | 1.58 | 1.51 |
| 81 | DA | 1921 | A | O4'-C1' | 5.89 | 1.49 | 1.41 |
| 78 | CA | 640 | U | O4'-C1' | 5.89 | 1.49 | 1.41 |
| 81 | DA | 356 | C | C2'-C1' | 5.89 | 1.59 | 1.53 |
| 81 | DA | 816 | A | C2'-C1' | -5.88 | 1.46 | 1.53 |
| 81 | DA | 2925 | C | O4'-C1' | 5.88 | 1.49 | 1.41 |
| 82 | DB | 88 | A | C2'-C1' | 5.88 | 1.59 | 1.53 |
| 33 | BD | 176 | SER | CA-CB | 5.88 | 1.61 | 1.52 |
| 81 | DA | 1870 | C | P-O5' | 5.88 | 1.65 | 1.59 |
| 81 | DA | 440 | A | O4'-C1' | 5.88 | 1.49 | 1.41 |
| 81 | DA | 862 | U | O4'-C1' | 5.88 | 1.49 | 1.41 |
| 81 | DA | 304 | G | O4'-C1' | -5.88 | 1.34 | 1.41 |
| 81 | DA | 796 | U | C2'-C1' | -5.88 | 1.46 | 1.53 |
| 31 | BB | 197 | PRO | N-CD | -5.88 | 1.39 | 1.47 |
| 81 | DA | 1368 | U | O4'-C1' | 5.88 | 1.49 | 1.41 |
| 51 | BZ | 70 | LYS | C-N | 5.87 | 1.47 | 1.34 |
| 78 | CA | 1306 | C | O4'-C1' | 5.87 | 1.49 | 1.41 |
| 81 | DA | 2665 | U | O4'-C1' | -5.87 | 1.34 | 1.41 |
| 81 | DA | 3290 | G | C2'-C1' | -5.87 | 1.46 | 1.53 |
| 17 | AQ | 89 | SER | CA-CB | 5.87 | 1.61 | 1.52 |
| 78 | CA | 873 | U | O4'-C1' | 5.87 | 1.49 | 1.41 |
| 78 | CA | 908 | U | O4'-C1' | 5.87 | 1.49 | 1.41 |
| 81 | DA | 2046 | U | C3'-O3' | -5.87 | 1.33 | 1.42 |
| 58 | Bg | 3 | GLY | N-CA | -5.87 | 1.37 | 1.46 |
| 61 | Bj | 18 | ARG | CZ-NH2 | 5.87 | 1.40 | 1.33 |
| 78 | CA | 1601 | G | P-O5' | -5.87 | 1.53 | 1.59 |
| 6 | AE | 168 | ARG | CD-NE | 5.87 | 1.56 | 1.46 |
| 18 | AP | 122 | ILE | N-CA | 5.87 | 1.58 | 1.46 |
| 81 | DA | 1122 | U | O4'-C1' | 5.87 | 1.49 | 1.41 |
| 81 | DA | 1380 | G | O4'-C1' | 5.87 | 1.49 | 1.41 |
| 81 | DA | 3051 | U | P-O5' | -5.86 | 1.53 | 1.59 |
| 78 | CA | 1340 | U | O3'-P | -5.86 | 1.54 | 1.61 |
| 81 | DA | 892 | U | C2'-C1' | -5.86 | 1.47 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 46 | BT | 151 | ARG | CD-NE | 5.86 | 1.56 | 1.46 |
| 81 | DA | 754 | G | C2'-C1' | -5.86 | 1.47 | 1.53 |
| 81 | DA | 1923 | C | C4'-C3' | -5.86 | 1.46 | 1.52 |
| 82 | DB | 98 | U | C4'-C3' | 5.86 | 1.59 | 1.53 |
| 66 | Bo | 36 | ARG | NE-CZ | 5.86 | 1.40 | 1.33 |
| 78 | CA | 164 | A | O3'-P | -5.86 | 1.54 | 1.61 |
| 81 | DA | 1655 | G | C2'-C1' | -5.86 | 1.47 | 1.53 |
| 46 | BT | 64 | ARG | NE-CZ | 5.86 | 1.40 | 1.33 |
| 12 | AK | 23 | PHE | N-CA | -5.85 | 1.34 | 1.46 |
| 35 | BG | 5 | LYS | C-N | 5.85 | 1.47 | 1.34 |
| 36 | BF | 173 | ARG | CZ-NH2 | 5.85 | 1.40 | 1.33 |
| 81 | DA | 107 | A | O4'-C1' | 5.85 | 1.49 | 1.41 |
| 14 | AM | 39 | GLY | CA-C | -5.85 | 1.42 | 1.51 |
| 39 | BJ | 75 | PRO | N-CA | 5.85 | 1.57 | 1.47 |
| 58 | Bg | 94 | GLU | N-CA | -5.85 | 1.34 | 1.46 |
| 78 | CA | 114 | C | O4'-C1' | 5.85 | 1.49 | 1.41 |
| 78 | CA | 1302 | U | C2'-C1' | 5.85 | 1.59 | 1.53 |
| 81 | DA | 689 | U | C2'-C1' | -5.85 | 1.47 | 1.53 |
| 81 | DA | 3235 | C | O4'-C1' | 5.85 | 1.49 | 1.41 |
| 6 | AE | 92 | ALA | C-N | 5.85 | 1.43 | 1.33 |
| 78 | CA | 1434 | U | P-O5' | -5.85 | 1.53 | 1.59 |
| 78 | CA | 1744 | A | O4'-C1' | 5.85 | 1.49 | 1.41 |
| 81 | DA | 2191 | U | O4'-C1' | 5.85 | 1.49 | 1.41 |
| 3 | AB | 78 | LYS | N-CA | 5.85 | 1.58 | 1.46 |
| 78 | CA | 1199 | G | O3'-P | -5.85 | 1.54 | 1.61 |
| 81 | DA | 1111 | U | C2'-C1' | -5.85 | 1.47 | 1.53 |
| 81 | DA | 3135 | U | O3'-P | -5.85 | 1.54 | 1.61 |
| 78 | CA | 1550 | A | C4'-O4' | -5.84 | 1.38 | 1.45 |
| 78 | CA | 1161 | C | C2'-C1' | -5.84 | 1.47 | 1.53 |
| 78 | CA | 588 | U | C4'-C3' | -5.84 | 1.46 | 1.52 |
| 78 | CA | 896 | U | O4'-C1' | 5.84 | 1.49 | 1.41 |
| 78 | CA | 1297 | G | C2'-C1' | 5.84 | 1.59 | 1.53 |
| 78 | CA | 59 | C | O4'-C1' | 5.84 | 1.49 | 1.41 |
| 78 | CA | 232 | U | C5'-C4' | 5.84 | 1.58 | 1.51 |
| 81 | DA | 3283 | U | O4'-C1' | 5.84 | 1.49 | 1.41 |
| 78 | CA | 1620 | C | C4'-C3' | -5.84 | 1.46 | 1.52 |
| 81 | DA | 2103 | U | C2'-C1' | -5.84 | 1.47 | 1.53 |
| 78 | CA | 1314 | U | O4'-C1' | 5.83 | 1.49 | 1.41 |
| 81 | DA | 982 | C | C5'-C4' | -5.83 | 1.44 | 1.51 |
| 63 | Bm | 87 | ARG | NE-CZ | 5.83 | 1.40 | 1.33 |
| 78 | CA | 150 | U | C4'-C3' | -5.83 | 1.46 | 1.52 |
| 78 | CA | 1053 | G | C2-N3 | 5.83 | 1.37 | 1.32 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 310 | U | C2'-C1' | -5.83 | 1.47 | 1.53 |
| 81 | DA | 2416 | U | C3'-O3' | -5.83 | 1.33 | 1.42 |
| 83 | DC | 81 | U | O4'-C1' | 5.83 | 1.49 | 1.41 |
| 18 | AP | 41 | GLY | CA-C | -5.83 | 1.42 | 1.51 |
| 33 | BD | 260 | GLN | CA-CB | 5.83 | 1.66 | 1.53 |
| 81 | DA | 1471 | U | C2'-C1' | -5.83 | 1.47 | 1.53 |
| 81 | DA | 1218 | U | O4'-C1' | 5.83 | 1.49 | 1.41 |
| 81 | DA | 1751 | G | C2'-C1' | -5.83 | 1.47 | 1.53 |
| 81 | DA | 2870 | C | O3'-P | -5.83 | 1.54 | 1.61 |
| 17 | AQ | 11 | ARG | CZ-NH1 | 5.83 | 1.40 | 1.33 |
| 78 | CA | 639 | U | O4'-C1' | 5.82 | 1.49 | 1.41 |
| 81 | DA | 17 | G | C2'-C1' | -5.82 | 1.47 | 1.53 |
| 81 | DA | 1369 | A | C2'-C1' | -5.82 | 1.47 | 1.53 |
| 81 | DA | 1584 | U | O3'-P | -5.82 | 1.54 | 1.61 |
| 74 | BQ | 123 | GLU | N-CA | -5.82 | 1.34 | 1.46 |
| 78 | CA | 379 | U | O4'-C1' | 5.82 | 1.49 | 1.41 |
| 78 | CA | 849 | C | C5'-C4' | 5.82 | 1.58 | 1.51 |
| 81 | DA | 2945 | G | C2'-C1' | -5.82 | 1.47 | 1.53 |
| 81 | DA | 3347 | A | C2'-C1' | -5.82 | 1.47 | 1.53 |
| 38 | Bs | 199 | SER | CA-CB | 5.82 | 1.61 | 1.52 |
| 69 | Br | 58 | PHE | CA-CB | -5.82 | 1.41 | 1.53 |
| 78 | CA | 390 | G | C2'-C1' | -5.82 | 1.47 | 1.53 |
| 81 | DA | 2344 | U | O4'-C1' | 5.82 | 1.49 | 1.41 |
| 53 | Ba | 75 | VAL | N-CA | -5.82 | 1.34 | 1.46 |
| 79 | CB | 21 | A | C2'-C1' | -5.82 | 1.47 | 1.53 |
| 81 | DA | 982 | C | C4'-C3' | 5.82 | 1.59 | 1.53 |
| 81 | DA | 992 | A | O4'-C1' | -5.82 | 1.34 | 1.41 |
| 81 | DA | 1129 | A | O4'-C1' | 5.82 | 1.49 | 1.41 |
| 65 | Bn | 34 | ALA | CA-CB | 5.82 | 1.64 | 1.52 |
| 78 | CA | 713 | A | P-O5' | -5.82 | 1.53 | 1.59 |
| 78 | CA | 1625 | C | C2'-C1' | -5.82 | 1.47 | 1.53 |
| 78 | CA | 1468 | U | C2'-C1' | -5.82 | 1.47 | 1.53 |
| 45 | BR | 13 | SER | N-CA | 5.81 | 1.57 | 1.46 |
| 49 | BV | 47 | TYR | CG-CD1 | 5.81 | 1.46 | 1.39 |
| 78 | CA | 1641 | C | O4'-C1' | 5.81 | 1.49 | 1.41 |
| 78 | CA | 1671 | A | O4'-C1' | 5.81 | 1.49 | 1.41 |
| 81 | DA | 283 | G | O4'-C1' | 5.81 | 1.49 | 1.41 |
| 78 | CA | 125 | U | C2'-C1' | -5.81 | 1.47 | 1.53 |
| 81 | DA | 52 | A | O4'-C1' | 5.81 | 1.49 | 1.41 |
| 81 | DA | 76 | G | C2'-C1' | 5.81 | 1.59 | 1.53 |
| 81 | DA | 1895 | A | O4'-C1' | -5.81 | 1.34 | 1.41 |
| 81 | DA | 2061 | G | O4'-C1' | -5.81 | 1.34 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 26 | AZ | 54 | ARG | CZ-NH2 | 5.81 | 1.40 | 1.33 |
| 41 | BN | 128 | ARG | NE-CZ | 5.81 | 1.40 | 1.33 |
| 49 | BV | 56 | ARG | NE-CZ | 5.81 | 1.40 | 1.33 |
| 81 | DA | 540 | U | O4'-C1' | 5.81 | 1.49 | 1.41 |
| 81 | DA | 2974 | U | O4'-C1' | 5.81 | 1.49 | 1.41 |
| 81 | DA | 378 | A | O4'-C1' | 5.81 | 1.49 | 1.41 |
| 78 | CA | 1260 | U | O4'-C1' | 5.81 | 1.49 | 1.41 |
| 81 | DA | 2200 | U | O4'-C1' | 5.81 | 1.49 | 1.41 |
| 81 | DA | 2477 | G | O4'-C1' | 5.81 | 1.49 | 1.41 |
| 16 | AO | 64 | ARG | N-CA | -5.80 | 1.34 | 1.46 |
| 78 | CA | 324 | U | O4'-C1' | 5.80 | 1.49 | 1.41 |
| 78 | CA | 560 | U | C4'-C3' | -5.80 | 1.46 | 1.52 |
| 81 | DA | 353 | G | C2'-C1' | 5.80 | 1.59 | 1.53 |
| 32 | BC | 334 | ARG | NE-CZ | 5.80 | 1.40 | 1.33 |
| 81 | DA | 453 | C | C2'-C1' | -5.80 | 1.47 | 1.53 |
| 78 | CA | 441 | A | O4'-C1' | 5.80 | 1.49 | 1.41 |
| 78 | CA | 1126 | G | O4'-C1' | 5.80 | 1.49 | 1.41 |
| 79 | CB | 23 | A | O4'-C1' | 5.80 | 1.49 | 1.41 |
| 81 | DA | 2771 | U | P-O5' | -5.80 | 1.53 | 1.59 |
| 53 | Ba | 8 | GLY | C-N | 5.80 | 1.47 | 1.34 |
| 81 | DA | 2507 | C | O3'-P | -5.80 | 1.54 | 1.61 |
| 82 | DB | 48 | A | O4'-C1' | 5.80 | 1.49 | 1.41 |
| 78 | CA | 642 | G | C3'-C2' | -5.80 | 1.46 | 1.52 |
| 22 | AV | 104 | ALA | CA-C | -5.80 | 1.37 | 1.52 |
| 39 | BJ | 97 | ASN | N-CA | -5.80 | 1.34 | 1.46 |
| 74 | BQ | 237 | GLU | C-N | 5.80 | 1.47 | 1.34 |
| 78 | CA | 600 | U | O4'-C1' | 5.80 | 1.49 | 1.41 |
| 78 | CA | 1468 | U | O4'-C1' | 5.80 | 1.49 | 1.41 |
| 81 | DA | 2374 | C | C2'-C1' | 5.80 | 1.59 | 1.53 |
| 81 | DA | 2919 | A | C2'-C1' | -5.80 | 1.47 | 1.53 |
| 81 | DA | 2923 | U | O4'-C1' | 5.80 | 1.49 | 1.41 |
| 81 | DA | 3385 | U | P-O5' | 5.80 | 1.65 | 1.59 |
| 35 | BG | 28 | GLN | N-CA | 5.79 | 1.57 | 1.46 |
| 78 | CA | 1136 | U | O4'-C1' | 5.79 | 1.49 | 1.41 |
| 82 | DB | 91 | C | O4'-C1' | 5.79 | 1.49 | 1.41 |
| 81 | DA | 231 | G | C2'-C1' | 5.79 | 1.59 | 1.53 |
| 81 | DA | 1435 | A | O4'-C1' | 5.79 | 1.49 | 1.41 |
| 40 | BK | 101 | ARG | CD-NE | 5.79 | 1.56 | 1.46 |
| 57 | Be | 234 | GLU | N-CA | -5.79 | 1.34 | 1.46 |
| 74 | BQ | 107 | ARG | CZ-NH2 | 5.79 | 1.40 | 1.33 |
| 78 | CA | 101 | U | C2'-C1' | -5.79 | 1.47 | 1.53 |
| 79 | CB | 50 | G | C2'-C1' | -5.79 | 1.47 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2960 | C | C2'-C1' | -5.79 | 1.47 | 1.53 |
| 82 | DB | 60 | U | C2'-C1' | 5.79 | 1.59 | 1.53 |
| 18 | AP | 115 | PHE | CB-CG | 5.79 | 1.61 | 1.51 |
| 78 | CA | 983 | A | C2'-C1' | -5.79 | 1.47 | 1.53 |
| 81 | DA | 898 | U | O4'-C1' | 5.79 | 1.49 | 1.41 |
| 82 | DB | 26 | U | O4'-C1' | 5.79 | 1.49 | 1.41 |
| 83 | DC | 56 | G | C2'-C1' | -5.79 | 1.47 | 1.53 |
| 65 | Bn | 77 | ARG | NE-CZ | 5.78 | 1.40 | 1.33 |
| 81 | DA | 2320 | A | C2'-C1' | -5.78 | 1.47 | 1.53 |
| 81 | DA | 3036 | G | P-O5' | -5.78 | 1.53 | 1.59 |
| 81 | DA | 2521 | U | O3'-P | -5.78 | 1.54 | 1.61 |
| 81 | DA | 2789 | U | O4'-C1' | 5.78 | 1.49 | 1.41 |
| 81 | DA | 2360 | C | O4'-C1' | 5.78 | 1.49 | 1.41 |
| 30 | BA | 26 | ARG | NE-CZ | 5.78 | 1.40 | 1.33 |
| 78 | CA | 1551 | U | C4'-C3' | -5.78 | 1.46 | 1.52 |
| 81 | DA | 225 | C | O4'-C1' | 5.78 | 1.49 | 1.41 |
| 5 | AC | 82 | ARG | NE-CZ | 5.78 | 1.40 | 1.33 |
| 81 | DA | 756 | U | O3'-P | -5.78 | 1.54 | 1.61 |
| 81 | DA | 2045 | G | O4'-C1' | 5.78 | 1.49 | 1.41 |
| 63 | Bm | 23 | ARG | NE-CZ | 5.77 | 1.40 | 1.33 |
| 65 | Bn | 16 | ARG | CZ-NH1 | 5.77 | 1.40 | 1.33 |
| 78 | CA | 1337 | A | C4'-O4' | 5.77 | 1.53 | 1.45 |
| 81 | DA | 2902 | A | O4'-C1' | 5.77 | 1.49 | 1.41 |
| 83 | DC | 90 | C | O4'-C1' | 5.77 | 1.49 | 1.41 |
| 17 | AQ | 26 | LEU | C-N | 5.77 | 1.47 | 1.34 |
| 81 | DA | 2357 | A | C2'-C1' | -5.77 | 1.47 | 1.53 |
| 46 | BT | 9 | ARG | CZ-NH1 | 5.77 | 1.40 | 1.33 |
| 78 | CA | 1453 | G | P-O5' | -5.77 | 1.53 | 1.59 |
| 78 | CA | 1755 | A | C2'-C1' | 5.77 | 1.59 | 1.53 |
| 81 | DA | 1270 | A | C2'-C1' | 5.77 | 1.59 | 1.53 |
| 81 | DA | 3362 | A | C2'-C1' | -5.77 | 1.47 | 1.53 |
| 81 | DA | 745 | C | P-O5' | -5.77 | 1.53 | 1.59 |
| 81 | DA | 315 | C | O4'-C1' | 5.76 | 1.49 | 1.41 |
| 81 | DA | 2981 | U | C2'-C1' | -5.76 | 1.47 | 1.53 |
| 81 | DA | 3356 | G | C2'-C1' | -5.76 | 1.47 | 1.53 |
| 81 | DA | 3199 | G | C4'-C3' | 5.76 | 1.59 | 1.53 |
| 78 | CA | 1555 | A | O4'-C1' | 5.76 | 1.49 | 1.41 |
| 81 | DA | 174 | C | C2'-C1' | -5.76 | 1.47 | 1.53 |
| 81 | DA | 199 | A | O4'-C1' | -5.76 | 1.34 | 1.41 |
| 81 | DA | 2607 | G | O3'-P | -5.76 | 1.54 | 1.61 |
| 10 | AI | 136 | SER | CA-CB | 5.76 | 1.61 | 1.52 |
| 43 | BP | 144 | ARG | CZ-NH1 | 5.76 | 1.40 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 175 | C | C2'-C1' | -5.76 | 1.47 | 1.53 |
| 81 | DA | 1387 | G | O4'-C1' | 5.76 | 1.49 | 1.41 |
| 81 | DA | 2453 | U | O4'-C1' | 5.76 | 1.49 | 1.41 |
| 81 | DA | 2814 | G | C2'-C1' | -5.76 | 1.47 | 1.53 |
| 43 | BP | 137 | PRO | CA-C | -5.76 | 1.41 | 1.52 |
| 2 | AA | 62 | ARG | CD-NE | 5.76 | 1.56 | 1.46 |
| 81 | DA | 22 | G | C2'-C1' | -5.76 | 1.47 | 1.53 |
| 81 | DA | 401 | U | C2'-C1' | 5.76 | 1.59 | 1.53 |
| 78 | CA | 474 | A | C2'-C1' | -5.75 | 1.47 | 1.53 |
| 81 | DA | 2868 | U | O4'-C1' | 5.75 | 1.49 | 1.41 |
| 4 | AD | 221 | ARG | NE-CZ | 5.75 | 1.40 | 1.33 |
| 13 | AL | 38 | PHE | C-N | 5.75 | 1.47 | 1.34 |
| 78 | CA | 1167 | G | O4'-C1' | -5.75 | 1.34 | 1.41 |
| 78 | CA | 1309 | C | C4'-O4' | -5.75 | 1.38 | 1.45 |
| 81 | DA | 1498 | A | O4'-C1' | 5.75 | 1.49 | 1.41 |
| 81 | DA | 2739 | A | O4'-C1' | 5.75 | 1.49 | 1.41 |
| 32 | BC | 370 | PHE | C-N | 5.75 | 1.47 | 1.34 |
| 81 | DA | 1976 | G | C2'-C1' | -5.75 | 1.47 | 1.53 |
| 78 | CA | 1598 | U | C4'-C3' | -5.75 | 1.46 | 1.52 |
| 19 | AR | 114 | HIS | CB-CG | 5.75 | 1.60 | 1.50 |
| 78 | CA | 870 | C | O4'-C1' | 5.75 | 1.49 | 1.41 |
| 81 | DA | 2519 | A | O3'-P | -5.75 | 1.54 | 1.61 |
| 81 | DA | 2529 | A | C5'-C4' | 5.75 | 1.58 | 1.51 |
| 78 | CA | 936 | G | C4'-O4' | -5.75 | 1.38 | 1.45 |
| 81 | DA | 351 | A | O4'-C1' | 5.75 | 1.49 | 1.41 |
| 78 | CA | 585 | A | C4'-O4' | -5.75 | 1.38 | 1.45 |
| 81 | DA | 1535 | A | O3'-P | -5.75 | 1.54 | 1.61 |
| 6 | AE | 175 | GLY | CA-C | -5.74 | 1.42 | 1.51 |
| 81 | DA | 724 | U | C4'-O4' | 5.74 | 1.53 | 1.45 |
| 83 | DC | 33 | U | C2'-C1' | -5.74 | 1.47 | 1.53 |
| 47 | BU | 102 | ARG | CD-NE | 5.74 | 1.56 | 1.46 |
| 81 | DA | 469 | G | C2'-C1' | -5.74 | 1.47 | 1.53 |
| 40 | BK | 135 | TYR | CE2-CZ | 5.74 | 1.46 | 1.38 |
| 81 | DA | 583 | G | O4'-C1' | -5.74 | 1.34 | 1.41 |
| 81 | DA | 2780 | A | O4'-C1' | 5.74 | 1.49 | 1.41 |
| 81 | DA | 1689 | U | C2'-C1' | 5.74 | 1.59 | 1.53 |
| 81 | DA | 1803 | C | C2'-C1' | -5.74 | 1.47 | 1.53 |
| 82 | DB | 127 | U | C2'-C1' | -5.74 | 1.47 | 1.53 |
| 78 | CA | 1393 | C | O3'-P | 5.73 | 1.68 | 1.61 |
| 78 | CA | 1740 | A | O4'-C1' | 5.73 | 1.49 | 1.41 |
| 81 | DA | 1990 | U | C2'-C1' | -5.73 | 1.47 | 1.53 |
| 33 | BD | 349 | THR | CA-CB | -5.73 | 1.38 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 79 | CB | 22 | G | O4'-C1' | 5.73 | 1.49 | 1.41 |
| 81 | DA | 2938 | G | O4'-C1' | 5.73 | 1.49 | 1.41 |
| 39 | BJ | 90 | ARG | CD-NE | 5.73 | 1.56 | 1.46 |
| 76 | BS | 74 | ILE | N-CA | -5.73 | 1.34 | 1.46 |
| 78 | CA | 1641 | C | C2'-C1' | -5.73 | 1.47 | 1.53 |
| 81 | DA | 161 | G | C3'-C2' | -5.73 | 1.46 | 1.52 |
| 81 | DA | 726 | G | O4'-C1' | 5.73 | 1.49 | 1.41 |
| 81 | DA | 2102 | U | O4'-C1' | 5.73 | 1.49 | 1.41 |
| 81 | DA | 2859 | U | O4'-C1' | -5.73 | 1.34 | 1.41 |
| 32 | BC | 37 | ARG | CZ-NH1 | 5.73 | 1.40 | 1.33 |
| 78 | CA | 1598 | U | C4'-O4' | -5.73 | 1.38 | 1.45 |
| 81 | DA | 1755 | C | O3'-P | -5.73 | 1.54 | 1.61 |
| 9 | AH | 71 | LYS | N-CA | -5.73 | 1.34 | 1.46 |
| 32 | BC | 65 | SER | CA-CB | 5.73 | 1.61 | 1.52 |
| 57 | Be | 132 | PRO | N-CA | -5.73 | 1.37 | 1.47 |
| 54 | Bd | 40 | ARG | CZ-NH2 | 5.72 | 1.40 | 1.33 |
| 78 | CA | 1653 | C | C2'-C1' | -5.72 | 1.47 | 1.53 |
| 81 | DA | 231 | G | C3'-O3' | 5.72 | 1.50 | 1.42 |
| 81 | DA | 1527 | C | P-O5' | -5.72 | 1.54 | 1.59 |
| 12 | AK | 20 | TYR | CG-CD1 | 5.72 | 1.46 | 1.39 |
| 43 | BP | 180 | PHE | N-CA | 5.72 | 1.57 | 1.46 |
| 48 | BW | 7 | ARG | NE-CZ | 5.72 | 1.40 | 1.33 |
| 81 | DA | 455 | C | C2'-C1' | -5.72 | 1.47 | 1.53 |
| 78 | CA | 193 | U | C2'-C1' | -5.72 | 1.47 | 1.53 |
| 78 | CA | 650 | U | C4'-O4' | -5.72 | 1.38 | 1.45 |
| 81 | DA | 746 | A | C2'-C1' | -5.72 | 1.47 | 1.53 |
| 81 | DA | 672 | A | C4'-O4' | 5.72 | 1.52 | 1.45 |
| 81 | DA | 1219 | C | O4'-C1' | 5.72 | 1.49 | 1.41 |
| 11 | AJ | 81 | THR | N-CA | -5.72 | 1.34 | 1.46 |
| 81 | DA | 1114 | U | C3'-C2' | 5.72 | 1.59 | 1.52 |
| 19 | AR | 77 | ARG | NE-CZ | 5.71 | 1.40 | 1.33 |
| 21 | AT | 13 | VAL | CB-CG2 | 5.71 | 1.64 | 1.52 |
| 81 | DA | 166 | C | P-OP2 | 5.71 | 1.58 | 1.49 |
| 81 | DA | 1680 | G | O3'-P | -5.71 | 1.54 | 1.61 |
| 81 | DA | 2824 | G | O4'-C1' | -5.71 | 1.34 | 1.41 |
| 5 | AC | 16 | LYS | CA-CB | 5.71 | 1.66 | 1.53 |
| 65 | Bn | 52 | TYR | CG-CD1 | 5.71 | 1.46 | 1.39 |
| 81 | DA | 1179 | A | O4'-C1' | -5.71 | 1.34 | 1.41 |
| 54 | Bd | 40 | ARG | CD-NE | 5.71 | 1.56 | 1.46 |
| 78 | CA | 701 | U | C4'-C3' | -5.71 | 1.46 | 1.52 |
| 81 | DA | 588 | G | O4'-C1' | -5.71 | 1.34 | 1.41 |
| 81 | DA | 2096 | A | O4'-C1' | 5.71 | 1.49 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2655 | U | C2'-C1' | -5.71 | 1.47 | 1.53 |
| 53 | Ba | 57 | HIS | CA-C | -5.71 | 1.38 | 1.52 |
| 78 | CA | 1394 | G | C4'-C3' | -5.71 | 1.46 | 1.52 |
| 78 | CA | 987 | G | O4'-C1' | 5.71 | 1.49 | 1.41 |
| 81 | DA | 25 | U | P-O5' | -5.71 | 1.54 | 1.59 |
| 81 | DA | 1632 | A | O4'-C1' | 5.71 | 1.49 | 1.41 |
| 5 | AC | 162 | SER | C-N | 5.71 | 1.45 | 1.34 |
| 81 | DA | 1446 | A | O3'-P | -5.71 | 1.54 | 1.61 |
| 81 | DA | 2646 | C | C4'-C3' | -5.71 | 1.46 | 1.52 |
| 33 | BD | 124 | SER | CA-CB | 5.71 | 1.61 | 1.52 |
| 45 | BR | 158 | HIS | N-CA | 5.71 | 1.57 | 1.46 |
| 81 | DA | 1269 | U | C2'-C1' | -5.71 | 1.47 | 1.53 |
| 81 | DA | 3047 | U | C4'-O4' | 5.70 | 1.52 | 1.45 |
| 74 | BQ | 197 | SER | N-CA | 5.70 | 1.57 | 1.46 |
| 78 | CA | 1573 | A | C3'-C2' | -5.70 | 1.46 | 1.52 |
| 78 | CA | 1794 | A | O4'-C1' | 5.70 | 1.49 | 1.41 |
| 78 | CA | 1100 | G | C4'-C3' | 5.70 | 1.59 | 1.53 |
| 81 | DA | 1164 | G | O4'-C1' | 5.70 | 1.49 | 1.41 |
| 11 | AJ | 102 | ARG | NE-CZ | 5.70 | 1.40 | 1.33 |
| 78 | CA | 1570 | A | O3'-P | -5.70 | 1.54 | 1.61 |
| 43 | BP | 29 | GLU | CG-CD | 5.70 | 1.60 | 1.51 |
| 81 | DA | 3353 | G | O4'-C1' | 5.69 | 1.49 | 1.41 |
| 32 | BC | 368 | GLY | C-N | 5.69 | 1.47 | 1.34 |
| 81 | DA | 1532 | C | C2'-C1' | -5.69 | 1.47 | 1.53 |
| 81 | DA | 2843 | U | O4'-C1' | 5.69 | 1.49 | 1.41 |
| 38 | Bs | 104 | ARG | NE-CZ | 5.69 | 1.40 | 1.33 |
| 78 | CA | 1477 | G | P-O5' | -5.69 | 1.54 | 1.59 |
| 24 | AX | 31 | TYR | CE1-CZ | 5.69 | 1.46 | 1.38 |
| 78 | CA | 320 | U | C2'-C1' | -5.69 | 1.47 | 1.53 |
| 78 | CA | 719 | U | C4'-C3' | -5.69 | 1.46 | 1.52 |
| 78 | CA | 1568 | C | C2'-C1' | 5.69 | 1.59 | 1.53 |
| 49 | BV | 69 | ARG | CZ-NH2 | 5.68 | 1.40 | 1.33 |
| 81 | DA | 482 | C | C2'-C1' | -5.68 | 1.47 | 1.53 |
| 81 | DA | 1378 | U | O3'-P | -5.68 | 1.54 | 1.61 |
| 81 | DA | 1768 | U | N3-C4 | 5.68 | 1.43 | 1.38 |
| 31 | BB | 38 | HIS | CB-CG | 5.68 | 1.60 | 1.50 |
| 78 | CA | 662 | U | C2'-C1' | -5.68 | 1.47 | 1.53 |
| 81 | DA | 809 | G | C2'-C1' | -5.68 | 1.47 | 1.53 |
| 81 | DA | 1596 | C | O4'-C1' | 5.68 | 1.49 | 1.41 |
| 78 | CA | 1451 | C | O4'-C1' | 5.68 | 1.49 | 1.41 |
| 6 | AE | 141 | ARG | CD-NE | 5.68 | 1.56 | 1.46 |
| 78 | CA | 1286 | U | C2'-C1' | -5.68 | 1.47 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 52 | BY | 51 | ARG | NE-CZ | 5.68 | 1.40 | 1.33 |
| 74 | BQ | 128 | GLU | C-N | 5.68 | 1.47 | 1.34 |
| 78 | CA | 376 | C | O4'-C1' | 5.68 | 1.49 | 1.41 |
| 81 | DA | 1284 | C | O4'-C1' | 5.68 | 1.49 | 1.41 |
| 62 | Bk | 64 | SER | CA-CB | 5.68 | 1.61 | 1.52 |
| 78 | CA | 633 | U | C2'-C1' | -5.68 | 1.47 | 1.53 |
| 83 | DC | 2 | G | P-O5' | -5.68 | 1.54 | 1.59 |
| 78 | CA | 1175 | U | C2'-C1' | -5.67 | 1.47 | 1.53 |
| 81 | DA | 380 | U | O4'-C1' | 5.67 | 1.49 | 1.41 |
| 31 | BB | 184 | ARG | CZ-NH1 | 5.67 | 1.40 | 1.33 |
| 78 | CA | 1411 | A | C2'-C1' | -5.67 | 1.47 | 1.53 |
| 81 | DA | 1666 | G | C2'-C1' | -5.67 | 1.47 | 1.53 |
| 32 | BC | 277 | SER | CA-CB | 5.67 | 1.61 | 1.52 |
| 78 | CA | 178 | U | C3'-O3' | -5.67 | 1.34 | 1.42 |
| 81 | DA | 1156 | C | O4'-C1' | 5.67 | 1.49 | 1.41 |
| 81 | DA | 2005 | G | C2'-C1' | -5.67 | 1.47 | 1.53 |
| 81 | DA | 2664 | C | C4'-C3' | 5.67 | 1.59 | 1.53 |
| 78 | CA | 1537 | C | O4'-C1' | 5.67 | 1.49 | 1.41 |
| 81 | DA | 181 | U | C2'-C1' | -5.67 | 1.47 | 1.53 |
| 81 | DA | 3041 | U | O4'-C1' | 5.67 | 1.49 | 1.41 |
| 41 | BN | 12 | TRP | CD2-CE2 | -5.67 | 1.34 | 1.41 |
| 57 | Be | 30 | ARG | CD-NE | 5.67 | 1.56 | 1.46 |
| 78 | CA | 385 | A | O4'-C1' | 5.67 | 1.49 | 1.41 |
| 78 | CA | 654 | C | O4'-C1' | 5.67 | 1.49 | 1.41 |
| 81 | DA | 2071 | A | O4'-C1' | 5.67 | 1.49 | 1.41 |
| 78 | CA | 1111 | G | O4'-C1' | 5.67 | 1.49 | 1.41 |
| 81 | DA | 774 | G | C5'-C4' | 5.67 | 1.58 | 1.51 |
| 81 | DA | 1941 | C | C2'-C1' | -5.67 | 1.47 | 1.53 |
| 81 | DA | 2723 | U | C3'-O3' | 5.67 | 1.50 | 1.42 |
| 42 | BM | 48 | ARG | CD-NE | 5.66 | 1.56 | 1.46 |
| 81 | DA | 636 | C | C4'-O4' | 5.66 | 1.52 | 1.45 |
| 2 | AA | 11 | PRO | C-N | 5.66 | 1.47 | 1.34 |
| 38 | Bs | 5 | ARG | C-N | 5.66 | 1.47 | 1.34 |
| 81 | DA | 1576 | G | C5'-C4' | 5.66 | 1.58 | 1.51 |
| 21 | AT | 87 | ARG | CZ-NH2 | 5.66 | 1.40 | 1.33 |
| 44 | BO | 62 | HIS | C-N | -5.66 | 1.21 | 1.34 |
| 74 | BQ | 123 | GLU | C-N | 5.66 | 1.47 | 1.34 |
| 81 | DA | 854 | G | C2'-C1' | -5.66 | 1.47 | 1.53 |
| 81 | DA | 2379 | U | C2'-C1' | -5.66 | 1.47 | 1.53 |
| 83 | DC | 47 | C | O5'-C5' | -5.66 | 1.33 | 1.42 |
| 8 | AF | 76 | ARG | CD-NE | 5.65 | 1.56 | 1.46 |
| 46 | BT | 176 | ARG | CD-NE | 5.65 | 1.56 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 47 | BU | 102 | ARG | CZ-NH1 | 5.65 | 1.40 | 1.33 |
| 81 | DA | 873 | C | C2'-C1' | -5.65 | 1.47 | 1.53 |
| 81 | DA | 1134 | G | O4'-C1' | -5.65 | 1.34 | 1.41 |
| 78 | CA | 959 | U | O3'-P | -5.65 | 1.54 | 1.61 |
| 78 | CA | 1241 | G | C4'-C3' | -5.65 | 1.46 | 1.52 |
| 81 | DA | 341 | G | O4'-C1' | 5.65 | 1.49 | 1.41 |
| 36 | BF | 46 | THR | C-N | 5.65 | 1.47 | 1.34 |
| 20 | AS | 91 | TYR | N-CA | 5.65 | 1.57 | 1.46 |
| 81 | DA | 1135 | A | O4'-C1' | 5.65 | 1.49 | 1.41 |
| 81 | DA | 3389 | U | C5'-C4' | 5.65 | 1.58 | 1.51 |
| 81 | DA | 100 | A | O4'-C1' | 5.65 | 1.49 | 1.41 |
| 83 | DC | 70 | A | C2'-C1' | -5.65 | 1.47 | 1.53 |
| 8 | AF | 148 | ARG | CD-NE | 5.65 | 1.56 | 1.46 |
| 31 | BB | 245 | LEU | C-O | -5.65 | 1.12 | 1.23 |
| 78 | CA | 1130 | G | C4'-C3' | -5.65 | 1.47 | 1.52 |
| 12 | AK | 107 | ARG | CD-NE | 5.64 | 1.56 | 1.46 |
| 78 | CA | 1394 | G | O3'-P | 5.64 | 1.68 | 1.61 |
| 81 | DA | 2883 | U | O4'-C1' | 5.64 | 1.49 | 1.41 |
| 81 | DA | 3107 | U | O4'-C1' | 5.64 | 1.49 | 1.41 |
| 78 | CA | 179 | A | C4'-O4' | 5.64 | 1.52 | 1.45 |
| 78 | CA | 587 | C | O4'-C1' | 5.64 | 1.49 | 1.41 |
| 78 | CA | 840 | U | C5'-C4' | 5.64 | 1.58 | 1.51 |
| 81 | DA | 910 | G | O4'-C1' | 5.64 | 1.49 | 1.41 |
| 81 | DA | 2673 | A | C2'-C1' | -5.64 | 1.47 | 1.53 |
| 78 | CA | 1558 | U | O4'-C1' | -5.64 | 1.34 | 1.41 |
| 78 | CA | 180 | A | O4'-C1' | 5.64 | 1.49 | 1.41 |
| 78 | CA | 1318 | G | C2'-C1' | -5.64 | 1.47 | 1.53 |
| 81 | DA | 637 | C | C3'-C2' | -5.64 | 1.46 | 1.52 |
| 81 | DA | 1263 | A | O4'-C1' | 5.64 | 1.49 | 1.41 |
| 81 | DA | 1678 | G | C4'-C3' | 5.64 | 1.59 | 1.53 |
| 81 | DA | 1742 | U | C2'-C1' | -5.64 | 1.47 | 1.53 |
| 81 | DA | 2689 | A | O3'-P | -5.64 | 1.54 | 1.61 |
| 78 | CA | 1085 | G | C2'-C1' | -5.64 | 1.47 | 1.53 |
| 78 | CA | 1113 | A | C2'-C1' | 5.64 | 1.59 | 1.53 |
| 81 | DA | 1006 | A | C4'-C3' | -5.64 | 1.47 | 1.52 |
| 81 | DA | 1077 | U | P-O5' | -5.64 | 1.54 | 1.59 |
| 69 | Br | 34 | SER | CA-CB | 5.63 | 1.61 | 1.52 |
| 81 | DA | 468 | G | O4'-C1' | 5.63 | 1.49 | 1.41 |
| 81 | DA | 549 | U | O4'-C1' | 5.63 | 1.49 | 1.41 |
| 81 | DA | 3313 | U | O4'-C1' | 5.63 | 1.49 | 1.41 |
| 6 | AE | 17 | ARG | NE-CZ | 5.63 | 1.40 | 1.33 |
| 78 | CA | 642 | G | C2'-C1' | 5.63 | 1.59 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 1005 | A | C4'-C3' | -5.63 | 1.47 | 1.52 |
| 78 | CA | 1195 | C | C2'-C1' | -5.63 | 1.47 | 1.53 |
| 81 | DA | 9 | U | O3'-P | -5.63 | 1.54 | 1.61 |
| 81 | DA | 2760 | C | O3'-P | -5.63 | 1.54 | 1.61 |
| 32 | BC | 297 | SER | C-N | 5.63 | 1.47 | 1.34 |
| 81 | DA | 1122 | U | C2'-C1' | -5.63 | 1.47 | 1.53 |
| 1 | Aa | 311 | ARG | CZ-NH2 | 5.63 | 1.40 | 1.33 |
| 47 | BU | 126 | VAL | CA-CB | 5.63 | 1.66 | 1.54 |
| 76 | BS | 89 | TYR | CE1-CZ | 5.63 | 1.45 | 1.38 |
| 78 | CA | 1025 | A | O4'-C1' | 5.63 | 1.49 | 1.41 |
| 81 | DA | 878 | G | O4'-C1' | 5.63 | 1.49 | 1.41 |
| 81 | DA | 1204 | A | O3'-P | -5.63 | 1.54 | 1.61 |
| 81 | DA | 1220 | U | O4'-C1' | 5.63 | 1.49 | 1.41 |
| 81 | DA | 1610 | G | O4'-C1' | 5.62 | 1.49 | 1.41 |
| 78 | CA | 563 | U | C4'-C3' | -5.62 | 1.47 | 1.52 |
| 81 | DA | 169 | U | O3'-P | -5.62 | 1.54 | 1.61 |
| 78 | CA | 384 | G | O4'-C1' | 5.62 | 1.49 | 1.41 |
| 81 | DA | 1067 | U | C2'-C1' | -5.62 | 1.47 | 1.53 |
| 81 | DA | 2413 | A | O4'-C1' | 5.62 | 1.49 | 1.41 |
| 78 | CA | 164 | A | C3'-C2' | -5.62 | 1.46 | 1.52 |
| 78 | CA | 1718 | G | C2'-C1' | -5.62 | 1.47 | 1.53 |
| 81 | DA | 2405 | C | O4'-C1' | 5.62 | 1.49 | 1.41 |
| 81 | DA | 2928 | C | O4'-C1' | 5.62 | 1.49 | 1.41 |
| 1 | Aa | 54 | PHE | N-CA | -5.62 | 1.35 | 1.46 |
| 3 | AB | 90 | ARG | CZ-NH1 | 5.62 | 1.40 | 1.33 |
| 81 | DA | 665 | A | O3'-P | -5.62 | 1.54 | 1.61 |
| 78 | CA | 238 | U | C3'-O3' | 5.61 | 1.50 | 1.42 |
| 81 | DA | 784 | A | C2'-C1' | 5.61 | 1.59 | 1.53 |
| 81 | DA | 2432 | A | C2'-C1' | -5.61 | 1.47 | 1.53 |
| 81 | DA | 2810 | C | O4'-C1' | 5.61 | 1.49 | 1.41 |
| 10 | AI | 54 | LEU | C-N | 5.61 | 1.47 | 1.34 |
| 32 | BC | 242 | THR | N-CA | -5.61 | 1.35 | 1.46 |
| 33 | BD | 324 | LEU | N-CA | 5.61 | 1.57 | 1.46 |
| 78 | CA | 1567 | U | C2'-C1' | -5.61 | 1.47 | 1.53 |
| 78 | CA | 1768 | G | O4'-C1' | 5.61 | 1.49 | 1.41 |
| 81 | DA | 222 | A | O4'-C1' | 5.61 | 1.49 | 1.41 |
| 81 | DA | 1919 | G | O4'-C1' | 5.61 | 1.49 | 1.41 |
| 4 | AD | 148 | ARG | CZ-NH2 | 5.61 | 1.40 | 1.33 |
| 81 | DA | 1832 | C | O3'-P | -5.61 | 1.54 | 1.61 |
| 81 | DA | 2682 | C | P-O5' | -5.61 | 1.54 | 1.59 |
| 81 | DA | 2899 | C | O3'-P | -5.61 | 1.54 | 1.61 |
| 81 | DA | 413 | U | C2'-C1' | -5.60 | 1.47 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2879 | C | C2'-C1' | -5.60 | 1.47 | 1.53 |
| 81 | DA | 695 | C | C2'-C1' | -5.60 | 1.47 | 1.53 |
| 81 | DA | 1296 | C | O3'-P | -5.60 | 1.54 | 1.61 |
| 78 | CA | 1271 | G | C2'-C1' | -5.60 | 1.47 | 1.53 |
| 81 | DA | 518 | G | O3'-P | -5.60 | 1.54 | 1.61 |
| 83 | DC | 93 | U | O4'-C1' | 5.60 | 1.49 | 1.41 |
| 65 | Bn | 39 | ARG | NE-CZ | 5.60 | 1.40 | 1.33 |
| 81 | DA | 434 | U | O4'-C1' | 5.60 | 1.49 | 1.41 |
| 81 | DA | 1329 | U | C2'-C1' | -5.60 | 1.47 | 1.53 |
| 81 | DA | 2006 | G | O4'-C1' | 5.60 | 1.49 | 1.41 |
| 52 | BY | 5 | SER | CA-CB | 5.59 | 1.61 | 1.52 |
| 78 | CA | 884 | A | C4'-C3' | -5.59 | 1.47 | 1.52 |
| 81 | DA | 2753 | G | C2'-C1' | -5.59 | 1.47 | 1.53 |
| 83 | DC | 107 | G | P-O5' | -5.59 | 1.54 | 1.59 |
| 34 | BE | 152 | HIS | CB-CG | 5.59 | 1.60 | 1.50 |
| 78 | CA | 525 | A | C4'-C3' | -5.59 | 1.47 | 1.52 |
| 81 | DA | 704 | U | C4'-C3' | -5.59 | 1.47 | 1.52 |
| 33 | BD | 31 | ARG | CZ-NH2 | 5.59 | 1.40 | 1.33 |
| 74 | BQ | 130 | GLU | CA-CB | 5.59 | 1.66 | 1.53 |
| 78 | CA | 1268 | G | C2'-C1' | -5.59 | 1.47 | 1.53 |
| 81 | DA | 1403 | C | O3'-P | -5.59 | 1.54 | 1.61 |
| 82 | DB | 145 | U | C2'-C1' | -5.59 | 1.47 | 1.53 |
| 78 | CA | 1404 | C | O4'-C1' | 5.59 | 1.49 | 1.41 |
| 10 | AI | 84 | ALA | CA-CB | 5.58 | 1.64 | 1.52 |
| 53 | Ba | 53 | VAL | CB-CG2 | 5.58 | 1.64 | 1.52 |
| 57 | Be | 224 | ILE | CA-CB | -5.58 | 1.42 | 1.54 |
| 78 | CA | 773 | C | O3'-P | -5.58 | 1.54 | 1.61 |
| 81 | DA | 2505 | U | C4'-C3' | -5.58 | 1.47 | 1.52 |
| 40 | BK | 37 | ARG | NE-CZ | 5.58 | 1.40 | 1.33 |
| 78 | CA | 660 | G | O4'-C1' | 5.58 | 1.49 | 1.41 |
| 78 | CA | 1366 | U | O4'-C1' | 5.58 | 1.49 | 1.41 |
| 81 | DA | 972 | A | C5'-C4' | 5.58 | 1.58 | 1.51 |
| 79 | CB | 39 | G | C2'-C1' | -5.58 | 1.47 | 1.53 |
| 81 | DA | 2018 | C | C2'-C1' | -5.58 | 1.47 | 1.53 |
| 81 | DA | 2718 | U | O4'-C1' | 5.58 | 1.49 | 1.41 |
| 81 | DA | 3023 | U | O4'-C1' | 5.58 | 1.49 | 1.41 |
| 3 | AB | 78 | LYS | C-N | 5.58 | 1.46 | 1.34 |
| 14 | AM | 77 | THR | C-N | 5.58 | 1.46 | 1.34 |
| 81 | DA | 3013 | U | O4'-C1' | 5.58 | 1.48 | 1.41 |
| 45 | BR | 140 | LEU | C-N | 5.57 | 1.46 | 1.34 |
| 78 | CA | 714 | G | P-O5' | -5.57 | 1.54 | 1.59 |
| 78 | CA | 1310 | U | O4'-C1' | 5.57 | 1.48 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 24 | G | C2'-C1' | 5.57 | 1.59 | 1.53 |
| 81 | DA | 842 | G | O4'-C1' | 5.57 | 1.48 | 1.41 |
| 78 | CA | 1036 | A | O4'-C1' | 5.57 | 1.48 | 1.41 |
| 81 | DA | 2389 | C | P-O5' | -5.57 | 1.54 | 1.59 |
| 81 | DA | 3112 | G | C2'-C1' | 5.57 | 1.59 | 1.53 |
| 74 | BQ | 50 | ARG | NE-CZ | 5.57 | 1.40 | 1.33 |
| 81 | DA | 585 | A | O4'-C1' | 5.57 | 1.48 | 1.41 |
| 81 | DA | 2159 | U | C2'-C1' | 5.57 | 1.59 | 1.53 |
| 78 | CA | 120 | U | C4'-C3' | 5.57 | 1.59 | 1.53 |
| 78 | CA | 590 | C | O4'-C1' | 5.57 | 1.48 | 1.41 |
| 78 | CA | 1269 | U | O4'-C1' | 5.57 | 1.48 | 1.41 |
| 81 | DA | 2704 | A | C2'-O2' | -5.57 | 1.34 | 1.41 |
| 78 | CA | 233 | C | O5'-C5' | -5.57 | 1.33 | 1.42 |
| 78 | CA | 1208 | A | C2'-C1' | -5.57 | 1.47 | 1.53 |
| 3 | AB | 215 | GLU | N-CA | 5.57 | 1.57 | 1.46 |
| 78 | CA | 143 | G | O4'-C1' | 5.57 | 1.48 | 1.41 |
| 81 | DA | 1791 | C | C3'-O3' | -5.57 | 1.34 | 1.42 |
| 78 | CA | 1459 | C | C4'-C3' | 5.56 | 1.59 | 1.53 |
| 78 | CA | 303 | U | O3'-P | -5.56 | 1.54 | 1.61 |
| 18 | AP | 93 | TYR | CG-CD2 | 5.56 | 1.46 | 1.39 |
| 33 | BD | 260 | GLN | C-N | 5.56 | 1.46 | 1.34 |
| 81 | DA | 3104 | U | C2'-C1' | 5.56 | 1.59 | 1.53 |
| 3 | AB | 206 | VAL | N-CA | 5.56 | 1.57 | 1.46 |
| 81 | DA | 2759 | U | O4'-C1' | 5.56 | 1.48 | 1.41 |
| 81 | DA | 1795 | U | C4'-O4' | -5.55 | 1.38 | 1.45 |
| 81 | DA | 3290 | G | O4'-C1' | 5.55 | 1.48 | 1.41 |
| 14 | AM | 16 | ARG | CZ-NH2 | 5.55 | 1.40 | 1.33 |
| 81 | DA | 234 | G | C3'-O3' | 5.55 | 1.50 | 1.42 |
| 81 | DA | 2303 | A | P-O5' | -5.55 | 1.54 | 1.59 |
| 52 | BY | 75 | ARG | NE-CZ | 5.55 | 1.40 | 1.33 |
| 78 | CA | 1160 | A | O4'-C1' | 5.55 | 1.48 | 1.41 |
| 81 | DA | 1491 | A | C2'-C1' | -5.55 | 1.47 | 1.53 |
| 81 | DA | 1793 | C | O3'-P | -5.55 | 1.54 | 1.61 |
| 83 | DC | 9 | C | C2'-C1' | -5.55 | 1.47 | 1.53 |
| 31 | BB | 34 | TYR | CE2-CZ | 5.55 | 1.45 | 1.38 |
| 81 | DA | 896 | A | C2'-C1' | 5.55 | 1.59 | 1.53 |
| 81 | DA | 1339 | C | P-O5' | -5.55 | 1.54 | 1.59 |
| 78 | CA | 1045 | C | C2'-C1' | -5.55 | 1.47 | 1.53 |
| 81 | DA | 2232 | A | O4'-C1' | 5.55 | 1.48 | 1.41 |
| 78 | CA | 223 | U | O4'-C1' | -5.55 | 1.34 | 1.41 |
| 81 | DA | 3217 | C | O4'-C1' | -5.55 | 1.34 | 1.41 |
| 83 | DC | 57 | C | C2'-C1' | 5.55 | 1.59 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 8 | AF | 69 | PHE | CE2-CZ | 5.54 | 1.47 | 1.37 |
| 63 | Bm | 66 | GLY | C-N | 5.54 | 1.43 | 1.33 |
| 78 | CA | 1293 | U | C2'-C1' | -5.54 | 1.47 | 1.53 |
| 81 | DA | 525 | C | O4'-C1' | 5.54 | 1.48 | 1.41 |
| 81 | DA | 1046 | A | C2'-C1' | 5.54 | 1.59 | 1.53 |
| 78 | CA | 465 | G | C2'-C1' | -5.54 | 1.47 | 1.53 |
| 78 | CA | 664 | U | O4'-C1' | 5.54 | 1.48 | 1.41 |
| 81 | DA | 185 | C | P-O5' | 5.54 | 1.65 | 1.59 |
| 81 | DA | 963 | G | C2'-C1' | -5.54 | 1.47 | 1.53 |
| 81 | DA | 1252 | A | C2'-C1' | -5.54 | 1.47 | 1.53 |
| 81 | DA | 2245 | C | O3'-P | -5.54 | 1.54 | 1.61 |
| 81 | DA | 2626 | A | C4'-C3' | 5.54 | 1.59 | 1.53 |
| 81 | DA | 857 | G | O3'-P | -5.54 | 1.54 | 1.61 |
| 37 | BH | 210 | ALA | N-CA | -5.54 | 1.35 | 1.46 |
| 81 | DA | 1152 | G | C2'-C1' | -5.54 | 1.47 | 1.53 |
| 81 | DA | 1705 | U | O4'-C1' | 5.54 | 1.48 | 1.41 |
| 32 | BC | 18 | PRO | CA-CB | -5.53 | 1.42 | 1.53 |
| 34 | BE | 52 | TYR | CG-CD1 | 5.53 | 1.46 | 1.39 |
| 47 | BU | 141 | VAL | C-O | -5.53 | 1.12 | 1.23 |
| 78 | CA | 1224 | A | C2'-O2' | 5.53 | 1.48 | 1.41 |
| 78 | CA | 996 | U | C2'-C1' | 5.53 | 1.59 | 1.53 |
| 81 | DA | 2980 | U | O4'-C1' | 5.53 | 1.48 | 1.41 |
| 62 | Bk | 78 | GLY | CA-C | -5.53 | 1.43 | 1.51 |
| 81 | DA | 991 | G | C2'-C1' | -5.53 | 1.47 | 1.53 |
| 78 | CA | 217 | A | C5'-C4' | 5.53 | 1.57 | 1.51 |
| 78 | CA | 226 | A | C4'-O4' | 5.53 | 1.52 | 1.45 |
| 78 | CA | 879 | G | C2'-C1' | 5.53 | 1.59 | 1.53 |
| 58 | Bg | 79 | ARG | CD-NE | 5.53 | 1.55 | 1.46 |
| 62 | Bk | 82 | ARG | N-CA | 5.53 | 1.57 | 1.46 |
| 78 | CA | 1184 | A | C2'-C1' | 5.53 | 1.59 | 1.53 |
| 81 | DA | 3356 | G | O4'-C1' | -5.53 | 1.34 | 1.41 |
| 82 | DB | 92 | A | O4'-C1' | 5.53 | 1.48 | 1.41 |
| 2 | AA | 209 | GLU | CB-CG | 5.53 | 1.62 | 1.52 |
| 78 | CA | 47 | A | O4'-C1' | 5.52 | 1.48 | 1.41 |
| 81 | DA | 214 | G | C2'-C1' | 5.52 | 1.59 | 1.53 |
| 78 | CA | 1246 | C | O4'-C1' | 5.52 | 1.48 | 1.41 |
| 81 | DA | 1602 | A | C2'-C1' | -5.52 | 1.47 | 1.53 |
| 81 | DA | 2119 | A | O4'-C1' | 5.52 | 1.48 | 1.41 |
| 81 | DA | 2783 | U | O3'-P | -5.52 | 1.54 | 1.61 |
| 81 | DA | 2953 | U | O4'-C1' | 5.52 | 1.48 | 1.41 |
| 82 | DB | 9 | A | O4'-C1' | 5.52 | 1.48 | 1.41 |
| 81 | DA | 273 | A | O4'-C1' | 5.52 | 1.48 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 952 | A | O4'-C1' | 5.52 | 1.48 | 1.41 |
| 81 | DA | 1293 | U | C2'-C1' | -5.52 | 1.47 | 1.53 |
| 81 | DA | 303 | G | C2'-C1' | -5.52 | 1.47 | 1.53 |
| 81 | DA | 914 | A | C3'-C2' | -5.52 | 1.46 | 1.52 |
| 81 | DA | 1458 | U | C2'-C1' | -5.52 | 1.47 | 1.53 |
| 78 | CA | 250 | C | C4'-C3' | 5.52 | 1.59 | 1.53 |
| 81 | DA | 2334 | U | O4'-C1' | -5.52 | 1.34 | 1.41 |
| 78 | CA | 837 | G | C3'-C2' | 5.51 | 1.59 | 1.52 |
| 78 | CA | 1047 | G | O4'-C1' | 5.51 | 1.48 | 1.41 |
| 81 | DA | 1387 | G | C2'-C1' | -5.51 | 1.47 | 1.53 |
| 81 | DA | 1417 | G | O4'-C1' | -5.51 | 1.34 | 1.41 |
| 81 | DA | 826 | G | C2'-C1' | -5.51 | 1.47 | 1.53 |
| 78 | CA | 1136 | U | C2'-C1' | 5.51 | 1.59 | 1.53 |
| 81 | DA | 764 | U | C5'-C4' | 5.51 | 1.57 | 1.51 |
| 42 | BM | 50 | PRO | N-CD | -5.51 | 1.40 | 1.47 |
| 76 | BS | 41 | SER | CA-CB | 5.51 | 1.61 | 1.52 |
| 78 | CA | 152 | U | C2'-C1' | 5.51 | 1.59 | 1.53 |
| 78 | CA | 1590 | G | C2'-C1' | -5.51 | 1.47 | 1.53 |
| 81 | DA | 933 | A | O3'-P | -5.51 | 1.54 | 1.61 |
| 81 | DA | 1823 | A | O3'-P | -5.51 | 1.54 | 1.61 |
| 81 | DA | 7 | C | O3'-P | -5.50 | 1.54 | 1.61 |
| 37 | BH | 135 | GLY | N-CA | -5.50 | 1.37 | 1.46 |
| 46 | BT | 82 | LYS | C-N | 5.50 | 1.43 | 1.33 |
| 81 | DA | 2757 | U | C2'-C1' | -5.50 | 1.47 | 1.53 |
| 81 | DA | 3393 | U | O4'-C1' | 5.50 | 1.48 | 1.41 |
| 78 | CA | 162 | A | C2'-C1' | -5.50 | 1.47 | 1.53 |
| 78 | CA | 252 | U | O3'-P | -5.50 | 1.54 | 1.61 |
| 81 | DA | 979 | U | C4'-C3' | 5.50 | 1.59 | 1.53 |
| 81 | DA | 1973 | G | C5'-C4' | 5.50 | 1.57 | 1.51 |
| 35 | BG | 113 | LYS | N-CA | -5.50 | 1.35 | 1.46 |
| 81 | DA | 802 | C | P-OP1 | -5.50 | 1.39 | 1.49 |
| 81 | DA | 1338 | C | C2'-C1' | 5.50 | 1.59 | 1.53 |
| 81 | DA | 1656 | A | C2'-C1' | -5.50 | 1.47 | 1.53 |
| 78 | CA | 1580 | C | P-O5' | -5.50 | 1.54 | 1.59 |
| 81 | DA | 1703 | U | C2'-C1' | 5.50 | 1.59 | 1.53 |
| 17 | AQ | 82 | ASP | C-N | 5.50 | 1.46 | 1.34 |
| 18 | AP | 99 | ARG | NE-CZ | 5.50 | 1.40 | 1.33 |
| 78 | CA | 231 | U | C2'-C1' | 5.50 | 1.59 | 1.53 |
| 81 | DA | 2777 | G | O4'-C1' | 5.50 | 1.48 | 1.41 |
| 17 | AQ | 19 | ARG | NE-CZ | 5.49 | 1.40 | 1.33 |
| 81 | DA | 897 | U | O4'-C1' | 5.49 | 1.48 | 1.41 |
| 81 | DA | 1546 | A | O4'-C1' | 5.49 | 1.48 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2071 | A | C3'-C2' | 5.49 | 1.58 | 1.52 |
| 82 | DB | 58 | G | O4'-C1' | -5.49 | 1.34 | 1.41 |
| 78 | CA | 1080 | U | C3'-O3' | -5.49 | 1.34 | 1.42 |
| 83 | DC | 106 | G | O3'-P | -5.49 | 1.54 | 1.61 |
| 40 | BK | 135 | TYR | CB-CG | 5.49 | 1.59 | 1.51 |
| 78 | CA | 821 | U | C5'-C4' | 5.49 | 1.57 | 1.51 |
| 81 | DA | 359 | U | O4'-C1' | 5.49 | 1.48 | 1.41 |
| 81 | DA | 2129 | U | O4'-C1' | 5.49 | 1.48 | 1.41 |
| 62 | Bk | 84 | LYS | N-CA | 5.49 | 1.57 | 1.46 |
| 6 | AE | 222 | TYR | CE1-CZ | 5.49 | 1.45 | 1.38 |
| 35 | BG | 31 | ARG | NE-CZ | 5.49 | 1.40 | 1.33 |
| 74 | BQ | 3 | PHE | CB-CG | 5.49 | 1.60 | 1.51 |
| 79 | CB | 11 | U | C2'-C1' | 5.49 | 1.59 | 1.53 |
| 81 | DA | 210 | U | O3'-P | -5.48 | 1.54 | 1.61 |
| 50 | BX | 103 | TYR | CB-CG | -5.48 | 1.43 | 1.51 |
| 78 | CA | 9 | U | O4'-C1' | 5.48 | 1.48 | 1.41 |
| 78 | CA | 1716 | C | C2'-C1' | -5.48 | 1.47 | 1.53 |
| 81 | DA | 1865 | A | O4'-C1' | 5.48 | 1.48 | 1.41 |
| 81 | DA | 1939 | G | O4'-C1' | 5.48 | 1.48 | 1.41 |
| 81 | DA | 234 | G | C2'-C1' | -5.48 | 1.47 | 1.53 |
| 81 | DA | 712 | G | O4'-C1' | 5.48 | 1.48 | 1.41 |
| 81 | DA | 2215 | A | O4'-C1' | 5.48 | 1.48 | 1.41 |
| 81 | DA | 602 | A | C2'-C1' | -5.48 | 1.47 | 1.53 |
| 81 | DA | 2633 | U | P-O5' | -5.48 | 1.54 | 1.59 |
| 83 | DC | 50 | U | C2'-C1' | -5.48 | 1.47 | 1.53 |
| 66 | Bo | 30 | ARG | CD-NE | 5.48 | 1.55 | 1.46 |
| 81 | DA | 704 | U | C3'-C2' | -5.48 | 1.46 | 1.52 |
| 81 | DA | 3313 | U | C3'-C2' | -5.48 | 1.46 | 1.52 |
| 46 | BT | 38 | ARG | NE-CZ | 5.47 | 1.40 | 1.33 |
| 78 | CA | 1081 | A | C3'-C2' | -5.47 | 1.46 | 1.52 |
| 78 | CA | 1317 | C | O4'-C1' | 5.47 | 1.48 | 1.41 |
| 81 | DA | 1101 | G | O3'-P | -5.47 | 1.54 | 1.61 |
| 81 | DA | 1532 | C | O4'-C1' | 5.47 | 1.48 | 1.41 |
| 78 | CA | 1779 | U | C2'-C1' | -5.47 | 1.47 | 1.53 |
| 81 | DA | 2962 | U | C2'-C1' | -5.47 | 1.47 | 1.53 |
| 20 | AS | 57 | ARG | CD-NE | 5.47 | 1.55 | 1.46 |
| 60 | Bi | 55 | SER | C-N | 5.47 | 1.46 | 1.34 |
| 81 | DA | 2369 | G | O3'-P | -5.47 | 1.54 | 1.61 |
| 78 | CA | 1506 | G | C2'-C1' | -5.47 | 1.47 | 1.53 |
| 81 | DA | 146 | U | C3'-O3' | 5.47 | 1.49 | 1.42 |
| 81 | DA | 155 | G | O3'-P | -5.47 | 1.54 | 1.61 |
| 81 | DA | 1471 | U | O4'-C1' | 5.47 | 1.48 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1607 | U | O4'-C1' | 5.47 | 1.48 | 1.41 |
| 81 | DA | 1750 | A | O4'-C1' | 5.47 | 1.48 | 1.41 |
| 78 | CA | 26 | A | C2'-C1' | 5.47 | 1.59 | 1.53 |
| 82 | DB | 57 | C | O4'-C1' | 5.47 | 1.48 | 1.41 |
| 66 | Bo | 8 | ARG | CZ-NH1 | 5.47 | 1.40 | 1.33 |
| 78 | CA | 1403 | C | C2'-C1' | -5.47 | 1.47 | 1.53 |
| 81 | DA | 171 | G | C5'-C4' | 5.47 | 1.57 | 1.51 |
| 17 | AQ | 71 | PHE | CA-CB | 5.46 | 1.66 | 1.53 |
| 35 | BG | 98 | VAL | C-N | 5.46 | 1.46 | 1.34 |
| 40 | BK | 185 | ALA | CA-CB | 5.46 | 1.64 | 1.52 |
| 81 | DA | 247 | C | O3'-P | -5.46 | 1.54 | 1.61 |
| 81 | DA | 1212 | A | C2'-C1' | -5.46 | 1.47 | 1.53 |
| 81 | DA | 2026 | A | O4'-C1' | 5.46 | 1.48 | 1.41 |
| 42 | BM | 78 | VAL | CA-CB | -5.46 | 1.43 | 1.54 |
| 65 | Bn | 17 | ARG | NE-CZ | 5.46 | 1.40 | 1.33 |
| 78 | CA | 737 | A | C4'-C3' | -5.46 | 1.47 | 1.52 |
| 78 | CA | 1550 | A | O3'-P | -5.46 | 1.54 | 1.61 |
| 81 | DA | 748 | U | C2'-C1' | 5.46 | 1.59 | 1.53 |
| 46 | BT | 151 | ARG | CZ-NH2 | 5.46 | 1.40 | 1.33 |
| 78 | CA | 405 | C | C2'-C1' | -5.46 | 1.47 | 1.53 |
| 78 | CA | 90 | C | O4'-C1' | 5.45 | 1.48 | 1.41 |
| 78 | CA | 1591 | C | C2'-C1' | -5.45 | 1.47 | 1.53 |
| 81 | DA | 1114 | U | O4'-C1' | -5.45 | 1.34 | 1.41 |
| 33 | BD | 321 | LYS | N-CA | -5.45 | 1.35 | 1.46 |
| 76 | BS | 162 | THR | N-CA | -5.45 | 1.35 | 1.46 |
| 81 | DA | 172 | G | C5'-C4' | 5.45 | 1.57 | 1.51 |
| 78 | CA | 1270 | G | O4'-C1' | 5.45 | 1.48 | 1.41 |
| 81 | DA | 3252 | G | O3'-P | -5.45 | 1.54 | 1.61 |
| 5 | AC | 9 | SER | CB-OG | -5.45 | 1.35 | 1.42 |
| 81 | DA | 549 | U | C2'-C1' | -5.45 | 1.47 | 1.53 |
| 44 | BO | 96 | LYS | C-N | -5.45 | 1.21 | 1.34 |
| 33 | BD | 31 | ARG | CD-NE | 5.45 | 1.55 | 1.46 |
| 78 | CA | 1096 | C | C4'-C3' | -5.45 | 1.47 | 1.52 |
| 81 | DA | 6 | A | O4'-C1' | 5.45 | 1.48 | 1.41 |
| 81 | DA | 2527 | G | P-O5' | -5.45 | 1.54 | 1.59 |
| 47 | BU | 137 | GLU | CD-OE1 | -5.44 | 1.19 | 1.25 |
| 81 | DA | 915 | A | C2'-C1' | -5.44 | 1.47 | 1.53 |
| 76 | BS | 151 | PHE | CG-CD2 | 5.44 | 1.47 | 1.38 |
| 78 | CA | 713 | A | O3'-P | -5.44 | 1.54 | 1.61 |
| 32 | BC | 18 | PRO | N-CA | 5.44 | 1.56 | 1.47 |
| 40 | BK | 94 | ARG | NE-CZ | 5.44 | 1.40 | 1.33 |
| 43 | BP | 162 | ARG | CZ-NH1 | 5.44 | 1.40 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 46 | BT | 62 | ARG | CZ-NH1 | 5.44 | 1.40 | 1.33 |
| 58 | Bg | 70 | ARG | CD-NE | 5.44 | 1.55 | 1.46 |
| 62 | Bk | 68 | ARG | CZ-NH1 | 5.44 | 1.40 | 1.33 |
| 78 | CA | 293 | U | O4'-C1' | 5.44 | 1.48 | 1.41 |
| 81 | DA | 160 | G | C4'-O4' | 5.44 | 1.52 | 1.45 |
| 21 | AT | 12 | TYR | CE2-CZ | 5.44 | 1.45 | 1.38 |
| 17 | AQ | 64 | GLY | CA-C | -5.44 | 1.43 | 1.51 |
| 32 | BC | 257 | PRO | N-CD | -5.44 | 1.40 | 1.47 |
| 47 | BU | 159 | PHE | CG-CD1 | 5.44 | 1.47 | 1.38 |
| 81 | DA | 1770 | G | O3'-P | -5.44 | 1.54 | 1.61 |
| 82 | DB | 27 | U | O4'-C1' | 5.44 | 1.48 | 1.41 |
| 81 | DA | 211 | A | O4'-C1' | 5.44 | 1.48 | 1.41 |
| 38 | Bs | 243 | TYR | CB-CG | -5.43 | 1.43 | 1.51 |
| 78 | CA | 1520 | U | C4'-C3' | -5.43 | 1.47 | 1.52 |
| 79 | CB | 27 | G | O4'-C1' | 5.43 | 1.48 | 1.41 |
| 56 | Bf | 59 | TYR | CG-CD1 | 5.43 | 1.46 | 1.39 |
| 81 | DA | 911 | C | O4'-C1' | 5.43 | 1.48 | 1.41 |
| 8 | AF | 102 | ARG | CZ-NH1 | 5.43 | 1.40 | 1.33 |
| 64 | Bl | 55 | ARG | CZ-NH2 | 5.43 | 1.40 | 1.33 |
| 81 | DA | 2421 | U | C2'-C1' | -5.43 | 1.47 | 1.53 |
| 42 | BM | 16 | GLY | CA-C | -5.43 | 1.43 | 1.51 |
| 76 | BS | 86 | ARG | CZ-NH2 | 5.43 | 1.40 | 1.33 |
| 78 | CA | 638 | U | O4'-C1' | 5.43 | 1.48 | 1.41 |
| 78 | CA | 1285 | U | O4'-C1' | 5.43 | 1.48 | 1.41 |
| 81 | DA | 985 | U | C2'-C1' | 5.43 | 1.59 | 1.53 |
| 82 | DB | 150 | G | O3'-P | -5.43 | 1.54 | 1.61 |
| 78 | CA | 586 | G | C4'-O4' | -5.43 | 1.38 | 1.45 |
| 39 | BJ | 114 | ARG | CZ-NH2 | 5.43 | 1.40 | 1.33 |
| 43 | BP | 71 | ARG | CZ-NH1 | 5.43 | 1.40 | 1.33 |
| 81 | DA | 886 | C | C2'-C1' | -5.43 | 1.47 | 1.53 |
| 81 | DA | 1463 | U | C2'-C1' | -5.43 | 1.47 | 1.53 |
| 81 | DA | 2116 | G | O4'-C1' | -5.43 | 1.34 | 1.41 |
| 51 | BZ | 48 | ARG | NE-CZ | 5.42 | 1.40 | 1.33 |
| 78 | CA | 824 | G | C2'-C1' | -5.42 | 1.47 | 1.53 |
| 78 | CA | 1049 | U | O4'-C1' | 5.42 | 1.48 | 1.41 |
| 81 | DA | 245 | U | C4'-O4' | 5.42 | 1.52 | 1.45 |
| 6 | AE | 224 | PHE | CB-CG | 5.42 | 1.60 | 1.51 |
| 78 | CA | 1566 | U | C4'-C3' | -5.42 | 1.47 | 1.52 |
| 81 | DA | 236 | G | C2'-C1' | 5.42 | 1.59 | 1.53 |
| 81 | DA | 2842 | U | O4'-C1' | 5.42 | 1.48 | 1.41 |
| 81 | DA | 3059 | G | C2'-C1' | -5.42 | 1.47 | 1.53 |
| 3 | AB | 40 | ARG | CZ-NH2 | 5.42 | 1.40 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 1546 | G | O4'-C1' | 5.42 | 1.48 | 1.41 |
| 81 | DA | 2588 | U | O4'-C1' | 5.42 | 1.48 | 1.41 |
| 83 | DC | 62 | A | C2'-C1' | 5.42 | 1.59 | 1.53 |
| 26 | AZ | 55 | ARG | NE-CZ | 5.42 | 1.40 | 1.33 |
| 39 | BJ | 75 | PRO | N-CD | -5.42 | 1.40 | 1.47 |
| 78 | CA | 1037 | C | O4'-C1' | 5.42 | 1.48 | 1.41 |
| 78 | CA | 289 | U | C5'-C4' | 5.42 | 1.57 | 1.51 |
| 81 | DA | 386 | A | O3'-P | -5.42 | 1.54 | 1.61 |
| 81 | DA | 1217 | A | O4'-C1' | 5.42 | 1.48 | 1.41 |
| 57 | Be | 60 | ARG | CD-NE | 5.42 | 1.55 | 1.46 |
| 81 | DA | 1895 | A | O3'-P | -5.42 | 1.54 | 1.61 |
| 78 | CA | 52 | U | C2'-C1' | -5.41 | 1.47 | 1.53 |
| 81 | DA | 1719 | G | C2'-C1' | -5.41 | 1.47 | 1.53 |
| 81 | DA | 1973 | G | P-O5' | 5.41 | 1.65 | 1.59 |
| 78 | CA | 501 | U | C2'-C1' | -5.41 | 1.47 | 1.53 |
| 78 | CA | 898 | A | O4'-C1' | 5.41 | 1.48 | 1.41 |
| 78 | CA | 1175 | U | O4'-C1' | 5.41 | 1.48 | 1.41 |
| 81 | DA | 601 | U | O4'-C1' | 5.41 | 1.48 | 1.41 |
| 81 | DA | 2030 | C | O3'-P | -5.41 | 1.54 | 1.61 |
| 81 | DA | 3087 | A | O4'-C1' | 5.41 | 1.48 | 1.41 |
| 83 | DC | 60 | G | O4'-C1' | -5.41 | 1.34 | 1.41 |
| 35 | BG | 31 | ARG | CD-NE | 5.41 | 1.55 | 1.46 |
| 78 | CA | 1242 | A | O3'-P | -5.41 | 1.54 | 1.61 |
| 78 | CA | 1652 | C | C4'-C3' | -5.41 | 1.47 | 1.52 |
| 81 | DA | 61 | A | O4'-C1' | 5.41 | 1.48 | 1.41 |
| 81 | DA | 157 | A | O3'-P | -5.41 | 1.54 | 1.61 |
| 81 | DA | 2015 | C | C2'-C1' | -5.41 | 1.47 | 1.53 |
| 33 | BD | 300 | ARG | CZ-NH2 | 5.41 | 1.40 | 1.33 |
| 14 | AM | 42 | TYR | CG-CD2 | -5.41 | 1.32 | 1.39 |
| 16 | AO | 106 | ARG | NE-CZ | 5.41 | 1.40 | 1.33 |
| 78 | CA | 733 | A | C4'-C3' | -5.41 | 1.47 | 1.52 |
| 78 | CA | 1151 | A | C2'-C1' | 5.41 | 1.59 | 1.53 |
| 81 | DA | 2805 | G | O4'-C1' | 5.41 | 1.48 | 1.41 |
| 53 | Ba | 8 | GLY | CA-C | 5.40 | 1.60 | 1.51 |
| 81 | DA | 2195 | C | O4'-C1' | 5.40 | 1.48 | 1.41 |
| 81 | DA | 2487 | U | O3'-P | 5.40 | 1.67 | 1.61 |
| 81 | DA | 1885 | U | C2'-C1' | -5.40 | 1.47 | 1.53 |
| 81 | DA | 2429 | G | C2'-C1' | -5.40 | 1.47 | 1.53 |
| 81 | DA | 2464 | U | O4'-C1' | 5.40 | 1.48 | 1.41 |
| 81 | DA | 2708 | C | P-O5' | -5.40 | 1.54 | 1.59 |
| 78 | CA | 944 | A | C2'-C1' | 5.40 | 1.59 | 1.53 |
| 78 | CA | 962 | C | O4'-C1' | 5.40 | 1.48 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 817 | A | C2'-C1' | -5.40 | 1.47 | 1.53 |
| 81 | DA | 1934 | G | C2'-C1' | -5.40 | 1.47 | 1.53 |
| 81 | DA | 2524 | A | P-O5' | 5.40 | 1.65 | 1.59 |
| 81 | DA | 2819 | A | O4'-C1' | 5.40 | 1.48 | 1.41 |
| 5 | AC | 3 | ARG | CD-NE | 5.40 | 1.55 | 1.46 |
| 11 | AJ | 28 | SER | CA-CB | 5.40 | 1.61 | 1.52 |
| 32 | BC | 32 | PHE | CB-CG | 5.40 | 1.60 | 1.51 |
| 60 | Bi | 4 | ARG | NE-CZ | 5.40 | 1.40 | 1.33 |
| 78 | CA | 13 | C | C3'-C2' | -5.40 | 1.46 | 1.52 |
| 81 | DA | 1634 | G | P-O5' | -5.40 | 1.54 | 1.59 |
| 81 | DA | 1396 | C | P-O5' | -5.40 | 1.54 | 1.59 |
| 81 | DA | 2939 | G | C2'-C1' | -5.40 | 1.47 | 1.53 |
| 52 | BY | 71 | SER | CA-CB | 5.40 | 1.61 | 1.52 |
| 81 | DA | 1628 | C | O4'-C1' | 5.40 | 1.48 | 1.41 |
| 81 | DA | 3068 | U | O4'-C1' | 5.40 | 1.48 | 1.41 |
| 22 | AV | 26 | LYS | N-CA | 5.39 | 1.57 | 1.46 |
| 78 | CA | 57 | G | O3'-P | -5.39 | 1.54 | 1.61 |
| 50 | BX | 44 | PRO | N-CD | -5.39 | 1.40 | 1.47 |
| 57 | Be | 33 | ARG | CZ-NH2 | 5.39 | 1.40 | 1.33 |
| 81 | DA | 3037 | U | C2'-C1' | -5.39 | 1.47 | 1.53 |
| 81 | DA | 3060 | C | C2'-C1' | -5.39 | 1.47 | 1.53 |
| 81 | DA | 1718 | G | O4'-C1' | 5.39 | 1.48 | 1.41 |
| 82 | DB | 143 | U | O4'-C1' | 5.39 | 1.48 | 1.41 |
| 81 | DA | 771 | A | C4'-C3' | 5.39 | 1.59 | 1.53 |
| 29 | AU | 19 | ALA | N-CA | -5.39 | 1.35 | 1.46 |
| 78 | CA | 1064 | G | C2-N3 | 5.39 | 1.37 | 1.32 |
| 79 | CB | 60 | C | O4'-C1' | 5.39 | 1.48 | 1.41 |
| 78 | CA | 613 | G | O4'-C1' | -5.38 | 1.34 | 1.41 |
| 81 | DA | 3028 | G | O4'-C1' | 5.38 | 1.48 | 1.41 |
| 81 | DA | 3361 | G | O3'-P | -5.38 | 1.54 | 1.61 |
| 43 | BP | 147 | ARG | CZ-NH2 | 5.38 | 1.40 | 1.33 |
| 78 | CA | 880 | C | C2'-O2' | -5.38 | 1.34 | 1.41 |
| 82 | DB | 121 | U | O4'-C1' | 5.38 | 1.48 | 1.41 |
| 82 | DB | 132 | G | O3'-P | -5.38 | 1.54 | 1.61 |
| 78 | CA | 358 | U | O4'-C1' | 5.38 | 1.48 | 1.41 |
| 78 | CA | 1088 | A | P-O5' | -5.38 | 1.54 | 1.59 |
| 81 | DA | 1317 | A | C2'-C1' | 5.38 | 1.59 | 1.53 |
| 18 | AP | 39 | GLY | N-CA | -5.38 | 1.38 | 1.46 |
| 78 | CA | 644 | C | O4'-C1' | 5.38 | 1.48 | 1.41 |
| 78 | CA | 1591 | C | P-O5' | -5.38 | 1.54 | 1.59 |
| 81 | DA | 607 | A | C4'-O4' | -5.38 | 1.38 | 1.45 |
| 81 | DA | 764 | U | O4'-C1' | 5.38 | 1.48 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1629 | U | O4'-C1' | 5.38 | 1.48 | 1.41 |
| 81 | DA | 1670 | C | C2'-C1' | -5.38 | 1.47 | 1.53 |
| 83 | DC | 8 | G | C2'-C1' | -5.38 | 1.47 | 1.53 |
| 81 | DA | 1862 | U | O4'-C1' | 5.38 | 1.48 | 1.41 |
| 35 | BG | 9 | TRP | N-CA | 5.37 | 1.57 | 1.46 |
| 78 | CA | 1450 | U | O4'-C1' | 5.37 | 1.48 | 1.41 |
| 81 | DA | 470 | G | O4'-C1' | 5.37 | 1.48 | 1.41 |
| 81 | DA | 3330 | A | P-OP2 | 5.37 | 1.58 | 1.49 |
| 3 | AB | 79 | TYR | N-CA | 5.37 | 1.57 | 1.46 |
| 44 | BO | 12 | ARG | NE-CZ | 5.37 | 1.40 | 1.33 |
| 78 | CA | 241 | U | O3'-P | -5.37 | 1.54 | 1.61 |
| 81 | DA | 367 | A | O4'-C1' | 5.37 | 1.48 | 1.41 |
| 81 | DA | 2238 | G | P-O5' | 5.37 | 1.65 | 1.59 |
| 31 | BB | 241 | ARG | CD-NE | 5.37 | 1.55 | 1.46 |
| 37 | BH | 216 | SER | N-CA | -5.37 | 1.35 | 1.46 |
| 38 | Bs | 48 | ARG | CZ-NH2 | 5.37 | 1.40 | 1.33 |
| 51 | BZ | 56 | ARG | NE-CZ | 5.37 | 1.40 | 1.33 |
| 53 | Ba | 13 | VAL | CA-CB | -5.37 | 1.43 | 1.54 |
| 78 | CA | 887 | A | O4'-C1' | 5.37 | 1.48 | 1.41 |
| 81 | DA | 988 | U | C3'-O3' | -5.37 | 1.34 | 1.42 |
| 81 | DA | 1820 | U | C4'-O4' | 5.37 | 1.52 | 1.45 |
| 81 | DA | 2635 | A | O4'-C1' | 5.37 | 1.48 | 1.41 |
| 81 | DA | 3243 | A | C5'-C4' | 5.37 | 1.57 | 1.51 |
| 38 | Bs | 5 | ARG | N-CA | 5.37 | 1.57 | 1.46 |
| 80 | CC | 20 | U | C1'-N1 | 5.37 | 1.56 | 1.48 |
| 81 | DA | 1125 | U | C2'-C1' | 5.37 | 1.59 | 1.53 |
| 59 | Bh | 125 | ARG | NE-CZ | 5.36 | 1.40 | 1.33 |
| 78 | CA | 835 | U | O4'-C1' | 5.36 | 1.48 | 1.41 |
| 78 | CA | 1093 | A | O4'-C1' | 5.36 | 1.48 | 1.41 |
| 81 | DA | 764 | U | C4'-C3' | 5.36 | 1.59 | 1.53 |
| 46 | BT | 170 | ARG | CZ-NH1 | 5.36 | 1.40 | 1.33 |
| 82 | DB | 40 | A | O4'-C1' | 5.36 | 1.48 | 1.41 |
| 24 | AX | 57 | GLU | CB-CG | 5.36 | 1.62 | 1.52 |
| 59 | Bh | 23 | ASP | C-O | -5.36 | 1.13 | 1.23 |
| 78 | CA | 446 | A | O4'-C1' | -5.36 | 1.34 | 1.41 |
| 81 | DA | 1926 | C | C4'-O4' | -5.36 | 1.38 | 1.45 |
| 81 | DA | 2969 | A | C2'-C1' | -5.36 | 1.47 | 1.53 |
| 48 | BW | 29 | ASP | CA-CB | 5.36 | 1.65 | 1.53 |
| 55 | Bc | 96 | GLU | C-O | -5.36 | 1.13 | 1.23 |
| 78 | CA | 447 | U | C3'-C2' | -5.36 | 1.46 | 1.52 |
| 78 | CA | 710 | U | C4'-C3' | -5.36 | 1.47 | 1.52 |
| 78 | CA | 719 | U | P-O5' | -5.36 | 1.54 | 1.59 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 930 | A | C3'-C2' | 5.36 | 1.58 | 1.52 |
| 81 | DA | 425 | G | P-O5' | -5.36 | 1.54 | 1.59 |
| 81 | DA | 1964 | C | C2'-C1' | -5.36 | 1.47 | 1.53 |
| 4 | AD | 59 | ARG | CZ-NH2 | 5.36 | 1.40 | 1.33 |
| 81 | DA | 3396 | U | C2'-C1' | 5.36 | 1.59 | 1.53 |
| 33 | BD | 326 | ARG | CZ-NH2 | 5.35 | 1.40 | 1.33 |
| 69 | Br | 59 | HIS | N-CA | 5.35 | 1.57 | 1.46 |
| 81 | DA | 2641 | U | O4'-C1' | 5.35 | 1.48 | 1.41 |
| 81 | DA | 3115 | C | C2'-C1' | -5.35 | 1.47 | 1.53 |
| 48 | BW | 104 | ARG | CZ-NH1 | 5.35 | 1.40 | 1.33 |
| 78 | CA | 119 | A | C3'-C2' | -5.35 | 1.46 | 1.52 |
| 78 | CA | 227 | U | O4'-C1' | 5.35 | 1.48 | 1.41 |
| 78 | CA | 399 | A | C2'-C1' | 5.35 | 1.59 | 1.53 |
| 78 | CA | 1083 | G | C2'-C1' | -5.35 | 1.47 | 1.53 |
| 78 | CA | 1319 | A | C4'-C3' | -5.35 | 1.47 | 1.52 |
| 81 | DA | 1850 | A | C4'-O4' | -5.35 | 1.38 | 1.45 |
| 57 | Be | 51 | TYR | CZ-OH | 5.35 | 1.47 | 1.37 |
| 78 | CA | 1221 | A | P-O5' | -5.35 | 1.54 | 1.59 |
| 81 | DA | 2850 | G | C2'-C1' | -5.35 | 1.47 | 1.53 |
| 14 | AM | 88 | ARG | CD-NE | 5.35 | 1.55 | 1.46 |
| 39 | BJ | 108 | GLU | CD-OE2 | -5.35 | 1.19 | 1.25 |
| 81 | DA | 2604 | U | O4'-C1' | 5.35 | 1.48 | 1.41 |
| 81 | DA | 2951 | G | O4'-C1' | 5.35 | 1.48 | 1.41 |
| 3 | AB | 79 | TYR | CA-C | -5.35 | 1.39 | 1.52 |
| 48 | BW | 36 | TYR | CE1-CZ | 5.34 | 1.45 | 1.38 |
| 78 | CA | 244 | A | P-O5' | 5.34 | 1.65 | 1.59 |
| 46 | BT | 98 | ARG | NE-CZ | 5.34 | 1.40 | 1.33 |
| 78 | CA | 1030 | A | C2'-C1' | 5.34 | 1.59 | 1.53 |
| 10 | AI | 54 | LEU | CA-CB | 5.34 | 1.66 | 1.53 |
| 81 | DA | 707 | U | C2'-C1' | -5.34 | 1.47 | 1.53 |
| 81 | DA | 1868 | G | O4'-C1' | 5.34 | 1.48 | 1.41 |
| 78 | CA | 1479 | A | C3'-C2' | -5.34 | 1.46 | 1.52 |
| 19 | AR | 115 | TYR | CB-CG | -5.34 | 1.43 | 1.51 |
| 74 | BQ | 248 | ARG | N-CA | -5.34 | 1.35 | 1.46 |
| 81 | DA | 2082 | U | O4'-C1' | 5.34 | 1.48 | 1.41 |
| 5 | AC | 54 | ARG | NE-CZ | 5.34 | 1.40 | 1.33 |
| 78 | CA | 910 | C | C4'-C3' | -5.34 | 1.47 | 1.52 |
| 78 | CA | 1390 | U | O4'-C1' | 5.34 | 1.48 | 1.41 |
| 81 | DA | 670 | C | O3'-P | -5.34 | 1.54 | 1.61 |
| 78 | CA | 1091 | A | O4'-C1' | -5.33 | 1.34 | 1.41 |
| 81 | DA | 674 | G | O3'-P | -5.33 | 1.54 | 1.61 |
| 81 | DA | 798 | G | P-O5' | -5.33 | 1.54 | 1.59 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 6 | AE | 91 | ARG | CD-NE | 5.33 | 1.55 | 1.46 |
| 32 | BC | 289 | ASP | C-N | 5.33 | 1.46 | 1.34 |
| 78 | CA | 913 | G | O4'-C1' | -5.33 | 1.34 | 1.41 |
| 78 | CA | 935 | U | C4'-C3' | -5.33 | 1.47 | 1.52 |
| 81 | DA | 1320 | C | O3'-P | -5.33 | 1.54 | 1.61 |
| 81 | DA | 2573 | G | C2'-C1' | -5.33 | 1.47 | 1.53 |
| 74 | BQ | 111 | GLN | N-CA | -5.33 | 1.35 | 1.46 |
| 81 | DA | 368 | G | O4'-C1' | 5.33 | 1.48 | 1.41 |
| 18 | AP | 116 | ARG | CG-CD | 5.33 | 1.65 | 1.51 |
| 32 | BC | 381 | GLY | C-N | 5.33 | 1.46 | 1.34 |
| 81 | DA | 160 | G | C5'-C4' | 5.33 | 1.57 | 1.51 |
| 78 | CA | 1603 | U | C4'-C3' | -5.33 | 1.47 | 1.52 |
| 81 | DA | 2164 | A | O4'-C1' | 5.33 | 1.48 | 1.41 |
| 81 | DA | 2238 | G | C5'-C4' | 5.33 | 1.57 | 1.51 |
| 81 | DA | 3371 | G | O4'-C1' | 5.33 | 1.48 | 1.41 |
| 83 | DC | 68 | U | C2'-C1' | -5.33 | 1.47 | 1.53 |
| 42 | BM | 128 | ARG | CD-NE | 5.33 | 1.55 | 1.46 |
| 78 | CA | 1220 | C | C5'-C4' | 5.33 | 1.57 | 1.51 |
| 56 | Bf | 35 | ARG | CZ-NH1 | 5.32 | 1.40 | 1.33 |
| 81 | DA | 2387 | A | C2'-C1' | -5.32 | 1.47 | 1.53 |
| 14 | AM | 101 | LEU | CG-CD2 | -5.32 | 1.32 | 1.51 |
| 40 | BK | 160 | ARG | NE-CZ | 5.32 | 1.40 | 1.33 |
| 78 | CA | 1479 | A | C2'-C1' | 5.32 | 1.59 | 1.53 |
| 61 | Bj | 44 | TYR | CB-CG | -5.32 | 1.43 | 1.51 |
| 78 | CA | 34 | G | C2'-C1' | 5.32 | 1.59 | 1.53 |
| 81 | DA | 1662 | G | O3'-P | -5.32 | 1.54 | 1.61 |
| 81 | DA | 2043 | U | O3'-P | -5.32 | 1.54 | 1.61 |
| 81 | DA | 2992 | U | O4'-C1' | 5.32 | 1.48 | 1.41 |
| 81 | DA | 1075 | A | O3'-P | -5.32 | 1.54 | 1.61 |
| 81 | DA | 2414 | G | O4'-C1' | 5.31 | 1.48 | 1.41 |
| 3 | AB | 91 | VAL | CB-CG1 | 5.31 | 1.64 | 1.52 |
| 64 | Bl | 39 | TYR | CA-CB | -5.31 | 1.42 | 1.53 |
| 81 | DA | 42 | C | C2'-C1' | -5.31 | 1.47 | 1.53 |
| 83 | DC | 95 | C | O4'-C1' | 5.31 | 1.48 | 1.41 |
| 81 | DA | 2648 | G | C4'-O4' | 5.31 | 1.52 | 1.45 |
| 78 | CA | 882 | U | C2'-C1' | -5.31 | 1.47 | 1.53 |
| 78 | CA | 1441 | C | P-O5' | -5.31 | 1.54 | 1.59 |
| 5 | AC | 53 | ARG | CD-NE | 5.31 | 1.55 | 1.46 |
| 81 | DA | 507 | U | C2'-C1' | -5.31 | 1.47 | 1.53 |
| 78 | CA | 1355 | C | C2'-C1' | -5.31 | 1.47 | 1.53 |
| 78 | CA | 1673 | G | O3'-P | -5.31 | 1.54 | 1.61 |
| 81 | DA | 685 | G | C2'-C1' | -5.31 | 1.47 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1826 | C | O3'-P | -5.31 | 1.54 | 1.61 |
| 4 | AD | 94 | ALA | N-CA | 5.30 | 1.56 | 1.46 |
| 17 | AQ | 133 | ARG | CZ-NH1 | 5.30 | 1.40 | 1.33 |
| 31 | BB | 214 | GLY | N-CA | -5.30 | 1.38 | 1.46 |
| 78 | CA | 1049 | U | P-O5' | -5.30 | 1.54 | 1.59 |
| 82 | DB | 107 | G | O4'-C1' | 5.30 | 1.48 | 1.41 |
| 78 | CA | 1196 | A | C2'-C1' | 5.30 | 1.59 | 1.53 |
| 26 | AZ | 40 | TYR | CA-CB | -5.30 | 1.42 | 1.53 |
| 57 | Be | 132 | PRO | N-CD | 5.30 | 1.55 | 1.47 |
| 78 | CA | 528 | U | C3'-O3' | -5.30 | 1.34 | 1.42 |
| 81 | DA | 244 | G | C4'-O4' | 5.30 | 1.52 | 1.45 |
| 3 | AB | 94 | ARG | NE-CZ | 5.30 | 1.40 | 1.33 |
| 78 | CA | 1442 | U | O4'-C1' | 5.30 | 1.48 | 1.41 |
| 81 | DA | 60 | A | O4'-C1' | 5.30 | 1.48 | 1.41 |
| 81 | DA | 537 | A | C2'-C1' | -5.30 | 1.47 | 1.53 |
| 81 | DA | 667 | C | C2'-C1' | -5.30 | 1.47 | 1.53 |
| 81 | DA | 2879 | C | O4'-C1' | 5.30 | 1.48 | 1.41 |
| 47 | BU | 34 | TYR | CE2-CZ | 5.30 | 1.45 | 1.38 |
| 78 | CA | 1100 | G | P-O5' | 5.30 | 1.65 | 1.59 |
| 81 | DA | 975 | C | O4'-C1' | 5.30 | 1.48 | 1.41 |
| 35 | BG | 152 | THR | CA-CB | -5.30 | 1.39 | 1.53 |
| 53 | Ba | 7 | ALA | C-N | 5.30 | 1.42 | 1.33 |
| 81 | DA | 790 | U | C3'-C2' | -5.30 | 1.47 | 1.52 |
| 81 | DA | 2846 | U | C2'-C1' | -5.30 | 1.47 | 1.53 |
| 82 | DB | 126 | A | C2'-C1' | -5.30 | 1.47 | 1.53 |
| 3 | AB | 76 | ARG | CD-NE | 5.29 | 1.55 | 1.46 |
| 81 | DA | 537 | A | O3'-P | -5.29 | 1.54 | 1.61 |
| 4 | AD | 239 | PRO | N-CA | 5.29 | 1.56 | 1.47 |
| 74 | BQ | 288 | ALA | CA-CB | 5.29 | 1.63 | 1.52 |
| 81 | DA | 1463 | U | O4'-C1' | 5.29 | 1.48 | 1.41 |
| 81 | DA | 2013 | C | C2'-C1' | -5.29 | 1.47 | 1.53 |
| 81 | DA | 965 | A | C2'-C1' | -5.29 | 1.47 | 1.53 |
| 4 | AD | 191 | ARG | CZ-NH2 | 5.29 | 1.40 | 1.33 |
| 81 | DA | 171 | G | C3'-O3' | 5.29 | 1.49 | 1.42 |
| 32 | BC | 26 | ARG | CZ-NH1 | 5.29 | 1.40 | 1.33 |
| 78 | CA | 547 | U | C2'-C1' | -5.29 | 1.47 | 1.53 |
| 78 | CA | 1745 | G | O3'-P | -5.29 | 1.54 | 1.61 |
| 81 | DA | 262 | U | P-O5' | -5.29 | 1.54 | 1.59 |
| 81 | DA | 1838 | G | C2'-C1' | -5.29 | 1.47 | 1.53 |
| 11 | AJ | 23 | ARG | NE-CZ | 5.29 | 1.40 | 1.33 |
| 18 | AP | 67 | ARG | CD-NE | 5.29 | 1.55 | 1.46 |
| 81 | DA | 467 | U | O4'-C1' | 5.29 | 1.48 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2342 | U | C2'-C1' | -5.29 | 1.47 | 1.53 |
| 81 | DA | 668 | G | O4'-C1' | 5.29 | 1.48 | 1.41 |
| 81 | DA | 1794 | G | C3'-C2' | -5.29 | 1.47 | 1.52 |
| 14 | AM | 37 | GLY | N-CA | -5.28 | 1.38 | 1.46 |
| 31 | BB | 62 | VAL | C-N | 5.28 | 1.46 | 1.34 |
| 78 | CA | 256 | A | C5'-C4' | 5.28 | 1.57 | 1.51 |
| 78 | CA | 551 | G | O4'-C1' | 5.28 | 1.48 | 1.41 |
| 81 | DA | 2503 | G | C2'-C1' | -5.28 | 1.47 | 1.53 |
| 81 | DA | 3345 | G | O3'-P | -5.28 | 1.54 | 1.61 |
| 41 | BN | 55 | ARG | CD-NE | 5.28 | 1.55 | 1.46 |
| 78 | CA | 1556 | A | C5'-C4' | -5.28 | 1.45 | 1.51 |
| 79 | CB | 24 | A | C2'-C1' | 5.28 | 1.59 | 1.53 |
| 81 | DA | 10 | C | C2'-C1' | -5.28 | 1.47 | 1.53 |
| 81 | DA | 800 | G | C3'-C2' | -5.28 | 1.47 | 1.52 |
| 78 | CA | 64 | U | O4'-C1' | 5.28 | 1.48 | 1.41 |
| 78 | CA | 252 | U | C3'-O3' | -5.28 | 1.34 | 1.42 |
| 81 | DA | 319 | A | O4'-C1' | 5.28 | 1.48 | 1.41 |
| 81 | DA | 466 | G | O4'-C1' | 5.28 | 1.48 | 1.41 |
| 81 | DA | 837 | A | C2'-C1' | -5.28 | 1.47 | 1.53 |
| 78 | CA | 12 | U | C2'-C1' | -5.28 | 1.47 | 1.53 |
| 79 | CB | 5 | U | O4'-C1' | 5.28 | 1.48 | 1.41 |
| 81 | DA | 1241 | U | C2'-C1' | -5.28 | 1.47 | 1.53 |
| 46 | BT | 162 | ARG | NE-CZ | 5.28 | 1.40 | 1.33 |
| 64 | Bl | 65 | ARG | NE-CZ | 5.28 | 1.40 | 1.33 |
| 78 | CA | 713 | A | C4'-C3' | -5.28 | 1.47 | 1.52 |
| 78 | CA | 1547 | A | C5'-C4' | 5.28 | 1.57 | 1.51 |
| 78 | CA | 1616 | G | P-O5' | -5.28 | 1.54 | 1.59 |
| 79 | CB | 47 | U | C2'-C1' | 5.28 | 1.59 | 1.53 |
| 81 | DA | 758 | C | O3'-P | -5.28 | 1.54 | 1.61 |
| 81 | DA | 2483 | G | O3'-P | -5.28 | 1.54 | 1.61 |
| 81 | DA | 2703 | A | O4'-C1' | -5.28 | 1.34 | 1.41 |
| 5 | AC | 149 | ARG | CZ-NH1 | 5.27 | 1.40 | 1.33 |
| 42 | BM | 30 | GLY | CA-C | -5.27 | 1.43 | 1.51 |
| 69 | Br | 51 | GLY | N-CA | -5.27 | 1.38 | 1.46 |
| 78 | CA | 1109 | G | C2'-C1' | -5.27 | 1.47 | 1.53 |
| 81 | DA | 1237 | G | O4'-C1' | 5.27 | 1.48 | 1.41 |
| 78 | CA | 550 | A | C2'-C1' | -5.27 | 1.47 | 1.53 |
| 4 | AD | 235 | TYR | CB-CG | -5.27 | 1.43 | 1.51 |
| 9 | AH | 78 | ARG | CD-NE | 5.27 | 1.55 | 1.46 |
| 46 | BT | 162 | ARG | CD-NE | 5.27 | 1.55 | 1.46 |
| 81 | DA | 2367 | A | C4'-C3' | 5.27 | 1.58 | 1.53 |
| 38 | Bs | 73 | PHE | N-CA | 5.27 | 1.56 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 43 | BP | 78 | GLY | CA-C | -5.27 | 1.43 | 1.51 |
| 78 | CA | 539 | G | O3'-P | -5.27 | 1.54 | 1.61 |
| 78 | CA | 555 | A | C3'-C2' | -5.27 | 1.47 | 1.52 |
| 81 | DA | 1590 | G | O4'-C1' | 5.27 | 1.48 | 1.41 |
| 78 | CA | 216 | U | C4'-O4' | 5.27 | 1.52 | 1.45 |
| 3 | AB | 34 | TYR | CE2-CZ | 5.26 | 1.45 | 1.38 |
| 37 | BH | 226 | TYR | CZ-OH | 5.26 | 1.46 | 1.37 |
| 78 | CA | 1315 | U | O4'-C1' | 5.26 | 1.48 | 1.41 |
| 78 | CA | 1654 | G | O4'-C1' | 5.26 | 1.48 | 1.41 |
| 81 | DA | 645 | A | C2'-C1' | 5.26 | 1.59 | 1.53 |
| 81 | DA | 1130 | A | O4'-C1' | 5.26 | 1.48 | 1.41 |
| 81 | DA | 3369 | G | C2'-C1' | 5.26 | 1.59 | 1.53 |
| 22 | AV | 33 | LYS | CB-CG | -5.26 | 1.38 | 1.52 |
| 32 | BC | 167 | ARG | NE-CZ | 5.26 | 1.39 | 1.33 |
| 60 | Bi | 48 | GLY | N-CA | -5.26 | 1.38 | 1.46 |
| 78 | CA | 289 | U | O4'-C1' | 5.26 | 1.48 | 1.41 |
| 81 | DA | 2093 | A | O3'-P | -5.26 | 1.54 | 1.61 |
| 81 | DA | 3243 | A | C4'-C3' | 5.26 | 1.58 | 1.53 |
| 78 | CA | 879 | G | O4'-C1' | -5.26 | 1.34 | 1.41 |
| 81 | DA | 1262 | G | O4'-C1' | 5.26 | 1.48 | 1.41 |
| 57 | Be | 232 | ARG | CA-CB | 5.26 | 1.65 | 1.53 |
| 78 | CA | 1135 | U | C4'-C3' | -5.26 | 1.47 | 1.52 |
| 81 | DA | 273 | A | O3'-P | -5.26 | 1.54 | 1.61 |
| 40 | BK | 12 | LYS | C-N | 5.26 | 1.42 | 1.33 |
| 48 | BW | 71 | PHE | CG-CD1 | 5.26 | 1.46 | 1.38 |
| 58 | Bg | 94 | GLU | CD-OE2 | 5.26 | 1.31 | 1.25 |
| 78 | CA | 640 | U | C4'-O4' | -5.26 | 1.38 | 1.45 |
| 78 | CA | 1289 | U | O4'-C1' | 5.26 | 1.48 | 1.41 |
| 81 | DA | 40 | A | C2'-C1' | -5.25 | 1.47 | 1.53 |
| 81 | DA | 1465 | A | O4'-C1' | 5.25 | 1.48 | 1.41 |
| 81 | DA | 2563 | G | C2'-C1' | -5.25 | 1.47 | 1.53 |
| 81 | DA | 1989 | U | C2'-C1' | -5.25 | 1.47 | 1.53 |
| 81 | DA | 2241 | U | P-O5' | -5.25 | 1.54 | 1.59 |
| 81 | DA | 2743 | A | O3'-P | -5.25 | 1.54 | 1.61 |
| 83 | DC | 27 | A | P-O5' | -5.25 | 1.54 | 1.59 |
| 4 | AD | 95 | THR | N-CA | 5.25 | 1.56 | 1.46 |
| 33 | BD | 203 | ARG | NE-CZ | 5.25 | 1.39 | 1.33 |
| 81 | DA | 1749 | A | O4'-C1' | 5.25 | 1.48 | 1.41 |
| 35 | BG | 149 | ILE | N-CA | 5.25 | 1.56 | 1.46 |
| 81 | DA | 2416 | U | P-O5' | -5.25 | 1.54 | 1.59 |
| 51 | BZ | 30 | ARG | CZ-NH1 | 5.25 | 1.39 | 1.33 |
| 81 | DA | 1992 | U | O4'-C1' | 5.25 | 1.48 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 5 | AC | 78 | ARG | NE-CZ | 5.25 | 1.39 | 1.33 |
| 14 | AM | 68 | ARG | CZ-NH1 | 5.25 | 1.39 | 1.33 |
| 18 | AP | 56 | LYS | N-CA | 5.25 | 1.56 | 1.46 |
| 81 | DA | 1824 | U | C2'-C1' | -5.25 | 1.47 | 1.53 |
| 81 | DA | 3097 | C | C2'-C1' | -5.25 | 1.47 | 1.53 |
| 2 | AA | 238 | GLU | CG-CD | 5.25 | 1.59 | 1.51 |
| 40 | BK | 168 | TYR | CE2-CZ | 5.25 | 1.45 | 1.38 |
| 81 | DA | 424 | G | P-O5' | -5.25 | 1.54 | 1.59 |
| 21 | AT | 12 | TYR | CZ-OH | 5.24 | 1.46 | 1.37 |
| 52 | BY | 65 | GLY | N-CA | -5.24 | 1.38 | 1.46 |
| 81 | DA | 1780 | G | O4'-C1' | 5.24 | 1.48 | 1.41 |
| 81 | DA | 2470 | C | C2'-C1' | -5.24 | 1.47 | 1.53 |
| 81 | DA | 3380 | U | O4'-C1' | 5.24 | 1.48 | 1.41 |
| 78 | CA | 633 | U | O4'-C1' | 5.24 | 1.48 | 1.41 |
| 81 | DA | 2225 | U | C2'-C1' | -5.24 | 1.47 | 1.53 |
| 81 | DA | 3381 | U | C2'-C1' | -5.24 | 1.47 | 1.53 |
| 78 | CA | 1691 | A | O4'-C1' | 5.24 | 1.48 | 1.41 |
| 81 | DA | 221 | A | C2'-C1' | -5.24 | 1.47 | 1.53 |
| 5 | AC | 44 | ARG | NE-CZ | 5.24 | 1.39 | 1.33 |
| 15 | AN | 54 | LYS | C-O | -5.24 | 1.13 | 1.23 |
| 56 | Bf | 57 | GLU | CD-OE2 | 5.24 | 1.31 | 1.25 |
| 63 | Bm | 80 | ARG | CZ-NH1 | 5.24 | 1.39 | 1.33 |
| 78 | CA | 822 | U | P-O5' | -5.24 | 1.54 | 1.59 |
| 81 | DA | 1522 | U | O4'-C1' | 5.24 | 1.48 | 1.41 |
| 81 | DA | 2279 | A | P-O5' | 5.24 | 1.65 | 1.59 |
| 78 | CA | 928 | U | C3'-C2' | -5.24 | 1.47 | 1.52 |
| 38 | Bs | 91 | GLU | CD-OE1 | 5.24 | 1.31 | 1.25 |
| 60 | Bi | 80 | ARG | N-CA | 5.24 | 1.56 | 1.46 |
| 77 | BI | 119 | TRP | NE1-CE2 | 5.24 | 1.44 | 1.37 |
| 81 | DA | 1323 | G | O4'-C1' | -5.24 | 1.34 | 1.41 |
| 81 | DA | 2495 | C | C2'-C1' | -5.24 | 1.47 | 1.53 |
| 81 | DA | 3080 | G | O4'-C1' | 5.24 | 1.48 | 1.41 |
| 81 | DA | 564 | G | C2'-C1' | -5.23 | 1.47 | 1.53 |
| 81 | DA | 2045 | G | C2'-C1' | -5.23 | 1.47 | 1.53 |
| 35 | BG | 76 | LEU | N-CA | 5.23 | 1.56 | 1.46 |
| 69 | Br | 45 | ARG | CZ-NH1 | 5.23 | 1.39 | 1.33 |
| 78 | CA | 588 | U | P-O5' | -5.23 | 1.54 | 1.59 |
| 78 | CA | 669 | G | O4'-C1' | 5.23 | 1.48 | 1.41 |
| 78 | CA | 857 | U | C2'-C1' | -5.23 | 1.47 | 1.53 |
| 81 | DA | 1544 | G | O4'-C1' | 5.23 | 1.48 | 1.41 |
| 81 | DA | 2866 | U | C2'-C1' | 5.23 | 1.59 | 1.53 |
| 60 | Bi | 68 | THR | N-CA | -5.23 | 1.35 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 365 | G | C2'-C1' | -5.23 | 1.47 | 1.53 |
| 78 | CA | 461 | G | O4'-C1' | -5.23 | 1.34 | 1.41 |
| 39 | BJ | 57 | LYS | CA-C | -5.23 | 1.39 | 1.52 |
| 3 | AB | 27 | ARG | NE-CZ | 5.23 | 1.39 | 1.33 |
| 9 | AH | 69 | LEU | CA-CB | 5.23 | 1.65 | 1.53 |
| 81 | DA | 72 | C | C2'-C1' | 5.23 | 1.59 | 1.53 |
| 14 | AM | 128 | PHE | CG-CD2 | 5.23 | 1.46 | 1.38 |
| 39 | BJ | 16 | ARG | CZ-NH1 | 5.23 | 1.39 | 1.33 |
| 78 | CA | 854 | U | O3'-P | -5.23 | 1.54 | 1.61 |
| 33 | BD | 313 | LEU | CA-C | -5.22 | 1.39 | 1.52 |
| 37 | BH | 73 | PRO | CA-CB | 5.22 | 1.64 | 1.53 |
| 64 | Bl | 56 | ARG | CZ-NH2 | 5.22 | 1.39 | 1.33 |
| 81 | DA | 2598 | G | O4'-C1' | 5.22 | 1.48 | 1.41 |
| 78 | CA | 149 | C | C2'-C1' | -5.22 | 1.47 | 1.53 |
| 78 | CA | 1234 | A | O3'-P | -5.22 | 1.54 | 1.61 |
| 78 | CA | 410 | A | C4'-O4' | -5.22 | 1.38 | 1.45 |
| 78 | CA | 497 | G | P-O5' | -5.22 | 1.54 | 1.59 |
| 81 | DA | 1218 | U | C2'-C1' | -5.22 | 1.47 | 1.53 |
| 81 | DA | 2591 | A | C2'-C1' | -5.22 | 1.47 | 1.53 |
| 47 | BU | 126 | VAL | C-N | 5.22 | 1.46 | 1.34 |
| 74 | BQ | 197 | SER | C-N | 5.22 | 1.46 | 1.34 |
| 78 | CA | 25 | C | C2'-C1' | -5.22 | 1.47 | 1.53 |
| 78 | CA | 906 | A | O4'-C1' | 5.22 | 1.48 | 1.41 |
| 78 | CA | 1039 | A | C3'-C2' | -5.22 | 1.47 | 1.52 |
| 78 | CA | 1394 | G | C2'-C1' | 5.22 | 1.59 | 1.53 |
| 56 | Bf | 98 | SER | CA-CB | 5.21 | 1.60 | 1.52 |
| 64 | Bl | 55 | ARG | NE-CZ | 5.21 | 1.39 | 1.33 |
| 79 | CB | 52 | G | C2'-C1' | -5.21 | 1.47 | 1.53 |
| 81 | DA | 586 | C | C2'-C1' | -5.21 | 1.47 | 1.53 |
| 81 | DA | 701 | G | C5'-C4' | 5.21 | 1.57 | 1.51 |
| 81 | DA | 3057 | U | O4'-C1' | 5.21 | 1.48 | 1.41 |
| 81 | DA | 3309 | G | O4'-C1' | -5.21 | 1.34 | 1.41 |
| 74 | BQ | 198 | TYR | N-CA | 5.21 | 1.56 | 1.46 |
| 74 | BQ | 272 | TYR | CA-CB | 5.21 | 1.65 | 1.53 |
| 78 | CA | 376 | C | C4'-C3' | -5.21 | 1.47 | 1.52 |
| 78 | CA | 381 | C | C2'-C1' | -5.21 | 1.47 | 1.53 |
| 81 | DA | 988 | U | C5'-C4' | 5.21 | 1.57 | 1.51 |
| 81 | DA | 3327 | G | C2'-C1' | -5.21 | 1.47 | 1.53 |
| 78 | CA | 1170 | G | C2'-C1' | -5.21 | 1.47 | 1.53 |
| 81 | DA | 305 | U | O4'-C1' | 5.21 | 1.48 | 1.41 |
| 81 | DA | 363 | G | O4'-C1' | -5.21 | 1.34 | 1.41 |
| 81 | DA | 2460 | U | O4'-C1' | 5.21 | 1.48 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | BH | 249 | ARG | NE-CZ | 5.21 | 1.39 | 1.33 |
| 78 | CA | 1393 | C | P-O5' | -5.21 | 1.54 | 1.59 |
| 81 | DA | 1876 | U | O4'-C1' | 5.21 | 1.48 | 1.41 |
| 81 | DA | 2722 | U | C3'-C2' | 5.21 | 1.58 | 1.52 |
| 40 | BK | 4 | GLU | CD-OE2 | 5.21 | 1.31 | 1.25 |
| 78 | CA | 238 | U | C4'-C3' | -5.21 | 1.47 | 1.52 |
| 78 | CA | 1173 | C | O3'-P | -5.21 | 1.54 | 1.61 |
| 81 | DA | 1895 | A | P-O5' | -5.21 | 1.54 | 1.59 |
| 83 | DC | 6 | C | P-O5' | -5.21 | 1.54 | 1.59 |
| 8 | AF | 35 | GLN | C-N | 5.21 | 1.46 | 1.34 |
| 47 | BU | 65 | TYR | CG-CD2 | 5.21 | 1.46 | 1.39 |
| 78 | CA | 507 | U | O3'-P | -5.21 | 1.54 | 1.61 |
| 81 | DA | 2383 | C | O3'-P | -5.20 | 1.54 | 1.61 |
| 76 | BS | 65 | GLU | CB-CG | 5.20 | 1.62 | 1.52 |
| 81 | DA | 2649 | A | O4'-C1' | 5.20 | 1.48 | 1.41 |
| 2 | AA | 103 | THR | C-N | -5.20 | 1.24 | 1.34 |
| 49 | BV | 59 | PRO | N-CA | -5.20 | 1.38 | 1.47 |
| 62 | Bk | 55 | ARG | CZ-NH1 | 5.20 | 1.39 | 1.33 |
| 81 | DA | 1599 | G | O3'-P | -5.20 | 1.54 | 1.61 |
| 81 | DA | 1754 | G | C2-N3 | 5.20 | 1.36 | 1.32 |
| 33 | BD | 202 | ARG | NE-CZ | 5.20 | 1.39 | 1.33 |
| 81 | DA | 1522 | U | C2'-C1' | -5.20 | 1.47 | 1.53 |
| 81 | DA | 3147 | G | O3'-P | -5.20 | 1.54 | 1.61 |
| 81 | DA | 3214 | U | C5'-C4' | 5.20 | 1.57 | 1.51 |
| 63 | Bm | 84 | ARG | NE-CZ | 5.20 | 1.39 | 1.33 |
| 81 | DA | 309 | U | O3'-P | -5.20 | 1.54 | 1.61 |
| 81 | DA | 2843 | U | C2'-C1' | -5.20 | 1.47 | 1.53 |
| 78 | CA | 891 | A | C2'-C1' | -5.19 | 1.47 | 1.53 |
| 81 | DA | 2073 | A | O3'-P | -5.19 | 1.54 | 1.61 |
| 17 | AQ | 112 | SER | CA-CB | 5.19 | 1.60 | 1.52 |
| 32 | BC | 17 | LEU | N-CA | 5.19 | 1.56 | 1.46 |
| 38 | Bs | 10 | GLU | CG-CD | 5.19 | 1.59 | 1.51 |
| 78 | CA | 1143 | A | C2'-C1' | -5.19 | 1.47 | 1.53 |
| 6 | AE | 7 | GLN | C-N | 5.19 | 1.46 | 1.34 |
| 30 | BA | 48 | ARG | CZ-NH1 | 5.19 | 1.39 | 1.33 |
| 32 | BC | 339 | ARG | CZ-NH2 | 5.19 | 1.39 | 1.33 |
| 81 | DA | 723 | U | O4'-C1' | 5.19 | 1.48 | 1.41 |
| 81 | DA | 2656 | A | O4'-C1' | 5.19 | 1.48 | 1.41 |
| 81 | DA | 3148 | U | C2'-C1' | -5.19 | 1.47 | 1.53 |
| 81 | DA | 3199 | G | C5'-C4' | 5.19 | 1.57 | 1.51 |
| 24 | AX | 80 | ARG | CZ-NH1 | 5.19 | 1.39 | 1.33 |
| 53 | Ba | 10 | VAL | N-CA | 5.19 | 1.56 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 56 | U | C3'-C2' | 5.19 | 1.58 | 1.52 |
| 20 | AS | 57 | ARG | NE-CZ | 5.18 | 1.39 | 1.33 |
| 53 | Ba | 10 | VAL | CB-CG2 | 5.18 | 1.63 | 1.52 |
| 79 | CB | 8 | U | O4'-C1' | 5.18 | 1.48 | 1.41 |
| 81 | DA | 828 | A | O4'-C1' | 5.18 | 1.48 | 1.41 |
| 82 | DB | 60 | U | C2'-O2' | 5.18 | 1.48 | 1.41 |
| 32 | BC | 62 | ARG | CZ-NH2 | 5.18 | 1.39 | 1.33 |
| 32 | BC | 290 | ASP | CA-C | -5.18 | 1.39 | 1.52 |
| 78 | CA | 270 | C | O4'-C1' | 5.18 | 1.48 | 1.41 |
| 81 | DA | 249 | U | C5'-C4' | 5.18 | 1.57 | 1.51 |
| 81 | DA | 460 | C | C2'-C1' | -5.18 | 1.47 | 1.53 |
| 35 | BG | 75 | PRO | C-O | -5.18 | 1.12 | 1.23 |
| 78 | CA | 337 | G | O3'-P | -5.18 | 1.54 | 1.61 |
| 78 | CA | 853 | G | C5'-C4' | 5.18 | 1.57 | 1.51 |
| 81 | DA | 1804 | A | O4'-C1' | 5.18 | 1.48 | 1.41 |
| 9 | AH | 101 | TYR | CE2-CZ | 5.18 | 1.45 | 1.38 |
| 35 | BG | 153 | PRO | N-CA | 5.18 | 1.56 | 1.47 |
| 41 | BN | 75 | GLY | CA-C | -5.18 | 1.43 | 1.51 |
| 78 | CA | 1477 | G | C5'-C4' | 5.18 | 1.57 | 1.51 |
| 81 | DA | 389 | A | C2'-C1' | -5.18 | 1.47 | 1.53 |
| 81 | DA | 1359 | C | C2'-C1' | -5.18 | 1.47 | 1.53 |
| 81 | DA | 1932 | A | C2'-C1' | -5.18 | 1.47 | 1.53 |
| 81 | DA | 3331 | U | P-O5' | -5.18 | 1.54 | 1.59 |
| 21 | AT | 9 | VAL | C-N | 5.17 | 1.46 | 1.34 |
| 30 | BA | 43 | PRO | N-CA | -5.17 | 1.38 | 1.47 |
| 46 | BT | 62 | ARG | CZ-NH2 | 5.17 | 1.39 | 1.33 |
| 63 | Bm | 17 | ARG | CZ-NH2 | 5.17 | 1.39 | 1.33 |
| 78 | CA | 1422 | A | O4'-C1' | 5.17 | 1.48 | 1.41 |
| 33 | BD | 354 | VAL | C-O | -5.17 | 1.13 | 1.23 |
| 16 | AO | 67 | THR | CA-CB | 5.17 | 1.66 | 1.53 |
| 78 | CA | 1660 | A | O4'-C1' | 5.17 | 1.48 | 1.41 |
| 81 | DA | 559 | A | O3'-P | -5.17 | 1.54 | 1.61 |
| 81 | DA | 994 | G | O4'-C1' | 5.17 | 1.48 | 1.41 |
| 81 | DA | 1076 | C | O3'-P | -5.17 | 1.54 | 1.61 |
| 11 | AJ | 89 | ARG | CZ-NH1 | 5.17 | 1.39 | 1.33 |
| 81 | DA | 752 | C | C3'-O3' | 5.17 | 1.49 | 1.42 |
| 2 | AA | 101 | ARG | CZ-NH2 | 5.17 | 1.39 | 1.33 |
| 14 | AM | 139 | LYS | N-CA | -5.17 | 1.36 | 1.46 |
| 81 | DA | 1018 | G | C2'-C1' | 5.17 | 1.59 | 1.53 |
| 81 | DA | 1825 | G | O3'-P | -5.17 | 1.54 | 1.61 |
| 1 | Aa | 259 | GLY | CA-C | -5.17 | 1.43 | 1.51 |
| 78 | CA | 1039 | A | C4'-C3' | -5.17 | 1.47 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1255 | C | C2'-C1' | 5.17 | 1.59 | 1.53 |
| 81 | DA | 3038 | U | C2'-C1' | -5.17 | 1.47 | 1.53 |
| 44 | BO | 40 | HIS | C-N | 5.17 | 1.46 | 1.34 |
| 68 | Bq | 17 | ARG | CZ-NH2 | 5.17 | 1.39 | 1.33 |
| 78 | CA | 1477 | G | C4'-C3' | -5.17 | 1.47 | 1.52 |
| 78 | CA | 1423 | U | C2'-C1' | -5.16 | 1.47 | 1.53 |
| 78 | CA | 1538 | U | C4'-O4' | -5.16 | 1.38 | 1.45 |
| 81 | DA | 1606 | U | C2'-C1' | -5.16 | 1.47 | 1.53 |
| 34 | BE | 143 | ARG | NE-CZ | 5.16 | 1.39 | 1.33 |
| 36 | BF | 124 | ARG | CZ-NH2 | 5.16 | 1.39 | 1.33 |
| 45 | BR | 157 | PRO | C-N | 5.16 | 1.46 | 1.34 |
| 1 | Aa | 275 | ARG | NE-CZ | 5.16 | 1.39 | 1.33 |
| 78 | CA | 1600 | A | C2'-C1' | 5.16 | 1.59 | 1.53 |
| 81 | DA | 1002 | A | P-O5' | -5.16 | 1.54 | 1.59 |
| 81 | DA | 2047 | A | C2'-C1' | 5.16 | 1.59 | 1.53 |
| 81 | DA | 3121 | U | C2'-C1' | -5.16 | 1.47 | 1.53 |
| 26 | AZ | 18 | THR | CA-CB | -5.16 | 1.40 | 1.53 |
| 78 | CA | 835 | U | C2'-C1' | -5.16 | 1.47 | 1.53 |
| 78 | CA | 1584 | G | C4'-O4' | -5.16 | 1.38 | 1.45 |
| 81 | DA | 1624 | G | C5'-C4' | 5.16 | 1.57 | 1.51 |
| 81 | DA | 3092 | C | C5'-C4' | 5.16 | 1.57 | 1.51 |
| 81 | DA | 448 | U | C4'-C3' | 5.16 | 1.58 | 1.53 |
| 78 | CA | 164 | A | C5'-C4' | -5.16 | 1.45 | 1.51 |
| 78 | CA | 911 | U | O4'-C1' | 5.16 | 1.48 | 1.41 |
| 78 | CA | 1479 | A | C3'-O3' | -5.16 | 1.34 | 1.42 |
| 81 | DA | 2172 | A | C3'-C2' | -5.16 | 1.47 | 1.52 |
| 83 | DC | 73 | G | O4'-C1' | 5.16 | 1.48 | 1.41 |
| 81 | DA | 1793 | C | O4'-C1' | 5.15 | 1.48 | 1.41 |
| 81 | DA | 2909 | U | C2'-C1' | -5.15 | 1.47 | 1.53 |
| 15 | AN | 40 | ARG | CZ-NH2 | 5.15 | 1.39 | 1.33 |
| 46 | BT | 140 | GLU | CG-CD | 5.15 | 1.59 | 1.51 |
| 81 | DA | 56 | G | C2'-C1' | -5.15 | 1.47 | 1.53 |
| 81 | DA | 281 | G | O4'-C1' | 5.15 | 1.48 | 1.41 |
| 81 | DA | 1489 | A | O4'-C1' | 5.15 | 1.48 | 1.41 |
| 81 | DA | 2173 | U | C4'-C3' | 5.15 | 1.58 | 1.53 |
| 49 | BV | 76 | PHE | CG-CD1 | 5.15 | 1.46 | 1.38 |
| 78 | CA | 229 | U | C2'-C1' | 5.15 | 1.59 | 1.53 |
| 81 | DA | 1450 | G | C2'-C1' | -5.15 | 1.47 | 1.53 |
| 81 | DA | 2531 | C | N3-C4 | 5.15 | 1.37 | 1.33 |
| 83 | DC | 12 | U | O4'-C1' | 5.15 | 1.48 | 1.41 |
| 20 | AS | 96 | ALA | N-CA | 5.15 | 1.56 | 1.46 |
| 52 | BY | 7 | ASP | N-CA | -5.15 | 1.36 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 59 | Bh | 12 | LYS | N-CA | 5.15 | 1.56 | 1.46 |
| 78 | CA | 96 | G | O4'-C1' | -5.15 | 1.34 | 1.41 |
| 16 | AO | 64 | ARG | NE-CZ | 5.14 | 1.39 | 1.33 |
| 32 | BC | 239 | PRO | N-CA | -5.14 | 1.38 | 1.47 |
| 78 | CA | 149 | C | C4'-C3' | -5.14 | 1.47 | 1.52 |
| 78 | CA | 1406 | A | C4'-C3' | -5.14 | 1.47 | 1.52 |
| 81 | DA | 1494 | U | O4'-C1' | 5.14 | 1.48 | 1.41 |
| 81 | DA | 2892 | A | C2'-C1' | -5.14 | 1.47 | 1.53 |
| 81 | DA | 3087 | A | C2'-C1' | -5.14 | 1.47 | 1.53 |
| 78 | CA | 1725 | U | P-O5' | -5.14 | 1.54 | 1.59 |
| 81 | DA | 577 | C | C2'-C1' | -5.14 | 1.47 | 1.53 |
| 81 | DA | 817 | A | O4'-C1' | 5.14 | 1.48 | 1.41 |
| 81 | DA | 1869 | C | C2'-C1' | -5.14 | 1.47 | 1.53 |
| 81 | DA | 2327 | U | C2'-C1' | -5.14 | 1.47 | 1.53 |
| 82 | DB | 155 | A | O4'-C1' | 5.14 | 1.48 | 1.41 |
| 36 | BF | 69 | ARG | CZ-NH1 | 5.14 | 1.39 | 1.33 |
| 14 | AM | 98 | TYR | CZ-OH | 5.14 | 1.46 | 1.37 |
| 78 | CA | 646 | C | C2'-C1' | -5.14 | 1.47 | 1.53 |
| 81 | DA | 673 | U | O5'-C5' | -5.14 | 1.34 | 1.42 |
| 81 | DA | 1434 | G | O4'-C1' | 5.14 | 1.48 | 1.41 |
| 81 | DA | 1523 | U | C2'-C1' | 5.14 | 1.59 | 1.53 |
| 81 | DA | 2119 | A | C2'-C1' | -5.14 | 1.47 | 1.53 |
| 47 | BU | 145 | GLY | CA-C | -5.14 | 1.43 | 1.51 |
| 81 | DA | 2745 | G | O4'-C1' | -5.14 | 1.34 | 1.41 |
| 4 | AD | 200 | ARG | CD-NE | 5.14 | 1.55 | 1.46 |
| 46 | BT | 71 | ARG | CA-CB | -5.14 | 1.42 | 1.53 |
| 58 | Bg | 72 | ARG | NE-CZ | 5.14 | 1.39 | 1.33 |
| 81 | DA | 1924 | U | C4'-C3' | -5.14 | 1.47 | 1.52 |
| 81 | DA | 1947 | G | O3'-P | -5.14 | 1.54 | 1.61 |
| 81 | DA | 2664 | C | C5'-C4' | 5.14 | 1.57 | 1.51 |
| 15 | AN | 32 | ARG | CZ-NH1 | 5.13 | 1.39 | 1.33 |
| 44 | BO | 32 | ARG | CZ-NH1 | 5.13 | 1.39 | 1.33 |
| 69 | Br | 101 | GLY | CA-C | -5.13 | 1.43 | 1.51 |
| 81 | DA | 663 | C | O4'-C1' | 5.13 | 1.48 | 1.41 |
| 81 | DA | 1157 | G | C2'-C1' | -5.13 | 1.47 | 1.53 |
| 82 | DB | 22 | U | C2'-C1' | 5.13 | 1.58 | 1.53 |
| 17 | AQ | 60 | ARG | CZ-NH2 | 5.13 | 1.39 | 1.33 |
| 81 | DA | 243 | G | C4'-C3' | 5.13 | 1.58 | 1.53 |
| 81 | DA | 799 | G | O3'-P | -5.13 | 1.54 | 1.61 |
| 81 | DA | 3250 | U | P-O5' | -5.13 | 1.54 | 1.59 |
| 78 | CA | 1533 | C | O3'-P | -5.13 | 1.54 | 1.61 |
| 81 | DA | 1477 | A | O4'-C1' | 5.13 | 1.48 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 635 | G | C3'-C2' | -5.13 | 1.47 | 1.52 |
| 81 | DA | 970 | A | O4'-C1' | 5.13 | 1.48 | 1.41 |
| 17 | AQ | 135 | ARG | CZ-NH2 | 5.13 | 1.39 | 1.33 |
| 81 | DA | 2855 | U | O4'-C1' | 5.13 | 1.48 | 1.41 |
| 38 | Bs | 184 | GLY | C-N | 5.13 | 1.45 | 1.34 |
| 78 | CA | 1419 | G | O4'-C1' | 5.13 | 1.48 | 1.41 |
| 81 | DA | 1400 | G | C2'-C1' | 5.13 | 1.58 | 1.53 |
| 81 | DA | 2964 | G | C2'-C1' | 5.12 | 1.58 | 1.53 |
| 33 | BD | 198 | ARG | CZ-NH2 | 5.12 | 1.39 | 1.33 |
| 81 | DA | 1755 | C | C5'-C4' | 5.12 | 1.57 | 1.51 |
| 41 | BN | 117 | ARG | NE-CZ | 5.12 | 1.39 | 1.33 |
| 50 | BX | 64 | GLU | CD-OE1 | 5.12 | 1.31 | 1.25 |
| 81 | DA | 689 | U | O4'-C1' | 5.12 | 1.48 | 1.41 |
| 81 | DA | 776 | U | C4'-C3' | -5.12 | 1.47 | 1.52 |
| 81 | DA | 1427 | U | C2'-C1' | -5.12 | 1.47 | 1.53 |
| 52 | BY | 74 | TYR | CG-CD2 | 5.12 | 1.45 | 1.39 |
| 78 | CA | 1669 | U | C2'-C1' | -5.12 | 1.47 | 1.53 |
| 81 | DA | 195 | U | O4'-C1' | 5.12 | 1.48 | 1.41 |
| 81 | DA | 1783 | U | O3'-P | -5.12 | 1.55 | 1.61 |
| 21 | AT | 29 | HIS | N-CA | 5.12 | 1.56 | 1.46 |
| 81 | DA | 167 | U | C2'-C1' | 5.12 | 1.58 | 1.53 |
| 78 | CA | 1355 | C | O3'-P | -5.12 | 1.55 | 1.61 |
| 81 | DA | 2253 | G | C2'-C1' | -5.12 | 1.47 | 1.53 |
| 47 | BU | 92 | ARG | CZ-NH1 | 5.11 | 1.39 | 1.33 |
| 78 | CA | 116 | U | O4'-C1' | 5.11 | 1.48 | 1.41 |
| 79 | CB | 14 | A | C2'-C1' | -5.11 | 1.47 | 1.53 |
| 78 | CA | 998 | A | C2'-C1' | -5.11 | 1.47 | 1.53 |
| 81 | DA | 178 | U | C4'-O4' | -5.11 | 1.39 | 1.45 |
| 81 | DA | 1186 | G | C2'-C1' | -5.11 | 1.47 | 1.53 |
| 29 | AU | 8 | ARG | CZ-NH2 | 5.11 | 1.39 | 1.33 |
| 81 | DA | 99 | A | C2'-C1' | -5.11 | 1.47 | 1.53 |
| 81 | DA | 266 | A | C2'-C1' | 5.11 | 1.58 | 1.53 |
| 81 | DA | 1285 | G | O3'-P | -5.11 | 1.55 | 1.61 |
| 78 | CA | 1472 | C | C2'-C1' | 5.11 | 1.58 | 1.53 |
| 81 | DA | 624 | G | O4'-C1' | 5.11 | 1.48 | 1.41 |
| 81 | DA | 1606 | U | O4'-C1' | 5.11 | 1.48 | 1.41 |
| 81 | DA | 2497 | U | O3'-P | -5.11 | 1.55 | 1.61 |
| 26 | AZ | 43 | ARG | CZ-NH1 | 5.11 | 1.39 | 1.33 |
| 78 | CA | 1405 | G | C3'-C2' | -5.11 | 1.47 | 1.52 |
| 81 | DA | 740 | G | C6-N1 | 5.11 | 1.43 | 1.39 |
| 81 | DA | 2503 | G | O3'-P | -5.11 | 1.55 | 1.61 |
| 81 | DA | 2612 | U | C2'-C1' | -5.11 | 1.47 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 14 | AM | 120 | ARG | CZ-NH2 | 5.10 | 1.39 | 1.33 |
| 34 | BE | 52 | TYR | CA-C | 5.10 | 1.66 | 1.52 |
| 78 | CA | 46 | A | P-O5' | -5.10 | 1.54 | 1.59 |
| 81 | DA | 1805 | C | O3'-P | -5.10 | 1.55 | 1.61 |
| 81 | DA | 1529 | A | C2'-C1' | -5.10 | 1.47 | 1.53 |
| 82 | DB | 33 | A | O3'-P | -5.10 | 1.55 | 1.61 |
| 32 | BC | 348 | ARG | CZ-NH2 | 5.10 | 1.39 | 1.33 |
| 43 | BP | 129 | TYR | CZ-OH | 5.10 | 1.46 | 1.37 |
| 58 | Bg | 72 | ARG | CD-NE | 5.10 | 1.55 | 1.46 |
| 78 | CA | 362 | G | C2'-C1' | -5.10 | 1.47 | 1.53 |
| 78 | CA | 1677 | C | O3'-P | -5.10 | 1.55 | 1.61 |
| 6 | AE | 19 | ARG | CZ-NH2 | 5.10 | 1.39 | 1.33 |
| 78 | CA | 667 | U | O3'-P | -5.10 | 1.55 | 1.61 |
| 78 | CA | 1665 | U | O4'-C1' | 5.10 | 1.48 | 1.41 |
| 81 | DA | 435 | C | C5'-C4' | 5.10 | 1.57 | 1.51 |
| 82 | DB | 84 | C | C2'-C1' | 5.10 | 1.58 | 1.53 |
| 14 | AM | 65 | GLU | CG-CD | -5.10 | 1.44 | 1.51 |
| 32 | BC | 17 | LEU | C-N | 5.10 | 1.44 | 1.34 |
| 44 | BO | 7 | LYS | CA-CB | 5.10 | 1.65 | 1.53 |
| 78 | CA | 650 | U | O3'-P | -5.10 | 1.55 | 1.61 |
| 78 | CA | 345 | U | O4'-C1' | 5.10 | 1.48 | 1.41 |
| 81 | DA | 2561 | A | C3'-O3' | 5.10 | 1.49 | 1.42 |
| 13 | AL | 107 | PHE | CE1-CZ | 5.09 | 1.47 | 1.37 |
| 14 | AM | 126 | ARG | NE-CZ | 5.09 | 1.39 | 1.33 |
| 78 | CA | 1080 | U | C4'-C3' | -5.09 | 1.47 | 1.52 |
| 81 | DA | 1266 | G | C2'-C1' | -5.09 | 1.47 | 1.53 |
| 81 | DA | 2510 | U | P-O5' | -5.09 | 1.54 | 1.59 |
| 81 | DA | 1767 | C | O3'-P | -5.09 | 1.55 | 1.61 |
| 6 | AE | 184 | VAL | CB-CG2 | 5.09 | 1.63 | 1.52 |
| 10 | AI | 92 | TYR | CE1-CZ | 5.09 | 1.45 | 1.38 |
| 81 | DA | 177 | U | O4'-C1' | 5.09 | 1.48 | 1.41 |
| 32 | BC | 362 | ALA | N-CA | -5.09 | 1.36 | 1.46 |
| 34 | BE | 89 | TYR | C-N | 5.09 | 1.45 | 1.34 |
| 60 | Bi | 17 | SER | CA-C | -5.09 | 1.39 | 1.52 |
| 69 | Br | 95 | GLY | CA-C | -5.09 | 1.43 | 1.51 |
| 81 | DA | 37 | U | C2'-C1' | 5.09 | 1.58 | 1.53 |
| 81 | DA | 925 | A | C2'-C1' | 5.09 | 1.58 | 1.53 |
| 81 | DA | 1109 | U | O3'-P | -5.09 | 1.55 | 1.61 |
| 81 | DA | 2692 | A | O4'-C1' | 5.09 | 1.48 | 1.41 |
| 81 | DA | 2823 | G | O4'-C1' | 5.09 | 1.48 | 1.41 |
| 83 | DC | 10 | C | O3'-P | -5.09 | 1.55 | 1.61 |
| 81 | DA | 483 | G | C2'-C1' | -5.09 | 1.47 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 971 | G | C2'-C1' | -5.09 | 1.47 | 1.53 |
| 49 | BV | 90 | PHE | CB-CG | -5.09 | 1.42 | 1.51 |
| 64 | Bl | 39 | TYR | N-CA | 5.09 | 1.56 | 1.46 |
| 81 | DA | 1693 | C | O4'-C1' | 5.09 | 1.48 | 1.41 |
| 81 | DA | 2153 | U | O4'-C1' | 5.08 | 1.48 | 1.41 |
| 22 | AV | 74 | SER | CA-CB | 5.08 | 1.60 | 1.52 |
| 47 | BU | 139 | ARG | CA-C | 5.08 | 1.66 | 1.52 |
| 62 | Bk | 45 | ARG | CZ-NH1 | 5.08 | 1.39 | 1.33 |
| 78 | CA | 660 | G | C4'-O4' | 5.08 | 1.52 | 1.45 |
| 78 | CA | 935 | U | C3'-C2' | -5.08 | 1.47 | 1.52 |
| 78 | CA | 1553 | G | C4'-C3' | -5.08 | 1.47 | 1.52 |
| 81 | DA | 1048 | A | C2'-C1' | -5.08 | 1.47 | 1.53 |
| 78 | CA | 1599 | C | C4'-C3' | -5.08 | 1.47 | 1.52 |
| 81 | DA | 11 | A | C2'-C1' | -5.08 | 1.47 | 1.53 |
| 81 | DA | 459 | G | C2'-C1' | -5.08 | 1.47 | 1.53 |
| 81 | DA | 1679 | A | C3'-C2' | -5.08 | 1.47 | 1.52 |
| 81 | DA | 2826 | U | O4'-C1' | 5.08 | 1.48 | 1.41 |
| 81 | DA | 796 | U | O3'-P | -5.08 | 1.55 | 1.61 |
| 81 | DA | 2274 | U | C2'-C1' | -5.08 | 1.47 | 1.53 |
| 78 | CA | 1337 | A | P-O5' | -5.08 | 1.54 | 1.59 |
| 81 | DA | 257 | U | C2'-C1' | -5.08 | 1.47 | 1.53 |
| 81 | DA | 1754 | G | C4'-C3' | 5.08 | 1.58 | 1.53 |
| 81 | DA | 2769 | A | O4'-C1' | 5.08 | 1.48 | 1.41 |
| 22 | AV | 77 | ARG | CZ-NH1 | 5.08 | 1.39 | 1.33 |
| 79 | CB | 46 | A | O4'-C1' | 5.08 | 1.48 | 1.41 |
| 81 | DA | 2326 | A | O4'-C1' | 5.08 | 1.48 | 1.41 |
| 81 | DA | 3071 | U | O4'-C1' | 5.08 | 1.48 | 1.41 |
| 33 | BD | 88 | GLY | N-CA | -5.08 | 1.38 | 1.46 |
| 52 | BY | 34 | PRO | N-CD | -5.08 | 1.40 | 1.47 |
| 78 | CA | 222 | A | C2'-C1' | 5.08 | 1.58 | 1.53 |
| 78 | CA | 581 | U | C2'-C1' | 5.08 | 1.58 | 1.53 |
| 78 | CA | 1241 | G | O3'-P | -5.08 | 1.55 | 1.61 |
| 81 | DA | 1061 | A | C3'-C2' | -5.08 | 1.47 | 1.52 |
| 81 | DA | 1920 | U | O4'-C1' | 5.08 | 1.48 | 1.41 |
| 78 | CA | 141 | U | C2'-C1' | 5.07 | 1.58 | 1.53 |
| 81 | DA | 457 | C | C2'-C1' | -5.07 | 1.47 | 1.53 |
| 81 | DA | 594 | U | O3'-P | -5.07 | 1.55 | 1.61 |
| 5 | AC | 95 | TYR | CG-CD1 | 5.07 | 1.45 | 1.39 |
| 61 | Bj | 70 | LYS | N-CA | -5.07 | 1.36 | 1.46 |
| 67 | Bp | 37 | ARG | CZ-NH2 | 5.07 | 1.39 | 1.33 |
| 81 | DA | 19 | U | C2'-C1' | -5.07 | 1.47 | 1.53 |
| 8 | AF | 166 | ARG | CZ-NH1 | 5.07 | 1.39 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 34 | BE | 41 | SER | C-N | 5.07 | 1.42 | 1.33 |
| 58 | Bg | 62 | ARG | CZ-NH1 | 5.07 | 1.39 | 1.33 |
| 78 | CA | 857 | U | C4'-C3' | -5.07 | 1.47 | 1.52 |
| 81 | DA | 2526 | C | C2'-C1' | -5.07 | 1.47 | 1.53 |
| 2 | AA | 229 | LYS | N-CA | -5.07 | 1.36 | 1.46 |
| 9 | AH | 101 | TYR | CZ-OH | 5.07 | 1.46 | 1.37 |
| 63 | Bm | 92 | ALA | C-O | 5.07 | 1.32 | 1.23 |
| 78 | CA | 307 | G | O3'-P | -5.07 | 1.55 | 1.61 |
| 6 | AE | 140 | ARG | NE-CZ | 5.07 | 1.39 | 1.33 |
| 78 | CA | 574 | G | C2-N3 | 5.07 | 1.36 | 1.32 |
| 35 | BG | 2 | SER | CB-OG | -5.07 | 1.35 | 1.42 |
| 44 | BO | 31 | GLY | CA-C | 5.07 | 1.59 | 1.51 |
| 81 | DA | 2715 | A | O4'-C1' | 5.07 | 1.48 | 1.41 |
| 81 | DA | 3297 | U | C2'-C1' | -5.07 | 1.47 | 1.53 |
| 46 | BT | 76 | SER | CA-CB | 5.06 | 1.60 | 1.52 |
| 51 | BZ | 17 | ARG | CZ-NH1 | 5.06 | 1.39 | 1.33 |
| 78 | CA | 990 | C | C4'-O4' | -5.06 | 1.39 | 1.45 |
| 78 | CA | 204 | G | C5'-C4' | 5.06 | 1.57 | 1.51 |
| 81 | DA | 937 | G | O4'-C1' | 5.06 | 1.48 | 1.41 |
| 81 | DA | 1153 | A | C2'-C1' | -5.06 | 1.47 | 1.53 |
| 81 | DA | 2266 | U | O4'-C1' | 5.06 | 1.48 | 1.41 |
| 32 | BC | 167 | ARG | CD-NE | 5.06 | 1.55 | 1.46 |
| 78 | CA | 1039 | A | C4'-O4' | 5.06 | 1.52 | 1.45 |
| 78 | CA | 464 | A | C4'-C3' | -5.06 | 1.47 | 1.52 |
| 78 | CA | 946 | U | C4'-C3' | -5.06 | 1.47 | 1.52 |
| 41 | BN | 121 | MET | CG-SD | 5.05 | 1.94 | 1.81 |
| 81 | DA | 980 | A | C4'-C3' | 5.05 | 1.58 | 1.53 |
| 81 | DA | 2669 | G | C2'-C1' | -5.05 | 1.47 | 1.53 |
| 81 | DA | 3059 | G | O4'-C1' | 5.05 | 1.48 | 1.41 |
| 81 | DA | 3302 | U | C2'-C1' | -5.05 | 1.47 | 1.53 |
| 83 | DC | 79 | U | O4'-C1' | 5.05 | 1.48 | 1.41 |
| 76 | BS | 23 | HIS | N-CA | -5.05 | 1.36 | 1.46 |
| 78 | CA | 909 | U | O4'-C1' | 5.05 | 1.48 | 1.41 |
| 81 | DA | 94 | G | C2'-O2' | 5.05 | 1.48 | 1.41 |
| 81 | DA | 1869 | C | O3'-P | 5.05 | 1.67 | 1.61 |
| 40 | BK | 117 | ARG | CZ-NH2 | 5.05 | 1.39 | 1.33 |
| 78 | CA | 1713 | G | C2'-C1' | -5.05 | 1.47 | 1.53 |
| 81 | DA | 2647 | A | C2'-C1' | 5.05 | 1.58 | 1.53 |
| 46 | BT | 97 | ARG | CZ-NH1 | 5.05 | 1.39 | 1.33 |
| 76 | BS | 28 | ARG | CZ-NH1 | 5.05 | 1.39 | 1.33 |
| 81 | DA | 2114 | C | O3'-P | -5.05 | 1.55 | 1.61 |
| 1 | Aa | 275 | ARG | CD-NE | 5.05 | 1.55 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | AA | 115 | PHE | CB-CG | 5.05 | 1.59 | 1.51 |
| 39 | BJ | 90 | ARG | NE-CZ | 5.05 | 1.39 | 1.33 |
| 44 | BO | 8 | THR | CA-CB | 5.05 | 1.66 | 1.53 |
| 81 | DA | 1748 | G | O4'-C1' | -5.05 | 1.35 | 1.41 |
| 81 | DA | 1794 | G | C2'-C1' | 5.05 | 1.58 | 1.53 |
| 81 | DA | 1930 | A | O4'-C1' | 5.05 | 1.48 | 1.41 |
| 81 | DA | 3364 | C | P-O5' | -5.05 | 1.54 | 1.59 |
| 83 | DC | 89 | A | O4'-C1' | 5.04 | 1.48 | 1.41 |
| 78 | CA | 915 | A | O4'-C1' | 5.04 | 1.48 | 1.41 |
| 81 | DA | 940 | G | C2'-C1' | -5.04 | 1.47 | 1.53 |
| 81 | DA | 3211 | C | P-O5' | -5.04 | 1.54 | 1.59 |
| 81 | DA | 3339 | A | O4'-C1' | 5.04 | 1.48 | 1.41 |
| 4 | AD | 219 | VAL | CA-CB | 5.04 | 1.65 | 1.54 |
| 58 | Bg | 68 | GLU | CB-CG | 5.04 | 1.61 | 1.52 |
| 81 | DA | 3017 | A | O4'-C1' | 5.04 | 1.48 | 1.41 |
| 81 | DA | 947 | G | O3'-P | -5.04 | 1.55 | 1.61 |
| 32 | BC | 5 | LYS | CA-CB | -5.04 | 1.42 | 1.53 |
| 81 | DA | 659 | G | C2'-C1' | -5.04 | 1.47 | 1.53 |
| 81 | DA | 2056 | U | O4'-C1' | 5.04 | 1.48 | 1.41 |
| 81 | DA | 130 | A | O4'-C1' | 5.04 | 1.48 | 1.41 |
| 81 | DA | 212 | G | C2'-C1' | 5.04 | 1.58 | 1.53 |
| 78 | CA | 41 | A | O4'-C1' | 5.04 | 1.48 | 1.41 |
| 78 | CA | 219 | A | O3'-P | -5.04 | 1.55 | 1.61 |
| 78 | CA | 343 | C | C2'-C1' | -5.04 | 1.47 | 1.53 |
| 78 | CA | 969 | C | C2'-C1' | -5.04 | 1.47 | 1.53 |
| 81 | DA | 672 | A | C3'-O3' | -5.04 | 1.35 | 1.42 |
| 81 | DA | 696 | C | C2'-C1' | -5.04 | 1.47 | 1.53 |
| 81 | DA | 3201 | C | O3'-P | -5.04 | 1.55 | 1.61 |
| 78 | CA | 210 | A | P-O5' | -5.03 | 1.54 | 1.59 |
| 81 | DA | 1739 | U | P-O5' | -5.03 | 1.54 | 1.59 |
| 81 | DA | 2350 | C | O3'-P | -5.03 | 1.55 | 1.61 |
| 82 | DB | 156 | U | C2'-C1' | 5.03 | 1.58 | 1.53 |
| 81 | DA | 2328 | U | C2'-C1' | -5.03 | 1.47 | 1.53 |
| 81 | DA | 2993 | G | O4'-C1' | 5.03 | 1.48 | 1.41 |
| 62 | Bk | 36 | ARG | NE-CZ | 5.03 | 1.39 | 1.33 |
| 81 | DA | 747 | A | C3'-O3' | -5.03 | 1.35 | 1.42 |
| 81 | DA | 2049 | A | C2'-C1' | 5.03 | 1.58 | 1.53 |
| 81 | DA | 2472 | U | O4'-C1' | 5.03 | 1.48 | 1.41 |
| 37 | BH | 73 | PRO | C-N | 5.03 | 1.45 | 1.34 |
| 78 | CA | 1233 | G | C3'-O3' | -5.03 | 1.35 | 1.42 |
| 62 | Bk | 25 | LYS | N-CA | 5.03 | 1.56 | 1.46 |
| 78 | CA | 1551 | U | C3'-C2' | 5.03 | 1.58 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 736 | A | O3'-P | -5.03 | 1.55 | 1.61 |
| 81 | DA | 2099 | A | C3'-O3' | -5.03 | 1.35 | 1.42 |
| 81 | DA | 2132 | C | O4'-C1' | 5.03 | 1.48 | 1.41 |
| 6 | AE | 224 | PHE | CG-CD2 | 5.03 | 1.46 | 1.38 |
| 13 | AL | 47 | SER | CA-CB | 5.03 | 1.60 | 1.52 |
| 21 | AT | 87 | ARG | C-OXT | 5.03 | 1.32 | 1.23 |
| 76 | BS | 153 | LEU | CA-C | -5.03 | 1.39 | 1.52 |
| 78 | CA | 832 | U | C4'-O4' | -5.03 | 1.39 | 1.45 |
| 78 | CA | 1459 | C | C5'-C4' | 5.03 | 1.57 | 1.51 |
| 78 | CA | 1535 | U | P-O5' | -5.03 | 1.54 | 1.59 |
| 81 | DA | 408 | A | O4'-C1' | 5.03 | 1.48 | 1.41 |
| 81 | DA | 2307 | G | O4'-C1' | 5.03 | 1.48 | 1.41 |
| 81 | DA | 377 | A | C2'-C1' | -5.02 | 1.47 | 1.53 |
| 81 | DA | 1545 | A | O4'-C1' | 5.02 | 1.48 | 1.41 |
| 6 | AE | 74 | PRO | C-N | 5.02 | 1.42 | 1.33 |
| 62 | Bk | 55 | ARG | CZ-NH2 | 5.02 | 1.39 | 1.33 |
| 78 | CA | 384 | G | C2'-C1' | -5.02 | 1.47 | 1.53 |
| 78 | CA | 1089 | U | O4'-C1' | 5.02 | 1.48 | 1.41 |
| 78 | CA | 1321 | A | O3'-P | -5.02 | 1.55 | 1.61 |
| 81 | DA | 83 | U | O4'-C1' | 5.02 | 1.48 | 1.41 |
| 81 | DA | 1322 | U | C2'-C1' | -5.02 | 1.47 | 1.53 |
| 32 | BC | 210 | GLU | CB-CG | 5.02 | 1.61 | 1.52 |
| 37 | BH | 68 | ARG | CD-NE | 5.02 | 1.54 | 1.46 |
| 78 | CA | 1560 | U | C4'-C3' | -5.02 | 1.47 | 1.52 |
| 78 | CA | 1784 | C | O4'-C1' | 5.02 | 1.48 | 1.41 |
| 79 | CB | 50 | G | O4'-C1' | -5.02 | 1.35 | 1.41 |
| 81 | DA | 1468 | A | C2'-C1' | -5.02 | 1.47 | 1.53 |
| 81 | DA | 2608 | G | O4'-C1' | 5.02 | 1.48 | 1.41 |
| 81 | DA | 2810 | C | C2'-C1' | -5.02 | 1.47 | 1.53 |
| 82 | DB | 47 | C | O3'-P | -5.02 | 1.55 | 1.61 |
| 5 | AC | 132 | ARG | CZ-NH2 | 5.02 | 1.39 | 1.33 |
| 81 | DA | 2988 | C | C2'-C1' | 5.02 | 1.58 | 1.53 |
| 4 | AD | 54 | TYR | CZ-OH | 5.01 | 1.46 | 1.37 |
| 29 | AU | 90 | ARG | CZ-NH2 | 5.01 | 1.39 | 1.33 |
| 74 | BQ | 190 | ILE | C-N | 5.01 | 1.45 | 1.34 |
| 78 | CA | 1206 | U | C4'-C3' | -5.01 | 1.47 | 1.52 |
| 81 | DA | 884 | A | C2'-C1' | 5.01 | 1.58 | 1.53 |
| 81 | DA | 2487 | U | C3'-C2' | 5.01 | 1.58 | 1.52 |
| 78 | CA | 514 | G | C4'-C3' | -5.01 | 1.47 | 1.52 |
| 81 | DA | 1228 | C | C2'-C1' | -5.01 | 1.47 | 1.53 |
| 81 | DA | 1722 | U | O4'-C1' | 5.01 | 1.48 | 1.41 |
| 83 | DC | 33 | U | O4'-C1' | 5.01 | 1.48 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | AS | 80 | TYR | CZ-OH | 5.01 | 1.46 | 1.37 |
| 78 | CA | 1077 | C | O4'-C1' | 5.01 | 1.48 | 1.41 |
| 81 | DA | 1150 | A | C2'-C1' | -5.01 | 1.47 | 1.53 |
| 61 | Bj | 3 | GLU | CB-CG | 5.01 | 1.61 | 1.52 |
| 78 | CA | 1367 | G | O3'-P | -5.01 | 1.55 | 1.61 |
| 81 | DA | 474 | G | C2'-C1' | -5.01 | 1.47 | 1.53 |
| 81 | DA | 2925 | C | C4'-C3' | -5.01 | 1.47 | 1.52 |
| 81 | DA | 3355 | U | O4'-C1' | 5.01 | 1.48 | 1.41 |
| 78 | CA | 985 | G | C2'-C1' | -5.01 | 1.47 | 1.53 |
| 78 | CA | 1605 | G | C2'-C1' | -5.01 | 1.47 | 1.53 |
| 81 | DA | 22 | G | O4'-C1' | 5.01 | 1.48 | 1.41 |
| 81 | DA | 525 | C | C2'-C1' | 5.01 | 1.58 | 1.53 |
| 29 | AU | 10 | ARG | CZ-NH2 | 5.01 | 1.39 | 1.33 |
| 32 | BC | 6 | TYR | N-CA | 5.01 | 1.56 | 1.46 |
| 78 | CA | 826 | U | C4'-C3' | -5.01 | 1.47 | 1.52 |
| 81 | DA | 672 | A | C4'-C3' | -5.01 | 1.47 | 1.52 |
| 81 | DA | 919 | U | C2'-C1' | -5.01 | 1.47 | 1.53 |
| 81 | DA | 2500 | A | O3'-P | -5.01 | 1.55 | 1.61 |
| 59 | Bh | 44 | ARG | CZ-NH1 | 5.00 | 1.39 | 1.33 |
| 81 | DA | 519 | A | P-O5' | -5.00 | 1.54 | 1.59 |
| 81 | DA | 1865 | A | C2'-C1' | 5.00 | 1.58 | 1.53 |
| 81 | DA | 1959 | G | O4'-C1' | 5.00 | 1.48 | 1.41 |
| 32 | BC | 228 | GLY | CA-C | -5.00 | 1.43 | 1.51 |
| 43 | BP | 38 | ARG | CZ-NH2 | 5.00 | 1.39 | 1.33 |
| 56 | Bf | 54 | SER | CB-OG | 5.00 | 1.48 | 1.42 |
| 60 | Bi | 16 | ARG | CD-NE | 5.00 | 1.54 | 1.46 |
| 81 | DA | 1319 | G | O3'-P | -5.00 | 1.55 | 1.61 |
| 81 | DA | 2115 | G | O4'-C1' | 5.00 | 1.48 | 1.41 |

All (14979) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 32 | BC | 266 | ARG | NE-CZ-NH1 | -73.84 | 83.38 | 120.30 |
| 81 | DA | 3305 | A | P-O3'-C3' | 50.10 | 179.82 | 119.70 |
| 81 | DA | 3047 | U | P-O3'-C3' | 47.61 | 176.83 | 119.70 |
| 81 | DA | 2046 | U | P-O3'-C3' | 47.25 | 176.40 | 119.70 |
| 81 | DA | 2071 | A | P-O3'-C3' | 46.20 | 175.13 | 119.70 |
| 11 | AJ | 14 | GLN | CG-CD-OE1 | -45.24 | 31.12 | 121.60 |
| 81 | DA | 2079 | G | P-O3'-C3' | 44.97 | 173.66 | 119.70 |
| 81 | DA | 3215 | A | N9-C1'-C2' | 44.22 | 171.49 | 114.00 |
| 78 | CA | 1677 | C | P-O3'-C3' | 44.20 | 172.74 | 119.70 |
| 81 | DA | 1221 | A | O4'-C1'-N9 | 44.12 | 143.49 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 5 | AC | 142 | ASN | CB-CG-OD1 | -43.56 | 34.48 | 121.60 |
| 81 | DA | 2480 | A | P-O3'-C3' | 43.30 | 171.66 | 119.70 |
| 81 | DA | 2362 | C | O4'-C1'-N1 | 42.49 | 142.19 | 108.20 |
| 81 | DA | 2915 | U | P-O3'-C3' | 41.56 | 169.57 | 119.70 |
| 78 | CA | 46 | A | O4'-C1'-N9 | 40.67 | 140.74 | 108.20 |
| 81 | DA | 2870 | C | P-O3'-C3' | 39.77 | 167.42 | 119.70 |
| 78 | CA | 29 | U | P-O3'-C3' | 39.75 | 167.40 | 119.70 |
| 81 | DA | 2208 | A | P-O3'-C3' | 38.89 | 166.37 | 119.70 |
| 62 | Bk | 25 | LYS | O-C-N | -38.10 | 61.74 | 122.70 |
| 57 | Be | 202 | LEU | O-C-N | -37.88 | 62.10 | 122.70 |
| 81 | DA | 1755 | C | P-O3'-C3' | 37.73 | 164.98 | 119.70 |
| 55 | Bc | 104 | GLN | O-C-N | -37.62 | 62.51 | 122.70 |
| 78 | CA | 295 | A | O4'-C1'-N9 | 37.49 | 138.20 | 108.20 |
| 81 | DA | 3222 | U | P-O3'-C3' | 37.41 | 164.59 | 119.70 |
| 81 | DA | 1432 | C | O4'-C1'-N1 | 37.35 | 138.08 | 108.20 |
| 35 | BG | 5 | LYS | O-C-N | -37.12 | 63.30 | 122.70 |
| 74 | BQ | 197 | SER | O-C-N | -36.80 | 63.82 | 122.70 |
| 10 | AI | 54 | LEU | O-C-N | -36.80 | 63.82 | 122.70 |
| 22 | AV | 26 | LYS | O-C-N | -36.79 | 63.83 | 122.70 |
| 81 | DA | 855 | U | P-O3'-C3' | 36.76 | 163.81 | 119.70 |
| 65 | Bn | 71 | PRO | O-C-N | -36.61 | 64.12 | 122.70 |
| 40 | BK | 184 | THR | O-C-N | -36.55 | 64.23 | 122.70 |
| 21 | AT | 9 | VAL | O-C-N | -36.37 | 64.50 | 122.70 |
| 18 | AP | 57 | LYS | O-C-N | -36.28 | 64.66 | 122.70 |
| 81 | DA | 2279 | A | P-O3'-C3' | 36.19 | 163.12 | 119.70 |
| 2 | AA | 229 | LYS | O-C-N | -36.06 | 65.00 | 122.70 |
| 45 | BR | 157 | PRO | O-C-N | -36.06 | 65.00 | 122.70 |
| 81 | DA | 1771 | C | P-O3'-C3' | 35.90 | 162.78 | 119.70 |
| 31 | BB | 62 | VAL | O-C-N | -35.78 | 65.44 | 122.70 |
| 60 | Bi | 16 | ARG | O-C-N | -35.71 | 65.56 | 122.70 |
| 81 | DA | 858 | A | P-O3'-C3' | 35.62 | 162.45 | 119.70 |
| 32 | BC | 368 | GLY | O-C-N | -35.46 | 65.97 | 122.70 |
| 44 | BO | 40 | HIS | O-C-N | -35.43 | 66.01 | 122.70 |
| 38 | Bs | 5 | ARG | O-C-N | -35.30 | 66.21 | 122.70 |
| 45 | BR | 140 | LEU | O-C-N | -35.21 | 66.36 | 122.70 |
| 83 | DC | 48 | U | P-O3'-C3' | 35.17 | 161.90 | 119.70 |
| 3 | AB | 78 | LYS | O-C-N | -35.16 | 66.44 | 122.70 |
| 78 | CA | 1702 | A | O4'-C1'-N9 | 35.05 | 136.24 | 108.20 |
| 18 | AP | 122 | ILE | O-C-N | -35.03 | 66.65 | 122.70 |
| 44 | BO | 3 | SER | O-C-N | -34.97 | 66.75 | 122.70 |
| 81 | DA | 834 | U | P-O3'-C3' | 34.90 | 161.58 | 119.70 |
| 6 | AE | 7 | GLN | O-C-N | -34.81 | 67.00 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 26 | AZ | 44 | PHE | O-C-N | -34.67 | 67.23 | 122.70 |
| 74 | BQ | 123 | GLU | O-C-N | -34.42 | 67.62 | 122.70 |
| 81 | DA | 3221 | C | C3'-C2'-C1' | 34.38 | 129.00 | 101.50 |
| 32 | BC | 381 | GLY | O-C-N | -34.37 | 67.71 | 122.70 |
| 13 | AL | 34 | LEU | O-C-N | -34.30 | 64.89 | 123.20 |
| 81 | DA | 671 | U | P-O3'-C3' | 34.26 | 160.81 | 119.70 |
| 76 | BS | 15 | GLY | O-C-N | -34.08 | 68.17 | 122.70 |
| 81 | DA | 3382 | U | P-O3'-C3' | 33.95 | 160.43 | 119.70 |
| 2 | AA | 11 | PRO | O-C-N | -33.93 | 68.42 | 122.70 |
| 17 | AQ | 63 | LYS | O-C-N | -33.91 | 65.55 | 123.20 |
| 51 | BZ | 51 | TRP | O-C-N | -33.78 | 68.66 | 122.70 |
| 17 | AQ | 26 | LEU | O-C-N | -33.70 | 68.78 | 122.70 |
| 36 | BF | 2 | LYS | O-C-N | -33.64 | 68.88 | 122.70 |
| 74 | BQ | 238 | ASP | O-C-N | -33.62 | 68.91 | 122.70 |
| 81 | DA | 2174 | G | P-O3'-C3' | 33.44 | 159.83 | 119.70 |
| 14 | AM | 99 | HIS | O-C-N | -33.44 | 69.20 | 122.70 |
| 81 | DA | 2637 | A | O4'-C1'-N9 | 33.32 | 134.86 | 108.20 |
| 33 | BD | 331 | ALA | O-C-N | -33.17 | 69.63 | 122.70 |
| 17 | AQ | 81 | LYS | O-C-N | -33.16 | 69.64 | 122.70 |
| 74 | BQ | 237 | GLU | O-C-N | -33.10 | 69.75 | 122.70 |
| 81 | DA | 704 | U | P-O3'-C3' | 33.08 | 159.40 | 119.70 |
| 78 | CA | 1676 | U | P-O3'-C3' | 33.08 | 159.39 | 119.70 |
| 81 | DA | 2989 | U | O4'-C1'-C2' | -32.86 | 72.94 | 105.80 |
| 48 | BW | 93 | ILE | O-C-N | -32.77 | 70.27 | 122.70 |
| 44 | BO | 7 | LYS | O-C-N | -32.74 | 70.32 | 122.70 |
| 74 | BQ | 201 | GLY | O-C-N | -32.66 | 67.67 | 123.20 |
| 81 | DA | 2257 | C | O4'-C1'-N1 | 32.65 | 134.32 | 108.20 |
| 81 | DA | 1633 | C | P-O3'-C3' | 32.62 | 158.84 | 119.70 |
| 78 | CA | 636 | A | C1'-O4'-C4' | 32.49 | 135.89 | 109.90 |
| 74 | BQ | 115 | LEU | O-C-N | -32.42 | 70.83 | 122.70 |
| 69 | Br | 58 | PHE | O-C-N | -32.40 | 70.85 | 122.70 |
| 53 | Ba | 13 | VAL | O-C-N | -32.40 | 70.86 | 122.70 |
| 33 | BD | 78 | GLY | O-C-N | -32.28 | 68.32 | 123.20 |
| 26 | AZ | 40 | TYR | O-C-N | -32.22 | 71.15 | 122.70 |
| 4 | AD | 96 | ASN | O-C-N | -32.17 | 71.23 | 122.70 |
| 40 | BK | 63 | ALA | O-C-N | -32.14 | 71.27 | 122.70 |
| 34 | BE | 123 | PHE | O-C-N | -32.05 | 68.71 | 123.20 |
| 81 | DA | 2509 | U | P-O3'-C3' | 32.03 | 158.14 | 119.70 |
| 13 | AL | 134 | ALA | O-C-N | -31.99 | 71.52 | 122.70 |
| 81 | DA | 2648 | G | O4'-C1'-N9 | 31.96 | 133.77 | 108.20 |
| 45 | BR | 143 | PRO | O-C-N | -31.94 | 71.59 | 122.70 |
| 32 | BC | 362 | ALA | O-C-N | -31.93 | 71.60 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 11 | AJ | 119 | ALA | O-C-N | -31.89 | 71.67 | 122.70 |
| 5 | AC | 157 | ASP | O-C-N | -31.84 | 71.75 | 122.70 |
| 65 | Bn | 35 | GLY | O-C-N | -31.80 | 71.82 | 122.70 |
| 65 | Bn | 35 | GLY | CA-C-O | -31.79 | 63.37 | 120.60 |
| 81 | DA | 1256 | G | P-O3'-C3' | 31.79 | 157.85 | 119.70 |
| 45 | BR | 95 | GLU | O-C-N | -31.79 | 71.84 | 122.70 |
| 81 | DA | 1841 | A | P-O3'-C3' | 31.77 | 157.83 | 119.70 |
| 9 | AH | 66 | ASN | O-C-N | -31.75 | 69.23 | 123.20 |
| 31 | BB | 252 | THR | O-C-N | -31.74 | 71.92 | 122.70 |
| 60 | Bi | 68 | THR | O-C-N | -31.73 | 71.93 | 122.70 |
| 81 | DA | 3313 | U | P-O3'-C3' | 31.72 | 157.76 | 119.70 |
| 4 | AD | 153 | ASN | O-C-N | -31.65 | 72.06 | 122.70 |
| 74 | BQ | 201 | GLY | CA-C-O | -31.59 | 63.73 | 120.60 |
| 81 | DA | 2668 | U | P-O3'-C3' | 31.56 | 157.57 | 119.70 |
| 81 | DA | 2030 | C | P-O3'-C3' | 31.55 | 157.56 | 119.70 |
| 31 | BB | 249 | SER | O-C-N | -31.52 | 72.26 | 122.70 |
| 35 | BG | 27 | PRO | O-C-N | -31.48 | 72.32 | 122.70 |
| 81 | DA | 1989 | U | P-O3'-C3' | 31.45 | 157.44 | 119.70 |
| 33 | BD | 84 | ARG | O-C-N | -31.45 | 72.38 | 122.70 |
| 32 | BC | 297 | SER | O-C-N | -31.41 | 72.45 | 122.70 |
| 35 | BG | 38 | THR | O-C-N | -31.39 | 72.47 | 122.70 |
| 32 | BC | 3 | HIS | O-C-N | -31.39 | 72.48 | 122.70 |
| 81 | DA | 2865 | U | P-O3'-C3' | 31.37 | 157.34 | 119.70 |
| 32 | BC | 298 | PHE | O-C-N | -31.33 | 72.57 | 122.70 |
| 81 | DA | 3341 | U | P-O3'-C3' | 31.27 | 157.22 | 119.70 |
| 78 | CA | 141 | U | P-O3'-C3' | 31.26 | 157.21 | 119.70 |
| 40 | BK | 69 | GLY | CA-C-O | -31.18 | 64.47 | 120.60 |
| 81 | DA | 1233 | G | O4'-C1'-N9 | 31.18 | 133.14 | 108.20 |
| 81 | DA | 1261 | G | C1'-O4'-C4' | 31.13 | 134.80 | 109.90 |
| 78 | CA | 1190 | C | O5'-P-OP1 | 31.12 | 148.05 | 110.70 |
| 17 | AQ | 82 | ASP | O-C-N | -31.06 | 73.01 | 122.70 |
| 81 | DA | 594 | U | P-O3'-C3' | 31.04 | 156.95 | 119.70 |
| 81 | DA | 2899 | C | P-O3'-C3' | 31.03 | 156.93 | 119.70 |
| 81 | DA | 1261 | G | O4'-C1'-N9 | 31.02 | 133.02 | 108.20 |
| 46 | BT | 82 | LYS | O-C-N | -31.00 | 70.50 | 123.20 |
| 33 | BD | 89 | ALA | O-C-N | -30.99 | 73.11 | 122.70 |
| 61 | Bj | 8 | TYR | O-C-N | -30.95 | 73.18 | 122.70 |
| 4 | AD | 94 | ALA | O-C-N | -30.95 | 73.19 | 122.70 |
| 60 | Bi | 77 | GLY | O-C-N | -30.88 | 70.70 | 123.20 |
| 78 | CA | 178 | U | P-O3'-C3' | 30.88 | 156.76 | 119.70 |
| 32 | BC | 360 | ASP | O-C-N | -30.84 | 73.36 | 122.70 |
| 81 | DA | 3041 | U | P-O3'-C3' | 30.82 | 156.69 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1560 | G | P-O3'-C3' | 30.78 | 156.63 | 119.70 |
| 3 | AB | 205 | ALA | O-C-N | -30.76 | 73.48 | 122.70 |
| 62 | Bk | 81 | THR | CA-C-O | -30.73 | 55.56 | 120.10 |
| 81 | DA | 1990 | U | P-O5'-C5' | 30.68 | 169.99 | 120.90 |
| 81 | DA | 671 | U | O4'-C1'-N1 | 30.63 | 132.71 | 108.20 |
| 81 | DA | 1401 | A | O4'-C1'-N9 | 30.62 | 132.70 | 108.20 |
| 44 | BO | 8 | THR | O-C-N | -30.58 | 73.78 | 122.70 |
| 32 | BC | 130 | PHE | O-C-N | -30.51 | 73.89 | 122.70 |
| 74 | BQ | 121 | GLY | CA-C-O | -30.50 | 65.69 | 120.60 |
| 38 | Bs | 72 | ASP | O-C-N | -30.50 | 73.90 | 122.70 |
| 64 | Bl | 39 | TYR | O-C-N | -30.34 | 63.45 | 121.10 |
| 74 | BQ | 121 | GLY | O-C-N | -30.31 | 74.21 | 122.70 |
| 81 | DA | 3149 | G | O4'-C1'-N9 | 30.25 | 132.40 | 108.20 |
| 33 | BD | 321 | LYS | O-C-N | -30.24 | 74.32 | 122.70 |
| 20 | AS | 90 | PRO | O-C-N | -30.22 | 74.34 | 122.70 |
| 69 | Br | 89 | LYS | O-C-N | -30.19 | 74.40 | 122.70 |
| 78 | CA | 1546 | G | C3'-C2'-C1' | -30.16 | 77.37 | 101.50 |
| 60 | Bi | 78 | GLY | O-C-N | -30.15 | 74.46 | 122.70 |
| 81 | DA | 969 | C | O4'-C1'-N1 | 30.12 | 132.29 | 108.20 |
| 26 | AZ | 39 | LEU | O-C-N | -30.11 | 74.52 | 122.70 |
| 18 | AP | 40 | LEU | O-C-N | -30.11 | 72.02 | 123.20 |
| 34 | BE | 9 | MET | O-C-N | -30.09 | 74.55 | 122.70 |
| 46 | BT | 71 | ARG | O-C-N | -30.04 | 74.63 | 122.70 |
| 43 | BP | 80 | THR | O-C-N | -29.99 | 74.71 | 122.70 |
| 81 | DA | 2989 | U | N1-C1'-C2' | 29.95 | 152.94 | 114.00 |
| 74 | BQ | 128 | GLU | O-C-N | -29.94 | 74.80 | 122.70 |
| 59 | Bh | 12 | LYS | O-C-N | -29.90 | 74.87 | 122.70 |
| 60 | Bi | 78 | GLY | CA-C-O | -29.84 | 66.88 | 120.60 |
| 32 | BC | 289 | ASP | CA-C-O | -29.83 | 57.46 | 120.10 |
| 78 | CA | 1302 | U | P-O3'-C3' | 29.82 | 155.48 | 119.70 |
| 62 | Bk | 83 | ALA | CA-C-O | -29.81 | 57.50 | 120.10 |
| 81 | DA | 636 | C | P-O3'-C3' | 29.80 | 155.46 | 119.70 |
| 81 | DA | 220 | G | O4'-C1'-N9 | 29.80 | 132.04 | 108.20 |
| 33 | BD | 323 | VAL | O-C-N | -29.79 | 75.04 | 122.70 |
| 34 | BE | 89 | TYR | O-C-N | -29.78 | 75.05 | 122.70 |
| 2 | AA | 250 | VAL | O-C-N | -29.76 | 75.09 | 122.70 |
| 78 | CA | 1386 | G | O4'-C1'-N9 | 29.73 | 131.99 | 108.20 |
| 81 | DA | 1270 | A | O4'-C1'-N9 | 29.69 | 131.96 | 108.20 |
| 45 | BR | 98 | LYS | O-C-N | -29.67 | 75.23 | 122.70 |
| 32 | BC | 289 | ASP | O-C-N | -29.66 | 75.25 | 122.70 |
| 60 | Bi | 77 | GLY | CA-C-O | -29.64 | 67.24 | 120.60 |
| 79 | CB | 72 | G | O4'-C1'-N9 | 29.64 | 131.91 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 47 | BU | 126 | VAL | O-C-N | -29.58 | 75.38 | 122.70 |
| 82 | DB | 44 | A | P-O3'-C3' | 29.55 | 155.15 | 119.70 |
| 6 | AE | 4 | PRO | O-C-N | -29.52 | 75.46 | 122.70 |
| 60 | Bi | 79 | SER | O-C-N | -29.52 | 75.47 | 122.70 |
| 4 | AD | 93 | ASP | O-C-N | -29.50 | 75.49 | 122.70 |
| 81 | DA | 2737 | C | P-O3'-C3' | 29.50 | 155.11 | 119.70 |
| 60 | Bi | 108 | GLN | O-C-N | -29.47 | 75.55 | 122.70 |
| 81 | DA | 1207 | G | N9-C1'-C2' | 29.46 | 152.30 | 114.00 |
| 43 | BP | 74 | PRO | O-C-N | -29.44 | 75.59 | 122.70 |
| 48 | BW | 90 | ARG | O-C-N | -29.34 | 75.76 | 122.70 |
| 81 | DA | 1947 | G | O4'-C1'-N9 | 29.31 | 131.65 | 108.20 |
| 81 | DA | 2758 | A | O4'-C1'-N9 | 29.31 | 131.65 | 108.20 |
| 44 | BO | 142 | GLY | O-C-N | -29.25 | 73.48 | 123.20 |
| 74 | BQ | 129 | TYR | O-C-N | -29.23 | 75.93 | 122.70 |
| 65 | Bn | 34 | ALA | O-C-N | -29.19 | 73.58 | 123.20 |
| 81 | DA | 2956 | A | P-O3'-C3' | 29.19 | 154.72 | 119.70 |
| 81 | DA | 791 | A | P-O3'-C3' | 29.11 | 154.63 | 119.70 |
| 78 | CA | 1437 | U | P-O3'-C3' | 29.05 | 154.56 | 119.70 |
| 32 | BC | 5 | LYS | O-C-N | -29.04 | 76.23 | 122.70 |
| 20 | AS | 102 | ARG | NE-CZ-NH2 | -29.04 | 105.78 | 120.30 |
| 32 | BC | 368 | GLY | CA-C-O | -29.01 | 68.39 | 120.60 |
| 78 | CA | 1080 | U | P-O3'-C3' | 29.00 | 154.50 | 119.70 |
| 33 | BD | 78 | GLY | CA-C-O | -28.99 | 68.41 | 120.60 |
| 81 | DA | 3080 | G | P-O3'-C3' | 28.96 | 154.46 | 119.70 |
| 35 | BG | 8 | LYS | O-C-N | -28.96 | 76.36 | 122.70 |
| 35 | BG | 3 | ALA | O-C-N | -28.92 | 76.43 | 122.70 |
| 35 | BG | 148 | GLU | O-C-N | -28.92 | 76.43 | 122.70 |
| 32 | BC | 381 | GLY | CA-C-O | -28.89 | 68.59 | 120.60 |
| 16 | AO | 67 | THR | O-C-N | -28.82 | 74.20 | 123.20 |
| 58 | Bg | 107 | VAL | O-C-N | -28.80 | 76.62 | 122.70 |
| 83 | DC | 28 | C | P-O3'-C3' | 28.78 | 154.23 | 119.70 |
| 6 | AE | 92 | ALA | O-C-N | -28.75 | 74.32 | 123.20 |
| 74 | BQ | 190 | ILE | O-C-N | -28.69 | 76.80 | 122.70 |
| 37 | BH | 89 | GLU | O-C-N | -28.69 | 76.80 | 122.70 |
| 78 | CA | 837 | G | P-O3'-C3' | 28.62 | 154.04 | 119.70 |
| 81 | DA | 1259 | A | O4'-C1'-N9 | 28.61 | 131.09 | 108.20 |
| 33 | BD | 148 | ILE | O-C-N | -28.57 | 66.81 | 121.10 |
| 78 | CA | 636 | A | N9-C1'-C2' | -28.56 | 76.87 | 114.00 |
| 34 | BE | 55 | ARG | CA-C-N | 28.54 | 179.99 | 117.20 |
| 81 | DA | 2468 | A | P-O3'-C3' | 28.53 | 153.94 | 119.70 |
| 62 | Bk | 83 | ALA | O-C-N | -28.52 | 77.07 | 122.70 |
| 5 | AC | 162 | SER | CA-C-O | -28.45 | 60.36 | 120.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 368 | U | P-O3'-C3' | 28.43 | 153.82 | 119.70 |
| 78 | CA | 1321 | A | O4'-C1'-N9 | 28.37 | 130.89 | 108.20 |
| 78 | CA | 1235 | C | O4'-C1'-N1 | 28.34 | 130.87 | 108.20 |
| 35 | BG | 152 | THR | CA-C-O | -28.32 | 60.64 | 120.10 |
| 79 | CB | 55 | C | N1-C1'-C2' | 28.27 | 150.75 | 114.00 |
| 78 | CA | 179 | A | O4'-C1'-N9 | 28.17 | 130.74 | 108.20 |
| 81 | DA | 3345 | G | P-O3'-C3' | 28.09 | 153.41 | 119.70 |
| 81 | DA | 2689 | A | P-O3'-C3' | 28.07 | 153.38 | 119.70 |
| 44 | BO | 142 | GLY | CA-C-O | -28.05 | 70.11 | 120.60 |
| 81 | DA | 2735 | U | P-O3'-C3' | 27.97 | 153.26 | 119.70 |
| 45 | BR | 142 | GLY | CA-C-O | -27.95 | 70.29 | 120.60 |
| 34 | BE | 123 | PHE | CA-C-O | -27.93 | 61.46 | 120.10 |
| 37 | BH | 73 | PRO | O-C-N | -27.92 | 78.03 | 122.70 |
| 78 | CA | 173 | A | O4'-C1'-N9 | 27.89 | 130.51 | 108.20 |
| 32 | BC | 17 | LEU | O-C-N | -27.89 | 68.11 | 121.10 |
| 81 | DA | 637 | C | P-O3'-C3' | 27.88 | 153.15 | 119.70 |
| 81 | DA | 636 | C | P-O5'-C5' | 27.76 | 165.32 | 120.90 |
| 81 | DA | 1260 | A | O4'-C1'-N9 | 27.73 | 130.39 | 108.20 |
| 31 | BB | 73 | GLU | O-C-N | -27.68 | 78.41 | 122.70 |
| 2 | AA | 195 | TRP | O-C-N | -27.66 | 78.45 | 122.70 |
| 78 | CA | 886 | U | O4'-C1'-N1 | 27.58 | 130.27 | 108.20 |
| 13 | AL | 87 | VAL | O-C-N | -27.58 | 68.70 | 121.10 |
| 81 | DA | 2187 | G | O4'-C1'-N9 | 27.56 | 130.25 | 108.20 |
| 53 | Ba | 60 | LYS | O-C-N | -27.45 | 78.79 | 122.70 |
| 33 | BD | 12 | THR | O-C-N | -27.43 | 76.58 | 123.20 |
| 81 | DA | 2783 | U | P-O3'-C3' | 27.42 | 152.61 | 119.70 |
| 35 | BG | 148 | GLU | CA-C-O | -27.38 | 62.61 | 120.10 |
| 78 | CA | 1 | U | O5'-P-OP2 | 27.29 | 143.45 | 110.70 |
| 47 | BU | 126 | VAL | CA-C-O | -27.26 | 62.85 | 120.10 |
| 81 | DA | 2497 | U | P-O3'-C3' | 27.26 | 152.41 | 119.70 |
| 3 | AB | 205 | ALA | CA-C-O | -27.24 | 62.89 | 120.10 |
| 31 | BB | 127 | ALA | O-C-N | -27.23 | 79.14 | 122.70 |
| 62 | Bk | 25 | LYS | CA-C-O | -27.22 | 62.95 | 120.10 |
| 78 | CA | 1755 | A | O4'-C1'-N9 | 27.21 | 129.97 | 108.20 |
| 80 | CC | 18 | C | OP2-P-O3' | 27.21 | 165.06 | 105.20 |
| 58 | Bg | 107 | VAL | CA-C-O | -27.18 | 63.02 | 120.10 |
| 76 | BS | 15 | GLY | CA-C-O | -27.18 | 71.68 | 120.60 |
| 40 | BK | 184 | THR | CA-C-O | -27.17 | 63.05 | 120.10 |
| 82 | DB | 132 | G | P-O3'-C3' | 27.12 | 152.24 | 119.70 |
| 13 | AL | 38 | PHE | CB-CG-CD2 | -27.11 | 101.83 | 120.80 |
| 81 | DA | 1991 | G | O4'-C1'-N9 | 27.00 | 129.80 | 108.20 |
| 62 | Bk | 81 | THR | O-C-N | -26.95 | 79.57 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 82 | DB | 96 | A | P-O3'-C3' | 26.94 | 152.02 | 119.70 |
| 78 | CA | 452 | A | O4'-C1'-N9 | 26.91 | 129.73 | 108.20 |
| 48 | BW | 90 | ARG | CA-C-O | -26.89 | 63.63 | 120.10 |
| 55 | Bc | 94 | LYS | O-C-N | -26.87 | 79.71 | 122.70 |
| 20 | AS | 96 | ALA | O-C-N | -26.86 | 79.73 | 122.70 |
| 81 | DA | 2998 | U | O4'-C1'-N1 | 26.78 | 129.62 | 108.20 |
| 55 | Bc | 94 | LYS | CA-C-O | -26.76 | 63.90 | 120.10 |
| 33 | BD | 84 | ARG | CA-C-O | -26.76 | 63.91 | 120.10 |
| 74 | BQ | 123 | GLU | CA-C-O | -26.71 | 64.00 | 120.10 |
| 81 | DA | 2510 | U | O4'-C1'-N1 | 26.65 | 129.52 | 108.20 |
| 78 | CA | 1191 | U | O4'-C1'-N1 | 26.64 | 129.51 | 108.20 |
| 81 | DA | 2093 | A | P-O3'-C3' | 26.58 | 151.60 | 119.70 |
| 81 | DA | 2064 | C | P-O3'-C3' | 26.53 | 151.54 | 119.70 |
| 32 | BC | 297 | SER | CA-C-O | -26.43 | 64.61 | 120.10 |
| 34 | BE | 89 | TYR | CA-C-O | -26.38 | 64.71 | 120.10 |
| 31 | BB | 73 | GLU | CA-C-O | -26.33 | 64.81 | 120.10 |
| 78 | CA | 1108 | G | O4'-C1'-N9 | 26.31 | 129.25 | 108.20 |
| 31 | BB | 196 | TRP | CA-C-O | -26.29 | 64.89 | 120.10 |
| 81 | DA | 2319 | U | O4'-C1'-N1 | 26.29 | 129.23 | 108.20 |
| 81 | DA | 406 | G | O4'-C1'-N9 | 26.28 | 129.22 | 108.20 |
| 81 | DA | 521 | A | O4'-C1'-N9 | 26.25 | 129.20 | 108.20 |
| 81 | DA | 419 | G | O4'-C1'-N9 | 26.23 | 129.18 | 108.20 |
| 39 | BJ | 75 | PRO | O-C-N | -26.18 | 80.81 | 122.70 |
| 81 | DA | 3221 | C | O4'-C1'-C2' | -26.17 | 79.63 | 105.80 |
| 78 | CA | 138 | A | O4'-C1'-N9 | 26.16 | 129.12 | 108.20 |
| 16 | AO | 67 | THR | CA-C-O | -26.14 | 65.20 | 120.10 |
| 45 | BR | 95 | GLU | CA-C-O | -26.14 | 65.21 | 120.10 |
| 83 | DC | 8 | G | P-O3'-C3' | 26.08 | 150.99 | 119.70 |
| 32 | BC | 256 | HIS | O-C-N | -26.07 | 71.57 | 121.10 |
| 78 | CA | 337 | G | P-O3'-C3' | 26.02 | 150.93 | 119.70 |
| 36 | BF | 2 | LYS | CA-C-O | -25.99 | 65.52 | 120.10 |
| 78 | CA | 1529 | C | P-O3'-C3' | 25.98 | 150.88 | 119.70 |
| 17 | AQ | 82 | ASP | CA-C-O | -25.91 | 65.70 | 120.10 |
| 78 | CA | 529 | A | P-O3'-C3' | 25.84 | 150.70 | 119.70 |
| 45 | BR | 140 | LEU | CA-C-O | -25.83 | 65.85 | 120.10 |
| 32 | BC | 17 | LEU | CA-C-O | -25.82 | 65.89 | 120.10 |
| 21 | AT | 9 | VAL | CA-C-O | -25.78 | 65.96 | 120.10 |
| 60 | Bi | 108 | GLN | CA-C-O | -25.72 | 66.08 | 120.10 |
| 31 | BB | 196 | TRP | O-C-N | -25.72 | 72.23 | 121.10 |
| 81 | DA | 3224 | G | O4'-C1'-N9 | 25.69 | 128.75 | 108.20 |
| 81 | DA | 3252 | G | P-O3'-C3' | 25.68 | 150.51 | 119.70 |
| 81 | DA | 3215 | A | O4'-C1'-N9 | -25.63 | 87.69 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 64 | Bl | 39 | TYR | CA-C-O | -25.62 | 66.30 | 120.10 |
| 43 | BP | 80 | THR | CA-C-O | -25.61 | 66.32 | 120.10 |
| 78 | CA | 610 | G | O4'-C1'-N9 | 25.61 | 128.69 | 108.20 |
| 33 | BD | 89 | ALA | CA-C-O | -25.60 | 66.33 | 120.10 |
| 81 | DA | 2971 | A | O4'-C1'-N9 | 25.60 | 128.68 | 108.20 |
| 48 | BW | 93 | ILE | CA-C-O | -25.57 | 66.40 | 120.10 |
| 81 | DA | 962 | A | O4'-C1'-N9 | 25.57 | 128.66 | 108.20 |
| 17 | AQ | 26 | LEU | CA-C-O | -25.57 | 66.41 | 120.10 |
| 37 | BH | 158 | ASP | O-C-N | -25.55 | 72.55 | 121.10 |
| 81 | DA | 1571 | A | P-O3'-C3' | 25.52 | 150.32 | 119.70 |
| 11 | AJ | 119 | ALA | CA-C-O | -25.52 | 66.52 | 120.10 |
| 78 | CA | 1190 | C | C5'-C4'-O4' | -25.48 | 78.53 | 109.10 |
| 81 | DA | 1209 | G | C1'-O4'-C4' | 25.47 | 130.28 | 109.90 |
| 78 | CA | 45 | U | O4'-C1'-N1 | 25.44 | 128.56 | 108.20 |
| 81 | DA | 537 | A | P-O3'-C3' | 25.42 | 150.20 | 119.70 |
| 81 | DA | 1075 | A | P-O3'-C3' | 25.35 | 150.12 | 119.70 |
| 78 | CA | 141 | U | O4'-C1'-N1 | 25.33 | 128.46 | 108.20 |
| 81 | DA | 2114 | C | P-O3'-C3' | 25.30 | 150.06 | 119.70 |
| 9 | AH | 66 | ASN | CA-C-O | -25.28 | 67.02 | 120.10 |
| 35 | BG | 3 | ALA | CA-C-O | -25.27 | 67.02 | 120.10 |
| 31 | BB | 249 | SER | CA-C-O | -25.27 | 67.04 | 120.10 |
| 39 | BJ | 76 | SER | CA-C-O | -25.24 | 67.09 | 120.10 |
| 81 | DA | 3215 | A | C1'-O4'-C4' | -25.22 | 89.72 | 109.90 |
| 81 | DA | 673 | U | P-O3'-C3' | 25.21 | 149.95 | 119.70 |
| 78 | CA | 1473 | U | O4'-C1'-N1 | 25.20 | 128.36 | 108.20 |
| 78 | CA | 501 | U | P-O3'-C3' | 25.18 | 149.92 | 119.70 |
| 32 | BC | 256 | HIS | CA-C-O | -25.13 | 67.33 | 120.10 |
| 59 | Bh | 12 | LYS | CA-C-O | -25.12 | 67.36 | 120.10 |
| 78 | CA | 959 | U | O4'-C1'-N1 | 25.12 | 128.29 | 108.20 |
| 37 | BH | 73 | PRO | CA-C-O | -25.09 | 59.97 | 120.20 |
| 40 | BK | 69 | GLY | O-C-N | -25.06 | 73.48 | 121.10 |
| 53 | Ba | 13 | VAL | CA-C-O | -25.05 | 67.50 | 120.10 |
| 81 | DA | 383 | G | P-O3'-C3' | 25.03 | 149.74 | 119.70 |
| 61 | Bj | 8 | TYR | CA-C-O | -25.01 | 67.58 | 120.10 |
| 78 | CA | 1551 | U | P-O5'-C5' | 25.01 | 160.91 | 120.90 |
| 81 | DA | 2760 | C | P-O3'-C3' | 24.95 | 149.64 | 119.70 |
| 18 | AP | 57 | LYS | CA-C-O | -24.92 | 67.77 | 120.10 |
| 44 | BO | 8 | THR | CA-C-O | -24.89 | 67.82 | 120.10 |
| 40 | BK | 185 | ALA | N-CA-CB | -24.86 | 75.30 | 110.10 |
| 18 | AP | 122 | ILE | CA-C-O | -24.85 | 67.91 | 120.10 |
| 81 | DA | 736 | A | P-O3'-C3' | 24.81 | 149.47 | 119.70 |
| 81 | DA | 2989 | U | C3'-C2'-C1' | 24.79 | 121.33 | 101.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 74 | BQ | 115 | LEU | CA-C-O | -24.78 | 68.06 | 120.10 |
| 57 | Be | 202 | LEU | CA-C-O | -24.77 | 68.08 | 120.10 |
| 78 | CA | 1341 | A | O4'-C1'-N9 | 24.77 | 128.02 | 108.20 |
| 81 | DA | 995 | U | P-O3'-C3' | 24.75 | 149.40 | 119.70 |
| 6 | AE | 92 | ALA | CA-C-O | -24.69 | 68.25 | 120.10 |
| 5 | AC | 162 | SER | O-C-N | -24.66 | 74.24 | 121.10 |
| 74 | BQ | 128 | GLU | CA-C-O | -24.64 | 68.36 | 120.10 |
| 32 | BC | 298 | PHE | CA-C-O | -24.61 | 68.41 | 120.10 |
| 81 | DA | 2159 | U | O4'-C1'-N1 | 24.61 | 127.89 | 108.20 |
| 17 | AQ | 63 | LYS | CA-C-O | -24.59 | 68.47 | 120.10 |
| 40 | BK | 63 | ALA | CA-C-O | -24.57 | 68.51 | 120.10 |
| 81 | DA | 1288 | U | P-O3'-C3' | 24.55 | 149.16 | 119.70 |
| 44 | BO | 7 | LYS | CA-C-O | -24.52 | 68.60 | 120.10 |
| 78 | CA | 1199 | G | O4'-C1'-N9 | 24.51 | 127.81 | 108.20 |
| 65 | Bn | 34 | ALA | CA-C-O | -24.49 | 68.67 | 120.10 |
| 81 | DA | 2244 | A | P-O3'-C3' | 24.46 | 149.05 | 119.70 |
| 74 | BQ | 237 | GLU | CA-C-O | -24.43 | 68.80 | 120.10 |
| 78 | CA | 1551 | U | O5'-C5'-C4' | 24.39 | 158.05 | 111.70 |
| 81 | DA | 838 | G | O4'-C1'-N9 | 24.38 | 127.70 | 108.20 |
| 57 | Be | 220 | PHE | CB-CG-CD2 | -24.36 | 103.75 | 120.80 |
| 81 | DA | 2423 | U | P-O3'-C3' | 24.34 | 148.90 | 119.70 |
| 18 | AP | 40 | LEU | CA-C-O | -24.33 | 69.00 | 120.10 |
| 78 | CA | 630 | A | O4'-C1'-N9 | 24.33 | 127.66 | 108.20 |
| 78 | CA | 1437 | U | O4'-C1'-N1 | 24.32 | 127.66 | 108.20 |
| 81 | DA | 1623 | G | P-O3'-C3' | 24.32 | 148.89 | 119.70 |
| 81 | DA | 2228 | A | O4'-C1'-N9 | 24.27 | 127.61 | 108.20 |
| 32 | BC | 5 | LYS | CA-C-O | -24.26 | 69.15 | 120.10 |
| 81 | DA | 2614 | G | P-O3'-C3' | 24.25 | 148.81 | 119.70 |
| 69 | Br | 58 | PHE | CA-C-O | -24.23 | 69.22 | 120.10 |
| 80 | CC | 18 | C | O3'-P-O5' | -24.20 | 58.01 | 104.00 |
| 81 | DA | 71 | A | N9-C1'-C2' | 24.18 | 145.44 | 114.00 |
| 32 | BC | 3 | HIS | CA-C-O | -24.16 | 69.38 | 120.10 |
| 81 | DA | 674 | G | P-O3'-C3' | 24.14 | 148.66 | 119.70 |
| 78 | CA | 303 | U | P-O3'-C3' | 24.13 | 148.66 | 119.70 |
| 34 | BE | 54 | VAL | O-C-N | -24.13 | 84.09 | 122.70 |
| 83 | DC | 46 | A | P-O3'-C3' | 24.13 | 148.65 | 119.70 |
| 2 | AA | 195 | TRP | CA-C-O | -24.12 | 69.45 | 120.10 |
| 60 | Bi | 79 | SER | CA-C-O | -24.10 | 69.48 | 120.10 |
| 44 | BO | 40 | HIS | CA-C-O | -24.07 | 69.56 | 120.10 |
| 81 | DA | 1640 | G | P-O3'-C3' | 24.02 | 148.52 | 119.70 |
| 4 | AD | 93 | ASP | CA-C-O | -24.00 | 69.69 | 120.10 |
| 43 | BP | 74 | PRO | CA-C-O | -24.00 | 62.60 | 120.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 3221 | C | P-O3'-C3' | 23.99 | 148.49 | 119.70 |
| 81 | DA | 2647 | A | O4'-C1'-N9 | 23.97 | 127.38 | 108.20 |
| 81 | DA | 1603 | A | O5'-P-OP1 | -23.95 | 81.96 | 110.70 |
| 81 | DA | 1401 | A | N9-C1'-C2' | -23.94 | 82.88 | 114.00 |
| 2 | AA | 229 | LYS | CA-C-O | -23.93 | 69.84 | 120.10 |
| 33 | BD | 12 | THR | CA-C-O | -23.93 | 69.86 | 120.10 |
| 74 | BQ | 238 | ASP | CA-C-O | -23.91 | 69.89 | 120.10 |
| 81 | DA | 1770 | G | P-O3'-C3' | 23.90 | 148.38 | 119.70 |
| 32 | BC | 360 | ASP | CA-C-O | -23.88 | 69.95 | 120.10 |
| 45 | BR | 143 | PRO | CA-C-O | -23.88 | 62.89 | 120.20 |
| 81 | DA | 2858 | U | P-O3'-C3' | 23.76 | 148.22 | 119.70 |
| 74 | BQ | 190 | ILE | CA-C-O | -23.76 | 70.21 | 120.10 |
| 14 | AM | 99 | HIS | CA-C-O | -23.75 | 70.23 | 120.10 |
| 53 | Ba | 60 | LYS | CA-C-O | -23.65 | 70.43 | 120.10 |
| 39 | BJ | 76 | SER | O-C-N | -23.65 | 84.86 | 122.70 |
| 81 | DA | 1054 | A | O4'-C1'-N9 | 23.64 | 127.11 | 108.20 |
| 37 | BH | 89 | GLU | CA-C-O | -23.64 | 70.46 | 120.10 |
| 6 | AE | 7 | GLN | CA-C-O | -23.63 | 70.47 | 120.10 |
| 69 | Br | 89 | LYS | CA-C-O | -23.60 | 70.53 | 120.10 |
| 2 | AA | 11 | PRO | CA-C-O | -23.60 | 63.56 | 120.20 |
| 5 | AC | 157 | ASP | CA-C-O | -23.59 | 70.56 | 120.10 |
| 45 | BR | 142 | GLY | O-C-N | -23.59 | 76.29 | 121.10 |
| 13 | AL | 87 | VAL | CA-C-O | -23.58 | 70.59 | 120.10 |
| 35 | BG | 8 | LYS | CA-C-O | -23.57 | 70.60 | 120.10 |
| 37 | BH | 158 | ASP | CA-C-O | -23.57 | 70.61 | 120.10 |
| 78 | CA | 944 | A | O4'-C1'-N9 | 23.57 | 127.05 | 108.20 |
| 78 | CA | 1340 | U | P-O3'-C3' | 23.56 | 147.97 | 119.70 |
| 81 | DA | 2712 | U | P-O3'-C3' | 23.55 | 147.96 | 119.70 |
| 60 | Bi | 16 | ARG | CA-C-O | -23.54 | 70.67 | 120.10 |
| 81 | DA | 3145 | C | P-O3'-C3' | 23.53 | 147.94 | 119.70 |
| 81 | DA | 583 | G | O4'-C1'-N9 | 23.50 | 127.00 | 108.20 |
| 81 | DA | 228 | U | P-O3'-C3' | 23.48 | 147.88 | 119.70 |
| 78 | CA | 1081 | A | O4'-C1'-N9 | 23.47 | 126.98 | 108.20 |
| 81 | DA | 2304 | C | P-O3'-C3' | 23.47 | 147.86 | 119.70 |
| 38 | Bs | 72 | ASP | CA-C-O | -23.45 | 70.85 | 120.10 |
| 26 | AZ | 18 | THR | O-C-N | -23.40 | 76.64 | 121.10 |
| 83 | DC | 9 | C | P-O3'-C3' | 23.33 | 147.70 | 119.70 |
| 81 | DA | 2100 | A | N9-C1'-C2' | 23.32 | 144.32 | 114.00 |
| 81 | DA | 2736 | A | O4'-C1'-N9 | 23.32 | 126.86 | 108.20 |
| 3 | AB | 78 | LYS | CA-C-O | -23.31 | 71.15 | 120.10 |
| 81 | DA | 2439 | A | P-O3'-C3' | 23.29 | 147.64 | 119.70 |
| 26 | AZ | 39 | LEU | CA-C-O | -23.26 | 71.25 | 120.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2421 | U | P-O3'-C3' | 23.23 | 147.58 | 119.70 |
| 81 | DA | 1717 | U | P-O3'-C3' | 23.22 | 147.56 | 119.70 |
| 81 | DA | 2619 | G | P-O3'-C3' | 23.22 | 147.56 | 119.70 |
| 81 | DA | 1678 | G | O4'-C1'-N9 | 23.19 | 126.76 | 108.20 |
| 81 | DA | 1602 | A | O3'-P-O5' | -23.18 | 59.95 | 104.00 |
| 74 | BQ | 197 | SER | CA-C-O | -23.16 | 71.45 | 120.10 |
| 78 | CA | 174 | U | N1-C1'-C2' | 23.16 | 144.11 | 114.00 |
| 13 | AL | 34 | LEU | CA-C-O | -23.14 | 71.50 | 120.10 |
| 81 | DA | 1261 | G | N9-C1'-C2' | -23.14 | 83.92 | 114.00 |
| 26 | AZ | 44 | PHE | CA-C-O | -23.13 | 71.52 | 120.10 |
| 81 | DA | 701 | G | P-O3'-C3' | 23.12 | 147.44 | 119.70 |
| 6 | AE | 4 | PRO | CA-C-O | -23.09 | 64.78 | 120.20 |
| 26 | AZ | 40 | TYR | CA-C-O | -23.09 | 71.61 | 120.10 |
| 78 | CA | 191 | C | P-O3'-C3' | 23.07 | 147.39 | 119.70 |
| 81 | DA | 8 | C | P-O3'-C3' | 23.04 | 147.35 | 119.70 |
| 32 | BC | 362 | ALA | CA-C-O | -23.04 | 71.72 | 120.10 |
| 46 | BT | 82 | LYS | CA-C-O | -23.03 | 71.73 | 120.10 |
| 60 | Bi | 68 | THR | CA-C-O | -23.03 | 71.74 | 120.10 |
| 78 | CA | 1173 | C | P-O3'-C3' | 23.01 | 147.31 | 119.70 |
| 5 | AC | 23 | ARG | NE-CZ-NH2 | -22.95 | 108.83 | 120.30 |
| 31 | BB | 127 | ALA | CA-C-O | -22.94 | 71.94 | 120.10 |
| 81 | DA | 1195 | A | O4'-C1'-N9 | 22.92 | 126.54 | 108.20 |
| 81 | DA | 1338 | C | O4'-C1'-N1 | 22.91 | 126.52 | 108.20 |
| 34 | BE | 54 | VAL | C-N-CA | -22.84 | 64.60 | 121.70 |
| 81 | DA | 2229 | A | O4'-C1'-N9 | 22.83 | 126.47 | 108.20 |
| 5 | AC | 23 | ARG | NE-CZ-NH1 | -22.82 | 108.89 | 120.30 |
| 81 | DA | 1811 | G | O4'-C1'-N9 | 22.81 | 126.45 | 108.20 |
| 17 | AQ | 81 | LYS | CA-C-O | -22.78 | 72.26 | 120.10 |
| 79 | CB | 73 | C | P-O3'-C3' | 22.77 | 147.02 | 119.70 |
| 2 | AA | 250 | VAL | CA-C-O | -22.75 | 72.32 | 120.10 |
| 33 | BD | 145 | ILE | CA-C-O | -22.75 | 72.33 | 120.10 |
| 81 | DA | 2272 | G | O4'-C1'-N9 | 22.74 | 126.39 | 108.20 |
| 78 | CA | 387 | A | O4'-C1'-N9 | 22.62 | 126.29 | 108.20 |
| 81 | DA | 2484 | A | O4'-C1'-N9 | 22.60 | 126.28 | 108.20 |
| 78 | CA | 1355 | C | P-O3'-C3' | 22.59 | 146.81 | 119.70 |
| 10 | AI | 54 | LEU | CA-C-O | -22.58 | 72.68 | 120.10 |
| 81 | DA | 3368 | U | P-O3'-C3' | 22.56 | 146.77 | 119.70 |
| 78 | CA | 928 | U | O4'-C1'-N1 | 22.51 | 126.21 | 108.20 |
| 78 | CA | 1337 | A | O4'-C1'-N9 | 22.49 | 126.19 | 108.20 |
| 81 | DA | 2763 | U | O4'-C1'-N1 | 22.47 | 126.18 | 108.20 |
| 81 | DA | 2673 | A | P-O5'-C5' | 22.47 | 156.85 | 120.90 |
| 35 | BG | 99 | GLU | N-CA-CB | 22.46 | 151.03 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | BG | 69 | PHE | CD1-CE1-CZ | -22.45 | 93.16 | 120.10 |
| 81 | DA | 2988 | C | P-O3'-C3' | 22.44 | 146.63 | 119.70 |
| 81 | DA | 1786 | G | O4'-C1'-N9 | 22.40 | 126.12 | 108.20 |
| 81 | DA | 1320 | C | P-O3'-C3' | 22.40 | 146.58 | 119.70 |
| 81 | DA | 1753 | G | P-O3'-C3' | 22.40 | 146.58 | 119.70 |
| 34 | BE | 116 | TYR | CG-CD1-CE1 | -22.39 | 103.38 | 121.30 |
| 81 | DA | 1080 | A | O4'-C1'-N9 | 22.39 | 126.11 | 108.20 |
| 45 | BR | 98 | LYS | CA-C-O | -22.37 | 73.12 | 120.10 |
| 81 | DA | 2507 | C | P-O3'-C3' | 22.35 | 146.52 | 119.70 |
| 81 | DA | 310 | U | P-O3'-C3' | 22.34 | 146.51 | 119.70 |
| 81 | DA | 651 | G | P-O3'-C3' | 22.29 | 146.45 | 119.70 |
| 81 | DA | 1455 | U | O4'-C1'-N1 | 22.29 | 126.03 | 108.20 |
| 83 | DC | 49 | G | O5'-P-OP1 | -22.29 | 83.95 | 110.70 |
| 81 | DA | 3246 | G | P-O3'-C3' | 22.28 | 146.43 | 119.70 |
| 81 | DA | 1620 | U | P-O3'-C3' | 22.26 | 146.42 | 119.70 |
| 81 | DA | 186 | U | O4'-C1'-N1 | 22.24 | 125.99 | 108.20 |
| 81 | DA | 1261 | G | O4'-C1'-C2' | -22.24 | 83.56 | 105.80 |
| 81 | DA | 1506 | A | O4'-C1'-N9 | 22.21 | 125.97 | 108.20 |
| 44 | BO | 3 | SER | CA-C-O | -22.21 | 73.46 | 120.10 |
| 81 | DA | 861 | C | P-O3'-C3' | 22.19 | 146.33 | 119.70 |
| 83 | DC | 41 | G | P-O3'-C3' | 22.15 | 146.28 | 119.70 |
| 81 | DA | 1427 | U | P-O3'-C3' | 22.15 | 146.28 | 119.70 |
| 83 | DC | 107 | G | O4'-C1'-N9 | 22.14 | 125.91 | 108.20 |
| 13 | AL | 38 | PHE | CB-CG-CD1 | 22.11 | 136.27 | 120.80 |
| 81 | DA | 21 | G | O4'-C1'-N9 | 22.10 | 125.88 | 108.20 |
| 81 | DA | 3002 | C | P-O3'-C3' | 22.09 | 146.21 | 119.70 |
| 78 | CA | 856 | A | O4'-C1'-N9 | 22.06 | 125.85 | 108.20 |
| 81 | DA | 1826 | C | O4'-C1'-N1 | 22.04 | 125.83 | 108.20 |
| 81 | DA | 1483 | G | O4'-C1'-N9 | 22.01 | 125.81 | 108.20 |
| 81 | DA | 3296 | A | P-O3'-C3' | 21.99 | 146.09 | 119.70 |
| 81 | DA | 1538 | G | P-O3'-C3' | 21.98 | 146.07 | 119.70 |
| 55 | Bc | 104 | GLN | CA-C-O | -21.95 | 74.00 | 120.10 |
| 16 | AO | 65 | VAL | CG1-CB-CG2 | 21.94 | 146.01 | 110.90 |
| 83 | DC | 50 | U | P-O3'-C3' | 21.93 | 146.01 | 119.70 |
| 4 | AD | 153 | ASN | CA-C-O | -21.92 | 74.06 | 120.10 |
| 33 | BD | 323 | VAL | CA-C-O | -21.92 | 74.07 | 120.10 |
| 79 | CB | 12 | U | P-O3'-C3' | 21.91 | 146.00 | 119.70 |
| 34 | BE | 9 | MET | CA-C-O | -21.91 | 74.10 | 120.10 |
| 81 | DA | 2734 | A | P-O3'-C3' | 21.90 | 145.98 | 119.70 |
| 74 | BQ | 129 | TYR | CA-C-O | -21.90 | 74.11 | 120.10 |
| 78 | CA | 636 | A | O4'-C1'-C2' | -21.89 | 83.91 | 105.80 |
| 78 | CA | 661 | A | P-O3'-C3' | 21.89 | 145.97 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | AD | 94 | ALA | CA-C-O | -21.86 | 74.20 | 120.10 |
| 78 | CA | 1 | U | OP1-P-OP2 | -21.85 | 86.82 | 119.60 |
| 31 | BB | 252 | THR | CA-C-O | -21.84 | 74.23 | 120.10 |
| 78 | CA | 1340 | U | P-O5'-C5' | 21.84 | 155.84 | 120.90 |
| 81 | DA | 2267 | C | P-O3'-C3' | 21.82 | 145.89 | 119.70 |
| 81 | DA | 1689 | U | O4'-C1'-N1 | 21.81 | 125.65 | 108.20 |
| 35 | BG | 38 | THR | CA-C-O | -21.81 | 74.30 | 120.10 |
| 38 | Bs | 5 | ARG | CA-C-O | -21.81 | 74.30 | 120.10 |
| 81 | DA | 1657 | C | P-O3'-C3' | 21.80 | 145.86 | 119.70 |
| 34 | BE | 116 | TYR | CD1-CE1-CZ | 21.75 | 139.38 | 119.80 |
| 81 | DA | 63 | A | O4'-C1'-N9 | 21.75 | 125.60 | 108.20 |
| 33 | BD | 148 | ILE | CA-C-O | -21.74 | 74.45 | 120.10 |
| 81 | DA | 996 | A | P-O3'-C3' | 21.72 | 145.77 | 119.70 |
| 26 | AZ | 18 | THR | CA-C-O | -21.71 | 74.50 | 120.10 |
| 78 | CA | 1583 | A | O4'-C1'-N9 | -21.70 | 90.84 | 108.20 |
| 81 | DA | 2500 | A | P-O3'-C3' | 21.70 | 145.74 | 119.70 |
| 81 | DA | 720 | A | O4'-C1'-N9 | 21.68 | 125.55 | 108.20 |
| 15 | AN | 54 | LYS | CA-C-O | -21.64 | 74.66 | 120.10 |
| 74 | BQ | 158 | ARG | NH1-CZ-NH2 | -21.63 | 95.61 | 119.40 |
| 81 | DA | 1694 | U | O4'-C1'-N1 | 21.62 | 125.50 | 108.20 |
| 81 | DA | 2462 | A | P-O3'-C3' | 21.61 | 145.63 | 119.70 |
| 81 | DA | 1206 | G | O4'-C1'-N9 | 21.59 | 125.47 | 108.20 |
| 78 | CA | 1479 | A | P-O3'-C3' | 21.56 | 145.57 | 119.70 |
| 81 | DA | 1704 | A | O4'-C1'-N9 | 21.54 | 125.43 | 108.20 |
| 81 | DA | 2362 | C | N1-C1'-C2' | -21.52 | 86.02 | 114.00 |
| 78 | CA | 2 | A | O4'-C1'-N9 | 21.48 | 125.39 | 108.20 |
| 81 | DA | 636 | C | N1-C1'-C2' | 21.46 | 141.90 | 114.00 |
| 81 | DA | 914 | A | O4'-C1'-N9 | 21.46 | 125.37 | 108.20 |
| 33 | BD | 321 | LYS | CA-C-O | -21.44 | 75.08 | 120.10 |
| 81 | DA | 2886 | U | O4'-C1'-N1 | 21.42 | 125.34 | 108.20 |
| 61 | Bj | 20 | LYS | CA-C-O | -21.42 | 75.12 | 120.10 |
| 83 | DC | 101 | A | P-O5'-C5' | 21.41 | 155.15 | 120.90 |
| 78 | CA | 689 | G | P-O3'-C3' | 21.37 | 145.35 | 119.70 |
| 81 | DA | 2808 | A | O4'-C1'-N9 | 21.34 | 125.27 | 108.20 |
| 35 | BG | 152 | THR | O-C-N | -21.33 | 80.57 | 121.10 |
| 45 | BR | 157 | PRO | CA-C-O | -21.32 | 69.03 | 120.20 |
| 81 | DA | 1690 | C | P-O3'-C3' | 21.32 | 145.28 | 119.70 |
| 78 | CA | 1550 | A | P-O3'-C3' | 21.31 | 145.27 | 119.70 |
| 81 | DA | 2755 | C | P-O3'-C3' | 21.29 | 145.25 | 119.70 |
| 32 | BC | 130 | PHE | CA-C-O | -21.28 | 75.41 | 120.10 |
| 53 | Ba | 10 | VAL | CA-CB-CG2 | 21.23 | 142.75 | 110.90 |
| 81 | DA | 63 | A | P-O3'-C3' | 21.23 | 145.18 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 45 | U | C1'-O4'-C4' | 21.18 | 126.84 | 109.90 |
| 81 | DA | 1536 | G | P-O3'-C3' | 21.14 | 145.07 | 119.70 |
| 81 | DA | 2784 | G | P-O3'-C3' | 21.11 | 145.03 | 119.70 |
| 81 | DA | 1020 | G | P-O3'-C3' | 21.11 | 145.03 | 119.70 |
| 81 | DA | 419 | G | P-O3'-C3' | 21.08 | 144.99 | 119.70 |
| 81 | DA | 2047 | A | O4'-C1'-N9 | 21.08 | 125.06 | 108.20 |
| 81 | DA | 1701 | C | N1-C1'-C2' | 21.05 | 141.37 | 114.00 |
| 81 | DA | 2757 | U | P-O3'-C3' | 21.05 | 144.96 | 119.70 |
| 1 | Aa | 59 | ARG | N-CA-C | 20.99 | 167.67 | 111.00 |
| 81 | DA | 1535 | A | O4'-C1'-N9 | 20.98 | 124.98 | 108.20 |
| 81 | DA | 1528 | G | O4'-C1'-N9 | 20.95 | 124.96 | 108.20 |
| 81 | DA | 845 | G | O4'-C1'-N9 | 20.94 | 124.95 | 108.20 |
| 78 | CA | 1092 | A | O4'-C1'-N9 | 20.93 | 124.95 | 108.20 |
| 81 | DA | 1823 | A | P-O3'-C3' | 20.93 | 144.81 | 119.70 |
| 78 | CA | 650 | U | P-O3'-C3' | 20.92 | 144.81 | 119.70 |
| 83 | DC | 48 | U | O4'-C1'-N1 | 20.92 | 124.93 | 108.20 |
| 81 | DA | 2369 | G | P-O3'-C3' | 20.90 | 144.78 | 119.70 |
| 81 | DA | 1215 | U | P-O3'-C3' | 20.89 | 144.77 | 119.70 |
| 81 | DA | 3141 | A | P-O5'-C5' | 20.86 | 154.27 | 120.90 |
| 79 | CB | 55 | C | C1'-O4'-C4' | -20.84 | 93.23 | 109.90 |
| 81 | DA | 2866 | U | O4'-C1'-N1 | 20.84 | 124.87 | 108.20 |
| 81 | DA | 2506 | U | C3'-C2'-C1' | 20.81 | 118.15 | 101.50 |
| 81 | DA | 1208 | U | O4'-C1'-N1 | 20.80 | 124.84 | 108.20 |
| 78 | CA | 474 | A | P-O3'-C3' | 20.80 | 144.66 | 119.70 |
| 11 | AJ | 85 | ARG | NE-CZ-NH1 | 20.79 | 130.70 | 120.30 |
| 81 | DA | 860 | G | P-O3'-C3' | 20.79 | 144.64 | 119.70 |
| 81 | DA | 2489 | C | P-O3'-C3' | 20.78 | 144.64 | 119.70 |
| 81 | DA | 2041 | U | P-O3'-C3' | 20.76 | 144.62 | 119.70 |
| 81 | DA | 519 | A | O4'-C1'-N9 | 20.72 | 124.78 | 108.20 |
| 81 | DA | 3151 | U | O4'-C1'-N1 | 20.70 | 124.76 | 108.20 |
| 5 | AC | 23 | ARG | NH1-CZ-NH2 | 20.68 | 142.15 | 119.40 |
| 81 | DA | 1801 | U | P-O3'-C3' | 20.68 | 144.52 | 119.70 |
| 81 | DA | 2244 | A | O4'-C1'-N9 | 20.68 | 124.74 | 108.20 |
| 81 | DA | 263 | C | P-O3'-C3' | 20.67 | 144.51 | 119.70 |
| 81 | DA | 655 | C | P-O3'-C3' | 20.67 | 144.50 | 119.70 |
| 81 | DA | 1400 | G | P-O3'-C3' | 20.65 | 144.48 | 119.70 |
| 81 | DA | 2493 | U | O4'-C1'-N1 | 20.62 | 124.70 | 108.20 |
| 57 | Be | 120 | THR | CA-CB-CG2 | -20.60 | 83.57 | 112.40 |
| 74 | BQ | 158 | ARG | NE-CZ-NH2 | 20.59 | 130.60 | 120.30 |
| 81 | DA | 1872 | C | O4'-C1'-N1 | -20.55 | 91.76 | 108.20 |
| 35 | BG | 5 | LYS | CA-C-O | -20.55 | 76.96 | 120.10 |
| 33 | BD | 331 | ALA | CA-C-O | -20.54 | 76.97 | 120.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 79 | CB | 75 | A | O4'-C1'-N9 | 20.53 | 124.63 | 108.20 |
| 20 | AS | 90 | PRO | CA-C-O | -20.52 | 70.95 | 120.20 |
| 78 | CA | 1441 | C | P-O5'-C5' | 20.52 | 153.73 | 120.90 |
| 81 | DA | 1965 | C | P-O3'-C3' | 20.51 | 144.31 | 119.70 |
| 4 | AD | 96 | ASN | CA-C-O | -20.51 | 77.04 | 120.10 |
| 81 | DA | 1955 | U | O4'-C1'-N1 | 20.50 | 124.60 | 108.20 |
| 78 | CA | 1421 | A | O4'-C1'-N9 | 20.47 | 124.57 | 108.20 |
| 81 | DA | 1766 | G | P-O3'-C3' | 20.46 | 144.25 | 119.70 |
| 51 | BZ | 51 | TRP | CA-C-O | -20.44 | 77.18 | 120.10 |
| 78 | CA | 45 | U | N1-C1'-C2' | -20.43 | 87.44 | 114.00 |
| 81 | DA | 1 | G | O4'-C1'-N9 | 20.39 | 124.52 | 108.20 |
| 78 | CA | 1756 | A | O4'-C1'-N9 | 20.38 | 124.51 | 108.20 |
| 78 | CA | 1476 | C | P-O3'-C3' | 20.38 | 144.16 | 119.70 |
| 81 | DA | 1754 | G | P-O3'-C3' | 20.38 | 144.16 | 119.70 |
| 81 | DA | 1791 | C | P-O3'-C3' | 20.38 | 144.15 | 119.70 |
| 78 | CA | 400 | A | O4'-C1'-N9 | 20.37 | 124.50 | 108.20 |
| 81 | DA | 3242 | G | O4'-C1'-N9 | 20.35 | 124.48 | 108.20 |
| 78 | CA | 37 | U | O4'-C1'-N1 | 20.34 | 124.47 | 108.20 |
| 78 | CA | 1339 | C | P-O3'-C3' | 20.34 | 144.10 | 119.70 |
| 81 | DA | 3199 | G | P-O3'-C3' | 20.32 | 144.09 | 119.70 |
| 81 | DA | 2072 | G | O4'-C1'-N9 | 20.32 | 124.45 | 108.20 |
| 78 | CA | 469 | C | O4'-C1'-C2' | -20.30 | 85.50 | 105.80 |
| 81 | DA | 2434 | U | P-O3'-C3' | 20.30 | 144.06 | 119.70 |
| 81 | DA | 786 | A | O4'-C1'-N9 | 20.29 | 124.43 | 108.20 |
| 81 | DA | 1627 | U | O4'-C1'-N1 | 20.28 | 124.43 | 108.20 |
| 83 | DC | 29 | C | P-O3'-C3' | 20.28 | 144.04 | 119.70 |
| 81 | DA | 783 | A | O4'-C1'-N9 | 20.28 | 124.42 | 108.20 |
| 81 | DA | 1378 | U | P-O3'-C3' | 20.27 | 144.03 | 119.70 |
| 34 | BE | 55 | ARG | O-C-N | -20.27 | 90.27 | 122.70 |
| 83 | DC | 15 | C | P-O3'-C3' | 20.25 | 144.00 | 119.70 |
| 78 | CA | 1666 | U | O4'-C1'-N1 | 20.25 | 124.40 | 108.20 |
| 61 | Bj | 20 | LYS | O-C-N | -20.22 | 90.34 | 122.70 |
| 81 | DA | 1871 | U | O4'-C1'-N1 | 20.20 | 124.36 | 108.20 |
| 78 | CA | 164 | A | P-O5'-C5' | 20.20 | 153.21 | 120.90 |
| 81 | DA | 2363 | A | O4'-C1'-N9 | 20.18 | 124.34 | 108.20 |
| 83 | DC | 92 | A | P-O3'-C3' | 20.17 | 143.90 | 119.70 |
| 80 | CC | 12 | A | O4'-C1'-N9 | 20.14 | 124.31 | 108.20 |
| 81 | DA | 2416 | U | P-O3'-C3' | 20.11 | 143.83 | 119.70 |
| 81 | DA | 1255 | C | O4'-C1'-N1 | 20.11 | 124.29 | 108.20 |
| 40 | BK | 185 | ALA | CB-CA-C | -20.04 | 80.03 | 110.10 |
| 81 | DA | 2727 | A | O4'-C1'-N9 | 20.04 | 124.23 | 108.20 |
| 81 | DA | 3092 | C | O4'-C1'-N1 | -20.04 | 92.17 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 637 | C | O4'-C1'-N1 | 20.03 | 124.23 | 108.20 |
| 31 | BB | 62 | VAL | CA-C-O | -20.03 | 78.04 | 120.10 |
| 81 | DA | 2483 | G | P-O3'-C3' | 20.00 | 143.70 | 119.70 |
| 83 | DC | 22 | A | O4'-C1'-N9 | 19.98 | 124.18 | 108.20 |
| 81 | DA | 607 | A | C5'-C4'-C3' | 19.95 | 147.92 | 116.00 |
| 81 | DA | 3122 | A | O4'-C1'-N9 | 19.95 | 124.16 | 108.20 |
| 81 | DA | 2165 | G | O4'-C1'-N9 | 19.95 | 124.16 | 108.20 |
| 81 | DA | 2149 | A | O4'-C1'-N9 | 19.95 | 124.16 | 108.20 |
| 81 | DA | 1104 | G | O4'-C1'-N9 | 19.94 | 124.15 | 108.20 |
| 81 | DA | 2623 | G | O4'-C1'-N9 | 19.93 | 124.14 | 108.20 |
| 47 | BU | 116 | ARG | NE-CZ-NH1 | -19.90 | 110.35 | 120.30 |
| 78 | CA | 540 | G | P-O3'-C3' | 19.89 | 143.57 | 119.70 |
| 83 | DC | 53 | U | P-O3'-C3' | 19.89 | 143.56 | 119.70 |
| 81 | DA | 1528 | G | P-O3'-C3' | 19.88 | 143.56 | 119.70 |
| 22 | AV | 26 | LYS | CA-C-O | -19.84 | 78.44 | 120.10 |
| 81 | DA | 3041 | U | O3'-P-O5' | -19.83 | 66.33 | 104.00 |
| 81 | DA | 45 | A | P-O5'-C5' | 19.82 | 152.62 | 120.90 |
| 81 | DA | 1598 | G | O4'-C1'-N9 | 19.80 | 124.04 | 108.20 |
| 81 | DA | 1333 | C | P-O3'-C3' | 19.80 | 143.46 | 119.70 |
| 81 | DA | 1055 | A | O4'-C1'-C2' | -19.79 | 86.01 | 105.80 |
| 81 | DA | 2628 | A | O3'-P-O5' | -19.77 | 66.43 | 104.00 |
| 16 | AO | 64 | ARG | N-CA-CB | -19.77 | 75.02 | 110.60 |
| 46 | BT | 71 | ARG | CA-C-O | -19.74 | 78.65 | 120.10 |
| 81 | DA | 262 | U | O4'-C1'-N1 | 19.72 | 123.97 | 108.20 |
| 78 | CA | 1673 | G | P-O3'-C3' | 19.69 | 143.33 | 119.70 |
| 81 | DA | 2204 | C | P-O3'-C3' | 19.66 | 143.29 | 119.70 |
| 78 | CA | 1003 | A | O4'-C1'-N9 | 19.64 | 123.92 | 108.20 |
| 78 | CA | 462 | G | P-O3'-C3' | 19.64 | 143.27 | 119.70 |
| 78 | CA | 1337 | A | P-O5'-C5' | 19.62 | 152.29 | 120.90 |
| 78 | CA | 1534 | G | P-O5'-C5' | 19.62 | 152.29 | 120.90 |
| 78 | CA | 1091 | A | O4'-C1'-N9 | 19.61 | 123.89 | 108.20 |
| 81 | DA | 2503 | G | P-O3'-C3' | 19.61 | 143.23 | 119.70 |
| 81 | DA | 1688 | U | P-O5'-C5' | 19.59 | 152.24 | 120.90 |
| 81 | DA | 1250 | G | O4'-C1'-N9 | 19.58 | 123.87 | 108.20 |
| 81 | DA | 2606 | G | O4'-C1'-N9 | 19.56 | 123.85 | 108.20 |
| 81 | DA | 2275 | A | O4'-C1'-N9 | 19.56 | 123.84 | 108.20 |
| 81 | DA | 2061 | G | O4'-C1'-N9 | 19.49 | 123.79 | 108.20 |
| 82 | DB | 25 | G | O4'-C1'-N9 | 19.49 | 123.80 | 108.20 |
| 81 | DA | 313 | A | O4'-C1'-N9 | 19.49 | 123.79 | 108.20 |
| 81 | DA | 1656 | A | P-O3'-C3' | 19.49 | 143.08 | 119.70 |
| 81 | DA | 2043 | U | P-O3'-C3' | 19.48 | 143.08 | 119.70 |
| 81 | DA | 1061 | A | O4'-C1'-N9 | 19.45 | 123.76 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 27 | U | O4'-C1'-N1 | 19.45 | 123.76 | 108.20 |
| 78 | CA | 622 | A | P-O3'-C3' | 19.45 | 143.04 | 119.70 |
| 81 | DA | 3334 | U | O4'-C1'-N1 | 19.44 | 123.75 | 108.20 |
| 78 | CA | 104 | A | P-O3'-C3' | 19.44 | 143.02 | 119.70 |
| 34 | BE | 115 | LYS | CB-CA-C | -19.42 | 71.55 | 110.40 |
| 83 | DC | 51 | G | P-O3'-C3' | 19.41 | 142.99 | 119.70 |
| 81 | DA | 2648 | G | N9-C1'-C2' | -19.40 | 88.77 | 114.00 |
| 78 | CA | 373 | G | O4'-C1'-N9 | 19.36 | 123.68 | 108.20 |
| 78 | CA | 1222 | C | O4'-C1'-N1 | 19.34 | 123.67 | 108.20 |
| 81 | DA | 1883 | A | P-O3'-C3' | 19.34 | 142.91 | 119.70 |
| 81 | DA | 728 | G | P-O3'-C3' | 19.34 | 142.91 | 119.70 |
| 81 | DA | 2067 | U | O4'-C1'-N1 | 19.33 | 123.67 | 108.20 |
| 81 | DA | 2666 | C | P-O3'-C3' | 19.30 | 142.87 | 119.70 |
| 81 | DA | 2114 | C | O4'-C1'-N1 | 19.30 | 123.64 | 108.20 |
| 37 | BH | 204 | ARG | NE-CZ-NH1 | 19.27 | 129.94 | 120.30 |
| 78 | CA | 647 | G | O4'-C1'-N9 | 19.27 | 123.61 | 108.20 |
| 81 | DA | 1021 | G | P-O3'-C3' | 19.20 | 142.74 | 119.70 |
| 81 | DA | 1876 | U | P-O3'-C3' | 19.20 | 142.74 | 119.70 |
| 78 | CA | 297 | U | P-O3'-C3' | 19.16 | 142.69 | 119.70 |
| 81 | DA | 148 | G | P-O3'-C3' | 19.14 | 142.66 | 119.70 |
| 82 | DB | 3 | A | N9-C1'-C2' | 19.08 | 138.81 | 114.00 |
| 81 | DA | 1535 | A | P-O3'-C3' | 19.08 | 142.59 | 119.70 |
| 81 | DA | 2166 | A | C3'-C2'-C1' | 19.05 | 116.74 | 101.50 |
| 78 | CA | 960 | U | O4'-C1'-C2' | -19.03 | 86.77 | 105.80 |
| 78 | CA | 994 | G | O4'-C1'-N9 | 19.00 | 123.40 | 108.20 |
| 81 | DA | 1435 | A | P-O3'-C3' | 19.00 | 142.50 | 119.70 |
| 65 | Bn | 71 | PRO | CA-C-O | -18.99 | 74.63 | 120.20 |
| 33 | BD | 145 | ILE | O-C-N | -18.96 | 85.08 | 121.10 |
| 81 | DA | 2934 | A | C1'-O4'-C4' | 18.94 | 125.05 | 109.90 |
| 81 | DA | 2989 | U | C1'-O4'-C4' | 18.93 | 125.05 | 109.90 |
| 78 | CA | 295 | A | N9-C1'-C2' | -18.92 | 89.40 | 114.00 |
| 41 | BN | 108 | ARG | NE-CZ-NH1 | 18.91 | 129.75 | 120.30 |
| 81 | DA | 2624 | G | P-O3'-C3' | 18.90 | 142.38 | 119.70 |
| 81 | DA | 49 | A | O4'-C1'-N9 | 18.90 | 123.32 | 108.20 |
| 81 | DA | 487 | U | P-O5'-C5' | 18.90 | 151.14 | 120.90 |
| 81 | DA | 1756 | C | P-O5'-C5' | 18.87 | 151.09 | 120.90 |
| 81 | DA | 3240 | C | P-O3'-C3' | 18.86 | 142.33 | 119.70 |
| 78 | CA | 964 | U | O4'-C1'-N1 | 18.85 | 123.28 | 108.20 |
| 81 | DA | 2617 | U | P-O3'-C3' | 18.85 | 142.31 | 119.70 |
| 78 | CA | 1367 | G | P-O3'-C3' | 18.84 | 142.31 | 119.70 |
| 78 | CA | 667 | U | O4'-C1'-N1 | 18.84 | 123.27 | 108.20 |
| 81 | DA | 2194 | G | O4'-C1'-N9 | 18.82 | 123.26 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1343 | A | P-O3'-C3' | 18.80 | 142.27 | 119.70 |
| 81 | DA | 3222 | U | O4'-C1'-N1 | 18.80 | 123.24 | 108.20 |
| 78 | CA | 306 | U | O4'-C1'-C2' | -18.79 | 87.01 | 105.80 |
| 81 | DA | 1015 | U | O4'-C1'-N1 | 18.79 | 123.23 | 108.20 |
| 81 | DA | 784 | A | O4'-C1'-N9 | 18.77 | 123.22 | 108.20 |
| 40 | BK | 133 | ARG | NE-CZ-NH2 | 18.76 | 129.68 | 120.30 |
| 81 | DA | 2787 | G | P-O3'-C3' | 18.76 | 142.21 | 119.70 |
| 81 | DA | 104 | G | P-O3'-C3' | 18.74 | 142.19 | 119.70 |
| 31 | BB | 193 | ARG | NE-CZ-NH1 | 18.73 | 129.67 | 120.30 |
| 78 | CA | 825 | U | P-O3'-C3' | 18.72 | 142.17 | 119.70 |
| 81 | DA | 1773 | C | O4'-C1'-N1 | 18.72 | 123.18 | 108.20 |
| 81 | DA | 1063 | G | P-O3'-C3' | 18.70 | 142.14 | 119.70 |
| 81 | DA | 1390 | A | P-O3'-C3' | 18.70 | 142.14 | 119.70 |
| 78 | CA | 1164 | G | O4'-C1'-N9 | 18.70 | 123.16 | 108.20 |
| 81 | DA | 1774 | C | P-O3'-C3' | 18.69 | 142.13 | 119.70 |
| 81 | DA | 2450 | G | P-O3'-C3' | 18.68 | 142.11 | 119.70 |
| 81 | DA | 785 | G | O4'-C1'-N9 | 18.67 | 123.14 | 108.20 |
| 83 | DC | 51 | G | O4'-C1'-N9 | 18.67 | 123.14 | 108.20 |
| 78 | CA | 1528 | U | P-O3'-C3' | 18.66 | 142.09 | 119.70 |
| 78 | CA | 323 | A | O4'-C1'-N9 | 18.65 | 123.12 | 108.20 |
| 78 | CA | 1530 | C | O4'-C1'-N1 | 18.63 | 123.10 | 108.20 |
| 81 | DA | 3245 | A | N9-C1'-C2' | 18.61 | 138.19 | 114.00 |
| 81 | DA | 1641 | U | O4'-C1'-N1 | 18.59 | 123.07 | 108.20 |
| 81 | DA | 1247 | U | O4'-C1'-N1 | 18.58 | 123.06 | 108.20 |
| 82 | DB | 106 | C | P-O3'-C3' | 18.57 | 141.99 | 119.70 |
| 81 | DA | 1675 | G | O4'-C1'-N9 | 18.57 | 123.06 | 108.20 |
| 81 | DA | 1826 | C | P-O3'-C3' | 18.56 | 141.98 | 119.70 |
| 78 | CA | 683 | C | O4'-C1'-N1 | 18.56 | 123.05 | 108.20 |
| 81 | DA | 178 | U | P-O3'-C3' | 18.55 | 141.96 | 119.70 |
| 81 | DA | 2638 | C | N1-C1'-C2' | 18.55 | 138.11 | 114.00 |
| 78 | CA | 163 | G | P-O3'-C3' | 18.54 | 141.95 | 119.70 |
| 83 | DC | 40 | C | P-O3'-C3' | 18.54 | 141.94 | 119.70 |
| 78 | CA | 139 | C | P-O3'-C3' | 18.52 | 141.92 | 119.70 |
| 82 | DB | 98 | U | O5'-C5'-C4' | 18.52 | 146.88 | 111.70 |
| 81 | DA | 2499 | U | P-O5'-C5' | 18.51 | 150.51 | 120.90 |
| 81 | DA | 663 | C | P-O5'-C5' | 18.49 | 150.49 | 120.90 |
| 81 | DA | 2376 | G | P-O3'-C3' | 18.47 | 141.86 | 119.70 |
| 78 | CA | 1491 | U | P-O3'-C3' | 18.45 | 141.84 | 119.70 |
| 78 | CA | 1394 | G | O4'-C1'-N9 | 18.44 | 122.95 | 108.20 |
| 79 | CB | 67 | G | P-O3'-C3' | 18.43 | 141.82 | 119.70 |
| 81 | DA | 2322 | C | P-O3'-C3' | 18.42 | 141.81 | 119.70 |
| 82 | DB | 150 | G | P-O3'-C3' | 18.41 | 141.79 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 118 | U | P-O3'-C3' | 18.40 | 141.78 | 119.70 |
| 81 | DA | 1209 | G | N9-C1'-C2' | -18.40 | 90.08 | 114.00 |
| 81 | DA | 1675 | G | P-O3'-C3' | 18.39 | 141.77 | 119.70 |
| 81 | DA | 1233 | G | P-O3'-C3' | 18.34 | 141.71 | 119.70 |
| 81 | DA | 1500 | G | P-O3'-C3' | 18.33 | 141.70 | 119.70 |
| 81 | DA | 2166 | A | O4'-C1'-N9 | -18.32 | 93.54 | 108.20 |
| 81 | DA | 3042 | U | O5'-P-OP1 | -18.32 | 88.72 | 110.70 |
| 81 | DA | 3299 | A | O4'-C1'-N9 | 18.31 | 122.85 | 108.20 |
| 78 | CA | 1200 | G | N9-C1'-C2' | 18.30 | 137.79 | 114.00 |
| 78 | CA | 1546 | G | C1'-O4'-C4' | -18.30 | 95.26 | 109.90 |
| 81 | DA | 7 | C | P-O3'-C3' | 18.30 | 141.66 | 119.70 |
| 81 | DA | 555 | U | O4'-C1'-N1 | 18.29 | 122.83 | 108.20 |
| 81 | DA | 520 | U | P-O5'-C5' | 18.27 | 150.14 | 120.90 |
| 81 | DA | 1741 | A | P-O3'-C3' | 18.26 | 141.62 | 119.70 |
| 81 | DA | 3050 | U | P-O3'-C3' | 18.26 | 141.61 | 119.70 |
| 79 | CB | 27 | G | P-O3'-C3' | 18.24 | 141.59 | 119.70 |
| 81 | DA | 2827 | U | O4'-C1'-N1 | 18.23 | 122.78 | 108.20 |
| 78 | CA | 1546 | G | O4'-C1'-C2' | 18.22 | 124.02 | 105.80 |
| 78 | CA | 1285 | U | P-O3'-C3' | 18.20 | 141.54 | 119.70 |
| 43 | BP | 2 | GLY | N-CA-C | 18.18 | 158.56 | 113.10 |
| 78 | CA | 1735 | U | P-O3'-C3' | 18.17 | 141.51 | 119.70 |
| 81 | DA | 3242 | G | P-O5'-C5' | 18.12 | 149.90 | 120.90 |
| 81 | DA | 933 | A | O4'-C1'-N9 | 18.10 | 122.68 | 108.20 |
| 78 | CA | 234 | G | O4'-C1'-N9 | 18.09 | 122.67 | 108.20 |
| 78 | CA | 56 | U | O4'-C1'-N1 | 18.09 | 122.67 | 108.20 |
| 81 | DA | 2648 | G | C1'-O4'-C4' | 18.07 | 124.35 | 109.90 |
| 74 | BQ | 243 | ALA | N-CA-CB | 18.03 | 135.35 | 110.10 |
| 81 | DA | 983 | A | O4'-C1'-N9 | 18.01 | 122.61 | 108.20 |
| 81 | DA | 3137 | C | P-O3'-C3' | 18.01 | 141.31 | 119.70 |
| 81 | DA | 780 | A | P-O3'-C3' | 18.00 | 141.30 | 119.70 |
| 78 | CA | 1388 | A | P-O3'-C3' | 17.99 | 141.28 | 119.70 |
| 81 | DA | 2437 | G | O4'-C1'-N9 | 17.99 | 122.59 | 108.20 |
| 81 | DA | 2047 | A | C5'-C4'-O4' | 17.96 | 130.66 | 109.10 |
| 83 | DC | 44 | C | P-O3'-C3' | 17.93 | 141.22 | 119.70 |
| 81 | DA | 677 | A | C1'-O4'-C4' | 17.92 | 124.24 | 109.90 |
| 81 | DA | 666 | A | O4'-C1'-N9 | 17.91 | 122.53 | 108.20 |
| 78 | CA | 1477 | G | O4'-C1'-N9 | 17.91 | 122.53 | 108.20 |
| 31 | BB | 37 | ARG | O-C-N | -17.90 | 94.06 | 122.70 |
| 81 | DA | 579 | G | O4'-C1'-N9 | 17.89 | 122.51 | 108.20 |
| 83 | DC | 49 | G | P-O5'-C5' | 17.89 | 149.52 | 120.90 |
| 81 | DA | 2078 | C | P-O3'-C3' | 17.87 | 141.14 | 119.70 |
| 78 | CA | 219 | A | P-O3'-C3' | 17.86 | 141.13 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 1233 | G | P-O3'-C3' | 17.85 | 141.12 | 119.70 |
| 78 | CA | 1478 | G | O5'-P-OP1 | -17.85 | 89.28 | 110.70 |
| 81 | DA | 518 | G | P-O3'-C3' | 17.85 | 141.12 | 119.70 |
| 78 | CA | 478 | A | O4'-C1'-N9 | 17.84 | 122.47 | 108.20 |
| 81 | DA | 857 | G | P-O3'-C3' | 17.84 | 141.11 | 119.70 |
| 81 | DA | 3149 | G | N9-C1'-C2' | -17.84 | 90.81 | 114.00 |
| 81 | DA | 3099 | C | C5'-C4'-C3' | 17.84 | 144.54 | 116.00 |
| 81 | DA | 699 | A | O4'-C1'-C2' | -17.83 | 87.97 | 105.80 |
| 81 | DA | 1832 | C | P-O3'-C3' | 17.82 | 141.09 | 119.70 |
| 81 | DA | 385 | A | P-O3'-C3' | 17.79 | 141.05 | 119.70 |
| 78 | CA | 1568 | C | O4'-C1'-N1 | 17.76 | 122.41 | 108.20 |
| 39 | BJ | 75 | PRO | CA-C-O | -17.75 | 77.60 | 120.20 |
| 78 | CA | 891 | A | P-O3'-C3' | 17.75 | 140.99 | 119.70 |
| 81 | DA | 3300 | U | P-O3'-C3' | 17.73 | 140.97 | 119.70 |
| 38 | Bs | 243 | TYR | CB-CG-CD2 | -17.72 | 110.37 | 121.00 |
| 78 | CA | 348 | U | P-O5'-C5' | 17.71 | 149.24 | 120.90 |
| 78 | CA | 507 | U | P-O3'-C3' | 17.70 | 140.94 | 119.70 |
| 4 | AD | 148 | ARG | NE-CZ-NH1 | 17.69 | 129.15 | 120.30 |
| 81 | DA | 3130 | A | O4'-C1'-N9 | 17.69 | 122.35 | 108.20 |
| 81 | DA | 2682 | C | O4'-C1'-N1 | 17.68 | 122.34 | 108.20 |
| 78 | CA | 1583 | A | C3'-C2'-C1' | 17.68 | 115.64 | 101.50 |
| 81 | DA | 1588 | A | O4'-C1'-N9 | 17.67 | 122.34 | 108.20 |
| 81 | DA | 3001 | C | P-O3'-C3' | 17.66 | 140.90 | 119.70 |
| 81 | DA | 1292 | C | P-O3'-C3' | 17.65 | 140.88 | 119.70 |
| 57 | Be | 220 | PHE | CB-CG-CD1 | -17.64 | 108.45 | 120.80 |
| 78 | CA | 1356 | U | P-O3'-C3' | 17.63 | 140.85 | 119.70 |
| 78 | CA | 1202 | A | O4'-C1'-N9 | 17.63 | 122.30 | 108.20 |
| 81 | DA | 1144 | U | P-O3'-C3' | 17.61 | 140.84 | 119.70 |
| 81 | DA | 2463 | G | O4'-C1'-N9 | 17.61 | 122.29 | 108.20 |
| 81 | DA | 1060 | U | N1-C1'-C2' | 17.60 | 136.88 | 114.00 |
| 81 | DA | 3201 | C | P-O3'-C3' | 17.58 | 140.80 | 119.70 |
| 81 | DA | 1400 | G | O4'-C1'-N9 | 17.57 | 122.26 | 108.20 |
| 80 | CC | 18 | C | OP1-P-O3' | -17.57 | 66.54 | 105.20 |
| 78 | CA | 69 | G | O4'-C1'-N9 | 17.57 | 122.25 | 108.20 |
| 78 | CA | 501 | U | O4'-C1'-N1 | 17.57 | 122.25 | 108.20 |
| 39 | BJ | 76 | SER | CB-CA-C | 17.55 | 143.44 | 110.10 |
| 81 | DA | 374 | A | O4'-C1'-N9 | 17.53 | 122.22 | 108.20 |
| 81 | DA | 2445 | A | P-O5'-C5' | 17.52 | 148.93 | 120.90 |
| 78 | CA | 402 | C | O4'-C1'-N1 | -17.52 | 94.19 | 108.20 |
| 81 | DA | 3142 | A | C1'-O4'-C4' | 17.52 | 123.91 | 109.90 |
| 81 | DA | 2685 | C | P-O3'-C3' | 17.51 | 140.71 | 119.70 |
| 81 | DA | 1229 | G | O4'-C1'-N9 | 17.50 | 122.20 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 1040 | G | O4'-C1'-N9 | 17.50 | 122.20 | 108.20 |
| 74 | BQ | 158 | ARG | O-C-N | -17.48 | 94.73 | 122.70 |
| 81 | DA | 778 | U | O4'-C1'-N1 | 17.48 | 122.19 | 108.20 |
| 78 | CA | 1748 | G | P-O3'-C3' | 17.48 | 140.68 | 119.70 |
| 81 | DA | 1113 | G | O4'-C1'-N9 | 17.48 | 122.18 | 108.20 |
| 78 | CA | 294 | C | N1-C1'-C2' | 17.47 | 136.71 | 114.00 |
| 14 | AM | 12 | GLN | C-N-CA | 17.46 | 165.34 | 121.70 |
| 78 | CA | 990 | C | N1-C1'-C2' | 17.45 | 136.68 | 114.00 |
| 1 | Aa | 59 | ARG | CB-CA-C | -17.43 | 75.54 | 110.40 |
| 82 | DB | 33 | A | O4'-C1'-N9 | 17.43 | 122.14 | 108.20 |
| 78 | CA | 438 | A | P-O3'-C3' | 17.41 | 140.59 | 119.70 |
| 81 | DA | 456 | U | P-O3'-C3' | 17.41 | 140.59 | 119.70 |
| 78 | CA | 1528 | U | O4'-C1'-N1 | 17.40 | 122.12 | 108.20 |
| 78 | CA | 1389 | C | O4'-C1'-N1 | 17.40 | 122.12 | 108.20 |
| 81 | DA | 1819 | U | O4'-C1'-N1 | 17.39 | 122.11 | 108.20 |
| 78 | CA | 173 | A | P-O5'-C5' | 17.39 | 148.73 | 120.90 |
| 81 | DA | 1164 | G | P-O3'-C3' | 17.39 | 140.56 | 119.70 |
| 81 | DA | 2757 | U | O4'-C1'-C2' | -17.36 | 88.44 | 105.80 |
| 81 | DA | 541 | U | O4'-C1'-N1 | 17.34 | 122.08 | 108.20 |
| 81 | DA | 3331 | U | O4'-C1'-N1 | 17.34 | 122.07 | 108.20 |
| 82 | DB | 99 | C | O4'-C1'-N1 | 17.34 | 122.07 | 108.20 |
| 81 | DA | 3003 | G | O4'-C1'-N9 | 17.31 | 122.05 | 108.20 |
| 81 | DA | 2479 | C | O4'-C1'-N1 | 17.31 | 122.05 | 108.20 |
| 81 | DA | 2566 | C | P-O3'-C3' | 17.31 | 140.47 | 119.70 |
| 78 | CA | 1281 | G | P-O3'-C3' | 17.29 | 140.45 | 119.70 |
| 81 | DA | 1290 | A | O4'-C1'-N9 | 17.29 | 122.03 | 108.20 |
| 78 | CA | 1479 | A | O4'-C1'-N9 | 17.27 | 122.02 | 108.20 |
| 78 | CA | 1520 | U | C5'-C4'-C3' | 17.27 | 143.64 | 116.00 |
| 78 | CA | 773 | C | P-O3'-C3' | 17.26 | 140.42 | 119.70 |
| 81 | DA | 801 | A | O4'-C1'-N9 | 17.26 | 122.01 | 108.20 |
| 78 | CA | 1535 | U | O4'-C1'-N1 | 17.26 | 122.01 | 108.20 |
| 81 | DA | 1685 | C | N1-C1'-C2' | 17.26 | 136.43 | 114.00 |
| 81 | DA | 2669 | G | O4'-C1'-N9 | 17.24 | 121.99 | 108.20 |
| 78 | CA | 1547 | A | P-O3'-C3' | 17.23 | 140.38 | 119.70 |
| 78 | CA | 163 | G | O4'-C1'-N9 | 17.21 | 121.97 | 108.20 |
| 81 | DA | 3107 | U | C3'-C2'-C1' | 17.21 | 115.27 | 101.50 |
| 81 | DA | 3217 | C | O4'-C1'-N1 | 17.21 | 121.97 | 108.20 |
| 81 | DA | 338 | A | C3'-C2'-C1' | 17.20 | 115.26 | 101.50 |
| 81 | DA | 1788 | C | P-O3'-C3' | 17.20 | 140.34 | 119.70 |
| 81 | DA | 1413 | G | P-O3'-C3' | 17.19 | 140.33 | 119.70 |
| 81 | DA | 1208 | U | P-O3'-C3' | 17.16 | 140.29 | 119.70 |
| 81 | DA | 1571 | A | O4'-C1'-N9 | 17.16 | 121.93 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 1698 | G | P-O3'-C3' | 17.16 | 140.29 | 119.70 |
| 81 | DA | 1251 | A | N9-C1'-C2' | 17.14 | 136.29 | 114.00 |
| 81 | DA | 3345 | G | O4'-C1'-N9 | 17.14 | 121.91 | 108.20 |
| 81 | DA | 3092 | C | O4'-C1'-C2' | -17.14 | 88.66 | 105.80 |
| 81 | DA | 947 | G | P-O3'-C3' | 17.12 | 140.25 | 119.70 |
| 34 | BE | 52 | TYR | N-CA-C | 17.12 | 157.22 | 111.00 |
| 81 | DA | 3010 | U | O4'-C1'-N1 | 17.12 | 121.89 | 108.20 |
| 78 | CA | 1234 | A | O4'-C1'-N9 | 17.11 | 121.88 | 108.20 |
| 81 | DA | 1207 | G | O4'-C1'-N9 | -17.08 | 94.54 | 108.20 |
| 81 | DA | 109 | A | N9-C1'-C2' | 17.08 | 136.20 | 114.00 |
| 81 | DA | 2648 | G | P-O3'-C3' | 17.07 | 140.18 | 119.70 |
| 81 | DA | 278 | U | O4'-C1'-N1 | 17.06 | 121.85 | 108.20 |
| 78 | CA | 960 | U | C1'-O4'-C4' | 17.06 | 123.55 | 109.90 |
| 78 | CA | 1548 | G | O4'-C1'-N9 | 17.05 | 121.84 | 108.20 |
| 81 | DA | 1578 | C | P-O3'-C3' | 17.04 | 140.15 | 119.70 |
| 81 | DA | 2238 | G | O4'-C1'-N9 | 17.04 | 121.83 | 108.20 |
| 81 | DA | 1896 | A | N9-C1'-C2' | 17.04 | 136.15 | 114.00 |
| 81 | DA | 993 | G | N9-C1'-C2' | 17.03 | 136.14 | 114.00 |
| 83 | DC | 25 | G | O4'-C1'-N9 | 17.03 | 121.82 | 108.20 |
| 81 | DA | 1268 | G | P-O3'-C3' | 17.03 | 140.13 | 119.70 |
| 78 | CA | 369 | A | O4'-C1'-N9 | 17.02 | 121.82 | 108.20 |
| 81 | DA | 2880 | U | N1-C1'-C2' | 17.01 | 136.12 | 114.00 |
| 35 | BG | 27 | PRO | CA-C-O | -16.99 | 79.42 | 120.20 |
| 78 | CA | 1057 | U | P-O3'-C3' | 16.99 | 140.09 | 119.70 |
| 81 | DA | 1346 | G | O4'-C1'-N9 | 16.98 | 121.79 | 108.20 |
| 81 | DA | 1688 | U | O3'-P-O5' | -16.96 | 71.77 | 104.00 |
| 81 | DA | 1194 | G | P-O3'-C3' | 16.95 | 140.04 | 119.70 |
| 81 | DA | 1682 | U | O4'-C1'-C2' | -16.95 | 88.85 | 105.80 |
| 81 | DA | 2073 | A | P-O3'-C3' | 16.95 | 140.04 | 119.70 |
| 81 | DA | 2367 | A | P-O3'-C3' | 16.95 | 140.04 | 119.70 |
| 81 | DA | 3062 | G | P-O3'-C3' | 16.93 | 140.02 | 119.70 |
| 78 | CA | 1601 | G | P-O3'-C3' | 16.93 | 140.01 | 119.70 |
| 43 | BP | 127 | TYR | CB-CG-CD1 | -16.91 | 110.85 | 121.00 |
| 81 | DA | 896 | A | P-O3'-C3' | 16.91 | 139.99 | 119.70 |
| 81 | DA | 2470 | C | P-O3'-C3' | 16.90 | 139.98 | 119.70 |
| 78 | CA | 1566 | U | O4'-C1'-N1 | 16.90 | 121.72 | 108.20 |
| 81 | DA | 2505 | U | O4'-C1'-N1 | 16.89 | 121.71 | 108.20 |
| 81 | DA | 1217 | A | P-O5'-C5' | 16.89 | 147.92 | 120.90 |
| 34 | BE | 60 | ARG | O-C-N | -16.87 | 95.70 | 122.70 |
| 81 | DA | 1257 | C | O4'-C1'-N1 | 16.87 | 121.69 | 108.20 |
| 81 | DA | 2065 | U | P-O3'-C3' | 16.86 | 139.93 | 119.70 |
| 81 | DA | 670 | C | P-O3'-C3' | 16.86 | 139.93 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 83 | DC | 48 | U | O3'-P-O5' | 16.85 | 136.01 | 104.00 |
| 81 | DA | 1366 | A | N9-C1'-C2' | 16.85 | 135.90 | 114.00 |
| 81 | DA | 2075 | C | P-O3'-C3' | 16.84 | 139.91 | 119.70 |
| 78 | CA | 1393 | C | O4'-C1'-C2' | -16.84 | 88.96 | 105.80 |
| 81 | DA | 715 | A | O4'-C1'-N9 | 16.82 | 121.66 | 108.20 |
| 81 | DA | 1699 | A | O4'-C1'-N9 | 16.82 | 121.66 | 108.20 |
| 78 | CA | 946 | U | O4'-C1'-N1 | 16.82 | 121.65 | 108.20 |
| 78 | CA | 899 | G | C3'-C2'-C1' | -16.81 | 88.06 | 101.50 |
| 81 | DA | 675 | C | C3'-C2'-C1' | 16.81 | 114.94 | 101.50 |
| 81 | DA | 2614 | G | O4'-C1'-N9 | 16.80 | 121.64 | 108.20 |
| 79 | CB | 72 | G | P-O3'-C3' | 16.80 | 139.86 | 119.70 |
| 81 | DA | 1056 | U | O4'-C1'-N1 | 16.80 | 121.64 | 108.20 |
| 82 | DB | 60 | U | O4'-C1'-N1 | 16.77 | 121.62 | 108.20 |
| 82 | DB | 89 | A | P-O3'-C3' | 16.77 | 139.82 | 119.70 |
| 78 | CA | 1068 | C | P-O3'-C3' | 16.76 | 139.82 | 119.70 |
| 78 | CA | 1038 | U | O4'-C1'-N1 | 16.76 | 121.61 | 108.20 |
| 81 | DA | 1807 | G | O4'-C1'-N9 | 16.75 | 121.60 | 108.20 |
| 78 | CA | 1702 | A | C1'-O4'-C4' | 16.74 | 123.30 | 109.90 |
| 78 | CA | 1459 | C | O4'-C1'-N1 | 16.74 | 121.59 | 108.20 |
| 78 | CA | 411 | C | O4'-C1'-N1 | 16.72 | 121.58 | 108.20 |
| 78 | CA | 326 | G | C1'-O4'-C4' | -16.72 | 96.52 | 109.90 |
| 20 | AS | 95 | ASP | CA-C-O | -16.71 | 85.00 | 120.10 |
| 81 | DA | 1639 | C | P-O3'-C3' | 16.71 | 139.76 | 119.70 |
| 82 | DB | 2 | A | P-O3'-C3' | 16.71 | 139.75 | 119.70 |
| 81 | DA | 851 | C | P-O3'-C3' | 16.69 | 139.73 | 119.70 |
| 81 | DA | 2988 | C | O4'-C1'-C2' | -16.67 | 89.13 | 105.80 |
| 81 | DA | 2628 | A | P-O3'-C3' | 16.67 | 139.71 | 119.70 |
| 78 | CA | 245 | U | P-O3'-C3' | 16.66 | 139.70 | 119.70 |
| 78 | CA | 103 | A | P-O3'-C3' | 16.66 | 139.69 | 119.70 |
| 78 | CA | 1477 | G | C3'-C2'-C1' | -16.65 | 88.18 | 101.50 |
| 81 | DA | 1927 | G | O4'-C1'-N9 | 16.65 | 121.52 | 108.20 |
| 78 | CA | 304 | U | P-O3'-C3' | 16.64 | 139.67 | 119.70 |
| 81 | DA | 2446 | U | P-O3'-C3' | 16.64 | 139.67 | 119.70 |
| 81 | DA | 3138 | U | P-O3'-C3' | 16.64 | 139.67 | 119.70 |
| 81 | DA | 1615 | C | P-O3'-C3' | 16.63 | 139.66 | 119.70 |
| 78 | CA | 150 | U | P-O3'-C3' | 16.62 | 139.65 | 119.70 |
| 81 | DA | 311 | C | C5'-C4'-C3' | 16.62 | 142.59 | 116.00 |
| 78 | CA | 309 | C | P-O3'-C3' | 16.62 | 139.64 | 119.70 |
| 81 | DA | 2530 | G | O4'-C1'-N9 | 16.61 | 121.49 | 108.20 |
| 82 | DB | 3 | A | C1'-O4'-C4' | -16.61 | 96.62 | 109.90 |
| 81 | DA | 1602 | A | OP1-P-O3' | 16.60 | 141.72 | 105.20 |
| 81 | DA | 661 | G | O4'-C1'-N9 | 16.60 | 121.48 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 167 | U | O4'-C1'-N1 | 16.59 | 121.47 | 108.20 |
| 81 | DA | 2672 | G | P-O3'-C3' | 16.59 | 139.60 | 119.70 |
| 81 | DA | 468 | G | P-O3'-C3' | 16.58 | 139.60 | 119.70 |
| 81 | DA | 517 | G | N9-C1'-C2' | 16.58 | 135.55 | 114.00 |
| 81 | DA | 1209 | G | O4'-C1'-C2' | -16.57 | 89.23 | 105.80 |
| 81 | DA | 2781 | U | O4'-C1'-N1 | 16.57 | 121.45 | 108.20 |
| 81 | DA | 2187 | G | N9-C1'-C2' | -16.57 | 92.46 | 114.00 |
| 81 | DA | 2450 | G | O4'-C1'-N9 | 16.56 | 121.44 | 108.20 |
| 78 | CA | 585 | A | P-O3'-C3' | 16.54 | 139.55 | 119.70 |
| 78 | CA | 454 | U | O4'-C1'-N1 | 16.54 | 121.43 | 108.20 |
| 78 | CA | 838 | G | C3'-C2'-C1' | 16.53 | 114.73 | 101.50 |
| 81 | DA | 1480 | G | O4'-C1'-N9 | 16.53 | 121.43 | 108.20 |
| 78 | CA | 542 | A | P-O3'-C3' | 16.53 | 139.53 | 119.70 |
| 81 | DA | 1988 | C | P-O3'-C3' | 16.51 | 139.52 | 119.70 |
| 78 | CA | 311 | U | O4'-C1'-N1 | 16.51 | 121.41 | 108.20 |
| 81 | DA | 2665 | U | O4'-C1'-N1 | 16.51 | 121.41 | 108.20 |
| 81 | DA | 1967 | U | O4'-C1'-N1 | 16.50 | 121.40 | 108.20 |
| 81 | DA | 3009 | G | O4'-C1'-N9 | 16.49 | 121.39 | 108.20 |
| 81 | DA | 2719 | U | P-O3'-C3' | 16.49 | 139.48 | 119.70 |
| 78 | CA | 1477 | G | C1'-O4'-C4' | -16.48 | 96.71 | 109.90 |
| 81 | DA | 2596 | U | P-O3'-C3' | 16.47 | 139.46 | 119.70 |
| 82 | DB | 86 | U | O4'-C1'-N1 | 16.46 | 121.37 | 108.20 |
| 81 | DA | 261 | U | O4'-C1'-N1 | 16.45 | 121.36 | 108.20 |
| 78 | CA | 833 | U | O4'-C1'-N1 | 16.43 | 121.35 | 108.20 |
| 78 | CA | 713 | A | P-O3'-C3' | 16.43 | 139.42 | 119.70 |
| 81 | DA | 2899 | C | N1-C1'-C2' | 16.43 | 135.36 | 114.00 |
| 79 | CB | 13 | U | O4'-C1'-N1 | 16.42 | 121.34 | 108.20 |
| 81 | DA | 2491 | A | C4'-C3'-C2' | 16.42 | 119.02 | 102.60 |
| 81 | DA | 9 | U | P-O3'-C3' | 16.42 | 139.40 | 119.70 |
| 78 | CA | 306 | U | C1'-O4'-C4' | 16.41 | 123.03 | 109.90 |
| 81 | DA | 2745 | G | O4'-C1'-N9 | 16.41 | 121.33 | 108.20 |
| 78 | CA | 119 | A | O3'-P-O5' | 16.41 | 135.18 | 104.00 |
| 14 | AM | 12 | GLN | O-C-N | -16.39 | 96.48 | 122.70 |
| 81 | DA | 2720 | G | C3'-C2'-C1' | 16.39 | 114.61 | 101.50 |
| 81 | DA | 3372 | A | P-O3'-C3' | 16.37 | 139.35 | 119.70 |
| 81 | DA | 2393 | G | P-O5'-C5' | 16.36 | 147.08 | 120.90 |
| 81 | DA | 1677 | G | O4'-C1'-N9 | 16.36 | 121.29 | 108.20 |
| 81 | DA | 3383 | G | O4'-C1'-N9 | 16.36 | 121.29 | 108.20 |
| 78 | CA | 234 | G | P-O3'-C3' | 16.36 | 139.33 | 119.70 |
| 78 | CA | 714 | G | P-O3'-C3' | 16.35 | 139.32 | 119.70 |
| 81 | DA | 3169 | U | O4'-C1'-N1 | 16.35 | 121.28 | 108.20 |
| 81 | DA | 1974 | A | P-O3'-C3' | 16.34 | 139.30 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2627 | C | O5'-P-OP2 | -16.34 | 91.00 | 105.70 |
| 81 | DA | 1226 | G | P-O3'-C3' | 16.33 | 139.29 | 119.70 |
| 78 | CA | 1201 | G | O4'-C1'-N9 | -16.32 | 95.14 | 108.20 |
| 78 | CA | 1405 | G | O4'-C1'-N9 | 16.31 | 121.25 | 108.20 |
| 78 | CA | 590 | C | P-O3'-C3' | 16.31 | 139.27 | 119.70 |
| 81 | DA | 2581 | U | P-O3'-C3' | 16.31 | 139.27 | 119.70 |
| 81 | DA | 1942 | U | P-O3'-C3' | 16.30 | 139.26 | 119.70 |
| 78 | CA | 1528 | U | P-O5'-C5' | 16.30 | 146.98 | 120.90 |
| 81 | DA | 2816 | G | O4'-C1'-N9 | -16.30 | 95.16 | 108.20 |
| 81 | DA | 1617 | G | P-O3'-C3' | 16.30 | 139.26 | 119.70 |
| 78 | CA | 894 | U | P-O3'-C3' | 16.28 | 139.24 | 119.70 |
| 81 | DA | 3247 | G | O4'-C1'-N9 | 16.28 | 121.23 | 108.20 |
| 81 | DA | 2243 | A | O4'-C1'-N9 | 16.27 | 121.22 | 108.20 |
| 81 | DA | 1083 | G | O4'-C1'-N9 | 16.25 | 121.20 | 108.20 |
| 81 | DA | 1397 | C | P-O5'-C5' | 16.25 | 146.91 | 120.90 |
| 81 | DA | 534 | U | O4'-C1'-N1 | 16.25 | 121.20 | 108.20 |
| 81 | DA | 2928 | C | P-O3'-C3' | 16.25 | 139.20 | 119.70 |
| 78 | CA | 839 | U | O4'-C1'-N1 | 16.24 | 121.19 | 108.20 |
| 83 | DC | 3 | U | O4'-C1'-C2' | -16.24 | 89.56 | 105.80 |
| 81 | DA | 1684 | U | P-O3'-C3' | 16.24 | 139.19 | 119.70 |
| 81 | DA | 3241 | G | N9-C1'-C2' | 16.20 | 135.06 | 114.00 |
| 81 | DA | 2228 | A | P-O3'-C3' | 16.19 | 139.13 | 119.70 |
| 78 | CA | 613 | G | O4'-C1'-N9 | 16.18 | 121.15 | 108.20 |
| 81 | DA | 162 | G | O4'-C1'-N9 | 16.18 | 121.14 | 108.20 |
| 78 | CA | 1724 | U | O4'-C1'-N1 | 16.16 | 121.12 | 108.20 |
| 78 | CA | 1043 | A | O4'-C1'-N9 | 16.16 | 121.12 | 108.20 |
| 81 | DA | 424 | G | P-O3'-C3' | 16.14 | 139.07 | 119.70 |
| 78 | CA | 1351 | G | P-O3'-C3' | 16.14 | 139.06 | 119.70 |
| 78 | CA | 1541 | G | N9-C1'-C2' | 16.13 | 134.97 | 114.00 |
| 78 | CA | 631 | G | N9-C1'-C2' | -16.12 | 93.04 | 114.00 |
| 78 | CA | 1397 | U | P-O5'-C5' | 16.12 | 146.69 | 120.90 |
| 81 | DA | 1401 | A | C1'-O4'-C4' | 16.10 | 122.78 | 109.90 |
| 78 | CA | 631 | G | C1'-O4'-C4' | 16.10 | 122.78 | 109.90 |
| 81 | DA | 2046 | U | O3'-P-O5' | -16.10 | 73.41 | 104.00 |
| 81 | DA | 3041 | U | OP1-P-O3' | 16.10 | 140.61 | 105.20 |
| 78 | CA | 299 | A | O4'-C1'-N9 | 16.09 | 121.08 | 108.20 |
| 81 | DA | 1357 | G | O4'-C1'-N9 | 16.08 | 121.06 | 108.20 |
| 81 | DA | 2498 | U | O4'-C1'-N1 | 16.07 | 121.06 | 108.20 |
| 81 | DA | 2025 | G | P-O5'-C5' | 16.07 | 146.61 | 120.90 |
| 81 | DA | 3005 | A | O4'-C1'-N9 | 16.06 | 121.05 | 108.20 |
| 81 | DA | 1867 | A | O4'-C1'-N9 | 16.06 | 121.05 | 108.20 |
| 81 | DA | 2364 | G | P-O3'-C3' | 16.05 | 138.97 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2580 | A | O4'-C1'-N9 | 16.04 | 121.03 | 108.20 |
| 46 | BT | 88 | ARG | NE-CZ-NH2 | -16.03 | 112.28 | 120.30 |
| 81 | DA | 297 | G | O4'-C1'-N9 | 15.99 | 121.00 | 108.20 |
| 81 | DA | 1517 | G | P-O3'-C3' | 15.99 | 138.89 | 119.70 |
| 81 | DA | 2934 | A | N9-C1'-C2' | -15.99 | 93.22 | 114.00 |
| 34 | BE | 55 | ARG | C-N-CA | 15.98 | 161.65 | 121.70 |
| 81 | DA | 1661 | G | O4'-C1'-N9 | 15.98 | 120.98 | 108.20 |
| 78 | CA | 218 | A | P-O3'-C3' | 15.97 | 138.87 | 119.70 |
| 81 | DA | 677 | A | O4'-C1'-C2' | -15.97 | 89.83 | 105.80 |
| 82 | DB | 122 | U | O4'-C1'-N1 | 15.96 | 120.97 | 108.20 |
| 78 | CA | 1559 | A | O4'-C1'-N9 | 15.95 | 120.96 | 108.20 |
| 81 | DA | 1947 | G | P-O3'-C3' | 15.92 | 138.80 | 119.70 |
| 78 | CA | 1754 | A | P-O3'-C3' | 15.92 | 138.80 | 119.70 |
| 81 | DA | 680 | G | O4'-C1'-N9 | 15.90 | 120.92 | 108.20 |
| 78 | CA | 1436 | A | N9-C1'-C2' | 15.90 | 134.67 | 114.00 |
| 81 | DA | 1871 | U | C5'-C4'-O4' | -15.88 | 90.04 | 109.10 |
| 17 | AQ | 94 | SER | N-CA-CB | 15.88 | 134.32 | 110.50 |
| 33 | BD | 354 | VAL | O-C-N | -15.86 | 97.33 | 122.70 |
| 81 | DA | 1750 | A | P-O3'-C3' | 15.85 | 138.72 | 119.70 |
| 81 | DA | 1686 | U | O4'-C1'-C2' | -15.85 | 89.95 | 105.80 |
| 81 | DA | 2170 | U | O4'-C1'-N1 | 15.85 | 120.88 | 108.20 |
| 81 | DA | 2970 | C | P-O3'-C3' | 15.85 | 138.71 | 119.70 |
| 81 | DA | 2315 | G | P-O3'-C3' | 15.84 | 138.71 | 119.70 |
| 81 | DA | 2362 | C | C1'-O4'-C4' | 15.84 | 122.57 | 109.90 |
| 83 | DC | 8 | G | O4'-C1'-N9 | 15.84 | 120.87 | 108.20 |
| 81 | DA | 3051 | U | P-O3'-C3' | 15.83 | 138.70 | 119.70 |
| 78 | CA | 867 | G | O4'-C1'-N9 | 15.83 | 120.87 | 108.20 |
| 78 | CA | 336 | G | O4'-C1'-N9 | 15.82 | 120.86 | 108.20 |
| 81 | DA | 166 | C | P-O3'-C3' | 15.82 | 138.69 | 119.70 |
| 78 | CA | 853 | G | O4'-C1'-N9 | 15.82 | 120.85 | 108.20 |
| 78 | CA | 1089 | U | O4'-C1'-N1 | 15.81 | 120.85 | 108.20 |
| 6 | AE | 92 | ALA | CB-CA-C | -15.81 | 86.39 | 110.10 |
| 81 | DA | 1006 | A | O4'-C1'-N9 | 15.80 | 120.84 | 108.20 |
| 81 | DA | 2060 | A | P-O3'-C3' | 15.79 | 138.65 | 119.70 |
| 81 | DA | 1695 | U | O4'-C1'-N1 | 15.78 | 120.83 | 108.20 |
| 81 | DA | 1232 | C | P-O3'-C3' | 15.78 | 138.64 | 119.70 |
| 78 | CA | 1584 | G | C3'-C2'-C1' | -15.78 | 88.88 | 101.50 |
| 78 | CA | 631 | G | O4'-C1'-C2' | -15.75 | 90.05 | 105.80 |
| 81 | DA | 2637 | A | N9-C1'-C2' | -15.75 | 93.53 | 114.00 |
| 81 | DA | 73 | C | P-O3'-C3' | 15.75 | 138.59 | 119.70 |
| 81 | DA | 984 | G | O4'-C1'-N9 | 15.74 | 120.79 | 108.20 |
| 79 | CB | 64 | G | P-O3'-C3' | 15.73 | 138.58 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 3054 | U | P-O3'-C3' | 15.73 | 138.58 | 119.70 |
| 81 | DA | 3304 | U | C5'-C4'-C3' | -15.73 | 90.84 | 116.00 |
| 81 | DA | 1567 | U | P-O3'-C3' | 15.72 | 138.57 | 119.70 |
| 81 | DA | 1748 | G | P-O3'-C3' | 15.71 | 138.55 | 119.70 |
| 81 | DA | 3090 | U | C3'-C2'-C1' | 15.70 | 114.06 | 101.50 |
| 81 | DA | 2530 | G | P-O3'-C3' | 15.70 | 138.54 | 119.70 |
| 81 | DA | 1870 | C | P-O3'-C3' | 15.69 | 138.53 | 119.70 |
| 81 | DA | 1395 | G | P-O3'-C3' | 15.67 | 138.51 | 119.70 |
| 81 | DA | 1972 | A | P-O3'-C3' | 15.67 | 138.51 | 119.70 |
| 81 | DA | 2969 | A | P-O3'-C3' | 15.66 | 138.50 | 119.70 |
| 81 | DA | 1622 | U | O4'-C1'-N1 | 15.66 | 120.73 | 108.20 |
| 81 | DA | 1391 | C | C5'-C4'-C3' | 15.65 | 141.04 | 116.00 |
| 81 | DA | 1975 | C | O4'-C1'-C2' | -15.65 | 90.15 | 105.80 |
| 78 | CA | 1478 | G | O4'-C1'-C2' | 15.64 | 121.68 | 107.60 |
| 78 | CA | 1548 | G | C3'-C2'-C1' | -15.64 | 88.99 | 101.50 |
| 81 | DA | 2708 | C | P-O3'-C3' | 15.63 | 138.46 | 119.70 |
| 81 | DA | 2837 | A | O4'-C1'-N9 | 15.63 | 120.70 | 108.20 |
| 81 | DA | 1483 | G | P-O3'-C3' | 15.63 | 138.46 | 119.70 |
| 83 | DC | 60 | G | O4'-C1'-C2' | 15.62 | 121.66 | 107.60 |
| 78 | CA | 1419 | G | O4'-C1'-N9 | 15.61 | 120.69 | 108.20 |
| 81 | DA | 884 | A | O4'-C1'-N9 | 15.61 | 120.68 | 108.20 |
| 82 | DB | 93 | U | P-O3'-C3' | 15.60 | 138.42 | 119.70 |
| 81 | DA | 2859 | U | O4'-C1'-N1 | 15.60 | 120.68 | 108.20 |
| 81 | DA | 425 | G | P-O3'-C3' | 15.59 | 138.41 | 119.70 |
| 81 | DA | 2629 | U | O4'-C1'-N1 | 15.59 | 120.67 | 108.20 |
| 81 | DA | 328 | U | P-O3'-C3' | 15.59 | 138.40 | 119.70 |
| 81 | DA | 2207 | A | O4'-C1'-N9 | 15.59 | 120.67 | 108.20 |
| 83 | DC | 85 | G | O4'-C1'-N9 | 15.59 | 120.67 | 108.20 |
| 83 | DC | 26 | C | N1-C1'-C2' | 15.57 | 134.25 | 114.00 |
| 78 | CA | 222 | A | O4'-C1'-N9 | 15.57 | 120.66 | 108.20 |
| 81 | DA | 1668 | G | O4'-C1'-N9 | 15.57 | 120.66 | 108.20 |
| 4 | AD | 145 | ARG | NE-CZ-NH1 | 15.56 | 128.08 | 120.30 |
| 81 | DA | 2530 | G | O3'-P-O5' | -15.56 | 74.44 | 104.00 |
| 78 | CA | 820 | U | O4'-C1'-N1 | 15.55 | 120.64 | 108.20 |
| 81 | DA | 1281 | G | O4'-C1'-N9 | 15.53 | 120.62 | 108.20 |
| 81 | DA | 959 | C | P-O3'-C3' | 15.53 | 138.33 | 119.70 |
| 81 | DA | 2934 | A | O4'-C1'-N9 | 15.50 | 120.60 | 108.20 |
| 78 | CA | 304 | U | O4'-C1'-N1 | 15.46 | 120.56 | 108.20 |
| 78 | CA | 1584 | G | P-O5'-C5' | 15.45 | 145.62 | 120.90 |
| 81 | DA | 2508 | U | C3'-C2'-C1' | 15.44 | 113.85 | 101.50 |
| 81 | DA | 374 | A | P-O3'-C3' | 15.43 | 138.22 | 119.70 |
| 81 | DA | 1943 | C | P-O3'-C3' | 15.43 | 138.22 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 44 | BO | 57 | GLY | CA-C-O | -15.41 | 92.85 | 120.60 |
| 81 | DA | 1698 | C | O4'-C1'-N1 | 15.40 | 120.52 | 108.20 |
| 81 | DA | 2783 | U | O4'-C1'-N1 | 15.38 | 120.51 | 108.20 |
| 81 | DA | 3216 | G | O4'-C1'-N9 | 15.38 | 120.51 | 108.20 |
| 81 | DA | 1748 | G | O4'-C1'-N9 | 15.37 | 120.50 | 108.20 |
| 78 | CA | 868 | G | O4'-C1'-N9 | 15.37 | 120.50 | 108.20 |
| 81 | DA | 76 | G | O4'-C1'-N9 | 15.37 | 120.50 | 108.20 |
| 81 | DA | 3374 | U | P-O3'-C3' | 15.37 | 138.14 | 119.70 |
| 78 | CA | 1472 | C | P-O3'-C3' | 15.36 | 138.13 | 119.70 |
| 81 | DA | 437 | G | P-O3'-C3' | 15.35 | 138.12 | 119.70 |
| 81 | DA | 3332 | U | O4'-C1'-N1 | 15.35 | 120.48 | 108.20 |
| 81 | DA | 3354 | U | O4'-C1'-N1 | 15.34 | 120.47 | 108.20 |
| 78 | CA | 1601 | G | C1'-O4'-C4' | -15.34 | 97.63 | 109.90 |
| 78 | CA | 174 | U | P-O5'-C5' | 15.32 | 145.41 | 120.90 |
| 81 | DA | 1045 | C | O4'-C1'-N1 | 15.31 | 120.45 | 108.20 |
| 81 | DA | 602 | A | P-O3'-C3' | 15.31 | 138.07 | 119.70 |
| 78 | CA | 634 | G | O4'-C1'-N9 | 15.30 | 120.44 | 108.20 |
| 81 | DA | 2175 | U | C5'-C4'-C3' | -15.30 | 91.52 | 116.00 |
| 81 | DA | 1625 | A | P-O5'-C5' | 15.29 | 145.37 | 120.90 |
| 81 | DA | 169 | U | N1-C1'-C2' | -15.28 | 94.13 | 114.00 |
| 81 | DA | 2041 | U | O4'-C1'-N1 | 15.28 | 120.42 | 108.20 |
| 81 | DA | 2066 | C | P-O3'-C3' | 15.28 | 138.04 | 119.70 |
| 79 | CB | 40 | U | P-O3'-C3' | 15.28 | 138.04 | 119.70 |
| 81 | DA | 990 | U | O4'-C1'-N1 | 15.27 | 120.41 | 108.20 |
| 81 | DA | 2531 | C | C5'-C4'-C3' | 15.27 | 140.43 | 116.00 |
| 83 | DC | 113 | C | P-O5'-C5' | 15.26 | 145.32 | 120.90 |
| 78 | CA | 161 | U | P-O3'-C3' | 15.26 | 138.01 | 119.70 |
| 81 | DA | 1401 | A | O4'-C1'-C2' | -15.23 | 90.57 | 105.80 |
| 81 | DA | 3386 | G | P-O3'-C3' | 15.22 | 137.97 | 119.70 |
| 81 | DA | 1429 | G | O4'-C1'-N9 | -15.19 | 96.05 | 108.20 |
| 81 | DA | 1579 | C | C3'-C2'-C1' | 15.19 | 113.65 | 101.50 |
| 81 | DA | 2712 | U | O4'-C1'-N1 | 15.19 | 120.35 | 108.20 |
| 81 | DA | 1005 | G | O4'-C1'-N9 | 15.18 | 120.34 | 108.20 |
| 81 | DA | 989 | A | O4'-C1'-N9 | 15.17 | 120.34 | 108.20 |
| 78 | CA | 1507 | G | P-O3'-C3' | 15.17 | 137.90 | 119.70 |
| 81 | DA | 618 | C | P-O3'-C3' | 15.17 | 137.90 | 119.70 |
| 81 | DA | 2623 | G | N9-C1'-C2' | -15.17 | 94.28 | 114.00 |
| 81 | DA | 2266 | U | P-O3'-C3' | 15.16 | 137.89 | 119.70 |
| 81 | DA | 1115 | G | C3'-C2'-C1' | 15.15 | 113.62 | 101.50 |
| 81 | DA | 2531 | C | C5'-C4'-O4' | -15.14 | 90.93 | 109.10 |
| 55 | Bc | 108 | GLN | O-C-N | -15.13 | 98.49 | 122.70 |
| 81 | DA | 3131 | U | N1-C1'-C2' | 15.13 | 133.67 | 114.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1273 | A | P-O3'-C3' | 15.12 | 137.84 | 119.70 |
| 81 | DA | 401 | U | O4'-C1'-N1 | 15.11 | 120.29 | 108.20 |
| 81 | DA | 1236 | G | O4'-C1'-N9 | 15.11 | 120.29 | 108.20 |
| 81 | DA | 1 | G | P-O3'-C3' | 15.10 | 137.82 | 119.70 |
| 81 | DA | 1391 | C | O4'-C1'-N1 | 15.10 | 120.28 | 108.20 |
| 82 | DB | 38 | U | N1-C1'-C2' | 15.10 | 133.63 | 114.00 |
| 2 | AA | 10 | THR | C-N-CD | -15.10 | 87.39 | 120.60 |
| 78 | CA | 844 | A | N1-C6-N6 | 15.09 | 127.65 | 118.60 |
| 78 | CA | 1189 | A | P-O3'-C3' | 15.09 | 137.80 | 119.70 |
| 81 | DA | 721 | G | O4'-C1'-N9 | 15.09 | 120.27 | 108.20 |
| 81 | DA | 1014 | U | N1-C1'-C2' | 15.08 | 133.61 | 114.00 |
| 78 | CA | 1647 | U | P-O3'-C3' | 15.07 | 137.78 | 119.70 |
| 81 | DA | 899 | U | P-O3'-C3' | 15.07 | 137.78 | 119.70 |
| 83 | DC | 83 | U | P-O3'-C3' | 15.06 | 137.77 | 119.70 |
| 78 | CA | 1381 | U | P-O3'-C3' | 15.05 | 137.76 | 119.70 |
| 78 | CA | 610 | G | C3'-C2'-C1' | -15.05 | 89.46 | 101.50 |
| 81 | DA | 1579 | C | P-O3'-C3' | 15.04 | 137.75 | 119.70 |
| 81 | DA | 1198 | C | P-O3'-C3' | 15.04 | 137.75 | 119.70 |
| 81 | DA | 1293 | U | P-O3'-C3' | 15.03 | 137.74 | 119.70 |
| 81 | DA | 1291 | A | P-O3'-C3' | 15.02 | 137.73 | 119.70 |
| 81 | DA | 894 | G | O4'-C1'-N9 | 15.01 | 120.21 | 108.20 |
| 81 | DA | 2501 | U | P-O3'-C3' | 15.01 | 137.71 | 119.70 |
| 57 | Be | 220 | PHE | N-CA-CB | -15.00 | 83.59 | 110.60 |
| 81 | DA | 2046 | U | O4'-C1'-N1 | 15.00 | 120.20 | 108.20 |
| 81 | DA | 530 | G | O4'-C1'-N9 | 15.00 | 120.20 | 108.20 |
| 81 | DA | 3145 | C | O4'-C1'-N1 | 14.99 | 120.19 | 108.20 |
| 32 | BC | 6 | TYR | CB-CG-CD2 | 14.99 | 130.00 | 121.00 |
| 81 | DA | 887 | G | P-O3'-C3' | 14.98 | 137.68 | 119.70 |
| 81 | DA | 2889 | C | P-O3'-C3' | 14.98 | 137.68 | 119.70 |
| 81 | DA | 3306 | U | N1-C1'-C2' | 14.98 | 133.48 | 114.00 |
| 81 | DA | 933 | A | P-O3'-C3' | 14.97 | 137.67 | 119.70 |
| 78 | CA | 646 | C | P-O3'-C3' | 14.96 | 137.65 | 119.70 |
| 81 | DA | 2578 | U | P-O3'-C3' | 14.95 | 137.64 | 119.70 |
| 16 | AO | 40 | TYR | CB-CG-CD1 | 14.94 | 129.97 | 121.00 |
| 81 | DA | 2303 | A | N9-C1'-C2' | -14.94 | 94.58 | 114.00 |
| 81 | DA | 906 | A | O4'-C1'-N9 | 14.94 | 120.15 | 108.20 |
| 81 | DA | 550 | A | O4'-C1'-N9 | 14.93 | 120.14 | 108.20 |
| 78 | CA | 265 | A | P-O3'-C3' | 14.91 | 137.59 | 119.70 |
| 78 | CA | 1476 | C | O4'-C1'-C2' | -14.90 | 90.89 | 105.80 |
| 5 | AC | 114 | TYR | CB-CG-CD1 | -14.90 | 112.06 | 121.00 |
| 81 | DA | 2803 | A | O4'-C1'-N9 | 14.90 | 120.12 | 108.20 |
| 81 | DA | 1790 | G | O4'-C1'-N9 | 14.89 | 120.12 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 34 | BE | 51 | ARG | O-C-N | -14.88 | 98.89 | 122.70 |
| 81 | DA | 1825 | G | P-O3'-C3' | 14.88 | 137.55 | 119.70 |
| 81 | DA | 3003 | G | C3'-C2'-C1' | -14.88 | 89.60 | 101.50 |
| 81 | DA | 512 | U | N1-C1'-C2' | 14.87 | 133.33 | 114.00 |
| 82 | DB | 137 | C | P-O3'-C3' | 14.86 | 137.54 | 119.70 |
| 81 | DA | 705 | A | O4'-C1'-N9 | 14.86 | 120.09 | 108.20 |
| 81 | DA | 2445 | A | P-O3'-C3' | 14.86 | 137.53 | 119.70 |
| 81 | DA | 1527 | C | P-O3'-C3' | 14.85 | 137.52 | 119.70 |
| 81 | DA | 2463 | G | P-O3'-C3' | 14.85 | 137.52 | 119.70 |
| 81 | DA | 2683 | U | P-O3'-C3' | 14.85 | 137.51 | 119.70 |
| 78 | CA | 631 | G | O4'-C1'-N9 | 14.84 | 120.07 | 108.20 |
| 78 | CA | 1357 | A | P-O3'-C3' | 14.83 | 137.50 | 119.70 |
| 81 | DA | 3136 | G | O4'-C1'-N9 | 14.83 | 120.06 | 108.20 |
| 78 | CA | 680 | U | O4'-C1'-N1 | 14.82 | 120.06 | 108.20 |
| 81 | DA | 1686 | U | C3'-C2'-C1' | 14.82 | 113.36 | 101.50 |
| 81 | DA | 2186 | U | P-O3'-C3' | 14.82 | 137.48 | 119.70 |
| 81 | DA | 2824 | G | P-O3'-C3' | 14.81 | 137.47 | 119.70 |
| 83 | DC | 16 | U | O4'-C1'-N1 | 14.80 | 120.04 | 108.20 |
| 78 | CA | 1409 | G | P-O3'-C3' | 14.80 | 137.46 | 119.70 |
| 81 | DA | 1831 | U | N1-C1'-C2' | -14.80 | 94.76 | 114.00 |
| 81 | DA | 2513 | U | P-O3'-C3' | 14.79 | 137.45 | 119.70 |
| 78 | CA | 1238 | A | O4'-C1'-N9 | 14.79 | 120.03 | 108.20 |
| 81 | DA | 664 | U | O4'-C1'-N1 | 14.79 | 120.03 | 108.20 |
| 81 | DA | 160 | G | O4'-C1'-C2' | 14.78 | 120.90 | 107.60 |
| 11 | AJ | 85 | ARG | NH1-CZ-NH2 | -14.78 | 103.15 | 119.40 |
| 78 | CA | 515 | A | P-O3'-C3' | 14.78 | 137.43 | 119.70 |
| 81 | DA | 472 | A | P-O3'-C3' | 14.77 | 137.43 | 119.70 |
| 81 | DA | 2544 | U | P-O3'-C3' | 14.77 | 137.42 | 119.70 |
| 81 | DA | 2487 | U | O4'-C1'-C2' | -14.77 | 91.03 | 105.80 |
| 81 | DA | 2494 | A | O4'-C1'-N9 | 14.77 | 120.02 | 108.20 |
| 81 | DA | 3231 | U | P-O3'-C3' | 14.77 | 137.42 | 119.70 |
| 11 | AJ | 23 | ARG | NE-CZ-NH2 | -14.76 | 112.92 | 120.30 |
| 81 | DA | 338 | A | P-O3'-C3' | 14.76 | 137.41 | 119.70 |
| 81 | DA | 1078 | U | O4'-C1'-C2' | -14.76 | 91.04 | 105.80 |
| 81 | DA | 3004 | C | N1-C1'-C2' | 14.75 | 133.18 | 114.00 |
| 78 | CA | 1297 | G | O4'-C1'-N9 | 14.75 | 120.00 | 108.20 |
| 81 | DA | 1702 | U | O4'-C1'-N1 | 14.75 | 120.00 | 108.20 |
| 81 | DA | 799 | G | O4'-C1'-N9 | 14.74 | 120.00 | 108.20 |
| 78 | CA | 1615 | C | C3'-C2'-C1' | 14.74 | 113.29 | 101.50 |
| 81 | DA | 3214 | U | P-O3'-C3' | 14.74 | 137.39 | 119.70 |
| 81 | DA | 2710 | C | P-O3'-C3' | 14.73 | 137.38 | 119.70 |
| 78 | CA | 281 | G | P-O3'-C3' | 14.73 | 137.38 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 772 | U | O4'-C1'-N1 | 14.73 | 119.98 | 108.20 |
| 81 | DA | 2080 | C | P-O3'-C3' | 14.73 | 137.38 | 119.70 |
| 16 | AO | 104 | ARG | NE-CZ-NH2 | -14.72 | 112.94 | 120.30 |
| 81 | DA | 1222 | G | O4'-C1'-N9 | 14.72 | 119.97 | 108.20 |
| 81 | DA | 567 | G | O4'-C1'-N9 | 14.71 | 119.97 | 108.20 |
| 81 | DA | 581 | U | O4'-C1'-N1 | 14.71 | 119.97 | 108.20 |
| 78 | CA | 630 | A | N9-C1'-C2' | -14.71 | 94.88 | 114.00 |
| 81 | DA | 636 | C | O4'-C1'-C2' | -14.71 | 91.09 | 105.80 |
| 81 | DA | 1054 | A | N9-C1'-C2' | -14.71 | 94.88 | 114.00 |
| 78 | CA | 1401 | A | P-O3'-C3' | 14.71 | 137.35 | 119.70 |
| 81 | DA | 326 | U | P-O3'-C3' | 14.70 | 137.34 | 119.70 |
| 81 | DA | 729 | C | P-O3'-C3' | 14.70 | 137.34 | 119.70 |
| 78 | CA | 1547 | A | O5'-P-OP1 | 14.69 | 128.32 | 110.70 |
| 81 | DA | 2593 | A | P-O3'-C3' | 14.68 | 137.32 | 119.70 |
| 81 | DA | 1055 | A | N9-C1'-C2' | -14.68 | 94.92 | 114.00 |
| 81 | DA | 2698 | G | P-O3'-C3' | 14.68 | 137.31 | 119.70 |
| 81 | DA | 2377 | G | P-O5'-C5' | 14.67 | 144.38 | 120.90 |
| 81 | DA | 70 | A | N9-C1'-C2' | 14.67 | 133.07 | 114.00 |
| 78 | CA | 254 | A | O4'-C1'-N9 | 14.66 | 119.93 | 108.20 |
| 81 | DA | 3221 | C | O4'-C1'-N1 | -14.66 | 96.47 | 108.20 |
| 78 | CA | 965 | U | N1-C1'-C2' | 14.66 | 133.05 | 114.00 |
| 81 | DA | 2283 | G | P-O3'-C3' | 14.66 | 137.29 | 119.70 |
| 81 | DA | 3167 | A | O4'-C1'-N9 | 14.65 | 119.92 | 108.20 |
| 81 | DA | 638 | C | C5'-C4'-O4' | 14.65 | 126.67 | 109.10 |
| 81 | DA | 2869 | U | C1'-O4'-C4' | 14.64 | 121.61 | 109.90 |
| 81 | DA | 1013 | G | O4'-C1'-N9 | 14.64 | 119.91 | 108.20 |
| 44 | BO | 57 | GLY | CA-C-N | 14.64 | 149.40 | 117.20 |
| 81 | DA | 2186 | U | O4'-C1'-N1 | 14.64 | 119.91 | 108.20 |
| 78 | CA | 190 | C | P-O3'-C3' | 14.63 | 137.26 | 119.70 |
| 81 | DA | 2194 | G | P-O3'-C3' | 14.63 | 137.26 | 119.70 |
| 78 | CA | 1743 | U | O4'-C1'-N1 | 14.63 | 119.90 | 108.20 |
| 81 | DA | 1768 | U | P-O3'-C3' | 14.61 | 137.23 | 119.70 |
| 78 | CA | 504 | U | P-O3'-C3' | 14.60 | 137.22 | 119.70 |
| 81 | DA | 1692 | U | P-O3'-C3' | 14.60 | 137.22 | 119.70 |
| 81 | DA | 1203 | A | N9-C1'-C2' | 14.59 | 132.96 | 114.00 |
| 57 | Be | 98 | LYS | N-CA-CB | 14.57 | 136.83 | 110.60 |
| 81 | DA | 331 | G | C1'-O4'-C4' | 14.57 | 121.56 | 109.90 |
| 81 | DA | 996 | A | O4'-C1'-N9 | 14.56 | 119.85 | 108.20 |
| 81 | DA | 2546 | C | P-O3'-C3' | 14.56 | 137.17 | 119.70 |
| 81 | DA | 2860 | U | P-O3'-C3' | 14.56 | 137.17 | 119.70 |
| 81 | DA | 1076 | C | P-O3'-C3' | 14.55 | 137.17 | 119.70 |
| 81 | DA | 2726 | C | P-O3'-C3' | 14.55 | 137.16 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 185 | C | P-O3'-C3' | 14.55 | 137.16 | 119.70 |
| 81 | DA | 1965 | C | O4'-C1'-N1 | 14.55 | 119.84 | 108.20 |
| 78 | CA | 1480 | G | O4'-C1'-N9 | 14.55 | 119.84 | 108.20 |
| 81 | DA | 1575 | A | O4'-C1'-N9 | 14.55 | 119.84 | 108.20 |
| 81 | DA | 723 | U | O4'-C1'-N1 | 14.54 | 119.83 | 108.20 |
| 58 | Bg | 10 | ARG | NE-CZ-NH1 | 14.52 | 127.56 | 120.30 |
| 81 | DA | 2 | U | O4'-C1'-N1 | 14.51 | 119.81 | 108.20 |
| 78 | CA | 460 | A | O4'-C1'-N9 | 14.50 | 119.80 | 108.20 |
| 78 | CA | 1604 | U | O4'-C1'-N1 | 14.50 | 119.80 | 108.20 |
| 81 | DA | 2231 | C | N1-C1'-C2' | 14.50 | 132.85 | 114.00 |
| 41 | BN | 19 | ARG | NE-CZ-NH1 | 14.49 | 127.55 | 120.30 |
| 81 | DA | 752 | C | P-O3'-C3' | 14.49 | 137.09 | 119.70 |
| 81 | DA | 1789 | G | O4'-C1'-C2' | 14.48 | 120.63 | 107.60 |
| 81 | DA | 1585 | C | P-O3'-C3' | 14.47 | 137.07 | 119.70 |
| 81 | DA | 1778 | G | P-O3'-C3' | 14.47 | 137.07 | 119.70 |
| 81 | DA | 2350 | C | P-O3'-C3' | 14.47 | 137.06 | 119.70 |
| 81 | DA | 1704 | A | P-O3'-C3' | 14.47 | 137.06 | 119.70 |
| 34 | BE | 55 | ARG | CA-C-O | -14.46 | 89.73 | 120.10 |
| 81 | DA | 796 | U | P-O3'-C3' | 14.46 | 137.05 | 119.70 |
| 81 | DA | 1207 | G | O4'-C1'-C2' | -14.45 | 91.35 | 105.80 |
| 82 | DB | 16 | G | O4'-C1'-N9 | 14.45 | 119.76 | 108.20 |
| 78 | CA | 899 | G | O4'-C1'-N9 | 14.45 | 119.76 | 108.20 |
| 34 | BE | 60 | ARG | C-N-CA | -14.45 | 85.58 | 121.70 |
| 81 | DA | 2708 | C | P-O5'-C5' | 14.45 | 144.02 | 120.90 |
| 65 | Bn | 34 | ALA | N-CA-CB | 14.45 | 130.32 | 110.10 |
| 81 | DA | 149 | U | P-O5'-C5' | 14.45 | 144.01 | 120.90 |
| 2 | AA | 252 | TRP | CA-CB-CG | 14.44 | 141.14 | 113.70 |
| 81 | DA | 1262 | G | P-O3'-C3' | 14.44 | 137.03 | 119.70 |
| 81 | DA | 3142 | A | O4'-C1'-N9 | 14.44 | 119.75 | 108.20 |
| 81 | DA | 1622 | U | P-O3'-C3' | 14.44 | 137.02 | 119.70 |
| 81 | DA | 1078 | U | O4'-C1'-N1 | 14.43 | 119.75 | 108.20 |
| 78 | CA | 1359 | C | P-O3'-C3' | 14.43 | 137.01 | 119.70 |
| 32 | BC | 362 | ALA | CB-CA-C | -14.42 | 88.47 | 110.10 |
| 78 | CA | 1544 | U | C3'-C2'-C1' | -14.40 | 89.98 | 101.50 |
| 81 | DA | 2648 | G | O4'-C1'-C2' | -14.40 | 91.40 | 105.80 |
| 81 | DA | 997 | A | O4'-C1'-N9 | 14.40 | 119.72 | 108.20 |
| 81 | DA | 1627 | U | N1-C1'-C2' | -14.40 | 95.28 | 114.00 |
| 81 | DA | 678 | G | O4'-C1'-C2' | 14.39 | 120.56 | 107.60 |
| 81 | DA | 282 | G | P-O3'-C3' | 14.39 | 136.97 | 119.70 |
| 78 | CA | 57 | G | O3'-P-O5' | -14.39 | 76.67 | 104.00 |
| 81 | DA | 3258 | U | O4'-C1'-N1 | 14.38 | 119.71 | 108.20 |
| 81 | DA | 1774 | C | O4'-C1'-N1 | 14.38 | 119.71 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2354 | C | P-O3'-C3' | -14.38 | 102.44 | 119.70 |
| 81 | DA | 798 | G | P-O3'-C3' | 14.38 | 136.95 | 119.70 |
| 81 | DA | 1706 | C | P-O3'-C3' | 14.38 | 136.95 | 119.70 |
| 81 | DA | 3300 | U | O4'-C1'-N1 | 14.38 | 119.70 | 108.20 |
| 78 | CA | 1573 | A | O4'-C1'-N9 | 14.37 | 119.70 | 108.20 |
| 76 | BS | 73 | THR | O-C-N | -14.36 | 99.72 | 122.70 |
| 31 | BB | 40 | TYR | CB-CG-CD1 | 14.36 | 129.62 | 121.00 |
| 34 | BE | 61 | ARG | CB-CA-C | -14.36 | 81.68 | 110.40 |
| 78 | CA | 140 | A | N9-C1'-C2' | -14.35 | 95.34 | 114.00 |
| 81 | DA | 2757 | U | C5'-C4'-O4' | 14.35 | 126.32 | 109.10 |
| 81 | DA | 1500 | G | O4'-C1'-N9 | 14.34 | 119.67 | 108.20 |
| 81 | DA | 417 | A | O4'-C1'-N9 | 14.34 | 119.67 | 108.20 |
| 81 | DA | 2480 | A | O3'-P-O5' | -14.31 | 76.81 | 104.00 |
| 81 | DA | 2632 | G | O4'-C1'-N9 | 14.31 | 119.65 | 108.20 |
| 81 | DA | 473 | G | O4'-C1'-N9 | 14.31 | 119.64 | 108.20 |
| 78 | CA | 662 | U | P-O5'-C5' | 14.30 | 143.79 | 120.90 |
| 81 | DA | 766 | U | O4'-C1'-N1 | 14.30 | 119.64 | 108.20 |
| 45 | BR | 54 | LEU | CB-CG-CD1 | -14.30 | 86.69 | 111.00 |
| 78 | CA | 172 | C | P-O3'-C3' | 14.29 | 136.85 | 119.70 |
| 81 | DA | 276 | U | P-O5'-C5' | 14.27 | 143.74 | 120.90 |
| 81 | DA | 2410 | U | P-O3'-C3' | 14.27 | 136.83 | 119.70 |
| 81 | DA | 3320 | A | O4'-C1'-N9 | 14.27 | 119.62 | 108.20 |
| 3 | AB | 212 | LYS | CA-C-O | -14.27 | 90.13 | 120.10 |
| 78 | CA | 1398 | U | C1'-O4'-C4' | -14.27 | 98.48 | 109.90 |
| 81 | DA | 2209 | U | P-O3'-C3' | 14.27 | 136.82 | 119.70 |
| 62 | Bk | 55 | ARG | NE-CZ-NH2 | 14.26 | 127.43 | 120.30 |
| 78 | CA | 117 | U | P-O5'-C5' | 14.26 | 143.72 | 120.90 |
| 81 | DA | 1390 | A | O4'-C1'-N9 | 14.26 | 119.61 | 108.20 |
| 81 | DA | 2197 | C | O4'-C1'-C2' | -14.26 | 91.54 | 105.80 |
| 16 | AO | 64 | ARG | NE-CZ-NH2 | -14.26 | 113.17 | 120.30 |
| 78 | CA | 500 | C | P-O3'-C3' | 14.25 | 136.80 | 119.70 |
| 78 | CA | 205 | U | P-O3'-C3' | 14.25 | 136.80 | 119.70 |
| 78 | CA | 1602 | C | C3'-C2'-C1' | 14.25 | 112.90 | 101.50 |
| 47 | BU | 136 | ARG | NE-CZ-NH1 | 14.25 | 127.42 | 120.30 |
| 81 | DA | 699 | A | C3'-C2'-C1' | 14.24 | 112.89 | 101.50 |
| 81 | DA | 3107 | U | O4'-C1'-C2' | -14.24 | 91.56 | 105.80 |
| 81 | DA | 636 | C | C3'-C2'-C1' | 14.23 | 112.89 | 101.50 |
| 81 | DA | 2625 | C | C3'-C2'-C1' | 14.23 | 112.89 | 101.50 |
| 81 | DA | 298 | U | P-O3'-C3' | 14.23 | 136.78 | 119.70 |
| 81 | DA | 1534 | A | P-O3'-C3' | 14.22 | 136.76 | 119.70 |
| 81 | DA | 2369 | G | O4'-C1'-N9 | 14.21 | 119.57 | 108.20 |
| 78 | CA | 898 | A | P-O3'-C3' | 14.21 | 136.75 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 278 | U | P-O3'-C3' | 14.21 | 136.75 | 119.70 |
| 81 | DA | 434 | U | P-O3'-C3' | -14.20 | 102.66 | 119.70 |
| 83 | DC | 49 | G | C3'-C2'-C1' | 14.20 | 112.86 | 101.50 |
| 81 | DA | 1991 | G | C3'-C2'-C1' | -14.19 | 90.14 | 101.50 |
| 81 | DA | 675 | C | O4'-C1'-C2' | -14.19 | 91.61 | 105.80 |
| 81 | DA | 1414 | G | O4'-C1'-N9 | 14.19 | 119.55 | 108.20 |
| 81 | DA | 2166 | A | O4'-C1'-C2' | -14.19 | 91.61 | 105.80 |
| 81 | DA | 134 | U | O4'-C1'-N1 | 14.19 | 119.55 | 108.20 |
| 80 | CC | 18 | C | C3'-C2'-C1' | 14.17 | 112.84 | 101.50 |
| 81 | DA | 3389 | U | O4'-C1'-N1 | 14.17 | 119.53 | 108.20 |
| 81 | DA | 1831 | U | O4'-C1'-N1 | 14.16 | 119.53 | 108.20 |
| 78 | CA | 295 | A | C3'-C2'-C1' | -14.16 | 90.17 | 101.50 |
| 81 | DA | 1587 | A | O4'-C1'-N9 | 14.16 | 119.53 | 108.20 |
| 81 | DA | 1088 | U | P-O3'-C3' | 14.15 | 136.68 | 119.70 |
| 78 | CA | 1381 | U | O4'-C1'-N1 | 14.15 | 119.52 | 108.20 |
| 20 | AS | 60 | SER | CB-CA-C | 14.14 | 136.97 | 110.10 |
| 81 | DA | 409 | A | C3'-C2'-C1' | 14.14 | 112.81 | 101.50 |
| 82 | DB | 63 | G | P-O3'-C3' | 14.13 | 136.66 | 119.70 |
| 78 | CA | 1658 | G | O4'-C1'-N9 | 14.13 | 119.50 | 108.20 |
| 78 | CA | 1761 | U | P-O3'-C3' | 14.12 | 136.65 | 119.70 |
| 78 | CA | 1337 | A | N9-C1'-C2' | -14.12 | 95.65 | 114.00 |
| 81 | DA | 1966 | U | P-O3'-C3' | 14.12 | 136.64 | 119.70 |
| 81 | DA | 2508 | U | O4'-C1'-N1 | 14.11 | 119.49 | 108.20 |
| 81 | DA | 303 | G | P-O3'-C3' | 14.10 | 136.62 | 119.70 |
| 8 | AF | 225 | ARG | NE-CZ-NH1 | 14.10 | 127.35 | 120.30 |
| 81 | DA | 2172 | A | C3'-C2'-C1' | -14.09 | 90.22 | 101.50 |
| 78 | CA | 1570 | A | C3'-C2'-C1' | 14.09 | 112.77 | 101.50 |
| 81 | DA | 265 | A | P-O5'-C5' | 14.09 | 143.44 | 120.90 |
| 78 | CA | 894 | U | O4'-C1'-C2' | -14.08 | 91.72 | 105.80 |
| 78 | CA | 1690 | G | C5'-C4'-C3' | 14.08 | 138.53 | 116.00 |
| 82 | DB | 3 | A | P-O3'-C3' | 14.07 | 136.59 | 119.70 |
| 81 | DA | 3242 | G | N9-C1'-C2' | -14.06 | 95.72 | 114.00 |
| 81 | DA | 927 | C | P-O3'-C3' | 14.06 | 136.57 | 119.70 |
| 78 | CA | 1367 | G | P-O5'-C5' | 14.05 | 143.38 | 120.90 |
| 81 | DA | 943 | U | P-O3'-C3' | 14.05 | 136.56 | 119.70 |
| 81 | DA | 1644 | C | P-O3'-C3' | 14.05 | 136.56 | 119.70 |
| 81 | DA | 1662 | G | P-O3'-C3' | 14.05 | 136.56 | 119.70 |
| 81 | DA | 1095 | U | P-O3'-C3' | 14.04 | 136.55 | 119.70 |
| 78 | CA | 1141 | G | C1'-O4'-C4' | -14.04 | 98.67 | 109.90 |
| 81 | DA | 677 | A | O4'-C1'-N9 | 14.03 | 119.42 | 108.20 |
| 81 | DA | 1685 | C | P-O3'-C3' | 14.03 | 136.53 | 119.70 |
| 81 | DA | 2339 | C | C1'-O4'-C4' | 14.03 | 121.12 | 109.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 70 | C | P-O3'-C3' | 14.02 | 136.53 | 119.70 |
| 81 | DA | 1634 | G | P-O3'-C3' | 14.02 | 136.53 | 119.70 |
| 78 | CA | 1572 | G | O4'-C1'-N9 | 14.02 | 119.42 | 108.20 |
| 81 | DA | 1384 | U | O4'-C1'-N1 | 14.02 | 119.41 | 108.20 |
| 35 | BG | 69 | PHE | CE1-CZ-CE2 | 14.01 | 145.22 | 120.00 |
| 83 | DC | 54 | A | N9-C1'-C2' | 14.01 | 132.21 | 114.00 |
| 81 | DA | 1237 | G | P-O3'-C3' | 14.00 | 136.50 | 119.70 |
| 81 | DA | 1064 | A | P-O3'-C3' | 13.99 | 136.49 | 119.70 |
| 81 | DA | 71 | A | O4'-C1'-N9 | -13.99 | 97.01 | 108.20 |
| 78 | CA | 1702 | A | N9-C1'-C2' | -13.99 | 95.81 | 114.00 |
| 81 | DA | 275 | U | O4'-C1'-N1 | 13.99 | 119.39 | 108.20 |
| 81 | DA | 1902 | G | O4'-C1'-N9 | 13.98 | 119.38 | 108.20 |
| 78 | CA | 1113 | A | O4'-C1'-N9 | 13.98 | 119.38 | 108.20 |
| 74 | BQ | 252 | ALA | CB-CA-C | -13.97 | 89.14 | 110.10 |
| 78 | CA | 36 | C | P-O3'-C3' | 13.97 | 136.47 | 119.70 |
| 81 | DA | 2187 | G | C1'-O4'-C4' | 13.97 | 121.08 | 109.90 |
| 81 | DA | 1207 | G | C3'-C2'-C1' | 13.97 | 112.68 | 101.50 |
| 78 | CA | 1405 | G | N9-C1'-C2' | -13.97 | 95.84 | 114.00 |
| 9 | AH | 69 | LEU | N-CA-CB | 13.96 | 138.32 | 110.40 |
| 81 | DA | 1572 | U | C3'-C2'-C1' | 13.96 | 112.67 | 101.50 |
| 78 | CA | 1475 | A | P-O3'-C3' | -13.95 | 102.96 | 119.70 |
| 81 | DA | 1859 | A | O4'-C1'-C2' | -13.95 | 91.85 | 105.80 |
| 78 | CA | 621 | A | O4'-C1'-N9 | 13.94 | 119.35 | 108.20 |
| 81 | DA | 2451 | G | P-O5'-C5' | 13.94 | 143.20 | 120.90 |
| 78 | CA | 1393 | C | N1-C1'-C2' | -13.93 | 95.89 | 114.00 |
| 40 | BK | 101 | ARG | NE-CZ-NH1 | 13.93 | 127.26 | 120.30 |
| 78 | CA | 228 | G | C1'-O4'-C4' | 13.92 | 121.03 | 109.90 |
| 78 | CA | 1196 | A | O4'-C1'-N9 | 13.92 | 119.33 | 108.20 |
| 81 | DA | 2527 | G | O4'-C1'-N9 | 13.91 | 119.33 | 108.20 |
| 78 | CA | 1603 | U | O4'-C1'-N1 | 13.91 | 119.33 | 108.20 |
| 81 | DA | 639 | G | P-O3'-C3' | 13.90 | 136.38 | 119.70 |
| 74 | BQ | 242 | SER | CA-C-O | -13.90 | 90.91 | 120.10 |
| 82 | DB | 134 | G | P-O3'-C3' | 13.90 | 136.38 | 119.70 |
| 78 | CA | 1541 | G | C1'-O4'-C4' | -13.89 | 98.78 | 109.90 |
| 5 | AC | 53 | ARG | NE-CZ-NH1 | 13.89 | 127.24 | 120.30 |
| 81 | DA | 3050 | U | C3'-C2'-C1' | 13.88 | 112.61 | 101.50 |
| 78 | CA | 1338 | C | C5'-C4'-C3' | 13.87 | 138.20 | 116.00 |
| 81 | DA | 72 | C | P-O3'-C3' | 13.87 | 136.34 | 119.70 |
| 78 | CA | 959 | U | P-O3'-C3' | 13.87 | 136.34 | 119.70 |
| 81 | DA | 151 | A | P-O3'-C3' | 13.87 | 136.34 | 119.70 |
| 81 | DA | 843 | A | O4'-C1'-N9 | 13.86 | 119.28 | 108.20 |
| 78 | CA | 336 | G | P-O3'-C3' | -13.85 | 103.08 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 1546 | G | C5'-C4'-C3' | -13.85 | 93.83 | 116.00 |
| 78 | CA | 1489 | U | P-O3'-C3' | 13.84 | 136.31 | 119.70 |
| 81 | DA | 229 | G | P-O3'-C3' | 13.84 | 136.31 | 119.70 |
| 81 | DA | 258 | G | O4'-C1'-N9 | 13.84 | 119.27 | 108.20 |
| 81 | DA | 1185 | C | P-O3'-C3' | 13.84 | 136.31 | 119.70 |
| 49 | BV | 61 | ARG | NE-CZ-NH1 | 13.83 | 127.22 | 120.30 |
| 78 | CA | 46 | A | O3'-P-O5' | -13.83 | 77.72 | 104.00 |
| 81 | DA | 1789 | G | C1'-O4'-C4' | -13.83 | 98.83 | 109.90 |
| 78 | CA | 229 | U | O4'-C1'-N1 | 13.83 | 119.26 | 108.20 |
| 78 | CA | 1305 | U | P-O3'-C3' | 13.82 | 136.29 | 119.70 |
| 81 | DA | 2509 | U | O4'-C1'-N1 | 13.82 | 119.25 | 108.20 |
| 31 | BB | 38 | HIS | N-CA-CB | -13.82 | 85.73 | 110.60 |
| 35 | BG | 99 | GLU | N-CA-C | -13.82 | 73.69 | 111.00 |
| 58 | Bg | 19 | ARG | NE-CZ-NH1 | 13.82 | 127.21 | 120.30 |
| 13 | AL | 109 | ARG | NE-CZ-NH2 | -13.81 | 113.39 | 120.30 |
| 81 | DA | 1790 | G | O4'-C1'-C2' | 13.81 | 120.03 | 107.60 |
| 35 | BG | 98 | VAL | C-N-CA | 13.81 | 156.22 | 121.70 |
| 81 | DA | 1871 | U | O5'-C5'-C4' | 13.80 | 137.93 | 111.70 |
| 81 | DA | 2999 | U | O4'-C1'-N1 | 13.80 | 119.24 | 108.20 |
| 81 | DA | 3385 | U | O4'-C1'-N1 | 13.80 | 119.24 | 108.20 |
| 81 | DA | 734 | C | P-O3'-C3' | 13.80 | 136.26 | 119.70 |
| 81 | DA | 3062 | G | O4'-C1'-N9 | 13.79 | 119.23 | 108.20 |
| 81 | DA | 1181 | U | O4'-C1'-N1 | 13.79 | 119.23 | 108.20 |
| 78 | CA | 53 | G | P-O3'-C3' | 13.79 | 136.24 | 119.70 |
| 78 | CA | 374 | U | N1-C1'-C2' | 13.79 | 131.92 | 114.00 |
| 78 | CA | 1022 | C | C3'-C2'-C1' | 13.79 | 112.53 | 101.50 |
| 81 | DA | 3304 | U | O4'-C4'-C3' | -13.78 | 90.22 | 104.00 |
| 78 | CA | 1453 | G | P-O5'-C5' | 13.78 | 142.95 | 120.90 |
| 78 | CA | 69 | G | P-O3'-C3' | 13.77 | 136.23 | 119.70 |
| 81 | DA | 1785 | U | O4'-C1'-N1 | 13.77 | 119.21 | 108.20 |
| 81 | DA | 1870 | C | C5'-C4'-C3' | 13.76 | 138.01 | 116.00 |
| 81 | DA | 2025 | G | O4'-C1'-N9 | 13.76 | 119.21 | 108.20 |
| 81 | DA | 2206 | G | O4'-C1'-C2' | -13.75 | 92.05 | 105.80 |
| 81 | DA | 2993 | G | P-O3'-C3' | 13.75 | 136.20 | 119.70 |
| 83 | DC | 30 | G | O4'-C1'-N9 | 13.75 | 119.20 | 108.20 |
| 81 | DA | 1055 | A | P-O5'-C5' | 13.75 | 142.90 | 120.90 |
| 1 | Aa | 38 | ARG | NE-CZ-NH2 | -13.74 | 113.43 | 120.30 |
| 81 | DA | 1795 | U | O4'-C1'-N1 | 13.74 | 119.19 | 108.20 |
| 78 | CA | 1615 | C | O4'-C1'-N1 | -13.73 | 97.21 | 108.20 |
| 81 | DA | 1052 | U | O4'-C1'-N1 | 13.73 | 119.19 | 108.20 |
| 81 | DA | 1323 | G | O4'-C1'-N9 | 13.73 | 119.19 | 108.20 |
| 81 | DA | 2157 | G | C3'-C2'-C1' | 13.73 | 112.48 | 101.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2754 | G | P-O3'-C3' | 13.73 | 136.17 | 119.70 |
| 81 | DA | 1623 | G | C5'-C4'-C3' | 13.72 | 137.96 | 116.00 |
| 81 | DA | 3231 | U | O4'-C1'-N1 | 13.72 | 119.18 | 108.20 |
| 81 | DA | 1651 | U | O4'-C1'-N1 | 13.72 | 119.18 | 108.20 |
| 78 | CA | 1340 | U | O4'-C1'-N1 | 13.71 | 119.17 | 108.20 |
| 81 | DA | 1939 | G | P-O3'-C3' | 13.71 | 136.15 | 119.70 |
| 81 | DA | 2031 | U | P-O3'-C3' | 13.71 | 136.15 | 119.70 |
| 34 | BE | 61 | ARG | N-CA-CB | -13.71 | 85.93 | 110.60 |
| 82 | DB | 90 | U | O4'-C1'-N1 | 13.70 | 119.16 | 108.20 |
| 78 | CA | 400 | A | P-O3'-C3' | 13.70 | 136.14 | 119.70 |
| 81 | DA | 2535 | A | N1-C6-N6 | 13.70 | 126.82 | 118.60 |
| 83 | DC | 52 | U | O4'-C1'-N1 | 13.69 | 119.15 | 108.20 |
| 81 | DA | 248 | U | O4'-C1'-N1 | 13.68 | 119.15 | 108.20 |
| 78 | CA | 1310 | U | C5'-C4'-C3' | -13.68 | 94.11 | 116.00 |
| 81 | DA | 2157 | G | O4'-C1'-N9 | -13.68 | 97.26 | 108.20 |
| 81 | DA | 442 | G | P-O3'-C3' | 13.67 | 136.11 | 119.70 |
| 81 | DA | 2363 | A | N9-C1'-C2' | -13.66 | 96.24 | 114.00 |
| 81 | DA | 2469 | G | C5'-C4'-C3' | 13.66 | 137.86 | 116.00 |
| 81 | DA | 2618 | G | O4'-C1'-N9 | 13.65 | 119.12 | 108.20 |
| 81 | DA | 2233 | A | O4'-C1'-N9 | 13.65 | 119.12 | 108.20 |
| 81 | DA | 346 | C | O4'-C1'-N1 | -13.64 | 97.29 | 108.20 |
| 78 | CA | 1563 | C | N1-C1'-C2' | 13.64 | 131.73 | 114.00 |
| 82 | DB | 46 | G | C1'-O4'-C4' | -13.63 | 98.99 | 109.90 |
| 33 | BD | 354 | VAL | CA-C-N | 13.63 | 147.19 | 117.20 |
| 78 | CA | 1690 | G | O4'-C1'-C2' | -13.63 | 92.17 | 105.80 |
| 81 | DA | 975 | C | P-O3'-C3' | 13.63 | 136.06 | 119.70 |
| 78 | CA | 4 | C | P-O3'-C3' | 13.63 | 136.06 | 119.70 |
| 3 | AB | 18 | TYR | CB-CG-CD1 | -13.62 | 112.83 | 121.00 |
| 81 | DA | 647 | A | N9-C1'-C2' | 13.61 | 131.70 | 114.00 |
| 81 | DA | 640 | U | P-O3'-C3' | 13.61 | 136.03 | 119.70 |
| 81 | DA | 2157 | G | P-O3'-C3' | 13.61 | 136.03 | 119.70 |
| 82 | DB | 45 | C | P-O3'-C3' | 13.60 | 136.02 | 119.70 |
| 29 | AU | 70 | VAL | CA-CB-CG1 | -13.60 | 90.50 | 110.90 |
| 81 | DA | 3381 | U | P-O3'-C3' | 13.60 | 136.02 | 119.70 |
| 83 | DC | 116 | U | O4'-C1'-N1 | 13.60 | 119.08 | 108.20 |
| 81 | DA | 1702 | U | P-O3'-C3' | 13.59 | 136.01 | 119.70 |
| 81 | DA | 2476 | C | N1-C1'-C2' | 13.59 | 131.67 | 114.00 |
| 78 | CA | 894 | U | O3'-P-O5' | -13.58 | 78.19 | 104.00 |
| 40 | BK | 185 | ALA | N-CA-C | 13.57 | 147.64 | 111.00 |
| 78 | CA | 989 | U | N1-C1'-C2' | 13.56 | 131.63 | 114.00 |
| 33 | BD | 355 | PHE | N-CA-CB | 13.56 | 135.00 | 110.60 |
| 78 | CA | 713 | A | O3'-P-O5' | -13.55 | 78.25 | 104.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 48 | BW | 98 | THR | CA-CB-CG2 | 13.55 | 131.37 | 112.40 |
| 81 | DA | 2435 | G | P-O3'-C3' | 13.55 | 135.96 | 119.70 |
| 9 | AH | 23 | ARG | NE-CZ-NH2 | -13.55 | 113.53 | 120.30 |
| 78 | CA | 831 | U | C3'-C2'-C1' | -13.54 | 90.67 | 101.50 |
| 81 | DA | 768 | C | O4'-C1'-N1 | 13.54 | 119.03 | 108.20 |
| 81 | DA | 2844 | C | N1-C1'-C2' | 13.54 | 131.60 | 114.00 |
| 78 | CA | 1210 | C | N1-C1'-C2' | 13.54 | 131.60 | 114.00 |
| 83 | DC | 38 | U | O4'-C1'-N1 | 13.54 | 119.03 | 108.20 |
| 81 | DA | 2435 | G | N9-C1'-C2' | -13.54 | 96.40 | 114.00 |
| 81 | DA | 1115 | G | O4'-C1'-C2' | -13.53 | 92.27 | 105.80 |
| 83 | DC | 31 | U | O4'-C1'-N1 | 13.53 | 119.03 | 108.20 |
| 34 | BE | 55 | ARG | N-CA-C | 13.53 | 147.53 | 111.00 |
| 78 | CA | 462 | G | O4'-C1'-N9 | 13.53 | 119.02 | 108.20 |
| 81 | DA | 3212 | C | C3'-C2'-C1' | 13.53 | 112.32 | 101.50 |
| 81 | DA | 3309 | G | O4'-C1'-N9 | 13.53 | 119.02 | 108.20 |
| 78 | CA | 555 | A | P-O3'-C3' | 13.52 | 135.92 | 119.70 |
| 78 | CA | 839 | U | C1'-O4'-C4' | 13.51 | 120.71 | 109.90 |
| 81 | DA | 2928 | C | O4'-C1'-N1 | 13.51 | 119.01 | 108.20 |
| 78 | CA | 141 | U | N1-C1'-C2' | -13.51 | 96.44 | 114.00 |
| 82 | DB | 55 | U | O4'-C1'-N1 | 13.51 | 119.01 | 108.20 |
| 81 | DA | 316 | U | O4'-C1'-N1 | 13.51 | 119.01 | 108.20 |
| 81 | DA | 1630 | U | O4'-C1'-N1 | 13.49 | 119.00 | 108.20 |
| 81 | DA | 160 | G | C1'-O4'-C4' | -13.49 | 99.11 | 109.90 |
| 81 | DA | 352 | A | O4'-C1'-N9 | 13.49 | 118.99 | 108.20 |
| 78 | CA | 1614 | A | O4'-C1'-C2' | -13.48 | 92.31 | 105.80 |
| 81 | DA | 135 | C | O4'-C1'-N1 | 13.48 | 118.99 | 108.20 |
| 81 | DA | 1972 | A | O4'-C1'-N9 | 13.48 | 118.99 | 108.20 |
| 81 | DA | 1885 | U | O4'-C1'-N1 | 13.48 | 118.98 | 108.20 |
| 81 | DA | 2367 | A | N9-C1'-C2' | 13.48 | 131.53 | 114.00 |
| 83 | DC | 21 | G | O4'-C1'-N9 | 13.48 | 118.98 | 108.20 |
| 2 | AA | 11 | PRO | CA-N-CD | -13.48 | 92.63 | 111.50 |
| 78 | CA | 652 | G | N9-C1'-C2' | 13.47 | 131.51 | 114.00 |
| 82 | DB | 158 | U | O4'-C1'-N1 | 13.47 | 118.98 | 108.20 |
| 78 | CA | 1702 | A | P-O3'-C3' | 13.47 | 135.86 | 119.70 |
| 81 | DA | 1989 | U | O4'-C1'-N1 | 13.47 | 118.97 | 108.20 |
| 81 | DA | 3232 | G | O4'-C1'-N9 | 13.47 | 118.98 | 108.20 |
| 78 | CA | 1068 | C | O4'-C1'-N1 | 13.46 | 118.97 | 108.20 |
| 81 | DA | 2637 | A | P-O3'-C3' | 13.45 | 135.84 | 119.70 |
| 78 | CA | 177 | U | P-O3'-C3' | 13.45 | 135.84 | 119.70 |
| 83 | DC | 3 | U | P-O3'-C3' | 13.45 | 135.84 | 119.70 |
| 74 | BQ | 12 | TYR | CB-CG-CD1 | 13.45 | 129.07 | 121.00 |
| 81 | DA | 2181 | C | O4'-C1'-N1 | 13.44 | 118.95 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2504 | U | O4'-C1'-N1 | 13.44 | 118.95 | 108.20 |
| 44 | BO | 62 | HIS | CA-C-N | -13.44 | 87.63 | 117.20 |
| 78 | CA | 1601 | G | O4'-C1'-N9 | 13.43 | 118.95 | 108.20 |
| 81 | DA | 1542 | G | O4'-C1'-N9 | 13.43 | 118.95 | 108.20 |
| 81 | DA | 2495 | C | P-O3'-C3' | 13.43 | 135.81 | 119.70 |
| 78 | CA | 481 | A | P-O3'-C3' | 13.43 | 135.81 | 119.70 |
| 78 | CA | 1478 | G | C3'-C2'-C1' | -13.42 | 90.77 | 101.50 |
| 78 | CA | 183 | U | P-O3'-C3' | 13.41 | 135.80 | 119.70 |
| 81 | DA | 3136 | G | P-O3'-C3' | 13.41 | 135.79 | 119.70 |
| 1 | Aa | 54 | PHE | C-N-CA | 13.41 | 150.46 | 122.30 |
| 78 | CA | 302 | U | O4'-C1'-N1 | 13.41 | 118.93 | 108.20 |
| 81 | DA | 220 | G | C1'-O4'-C4' | 13.40 | 120.62 | 109.90 |
| 81 | DA | 449 | U | O4'-C1'-N1 | 13.40 | 118.92 | 108.20 |
| 81 | DA | 338 | A | O4'-C1'-C2' | -13.40 | 92.40 | 105.80 |
| 81 | DA | 3086 | A | P-O3'-C3' | 13.40 | 135.78 | 119.70 |
| 78 | CA | 312 | A | O4'-C1'-N9 | -13.39 | 97.48 | 108.20 |
| 78 | CA | 920 | U | P-O3'-C3' | 13.39 | 135.77 | 119.70 |
| 62 | Bk | 76 | ARG | NE-CZ-NH1 | 13.39 | 127.00 | 120.30 |
| 81 | DA | 1506 | A | N9-C1'-C2' | -13.39 | 96.59 | 114.00 |
| 82 | DB | 134 | G | O4'-C1'-N9 | 13.38 | 118.91 | 108.20 |
| 4 | AD | 148 | ARG | NE-CZ-NH2 | -13.38 | 113.61 | 120.30 |
| 78 | CA | 609 | U | O4'-C1'-N1 | -13.37 | 97.51 | 108.20 |
| 81 | DA | 2484 | A | P-O3'-C3' | 13.36 | 135.73 | 119.70 |
| 1 | Aa | 58 | VAL | CA-C-O | -13.35 | 92.06 | 120.10 |
| 5 | AC | 8 | TYR | CB-CG-CD2 | -13.35 | 112.99 | 121.00 |
| 16 | AO | 64 | ARG | CB-CA-C | 13.35 | 137.11 | 110.40 |
| 78 | CA | 326 | G | O4'-C4'-C3' | 13.35 | 117.35 | 104.00 |
| 45 | BR | 13 | SER | CA-C-O | -13.35 | 92.07 | 120.10 |
| 60 | Bi | 41 | ARG | NE-CZ-NH1 | 13.34 | 126.97 | 120.30 |
| 81 | DA | 1507 | G | O4'-C1'-N9 | 13.34 | 118.87 | 108.20 |
| 81 | DA | 2175 | U | C3'-C2'-C1' | 13.34 | 112.17 | 101.50 |
| 81 | DA | 124 | U | O4'-C1'-C2' | -13.34 | 92.46 | 105.80 |
| 78 | CA | 169 | A | C1'-O4'-C4' | 13.33 | 120.57 | 109.90 |
| 81 | DA | 993 | G | C1'-O4'-C4' | -13.33 | 99.23 | 109.90 |
| 78 | CA | 152 | U | O4'-C1'-N1 | 13.33 | 118.86 | 108.20 |
| 76 | BS | 52 | LYS | CB-CA-C | -13.33 | 83.75 | 110.40 |
| 78 | CA | 1387 | G | P-O5'-C5' | 13.33 | 142.22 | 120.90 |
| 81 | DA | 161 | G | P-O3'-C3' | 13.32 | 135.69 | 119.70 |
| 2 | AA | 11 | PRO | N-CA-CB | 13.30 | 119.27 | 103.30 |
| 81 | DA | 3020 | U | O4'-C1'-N1 | 13.30 | 118.84 | 108.20 |
| 81 | DA | 169 | U | O4'-C1'-N1 | 13.30 | 118.84 | 108.20 |
| 81 | DA | 266 | A | O4'-C1'-N9 | 13.30 | 118.84 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1648 | A | O4'-C1'-N9 | 13.30 | 118.84 | 108.20 |
| 78 | CA | 455 | C | O4'-C1'-N1 | 13.29 | 118.83 | 108.20 |
| 81 | DA | 608 | A | P-O3'-C3' | 13.29 | 135.65 | 119.70 |
| 78 | CA | 1622 | G | O4'-C1'-N9 | 13.29 | 118.83 | 108.20 |
| 81 | DA | 331 | G | O4'-C1'-C2' | -13.28 | 92.52 | 105.80 |
| 81 | DA | 1790 | G | C1'-O4'-C4' | -13.29 | 99.27 | 109.90 |
| 78 | CA | 558 | U | N1-C1'-C2' | 13.28 | 131.26 | 114.00 |
| 81 | DA | 1403 | C | P-O3'-C3' | 13.28 | 135.63 | 119.70 |
| 83 | DC | 114 | A | O4'-C1'-C2' | 13.28 | 119.55 | 107.60 |
| 78 | CA | 368 | U | N1-C1'-C2' | 13.28 | 131.26 | 114.00 |
| 78 | CA | 350 | U | O4'-C1'-N1 | 13.27 | 118.82 | 108.20 |
| 81 | DA | 1698 | C | N1-C1'-C2' | -13.27 | 96.75 | 114.00 |
| 81 | DA | 2001 | U | O4'-C1'-N1 | 13.27 | 118.82 | 108.20 |
| 81 | DA | 1263 | A | N9-C1'-C2' | 13.27 | 131.25 | 114.00 |
| 78 | CA | 312 | A | P-O3'-C3' | 13.26 | 135.62 | 119.70 |
| 81 | DA | 1694 | U | N1-C1'-C2' | -13.26 | 96.76 | 114.00 |
| 82 | DB | 90 | U | P-O3'-C3' | 13.25 | 135.60 | 119.70 |
| 81 | DA | 531 | G | C3'-C2'-C1' | 13.25 | 112.10 | 101.50 |
| 78 | CA | 1653 | C | P-O3'-C3' | 13.24 | 135.59 | 119.70 |
| 81 | DA | 2177 | G | C3'-C2'-C1' | 13.24 | 112.09 | 101.50 |
| 81 | DA | 2768 | U | O4'-C1'-N1 | 13.24 | 118.79 | 108.20 |
| 81 | DA | 3224 | G | P-O3'-C3' | 13.23 | 135.58 | 119.70 |
| 81 | DA | 1034 | U | P-O3'-C3' | 13.23 | 135.58 | 119.70 |
| 81 | DA | 2770 | G | O4'-C1'-N9 | -13.22 | 97.62 | 108.20 |
| 78 | CA | 123 | G | O3'-P-O5' | -13.22 | 78.88 | 104.00 |
| 78 | CA | 1386 | G | N9-C1'-C2' | -13.22 | 96.81 | 114.00 |
| 83 | DC | 46 | A | N9-C1'-C2' | -13.22 | 96.81 | 114.00 |
| 81 | DA | 2493 | U | P-O5'-C5' | 13.21 | 142.04 | 120.90 |
| 81 | DA | 3306 | U | C5'-C4'-O4' | 13.22 | 124.96 | 109.10 |
| 81 | DA | 3394 | U | P-O3'-C3' | 13.21 | 135.56 | 119.70 |
| 78 | CA | 1137 | A | P-O3'-C3' | 13.21 | 135.55 | 119.70 |
| 81 | DA | 1250 | G | N9-C1'-C2' | -13.21 | 96.83 | 114.00 |
| 81 | DA | 2165 | G | P-O3'-C3' | 13.20 | 135.54 | 119.70 |
| 83 | DC | 114 | A | P-O3'-C3' | 13.20 | 135.54 | 119.70 |
| 78 | CA | 178 | U | O3'-P-O5' | -13.20 | 78.92 | 104.00 |
| 78 | CA | 1792 | G | O4'-C1'-N9 | 13.19 | 118.75 | 108.20 |
| 81 | DA | 2801 | A | O4'-C1'-N9 | 13.19 | 118.75 | 108.20 |
| 78 | CA | 1453 | G | O4'-C1'-C2' | -13.18 | 92.62 | 105.80 |
| 81 | DA | 1687 | U | N1-C1'-C2' | 13.18 | 131.13 | 114.00 |
| 81 | DA | 2950 | G | O4'-C1'-N9 | 13.17 | 118.74 | 108.20 |
| 78 | CA | 1527 | C | P-O3'-C3' | 13.17 | 135.50 | 119.70 |
| 81 | DA | 2390 | A | P-O5'-C5' | 13.17 | 141.97 | 120.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2770 | G | N9-C1'-C2' | 13.17 | 131.12 | 114.00 |
| 81 | DA | 2716 | U | P-O3'-C3' | 13.17 | 135.50 | 119.70 |
| 78 | CA | 1356 | U | P-O5'-C5' | 13.16 | 141.96 | 120.90 |
| 78 | CA | 607 | G | P-O3'-C3' | 13.16 | 135.50 | 119.70 |
| 81 | DA | 3234 | A | O4'-C1'-N9 | 13.16 | 118.73 | 108.20 |
| 78 | CA | 1549 | C | P-O3'-C3' | 13.16 | 135.49 | 119.70 |
| 81 | DA | 1746 | U | O4'-C1'-N1 | 13.15 | 118.72 | 108.20 |
| 81 | DA | 1569 | U | P-O3'-C3' | 13.15 | 135.48 | 119.70 |
| 78 | CA | 1720 | G | O4'-C1'-N9 | 13.15 | 118.72 | 108.20 |
| 81 | DA | 1056 | U | P-O5'-C5' | 13.14 | 141.93 | 120.90 |
| 78 | CA | 1190 | C | O5'-C5'-C4' | 13.13 | 136.65 | 111.70 |
| 78 | CA | 1584 | G | O4'-C1'-C2' | 13.13 | 119.42 | 107.60 |
| 81 | DA | 2217 | U | O4'-C1'-N1 | 13.13 | 118.71 | 108.20 |
| 82 | DB | 50 | C | C1'-O4'-C4' | 13.13 | 120.40 | 109.90 |
| 78 | CA | 897 | C | O4'-C1'-C2' | -13.12 | 92.68 | 105.80 |
| 81 | DA | 690 | A | P-O3'-C3' | 13.12 | 135.44 | 119.70 |
| 81 | DA | 1963 | G | O4'-C1'-N9 | 13.11 | 118.69 | 108.20 |
| 81 | DA | 2591 | A | O4'-C1'-N9 | 13.11 | 118.69 | 108.20 |
| 39 | BJ | 76 | SER | N-CA-CB | 13.11 | 130.16 | 110.50 |
| 81 | DA | 209 | A | C1'-O4'-C4' | 13.11 | 120.38 | 109.90 |
| 81 | DA | 1826 | C | N1-C1'-C2' | -13.10 | 96.97 | 114.00 |
| 81 | DA | 2368 | A | O4'-C1'-N9 | 13.10 | 118.68 | 108.20 |
| 78 | CA | 1579 | U | P-O5'-C5' | 13.10 | 141.85 | 120.90 |
| 81 | DA | 800 | G | O4'-C1'-N9 | 13.10 | 118.68 | 108.20 |
| 50 | BX | 93 | TYR | CB-CG-CD2 | 13.09 | 128.85 | 121.00 |
| 78 | CA | 967 | A | O4'-C1'-N9 | 13.09 | 118.67 | 108.20 |
| 81 | DA | 155 | G | P-O3'-C3' | 13.09 | 135.41 | 119.70 |
| 43 | BP | 148 | TYR | CB-CG-CD1 | -13.09 | 113.15 | 121.00 |
| 81 | DA | 414 | U | O4'-C1'-N1 | 13.09 | 118.67 | 108.20 |
| 82 | DB | 103 | G | N9-C1'-C2' | 13.09 | 131.02 | 114.00 |
| 81 | DA | 1679 | A | C5'-C4'-C3' | 13.09 | 136.94 | 116.00 |
| 81 | DA | 2081 | U | O4'-C1'-N1 | 13.09 | 118.67 | 108.20 |
| 78 | CA | 1547 | A | OP1-P-OP2 | -13.09 | 99.97 | 119.60 |
| 81 | DA | 1793 | C | P-O3'-C3' | 13.09 | 135.40 | 119.70 |
| 81 | DA | 531 | G | N9-C1'-C2' | 13.08 | 131.01 | 114.00 |
| 81 | DA | 2361 | A | P-O3'-C3' | 13.08 | 135.39 | 119.70 |
| 35 | BG | 153 | PRO | N-CA-CB | -13.07 | 87.61 | 103.30 |
| 78 | CA | 465 | G | O4'-C1'-N9 | 13.07 | 118.66 | 108.20 |
| 81 | DA | 1499 | C | P-O3'-C3' | 13.07 | 135.38 | 119.70 |
| 81 | DA | 3090 | U | P-O3'-C3' | 13.07 | 135.38 | 119.70 |
| 81 | DA | 2475 | G | O4'-C1'-C2' | -13.06 | 92.74 | 105.80 |
| 83 | DC | 45 | A | P-O3'-C3' | -13.05 | 104.04 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|---|---|---|---|---|---|---|---|
| 1 | Aa | 58 | VAL | CA-C-N | 13.04 | 145.89 | 117.20 |
| 81 | DA | 1561 | G | C1'-O4'-C4' | -13.04 | 99.47 | 109.90 |
| 81 | DA | 3034 | C | O4'-C1'-C2' | -13.04 | 92.76 | 105.80 |
| 78 | CA | 677 | G | O4'-C1'-N9 | 13.03 | 118.63 | 108.20 |
| 81 | DA | 3304 | U | C5'-C4'-O4' | -13.03 | 93.46 | 109.10 |
| 81 | DA | 608 | A | N9-C1'-C2' | 13.03 | 130.94 | 114.00 |
| 78 | CA | 453 | U | O4'-C1'-N1 | 13.03 | 118.62 | 108.20 |
| 81 | DA | 1282 | G | P-O3'-C3' | 13.03 | 135.33 | 119.70 |
| 81 | DA | 3282 | U | N1-C1'-C2' | 13.02 | 130.92 | 114.00 |
| 81 | DA | 2770 | G | C3'-C2'-C1' | 13.01 | 111.91 | 101.50 |
| 37 | BH | 236 | GLY | CA-C-O | -13.01 | 97.18 | 120.60 |
| 79 | CB | 55 | C | O4'-C1'-N1 | -13.01 | 97.79 | 108.20 |
| 81 | DA | 309 | U | P-O3'-C3' | 13.00 | 135.29 | 119.70 |
| 81 | DA | 3051 | U | O4'-C1'-N1 | 12.99 | 118.60 | 108.20 |
| 78 | CA | 1746 | A | P-O3'-C3' | 12.99 | 135.28 | 119.70 |
| 78 | CA | 546 | U | P-O3'-C3' | 12.98 | 135.28 | 119.70 |
| 81 | DA | 2815 | G | P-O3'-C3' | 12.98 | 135.28 | 119.70 |
| 78 | CA | 853 | G | N9-C1'-C2' | -12.98 | 97.13 | 114.00 |
| 78 | CA | 681 | U | O4'-C1'-N1 | 12.98 | 118.58 | 108.20 |
| 81 | DA | 3149 | G | C3'-C2'-C1' | -12.98 | 91.12 | 101.50 |
| 78 | CA | 1302 | U | O4'-C1'-N1 | 12.97 | 118.58 | 108.20 |
| 81 | DA | 702 | C | C3'-C2'-C1' | 12.97 | 111.88 | 101.50 |
| 40 | BK | 48 | PHE | CB-CG-CD1 | -12.97 | 111.72 | 120.80 |
| 78 | CA | 1426 | C | P-O3'-C3' | 12.97 | 135.26 | 119.70 |
| 82 | DB | 95 | G | P-O3'-C3' | 12.96 | 135.26 | 119.70 |
| 81 | DA | 1446 | A | P-O3'-C3' | 12.96 | 135.25 | 119.70 |
| 78 | CA | 374 | U | C1'-O4'-C4' | -12.96 | 99.53 | 109.90 |
| 81 | DA | 1938 | U | O4'-C1'-N1 | 12.96 | 118.57 | 108.20 |
| 81 | DA | 3051 | U | C5'-C4'-C3' | 12.96 | 136.73 | 116.00 |
| 81 | DA | 2799 | A | P-O3'-C3' | 12.95 | 135.24 | 119.70 |
| 81 | DA | 3000 | A | P-O3'-C3' | 12.95 | 135.24 | 119.70 |
| 82 | DB | 153 | U | O4'-C1'-N1 | 12.94 | 118.55 | 108.20 |
| 32 | BC | 100 | ARG | NE-CZ-NH2 | -12.94 | 113.83 | 120.30 |
| 81 | DA | 3325 | G | O4'-C1'-N9 | 12.94 | 118.55 | 108.20 |
| 78 | CA | 591 | A | N9-C1'-C2' | 12.94 | 130.82 | 114.00 |
| 78 | CA | 492 | A | N1-C6-N6 | 12.94 | 126.36 | 118.60 |
| 78 | CA | 1791 | A | O4'-C1'-C2' | -12.94 | 92.86 | 105.80 |
| 81 | DA | 353 | G | O4'-C1'-N9 | 12.93 | 118.55 | 108.20 |
| 81 | DA | 2757 | U | N1-C1'-C2' | 12.93 | 130.81 | 114.00 |
| 81 | DA | 1948 | G | P-O3'-C3' | 12.93 | 135.22 | 119.70 |
| 21 | AT | 54 | ALA | O-C-N | -12.93 | 102.01 | 122.70 |
| 78 | CA | 1478 | G | P-O5'-C5' | 12.93 | 141.59 | 120.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1831 | U | C1'-O4'-C4' | 12.93 | 120.24 | 109.90 |
| 78 | CA | 178 | U | O4'-C4'-C3' | -12.92 | 91.08 | 104.00 |
| 82 | DB | 152 | G | O4'-C1'-N9 | 12.92 | 118.53 | 108.20 |
| 78 | CA | 1537 | C | P-O3'-C3' | 12.91 | 135.20 | 119.70 |
| 81 | DA | 658 | G | O4'-C1'-C2' | 12.90 | 119.21 | 107.60 |
| 81 | DA | 1055 | A | C1'-O4'-C4' | 12.90 | 120.22 | 109.90 |
| 81 | DA | 1717 | U | O4'-C1'-N1 | 12.90 | 118.52 | 108.20 |
| 81 | DA | 1832 | C | P-O5'-C5' | 12.90 | 141.54 | 120.90 |
| 81 | DA | 2208 | A | O4'-C1'-C2' | -12.90 | 92.90 | 105.80 |
| 81 | DA | 3141 | A | P-O3'-C3' | 12.89 | 135.17 | 119.70 |
| 78 | CA | 1612 | U | O4'-C1'-N1 | 12.89 | 118.51 | 108.20 |
| 35 | BG | 3 | ALA | N-CA-CB | -12.88 | 92.06 | 110.10 |
| 81 | DA | 860 | G | O4'-C1'-N9 | 12.88 | 118.51 | 108.20 |
| 81 | DA | 1791 | C | O3'-P-O5' | -12.88 | 79.52 | 104.00 |
| 81 | DA | 2514 | U | O4'-C1'-C2' | -12.88 | 92.92 | 105.80 |
| 81 | DA | 2405 | C | O4'-C1'-N1 | 12.88 | 118.50 | 108.20 |
| 5 | AC | 183 | ALA | N-CA-CB | -12.87 | 92.08 | 110.10 |
| 82 | DB | 98 | U | O5'-P-OP1 | -12.87 | 94.12 | 105.70 |
| 81 | DA | 1332 | A | N9-C1'-C2' | 12.87 | 130.73 | 114.00 |
| 81 | DA | 1221 | A | N9-C1'-C2' | -12.86 | 97.28 | 114.00 |
| 81 | DA | 785 | G | P-O3'-C3' | 12.86 | 135.13 | 119.70 |
| 78 | CA | 32 | U | N1-C1'-C2' | -12.85 | 97.29 | 114.00 |
| 78 | CA | 1263 | G | O4'-C1'-N9 | 12.85 | 118.48 | 108.20 |
| 81 | DA | 1674 | G | O4'-C1'-N9 | 12.85 | 118.48 | 108.20 |
| 81 | DA | 1682 | U | P-O3'-C3' | 12.85 | 135.12 | 119.70 |
| 78 | CA | 1562 | G | O4'-C1'-C2' | -12.85 | 92.95 | 105.80 |
| 81 | DA | 969 | C | N1-C1'-C2' | -12.85 | 97.29 | 114.00 |
| 81 | DA | 2683 | U | O4'-C1'-N1 | 12.85 | 118.48 | 108.20 |
| 81 | DA | 304 | G | O4'-C1'-N9 | 12.85 | 118.48 | 108.20 |
| 78 | CA | 1214 | U | O4'-C1'-N1 | 12.84 | 118.47 | 108.20 |
| 83 | DC | 70 | A | P-O3'-C3' | 12.84 | 135.11 | 119.70 |
| 81 | DA | 2406 | C | O4'-C1'-N1 | 12.83 | 118.47 | 108.20 |
| 81 | DA | 745 | C | N1-C1'-C2' | 12.83 | 130.68 | 114.00 |
| 78 | CA | 1613 | U | O4'-C1'-N1 | 12.82 | 118.46 | 108.20 |
| 81 | DA | 3330 | A | O5'-P-OP2 | -12.82 | 94.16 | 105.70 |
| 79 | CB | 30 | G | P-O3'-C3' | 12.82 | 135.08 | 119.70 |
| 81 | DA | 1324 | U | O4'-C1'-N1 | 12.82 | 118.45 | 108.20 |
| 82 | DB | 2 | A | O4'-C1'-N9 | 12.82 | 118.46 | 108.20 |
| 78 | CA | 948 | G | C1'-O4'-C4' | -12.82 | 99.65 | 109.90 |
| 78 | CA | 485 | A | N1-C6-N6 | 12.81 | 126.29 | 118.60 |
| 81 | DA | 1637 | A | P-O3'-C3' | 12.81 | 135.07 | 119.70 |
| 81 | DA | 2334 | U | O4'-C1'-N1 | 12.81 | 118.45 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 760 | G | C1'-O4'-C4' | -12.80 | 99.66 | 109.90 |
| 78 | CA | 140 | A | C1'-O4'-C4' | 12.80 | 120.14 | 109.90 |
| 78 | CA | 824 | G | P-O3'-C3' | 12.80 | 135.06 | 119.70 |
| 78 | CA | 1398 | U | O4'-C1'-C2' | 12.79 | 119.11 | 107.60 |
| 81 | DA | 71 | A | P-O3'-C3' | 12.79 | 135.04 | 119.70 |
| 81 | DA | 1805 | C | P-O3'-C3' | 12.79 | 135.04 | 119.70 |
| 51 | BZ | 56 | ARG | NE-CZ-NH2 | -12.79 | 113.91 | 120.30 |
| 83 | DC | 16 | U | P-O3'-C3' | 12.78 | 135.04 | 119.70 |
| 38 | Bs | 179 | SER | C-N-CD | -12.78 | 92.48 | 120.60 |
| 81 | DA | 1825 | G | C3'-C2'-C1' | -12.78 | 91.28 | 101.50 |
| 81 | DA | 2403 | G | O4'-C1'-C2' | -12.78 | 93.03 | 105.80 |
| 81 | DA | 3383 | G | P-O3'-C3' | 12.77 | 135.03 | 119.70 |
| 52 | BY | 13 | ARG | NE-CZ-NH2 | 12.77 | 126.69 | 120.30 |
| 81 | DA | 2163 | C | O4'-C1'-C2' | -12.77 | 93.03 | 105.80 |
| 81 | DA | 3189 | G | P-O3'-C3' | 12.77 | 135.03 | 119.70 |
| 81 | DA | 1678 | G | N9-C1'-C2' | -12.77 | 97.40 | 114.00 |
| 81 | DA | 3034 | C | C3'-C2'-C1' | 12.77 | 111.72 | 101.50 |
| 78 | CA | 667 | U | P-O3'-C3' | 12.77 | 135.02 | 119.70 |
| 5 | AC | 95 | TYR | CB-CG-CD2 | -12.76 | 113.34 | 121.00 |
| 78 | CA | 822 | U | O4'-C1'-N1 | 12.75 | 118.40 | 108.20 |
| 82 | DB | 149 | A | P-O3'-C3' | 12.75 | 135.00 | 119.70 |
| 78 | CA | 1580 | C | N1-C1'-C2' | 12.75 | 130.58 | 114.00 |
| 81 | DA | 1277 | C | P-O3'-C3' | 12.75 | 135.00 | 119.70 |
| 83 | DC | 7 | G | P-O3'-C3' | 12.75 | 135.00 | 119.70 |
| 81 | DA | 935 | U | O4'-C1'-N1 | 12.74 | 118.39 | 108.20 |
| 81 | DA | 1208 | U | C5'-C4'-C3' | 12.74 | 136.38 | 116.00 |
| 49 | BV | 162 | GLU | O-C-N | -12.74 | 102.32 | 122.70 |
| 81 | DA | 1303 | A | O4'-C1'-N9 | 12.73 | 118.39 | 108.20 |
| 81 | DA | 3361 | G | O4'-C1'-C2' | -12.73 | 93.07 | 105.80 |
| 81 | DA | 209 | A | N9-C1'-C2' | -12.73 | 97.45 | 114.00 |
| 81 | DA | 3163 | A | P-O3'-C3' | 12.72 | 134.97 | 119.70 |
| 81 | DA | 783 | A | P-O3'-C3' | 12.72 | 134.96 | 119.70 |
| 81 | DA | 2174 | G | O3'-P-O5' | -12.72 | 79.83 | 104.00 |
| 16 | AO | 104 | ARG | NE-CZ-NH1 | 12.72 | 126.66 | 120.30 |
| 81 | DA | 2741 | C | C3'-C2'-C1' | 12.72 | 111.67 | 101.50 |
| 81 | DA | 2677 | G | O4'-C1'-C2' | -12.71 | 93.09 | 105.80 |
| 83 | DC | 47 | C | O5'-P-OP2 | -12.71 | 94.27 | 105.70 |
| 32 | BC | 156 | SER | N-CA-CB | 12.70 | 129.55 | 110.50 |
| 76 | BS | 160 | PRO | CA-C-N | 12.69 | 152.64 | 117.10 |
| 81 | DA | 566 | G | P-O3'-C3' | 12.70 | 134.93 | 119.70 |
| 81 | DA | 894 | G | P-O3'-C3' | 12.69 | 134.93 | 119.70 |
| 81 | DA | 1569 | U | O4'-C1'-N1 | 12.69 | 118.36 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2502 | A | O4'-C1'-N9 | 12.69 | 118.36 | 108.20 |
| 78 | CA | 267 | U | O4'-C1'-C2' | -12.69 | 93.11 | 105.80 |
| 81 | DA | 2437 | G | P-O3'-C3' | 12.69 | 134.93 | 119.70 |
| 78 | CA | 1420 | C | C3'-C2'-C1' | 12.69 | 111.65 | 101.50 |
| 81 | DA | 798 | G | O4'-C1'-N9 | 12.69 | 118.35 | 108.20 |
| 81 | DA | 1221 | A | O4'-C1'-C2' | 12.69 | 119.02 | 107.60 |
| 81 | DA | 2682 | C | P-O3'-C3' | 12.69 | 134.92 | 119.70 |
| 81 | DA | 3361 | G | P-O3'-C3' | 12.69 | 134.92 | 119.70 |
| 81 | DA | 1859 | A | N9-C1'-C2' | -12.67 | 97.53 | 114.00 |
| 78 | CA | 327 | U | O4'-C1'-N1 | 12.67 | 118.34 | 108.20 |
| 81 | DA | 673 | U | O4'-C1'-N1 | 12.67 | 118.34 | 108.20 |
| 81 | DA | 2998 | U | N1-C1'-C2' | -12.67 | 97.53 | 114.00 |
| 81 | DA | 1362 | G | O4'-C1'-N9 | 12.66 | 118.33 | 108.20 |
| 81 | DA | 2627 | C | C5'-C4'-C3' | -12.66 | 95.74 | 116.00 |
| 81 | DA | 1209 | G | P-O3'-C3' | 12.66 | 134.90 | 119.70 |
| 63 | Bm | 85 | ARG | NE-CZ-NH2 | -12.66 | 113.97 | 120.30 |
| 78 | CA | 838 | G | O4'-C1'-C2' | -12.66 | 93.14 | 105.80 |
| 81 | DA | 545 | U | O4'-C1'-N1 | 12.65 | 118.32 | 108.20 |
| 81 | DA | 3091 | A | P-O3'-C3' | 12.65 | 134.88 | 119.70 |
| 32 | BC | 344 | THR | N-CA-CB | 12.65 | 134.33 | 110.30 |
| 81 | DA | 2172 | A | C1'-O4'-C4' | -12.65 | 99.78 | 109.90 |
| 83 | DC | 21 | G | C3'-C2'-C1' | -12.64 | 91.39 | 101.50 |
| 32 | BC | 284 | ARG | NE-CZ-NH2 | -12.64 | 113.98 | 120.30 |
| 78 | CA | 719 | U | P-O3'-C3' | 12.64 | 134.86 | 119.70 |
| 78 | CA | 123 | G | O4'-C1'-C2' | -12.63 | 93.17 | 105.80 |
| 78 | CA | 1395 | G | P-O3'-C3' | 12.63 | 134.86 | 119.70 |
| 81 | DA | 2086 | A | P-O3'-C3' | 12.63 | 134.86 | 119.70 |
| 81 | DA | 3091 | A | O4'-C1'-C2' | -12.63 | 93.17 | 105.80 |
| 81 | DA | 2160 | G | N9-C1'-C2' | 12.63 | 130.42 | 114.00 |
| 78 | CA | 219 | A | O4'-C1'-N9 | 12.63 | 118.30 | 108.20 |
| 38 | Bs | 42 | ARG | NE-CZ-NH1 | 12.62 | 126.61 | 120.30 |
| 78 | CA | 729 | G | P-O3'-C3' | 12.62 | 134.84 | 119.70 |
| 81 | DA | 1309 | U | O4'-C1'-N1 | 12.62 | 118.30 | 108.20 |
| 81 | DA | 1740 | U | O4'-C1'-N1 | 12.62 | 118.30 | 108.20 |
| 81 | DA | 3302 | U | O4'-C1'-N1 | 12.61 | 118.29 | 108.20 |
| 78 | CA | 885 | G | N9-C1'-C2' | 12.61 | 130.39 | 114.00 |
| 39 | BJ | 76 | SER | N-CA-C | -12.60 | 76.97 | 111.00 |
| 78 | CA | 1670 | G | O4'-C1'-N9 | 12.60 | 118.28 | 108.20 |
| 78 | CA | 957 | G | O4'-C1'-N9 | 12.60 | 118.28 | 108.20 |
| 78 | CA | 1348 | A | N9-C1'-C2' | 12.60 | 130.38 | 114.00 |
| 81 | DA | 491 | C | P-O3'-C3' | 12.59 | 134.81 | 119.70 |
| 81 | DA | 1335 | C | P-O3'-C3' | 12.59 | 134.81 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2754 | G | O4'-C1'-N9 | 12.59 | 118.27 | 108.20 |
| 11 | AJ | 85 | ARG | CD-NE-CZ | 12.59 | 141.22 | 123.60 |
| 78 | CA | 970 | A | O4'-C1'-N9 | 12.58 | 118.27 | 108.20 |
| 67 | Bp | 31 | ALA | N-CA-CB | 12.58 | 127.71 | 110.10 |
| 81 | DA | 1180 | A | O4'-C1'-N9 | 12.58 | 118.26 | 108.20 |
| 78 | CA | 1058 | U | P-O3'-C3' | 12.58 | 134.79 | 119.70 |
| 81 | DA | 2176 | U | N1-C1'-C2' | 12.58 | 130.35 | 114.00 |
| 81 | DA | 2402 | A | O4'-C1'-N9 | 12.57 | 118.26 | 108.20 |
| 47 | BU | 142 | SER | N-CA-CB | 12.56 | 129.35 | 110.50 |
| 81 | DA | 3357 | U | P-O3'-C3' | 12.56 | 134.77 | 119.70 |
| 81 | DA | 1776 | G | O4'-C1'-N9 | 12.56 | 118.25 | 108.20 |
| 81 | DA | 65 | A | P-O3'-C3' | 12.56 | 134.77 | 119.70 |
| 78 | CA | 1108 | G | N9-C1'-C2' | -12.56 | 97.67 | 114.00 |
| 81 | DA | 1926 | C | O4'-C1'-N1 | 12.55 | 118.24 | 108.20 |
| 78 | CA | 894 | U | O4'-C1'-N1 | 12.55 | 118.24 | 108.20 |
| 81 | DA | 1820 | U | O4'-C1'-C2' | -12.55 | 93.25 | 105.80 |
| 81 | DA | 1842 | A | O4'-C1'-C2' | -12.55 | 93.25 | 105.80 |
| 81 | DA | 2796 | G | O4'-C1'-N9 | 12.55 | 118.24 | 108.20 |
| 81 | DA | 20 | A | P-O3'-C3' | 12.54 | 134.75 | 119.70 |
| 81 | DA | 3348 | G | O4'-C1'-N9 | 12.54 | 118.23 | 108.20 |
| 78 | CA | 529 | A | P-O5'-C5' | -12.54 | 100.84 | 120.90 |
| 81 | DA | 768 | C | P-O3'-C3' | 12.54 | 134.74 | 119.70 |
| 78 | CA | 874 | C | N1-C1'-C2' | 12.53 | 130.29 | 114.00 |
| 78 | CA | 1736 | G | O4'-C1'-N9 | 12.53 | 118.23 | 108.20 |
| 81 | DA | 422 | A | C1'-O4'-C4' | 12.53 | 119.93 | 109.90 |
| 81 | DA | 1160 | C | P-O3'-C3' | 12.53 | 134.74 | 119.70 |
| 81 | DA | 2348 | A | N9-C1'-C2' | 12.52 | 130.28 | 114.00 |
| 78 | CA | 651 | G | N9-C1'-C2' | 12.52 | 130.28 | 114.00 |
| 81 | DA | 3349 | C | P-O3'-C3' | 12.52 | 134.73 | 119.70 |
| 81 | DA | 3107 | U | N1-C1'-C2' | 12.52 | 130.28 | 114.00 |
| 81 | DA | 1316 | C | N1-C1'-C2' | 12.52 | 130.27 | 114.00 |
| 78 | CA | 505 | A | N1-C6-N6 | 12.52 | 126.11 | 118.60 |
| 83 | DC | 42 | A | C3'-C2'-C1' | 12.51 | 111.51 | 101.50 |
| 78 | CA | 1364 | G | P-O3'-C3' | 12.51 | 134.71 | 119.70 |
| 81 | DA | 2001 | U | O4'-C1'-C2' | -12.50 | 93.30 | 105.80 |
| 81 | DA | 2672 | G | O3'-P-O5' | -12.49 | 80.26 | 104.00 |
| 81 | DA | 2525 | G | P-O3'-C3' | 12.48 | 134.68 | 119.70 |
| 78 | CA | 1393 | C | C1'-O4'-C4' | 12.48 | 119.89 | 109.90 |
| 78 | CA | 650 | U | C1'-O4'-C4' | 12.47 | 119.88 | 109.90 |
| 81 | DA | 2107 | A | P-O3'-C3' | 12.47 | 134.67 | 119.70 |
| 81 | DA | 2363 | A | P-O3'-C3' | 12.47 | 134.66 | 119.70 |
| 81 | DA | 2916 | U | C5'-C4'-C3' | 12.47 | 135.95 | 116.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 83 | DC | 102 | C | C3'-C2'-C1' | 12.47 | 111.47 | 101.50 |
| 78 | CA | 951 | A | O4'-C1'-N9 | 12.47 | 118.17 | 108.20 |
| 53 | Ba | 55 | LYS | C-N-CA | 12.46 | 152.85 | 121.70 |
| 81 | DA | 1455 | U | C1'-O4'-C4' | 12.46 | 119.87 | 109.90 |
| 81 | DA | 665 | A | O4'-C1'-N9 | -12.46 | 98.23 | 108.20 |
| 4 | AD | 108 | ARG | NE-CZ-NH2 | -12.45 | 114.07 | 120.30 |
| 81 | DA | 634 | C | N1-C1'-C2' | 12.45 | 130.19 | 114.00 |
| 10 | AI | 138 | PHE | CB-CG-CD1 | 12.45 | 129.51 | 120.80 |
| 81 | DA | 2141 | U | O4'-C1'-N1 | -12.45 | 98.24 | 108.20 |
| 81 | DA | 2192 | C | P-O3'-C3' | 12.45 | 134.64 | 119.70 |
| 82 | DB | 65 | A | P-O3'-C3' | 12.45 | 134.63 | 119.70 |
| 53 | Ba | 9 | LYS | N-CA-CB | -12.44 | 88.21 | 110.60 |
| 81 | DA | 70 | A | C3'-C2'-C1' | 12.44 | 111.45 | 101.50 |
| 81 | DA | 689 | U | O4'-C1'-N1 | 12.44 | 118.15 | 108.20 |
| 78 | CA | 295 | A | C1'-O4'-C4' | 12.43 | 119.84 | 109.90 |
| 81 | DA | 1007 | U | C1'-O4'-C4' | -12.43 | 99.96 | 109.90 |
| 83 | DC | 69 | G | P-O3'-C3' | 12.42 | 134.61 | 119.70 |
| 81 | DA | 1008 | U | P-O3'-C3' | 12.42 | 134.60 | 119.70 |
| 32 | BC | 130 | PHE | N-CA-C | -12.41 | 77.49 | 111.00 |
| 78 | CA | 478 | A | P-O3'-C3' | 12.41 | 134.59 | 119.70 |
| 78 | CA | 1009 | U | P-O3'-C3' | 12.40 | 134.59 | 119.70 |
| 81 | DA | 169 | U | C1'-O4'-C4' | 12.40 | 119.82 | 109.90 |
| 78 | CA | 1386 | G | C3'-C2'-C1' | -12.40 | 91.58 | 101.50 |
| 81 | DA | 637 | C | C3'-C2'-C1' | 12.40 | 111.42 | 101.50 |
| 81 | DA | 1073 | U | O4'-C1'-N1 | 12.40 | 118.12 | 108.20 |
| 81 | DA | 2280 | A | P-O3'-C3' | 12.40 | 134.58 | 119.70 |
| 82 | DB | 58 | G | P-O3'-C3' | 12.40 | 134.58 | 119.70 |
| 81 | DA | 2479 | C | C3'-C2'-C1' | -12.39 | 91.58 | 101.50 |
| 78 | CA | 583 | C | N1-C1'-C2' | 12.39 | 130.11 | 114.00 |
| 81 | DA | 916 | G | P-O3'-C3' | 12.39 | 134.57 | 119.70 |
| 78 | CA | 858 | G | O4'-C1'-N9 | 12.39 | 118.11 | 108.20 |
| 78 | CA | 1453 | G | O4'-C1'-N9 | 12.38 | 118.11 | 108.20 |
| 32 | BC | 6 | TYR | CB-CG-CD1 | -12.38 | 113.57 | 121.00 |
| 81 | DA | 2254 | U | C1'-O4'-C4' | 12.38 | 119.81 | 109.90 |
| 78 | CA | 1396 | U | P-O3'-C3' | 12.38 | 134.55 | 119.70 |
| 81 | DA | 2294 | U | O4'-C1'-N1 | 12.38 | 118.10 | 108.20 |
| 78 | CA | 1419 | G | C3'-C2'-C1' | -12.36 | 91.61 | 101.50 |
| 81 | DA | 2988 | C | C3'-C2'-C1' | 12.36 | 111.39 | 101.50 |
| 81 | DA | 769 | G | P-O3'-C3' | 12.36 | 134.53 | 119.70 |
| 81 | DA | 1730 | G | O4'-C1'-N9 | 12.35 | 118.08 | 108.20 |
| 78 | CA | 689 | G | O4'-C1'-N9 | 12.35 | 118.08 | 108.20 |
| 78 | CA | 1433 | G | O4'-C1'-C2' | -12.35 | 93.45 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1314 | C | C3'-C2'-C1' | 12.34 | 111.37 | 101.50 |
| 81 | DA | 448 | U | P-O3'-C3' | 12.34 | 134.51 | 119.70 |
| 78 | CA | 1086 | A | N9-C1'-C2' | 12.34 | 130.03 | 114.00 |
| 74 | BQ | 136 | GLU | O-C-N | 12.33 | 142.44 | 122.70 |
| 81 | DA | 1757 | A | P-O3'-C3' | 12.33 | 134.50 | 119.70 |
| 78 | CA | 483 | A | N1-C6-N6 | 12.33 | 126.00 | 118.60 |
| 78 | CA | 1348 | A | C1'-O4'-C4' | -12.32 | 100.04 | 109.90 |
| 81 | DA | 2631 | U | P-O3'-C3' | 12.32 | 134.49 | 119.70 |
| 81 | DA | 1235 | U | P-O3'-C3' | 12.31 | 134.48 | 119.70 |
| 29 | AU | 62 | THR | CA-CB-CG2 | -12.31 | 95.16 | 112.40 |
| 81 | DA | 1879 | A | P-O3'-C3' | 12.31 | 134.47 | 119.70 |
| 81 | DA | 2072 | G | P-O3'-C3' | 12.30 | 134.46 | 119.70 |
| 78 | CA | 1635 | A | N1-C6-N6 | 12.30 | 125.98 | 118.60 |
| 81 | DA | 2185 | G | O4'-C1'-N9 | 12.30 | 118.04 | 108.20 |
| 81 | DA | 2627 | C | C3'-C2'-C1' | 12.29 | 111.33 | 101.50 |
| 78 | CA | 1190 | C | O4'-C1'-N1 | 12.29 | 118.03 | 108.20 |
| 81 | DA | 1673 | G | P-O3'-C3' | 12.29 | 134.45 | 119.70 |
| 81 | DA | 2907 | G | O4'-C1'-N9 | 12.29 | 118.03 | 108.20 |
| 78 | CA | 1027 | A | O4'-C1'-N9 | 12.29 | 118.03 | 108.20 |
| 78 | CA | 1338 | C | P-O3'-C3' | 12.28 | 134.44 | 119.70 |
| 78 | CA | 1458 | G | C1'-O4'-C4' | -12.28 | 100.08 | 109.90 |
| 81 | DA | 3252 | G | O4'-C1'-N9 | 12.28 | 118.02 | 108.20 |
| 81 | DA | 2527 | G | C3'-C2'-C1' | -12.28 | 91.68 | 101.50 |
| 81 | DA | 2617 | U | N1-C1'-C2' | -12.28 | 98.04 | 114.00 |
| 81 | DA | 2757 | U | C4'-C3'-C2' | -12.28 | 90.32 | 102.60 |
| 81 | DA | 2763 | U | N1-C1'-C2' | -12.27 | 98.05 | 114.00 |
| 78 | CA | 513 | U | P-O3'-C3' | 12.27 | 134.42 | 119.70 |
| 81 | DA | 1871 | U | P-O5'-C5' | 12.27 | 140.52 | 120.90 |
| 78 | CA | 81 | G | C1'-O4'-C4' | -12.26 | 100.09 | 109.90 |
| 81 | DA | 1410 | U | O4'-C1'-N1 | 12.26 | 118.01 | 108.20 |
| 81 | DA | 2067 | U | N1-C1'-C2' | -12.26 | 98.06 | 114.00 |
| 81 | DA | 2676 | A | P-O3'-C3' | 12.26 | 134.42 | 119.70 |
| 81 | DA | 2632 | G | P-O3'-C3' | -12.26 | 104.99 | 119.70 |
| 64 | Bl | 63 | ARG | CB-CG-CD | 12.26 | 143.47 | 111.60 |
| 81 | DA | 70 | A | O4'-C1'-N9 | -12.26 | 98.39 | 108.20 |
| 81 | DA | 606 | C | P-O3'-C3' | 12.26 | 134.41 | 119.70 |
| 82 | DB | 33 | A | P-O3'-C3' | 12.26 | 134.41 | 119.70 |
| 55 | Bc | 70 | TYR | CB-CG-CD1 | 12.25 | 128.35 | 121.00 |
| 83 | DC | 45 | A | O4'-C1'-C2' | -12.25 | 93.55 | 105.80 |
| 81 | DA | 982 | C | O4'-C1'-C2' | -12.24 | 93.56 | 105.80 |
| 81 | DA | 2452 | G | O4'-C1'-C2' | -12.24 | 93.56 | 105.80 |
| 82 | DB | 32 | C | N1-C1'-C2' | 12.24 | 129.91 | 114.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 83 | DC | 108 | U | P-O5'-C5' | 12.24 | 140.49 | 120.90 |
| 13 | AL | 1 | MET | C-N-CA | 12.24 | 148.00 | 122.30 |
| 3 | AB | 34 | TYR | CB-CG-CD2 | -12.23 | 113.66 | 121.00 |
| 20 | AS | 102 | ARG | NH1-CZ-NH2 | 12.23 | 132.86 | 119.40 |
| 81 | DA | 1209 | G | O4'-C1'-N9 | 12.23 | 117.98 | 108.20 |
| 81 | DA | 2510 | U | P-O5'-C5' | 12.23 | 140.47 | 120.90 |
| 81 | DA | 1998 | G | O4'-C1'-N9 | 12.23 | 117.98 | 108.20 |
| 39 | BJ | 92 | ARG | NE-CZ-NH2 | -12.22 | 114.19 | 120.30 |
| 78 | CA | 49 | C | P-O3'-C3' | -12.22 | 105.04 | 119.70 |
| 81 | DA | 2934 | A | O4'-C1'-C2' | -12.22 | 93.58 | 105.80 |
| 35 | BG | 75 | PRO | N-CA-C | 12.22 | 143.87 | 112.10 |
| 78 | CA | 355 | G | O4'-C1'-N9 | 12.22 | 117.97 | 108.20 |
| 81 | DA | 2540 | A | N1-C6-N6 | 12.22 | 125.93 | 118.60 |
| 81 | DA | 1127 | G | O4'-C1'-N9 | 12.22 | 117.97 | 108.20 |
| 78 | CA | 1608 | U | O4'-C1'-N1 | 12.21 | 117.97 | 108.20 |
| 81 | DA | 672 | A | C1'-O4'-C4' | -12.21 | 100.14 | 109.90 |
| 78 | CA | 489 | C | O4'-C1'-N1 | 12.20 | 117.96 | 108.20 |
| 81 | DA | 2818 | U | O4'-C1'-N1 | 12.20 | 117.96 | 108.20 |
| 31 | BB | 245 | LEU | CA-C-N | 12.20 | 144.04 | 117.20 |
| 81 | DA | 1298 | C | P-O3'-C3' | 12.20 | 134.34 | 119.70 |
| 81 | DA | 1298 | C | N1-C1'-C2' | 12.19 | 129.85 | 114.00 |
| 69 | Br | 104 | LEU | C-N-CA | 12.19 | 152.18 | 121.70 |
| 81 | DA | 3212 | C | O4'-C1'-C2' | -12.19 | 93.61 | 105.80 |
| 83 | DC | 61 | U | O4'-C1'-N1 | 12.19 | 117.95 | 108.20 |
| 81 | DA | 2254 | U | O4'-C1'-C2' | -12.19 | 93.61 | 105.80 |
| 81 | DA | 740 | G | N1-C6-O6 | 12.19 | 127.21 | 119.90 |
| 81 | DA | 1847 | A | P-O3'-C3' | 12.19 | 134.33 | 119.70 |
| 81 | DA | 3203 | U | P-O3'-C3' | 12.19 | 134.32 | 119.70 |
| 26 | AZ | 54 | ARG | NE-CZ-NH2 | -12.19 | 114.21 | 120.30 |
| 20 | AS | 96 | ALA | CA-C-N | 12.18 | 144.00 | 117.20 |
| 63 | Bm | 36 | ARG | NE-CZ-NH2 | 12.18 | 126.39 | 120.30 |
| 81 | DA | 680 | G | P-O3'-C3' | 12.18 | 134.32 | 119.70 |
| 78 | CA | 1584 | G | P-O3'-C3' | 12.18 | 134.31 | 119.70 |
| 78 | CA | 1107 | G | C3'-C2'-C1' | 12.17 | 111.24 | 101.50 |
| 79 | CB | 11 | U | P-O3'-C3' | 12.17 | 134.30 | 119.70 |
| 78 | CA | 630 | A | P-O3'-C3' | 12.16 | 134.30 | 119.70 |
| 78 | CA | 1419 | G | C5'-C4'-C3' | 12.16 | 135.46 | 116.00 |
| 81 | DA | 157 | A | P-O3'-C3' | 12.16 | 134.29 | 119.70 |
| 81 | DA | 3103 | A | C3'-C2'-C1' | 12.16 | 111.23 | 101.50 |
| 81 | DA | 2840 | C | O4'-C1'-C2' | -12.16 | 93.64 | 105.80 |
| 81 | DA | 2633 | U | P-O5'-C5' | 12.15 | 140.35 | 120.90 |
| 78 | CA | 1129 | U | O4'-C1'-N1 | 12.15 | 117.92 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 594 | A | O4'-C1'-N9 | 12.15 | 117.92 | 108.20 |
| 82 | DB | 139 | U | O4'-C1'-N1 | 12.15 | 117.92 | 108.20 |
| 81 | DA | 136 | G | C5'-C4'-C3' | 12.14 | 135.43 | 116.00 |
| 81 | DA | 1885 | U | P-O3'-C3' | 12.14 | 134.27 | 119.70 |
| 78 | CA | 955 | A | O4'-C1'-N9 | 12.14 | 117.91 | 108.20 |
| 81 | DA | 1668 | G | P-O3'-C3' | 12.14 | 134.27 | 119.70 |
| 81 | DA | 2175 | U | O5'-C5'-C4' | -12.14 | 88.64 | 111.70 |
| 82 | DB | 91 | C | O4'-C1'-C2' | -12.14 | 93.66 | 105.80 |
| 81 | DA | 2779 | A | P-O3'-C3' | 12.14 | 134.26 | 119.70 |
| 82 | DB | 121 | U | P-O3'-C3' | 12.14 | 134.26 | 119.70 |
| 81 | DA | 451 | U | O4'-C1'-N1 | 12.13 | 117.91 | 108.20 |
| 33 | BD | 194 | TYR | CB-CG-CD2 | -12.13 | 113.72 | 121.00 |
| 81 | DA | 2001 | U | C1'-O4'-C4' | 12.13 | 119.60 | 109.90 |
| 81 | DA | 182 | U | O4'-C1'-N1 | 12.13 | 117.90 | 108.20 |
| 81 | DA | 1789 | G | C3'-C2'-C1' | -12.13 | 91.80 | 101.50 |
| 81 | DA | 2436 | U | O3'-P-O5' | -12.12 | 80.96 | 104.00 |
| 81 | DA | 623 | U | P-O3'-C3' | 12.12 | 134.25 | 119.70 |
| 81 | DA | 408 | A | P-O3'-C3' | 12.12 | 134.24 | 119.70 |
| 81 | DA | 3387 | U | O4'-C1'-N1 | 12.12 | 117.90 | 108.20 |
| 79 | CB | 25 | U | P-O3'-C3' | 12.11 | 134.24 | 119.70 |
| 81 | DA | 2869 | U | O4'-C1'-C2' | -12.12 | 93.69 | 105.80 |
| 81 | DA | 2663 | G | P-O3'-C3' | 12.11 | 134.23 | 119.70 |
| 78 | CA | 1181 | U | O4'-C1'-N1 | 12.11 | 117.89 | 108.20 |
| 78 | CA | 393 | C | P-O3'-C3' | 12.11 | 134.23 | 119.70 |
| 81 | DA | 250 | U | P-O3'-C3' | 12.11 | 134.23 | 119.70 |
| 81 | DA | 2763 | U | O4'-C1'-C2' | -12.10 | 93.70 | 105.80 |
| 81 | DA | 2323 | G | O4'-C1'-N9 | 12.10 | 117.88 | 108.20 |
| 82 | DB | 131 | A | O4'-C1'-N9 | 12.10 | 117.88 | 108.20 |
| 76 | BS | 160 | PRO | O-C-N | -12.10 | 98.12 | 121.10 |
| 78 | CA | 630 | A | C1'-O4'-C4' | 12.10 | 119.58 | 109.90 |
| 81 | DA | 1191 | U | O4'-C1'-C2' | -12.10 | 93.70 | 105.80 |
| 83 | DC | 111 | U | O4'-C1'-N1 | 12.10 | 117.88 | 108.20 |
| 81 | DA | 688 | G | P-O3'-C3' | 12.09 | 134.21 | 119.70 |
| 26 | AZ | 33 | ARG | NE-CZ-NH1 | 12.09 | 126.35 | 120.30 |
| 78 | CA | 1322 | A | O5'-C5'-C4' | 12.09 | 134.66 | 111.70 |
| 81 | DA | 1955 | U | N1-C1'-C2' | -12.09 | 98.29 | 114.00 |
| 78 | CA | 1633 | A | N1-C6-N6 | 12.08 | 125.85 | 118.60 |
| 78 | CA | 1701 | A | P-O3'-C3' | 12.08 | 134.20 | 119.70 |
| 81 | DA | 2511 | A | P-O5'-C5' | 12.08 | 140.23 | 120.90 |
| 78 | CA | 932 | U | O4'-C1'-N1 | 12.08 | 117.86 | 108.20 |
| 78 | CA | 882 | U | O4'-C1'-N1 | 12.08 | 117.86 | 108.20 |
| 81 | DA | 2179 | C | P-O3'-C3' | 12.08 | 134.19 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1293 | U | O4'-C1'-N1 | 12.07 | 117.86 | 108.20 |
| 81 | DA | 149 | U | P-O3'-C3' | 12.07 | 134.18 | 119.70 |
| 81 | DA | 2263 | C | P-O3'-C3' | 12.07 | 134.18 | 119.70 |
| 81 | DA | 73 | C | O4'-C1'-N1 | 12.07 | 117.85 | 108.20 |
| 53 | Ba | 10 | VAL | C-N-CA | 12.06 | 151.86 | 121.70 |
| 78 | CA | 140 | A | O4'-C1'-C2' | -12.06 | 93.74 | 105.80 |
| 81 | DA | 2644 | C | O4'-C1'-N1 | 12.06 | 117.85 | 108.20 |
| 81 | DA | 330 | G | O4'-C1'-N9 | 12.05 | 117.84 | 108.20 |
| 82 | DB | 93 | U | O4'-C1'-N1 | 12.05 | 117.84 | 108.20 |
| 78 | CA | 1096 | C | C3'-C2'-C1' | 12.05 | 111.14 | 101.50 |
| 78 | CA | 931 | C | P-O5'-C5' | 12.04 | 140.17 | 120.90 |
| 81 | DA | 1467 | A | O4'-C1'-N9 | 12.04 | 117.83 | 108.20 |
| 81 | DA | 1659 | U | O4'-C1'-N1 | 12.04 | 117.83 | 108.20 |
| 81 | DA | 1579 | C | O4'-C1'-C2' | -12.04 | 93.76 | 105.80 |
| 78 | CA | 632 | U | O4'-C1'-C2' | -12.02 | 93.78 | 105.80 |
| 79 | CB | 40 | U | O4'-C1'-N1 | 12.02 | 117.82 | 108.20 |
| 81 | DA | 1811 | G | N9-C1'-C2' | -12.02 | 98.37 | 114.00 |
| 78 | CA | 32 | U | O4'-C1'-N1 | 12.02 | 117.82 | 108.20 |
| 81 | DA | 1388 | U | O4'-C1'-N1 | 12.02 | 117.81 | 108.20 |
| 81 | DA | 1478 | C | P-O3'-C3' | 12.02 | 134.12 | 119.70 |
| 60 | Bi | 62 | TYR | CB-CG-CD1 | -12.02 | 113.79 | 121.00 |
| 81 | DA | 508 | U | O4'-C1'-N1 | 12.02 | 117.81 | 108.20 |
| 81 | DA | 310 | U | O3'-P-O5' | -12.01 | 81.18 | 104.00 |
| 31 | BB | 34 | TYR | CB-CG-CD2 | -12.01 | 113.80 | 121.00 |
| 81 | DA | 124 | U | C3'-C2'-C1' | 12.01 | 111.11 | 101.50 |
| 78 | CA | 887 | A | C3'-C2'-C1' | 12.00 | 111.10 | 101.50 |
| 81 | DA | 1179 | A | O4'-C1'-N9 | 12.00 | 117.80 | 108.20 |
| 78 | CA | 1078 | C | N1-C1'-C2' | 12.00 | 129.60 | 114.00 |
| 79 | CB | 72 | G | N9-C1'-C2' | -12.00 | 98.40 | 114.00 |
| 81 | DA | 2420 | C | C3'-C2'-C1' | 12.00 | 111.10 | 101.50 |
| 29 | AU | 62 | THR | CA-C-O | -11.99 | 94.91 | 120.10 |
| 78 | CA | 1648 | A | O5'-C5'-C4' | 11.99 | 134.49 | 111.70 |
| 81 | DA | 738 | A | N1-C6-N6 | 11.99 | 125.80 | 118.60 |
| 78 | CA | 347 | G | P-O3'-C3' | -11.99 | 105.31 | 119.70 |
| 78 | CA | 976 | G | O4'-C1'-N9 | 11.99 | 117.79 | 108.20 |
| 81 | DA | 2116 | G | O4'-C1'-N9 | 11.99 | 117.79 | 108.20 |
| 78 | CA | 1478 | G | O4'-C1'-N9 | 11.98 | 117.79 | 108.20 |
| 81 | DA | 1551 | C | N1-C1'-C2' | 11.98 | 129.58 | 114.00 |
| 81 | DA | 199 | A | O4'-C1'-N9 | 11.98 | 117.79 | 108.20 |
| 81 | DA | 830 | A | O4'-C1'-N9 | 11.98 | 117.78 | 108.20 |
| 82 | DB | 58 | G | O4'-C1'-N9 | 11.98 | 117.78 | 108.20 |
| 53 | Ba | 57 | HIS | N-CA-CB | 11.98 | 132.16 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | AD | 68 | ARG | NE-CZ-NH2 | -11.98 | 114.31 | 120.30 |
| 78 | CA | 88 | U | P-O3'-C3' | 11.98 | 134.07 | 119.70 |
| 78 | CA | 620 | A | P-O3'-C3' | 11.96 | 134.06 | 119.70 |
| 78 | CA | 1417 | A | C3'-C2'-C1' | 11.96 | 111.07 | 101.50 |
| 83 | DC | 112 | G | O4'-C1'-N9 | 11.97 | 117.77 | 108.20 |
| 78 | CA | 1087 | A | P-O3'-C3' | 11.96 | 134.06 | 119.70 |
| 81 | DA | 2840 | C | O4'-C1'-N1 | 11.96 | 117.77 | 108.20 |
| 83 | DC | 46 | A | O4'-C1'-C2' | -11.96 | 93.84 | 105.80 |
| 81 | DA | 3142 | A | N9-C1'-C2' | -11.96 | 98.46 | 114.00 |
| 81 | DA | 588 | G | O4'-C1'-N9 | 11.96 | 117.76 | 108.20 |
| 79 | CB | 37 | G | P-O3'-C3' | 11.95 | 134.04 | 119.70 |
| 81 | DA | 2157 | G | O4'-C1'-C2' | -11.95 | 93.85 | 105.80 |
| 81 | DA | 1300 | G | O4'-C1'-N9 | 11.95 | 117.76 | 108.20 |
| 81 | DA | 3244 | A | N9-C1'-C2' | 11.95 | 129.53 | 114.00 |
| 81 | DA | 2697 | A | C3'-C2'-C1' | 11.95 | 111.06 | 101.50 |
| 77 | BI | 107 | GLY | C-N-CA | 11.93 | 151.53 | 121.70 |
| 81 | DA | 664 | U | O5'-P-OP1 | -11.93 | 94.96 | 105.70 |
| 78 | CA | 842 | C | P-O3'-C3' | 11.92 | 134.01 | 119.70 |
| 81 | DA | 1694 | U | P-O3'-C3' | 11.92 | 134.00 | 119.70 |
| 81 | DA | 2279 | A | O3'-P-O5' | -11.91 | 81.36 | 104.00 |
| 81 | DA | 1004 | U | N1-C1'-C2' | 11.91 | 129.48 | 114.00 |
| 81 | DA | 3288 | G | P-O3'-C3' | 11.91 | 133.99 | 119.70 |
| 81 | DA | 1688 | U | O4'-C1'-N1 | -11.91 | 98.67 | 108.20 |
| 78 | CA | 1478 | G | C1'-O4'-C4' | -11.90 | 100.38 | 109.90 |
| 81 | DA | 1297 | C | P-O3'-C3' | 11.90 | 133.98 | 119.70 |
| 81 | DA | 1314 | C | O4'-C1'-N1 | -11.90 | 98.68 | 108.20 |
| 81 | DA | 1405 | U | N1-C1'-C2' | 11.90 | 129.47 | 114.00 |
| 81 | DA | 1898 | G | O4'-C1'-N9 | 11.90 | 117.72 | 108.20 |
| 81 | DA | 1535 | A | N9-C1'-C2' | -11.90 | 98.53 | 114.00 |
| 81 | DA | 1432 | C | N1-C1'-C2' | -11.89 | 98.54 | 114.00 |
| 47 | BU | 88 | ARG | NE-CZ-NH1 | 11.89 | 126.25 | 120.30 |
| 74 | BQ | 145 | PHE | CB-CG-CD1 | -11.89 | 112.48 | 120.80 |
| 81 | DA | 2163 | C | C3'-C2'-C1' | 11.89 | 111.01 | 101.50 |
| 81 | DA | 3283 | U | P-O3'-C3' | 11.89 | 133.97 | 119.70 |
| 78 | CA | 46 | A | N9-C1'-C2' | -11.88 | 98.55 | 114.00 |
| 81 | DA | 1623 | G | C5'-C4'-O4' | -11.88 | 94.84 | 109.10 |
| 78 | CA | 1501 | C | O4'-C1'-N1 | 11.88 | 117.70 | 108.20 |
| 81 | DA | 382 | U | O4'-C1'-N1 | 11.88 | 117.70 | 108.20 |
| 81 | DA | 164 | A | N1-C6-N6 | 11.87 | 125.72 | 118.60 |
| 83 | DC | 60 | G | C1'-O4'-C4' | -11.87 | 100.40 | 109.90 |
| 81 | DA | 2108 | C | C3'-C2'-C1' | 11.86 | 110.99 | 101.50 |
| 83 | DC | 46 | A | O5'-C5'-C4' | 11.86 | 134.24 | 111.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 571 | G | N9-C1'-C2' | 11.86 | 129.42 | 114.00 |
| 81 | DA | 1113 | G | P-O3'-C3' | -11.86 | 105.47 | 119.70 |
| 83 | DC | 115 | A | O4'-C1'-N9 | 11.86 | 117.69 | 108.20 |
| 74 | BQ | 79 | TYR | CB-CG-CD2 | 11.86 | 128.11 | 121.00 |
| 81 | DA | 1876 | U | O4'-C1'-N1 | 11.86 | 117.68 | 108.20 |
| 81 | DA | 2693 | C | P-O3'-C3' | 11.85 | 133.92 | 119.70 |
| 81 | DA | 2265 | C | P-O3'-C3' | -11.85 | 105.48 | 119.70 |
| 81 | DA | 2760 | C | C5'-C4'-C3' | 11.85 | 134.96 | 116.00 |
| 2 | AA | 110 | TYR | CB-CG-CD2 | -11.85 | 113.89 | 121.00 |
| 81 | DA | 1853 | U | O4'-C1'-N1 | 11.85 | 117.68 | 108.20 |
| 78 | CA | 446 | A | O4'-C1'-N9 | 11.85 | 117.68 | 108.20 |
| 81 | DA | 730 | C | P-O3'-C3' | 11.85 | 133.91 | 119.70 |
| 83 | DC | 44 | C | O4'-C1'-N1 | 11.85 | 117.68 | 108.20 |
| 12 | AK | 124 | ASP | CB-CG-OD1 | -11.84 | 107.64 | 118.30 |
| 81 | DA | 2374 | C | O4'-C1'-C2' | -11.84 | 93.96 | 105.80 |
| 81 | DA | 3304 | U | P-O3'-C3' | 11.84 | 133.91 | 119.70 |
| 81 | DA | 441 | U | O4'-C1'-N1 | 11.84 | 117.67 | 108.20 |
| 56 | Bf | 27 | TYR | CB-CG-CD1 | 11.83 | 128.10 | 121.00 |
| 81 | DA | 1937 | U | P-O3'-C3' | 11.83 | 133.89 | 119.70 |
| 81 | DA | 1766 | G | O4'-C1'-N9 | 11.82 | 117.66 | 108.20 |
| 81 | DA | 2755 | C | C3'-C2'-C1' | 11.82 | 110.96 | 101.50 |
| 81 | DA | 1329 | U | C3'-C2'-C1' | 11.82 | 110.96 | 101.50 |
| 78 | CA | 1080 | U | O4'-C1'-N1 | 11.82 | 117.65 | 108.20 |
| 78 | CA | 650 | U | O5'-P-OP1 | 11.81 | 124.87 | 110.70 |
| 78 | CA | 1062 | A | N1-C6-N6 | 11.81 | 125.69 | 118.60 |
| 81 | DA | 671 | U | C3'-C2'-C1' | -11.81 | 92.05 | 101.50 |
| 78 | CA | 235 | G | C1'-O4'-C4' | -11.80 | 100.46 | 109.90 |
| 81 | DA | 2651 | G | P-O3'-C3' | 11.81 | 133.87 | 119.70 |
| 78 | CA | 1628 | U | P-O3'-C3' | 11.80 | 133.86 | 119.70 |
| 35 | BG | 75 | PRO | CA-C-O | -11.80 | 91.88 | 120.20 |
| 81 | DA | 1188 | U | O4'-C1'-N1 | 11.80 | 117.64 | 108.20 |
| 43 | BP | 180 | PHE | CB-CG-CD1 | -11.79 | 112.54 | 120.80 |
| 78 | CA | 312 | A | C3'-C2'-C1' | 11.79 | 110.93 | 101.50 |
| 78 | CA | 461 | G | O4'-C1'-N9 | 11.79 | 117.63 | 108.20 |
| 81 | DA | 2173 | U | N1-C1'-C2' | 11.79 | 129.33 | 114.00 |
| 41 | BN | 108 | ARG | CB-CG-CD | 11.78 | 142.22 | 111.60 |
| 81 | DA | 2423 | U | O4'-C1'-N1 | 11.78 | 117.62 | 108.20 |
| 81 | DA | 1245 | A | O4'-C1'-N9 | 11.77 | 117.62 | 108.20 |
| 81 | DA | 1298 | C | P-O5'-C5' | 11.77 | 139.74 | 120.90 |
| 78 | CA | 947 | U | O4'-C1'-N1 | 11.77 | 117.62 | 108.20 |
| 81 | DA | 147 | U | P-O3'-C3' | 11.77 | 133.82 | 119.70 |
| 82 | DB | 85 | G | O4'-C1'-N9 | -11.77 | 98.78 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2917 | G | O4'-C1'-C2' | 11.76 | 118.19 | 107.60 |
| 81 | DA | 518 | G | P-O5'-C5' | 11.76 | 139.72 | 120.90 |
| 81 | DA | 1693 | C | O4'-C1'-N1 | 11.76 | 117.61 | 108.20 |
| 81 | DA | 2547 | A | N1-C6-N6 | 11.76 | 125.66 | 118.60 |
| 82 | DB | 78 | G | P-O3'-C3' | 11.76 | 133.81 | 119.70 |
| 81 | DA | 932 | U | O4'-C1'-N1 | 11.76 | 117.60 | 108.20 |
| 21 | AT | 62 | ARG | NE-CZ-NH2 | -11.75 | 114.42 | 120.30 |
| 78 | CA | 1236 | A | O4'-C1'-N9 | 11.75 | 117.60 | 108.20 |
| 81 | DA | 638 | C | P-O5'-C5' | 11.75 | 139.70 | 120.90 |
| 81 | DA | 1744 | G | O4'-C1'-N9 | 11.75 | 117.60 | 108.20 |
| 81 | DA | 1739 | U | O4'-C1'-N1 | 11.75 | 117.60 | 108.20 |
| 78 | CA | 213 | A | P-O3'-C3' | -11.75 | 105.61 | 119.70 |
| 78 | CA | 666 | U | N1-C1'-C2' | 11.75 | 129.27 | 114.00 |
| 78 | CA | 1063 | U | P-O3'-C3' | 11.75 | 133.80 | 119.70 |
| 78 | CA | 786 | C | P-O3'-C3' | 11.75 | 133.79 | 119.70 |
| 81 | DA | 742 | G | O4'-C1'-N9 | 11.74 | 117.60 | 108.20 |
| 78 | CA | 1570 | A | O4'-C1'-C2' | -11.74 | 94.06 | 105.80 |
| 29 | AU | 36 | SER | C-N-CA | 11.74 | 151.05 | 121.70 |
| 61 | Bj | 89 | LEU | CA-C-N | 11.74 | 149.97 | 117.10 |
| 81 | DA | 156 | G | P-O3'-C3' | 11.73 | 133.78 | 119.70 |
| 81 | DA | 597 | G | C1'-O4'-C4' | -11.73 | 100.51 | 109.90 |
| 81 | DA | 431 | U | O4'-C1'-N1 | 11.73 | 117.59 | 108.20 |
| 61 | Bj | 37 | THR | CA-C-O | -11.73 | 95.47 | 120.10 |
| 78 | CA | 689 | G | C3'-C2'-C1' | -11.73 | 92.12 | 101.50 |
| 78 | CA | 1606 | C | P-O5'-C5' | 11.73 | 139.66 | 120.90 |
| 81 | DA | 3248 | C | P-O3'-C3' | 11.73 | 133.78 | 119.70 |
| 81 | DA | 1306 | G | P-O3'-C3' | 11.72 | 133.77 | 119.70 |
| 16 | AO | 130 | ARG | NE-CZ-NH1 | 11.72 | 126.16 | 120.30 |
| 81 | DA | 873 | C | C3'-C2'-C1' | 11.71 | 110.87 | 101.50 |
| 81 | DA | 1686 | U | P-O5'-C5' | 11.71 | 139.64 | 120.90 |
| 81 | DA | 3240 | C | P-O5'-C5' | 11.71 | 139.64 | 120.90 |
| 81 | DA | 2307 | G | P-O3'-C3' | 11.71 | 133.75 | 119.70 |
| 81 | DA | 1338 | C | C1'-O4'-C4' | 11.71 | 119.27 | 109.90 |
| 81 | DA | 1002 | A | P-O5'-C5' | 11.71 | 139.63 | 120.90 |
| 81 | DA | 2663 | G | O4'-C1'-N9 | 11.71 | 117.56 | 108.20 |
| 81 | DA | 3328 | G | O4'-C1'-N9 | 11.71 | 117.56 | 108.20 |
| 78 | CA | 1533 | C | O4'-C1'-N1 | 11.70 | 117.56 | 108.20 |
| 81 | DA | 2386 | A | P-O3'-C3' | 11.70 | 133.74 | 119.70 |
| 81 | DA | 185 | C | C1'-O4'-C4' | -11.70 | 100.54 | 109.90 |
| 81 | DA | 1242 | G | O4'-C1'-N9 | 11.69 | 117.55 | 108.20 |
| 82 | DB | 131 | A | P-O3'-C3' | 11.69 | 133.73 | 119.70 |
| 76 | BS | 166 | LYS | CB-CA-C | -11.69 | 87.02 | 110.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1971 | C | O4'-C1'-C2' | -11.69 | 94.11 | 105.80 |
| 81 | DA | 3382 | U | N1-C1'-C2' | 11.69 | 129.19 | 114.00 |
| 81 | DA | 3092 | C | C3'-C2'-C1' | 11.68 | 110.84 | 101.50 |
| 82 | DB | 128 | U | O4'-C1'-C2' | -11.68 | 94.12 | 105.80 |
| 78 | CA | 1545 | A | O4'-C1'-N9 | 11.68 | 117.54 | 108.20 |
| 81 | DA | 2137 | U | O4'-C1'-N1 | 11.68 | 117.54 | 108.20 |
| 78 | CA | 1412 | G | O4'-C1'-N9 | -11.67 | 98.86 | 108.20 |
| 81 | DA | 3303 | G | P-O3'-C3' | 11.67 | 133.71 | 119.70 |
| 78 | CA | 1586 | A | O3'-P-O5' | 11.66 | 126.15 | 104.00 |
| 81 | DA | 1481 | A | P-O3'-C3' | 11.66 | 133.69 | 119.70 |
| 81 | DA | 974 | G | O4'-C1'-N9 | 11.66 | 117.52 | 108.20 |
| 81 | DA | 2917 | G | C1'-O4'-C4' | -11.65 | 100.58 | 109.90 |
| 78 | CA | 1480 | G | O5'-P-OP2 | -11.65 | 95.21 | 105.70 |
| 81 | DA | 1866 | C | C3'-C2'-C1' | 11.65 | 110.82 | 101.50 |
| 81 | DA | 3106 | A | P-O3'-C3' | -11.65 | 105.72 | 119.70 |
| 81 | DA | 1744 | G | P-O3'-C3' | 11.65 | 133.68 | 119.70 |
| 81 | DA | 1057 | A | O4'-C1'-N9 | 11.64 | 117.52 | 108.20 |
| 81 | DA | 212 | G | O4'-C1'-N9 | 11.64 | 117.51 | 108.20 |
| 81 | DA | 1595 | U | O4'-C1'-N1 | 11.64 | 117.51 | 108.20 |
| 81 | DA | 1790 | G | C3'-C2'-C1' | -11.64 | 92.19 | 101.50 |
| 81 | DA | 2504 | U | N1-C1'-C2' | -11.64 | 98.87 | 114.00 |
| 81 | DA | 572 | A | P-O3'-C3' | 11.63 | 133.66 | 119.70 |
| 81 | DA | 2771 | U | O4'-C1'-N1 | 11.63 | 117.51 | 108.20 |
| 81 | DA | 1406 | A | P-O3'-C3' | 11.63 | 133.66 | 119.70 |
| 81 | DA | 735 | A | N1-C6-N6 | 11.63 | 125.58 | 118.60 |
| 81 | DA | 1947 | G | N9-C1'-C2' | -11.63 | 98.88 | 114.00 |
| 81 | DA | 2569 | A | N1-C6-N6 | 11.63 | 125.58 | 118.60 |
| 82 | DB | 156 | U | O4'-C1'-N1 | 11.63 | 117.50 | 108.20 |
| 78 | CA | 1565 | C | C3'-C2'-C1' | 11.63 | 110.80 | 101.50 |
| 78 | CA | 1589 | C | C3'-C2'-C1' | 11.63 | 110.80 | 101.50 |
| 81 | DA | 2623 | G | C1'-O4'-C4' | 11.63 | 119.20 | 109.90 |
| 43 | BP | 127 | TYR | CB-CG-CD2 | 11.62 | 127.97 | 121.00 |
| 81 | DA | 2049 | A | C3'-C2'-C1' | 11.62 | 110.80 | 101.50 |
| 39 | BJ | 67 | ARG | NE-CZ-NH2 | -11.62 | 114.49 | 120.30 |
| 78 | CA | 392 | G | P-O3'-C3' | 11.62 | 133.64 | 119.70 |
| 81 | DA | 2619 | G | N9-C1'-C2' | 11.61 | 129.09 | 114.00 |
| 76 | BS | 70 | ASN | N-CA-CB | 11.61 | 131.50 | 110.60 |
| 81 | DA | 1877 | U | P-O3'-C3' | 11.61 | 133.63 | 119.70 |
| 81 | DA | 1603 | A | O5'-P-OP2 | 11.61 | 124.63 | 110.70 |
| 81 | DA | 2579 | G | O4'-C1'-N9 | 11.61 | 117.48 | 108.20 |
| 81 | DA | 2177 | G | O4'-C1'-N9 | 11.61 | 117.48 | 108.20 |
| 78 | CA | 1066 | C | O4'-C1'-N1 | 11.60 | 117.48 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 306 | A | N9-C1'-C2' | -11.60 | 98.92 | 114.00 |
| 78 | CA | 900 | A | O4'-C4'-C3' | 11.60 | 115.60 | 104.00 |
| 78 | CA | 1404 | C | P-O3'-C3' | 11.60 | 133.61 | 119.70 |
| 81 | DA | 474 | G | P-O3'-C3' | 11.60 | 133.62 | 119.70 |
| 78 | CA | 1680 | G | P-O3'-C3' | 11.59 | 133.61 | 119.70 |
| 81 | DA | 2372 | A | C3'-C2'-C1' | 11.59 | 110.78 | 101.50 |
| 81 | DA | 1757 | A | O5'-C5'-C4' | 11.59 | 133.72 | 111.70 |
| 5 | AC | 8 | TYR | CB-CG-CD1 | 11.59 | 127.95 | 121.00 |
| 81 | DA | 1551 | C | P-O3'-C3' | 11.59 | 133.60 | 119.70 |
| 47 | BU | 140 | ILE | O-C-N | -11.58 | 104.17 | 122.70 |
| 81 | DA | 2339 | C | O4'-C1'-C2' | -11.58 | 94.22 | 105.80 |
| 78 | CA | 1585 | U | O4'-C1'-C2' | -11.58 | 94.22 | 105.80 |
| 81 | DA | 1810 | A | P-O3'-C3' | 11.58 | 133.60 | 119.70 |
| 81 | DA | 2070 | U | O4'-C1'-N1 | 11.58 | 117.46 | 108.20 |
| 81 | DA | 3387 | U | O4'-C1'-C2' | -11.58 | 94.22 | 105.80 |
| 78 | CA | 1753 | A | P-O3'-C3' | 11.58 | 133.59 | 119.70 |
| 74 | BQ | 242 | SER | N-CA-CB | 11.57 | 127.86 | 110.50 |
| 78 | CA | 588 | U | O5'-P-OP2 | -11.57 | 95.28 | 105.70 |
| 81 | DA | 3385 | U | P-O3'-C3' | 11.57 | 133.59 | 119.70 |
| 81 | DA | 1437 | C | O4'-C1'-C2' | -11.56 | 94.24 | 105.80 |
| 78 | CA | 301 | A | P-O3'-C3' | 11.56 | 133.57 | 119.70 |
| 81 | DA | 3142 | A | O4'-C1'-C2' | -11.56 | 94.24 | 105.80 |
| 80 | CC | 22 | A | N1-C6-N6 | 11.55 | 125.53 | 118.60 |
| 81 | DA | 49 | A | P-O3'-C3' | 11.56 | 133.57 | 119.70 |
| 81 | DA | 626 | U | O4'-C1'-N1 | 11.55 | 117.44 | 108.20 |
| 81 | DA | 235 | A | O4'-C1'-N9 | 11.55 | 117.44 | 108.20 |
| 78 | CA | 567 | A | N1-C6-N6 | 11.54 | 125.53 | 118.60 |
| 81 | DA | 1556 | C | P-O3'-C3' | 11.54 | 133.55 | 119.70 |
| 83 | DC | 27 | A | C3'-C2'-C1' | 11.54 | 110.74 | 101.50 |
| 78 | CA | 296 | U | O4'-C1'-C2' | -11.54 | 94.26 | 105.80 |
| 78 | CA | 689 | G | O4'-C1'-C2' | 11.54 | 117.99 | 107.60 |
| 81 | DA | 595 | G | O4'-C1'-N9 | 11.54 | 117.43 | 108.20 |
| 78 | CA | 640 | U | O4'-C1'-N1 | 11.53 | 117.43 | 108.20 |
| 81 | DA | 3303 | G | C1'-O4'-C4' | -11.53 | 100.67 | 109.90 |
| 81 | DA | 513 | G | O4'-C1'-N9 | 11.53 | 117.42 | 108.20 |
| 81 | DA | 769 | G | O4'-C1'-N9 | 11.53 | 117.42 | 108.20 |
| 81 | DA | 2057 | G | O4'-C1'-N9 | 11.53 | 117.42 | 108.20 |
| 81 | DA | 3006 | A | N9-C1'-C2' | 11.53 | 128.98 | 114.00 |
| 78 | CA | 1162 | C | N1-C1'-C2' | 11.52 | 128.98 | 114.00 |
| 81 | DA | 2854 | U | O4'-C1'-N1 | 11.52 | 117.42 | 108.20 |
| 74 | BQ | 242 | SER | CA-C-N | 11.52 | 142.54 | 117.20 |
| 78 | CA | 1133 | A | C1'-O4'-C4' | -11.52 | 100.69 | 109.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1632 | A | P-O5'-C5' | 11.52 | 139.33 | 120.90 |
| 81 | DA | 1817 | G | O4'-C1'-N9 | 11.52 | 117.41 | 108.20 |
| 78 | CA | 1099 | U | P-O3'-C3' | 11.52 | 133.52 | 119.70 |
| 3 | AB | 18 | TYR | CB-CG-CD2 | 11.51 | 127.91 | 121.00 |
| 49 | BV | 162 | GLU | C-N-CA | 11.51 | 150.48 | 121.70 |
| 78 | CA | 912 | U | O4'-C1'-N1 | 11.51 | 117.41 | 108.20 |
| 81 | DA | 198 | A | C3'-C2'-C1' | 11.51 | 110.71 | 101.50 |
| 81 | DA | 3051 | U | O4'-C4'-C3' | -11.51 | 92.49 | 104.00 |
| 83 | DC | 2 | G | N9-C1'-C2' | -11.51 | 99.04 | 114.00 |
| 31 | BB | 252 | THR | N-CA-C | -11.50 | 79.96 | 111.00 |
| 81 | DA | 1214 | U | P-O3'-C3' | 11.50 | 133.50 | 119.70 |
| 81 | DA | 740 | G | P-O3'-C3' | 11.50 | 133.50 | 119.70 |
| 81 | DA | 2422 | C | P-O3'-C3' | 11.50 | 133.50 | 119.70 |
| 81 | DA | 2479 | C | C1'-O4'-C4' | -11.50 | 100.70 | 109.90 |
| 82 | DB | 39 | G | O4'-C1'-C2' | -11.50 | 94.30 | 105.80 |
| 45 | BR | 96 | PHE | N-CA-CB | -11.49 | 89.91 | 110.60 |
| 78 | CA | 1546 | G | O4'-C4'-C3' | -11.49 | 92.51 | 104.00 |
| 81 | DA | 853 | G | O4'-C1'-N9 | 11.49 | 117.39 | 108.20 |
| 81 | DA | 2880 | U | C1'-O4'-C4' | -11.49 | 100.71 | 109.90 |
| 34 | BE | 53 | THR | N-CA-C | 11.49 | 142.03 | 111.00 |
| 78 | CA | 1338 | C | O5'-C5'-C4' | 11.49 | 133.53 | 111.70 |
| 81 | DA | 1570 | U | O4'-C1'-N1 | 11.48 | 117.39 | 108.20 |
| 83 | DC | 29 | C | C3'-C2'-C1' | 11.48 | 110.69 | 101.50 |
| 81 | DA | 2720 | G | N9-C1'-C2' | 11.48 | 128.93 | 114.00 |
| 76 | BS | 46 | PHE | CB-CG-CD1 | -11.48 | 112.76 | 120.80 |
| 78 | CA | 288 | A | O4'-C1'-C2' | -11.48 | 94.32 | 105.80 |
| 81 | DA | 1152 | G | P-O3'-C3' | 11.47 | 133.47 | 119.70 |
| 81 | DA | 2652 | U | N1-C1'-C2' | 11.47 | 128.91 | 114.00 |
| 83 | DC | 93 | U | P-O3'-C3' | 11.47 | 133.46 | 119.70 |
| 78 | CA | 318 | U | P-O3'-C3' | 11.46 | 133.45 | 119.70 |
| 81 | DA | 1783 | U | O4'-C1'-N1 | 11.45 | 117.36 | 108.20 |
| 81 | DA | 3047 | U | C3'-C2'-C1' | 11.45 | 110.66 | 101.50 |
| 78 | CA | 1087 | A | O3'-P-O5' | -11.44 | 82.26 | 104.00 |
| 81 | DA | 246 | U | O4'-C1'-N1 | 11.44 | 117.36 | 108.20 |
| 78 | CA | 1548 | G | C1'-O4'-C4' | -11.44 | 100.75 | 109.90 |
| 81 | DA | 104 | G | O4'-C1'-N9 | 11.44 | 117.35 | 108.20 |
| 81 | DA | 1649 | U | O4'-C1'-N1 | 11.44 | 117.35 | 108.20 |
| 81 | DA | 2755 | C | O3'-P-O5' | -11.44 | 82.27 | 104.00 |
| 32 | BC | 344 | THR | CA-C-O | -11.43 | 96.09 | 120.10 |
| 76 | BS | 45 | TYR | CB-CG-CD1 | 11.43 | 127.86 | 121.00 |
| 78 | CA | 623 | A | N9-C1'-C2' | -11.43 | 99.14 | 114.00 |
| 78 | CA | 1554 | U | O4'-C1'-N1 | 11.42 | 117.34 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 79 | CB | 28 | G | O4'-C1'-N9 | 11.42 | 117.33 | 108.20 |
| 6 | AE | 70 | ASP | O-C-N | -11.42 | 104.43 | 122.70 |
| 81 | DA | 842 | G | P-O3'-C3' | 11.41 | 133.40 | 119.70 |
| 81 | DA | 518 | G | C3'-C2'-C1' | 11.41 | 110.63 | 101.50 |
| 81 | DA | 1039 | U | P-O3'-C3' | 11.41 | 133.39 | 119.70 |
| 44 | BO | 21 | ARG | C-N-CA | 11.41 | 150.22 | 121.70 |
| 81 | DA | 2491 | A | O4'-C4'-C3' | -11.40 | 92.59 | 104.00 |
| 78 | CA | 354 | C | C3'-C2'-C1' | 11.40 | 110.62 | 101.50 |
| 78 | CA | 508 | U | P-O5'-C5' | 11.40 | 139.14 | 120.90 |
| 81 | DA | 1561 | G | O4'-C1'-C2' | 11.39 | 117.85 | 107.60 |
| 78 | CA | 1444 | A | O4'-C1'-N9 | 11.39 | 117.31 | 108.20 |
| 78 | CA | 1503 | A | N1-C6-N6 | 11.39 | 125.43 | 118.60 |
| 78 | CA | 1081 | A | C1'-O4'-C4' | 11.39 | 119.01 | 109.90 |
| 78 | CA | 29 | U | N1-C1'-C2' | 11.38 | 128.80 | 114.00 |
| 81 | DA | 782 | U | O4'-C1'-N1 | 11.38 | 117.31 | 108.20 |
| 81 | DA | 1821 | U | N1-C1'-C2' | 11.38 | 128.80 | 114.00 |
| 78 | CA | 497 | G | P-O5'-C5' | 11.38 | 139.11 | 120.90 |
| 45 | BR | 54 | LEU | CB-CG-CD2 | 11.38 | 130.35 | 111.00 |
| 78 | CA | 1066 | C | P-O3'-C3' | 11.38 | 133.36 | 119.70 |
| 81 | DA | 2031 | U | O4'-C1'-N1 | 11.38 | 117.30 | 108.20 |
| 81 | DA | 352 | A | O4'-C1'-C2' | -11.38 | 94.42 | 105.80 |
| 81 | DA | 1258 | U | O4'-C1'-N1 | 11.38 | 117.30 | 108.20 |
| 81 | DA | 103 | G | O4'-C1'-C2' | -11.38 | 94.42 | 105.80 |
| 78 | CA | 947 | U | O4'-C1'-C2' | -11.37 | 94.43 | 105.80 |
| 1 | Aa | 38 | ARG | NE-CZ-NH1 | 11.37 | 125.98 | 120.30 |
| 78 | CA | 1267 | G | P-O3'-C3' | 11.37 | 133.34 | 119.70 |
| 83 | DC | 46 | A | C1'-O4'-C4' | 11.36 | 118.99 | 109.90 |
| 79 | CB | 41 | G | N9-C1'-C2' | 11.36 | 128.77 | 114.00 |
| 81 | DA | 310 | U | O4'-C1'-N1 | 11.36 | 117.29 | 108.20 |
| 81 | DA | 858 | A | O3'-P-O5' | -11.36 | 82.42 | 104.00 |
| 81 | DA | 2040 | U | P-O3'-C3' | 11.36 | 133.33 | 119.70 |
| 2 | AA | 241 | GLU | N-CA-CB | 11.36 | 131.04 | 110.60 |
| 78 | CA | 196 | G | C1'-O4'-C4' | -11.35 | 100.82 | 109.90 |
| 78 | CA | 29 | U | C3'-C2'-C1' | 11.35 | 110.58 | 101.50 |
| 81 | DA | 708 | G | P-O3'-C3' | 11.35 | 133.32 | 119.70 |
| 81 | DA | 1814 | A | O4'-C1'-N9 | 11.35 | 117.28 | 108.20 |
| 81 | DA | 1820 | U | O4'-C4'-C3' | -11.35 | 92.65 | 104.00 |
| 78 | CA | 235 | G | N9-C1'-C2' | 11.35 | 128.75 | 114.00 |
| 81 | DA | 469 | G | P-O3'-C3' | 11.35 | 133.32 | 119.70 |
| 81 | DA | 2258 | U | O4'-C1'-N1 | 11.34 | 117.28 | 108.20 |
| 81 | DA | 402 | A | P-O3'-C3' | 11.34 | 133.31 | 119.70 |
| 78 | CA | 297 | U | N1-C1'-C2' | 11.34 | 128.74 | 114.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 1785 | U | O4'-C1'-N1 | 11.34 | 117.27 | 108.20 |
| 81 | DA | 968 | G | P-O3'-C3' | 11.33 | 133.30 | 119.70 |
| 78 | CA | 226 | A | C1'-O4'-C4' | -11.33 | 100.83 | 109.90 |
| 78 | CA | 1091 | A | C1'-O4'-C4' | 11.33 | 118.97 | 109.90 |
| 81 | DA | 1001 | G | C3'-C2'-C1' | -11.33 | 92.44 | 101.50 |
| 81 | DA | 1582 | C | N1-C1'-C2' | 11.33 | 128.73 | 114.00 |
| 81 | DA | 2041 | U | O4'-C1'-C2' | -11.33 | 94.47 | 105.80 |
| 83 | DC | 30 | G | P-O3'-C3' | 11.32 | 133.29 | 119.70 |
| 78 | CA | 1630 | U | O4'-C1'-N1 | 11.32 | 117.26 | 108.20 |
| 15 | AN | 53 | ASN | C-N-CA | -11.32 | 93.40 | 121.70 |
| 82 | DB | 38 | U | C3'-C2'-C1' | 11.32 | 110.56 | 101.50 |
| 81 | DA | 429 | U | P-O3'-C3' | 11.32 | 133.28 | 119.70 |
| 81 | DA | 3395 | G | P-O3'-C3' | 11.32 | 133.28 | 119.70 |
| 81 | DA | 1552 | G | N9-C1'-C2' | 11.31 | 128.70 | 114.00 |
| 81 | DA | 1820 | U | P-O3'-C3' | 11.31 | 133.28 | 119.70 |
| 81 | DA | 3111 | U | O4'-C1'-N1 | 11.31 | 117.25 | 108.20 |
| 81 | DA | 3296 | A | C5'-C4'-C3' | 11.31 | 134.10 | 116.00 |
| 81 | DA | 3389 | U | C5'-C4'-C3' | 11.31 | 134.10 | 116.00 |
| 32 | BC | 196 | ARG | NE-CZ-NH2 | -11.31 | 114.65 | 120.30 |
| 81 | DA | 230 | U | O4'-C1'-N1 | 11.31 | 117.25 | 108.20 |
| 81 | DA | 2563 | G | O4'-C1'-N9 | 11.31 | 117.25 | 108.20 |
| 81 | DA | 2816 | G | C1'-O4'-C4' | -11.30 | 100.86 | 109.90 |
| 82 | DB | 84 | C | O4'-C1'-N1 | 11.30 | 117.24 | 108.20 |
| 81 | DA | 3221 | C | P-O5'-C5' | 11.30 | 138.98 | 120.90 |
| 81 | DA | 2684 | C | P-O3'-C3' | 11.30 | 133.26 | 119.70 |
| 78 | CA | 46 | A | C3'-C2'-C1' | -11.30 | 92.46 | 101.50 |
| 81 | DA | 580 | C | N1-C1'-C2' | 11.30 | 128.68 | 114.00 |
| 81 | DA | 2672 | G | O4'-C1'-N9 | 11.29 | 117.24 | 108.20 |
| 81 | DA | 1666 | G | P-O3'-C3' | 11.29 | 133.24 | 119.70 |
| 82 | DB | 134 | G | N9-C1'-C2' | -11.28 | 99.33 | 114.00 |
| 82 | DB | 153 | U | P-O3'-C3' | 11.28 | 133.24 | 119.70 |
| 10 | AI | 66 | ARG | NE-CZ-NH2 | -11.28 | 114.66 | 120.30 |
| 79 | CB | 13 | U | P-O3'-C3' | 11.28 | 133.24 | 119.70 |
| 81 | DA | 320 | G | O4'-C1'-N9 | 11.28 | 117.22 | 108.20 |
| 81 | DA | 779 | G | O4'-C1'-N9 | 11.28 | 117.22 | 108.20 |
| 81 | DA | 2437 | G | N9-C1'-C2' | -11.28 | 99.34 | 114.00 |
| 81 | DA | 2795 | U | O4'-C1'-N1 | 11.28 | 117.22 | 108.20 |
| 78 | CA | 275 | C | P-O3'-C3' | 11.28 | 133.23 | 119.70 |
| 81 | DA | 1847 | A | O4'-C1'-N9 | 11.28 | 117.22 | 108.20 |
| 13 | AL | 93 | LEU | N-CA-CB | -11.27 | 87.86 | 110.40 |
| 78 | CA | 1580 | C | C3'-C2'-C1' | 11.27 | 110.52 | 101.50 |
| 78 | CA | 1583 | A | N9-C1'-C2' | 11.27 | 128.65 | 114.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2509 | U | O3'-P-O5' | -11.26 | 82.60 | 104.00 |
| 81 | DA | 218 | G | O4'-C1'-N9 | 11.26 | 117.21 | 108.20 |
| 81 | DA | 1339 | C | P-O5'-C5' | 11.26 | 138.91 | 120.90 |
| 81 | DA | 299 | G | P-O5'-C5' | 11.25 | 138.91 | 120.90 |
| 81 | DA | 2014 | U | O4'-C1'-N1 | 11.25 | 117.20 | 108.20 |
| 78 | CA | 826 | U | C1'-O4'-C4' | -11.25 | 100.90 | 109.90 |
| 69 | Br | 104 | LEU | O-C-N | -11.25 | 104.70 | 122.70 |
| 78 | CA | 579 | A | N1-C6-N6 | 11.24 | 125.35 | 118.60 |
| 4 | AD | 153 | ASN | CB-CA-C | -11.24 | 87.92 | 110.40 |
| 78 | CA | 1130 | G | O4'-C1'-N9 | 11.24 | 117.19 | 108.20 |
| 78 | CA | 1582 | U | O4'-C1'-N1 | 11.24 | 117.19 | 108.20 |
| 81 | DA | 2439 | A | C3'-C2'-C1' | 11.24 | 110.49 | 101.50 |
| 78 | CA | 824 | G | O4'-C1'-N9 | 11.23 | 117.18 | 108.20 |
| 29 | AU | 62 | THR | CA-C-N | 11.23 | 141.90 | 117.20 |
| 78 | CA | 44 | U | P-O3'-C3' | 11.23 | 133.17 | 119.70 |
| 24 | AX | 32 | PHE | CB-CG-CD2 | -11.22 | 112.94 | 120.80 |
| 31 | BB | 84 | THR | C-N-CA | 11.22 | 145.87 | 122.30 |
| 81 | DA | 638 | C | O4'-C1'-N1 | 11.22 | 117.18 | 108.20 |
| 81 | DA | 1540 | U | O4'-C1'-N1 | 11.22 | 117.18 | 108.20 |
| 81 | DA | 3056 | U | C3'-C2'-C1' | 11.22 | 110.48 | 101.50 |
| 81 | DA | 3104 | U | O4'-C1'-N1 | 11.22 | 117.18 | 108.20 |
| 32 | BC | 137 | TYR | CB-CG-CD2 | -11.22 | 114.27 | 121.00 |
| 78 | CA | 45 | U | O4'-C1'-C2' | -11.21 | 94.59 | 105.80 |
| 78 | CA | 1106 | U | O4'-C1'-N1 | 11.21 | 117.17 | 108.20 |
| 81 | DA | 1316 | C | C3'-C2'-C1' | 11.21 | 110.47 | 101.50 |
| 81 | DA | 1869 | C | O3'-P-O5' | 11.21 | 125.29 | 104.00 |
| 81 | DA | 594 | U | O4'-C1'-C2' | -11.20 | 94.60 | 105.80 |
| 78 | CA | 1208 | A | O4'-C1'-N9 | 11.20 | 117.16 | 108.20 |
| 81 | DA | 1535 | A | C1'-O4'-C4' | 11.20 | 118.86 | 109.90 |
| 81 | DA | 2466 | G | N9-C1'-C2' | 11.20 | 128.56 | 114.00 |
| 78 | CA | 528 | U | P-O3'-C3' | 11.20 | 133.14 | 119.70 |
| 81 | DA | 604 | G | O4'-C1'-N9 | 11.20 | 117.16 | 108.20 |
| 81 | DA | 3214 | U | O4'-C1'-N1 | 11.20 | 117.16 | 108.20 |
| 81 | DA | 1756 | C | O4'-C1'-N1 | 11.19 | 117.15 | 108.20 |
| 81 | DA | 2375 | G | O4'-C1'-C2' | -11.19 | 94.61 | 105.80 |
| 81 | DA | 3050 | U | N1-C1'-C2' | 11.19 | 128.55 | 114.00 |
| 78 | CA | 652 | G | C1'-O4'-C4' | -11.19 | 100.95 | 109.90 |
| 78 | CA | 1221 | A | P-O5'-C5' | 11.19 | 138.80 | 120.90 |
| 81 | DA | 3334 | U | P-O3'-C3' | 11.18 | 133.12 | 119.70 |
| 53 | Ba | 16 | GLY | O-C-N | -11.18 | 104.81 | 122.70 |
| 81 | DA | 3313 | U | C5'-C4'-C3' | -11.18 | 98.12 | 116.00 |
| 81 | DA | 3334 | U | N1-C1'-C2' | -11.16 | 99.49 | 114.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 786 | A | N9-C1'-C2' | -11.16 | 99.49 | 114.00 |
| 81 | DA | 24 | G | O4'-C1'-N9 | 11.16 | 117.12 | 108.20 |
| 78 | CA | 1578 | U | O4'-C1'-N1 | 11.15 | 117.12 | 108.20 |
| 78 | CA | 856 | A | C1'-O4'-C4' | 11.15 | 118.82 | 109.90 |
| 78 | CA | 1069 | A | N1-C6-N6 | 11.15 | 125.29 | 118.60 |
| 81 | DA | 409 | A | O4'-C1'-C2' | -11.15 | 94.65 | 105.80 |
| 49 | BV | 139 | TYR | CB-CG-CD2 | -11.14 | 114.31 | 121.00 |
| 81 | DA | 1409 | G | O3'-P-O5' | -11.14 | 82.83 | 104.00 |
| 81 | DA | 2887 | A | N9-C1'-C2' | 11.14 | 128.48 | 114.00 |
| 78 | CA | 284 | G | O4'-C1'-N9 | 11.14 | 117.11 | 108.20 |
| 40 | BK | 64 | PHE | CB-CG-CD1 | -11.14 | 113.00 | 120.80 |
| 81 | DA | 1338 | C | C3'-C2'-C1' | 11.14 | 110.41 | 101.50 |
| 14 | AM | 88 | ARG | NE-CZ-NH2 | 11.13 | 125.87 | 120.30 |
| 81 | DA | 3219 | G | O4'-C1'-N9 | 11.13 | 117.11 | 108.20 |
| 83 | DC | 2 | G | O4'-C1'-C2' | -11.13 | 94.67 | 105.80 |
| 81 | DA | 1178 | G | C3'-C2'-C1' | 11.13 | 110.40 | 101.50 |
| 78 | CA | 194 | U | O4'-C1'-N1 | 11.13 | 117.10 | 108.20 |
| 78 | CA | 628 | G | P-O3'-C3' | 11.12 | 133.05 | 119.70 |
| 78 | CA | 1642 | G | O4'-C1'-N9 | 11.12 | 117.10 | 108.20 |
| 78 | CA | 220 | A | P-O3'-C3' | 11.11 | 133.04 | 119.70 |
| 81 | DA | 1851 | G | P-O3'-C3' | 11.12 | 133.04 | 119.70 |
| 81 | DA | 1455 | U | P-O3'-C3' | 11.11 | 133.03 | 119.70 |
| 16 | AO | 112 | LYS | N-CA-CB | -11.11 | 90.61 | 110.60 |
| 38 | Bs | 61 | ARG | NE-CZ-NH1 | 11.11 | 125.85 | 120.30 |
| 78 | CA | 1394 | G | P-O3'-C3' | -11.11 | 106.37 | 119.70 |
| 81 | DA | 2041 | U | N1-C1'-C2' | -11.11 | 99.56 | 114.00 |
| 81 | DA | 2830 | G | P-O3'-C3' | 11.11 | 133.03 | 119.70 |
| 78 | CA | 1547 | A | O5'-P-OP2 | 11.10 | 124.02 | 110.70 |
| 81 | DA | 560 | G | N9-C1'-C2' | -11.10 | 99.57 | 114.00 |
| 78 | CA | 25 | C | P-O3'-C3' | 11.10 | 133.02 | 119.70 |
| 78 | CA | 659 | C | P-O3'-C3' | -11.10 | 106.38 | 119.70 |
| 81 | DA | 298 | U | N1-C1'-C2' | 11.10 | 128.43 | 114.00 |
| 78 | CA | 1301 | U | O3'-P-O5' | -11.10 | 82.92 | 104.00 |
| 81 | DA | 839 | C | P-O3'-C3' | 11.10 | 133.01 | 119.70 |
| 81 | DA | 3042 | U | O5'-P-OP2 | 11.09 | 124.01 | 110.70 |
| 83 | DC | 31 | U | P-O3'-C3' | 11.09 | 133.01 | 119.70 |
| 78 | CA | 1392 | U | O4'-C1'-N1 | 11.09 | 117.07 | 108.20 |
| 78 | CA | 172 | C | N1-C1'-C2' | 11.09 | 128.42 | 114.00 |
| 78 | CA | 1584 | G | C1'-O4'-C4' | -11.09 | 101.03 | 109.90 |
| 81 | DA | 1609 | C | C3'-C2'-C1' | 11.09 | 110.37 | 101.50 |
| 78 | CA | 296 | U | C3'-C2'-C1' | 11.08 | 110.37 | 101.50 |
| 78 | CA | 1187 | U | O4'-C1'-N1 | 11.08 | 117.07 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 316 | U | P-O3'-C3' | 11.08 | 133.00 | 119.70 |
| 81 | DA | 1275 | C | O4'-C1'-N1 | 11.08 | 117.07 | 108.20 |
| 78 | CA | 514 | G | O5'-P-OP2 | -11.08 | 95.73 | 105.70 |
| 81 | DA | 773 | G | O4'-C1'-N9 | 11.08 | 117.06 | 108.20 |
| 81 | DA | 265 | A | O4'-C1'-N9 | 11.08 | 117.06 | 108.20 |
| 81 | DA | 337 | G | N9-C1'-C2' | -11.08 | 99.60 | 114.00 |
| 78 | CA | 15 | U | N1-C1'-C2' | 11.08 | 128.40 | 114.00 |
| 35 | BG | 100 | LYS | N-CA-CB | -11.08 | 90.66 | 110.60 |
| 78 | CA | 489 | C | P-O3'-C3' | 11.08 | 132.99 | 119.70 |
| 78 | CA | 1530 | C | P-O3'-C3' | 11.08 | 132.99 | 119.70 |
| 42 | BM | 128 | ARG | NE-CZ-NH1 | -11.07 | 114.76 | 120.30 |
| 78 | CA | 580 | A | N1-C6-N6 | 11.07 | 125.25 | 118.60 |
| 81 | DA | 986 | U | O4'-C1'-N1 | 11.07 | 117.06 | 108.20 |
| 81 | DA | 2994 | A | O4'-C1'-N9 | 11.07 | 117.06 | 108.20 |
| 78 | CA | 650 | U | N1-C1'-C2' | -11.07 | 99.61 | 114.00 |
| 78 | CA | 1375 | A | C3'-C2'-C1' | 11.07 | 110.36 | 101.50 |
| 81 | DA | 2000 | U | O4'-C1'-N1 | 11.07 | 117.06 | 108.20 |
| 81 | DA | 635 | G | C5'-C4'-C3' | -11.07 | 98.28 | 116.00 |
| 81 | DA | 673 | U | P-O5'-C5' | 11.07 | 138.61 | 120.90 |
| 29 | AU | 36 | SER | CA-C-O | -11.06 | 96.86 | 120.10 |
| 81 | DA | 834 | U | O4'-C1'-N1 | 11.06 | 117.05 | 108.20 |
| 81 | DA | 681 | U | N1-C1'-C2' | 11.06 | 128.38 | 114.00 |
| 78 | CA | 309 | C | O4'-C1'-N1 | 11.06 | 117.05 | 108.20 |
| 4 | AD | 239 | PRO | CB-CA-C | 11.05 | 139.64 | 112.00 |
| 76 | BS | 46 | PHE | CB-CG-CD2 | 11.05 | 128.54 | 120.80 |
| 81 | DA | 1508 | C | C3'-C2'-C1' | 11.05 | 110.34 | 101.50 |
| 81 | DA | 2136 | C | N1-C1'-C2' | 11.05 | 128.37 | 114.00 |
| 81 | DA | 1692 | U | O4'-C1'-N1 | 11.05 | 117.04 | 108.20 |
| 79 | CB | 50 | G | O4'-C1'-N9 | 11.05 | 117.04 | 108.20 |
| 81 | DA | 1081 | U | O4'-C1'-N1 | 11.05 | 117.04 | 108.20 |
| 81 | DA | 2720 | G | P-O3'-C3' | 11.05 | 132.96 | 119.70 |
| 81 | DA | 3217 | C | C1'-O4'-C4' | 11.05 | 118.74 | 109.90 |
| 29 | AU | 72 | PHE | CB-CG-CD1 | 11.04 | 128.53 | 120.80 |
| 81 | DA | 1280 | C | O4'-C1'-N1 | 11.04 | 117.04 | 108.20 |
| 44 | BO | 73 | LEU | CA-C-N | 11.04 | 141.49 | 117.20 |
| 78 | CA | 894 | U | C1'-O4'-C4' | 11.04 | 118.73 | 109.90 |
| 3 | AB | 212 | LYS | CA-C-N | 11.04 | 141.48 | 117.20 |
| 78 | CA | 1337 | A | C1'-O4'-C4' | 11.04 | 118.73 | 109.90 |
| 81 | DA | 571 | U | N1-C1'-C2' | 11.04 | 128.35 | 114.00 |
| 78 | CA | 1375 | A | N9-C1'-C2' | 11.03 | 128.34 | 114.00 |
| 81 | DA | 516 | A | C3'-C2'-C1' | 11.04 | 110.33 | 101.50 |
| 78 | CA | 1613 | U | N1-C1'-C2' | -11.03 | 99.66 | 114.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2089 | A | P-O3'-C3' | 11.02 | 132.93 | 119.70 |
| 81 | DA | 2760 | C | C3'-C2'-C1' | 11.02 | 110.32 | 101.50 |
| 81 | DA | 740 | G | C5-C6-O6 | -11.02 | 121.99 | 128.60 |
| 78 | CA | 178 | U | O4'-C1'-N1 | 11.02 | 117.01 | 108.20 |
| 81 | DA | 2607 | G | N9-C1'-C2' | 11.02 | 128.32 | 114.00 |
| 12 | AK | 60 | ALA | N-CA-CB | 11.02 | 125.52 | 110.10 |
| 81 | DA | 1914 | G | N9-C1'-C2' | 11.01 | 128.32 | 114.00 |
| 81 | DA | 2578 | U | O4'-C1'-N1 | 11.01 | 117.01 | 108.20 |
| 81 | DA | 3167 | A | P-O5'-C5' | 11.01 | 138.52 | 120.90 |
| 82 | DB | 106 | C | C3'-C2'-C1' | 11.01 | 110.31 | 101.50 |
| 81 | DA | 3212 | C | P-O3'-C3' | -11.01 | 106.49 | 119.70 |
| 6 | AE | 24 | ARG | NE-CZ-NH2 | 11.01 | 125.81 | 120.30 |
| 81 | DA | 1320 | C | O4'-C1'-N1 | 11.01 | 117.01 | 108.20 |
| 81 | DA | 3243 | A | P-O5'-C5' | 11.01 | 138.51 | 120.90 |
| 81 | DA | 1005 | G | N9-C1'-C2' | -11.01 | 99.69 | 114.00 |
| 78 | CA | 588 | U | P-O3'-C3' | 11.00 | 132.90 | 119.70 |
| 78 | CA | 1767 | G | P-O3'-C3' | 11.00 | 132.90 | 119.70 |
| 78 | CA | 490 | C | P-O3'-C3' | 11.00 | 132.90 | 119.70 |
| 81 | DA | 1884 | A | C5'-C4'-O4' | -10.99 | 95.91 | 109.10 |
| 81 | DA | 2392 | C | O3'-P-O5' | -10.99 | 83.12 | 104.00 |
| 81 | DA | 3255 | U | N1-C1'-C2' | 10.99 | 128.29 | 114.00 |
| 81 | DA | 572 | A | O4'-C1'-N9 | 10.99 | 116.99 | 108.20 |
| 81 | DA | 2677 | G | O4'-C1'-N9 | 10.99 | 116.99 | 108.20 |
| 81 | DA | 2049 | A | O4'-C1'-C2' | -10.98 | 94.82 | 105.80 |
| 81 | DA | 255 | A | N9-C1'-C2' | -10.98 | 99.72 | 114.00 |
| 81 | DA | 1110 | U | O4'-C1'-N1 | 10.98 | 116.98 | 108.20 |
| 81 | DA | 2408 | U | N1-C1'-C2' | 10.98 | 128.28 | 114.00 |
| 78 | CA | 1065 | A | N1-C6-N6 | 10.98 | 125.19 | 118.60 |
| 13 | AL | 10 | ASN | O-C-N | -10.98 | 105.14 | 122.70 |
| 79 | CB | 71 | A | P-O3'-C3' | 10.98 | 132.87 | 119.70 |
| 81 | DA | 1652 | G | P-O3'-C3' | 10.98 | 132.87 | 119.70 |
| 78 | CA | 629 | U | P-O3'-C3' | 10.97 | 132.87 | 119.70 |
| 81 | DA | 2208 | A | N9-C1'-C2' | -10.97 | 99.73 | 114.00 |
| 81 | DA | 2253 | G | O4'-C1'-N9 | 10.97 | 116.98 | 108.20 |
| 78 | CA | 486 | G | N1-C6-O6 | 10.97 | 126.48 | 119.90 |
| 81 | DA | 2917 | G | C3'-C2'-C1' | -10.97 | 92.72 | 101.50 |
| 81 | DA | 303 | G | O4'-C1'-N9 | 10.97 | 116.98 | 108.20 |
| 78 | CA | 1735 | U | C3'-C2'-C1' | 10.97 | 110.27 | 101.50 |
| 83 | DC | 48 | U | OP1-P-O3' | -10.97 | 81.07 | 105.20 |
| 47 | BU | 139 | ARG | C-N-CA | 10.96 | 149.11 | 121.70 |
| 78 | CA | 1768 | G | P-O5'-C5' | 10.96 | 138.44 | 120.90 |
| 43 | BP | 13 | LYS | CB-CA-C | 10.96 | 132.31 | 110.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 1794 | A | O4'-C1'-C2' | -10.96 | 94.84 | 105.80 |
| 81 | DA | 2444 | C | P-O3'-C3' | -10.96 | 106.55 | 119.70 |
| 38 | Bs | 55 | LYS | CA-CB-CG | 10.95 | 137.49 | 113.40 |
| 81 | DA | 2303 | A | C5'-C4'-C3' | 10.95 | 133.52 | 116.00 |
| 81 | DA | 3336 | A | O4'-C1'-N9 | 10.95 | 116.96 | 108.20 |
| 82 | DB | 69 | U | P-O3'-C3' | 10.95 | 132.84 | 119.70 |
| 83 | DC | 72 | C | O4'-C1'-N1 | 10.95 | 116.96 | 108.20 |
| 79 | CB | 36 | C | N1-C1'-C2' | 10.95 | 128.23 | 114.00 |
| 81 | DA | 369 | A | P-O3'-C3' | 10.95 | 132.84 | 119.70 |
| 81 | DA | 1297 | C | O4'-C1'-C2' | -10.95 | 94.85 | 105.80 |
| 24 | AX | 32 | PHE | CB-CG-CD1 | 10.94 | 128.46 | 120.80 |
| 57 | Be | 98 | LYS | CA-C-O | 10.94 | 143.08 | 120.10 |
| 11 | AJ | 85 | ARG | NE-CZ-NH2 | 10.94 | 125.77 | 120.30 |
| 81 | DA | 852 | U | O4'-C1'-N1 | 10.94 | 116.95 | 108.20 |
| 81 | DA | 2440 | G | N9-C1'-C2' | 10.94 | 128.22 | 114.00 |
| 81 | DA | 2705 | A | N9-C1'-C2' | -10.94 | 99.78 | 114.00 |
| 78 | CA | 510 | G | P-O3'-C3' | 10.94 | 132.82 | 119.70 |
| 81 | DA | 1990 | U | C3'-C2'-C1' | 10.94 | 110.25 | 101.50 |
| 81 | DA | 2487 | U | O4'-C1'-N1 | 10.94 | 116.95 | 108.20 |
| 78 | CA | 46 | A | P-O5'-C5' | 10.93 | 138.39 | 120.90 |
| 81 | DA | 1123 | U | O4'-C1'-N1 | 10.93 | 116.95 | 108.20 |
| 81 | DA | 1819 | U | P-O3'-C3' | 10.93 | 132.82 | 119.70 |
| 81 | DA | 3374 | U | N1-C1'-C2' | 10.93 | 128.21 | 114.00 |
| 83 | DC | 49 | G | O4'-C1'-N9 | -10.93 | 99.45 | 108.20 |
| 78 | CA | 1379 | C | P-O3'-C3' | -10.93 | 106.59 | 119.70 |
| 81 | DA | 3242 | G | C1'-O4'-C4' | 10.93 | 118.64 | 109.90 |
| 81 | DA | 1506 | A | C1'-O4'-C4' | 10.92 | 118.64 | 109.90 |
| 78 | CA | 1220 | C | O4'-C1'-N1 | 10.92 | 116.94 | 108.20 |
| 81 | DA | 1257 | C | P-O3'-C3' | 10.92 | 132.80 | 119.70 |
| 2 | AA | 66 | ALA | CB-CA-C | -10.92 | 93.72 | 110.10 |
| 81 | DA | 3306 | U | O4'-C1'-N1 | 10.92 | 116.93 | 108.20 |
| 78 | CA | 580 | A | P-O3'-C3' | 10.91 | 132.80 | 119.70 |
| 81 | DA | 1895 | A | C1'-O4'-C4' | 10.91 | 118.63 | 109.90 |
| 81 | DA | 1686 | U | C1'-O4'-C4' | 10.91 | 118.63 | 109.90 |
| 81 | DA | 311 | C | C5'-C4'-O4' | -10.91 | 96.01 | 109.10 |
| 78 | CA | 1477 | G | O5'-P-OP1 | 10.91 | 123.79 | 110.70 |
| 78 | CA | 92 | A | C5'-C4'-C3' | 10.90 | 133.44 | 116.00 |
| 81 | DA | 492 | U | O4'-C1'-N1 | 10.90 | 116.92 | 108.20 |
| 81 | DA | 2561 | A | O5'-P-OP2 | -10.90 | 95.89 | 105.70 |
| 78 | CA | 1079 | U | O4'-C1'-N1 | 10.89 | 116.91 | 108.20 |
| 81 | DA | 419 | G | N9-C1'-C2' | -10.89 | 99.85 | 114.00 |
| 81 | DA | 1285 | G | O4'-C1'-C2' | -10.89 | 94.91 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1895 | A | N9-C1'-C2' | -10.88 | 99.85 | 114.00 |
| 78 | CA | 1305 | U | O3'-P-O5' | 10.88 | 124.67 | 104.00 |
| 81 | DA | 1 | G | N9-C1'-C2' | -10.88 | 99.86 | 114.00 |
| 81 | DA | 2705 | A | O4'-C1'-N9 | 10.88 | 116.90 | 108.20 |
| 44 | BO | 58 | MET | N-CA-CB | 10.88 | 130.18 | 110.60 |
| 82 | DB | 105 | A | N9-C1'-C2' | 10.88 | 128.14 | 114.00 |
| 81 | DA | 983 | A | N9-C1'-C2' | -10.88 | 99.86 | 114.00 |
| 81 | DA | 2500 | A | O4'-C1'-N9 | 10.87 | 116.90 | 108.20 |
| 78 | CA | 1737 | G | O4'-C1'-N9 | 10.87 | 116.90 | 108.20 |
| 81 | DA | 1583 | A | P-O3'-C3' | 10.87 | 132.75 | 119.70 |
| 83 | DC | 14 | U | C3'-C2'-C1' | 10.87 | 110.20 | 101.50 |
| 78 | CA | 1643 | U | O4'-C1'-N1 | 10.87 | 116.90 | 108.20 |
| 78 | CA | 660 | G | O4'-C1'-N9 | 10.86 | 116.89 | 108.20 |
| 78 | CA | 1658 | G | P-O3'-C3' | 10.87 | 132.74 | 119.70 |
| 40 | BK | 63 | ALA | CB-CA-C | -10.86 | 93.81 | 110.10 |
| 81 | DA | 1050 | U | O4'-C1'-N1 | 10.86 | 116.89 | 108.20 |
| 81 | DA | 1331 | U | O4'-C1'-N1 | -10.86 | 99.51 | 108.20 |
| 81 | DA | 3355 | U | O4'-C1'-C2' | -10.86 | 94.94 | 105.80 |
| 78 | CA | 123 | G | N9-C1'-C2' | 10.86 | 128.11 | 114.00 |
| 81 | DA | 1319 | G | O4'-C1'-C2' | 10.86 | 117.37 | 107.60 |
| 83 | DC | 2 | G | C1'-O4'-C4' | 10.86 | 118.58 | 109.90 |
| 81 | DA | 1627 | U | O4'-C1'-C2' | -10.85 | 94.95 | 105.80 |
| 81 | DA | 574 | U | O4'-C1'-N1 | 10.85 | 116.88 | 108.20 |
| 81 | DA | 1277 | C | C1'-O4'-C4' | -10.85 | 101.22 | 109.90 |
| 83 | DC | 23 | A | P-O3'-C3' | 10.85 | 132.72 | 119.70 |
| 4 | AD | 235 | TYR | CB-CG-CD1 | -10.85 | 114.49 | 121.00 |
| 81 | DA | 598 | A | C4'-C3'-C2' | -10.85 | 91.75 | 102.60 |
| 76 | BS | 159 | ARG | NE-CZ-NH1 | 10.85 | 125.72 | 120.30 |
| 78 | CA | 1562 | G | C1'-O4'-C4' | 10.85 | 118.58 | 109.90 |
| 78 | CA | 435 | C | N1-C1'-C2' | 10.84 | 128.10 | 114.00 |
| 78 | CA | 346 | G | N9-C1'-C2' | 10.84 | 128.09 | 114.00 |
| 81 | DA | 1487 | G | O4'-C1'-N9 | 10.84 | 116.87 | 108.20 |
| 81 | DA | 277 | G | O4'-C1'-N9 | 10.84 | 116.87 | 108.20 |
| 81 | DA | 3108 | G | P-O3'-C3' | 10.84 | 132.71 | 119.70 |
| 81 | DA | 2319 | U | C3'-C2'-C1' | -10.84 | 92.83 | 101.50 |
| 16 | AO | 65 | VAL | CB-CA-C | -10.83 | 90.82 | 111.40 |
| 81 | DA | 2203 | U | O4'-C1'-N1 | 10.83 | 116.86 | 108.20 |
| 81 | DA | 2513 | U | O4'-C1'-N1 | 10.83 | 116.86 | 108.20 |
| 81 | DA | 551 | A | O4'-C1'-N9 | 10.83 | 116.86 | 108.20 |
| 81 | DA | 594 | U | C3'-C2'-C1' | 10.83 | 110.16 | 101.50 |
| 81 | DA | 1699 | A | O4'-C1'-C2' | -10.82 | 94.98 | 105.80 |
| 81 | DA | 2466 | G | C1'-O4'-C4' | -10.82 | 101.24 | 109.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 460 | A | P-O3'-C3' | 10.82 | 132.68 | 119.70 |
| 81 | DA | 1170 | A | P-O3'-C3' | 10.82 | 132.68 | 119.70 |
| 82 | DB | 126 | A | O4'-C1'-N9 | 10.82 | 116.85 | 108.20 |
| 81 | DA | 524 | U | O4'-C1'-N1 | 10.81 | 116.85 | 108.20 |
| 78 | CA | 16 | G | C1'-O4'-C4' | 10.81 | 118.55 | 109.90 |
| 79 | CB | 42 | C | P-O3'-C3' | 10.81 | 132.68 | 119.70 |
| 78 | CA | 1548 | G | O4'-C1'-C2' | 10.81 | 117.33 | 107.60 |
| 32 | BC | 379 | PHE | CB-CG-CD1 | -10.81 | 113.23 | 120.80 |
| 78 | CA | 1264 | G | O4'-C1'-N9 | 10.81 | 116.85 | 108.20 |
| 78 | CA | 1611 | A | N9-C1'-C2' | -10.81 | 99.95 | 114.00 |
| 81 | DA | 553 | U | O4'-C1'-N1 | 10.81 | 116.85 | 108.20 |
| 81 | DA | 1847 | A | N9-C1'-C2' | -10.81 | 99.95 | 114.00 |
| 81 | DA | 1890 | U | O4'-C1'-N1 | 10.81 | 116.84 | 108.20 |
| 81 | DA | 1572 | U | P-O3'-C3' | 10.80 | 132.67 | 119.70 |
| 81 | DA | 3018 | C | O3'-P-O5' | -10.80 | 83.47 | 104.00 |
| 38 | Bs | 242 | ASN | CB-CG-OD1 | 10.80 | 143.20 | 121.60 |
| 81 | DA | 1870 | C | C4'-C3'-O3' | 10.80 | 134.60 | 113.00 |
| 5 | AC | 168 | ARG | O-C-N | -10.80 | 100.58 | 121.10 |
| 49 | BV | 152 | GLU | O-C-N | -10.80 | 105.42 | 122.70 |
| 81 | DA | 1861 | G | O4'-C1'-N9 | 10.80 | 116.84 | 108.20 |
| 81 | DA | 1562 | C | P-O3'-C3' | 10.80 | 132.66 | 119.70 |
| 81 | DA | 1526 | U | P-O3'-C3' | 10.80 | 132.66 | 119.70 |
| 22 | AV | 104 | ALA | N-CA-CB | 10.79 | 125.21 | 110.10 |
| 81 | DA | 420 | G | O4'-C1'-N9 | 10.79 | 116.83 | 108.20 |
| 5 | AC | 149 | ARG | NE-CZ-NH1 | 10.79 | 125.69 | 120.30 |
| 81 | DA | 596 | C | P-O3'-C3' | 10.79 | 132.65 | 119.70 |
| 81 | DA | 1078 | U | C1'-O4'-C4' | 10.79 | 118.53 | 109.90 |
| 81 | DA | 1459 | C | O4'-C1'-N1 | 10.79 | 116.83 | 108.20 |
| 17 | AQ | 47 | ARG | NE-CZ-NH2 | -10.79 | 114.91 | 120.30 |
| 81 | DA | 2138 | A | O4'-C1'-N9 | 10.78 | 116.83 | 108.20 |
| 83 | DC | 25 | G | N9-C1'-C2' | -10.78 | 99.98 | 114.00 |
| 83 | DC | 115 | A | N9-C1'-C2' | -10.79 | 99.98 | 114.00 |
| 78 | CA | 1394 | G | N9-C1'-C2' | -10.78 | 99.98 | 114.00 |
| 81 | DA | 764 | U | O4'-C1'-N1 | 10.78 | 116.83 | 108.20 |
| 78 | CA | 1141 | G | N9-C1'-C2' | 10.78 | 128.01 | 114.00 |
| 81 | DA | 1585 | C | N1-C1'-C2' | 10.78 | 128.01 | 114.00 |
| 81 | DA | 2688 | U | O4'-C1'-N1 | 10.78 | 116.82 | 108.20 |
| 81 | DA | 1257 | C | C4'-C3'-C2' | -10.78 | 91.82 | 102.60 |
| 81 | DA | 1314 | C | N1-C1'-C2' | 10.78 | 128.01 | 114.00 |
| 81 | DA | 2717 | U | P-O3'-C3' | 10.77 | 132.63 | 119.70 |
| 81 | DA | 1319 | G | P-O3'-C3' | 10.77 | 132.62 | 119.70 |
| 81 | DA | 1681 | U | P-O5'-C5' | 10.77 | 138.13 | 120.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 1340 | U | N1-C1'-C2' | -10.77 | 100.00 | 114.00 |
| 78 | CA | 1548 | G | P-O3'-C3' | 10.77 | 132.62 | 119.70 |
| 5 | AC | 53 | ARG | NE-CZ-NH2 | -10.76 | 114.92 | 120.30 |
| 78 | CA | 1580 | C | O4'-C1'-N1 | -10.76 | 99.59 | 108.20 |
| 81 | DA | 2467 | G | P-O3'-C3' | 10.76 | 132.61 | 119.70 |
| 81 | DA | 588 | G | P-O3'-C3' | 10.75 | 132.60 | 119.70 |
| 78 | CA | 1466 | G | P-O3'-C3' | 10.75 | 132.60 | 119.70 |
| 79 | CB | 58 | U | O4'-C1'-N1 | 10.75 | 116.80 | 108.20 |
| 82 | DB | 62 | C | N1-C1'-C2' | 10.75 | 127.98 | 114.00 |
| 44 | BO | 21 | ARG | O-C-N | -10.75 | 105.50 | 122.70 |
| 78 | CA | 369 | A | N9-C1'-C2' | -10.75 | 100.03 | 114.00 |
| 43 | BP | 178 | HIS | CA-CB-CG | 10.74 | 131.86 | 113.60 |
| 83 | DC | 60 | G | C3'-C2'-C1' | -10.74 | 92.90 | 101.50 |
| 43 | BP | 180 | PHE | CB-CG-CD2 | 10.74 | 128.32 | 120.80 |
| 81 | DA | 2898 | G | P-O3'-C3' | 10.74 | 132.59 | 119.70 |
| 78 | CA | 1441 | C | P-O3'-C3' | 10.74 | 132.59 | 119.70 |
| 78 | CA | 1506 | G | O4'-C1'-N9 | 10.74 | 116.79 | 108.20 |
| 78 | CA | 597 | G | P-O3'-C3' | 10.73 | 132.58 | 119.70 |
| 81 | DA | 3125 | U | P-O3'-C3' | 10.73 | 132.58 | 119.70 |
| 83 | DC | 29 | C | P-O5'-C5' | 10.73 | 138.07 | 120.90 |
| 81 | DA | 2141 | U | C3'-C2'-C1' | 10.73 | 110.08 | 101.50 |
| 81 | DA | 825 | U | O4'-C1'-N1 | 10.72 | 116.78 | 108.20 |
| 32 | BC | 345 | ASN | N-CA-CB | 10.72 | 129.90 | 110.60 |
| 43 | BP | 30 | TYR | CB-CG-CD1 | 10.72 | 127.43 | 121.00 |
| 61 | Bj | 73 | ARG | NE-CZ-NH2 | -10.72 | 114.94 | 120.30 |
| 78 | CA | 626 | U | O4'-C1'-N1 | 10.72 | 116.78 | 108.20 |
| 78 | CA | 1452 | U | O3'-P-O5' | -10.72 | 83.63 | 104.00 |
| 81 | DA | 9 | U | O3'-P-O5' | -10.72 | 83.63 | 104.00 |
| 81 | DA | 573 | C | P-O5'-C5' | 10.72 | 138.05 | 120.90 |
| 37 | BH | 80 | TYR | CB-CG-CD2 | 10.72 | 127.43 | 121.00 |
| 38 | Bs | 248 | ALA | N-CA-CB | -10.72 | 95.10 | 110.10 |
| 81 | DA | 1482 | A | P-O3'-C3' | 10.72 | 132.56 | 119.70 |
| 81 | DA | 2197 | C | O4'-C1'-N1 | -10.71 | 99.63 | 108.20 |
| 79 | CB | 56 | A | P-O5'-C5' | 10.71 | 138.04 | 120.90 |
| 78 | CA | 1347 | U | O4'-C1'-N1 | 10.71 | 116.77 | 108.20 |
| 78 | CA | 155 | U | N1-C1'-C2' | -10.71 | 100.08 | 114.00 |
| 78 | CA | 1452 | U | N1-C1'-C2' | 10.71 | 127.92 | 114.00 |
| 78 | CA | 1688 | U | O4'-C1'-N1 | 10.71 | 116.77 | 108.20 |
| 81 | DA | 1343 | A | O4'-C1'-N9 | 10.71 | 116.77 | 108.20 |
| 12 | AK | 123 | SER | N-CA-CB | 10.71 | 126.56 | 110.50 |
| 81 | DA | 512 | U | C3'-C2'-C1' | 10.71 | 110.06 | 101.50 |
| 81 | DA | 1755 | C | O3'-P-O5' | -10.71 | 83.66 | 104.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 3107 | U | C1'-O4'-C4' | 10.71 | 118.46 | 109.90 |
| 35 | BG | 25 | ALA | CB-CA-C | -10.70 | 94.05 | 110.10 |
| 78 | CA | 10 | G | C5'-C4'-C3' | -10.70 | 98.88 | 116.00 |
| 4 | AD | 219 | VAL | CB-CA-C | 10.70 | 131.73 | 111.40 |
| 78 | CA | 116 | U | P-O3'-C3' | -10.70 | 106.86 | 119.70 |
| 81 | DA | 1732 | U | O4'-C1'-N1 | 10.70 | 116.76 | 108.20 |
| 78 | CA | 926 | A | O4'-C1'-N9 | 10.69 | 116.75 | 108.20 |
| 81 | DA | 598 | A | O4'-C1'-N9 | 10.69 | 116.75 | 108.20 |
| 78 | CA | 1238 | A | C1'-O4'-C4' | 10.69 | 118.45 | 109.90 |
| 81 | DA | 1871 | U | C4'-C3'-O3' | 10.69 | 134.38 | 113.00 |
| 81 | DA | 2469 | G | P-O3'-C3' | 10.69 | 132.53 | 119.70 |
| 81 | DA | 3034 | C | P-O3'-C3' | 10.69 | 132.53 | 119.70 |
| 81 | DA | 665 | A | N9-C1'-C2' | 10.69 | 127.90 | 114.00 |
| 82 | DB | 16 | G | P-O3'-C3' | 10.69 | 132.53 | 119.70 |
| 81 | DA | 1792 | C | P-O3'-C3' | 10.69 | 132.53 | 119.70 |
| 13 | AL | 87 | VAL | CB-CA-C | 10.69 | 131.70 | 111.40 |
| 33 | BD | 89 | ALA | CB-CA-C | -10.68 | 94.08 | 110.10 |
| 32 | BC | 275 | ARG | NE-CZ-NH1 | 10.68 | 125.64 | 120.30 |
| 33 | BD | 310 | THR | CA-CB-CG2 | -10.68 | 97.44 | 112.40 |
| 78 | CA | 649 | U | O4'-C1'-N1 | 10.68 | 116.75 | 108.20 |
| 81 | DA | 362 | U | O4'-C1'-N1 | 10.68 | 116.75 | 108.20 |
| 81 | DA | 162 | G | C1'-O4'-C4' | 10.68 | 118.44 | 109.90 |
| 81 | DA | 1525 | G | P-O3'-C3' | 10.68 | 132.51 | 119.70 |
| 81 | DA | 2416 | U | P-O5'-C5' | 10.68 | 137.98 | 120.90 |
| 74 | BQ | 15 | ARG | NE-CZ-NH1 | -10.67 | 114.96 | 120.30 |
| 78 | CA | 429 | G | O4'-C1'-N9 | 10.67 | 116.74 | 108.20 |
| 81 | DA | 2487 | U | P-O5'-C5' | 10.67 | 137.98 | 120.90 |
| 78 | CA | 1736 | G | P-O3'-C3' | 10.67 | 132.51 | 119.70 |
| 78 | CA | 352 | A | O4'-C1'-N9 | 10.67 | 116.74 | 108.20 |
| 81 | DA | 1088 | U | O4'-C1'-N1 | 10.67 | 116.74 | 108.20 |
| 81 | DA | 821 | U | O4'-C1'-N1 | 10.67 | 116.73 | 108.20 |
| 78 | CA | 1677 | C | O5'-C5'-C4' | 10.67 | 131.97 | 111.70 |
| 81 | DA | 1624 | G | O4'-C1'-C2' | -10.67 | 95.13 | 105.80 |
| 81 | DA | 2281 | A | P-O3'-C3' | 10.67 | 132.50 | 119.70 |
| 81 | DA | 1439 | U | O4'-C1'-N1 | 10.66 | 116.73 | 108.20 |
| 81 | DA | 1627 | U | C1'-O4'-C4' | 10.66 | 118.43 | 109.90 |
| 12 | AK | 59 | ALA | N-CA-CB | 10.66 | 125.02 | 110.10 |
| 78 | CA | 689 | G | C1'-O4'-C4' | -10.65 | 101.38 | 109.90 |
| 79 | CB | 34 | G | N1-C6-O6 | 10.65 | 126.29 | 119.90 |
| 82 | DB | 98 | U | C5'-C4'-O4' | 10.65 | 121.88 | 109.10 |
| 42 | BM | 94 | TYR | CB-CG-CD1 | -10.65 | 114.61 | 121.00 |
| 78 | CA | 1357 | A | O4'-C1'-N9 | 10.65 | 116.72 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1317 | A | O4'-C1'-N9 | 10.65 | 116.72 | 108.20 |
| 81 | DA | 2763 | U | C1'-O4'-C4' | 10.65 | 118.42 | 109.90 |
| 81 | DA | 1296 | C | P-O5'-C5' | 10.65 | 137.94 | 120.90 |
| 32 | BC | 232 | ARG | NE-CZ-NH2 | -10.65 | 114.98 | 120.30 |
| 81 | DA | 220 | G | N9-C1'-C2' | -10.65 | 100.16 | 114.00 |
| 78 | CA | 874 | C | C3'-C2'-C1' | 10.64 | 110.01 | 101.50 |
| 81 | DA | 1338 | C | C5'-C4'-O4' | -10.64 | 96.33 | 109.10 |
| 78 | CA | 1725 | U | P-O5'-C5' | 10.64 | 137.92 | 120.90 |
| 81 | DA | 1001 | G | O4'-C1'-N9 | 10.64 | 116.71 | 108.20 |
| 81 | DA | 1215 | U | O4'-C1'-N1 | 10.64 | 116.71 | 108.20 |
| 81 | DA | 2340 | U | O4'-C1'-N1 | 10.64 | 116.71 | 108.20 |
| 82 | DB | 111 | A | O4'-C1'-N9 | 10.64 | 116.71 | 108.20 |
| 8 | AF | 185 | ARG | NE-CZ-NH1 | 10.63 | 125.62 | 120.30 |
| 60 | Bi | 67 | LYS | CD-CE-NZ | 10.63 | 136.16 | 111.70 |
| 81 | DA | 204 | A | O4'-C1'-N9 | 10.63 | 116.71 | 108.20 |
| 81 | DA | 604 | G | N9-C1'-C2' | -10.63 | 100.18 | 114.00 |
| 81 | DA | 2818 | U | N1-C1'-C2' | -10.63 | 100.18 | 114.00 |
| 34 | BE | 52 | TYR | C-N-CA | 10.63 | 148.27 | 121.70 |
| 60 | Bi | 79 | SER | N-CA-C | -10.63 | 82.30 | 111.00 |
| 81 | DA | 1775 | G | O4'-C1'-N9 | 10.63 | 116.70 | 108.20 |
| 81 | DA | 2963 | C | P-O3'-C3' | 10.63 | 132.46 | 119.70 |
| 81 | DA | 2487 | U | C1'-O4'-C4' | 10.63 | 118.40 | 109.90 |
| 17 | AQ | 59 | LYS | CB-CA-C | 10.62 | 131.65 | 110.40 |
| 17 | AQ | 67 | ARG | NE-CZ-NH1 | 10.62 | 125.61 | 120.30 |
| 81 | DA | 275 | U | P-O3'-C3' | -10.62 | 106.95 | 119.70 |
| 81 | DA | 1360 | C | P-O3'-C3' | 10.62 | 132.45 | 119.70 |
| 1 | Aa | 305 | TYR | CB-CG-CD1 | 10.62 | 127.37 | 121.00 |
| 83 | DC | 3 | U | C1'-O4'-C4' | 10.62 | 118.40 | 109.90 |
| 81 | DA | 3003 | G | O4'-C1'-C2' | 10.62 | 117.16 | 107.60 |
| 21 | AT | 45 | ALA | N-CA-CB | 10.62 | 124.96 | 110.10 |
| 78 | CA | 1453 | G | P-O3'-C3' | 10.62 | 132.44 | 119.70 |
| 81 | DA | 1633 | C | O3'-P-O5' | -10.62 | 83.83 | 104.00 |
| 81 | DA | 1551 | C | C3'-C2'-C1' | 10.62 | 109.99 | 101.50 |
| 78 | CA | 1167 | G | O4'-C1'-N9 | 10.61 | 116.69 | 108.20 |
| 14 | AM | 12 | GLN | CA-C-N | 10.61 | 140.54 | 117.20 |
| 78 | CA | 1133 | A | N9-C1'-C2' | 10.61 | 127.79 | 114.00 |
| 40 | BK | 63 | ALA | N-CA-CB | -10.61 | 95.25 | 110.10 |
| 81 | DA | 832 | G | O4'-C1'-N9 | 10.61 | 116.69 | 108.20 |
| 81 | DA | 2789 | U | O4'-C1'-N1 | 10.61 | 116.69 | 108.20 |
| 13 | AL | 10 | ASN | CB-CA-C | 10.61 | 131.61 | 110.40 |
| 78 | CA | 305 | C | O4'-C1'-C2' | -10.61 | 95.19 | 105.80 |
| 83 | DC | 46 | A | O4'-C1'-N9 | 10.61 | 116.69 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2873 | U | C3'-C2'-C1' | 10.61 | 109.98 | 101.50 |
| 78 | CA | 1462 | G | P-O3'-C3' | 10.60 | 132.43 | 119.70 |
| 81 | DA | 74 | G | O4'-C1'-N9 | 10.60 | 116.68 | 108.20 |
| 78 | CA | 1544 | U | O4'-C1'-N1 | 10.60 | 116.68 | 108.20 |
| 81 | DA | 2208 | A | C1'-O4'-C4' | -10.60 | 101.42 | 109.90 |
| 78 | CA | 174 | U | C3'-C2'-C1' | 10.60 | 109.98 | 101.50 |
| 31 | BB | 66 | PRO | C-N-CA | 10.60 | 148.19 | 121.70 |
| 81 | DA | 2382 | G | O4'-C1'-N9 | 10.59 | 116.67 | 108.20 |
| 40 | BK | 101 | ARG | NE-CZ-NH2 | -10.59 | 115.01 | 120.30 |
| 78 | CA | 218 | A | O4'-C1'-C2' | 10.59 | 117.13 | 107.60 |
| 61 | Bj | 21 | ARG | CA-C-N | 10.58 | 140.48 | 117.20 |
| 81 | DA | 2699 | G | P-O5'-C5' | 10.58 | 137.84 | 120.90 |
| 55 | Bc | 41 | LEU | CD1-CG-CD2 | 10.58 | 142.24 | 110.50 |
| 79 | CB | 74 | C | P-O3'-C3' | 10.58 | 132.40 | 119.70 |
| 81 | DA | 1607 | U | P-O3'-C3' | 10.58 | 132.39 | 119.70 |
| 81 | DA | 2827 | U | N1-C1'-C2' | -10.58 | 100.25 | 114.00 |
| 83 | DC | 4 | U | O4'-C1'-N1 | 10.58 | 116.66 | 108.20 |
| 78 | CA | 1295 | G | O4'-C1'-N9 | 10.58 | 116.66 | 108.20 |
| 81 | DA | 577 | C | O4'-C1'-C2' | -10.57 | 95.22 | 105.80 |
| 81 | DA | 1842 | A | N9-C1'-C2' | -10.57 | 100.25 | 114.00 |
| 81 | DA | 1414 | G | C1'-O4'-C4' | 10.57 | 118.36 | 109.90 |
| 77 | BI | 106 | ALA | N-CA-C | 10.57 | 139.54 | 111.00 |
| 81 | DA | 1009 | A | O5'-C5'-C4' | 10.57 | 131.78 | 111.70 |
| 81 | DA | 3094 | A | N9-C1'-C2' | 10.57 | 127.74 | 114.00 |
| 13 | AL | 5 | LYS | O-C-N | -10.57 | 101.02 | 121.10 |
| 78 | CA | 306 | U | C3'-C2'-C1' | 10.57 | 109.95 | 101.50 |
| 81 | DA | 1576 | G | O4'-C1'-N9 | 10.56 | 116.65 | 108.20 |
| 81 | DA | 2759 | U | C5'-C4'-C3' | 10.56 | 132.90 | 116.00 |
| 81 | DA | 261 | U | C1'-O4'-C4' | -10.56 | 101.45 | 109.90 |
| 81 | DA | 388 | G | O4'-C1'-N9 | 10.56 | 116.65 | 108.20 |
| 81 | DA | 1411 | C | P-O3'-C3' | 10.56 | 132.37 | 119.70 |
| 81 | DA | 2514 | U | O4'-C1'-N1 | 10.56 | 116.65 | 108.20 |
| 81 | DA | 3049 | A | P-O3'-C3' | -10.56 | 107.03 | 119.70 |
| 78 | CA | 287 | G | N9-C1'-C2' | 10.56 | 127.73 | 114.00 |
| 78 | CA | 1066 | C | P-O5'-C5' | 10.56 | 137.79 | 120.90 |
| 81 | DA | 1970 | U | O4'-C1'-N1 | 10.56 | 116.65 | 108.20 |
| 78 | CA | 171 | A | P-O3'-C3' | 10.55 | 132.37 | 119.70 |
| 81 | DA | 741 | U | P-O3'-C3' | 10.55 | 132.37 | 119.70 |
| 4 | AD | 154 | ILE | N-CA-CB | 10.55 | 135.07 | 110.80 |
| 83 | DC | 75 | G | P-O3'-C3' | 10.55 | 132.36 | 119.70 |
| 81 | DA | 2567 | C | P-O3'-C3' | -10.55 | 107.04 | 119.70 |
| 74 | BQ | 136 | GLU | CA-C-N | -10.55 | 93.99 | 117.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1806 | A | P-O3'-C3' | 10.55 | 132.36 | 119.70 |
| 78 | CA | 1420 | C | O4'-C1'-C2' | -10.55 | 95.25 | 105.80 |
| 81 | DA | 1957 | G | O4'-C1'-N9 | 10.54 | 116.64 | 108.20 |
| 78 | CA | 650 | U | O4'-C1'-C2' | -10.54 | 95.26 | 105.80 |
| 4 | AD | 109 | PHE | CB-CG-CD2 | 10.54 | 128.18 | 120.80 |
| 78 | CA | 893 | U | O4'-C1'-N1 | 10.54 | 116.63 | 108.20 |
| 81 | DA | 969 | C | C1'-O4'-C4' | 10.54 | 118.33 | 109.90 |
| 4 | AD | 238 | LEU | CB-CA-C | -10.54 | 90.18 | 110.20 |
| 81 | DA | 3363 | U | O4'-C1'-C2' | -10.54 | 95.26 | 105.80 |
| 78 | CA | 871 | G | P-O3'-C3' | 10.54 | 132.34 | 119.70 |
| 81 | DA | 2563 | G | P-O3'-C3' | 10.54 | 132.34 | 119.70 |
| 78 | CA | 1023 | A | O4'-C1'-N9 | 10.53 | 116.62 | 108.20 |
| 82 | DB | 132 | G | N9-C1'-C2' | -10.53 | 100.31 | 114.00 |
| 31 | BB | 128 | ARG | NE-CZ-NH2 | 10.53 | 125.56 | 120.30 |
| 76 | BS | 6 | PHE | CB-CG-CD1 | 10.52 | 128.17 | 120.80 |
| 78 | CA | 307 | G | P-O3'-C3' | 10.52 | 132.33 | 119.70 |
| 81 | DA | 1575 | A | N9-C1'-C2' | -10.52 | 100.32 | 114.00 |
| 81 | DA | 1760 | A | N1-C6-N6 | 10.52 | 124.91 | 118.60 |
| 81 | DA | 1213 | G | O4'-C1'-N9 | 10.52 | 116.61 | 108.20 |
| 81 | DA | 1612 | A | O4'-C1'-N9 | 10.52 | 116.61 | 108.20 |
| 81 | DA | 3233 | C | P-O5'-C5' | 10.52 | 137.73 | 120.90 |
| 47 | BU | 136 | ARG | NE-CZ-NH2 | -10.51 | 115.04 | 120.30 |
| 81 | DA | 671 | U | C5'-C4'-C3' | 10.51 | 132.82 | 116.00 |
| 81 | DA | 1890 | U | P-O5'-C5' | 10.51 | 137.72 | 120.90 |
| 81 | DA | 2451 | G | P-O3'-C3' | 10.51 | 132.31 | 119.70 |
| 74 | BQ | 238 | ASP | N-CA-CB | 10.51 | 129.51 | 110.60 |
| 81 | DA | 1527 | C | O4'-C1'-N1 | 10.51 | 116.60 | 108.20 |
| 81 | DA | 3370 | A | P-O3'-C3' | 10.51 | 132.31 | 119.70 |
| 78 | CA | 374 | U | C3'-C2'-C1' | -10.50 | 93.10 | 101.50 |
| 81 | DA | 2228 | A | N9-C1'-C2' | -10.50 | 100.35 | 114.00 |
| 74 | BQ | 172 | TYR | CB-CG-CD2 | 10.50 | 127.30 | 121.00 |
| 81 | DA | 955 | U | O4'-C1'-N1 | 10.50 | 116.60 | 108.20 |
| 8 | AF | 112 | ARG | NE-CZ-NH2 | -10.50 | 115.05 | 120.30 |
| 78 | CA | 466 | U | O4'-C1'-N1 | 10.50 | 116.60 | 108.20 |
| 78 | CA | 496 | G | N1-C6-O6 | 10.50 | 126.20 | 119.90 |
| 81 | DA | 3253 | G | P-O5'-C5' | 10.50 | 137.70 | 120.90 |
| 32 | BC | 67 | PHE | CB-CG-CD2 | 10.50 | 128.15 | 120.80 |
| 78 | CA | 182 | A | O4'-C1'-N9 | 10.50 | 116.60 | 108.20 |
| 81 | DA | 1638 | A | O4'-C1'-N9 | 10.50 | 116.60 | 108.20 |
| 78 | CA | 482 | U | O4'-C1'-N1 | 10.50 | 116.60 | 108.20 |
| 81 | DA | 2303 | A | C1'-O4'-C4' | 10.50 | 118.30 | 109.90 |
| 81 | DA | 743 | C | N1-C1'-C2' | 10.49 | 127.64 | 114.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2118 | C | N1-C1'-C2' | 10.49 | 127.64 | 114.00 |
| 78 | CA | 1186 | U | O4'-C1'-N1 | 10.49 | 116.59 | 108.20 |
| 78 | CA | 1350 | U | P-O3'-C3' | 10.49 | 132.29 | 119.70 |
| 81 | DA | 1591 | G | C1'-O4'-C4' | -10.49 | 101.51 | 109.90 |
| 34 | BE | 61 | ARG | N-CA-C | 10.48 | 139.31 | 111.00 |
| 81 | DA | 1621 | A | O4'-C1'-N9 | 10.48 | 116.59 | 108.20 |
| 81 | DA | 3333 | G | O4'-C1'-C2' | 10.48 | 117.04 | 107.60 |
| 81 | DA | 556 | U | P-O3'-C3' | 10.48 | 132.28 | 119.70 |
| 81 | DA | 1341 | U | P-O3'-C3' | 10.48 | 132.27 | 119.70 |
| 6 | AE | 81 | MET | CB-CA-C | -10.48 | 89.45 | 110.40 |
| 81 | DA | 486 | U | O3'-P-O5' | 10.47 | 123.90 | 104.00 |
| 47 | BU | 140 | ILE | C-N-CA | -10.47 | 95.52 | 121.70 |
| 81 | DA | 1577 | G | O4'-C1'-N9 | 10.47 | 116.58 | 108.20 |
| 81 | DA | 2471 | U | O4'-C1'-N1 | 10.47 | 116.58 | 108.20 |
| 78 | CA | 231 | U | O4'-C1'-N1 | 10.47 | 116.58 | 108.20 |
| 81 | DA | 2393 | G | O4'-C1'-N9 | 10.46 | 116.57 | 108.20 |
| 12 | AK | 59 | ALA | CB-CA-C | -10.46 | 94.41 | 110.10 |
| 47 | BU | 126 | VAL | N-CA-C | 10.46 | 139.25 | 111.00 |
| 78 | CA | 54 | C | P-O5'-C5' | 10.46 | 137.64 | 120.90 |
| 81 | DA | 475 | G | P-O3'-C3' | 10.46 | 132.25 | 119.70 |
| 78 | CA | 874 | C | O4'-C1'-N1 | -10.46 | 99.83 | 108.20 |
| 81 | DA | 752 | C | N1-C1'-C2' | 10.46 | 127.60 | 114.00 |
| 81 | DA | 1888 | U | O4'-C1'-N1 | 10.46 | 116.57 | 108.20 |
| 69 | Br | 89 | LYS | CB-CA-C | 10.46 | 131.31 | 110.40 |
| 81 | DA | 2528 | G | N9-C1'-C2' | -10.46 | 100.41 | 114.00 |
| 81 | DA | 2254 | U | O4'-C1'-N1 | 10.45 | 116.56 | 108.20 |
| 78 | CA | 589 | C | N1-C1'-C2' | 10.45 | 127.59 | 114.00 |
| 81 | DA | 1542 | G | P-O3'-C3' | 10.45 | 132.24 | 119.70 |
| 83 | DC | 94 | A | P-O3'-C3' | 10.45 | 132.24 | 119.70 |
| 78 | CA | 267 | U | C3'-C2'-C1' | 10.45 | 109.86 | 101.50 |
| 78 | CA | 650 | U | O4'-C1'-N1 | 10.45 | 116.56 | 108.20 |
| 81 | DA | 672 | A | O5'-C5'-C4' | -10.45 | 91.85 | 111.70 |
| 81 | DA | 2376 | G | P-O5'-C5' | 10.45 | 137.62 | 120.90 |
| 81 | DA | 2612 | U | O4'-C1'-N1 | 10.45 | 116.56 | 108.20 |
| 44 | BO | 117 | ARG | NE-CZ-NH2 | -10.44 | 115.08 | 120.30 |
| 82 | DB | 132 | G | O4'-C1'-N9 | 10.44 | 116.55 | 108.20 |
| 81 | DA | 1624 | G | O4'-C1'-N9 | 10.44 | 116.55 | 108.20 |
| 82 | DB | 52 | A | O4'-C1'-C2' | -10.44 | 95.36 | 105.80 |
| 78 | CA | 434 | G | P-O3'-C3' | 10.43 | 132.22 | 119.70 |
| 78 | CA | 1735 | U | O4'-C1'-C2' | -10.43 | 95.37 | 105.80 |
| 13 | AL | 1 | MET | N-CA-CB | -10.43 | 91.83 | 110.60 |
| 78 | CA | 1185 | U | N1-C1'-C2' | 10.43 | 127.56 | 114.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 1425 | A | N1-C6-N6 | 10.43 | 124.86 | 118.60 |
| 15 | AN | 14 | TYR | CB-CG-CD1 | 10.43 | 127.26 | 121.00 |
| 81 | DA | 697 | A | P-O3'-C3' | 10.43 | 132.22 | 119.70 |
| 81 | DA | 2279 | A | O4'-C1'-C2' | 10.43 | 116.99 | 107.60 |
| 81 | DA | 3238 | G | O4'-C1'-N9 | 10.43 | 116.54 | 108.20 |
| 78 | CA | 1605 | G | O4'-C1'-N9 | 10.43 | 116.54 | 108.20 |
| 81 | DA | 56 | G | O4'-C1'-N9 | 10.43 | 116.54 | 108.20 |
| 81 | DA | 1688 | U | N1-C1'-C2' | 10.43 | 127.55 | 114.00 |
| 76 | BS | 120 | PHE | N-CA-CB | 10.42 | 129.36 | 110.60 |
| 81 | DA | 2754 | G | N9-C1'-C2' | -10.42 | 100.46 | 114.00 |
| 55 | Bc | 109 | ILE | N-CA-CB | 10.41 | 134.76 | 110.80 |
| 81 | DA | 1754 | G | O4'-C4'-C3' | -10.41 | 93.59 | 104.00 |
| 82 | DB | 97 | A | P-O3'-C3' | 10.41 | 132.19 | 119.70 |
| 14 | AM | 68 | ARG | NE-CZ-NH1 | -10.41 | 115.10 | 120.30 |
| 81 | DA | 2634 | U | N1-C1'-C2' | 10.41 | 127.53 | 114.00 |
| 81 | DA | 2992 | U | P-O3'-C3' | 10.41 | 132.19 | 119.70 |
| 81 | DA | 765 | C | C3'-C2'-C1' | 10.40 | 109.82 | 101.50 |
| 81 | DA | 3123 | A | O4'-C1'-N9 | 10.40 | 116.52 | 108.20 |
| 81 | DA | 3355 | U | C1'-O4'-C4' | 10.40 | 118.22 | 109.90 |
| 15 | AN | 54 | LYS | O-C-N | 10.40 | 139.34 | 122.70 |
| 57 | Be | 97 | PRO | C-N-CA | 10.40 | 147.71 | 121.70 |
| 81 | DA | 2526 | C | O4'-C1'-N1 | 10.40 | 116.52 | 108.20 |
| 78 | CA | 1698 | G | O4'-C1'-N9 | 10.40 | 116.52 | 108.20 |
| 81 | DA | 1916 | U | P-O5'-C5' | 10.40 | 137.54 | 120.90 |
| 16 | AO | 40 | TYR | CB-CG-CD2 | -10.40 | 114.76 | 121.00 |
| 81 | DA | 702 | C | O4'-C1'-N1 | -10.40 | 99.88 | 108.20 |
| 81 | DA | 2483 | G | O4'-C1'-N9 | 10.40 | 116.52 | 108.20 |
| 43 | BP | 159 | ARG | NE-CZ-NH1 | 10.39 | 125.50 | 120.30 |
| 82 | DB | 20 | U | P-O3'-C3' | 10.39 | 132.17 | 119.70 |
| 81 | DA | 1054 | A | C1'-O4'-C4' | 10.39 | 118.21 | 109.90 |
| 81 | DA | 3004 | C | C1'-O4'-C4' | -10.39 | 101.59 | 109.90 |
| 74 | BQ | 176 | SER | N-CA-CB | 10.39 | 126.08 | 110.50 |
| 78 | CA | 169 | A | N9-C1'-C2' | -10.39 | 100.49 | 114.00 |
| 78 | CA | 1570 | A | N9-C1'-C2' | -10.39 | 100.49 | 114.00 |
| 81 | DA | 242 | C | C3'-C2'-C1' | 10.39 | 109.81 | 101.50 |
| 81 | DA | 1116 | G | P-O3'-C3' | 10.39 | 132.16 | 119.70 |
| 81 | DA | 2788 | C | N1-C1'-C2' | 10.38 | 127.50 | 114.00 |
| 81 | DA | 2798 | C | N1-C1'-C2' | 10.38 | 127.49 | 114.00 |
| 81 | DA | 1698 | C | O4'-C1'-C2' | -10.38 | 95.42 | 105.80 |
| 78 | CA | 299 | A | N9-C1'-C2' | -10.38 | 100.51 | 114.00 |
| 81 | DA | 1933 | A | O4'-C1'-N9 | 10.37 | 116.50 | 108.20 |
| 81 | DA | 698 | U | O4'-C1'-N1 | 10.37 | 116.50 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1883 | A | O4'-C1'-N9 | 10.37 | 116.50 | 108.20 |
| 81 | DA | 2040 | U | O4'-C1'-N1 | 10.37 | 116.50 | 108.20 |
| 78 | CA | 838 | G | C1'-O4'-C4' | 10.37 | 118.19 | 109.90 |
| 81 | DA | 607 | A | C1'-O4'-C4' | -10.37 | 101.61 | 109.90 |
| 81 | DA | 1523 | U | O4'-C1'-N1 | 10.37 | 116.50 | 108.20 |
| 81 | DA | 1870 | C | O4'-C1'-N1 | 10.37 | 116.50 | 108.20 |
| 78 | CA | 661 | A | O4'-C1'-N9 | 10.37 | 116.49 | 108.20 |
| 78 | CA | 399 | A | O4'-C1'-N9 | 10.37 | 116.49 | 108.20 |
| 78 | CA | 627 | C | O4'-C1'-N1 | 10.37 | 116.49 | 108.20 |
| 81 | DA | 2889 | C | O4'-C1'-N1 | 10.36 | 116.49 | 108.20 |
| 52 | BY | 3 | LYS | N-CA-CB | 10.36 | 129.25 | 110.60 |
| 81 | DA | 2681 | U | O4'-C1'-N1 | 10.36 | 116.49 | 108.20 |
| 61 | Bj | 89 | LEU | O-C-N | -10.36 | 101.41 | 121.10 |
| 78 | CA | 123 | G | C3'-C2'-C1' | 10.36 | 109.79 | 101.50 |
| 51 | BZ | 67 | VAL | CA-C-N | 10.36 | 139.99 | 117.20 |
| 78 | CA | 1366 | U | P-O3'-C3' | 10.36 | 132.13 | 119.70 |
| 4 | AD | 86 | PHE | CB-CG-CD1 | 10.36 | 128.05 | 120.80 |
| 78 | CA | 1200 | G | C1'-O4'-C4' | -10.36 | 101.62 | 109.90 |
| 78 | CA | 1343 | U | P-O3'-C3' | 10.35 | 132.12 | 119.70 |
| 81 | DA | 464 | U | O4'-C1'-N1 | 10.35 | 116.48 | 108.20 |
| 82 | DB | 45 | C | N1-C1'-C2' | 10.35 | 127.46 | 114.00 |
| 30 | BA | 190 | PHE | CB-CA-C | 10.35 | 131.09 | 110.40 |
| 81 | DA | 3099 | C | O3'-P-O5' | -10.35 | 84.34 | 104.00 |
| 78 | CA | 1394 | G | C4'-C3'-C2' | -10.35 | 92.25 | 102.60 |
| 83 | DC | 49 | G | O4'-C1'-C2' | -10.35 | 95.45 | 105.80 |
| 74 | BQ | 248 | ARG | NE-CZ-NH1 | 10.34 | 125.47 | 120.30 |
| 81 | DA | 2070 | U | P-O3'-C3' | 10.34 | 132.11 | 119.70 |
| 81 | DA | 3126 | C | P-O3'-C3' | 10.34 | 132.11 | 119.70 |
| 81 | DA | 625 | G | O4'-C1'-N9 | 10.34 | 116.47 | 108.20 |
| 81 | DA | 1641 | U | P-O5'-C5' | 10.34 | 137.44 | 120.90 |
| 78 | CA | 1743 | U | P-O3'-C3' | 10.34 | 132.11 | 119.70 |
| 81 | DA | 1784 | G | O4'-C1'-N9 | 10.34 | 116.47 | 108.20 |
| 81 | DA | 3313 | U | C3'-C2'-C1' | -10.34 | 93.23 | 101.50 |
| 2 | AA | 10 | THR | N-CA-CB | 10.34 | 129.94 | 110.30 |
| 78 | CA | 255 | U | C4'-C3'-C2' | -10.34 | 92.27 | 102.60 |
| 81 | DA | 775 | A | O4'-C1'-N9 | 10.33 | 116.46 | 108.20 |
| 81 | DA | 2149 | A | C1'-O4'-C4' | 10.33 | 118.16 | 109.90 |
| 83 | DC | 50 | U | P-O5'-C5' | 10.33 | 137.42 | 120.90 |
| 81 | DA | 1005 | G | C4'-C3'-C2' | -10.32 | 92.28 | 102.60 |
| 82 | DB | 38 | U | P-O3'-C3' | 10.32 | 132.09 | 119.70 |
| 81 | DA | 2451 | G | O4'-C1'-N9 | 10.32 | 116.46 | 108.20 |
| 81 | DA | 1131 | G | P-O3'-C3' | 10.32 | 132.08 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 57 | G | O4'-C1'-N9 | 10.32 | 116.45 | 108.20 |
| 78 | CA | 1080 | U | O3'-P-O5' | -10.32 | 84.40 | 104.00 |
| 78 | CA | 1400 | A | O4'-C1'-N9 | -10.32 | 99.95 | 108.20 |
| 81 | DA | 2698 | G | O4'-C1'-N9 | 10.32 | 116.45 | 108.20 |
| 78 | CA | 163 | G | O3'-P-O5' | -10.31 | 84.40 | 104.00 |
| 81 | DA | 872 | U | P-O3'-C3' | 10.31 | 132.08 | 119.70 |
| 78 | CA | 268 | C | N1-C1'-C2' | 10.31 | 127.41 | 114.00 |
| 81 | DA | 1253 | U | O4'-C1'-N1 | 10.31 | 116.45 | 108.20 |
| 81 | DA | 1534 | A | O4'-C1'-N9 | 10.31 | 116.45 | 108.20 |
| 81 | DA | 2816 | G | P-O3'-C3' | 10.31 | 132.07 | 119.70 |
| 78 | CA | 1103 | U | O4'-C1'-N1 | 10.30 | 116.44 | 108.20 |
| 78 | CA | 1546 | G | C4'-C3'-C2' | 10.30 | 112.91 | 102.60 |
| 53 | Ba | 9 | LYS | N-CA-C | 10.30 | 138.81 | 111.00 |
| 81 | DA | 521 | A | N9-C1'-C2' | -10.30 | 100.61 | 114.00 |
| 81 | DA | 1074 | U | P-O5'-C5' | 10.30 | 137.38 | 120.90 |
| 81 | DA | 3241 | G | O4'-C1'-N9 | -10.30 | 99.96 | 108.20 |
| 82 | DB | 122 | U | P-O5'-C5' | 10.30 | 137.38 | 120.90 |
| 13 | AL | 39 | LYS | N-CA-CB | 10.30 | 129.14 | 110.60 |
| 81 | DA | 2492 | C | C3'-C2'-C1' | 10.30 | 109.74 | 101.50 |
| 81 | DA | 2690 | G | O4'-C1'-N9 | 10.30 | 116.44 | 108.20 |
| 81 | DA | 2510 | U | O4'-C1'-C2' | -10.29 | 95.50 | 105.80 |
| 79 | CB | 47 | U | O4'-C1'-N1 | 10.29 | 116.43 | 108.20 |
| 41 | BN | 39 | ILE | CG1-CB-CG2 | 10.29 | 134.04 | 111.40 |
| 78 | CA | 629 | U | O4'-C1'-N1 | 10.29 | 116.43 | 108.20 |
| 81 | DA | 1695 | U | N1-C1'-C2' | -10.29 | 100.62 | 114.00 |
| 78 | CA | 984 | G | O4'-C1'-N9 | 10.28 | 116.43 | 108.20 |
| 78 | CA | 1375 | A | O4'-C1'-N9 | -10.29 | 99.97 | 108.20 |
| 81 | DA | 1087 | G | O4'-C1'-N9 | 10.29 | 116.43 | 108.20 |
| 81 | DA | 992 | A | N9-C1'-C2' | -10.28 | 100.64 | 114.00 |
| 81 | DA | 3307 | A | O4'-C1'-N9 | 10.28 | 116.42 | 108.20 |
| 83 | DC | 26 | C | C1'-O4'-C4' | -10.28 | 101.68 | 109.90 |
| 56 | Bf | 27 | TYR | CB-CG-CD2 | -10.28 | 114.83 | 121.00 |
| 81 | DA | 3352 | U | N1-C1'-C2' | 10.28 | 127.36 | 114.00 |
| 13 | AL | 6 | PRO | N-CD-CG | 10.27 | 118.61 | 103.20 |
| 40 | BK | 130 | LYS | CA-C-O | -10.27 | 98.53 | 120.10 |
| 47 | BU | 17 | ARG | NE-CZ-NH2 | 10.27 | 125.44 | 120.30 |
| 78 | CA | 280 | U | N1-C1'-C2' | 10.27 | 127.36 | 114.00 |
| 78 | CA | 1573 | A | N9-C1'-C2' | -10.27 | 100.65 | 114.00 |
| 81 | DA | 1640 | G | O3'-P-O5' | -10.27 | 84.48 | 104.00 |
| 81 | DA | 1715 | A | O4'-C1'-N9 | 10.27 | 116.42 | 108.20 |
| 81 | DA | 566 | G | N9-C1'-C2' | 10.27 | 127.34 | 114.00 |
| 81 | DA | 2607 | G | C1'-O4'-C4' | -10.27 | 101.69 | 109.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 60 | Bi | 43 | LYS | N-CA-CB | 10.26 | 129.07 | 110.60 |
| 81 | DA | 671 | U | O3'-P-O5' | -10.26 | 84.50 | 104.00 |
| 81 | DA | 2445 | A | N9-C1'-C2' | 10.26 | 127.34 | 114.00 |
| 13 | AL | 134 | ALA | C-N-CA | -10.26 | 96.05 | 121.70 |
| 81 | DA | 299 | G | O4'-C1'-N9 | 10.26 | 116.41 | 108.20 |
| 81 | DA | 2406 | C | C3'-C2'-C1' | 10.26 | 109.71 | 101.50 |
| 78 | CA | 593 | U | O4'-C1'-N1 | 10.26 | 116.41 | 108.20 |
| 78 | CA | 1192 | C | N1-C1'-C2' | 10.26 | 127.33 | 114.00 |
| 81 | DA | 3066 | U | O4'-C1'-N1 | 10.26 | 116.40 | 108.20 |
| 81 | DA | 1697 | A | P-O3'-C3' | 10.25 | 132.00 | 119.70 |
| 78 | CA | 1081 | A | O4'-C1'-C2' | -10.25 | 95.55 | 105.80 |
| 81 | DA | 109 | A | C3'-C2'-C1' | 10.25 | 109.70 | 101.50 |
| 81 | DA | 848 | A | P-O3'-C3' | 10.25 | 132.00 | 119.70 |
| 81 | DA | 1695 | U | P-O3'-C3' | 10.25 | 132.00 | 119.70 |
| 81 | DA | 855 | U | O3'-P-O5' | -10.25 | 84.53 | 104.00 |
| 78 | CA | 194 | U | P-O3'-C3' | 10.24 | 131.99 | 119.70 |
| 35 | BG | 99 | GLU | CA-CB-CG | 10.24 | 135.93 | 113.40 |
| 35 | BG | 14 | ASP | C-N-CA | 10.24 | 147.30 | 121.70 |
| 78 | CA | 880 | C | O4'-C1'-N1 | 10.24 | 116.39 | 108.20 |
| 81 | DA | 1422 | G | C1'-O4'-C4' | -10.24 | 101.71 | 109.90 |
| 5 | AC | 164 | PHE | C-N-CA | 10.23 | 143.79 | 122.30 |
| 79 | CB | 25 | U | O4'-C1'-N1 | 10.23 | 116.39 | 108.20 |
| 81 | DA | 384 | A | P-O3'-C3' | 10.23 | 131.98 | 119.70 |
| 81 | DA | 2999 | U | P-O3'-C3' | 10.23 | 131.98 | 119.70 |
| 81 | DA | 1259 | A | P-O3'-C3' | 10.23 | 131.98 | 119.70 |
| 81 | DA | 2339 | C | O4'-C1'-N1 | 10.23 | 116.39 | 108.20 |
| 81 | DA | 250 | U | C1'-O4'-C4' | 10.23 | 118.08 | 109.90 |
| 81 | DA | 2362 | C | O4'-C1'-C2' | -10.23 | 95.57 | 105.80 |
| 81 | DA | 2899 | C | C1'-O4'-C4' | -10.23 | 101.72 | 109.90 |
| 81 | DA | 834 | U | O3'-P-O5' | -10.22 | 84.58 | 104.00 |
| 81 | DA | 1134 | G | O4'-C1'-N9 | 10.22 | 116.38 | 108.20 |
| 81 | DA | 774 | G | C1'-O4'-C4' | -10.22 | 101.72 | 109.90 |
| 50 | BX | 93 | TYR | CB-CG-CD1 | -10.22 | 114.87 | 121.00 |
| 81 | DA | 2740 | A | O4'-C1'-N9 | 10.22 | 116.37 | 108.20 |
| 81 | DA | 1001 | G | P-O3'-C3' | -10.21 | 107.44 | 119.70 |
| 74 | BQ | 40 | HIS | CA-C-N | -10.21 | 94.74 | 117.20 |
| 81 | DA | 522 | A | O4'-C1'-N9 | 10.21 | 116.37 | 108.20 |
| 78 | CA | 1447 | C | O4'-C1'-C2' | -10.21 | 95.59 | 105.80 |
| 81 | DA | 187 | A | P-O5'-C5' | 10.21 | 137.23 | 120.90 |
| 41 | BN | 77 | ARG | N-CA-CB | 10.20 | 128.96 | 110.60 |
| 78 | CA | 831 | U | O4'-C1'-N1 | 10.20 | 116.36 | 108.20 |
| 78 | CA | 1326 | A | P-O3'-C3' | 10.20 | 131.94 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1084 | A | P-O3'-C3' | 10.20 | 131.94 | 119.70 |
| 81 | DA | 1296 | C | O4'-C1'-N1 | 10.20 | 116.36 | 108.20 |
| 40 | BK | 48 | PHE | CB-CG-CD2 | 10.20 | 127.94 | 120.80 |
| 59 | Bh | 20 | HIS | C-N-CA | 10.20 | 147.20 | 121.70 |
| 78 | CA | 1310 | U | O5'-C5'-C4' | 10.20 | 131.08 | 111.70 |
| 81 | DA | 1138 | U | O4'-C1'-N1 | 10.20 | 116.36 | 108.20 |
| 81 | DA | 971 | G | O4'-C1'-N9 | 10.20 | 116.36 | 108.20 |
| 81 | DA | 1771 | C | O3'-P-O5' | -10.20 | 84.63 | 104.00 |
| 81 | DA | 1513 | G | O4'-C1'-C2' | 10.19 | 116.77 | 107.60 |
| 81 | DA | 2941 | A | N9-C1'-C2' | -10.20 | 100.75 | 114.00 |
| 35 | BG | 49 | GLY | N-CA-C | 10.19 | 138.58 | 113.10 |
| 38 | Bs | 136 | PHE | CB-CG-CD2 | -10.19 | 113.67 | 120.80 |
| 78 | CA | 782 | U | P-O3'-C3' | 10.19 | 131.93 | 119.70 |
| 78 | CA | 1265 | G | O4'-C1'-N9 | 10.19 | 116.35 | 108.20 |
| 81 | DA | 2426 | U | O4'-C1'-N1 | 10.19 | 116.35 | 108.20 |
| 81 | DA | 3242 | G | O4'-C1'-C2' | -10.19 | 95.61 | 105.80 |
| 82 | DB | 151 | C | C3'-C2'-C1' | 10.19 | 109.65 | 101.50 |
| 16 | AO | 124 | ARG | NE-CZ-NH1 | -10.19 | 115.21 | 120.30 |
| 78 | CA | 856 | A | N9-C1'-C2' | -10.19 | 100.76 | 114.00 |
| 13 | AL | 23 | ARG | CB-CA-C | 10.19 | 130.77 | 110.40 |
| 78 | CA | 1340 | U | C5'-C4'-O4' | 10.19 | 121.32 | 109.10 |
| 74 | BQ | 30 | TYR | CB-CG-CD2 | -10.18 | 114.89 | 121.00 |
| 78 | CA | 123 | G | P-O3'-C3' | 10.18 | 131.92 | 119.70 |
| 81 | DA | 903 | U | O4'-C1'-N1 | 10.18 | 116.34 | 108.20 |
| 81 | DA | 1996 | C | O4'-C1'-C2' | -10.18 | 95.62 | 105.80 |
| 82 | DB | 49 | G | O4'-C1'-N9 | 10.18 | 116.34 | 108.20 |
| 81 | DA | 2153 | U | P-O5'-C5' | 10.18 | 137.18 | 120.90 |
| 10 | AI | 138 | PHE | CB-CG-CD2 | -10.17 | 113.68 | 120.80 |
| 81 | DA | 678 | G | P-O3'-C3' | 10.17 | 131.91 | 119.70 |
| 81 | DA | 1321 | G | P-O3'-C3' | 10.17 | 131.91 | 119.70 |
| 78 | CA | 1617 | U | O4'-C1'-N1 | 10.17 | 116.34 | 108.20 |
| 78 | CA | 1280 | C | P-O3'-C3' | 10.17 | 131.90 | 119.70 |
| 78 | CA | 32 | U | O4'-C1'-C2' | -10.17 | 95.63 | 105.80 |
| 41 | BN | 108 | ARG | NE-CZ-NH2 | -10.16 | 115.22 | 120.30 |
| 43 | BP | 30 | TYR | CB-CG-CD2 | -10.16 | 114.90 | 121.00 |
| 78 | CA | 418 | G | O4'-C1'-N9 | 10.16 | 116.33 | 108.20 |
| 81 | DA | 1948 | G | C5'-C4'-C3' | 10.16 | 132.26 | 116.00 |
| 12 | AK | 124 | ASP | CB-CG-OD2 | 10.16 | 127.45 | 118.30 |
| 81 | DA | 2036 | U | O4'-C1'-N1 | 10.16 | 116.33 | 108.20 |
| 81 | DA | 2280 | A | P-O5'-C5' | 10.16 | 137.16 | 120.90 |
| 35 | BG | 132 | ALA | N-CA-CB | -10.16 | 95.88 | 110.10 |
| 78 | CA | 609 | U | C3'-C2'-C1' | 10.16 | 109.63 | 101.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1614 | C | O4'-C1'-N1 | 10.16 | 116.33 | 108.20 |
| 81 | DA | 1720 | U | O4'-C1'-N1 | 10.16 | 116.33 | 108.20 |
| 81 | DA | 2736 | A | N9-C1'-C2' | -10.16 | 100.79 | 114.00 |
| 14 | AM | 120 | ARG | N-CA-CB | 10.16 | 128.88 | 110.60 |
| 21 | AT | 12 | TYR | CB-CG-CD1 | 10.16 | 127.09 | 121.00 |
| 79 | CB | 5 | U | O4'-C1'-N1 | 10.15 | 116.32 | 108.20 |
| 81 | DA | 74 | G | C5'-C4'-C3' | 10.15 | 132.24 | 116.00 |
| 81 | DA | 922 | U | O4'-C1'-N1 | -10.15 | 100.08 | 108.20 |
| 81 | DA | 725 | G | P-O3'-C3' | 10.15 | 131.88 | 119.70 |
| 78 | CA | 252 | U | C1'-O4'-C4' | 10.15 | 118.02 | 109.90 |
| 81 | DA | 1624 | G | P-O3'-C3' | 10.15 | 131.88 | 119.70 |
| 79 | CB | 11 | U | O4'-C1'-N1 | 10.14 | 116.31 | 108.20 |
| 81 | DA | 450 | G | P-O3'-C3' | 10.14 | 131.87 | 119.70 |
| 38 | Bs | 197 | PHE | CB-CG-CD1 | -10.14 | 113.70 | 120.80 |
| 81 | DA | 249 | U | P-O3'-C3' | 10.14 | 131.87 | 119.70 |
| 81 | DA | 751 | A | O4'-C1'-N9 | 10.14 | 116.31 | 108.20 |
| 81 | DA | 1542 | G | C3'-C2'-C1' | -10.14 | 93.39 | 101.50 |
| 81 | DA | 3391 | A | P-O3'-C3' | 10.14 | 131.87 | 119.70 |
| 78 | CA | 630 | A | O4'-C1'-C2' | -10.14 | 95.66 | 105.80 |
| 81 | DA | 2840 | C | N1-C1'-C2' | -10.14 | 100.82 | 114.00 |
| 81 | DA | 306 | A | P-O3'-C3' | 10.14 | 131.86 | 119.70 |
| 81 | DA | 1986 | U | O4'-C1'-N1 | 10.14 | 116.31 | 108.20 |
| 81 | DA | 1829 | G | O4'-C1'-N9 | 10.13 | 116.31 | 108.20 |
| 81 | DA | 1947 | G | C3'-C2'-C1' | -10.14 | 93.39 | 101.50 |
| 78 | CA | 1545 | A | C3'-C2'-C1' | -10.13 | 93.39 | 101.50 |
| 81 | DA | 605 | U | O4'-C1'-N1 | 10.13 | 116.31 | 108.20 |
| 81 | DA | 2124 | G | O4'-C1'-N9 | 10.13 | 116.31 | 108.20 |
| 81 | DA | 3218 | A | O4'-C1'-N9 | 10.13 | 116.31 | 108.20 |
| 78 | CA | 488 | G | O4'-C1'-N9 | 10.13 | 116.30 | 108.20 |
| 81 | DA | 1408 | G | P-O3'-C3' | 10.13 | 131.86 | 119.70 |
| 81 | DA | 169 | U | O4'-C1'-C2' | -10.13 | 95.67 | 105.80 |
| 81 | DA | 1397 | C | C3'-C2'-C1' | 10.13 | 109.60 | 101.50 |
| 81 | DA | 2475 | G | C1'-O4'-C4' | 10.12 | 118.00 | 109.90 |
| 81 | DA | 2491 | A | N9-C1'-C2' | 10.12 | 127.16 | 114.00 |
| 78 | CA | 635 | A | O4'-C1'-C2' | -10.12 | 95.68 | 105.80 |
| 81 | DA | 2968 | G | O4'-C1'-N9 | 10.12 | 116.30 | 108.20 |
| 11 | AJ | 84 | MET | CB-CA-C | -10.12 | 90.16 | 110.40 |
| 81 | DA | 435 | C | C3'-C2'-C1' | 10.12 | 109.60 | 101.50 |
| 81 | DA | 2013 | C | C3'-C2'-C1' | 10.12 | 109.59 | 101.50 |
| 81 | DA | 2231 | C | C3'-C2'-C1' | 10.12 | 109.59 | 101.50 |
| 81 | DA | 1071 | U | O4'-C1'-N1 | 10.11 | 116.29 | 108.20 |
| 81 | DA | 1168 | U | O4'-C1'-N1 | 10.12 | 116.29 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1263 | A | O4'-C1'-C2' | 10.11 | 116.70 | 107.60 |
| 78 | CA | 1337 | A | C4'-C3'-C2' | 10.11 | 112.71 | 102.60 |
| 81 | DA | 2487 | U | C3'-C2'-C1' | 10.11 | 109.59 | 101.50 |
| 78 | CA | 1113 | A | N9-C1'-C2' | -10.11 | 100.86 | 114.00 |
| 78 | CA | 1461 | C | O4'-C1'-N1 | 10.11 | 116.29 | 108.20 |
| 81 | DA | 2025 | G | C4'-C3'-C2' | -10.11 | 92.49 | 102.60 |
| 74 | BQ | 253 | PHE | CB-CG-CD1 | -10.11 | 113.73 | 120.80 |
| 20 | AS | 97 | SER | N-CA-CB | 10.10 | 125.65 | 110.50 |
| 81 | DA | 1684 | U | O4'-C1'-N1 | -10.10 | 100.12 | 108.20 |
| 81 | DA | 2345 | A | C1'-O4'-C4' | -10.10 | 101.82 | 109.90 |
| 81 | DA | 1564 | U | N1-C1'-C2' | 10.10 | 127.13 | 114.00 |
| 35 | BG | 75 | PRO | CA-C-N | 10.09 | 139.40 | 117.20 |
| 78 | CA | 1085 | G | O4'-C1'-N9 | 10.09 | 116.27 | 108.20 |
| 81 | DA | 2520 | A | O4'-C1'-N9 | 10.09 | 116.28 | 108.20 |
| 81 | DA | 2870 | C | C3'-C2'-C1' | 10.09 | 109.58 | 101.50 |
| 39 | BJ | 16 | ARG | NE-CZ-NH1 | 10.09 | 125.35 | 120.30 |
| 81 | DA | 730 | C | O4'-C1'-N1 | 10.09 | 116.27 | 108.20 |
| 81 | DA | 2613 | U | P-O3'-C3' | 10.09 | 131.81 | 119.70 |
| 17 | AQ | 82 | ASP | N-CA-CB | 10.09 | 128.75 | 110.60 |
| 42 | BM | 86 | ARG | NE-CZ-NH1 | 10.09 | 125.34 | 120.30 |
| 81 | DA | 3022 | G | N9-C1'-C2' | 10.09 | 127.11 | 114.00 |
| 76 | BS | 151 | PHE | CB-CG-CD2 | -10.08 | 113.74 | 120.80 |
| 83 | DC | 16 | U | O3'-P-O5' | 10.08 | 123.16 | 104.00 |
| 78 | CA | 1000 | C | O4'-C1'-N1 | 10.08 | 116.26 | 108.20 |
| 81 | DA | 789 | A | P-O3'-C3' | 10.08 | 131.79 | 119.70 |
| 81 | DA | 2760 | C | N1-C1'-C2' | 10.08 | 127.10 | 114.00 |
| 81 | DA | 1401 | A | C4'-C3'-C2' | -10.08 | 92.52 | 102.60 |
| 81 | DA | 2381 | G | P-O3'-C3' | 10.07 | 131.79 | 119.70 |
| 48 | BW | 107 | PHE | CB-CG-CD1 | 10.07 | 127.85 | 120.80 |
| 81 | DA | 209 | A | O4'-C1'-N9 | 10.07 | 116.26 | 108.20 |
| 81 | DA | 1003 | A | O4'-C1'-N9 | 10.07 | 116.26 | 108.20 |
| 83 | DC | 83 | U | O4'-C1'-N1 | 10.07 | 116.26 | 108.20 |
| 1 | Aa | 54 | PHE | CB-CA-C | 10.07 | 130.54 | 110.40 |
| 78 | CA | 1225 | U | P-O3'-C3' | 10.07 | 131.78 | 119.70 |
| 78 | CA | 1508 | U | P-O3'-C3' | 10.07 | 131.78 | 119.70 |
| 81 | DA | 62 | A | P-O3'-C3' | 10.07 | 131.78 | 119.70 |
| 81 | DA | 806 | A | O4'-C1'-C2' | -10.07 | 95.73 | 105.80 |
| 81 | DA | 1055 | A | P-O3'-C3' | 10.07 | 131.78 | 119.70 |
| 78 | CA | 1770 | U | O4'-C1'-N1 | 10.06 | 116.25 | 108.20 |
| 78 | CA | 591 | A | P-O3'-C3' | 10.06 | 131.78 | 119.70 |
| 81 | DA | 1076 | C | N1-C1'-C2' | 10.06 | 127.07 | 114.00 |
| 81 | DA | 2788 | C | C3'-C2'-C1' | 10.06 | 109.55 | 101.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 82 | DB | 124 | G | P-O3'-C3' | 10.06 | 131.77 | 119.70 |
| 81 | DA | 71 | A | C3'-C2'-C1' | 10.05 | 109.54 | 101.50 |
| 81 | DA | 813 | G | O4'-C1'-N9 | 10.05 | 116.24 | 108.20 |
| 2 | AA | 252 | TRP | N-CA-CB | 10.05 | 128.69 | 110.60 |
| 40 | BK | 133 | ARG | CD-NE-CZ | 10.05 | 137.67 | 123.60 |
| 81 | DA | 995 | U | O4'-C1'-N1 | 10.05 | 116.24 | 108.20 |
| 81 | DA | 1690 | C | O4'-C1'-N1 | 10.05 | 116.24 | 108.20 |
| 81 | DA | 2757 | U | P-O5'-C5' | 10.05 | 136.98 | 120.90 |
| 81 | DA | 1339 | C | O4'-C1'-N1 | 10.04 | 116.24 | 108.20 |
| 30 | BA | 122 | ARG | NE-CZ-NH1 | -10.04 | 115.28 | 120.30 |
| 8 | AF | 30 | PRO | CA-N-CD | -10.04 | 97.45 | 111.50 |
| 77 | BI | 106 | ALA | CA-C-N | 10.04 | 136.27 | 116.20 |
| 81 | DA | 2169 | G | O4'-C1'-N9 | 10.04 | 116.23 | 108.20 |
| 81 | DA | 2562 | A | N1-C6-N6 | 10.04 | 124.62 | 118.60 |
| 81 | DA | 1990 | U | O3'-P-O5' | -10.04 | 84.93 | 104.00 |
| 79 | CB | 43 | C | N1-C1'-C2' | 10.03 | 127.04 | 114.00 |
| 81 | DA | 1758 | G | N1-C6-O6 | 10.03 | 125.92 | 119.90 |
| 81 | DA | 2700 | G | C1'-O4'-C4' | -10.03 | 101.88 | 109.90 |
| 2 | AA | 195 | TRP | N-CA-C | -10.03 | 83.92 | 111.00 |
| 81 | DA | 2917 | G | O4'-C1'-N9 | 10.03 | 116.22 | 108.20 |
| 82 | DB | 112 | U | C1'-O4'-C4' | 10.03 | 117.92 | 109.90 |
| 38 | Bs | 243 | TYR | CB-CA-C | -10.03 | 90.35 | 110.40 |
| 83 | DC | 29 | C | C4'-C3'-C2' | -10.03 | 92.57 | 102.60 |
| 81 | DA | 2446 | U | N1-C1'-C2' | 10.02 | 127.03 | 114.00 |
| 78 | CA | 1015 | U | O4'-C1'-N1 | -10.02 | 100.19 | 108.20 |
| 81 | DA | 1390 | A | C5'-C4'-C3' | 10.02 | 132.03 | 116.00 |
| 81 | DA | 186 | U | P-O3'-C3' | 10.01 | 131.72 | 119.70 |
| 81 | DA | 1872 | C | C3'-C2'-C1' | 10.01 | 109.51 | 101.50 |
| 81 | DA | 2491 | A | C5'-C4'-C3' | 10.01 | 132.02 | 116.00 |
| 81 | DA | 2966 | G | N9-C1'-C2' | 10.01 | 127.02 | 114.00 |
| 5 | AC | 162 | SER | N-CA-C | 10.01 | 138.03 | 111.00 |
| 53 | Ba | 42 | LEU | CB-CA-C | -10.01 | 91.18 | 110.20 |
| 78 | CA | 156 | A | O4'-C1'-N9 | 10.01 | 116.21 | 108.20 |
| 78 | CA | 1632 | C | N1-C1'-C2' | 10.01 | 127.01 | 114.00 |
| 81 | DA | 3217 | C | P-O3'-C3' | 10.01 | 131.71 | 119.70 |
| 78 | CA | 943 | C | N1-C1'-C2' | 10.01 | 127.01 | 114.00 |
| 78 | CA | 1061 | A | N1-C6-N6 | 10.01 | 124.60 | 118.60 |
| 81 | DA | 1688 | U | C3'-C2'-C1' | 10.01 | 109.50 | 101.50 |
| 81 | DA | 1228 | C | O4'-C1'-N1 | 10.00 | 116.20 | 108.20 |
| 81 | DA | 1712 | G | P-O3'-C3' | 10.00 | 131.70 | 119.70 |
| 81 | DA | 1428 | A | O4'-C1'-C2' | -10.00 | 95.80 | 105.80 |
| 81 | DA | 1513 | G | C1'-O4'-C4' | -10.00 | 101.90 | 109.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1944 | U | P-O3'-C3' | 10.00 | 131.70 | 119.70 |
| 48 | BW | 107 | PHE | CB-CG-CD2 | -9.99 | 113.80 | 120.80 |
| 76 | BS | 9 | TYR | CB-CG-CD1 | 9.99 | 127.00 | 121.00 |
| 81 | DA | 2063 | U | O4'-C1'-C2' | -9.99 | 95.81 | 105.80 |
| 81 | DA | 2224 | A | P-O3'-C3' | 9.99 | 131.69 | 119.70 |
| 81 | DA | 1709 | C | C3'-C2'-C1' | 9.99 | 109.49 | 101.50 |
| 81 | DA | 2665 | U | N1-C1'-C2' | -9.99 | 101.01 | 112.00 |
| 82 | DB | 132 | G | C5'-C4'-C3' | 9.99 | 131.98 | 116.00 |
| 30 | BA | 152 | ARG | NE-CZ-NH2 | -9.99 | 115.31 | 120.30 |
| 43 | BP | 123 | GLN | N-CA-C | 9.99 | 137.96 | 111.00 |
| 78 | CA | 996 | U | O4'-C1'-N1 | 9.98 | 116.19 | 108.20 |
| 81 | DA | 2165 | G | N9-C1'-C2' | -9.98 | 101.02 | 112.00 |
| 60 | Bi | 9 | ARG | NE-CZ-NH2 | -9.98 | 115.31 | 120.30 |
| 50 | BX | 54 | TYR | CB-CG-CD2 | -9.98 | 115.01 | 121.00 |
| 81 | DA | 2801 | A | O4'-C1'-C2' | 9.98 | 116.58 | 107.60 |
| 78 | CA | 1096 | C | O4'-C1'-C2' | -9.97 | 95.83 | 105.80 |
| 78 | CA | 1525 | A | P-O3'-C3' | 9.97 | 131.66 | 119.70 |
| 81 | DA | 43 | A | C3'-C2'-C1' | -9.97 | 93.53 | 101.50 |
| 81 | DA | 329 | U | O4'-C1'-N1 | 9.96 | 116.17 | 108.20 |
| 81 | DA | 1681 | U | C3'-C2'-C1' | 9.96 | 109.47 | 101.50 |
| 83 | DC | 55 | A | O4'-C1'-C2' | -9.96 | 95.84 | 105.80 |
| 81 | DA | 2115 | G | P-O5'-C5' | -9.96 | 104.97 | 120.90 |
| 81 | DA | 3211 | C | C5'-C4'-C3' | 9.96 | 131.94 | 116.00 |
| 81 | DA | 586 | C | P-O3'-C3' | 9.96 | 131.65 | 119.70 |
| 81 | DA | 1321 | G | O4'-C1'-N9 | 9.96 | 116.16 | 108.20 |
| 81 | DA | 2566 | C | O4'-C1'-N1 | 9.96 | 116.16 | 108.20 |
| 78 | CA | 440 | U | O4'-C1'-N1 | 9.95 | 116.16 | 108.20 |
| 81 | DA | 1400 | G | N9-C1'-C2' | -9.95 | 101.06 | 112.00 |
| 81 | DA | 2130 | G | O4'-C1'-N9 | 9.95 | 116.16 | 108.20 |
| 78 | CA | 120 | U | P-O5'-C5' | 9.95 | 136.81 | 120.90 |
| 78 | CA | 224 | C | O4'-C1'-N1 | 9.95 | 116.16 | 108.20 |
| 81 | DA | 2335 | G | O4'-C1'-N9 | 9.94 | 116.16 | 108.20 |
| 81 | DA | 559 | A | O4'-C1'-N9 | 9.94 | 116.15 | 108.20 |
| 81 | DA | 612 | U | O4'-C1'-N1 | 9.94 | 116.15 | 108.20 |
| 81 | DA | 1734 | G | O4'-C1'-N9 | 9.94 | 116.15 | 108.20 |
| 78 | CA | 32 | U | C1'-O4'-C4' | 9.94 | 117.85 | 109.90 |
| 44 | BO | 87 | ARG | NE-CZ-NH2 | -9.94 | 115.33 | 120.30 |
| 78 | CA | 295 | A | C5'-C4'-C3' | 9.94 | 131.90 | 116.00 |
| 78 | CA | 648 | G | C5'-C4'-C3' | 9.94 | 131.90 | 116.00 |
| 81 | DA | 93 | C | C3'-C2'-C1' | 9.94 | 109.45 | 101.50 |
| 35 | BG | 163 | PHE | CB-CG-CD1 | 9.94 | 127.76 | 120.80 |
| 79 | CB | 32 | U | O4'-C1'-N1 | 9.94 | 116.15 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 111 | C | N1-C1'-C2' | 9.94 | 126.92 | 114.00 |
| 81 | DA | 3350 | C | N1-C1'-C2' | 9.94 | 126.92 | 114.00 |
| 78 | CA | 1342 | C | P-O3'-C3' | 9.93 | 131.62 | 119.70 |
| 37 | BH | 204 | ARG | NE-CZ-NH2 | -9.93 | 115.33 | 120.30 |
| 78 | CA | 49 | C | O4'-C1'-N1 | 9.93 | 116.15 | 108.20 |
| 81 | DA | 576 | C | C3'-C2'-C1' | 9.93 | 109.45 | 101.50 |
| 81 | DA | 609 | G | O4'-C1'-N9 | 9.93 | 116.15 | 108.20 |
| 82 | DB | 154 | C | C3'-C2'-C1' | 9.93 | 109.45 | 101.50 |
| 81 | DA | 2689 | A | C3'-C2'-C1' | 9.93 | 109.45 | 101.50 |
| 81 | DA | 994 | G | P-O3'-C3' | 9.93 | 131.61 | 119.70 |
| 81 | DA | 2567 | C | O4'-C1'-N1 | 9.93 | 116.14 | 108.20 |
| 81 | DA | 2679 | A | P-O3'-C3' | 9.93 | 131.62 | 119.70 |
| 82 | DB | 51 | G | P-O3'-C3' | 9.93 | 131.61 | 119.70 |
| 17 | AQ | 135 | ARG | NE-CZ-NH1 | 9.92 | 125.26 | 120.30 |
| 29 | AU | 62 | THR | N-CA-CB | 9.92 | 129.15 | 110.30 |
| 78 | CA | 932 | U | N1-C1'-C2' | -9.92 | 101.09 | 112.00 |
| 81 | DA | 287 | G | O4'-C1'-N9 | 9.92 | 116.14 | 108.20 |
| 81 | DA | 1844 | C | O4'-C1'-N1 | 9.92 | 116.14 | 108.20 |
| 81 | DA | 2508 | U | O4'-C1'-C2' | -9.92 | 95.88 | 105.80 |
| 81 | DA | 2736 | A | P-O3'-C3' | 9.92 | 131.61 | 119.70 |
| 46 | BT | 162 | ARG | NE-CZ-NH1 | -9.92 | 115.34 | 120.30 |
| 78 | CA | 868 | G | C3'-C2'-C1' | -9.92 | 93.56 | 101.50 |
| 81 | DA | 3055 | U | O4'-C1'-N1 | 9.92 | 116.14 | 108.20 |
| 78 | CA | 839 | U | O4'-C1'-C2' | -9.92 | 95.88 | 105.80 |
| 78 | CA | 971 | A | O4'-C1'-N9 | 9.92 | 116.13 | 108.20 |
| 81 | DA | 292 | U | O4'-C1'-N1 | 9.92 | 116.13 | 108.20 |
| 81 | DA | 2693 | C | C3'-C2'-C1' | 9.92 | 109.43 | 101.50 |
| 50 | BX | 60 | TYR | CG-CD1-CE1 | -9.91 | 113.37 | 121.30 |
| 81 | DA | 1249 | G | O4'-C1'-N9 | 9.91 | 116.13 | 108.20 |
| 78 | CA | 349 | U | O4'-C1'-N1 | 9.91 | 116.13 | 108.20 |
| 81 | DA | 2630 | C | C3'-C2'-C1' | 9.91 | 109.43 | 101.50 |
| 78 | CA | 990 | C | C1'-O4'-C4' | -9.91 | 101.97 | 109.90 |
| 78 | CA | 831 | U | N1-C1'-C2' | -9.91 | 101.10 | 112.00 |
| 18 | AP | 99 | ARG | NE-CZ-NH1 | 9.91 | 125.25 | 120.30 |
| 79 | CB | 71 | A | N9-C1'-C2' | 9.91 | 126.88 | 114.00 |
| 81 | DA | 2378 | C | N1-C1'-C2' | 9.91 | 126.88 | 114.00 |
| 81 | DA | 3054 | U | O3'-P-O5' | -9.91 | 85.18 | 104.00 |
| 81 | DA | 1079 | A | O4'-C1'-C2' | -9.90 | 95.90 | 105.80 |
| 81 | DA | 2576 | G | N1-C6-O6 | 9.90 | 125.84 | 119.90 |
| 81 | DA | 3296 | A | N9-C1'-C2' | 9.90 | 126.87 | 114.00 |
| 10 | AI | 84 | ALA | N-CA-CB | 9.90 | 123.96 | 110.10 |
| 81 | DA | 1362 | G | O4'-C1'-C2' | 9.90 | 116.51 | 107.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 32 | BC | 250 | ALA | CB-CA-C | -9.90 | 95.26 | 110.10 |
| 78 | CA | 423 | G | O4'-C1'-N9 | 9.90 | 116.12 | 108.20 |
| 81 | DA | 3193 | C | P-O3'-C3' | 9.90 | 131.58 | 119.70 |
| 83 | DC | 109 | G | O4'-C1'-N9 | 9.90 | 116.12 | 108.20 |
| 4 | AD | 239 | PRO | CA-N-CD | -9.89 | 97.65 | 111.50 |
| 78 | CA | 476 | U | P-O3'-C3' | 9.89 | 131.57 | 119.70 |
| 81 | DA | 2625 | C | O4'-C1'-C2' | -9.89 | 95.91 | 105.80 |
| 81 | DA | 461 | U | O4'-C1'-N1 | 9.89 | 116.11 | 108.20 |
| 81 | DA | 819 | U | O4'-C1'-N1 | 9.89 | 116.11 | 108.20 |
| 81 | DA | 1862 | U | O4'-C1'-N1 | 9.89 | 116.11 | 108.20 |
| 72 | Bt | 60 | ASN | CB-CA-C | -9.88 | 90.63 | 110.40 |
| 78 | CA | 252 | U | O4'-C1'-C2' | -9.88 | 95.92 | 105.80 |
| 78 | CA | 1222 | C | P-O3'-C3' | 9.88 | 131.56 | 119.70 |
| 81 | DA | 2477 | G | O4'-C1'-N9 | 9.88 | 116.11 | 108.20 |
| 74 | BQ | 198 | TYR | CB-CG-CD2 | 9.88 | 126.93 | 121.00 |
| 81 | DA | 2447 | A | P-O3'-C3' | 9.88 | 131.56 | 119.70 |
| 81 | DA | 2520 | A | N9-C1'-C2' | -9.88 | 101.13 | 112.00 |
| 81 | DA | 3220 | G | O4'-C1'-N9 | 9.88 | 116.10 | 108.20 |
| 81 | DA | 2132 | C | O4'-C1'-N1 | 9.87 | 116.10 | 108.20 |
| 78 | CA | 842 | C | O4'-C1'-N1 | 9.87 | 116.10 | 108.20 |
| 81 | DA | 2618 | G | P-O3'-C3' | 9.87 | 131.54 | 119.70 |
| 81 | DA | 2645 | G | O4'-C1'-N9 | 9.87 | 116.09 | 108.20 |
| 78 | CA | 16 | G | N9-C1'-C2' | -9.87 | 101.15 | 112.00 |
| 82 | DB | 46 | G | N9-C1'-C2' | 9.87 | 126.83 | 114.00 |
| 81 | DA | 2596 | U | O4'-C1'-N1 | 9.86 | 116.09 | 108.20 |
| 81 | DA | 924 | G | C3'-C2'-C1' | 9.86 | 109.39 | 101.50 |
| 1 | Aa | 48 | THR | C-N-CA | -9.86 | 101.60 | 122.30 |
| 18 | AP | 57 | LYS | N-CA-C | -9.86 | 84.38 | 111.00 |
| 61 | Bj | 21 | ARG | CA-C-O | -9.86 | 99.40 | 120.10 |
| 78 | CA | 1551 | U | O5'-P-OP2 | 9.86 | 122.53 | 110.70 |
| 81 | DA | 2948 | C | N1-C1'-C2' | 9.86 | 126.82 | 114.00 |
| 78 | CA | 1741 | U | O4'-C1'-N1 | 9.85 | 116.08 | 108.20 |
| 81 | DA | 1850 | A | O4'-C1'-N9 | 9.85 | 116.08 | 108.20 |
| 4 | AD | 235 | TYR | CA-C-O | -9.85 | 99.42 | 120.10 |
| 5 | AC | 82 | ARG | NE-CZ-NH1 | 9.85 | 125.22 | 120.30 |
| 22 | AV | 105 | THR | CA-C-O | -9.85 | 99.42 | 120.10 |
| 78 | CA | 1254 | U | P-O3'-C3' | -9.85 | 107.88 | 119.70 |
| 81 | DA | 677 | A | P-O5'-C5' | 9.85 | 136.66 | 120.90 |
| 13 | AL | 34 | LEU | N-CA-C | -9.85 | 84.41 | 111.00 |
| 81 | DA | 1513 | G | N9-C1'-C2' | 9.85 | 126.80 | 114.00 |
| 81 | DA | 1728 | G | O4'-C1'-C2' | 9.85 | 116.46 | 107.60 |
| 81 | DA | 1777 | U | P-O3'-C3' | 9.85 | 131.52 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2775 | U | O4'-C1'-N1 | 9.84 | 116.08 | 108.20 |
| 78 | CA | 887 | A | P-O3'-C3' | 9.84 | 131.51 | 119.70 |
| 78 | CA | 1547 | A | C5'-C4'-C3' | 9.84 | 131.75 | 116.00 |
| 82 | DB | 50 | C | O4'-C1'-N1 | 9.84 | 116.07 | 108.20 |
| 81 | DA | 1992 | U | O4'-C1'-N1 | 9.83 | 116.07 | 108.20 |
| 20 | AS | 91 | TYR | CB-CG-CD2 | -9.83 | 115.10 | 121.00 |
| 78 | CA | 105 | A | N9-C1'-C2' | 9.83 | 126.78 | 114.00 |
| 78 | CA | 1479 | A | C3'-C2'-C1' | -9.83 | 93.64 | 101.50 |
| 81 | DA | 3253 | G | N9-C1'-C2' | 9.83 | 126.78 | 114.00 |
| 1 | Aa | 61 | PHE | CB-CG-CD2 | 9.83 | 127.68 | 120.80 |
| 81 | DA | 1682 | U | C1'-O4'-C4' | 9.83 | 117.76 | 109.90 |
| 81 | DA | 2403 | G | O4'-C1'-N9 | 9.83 | 116.06 | 108.20 |
| 81 | DA | 2682 | C | O4'-C4'-C3' | -9.83 | 94.17 | 104.00 |
| 69 | Br | 104 | LEU | CA-C-N | 9.82 | 138.81 | 117.20 |
| 81 | DA | 1984 | C | P-O3'-C3' | 9.82 | 131.49 | 119.70 |
| 78 | CA | 1449 | U | O4'-C1'-N1 | 9.82 | 116.06 | 108.20 |
| 32 | BC | 379 | PHE | CB-CG-CD2 | 9.82 | 127.67 | 120.80 |
| 40 | BK | 46 | GLU | N-CA-CB | 9.82 | 128.27 | 110.60 |
| 78 | CA | 1338 | C | P-O5'-C5' | -9.82 | 105.19 | 120.90 |
| 81 | DA | 2988 | C | C1'-O4'-C4' | 9.82 | 117.75 | 109.90 |
| 82 | DB | 151 | C | P-O3'-C3' | 9.82 | 131.48 | 119.70 |
| 78 | CA | 95 | G | O4'-C1'-N9 | 9.81 | 116.05 | 108.20 |
| 78 | CA | 221 | A | O4'-C1'-N9 | 9.81 | 116.05 | 108.20 |
| 79 | CB | 41 | G | C1'-O4'-C4' | -9.81 | 102.05 | 109.90 |
| 81 | DA | 1044 | U | O4'-C1'-N1 | 9.81 | 116.05 | 108.20 |
| 81 | DA | 2657 | A | O4'-C1'-C2' | -9.81 | 95.99 | 105.80 |
| 81 | DA | 2233 | A | N9-C1'-C2' | -9.81 | 101.21 | 112.00 |
| 78 | CA | 845 | G | N1-C6-O6 | 9.80 | 125.78 | 119.90 |
| 81 | DA | 985 | U | O4'-C1'-N1 | 9.80 | 116.04 | 108.20 |
| 82 | DB | 144 | G | P-O3'-C3' | 9.80 | 131.47 | 119.70 |
| 32 | BC | 365 | PHE | CB-CG-CD1 | -9.80 | 113.94 | 120.80 |
| 81 | DA | 1859 | A | O4'-C1'-N9 | 9.80 | 116.04 | 108.20 |
| 81 | DA | 3313 | U | O4'-C1'-N1 | 9.80 | 116.04 | 108.20 |
| 81 | DA | 973 | A | C1'-O4'-C4' | -9.80 | 102.06 | 109.90 |
| 81 | DA | 1404 | G | C4'-C3'-C2' | -9.80 | 92.80 | 102.60 |
| 81 | DA | 2531 | C | C1'-O4'-C4' | 9.80 | 117.74 | 109.90 |
| 78 | CA | 900 | A | O5'-P-OP2 | -9.79 | 96.89 | 105.70 |
| 78 | CA | 1790 | A | P-O3'-C3' | -9.79 | 107.95 | 119.70 |
| 81 | DA | 562 | C | P-O3'-C3' | 9.79 | 131.45 | 119.70 |
| 81 | DA | 1873 | U | N1-C1'-C2' | 9.79 | 126.73 | 114.00 |
| 81 | DA | 1981 | G | O4'-C1'-N9 | 9.80 | 116.04 | 108.20 |
| 81 | DA | 3085 | G | O4'-C1'-C2' | 9.79 | 116.42 | 107.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|---|---|---|---|---|---|---|---|
| 59 | Bh | 127 | ALA | N-CA-CB | -9.79 | 96.39 | 110.10 |
| 78 | CA | 1462 | G | O4'-C1'-N9 | 9.79 | 116.03 | 108.20 |
| 81 | DA | 688 | G | O4'-C1'-N9 | 9.79 | 116.03 | 108.20 |
| 81 | DA | 2682 | C | O4'-C1'-C2' | -9.79 | 96.01 | 105.80 |
| 10 | AI | 112 | TYR | CB-CG-CD2 | -9.79 | 115.13 | 121.00 |
| 78 | CA | 1301 | U | P-O3'-C3' | 9.79 | 131.44 | 119.70 |
| 20 | AS | 56 | LYS | CB-CA-C | 9.78 | 129.96 | 110.40 |
| 81 | DA | 593 | C | O4'-C1'-N1 | 9.78 | 116.03 | 108.20 |
| 81 | DA | 2901 | G | O4'-C1'-C2' | 9.78 | 116.40 | 107.60 |
| 81 | DA | 1404 | G | O4'-C1'-N9 | 9.78 | 116.02 | 108.20 |
| 81 | DA | 2140 | U | O4'-C1'-N1 | 9.78 | 116.02 | 108.20 |
| 69 | Br | 47 | GLN | C-N-CA | 9.78 | 146.15 | 121.70 |
| 81 | DA | 1794 | G | O4'-C1'-N9 | 9.78 | 116.02 | 108.20 |
| 81 | DA | 513 | G | P-O3'-C3' | 9.78 | 131.43 | 119.70 |
| 81 | DA | 1221 | A | C3'-C2'-C1' | -9.78 | 93.68 | 101.50 |
| 78 | CA | 437 | A | O4'-C1'-N9 | 9.78 | 116.02 | 108.20 |
| 81 | DA | 3239 | G | N9-C1'-C2' | 9.78 | 126.71 | 114.00 |
| 40 | BK | 178 | VAL | CA-CB-CG1 | 9.77 | 125.56 | 110.90 |
| 78 | CA | 852 | C | P-O3'-C3' | 9.77 | 131.43 | 119.70 |
| 78 | CA | 1233 | G | C1'-O4'-C4' | 9.77 | 117.72 | 109.90 |
| 81 | DA | 3247 | G | P-O3'-C3' | 9.77 | 131.43 | 119.70 |
| 16 | AO | 113 | PHE | CB-CG-CD2 | 9.77 | 127.64 | 120.80 |
| 78 | CA | 1647 | U | O4'-C1'-N1 | 9.77 | 116.01 | 108.20 |
| 78 | CA | 1049 | U | P-O5'-C5' | 9.77 | 136.52 | 120.90 |
| 78 | CA | 484 | C | O4'-C1'-N1 | 9.76 | 116.01 | 108.20 |
| 81 | DA | 295 | A | C3'-C2'-C1' | 9.76 | 109.31 | 101.50 |
| 81 | DA | 2149 | A | N9-C1'-C2' | -9.76 | 101.26 | 112.00 |
| 78 | CA | 1672 | G | O4'-C1'-N9 | 9.76 | 116.01 | 108.20 |
| 81 | DA | 1686 | U | P-O3'-C3' | 9.76 | 131.41 | 119.70 |
| 81 | DA | 1951 | C | P-O3'-C3' | 9.76 | 131.41 | 119.70 |
| 81 | DA | 3254 | G | P-O3'-C3' | -9.76 | 107.99 | 119.70 |
| 81 | DA | 3045 | G | O4'-C1'-N9 | 9.76 | 116.00 | 108.20 |
| 42 | BM | 64 | LYS | CB-CA-C | 9.75 | 129.91 | 110.40 |
| 79 | CB | 19 | U | O4'-C1'-N1 | 9.75 | 116.00 | 108.20 |
| 81 | DA | 1017 | C | P-O3'-C3' | 9.75 | 131.40 | 119.70 |
| 81 | DA | 1870 | C | C4'-C3'-C2' | 9.75 | 112.35 | 102.60 |
| 18 | AP | 40 | LEU | CB-CA-C | 9.75 | 128.72 | 110.20 |
| 81 | DA | 1818 | U | O4'-C1'-N1 | 9.75 | 116.00 | 108.20 |
| 81 | DA | 1832 | C | O4'-C1'-N1 | 9.75 | 116.00 | 108.20 |
| 81 | DA | 2546 | C | O4'-C1'-N1 | 9.75 | 116.00 | 108.20 |
| 76 | BS | 117 | ARG | N-CA-CB | 9.75 | 128.14 | 110.60 |
| 78 | CA | 552 | G | O4'-C1'-N9 | 9.75 | 116.00 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1623 | G | O4'-C1'-N9 | 9.75 | 116.00 | 108.20 |
| 82 | DB | 125 | U | O4'-C1'-N1 | 9.75 | 116.00 | 108.20 |
| 81 | DA | 1230 | G | O4'-C1'-N9 | 9.74 | 116.00 | 108.20 |
| 81 | DA | 7 | C | C3'-C2'-C1' | 9.74 | 109.29 | 101.50 |
| 81 | DA | 126 | U | O4'-C1'-N1 | 9.74 | 115.99 | 108.20 |
| 78 | CA | 284 | G | C5'-C4'-C3' | 9.74 | 131.58 | 116.00 |
| 81 | DA | 160 | G | C3'-C2'-C1' | -9.74 | 93.71 | 101.50 |
| 83 | DC | 56 | G | O4'-C1'-N9 | 9.74 | 115.99 | 108.20 |
| 79 | CB | 11 | U | N1-C1'-C2' | -9.74 | 101.29 | 112.00 |
| 81 | DA | 2786 | G | O4'-C1'-N9 | 9.74 | 115.99 | 108.20 |
| 81 | DA | 2180 | G | O4'-C1'-C2' | 9.73 | 116.36 | 107.60 |
| 66 | Bo | 21 | ARG | NE-CZ-NH1 | 9.73 | 125.17 | 120.30 |
| 78 | CA | 222 | A | P-O3'-C3' | 9.73 | 131.38 | 119.70 |
| 78 | CA | 1427 | A | N1-C6-N6 | 9.73 | 124.44 | 118.60 |
| 81 | DA | 179 | C | C1'-O4'-C4' | -9.73 | 102.12 | 109.90 |
| 81 | DA | 720 | A | OP1-P-OP2 | -9.73 | 105.00 | 119.60 |
| 81 | DA | 741 | U | O4'-C1'-N1 | 9.73 | 115.98 | 108.20 |
| 81 | DA | 1895 | A | O4'-C1'-N9 | 9.73 | 115.98 | 108.20 |
| 81 | DA | 466 | G | P-O3'-C3' | 9.72 | 131.37 | 119.70 |
| 78 | CA | 623 | A | O4'-C1'-N9 | 9.72 | 115.98 | 108.20 |
| 78 | CA | 1053 | G | P-O3'-C3' | 9.72 | 131.37 | 119.70 |
| 81 | DA | 599 | C | C3'-C2'-C1' | 9.72 | 109.28 | 101.50 |
| 82 | DB | 120 | C | P-O3'-C3' | 9.72 | 131.36 | 119.70 |
| 78 | CA | 1091 | A | N9-C1'-C2' | -9.72 | 101.31 | 112.00 |
| 81 | DA | 721 | G | N9-C1'-C2' | -9.72 | 101.31 | 112.00 |
| 81 | DA | 2748 | A | C1'-O4'-C4' | 9.72 | 117.67 | 109.90 |
| 81 | DA | 1770 | G | N1-C6-O6 | 9.71 | 125.73 | 119.90 |
| 43 | BP | 13 | LYS | C-N-CA | 9.71 | 145.98 | 121.70 |
| 78 | CA | 280 | U | C3'-C2'-C1' | 9.71 | 109.27 | 101.50 |
| 78 | CA | 1091 | A | O4'-C1'-C2' | -9.71 | 96.09 | 105.80 |
| 81 | DA | 1474 | A | P-O3'-C3' | 9.71 | 131.35 | 119.70 |
| 82 | DB | 50 | C | O4'-C1'-C2' | -9.71 | 96.09 | 105.80 |
| 83 | DC | 21 | G | C1'-O4'-C4' | -9.71 | 102.14 | 109.90 |
| 51 | BZ | 70 | LYS | CA-C-O | -9.71 | 99.72 | 120.10 |
| 81 | DA | 1430 | U | O4'-C1'-N1 | 9.71 | 115.97 | 108.20 |
| 78 | CA | 503 | G | N1-C6-O6 | 9.70 | 125.72 | 119.90 |
| 81 | DA | 113 | C | C3'-C2'-C1' | 9.70 | 109.26 | 101.50 |
| 32 | BC | 300 | ARG | NE-CZ-NH2 | -9.70 | 115.45 | 120.30 |
| 81 | DA | 547 | G | P-O3'-C3' | 9.70 | 131.34 | 119.70 |
| 37 | BH | 84 | ARG | NE-CZ-NH1 | 9.70 | 125.15 | 120.30 |
| 81 | DA | 1222 | G | C1'-O4'-C4' | 9.70 | 117.66 | 109.90 |
| 40 | BK | 128 | ARG | C-N-CA | 9.70 | 145.94 | 121.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 3076 | C | N1-C1'-C2' | 9.70 | 126.60 | 114.00 |
| 40 | BK | 128 | ARG | O-C-N | -9.69 | 107.19 | 122.70 |
| 81 | DA | 736 | A | N1-C6-N6 | 9.69 | 124.42 | 118.60 |
| 78 | CA | 1451 | C | N1-C1'-C2' | 9.69 | 126.60 | 114.00 |
| 81 | DA | 1747 | G | P-O5'-C5' | 9.69 | 136.40 | 120.90 |
| 15 | AN | 47 | ALA | C-N-CA | 9.69 | 145.92 | 121.70 |
| 78 | CA | 93 | A | O4'-C1'-C2' | 9.69 | 116.32 | 107.60 |
| 67 | Bp | 34 | CYS | CB-CA-C | -9.68 | 91.03 | 110.40 |
| 78 | CA | 151 | G | C5'-C4'-C3' | -9.68 | 100.51 | 116.00 |
| 78 | CA | 299 | A | C1'-O4'-C4' | 9.68 | 117.65 | 109.90 |
| 81 | DA | 147 | U | C5'-C4'-C3' | 9.68 | 131.48 | 116.00 |
| 81 | DA | 2674 | A | C1'-O4'-C4' | -9.68 | 102.16 | 109.90 |
| 81 | DA | 2531 | C | O4'-C1'-N1 | 9.68 | 115.94 | 108.20 |
| 8 | AF | 29 | ILE | CB-CA-C | 9.67 | 130.94 | 111.60 |
| 61 | Bj | 20 | LYS | N-CA-C | -9.67 | 84.88 | 111.00 |
| 81 | DA | 2901 | G | O4'-C1'-N9 | 9.67 | 115.94 | 108.20 |
| 78 | CA | 386 | G | N9-C1'-C2' | 9.67 | 126.57 | 114.00 |
| 81 | DA | 298 | U | C3'-C2'-C1' | 9.67 | 109.23 | 101.50 |
| 83 | DC | 102 | C | O4'-C1'-N1 | -9.67 | 100.47 | 108.20 |
| 81 | DA | 2388 | U | O4'-C1'-N1 | 9.66 | 115.93 | 108.20 |
| 29 | AU | 94 | TYR | CB-CG-CD1 | -9.66 | 115.20 | 121.00 |
| 78 | CA | 1623 | C | P-O3'-C3' | 9.66 | 131.30 | 119.70 |
| 81 | DA | 1287 | A | O4'-C1'-C2' | -9.66 | 96.14 | 105.80 |
| 81 | DA | 2264 | U | N1-C1'-C2' | 9.66 | 126.56 | 114.00 |
| 81 | DA | 2656 | A | N9-C1'-C2' | 9.66 | 126.56 | 114.00 |
| 72 | Bu | 60 | ASN | CB-CA-C | -9.66 | 91.08 | 110.40 |
| 81 | DA | 2041 | U | C1'-O4'-C4' | 9.66 | 117.63 | 109.90 |
| 81 | DA | 635 | G | P-O5'-C5' | -9.66 | 105.44 | 120.90 |
| 78 | CA | 227 | U | P-O3'-C3' | -9.66 | 108.11 | 119.70 |
| 79 | CB | 44 | A | O4'-C1'-N9 | 9.66 | 115.93 | 108.20 |
| 81 | DA | 1291 | A | O4'-C1'-N9 | 9.66 | 115.93 | 108.20 |
| 81 | DA | 2791 | G | O4'-C1'-N9 | 9.66 | 115.93 | 108.20 |
| 74 | BQ | 12 | TYR | CB-CG-CD2 | -9.66 | 115.20 | 121.00 |
| 81 | DA | 1782 | U | C5'-C4'-C3' | -9.66 | 100.55 | 116.00 |
| 14 | AM | 120 | ARG | NE-CZ-NH1 | 9.66 | 125.13 | 120.30 |
| 81 | DA | 211 | A | O4'-C1'-C2' | -9.66 | 96.14 | 105.80 |
| 79 | CB | 7 | A | P-O3'-C3' | 9.65 | 131.28 | 119.70 |
| 32 | BC | 123 | TYR | N-CA-CB | 9.65 | 127.97 | 110.60 |
| 81 | DA | 236 | G | O4'-C1'-N9 | 9.65 | 115.92 | 108.20 |
| 82 | DB | 41 | A | O4'-C1'-C2' | 9.65 | 116.28 | 107.60 |
| 81 | DA | 3168 | A | O4'-C1'-N9 | 9.65 | 115.92 | 108.20 |
| 42 | BM | 64 | LYS | O-C-N | -9.65 | 106.80 | 123.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1169 | A | N9-C1'-C2' | 9.65 | 126.54 | 114.00 |
| 81 | DA | 3245 | A | C1'-O4'-C4' | -9.65 | 102.18 | 109.90 |
| 2 | AA | 179 | ARG | NE-CZ-NH2 | -9.64 | 115.48 | 120.30 |
| 57 | Be | 41 | ARG | NE-CZ-NH2 | -9.64 | 115.48 | 120.30 |
| 78 | CA | 221 | A | P-O3'-C3' | 9.64 | 131.28 | 119.70 |
| 81 | DA | 250 | U | C5'-C4'-C3' | 9.64 | 131.43 | 116.00 |
| 81 | DA | 3283 | U | O4'-C1'-N1 | 9.64 | 115.92 | 108.20 |
| 78 | CA | 1220 | C | C5'-C4'-C3' | 9.64 | 131.42 | 116.00 |
| 81 | DA | 831 | G | O4'-C1'-N9 | 9.64 | 115.91 | 108.20 |
| 81 | DA | 3221 | C | C4'-C3'-C2' | -9.64 | 92.96 | 102.60 |
| 20 | AS | 53 | TRP | CA-C-N | -9.63 | 96.01 | 117.20 |
| 81 | DA | 3251 | U | O4'-C1'-N1 | 9.63 | 115.91 | 108.20 |
| 78 | CA | 1432 | U | P-O3'-C3' | 9.63 | 131.25 | 119.70 |
| 37 | BH | 158 | ASP | CB-CA-C | -9.63 | 91.15 | 110.40 |
| 78 | CA | 658 | C | P-O3'-C3' | 9.62 | 131.25 | 119.70 |
| 81 | DA | 672 | A | O3'-P-O5' | -9.62 | 85.72 | 104.00 |
| 74 | BQ | 260 | PHE | CB-CG-CD2 | 9.62 | 127.54 | 120.80 |
| 39 | BJ | 90 | ARG | NE-CZ-NH2 | -9.62 | 115.49 | 120.30 |
| 76 | BS | 156 | ARG | NE-CZ-NH2 | -9.62 | 115.49 | 120.30 |
| 78 | CA | 432 | G | O4'-C1'-N9 | 9.61 | 115.89 | 108.20 |
| 78 | CA | 836 | U | O4'-C1'-N1 | 9.62 | 115.89 | 108.20 |
| 78 | CA | 899 | G | C1'-O4'-C4' | -9.62 | 102.21 | 109.90 |
| 81 | DA | 2428 | U | O4'-C1'-N1 | 9.62 | 115.89 | 108.20 |
| 83 | DC | 71 | C | O4'-C1'-C2' | -9.61 | 96.19 | 105.80 |
| 4 | AD | 86 | PHE | CB-CG-CD2 | -9.61 | 114.07 | 120.80 |
| 17 | AQ | 63 | LYS | N-CA-C | 9.61 | 136.95 | 111.00 |
| 72 | Bt | 60 | ASN | O-C-N | -9.61 | 107.33 | 122.70 |
| 78 | CA | 961 | U | O4'-C1'-N1 | 9.61 | 115.89 | 108.20 |
| 81 | DA | 3320 | A | P-O3'-C3' | 9.61 | 131.23 | 119.70 |
| 83 | DC | 32 | U | N1-C1'-C2' | 9.61 | 126.49 | 114.00 |
| 26 | AZ | 58 | PRO | CA-N-CD | -9.61 | 98.05 | 111.50 |
| 4 | AD | 235 | TYR | CB-CA-C | -9.60 | 91.19 | 110.40 |
| 81 | DA | 607 | A | N9-C1'-C2' | -9.60 | 101.44 | 112.00 |
| 81 | DA | 3148 | U | P-O3'-C3' | 9.60 | 131.22 | 119.70 |
| 81 | DA | 1802 | C | O4'-C1'-C2' | -9.60 | 96.20 | 105.80 |
| 81 | DA | 1948 | G | O4'-C1'-N9 | 9.60 | 115.88 | 108.20 |
| 82 | DB | 46 | G | C3'-C2'-C1' | -9.60 | 93.82 | 101.50 |
| 4 | AD | 93 | ASP | N-CA-CB | -9.60 | 93.33 | 110.60 |
| 78 | CA | 1592 | A | O4'-C1'-N9 | 9.60 | 115.88 | 108.20 |
| 57 | Be | 51 | TYR | CB-CG-CD2 | -9.60 | 115.24 | 121.00 |
| 78 | CA | 953 | G | O4'-C1'-N9 | 9.60 | 115.88 | 108.20 |
| 37 | BH | 89 | GLU | OE1-CD-OE2 | -9.59 | 111.79 | 123.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 955 | A | O4'-C1'-C2' | -9.59 | 96.21 | 105.80 |
| 78 | CA | 288 | A | N9-C1'-C2' | -9.59 | 101.45 | 112.00 |
| 81 | DA | 392 | G | O4'-C1'-N9 | 9.59 | 115.87 | 108.20 |
| 5 | AC | 62 | ARG | NE-CZ-NH2 | -9.59 | 115.51 | 120.30 |
| 78 | CA | 626 | U | P-O3'-C3' | 9.59 | 131.20 | 119.70 |
| 81 | DA | 1128 | U | N1-C1'-C2' | 9.59 | 126.46 | 114.00 |
| 81 | DA | 854 | G | P-O3'-C3' | 9.58 | 131.20 | 119.70 |
| 81 | DA | 1786 | G | C3'-C2'-C1' | -9.58 | 93.83 | 101.50 |
| 81 | DA | 2375 | G | P-O3'-C3' | 9.58 | 131.20 | 119.70 |
| 55 | Bc | 67 | ARG | NE-CZ-NH2 | -9.58 | 115.51 | 120.30 |
| 81 | DA | 363 | G | O4'-C1'-N9 | 9.58 | 115.86 | 108.20 |
| 81 | DA | 1358 | C | N1-C1'-C2' | 9.58 | 126.45 | 114.00 |
| 78 | CA | 1765 | A | N9-C1'-C2' | 9.58 | 126.45 | 114.00 |
| 74 | BQ | 158 | ARG | NE-CZ-NH1 | 9.58 | 125.09 | 120.30 |
| 78 | CA | 1520 | U | C4'-C3'-O3' | -9.57 | 89.29 | 109.40 |
| 79 | CB | 26 | G | O4'-C1'-N9 | 9.57 | 115.86 | 108.20 |
| 82 | DB | 116 | G | O4'-C1'-N9 | 9.57 | 115.86 | 108.20 |
| 78 | CA | 81 | G | N9-C1'-C2' | 9.57 | 126.44 | 114.00 |
| 78 | CA | 913 | G | O4'-C1'-N9 | 9.57 | 115.86 | 108.20 |
| 78 | CA | 54 | C | O4'-C1'-N1 | 9.57 | 115.86 | 108.20 |
| 79 | CB | 2 | C | N1-C1'-C2' | 9.57 | 126.44 | 114.00 |
| 81 | DA | 25 | U | P-O5'-C5' | 9.57 | 136.21 | 120.90 |
| 81 | DA | 30 | G | O4'-C1'-N9 | 9.57 | 115.86 | 108.20 |
| 22 | AV | 106 | ALA | N-CA-CB | 9.57 | 123.49 | 110.10 |
| 78 | CA | 921 | U | O4'-C1'-N1 | 9.57 | 115.86 | 108.20 |
| 60 | Bi | 55 | SER | CA-C-O | -9.57 | 100.01 | 120.10 |
| 81 | DA | 2231 | C | O4'-C1'-N1 | -9.57 | 100.55 | 108.20 |
| 83 | DC | 79 | U | O4'-C1'-N1 | 9.57 | 115.85 | 108.20 |
| 78 | CA | 154 | G | C3'-C2'-C1' | 9.56 | 109.15 | 101.50 |
| 81 | DA | 299 | G | C5'-C4'-C3' | 9.56 | 131.30 | 116.00 |
| 81 | DA | 3048 | A | C3'-C2'-C1' | 9.56 | 109.15 | 101.50 |
| 81 | DA | 736 | A | P-O5'-C5' | 9.56 | 136.20 | 120.90 |
| 8 | AF | 27 | THR | CB-CA-C | 9.56 | 137.41 | 111.60 |
| 13 | AL | 7 | ARG | NE-CZ-NH2 | -9.56 | 115.52 | 120.30 |
| 81 | DA | 1624 | G | C3'-C2'-C1' | 9.56 | 109.14 | 101.50 |
| 81 | DA | 3237 | U | O4'-C1'-N1 | 9.56 | 115.85 | 108.20 |
| 81 | DA | 816 | A | O4'-C1'-N9 | -9.56 | 100.56 | 108.20 |
| 78 | CA | 165 | G | O4'-C1'-N9 | 9.55 | 115.84 | 108.20 |
| 81 | DA | 2016 | U | O4'-C1'-N1 | 9.55 | 115.84 | 108.20 |
| 81 | DA | 2176 | U | C1'-O4'-C4' | 9.55 | 117.54 | 109.90 |
| 81 | DA | 576 | C | N1-C1'-C2' | 9.55 | 126.42 | 114.00 |
| 82 | DB | 4 | C | O4'-C1'-N1 | 9.55 | 115.84 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | AD | 218 | PHE | C-N-CA | 9.55 | 145.57 | 121.70 |
| 38 | Bs | 180 | PRO | CB-CA-C | -9.55 | 88.13 | 112.00 |
| 81 | DA | 1448 | U | O4'-C1'-N1 | 9.55 | 115.84 | 108.20 |
| 55 | Bc | 89 | ARG | NE-CZ-NH1 | 9.54 | 125.07 | 120.30 |
| 78 | CA | 1235 | C | C3'-C2'-C1' | -9.54 | 93.86 | 101.50 |
| 78 | CA | 1700 | C | P-O3'-C3' | 9.54 | 131.15 | 119.70 |
| 81 | DA | 317 | A | N9-C1'-C2' | 9.54 | 126.41 | 114.00 |
| 81 | DA | 2803 | A | N9-C1'-C2' | -9.55 | 101.50 | 112.00 |
| 78 | CA | 93 | A | O4'-C1'-N9 | 9.54 | 115.83 | 108.20 |
| 81 | DA | 687 | U | P-O3'-C3' | 9.54 | 131.15 | 119.70 |
| 78 | CA | 1123 | C | C3'-C2'-C1' | 9.54 | 109.13 | 101.50 |
| 81 | DA | 1533 | U | O4'-C1'-N1 | 9.54 | 115.83 | 108.20 |
| 81 | DA | 1586 | G | P-O3'-C3' | 9.54 | 131.15 | 119.70 |
| 29 | AU | 5 | VAL | N-CA-CB | 9.54 | 132.49 | 111.50 |
| 78 | CA | 315 | A | O4'-C1'-N9 | 9.54 | 115.83 | 108.20 |
| 81 | DA | 506 | U | P-O3'-C3' | 9.54 | 131.15 | 119.70 |
| 81 | DA | 734 | C | O4'-C1'-N1 | 9.54 | 115.83 | 108.20 |
| 81 | DA | 314 | U | O4'-C1'-N1 | 9.54 | 115.83 | 108.20 |
| 81 | DA | 1677 | G | C3'-C2'-C1' | -9.54 | 93.87 | 101.50 |
| 43 | BP | 180 | PHE | O-C-N | -9.53 | 107.45 | 122.70 |
| 81 | DA | 177 | U | P-O3'-C3' | -9.53 | 108.26 | 119.70 |
| 81 | DA | 3169 | U | P-O3'-C3' | 9.53 | 131.14 | 119.70 |
| 26 | AZ | 54 | ARG | NE-CZ-NH1 | 9.53 | 125.06 | 120.30 |
| 81 | DA | 2130 | G | O4'-C1'-C2' | -9.53 | 96.27 | 105.80 |
| 78 | CA | 457 | G | C1'-O4'-C4' | -9.53 | 102.28 | 109.90 |
| 81 | DA | 2334 | U | P-O3'-C3' | 9.53 | 131.13 | 119.70 |
| 81 | DA | 1686 | U | O4'-C1'-N1 | 9.53 | 115.82 | 108.20 |
| 81 | DA | 1724 | U | O4'-C1'-N1 | 9.53 | 115.82 | 108.20 |
| 81 | DA | 1446 | A | N9-C1'-C2' | -9.52 | 101.53 | 112.00 |
| 81 | DA | 2372 | A | O4'-C1'-N9 | -9.52 | 100.58 | 108.20 |
| 78 | CA | 651 | G | C5'-C4'-C3' | 9.52 | 131.23 | 116.00 |
| 81 | DA | 2697 | A | P-O3'-C3' | 9.52 | 131.12 | 119.70 |
| 81 | DA | 2991 | A | O4'-C1'-N9 | 9.52 | 115.82 | 108.20 |
| 78 | CA | 849 | C | C1'-O4'-C4' | -9.52 | 102.29 | 109.90 |
| 39 | BJ | 14 | TYR | CB-CA-C | 9.52 | 129.43 | 110.40 |
| 78 | CA | 1565 | C | O4'-C1'-C2' | -9.52 | 96.28 | 105.80 |
| 81 | DA | 1256 | G | O3'-P-O5' | -9.52 | 85.92 | 104.00 |
| 78 | CA | 1288 | G | P-O3'-C3' | 9.51 | 131.12 | 119.70 |
| 81 | DA | 2794 | G | P-O3'-C3' | 9.51 | 131.12 | 119.70 |
| 78 | CA | 177 | U | O4'-C1'-N1 | 9.51 | 115.81 | 108.20 |
| 78 | CA | 607 | G | O4'-C1'-N9 | 9.51 | 115.81 | 108.20 |
| 37 | BH | 232 | HIS | N-CA-CB | 9.51 | 127.72 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 1712 | A | O4'-C1'-N9 | 9.51 | 115.81 | 108.20 |
| 81 | DA | 2444 | C | C4'-C3'-C2' | -9.51 | 93.09 | 102.60 |
| 81 | DA | 2915 | U | O3'-P-O5' | 9.51 | 122.07 | 104.00 |
| 81 | DA | 3215 | A | O4'-C1'-C2' | -9.51 | 96.29 | 105.80 |
| 53 | Ba | 85 | TYR | CB-CG-CD2 | -9.51 | 115.30 | 121.00 |
| 81 | DA | 774 | G | N9-C1'-C2' | 9.51 | 126.36 | 114.00 |
| 81 | DA | 1100 | U | O4'-C1'-N1 | 9.51 | 115.81 | 108.20 |
| 6 | AE | 98 | PHE | CB-CG-CD1 | -9.50 | 114.15 | 120.80 |
| 78 | CA | 1419 | G | O3'-P-O5' | -9.50 | 85.94 | 104.00 |
| 81 | DA | 693 | A | P-O3'-C3' | 9.50 | 131.10 | 119.70 |
| 81 | DA | 2062 | G | O4'-C1'-N9 | 9.50 | 115.80 | 108.20 |
| 78 | CA | 86 | A | P-O3'-C3' | 9.50 | 131.10 | 119.70 |
| 78 | CA | 610 | G | O4'-C1'-C2' | 9.50 | 116.15 | 107.60 |
| 81 | DA | 833 | G | O4'-C1'-N9 | 9.50 | 115.80 | 108.20 |
| 81 | DA | 3035 | A | O4'-C1'-N9 | 9.50 | 115.80 | 108.20 |
| 78 | CA | 1088 | A | O4'-C1'-N9 | 9.49 | 115.80 | 108.20 |
| 5 | AC | 194 | ALA | C-N-CA | 9.49 | 145.43 | 121.70 |
| 78 | CA | 679 | U | P-O3'-C3' | -9.49 | 108.31 | 119.70 |
| 78 | CA | 1201 | G | C3'-C2'-C1' | 9.49 | 109.09 | 101.50 |
| 81 | DA | 628 | A | O4'-C1'-N9 | 9.49 | 115.79 | 108.20 |
| 81 | DA | 1680 | G | O4'-C1'-N9 | 9.49 | 115.80 | 108.20 |
| 81 | DA | 758 | C | O4'-C1'-N1 | 9.49 | 115.79 | 108.20 |
| 82 | DB | 45 | C | C3'-C2'-C1' | 9.49 | 109.09 | 101.50 |
| 78 | CA | 955 | A | C1'-O4'-C4' | 9.49 | 117.49 | 109.90 |
| 81 | DA | 147 | U | O5'-P-OP2 | -9.49 | 97.16 | 105.70 |
| 81 | DA | 3351 | U | O4'-C1'-N1 | 9.49 | 115.79 | 108.20 |
| 81 | DA | 161 | G | O4'-C1'-N9 | 9.49 | 115.79 | 108.20 |
| 81 | DA | 658 | G | C1'-O4'-C4' | -9.49 | 102.31 | 109.90 |
| 81 | DA | 2591 | A | P-O3'-C3' | 9.49 | 131.08 | 119.70 |
| 35 | BG | 158 | TYR | CB-CG-CD1 | 9.48 | 126.69 | 121.00 |
| 81 | DA | 113 | C | N1-C1'-C2' | 9.48 | 126.33 | 114.00 |
| 78 | CA | 1615 | C | O4'-C1'-C2' | -9.48 | 96.32 | 105.80 |
| 13 | AL | 6 | PRO | CA-N-CD | -9.48 | 98.23 | 111.50 |
| 78 | CA | 288 | A | C1'-O4'-C4' | 9.48 | 117.48 | 109.90 |
| 81 | DA | 2152 | A | C5'-C4'-C3' | 9.48 | 131.16 | 116.00 |
| 52 | BY | 27 | ARG | NE-CZ-NH1 | 9.47 | 125.04 | 120.30 |
| 81 | DA | 570 | A | O4'-C1'-N9 | 9.47 | 115.78 | 108.20 |
| 82 | DB | 28 | C | P-O3'-C3' | -9.47 | 108.33 | 119.70 |
| 81 | DA | 250 | U | O4'-C1'-N1 | 9.47 | 115.78 | 108.20 |
| 81 | DA | 672 | A | P-O5'-C5' | 9.47 | 136.06 | 120.90 |
| 57 | Be | 176 | TYR | CB-CG-CD2 | 9.47 | 126.68 | 121.00 |
| 81 | DA | 1767 | C | O4'-C1'-N1 | 9.47 | 115.78 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | BG | 101 | PHE | N-CA-CB | 9.47 | 127.64 | 110.60 |
| 79 | CB | 33 | U | O4'-C1'-N1 | 9.47 | 115.77 | 108.20 |
| 37 | BH | 84 | ARG | NE-CZ-NH2 | -9.47 | 115.57 | 120.30 |
| 37 | BH | 128 | LYS | C-N-CD | -9.46 | 99.78 | 120.60 |
| 81 | DA | 2026 | A | P-O5'-C5' | 9.46 | 136.04 | 120.90 |
| 31 | BB | 66 | PRO | O-C-N | 9.46 | 137.84 | 122.70 |
| 81 | DA | 1299 | U | O4'-C1'-N1 | 9.46 | 115.77 | 108.20 |
| 81 | DA | 3010 | U | C1'-O4'-C4' | 9.46 | 117.47 | 109.90 |
| 31 | BB | 196 | TRP | CB-CA-C | -9.46 | 91.48 | 110.40 |
| 81 | DA | 1393 | A | P-O3'-C3' | 9.46 | 131.05 | 119.70 |
| 81 | DA | 1675 | G | O4'-C1'-C2' | 9.46 | 116.11 | 107.60 |
| 81 | DA | 1788 | C | O4'-C1'-N1 | 9.46 | 115.77 | 108.20 |
| 78 | CA | 10 | G | C3'-C2'-C1' | 9.46 | 109.07 | 101.50 |
| 81 | DA | 557 | A | O4'-C1'-N9 | 9.46 | 115.77 | 108.20 |
| 81 | DA | 3324 | C | C5'-C4'-C3' | 9.46 | 131.13 | 116.00 |
| 81 | DA | 1839 | A | N9-C1'-C2' | 9.46 | 126.29 | 114.00 |
| 78 | CA | 230 | C | C3'-C2'-C1' | 9.46 | 109.06 | 101.50 |
| 81 | DA | 2209 | U | O4'-C1'-N1 | 9.46 | 115.77 | 108.20 |
| 81 | DA | 2677 | G | P-O3'-C3' | 9.46 | 131.05 | 119.70 |
| 81 | DA | 2875 | U | O4'-C1'-N1 | 9.46 | 115.76 | 108.20 |
| 45 | BR | 96 | PHE | CB-CG-CD1 | -9.45 | 114.18 | 120.80 |
| 81 | DA | 1767 | C | P-O3'-C3' | 9.45 | 131.04 | 119.70 |
| 3 | AB | 75 | LYS | CB-CA-C | -9.45 | 91.50 | 110.40 |
| 45 | BR | 105 | ARG | NE-CZ-NH2 | 9.45 | 125.03 | 120.30 |
| 78 | CA | 1502 | G | P-O3'-C3' | 9.45 | 131.04 | 119.70 |
| 81 | DA | 3103 | A | O4'-C1'-C2' | -9.45 | 96.35 | 105.80 |
| 19 | AR | 54 | ALA | N-CA-CB | 9.44 | 123.32 | 110.10 |
| 34 | BE | 116 | TYR | CE1-CZ-CE2 | -9.45 | 104.69 | 119.80 |
| 58 | Bg | 93 | VAL | N-CA-CB | 9.45 | 132.28 | 111.50 |
| 78 | CA | 647 | G | O5'-P-OP2 | -9.45 | 97.20 | 105.70 |
| 81 | DA | 2731 | U | O4'-C1'-N1 | 9.45 | 115.76 | 108.20 |
| 81 | DA | 1677 | G | O4'-C1'-C2' | 9.44 | 116.10 | 107.60 |
| 6 | AE | 7 | GLN | CB-CA-C | 9.44 | 129.28 | 110.40 |
| 78 | CA | 1549 | C | C3'-C2'-C1' | 9.44 | 109.05 | 101.50 |
| 78 | CA | 1230 | A | P-O5'-C5' | 9.44 | 136.00 | 120.90 |
| 78 | CA | 1614 | A | C3'-C2'-C1' | 9.44 | 109.05 | 101.50 |
| 81 | DA | 259 | C | C3'-C2'-C1' | 9.44 | 109.05 | 101.50 |
| 81 | DA | 2019 | U | O4'-C1'-N1 | 9.44 | 115.75 | 108.20 |
| 78 | CA | 1672 | G | P-O3'-C3' | 9.44 | 131.02 | 119.70 |
| 81 | DA | 44 | U | P-O3'-C3' | -9.44 | 108.38 | 119.70 |
| 81 | DA | 471 | U | O4'-C1'-N1 | 9.44 | 115.75 | 108.20 |
| 81 | DA | 750 | G | P-O3'-C3' | 9.44 | 131.02 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 384 | A | N9-C1'-C2' | 9.43 | 126.27 | 114.00 |
| 81 | DA | 1008 | U | O4'-C1'-N1 | 9.43 | 115.75 | 108.20 |
| 81 | DA | 2131 | A | C1'-O4'-C4' | -9.43 | 102.35 | 109.90 |
| 83 | DC | 22 | A | P-O3'-C3' | 9.43 | 131.02 | 119.70 |
| 78 | CA | 1440 | C | P-O3'-C3' | -9.43 | 108.38 | 119.70 |
| 81 | DA | 294 | U | O4'-C1'-N1 | 9.43 | 115.75 | 108.20 |
| 81 | DA | 2266 | U | C3'-C2'-C1' | 9.43 | 109.05 | 101.50 |
| 81 | DA | 269 | G | O4'-C1'-N9 | 9.43 | 115.75 | 108.20 |
| 81 | DA | 1055 | A | C3'-C2'-C1' | 9.43 | 109.05 | 101.50 |
| 78 | CA | 1583 | A | P-O3'-C3' | 9.43 | 131.01 | 119.70 |
| 78 | CA | 924 | A | O4'-C1'-N9 | 9.43 | 115.74 | 108.20 |
| 81 | DA | 1493 | G | N9-C1'-C2' | -9.43 | 101.63 | 112.00 |
| 59 | Bh | 20 | HIS | CB-CA-C | -9.42 | 91.55 | 110.40 |
| 81 | DA | 709 | A | P-O3'-C3' | 9.42 | 131.01 | 119.70 |
| 81 | DA | 2248 | C | C3'-C2'-C1' | 9.42 | 109.04 | 101.50 |
| 81 | DA | 3041 | U | O4'-C1'-N1 | 9.42 | 115.74 | 108.20 |
| 78 | CA | 24 | U | O4'-C1'-N1 | 9.42 | 115.74 | 108.20 |
| 81 | DA | 1397 | C | N1-C1'-C2' | 9.42 | 126.25 | 114.00 |
| 81 | DA | 48 | A | O4'-C1'-N9 | 9.42 | 115.74 | 108.20 |
| 81 | DA | 671 | U | C4'-C3'-C2' | -9.42 | 93.18 | 102.60 |
| 78 | CA | 837 | G | O4'-C1'-N9 | 9.42 | 115.73 | 108.20 |
| 81 | DA | 810 | A | O4'-C1'-N9 | 9.42 | 115.73 | 108.20 |
| 78 | CA | 639 | U | O4'-C1'-N1 | 9.41 | 115.73 | 108.20 |
| 78 | CA | 656 | G | O4'-C1'-N9 | 9.41 | 115.73 | 108.20 |
| 81 | DA | 328 | U | O4'-C1'-N1 | 9.41 | 115.73 | 108.20 |
| 81 | DA | 2085 | U | C5'-C4'-C3' | 9.41 | 131.06 | 116.00 |
| 37 | BH | 222 | PHE | CB-CG-CD1 | -9.41 | 114.21 | 120.80 |
| 78 | CA | 1650 | U | O4'-C1'-N1 | 9.41 | 115.73 | 108.20 |
| 81 | DA | 234 | G | O4'-C1'-N9 | 9.41 | 115.73 | 108.20 |
| 52 | BY | 40 | ARG | NE-CZ-NH1 | 9.41 | 125.00 | 120.30 |
| 20 | AS | 123 | ARG | NE-CZ-NH1 | 9.41 | 125.00 | 120.30 |
| 78 | CA | 497 | G | N1-C6-O6 | 9.41 | 125.54 | 119.90 |
| 81 | DA | 845 | G | C3'-C2'-C1' | -9.41 | 93.97 | 101.50 |
| 81 | DA | 1302 | A | O4'-C1'-N9 | 9.40 | 115.72 | 108.20 |
| 81 | DA | 1889 | G | C1'-O4'-C4' | -9.40 | 102.38 | 109.90 |
| 33 | BD | 318 | LEU | C-N-CA | 9.40 | 145.20 | 121.70 |
| 78 | CA | 1601 | G | N9-C1'-C2' | 9.40 | 126.22 | 114.00 |
| 82 | DB | 4 | C | C5'-C4'-C3' | 9.40 | 131.04 | 116.00 |
| 82 | DB | 43 | A | O4'-C1'-N9 | 9.40 | 115.72 | 108.20 |
| 78 | CA | 38 | C | C3'-C2'-C1' | 9.40 | 109.02 | 101.50 |
| 81 | DA | 728 | G | N1-C6-O6 | 9.40 | 125.54 | 119.90 |
| 81 | DA | 1700 | G | O4'-C1'-N9 | 9.40 | 115.72 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1798 | A | O4'-C1'-N9 | 9.40 | 115.72 | 108.20 |
| 81 | DA | 2769 | A | P-O3'-C3' | -9.40 | 108.42 | 119.70 |
| 81 | DA | 3390 | G | C5'-C4'-C3' | 9.40 | 131.03 | 116.00 |
| 81 | DA | 2837 | A | N9-C1'-C2' | -9.39 | 101.67 | 112.00 |
| 78 | CA | 1158 | C | O4'-C1'-C2' | -9.39 | 96.41 | 105.80 |
| 61 | Bj | 8 | TYR | CB-CG-CD2 | 9.39 | 126.64 | 121.00 |
| 78 | CA | 63 | G | O4'-C1'-N9 | 9.39 | 115.71 | 108.20 |
| 81 | DA | 916 | G | O4'-C1'-N9 | 9.39 | 115.71 | 108.20 |
| 78 | CA | 175 | G | O4'-C1'-N9 | 9.39 | 115.71 | 108.20 |
| 78 | CA | 960 | U | N1-C1'-C2' | -9.39 | 101.67 | 112.00 |
| 81 | DA | 2098 | C | P-O3'-C3' | 9.39 | 130.97 | 119.70 |
| 81 | DA | 850 | U | O4'-C1'-N1 | 9.39 | 115.71 | 108.20 |
| 81 | DA | 1983 | G | P-O3'-C3' | 9.39 | 130.97 | 119.70 |
| 83 | DC | 31 | U | N1-C1'-C2' | -9.39 | 101.67 | 112.00 |
| 78 | CA | 841 | U | C5'-C4'-C3' | 9.39 | 131.02 | 116.00 |
| 81 | DA | 1699 | A | C1'-O4'-C4' | 9.39 | 117.41 | 109.90 |
| 81 | DA | 2971 | A | P-O3'-C3' | 9.38 | 130.96 | 119.70 |
| 48 | BW | 93 | ILE | CB-CA-C | -9.38 | 92.83 | 111.60 |
| 78 | CA | 1536 | G | N9-C1'-C2' | 9.38 | 126.20 | 114.00 |
| 81 | DA | 1769 | G | N1-C6-O6 | 9.38 | 125.53 | 119.90 |
| 81 | DA | 2516 | U | O4'-C1'-N1 | 9.38 | 115.71 | 108.20 |
| 81 | DA | 1759 | C | O4'-C1'-N1 | 9.38 | 115.70 | 108.20 |
| 81 | DA | 1830 | G | O4'-C1'-N9 | 9.38 | 115.70 | 108.20 |
| 81 | DA | 1909 | A | O4'-C1'-N9 | 9.38 | 115.70 | 108.20 |
| 78 | CA | 1613 | U | C1'-O4'-C4' | 9.38 | 117.40 | 109.90 |
| 81 | DA | 606 | C | N1-C1'-C2' | 9.38 | 126.19 | 114.00 |
| 81 | DA | 1904 | C | N1-C1'-C2' | 9.38 | 126.19 | 114.00 |
| 78 | CA | 636 | A | O4'-C1'-N9 | 9.38 | 115.70 | 108.20 |
| 81 | DA | 2255 | A | O4'-C1'-N9 | 9.37 | 115.70 | 108.20 |
| 3 | AB | 54 | ARG | NE-CZ-NH2 | -9.37 | 115.61 | 120.30 |
| 35 | BG | 76 | LEU | CD1-CG-CD2 | 9.37 | 138.62 | 110.50 |
| 78 | CA | 415 | C | C1'-O4'-C4' | 9.37 | 117.40 | 109.90 |
| 81 | DA | 960 | U | N1-C1'-C2' | 9.37 | 126.18 | 114.00 |
| 83 | DC | 33 | U | O4'-C1'-N1 | 9.37 | 115.70 | 108.20 |
| 33 | BD | 330 | TYR | CB-CG-CD2 | -9.37 | 115.38 | 121.00 |
| 78 | CA | 1134 | C | N1-C1'-C2' | 9.37 | 126.18 | 114.00 |
| 78 | CA | 1649 | G | N9-C1'-C2' | -9.37 | 101.69 | 112.00 |
| 81 | DA | 276 | U | O4'-C1'-N1 | 9.37 | 115.69 | 108.20 |
| 81 | DA | 3107 | U | C4'-C3'-C2' | -9.37 | 93.23 | 102.60 |
| 81 | DA | 3344 | A | O4'-C1'-N9 | 9.37 | 115.69 | 108.20 |
| 78 | CA | 283 | U | O4'-C1'-N1 | 9.36 | 115.69 | 108.20 |
| 78 | CA | 434 | G | O4'-C1'-N9 | 9.36 | 115.69 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 997 | A | N9-C1'-C2' | -9.36 | 101.70 | 112.00 |
| 81 | DA | 1688 | U | P-O3'-C3' | 9.36 | 130.94 | 119.70 |
| 81 | DA | 2163 | C | C5'-C4'-C3' | 9.36 | 130.98 | 116.00 |
| 81 | DA | 2617 | U | C1'-O4'-C4' | 9.36 | 117.39 | 109.90 |
| 81 | DA | 3050 | U | P-O5'-C5' | 9.36 | 135.88 | 120.90 |
| 78 | CA | 1602 | C | O4'-C1'-N1 | -9.36 | 100.71 | 108.20 |
| 81 | DA | 2476 | C | C5'-C4'-C3' | 9.36 | 130.97 | 116.00 |
| 78 | CA | 714 | G | P-O5'-C5' | 9.36 | 135.87 | 120.90 |
| 81 | DA | 1893 | A | O4'-C1'-N9 | 9.36 | 115.69 | 108.20 |
| 81 | DA | 3363 | U | O4'-C1'-N1 | 9.36 | 115.68 | 108.20 |
| 65 | Bn | 7 | ASP | CB-CG-OD2 | -9.35 | 109.88 | 118.30 |
| 68 | Bq | 11 | ARG | NE-CZ-NH2 | -9.35 | 115.62 | 120.30 |
| 81 | DA | 1335 | C | C3'-C2'-C1' | 9.35 | 108.98 | 101.50 |
| 78 | CA | 1385 | G | O4'-C1'-N9 | 9.35 | 115.68 | 108.20 |
| 81 | DA | 2381 | G | O4'-C1'-N9 | 9.35 | 115.68 | 108.20 |
| 82 | DB | 128 | U | P-O3'-C3' | 9.35 | 130.92 | 119.70 |
| 82 | DB | 154 | C | N1-C1'-C2' | 9.35 | 126.15 | 114.00 |
| 81 | DA | 2238 | G | C5'-C4'-O4' | -9.35 | 97.88 | 109.10 |
| 81 | DA | 742 | G | N9-C1'-C2' | -9.35 | 101.72 | 112.00 |
| 81 | DA | 640 | U | O4'-C1'-N1 | 9.34 | 115.67 | 108.20 |
| 44 | BO | 60 | TYR | N-CA-CB | 9.34 | 127.42 | 110.60 |
| 78 | CA | 179 | A | C1'-O4'-C4' | 9.34 | 117.37 | 109.90 |
| 78 | CA | 1409 | G | O4'-C1'-N9 | 9.34 | 115.67 | 108.20 |
| 81 | DA | 370 | U | O4'-C1'-N1 | 9.34 | 115.67 | 108.20 |
| 81 | DA | 2172 | A | O4'-C1'-C2' | 9.34 | 116.01 | 107.60 |
| 78 | CA | 1391 | A | O4'-C1'-N9 | 9.34 | 115.67 | 108.20 |
| 81 | DA | 1613 | A | O4'-C1'-N9 | 9.34 | 115.67 | 108.20 |
| 61 | Bj | 3 | GLU | N-CA-CB | 9.34 | 127.41 | 110.60 |
| 78 | CA | 469 | C | C3'-C2'-C1' | 9.34 | 108.97 | 101.50 |
| 81 | DA | 2362 | C | C4'-C3'-C2' | 9.34 | 111.94 | 102.60 |
| 3 | AB | 79 | TYR | CB-CG-CD2 | -9.33 | 115.40 | 121.00 |
| 35 | BG | 77 | ARG | CD-NE-CZ | -9.33 | 110.53 | 123.60 |
| 78 | CA | 448 | C | P-O3'-C3' | 9.33 | 130.90 | 119.70 |
| 81 | DA | 736 | A | C5'-C4'-C3' | 9.33 | 130.93 | 116.00 |
| 81 | DA | 2657 | A | C3'-C2'-C1' | 9.33 | 108.97 | 101.50 |
| 78 | CA | 1161 | C | O4'-C1'-C2' | -9.33 | 96.47 | 105.80 |
| 78 | CA | 848 | C | O4'-C1'-N1 | 9.32 | 115.66 | 108.20 |
| 78 | CA | 879 | G | O4'-C1'-N9 | 9.32 | 115.66 | 108.20 |
| 3 | AB | 34 | TYR | CB-CG-CD1 | 9.32 | 126.59 | 121.00 |
| 22 | AV | 106 | ALA | CB-CA-C | -9.32 | 96.12 | 110.10 |
| 78 | CA | 855 | A | C1'-O4'-C4' | -9.32 | 102.44 | 109.90 |
| 78 | CA | 1534 | G | P-O3'-C3' | -9.32 | 108.52 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 958 | C | O4'-C1'-N1 | 9.32 | 115.66 | 108.20 |
| 81 | DA | 2536 | A | N1-C6-N6 | 9.32 | 124.19 | 118.60 |
| 81 | DA | 2269 | U | O4'-C1'-C2' | -9.32 | 96.48 | 105.80 |
| 78 | CA | 1479 | A | N9-C1'-C2' | -9.32 | 101.75 | 112.00 |
| 78 | CA | 393 | C | C3'-C2'-C1' | 9.31 | 108.95 | 101.50 |
| 78 | CA | 564 | G | N1-C6-O6 | 9.31 | 125.49 | 119.90 |
| 81 | DA | 2877 | G | O4'-C1'-N9 | 9.31 | 115.65 | 108.20 |
| 44 | BO | 7 | LYS | N-CA-CB | 9.31 | 127.36 | 110.60 |
| 61 | Bj | 2 | ALA | CA-C-O | -9.31 | 100.55 | 120.10 |
| 78 | CA | 16 | G | O4'-C1'-N9 | 9.31 | 115.65 | 108.20 |
| 81 | DA | 997 | A | P-O3'-C3' | -9.31 | 108.53 | 119.70 |
| 81 | DA | 3167 | A | C3'-C2'-C1' | 9.31 | 108.95 | 101.50 |
| 81 | DA | 3071 | U | O4'-C1'-N1 | 9.31 | 115.64 | 108.20 |
| 78 | CA | 989 | U | C1'-O4'-C4' | -9.30 | 102.46 | 109.90 |
| 22 | AV | 29 | LYS | CA-C-N | 9.30 | 137.67 | 117.20 |
| 81 | DA | 26 | A | O4'-C1'-N9 | 9.30 | 115.64 | 108.20 |
| 78 | CA | 672 | U | O3'-P-O5' | -9.30 | 86.33 | 104.00 |
| 81 | DA | 3222 | U | O3'-P-O5' | -9.30 | 86.33 | 104.00 |
| 82 | DB | 105 | A | P-O3'-C3' | 9.30 | 130.86 | 119.70 |
| 81 | DA | 1401 | A | O4'-C4'-C3' | -9.30 | 94.70 | 104.00 |
| 43 | BP | 63 | ARG | NE-CZ-NH2 | -9.29 | 115.65 | 120.30 |
| 81 | DA | 3258 | U | N1-C1'-C2' | -9.29 | 101.78 | 112.00 |
| 78 | CA | 1662 | G | O4'-C1'-N9 | 9.29 | 115.63 | 108.20 |
| 78 | CA | 1599 | C | C3'-C2'-C1' | 9.29 | 108.93 | 101.50 |
| 81 | DA | 253 | A | C1'-O4'-C4' | 9.29 | 117.33 | 109.90 |
| 81 | DA | 2004 | U | O4'-C1'-N1 | 9.29 | 115.63 | 108.20 |
| 78 | CA | 891 | A | O4'-C1'-N9 | 9.29 | 115.63 | 108.20 |
| 78 | CA | 1765 | A | C3'-C2'-C1' | 9.29 | 108.93 | 101.50 |
| 81 | DA | 2944 | U | C3'-C2'-C1' | 9.29 | 108.93 | 101.50 |
| 83 | DC | 3 | U | P-O5'-C5' | 9.29 | 135.76 | 120.90 |
| 81 | DA | 554 | A | P-O3'-C3' | 9.29 | 130.84 | 119.70 |
| 34 | BE | 53 | THR | CA-CB-CG2 | 9.28 | 125.40 | 112.40 |
| 46 | BT | 81 | ARG | NE-CZ-NH1 | 9.28 | 124.94 | 120.30 |
| 78 | CA | 1409 | G | C1'-O4'-C4' | 9.28 | 117.33 | 109.90 |
| 81 | DA | 2363 | A | C1'-O4'-C4' | 9.28 | 117.33 | 109.90 |
| 81 | DA | 1754 | G | N1-C6-O6 | 9.28 | 125.47 | 119.90 |
| 81 | DA | 3010 | U | O4'-C1'-C2' | -9.28 | 96.52 | 105.80 |
| 78 | CA | 1583 | A | C1'-O4'-C4' | -9.28 | 102.48 | 109.90 |
| 81 | DA | 786 | A | O4'-C1'-C2' | -9.28 | 96.52 | 105.80 |
| 81 | DA | 1737 | U | OP1-P-OP2 | -9.28 | 105.68 | 119.60 |
| 81 | DA | 1701 | C | C1'-O4'-C4' | -9.28 | 102.48 | 109.90 |
| 47 | BU | 141 | VAL | CA-CB-CG1 | 9.27 | 124.81 | 110.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 114 | A | C1'-O4'-C4' | 9.27 | 117.32 | 109.90 |
| 81 | DA | 1819 | U | N1-C1'-C2' | -9.27 | 101.80 | 112.00 |
| 81 | DA | 2236 | G | P-O3'-C3' | 9.27 | 130.82 | 119.70 |
| 81 | DA | 2283 | G | C2'-C3'-O3' | 9.27 | 129.90 | 109.50 |
| 58 | Bg | 107 | VAL | C-N-CA | -9.27 | 98.53 | 121.70 |
| 81 | DA | 1711 | C | N1-C1'-C2' | 9.27 | 126.05 | 114.00 |
| 81 | DA | 2242 | A | O4'-C1'-N9 | -9.27 | 100.79 | 108.20 |
| 81 | DA | 1251 | A | P-O3'-C3' | 9.26 | 130.82 | 119.70 |
| 81 | DA | 1987 | G | O4'-C1'-N9 | 9.26 | 115.61 | 108.20 |
| 81 | DA | 2114 | C | O3'-P-O5' | 9.26 | 121.60 | 104.00 |
| 81 | DA | 777 | U | C1'-O4'-C4' | -9.26 | 102.49 | 109.90 |
| 81 | DA | 2886 | U | N1-C1'-C2' | -9.26 | 101.81 | 112.00 |
| 81 | DA | 2475 | G | C3'-C2'-C1' | 9.26 | 108.90 | 101.50 |
| 43 | BP | 166 | ALA | CB-CA-C | -9.25 | 96.22 | 110.10 |
| 78 | CA | 487 | G | N1-C6-O6 | 9.25 | 125.45 | 119.90 |
| 81 | DA | 1238 | C | C5'-C4'-C3' | 9.25 | 130.80 | 116.00 |
| 81 | DA | 2421 | U | O4'-C1'-N1 | 9.25 | 115.60 | 108.20 |
| 82 | DB | 82 | U | O4'-C1'-N1 | 9.25 | 115.60 | 108.20 |
| 78 | CA | 196 | G | N9-C1'-C2' | 9.25 | 126.02 | 114.00 |
| 78 | CA | 1241 | G | C1'-O4'-C4' | 9.25 | 117.30 | 109.90 |
| 81 | DA | 2084 | C | O4'-C1'-N1 | 9.25 | 115.60 | 108.20 |
| 81 | DA | 2646 | C | C3'-C2'-C1' | -9.25 | 94.10 | 101.50 |
| 78 | CA | 154 | G | O4'-C1'-N9 | -9.25 | 100.80 | 108.20 |
| 81 | DA | 82 | C | C3'-C2'-C1' | 9.25 | 108.90 | 101.50 |
| 81 | DA | 1687 | U | C5'-C4'-C3' | 9.25 | 130.80 | 116.00 |
| 81 | DA | 2350 | C | O4'-C1'-N1 | 9.25 | 115.60 | 108.20 |
| 81 | DA | 3168 | A | P-O3'-C3' | 9.25 | 130.80 | 119.70 |
| 21 | AT | 53 | TYR | N-CA-C | -9.24 | 86.04 | 111.00 |
| 78 | CA | 1545 | A | N9-C1'-C2' | -9.24 | 101.83 | 112.00 |
| 81 | DA | 3132 | C | N1-C1'-C2' | 9.24 | 126.02 | 114.00 |
| 74 | BQ | 137 | ASP | N-CA-C | 9.24 | 135.95 | 111.00 |
| 81 | DA | 1871 | U | O5'-P-OP1 | -9.24 | 97.38 | 105.70 |
| 83 | DC | 8 | G | C3'-C2'-C1' | -9.24 | 94.11 | 101.50 |
| 83 | DC | 12 | U | P-O3'-C3' | 9.24 | 130.79 | 119.70 |
| 81 | DA | 798 | G | O4'-C1'-C2' | 9.24 | 115.92 | 107.60 |
| 81 | DA | 3286 | G | O4'-C1'-N9 | 9.24 | 115.59 | 108.20 |
| 5 | AC | 15 | PRO | CA-N-CD | -9.24 | 98.57 | 111.50 |
| 35 | BG | 15 | VAL | CA-C-O | -9.24 | 100.70 | 120.10 |
| 40 | BK | 184 | THR | N-CA-C | -9.24 | 86.06 | 111.00 |
| 78 | CA | 1365 | C | P-O3'-C3' | 9.24 | 130.78 | 119.70 |
| 81 | DA | 2064 | C | O4'-C1'-N1 | 9.24 | 115.59 | 108.20 |
| 81 | DA | 3282 | U | C3'-C2'-C1' | 9.24 | 108.89 | 101.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 16 | AO | 128 | TYR | CB-CG-CD1 | -9.23 | 115.46 | 121.00 |
| 81 | DA | 1530 | U | O4'-C1'-N1 | 9.23 | 115.59 | 108.20 |
| 81 | DA | 3048 | A | O5'-C5'-C4' | 9.23 | 129.24 | 111.70 |
| 81 | DA | 3050 | U | C5'-C4'-C3' | -9.23 | 101.23 | 116.00 |
| 81 | DA | 3303 | G | N9-C1'-C2' | 9.23 | 126.00 | 114.00 |
| 4 | AD | 108 | ARG | NE-CZ-NH1 | 9.23 | 124.91 | 120.30 |
| 81 | DA | 2621 | G | P-O5'-C5' | 9.23 | 135.66 | 120.90 |
| 78 | CA | 1398 | U | P-O5'-C5' | -9.22 | 106.14 | 120.90 |
| 57 | Be | 138 | TYR | CB-CG-CD2 | -9.22 | 115.47 | 121.00 |
| 81 | DA | 231 | G | N9-C1'-C2' | -9.22 | 101.86 | 112.00 |
| 81 | DA | 1282 | G | O4'-C1'-N9 | 9.22 | 115.58 | 108.20 |
| 81 | DA | 1788 | C | C5'-C4'-C3' | 9.22 | 130.75 | 116.00 |
| 81 | DA | 3011 | A | P-O5'-C5' | -9.22 | 106.15 | 120.90 |
| 81 | DA | 2424 | A | O4'-C1'-N9 | 9.21 | 115.57 | 108.20 |
| 81 | DA | 835 | G | O4'-C1'-N9 | 9.21 | 115.57 | 108.20 |
| 78 | CA | 1775 | U | O4'-C1'-N1 | 9.21 | 115.57 | 108.20 |
| 81 | DA | 1314 | C | C1'-O4'-C4' | -9.21 | 102.53 | 109.90 |
| 81 | DA | 745 | C | C1'-O4'-C4' | -9.21 | 102.53 | 109.90 |
| 81 | DA | 2901 | G | C3'-C2'-C1' | -9.21 | 94.13 | 101.50 |
| 38 | Bs | 42 | ARG | CB-CA-C | 9.21 | 128.82 | 110.40 |
| 78 | CA | 1240 | U | O4'-C1'-N1 | 9.21 | 115.57 | 108.20 |
| 81 | DA | 129 | U | O4'-C1'-N1 | 9.21 | 115.57 | 108.20 |
| 81 | DA | 1387 | G | OP1-P-OP2 | -9.21 | 105.79 | 119.60 |
| 81 | DA | 2854 | U | P-O3'-C3' | 9.20 | 130.74 | 119.70 |
| 78 | CA | 106 | U | O4'-C1'-N1 | 9.20 | 115.56 | 108.20 |
| 78 | CA | 466 | U | P-O3'-C3' | -9.20 | 108.66 | 119.70 |
| 78 | CA | 1558 | U | O4'-C1'-N1 | 9.20 | 115.56 | 108.20 |
| 81 | DA | 1716 | U | P-O3'-C3' | 9.20 | 130.74 | 119.70 |
| 81 | DA | 1988 | C | O4'-C1'-N1 | 9.20 | 115.56 | 108.20 |
| 81 | DA | 2876 | C | N1-C1'-C2' | 9.20 | 125.96 | 114.00 |
| 42 | BM | 64 | LYS | CA-C-N | 9.20 | 134.60 | 116.20 |
| 43 | BP | 99 | ARG | NE-CZ-NH2 | 9.20 | 124.90 | 120.30 |
| 78 | CA | 1112 | G | C1'-O4'-C4' | -9.20 | 102.54 | 109.90 |
| 81 | DA | 233 | C | O4'-C1'-C2' | -9.20 | 96.60 | 105.80 |
| 81 | DA | 732 | C | O4'-C1'-N1 | 9.20 | 115.56 | 108.20 |
| 81 | DA | 759 | U | O4'-C1'-N1 | 9.20 | 115.56 | 108.20 |
| 81 | DA | 2169 | G | OP1-P-OP2 | -9.20 | 105.80 | 119.60 |
| 43 | BP | 16 | SER | CB-CA-C | -9.20 | 92.63 | 110.10 |
| 81 | DA | 2762 | A | P-O3'-C3' | 9.20 | 130.73 | 119.70 |
| 81 | DA | 3125 | U | O4'-C1'-N1 | 9.19 | 115.56 | 108.20 |
| 81 | DA | 2869 | U | P-O3'-C3' | -9.19 | 108.67 | 119.70 |
| 81 | DA | 331 | G | N9-C1'-C2' | -9.19 | 101.89 | 112.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 3224 | G | N9-C1'-C2' | -9.19 | 101.89 | 112.00 |
| 83 | DC | 20 | A | O4'-C1'-C2' | 9.19 | 115.87 | 107.60 |
| 78 | CA | 87 | C | P-O3'-C3' | -9.19 | 108.68 | 119.70 |
| 78 | CA | 1542 | G | O4'-C1'-N9 | 9.19 | 115.55 | 108.20 |
| 81 | DA | 3224 | G | C3'-C2'-C1' | -9.19 | 94.15 | 101.50 |
| 81 | DA | 3325 | G | C5'-C4'-C3' | 9.19 | 130.70 | 116.00 |
| 81 | DA | 2142 | A | O4'-C1'-C2' | -9.18 | 96.62 | 105.80 |
| 43 | BP | 180 | PHE | CA-C-N | 9.18 | 137.39 | 117.20 |
| 74 | BQ | 158 | ARG | C-N-CA | 9.18 | 144.64 | 121.70 |
| 78 | CA | 228 | G | N9-C1'-C2' | -9.18 | 101.90 | 112.00 |
| 33 | BD | 12 | THR | N-CA-C | -9.18 | 86.23 | 111.00 |
| 11 | AJ | 85 | ARG | CB-CG-CD | 9.17 | 135.45 | 111.60 |
| 78 | CA | 44 | U | OP1-P-OP2 | -9.17 | 105.84 | 119.60 |
| 81 | DA | 257 | U | O4'-C1'-N1 | 9.17 | 115.54 | 108.20 |
| 81 | DA | 1304 | A | O4'-C1'-N9 | 9.17 | 115.54 | 108.20 |
| 81 | DA | 1432 | C | C1'-O4'-C4' | 9.17 | 117.23 | 109.90 |
| 81 | DA | 2627 | C | P-O3'-C3' | -9.17 | 108.70 | 119.70 |
| 30 | BA | 41 | TYR | CB-CG-CD2 | -9.17 | 115.50 | 121.00 |
| 39 | BJ | 14 | TYR | CB-CG-CD2 | 9.17 | 126.50 | 121.00 |
| 78 | CA | 1721 | A | O4'-C1'-C2' | -9.17 | 96.63 | 105.80 |
| 81 | DA | 2957 | G | P-O3'-C3' | -9.17 | 108.70 | 119.70 |
| 83 | DC | 31 | U | C1'-O4'-C4' | 9.17 | 117.23 | 109.90 |
| 83 | DC | 54 | A | P-O3'-C3' | -9.17 | 108.70 | 119.70 |
| 4 | AD | 113 | ARG | NE-CZ-NH2 | -9.16 | 115.72 | 120.30 |
| 56 | Bf | 85 | PHE | CB-CG-CD1 | 9.16 | 127.21 | 120.80 |
| 78 | CA | 1406 | A | C1'-O4'-C4' | -9.16 | 102.57 | 109.90 |
| 78 | CA | 1424 | A | P-O3'-C3' | 9.16 | 130.70 | 119.70 |
| 81 | DA | 3115 | C | O4'-C1'-C2' | -9.16 | 96.64 | 105.80 |
| 82 | DB | 36 | G | O4'-C1'-N9 | 9.16 | 115.53 | 108.20 |
| 81 | DA | 597 | G | O4'-C1'-C2' | 9.16 | 115.84 | 107.60 |
| 82 | DB | 122 | U | C1'-O4'-C4' | 9.16 | 117.23 | 109.90 |
| 78 | CA | 47 | A | O4'-C1'-N9 | 9.16 | 115.53 | 108.20 |
| 81 | DA | 529 | A | N9-C1'-C2' | 9.16 | 125.90 | 114.00 |
| 81 | DA | 2243 | A | N9-C1'-C2' | -9.16 | 101.93 | 112.00 |
| 81 | DA | 902 | G | P-O3'-C3' | 9.16 | 130.69 | 119.70 |
| 81 | DA | 3249 | C | N1-C1'-C2' | 9.16 | 125.90 | 114.00 |
| 78 | CA | 503 | G | P-O3'-C3' | 9.15 | 130.68 | 119.70 |
| 81 | DA | 1006 | A | C5'-C4'-O4' | 9.15 | 120.08 | 109.10 |
| 1 | Aa | 53 | LYS | C-N-CA | 9.15 | 144.57 | 121.70 |
| 79 | CB | 54 | U | O4'-C1'-N1 | 9.15 | 115.52 | 108.20 |
| 81 | DA | 1974 | A | C5'-C4'-C3' | 9.15 | 130.64 | 116.00 |
| 81 | DA | 2421 | U | C3'-C2'-C1' | 9.15 | 108.82 | 101.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 60 | Bi | 55 | SER | C-N-CA | 9.15 | 144.57 | 121.70 |
| 81 | DA | 1634 | G | P-O5'-C5' | 9.15 | 135.54 | 120.90 |
| 61 | Bj | 9 | VAL | N-CA-CB | 9.15 | 131.62 | 111.50 |
| 81 | DA | 1039 | U | O4'-C1'-C2' | -9.15 | 96.65 | 105.80 |
| 81 | DA | 1094 | U | O4'-C1'-N1 | 9.15 | 115.52 | 108.20 |
| 81 | DA | 1216 | C | P-O3'-C3' | -9.15 | 108.72 | 119.70 |
| 74 | BQ | 40 | HIS | C-N-CA | -9.14 | 98.84 | 121.70 |
| 83 | DC | 32 | U | O4'-C1'-N1 | 9.14 | 115.52 | 108.20 |
| 81 | DA | 608 | A | C3'-C2'-C1' | 9.14 | 108.81 | 101.50 |
| 81 | DA | 1288 | U | O3'-P-O5' | -9.14 | 86.63 | 104.00 |
| 61 | Bj | 73 | ARG | NE-CZ-NH1 | 9.14 | 124.87 | 120.30 |
| 78 | CA | 682 | C | O4'-C1'-N1 | 9.14 | 115.51 | 108.20 |
| 81 | DA | 3296 | A | O4'-C1'-N9 | -9.14 | 100.89 | 108.20 |
| 81 | DA | 1400 | G | O3'-P-O5' | -9.14 | 86.64 | 104.00 |
| 31 | BB | 38 | HIS | N-CA-C | 9.14 | 135.67 | 111.00 |
| 61 | Bj | 12 | LYS | CB-CA-C | -9.14 | 92.13 | 110.40 |
| 78 | CA | 1392 | U | O4'-C1'-C2' | -9.14 | 96.66 | 105.80 |
| 81 | DA | 813 | G | P-O3'-C3' | 9.14 | 130.66 | 119.70 |
| 81 | DA | 2988 | C | O3'-P-O5' | 9.14 | 121.36 | 104.00 |
| 22 | AV | 26 | LYS | N-CA-CB | 9.13 | 127.04 | 110.60 |
| 78 | CA | 227 | U | O4'-C1'-N1 | 9.13 | 115.51 | 108.20 |
| 31 | BB | 42 | ARG | NE-CZ-NH2 | -9.13 | 115.73 | 120.30 |
| 81 | DA | 1694 | U | O4'-C1'-C2' | -9.13 | 96.67 | 105.80 |
| 6 | AE | 24 | ARG | CA-CB-CG | 9.13 | 133.49 | 113.40 |
| 31 | BB | 89 | TYR | CB-CG-CD1 | -9.13 | 115.52 | 121.00 |
| 78 | CA | 566 | C | O4'-C1'-N1 | 9.13 | 115.50 | 108.20 |
| 5 | AC | 82 | ARG | NE-CZ-NH2 | -9.13 | 115.74 | 120.30 |
| 20 | AS | 90 | PRO | CA-N-CD | -9.13 | 98.72 | 111.50 |
| 81 | DA | 3035 | A | O4'-C1'-C2' | -9.13 | 96.67 | 105.80 |
| 83 | DC | 27 | A | O4'-C1'-N9 | -9.13 | 100.90 | 108.20 |
| 81 | DA | 132 | C | O4'-C1'-C2' | -9.13 | 96.67 | 105.80 |
| 81 | DA | 562 | C | N1-C1'-C2' | 9.13 | 125.87 | 114.00 |
| 81 | DA | 1802 | C | N1-C1'-C2' | 9.13 | 125.87 | 114.00 |
| 81 | DA | 3041 | U | C1'-O4'-C4' | -9.13 | 102.60 | 109.90 |
| 81 | DA | 701 | G | O4'-C1'-N9 | 9.12 | 115.50 | 108.20 |
| 81 | DA | 3074 | G | P-O5'-C5' | 9.12 | 135.50 | 120.90 |
| 81 | DA | 2862 | U | O4'-C1'-N1 | 9.12 | 115.50 | 108.20 |
| 81 | DA | 3219 | G | P-O3'-C3' | 9.12 | 130.65 | 119.70 |
| 78 | CA | 138 | A | OP1-P-OP2 | -9.12 | 105.92 | 119.60 |
| 81 | DA | 1260 | A | P-O5'-C5' | -9.12 | 106.31 | 120.90 |
| 81 | DA | 1661 | G | P-O3'-C3' | 9.12 | 130.64 | 119.70 |
| 78 | CA | 668 | C | N1-C1'-C2' | 9.12 | 125.85 | 114.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 1666 | U | O4'-C1'-C2' | -9.12 | 96.68 | 105.80 |
| 79 | CB | 1 | U | P-O3'-C3' | 9.12 | 130.64 | 119.70 |
| 81 | DA | 1147 | G | O4'-C1'-N9 | 9.12 | 115.49 | 108.20 |
| 81 | DA | 1591 | G | O4'-C1'-C2' | 9.12 | 115.81 | 107.60 |
| 81 | DA | 1600 | U | O4'-C1'-N1 | 9.12 | 115.49 | 108.20 |
| 78 | CA | 1233 | G | O4'-C1'-N9 | 9.11 | 115.49 | 108.20 |
| 81 | DA | 2344 | U | O4'-C1'-N1 | 9.11 | 115.49 | 108.20 |
| 81 | DA | 2515 | A | P-O3'-C3' | 9.11 | 130.63 | 119.70 |
| 32 | BC | 35 | ASP | CB-CG-OD1 | 9.11 | 126.50 | 118.30 |
| 61 | Bj | 89 | LEU | CB-CA-C | -9.11 | 92.89 | 110.20 |
| 78 | CA | 1756 | A | C3'-C2'-C1' | -9.11 | 94.21 | 101.50 |
| 79 | CB | 24 | A | O4'-C1'-N9 | 9.11 | 115.49 | 108.20 |
| 78 | CA | 1478 | G | O3'-P-O5' | 9.11 | 121.30 | 104.00 |
| 81 | DA | 1338 | C | N1-C1'-C2' | -9.11 | 101.98 | 112.00 |
| 81 | DA | 1506 | A | O4'-C1'-C2' | -9.11 | 96.69 | 105.80 |
| 81 | DA | 3321 | C | P-O3'-C3' | 9.11 | 130.63 | 119.70 |
| 78 | CA | 179 | A | O4'-C4'-C3' | -9.10 | 94.90 | 104.00 |
| 78 | CA | 387 | A | N9-C1'-C2' | -9.10 | 101.99 | 112.00 |
| 78 | CA | 1112 | G | N9-C1'-C2' | 9.10 | 125.83 | 114.00 |
| 81 | DA | 183 | G | O4'-C1'-C2' | 9.10 | 115.79 | 107.60 |
| 81 | DA | 2189 | U | C1'-O4'-C4' | 9.10 | 117.18 | 109.90 |
| 49 | BV | 165 | VAL | CA-C-O | -9.10 | 101.00 | 120.10 |
| 81 | DA | 3311 | C | P-O3'-C3' | 9.09 | 130.61 | 119.70 |
| 30 | BA | 41 | TYR | CB-CG-CD1 | 9.09 | 126.45 | 121.00 |
| 78 | CA | 1343 | U | O4'-C1'-N1 | 9.09 | 115.47 | 108.20 |
| 79 | CB | 22 | G | N9-C1'-C2' | 9.09 | 125.82 | 114.00 |
| 78 | CA | 1725 | U | O4'-C1'-N1 | 9.09 | 115.47 | 108.20 |
| 78 | CA | 364 | G | O4'-C1'-N9 | 9.09 | 115.47 | 108.20 |
| 81 | DA | 1379 | G | C1'-O4'-C4' | -9.09 | 102.63 | 109.90 |
| 83 | DC | 50 | U | O4'-C1'-N1 | 9.09 | 115.47 | 108.20 |
| 81 | DA | 521 | A | P-O5'-C5' | 9.09 | 135.44 | 120.90 |
| 81 | DA | 1625 | A | O4'-C1'-N9 | -9.09 | 100.93 | 108.20 |
| 82 | DB | 91 | C | C1'-O4'-C4' | 9.09 | 117.17 | 109.90 |
| 43 | BP | 44 | ARG | NE-CZ-NH1 | 9.08 | 124.84 | 120.30 |
| 53 | Ba | 74 | VAL | CA-CB-CG2 | -9.08 | 97.28 | 110.90 |
| 83 | DC | 90 | C | O4'-C1'-N1 | 9.08 | 115.47 | 108.20 |
| 83 | DC | 98 | G | P-O3'-C3' | 9.08 | 130.60 | 119.70 |
| 81 | DA | 2305 | G | P-O5'-C5' | 9.08 | 135.43 | 120.90 |
| 2 | AA | 185 | ARG | NE-CZ-NH2 | -9.08 | 115.76 | 120.30 |
| 78 | CA | 501 | U | C5'-C4'-O4' | -9.08 | 98.21 | 109.10 |
| 13 | AL | 13 | ARG | CG-CD-NE | 9.07 | 130.85 | 111.80 |
| 78 | CA | 218 | A | N9-C1'-C2' | 9.07 | 125.80 | 114.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 1458 | G | O4'-C1'-C2' | 9.07 | 115.77 | 107.60 |
| 81 | DA | 311 | C | O4'-C4'-C3' | -9.07 | 94.92 | 104.00 |
| 81 | DA | 1703 | U | O4'-C1'-C2' | -9.07 | 96.72 | 105.80 |
| 81 | DA | 1362 | G | C3'-C2'-C1' | -9.07 | 94.24 | 101.50 |
| 81 | DA | 2403 | G | N9-C1'-C2' | -9.07 | 102.02 | 112.00 |
| 76 | BS | 113 | ALA | N-CA-CB | -9.07 | 97.40 | 110.10 |
| 78 | CA | 1242 | A | P-O3'-C3' | 9.07 | 130.58 | 119.70 |
| 81 | DA | 3310 | A | P-O3'-C3' | -9.07 | 108.82 | 119.70 |
| 81 | DA | 1818 | U | P-O3'-C3' | 9.07 | 130.58 | 119.70 |
| 33 | BD | 242 | ALA | N-CA-CB | 9.06 | 122.79 | 110.10 |
| 78 | CA | 558 | U | P-O3'-C3' | 9.06 | 130.58 | 119.70 |
| 81 | DA | 1446 | A | O4'-C1'-C2' | -9.06 | 96.73 | 105.80 |
| 81 | DA | 2322 | C | O4'-C1'-N1 | 9.06 | 115.45 | 108.20 |
| 81 | DA | 2509 | U | C4'-C3'-C2' | -9.06 | 93.54 | 102.60 |
| 81 | DA | 1814 | A | N9-C1'-C2' | -9.06 | 102.03 | 112.00 |
| 78 | CA | 1529 | C | O4'-C1'-N1 | 9.06 | 115.45 | 108.20 |
| 13 | AL | 135 | LEU | C-N-CA | 9.05 | 144.34 | 121.70 |
| 81 | DA | 2630 | C | P-O3'-C3' | -9.06 | 108.83 | 119.70 |
| 11 | AJ | 85 | ARG | CB-CA-C | -9.05 | 92.29 | 110.40 |
| 35 | BG | 75 | PRO | N-CA-CB | 9.05 | 114.17 | 103.30 |
| 78 | CA | 325 | G | N9-C1'-C2' | -9.05 | 102.04 | 112.00 |
| 81 | DA | 2842 | U | O4'-C1'-N1 | 9.05 | 115.44 | 108.20 |
| 81 | DA | 198 | A | O4'-C1'-C2' | -9.05 | 96.75 | 105.80 |
| 81 | DA | 898 | U | O4'-C1'-N1 | 9.05 | 115.44 | 108.20 |
| 81 | DA | 1341 | U | N1-C1'-C2' | 9.05 | 125.77 | 114.00 |
| 78 | CA | 105 | A | O4'-C1'-N9 | -9.05 | 100.96 | 108.20 |
| 81 | DA | 2592 | G | P-O3'-C3' | 9.05 | 130.56 | 119.70 |
| 78 | CA | 1458 | G | N9-C1'-C2' | 9.05 | 125.76 | 114.00 |
| 81 | DA | 182 | U | C1'-O4'-C4' | 9.04 | 117.14 | 109.90 |
| 81 | DA | 2705 | A | P-O3'-C3' | 9.04 | 130.55 | 119.70 |
| 81 | DA | 42 | C | O3'-P-O5' | -9.04 | 86.82 | 104.00 |
| 81 | DA | 252 | U | O4'-C1'-N1 | 9.04 | 115.43 | 108.20 |
| 81 | DA | 1446 | A | C1'-O4'-C4' | 9.04 | 117.13 | 109.90 |
| 79 | CB | 44 | A | P-O3'-C3' | 9.04 | 130.55 | 119.70 |
| 81 | DA | 2824 | G | O4'-C1'-N9 | 9.04 | 115.43 | 108.20 |
| 81 | DA | 636 | C | C4'-C3'-C2' | 9.04 | 111.64 | 102.60 |
| 81 | DA | 2211 | U | O4'-C1'-N1 | 9.04 | 115.43 | 108.20 |
| 81 | DA | 1825 | G | O4'-C1'-N9 | 9.04 | 115.43 | 108.20 |
| 43 | BP | 2 | GLY | CA-C-O | -9.03 | 104.34 | 120.60 |
| 62 | Bk | 82 | ARG | CA-C-O | -9.03 | 101.13 | 120.10 |
| 81 | DA | 1207 | G | P-O5'-C5' | 9.04 | 135.35 | 120.90 |
| 81 | DA | 1399 | A | OP1-P-OP2 | -9.04 | 106.05 | 119.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 3005 | A | N9-C1'-C2' | -9.04 | 102.06 | 112.00 |
| 22 | AV | 58 | ARG | NE-CZ-NH2 | -9.03 | 115.78 | 120.30 |
| 35 | BG | 10 | TYR | CB-CA-C | -9.03 | 92.34 | 110.40 |
| 83 | DC | 22 | A | C3'-C2'-C1' | -9.03 | 94.27 | 101.50 |
| 78 | CA | 166 | C | O4'-C1'-N1 | -9.03 | 100.97 | 108.20 |
| 78 | CA | 893 | U | P-O5'-C5' | 9.03 | 135.35 | 120.90 |
| 78 | CA | 1464 | G | O4'-C1'-N9 | 9.03 | 115.42 | 108.20 |
| 78 | CA | 1772 | C | P-O5'-C5' | 9.03 | 135.35 | 120.90 |
| 81 | DA | 1825 | G | C1'-O4'-C4' | -9.03 | 102.68 | 109.90 |
| 78 | CA | 662 | U | O4'-C4'-C3' | -9.03 | 94.97 | 104.00 |
| 58 | Bg | 12 | TYR | CB-CG-CD1 | -9.03 | 115.58 | 121.00 |
| 78 | CA | 1355 | C | O3'-P-O5' | -9.03 | 86.85 | 104.00 |
| 78 | CA | 1656 | U | O4'-C1'-N1 | 9.02 | 115.42 | 108.20 |
| 78 | CA | 1498 | G | N1-C6-O6 | 9.02 | 125.31 | 119.90 |
| 53 | Ba | 27 | LYS | C-N-CD | -9.02 | 100.75 | 120.60 |
| 78 | CA | 218 | A | C1'-O4'-C4' | -9.02 | 102.69 | 109.90 |
| 78 | CA | 281 | G | O4'-C1'-N9 | 9.02 | 115.42 | 108.20 |
| 78 | CA | 646 | C | C3'-C2'-C1' | -9.02 | 94.29 | 101.50 |
| 78 | CA | 1124 | A | O4'-C1'-N9 | 9.02 | 115.41 | 108.20 |
| 81 | DA | 459 | G | O4'-C1'-N9 | 9.02 | 115.41 | 108.20 |
| 81 | DA | 637 | C | O5'-P-OP2 | -9.02 | 97.58 | 105.70 |
| 81 | DA | 1288 | U | O4'-C1'-N1 | 9.02 | 115.41 | 108.20 |
| 81 | DA | 2744 | U | N1-C1'-C2' | 9.02 | 125.72 | 114.00 |
| 78 | CA | 96 | G | P-O3'-C3' | 9.02 | 130.52 | 119.70 |
| 81 | DA | 2452 | G | N9-C1'-C2' | -9.01 | 102.08 | 112.00 |
| 57 | Be | 27 | ALA | CB-CA-C | -9.01 | 96.58 | 110.10 |
| 81 | DA | 2071 | A | C1'-O4'-C4' | 9.01 | 117.11 | 109.90 |
| 16 | AO | 63 | ALA | C-N-CA | 9.01 | 144.23 | 121.70 |
| 16 | AO | 75 | LEU | N-CA-CB | 9.01 | 128.42 | 110.40 |
| 78 | CA | 288 | A | P-O3'-C3' | 9.01 | 130.51 | 119.70 |
| 59 | Bh | 17 | PHE | CB-CG-CD2 | 9.01 | 127.11 | 120.80 |
| 81 | DA | 1789 | G | O4'-C1'-N9 | 9.01 | 115.41 | 108.20 |
| 2 | AA | 174 | TRP | CB-CG-CD2 | -9.01 | 114.89 | 126.60 |
| 74 | BQ | 40 | HIS | O-C-N | 9.00 | 137.10 | 122.70 |
| 81 | DA | 2233 | A | C1'-O4'-C4' | 9.00 | 117.10 | 109.90 |
| 81 | DA | 3093 | C | P-O3'-C3' | 9.00 | 130.50 | 119.70 |
| 79 | CB | 34 | G | C5-C6-O6 | -9.00 | 123.20 | 128.60 |
| 81 | DA | 479 | U | P-O3'-C3' | 9.00 | 130.50 | 119.70 |
| 81 | DA | 814 | U | O4'-C1'-N1 | 9.00 | 115.40 | 108.20 |
| 81 | DA | 2043 | U | O4'-C1'-N1 | 9.00 | 115.40 | 108.20 |
| 81 | DA | 3366 | G | O4'-C1'-N9 | 9.00 | 115.40 | 108.20 |
| 82 | DB | 2 | A | OP1-P-OP2 | -9.00 | 106.10 | 119.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 540 | U | O4'-C1'-N1 | 9.00 | 115.40 | 108.20 |
| 61 | Bj | 8 | TYR | N-CA-C | -9.00 | 86.71 | 111.00 |
| 78 | CA | 662 | U | O4'-C1'-C2' | -9.00 | 96.80 | 105.80 |
| 81 | DA | 1591 | G | P-O3'-C3' | 9.00 | 130.50 | 119.70 |
| 81 | DA | 2573 | G | N1-C6-O6 | 9.00 | 125.30 | 119.90 |
| 81 | DA | 249 | U | O4'-C1'-N1 | 8.99 | 115.40 | 108.20 |
| 29 | AU | 72 | PHE | CB-CG-CD2 | -8.99 | 114.50 | 120.80 |
| 3 | AB | 72 | LEU | O-C-N | -8.99 | 108.31 | 122.70 |
| 78 | CA | 145 | A | OP1-P-OP2 | -8.99 | 106.11 | 119.60 |
| 78 | CA | 617 | U | N1-C1'-C2' | 8.99 | 125.69 | 114.00 |
| 31 | BB | 193 | ARG | NH1-CZ-NH2 | -8.99 | 109.52 | 119.40 |
| 35 | BG | 76 | LEU | CB-CA-C | -8.99 | 93.12 | 110.20 |
| 81 | DA | 1429 | G | N9-C1'-C2' | 8.99 | 125.68 | 114.00 |
| 57 | Be | 132 | PRO | O-C-N | -8.99 | 108.32 | 122.70 |
| 81 | DA | 637 | C | P-O5'-C5' | -8.99 | 106.52 | 120.90 |
| 81 | DA | 1821 | U | C3'-C2'-C1' | 8.99 | 108.69 | 101.50 |
| 81 | DA | 1897 | G | P-O3'-C3' | 8.99 | 130.49 | 119.70 |
| 83 | DC | 31 | U | O4'-C1'-C2' | -8.99 | 96.81 | 105.80 |
| 81 | DA | 2028 | U | O4'-C1'-N1 | 8.99 | 115.39 | 108.20 |
| 81 | DA | 2700 | G | P-O3'-C3' | 8.99 | 130.48 | 119.70 |
| 78 | CA | 948 | G | O4'-C1'-C2' | 8.98 | 115.69 | 107.60 |
| 81 | DA | 1864 | A | O4'-C1'-N9 | 8.98 | 115.39 | 108.20 |
| 81 | DA | 3099 | C | P-O3'-C3' | 8.98 | 130.48 | 119.70 |
| 81 | DA | 375 | A | O4'-C1'-C2' | -8.98 | 96.82 | 105.80 |
| 81 | DA | 683 | U | O4'-C1'-N1 | 8.98 | 115.39 | 108.20 |
| 81 | DA | 2209 | U | C5'-C4'-C3' | 8.98 | 130.37 | 116.00 |
| 81 | DA | 739 | G | N1-C6-O6 | 8.98 | 125.29 | 119.90 |
| 81 | DA | 1426 | C | O4'-C1'-N1 | 8.98 | 115.38 | 108.20 |
| 81 | DA | 1 | G | OP1-P-OP2 | -8.98 | 106.14 | 119.60 |
| 81 | DA | 1414 | G | O4'-C1'-C2' | -8.98 | 96.82 | 105.80 |
| 81 | DA | 2200 | U | O4'-C1'-N1 | 8.98 | 115.38 | 108.20 |
| 81 | DA | 3241 | G | O3'-P-O5' | -8.98 | 86.94 | 104.00 |
| 32 | BC | 5 | LYS | CB-CA-C | 8.97 | 128.35 | 110.40 |
| 41 | BN | 115 | PHE | N-CA-CB | -8.97 | 94.45 | 110.60 |
| 81 | DA | 2681 | U | O4'-C1'-C2' | -8.97 | 96.83 | 105.80 |
| 81 | DA | 1033 | U | O4'-C1'-N1 | 8.97 | 115.38 | 108.20 |
| 81 | DA | 2179 | C | C3'-C2'-C1' | 8.97 | 108.68 | 101.50 |
| 81 | DA | 3012 | A | P-O3'-C3' | -8.97 | 108.93 | 119.70 |
| 34 | BE | 89 | TYR | CB-CA-C | -8.97 | 92.46 | 110.40 |
| 78 | CA | 646 | C | O3'-P-O5' | 8.97 | 121.04 | 104.00 |
| 82 | DB | 100 | U | N1-C1'-C2' | 8.97 | 125.66 | 114.00 |
| 78 | CA | 591 | A | O4'-C1'-C2' | -8.97 | 96.83 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 1702 | A | O4'-C1'-C2' | -8.97 | 96.83 | 105.80 |
| 81 | DA | 737 | G | P-O3'-C3' | 8.97 | 130.46 | 119.70 |
| 81 | DA | 2942 | C | C3'-C2'-C1' | 8.97 | 108.68 | 101.50 |
| 81 | DA | 1438 | U | O3'-P-O5' | -8.97 | 86.96 | 104.00 |
| 81 | DA | 1508 | C | N1-C1'-C2' | 8.97 | 125.66 | 114.00 |
| 67 | Bp | 26 | ARG | NE-CZ-NH2 | -8.97 | 115.82 | 120.30 |
| 81 | DA | 2708 | C | N1-C1'-C2' | 8.97 | 125.66 | 114.00 |
| 78 | CA | 547 | U | O4'-C1'-N1 | 8.96 | 115.37 | 108.20 |
| 78 | CA | 886 | U | C3'-C2'-C1' | -8.96 | 94.33 | 101.50 |
| 81 | DA | 1178 | G | N9-C1'-C2' | 8.96 | 125.65 | 114.00 |
| 81 | DA | 1800 | A | O4'-C1'-N9 | 8.97 | 115.37 | 108.20 |
| 81 | DA | 2392 | C | O4'-C1'-C2' | -8.97 | 96.83 | 105.80 |
| 81 | DA | 1754 | G | C5'-C4'-C3' | 8.96 | 130.34 | 116.00 |
| 81 | DA | 2561 | A | OP1-P-OP2 | -8.96 | 106.15 | 119.60 |
| 78 | CA | 142 | G | C3'-C2'-C1' | 8.96 | 108.67 | 101.50 |
| 78 | CA | 1057 | U | O4'-C1'-N1 | 8.96 | 115.37 | 108.20 |
| 78 | CA | 1663 | G | O4'-C1'-N9 | 8.96 | 115.37 | 108.20 |
| 81 | DA | 233 | C | O4'-C1'-N1 | 8.96 | 115.37 | 108.20 |
| 81 | DA | 1285 | G | C3'-C2'-C1' | 8.96 | 108.67 | 101.50 |
| 34 | BE | 123 | PHE | N-CA-C | -8.96 | 86.81 | 111.00 |
| 62 | Bk | 82 | ARG | C-N-CA | 8.96 | 144.09 | 121.70 |
| 78 | CA | 844 | A | C5-C6-N6 | -8.96 | 116.53 | 123.70 |
| 78 | CA | 1551 | U | C5'-C4'-C3' | 8.96 | 130.33 | 116.00 |
| 81 | DA | 2377 | G | P-O3'-C3' | 8.96 | 130.45 | 119.70 |
| 78 | CA | 354 | C | O4'-C1'-C2' | -8.96 | 96.84 | 105.80 |
| 78 | CA | 1341 | A | N9-C1'-C2' | -8.95 | 102.15 | 112.00 |
| 82 | DB | 148 | G | O4'-C1'-N9 | 8.96 | 115.36 | 108.20 |
| 82 | DB | 86 | U | N1-C1'-C2' | -8.95 | 102.15 | 112.00 |
| 9 | AH | 101 | TYR | CB-CG-CD1 | -8.95 | 115.63 | 121.00 |
| 39 | BJ | 123 | ARG | NE-CZ-NH1 | -8.95 | 115.83 | 120.30 |
| 81 | DA | 540 | U | P-O3'-C3' | 8.95 | 130.44 | 119.70 |
| 3 | AB | 22 | ASN | N-CA-CB | 8.95 | 126.70 | 110.60 |
| 81 | DA | 3055 | U | C1'-O4'-C4' | 8.95 | 117.06 | 109.90 |
| 81 | DA | 3241 | G | O4'-C1'-C2' | -8.95 | 96.85 | 105.80 |
| 41 | BN | 125 | LYS | N-CA-CB | 8.94 | 126.70 | 110.60 |
| 81 | DA | 2594 | C | N1-C1'-C2' | 8.94 | 125.63 | 114.00 |
| 78 | CA | 163 | G | C2'-C3'-O3' | 8.94 | 129.17 | 109.50 |
| 81 | DA | 1768 | U | O4'-C1'-N1 | 8.94 | 115.35 | 108.20 |
| 81 | DA | 2788 | C | O3'-P-O5' | -8.94 | 87.02 | 104.00 |
| 81 | DA | 2073 | A | C3'-C2'-C1' | 8.94 | 108.65 | 101.50 |
| 78 | CA | 866 | G | OP1-P-OP2 | -8.94 | 106.20 | 119.60 |
| 81 | DA | 7 | C | N1-C1'-C2' | 8.94 | 125.61 | 114.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 961 | C | C3'-C2'-C1' | 8.94 | 108.65 | 101.50 |
| 32 | BC | 17 | LEU | CB-CA-C | 8.93 | 127.17 | 110.20 |
| 77 | BI | 119 | TRP | CA-CB-CG | 8.93 | 130.67 | 113.70 |
| 78 | CA | 228 | G | O4'-C1'-C2' | -8.93 | 96.87 | 105.80 |
| 78 | CA | 145 | A | O4'-C1'-N9 | 8.93 | 115.35 | 108.20 |
| 78 | CA | 854 | U | O4'-C1'-N1 | 8.93 | 115.35 | 108.20 |
| 81 | DA | 2996 | U | OP1-P-OP2 | -8.93 | 106.20 | 119.60 |
| 81 | DA | 3065 | G | OP1-P-OP2 | -8.93 | 106.20 | 119.60 |
| 78 | CA | 1446 | A | OP1-P-OP2 | -8.93 | 106.20 | 119.60 |
| 81 | DA | 1319 | G | C1'-O4'-C4' | -8.93 | 102.75 | 109.90 |
| 81 | DA | 1831 | U | O4'-C1'-C2' | -8.93 | 96.87 | 105.80 |
| 81 | DA | 2492 | C | P-O3'-C3' | 8.93 | 130.42 | 119.70 |
| 82 | DB | 156 | U | P-O3'-C3' | 8.93 | 130.42 | 119.70 |
| 55 | Bc | 104 | GLN | CB-CA-C | 8.93 | 128.26 | 110.40 |
| 81 | DA | 597 | G | O4'-C1'-N9 | 8.93 | 115.34 | 108.20 |
| 81 | DA | 1866 | C | N1-C1'-C2' | 8.93 | 125.61 | 114.00 |
| 78 | CA | 1746 | A | OP1-P-O3' | 8.92 | 124.83 | 105.20 |
| 81 | DA | 2693 | C | O4'-C1'-C2' | -8.92 | 96.88 | 105.80 |
| 81 | DA | 2790 | A | P-O3'-C3' | -8.92 | 109.00 | 119.70 |
| 81 | DA | 2872 | A | O4'-C1'-N9 | 8.92 | 115.33 | 108.20 |
| 81 | DA | 2607 | G | C3'-C2'-C1' | -8.92 | 94.37 | 101.50 |
| 78 | CA | 289 | U | O4'-C1'-N1 | 8.92 | 115.33 | 108.20 |
| 78 | CA | 378 | A | O4'-C1'-N9 | 8.92 | 115.33 | 108.20 |
| 81 | DA | 2681 | U | O3'-P-O5' | -8.92 | 87.06 | 104.00 |
| 78 | CA | 949 | C | P-O3'-C3' | 8.91 | 130.40 | 119.70 |
| 19 | AR | 130 | ARG | CB-CA-C | -8.91 | 92.58 | 110.40 |
| 35 | BG | 169 | ASP | CB-CA-C | -8.91 | 92.58 | 110.40 |
| 78 | CA | 304 | U | C5'-C4'-C3' | 8.91 | 130.26 | 116.00 |
| 81 | DA | 1685 | C | C3'-C2'-C1' | 8.91 | 108.63 | 101.50 |
| 78 | CA | 1586 | A | C1'-O4'-C4' | -8.91 | 102.77 | 109.90 |
| 78 | CA | 1083 | G | OP1-P-OP2 | -8.91 | 106.24 | 119.60 |
| 81 | DA | 3221 | C | O5'-C5'-C4' | -8.91 | 94.77 | 111.70 |
| 4 | AD | 164 | LEU | CB-CA-C | -8.91 | 93.28 | 110.20 |
| 83 | DC | 9 | C | O4'-C1'-N1 | 8.91 | 115.33 | 108.20 |
| 78 | CA | 415 | C | O4'-C1'-N1 | 8.91 | 115.33 | 108.20 |
| 81 | DA | 2646 | C | O4'-C4'-C3' | -8.90 | 95.09 | 104.00 |
| 78 | CA | 222 | A | O4'-C4'-C3' | -8.90 | 95.10 | 104.00 |
| 81 | DA | 3380 | U | OP1-P-OP2 | -8.90 | 106.24 | 119.60 |
| 59 | Bh | 27 | ARG | NE-CZ-NH2 | -8.90 | 115.85 | 120.30 |
| 78 | CA | 191 | C | O4'-C1'-C2' | -8.90 | 96.90 | 105.80 |
| 81 | DA | 1884 | A | N9-C1'-C2' | 8.90 | 125.57 | 114.00 |
| 47 | BU | 140 | ILE | N-CA-C | -8.90 | 86.97 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 74 | BQ | 238 | ASP | CB-CG-OD1 | 8.90 | 126.31 | 118.30 |
| 78 | CA | 293 | U | P-O3'-C3' | 8.90 | 130.38 | 119.70 |
| 78 | CA | 1017 | U | O4'-C1'-N1 | 8.90 | 115.32 | 108.20 |
| 78 | CA | 323 | A | OP1-P-OP2 | -8.90 | 106.25 | 119.60 |
| 81 | DA | 1649 | U | O4'-C1'-C2' | -8.90 | 96.90 | 105.80 |
| 81 | DA | 73 | C | O4'-C1'-C2' | -8.89 | 96.91 | 105.80 |
| 82 | DB | 114 | G | O4'-C1'-N9 | 8.89 | 115.31 | 108.20 |
| 78 | CA | 577 | G | N1-C6-O6 | 8.89 | 125.23 | 119.90 |
| 78 | CA | 1275 | A | N1-C6-N6 | 8.89 | 123.93 | 118.60 |
| 16 | AO | 67 | THR | N-CA-C | 8.89 | 135.00 | 111.00 |
| 78 | CA | 120 | U | O4'-C1'-N1 | 8.89 | 115.31 | 108.20 |
| 81 | DA | 1070 | U | O4'-C1'-N1 | 8.89 | 115.31 | 108.20 |
| 81 | DA | 2685 | C | N1-C1'-C2' | 8.89 | 125.55 | 114.00 |
| 81 | DA | 2773 | C | OP1-P-OP2 | -8.89 | 106.27 | 119.60 |
| 74 | BQ | 136 | GLU | C-N-CA | -8.88 | 99.49 | 121.70 |
| 78 | CA | 561 | G | O4'-C1'-N9 | 8.89 | 115.31 | 108.20 |
| 78 | CA | 1090 | C | N1-C1'-C2' | 8.89 | 125.55 | 114.00 |
| 81 | DA | 209 | A | O4'-C1'-C2' | -8.88 | 96.92 | 105.80 |
| 81 | DA | 2509 | U | O4'-C4'-C3' | -8.88 | 95.12 | 104.00 |
| 81 | DA | 3036 | G | N9-C1'-C2' | 8.88 | 125.55 | 114.00 |
| 81 | DA | 3107 | U | P-O5'-C5' | 8.88 | 135.11 | 120.90 |
| 11 | AJ | 82 | TYR | CB-CG-CD1 | 8.88 | 126.33 | 121.00 |
| 40 | BK | 178 | VAL | CA-C-N | 8.88 | 136.73 | 117.20 |
| 45 | BR | 143 | PRO | CA-N-CD | 8.88 | 124.13 | 111.70 |
| 51 | BZ | 56 | ARG | NE-CZ-NH1 | 8.88 | 124.74 | 120.30 |
| 81 | DA | 1562 | C | C3'-C2'-C1' | 8.88 | 108.60 | 101.50 |
| 81 | DA | 3055 | U | O4'-C1'-C2' | -8.88 | 96.92 | 105.80 |
| 81 | DA | 1773 | C | P-O3'-C3' | 8.88 | 130.35 | 119.70 |
| 81 | DA | 3303 | G | C3'-C2'-C1' | -8.87 | 94.40 | 101.50 |
| 81 | DA | 1437 | C | C3'-C2'-C1' | 8.87 | 108.60 | 101.50 |
| 81 | DA | 3236 | U | P-O3'-C3' | 8.87 | 130.34 | 119.70 |
| 34 | BE | 58 | GLY | O-C-N | -8.87 | 108.51 | 122.70 |
| 78 | CA | 481 | A | O4'-C1'-N9 | 8.87 | 115.29 | 108.20 |
| 78 | CA | 1458 | G | C3'-C2'-C1' | -8.87 | 94.41 | 101.50 |
| 79 | CB | 61 | C | N1-C1'-C2' | 8.87 | 125.53 | 114.00 |
| 81 | DA | 814 | U | P-O3'-C3' | 8.86 | 130.34 | 119.70 |
| 81 | DA | 1214 | U | O4'-C1'-N1 | 8.86 | 115.29 | 108.20 |
| 81 | DA | 1663 | C | P-O3'-C3' | 8.87 | 130.34 | 119.70 |
| 81 | DA | 2446 | U | P-O5'-C5' | 8.87 | 135.09 | 120.90 |
| 81 | DA | 613 | G | O4'-C1'-N9 | 8.86 | 115.29 | 108.20 |
| 81 | DA | 672 | A | P-O3'-C3' | 8.86 | 130.33 | 119.70 |
| 81 | DA | 1258 | U | P-O3'-C3' | 8.86 | 130.34 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 683 | C | O4'-C1'-C2' | -8.86 | 96.94 | 105.80 |
| 81 | DA | 495 | G | P-O3'-C3' | 8.86 | 130.33 | 119.70 |
| 81 | DA | 2661 | G | P-O3'-C3' | 8.86 | 130.33 | 119.70 |
| 33 | BD | 321 | LYS | CB-CA-C | -8.86 | 92.69 | 110.40 |
| 81 | DA | 1408 | G | O4'-C1'-N9 | 8.86 | 115.29 | 108.20 |
| 49 | BV | 139 | TYR | CB-CG-CD1 | 8.86 | 126.31 | 121.00 |
| 81 | DA | 1975 | C | P-O3'-C3' | -8.86 | 109.07 | 119.70 |
| 78 | CA | 1476 | C | C1'-O4'-C4' | 8.85 | 116.98 | 109.90 |
| 78 | CA | 1785 | U | P-O3'-C3' | 8.85 | 130.32 | 119.70 |
| 81 | DA | 3010 | U | C5'-C4'-C3' | 8.85 | 130.16 | 116.00 |
| 81 | DA | 1621 | A | O3'-P-O5' | -8.85 | 87.19 | 104.00 |
| 81 | DA | 924 | G | O4'-C1'-N9 | -8.85 | 101.12 | 108.20 |
| 81 | DA | 2149 | A | P-O3'-C3' | 8.85 | 130.32 | 119.70 |
| 80 | CC | 12 | A | OP1-P-OP2 | -8.85 | 106.33 | 119.60 |
| 81 | DA | 521 | A | C5'-C4'-C3' | 8.84 | 130.15 | 116.00 |
| 78 | CA | 177 | U | OP1-P-OP2 | -8.84 | 106.34 | 119.60 |
| 81 | DA | 595 | G | P-O3'-C3' | -8.84 | 109.09 | 119.70 |
| 81 | DA | 3355 | U | O4'-C1'-N1 | 8.84 | 115.27 | 108.20 |
| 78 | CA | 993 | A | P-O5'-C5' | 8.84 | 135.04 | 120.90 |
| 81 | DA | 3385 | U | C5'-C4'-O4' | -8.84 | 98.49 | 109.10 |
| 78 | CA | 1600 | A | O4'-C1'-N9 | 8.84 | 115.27 | 108.20 |
| 21 | AT | 12 | TYR | CB-CG-CD2 | -8.84 | 115.70 | 121.00 |
| 72 | Bu | 60 | ASN | O-C-N | -8.84 | 108.56 | 122.70 |
| 81 | DA | 1433 | A | O4'-C1'-C2' | -8.84 | 96.96 | 105.80 |
| 81 | DA | 3384 | U | O4'-C1'-N1 | 8.84 | 115.27 | 108.20 |
| 78 | CA | 645 | C | O4'-C1'-C2' | -8.84 | 96.97 | 105.80 |
| 78 | CA | 1750 | A | P-O3'-C3' | 8.84 | 130.30 | 119.70 |
| 81 | DA | 273 | A | O3'-P-O5' | -8.84 | 87.21 | 104.00 |
| 81 | DA | 2629 | U | P-O5'-C5' | 8.84 | 135.04 | 120.90 |
| 33 | BD | 84 | ARG | CB-CA-C | 8.83 | 128.07 | 110.40 |
| 81 | DA | 30 | G | OP1-P-OP2 | -8.83 | 106.35 | 119.60 |
| 81 | DA | 3255 | U | P-O5'-C5' | 8.83 | 135.03 | 120.90 |
| 1 | Aa | 278 | PHE | CB-CG-CD2 | 8.83 | 126.98 | 120.80 |
| 81 | DA | 3244 | A | C1'-O4'-C4' | -8.83 | 102.83 | 109.90 |
| 78 | CA | 1508 | U | O4'-C1'-N1 | 8.83 | 115.26 | 108.20 |
| 78 | CA | 164 | A | N9-C1'-C2' | 8.82 | 125.47 | 114.00 |
| 78 | CA | 1297 | G | C3'-C2'-C1' | -8.82 | 94.44 | 101.50 |
| 81 | DA | 66 | A | O4'-C1'-C2' | -8.82 | 96.98 | 105.80 |
| 81 | DA | 673 | U | C5'-C4'-O4' | 8.82 | 119.69 | 109.10 |
| 78 | CA | 1565 | C | P-O5'-C5' | 8.82 | 135.01 | 120.90 |
| 81 | DA | 1298 | C | C1'-O4'-C4' | -8.82 | 102.84 | 109.90 |
| 78 | CA | 1690 | G | O4'-C4'-C3' | -8.82 | 95.18 | 104.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 51 | BZ | 40 | PHE | CB-CG-CD1 | -8.82 | 114.63 | 120.80 |
| 78 | CA | 393 | C | N1-C1'-C2' | 8.82 | 125.46 | 114.00 |
| 78 | CA | 1665 | U | O4'-C1'-N1 | 8.82 | 115.25 | 108.20 |
| 81 | DA | 1403 | C | OP1-P-OP2 | -8.82 | 106.38 | 119.60 |
| 15 | AN | 32 | ARG | NE-CZ-NH1 | 8.81 | 124.71 | 120.30 |
| 33 | BD | 354 | VAL | C-N-CA | -8.81 | 99.66 | 121.70 |
| 72 | Bt | 60 | ASN | CA-C-N | 8.81 | 136.59 | 117.20 |
| 78 | CA | 685 | A | P-O3'-C3' | 8.81 | 130.28 | 119.70 |
| 81 | DA | 1287 | A | C3'-C2'-C1' | 8.81 | 108.55 | 101.50 |
| 81 | DA | 3374 | U | O4'-C1'-N1 | 8.81 | 115.25 | 108.20 |
| 78 | CA | 538 | A | P-O3'-C3' | 8.81 | 130.27 | 119.70 |
| 17 | AQ | 53 | TYR | CB-CG-CD1 | -8.81 | 115.71 | 121.00 |
| 60 | Bi | 60 | ARG | NE-CZ-NH1 | 8.81 | 124.70 | 120.30 |
| 81 | DA | 1198 | C | O4'-C1'-C2' | -8.81 | 96.99 | 105.80 |
| 78 | CA | 283 | U | O4'-C1'-C2' | -8.81 | 96.99 | 105.80 |
| 81 | DA | 3346 | U | O4'-C1'-N1 | 8.81 | 115.25 | 108.20 |
| 82 | DB | 121 | U | O4'-C1'-N1 | 8.81 | 115.25 | 108.20 |
| 30 | BA | 208 | SER | N-CA-CB | 8.81 | 123.71 | 110.50 |
| 76 | BS | 82 | ARG | NE-CZ-NH2 | -8.81 | 115.90 | 120.30 |
| 78 | CA | 1458 | G | OP1-P-OP2 | -8.81 | 106.39 | 119.60 |
| 38 | Bs | 34 | SER | N-CA-CB | 8.80 | 123.71 | 110.50 |
| 78 | CA | 1393 | C | P-O3'-C3' | -8.80 | 109.14 | 119.70 |
| 79 | CB | 51 | G | O4'-C1'-N9 | 8.80 | 115.24 | 108.20 |
| 81 | DA | 1375 | G | O4'-C1'-N9 | 8.80 | 115.24 | 108.20 |
| 81 | DA | 2487 | U | C5'-C4'-O4' | -8.80 | 98.54 | 109.10 |
| 78 | CA | 164 | A | C1'-O4'-C4' | -8.80 | 102.86 | 109.90 |
| 78 | CA | 236 | A | C1'-O4'-C4' | 8.80 | 116.94 | 109.90 |
| 78 | CA | 885 | G | C5'-C4'-C3' | -8.80 | 101.92 | 116.00 |
| 78 | CA | 1133 | A | C3'-C2'-C1' | -8.80 | 94.46 | 101.50 |
| 81 | DA | 821 | U | P-O3'-C3' | -8.80 | 109.14 | 119.70 |
| 38 | Bs | 191 | TYR | CB-CG-CD2 | -8.80 | 115.72 | 121.00 |
| 43 | BP | 13 | LYS | CA-C-O | -8.80 | 101.62 | 120.10 |
| 81 | DA | 2135 | U | O4'-C1'-N1 | 8.80 | 115.24 | 108.20 |
| 83 | DC | 2 | G | P-O5'-C5' | 8.80 | 134.98 | 120.90 |
| 81 | DA | 919 | U | N1-C1'-C2' | 8.80 | 125.44 | 114.00 |
| 81 | DA | 1779 | C | O4'-C1'-C2' | -8.80 | 97.00 | 105.80 |
| 83 | DC | 18 | C | O4'-C1'-N1 | 8.80 | 115.24 | 108.20 |
| 31 | BB | 245 | LEU | CA-C-O | -8.79 | 101.64 | 120.10 |
| 81 | DA | 1192 | C | O4'-C1'-C2' | -8.79 | 97.01 | 105.80 |
| 81 | DA | 1496 | C | N1-C1'-C2' | 8.79 | 125.43 | 114.00 |
| 81 | DA | 2466 | G | O5'-C5'-C4' | 8.79 | 128.40 | 111.70 |
| 81 | DA | 2532 | U | O4'-C1'-N1 | 8.79 | 115.23 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | AS | 12 | GLN | N-CA-CB | -8.79 | 94.78 | 110.60 |
| 81 | DA | 1525 | G | N9-C1'-C2' | 8.79 | 125.42 | 114.00 |
| 81 | DA | 1997 | U | O4'-C1'-N1 | 8.79 | 115.23 | 108.20 |
| 83 | DC | 42 | A | O4'-C1'-C2' | -8.79 | 97.01 | 105.80 |
| 81 | DA | 722 | G | C3'-C2'-C1' | 8.79 | 108.53 | 101.50 |
| 83 | DC | 17 | A | N9-C1'-C2' | 8.79 | 125.42 | 114.00 |
| 82 | DB | 122 | U | O4'-C1'-C2' | -8.78 | 97.02 | 105.80 |
| 5 | AC | 19 | TYR | N-CA-CB | 8.78 | 126.41 | 110.60 |
| 35 | BG | 5 | LYS | CB-CA-C | 8.78 | 127.97 | 110.40 |
| 78 | CA | 1570 | A | O4'-C1'-N9 | -8.78 | 101.17 | 108.20 |
| 81 | DA | 3 | U | O4'-C1'-N1 | 8.78 | 115.23 | 108.20 |
| 81 | DA | 1010 | G | O4'-C1'-N9 | 8.78 | 115.23 | 108.20 |
| 81 | DA | 1620 | U | OP1-P-OP2 | -8.78 | 106.43 | 119.60 |
| 82 | DB | 59 | A | P-O3'-C3' | 8.78 | 130.24 | 119.70 |
| 33 | BD | 31 | ARG | NE-CZ-NH1 | 8.78 | 124.69 | 120.30 |
| 78 | CA | 668 | C | C3'-C2'-C1' | 8.78 | 108.52 | 101.50 |
| 40 | BK | 180 | SER | N-CA-CB | 8.78 | 123.67 | 110.50 |
| 78 | CA | 1340 | U | C5'-C4'-C3' | 8.78 | 130.05 | 116.00 |
| 81 | DA | 337 | G | O4'-C1'-C2' | -8.78 | 97.02 | 105.80 |
| 81 | DA | 672 | A | O4'-C1'-N9 | 8.78 | 115.22 | 108.20 |
| 81 | DA | 1698 | C | C1'-O4'-C4' | 8.78 | 116.92 | 109.90 |
| 57 | Be | 55 | TYR | CB-CG-CD1 | -8.78 | 115.73 | 121.00 |
| 81 | DA | 3044 | G | O4'-C1'-N9 | 8.78 | 115.22 | 108.20 |
| 81 | DA | 3140 | G | O4'-C1'-N9 | 8.78 | 115.22 | 108.20 |
| 35 | BG | 141 | VAL | O-C-N | -8.77 | 108.66 | 122.70 |
| 81 | DA | 319 | A | O4'-C1'-N9 | 8.77 | 115.22 | 108.20 |
| 81 | DA | 1120 | A | P-O3'-C3' | 8.77 | 130.22 | 119.70 |
| 81 | DA | 3002 | C | C3'-C2'-C1' | 8.77 | 108.51 | 101.50 |
| 78 | CA | 587 | C | O3'-P-O5' | 8.76 | 120.65 | 104.00 |
| 78 | CA | 1379 | C | N1-C1'-C2' | 8.76 | 125.39 | 114.00 |
| 81 | DA | 4 | U | O4'-C1'-N1 | 8.76 | 115.21 | 108.20 |
| 81 | DA | 2520 | A | C1'-O4'-C4' | 8.76 | 116.91 | 109.90 |
| 78 | CA | 1576 | A | C1'-O4'-C4' | 8.76 | 116.91 | 109.90 |
| 81 | DA | 452 | G | P-O3'-C3' | 8.76 | 130.21 | 119.70 |
| 81 | DA | 2899 | C | C3'-C2'-C1' | 8.76 | 108.51 | 101.50 |
| 81 | DA | 575 | G | O4'-C1'-N9 | 8.76 | 115.21 | 108.20 |
| 81 | DA | 1689 | U | C4'-C3'-C2' | -8.76 | 93.84 | 102.60 |
| 83 | DC | 12 | U | O4'-C1'-N1 | 8.76 | 115.21 | 108.20 |
| 33 | BD | 305 | ALA | CB-CA-C | -8.76 | 96.97 | 110.10 |
| 81 | DA | 186 | U | P-O5'-C5' | 8.76 | 134.91 | 120.90 |
| 78 | CA | 712 | G | P-O3'-C3' | -8.75 | 109.20 | 119.70 |
| 78 | CA | 1070 | C | O4'-C1'-N1 | 8.75 | 115.20 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1820 | U | N1-C1'-C2' | 8.75 | 125.38 | 114.00 |
| 81 | DA | 2800 | G | C1'-O4'-C4' | 8.75 | 116.90 | 109.90 |
| 78 | CA | 467 | G | P-O5'-C5' | 8.75 | 134.90 | 120.90 |
| 81 | DA | 2469 | G | O3'-P-O5' | -8.75 | 87.37 | 104.00 |
| 78 | CA | 1490 | C | C5'-C4'-C3' | 8.75 | 130.00 | 116.00 |
| 83 | DC | 118 | U | N1-C1'-C2' | 8.75 | 125.37 | 114.00 |
| 43 | BP | 122 | ASN | N-CA-C | 8.75 | 134.62 | 111.00 |
| 78 | CA | 1282 | U | N1-C1'-C2' | 8.75 | 125.37 | 114.00 |
| 78 | CA | 899 | G | O4'-C1'-C2' | 8.74 | 115.47 | 107.60 |
| 81 | DA | 518 | G | O3'-P-O5' | -8.74 | 87.39 | 104.00 |
| 57 | Be | 98 | LYS | CA-CB-CG | 8.74 | 132.63 | 113.40 |
| 20 | AS | 96 | ALA | N-CA-CB | 8.74 | 122.34 | 110.10 |
| 2 | AA | 252 | TRP | CB-CA-C | -8.74 | 92.92 | 110.40 |
| 10 | AI | 68 | ARG | NE-CZ-NH1 | -8.74 | 115.93 | 120.30 |
| 79 | CB | 59 | U | O4'-C1'-N1 | 8.74 | 115.19 | 108.20 |
| 81 | DA | 2894 | C | O4'-C1'-N1 | 8.74 | 115.19 | 108.20 |
| 32 | BC | 199 | PHE | N-CA-CB | 8.74 | 126.33 | 110.60 |
| 81 | DA | 502 | U | O4'-C1'-N1 | 8.74 | 115.19 | 108.20 |
| 81 | DA | 1994 | G | P-O3'-C3' | 8.74 | 130.19 | 119.70 |
| 81 | DA | 1414 | G | P-O3'-C3' | -8.74 | 109.22 | 119.70 |
| 81 | DA | 1719 | G | O4'-C1'-N9 | 8.74 | 115.19 | 108.20 |
| 81 | DA | 37 | U | O4'-C1'-N1 | 8.73 | 115.19 | 108.20 |
| 55 | Bc | 38 | ARG | NE-CZ-NH2 | -8.73 | 115.93 | 120.30 |
| 78 | CA | 499 | U | O4'-C1'-N1 | 8.73 | 115.18 | 108.20 |
| 81 | DA | 2473 | C | O4'-C1'-N1 | 8.73 | 115.18 | 108.20 |
| 78 | CA | 572 | C | N1-C1'-C2' | 8.73 | 125.34 | 114.00 |
| 81 | DA | 573 | C | C3'-C2'-C1' | 8.73 | 108.48 | 101.50 |
| 81 | DA | 2968 | G | N9-C1'-C2' | -8.73 | 102.40 | 112.00 |
| 78 | CA | 88 | U | O4'-C1'-N1 | 8.72 | 115.18 | 108.20 |
| 81 | DA | 1241 | U | P-O3'-C3' | 8.72 | 130.17 | 119.70 |
| 78 | CA | 1530 | C | C5'-C4'-O4' | -8.72 | 98.63 | 109.10 |
| 81 | DA | 962 | A | C1'-O4'-C4' | 8.72 | 116.88 | 109.90 |
| 83 | DC | 37 | G | C3'-C2'-C1' | 8.72 | 108.48 | 101.50 |
| 81 | DA | 598 | A | P-O3'-C3' | -8.72 | 109.24 | 119.70 |
| 34 | BE | 111 | ASP | N-CA-CB | 8.72 | 126.29 | 110.60 |
| 81 | DA | 1605 | A | O4'-C1'-N9 | 8.72 | 115.18 | 108.20 |
| 83 | DC | 49 | G | C2'-C3'-O3' | 8.72 | 128.68 | 109.50 |
| 78 | CA | 120 | U | O5'-C5'-C4' | 8.72 | 128.26 | 111.70 |
| 78 | CA | 1436 | A | C5'-C4'-C3' | 8.71 | 129.94 | 116.00 |
| 62 | Bk | 27 | SER | N-CA-CB | 8.71 | 123.57 | 110.50 |
| 62 | Bk | 82 | ARG | N-CA-CB | -8.71 | 94.92 | 110.60 |
| 78 | CA | 170 | U | O4'-C1'-N1 | 8.71 | 115.17 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 469 | C | C1'-O4'-C4' | 8.71 | 116.87 | 109.90 |
| 20 | AS | 24 | ARG | NE-CZ-NH1 | 8.71 | 124.65 | 120.30 |
| 78 | CA | 1505 | A | N1-C6-N6 | 8.71 | 123.83 | 118.60 |
| 81 | DA | 691 | A | O4'-C1'-N9 | 8.71 | 115.17 | 108.20 |
| 46 | BT | 124 | TYR | CB-CG-CD2 | -8.71 | 115.78 | 121.00 |
| 81 | DA | 3107 | U | P-O3'-C3' | 8.71 | 130.15 | 119.70 |
| 78 | CA | 1744 | A | P-O3'-C3' | 8.71 | 130.15 | 119.70 |
| 81 | DA | 1078 | U | N1-C1'-C2' | -8.71 | 102.42 | 112.00 |
| 78 | CA | 851 | U | N1-C1'-C2' | 8.70 | 125.31 | 114.00 |
| 81 | DA | 733 | G | N1-C6-O6 | 8.70 | 125.12 | 119.90 |
| 81 | DA | 802 | C | O5'-P-OP1 | -8.70 | 97.87 | 105.70 |
| 81 | DA | 2681 | U | P-O3'-C3' | 8.70 | 130.14 | 119.70 |
| 3 | AB | 78 | LYS | N-CA-CB | 8.70 | 126.25 | 110.60 |
| 78 | CA | 1452 | U | P-O3'-C3' | 8.70 | 130.14 | 119.70 |
| 81 | DA | 1234 | G | C1'-O4'-C4' | -8.70 | 102.94 | 109.90 |
| 78 | CA | 1562 | G | N9-C1'-C2' | -8.69 | 102.44 | 112.00 |
| 81 | DA | 2710 | C | C3'-C2'-C1' | 8.70 | 108.46 | 101.50 |
| 6 | AE | 66 | PHE | CB-CG-CD2 | -8.69 | 114.72 | 120.80 |
| 78 | CA | 1339 | C | O3'-P-O5' | -8.69 | 87.48 | 104.00 |
| 83 | DC | 1 | G | N9-C1'-C2' | -8.69 | 102.44 | 112.00 |
| 32 | BC | 102 | LEU | CB-CA-C | 8.69 | 126.71 | 110.20 |
| 78 | CA | 1666 | U | C1'-O4'-C4' | 8.69 | 116.85 | 109.90 |
| 81 | DA | 240 | U | N1-C1'-C2' | 8.69 | 125.30 | 114.00 |
| 78 | CA | 151 | G | C1'-O4'-C4' | -8.69 | 102.95 | 109.90 |
| 78 | CA | 306 | U | N1-C1'-C2' | -8.69 | 102.44 | 112.00 |
| 78 | CA | 1623 | C | C3'-C2'-C1' | 8.69 | 108.45 | 101.50 |
| 81 | DA | 974 | G | C5'-C4'-C3' | 8.69 | 129.90 | 116.00 |
| 81 | DA | 2229 | A | P-O3'-C3' | 8.69 | 130.13 | 119.70 |
| 13 | AL | 86 | PHE | CB-CG-CD2 | 8.69 | 126.88 | 120.80 |
| 81 | DA | 2260 | U | O4'-C1'-N1 | 8.69 | 115.15 | 108.20 |
| 4 | AD | 150 | PRO | N-CA-CB | 8.69 | 113.72 | 103.30 |
| 81 | DA | 206 | G | O4'-C1'-N9 | 8.69 | 115.15 | 108.20 |
| 81 | DA | 2221 | G | C3'-C2'-C1' | 8.68 | 108.45 | 101.50 |
| 78 | CA | 1415 | U | OP1-P-OP2 | -8.68 | 106.58 | 119.60 |
| 81 | DA | 50 | U | O4'-C1'-C2' | -8.68 | 97.12 | 105.80 |
| 81 | DA | 2514 | U | C1'-O4'-C4' | 8.68 | 116.85 | 109.90 |
| 81 | DA | 254 | A | C3'-C2'-C1' | 8.68 | 108.45 | 101.50 |
| 78 | CA | 30 | G | C5'-C4'-C3' | 8.68 | 129.89 | 116.00 |
| 83 | DC | 1 | G | OP1-P-OP2 | -8.68 | 106.58 | 119.60 |
| 15 | AN | 47 | ALA | O-C-N | -8.68 | 108.81 | 122.70 |
| 78 | CA | 866 | G | O4'-C1'-N9 | 8.68 | 115.14 | 108.20 |
| 78 | CA | 1761 | U | O4'-C1'-N1 | 8.68 | 115.14 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2529 | A | P-O3'-C3' | 8.68 | 130.11 | 119.70 |
| 81 | DA | 528 | U | O4'-C1'-N1 | 8.67 | 115.14 | 108.20 |
| 18 | AP | 108 | PRO | C-N-CA | 8.67 | 143.38 | 121.70 |
| 33 | BD | 148 | ILE | CB-CA-C | 8.67 | 128.95 | 111.60 |
| 78 | CA | 298 | C | C3'-C2'-C1' | 8.67 | 108.44 | 101.50 |
| 78 | CA | 1274 | C | O4'-C1'-N1 | 8.67 | 115.14 | 108.20 |
| 78 | CA | 1617 | U | N1-C1'-C2' | -8.67 | 102.46 | 112.00 |
| 81 | DA | 1571 | A | C1'-O4'-C4' | 8.67 | 116.84 | 109.90 |
| 81 | DA | 1612 | A | N9-C1'-C2' | -8.67 | 102.46 | 112.00 |
| 78 | CA | 1495 | C | O4'-C1'-N1 | 8.67 | 115.14 | 108.20 |
| 81 | DA | 1174 | G | C1'-O4'-C4' | -8.67 | 102.96 | 109.90 |
| 81 | DA | 2534 | G | N1-C6-O6 | 8.67 | 125.10 | 119.90 |
| 82 | DB | 126 | A | P-O3'-C3' | 8.67 | 130.10 | 119.70 |
| 43 | BP | 81 | TYR | CB-CG-CD2 | -8.67 | 115.80 | 121.00 |
| 78 | CA | 447 | U | C1'-O4'-C4' | -8.67 | 102.97 | 109.90 |
| 81 | DA | 162 | G | O4'-C1'-C2' | -8.67 | 97.13 | 105.80 |
| 81 | DA | 1561 | G | P-O5'-C5' | 8.67 | 134.76 | 120.90 |
| 81 | DA | 1599 | G | O4'-C1'-N9 | 8.67 | 115.13 | 108.20 |
| 81 | DA | 2099 | A | O3'-P-O5' | 8.67 | 120.47 | 104.00 |
| 81 | DA | 2086 | A | C5'-C4'-C3' | 8.66 | 129.86 | 116.00 |
| 78 | CA | 1729 | C | O4'-C1'-N1 | 8.66 | 115.13 | 108.20 |
| 78 | CA | 1746 | A | C1'-O4'-C4' | 8.66 | 116.83 | 109.90 |
| 81 | DA | 1041 | U | O4'-C1'-N1 | 8.66 | 115.13 | 108.20 |
| 81 | DA | 1057 | A | P-O3'-C3' | 8.66 | 130.10 | 119.70 |
| 81 | DA | 2616 | C | N1-C1'-C2' | 8.66 | 125.27 | 114.00 |
| 81 | DA | 404 | G | O4'-C1'-N9 | 8.66 | 115.13 | 108.20 |
| 81 | DA | 1171 | G | P-O3'-C3' | 8.66 | 130.09 | 119.70 |
| 1 | Aa | 10 | ARG | NE-CZ-NH2 | -8.66 | 115.97 | 120.30 |
| 17 | AQ | 67 | ARG | NE-CZ-NH2 | -8.66 | 115.97 | 120.30 |
| 34 | BE | 61 | ARG | O-C-N | -8.66 | 108.84 | 122.70 |
| 52 | BY | 51 | ARG | NE-CZ-NH1 | -8.66 | 115.97 | 120.30 |
| 81 | DA | 1306 | G | N9-C1'-C2' | 8.66 | 125.26 | 114.00 |
| 81 | DA | 1901 | A | N9-C1'-C2' | 8.66 | 125.26 | 114.00 |
| 81 | DA | 2509 | U | C5'-C4'-C3' | 8.66 | 129.86 | 116.00 |
| 81 | DA | 3099 | C | O4'-C4'-C3' | -8.66 | 95.34 | 104.00 |
| 78 | CA | 240 | U | P-O3'-C3' | -8.66 | 109.31 | 119.70 |
| 81 | DA | 2624 | G | N9-C1'-C2' | 8.66 | 125.26 | 114.00 |
| 81 | DA | 3214 | U | C5'-C4'-C3' | 8.66 | 129.85 | 116.00 |
| 83 | DC | 76 | U | O4'-C1'-C2' | -8.66 | 97.14 | 105.80 |
| 79 | CB | 1 | U | OP1-P-OP2 | -8.65 | 106.62 | 119.60 |
| 81 | DA | 490 | A | C4'-C3'-C2' | -8.65 | 93.95 | 102.60 |
| 78 | CA | 498 | G | N1-C6-O6 | 8.65 | 125.09 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 1787 | C | C3'-C2'-C1' | 8.65 | 108.42 | 101.50 |
| 81 | DA | 672 | A | C3'-C2'-C1' | -8.65 | 94.58 | 101.50 |
| 81 | DA | 2501 | U | O4'-C1'-N1 | 8.65 | 115.12 | 108.20 |
| 82 | DB | 105 | A | C1'-O4'-C4' | -8.65 | 102.98 | 109.90 |
| 78 | CA | 1041 | G | O4'-C1'-N9 | 8.65 | 115.12 | 108.20 |
| 78 | CA | 213 | A | N1-C6-N6 | 8.65 | 123.79 | 118.60 |
| 78 | CA | 369 | A | C1'-O4'-C4' | 8.65 | 116.82 | 109.90 |
| 81 | DA | 2267 | C | C3'-C2'-C1' | 8.65 | 108.42 | 101.50 |
| 43 | BP | 12 | ARG | NE-CZ-NH2 | -8.64 | 115.98 | 120.30 |
| 78 | CA | 609 | U | O4'-C1'-C2' | -8.64 | 97.16 | 105.80 |
| 81 | DA | 112 | U | O4'-C1'-N1 | 8.64 | 115.12 | 108.20 |
| 81 | DA | 238 | A | C3'-C2'-C1' | 8.64 | 108.42 | 101.50 |
| 81 | DA | 2425 | G | O4'-C1'-N9 | 8.64 | 115.11 | 108.20 |
| 78 | CA | 1472 | C | O4'-C1'-C2' | -8.64 | 97.16 | 105.80 |
| 68 | Bq | 20 | VAL | CA-CB-CG1 | 8.64 | 123.86 | 110.90 |
| 78 | CA | 1563 | C | C1'-O4'-C4' | -8.64 | 102.99 | 109.90 |
| 63 | Bm | 69 | TYR | CB-CG-CD1 | -8.64 | 115.82 | 121.00 |
| 74 | BQ | 79 | TYR | CB-CG-CD1 | -8.64 | 115.82 | 121.00 |
| 78 | CA | 1121 | C | O4'-C1'-N1 | 8.64 | 115.11 | 108.20 |
| 81 | DA | 2206 | G | P-O3'-C3' | 8.64 | 130.07 | 119.70 |
| 38 | Bs | 197 | PHE | CB-CG-CD2 | 8.64 | 126.85 | 120.80 |
| 76 | BS | 120 | PHE | CB-CG-CD1 | -8.64 | 114.75 | 120.80 |
| 78 | CA | 1642 | G | N9-C1'-C2' | -8.64 | 102.50 | 112.00 |
| 79 | CB | 29 | C | O3'-P-O5' | -8.64 | 87.59 | 104.00 |
| 78 | CA | 192 | U | O4'-C1'-N1 | 8.64 | 115.11 | 108.20 |
| 81 | DA | 2494 | A | P-O3'-C3' | 8.63 | 130.06 | 119.70 |
| 83 | DC | 27 | A | O4'-C1'-C2' | -8.63 | 97.17 | 105.80 |
| 81 | DA | 2949 | U | O4'-C1'-N1 | 8.63 | 115.11 | 108.20 |
| 81 | DA | 1524 | A | P-O3'-C3' | 8.63 | 130.06 | 119.70 |
| 81 | DA | 3005 | A | C1'-O4'-C4' | 8.63 | 116.81 | 109.90 |
| 78 | CA | 272 | U | O4'-C1'-N1 | 8.63 | 115.10 | 108.20 |
| 81 | DA | 1775 | G | P-O3'-C3' | -8.63 | 109.35 | 119.70 |
| 81 | DA | 1806 | A | C3'-C2'-C1' | 8.63 | 108.40 | 101.50 |
| 81 | DA | 1850 | A | N9-C1'-C2' | -8.63 | 102.51 | 112.00 |
| 81 | DA | 2510 | U | O4'-C4'-C3' | -8.63 | 95.37 | 104.00 |
| 81 | DA | 2435 | G | O4'-C1'-N9 | 8.63 | 115.10 | 108.20 |
| 81 | DA | 375 | A | C1'-O4'-C4' | 8.62 | 116.80 | 109.90 |
| 81 | DA | 1234 | G | C5'-C4'-C3' | -8.62 | 102.21 | 116.00 |
| 81 | DA | 2111 | G | O4'-C1'-N9 | 8.62 | 115.10 | 108.20 |
| 76 | BS | 159 | ARG | NE-CZ-NH2 | -8.62 | 115.99 | 120.30 |
| 78 | CA | 68 | A | C1'-O4'-C4' | -8.62 | 103.00 | 109.90 |
| 78 | CA | 407 | A | O4'-C1'-N9 | 8.62 | 115.09 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 560 | G | O4'-C1'-N9 | 8.62 | 115.09 | 108.20 |
| 78 | CA | 1324 | G | O4'-C1'-N9 | -8.62 | 101.31 | 108.20 |
| 81 | DA | 531 | G | P-O3'-C3' | 8.62 | 130.04 | 119.70 |
| 81 | DA | 1193 | A | N9-C1'-C2' | -8.62 | 102.52 | 112.00 |
| 81 | DA | 2133 | U | O4'-C1'-N1 | 8.62 | 115.09 | 108.20 |
| 81 | DA | 2883 | U | O4'-C1'-N1 | 8.62 | 115.09 | 108.20 |
| 83 | DC | 78 | G | O4'-C1'-N9 | 8.62 | 115.09 | 108.20 |
| 82 | DB | 54 | A | P-O3'-C3' | 8.61 | 130.04 | 119.70 |
| 78 | CA | 216 | U | O4'-C1'-N1 | 8.61 | 115.09 | 108.20 |
| 81 | DA | 2990 | G | O4'-C1'-N9 | 8.61 | 115.09 | 108.20 |
| 26 | AZ | 33 | ARG | NE-CZ-NH2 | -8.61 | 116.00 | 120.30 |
| 49 | BV | 64 | ASN | N-CA-CB | -8.61 | 95.10 | 110.60 |
| 58 | Bg | 19 | ARG | NE-CZ-NH2 | -8.61 | 116.00 | 120.30 |
| 76 | BS | 74 | ILE | N-CA-C | -8.61 | 87.76 | 111.00 |
| 79 | CB | 55 | C | C4'-C3'-C2' | -8.61 | 93.99 | 102.60 |
| 81 | DA | 1828 | A | O4'-C1'-N9 | 8.61 | 115.09 | 108.20 |
| 81 | DA | 1898 | G | P-O3'-C3' | 8.61 | 130.03 | 119.70 |
| 78 | CA | 573 | C | N1-C1'-C2' | 8.61 | 125.19 | 114.00 |
| 47 | BU | 159 | PHE | CB-CG-CD1 | 8.61 | 126.82 | 120.80 |
| 81 | DA | 1828 | A | P-O3'-C3' | 8.61 | 130.03 | 119.70 |
| 78 | CA | 161 | U | O4'-C1'-N1 | 8.60 | 115.08 | 108.20 |
| 16 | AO | 63 | ALA | CA-C-N | -8.60 | 98.28 | 117.20 |
| 78 | CA | 1102 | G | O4'-C1'-N9 | 8.60 | 115.08 | 108.20 |
| 78 | CA | 1339 | C | C1'-O4'-C4' | -8.60 | 103.02 | 109.90 |
| 78 | CA | 1528 | U | C1'-O4'-C4' | 8.60 | 116.78 | 109.90 |
| 81 | DA | 511 | G | O4'-C1'-N9 | 8.60 | 115.08 | 108.20 |
| 81 | DA | 526 | C | N1-C1'-C2' | 8.60 | 125.18 | 114.00 |
| 81 | DA | 273 | A | P-O3'-C3' | 8.60 | 130.02 | 119.70 |
| 81 | DA | 1412 | G | O4'-C1'-N9 | 8.60 | 115.08 | 108.20 |
| 13 | AL | 5 | LYS | CA-C-N | 8.60 | 141.17 | 117.10 |
| 81 | DA | 2378 | C | C3'-C2'-C1' | 8.60 | 108.38 | 101.50 |
| 35 | BG | 15 | VAL | N-CA-CB | -8.60 | 92.59 | 111.50 |
| 81 | DA | 2001 | U | N1-C1'-C2' | -8.60 | 102.55 | 112.00 |
| 81 | DA | 3063 | C | C3'-C2'-C1' | 8.60 | 108.38 | 101.50 |
| 81 | DA | 2768 | U | P-O3'-C3' | -8.59 | 109.39 | 119.70 |
| 81 | DA | 419 | G | C1'-O4'-C4' | 8.59 | 116.77 | 109.90 |
| 15 | AN | 53 | ASN | N-CA-C | -8.59 | 87.81 | 111.00 |
| 81 | DA | 1651 | U | C4'-C3'-C2' | -8.59 | 94.01 | 102.60 |
| 81 | DA | 2099 | A | P-O5'-C5' | 8.59 | 134.64 | 120.90 |
| 81 | DA | 3105 | U | N1-C1'-C2' | 8.59 | 125.17 | 114.00 |
| 81 | DA | 3345 | G | N9-C1'-C2' | -8.59 | 102.55 | 112.00 |
| 82 | DB | 47 | C | O4'-C1'-N1 | 8.59 | 115.07 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 1441 | C | O3'-P-O5' | -8.59 | 87.68 | 104.00 |
| 81 | DA | 597 | G | C3'-C2'-C1' | -8.59 | 94.63 | 101.50 |
| 83 | DC | 27 | A | C5'-C4'-C3' | -8.59 | 102.26 | 116.00 |
| 81 | DA | 2638 | C | O4'-C1'-C2' | -8.59 | 97.22 | 105.80 |
| 81 | DA | 2699 | G | N9-C1'-C2' | 8.59 | 125.16 | 114.00 |
| 51 | BZ | 60 | LYS | CA-C-O | -8.58 | 102.07 | 120.10 |
| 81 | DA | 2368 | A | O3'-P-O5' | -8.58 | 87.69 | 104.00 |
| 81 | DA | 2632 | G | O4'-C4'-C3' | -8.58 | 95.42 | 104.00 |
| 20 | AS | 91 | TYR | CB-CG-CD1 | 8.58 | 126.15 | 121.00 |
| 81 | DA | 836 | A | O4'-C1'-C2' | -8.58 | 97.22 | 105.80 |
| 78 | CA | 1011 | G | O4'-C1'-N9 | 8.58 | 115.06 | 108.20 |
| 81 | DA | 3014 | U | O4'-C1'-N1 | 8.58 | 115.06 | 108.20 |
| 81 | DA | 547 | G | N9-C1'-C2' | 8.58 | 125.15 | 114.00 |
| 81 | DA | 2241 | U | O4'-C1'-N1 | 8.58 | 115.06 | 108.20 |
| 81 | DA | 2496 | C | N1-C1'-C2' | 8.58 | 125.15 | 114.00 |
| 81 | DA | 2992 | U | O4'-C1'-N1 | 8.58 | 115.06 | 108.20 |
| 19 | AR | 127 | ARG | NE-CZ-NH1 | 8.57 | 124.59 | 120.30 |
| 33 | BD | 300 | ARG | NE-CZ-NH2 | -8.57 | 116.01 | 120.30 |
| 78 | CA | 463 | U | O4'-C1'-N1 | 8.57 | 115.06 | 108.20 |
| 79 | CB | 53 | U | O4'-C1'-N1 | 8.57 | 115.06 | 108.20 |
| 81 | DA | 1615 | C | N1-C1'-C2' | 8.57 | 125.15 | 114.00 |
| 81 | DA | 2265 | C | O4'-C1'-N1 | 8.57 | 115.06 | 108.20 |
| 81 | DA | 2620 | G | O4'-C1'-N9 | 8.57 | 115.06 | 108.20 |
| 81 | DA | 631 | U | O4'-C1'-N1 | 8.57 | 115.06 | 108.20 |
| 81 | DA | 1049 | C | C3'-C2'-C1' | 8.57 | 108.36 | 101.50 |
| 81 | DA | 2403 | G | C1'-O4'-C4' | 8.57 | 116.76 | 109.90 |
| 81 | DA | 2699 | G | C1'-O4'-C4' | -8.57 | 103.04 | 109.90 |
| 82 | DB | 151 | C | O5'-C5'-C4' | 8.57 | 127.98 | 111.70 |
| 78 | CA | 1468 | U | O4'-C1'-N1 | 8.57 | 115.05 | 108.20 |
| 81 | DA | 2570 | U | P-O3'-C3' | 8.57 | 129.98 | 119.70 |
| 81 | DA | 3258 | U | C1'-O4'-C4' | 8.57 | 116.75 | 109.90 |
| 81 | DA | 210 | U | O4'-C1'-N1 | 8.56 | 115.05 | 108.20 |
| 81 | DA | 1470 | U | O4'-C1'-N1 | 8.56 | 115.05 | 108.20 |
| 81 | DA | 2308 | C | C3'-C2'-C1' | 8.56 | 108.35 | 101.50 |
| 81 | DA | 3218 | A | O4'-C1'-C2' | -8.56 | 97.24 | 105.80 |
| 50 | BX | 60 | TYR | CB-CG-CD2 | -8.56 | 115.86 | 121.00 |
| 78 | CA | 1065 | A | P-O3'-C3' | 8.56 | 129.97 | 119.70 |
| 6 | AE | 66 | PHE | CB-CG-CD1 | 8.56 | 126.79 | 120.80 |
| 78 | CA | 1644 | C | P-O3'-C3' | 8.55 | 129.96 | 119.70 |
| 81 | DA | 1738 | C | C3'-C2'-C1' | 8.55 | 108.34 | 101.50 |
| 43 | BP | 81 | TYR | CB-CG-CD1 | 8.55 | 126.13 | 121.00 |
| 78 | CA | 1292 | G | O4'-C1'-N9 | 8.55 | 115.04 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 72 | C | O4'-C1'-N1 | 8.55 | 115.04 | 108.20 |
| 81 | DA | 556 | U | N1-C1'-C2' | 8.55 | 125.12 | 114.00 |
| 81 | DA | 1382 | G | C4'-C3'-C2' | -8.55 | 94.05 | 102.60 |
| 81 | DA | 2626 | A | N9-C1'-C2' | 8.55 | 125.11 | 114.00 |
| 81 | DA | 3234 | A | C1'-O4'-C4' | 8.55 | 116.74 | 109.90 |
| 78 | CA | 1156 | C | N1-C1'-C2' | 8.55 | 125.11 | 114.00 |
| 32 | BC | 137 | TYR | CG-CD2-CE2 | -8.55 | 114.46 | 121.30 |
| 78 | CA | 606 | A | C1'-O4'-C4' | -8.55 | 103.06 | 109.90 |
| 78 | CA | 840 | U | P-O3'-C3' | -8.55 | 109.44 | 119.70 |
| 81 | DA | 3234 | A | N9-C1'-C2' | -8.55 | 102.60 | 112.00 |
| 21 | AT | 9 | VAL | C-N-CA | -8.54 | 100.34 | 121.70 |
| 81 | DA | 360 | G | N9-C1'-C2' | 8.54 | 125.11 | 114.00 |
| 81 | DA | 2165 | G | C3'-C2'-C1' | -8.54 | 94.67 | 101.50 |
| 81 | DA | 2989 | U | P-O5'-C5' | 8.54 | 134.57 | 120.90 |
| 81 | DA | 3253 | G | C1'-O4'-C4' | -8.54 | 103.06 | 109.90 |
| 81 | DA | 1669 | C | P-O5'-C5' | 8.54 | 134.56 | 120.90 |
| 38 | Bs | 39 | HIS | CB-CA-C | 8.54 | 127.48 | 110.40 |
| 81 | DA | 1699 | A | C5'-C4'-C3' | 8.54 | 129.66 | 116.00 |
| 81 | DA | 2793 | G | O4'-C1'-N9 | 8.54 | 115.03 | 108.20 |
| 83 | DC | 21 | G | N9-C1'-C2' | 8.54 | 125.10 | 114.00 |
| 78 | CA | 1687 | U | O4'-C1'-N1 | 8.54 | 115.03 | 108.20 |
| 83 | DC | 40 | C | C3'-C2'-C1' | 8.54 | 108.33 | 101.50 |
| 78 | CA | 1136 | U | O4'-C1'-N1 | 8.53 | 115.03 | 108.20 |
| 81 | DA | 203 | G | C1'-O4'-C4' | -8.54 | 103.07 | 109.90 |
| 81 | DA | 356 | C | O4'-C1'-N1 | 8.54 | 115.03 | 108.20 |
| 53 | Ba | 10 | VAL | N-CA-C | 8.53 | 134.04 | 111.00 |
| 78 | CA | 1151 | A | O4'-C1'-N9 | 8.53 | 115.03 | 108.20 |
| 81 | DA | 2188 | A | P-O3'-C3' | 8.53 | 129.94 | 119.70 |
| 81 | DA | 2802 | A | P-O3'-C3' | 8.53 | 129.94 | 119.70 |
| 78 | CA | 101 | U | O4'-C1'-N1 | 8.53 | 115.03 | 108.20 |
| 32 | BC | 119 | TYR | CB-CG-CD2 | -8.53 | 115.88 | 121.00 |
| 81 | DA | 166 | C | N1-C1'-C2' | 8.53 | 125.09 | 114.00 |
| 81 | DA | 1062 | A | O4'-C1'-N9 | 8.53 | 115.02 | 108.20 |
| 81 | DA | 1401 | A | C5'-C4'-C3' | 8.53 | 129.65 | 116.00 |
| 81 | DA | 524 | U | N1-C1'-C2' | -8.53 | 102.62 | 112.00 |
| 66 | Bo | 44 | TRP | CB-CG-CD2 | -8.52 | 115.52 | 126.60 |
| 78 | CA | 1427 | A | C5'-C4'-C3' | 8.52 | 129.64 | 116.00 |
| 81 | DA | 1823 | A | OP1-P-OP2 | -8.52 | 106.81 | 119.60 |
| 78 | CA | 533 | U | P-O3'-C3' | -8.52 | 109.47 | 119.70 |
| 81 | DA | 1811 | G | C1'-O4'-C4' | 8.52 | 116.72 | 109.90 |
| 78 | CA | 1753 | A | O4'-C1'-N9 | 8.52 | 115.02 | 108.20 |
| 78 | CA | 678 | A | C3'-C2'-C1' | 8.52 | 108.32 | 101.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 842 | C | C6-N1-C2 | -8.52 | 116.89 | 120.30 |
| 78 | CA | 1058 | U | O4'-C1'-N1 | 8.52 | 115.02 | 108.20 |
| 4 | AD | 145 | ARG | NE-CZ-NH2 | -8.52 | 116.04 | 120.30 |
| 10 | AI | 107 | LYS | CG-CD-CE | 8.52 | 137.45 | 111.90 |
| 78 | CA | 1394 | G | O4'-C1'-C2' | 8.52 | 115.26 | 107.60 |
| 81 | DA | 2674 | A | N9-C1'-C2' | 8.52 | 125.07 | 114.00 |
| 81 | DA | 3089 | C | N1-C1'-C2' | 8.52 | 125.07 | 114.00 |
| 74 | BQ | 129 | TYR | CB-CG-CD2 | -8.51 | 115.89 | 121.00 |
| 81 | DA | 492 | U | P-O3'-C3' | 8.51 | 129.92 | 119.70 |
| 81 | DA | 1645 | U | N1-C1'-C2' | 8.51 | 125.07 | 114.00 |
| 81 | DA | 2056 | U | O4'-C1'-N1 | 8.51 | 115.01 | 108.20 |
| 81 | DA | 2704 | A | C3'-C2'-C1' | 8.51 | 108.31 | 101.50 |
| 78 | CA | 1043 | A | N9-C1'-C2' | -8.51 | 102.64 | 112.00 |
| 81 | DA | 3373 | U | P-O3'-C3' | 8.51 | 129.91 | 119.70 |
| 83 | DC | 118 | U | C1'-O4'-C4' | -8.51 | 103.09 | 109.90 |
| 78 | CA | 1589 | C | O4'-C1'-C2' | -8.51 | 97.29 | 105.80 |
| 81 | DA | 1222 | G | P-O5'-C5' | 8.51 | 134.51 | 120.90 |
| 81 | DA | 2244 | A | N9-C1'-C2' | -8.51 | 102.64 | 112.00 |
| 81 | DA | 1825 | G | O4'-C1'-C2' | 8.51 | 115.25 | 107.60 |
| 81 | DA | 2242 | A | C3'-C2'-C1' | 8.51 | 108.30 | 101.50 |
| 83 | DC | 61 | U | N1-C1'-C2' | -8.51 | 102.64 | 112.00 |
| 21 | AT | 29 | HIS | N-CA-CB | 8.50 | 125.91 | 110.60 |
| 72 | Bt | 60 | ASN | N-CA-CB | -8.50 | 95.29 | 110.60 |
| 78 | CA | 1492 | A | C5'-C4'-C3' | 8.50 | 129.60 | 116.00 |
| 81 | DA | 444 | U | P-O3'-C3' | 8.50 | 129.91 | 119.70 |
| 81 | DA | 1687 | U | O4'-C4'-C3' | -8.50 | 95.50 | 104.00 |
| 81 | DA | 663 | C | C5'-C4'-C3' | 8.50 | 129.60 | 116.00 |
| 81 | DA | 2434 | U | N1-C1'-C2' | 8.50 | 125.05 | 114.00 |
| 33 | BD | 145 | ILE | N-CA-CB | -8.50 | 91.26 | 110.80 |
| 37 | BH | 62 | LYS | N-CA-CB | 8.49 | 125.89 | 110.60 |
| 43 | BP | 116 | LEU | CA-C-O | -8.49 | 102.26 | 120.10 |
| 60 | Bi | 106 | LYS | N-CA-CB | 8.49 | 125.89 | 110.60 |
| 32 | BC | 3 | HIS | CB-CA-C | -8.49 | 93.42 | 110.40 |
| 47 | BU | 139 | ARG | N-CA-C | -8.49 | 88.07 | 111.00 |
| 78 | CA | 202 | A | C3'-C2'-C1' | 8.49 | 108.29 | 101.50 |
| 78 | CA | 1044 | U | O4'-C1'-N1 | -8.49 | 101.41 | 108.20 |
| 78 | CA | 1538 | U | O4'-C1'-N1 | 8.49 | 115.00 | 108.20 |
| 81 | DA | 2770 | G | C1'-O4'-C4' | -8.49 | 103.11 | 109.90 |
| 78 | CA | 900 | A | O5'-C5'-C4' | 8.49 | 127.83 | 111.70 |
| 81 | DA | 756 | U | C3'-C2'-C1' | 8.49 | 108.29 | 101.50 |
| 81 | DA | 2169 | G | P-O3'-C3' | 8.49 | 129.89 | 119.70 |
| 81 | DA | 2574 | G | N1-C6-O6 | 8.49 | 124.99 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 3013 | U | P-O5'-C5' | 8.49 | 134.48 | 120.90 |
| 78 | CA | 1779 | U | O4'-C1'-N1 | 8.49 | 114.99 | 108.20 |
| 81 | DA | 2579 | G | N1-C6-O6 | 8.49 | 124.99 | 119.90 |
| 36 | BF | 3 | TYR | CB-CG-CD2 | 8.48 | 126.09 | 121.00 |
| 81 | DA | 3254 | G | O4'-C1'-C2' | -8.48 | 97.31 | 105.80 |
| 43 | BP | 68 | ARG | NE-CZ-NH2 | -8.48 | 116.06 | 120.30 |
| 81 | DA | 1220 | U | P-O3'-C3' | 8.48 | 129.88 | 119.70 |
| 81 | DA | 1623 | G | O4'-C4'-C3' | -8.48 | 95.52 | 104.00 |
| 81 | DA | 2487 | U | O5'-P-OP1 | -8.48 | 98.07 | 105.70 |
| 81 | DA | 427 | C | N1-C1'-C2' | 8.48 | 125.02 | 114.00 |
| 81 | DA | 865 | U | O4'-C1'-N1 | 8.48 | 114.98 | 108.20 |
| 81 | DA | 1657 | C | C1'-O4'-C4' | 8.48 | 116.68 | 109.90 |
| 83 | DC | 53 | U | C3'-C2'-C1' | 8.48 | 108.28 | 101.50 |
| 81 | DA | 405 | U | N1-C1'-C2' | 8.47 | 125.02 | 114.00 |
| 45 | BR | 111 | ARG | NE-CZ-NH2 | -8.47 | 116.06 | 120.30 |
| 78 | CA | 1337 | A | O5'-C5'-C4' | -8.47 | 95.61 | 111.70 |
| 78 | CA | 1578 | U | P-O3'-C3' | 8.47 | 129.86 | 119.70 |
| 81 | DA | 678 | G | C3'-C2'-C1' | -8.47 | 94.72 | 101.50 |
| 81 | DA | 1783 | U | C5'-C4'-O4' | -8.47 | 98.94 | 109.10 |
| 77 | BI | 119 | TRP | N-CA-CB | 8.46 | 125.83 | 110.60 |
| 78 | CA | 34 | G | O4'-C1'-N9 | 8.46 | 114.97 | 108.20 |
| 81 | DA | 201 | A | N9-C1'-C2' | 8.47 | 125.01 | 114.00 |
| 81 | DA | 3217 | C | O4'-C1'-C2' | -8.46 | 97.33 | 105.80 |
| 2 | AA | 101 | ARG | CB-CA-C | 8.46 | 127.32 | 110.40 |
| 12 | AK | 20 | TYR | CB-CG-CD1 | -8.46 | 115.92 | 121.00 |
| 81 | DA | 3050 | U | O4'-C1'-C2' | -8.46 | 97.34 | 105.80 |
| 81 | DA | 1647 | A | C3'-C2'-C1' | 8.46 | 108.27 | 101.50 |
| 81 | DA | 2515 | A | C5'-C4'-C3' | 8.46 | 129.54 | 116.00 |
| 81 | DA | 2468 | A | O4'-C1'-N9 | 8.46 | 114.97 | 108.20 |
| 81 | DA | 3236 | U | N1-C1'-C2' | 8.46 | 125.00 | 114.00 |
| 61 | Bj | 20 | LYS | CA-C-N | 8.46 | 135.81 | 117.20 |
| 78 | CA | 852 | C | C3'-C2'-C1' | 8.46 | 108.27 | 101.50 |
| 78 | CA | 1161 | C | C3'-C2'-C1' | 8.46 | 108.27 | 101.50 |
| 78 | CA | 1050 | G | N1-C6-O6 | 8.45 | 124.97 | 119.90 |
| 78 | CA | 1238 | A | N9-C1'-C2' | -8.46 | 102.70 | 112.00 |
| 81 | DA | 2704 | A | O4'-C1'-C2' | -8.46 | 97.34 | 105.80 |
| 81 | DA | 3219 | G | P-O5'-C5' | 8.45 | 134.43 | 120.90 |
| 57 | Be | 176 | TYR | CB-CG-CD1 | -8.45 | 115.93 | 121.00 |
| 78 | CA | 486 | G | C5-C6-O6 | -8.45 | 123.53 | 128.60 |
| 78 | CA | 1438 | G | O5'-C5'-C4' | 8.45 | 127.76 | 111.70 |
| 81 | DA | 957 | C | C3'-C2'-C1' | 8.45 | 108.26 | 101.50 |
| 81 | DA | 2073 | A | O4'-C1'-C2' | -8.45 | 97.35 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 66 | Bo | 12 | LYS | CA-CB-CG | -8.45 | 94.81 | 113.40 |
| 78 | CA | 1214 | U | O4'-C1'-C2' | -8.45 | 97.35 | 105.80 |
| 78 | CA | 1220 | C | N1-C1'-C2' | -8.45 | 102.71 | 112.00 |
| 78 | CA | 1550 | A | O3'-P-O5' | -8.45 | 87.95 | 104.00 |
| 81 | DA | 3313 | U | C1'-O4'-C4' | -8.45 | 103.14 | 109.90 |
| 81 | DA | 3387 | U | N1-C1'-C2' | -8.45 | 102.71 | 112.00 |
| 31 | BB | 34 | TYR | CB-CG-CD1 | 8.45 | 126.07 | 121.00 |
| 78 | CA | 119 | A | P-O3'-C3' | 8.45 | 129.84 | 119.70 |
| 81 | DA | 1089 | G | O4'-C1'-N9 | 8.45 | 114.96 | 108.20 |
| 69 | Br | 63 | LYS | N-CA-CB | 8.44 | 125.80 | 110.60 |
| 45 | BR | 95 | GLU | CB-CA-C | 8.44 | 127.28 | 110.40 |
| 81 | DA | 2466 | G | O4'-C1'-N9 | -8.44 | 101.45 | 108.20 |
| 49 | BV | 21 | TYR | CB-CG-CD2 | -8.44 | 115.94 | 121.00 |
| 78 | CA | 1064 | G | N1-C6-O6 | 8.44 | 124.96 | 119.90 |
| 81 | DA | 169 | U | P-O3'-C3' | 8.44 | 129.83 | 119.70 |
| 38 | Bs | 35 | SER | N-CA-CB | 8.44 | 123.16 | 110.50 |
| 76 | BS | 82 | ARG | NE-CZ-NH1 | 8.44 | 124.52 | 120.30 |
| 78 | CA | 292 | U | O4'-C1'-N1 | 8.44 | 114.95 | 108.20 |
| 81 | DA | 2065 | U | O4'-C1'-N1 | 8.44 | 114.95 | 108.20 |
| 17 | AQ | 21 | TYR | CB-CG-CD2 | -8.43 | 115.94 | 121.00 |
| 81 | DA | 638 | C | O4'-C4'-C3' | -8.43 | 95.57 | 104.00 |
| 78 | CA | 638 | U | N1-C1'-C2' | 8.43 | 124.96 | 114.00 |
| 78 | CA | 1534 | G | O4'-C1'-N9 | 8.43 | 114.94 | 108.20 |
| 81 | DA | 637 | C | C5'-C4'-O4' | -8.43 | 98.98 | 109.10 |
| 15 | AN | 14 | TYR | CB-CG-CD2 | -8.43 | 115.94 | 121.00 |
| 32 | BC | 297 | SER | CB-CA-C | -8.43 | 94.09 | 110.10 |
| 53 | Ba | 8 | GLY | CA-C-O | -8.43 | 105.43 | 120.60 |
| 81 | DA | 1061 | A | C1'-O4'-C4' | -8.43 | 103.16 | 109.90 |
| 81 | DA | 2011 | U | O4'-C1'-N1 | 8.43 | 114.94 | 108.20 |
| 82 | DB | 96 | A | O4'-C1'-N9 | 8.43 | 114.94 | 108.20 |
| 34 | BE | 52 | TYR | CA-CB-CG | 8.42 | 129.40 | 113.40 |
| 41 | BN | 40 | ASP | N-CA-CB | 8.42 | 125.76 | 110.60 |
| 81 | DA | 80 | G | C1'-O4'-C4' | -8.42 | 103.16 | 109.90 |
| 81 | DA | 757 | C | O4'-C1'-N1 | 8.42 | 114.94 | 108.20 |
| 38 | Bs | 213 | PHE | CB-CG-CD1 | -8.42 | 114.91 | 120.80 |
| 81 | DA | 813 | G | P-O5'-C5' | 8.42 | 134.37 | 120.90 |
| 81 | DA | 1346 | G | N9-C1'-C2' | -8.42 | 102.74 | 112.00 |
| 81 | DA | 3077 | A | C3'-C2'-C1' | 8.42 | 108.23 | 101.50 |
| 81 | DA | 2466 | G | C4'-C3'-C2' | -8.42 | 94.18 | 102.60 |
| 81 | DA | 2505 | U | C1'-O4'-C4' | 8.42 | 116.63 | 109.90 |
| 81 | DA | 1660 | C | N1-C1'-C2' | 8.41 | 124.94 | 114.00 |
| 81 | DA | 3247 | G | O4'-C4'-C3' | -8.41 | 95.59 | 104.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 82 | DB | 49 | G | P-O3'-C3' | 8.41 | 129.80 | 119.70 |
| 82 | DB | 152 | G | C5'-C4'-C3' | -8.41 | 102.54 | 116.00 |
| 59 | Bh | 24 | ARG | NE-CZ-NH2 | -8.41 | 116.09 | 120.30 |
| 78 | CA | 834 | G | N9-C1'-C2' | 8.41 | 124.94 | 114.00 |
| 81 | DA | 3311 | C | P-O5'-C5' | 8.41 | 134.36 | 120.90 |
| 57 | Be | 110 | ARG | NE-CZ-NH2 | -8.41 | 116.09 | 120.30 |
| 78 | CA | 213 | A | O4'-C1'-N9 | 8.41 | 114.93 | 108.20 |
| 78 | CA | 287 | G | P-O3'-C3' | 8.41 | 129.79 | 119.70 |
| 78 | CA | 823 | G | N1-C6-O6 | 8.41 | 124.95 | 119.90 |
| 78 | CA | 1289 | U | P-O3'-C3' | 8.41 | 129.79 | 119.70 |
| 78 | CA | 1752 | U | N1-C1'-C2' | 8.41 | 124.93 | 114.00 |
| 81 | DA | 2735 | U | C1'-O4'-C4' | -8.41 | 103.17 | 109.90 |
| 20 | AS | 95 | ASP | CA-C-N | 8.41 | 135.70 | 117.20 |
| 48 | BW | 15 | PHE | CB-CG-CD1 | -8.41 | 114.91 | 120.80 |
| 78 | CA | 53 | G | O4'-C1'-N9 | 8.41 | 114.93 | 108.20 |
| 78 | CA | 1338 | C | C2'-C3'-O3' | 8.41 | 128.00 | 109.50 |
| 78 | CA | 1783 | C | P-O3'-C3' | 8.41 | 129.79 | 119.70 |
| 81 | DA | 1633 | C | N1-C1'-C2' | 8.41 | 124.93 | 114.00 |
| 81 | DA | 2748 | A | O4'-C1'-C2' | -8.41 | 97.39 | 105.80 |
| 81 | DA | 3006 | A | C1'-O4'-C4' | -8.41 | 103.17 | 109.90 |
| 19 | AR | 130 | ARG | CD-NE-CZ | 8.40 | 135.37 | 123.60 |
| 78 | CA | 383 | G | O4'-C1'-N9 | 8.40 | 114.92 | 108.20 |
| 81 | DA | 2800 | G | O4'-C1'-C2' | -8.40 | 97.39 | 105.80 |
| 22 | AV | 105 | THR | CB-CA-C | -8.40 | 88.91 | 111.60 |
| 79 | CB | 20 | C | O4'-C1'-N1 | 8.40 | 114.92 | 108.20 |
| 1 | Aa | 59 | ARG | NE-CZ-NH1 | 8.40 | 124.50 | 120.30 |
| 78 | CA | 114 | C | O4'-C1'-N1 | 8.40 | 114.92 | 108.20 |
| 78 | CA | 298 | C | O3'-P-O5' | -8.40 | 88.04 | 104.00 |
| 78 | CA | 1539 | G | C1'-O4'-C4' | 8.40 | 116.62 | 109.90 |
| 78 | CA | 1677 | C | C5'-C4'-O4' | 8.40 | 119.18 | 109.10 |
| 81 | DA | 1154 | A | C1'-O4'-C4' | 8.40 | 116.62 | 109.90 |
| 81 | DA | 2765 | C | O4'-C1'-N1 | 8.40 | 114.92 | 108.20 |
| 81 | DA | 3239 | G | C1'-O4'-C4' | -8.40 | 103.18 | 109.90 |
| 31 | BB | 23 | ARG | NE-CZ-NH2 | -8.40 | 116.10 | 120.30 |
| 78 | CA | 29 | U | O4'-C1'-C2' | -8.40 | 97.40 | 105.80 |
| 81 | DA | 2760 | C | O3'-P-O5' | -8.40 | 88.04 | 104.00 |
| 81 | DA | 626 | U | C5'-C4'-C3' | -8.40 | 102.57 | 116.00 |
| 57 | Be | 132 | PRO | C-N-CA | 8.39 | 142.69 | 121.70 |
| 74 | BQ | 190 | ILE | CB-CA-C | 8.39 | 128.39 | 111.60 |
| 78 | CA | 1333 | C | O4'-C1'-N1 | 8.39 | 114.92 | 108.20 |
| 81 | DA | 533 | A | O4'-C1'-N9 | 8.39 | 114.91 | 108.20 |
| 5 | AC | 114 | TYR | CB-CG-CD2 | 8.39 | 126.03 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 36 | BF | 3 | TYR | CB-CG-CD1 | -8.39 | 115.97 | 121.00 |
| 45 | BR | 3 | ILE | CA-C-O | -8.39 | 102.48 | 120.10 |
| 81 | DA | 1403 | C | N1-C1'-C2' | 8.39 | 124.91 | 114.00 |
| 81 | DA | 2628 | A | C5'-C4'-C3' | 8.39 | 129.42 | 116.00 |
| 34 | BE | 116 | TYR | CB-CG-CD2 | 8.39 | 126.03 | 121.00 |
| 81 | DA | 1055 | A | O3'-P-O5' | -8.39 | 88.07 | 104.00 |
| 81 | DA | 2577 | C | O4'-C1'-N1 | 8.38 | 114.91 | 108.20 |
| 81 | DA | 2634 | U | C1'-O4'-C4' | -8.38 | 103.19 | 109.90 |
| 81 | DA | 2766 | U | P-O5'-C5' | 8.38 | 134.31 | 120.90 |
| 14 | AM | 22 | VAL | N-CA-CB | 8.38 | 129.94 | 111.50 |
| 81 | DA | 31 | C | O4'-C1'-N1 | 8.38 | 114.90 | 108.20 |
| 81 | DA | 702 | C | N1-C1'-C2' | 8.38 | 124.89 | 114.00 |
| 81 | DA | 992 | A | O4'-C1'-N9 | 8.38 | 114.91 | 108.20 |
| 83 | DC | 13 | A | P-O3'-C3' | -8.38 | 109.64 | 119.70 |
| 16 | AO | 130 | ARG | NE-CZ-NH2 | -8.38 | 116.11 | 120.30 |
| 68 | Bq | 17 | ARG | NE-CZ-NH1 | 8.38 | 124.49 | 120.30 |
| 78 | CA | 1259 | U | O4'-C1'-N1 | 8.38 | 114.90 | 108.20 |
| 81 | DA | 2464 | U | P-O3'-C3' | 8.38 | 129.75 | 119.70 |
| 81 | DA | 2935 | U | O4'-C1'-N1 | 8.38 | 114.90 | 108.20 |
| 81 | DA | 1620 | U | N1-C1'-C2' | 8.38 | 124.89 | 114.00 |
| 81 | DA | 2581 | U | O4'-C1'-N1 | 8.38 | 114.90 | 108.20 |
| 32 | BC | 122 | TRP | N-CA-CB | 8.37 | 125.67 | 110.60 |
| 39 | BJ | 14 | TYR | CB-CG-CD1 | -8.37 | 115.98 | 121.00 |
| 78 | CA | 120 | U | C4'-C3'-C2' | -8.37 | 94.23 | 102.60 |
| 81 | DA | 2275 | A | C3'-C2'-C1' | -8.37 | 94.80 | 101.50 |
| 22 | AV | 31 | SER | O-C-N | -8.37 | 109.31 | 122.70 |
| 78 | CA | 664 | U | P-O3'-C3' | 8.37 | 129.74 | 119.70 |
| 81 | DA | 1007 | U | C3'-C2'-C1' | -8.37 | 94.81 | 101.50 |
| 81 | DA | 2487 | U | P-O3'-C3' | -8.37 | 109.66 | 119.70 |
| 2 | AA | 251 | GLU | CA-C-O | -8.37 | 102.53 | 120.10 |
| 81 | DA | 406 | G | N9-C1'-C2' | -8.37 | 102.80 | 112.00 |
| 81 | DA | 1441 | G | O4'-C1'-N9 | 8.37 | 114.89 | 108.20 |
| 81 | DA | 2334 | U | O3'-P-O5' | 8.37 | 119.89 | 104.00 |
| 81 | DA | 259 | C | O4'-C1'-C2' | -8.36 | 97.44 | 105.80 |
| 81 | DA | 843 | A | N9-C1'-C2' | -8.36 | 102.80 | 112.00 |
| 26 | AZ | 55 | ARG | NE-CZ-NH2 | -8.36 | 116.12 | 120.30 |
| 81 | DA | 1387 | G | O4'-C1'-N9 | 8.36 | 114.89 | 108.20 |
| 81 | DA | 2486 | A | P-O3'-C3' | 8.36 | 129.74 | 119.70 |
| 83 | DC | 1 | G | O4'-C1'-C2' | -8.36 | 97.44 | 105.80 |
| 44 | BO | 56 | VAL | CA-C-O | -8.36 | 102.54 | 120.10 |
| 81 | DA | 161 | G | C3'-C2'-C1' | -8.36 | 94.81 | 101.50 |
| 81 | DA | 3090 | U | P-O5'-C5' | 8.36 | 134.27 | 120.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 83 | DC | 96 | G | O4'-C1'-N9 | 8.36 | 114.89 | 108.20 |
| 18 | AP | 53 | TYR | O-C-N | -8.36 | 109.33 | 122.70 |
| 81 | DA | 2724 | U | P-O3'-C3' | -8.36 | 109.67 | 119.70 |
| 31 | BB | 6 | ARG | NE-CZ-NH2 | -8.35 | 116.12 | 120.30 |
| 34 | BE | 53 | THR | CA-C-O | -8.35 | 102.56 | 120.10 |
| 81 | DA | 627 | U | P-O5'-C5' | 8.35 | 134.27 | 120.90 |
| 78 | CA | 288 | A | O4'-C1'-N9 | 8.35 | 114.88 | 108.20 |
| 81 | DA | 924 | G | N9-C1'-C2' | 8.35 | 124.86 | 114.00 |
| 81 | DA | 2224 | A | O4'-C1'-N9 | 8.35 | 114.88 | 108.20 |
| 81 | DA | 2644 | C | C1'-O4'-C4' | 8.35 | 116.58 | 109.90 |
| 32 | BC | 93 | VAL | CA-CB-CG1 | -8.35 | 98.38 | 110.90 |
| 35 | BG | 76 | LEU | N-CA-CB | 8.35 | 127.09 | 110.40 |
| 69 | Br | 62 | ALA | O-C-N | -8.35 | 109.35 | 122.70 |
| 81 | DA | 159 | A | N9-C1'-C2' | -8.35 | 102.82 | 112.00 |
| 81 | DA | 1036 | A | N9-C1'-C2' | -8.35 | 102.82 | 112.00 |
| 83 | DC | 39 | C | N1-C1'-C2' | 8.35 | 124.85 | 114.00 |
| 81 | DA | 1872 | C | C1'-O4'-C4' | -8.35 | 103.22 | 109.90 |
| 50 | BX | 38 | LEU | CB-CA-C | 8.34 | 126.05 | 110.20 |
| 81 | DA | 829 | U | N1-C1'-C2' | 8.34 | 124.85 | 114.00 |
| 81 | DA | 2647 | A | N9-C1'-C2' | -8.34 | 102.82 | 112.00 |
| 78 | CA | 624 | G | O4'-C1'-N9 | 8.34 | 114.87 | 108.20 |
| 78 | CA | 1639 | C | O4'-C1'-N1 | 8.34 | 114.87 | 108.20 |
| 81 | DA | 1939 | G | N9-C1'-C2' | 8.34 | 124.84 | 114.00 |
| 81 | DA | 1969 | G | O4'-C1'-N9 | 8.34 | 114.87 | 108.20 |
| 81 | DA | 2195 | C | C5'-C4'-C3' | -8.34 | 102.66 | 116.00 |
| 81 | DA | 2898 | G | C3'-C2'-C1' | 8.34 | 108.17 | 101.50 |
| 22 | AV | 26 | LYS | CB-CA-C | 8.34 | 127.08 | 110.40 |
| 53 | Ba | 9 | LYS | C-N-CA | 8.34 | 142.54 | 121.70 |
| 56 | Bf | 50 | VAL | CB-CA-C | 8.34 | 127.24 | 111.40 |
| 81 | DA | 2493 | U | P-O3'-C3' | 8.34 | 129.70 | 119.70 |
| 10 | AI | 135 | ARG | NE-CZ-NH2 | 8.33 | 124.47 | 120.30 |
| 81 | DA | 1076 | C | O3'-P-O5' | -8.33 | 88.17 | 104.00 |
| 78 | CA | 871 | G | O4'-C1'-N9 | 8.33 | 114.87 | 108.20 |
| 78 | CA | 905 | A | O5'-P-OP1 | 8.33 | 120.70 | 110.70 |
| 78 | CA | 1300 | A | C1'-O4'-C4' | 8.33 | 116.57 | 109.90 |
| 83 | DC | 55 | A | N9-C1'-C2' | -8.33 | 102.83 | 112.00 |
| 35 | BG | 75 | PRO | CA-N-CD | -8.33 | 99.84 | 111.50 |
| 51 | BZ | 8 | PHE | CB-CG-CD2 | 8.33 | 126.63 | 120.80 |
| 81 | DA | 415 | G | C1'-O4'-C4' | -8.33 | 103.24 | 109.90 |
| 81 | DA | 1572 | U | O4'-C1'-C2' | -8.33 | 97.47 | 105.80 |
| 81 | DA | 2928 | C | C5'-C4'-C3' | -8.33 | 102.67 | 116.00 |
| 12 | AK | 123 | SER | CA-C-O | -8.33 | 102.61 | 120.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 646 | C | C1'-O4'-C4' | -8.33 | 103.24 | 109.90 |
| 78 | CA | 472 | U | O4'-C1'-N1 | 8.32 | 114.86 | 108.20 |
| 78 | CA | 611 | U | O4'-C1'-N1 | 8.32 | 114.86 | 108.20 |
| 78 | CA | 1539 | G | O4'-C1'-C2' | -8.32 | 97.48 | 105.80 |
| 81 | DA | 3056 | U | O4'-C1'-C2' | -8.32 | 97.48 | 105.80 |
| 83 | DC | 3 | U | N1-C1'-C2' | -8.32 | 102.84 | 112.00 |
| 82 | DB | 122 | U | N1-C1'-C2' | -8.32 | 102.84 | 112.00 |
| 5 | AC | 168 | ARG | CA-C-N | 8.32 | 140.40 | 117.10 |
| 81 | DA | 2422 | C | O4'-C1'-N1 | 8.32 | 114.86 | 108.20 |
| 81 | DA | 2505 | U | O4'-C1'-C2' | -8.32 | 97.48 | 105.80 |
| 35 | BG | 38 | THR | CB-CA-C | -8.32 | 89.14 | 111.60 |
| 81 | DA | 1517 | G | O4'-C1'-N9 | 8.32 | 114.86 | 108.20 |
| 33 | BD | 69 | ARG | NE-CZ-NH1 | 8.32 | 124.46 | 120.30 |
| 78 | CA | 598 | U | O4'-C1'-N1 | 8.32 | 114.85 | 108.20 |
| 78 | CA | 1328 | G | O4'-C1'-N9 | 8.32 | 114.85 | 108.20 |
| 81 | DA | 3305 | A | OP1-P-O3' | 8.32 | 123.50 | 105.20 |
| 78 | CA | 1546 | G | N9-C1'-C2' | 8.31 | 124.81 | 114.00 |
| 82 | DB | 5 | U | O4'-C1'-N1 | 8.31 | 114.85 | 108.20 |
| 78 | CA | 255 | U | O4'-C1'-N1 | 8.31 | 114.85 | 108.20 |
| 78 | CA | 576 | G | N1-C6-O6 | 8.31 | 124.89 | 119.90 |
| 81 | DA | 2891 | U | O4'-C1'-N1 | 8.31 | 114.85 | 108.20 |
| 81 | DA | 2284 | C | C3'-C2'-C1' | 8.31 | 108.15 | 101.50 |
| 30 | BA | 151 | VAL | N-CA-CB | 8.31 | 129.77 | 111.50 |
| 35 | BG | 8 | LYS | N-CA-C | 8.31 | 133.43 | 111.00 |
| 55 | Bc | 81 | ARG | NE-CZ-NH2 | -8.31 | 116.15 | 120.30 |
| 60 | Bi | 41 | ARG | CA-C-N | 8.31 | 140.36 | 117.10 |
| 78 | CA | 885 | G | O4'-C1'-C2' | -8.31 | 97.49 | 105.80 |
| 78 | CA | 1767 | G | O4'-C1'-N9 | -8.31 | 101.56 | 108.20 |
| 68 | Bq | 2 | ARG | NE-CZ-NH1 | -8.31 | 116.15 | 120.30 |
| 78 | CA | 444 | C | C3'-C2'-C1' | 8.31 | 108.14 | 101.50 |
| 44 | BO | 73 | LEU | CA-C-O | -8.30 | 102.66 | 120.10 |
| 78 | CA | 660 | G | P-O5'-C5' | -8.30 | 107.61 | 120.90 |
| 81 | DA | 874 | U | C1'-O4'-C4' | -8.30 | 103.26 | 109.90 |
| 81 | DA | 2025 | G | N9-C1'-C2' | -8.30 | 102.86 | 112.00 |
| 81 | DA | 2045 | G | O3'-P-O5' | -8.30 | 88.22 | 104.00 |
| 81 | DA | 2178 | A | P-O3'-C3' | 8.31 | 129.67 | 119.70 |
| 81 | DA | 3281 | U | O4'-C1'-N1 | 8.31 | 114.84 | 108.20 |
| 82 | DB | 63 | G | O4'-C1'-C2' | -8.30 | 97.50 | 105.80 |
| 45 | BR | 3 | ILE | C-N-CA | 8.30 | 142.45 | 121.70 |
| 81 | DA | 2420 | C | P-O3'-C3' | 8.30 | 129.66 | 119.70 |
| 78 | CA | 916 | U | N1-C1'-C2' | 8.30 | 124.79 | 114.00 |
| 78 | CA | 1158 | C | C3'-C2'-C1' | 8.30 | 108.14 | 101.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 740 | G | O4'-C1'-N9 | 8.30 | 114.84 | 108.20 |
| 81 | DA | 3393 | U | O4'-C1'-N1 | 8.30 | 114.84 | 108.20 |
| 35 | BG | 61 | ASN | N-CA-CB | 8.30 | 125.54 | 110.60 |
| 81 | DA | 1295 | G | C1'-O4'-C4' | -8.30 | 103.26 | 109.90 |
| 81 | DA | 1943 | C | N1-C1'-C2' | 8.30 | 124.79 | 114.00 |
| 81 | DA | 1649 | U | N1-C1'-C2' | -8.30 | 102.88 | 112.00 |
| 3 | AB | 72 | LEU | N-CA-CB | 8.29 | 126.99 | 110.40 |
| 66 | Bo | 41 | ARG | CA-C-O | -8.29 | 102.68 | 120.10 |
| 74 | BQ | 242 | SER | C-N-CA | -8.29 | 100.97 | 121.70 |
| 78 | CA | 177 | U | C3'-C2'-C1' | 8.29 | 108.14 | 101.50 |
| 81 | DA | 1755 | C | C4'-C3'-O3' | 8.29 | 129.59 | 113.00 |
| 81 | DA | 2573 | G | O4'-C1'-N9 | 8.29 | 114.84 | 108.20 |
| 81 | DA | 3073 | A | O3'-P-O5' | -8.29 | 88.24 | 104.00 |
| 78 | CA | 1577 | A | O4'-C1'-N9 | 8.29 | 114.83 | 108.20 |
| 81 | DA | 763 | G | O4'-C1'-N9 | 8.29 | 114.83 | 108.20 |
| 83 | DC | 102 | C | O4'-C1'-C2' | -8.29 | 97.51 | 105.80 |
| 78 | CA | 1591 | C | O5'-P-OP2 | -8.29 | 98.24 | 105.70 |
| 81 | DA | 2100 | A | C3'-C2'-C1' | 8.29 | 108.13 | 101.50 |
| 51 | BZ | 51 | TRP | CB-CA-C | 8.29 | 126.98 | 110.40 |
| 78 | CA | 347 | G | O4'-C1'-N9 | 8.29 | 114.83 | 108.20 |
| 78 | CA | 1382 | A | O4'-C1'-N9 | 8.29 | 114.83 | 108.20 |
| 81 | DA | 1002 | A | C4'-C3'-C2' | -8.28 | 94.32 | 102.60 |
| 81 | DA | 1608 | C | N1-C1'-C2' | 8.29 | 124.77 | 114.00 |
| 81 | DA | 2218 | G | C1'-O4'-C4' | -8.29 | 103.27 | 109.90 |
| 81 | DA | 3030 | G | N9-C1'-C2' | 8.28 | 124.77 | 114.00 |
| 82 | DB | 133 | G | O4'-C1'-N9 | 8.28 | 114.83 | 108.20 |
| 24 | AX | 77 | THR | N-CA-CB | 8.28 | 126.03 | 110.30 |
| 37 | BH | 131 | ALA | N-CA-CB | 8.28 | 121.69 | 110.10 |
| 81 | DA | 429 | U | O4'-C1'-N1 | 8.28 | 114.82 | 108.20 |
| 81 | DA | 2072 | G | C5'-C4'-C3' | -8.28 | 102.75 | 116.00 |
| 81 | DA | 2323 | G | N9-C1'-C2' | -8.28 | 102.89 | 112.00 |
| 81 | DA | 2565 | U | O4'-C1'-N1 | 8.28 | 114.83 | 108.20 |
| 81 | DA | 432 | G | P-O3'-C3' | 8.28 | 129.64 | 119.70 |
| 81 | DA | 1877 | U | O4'-C1'-N1 | 8.28 | 114.82 | 108.20 |
| 82 | DB | 52 | A | P-O5'-C5' | 8.28 | 134.14 | 120.90 |
| 45 | BR | 143 | PRO | N-CA-CB | -8.28 | 93.37 | 103.30 |
| 78 | CA | 1731 | A | P-O3'-C3' | 8.28 | 129.63 | 119.70 |
| 78 | CA | 280 | U | C1'-O4'-C4' | -8.27 | 103.28 | 109.90 |
| 78 | CA | 70 | C | C3'-C2'-C1' | 8.27 | 108.12 | 101.50 |
| 78 | CA | 1509 | C | N3-C4-N4 | 8.27 | 123.79 | 118.00 |
| 81 | DA | 1703 | U | O4'-C1'-N1 | 8.27 | 114.82 | 108.20 |
| 81 | DA | 3149 | G | C1'-O4'-C4' | 8.27 | 116.52 | 109.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 170 | G | O4'-C1'-C2' | -8.27 | 97.53 | 105.80 |
| 81 | DA | 1050 | U | C1'-O4'-C4' | 8.27 | 116.52 | 109.90 |
| 83 | DC | 38 | U | P-O5'-C5' | 8.27 | 134.13 | 120.90 |
| 78 | CA | 451 | A | P-O3'-C3' | 8.27 | 129.62 | 119.70 |
| 81 | DA | 1417 | G | O4'-C1'-N9 | 8.27 | 114.82 | 108.20 |
| 81 | DA | 2669 | G | O4'-C1'-C2' | 8.27 | 115.04 | 107.60 |
| 81 | DA | 1007 | U | C5'-C4'-O4' | 8.27 | 119.02 | 109.10 |
| 82 | DB | 153 | U | N1-C1'-C2' | -8.27 | 102.90 | 112.00 |
| 78 | CA | 179 | A | P-O5'-C5' | 8.27 | 134.13 | 120.90 |
| 78 | CA | 1009 | U | O4'-C1'-N1 | 8.27 | 114.81 | 108.20 |
| 81 | DA | 671 | U | C4'-C3'-O3' | 8.27 | 129.53 | 113.00 |
| 81 | DA | 1216 | C | C4'-C3'-C2' | -8.27 | 94.33 | 102.60 |
| 81 | DA | 1879 | A | N9-C1'-C2' | 8.27 | 124.75 | 114.00 |
| 81 | DA | 2030 | C | O4'-C1'-N1 | 8.27 | 114.81 | 108.20 |
| 81 | DA | 2807 | U | O4'-C1'-N1 | 8.27 | 114.81 | 108.20 |
| 32 | BC | 17 | LEU | N-CA-C | -8.26 | 88.69 | 111.00 |
| 81 | DA | 800 | G | N9-C1'-C2' | -8.26 | 102.91 | 112.00 |
| 81 | DA | 993 | G | C3'-C2'-C1' | -8.26 | 94.89 | 101.50 |
| 81 | DA | 1819 | U | C1'-O4'-C4' | 8.26 | 116.51 | 109.90 |
| 81 | DA | 3325 | G | C1'-O4'-C4' | 8.26 | 116.51 | 109.90 |
| 14 | AM | 110 | ARG | NE-CZ-NH1 | -8.26 | 116.17 | 120.30 |
| 34 | BE | 10 | ARG | N-CA-CB | 8.26 | 125.47 | 110.60 |
| 81 | DA | 3095 | U | P-O3'-C3' | 8.26 | 129.61 | 119.70 |
| 76 | BS | 41 | SER | CB-CA-C | -8.26 | 94.41 | 110.10 |
| 81 | DA | 531 | G | O4'-C1'-N9 | -8.26 | 101.59 | 108.20 |
| 81 | DA | 2206 | G | N9-C1'-C2' | -8.26 | 102.91 | 112.00 |
| 81 | DA | 1285 | G | P-O3'-C3' | 8.26 | 129.61 | 119.70 |
| 78 | CA | 200 | A | P-O3'-C3' | 8.26 | 129.61 | 119.70 |
| 78 | CA | 1439 | C | P-O3'-C3' | -8.26 | 109.79 | 119.70 |
| 81 | DA | 481 | U | O4'-C1'-N1 | 8.26 | 114.81 | 108.20 |
| 81 | DA | 1256 | G | C1'-O4'-C4' | -8.26 | 103.29 | 109.90 |
| 81 | DA | 1361 | U | O4'-C1'-C2' | -8.26 | 97.54 | 105.80 |
| 81 | DA | 2869 | U | O4'-C1'-N1 | 8.26 | 114.81 | 108.20 |
| 81 | DA | 3035 | A | P-O3'-C3' | 8.26 | 129.61 | 119.70 |
| 81 | DA | 3344 | A | C1'-O4'-C4' | 8.26 | 116.50 | 109.90 |
| 33 | BD | 84 | ARG | N-CA-CB | 8.25 | 125.45 | 110.60 |
| 81 | DA | 577 | C | C3'-C2'-C1' | 8.25 | 108.10 | 101.50 |
| 81 | DA | 1199 | C | C3'-C2'-C1' | 8.25 | 108.10 | 101.50 |
| 81 | DA | 2020 | A | O4'-C1'-C2' | -8.25 | 97.55 | 105.80 |
| 81 | DA | 2370 | G | O4'-C1'-N9 | 8.25 | 114.80 | 108.20 |
| 81 | DA | 331 | G | C3'-C2'-C1' | 8.25 | 108.10 | 101.50 |
| 81 | DA | 596 | C | C5'-C4'-C3' | 8.25 | 129.20 | 116.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1361 | U | C1'-O4'-C4' | 8.25 | 116.50 | 109.90 |
| 31 | BB | 246 | LEU | N-CA-C | -8.25 | 88.73 | 111.00 |
| 77 | BI | 4 | ARG | NE-CZ-NH1 | 8.25 | 124.42 | 120.30 |
| 78 | CA | 679 | U | C1'-O4'-C4' | 8.25 | 116.50 | 109.90 |
| 81 | DA | 624 | G | P-O3'-C3' | 8.25 | 129.60 | 119.70 |
| 81 | DA | 1985 | G | O4'-C1'-N9 | 8.25 | 114.80 | 108.20 |
| 81 | DA | 2544 | U | O4'-C1'-N1 | 8.25 | 114.80 | 108.20 |
| 83 | DC | 114 | A | P-O5'-C5' | 8.25 | 134.09 | 120.90 |
| 78 | CA | 257 | A | O4'-C1'-N9 | 8.24 | 114.80 | 108.20 |
| 78 | CA | 857 | U | O4'-C1'-N1 | 8.24 | 114.80 | 108.20 |
| 78 | CA | 1173 | C | O4'-C1'-N1 | 8.24 | 114.80 | 108.20 |
| 81 | DA | 948 | C | C3'-C2'-C1' | 8.24 | 108.09 | 101.50 |
| 59 | Bh | 21 | HIS | CA-CB-CG | 8.24 | 127.61 | 113.60 |
| 1 | Aa | 53 | LYS | CB-CA-C | -8.24 | 93.92 | 110.40 |
| 26 | AZ | 18 | THR | CB-CA-C | 8.24 | 133.85 | 111.60 |
| 45 | BR | 39 | ARG | N-CA-CB | 8.24 | 125.43 | 110.60 |
| 60 | Bi | 16 | ARG | CB-CA-C | -8.24 | 93.92 | 110.40 |
| 81 | DA | 1624 | G | C5'-C4'-O4' | -8.24 | 99.21 | 109.10 |
| 81 | DA | 3231 | U | C5'-C4'-C3' | -8.24 | 102.82 | 116.00 |
| 83 | DC | 102 | C | N1-C1'-C2' | 8.24 | 124.71 | 114.00 |
| 59 | Bh | 17 | PHE | CB-CG-CD1 | -8.24 | 115.03 | 120.80 |
| 78 | CA | 1441 | C | N1-C1'-C2' | 8.24 | 124.71 | 114.00 |
| 81 | DA | 361 | A | O4'-C1'-N9 | 8.24 | 114.79 | 108.20 |
| 81 | DA | 2741 | C | O4'-C1'-C2' | -8.24 | 97.56 | 105.80 |
| 1 | Aa | 212 | ALA | N-CA-CB | 8.23 | 121.63 | 110.10 |
| 81 | DA | 401 | U | N1-C1'-C2' | -8.23 | 102.94 | 112.00 |
| 81 | DA | 1251 | A | C1'-O4'-C4' | -8.23 | 103.31 | 109.90 |
| 78 | CA | 574 | G | N1-C6-O6 | 8.23 | 124.84 | 119.90 |
| 78 | CA | 1337 | A | C5'-C4'-O4' | -8.23 | 99.22 | 109.10 |
| 81 | DA | 1688 | U | O4'-C1'-C2' | -8.23 | 97.57 | 105.80 |
| 81 | DA | 1757 | A | C5-C6-N1 | -8.23 | 113.58 | 117.70 |
| 65 | Bn | 40 | GLN | N-CA-C | 8.23 | 133.22 | 111.00 |
| 81 | DA | 495 | G | O4'-C1'-N9 | 8.23 | 114.78 | 108.20 |
| 81 | DA | 899 | U | O4'-C1'-N1 | 8.23 | 114.78 | 108.20 |
| 3 | AB | 27 | ARG | NE-CZ-NH1 | -8.23 | 116.19 | 120.30 |
| 78 | CA | 304 | U | N1-C1'-C2' | 8.23 | 124.69 | 114.00 |
| 78 | CA | 591 | A | O3'-P-O5' | -8.23 | 88.37 | 104.00 |
| 81 | DA | 2656 | A | P-O3'-C3' | 8.23 | 129.57 | 119.70 |
| 81 | DA | 3287 | U | P-O3'-C3' | 8.23 | 129.57 | 119.70 |
| 44 | BO | 42 | ARG | NE-CZ-NH2 | 8.22 | 124.41 | 120.30 |
| 55 | Bc | 94 | LYS | N-CA-CB | 8.22 | 125.41 | 110.60 |
| 78 | CA | 1086 | A | O4'-C1'-N9 | -8.22 | 101.62 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 39 | BJ | 123 | ARG | CA-CB-CG | 8.22 | 131.49 | 113.40 |
| 78 | CA | 1301 | U | O4'-C1'-C2' | -8.22 | 97.58 | 105.80 |
| 79 | CB | 12 | U | O4'-C1'-N1 | 8.22 | 114.78 | 108.20 |
| 81 | DA | 707 | U | O4'-C1'-N1 | 8.22 | 114.78 | 108.20 |
| 79 | CB | 67 | G | O4'-C1'-N9 | 8.22 | 114.78 | 108.20 |
| 81 | DA | 3166 | C | O4'-C1'-N1 | 8.22 | 114.78 | 108.20 |
| 81 | DA | 1976 | G | C5'-C4'-C3' | 8.22 | 129.15 | 116.00 |
| 81 | DA | 2562 | A | O4'-C1'-N9 | 8.22 | 114.78 | 108.20 |
| 81 | DA | 2978 | U | O4'-C1'-N1 | 8.22 | 114.78 | 108.20 |
| 35 | BG | 96 | VAL | N-CA-C | -8.22 | 88.81 | 111.00 |
| 72 | Bu | 60 | ASN | CA-C-N | 8.22 | 135.28 | 117.20 |
| 78 | CA | 8 | U | O4'-C1'-N1 | 8.22 | 114.78 | 108.20 |
| 81 | DA | 914 | A | N9-C1'-C2' | -8.22 | 102.96 | 112.00 |
| 81 | DA | 2150 | G | C5'-C4'-C3' | -8.22 | 102.86 | 116.00 |
| 81 | DA | 3311 | C | N1-C1'-C2' | 8.22 | 124.68 | 114.00 |
| 78 | CA | 1049 | U | O4'-C1'-N1 | 8.21 | 114.77 | 108.20 |
| 78 | CA | 256 | A | O4'-C1'-C2' | -8.21 | 97.59 | 105.80 |
| 81 | DA | 2628 | A | O4'-C4'-C3' | -8.21 | 95.79 | 104.00 |
| 81 | DA | 3102 | G | O4'-C1'-N9 | 8.21 | 114.77 | 108.20 |
| 78 | CA | 1022 | C | O4'-C1'-C2' | -8.21 | 97.59 | 105.80 |
| 78 | CA | 1260 | U | O4'-C1'-N1 | 8.21 | 114.77 | 108.20 |
| 78 | CA | 1310 | U | C3'-C2'-C1' | 8.21 | 108.07 | 101.50 |
| 17 | AQ | 30 | THR | CA-CB-CG2 | -8.21 | 100.91 | 112.40 |
| 81 | DA | 1528 | G | C3'-C2'-C1' | -8.21 | 94.93 | 101.50 |
| 81 | DA | 2194 | G | C5'-C4'-C3' | -8.21 | 102.87 | 116.00 |
| 81 | DA | 2675 | C | C3'-C2'-C1' | 8.21 | 108.07 | 101.50 |
| 4 | AD | 153 | ASN | N-CA-CB | -8.21 | 95.83 | 110.60 |
| 81 | DA | 1762 | C | O4'-C1'-N1 | 8.20 | 114.76 | 108.20 |
| 81 | DA | 1827 | C | C3'-C2'-C1' | 8.21 | 108.06 | 101.50 |
| 42 | BM | 97 | ASP | CB-CG-OD1 | 8.20 | 125.68 | 118.30 |
| 78 | CA | 169 | A | O4'-C1'-N9 | 8.20 | 114.76 | 108.20 |
| 78 | CA | 1350 | U | O4'-C1'-N1 | 8.20 | 114.76 | 108.20 |
| 81 | DA | 519 | A | P-O5'-C5' | 8.20 | 134.03 | 120.90 |
| 81 | DA | 790 | U | C1'-O4'-C4' | -8.20 | 103.34 | 109.90 |
| 81 | DA | 1956 | A | O4'-C1'-N9 | 8.20 | 114.76 | 108.20 |
| 81 | DA | 2950 | G | P-O3'-C3' | 8.20 | 129.54 | 119.70 |
| 81 | DA | 2967 | A | O4'-C1'-N9 | 8.20 | 114.76 | 108.20 |
| 81 | DA | 3326 | G | O4'-C1'-C2' | -8.20 | 97.60 | 105.80 |
| 36 | BF | 88 | TYR | CB-CG-CD1 | 8.20 | 125.92 | 121.00 |
| 83 | DC | 32 | U | P-O3'-C3' | 8.20 | 129.54 | 119.70 |
| 81 | DA | 1689 | U | P-O3'-C3' | 8.20 | 129.53 | 119.70 |
| 81 | DA | 3373 | U | P-O5'-C5' | 8.20 | 134.02 | 120.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 6 | AE | 70 | ASP | CA-C-N | 8.19 | 135.23 | 117.20 |
| 81 | DA | 275 | U | C4'-C3'-C2' | -8.19 | 94.41 | 102.60 |
| 81 | DA | 1291 | A | O4'-C1'-C2' | -8.19 | 97.61 | 105.80 |
| 81 | DA | 2588 | U | O4'-C1'-N1 | 8.19 | 114.75 | 108.20 |
| 81 | DA | 161 | G | O3'-P-O5' | -8.19 | 88.44 | 104.00 |
| 53 | Ba | 13 | VAL | CB-CA-C | 8.19 | 126.96 | 111.40 |
| 78 | CA | 988 | A | O4'-C1'-C2' | -8.19 | 97.61 | 105.80 |
| 78 | CA | 1380 | U | O3'-P-O5' | -8.19 | 88.44 | 104.00 |
| 81 | DA | 97 | U | O4'-C1'-N1 | 8.19 | 114.75 | 108.20 |
| 81 | DA | 973 | A | O4'-C1'-N9 | 8.19 | 114.75 | 108.20 |
| 82 | DB | 23 | U | O4'-C1'-N1 | 8.19 | 114.75 | 108.20 |
| 78 | CA | 16 | G | O4'-C1'-C2' | -8.19 | 97.61 | 105.80 |
| 78 | CA | 1067 | C | P-O3'-C3' | 8.19 | 129.52 | 119.70 |
| 81 | DA | 2319 | U | P-O3'-C3' | 8.19 | 129.52 | 119.70 |
| 78 | CA | 1476 | C | OP1-P-O3' | -8.19 | 87.19 | 105.20 |
| 81 | DA | 2465 | G | N9-C1'-C2' | 8.19 | 124.64 | 114.00 |
| 5 | AC | 169 | PRO | C-N-CA | 8.18 | 139.49 | 122.30 |
| 81 | DA | 892 | U | O4'-C1'-N1 | 8.18 | 114.75 | 108.20 |
| 81 | DA | 2308 | C | N1-C1'-C2' | 8.18 | 124.64 | 114.00 |
| 81 | DA | 2806 | U | O4'-C1'-N1 | 8.18 | 114.75 | 108.20 |
| 78 | CA | 1336 | A | N9-C1'-C2' | 8.18 | 124.64 | 114.00 |
| 81 | DA | 229 | G | O4'-C1'-C2' | 8.18 | 114.96 | 107.60 |
| 81 | DA | 855 | U | O4'-C1'-N1 | 8.18 | 114.74 | 108.20 |
| 81 | DA | 2448 | G | O4'-C1'-N9 | 8.18 | 114.75 | 108.20 |
| 14 | AM | 128 | PHE | CB-CG-CD2 | 8.18 | 126.53 | 120.80 |
| 78 | CA | 1599 | C | O4'-C1'-C2' | -8.18 | 97.62 | 105.80 |
| 81 | DA | 877 | C | N1-C1'-C2' | 8.18 | 124.63 | 114.00 |
| 81 | DA | 3337 | G | O4'-C1'-N9 | 8.18 | 114.74 | 108.20 |
| 45 | BR | 14 | GLY | N-CA-C | 8.18 | 133.54 | 113.10 |
| 78 | CA | 894 | U | O4'-C4'-C3' | -8.17 | 95.83 | 104.00 |
| 78 | CA | 1078 | C | O4'-C1'-N1 | 8.17 | 114.74 | 108.20 |
| 81 | DA | 2496 | C | O4'-C1'-N1 | 8.17 | 114.74 | 108.20 |
| 78 | CA | 1111 | G | C1'-O4'-C4' | -8.17 | 103.37 | 109.90 |
| 5 | AC | 38 | ASN | N-CA-CB | 8.17 | 125.30 | 110.60 |
| 81 | DA | 666 | A | O4'-C1'-C2' | 8.17 | 114.95 | 107.60 |
| 81 | DA | 1283 | C | C3'-C2'-C1' | 8.17 | 108.03 | 101.50 |
| 81 | DA | 2492 | C | C4'-C3'-C2' | -8.17 | 94.43 | 102.60 |
| 34 | BE | 9 | MET | CB-CA-C | -8.16 | 94.07 | 110.40 |
| 78 | CA | 649 | U | C3'-C2'-C1' | -8.16 | 94.97 | 101.50 |
| 81 | DA | 2099 | A | OP1-P-O3' | -8.16 | 87.24 | 105.20 |
| 78 | CA | 1784 | C | P-O3'-C3' | 8.16 | 129.50 | 119.70 |
| 81 | DA | 3357 | U | O4'-C1'-N1 | 8.16 | 114.73 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2797 | C | O4'-C1'-C2' | -8.16 | 97.64 | 105.80 |
| 81 | DA | 2130 | G | C4'-C3'-C2' | -8.16 | 94.44 | 102.60 |
| 18 | AP | 93 | TYR | CG-CD1-CE1 | -8.16 | 114.78 | 121.30 |
| 60 | Bi | 68 | THR | CB-CA-C | -8.16 | 89.58 | 111.60 |
| 81 | DA | 83 | U | O4'-C1'-N1 | 8.16 | 114.72 | 108.20 |
| 81 | DA | 1679 | A | N9-C1'-C2' | 8.16 | 124.60 | 114.00 |
| 78 | CA | 1640 | C | O4'-C1'-N1 | 8.15 | 114.72 | 108.20 |
| 81 | DA | 2737 | C | N1-C1'-C2' | 8.15 | 124.60 | 114.00 |
| 78 | CA | 1727 | G | O4'-C1'-N9 | 8.15 | 114.72 | 108.20 |
| 81 | DA | 1316 | C | O4'-C1'-N1 | -8.15 | 101.68 | 108.20 |
| 81 | DA | 3048 | A | O4'-C1'-C2' | -8.15 | 97.65 | 105.80 |
| 10 | AI | 119 | ALA | CA-C-O | -8.15 | 102.98 | 120.10 |
| 82 | DB | 3 | A | C3'-C2'-C1' | -8.15 | 94.98 | 101.50 |
| 78 | CA | 1234 | A | C3'-C2'-C1' | -8.15 | 94.98 | 101.50 |
| 14 | AM | 110 | ARG | NE-CZ-NH2 | 8.15 | 124.37 | 120.30 |
| 81 | DA | 2827 | U | C1'-O4'-C4' | 8.15 | 116.42 | 109.90 |
| 81 | DA | 2830 | G | O4'-C1'-N9 | 8.15 | 114.72 | 108.20 |
| 81 | DA | 1842 | A | P-O5'-C5' | 8.14 | 133.93 | 120.90 |
| 81 | DA | 3387 | U | C1'-O4'-C4' | 8.14 | 116.42 | 109.90 |
| 81 | DA | 807 | A | O4'-C1'-N9 | 8.14 | 114.71 | 108.20 |
| 81 | DA | 1966 | U | O4'-C1'-N1 | 8.14 | 114.71 | 108.20 |
| 81 | DA | 2465 | G | P-O5'-C5' | -8.14 | 107.87 | 120.90 |
| 81 | DA | 2942 | C | N1-C1'-C2' | 8.14 | 124.59 | 114.00 |
| 81 | DA | 3337 | G | C1'-O4'-C4' | -8.14 | 103.39 | 109.90 |
| 46 | BT | 86 | GLU | CB-CA-C | 8.14 | 126.68 | 110.40 |
| 78 | CA | 591 | A | O4'-C4'-C3' | -8.14 | 95.86 | 104.00 |
| 81 | DA | 2148 | U | P-O3'-C3' | 8.14 | 129.47 | 119.70 |
| 81 | DA | 2380 | U | O4'-C1'-N1 | 8.14 | 114.71 | 108.20 |
| 81 | DA | 2440 | G | C1'-O4'-C4' | -8.14 | 103.39 | 109.90 |
| 81 | DA | 330 | G | P-O5'-C5' | -8.14 | 107.88 | 120.90 |
| 81 | DA | 1125 | U | O4'-C1'-N1 | 8.14 | 114.71 | 108.20 |
| 12 | AK | 107 | ARG | NE-CZ-NH2 | -8.13 | 116.23 | 120.30 |
| 81 | DA | 2093 | A | O3'-P-O5' | -8.14 | 88.54 | 104.00 |
| 83 | DC | 88 | G | O4'-C1'-N9 | 8.14 | 114.71 | 108.20 |
| 47 | BU | 156 | TYR | CB-CG-CD1 | 8.13 | 125.88 | 121.00 |
| 81 | DA | 184 | U | O4'-C1'-C2' | -8.13 | 97.67 | 105.80 |
| 81 | DA | 1637 | A | OP1-P-OP2 | -8.13 | 107.40 | 119.60 |
| 81 | DA | 3115 | C | O4'-C1'-N1 | -8.13 | 101.69 | 108.20 |
| 78 | CA | 655 | G | O4'-C1'-N9 | 8.13 | 114.70 | 108.20 |
| 81 | DA | 1260 | A | N9-C1'-C2' | -8.13 | 103.06 | 112.00 |
| 81 | DA | 2332 | A | C1'-O4'-C4' | -8.13 | 103.40 | 109.90 |
| 17 | AQ | 60 | ARG | NE-CZ-NH1 | 8.13 | 124.36 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 65 | Bn | 72 | THR | N-CA-CB | 8.13 | 125.74 | 110.30 |
| 78 | CA | 1394 | G | C5'-C4'-O4' | 8.13 | 118.85 | 109.10 |
| 81 | DA | 2510 | U | C4'-C3'-C2' | -8.13 | 94.47 | 102.60 |
| 81 | DA | 1637 | A | C1'-O4'-C4' | -8.13 | 103.40 | 109.90 |
| 81 | DA | 2172 | A | P-O3'-C3' | 8.13 | 129.45 | 119.70 |
| 78 | CA | 470 | A | O4'-C1'-C2' | -8.13 | 97.67 | 105.80 |
| 50 | BX | 48 | SER | N-CA-CB | 8.12 | 122.69 | 110.50 |
| 45 | BR | 143 | PRO | CB-CA-C | -8.12 | 91.69 | 112.00 |
| 78 | CA | 7 | G | O4'-C1'-N9 | 8.12 | 114.70 | 108.20 |
| 57 | Be | 23 | ALA | CB-CA-C | 8.12 | 122.28 | 110.10 |
| 57 | Be | 51 | TYR | CB-CG-CD1 | 8.12 | 125.87 | 121.00 |
| 78 | CA | 303 | U | O4'-C1'-C2' | -8.12 | 97.68 | 105.80 |
| 78 | CA | 1475 | A | O4'-C1'-C2' | -8.12 | 97.68 | 105.80 |
| 74 | BQ | 198 | TYR | N-CA-CB | 8.12 | 125.22 | 110.60 |
| 81 | DA | 1576 | G | O5'-C5'-C4' | 8.12 | 127.13 | 111.70 |
| 81 | DA | 2616 | C | C3'-C2'-C1' | 8.12 | 107.99 | 101.50 |
| 2 | AA | 113 | ARG | NE-CZ-NH1 | 8.12 | 124.36 | 120.30 |
| 81 | DA | 2535 | A | O4'-C1'-N9 | 8.12 | 114.69 | 108.20 |
| 16 | AO | 109 | LYS | CB-CA-C | 8.11 | 126.62 | 110.40 |
| 43 | BP | 17 | ASP | CB-CG-OD2 | -8.11 | 111.00 | 118.30 |
| 78 | CA | 61 | A | C3'-C2'-C1' | 8.11 | 107.99 | 101.50 |
| 81 | DA | 681 | U | C3'-C2'-C1' | 8.11 | 107.99 | 101.50 |
| 81 | DA | 1437 | C | C1'-O4'-C4' | 8.11 | 116.39 | 109.90 |
| 81 | DA | 2376 | G | O4'-C1'-C2' | -8.11 | 97.69 | 105.80 |
| 81 | DA | 2431 | C | C3'-C2'-C1' | 8.11 | 107.99 | 101.50 |
| 16 | AO | 106 | ARG | NE-CZ-NH1 | 8.11 | 124.36 | 120.30 |
| 17 | AQ | 33 | ARG | NE-CZ-NH2 | -8.11 | 116.25 | 120.30 |
| 78 | CA | 1473 | U | C1'-O4'-C4' | 8.11 | 116.39 | 109.90 |
| 81 | DA | 311 | C | O4'-C1'-C2' | -8.11 | 97.69 | 105.80 |
| 81 | DA | 498 | A | C3'-C2'-C1' | 8.11 | 107.99 | 101.50 |
| 81 | DA | 2241 | U | P-O3'-C3' | 8.11 | 129.43 | 119.70 |
| 82 | DB | 112 | U | O4'-C1'-N1 | 8.11 | 114.69 | 108.20 |
| 81 | DA | 2279 | A | O5'-C5'-C4' | 8.11 | 127.11 | 111.70 |
| 5 | AC | 16 | LYS | CA-CB-CG | 8.11 | 131.24 | 113.40 |
| 67 | Bp | 34 | CYS | O-C-N | -8.11 | 109.73 | 122.70 |
| 81 | DA | 49 | A | N9-C1'-C2' | -8.11 | 103.08 | 112.00 |
| 83 | DC | 77 | A | O4'-C1'-C2' | -8.11 | 97.69 | 105.80 |
| 47 | BU | 135 | PRO | N-CA-CB | 8.10 | 113.02 | 103.30 |
| 76 | BS | 165 | LEU | CB-CG-CD2 | 8.10 | 124.78 | 111.00 |
| 81 | DA | 2564 | G | N1-C6-O6 | 8.10 | 124.76 | 119.90 |
| 81 | DA | 3061 | G | P-O5'-C5' | 8.10 | 133.87 | 120.90 |
| 65 | Bn | 36 | LYS | N-CA-C | -8.10 | 89.12 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 1649 | G | C1'-O4'-C4' | 8.10 | 116.38 | 109.90 |
| 78 | CA | 1689 | A | P-O3'-C3' | 8.10 | 129.42 | 119.70 |
| 78 | CA | 363 | G | O4'-C1'-N9 | 8.10 | 114.68 | 108.20 |
| 78 | CA | 568 | G | N1-C6-O6 | 8.10 | 124.76 | 119.90 |
| 81 | DA | 2498 | U | N1-C1'-C2' | -8.10 | 103.09 | 112.00 |
| 78 | CA | 1522 | U | P-O3'-C3' | 8.10 | 129.42 | 119.70 |
| 81 | DA | 1547 | G | C3'-C2'-C1' | 8.10 | 107.98 | 101.50 |
| 81 | DA | 2444 | C | O4'-C1'-C2' | -8.10 | 97.70 | 105.80 |
| 81 | DA | 2914 | G | O4'-C1'-N9 | 8.10 | 114.68 | 108.20 |
| 8 | AF | 35 | GLN | CA-C-O | -8.10 | 103.10 | 120.10 |
| 78 | CA | 1149 | G | N9-C1'-C2' | 8.10 | 124.52 | 114.00 |
| 81 | DA | 217 | U | O4'-C1'-N1 | 8.10 | 114.68 | 108.20 |
| 81 | DA | 2914 | G | OP1-P-OP2 | -8.10 | 107.46 | 119.60 |
| 1 | Aa | 86 | ASP | CB-CG-OD1 | 8.09 | 125.58 | 118.30 |
| 39 | BJ | 59 | THR | N-CA-CB | 8.09 | 125.67 | 110.30 |
| 61 | Bj | 37 | THR | CA-C-N | 8.09 | 139.76 | 117.10 |
| 74 | BQ | 158 | ARG | CD-NE-CZ | 8.09 | 134.93 | 123.60 |
| 78 | CA | 852 | C | O4'-C1'-C2' | -8.09 | 97.71 | 105.80 |
| 81 | DA | 1790 | G | P-O5'-C5' | 8.09 | 133.85 | 120.90 |
| 81 | DA | 1948 | G | C5'-C4'-O4' | -8.09 | 99.39 | 109.10 |
| 78 | CA | 368 | U | C1'-O4'-C4' | -8.09 | 103.43 | 109.90 |
| 78 | CA | 683 | C | C5'-C4'-O4' | -8.09 | 99.39 | 109.10 |
| 78 | CA | 1010 | C | O4'-C1'-N1 | -8.09 | 101.73 | 108.20 |
| 78 | CA | 1051 | G | N1-C6-O6 | 8.09 | 124.75 | 119.90 |
| 81 | DA | 1563 | C | O4'-C1'-C2' | -8.09 | 97.71 | 105.80 |
| 22 | AV | 104 | ALA | CA-C-O | -8.09 | 103.12 | 120.10 |
| 33 | BD | 103 | THR | N-CA-CB | 8.09 | 125.67 | 110.30 |
| 81 | DA | 2533 | G | N1-C6-O6 | 8.09 | 124.75 | 119.90 |
| 78 | CA | 507 | U | O4'-C1'-N1 | 8.08 | 114.67 | 108.20 |
| 82 | DB | 37 | A | C1'-O4'-C4' | 8.08 | 116.37 | 109.90 |
| 46 | BT | 98 | ARG | NE-CZ-NH1 | -8.08 | 116.26 | 120.30 |
| 78 | CA | 117 | U | O4'-C1'-N1 | 8.08 | 114.66 | 108.20 |
| 78 | CA | 1029 | U | O4'-C1'-N1 | 8.08 | 114.66 | 108.20 |
| 81 | DA | 3240 | C | C1'-O4'-C4' | -8.08 | 103.44 | 109.90 |
| 81 | DA | 3365 | U | P-O3'-C3' | 8.08 | 129.40 | 119.70 |
| 81 | DA | 18 | G | O4'-C1'-N9 | 8.08 | 114.66 | 108.20 |
| 81 | DA | 3053 | G | O4'-C1'-N9 | 8.08 | 114.66 | 108.20 |
| 74 | BQ | 55 | PHE | C-N-CA | 8.08 | 141.89 | 121.70 |
| 78 | CA | 1541 | G | O4'-C1'-N9 | -8.08 | 101.74 | 108.20 |
| 81 | DA | 664 | U | C3'-C2'-C1' | -8.07 | 95.04 | 101.50 |
| 81 | DA | 3142 | A | P-O3'-C3' | 8.07 | 129.39 | 119.70 |
| 81 | DA | 1010 | G | P-O3'-C3' | 8.07 | 129.38 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 16 | AO | 106 | ARG | CB-CA-C | -8.07 | 94.27 | 110.40 |
| 81 | DA | 2240 | G | O4'-C1'-N9 | 8.07 | 114.65 | 108.20 |
| 58 | Bg | 91 | SER | CB-CA-C | -8.07 | 94.77 | 110.10 |
| 74 | BQ | 197 | SER | CB-CA-C | 8.07 | 125.43 | 110.10 |
| 78 | CA | 504 | U | O4'-C1'-N1 | 8.07 | 114.65 | 108.20 |
| 79 | CB | 16 | U | P-O3'-C3' | 8.07 | 129.38 | 119.70 |
| 81 | DA | 2455 | U | O4'-C1'-C2' | -8.07 | 97.73 | 105.80 |
| 83 | DC | 57 | C | O4'-C1'-C2' | -8.06 | 97.73 | 105.80 |
| 6 | AE | 82 | ASN | N-CA-CB | 8.06 | 125.11 | 110.60 |
| 72 | Bt | 36 | PRO | CA-N-CD | -8.06 | 100.21 | 111.50 |
| 78 | CA | 1735 | U | O5'-C5'-C4' | 8.06 | 127.02 | 111.70 |
| 81 | DA | 14 | U | O4'-C1'-N1 | 8.06 | 114.65 | 108.20 |
| 81 | DA | 200 | C | O4'-C1'-C2' | -8.06 | 97.73 | 105.80 |
| 81 | DA | 342 | A | O4'-C1'-N9 | 8.06 | 114.65 | 108.20 |
| 81 | DA | 241 | G | P-O5'-C5' | 8.06 | 133.80 | 120.90 |
| 81 | DA | 737 | G | N1-C6-O6 | 8.06 | 124.74 | 119.90 |
| 81 | DA | 788 | C | P-O3'-C3' | 8.06 | 129.38 | 119.70 |
| 82 | DB | 151 | C | C5'-C4'-C3' | -8.06 | 103.10 | 116.00 |
| 58 | Bg | 93 | VAL | C-N-CA | 8.06 | 141.85 | 121.70 |
| 81 | DA | 1833 | G | O4'-C1'-N9 | 8.06 | 114.65 | 108.20 |
| 82 | DB | 132 | G | C1'-O4'-C4' | 8.06 | 116.35 | 109.90 |
| 78 | CA | 1680 | G | C1'-O4'-C4' | 8.06 | 116.34 | 109.90 |
| 81 | DA | 177 | U | C4'-C3'-C2' | -8.06 | 94.54 | 102.60 |
| 81 | DA | 3085 | G | O4'-C1'-N9 | 8.06 | 114.64 | 108.20 |
| 5 | AC | 175 | ARG | NE-CZ-NH1 | -8.05 | 116.27 | 120.30 |
| 47 | BU | 84 | TYR | CB-CG-CD2 | -8.06 | 116.17 | 121.00 |
| 81 | DA | 202 | G | N9-C1'-C2' | 8.05 | 124.47 | 114.00 |
| 82 | DB | 127 | U | N1-C1'-C2' | 8.06 | 124.47 | 114.00 |
| 53 | Ba | 44 | ALA | C-N-CA | -8.05 | 105.39 | 122.30 |
| 78 | CA | 1241 | G | O4'-C1'-C2' | -8.05 | 97.75 | 105.80 |
| 78 | CA | 1428 | G | N1-C6-O6 | 8.05 | 124.73 | 119.90 |
| 83 | DC | 28 | C | O4'-C1'-N1 | 8.05 | 114.64 | 108.20 |
| 33 | BD | 328 | ASN | C-N-CD | -8.05 | 102.89 | 120.60 |
| 78 | CA | 146 | U | C3'-C2'-C1' | 8.05 | 107.94 | 101.50 |
| 81 | DA | 2487 | U | N1-C1'-C2' | -8.05 | 103.14 | 112.00 |
| 81 | DA | 837 | A | O4'-C1'-N9 | 8.05 | 114.64 | 108.20 |
| 81 | DA | 2503 | G | O3'-P-O5' | -8.05 | 88.71 | 104.00 |
| 81 | DA | 3148 | U | O4'-C1'-C2' | -8.05 | 97.75 | 105.80 |
| 4 | AD | 240 | LYS | C-N-CA | -8.05 | 105.40 | 122.30 |
| 35 | BG | 163 | PHE | CB-CG-CD2 | -8.04 | 115.17 | 120.80 |
| 76 | BS | 52 | LYS | N-CA-C | 8.05 | 132.72 | 111.00 |
| 78 | CA | 12 | U | O4'-C1'-N1 | 8.04 | 114.64 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 570 | A | O4'-C1'-N9 | 8.04 | 114.64 | 108.20 |
| 78 | CA | 839 | U | N1-C1'-C2' | -8.05 | 103.15 | 112.00 |
| 78 | CA | 1431 | C | O4'-C1'-N1 | 8.04 | 114.64 | 108.20 |
| 81 | DA | 40 | A | O4'-C1'-N9 | 8.04 | 114.64 | 108.20 |
| 81 | DA | 2408 | U | C1'-O4'-C4' | -8.04 | 103.47 | 109.90 |
| 81 | DA | 3151 | U | C1'-O4'-C4' | 8.04 | 116.34 | 109.90 |
| 43 | BP | 16 | SER | CA-C-O | -8.04 | 103.21 | 120.10 |
| 72 | Bu | 36 | PRO | CA-N-CD | -8.04 | 100.24 | 111.50 |
| 77 | BI | 111 | LEU | CB-CA-C | -8.04 | 94.92 | 110.20 |
| 78 | CA | 638 | U | O4'-C1'-N1 | 8.04 | 114.63 | 108.20 |
| 78 | CA | 684 | A | C4'-C3'-C2' | -8.04 | 94.56 | 102.60 |
| 81 | DA | 1816 | A | O4'-C1'-N9 | 8.04 | 114.63 | 108.20 |
| 81 | DA | 1856 | C | C3'-C2'-C1' | 8.04 | 107.93 | 101.50 |
| 81 | DA | 2216 | G | P-O3'-C3' | 8.04 | 129.34 | 119.70 |
| 81 | DA | 2303 | A | O4'-C1'-N9 | 8.04 | 114.63 | 108.20 |
| 81 | DA | 2010 | U | O4'-C1'-N1 | 8.04 | 114.63 | 108.20 |
| 81 | DA | 2998 | U | C1'-O4'-C4' | 8.04 | 116.33 | 109.90 |
| 82 | DB | 98 | U | C4'-C3'-C2' | 8.04 | 110.64 | 102.60 |
| 81 | DA | 2823 | G | O4'-C1'-N9 | 8.03 | 114.63 | 108.20 |
| 83 | DC | 18 | C | C4'-C3'-C2' | -8.03 | 94.57 | 102.60 |
| 37 | BH | 226 | TYR | CB-CG-CD1 | -8.03 | 116.18 | 121.00 |
| 81 | DA | 1653 | G | C3'-C2'-C1' | 8.03 | 107.92 | 101.50 |
| 81 | DA | 2136 | C | C3'-C2'-C1' | 8.03 | 107.92 | 101.50 |
| 2 | AA | 5 | ALA | CA-C-N | 8.03 | 134.86 | 117.20 |
| 78 | CA | 942 | G | O4'-C1'-N9 | 8.03 | 114.62 | 108.20 |
| 78 | CA | 1794 | A | C1'-O4'-C4' | 8.03 | 116.32 | 109.90 |
| 81 | DA | 1082 | U | O4'-C1'-C2' | -8.03 | 97.77 | 105.80 |
| 81 | DA | 2964 | G | O4'-C1'-N9 | 8.03 | 114.62 | 108.20 |
| 81 | DA | 3047 | U | O4'-C1'-N1 | 8.03 | 114.62 | 108.20 |
| 81 | DA | 3325 | G | N9-C1'-C2' | -8.03 | 103.17 | 112.00 |
| 81 | DA | 966 | U | O4'-C1'-N1 | 8.03 | 114.62 | 108.20 |
| 81 | DA | 2989 | U | O5'-P-OP2 | -8.03 | 98.48 | 105.70 |
| 37 | BH | 223 | ALA | N-CA-CB | -8.02 | 98.87 | 110.10 |
| 81 | DA | 675 | C | P-O3'-C3' | 8.02 | 129.33 | 119.70 |
| 81 | DA | 2541 | U | O4'-C1'-N1 | 8.02 | 114.62 | 108.20 |
| 20 | AS | 53 | TRP | CB-CG-CD1 | -8.02 | 116.57 | 127.00 |
| 78 | CA | 660 | G | O4'-C4'-C3' | -8.02 | 95.98 | 104.00 |
| 78 | CA | 1783 | C | O3'-P-O5' | -8.02 | 88.76 | 104.00 |
| 81 | DA | 977 | C | O4'-C1'-N1 | 8.02 | 114.62 | 108.20 |
| 81 | DA | 1391 | C | O4'-C4'-C3' | -8.02 | 95.98 | 104.00 |
| 81 | DA | 1761 | C | O4'-C1'-N1 | 8.02 | 114.62 | 108.20 |
| 81 | DA | 2323 | G | O4'-C1'-C2' | -8.02 | 97.78 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1109 | U | C1'-O4'-C4' | 8.02 | 116.31 | 109.90 |
| 81 | DA | 1420 | C | N1-C1'-C2' | 8.02 | 124.42 | 114.00 |
| 78 | CA | 1342 | C | C5'-C4'-C3' | 8.02 | 128.82 | 116.00 |
| 81 | DA | 1725 | C | N1-C1'-C2' | 8.01 | 124.42 | 114.00 |
| 81 | DA | 941 | G | O4'-C1'-N9 | 8.01 | 114.61 | 108.20 |
| 2 | AA | 252 | TRP | CD1-CG-CD2 | -8.01 | 99.89 | 106.30 |
| 49 | BV | 100 | ALA | N-CA-CB | 8.01 | 121.31 | 110.10 |
| 78 | CA | 480 | G | O4'-C1'-N9 | 8.01 | 114.61 | 108.20 |
| 81 | DA | 316 | U | N1-C1'-C2' | -8.01 | 103.19 | 112.00 |
| 81 | DA | 779 | G | C4'-C3'-C2' | -8.01 | 94.59 | 102.60 |
| 81 | DA | 2351 | U | O4'-C1'-N1 | 8.01 | 114.61 | 108.20 |
| 81 | DA | 2506 | U | P-O3'-C3' | -8.01 | 110.09 | 119.70 |
| 81 | DA | 251 | G | P-O5'-C5' | -8.01 | 108.09 | 120.90 |
| 81 | DA | 1049 | C | P-O5'-C5' | 8.01 | 133.71 | 120.90 |
| 81 | DA | 3288 | G | O4'-C1'-N9 | 8.01 | 114.60 | 108.20 |
| 67 | Bp | 41 | HIS | CA-CB-CG | 8.00 | 127.20 | 113.60 |
| 81 | DA | 1090 | G | O4'-C1'-N9 | 8.00 | 114.60 | 108.20 |
| 81 | DA | 2271 | A | C1'-O4'-C4' | 8.00 | 116.30 | 109.90 |
| 81 | DA | 3122 | A | P-O3'-C3' | 8.00 | 129.30 | 119.70 |
| 43 | BP | 17 | ASP | CB-CG-OD1 | 8.00 | 125.50 | 118.30 |
| 59 | Bh | 13 | HIS | CB-CA-C | 8.00 | 126.40 | 110.40 |
| 81 | DA | 3333 | G | C1'-O4'-C4' | -8.00 | 103.50 | 109.90 |
| 5 | AC | 95 | TYR | CG-CD1-CE1 | -8.00 | 114.90 | 121.30 |
| 78 | CA | 1297 | G | N9-C1'-C2' | -8.00 | 103.20 | 112.00 |
| 78 | CA | 1700 | C | C3'-C2'-C1' | 8.00 | 107.90 | 101.50 |
| 81 | DA | 2115 | G | N9-C1'-C2' | 8.00 | 124.40 | 114.00 |
| 81 | DA | 2181 | C | C5'-C4'-O4' | -8.00 | 99.50 | 109.10 |
| 81 | DA | 3295 | A | C5'-C4'-C3' | -8.00 | 103.20 | 116.00 |
| 83 | DC | 100 | A | O3'-P-O5' | -8.00 | 88.80 | 104.00 |
| 78 | CA | 670 | U | P-O3'-C3' | 8.00 | 129.29 | 119.70 |
| 78 | CA | 988 | A | C3'-C2'-C1' | 7.99 | 107.89 | 101.50 |
| 81 | DA | 3164 | C | O4'-C1'-N1 | 7.99 | 114.59 | 108.20 |
| 83 | DC | 74 | A | O4'-C1'-N9 | 7.99 | 114.59 | 108.20 |
| 78 | CA | 684 | A | C1'-O4'-C4' | -7.99 | 103.51 | 109.90 |
| 81 | DA | 2072 | G | C4'-C3'-C2' | -7.99 | 94.61 | 102.60 |
| 21 | AT | 54 | ALA | C-N-CA | 7.99 | 141.67 | 121.70 |
| 39 | BJ | 75 | PRO | CA-C-N | 7.99 | 134.78 | 117.20 |
| 51 | BZ | 67 | VAL | N-CA-CB | 7.99 | 129.07 | 111.50 |
| 81 | DA | 186 | U | C1'-O4'-C4' | 7.99 | 116.29 | 109.90 |
| 81 | DA | 2486 | A | C5'-C4'-C3' | 7.99 | 128.78 | 116.00 |
| 81 | DA | 2545 | C | O4'-C1'-N1 | 7.99 | 114.59 | 108.20 |
| 81 | DA | 984 | G | C1'-O4'-C4' | 7.99 | 116.29 | 109.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 1161 | C | N1-C1'-C2' | 7.99 | 124.38 | 114.00 |
| 62 | Bk | 81 | THR | CB-CA-C | -7.98 | 90.04 | 111.60 |
| 78 | CA | 1560 | U | C3'-C2'-C1' | 7.98 | 107.89 | 101.50 |
| 81 | DA | 3361 | G | C5'-C4'-O4' | 7.98 | 118.68 | 109.10 |
| 9 | AH | 57 | ARG | N-CA-CB | 7.98 | 124.97 | 110.60 |
| 81 | DA | 541 | U | N1-C1'-C2' | -7.98 | 103.22 | 112.00 |
| 82 | DB | 97 | A | C5'-C4'-C3' | 7.98 | 128.77 | 116.00 |
| 43 | BP | 172 | ARG | NE-CZ-NH2 | -7.98 | 116.31 | 120.30 |
| 78 | CA | 1399 | C | O4'-C1'-N1 | -7.98 | 101.82 | 108.20 |
| 40 | BK | 57 | PHE | CB-CG-CD1 | 7.98 | 126.38 | 120.80 |
| 72 | Bu | 60 | ASN | N-CA-CB | -7.98 | 96.24 | 110.60 |
| 78 | CA | 1267 | G | N9-C1'-C2' | 7.98 | 124.37 | 114.00 |
| 78 | CA | 1300 | A | O4'-C1'-N9 | 7.98 | 114.58 | 108.20 |
| 78 | CA | 1437 | U | C5'-C4'-O4' | -7.98 | 99.53 | 109.10 |
| 81 | DA | 2253 | G | O4'-C1'-C2' | 7.98 | 114.78 | 107.60 |
| 65 | Bn | 17 | ARG | NE-CZ-NH2 | -7.98 | 116.31 | 120.30 |
| 5 | AC | 164 | PHE | N-CA-C | -7.97 | 89.47 | 111.00 |
| 31 | BB | 35 | ALA | CB-CA-C | 7.97 | 122.06 | 110.10 |
| 74 | BQ | 130 | GLU | N-CA-CB | 7.97 | 124.95 | 110.60 |
| 81 | DA | 1667 | A | O4'-C1'-C2' | -7.97 | 97.83 | 105.80 |
| 81 | DA | 2175 | U | O4'-C1'-C2' | -7.97 | 97.83 | 105.80 |
| 81 | DA | 2415 | C | C4'-C3'-C2' | -7.97 | 94.63 | 102.60 |
| 65 | Bn | 71 | PRO | N-CA-CB | 7.97 | 112.87 | 103.30 |
| 81 | DA | 3113 | A | O4'-C1'-N9 | -7.97 | 101.82 | 108.20 |
| 74 | BQ | 107 | ARG | NE-CZ-NH2 | -7.97 | 116.31 | 120.30 |
| 78 | CA | 285 | G | C1'-O4'-C4' | -7.97 | 103.52 | 109.90 |
| 78 | CA | 506 | A | N1-C6-N6 | 7.97 | 123.38 | 118.60 |
| 81 | DA | 1855 | U | O4'-C1'-N1 | 7.97 | 114.58 | 108.20 |
| 36 | BF | 186 | PHE | CB-CG-CD2 | 7.97 | 126.38 | 120.80 |
| 78 | CA | 1507 | G | O4'-C1'-N9 | 7.97 | 114.58 | 108.20 |
| 81 | DA | 2988 | C | C5'-C4'-C3' | 7.97 | 128.75 | 116.00 |
| 20 | AS | 52 | GLY | CA-C-N | -7.97 | 99.67 | 117.20 |
| 35 | BG | 169 | ASP | CA-CB-CG | -7.97 | 95.87 | 113.40 |
| 81 | DA | 773 | G | P-O5'-C5' | 7.97 | 133.65 | 120.90 |
| 5 | AC | 157 | ASP | N-CA-CB | -7.97 | 96.26 | 110.60 |
| 78 | CA | 559 | C | O4'-C1'-N1 | 7.97 | 114.57 | 108.20 |
| 78 | CA | 1477 | G | P-O3'-C3' | -7.97 | 110.14 | 119.70 |
| 81 | DA | 1130 | A | P-O3'-C3' | 7.97 | 129.26 | 119.70 |
| 81 | DA | 1149 | G | O4'-C1'-N9 | 7.97 | 114.57 | 108.20 |
| 81 | DA | 2563 | G | N1-C6-O6 | 7.97 | 124.68 | 119.90 |
| 81 | DA | 3037 | U | O4'-C1'-N1 | 7.97 | 114.57 | 108.20 |
| 81 | DA | 3100 | U | C5'-C4'-C3' | 7.97 | 128.75 | 116.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 3212 | C | P-O5'-C5' | -7.97 | 108.15 | 120.90 |
| 78 | CA | 1003 | A | N9-C1'-C2' | -7.96 | 103.24 | 112.00 |
| 81 | DA | 925 | A | O4'-C1'-N9 | 7.96 | 114.57 | 108.20 |
| 81 | DA | 932 | U | P-O3'-C3' | 7.96 | 129.26 | 119.70 |
| 81 | DA | 972 | A | N9-C1'-C2' | 7.96 | 124.35 | 114.00 |
| 81 | DA | 1956 | A | N9-C1'-C2' | -7.96 | 103.24 | 112.00 |
| 17 | AQ | 93 | LEU | C-N-CA | -7.96 | 101.80 | 121.70 |
| 78 | CA | 591 | A | C5'-C4'-C3' | 7.96 | 128.74 | 116.00 |
| 81 | DA | 1492 | G | P-O3'-C3' | 7.96 | 129.25 | 119.70 |
| 81 | DA | 2050 | C | O4'-C1'-C2' | -7.96 | 97.84 | 105.80 |
| 81 | DA | 2628 | A | N9-C1'-C2' | 7.96 | 124.35 | 114.00 |
| 83 | DC | 46 | A | C3'-C2'-C1' | -7.96 | 95.13 | 101.50 |
| 34 | BE | 59 | ILE | N-CA-C | 7.96 | 132.49 | 111.00 |
| 81 | DA | 306 | A | O4'-C1'-N9 | 7.96 | 114.57 | 108.20 |
| 81 | DA | 1422 | G | O4'-C1'-C2' | 7.96 | 114.76 | 107.60 |
| 34 | BE | 52 | TYR | N-CA-CB | -7.96 | 96.28 | 110.60 |
| 81 | DA | 456 | U | O4'-C1'-N1 | 7.96 | 114.57 | 108.20 |
| 81 | DA | 674 | G | C5'-C4'-C3' | -7.96 | 103.27 | 116.00 |
| 81 | DA | 2174 | G | C4'-C3'-O3' | 7.96 | 128.91 | 113.00 |
| 81 | DA | 3193 | C | P-O5'-C5' | 7.96 | 133.63 | 120.90 |
| 81 | DA | 3344 | A | N9-C1'-C2' | -7.96 | 103.25 | 112.00 |
| 76 | BS | 70 | ASN | CA-C-N | 7.95 | 139.37 | 117.10 |
| 81 | DA | 1575 | A | C4'-C3'-C2' | -7.95 | 94.65 | 102.60 |
| 81 | DA | 1867 | A | C1'-O4'-C4' | 7.95 | 116.26 | 109.90 |
| 53 | Ba | 10 | VAL | CB-CA-C | -7.95 | 96.29 | 111.40 |
| 78 | CA | 613 | G | C1'-O4'-C4' | 7.95 | 116.26 | 109.90 |
| 81 | DA | 938 | C | O4'-C1'-N1 | 7.95 | 114.56 | 108.20 |
| 78 | CA | 388 | G | O4'-C1'-N9 | 7.95 | 114.56 | 108.20 |
| 78 | CA | 1191 | U | C3'-C2'-C1' | -7.95 | 95.14 | 101.50 |
| 78 | CA | 942 | G | N9-C1'-C2' | 7.95 | 124.33 | 114.00 |
| 81 | DA | 884 | A | N9-C1'-C2' | -7.95 | 103.26 | 112.00 |
| 16 | AO | 42 | ARG | C-N-CA | 7.94 | 141.56 | 121.70 |
| 81 | DA | 27 | C | C3'-C2'-C1' | 7.94 | 107.86 | 101.50 |
| 81 | DA | 3249 | C | C1'-O4'-C4' | -7.94 | 103.55 | 109.90 |
| 78 | CA | 1496 | U | O4'-C1'-N1 | 7.94 | 114.56 | 108.20 |
| 81 | DA | 1076 | C | C1'-O4'-C4' | -7.94 | 103.55 | 109.90 |
| 81 | DA | 1509 | A | N9-C1'-C2' | 7.94 | 124.33 | 114.00 |
| 81 | DA | 1576 | G | C5'-C4'-C3' | 7.94 | 128.71 | 116.00 |
| 81 | DA | 2800 | G | C3'-C2'-C1' | 7.94 | 107.85 | 101.50 |
| 34 | BE | 61 | ARG | CA-C-N | 7.94 | 134.67 | 117.20 |
| 40 | BK | 130 | LYS | CA-C-N | 7.94 | 139.33 | 117.10 |
| 78 | CA | 280 | U | O4'-C1'-N1 | -7.94 | 101.85 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 326 | G | P-O3'-C3' | -7.94 | 110.17 | 119.70 |
| 81 | DA | 2442 | G | O4'-C1'-C2' | -7.94 | 97.86 | 105.80 |
| 81 | DA | 2916 | U | C3'-C2'-C1' | 7.94 | 107.85 | 101.50 |
| 81 | DA | 3295 | A | OP1-P-OP2 | -7.94 | 107.69 | 119.60 |
| 81 | DA | 982 | C | P-O3'-C3' | 7.94 | 129.23 | 119.70 |
| 35 | BG | 143 | LYS | N-CA-CB | 7.94 | 124.89 | 110.60 |
| 81 | DA | 2045 | G | O4'-C1'-N9 | 7.94 | 114.55 | 108.20 |
| 81 | DA | 2345 | A | N9-C1'-C2' | 7.94 | 124.32 | 114.00 |
| 81 | DA | 635 | G | C3'-C2'-C1' | -7.94 | 95.15 | 101.50 |
| 78 | CA | 730 | G | C5'-C4'-C3' | 7.93 | 128.69 | 116.00 |
| 81 | DA | 3145 | C | P-O5'-C5' | 7.93 | 133.60 | 120.90 |
| 78 | CA | 1665 | U | P-O3'-C3' | -7.93 | 110.18 | 119.70 |
| 82 | DB | 6 | U | N1-C1'-C2' | 7.93 | 124.31 | 114.00 |
| 3 | AB | 205 | ALA | N-CA-C | -7.93 | 89.59 | 111.00 |
| 78 | CA | 401 | A | O4'-C1'-C2' | -7.93 | 97.87 | 105.80 |
| 78 | CA | 1677 | C | P-O5'-C5' | 7.93 | 133.59 | 120.90 |
| 81 | DA | 510 | G | N9-C1'-C2' | 7.93 | 124.31 | 114.00 |
| 81 | DA | 1495 | U | O4'-C1'-N1 | 7.93 | 114.54 | 108.20 |
| 5 | AC | 26 | ALA | N-CA-CB | 7.93 | 121.20 | 110.10 |
| 81 | DA | 2230 | C | C3'-C2'-C1' | 7.93 | 107.84 | 101.50 |
| 82 | DB | 98 | U | P-O3'-C3' | -7.93 | 110.19 | 119.70 |
| 78 | CA | 637 | C | C1'-O4'-C4' | 7.93 | 116.24 | 109.90 |
| 78 | CA | 1638 | G | N1-C6-O6 | 7.93 | 124.66 | 119.90 |
| 80 | CC | 16 | G | N9-C1'-C2' | -7.93 | 103.28 | 112.00 |
| 81 | DA | 436 | A | P-O3'-C3' | 7.93 | 129.21 | 119.70 |
| 42 | BM | 94 | TYR | CB-CG-CD2 | 7.92 | 125.75 | 121.00 |
| 81 | DA | 238 | A | O4'-C1'-C2' | -7.92 | 97.88 | 105.80 |
| 83 | DC | 55 | A | C1'-O4'-C4' | 7.92 | 116.24 | 109.90 |
| 45 | BR | 155 | MET | N-CA-CB | 7.92 | 124.86 | 110.60 |
| 74 | BQ | 15 | ARG | NE-CZ-NH2 | 7.92 | 124.26 | 120.30 |
| 81 | DA | 181 | U | P-O5'-C5' | -7.92 | 108.23 | 120.90 |
| 81 | DA | 2044 | U | P-O3'-C3' | 7.92 | 129.20 | 119.70 |
| 81 | DA | 2229 | A | P-O5'-C5' | 7.92 | 133.57 | 120.90 |
| 60 | Bi | 41 | ARG | O-C-N | -7.92 | 106.06 | 121.10 |
| 78 | CA | 171 | A | N9-C1'-C2' | -7.92 | 103.29 | 112.00 |
| 81 | DA | 1611 | G | O4'-C1'-N9 | 7.92 | 114.54 | 108.20 |
| 81 | DA | 2462 | A | O3'-P-O5' | -7.92 | 88.95 | 104.00 |
| 83 | DC | 10 | C | O4'-C1'-N1 | 7.92 | 114.53 | 108.20 |
| 81 | DA | 930 | U | O4'-C1'-N1 | 7.92 | 114.53 | 108.20 |
| 81 | DA | 2506 | U | P-O5'-C5' | 7.92 | 133.56 | 120.90 |
| 76 | BS | 6 | PHE | CB-CG-CD2 | -7.91 | 115.26 | 120.80 |
| 81 | DA | 501 | A | O4'-C1'-N9 | 7.91 | 114.53 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1199 | C | N1-C1'-C2' | 7.91 | 124.29 | 114.00 |
| 81 | DA | 2187 | G | O4'-C1'-C2' | -7.91 | 97.89 | 105.80 |
| 83 | DC | 116 | U | P-O3'-C3' | 7.91 | 129.20 | 119.70 |
| 56 | Bf | 59 | TYR | CB-CG-CD1 | 7.91 | 125.75 | 121.00 |
| 81 | DA | 2253 | G | C3'-C2'-C1' | -7.91 | 95.17 | 101.50 |
| 81 | DA | 2886 | U | P-O3'-C3' | 7.91 | 129.19 | 119.70 |
| 81 | DA | 2249 | G | O4'-C1'-N9 | 7.91 | 114.53 | 108.20 |
| 17 | AQ | 82 | ASP | CB-CA-C | -7.91 | 94.59 | 110.40 |
| 40 | BK | 135 | TYR | CB-CG-CD2 | -7.91 | 116.26 | 121.00 |
| 78 | CA | 305 | C | C3'-C2'-C1' | 7.91 | 107.82 | 101.50 |
| 81 | DA | 463 | C | C3'-C2'-C1' | 7.91 | 107.83 | 101.50 |
| 81 | DA | 2358 | A | O4'-C1'-N9 | 7.91 | 114.52 | 108.20 |
| 82 | DB | 59 | A | O4'-C1'-N9 | 7.91 | 114.52 | 108.20 |
| 82 | DB | 64 | U | O4'-C1'-N1 | 7.91 | 114.53 | 108.20 |
| 60 | Bi | 60 | ARG | NE-CZ-NH2 | -7.90 | 116.35 | 120.30 |
| 81 | DA | 624 | G | N9-C1'-C2' | 7.90 | 124.27 | 114.00 |
| 78 | CA | 1241 | G | N9-C1'-C2' | -7.90 | 103.31 | 112.00 |
| 78 | CA | 1684 | U | O4'-C1'-N1 | 7.90 | 114.52 | 108.20 |
| 81 | DA | 607 | A | C4'-C3'-C2' | -7.90 | 94.70 | 102.60 |
| 81 | DA | 2625 | C | O4'-C1'-N1 | -7.90 | 101.88 | 108.20 |
| 78 | CA | 1764 | C | C3'-C2'-C1' | 7.90 | 107.82 | 101.50 |
| 64 | Bl | 63 | ARG | N-CA-CB | 7.90 | 124.81 | 110.60 |
| 81 | DA | 1203 | A | C1'-O4'-C4' | -7.90 | 103.58 | 109.90 |
| 81 | DA | 1989 | U | O3'-P-O5' | 7.90 | 119.00 | 104.00 |
| 4 | AD | 221 | ARG | N-CA-CB | 7.89 | 124.81 | 110.60 |
| 78 | CA | 288 | A | O3'-P-O5' | -7.89 | 89.00 | 104.00 |
| 81 | DA | 2886 | U | C1'-O4'-C4' | 7.89 | 116.22 | 109.90 |
| 2 | AA | 6 | THR | O-C-N | -7.89 | 110.07 | 122.70 |
| 78 | CA | 768 | C | P-O3'-C3' | 7.89 | 129.17 | 119.70 |
| 78 | CA | 277 | U | O4'-C1'-N1 | 7.89 | 114.51 | 108.20 |
| 81 | DA | 2704 | A | O4'-C1'-N9 | 7.89 | 114.51 | 108.20 |
| 43 | BP | 175 | ASN | O-C-N | -7.89 | 110.08 | 122.70 |
| 81 | DA | 1812 | G | O4'-C1'-N9 | 7.89 | 114.51 | 108.20 |
| 81 | DA | 2406 | C | C5'-C4'-O4' | -7.89 | 99.63 | 109.10 |
| 81 | DA | 3144 | G | P-O3'-C3' | 7.89 | 129.17 | 119.70 |
| 8 | AF | 28 | PRO | N-CD-CG | 7.89 | 115.03 | 103.20 |
| 78 | CA | 1339 | C | C5'-C4'-O4' | 7.89 | 118.57 | 109.10 |
| 74 | BQ | 242 | SER | CB-CA-C | 7.89 | 125.08 | 110.10 |
| 81 | DA | 529 | A | C3'-C2'-C1' | 7.89 | 107.81 | 101.50 |
| 1 | Aa | 10 | ARG | NE-CZ-NH1 | 7.88 | 124.24 | 120.30 |
| 6 | AE | 174 | ARG | C-N-CA | -7.88 | 105.74 | 122.30 |
| 16 | AO | 112 | LYS | CB-CA-C | -7.88 | 94.63 | 110.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 33 | BD | 331 | ALA | N-CA-CB | -7.88 | 99.06 | 110.10 |
| 81 | DA | 799 | G | C3'-C2'-C1' | 7.88 | 107.81 | 101.50 |
| 81 | DA | 2172 | A | C5'-C4'-O4' | 7.88 | 118.56 | 109.10 |
| 81 | DA | 3058 | U | C5'-C4'-C3' | 7.88 | 128.62 | 116.00 |
| 78 | CA | 1601 | G | O4'-C1'-C2' | 7.88 | 114.69 | 107.60 |
| 81 | DA | 207 | U | O4'-C1'-N1 | 7.88 | 114.50 | 108.20 |
| 81 | DA | 1563 | C | C5'-C4'-O4' | 7.88 | 118.56 | 109.10 |
| 81 | DA | 2175 | U | C4'-C3'-C2' | -7.88 | 94.72 | 102.60 |
| 81 | DA | 3334 | U | C1'-O4'-C4' | 7.88 | 116.21 | 109.90 |
| 35 | BG | 148 | GLU | CB-CA-C | 7.88 | 126.16 | 110.40 |
| 78 | CA | 1295 | G | C3'-C2'-C1' | -7.88 | 95.20 | 101.50 |
| 81 | DA | 1177 | G | N9-C1'-C2' | 7.88 | 124.24 | 114.00 |
| 78 | CA | 662 | U | O4'-C1'-N1 | 7.88 | 114.50 | 108.20 |
| 81 | DA | 1230 | G | P-O3'-C3' | 7.88 | 129.15 | 119.70 |
| 81 | DA | 1976 | G | O4'-C1'-C2' | 7.88 | 114.69 | 107.60 |
| 33 | BD | 29 | PRO | O-C-N | -7.88 | 110.10 | 122.70 |
| 81 | DA | 984 | G | P-O3'-C3' | 7.88 | 129.15 | 119.70 |
| 78 | CA | 367 | A | O4'-C1'-N9 | 7.88 | 114.50 | 108.20 |
| 78 | CA | 1002 | G | O4'-C1'-N9 | 7.88 | 114.50 | 108.20 |
| 78 | CA | 1600 | A | P-O3'-C3' | 7.88 | 129.15 | 119.70 |
| 81 | DA | 1208 | U | N1-C1'-C2' | -7.88 | 103.34 | 112.00 |
| 81 | DA | 1391 | C | C5'-C4'-O4' | -7.88 | 99.65 | 109.10 |
| 46 | BT | 35 | ALA | N-CA-CB | 7.87 | 121.12 | 110.10 |
| 81 | DA | 1216 | C | O4'-C1'-N1 | 7.87 | 114.50 | 108.20 |
| 81 | DA | 3283 | U | O3'-P-O5' | -7.87 | 89.04 | 104.00 |
| 14 | AM | 141 | THR | N-CA-CB | 7.87 | 125.26 | 110.30 |
| 18 | AP | 82 | ARG | NE-CZ-NH1 | 7.87 | 124.23 | 120.30 |
| 20 | AS | 63 | ARG | NE-CZ-NH1 | -7.87 | 116.36 | 120.30 |
| 81 | DA | 352 | A | N9-C1'-C2' | -7.87 | 103.34 | 112.00 |
| 43 | BP | 21 | PHE | CB-CG-CD2 | -7.87 | 115.29 | 120.80 |
| 81 | DA | 791 | A | O3'-P-O5' | -7.87 | 89.05 | 104.00 |
| 81 | DA | 1347 | U | O4'-C1'-N1 | 7.87 | 114.50 | 108.20 |
| 81 | DA | 1549 | U | O4'-C1'-N1 | 7.87 | 114.50 | 108.20 |
| 81 | DA | 2511 | A | C4'-C3'-C2' | -7.87 | 94.73 | 102.60 |
| 22 | AV | 105 | THR | CA-C-N | 7.87 | 134.51 | 117.20 |
| 31 | BB | 246 | LEU | N-CA-CB | 7.87 | 126.14 | 110.40 |
| 38 | Bs | 222 | SER | CA-CB-OG | 7.87 | 132.44 | 111.20 |
| 81 | DA | 346 | C | C3'-C2'-C1' | 7.87 | 107.80 | 101.50 |
| 81 | DA | 552 | G | O4'-C1'-N9 | 7.87 | 114.50 | 108.20 |
| 81 | DA | 1949 | G | P-O3'-C3' | 7.87 | 129.14 | 119.70 |
| 81 | DA | 2901 | G | C1'-O4'-C4' | -7.87 | 103.61 | 109.90 |
| 81 | DA | 1036 | A | O4'-C1'-N9 | 7.87 | 114.49 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1722 | U | O4'-C1'-N1 | 7.87 | 114.49 | 108.20 |
| 60 | Bi | 62 | TYR | CB-CG-CD2 | 7.86 | 125.72 | 121.00 |
| 81 | DA | 89 | A | O4'-C1'-C2' | -7.86 | 97.94 | 105.80 |
| 81 | DA | 249 | U | O4'-C4'-C3' | -7.86 | 96.14 | 104.00 |
| 78 | CA | 30 | G | O4'-C4'-C3' | -7.86 | 96.14 | 104.00 |
| 81 | DA | 747 | A | O4'-C1'-N9 | 7.86 | 114.49 | 108.20 |
| 81 | DA | 2604 | U | O4'-C1'-N1 | 7.86 | 114.49 | 108.20 |
| 81 | DA | 2997 | G | P-O3'-C3' | 7.86 | 129.13 | 119.70 |
| 81 | DA | 3091 | A | O5'-C5'-C4' | 7.86 | 126.63 | 111.70 |
| 78 | CA | 603 | U | O4'-C1'-N1 | 7.86 | 114.49 | 108.20 |
| 11 | AJ | 85 | ARG | N-CA-CB | 7.86 | 124.74 | 110.60 |
| 37 | BH | 227 | ASP | CB-CG-OD1 | -7.86 | 111.23 | 118.30 |
| 43 | BP | 74 | PRO | CB-CA-C | -7.86 | 92.36 | 112.00 |
| 78 | CA | 1274 | C | C2-N1-C1' | 7.86 | 127.44 | 118.80 |
| 81 | DA | 572 | A | O3'-P-O5' | -7.86 | 89.07 | 104.00 |
| 82 | DB | 37 | A | N9-C1'-C2' | -7.86 | 103.36 | 112.00 |
| 78 | CA | 160 | C | P-O3'-C3' | 7.85 | 129.12 | 119.70 |
| 81 | DA | 1467 | A | O4'-C1'-C2' | -7.85 | 97.95 | 105.80 |
| 78 | CA | 1761 | U | C3'-C2'-C1' | 7.85 | 107.78 | 101.50 |
| 81 | DA | 255 | A | O4'-C1'-N9 | 7.85 | 114.48 | 108.20 |
| 20 | AS | 55 | TYR | CB-CG-CD1 | 7.85 | 125.71 | 121.00 |
| 78 | CA | 1239 | U | O4'-C1'-N1 | 7.85 | 114.48 | 108.20 |
| 81 | DA | 263 | C | C4'-C3'-C2' | -7.85 | 94.75 | 102.60 |
| 81 | DA | 1400 | G | C3'-C2'-C1' | -7.85 | 95.22 | 101.50 |
| 22 | AV | 29 | LYS | CB-CA-C | 7.85 | 126.09 | 110.40 |
| 81 | DA | 521 | A | C4'-C3'-C2' | -7.85 | 94.75 | 102.60 |
| 81 | DA | 2338 | C | P-O3'-C3' | 7.85 | 129.12 | 119.70 |
| 9 | AH | 87 | GLU | N-CA-CB | 7.84 | 124.72 | 110.60 |
| 30 | BA | 54 | LYS | N-CA-CB | 7.84 | 124.72 | 110.60 |
| 81 | DA | 1364 | C | C5'-C4'-C3' | 7.84 | 128.55 | 116.00 |
| 81 | DA | 3325 | G | C5'-C4'-O4' | -7.84 | 99.69 | 109.10 |
| 81 | DA | 248 | U | C2'-C3'-O3' | 7.84 | 126.75 | 109.50 |
| 81 | DA | 838 | G | O4'-C1'-C2' | 7.84 | 114.66 | 107.60 |
| 17 | AQ | 19 | ARG | NE-CZ-NH2 | -7.84 | 116.38 | 120.30 |
| 32 | BC | 314 | TYR | CB-CG-CD1 | -7.84 | 116.30 | 121.00 |
| 35 | BG | 4 | GLN | N-CA-CB | 7.84 | 124.72 | 110.60 |
| 81 | DA | 2476 | C | P-O3'-C3' | 7.84 | 129.11 | 119.70 |
| 34 | BE | 52 | TYR | CB-CA-C | -7.84 | 94.72 | 110.40 |
| 78 | CA | 869 | A | C1'-O4'-C4' | -7.84 | 103.63 | 109.90 |
| 81 | DA | 305 | U | O4'-C1'-N1 | 7.84 | 114.47 | 108.20 |
| 78 | CA | 928 | U | N1-C1'-C2' | -7.84 | 103.38 | 112.00 |
| 81 | DA | 2689 | A | N9-C1'-C2' | 7.84 | 124.19 | 114.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 83 | DC | 107 | G | N9-C1'-C2' | -7.84 | 103.38 | 112.00 |
| 35 | BG | 13 | GLU | C-N-CA | 7.84 | 141.29 | 121.70 |
| 78 | CA | 267 | U | C1'-O4'-C4' | 7.84 | 116.17 | 109.90 |
| 40 | BK | 4 | GLU | C-N-CD | -7.83 | 103.37 | 120.60 |
| 81 | DA | 1638 | A | C3'-C2'-C1' | -7.83 | 95.23 | 101.50 |
| 81 | DA | 2248 | C | N1-C1'-C2' | 7.83 | 124.18 | 114.00 |
| 82 | DB | 106 | C | N1-C1'-C2' | 7.83 | 124.18 | 114.00 |
| 15 | AN | 40 | ARG | NE-CZ-NH2 | 7.83 | 124.22 | 120.30 |
| 78 | CA | 172 | C | O4'-C1'-C2' | -7.83 | 97.97 | 105.80 |
| 81 | DA | 1725 | C | O4'-C1'-C2' | -7.83 | 97.97 | 105.80 |
| 78 | CA | 490 | C | O4'-C1'-N1 | 7.83 | 114.46 | 108.20 |
| 78 | CA | 843 | U | O4'-C1'-N1 | 7.83 | 114.46 | 108.20 |
| 81 | DA | 1128 | U | C1'-O4'-C4' | -7.83 | 103.64 | 109.90 |
| 81 | DA | 1294 | A | O4'-C1'-N9 | 7.83 | 114.46 | 108.20 |
| 81 | DA | 2874 | G | C1'-O4'-C4' | -7.83 | 103.64 | 109.90 |
| 81 | DA | 1539 | A | P-O3'-C3' | 7.83 | 129.09 | 119.70 |
| 81 | DA | 2264 | U | O4'-C1'-C2' | -7.83 | 97.97 | 105.80 |
| 81 | DA | 2422 | C | N1-C1'-C2' | 7.83 | 124.17 | 114.00 |
| 81 | DA | 311 | C | P-O3'-C3' | -7.83 | 110.31 | 119.70 |
| 81 | DA | 1234 | G | O4'-C1'-N9 | 7.83 | 114.46 | 108.20 |
| 81 | DA | 2767 | U | O4'-C1'-N1 | 7.83 | 114.46 | 108.20 |
| 35 | BG | 96 | VAL | CB-CA-C | -7.82 | 96.53 | 111.40 |
| 55 | Bc | 48 | ARG | NE-CZ-NH2 | -7.82 | 116.39 | 120.30 |
| 81 | DA | 995 | U | O4'-C1'-C2' | -7.82 | 97.98 | 105.80 |
| 81 | DA | 1265 | U | N1-C1'-C2' | 7.82 | 124.17 | 114.00 |
| 81 | DA | 1670 | C | O4'-C1'-N1 | 7.82 | 114.46 | 108.20 |
| 81 | DA | 1713 | G | N9-C1'-C2' | 7.82 | 124.17 | 114.00 |
| 81 | DA | 3396 | U | O4'-C1'-N1 | 7.82 | 114.46 | 108.20 |
| 78 | CA | 1394 | G | O4'-C4'-C3' | 7.82 | 112.36 | 106.10 |
| 36 | BF | 42 | ASP | CB-CG-OD2 | -7.82 | 111.26 | 118.30 |
| 40 | BK | 180 | SER | C-N-CA | -7.82 | 102.15 | 121.70 |
| 78 | CA | 1085 | G | C3'-C2'-C1' | -7.82 | 95.25 | 101.50 |
| 78 | CA | 1355 | C | O4'-C1'-C2' | -7.82 | 97.98 | 105.80 |
| 78 | CA | 1733 | C | C3'-C2'-C1' | 7.82 | 107.75 | 101.50 |
| 81 | DA | 896 | A | O4'-C1'-N9 | 7.82 | 114.45 | 108.20 |
| 47 | BU | 8 | ARG | N-CA-CB | 7.82 | 124.67 | 110.60 |
| 81 | DA | 430 | U | N1-C1'-C2' | 7.82 | 124.16 | 114.00 |
| 81 | DA | 1114 | U | C4'-C3'-C2' | -7.82 | 94.78 | 102.60 |
| 81 | DA | 1267 | U | O4'-C1'-C2' | -7.82 | 97.98 | 105.80 |
| 83 | DC | 17 | A | O4'-C1'-N9 | -7.82 | 101.95 | 108.20 |
| 78 | CA | 61 | A | O4'-C1'-C2' | -7.82 | 97.98 | 105.80 |
| 78 | CA | 1088 | A | N9-C1'-C2' | -7.82 | 103.40 | 112.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 454 | C | N1-C1'-C2' | 7.82 | 124.16 | 114.00 |
| 81 | DA | 748 | U | O4'-C1'-N1 | 7.82 | 114.45 | 108.20 |
| 81 | DA | 1649 | U | C1'-O4'-C4' | 7.82 | 116.15 | 109.90 |
| 81 | DA | 1773 | C | O4'-C1'-C2' | -7.82 | 97.98 | 105.80 |
| 81 | DA | 2789 | U | P-O3'-C3' | -7.82 | 110.32 | 119.70 |
| 83 | DC | 50 | U | N1-C1'-C2' | 7.82 | 124.16 | 114.00 |
| 12 | AK | 22 | SER | CA-C-O | -7.81 | 103.69 | 120.10 |
| 78 | CA | 896 | U | P-O3'-C3' | 7.81 | 129.08 | 119.70 |
| 78 | CA | 1299 | G | P-O3'-C3' | 7.81 | 129.08 | 119.70 |
| 81 | DA | 9 | U | N1-C1'-C2' | 7.81 | 124.16 | 114.00 |
| 81 | DA | 854 | G | O4'-C1'-N9 | 7.81 | 114.45 | 108.20 |
| 61 | Bj | 65 | ARG | NE-CZ-NH1 | -7.81 | 116.39 | 120.30 |
| 78 | CA | 569 | C | O4'-C1'-N1 | 7.81 | 114.45 | 108.20 |
| 81 | DA | 1737 | U | O4'-C1'-N1 | 7.81 | 114.45 | 108.20 |
| 81 | DA | 2736 | A | C4'-C3'-C2' | -7.81 | 94.79 | 102.60 |
| 38 | Bs | 248 | ALA | N-CA-C | 7.81 | 132.09 | 111.00 |
| 81 | DA | 1129 | A | P-O3'-C3' | 7.81 | 129.07 | 119.70 |
| 81 | DA | 1641 | U | P-O3'-C3' | 7.81 | 129.07 | 119.70 |
| 81 | DA | 2952 | G | C1'-O4'-C4' | -7.81 | 103.65 | 109.90 |
| 81 | DA | 3330 | A | OP1-P-OP2 | -7.81 | 107.89 | 119.60 |
| 32 | BC | 345 | ASN | C-N-CA | -7.81 | 102.18 | 121.70 |
| 81 | DA | 369 | A | N9-C1'-C2' | -7.81 | 103.41 | 112.00 |
| 81 | DA | 465 | U | O4'-C1'-N1 | 7.81 | 114.45 | 108.20 |
| 81 | DA | 3313 | U | C5'-C4'-O4' | 7.81 | 118.47 | 109.10 |
| 32 | BC | 19 | ARG | NE-CZ-NH2 | -7.80 | 116.40 | 120.30 |
| 34 | BE | 60 | ARG | NE-CZ-NH2 | -7.80 | 116.40 | 120.30 |
| 78 | CA | 54 | C | C4'-C3'-C2' | -7.80 | 94.80 | 102.60 |
| 81 | DA | 2066 | C | C3'-C2'-C1' | 7.80 | 107.74 | 101.50 |
| 81 | DA | 2673 | A | N9-C1'-C2' | 7.80 | 124.14 | 114.00 |
| 34 | BE | 115 | LYS | N-CA-CB | 7.80 | 124.65 | 110.60 |
| 78 | CA | 851 | U | C1'-O4'-C4' | -7.80 | 103.66 | 109.90 |
| 81 | DA | 214 | G | N9-C1'-C2' | -7.80 | 103.42 | 112.00 |
| 81 | DA | 1207 | G | O3'-P-O5' | -7.80 | 89.17 | 104.00 |
| 81 | DA | 3321 | C | O4'-C1'-N1 | 7.80 | 114.44 | 108.20 |
| 81 | DA | 158 | G | P-O3'-C3' | -7.80 | 110.34 | 119.70 |
| 81 | DA | 2416 | U | C1'-O4'-C4' | -7.80 | 103.66 | 109.90 |
| 15 | AN | 43 | PHE | CB-CG-CD1 | 7.80 | 126.26 | 120.80 |
| 74 | BQ | 236 | LEU | N-CA-CB | 7.80 | 126.00 | 110.40 |
| 81 | DA | 573 | C | O4'-C1'-C2' | -7.80 | 98.00 | 105.80 |
| 81 | DA | 1819 | U | P-O5'-C5' | 7.80 | 133.38 | 120.90 |
| 13 | AL | 1 | MET | N-CA-C | 7.80 | 132.05 | 111.00 |
| 78 | CA | 1383 | G | P-O3'-C3' | 7.80 | 129.06 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 83 | DC | 72 | C | C5'-C4'-C3' | 7.80 | 128.48 | 116.00 |
| 40 | BK | 135 | TYR | CB-CG-CD1 | 7.80 | 125.68 | 121.00 |
| 62 | Bk | 82 | ARG | O-C-N | -7.80 | 110.23 | 122.70 |
| 81 | DA | 1869 | C | C4'-C3'-C2' | -7.79 | 94.81 | 102.60 |
| 81 | DA | 792 | G | O4'-C1'-N9 | 7.79 | 114.44 | 108.20 |
| 81 | DA | 2489 | C | N1-C1'-C2' | 7.79 | 124.13 | 114.00 |
| 82 | DB | 140 | G | O4'-C1'-N9 | 7.79 | 114.44 | 108.20 |
| 33 | BD | 354 | VAL | N-CA-CB | 7.79 | 128.64 | 111.50 |
| 81 | DA | 406 | G | C1'-O4'-C4' | 7.79 | 116.13 | 109.90 |
| 81 | DA | 2238 | G | O5'-C5'-C4' | 7.79 | 126.51 | 111.70 |
| 81 | DA | 3241 | G | C3'-C2'-C1' | 7.79 | 107.73 | 101.50 |
| 50 | BX | 85 | GLN | N-CA-CB | 7.79 | 124.62 | 110.60 |
| 81 | DA | 1563 | C | O4'-C1'-N1 | 7.79 | 114.43 | 108.20 |
| 64 | Bl | 39 | TYR | N-CA-C | -7.79 | 89.97 | 111.00 |
| 81 | DA | 2079 | G | O3'-P-O5' | 7.79 | 118.80 | 104.00 |
| 78 | CA | 1324 | G | C1'-O4'-C4' | -7.79 | 103.67 | 109.90 |
| 81 | DA | 2 | U | N1-C1'-C2' | -7.79 | 103.44 | 112.00 |
| 78 | CA | 496 | G | C5-C6-O6 | -7.78 | 123.93 | 128.60 |
| 78 | CA | 886 | U | O4'-C1'-C2' | -7.78 | 98.02 | 105.80 |
| 81 | DA | 647 | A | C3'-C2'-C1' | 7.78 | 107.73 | 101.50 |
| 81 | DA | 1420 | C | C3'-C2'-C1' | 7.78 | 107.73 | 101.50 |
| 83 | DC | 48 | U | C1'-O4'-C4' | -7.78 | 103.67 | 109.90 |
| 37 | BH | 63 | LYS | O-C-N | -7.78 | 110.25 | 122.70 |
| 81 | DA | 3330 | A | P-O3'-C3' | -7.78 | 110.36 | 119.70 |
| 48 | BW | 96 | VAL | N-CA-C | -7.78 | 89.99 | 111.00 |
| 74 | BQ | 198 | TYR | CB-CG-CD1 | -7.78 | 116.33 | 121.00 |
| 78 | CA | 275 | C | O4'-C1'-C2' | -7.78 | 98.02 | 105.80 |
| 78 | CA | 1736 | G | C5'-C4'-C3' | 7.78 | 128.45 | 116.00 |
| 81 | DA | 2737 | C | P-O5'-C5' | 7.78 | 133.35 | 120.90 |
| 81 | DA | 2858 | U | N1-C1'-C2' | 7.78 | 124.11 | 114.00 |
| 78 | CA | 217 | A | N9-C1'-C2' | -7.78 | 103.44 | 112.00 |
| 78 | CA | 1233 | G | N9-C1'-C2' | -7.78 | 103.44 | 112.00 |
| 81 | DA | 309 | U | O3'-P-O5' | -7.78 | 89.22 | 104.00 |
| 81 | DA | 767 | U | O4'-C1'-C2' | -7.78 | 98.02 | 105.80 |
| 81 | DA | 1114 | U | O4'-C1'-N1 | 7.78 | 114.42 | 108.20 |
| 81 | DA | 1890 | U | P-O3'-C3' | 7.78 | 129.03 | 119.70 |
| 78 | CA | 1500 | C | O4'-C1'-N1 | 7.78 | 114.42 | 108.20 |
| 81 | DA | 2721 | A | O4'-C1'-N9 | -7.78 | 101.98 | 108.20 |
| 82 | DB | 120 | C | O4'-C1'-C2' | -7.78 | 98.02 | 105.80 |
| 78 | CA | 395 | U | O4'-C1'-N1 | 7.77 | 114.42 | 108.20 |
| 56 | Bf | 68 | TYR | CB-CG-CD2 | -7.77 | 116.34 | 121.00 |
| 78 | CA | 64 | U | O4'-C1'-N1 | 7.77 | 114.42 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2864 | A | O4'-C1'-N9 | 7.77 | 114.42 | 108.20 |
| 81 | DA | 2507 | C | C5'-C4'-C3' | -7.77 | 103.57 | 116.00 |
| 32 | BC | 360 | ASP | CB-CA-C | -7.77 | 94.87 | 110.40 |
| 79 | CB | 12 | U | C4'-C3'-C2' | -7.77 | 94.83 | 102.60 |
| 81 | DA | 2421 | U | O4'-C1'-C2' | -7.77 | 98.03 | 105.80 |
| 81 | DA | 2461 | A | O4'-C1'-N9 | 7.77 | 114.41 | 108.20 |
| 81 | DA | 2968 | G | C1'-O4'-C4' | 7.77 | 116.11 | 109.90 |
| 78 | CA | 1133 | A | O4'-C1'-N9 | 7.77 | 114.41 | 108.20 |
| 11 | AJ | 87 | HIS | N-CA-CB | 7.76 | 124.58 | 110.60 |
| 15 | AN | 53 | ASN | O-C-N | -7.76 | 110.28 | 122.70 |
| 35 | BG | 100 | LYS | N-CA-C | -7.76 | 90.03 | 111.00 |
| 43 | BP | 44 | ARG | N-CA-C | 7.76 | 131.96 | 111.00 |
| 43 | BP | 94 | TYR | CB-CG-CD1 | 7.76 | 125.66 | 121.00 |
| 76 | BS | 66 | ILE | N-CA-CB | 7.76 | 128.66 | 110.80 |
| 78 | CA | 82 | U | O4'-C1'-N1 | 7.76 | 114.41 | 108.20 |
| 38 | Bs | 36 | GLN | CA-CB-CG | 7.76 | 130.48 | 113.40 |
| 81 | DA | 2895 | G | P-O5'-C5' | 7.76 | 133.32 | 120.90 |
| 78 | CA | 1280 | C | C3'-C2'-C1' | 7.76 | 107.71 | 101.50 |
| 81 | DA | 3211 | C | O4'-C1'-N1 | 7.76 | 114.41 | 108.20 |
| 81 | DA | 2316 | G | C1'-O4'-C4' | -7.76 | 103.69 | 109.90 |
| 81 | DA | 2892 | A | C3'-C2'-C1' | 7.76 | 107.71 | 101.50 |
| 45 | BR | 142 | GLY | N-CA-C | -7.76 | 93.71 | 113.10 |
| 78 | CA | 189 | C | O4'-C1'-C2' | -7.76 | 98.04 | 105.80 |
| 81 | DA | 2746 | A | N9-C1'-C2' | 7.76 | 124.08 | 114.00 |
| 33 | BD | 194 | TYR | CZ-CE2-CD2 | 7.75 | 126.78 | 119.80 |
| 61 | Bj | 2 | ALA | N-CA-CB | 7.75 | 120.96 | 110.10 |
| 81 | DA | 3236 | U | C5'-C4'-C3' | -7.75 | 103.59 | 116.00 |
| 52 | BY | 10 | SER | N-CA-CB | 7.75 | 122.13 | 110.50 |
| 78 | CA | 1338 | C | N1-C1'-C2' | 7.75 | 124.08 | 114.00 |
| 78 | CA | 1548 | G | O3'-P-O5' | 7.75 | 118.73 | 104.00 |
| 81 | DA | 2630 | C | N1-C1'-C2' | 7.75 | 124.08 | 114.00 |
| 31 | BB | 36 | GLU | N-CA-CB | 7.75 | 124.55 | 110.60 |
| 81 | DA | 2664 | C | N1-C1'-C2' | 7.75 | 124.08 | 114.00 |
| 81 | DA | 754 | G | O4'-C1'-N9 | 7.75 | 114.40 | 108.20 |
| 53 | Ba | 62 | VAL | CB-CA-C | -7.75 | 96.68 | 111.40 |
| 78 | CA | 303 | U | C3'-C2'-C1' | 7.75 | 107.70 | 101.50 |
| 78 | CA | 495 | C | O4'-C1'-N1 | 7.75 | 114.40 | 108.20 |
| 81 | DA | 110 | G | C1'-O4'-C4' | -7.75 | 103.70 | 109.90 |
| 81 | DA | 882 | A | N9-C1'-C2' | 7.75 | 124.07 | 114.00 |
| 81 | DA | 2173 | U | C5'-C4'-C3' | 7.75 | 128.40 | 116.00 |
| 81 | DA | 1331 | U | N1-C1'-C2' | 7.75 | 124.07 | 114.00 |
| 41 | BN | 55 | ARG | NE-CZ-NH1 | 7.74 | 124.17 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 66 | Bo | 28 | ARG | NE-CZ-NH1 | -7.74 | 116.43 | 120.30 |
| 81 | DA | 2916 | U | P-O3'-C3' | -7.74 | 110.41 | 119.70 |
| 22 | AV | 29 | LYS | C-N-CA | -7.74 | 102.34 | 121.70 |
| 55 | Bc | 31 | LEU | CB-CA-C | 7.74 | 124.91 | 110.20 |
| 78 | CA | 427 | C | N1-C1'-C2' | 7.74 | 124.06 | 114.00 |
| 78 | CA | 1114 | G | O4'-C1'-N9 | 7.74 | 114.39 | 108.20 |
| 61 | Bj | 21 | ARG | CB-CA-C | 7.74 | 125.88 | 110.40 |
| 35 | BG | 97 | ASN | N-CA-CB | 7.74 | 124.53 | 110.60 |
| 51 | BZ | 67 | VAL | O-C-N | -7.74 | 110.32 | 122.70 |
| 78 | CA | 1090 | C | C2'-C3'-O3' | 7.74 | 126.52 | 109.50 |
| 81 | DA | 1763 | U | O4'-C1'-N1 | 7.74 | 114.39 | 108.20 |
| 65 | Bn | 29 | LYS | CB-CA-C | -7.73 | 94.93 | 110.40 |
| 78 | CA | 1124 | A | N9-C1'-C2' | -7.73 | 103.49 | 112.00 |
| 81 | DA | 443 | G | O4'-C1'-N9 | 7.73 | 114.39 | 108.20 |
| 81 | DA | 600 | G | P-O3'-C3' | 7.73 | 128.98 | 119.70 |
| 81 | DA | 2722 | U | O4'-C1'-N1 | 7.73 | 114.39 | 108.20 |
| 78 | CA | 1510 | U | O4'-C1'-N1 | 7.73 | 114.38 | 108.20 |
| 81 | DA | 3364 | C | P-O5'-C5' | 7.73 | 133.27 | 120.90 |
| 78 | CA | 304 | U | C3'-C2'-C1' | 7.73 | 107.68 | 101.50 |
| 81 | DA | 973 | A | C4'-C3'-C2' | -7.73 | 94.87 | 102.60 |
| 81 | DA | 2575 | G | N1-C6-O6 | 7.73 | 124.54 | 119.90 |
| 81 | DA | 2720 | G | O4'-C1'-C2' | -7.73 | 98.07 | 105.80 |
| 53 | Ba | 8 | GLY | C-N-CA | 7.73 | 141.02 | 121.70 |
| 78 | CA | 291 | G | C1'-O4'-C4' | -7.73 | 103.72 | 109.90 |
| 78 | CA | 1681 | A | O4'-C1'-N9 | 7.73 | 114.38 | 108.20 |
| 78 | CA | 1755 | A | C3'-C2'-C1' | -7.73 | 95.32 | 101.50 |
| 81 | DA | 763 | G | N1-C6-O6 | 7.73 | 124.54 | 119.90 |
| 82 | DB | 74 | U | P-O3'-C3' | 7.73 | 128.97 | 119.70 |
| 82 | DB | 98 | U | P-O5'-C5' | 7.73 | 133.26 | 120.90 |
| 78 | CA | 124 | A | C3'-C2'-C1' | 7.72 | 107.68 | 101.50 |
| 81 | DA | 3140 | G | O4'-C1'-C2' | -7.72 | 98.08 | 105.80 |
| 81 | DA | 3120 | C | P-O3'-C3' | -7.72 | 110.43 | 119.70 |
| 78 | CA | 1602 | C | C1'-O4'-C4' | -7.72 | 103.72 | 109.90 |
| 81 | DA | 181 | U | O4'-C1'-N1 | 7.72 | 114.38 | 108.20 |
| 78 | CA | 53 | G | O3'-P-O5' | 7.72 | 118.67 | 104.00 |
| 81 | DA | 1063 | G | O4'-C1'-N9 | 7.72 | 114.38 | 108.20 |
| 81 | DA | 1772 | U | O4'-C1'-N1 | 7.72 | 114.38 | 108.20 |
| 81 | DA | 3019 | U | N1-C1'-C2' | 7.72 | 124.03 | 114.00 |
| 81 | DA | 3137 | C | O4'-C1'-N1 | 7.72 | 114.38 | 108.20 |
| 82 | DB | 52 | A | C3'-C2'-C1' | 7.72 | 107.68 | 101.50 |
| 81 | DA | 2267 | C | O4'-C1'-N1 | 7.72 | 114.38 | 108.20 |
| 81 | DA | 2313 | A | O4'-C1'-C2' | -7.72 | 98.08 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 83 | DC | 26 | C | O4'-C1'-N1 | -7.72 | 102.03 | 108.20 |
| 50 | BX | 54 | TYR | N-CA-CB | 7.72 | 124.49 | 110.60 |
| 53 | Ba | 71 | PHE | CB-CG-CD1 | 7.72 | 126.20 | 120.80 |
| 81 | DA | 693 | A | C1'-O4'-C4' | 7.72 | 116.07 | 109.90 |
| 81 | DA | 1206 | G | C1'-O4'-C4' | -7.72 | 103.73 | 109.90 |
| 81 | DA | 3146 | G | P-O3'-C3' | 7.72 | 128.96 | 119.70 |
| 2 | AA | 195 | TRP | CB-CA-C | 7.71 | 125.83 | 110.40 |
| 32 | BC | 296 | THR | N-CA-CB | 7.71 | 124.96 | 110.30 |
| 35 | BG | 158 | TYR | CB-CG-CD2 | -7.71 | 116.37 | 121.00 |
| 81 | DA | 1728 | G | C1'-O4'-C4' | -7.71 | 103.73 | 109.90 |
| 78 | CA | 157 | A | C3'-C2'-C1' | 7.71 | 107.67 | 101.50 |
| 81 | DA | 329 | U | C3'-C2'-C1' | -7.71 | 95.33 | 101.50 |
| 9 | AH | 130 | TYR | CB-CG-CD1 | -7.71 | 116.38 | 121.00 |
| 78 | CA | 920 | U | O4'-C1'-N1 | 7.71 | 114.37 | 108.20 |
| 78 | CA | 1258 | U | O4'-C1'-N1 | 7.71 | 114.37 | 108.20 |
| 81 | DA | 521 | A | O5'-C5'-C4' | -7.71 | 97.06 | 111.70 |
| 81 | DA | 536 | U | N1-C1'-C2' | 7.71 | 124.02 | 114.00 |
| 81 | DA | 1046 | A | N9-C1'-C2' | -7.71 | 103.52 | 112.00 |
| 81 | DA | 1208 | U | C1'-O4'-C4' | 7.71 | 116.07 | 109.90 |
| 5 | AC | 168 | ARG | NE-CZ-NH1 | 7.71 | 124.15 | 120.30 |
| 19 | AR | 133 | ALA | N-CA-CB | 7.71 | 120.89 | 110.10 |
| 78 | CA | 1580 | C | P-O5'-C5' | 7.71 | 133.23 | 120.90 |
| 80 | CC | 18 | C | P-O3'-C3' | -7.71 | 110.45 | 119.70 |
| 81 | DA | 3031 | G | N9-C1'-C2' | 7.71 | 124.02 | 114.00 |
| 81 | DA | 3230 | G | C4'-C3'-C2' | -7.71 | 94.89 | 102.60 |
| 83 | DC | 47 | C | P-O3'-C3' | -7.71 | 110.45 | 119.70 |
| 49 | BV | 152 | GLU | C-N-CA | 7.71 | 140.96 | 121.70 |
| 81 | DA | 158 | G | C4'-C3'-C2' | -7.70 | 94.90 | 102.60 |
| 81 | DA | 341 | G | P-O3'-C3' | 7.70 | 128.94 | 119.70 |
| 81 | DA | 1754 | G | C2'-C3'-O3' | 7.70 | 126.45 | 109.50 |
| 82 | DB | 32 | C | C3'-C2'-C1' | 7.70 | 107.66 | 101.50 |
| 44 | BO | 9 | ARG | NE-CZ-NH2 | -7.70 | 116.45 | 120.30 |
| 81 | DA | 1505 | C | P-O3'-C3' | 7.70 | 128.94 | 119.70 |
| 81 | DA | 2539 | C | O4'-C1'-N1 | 7.70 | 114.36 | 108.20 |
| 81 | DA | 3090 | U | O5'-C5'-C4' | 7.70 | 126.33 | 111.70 |
| 81 | DA | 3304 | U | C2'-C3'-O3' | 7.70 | 126.44 | 109.50 |
| 35 | BG | 98 | VAL | CA-CB-CG1 | 7.70 | 122.45 | 110.90 |
| 48 | BW | 97 | SER | N-CA-CB | -7.70 | 98.95 | 110.50 |
| 51 | BZ | 69 | LYS | C-N-CA | 7.70 | 140.95 | 121.70 |
| 81 | DA | 175 | C | P-O5'-C5' | -7.70 | 108.58 | 120.90 |
| 83 | DC | 82 | A | P-O3'-C3' | -7.70 | 110.46 | 119.70 |
| 81 | DA | 2957 | G | C1'-O4'-C4' | -7.70 | 103.74 | 109.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 5 | AC | 107 | ARG | NE-CZ-NH1 | 7.70 | 124.15 | 120.30 |
| 57 | Be | 200 | ASN | N-CA-C | -7.70 | 90.22 | 111.00 |
| 81 | DA | 447 | U | P-O3'-C3' | 7.70 | 128.94 | 119.70 |
| 81 | DA | 997 | A | C1'-O4'-C4' | 7.69 | 116.06 | 109.90 |
| 81 | DA | 1194 | G | O4'-C1'-N9 | 7.69 | 114.35 | 108.20 |
| 78 | CA | 1649 | G | O4'-C1'-C2' | -7.69 | 98.11 | 105.80 |
| 81 | DA | 672 | A | O4'-C4'-C3' | -7.69 | 96.31 | 104.00 |
| 81 | DA | 2611 | U | O4'-C1'-N1 | 7.69 | 114.35 | 108.20 |
| 81 | DA | 3135 | U | O4'-C1'-N1 | 7.69 | 114.35 | 108.20 |
| 78 | CA | 1344 | A | O4'-C1'-N9 | 7.69 | 114.35 | 108.20 |
| 81 | DA | 1679 | A | O3'-P-O5' | -7.69 | 89.39 | 104.00 |
| 38 | Bs | 5 | ARG | CB-CA-C | 7.69 | 125.77 | 110.40 |
| 40 | BK | 128 | ARG | CA-C-N | 7.69 | 134.11 | 117.20 |
| 56 | Bf | 58 | TYR | CB-CG-CD2 | 7.69 | 125.61 | 121.00 |
| 79 | CB | 26 | G | O4'-C1'-C2' | 7.69 | 114.52 | 107.60 |
| 81 | DA | 2106 | A | P-O3'-C3' | 7.69 | 128.93 | 119.70 |
| 81 | DA | 3067 | C | O4'-C1'-C2' | -7.69 | 98.11 | 105.80 |
| 83 | DC | 18 | C | P-O3'-C3' | 7.69 | 128.92 | 119.70 |
| 81 | DA | 2895 | G | O4'-C1'-C2' | 7.68 | 114.52 | 107.60 |
| 42 | BM | 48 | ARG | NE-CZ-NH1 | 7.68 | 124.14 | 120.30 |
| 78 | CA | 647 | G | O4'-C1'-C2' | -7.68 | 98.12 | 105.80 |
| 81 | DA | 1167 | U | O4'-C1'-N1 | 7.68 | 114.34 | 108.20 |
| 81 | DA | 1409 | G | O4'-C1'-N9 | 7.68 | 114.35 | 108.20 |
| 81 | DA | 1941 | C | O4'-C1'-N1 | 7.68 | 114.35 | 108.20 |
| 81 | DA | 1180 | A | C1'-O4'-C4' | 7.68 | 116.05 | 109.90 |
| 11 | AJ | 14 | GLN | OE1-CD-NE2 | 7.68 | 139.56 | 121.90 |
| 60 | Bi | 19 | LYS | N-CA-C | -7.68 | 90.27 | 111.00 |
| 78 | CA | 1052 | U | O4'-C1'-N1 | 7.68 | 114.34 | 108.20 |
| 81 | DA | 2118 | C | C3'-C2'-C1' | 7.68 | 107.64 | 101.50 |
| 81 | DA | 2466 | G | O4'-C1'-C2' | 7.68 | 114.51 | 107.60 |
| 81 | DA | 2724 | U | N1-C1'-C2' | 7.68 | 123.98 | 114.00 |
| 6 | AE | 126 | ARG | CB-CA-C | 7.68 | 125.76 | 110.40 |
| 57 | Be | 71 | ALA | N-CA-CB | 7.68 | 120.85 | 110.10 |
| 78 | CA | 1450 | U | O4'-C1'-N1 | 7.68 | 114.34 | 108.20 |
| 78 | CA | 887 | A | P-O5'-C5' | -7.68 | 108.62 | 120.90 |
| 78 | CA | 1747 | G | O4'-C1'-N9 | 7.68 | 114.34 | 108.20 |
| 81 | DA | 1652 | G | O4'-C1'-N9 | 7.68 | 114.34 | 108.20 |
| 81 | DA | 2119 | A | P-O3'-C3' | 7.68 | 128.91 | 119.70 |
| 81 | DA | 2310 | U | N1-C1'-C2' | 7.68 | 123.98 | 114.00 |
| 6 | AE | 207 | LEU | CB-CG-CD2 | 7.67 | 124.05 | 111.00 |
| 76 | BS | 155 | TYR | N-CA-CB | 7.67 | 124.41 | 110.60 |
| 78 | CA | 818 | C | OP1-P-OP2 | -7.67 | 108.09 | 119.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 881 | A | O4'-C1'-N9 | 7.67 | 114.34 | 108.20 |
| 78 | CA | 955 | A | N9-C1'-C2' | -7.67 | 103.56 | 112.00 |
| 81 | DA | 1698 | C | C4'-C3'-C2' | -7.67 | 94.92 | 102.60 |
| 81 | DA | 1882 | G | O4'-C1'-C2' | 7.67 | 114.51 | 107.60 |
| 81 | DA | 2952 | G | O4'-C1'-C2' | 7.67 | 114.51 | 107.60 |
| 53 | Ba | 54 | THR | N-CA-CB | 7.67 | 124.88 | 110.30 |
| 81 | DA | 175 | C | O4'-C1'-N1 | 7.67 | 114.34 | 108.20 |
| 81 | DA | 661 | G | N9-C1'-C2' | -7.67 | 103.56 | 112.00 |
| 81 | DA | 1856 | C | O4'-C1'-N1 | 7.67 | 114.34 | 108.20 |
| 42 | BM | 64 | LYS | C-N-CA | -7.67 | 106.19 | 122.30 |
| 55 | Bc | 116 | TYR | CZ-CE2-CD2 | 7.67 | 126.70 | 119.80 |
| 61 | Bj | 38 | PRO | N-CA-C | 7.67 | 132.05 | 112.10 |
| 81 | DA | 1777 | U | O4'-C1'-N1 | 7.67 | 114.34 | 108.20 |
| 47 | BU | 84 | TYR | CB-CG-CD1 | -7.67 | 116.40 | 121.00 |
| 81 | DA | 989 | A | C1'-O4'-C4' | 7.67 | 116.03 | 109.90 |
| 81 | DA | 1058 | U | P-O5'-C5' | 7.67 | 133.17 | 120.90 |
| 81 | DA | 1745 | C | O4'-C1'-N1 | 7.67 | 114.33 | 108.20 |
| 81 | DA | 2899 | C | O4'-C1'-N1 | -7.67 | 102.06 | 108.20 |
| 56 | Bf | 85 | PHE | CB-CG-CD2 | -7.67 | 115.43 | 120.80 |
| 78 | CA | 1427 | A | P-O5'-C5' | -7.67 | 108.63 | 120.90 |
| 78 | CA | 313 | U | O4'-C1'-N1 | 7.66 | 114.33 | 108.20 |
| 81 | DA | 565 | U | O4'-C1'-N1 | 7.66 | 114.33 | 108.20 |
| 81 | DA | 1038 | C | O4'-C1'-C2' | -7.66 | 98.14 | 105.80 |
| 81 | DA | 2059 | U | N1-C1'-C2' | 7.66 | 123.96 | 114.00 |
| 4 | AD | 97 | GLU | N-CA-CB | 7.66 | 124.39 | 110.60 |
| 66 | Bo | 30 | ARG | NE-CZ-NH2 | -7.66 | 116.47 | 120.30 |
| 81 | DA | 301 | G | O4'-C1'-N9 | 7.66 | 114.33 | 108.20 |
| 81 | DA | 436 | A | C3'-C2'-C1' | 7.66 | 107.63 | 101.50 |
| 81 | DA | 637 | C | C4'-C3'-C2' | 7.66 | 110.26 | 102.60 |
| 53 | Ba | 13 | VAL | N-CA-CB | 7.66 | 128.35 | 111.50 |
| 81 | DA | 633 | C | N1-C1'-C2' | 7.66 | 123.96 | 114.00 |
| 81 | DA | 801 | A | P-O3'-C3' | -7.66 | 110.51 | 119.70 |
| 81 | DA | 1333 | C | C3'-C2'-C1' | 7.66 | 107.63 | 101.50 |
| 83 | DC | 112 | G | P-O3'-C3' | -7.66 | 110.51 | 119.70 |
| 81 | DA | 1725 | C | C3'-C2'-C1' | 7.66 | 107.62 | 101.50 |
| 32 | BC | 344 | THR | C-N-CA | -7.66 | 102.56 | 121.70 |
| 40 | BK | 134 | LYS | N-CA-C | -7.66 | 90.33 | 111.00 |
| 42 | BM | 64 | LYS | N-CA-C | -7.66 | 90.33 | 111.00 |
| 81 | DA | 2245 | C | C3'-C2'-C1' | 7.66 | 107.62 | 101.50 |
| 81 | DA | 2937 | G | O4'-C1'-N9 | 7.66 | 114.33 | 108.20 |
| 81 | DA | 1854 | C | O4'-C1'-C2' | -7.65 | 98.15 | 105.80 |
| 81 | DA | 2268 | U | O4'-C1'-N1 | 7.65 | 114.32 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 893 | U | P-O3'-C3' | -7.65 | 110.52 | 119.70 |
| 78 | CA | 123 | G | O4'-C4'-C3' | -7.65 | 96.35 | 104.00 |
| 78 | CA | 236 | A | O4'-C1'-N9 | 7.65 | 114.32 | 108.20 |
| 78 | CA | 1087 | A | C5'-C4'-O4' | 7.65 | 118.28 | 109.10 |
| 78 | CA | 164 | A | O5'-P-OP1 | 7.65 | 119.88 | 110.70 |
| 78 | CA | 588 | U | P-O5'-C5' | -7.65 | 108.66 | 120.90 |
| 81 | DA | 3220 | G | P-O5'-C5' | 7.65 | 133.14 | 120.90 |
| 5 | AC | 18 | PRO | C-N-CA | 7.65 | 140.82 | 121.70 |
| 81 | DA | 1462 | A | O3'-P-O5' | -7.65 | 89.47 | 104.00 |
| 81 | DA | 3108 | G | C1'-O4'-C4' | -7.65 | 103.78 | 109.90 |
| 51 | BZ | 67 | VAL | CA-C-O | -7.65 | 104.04 | 120.10 |
| 81 | DA | 739 | G | O4'-C1'-N9 | 7.65 | 114.32 | 108.20 |
| 81 | DA | 1037 | C | C3'-C2'-C1' | 7.65 | 107.62 | 101.50 |
| 78 | CA | 950 | C | N1-C1'-C2' | 7.64 | 123.94 | 114.00 |
| 78 | CA | 1144 | U | C5'-C4'-C3' | -7.64 | 103.77 | 116.00 |
| 3 | AB | 78 | LYS | CB-CA-C | 7.64 | 125.69 | 110.40 |
| 6 | AE | 30 | THR | CA-CB-CG2 | -7.64 | 101.70 | 112.40 |
| 10 | AI | 142 | TYR | CB-CG-CD2 | 7.64 | 125.59 | 121.00 |
| 59 | Bh | 24 | ARG | CD-NE-CZ | -7.64 | 112.90 | 123.60 |
| 78 | CA | 827 | C | O4'-C1'-N1 | 7.64 | 114.31 | 108.20 |
| 81 | DA | 678 | G | C1'-O4'-C4' | -7.64 | 103.79 | 109.90 |
| 81 | DA | 1698 | C | C5'-C4'-O4' | -7.64 | 99.93 | 109.10 |
| 81 | DA | 2776 | C | C3'-C2'-C1' | 7.64 | 107.61 | 101.50 |
| 44 | BO | 15 | VAL | N-CA-CB | 7.64 | 128.31 | 111.50 |
| 81 | DA | 2172 | A | C5'-C4'-C3' | -7.64 | 103.78 | 116.00 |
| 81 | DA | 3361 | G | C2'-C3'-O3' | 7.64 | 126.31 | 109.50 |
| 37 | BH | 228 | GLU | CB-CA-C | -7.64 | 95.12 | 110.40 |
| 83 | DC | 43 | U | N1-C1'-C2' | 7.64 | 123.93 | 114.00 |
| 78 | CA | 868 | G | O4'-C1'-C2' | 7.64 | 114.47 | 107.60 |
| 81 | DA | 1265 | U | C1'-O4'-C4' | -7.64 | 103.79 | 109.90 |
| 81 | DA | 1512 | U | O4'-C1'-N1 | 7.64 | 114.31 | 108.20 |
| 83 | DC | 32 | U | C1'-O4'-C4' | -7.64 | 103.79 | 109.90 |
| 74 | BQ | 128 | GLU | CB-CA-C | -7.63 | 95.13 | 110.40 |
| 78 | CA | 1459 | C | C4'-C3'-C2' | 7.63 | 110.23 | 102.60 |
| 81 | DA | 728 | G | C5-C6-O6 | -7.63 | 124.02 | 128.60 |
| 81 | DA | 858 | A | C5'-C4'-C3' | -7.63 | 103.79 | 116.00 |
| 81 | DA | 2922 | G | N9-C1'-C2' | 7.63 | 123.92 | 114.00 |
| 81 | DA | 3308 | C | C3'-C2'-C1' | 7.63 | 107.61 | 101.50 |
| 36 | BF | 141 | LYS | N-CA-CB | 7.63 | 124.34 | 110.60 |
| 81 | DA | 425 | G | P-O5'-C5' | 7.63 | 133.11 | 120.90 |
| 81 | DA | 1690 | C | O3'-P-O5' | -7.63 | 89.50 | 104.00 |
| 12 | AK | 67 | VAL | CB-CA-C | 7.63 | 125.90 | 111.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 58 | Bg | 79 | ARG | N-CA-CB | 7.63 | 124.33 | 110.60 |
| 61 | Bj | 21 | ARG | C-N-CA | -7.63 | 102.62 | 121.70 |
| 82 | DB | 39 | G | C5'-C4'-O4' | -7.63 | 99.94 | 109.10 |
| 78 | CA | 1577 | A | N9-C1'-C2' | -7.63 | 103.61 | 112.00 |
| 81 | DA | 962 | A | N9-C1'-C2' | -7.63 | 103.61 | 112.00 |
| 4 | AD | 235 | TYR | CA-C-N | 7.63 | 133.98 | 117.20 |
| 32 | BC | 256 | HIS | CB-CA-C | 7.63 | 125.66 | 110.40 |
| 34 | BE | 87 | LYS | N-CA-CB | 7.63 | 124.33 | 110.60 |
| 78 | CA | 1214 | U | C1'-O4'-C4' | 7.63 | 116.00 | 109.90 |
| 81 | DA | 1730 | G | N9-C1'-C2' | -7.63 | 103.61 | 112.00 |
| 50 | BX | 27 | ARG | NE-CZ-NH1 | 7.63 | 124.11 | 120.30 |
| 78 | CA | 383 | G | C1'-O4'-C4' | -7.63 | 103.80 | 109.90 |
| 81 | DA | 1 | G | C1'-O4'-C4' | 7.63 | 116.00 | 109.90 |
| 81 | DA | 1784 | G | P-O5'-C5' | 7.63 | 133.10 | 120.90 |
| 82 | DB | 57 | C | P-O3'-C3' | 7.63 | 128.85 | 119.70 |
| 78 | CA | 1460 | A | O4'-C1'-N9 | 7.62 | 114.30 | 108.20 |
| 78 | CA | 1755 | A | O4'-C1'-C2' | 7.62 | 114.46 | 107.60 |
| 78 | CA | 1783 | C | O4'-C1'-C2' | -7.62 | 98.17 | 105.80 |
| 81 | DA | 2002 | G | O4'-C1'-N9 | 7.62 | 114.30 | 108.20 |
| 4 | AD | 130 | GLN | CA-C-N | -7.62 | 100.43 | 117.20 |
| 81 | DA | 1219 | C | O4'-C1'-C2' | -7.62 | 98.18 | 105.80 |
| 81 | DA | 1495 | U | N1-C1'-C2' | 7.62 | 123.91 | 114.00 |
| 81 | DA | 1972 | A | C5'-C4'-C3' | 7.62 | 128.20 | 116.00 |
| 83 | DC | 9 | C | O3'-P-O5' | -7.62 | 89.52 | 104.00 |
| 81 | DA | 1289 | G | O4'-C1'-N9 | 7.62 | 114.30 | 108.20 |
| 81 | DA | 1562 | C | C5'-C4'-C3' | -7.62 | 103.81 | 116.00 |
| 81 | DA | 1869 | C | O4'-C1'-C2' | -7.62 | 98.18 | 105.80 |
| 78 | CA | 20 | G | O4'-C1'-N9 | 7.62 | 114.30 | 108.20 |
| 78 | CA | 1107 | G | N9-C1'-C2' | 7.62 | 123.90 | 114.00 |
| 78 | CA | 1596 | C | O4'-C1'-N1 | 7.62 | 114.30 | 108.20 |
| 81 | DA | 2486 | A | O3'-P-O5' | 7.62 | 118.48 | 104.00 |
| 57 | Be | 120 | THR | CA-CB-OG1 | 7.62 | 124.99 | 109.00 |
| 78 | CA | 1321 | A | N9-C1'-C2' | -7.62 | 103.62 | 112.00 |
| 78 | CA | 1649 | G | O4'-C1'-N9 | 7.62 | 114.29 | 108.20 |
| 81 | DA | 2195 | C | C4'-C3'-C2' | -7.62 | 94.98 | 102.60 |
| 81 | DA | 2874 | G | N9-C1'-C2' | 7.62 | 123.90 | 114.00 |
| 6 | AE | 241 | ASP | N-CA-CB | 7.61 | 124.30 | 110.60 |
| 10 | AI | 140 | LYS | N-CA-C | -7.61 | 90.44 | 111.00 |
| 36 | BF | 117 | PHE | CB-CG-CD1 | -7.61 | 115.47 | 120.80 |
| 61 | Bj | 8 | TYR | CB-CG-CD1 | -7.61 | 116.43 | 121.00 |
| 78 | CA | 1141 | G | C3'-C2'-C1' | -7.61 | 95.41 | 101.50 |
| 78 | CA | 1087 | A | C5'-C4'-C3' | -7.61 | 103.82 | 116.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 64 | Bl | 74 | PHE | CB-CG-CD2 | -7.61 | 115.47 | 120.80 |
| 81 | DA | 520 | U | O4'-C1'-N1 | 7.61 | 114.29 | 108.20 |
| 81 | DA | 1206 | G | C4'-C3'-C2' | -7.61 | 94.99 | 102.60 |
| 81 | DA | 2208 | A | C5'-C4'-C3' | -7.61 | 103.82 | 116.00 |
| 81 | DA | 3099 | C | N1-C1'-C2' | 7.61 | 123.89 | 114.00 |
| 81 | DA | 3385 | U | O5'-C5'-C4' | 7.61 | 126.16 | 111.70 |
| 22 | AV | 31 | SER | C-N-CA | 7.61 | 140.72 | 121.70 |
| 15 | AN | 43 | PHE | CB-CG-CD2 | -7.61 | 115.47 | 120.80 |
| 81 | DA | 1516 | C | P-O3'-C3' | 7.61 | 128.83 | 119.70 |
| 81 | DA | 2664 | C | C3'-C2'-C1' | 7.61 | 107.59 | 101.50 |
| 39 | BJ | 16 | ARG | NE-CZ-NH2 | -7.61 | 116.50 | 120.30 |
| 78 | CA | 1554 | U | N1-C1'-C2' | -7.61 | 103.64 | 112.00 |
| 81 | DA | 183 | G | C1'-O4'-C4' | -7.61 | 103.81 | 109.90 |
| 81 | DA | 1391 | C | P-O3'-C3' | 7.61 | 128.82 | 119.70 |
| 81 | DA | 1788 | C | C4'-C3'-C2' | -7.61 | 94.99 | 102.60 |
| 55 | Bc | 81 | ARG | CB-CA-C | -7.60 | 95.19 | 110.40 |
| 81 | DA | 160 | G | P-O5'-C5' | -7.60 | 108.74 | 120.90 |
| 81 | DA | 535 | G | P-O3'-C3' | 7.60 | 128.82 | 119.70 |
| 81 | DA | 2735 | U | C4'-C3'-C2' | -7.60 | 95.00 | 102.60 |
| 79 | CB | 75 | A | N9-C1'-C2' | -7.60 | 103.64 | 112.00 |
| 81 | DA | 2229 | A | C5'-C4'-O4' | -7.60 | 99.98 | 109.10 |
| 45 | BR | 53 | PHE | CB-CG-CD1 | -7.60 | 115.48 | 120.80 |
| 78 | CA | 1511 | U | O4'-C1'-N1 | 7.60 | 114.28 | 108.20 |
| 35 | BG | 77 | ARG | NE-CZ-NH1 | -7.59 | 116.50 | 120.30 |
| 78 | CA | 369 | A | O4'-C1'-C2' | -7.59 | 98.20 | 105.80 |
| 78 | CA | 641 | G | C1'-O4'-C4' | -7.59 | 103.82 | 109.90 |
| 81 | DA | 513 | G | O4'-C1'-C2' | 7.59 | 114.43 | 107.60 |
| 81 | DA | 2915 | U | C4'-C3'-C2' | -7.59 | 95.00 | 102.60 |
| 78 | CA | 1180 | C | C3'-C2'-C1' | 7.59 | 107.57 | 101.50 |
| 81 | DA | 1246 | G | O4'-C1'-N9 | 7.59 | 114.28 | 108.20 |
| 32 | BC | 61 | ASP | CB-CG-OD2 | -7.59 | 111.47 | 118.30 |
| 45 | BR | 98 | LYS | N-CA-C | -7.59 | 90.50 | 111.00 |
| 81 | DA | 1947 | G | C1'-O4'-C4' | 7.59 | 115.97 | 109.90 |
| 81 | DA | 393 | U | N1-C1'-C2' | 7.59 | 123.86 | 114.00 |
| 81 | DA | 1710 | C | O4'-C1'-N1 | 7.59 | 114.27 | 108.20 |
| 81 | DA | 2339 | C | C3'-C2'-C1' | 7.59 | 107.57 | 101.50 |
| 81 | DA | 2496 | C | O3'-P-O5' | -7.59 | 89.58 | 104.00 |
| 81 | DA | 2669 | G | C3'-C2'-C1' | -7.59 | 95.43 | 101.50 |
| 81 | DA | 1060 | U | C3'-C2'-C1' | 7.58 | 107.57 | 101.50 |
| 78 | CA | 1352 | G | O4'-C1'-N9 | 7.58 | 114.27 | 108.20 |
| 81 | DA | 1453 | A | O4'-C1'-N9 | 7.58 | 114.27 | 108.20 |
| 81 | DA | 2884 | C | N1-C1'-C2' | 7.58 | 123.86 | 114.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 83 | DC | 13 | A | C3'-C2'-C1' | 7.58 | 107.57 | 101.50 |
| 74 | BQ | 128 | GLU | N-CA-CB | -7.58 | 96.95 | 110.60 |
| 74 | BQ | 243 | ALA | CB-CA-C | -7.58 | 98.73 | 110.10 |
| 78 | CA | 398 | G | O4'-C1'-N9 | 7.58 | 114.27 | 108.20 |
| 81 | DA | 788 | C | C3'-C2'-C1' | 7.58 | 107.56 | 101.50 |
| 81 | DA | 848 | A | O4'-C1'-N9 | 7.58 | 114.27 | 108.20 |
| 81 | DA | 228 | U | O4'-C1'-N1 | 7.58 | 114.26 | 108.20 |
| 81 | DA | 2719 | U | O4'-C1'-N1 | 7.58 | 114.26 | 108.20 |
| 1 | Aa | 59 | ARG | N-CA-CB | -7.58 | 96.96 | 110.60 |
| 24 | AX | 47 | PHE | CB-CG-CD2 | -7.58 | 115.50 | 120.80 |
| 78 | CA | 1505 | A | C5-C6-N1 | -7.58 | 113.91 | 117.70 |
| 81 | DA | 390 | G | O4'-C1'-N9 | 7.58 | 114.26 | 108.20 |
| 81 | DA | 671 | U | C5'-C4'-O4' | -7.58 | 100.01 | 109.10 |
| 78 | CA | 1791 | A | C3'-C2'-C1' | 7.58 | 107.56 | 101.50 |
| 81 | DA | 7 | C | O4'-C1'-C2' | -7.58 | 98.22 | 105.80 |
| 81 | DA | 135 | C | C1'-O4'-C4' | 7.58 | 115.96 | 109.90 |
| 81 | DA | 1609 | C | P-O3'-C3' | 7.58 | 128.79 | 119.70 |
| 78 | CA | 173 | A | P-O3'-C3' | -7.58 | 110.61 | 119.70 |
| 81 | DA | 1357 | G | P-O5'-C5' | 7.58 | 133.02 | 120.90 |
| 82 | DB | 40 | A | C1'-O4'-C4' | -7.58 | 103.84 | 109.90 |
| 5 | AC | 5 | PRO | N-CA-CB | 7.57 | 112.39 | 103.30 |
| 29 | AU | 33 | ALA | CB-CA-C | -7.57 | 98.74 | 110.10 |
| 35 | BG | 77 | ARG | CB-CA-C | -7.57 | 95.25 | 110.40 |
| 38 | Bs | 72 | ASP | N-CA-C | -7.57 | 90.55 | 111.00 |
| 78 | CA | 338 | C | N1-C1'-C2' | 7.57 | 123.84 | 114.00 |
| 78 | CA | 1772 | C | N1-C1'-C2' | 7.57 | 123.84 | 114.00 |
| 78 | CA | 1782 | A | P-O3'-C3' | -7.57 | 110.61 | 119.70 |
| 78 | CA | 496 | G | O3'-P-O5' | -7.57 | 89.61 | 104.00 |
| 78 | CA | 1558 | U | O4'-C4'-C3' | 7.57 | 112.16 | 106.10 |
| 81 | DA | 2879 | C | P-O5'-C5' | 7.57 | 133.01 | 120.90 |
| 81 | DA | 3299 | A | C5'-C4'-O4' | -7.57 | 100.01 | 109.10 |
| 81 | DA | 2530 | G | C3'-C2'-C1' | -7.57 | 95.44 | 101.50 |
| 78 | CA | 368 | U | C3'-C2'-C1' | -7.57 | 95.44 | 101.50 |
| 78 | CA | 1555 | A | O4'-C1'-N9 | 7.57 | 114.25 | 108.20 |
| 78 | CA | 1570 | A | C5'-C4'-C3' | 7.57 | 128.11 | 116.00 |
| 81 | DA | 1483 | G | C3'-C2'-C1' | -7.57 | 95.44 | 101.50 |
| 6 | AE | 197 | TYR | CB-CG-CD1 | -7.57 | 116.46 | 121.00 |
| 81 | DA | 1405 | U | O4'-C1'-N1 | 7.57 | 114.25 | 108.20 |
| 38 | Bs | 22 | TYR | CB-CG-CD1 | -7.57 | 116.46 | 121.00 |
| 33 | BD | 296 | GLN | N-CA-CB | 7.56 | 124.22 | 110.60 |
| 81 | DA | 907 | G | P-O3'-C3' | 7.56 | 128.78 | 119.70 |
| 78 | CA | 1054 | U | O4'-C1'-N1 | 7.56 | 114.25 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 418 | A | O4'-C1'-N9 | 7.56 | 114.25 | 108.20 |
| 81 | DA | 1795 | U | N1-C1'-C2' | -7.56 | 103.68 | 112.00 |
| 81 | DA | 2502 | A | C1'-O4'-C4' | 7.56 | 115.95 | 109.90 |
| 81 | DA | 241 | G | C3'-C2'-C1' | -7.56 | 95.45 | 101.50 |
| 81 | DA | 1560 | G | O3'-P-O5' | -7.56 | 89.63 | 104.00 |
| 81 | DA | 2728 | G | P-O3'-C3' | 7.56 | 128.77 | 119.70 |
| 20 | AS | 45 | MET | CA-C-N | 7.56 | 138.27 | 117.10 |
| 78 | CA | 485 | A | P-O3'-C3' | 7.56 | 128.77 | 119.70 |
| 78 | CA | 1542 | G | N9-C1'-C2' | -7.56 | 103.68 | 112.00 |
| 81 | DA | 708 | G | O4'-C1'-N9 | 7.56 | 114.25 | 108.20 |
| 9 | AH | 108 | ALA | N-CA-CB | 7.56 | 120.68 | 110.10 |
| 32 | BC | 209 | PHE | CB-CG-CD2 | -7.56 | 115.51 | 120.80 |
| 32 | BC | 364 | LYS | N-CA-CB | -7.56 | 97.00 | 110.60 |
| 81 | DA | 1603 | A | OP1-P-OP2 | -7.56 | 108.26 | 119.60 |
| 78 | CA | 113 | U | O4'-C1'-N1 | 7.56 | 114.25 | 108.20 |
| 81 | DA | 3296 | A | C2'-C3'-O3' | 7.56 | 126.12 | 109.50 |
| 13 | AL | 135 | LEU | CA-C-N | -7.55 | 100.58 | 117.20 |
| 35 | BG | 96 | VAL | CA-CB-CG1 | -7.55 | 99.57 | 110.90 |
| 81 | DA | 960 | U | O4'-C1'-N1 | 7.55 | 114.24 | 108.20 |
| 81 | DA | 1794 | G | N9-C1'-C2' | -7.55 | 103.69 | 112.00 |
| 42 | BM | 40 | LYS | O-C-N | -7.55 | 110.36 | 123.20 |
| 55 | Bc | 6 | ALA | CB-CA-C | 7.55 | 121.43 | 110.10 |
| 81 | DA | 1664 | G | C1'-O4'-C4' | -7.55 | 103.86 | 109.90 |
| 81 | DA | 1144 | U | C3'-C2'-C1' | 7.55 | 107.54 | 101.50 |
| 12 | AK | 59 | ALA | CA-C-O | -7.55 | 104.24 | 120.10 |
| 61 | Bj | 85 | PHE | CA-C-N | -7.55 | 100.59 | 117.20 |
| 81 | DA | 940 | G | O4'-C1'-N9 | 7.55 | 114.24 | 108.20 |
| 81 | DA | 1848 | G | O4'-C1'-N9 | -7.55 | 102.16 | 108.20 |
| 80 | CC | 18 | C | O4'-C1'-N1 | -7.55 | 102.16 | 108.20 |
| 81 | DA | 2163 | C | C1'-O4'-C4' | 7.55 | 115.94 | 109.90 |
| 81 | DA | 2761 | G | C5'-C4'-C3' | 7.55 | 128.08 | 116.00 |
| 59 | Bh | 12 | LYS | N-CA-CB | -7.55 | 97.02 | 110.60 |
| 79 | CB | 17 | G | C3'-C2'-C1' | 7.55 | 107.54 | 101.50 |
| 81 | DA | 3111 | U | N1-C1'-C2' | -7.55 | 103.70 | 112.00 |
| 81 | DA | 2482 | U | O4'-C1'-N1 | 7.54 | 114.24 | 108.20 |
| 59 | Bh | 20 | HIS | CA-C-O | -7.54 | 104.26 | 120.10 |
| 78 | CA | 1579 | U | P-O3'-C3' | -7.54 | 110.65 | 119.70 |
| 81 | DA | 2148 | U | O4'-C1'-N1 | 7.54 | 114.23 | 108.20 |
| 81 | DA | 3192 | U | P-O5'-C5' | 7.54 | 132.97 | 120.90 |
| 78 | CA | 195 | G | P-O3'-C3' | 7.54 | 128.75 | 119.70 |
| 81 | DA | 1212 | A | O4'-C1'-N9 | 7.54 | 114.23 | 108.20 |
| 81 | DA | 2774 | C | P-O3'-C3' | -7.54 | 110.65 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 3023 | U | O4'-C1'-N1 | 7.54 | 114.23 | 108.20 |
| 78 | CA | 1222 | C | C5'-C4'-C3' | -7.54 | 103.94 | 116.00 |
| 78 | CA | 377 | G | N9-C1'-C2' | -7.54 | 103.71 | 112.00 |
| 81 | DA | 1754 | G | C3'-C2'-C1' | -7.54 | 95.47 | 101.50 |
| 81 | DA | 2227 | C | O4'-C1'-N1 | 7.54 | 114.23 | 108.20 |
| 81 | DA | 2434 | U | C3'-C2'-C1' | 7.54 | 107.53 | 101.50 |
| 78 | CA | 520 | A | P-O3'-C3' | -7.54 | 110.66 | 119.70 |
| 78 | CA | 837 | G | O3'-P-O5' | -7.54 | 89.68 | 104.00 |
| 81 | DA | 889 | U | O4'-C1'-N1 | 7.54 | 114.23 | 108.20 |
| 78 | CA | 855 | A | O4'-C1'-C2' | 7.53 | 114.38 | 107.60 |
| 81 | DA | 489 | C | C3'-C2'-C1' | 7.53 | 107.53 | 101.50 |
| 82 | DB | 41 | A | C3'-C2'-C1' | -7.53 | 95.47 | 101.50 |
| 44 | BO | 139 | ARG | NE-CZ-NH1 | 7.53 | 124.07 | 120.30 |
| 81 | DA | 1701 | C | C5'-C4'-C3' | 7.53 | 128.05 | 116.00 |
| 35 | BG | 31 | ARG | NE-CZ-NH1 | 7.53 | 124.07 | 120.30 |
| 43 | BP | 63 | ARG | NE-CZ-NH1 | 7.53 | 124.07 | 120.30 |
| 81 | DA | 1210 | U | C3'-C2'-C1' | 7.53 | 107.53 | 101.50 |
| 81 | DA | 2130 | G | C5'-C4'-C3' | -7.53 | 103.95 | 116.00 |
| 39 | BJ | 77 | ALA | C-N-CA | 7.53 | 140.52 | 121.70 |
| 78 | CA | 1610 | G | C1'-O4'-C4' | -7.53 | 103.88 | 109.90 |
| 81 | DA | 3304 | U | O4'-C1'-C2' | -7.53 | 98.27 | 105.80 |
| 43 | BP | 129 | TYR | CB-CG-CD2 | -7.53 | 116.48 | 121.00 |
| 78 | CA | 31 | C | C3'-C2'-C1' | 7.53 | 107.52 | 101.50 |
| 78 | CA | 207 | U | O4'-C1'-N1 | 7.53 | 114.22 | 108.20 |
| 78 | CA | 637 | C | C3'-C2'-C1' | 7.53 | 107.52 | 101.50 |
| 81 | DA | 606 | C | C3'-C2'-C1' | -7.53 | 95.48 | 101.50 |
| 81 | DA | 2139 | A | N9-C1'-C2' | 7.53 | 123.78 | 114.00 |
| 17 | AQ | 25 | THR | C-N-CA | 7.53 | 140.52 | 121.70 |
| 81 | DA | 178 | U | O4'-C1'-N1 | 7.53 | 114.22 | 108.20 |
| 81 | DA | 1216 | C | O4'-C1'-C2' | -7.53 | 98.28 | 105.80 |
| 81 | DA | 2615 | G | O4'-C1'-N9 | 7.53 | 114.22 | 108.20 |
| 81 | DA | 3147 | G | N9-C1'-C2' | 7.53 | 123.78 | 114.00 |
| 14 | AM | 126 | ARG | N-CA-CB | 7.52 | 124.14 | 110.60 |
| 81 | DA | 744 | A | C5'-C4'-C3' | 7.52 | 128.04 | 116.00 |
| 81 | DA | 2486 | A | C2'-C3'-O3' | 7.52 | 126.05 | 109.50 |
| 81 | DA | 3121 | U | O4'-C1'-C2' | -7.52 | 98.28 | 105.80 |
| 78 | CA | 1790 | A | O4'-C1'-N9 | 7.52 | 114.22 | 108.20 |
| 81 | DA | 720 | A | C5'-C4'-C3' | 7.52 | 128.03 | 116.00 |
| 81 | DA | 1447 | G | O4'-C1'-N9 | -7.52 | 102.18 | 108.20 |
| 81 | DA | 1475 | A | C4'-C3'-C2' | -7.52 | 95.08 | 102.60 |
| 81 | DA | 2165 | G | O4'-C1'-C2' | 7.52 | 114.37 | 107.60 |
| 78 | CA | 1492 | A | P-O5'-C5' | 7.52 | 132.93 | 120.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1072 | G | P-O3'-C3' | 7.52 | 128.72 | 119.70 |
| 82 | DB | 88 | A | N9-C1'-C2' | -7.52 | 103.73 | 112.00 |
| 81 | DA | 53 | G | O4'-C1'-N9 | 7.52 | 114.22 | 108.20 |
| 81 | DA | 1757 | A | C5'-C4'-O4' | 7.52 | 118.12 | 109.10 |
| 81 | DA | 1869 | C | C3'-C2'-C1' | 7.52 | 107.52 | 101.50 |
| 78 | CA | 38 | C | P-O5'-C5' | 7.52 | 132.93 | 120.90 |
| 78 | CA | 497 | G | C5-C6-O6 | -7.52 | 124.09 | 128.60 |
| 51 | BZ | 23 | ARG | NE-CZ-NH2 | -7.52 | 116.54 | 120.30 |
| 81 | DA | 160 | G | O4'-C1'-N9 | 7.52 | 114.21 | 108.20 |
| 78 | CA | 223 | U | N1-C1'-C2' | -7.51 | 103.73 | 112.00 |
| 81 | DA | 491 | C | C3'-C2'-C1' | 7.51 | 107.51 | 101.50 |
| 81 | DA | 1472 | U | O4'-C1'-N1 | 7.51 | 114.21 | 108.20 |
| 64 | Bl | 62 | GLY | N-CA-C | 7.51 | 131.88 | 113.10 |
| 81 | DA | 1621 | A | P-O3'-C3' | 7.51 | 128.71 | 119.70 |
| 37 | BH | 73 | PRO | CA-N-CD | -7.51 | 100.99 | 111.50 |
| 81 | DA | 515 | C | N1-C1'-C2' | 7.51 | 123.76 | 114.00 |
| 81 | DA | 623 | U | O4'-C1'-N1 | 7.51 | 114.21 | 108.20 |
| 81 | DA | 996 | A | C1'-O4'-C4' | 7.51 | 115.91 | 109.90 |
| 81 | DA | 1296 | C | O3'-P-O5' | -7.51 | 89.73 | 104.00 |
| 81 | DA | 1360 | C | C1'-O4'-C4' | -7.51 | 103.89 | 109.90 |
| 58 | Bg | 6 | ASP | N-CA-CB | 7.51 | 124.11 | 110.60 |
| 78 | CA | 269 | G | C1'-O4'-C4' | -7.51 | 103.90 | 109.90 |
| 81 | DA | 359 | U | O4'-C1'-N1 | 7.51 | 114.20 | 108.20 |
| 81 | DA | 647 | A | P-O3'-C3' | 7.51 | 128.71 | 119.70 |
| 81 | DA | 1765 | U | P-O3'-C3' | 7.51 | 128.71 | 119.70 |
| 81 | DA | 3305 | A | O3'-P-O5' | -7.51 | 89.74 | 104.00 |
| 37 | BH | 130 | TYR | CB-CG-CD1 | 7.50 | 125.50 | 121.00 |
| 81 | DA | 330 | G | O4'-C1'-C2' | -7.50 | 98.30 | 105.80 |
| 81 | DA | 568 | G | O4'-C1'-N9 | 7.50 | 114.20 | 108.20 |
| 81 | DA | 706 | A | O4'-C1'-N9 | 7.50 | 114.20 | 108.20 |
| 81 | DA | 2574 | G | O4'-C1'-N9 | 7.50 | 114.20 | 108.20 |
| 22 | AV | 33 | LYS | CA-CB-CG | -7.50 | 96.89 | 113.40 |
| 76 | BS | 71 | PRO | N-CA-C | 7.50 | 131.60 | 112.10 |
| 83 | DC | 49 | G | O5'-C5'-C4' | -7.50 | 97.45 | 111.70 |
| 78 | CA | 37 | U | N1-C1'-C2' | -7.50 | 103.75 | 112.00 |
| 78 | CA | 947 | U | C1'-O4'-C4' | 7.50 | 115.90 | 109.90 |
| 81 | DA | 1233 | G | C3'-C2'-C1' | -7.50 | 95.50 | 101.50 |
| 81 | DA | 1258 | U | C5'-C4'-C3' | -7.50 | 104.00 | 116.00 |
| 81 | DA | 1565 | G | O4'-C1'-N9 | 7.50 | 114.20 | 108.20 |
| 82 | DB | 37 | A | P-O3'-C3' | 7.50 | 128.70 | 119.70 |
| 81 | DA | 264 | G | O4'-C1'-C2' | -7.50 | 98.30 | 105.80 |
| 81 | DA | 847 | A | P-O3'-C3' | 7.50 | 128.70 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2640 | A | C5'-C4'-O4' | 7.50 | 118.10 | 109.10 |
| 81 | DA | 2759 | U | O4'-C1'-C2' | -7.50 | 98.31 | 105.80 |
| 50 | BX | 29 | SER | N-CA-CB | 7.49 | 121.74 | 110.50 |
| 50 | BX | 56 | ARG | NE-CZ-NH1 | 7.49 | 124.05 | 120.30 |
| 78 | CA | 27 | U | O3'-P-O5' | 7.49 | 118.22 | 104.00 |
| 78 | CA | 509 | G | N1-C6-O6 | 7.49 | 124.39 | 119.90 |
| 81 | DA | 241 | G | O4'-C1'-C2' | 7.49 | 114.34 | 107.60 |
| 81 | DA | 535 | G | N9-C1'-C2' | 7.49 | 123.73 | 114.00 |
| 81 | DA | 798 | G | C5'-C4'-C3' | 7.49 | 127.97 | 116.00 |
| 81 | DA | 1279 | C | C3'-C2'-C1' | 7.49 | 107.49 | 101.50 |
| 81 | DA | 1842 | A | O4'-C1'-N9 | -7.49 | 102.21 | 108.20 |
| 81 | DA | 2153 | U | N1-C1'-C2' | 7.49 | 123.73 | 114.00 |
| 81 | DA | 1216 | C | C3'-C2'-C1' | 7.48 | 107.49 | 101.50 |
| 81 | DA | 2587 | U | O4'-C1'-N1 | 7.48 | 114.19 | 108.20 |
| 83 | DC | 105 | A | O4'-C1'-N9 | 7.48 | 114.19 | 108.20 |
| 46 | BT | 98 | ARG | NE-CZ-NH2 | 7.48 | 124.04 | 120.30 |
| 76 | BS | 123 | ILE | O-C-N | -7.48 | 110.73 | 122.70 |
| 78 | CA | 185 | U | O4'-C1'-N1 | 7.48 | 114.19 | 108.20 |
| 78 | CA | 553 | G | C1'-O4'-C4' | -7.48 | 103.91 | 109.90 |
| 81 | DA | 178 | U | P-O5'-C5' | 7.48 | 132.87 | 120.90 |
| 81 | DA | 516 | A | P-O5'-C5' | 7.48 | 132.87 | 120.90 |
| 81 | DA | 3236 | U | C1'-O4'-C4' | -7.48 | 103.92 | 109.90 |
| 82 | DB | 37 | A | O4'-C1'-N9 | 7.48 | 114.19 | 108.20 |
| 78 | CA | 30 | G | O4'-C1'-N9 | -7.48 | 102.22 | 108.20 |
| 78 | CA | 831 | U | C4'-C3'-C2' | 7.48 | 110.08 | 102.60 |
| 78 | CA | 1108 | G | P-O3'-C3' | 7.48 | 128.68 | 119.70 |
| 78 | CA | 1770 | U | N1-C1'-C2' | -7.48 | 103.77 | 112.00 |
| 81 | DA | 605 | U | O4'-C1'-C2' | -7.48 | 98.32 | 105.80 |
| 81 | DA | 270 | U | C1'-O4'-C4' | 7.48 | 115.88 | 109.90 |
| 33 | BD | 297 | SER | N-CA-CB | -7.48 | 99.28 | 110.50 |
| 49 | BV | 83 | TRP | CG-CD2-CE3 | -7.48 | 127.17 | 133.90 |
| 78 | CA | 477 | A | C3'-C2'-C1' | 7.48 | 107.48 | 101.50 |
| 78 | CA | 1674 | C | C3'-C2'-C1' | 7.48 | 107.48 | 101.50 |
| 78 | CA | 1 | U | O4'-C1'-N1 | 7.47 | 114.18 | 108.20 |
| 81 | DA | 2325 | G | O4'-C1'-N9 | 7.47 | 114.18 | 108.20 |
| 81 | DA | 2648 | G | O4'-C4'-C3' | -7.47 | 96.53 | 104.00 |
| 78 | CA | 571 | G | O4'-C1'-N9 | -7.47 | 102.22 | 108.20 |
| 78 | CA | 1362 | U | P-O3'-C3' | 7.47 | 128.67 | 119.70 |
| 81 | DA | 73 | C | C1'-O4'-C4' | 7.47 | 115.88 | 109.90 |
| 81 | DA | 1631 | C | C3'-C2'-C1' | 7.47 | 107.48 | 101.50 |
| 81 | DA | 1695 | U | C1'-O4'-C4' | 7.47 | 115.88 | 109.90 |
| 81 | DA | 2681 | U | C4'-C3'-C2' | -7.47 | 95.13 | 102.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 905 | U | O4'-C1'-N1 | 7.47 | 114.18 | 108.20 |
| 81 | DA | 1085 | A | O4'-C1'-C2' | -7.47 | 98.33 | 105.80 |
| 59 | Bh | 27 | ARG | CB-CA-C | -7.47 | 95.46 | 110.40 |
| 78 | CA | 1678 | A | P-O5'-C5' | 7.47 | 132.85 | 120.90 |
| 81 | DA | 31 | C | C3'-C2'-C1' | 7.47 | 107.47 | 101.50 |
| 81 | DA | 704 | U | C2'-C3'-O3' | 7.47 | 125.93 | 109.50 |
| 81 | DA | 767 | U | O4'-C4'-C3' | -7.47 | 96.53 | 104.00 |
| 81 | DA | 1601 | U | O4'-C1'-N1 | 7.47 | 114.18 | 108.20 |
| 81 | DA | 2536 | A | C5'-C4'-C3' | 7.47 | 127.95 | 116.00 |
| 81 | DA | 2989 | U | O4'-C1'-N1 | 7.47 | 114.18 | 108.20 |
| 81 | DA | 3113 | A | C3'-C2'-C1' | 7.47 | 107.48 | 101.50 |
| 78 | CA | 1440 | C | C3'-C2'-C1' | 7.47 | 107.47 | 101.50 |
| 41 | BN | 11 | ASN | C-N-CA | 7.47 | 140.37 | 121.70 |
| 81 | DA | 2543 | U | O4'-C1'-N1 | 7.47 | 114.17 | 108.20 |
| 45 | BR | 157 | PRO | CA-N-CD | -7.46 | 101.05 | 111.50 |
| 81 | DA | 214 | G | O4'-C1'-C2' | -7.46 | 98.33 | 105.80 |
| 78 | CA | 172 | C | C3'-C2'-C1' | 7.46 | 107.47 | 101.50 |
| 35 | BG | 78 | ARG | NE-CZ-NH2 | -7.46 | 116.57 | 120.30 |
| 67 | Bp | 37 | ARG | NE-CZ-NH2 | -7.46 | 116.57 | 120.30 |
| 38 | Bs | 101 | VAL | CG1-CB-CG2 | 7.46 | 122.83 | 110.90 |
| 81 | DA | 1270 | A | C3'-C2'-C1' | -7.46 | 95.53 | 101.50 |
| 81 | DA | 2085 | U | O4'-C1'-N1 | 7.46 | 114.17 | 108.20 |
| 5 | AC | 172 | VAL | CG1-CB-CG2 | 7.46 | 122.83 | 110.90 |
| 78 | CA | 880 | C | C3'-C2'-C1' | 7.46 | 107.47 | 101.50 |
| 81 | DA | 1057 | A | N9-C1'-C2' | -7.46 | 103.80 | 112.00 |
| 81 | DA | 1383 | G | O4'-C1'-N9 | 7.46 | 114.17 | 108.20 |
| 82 | DB | 104 | A | C3'-C2'-C1' | 7.46 | 107.47 | 101.50 |
| 20 | AS | 52 | GLY | O-C-N | 7.46 | 134.63 | 122.70 |
| 74 | BQ | 39 | GLN | O-C-N | -7.46 | 110.77 | 122.70 |
| 78 | CA | 502 | U | O4'-C1'-N1 | 7.46 | 114.17 | 108.20 |
| 81 | DA | 251 | G | C5'-C4'-C3' | 7.46 | 127.93 | 116.00 |
| 81 | DA | 1018 | G | O4'-C1'-C2' | -7.46 | 98.34 | 105.80 |
| 81 | DA | 1429 | G | P-O3'-C3' | 7.46 | 128.65 | 119.70 |
| 81 | DA | 2406 | C | C1'-O4'-C4' | 7.46 | 115.86 | 109.90 |
| 60 | Bi | 42 | PRO | O-C-N | -7.46 | 110.77 | 122.70 |
| 3 | AB | 78 | LYS | N-CA-C | -7.45 | 90.88 | 111.00 |
| 33 | BD | 354 | VAL | CA-C-O | -7.45 | 104.45 | 120.10 |
| 45 | BR | 14 | GLY | C-N-CA | 7.45 | 140.33 | 121.70 |
| 68 | Bq | 21 | ARG | NE-CZ-NH1 | 7.45 | 124.03 | 120.30 |
| 78 | CA | 1749 | A | O4'-C1'-C2' | -7.45 | 98.35 | 105.80 |
| 81 | DA | 2854 | U | C5'-C4'-C3' | -7.45 | 104.08 | 116.00 |
| 81 | DA | 3348 | G | C5'-C4'-C3' | 7.45 | 127.92 | 116.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 33 | BD | 341 | SER | CB-CA-C | -7.45 | 95.94 | 110.10 |
| 78 | CA | 199 | G | P-O3'-C3' | 7.45 | 128.64 | 119.70 |
| 81 | DA | 907 | G | C1'-O4'-C4' | -7.45 | 103.94 | 109.90 |
| 81 | DA | 2452 | G | C1'-O4'-C4' | 7.45 | 115.86 | 109.90 |
| 29 | AU | 63 | GLN | N-CA-CB | 7.45 | 124.01 | 110.60 |
| 78 | CA | 1295 | G | C5'-C4'-C3' | 7.45 | 127.92 | 116.00 |
| 81 | DA | 874 | U | N1-C1'-C2' | 7.45 | 123.69 | 114.00 |
| 81 | DA | 2162 | U | O4'-C1'-N1 | 7.45 | 114.16 | 108.20 |
| 81 | DA | 2873 | U | N1-C1'-C2' | 7.45 | 123.68 | 114.00 |
| 81 | DA | 2945 | G | O4'-C1'-N9 | 7.45 | 114.16 | 108.20 |
| 81 | DA | 1755 | C | O4'-C1'-N1 | 7.45 | 114.16 | 108.20 |
| 81 | DA | 3003 | G | P-O3'-C3' | 7.45 | 128.64 | 119.70 |
| 57 | Be | 208 | SER | N-CA-CB | 7.45 | 121.67 | 110.50 |
| 78 | CA | 1674 | C | P-O5'-C5' | 7.45 | 132.82 | 120.90 |
| 81 | DA | 2481 | G | C3'-C2'-C1' | 7.45 | 107.46 | 101.50 |
| 43 | BP | 21 | PHE | CB-CG-CD1 | 7.45 | 126.01 | 120.80 |
| 81 | DA | 864 | G | O4'-C1'-N9 | 7.45 | 114.16 | 108.20 |
| 81 | DA | 1758 | G | C5-C6-O6 | -7.45 | 124.13 | 128.60 |
| 81 | DA | 1889 | G | C4'-C3'-C2' | -7.45 | 95.16 | 102.60 |
| 83 | DC | 100 | A | P-O3'-C3' | 7.45 | 128.63 | 119.70 |
| 83 | DC | 57 | C | C3'-C2'-C1' | 7.44 | 107.45 | 101.50 |
| 44 | BO | 21 | ARG | NE-CZ-NH2 | -7.44 | 116.58 | 120.30 |
| 57 | Be | 85 | PHE | CB-CG-CD1 | 7.44 | 126.01 | 120.80 |
| 78 | CA | 204 | G | C1'-O4'-C4' | -7.44 | 103.94 | 109.90 |
| 78 | CA | 643 | G | O4'-C1'-N9 | 7.44 | 114.16 | 108.20 |
| 81 | DA | 1250 | G | P-O3'-C3' | -7.44 | 110.77 | 119.70 |
| 81 | DA | 186 | U | N1-C1'-C2' | -7.44 | 103.81 | 112.00 |
| 81 | DA | 841 | A | C1'-O4'-C4' | -7.44 | 103.95 | 109.90 |
| 81 | DA | 869 | G | O4'-C1'-N9 | 7.44 | 114.15 | 108.20 |
| 81 | DA | 1409 | G | C3'-C2'-C1' | -7.44 | 95.55 | 101.50 |
| 83 | DC | 58 | U | O4'-C1'-N1 | 7.44 | 114.15 | 108.20 |
| 81 | DA | 1786 | G | P-O3'-C3' | -7.44 | 110.77 | 119.70 |
| 26 | AZ | 5 | HIS | N-CA-CB | 7.44 | 123.99 | 110.60 |
| 31 | BB | 21 | ARG | NE-CZ-NH1 | 7.44 | 124.02 | 120.30 |
| 78 | CA | 645 | C | O4'-C1'-N1 | 7.44 | 114.15 | 108.20 |
| 81 | DA | 838 | G | N9-C1'-C2' | -7.44 | 103.82 | 112.00 |
| 81 | DA | 1420 | C | P-O3'-C3' | 7.44 | 128.62 | 119.70 |
| 82 | DB | 87 | G | P-O3'-C3' | 7.44 | 128.63 | 119.70 |
| 9 | AH | 107 | SER | N-CA-CB | 7.44 | 121.65 | 110.50 |
| 81 | DA | 1035 | G | O4'-C1'-N9 | 7.44 | 114.15 | 108.20 |
| 44 | BO | 21 | ARG | CA-C-N | 7.43 | 133.56 | 117.20 |
| 79 | CB | 68 | C | N1-C1'-C2' | 7.43 | 123.66 | 114.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1295 | G | P-O3'-C3' | -7.43 | 110.78 | 119.70 |
| 81 | DA | 1378 | U | P-O5'-C5' | 7.43 | 132.80 | 120.90 |
| 81 | DA | 2625 | C | P-O3'-C3' | 7.43 | 128.62 | 119.70 |
| 81 | DA | 2245 | C | N1-C1'-C2' | 7.43 | 123.66 | 114.00 |
| 83 | DC | 53 | U | O4'-C1'-N1 | -7.43 | 102.25 | 108.20 |
| 78 | CA | 573 | C | C3'-C2'-O2' | -7.43 | 91.76 | 113.30 |
| 78 | CA | 1460 | A | P-O3'-C3' | 7.43 | 128.61 | 119.70 |
| 81 | DA | 2971 | A | O4'-C1'-C2' | -7.43 | 98.37 | 105.80 |
| 55 | Bc | 41 | LEU | CA-C-N | 7.43 | 137.90 | 117.10 |
| 55 | Bc | 67 | ARG | NE-CZ-NH1 | 7.43 | 124.01 | 120.30 |
| 81 | DA | 1826 | C | C4'-C3'-C2' | -7.43 | 95.17 | 102.60 |
| 83 | DC | 67 | C | N1-C1'-C2' | 7.43 | 123.66 | 114.00 |
| 18 | AP | 99 | ARG | NE-CZ-NH2 | -7.42 | 116.59 | 120.30 |
| 78 | CA | 253 | A | C5'-C4'-O4' | 7.42 | 118.01 | 109.10 |
| 78 | CA | 869 | A | C4'-C3'-C2' | -7.42 | 95.17 | 102.60 |
| 81 | DA | 1082 | U | C3'-C2'-C1' | 7.42 | 107.44 | 101.50 |
| 78 | CA | 411 | C | N1-C1'-C2' | -7.42 | 103.83 | 112.00 |
| 81 | DA | 2101 | C | P-O3'-C3' | -7.42 | 110.79 | 119.70 |
| 58 | Bg | 31 | ARG | NE-CZ-NH2 | -7.42 | 116.59 | 120.30 |
| 78 | CA | 46 | A | C5'-C4'-C3' | -7.42 | 104.13 | 116.00 |
| 81 | DA | 2052 | G | O4'-C1'-N9 | 7.42 | 114.14 | 108.20 |
| 36 | BF | 62 | ARG | NE-CZ-NH1 | 7.42 | 124.01 | 120.30 |
| 2 | AA | 250 | VAL | CA-CB-CG2 | 7.42 | 122.03 | 110.90 |
| 40 | BK | 199 | TYR | CB-CG-CD2 | -7.42 | 116.55 | 121.00 |
| 81 | DA | 1562 | C | C4'-C3'-C2' | -7.42 | 95.18 | 102.60 |
| 81 | DA | 2465 | G | C1'-O4'-C4' | -7.42 | 103.97 | 109.90 |
| 81 | DA | 2684 | C | C3'-C2'-C1' | 7.42 | 107.44 | 101.50 |
| 78 | CA | 1602 | C | O4'-C1'-C2' | -7.42 | 98.38 | 105.80 |
| 81 | DA | 530 | G | P-O3'-C3' | -7.42 | 110.80 | 119.70 |
| 81 | DA | 2376 | G | O3'-P-O5' | -7.42 | 89.91 | 104.00 |
| 6 | AE | 25 | ARG | NE-CZ-NH1 | 7.42 | 124.01 | 120.30 |
| 78 | CA | 416 | A | O4'-C1'-C2' | -7.42 | 98.39 | 105.80 |
| 78 | CA | 1406 | A | O4'-C1'-N9 | 7.42 | 114.13 | 108.20 |
| 81 | DA | 32 | U | P-O3'-C3' | 7.42 | 128.60 | 119.70 |
| 1 | Aa | 56 | VAL | O-C-N | -7.41 | 107.01 | 121.10 |
| 45 | BR | 124 | LEU | CB-CG-CD1 | 7.41 | 123.60 | 111.00 |
| 60 | Bi | 80 | ARG | N-CA-CB | 7.41 | 123.94 | 110.60 |
| 81 | DA | 490 | A | O4'-C1'-N9 | 7.41 | 114.13 | 108.20 |
| 81 | DA | 1631 | C | N1-C1'-C2' | 7.41 | 123.64 | 114.00 |
| 81 | DA | 1958 | U | O4'-C1'-N1 | 7.41 | 114.13 | 108.20 |
| 78 | CA | 155 | U | P-O3'-C3' | 7.41 | 128.59 | 119.70 |
| 81 | DA | 312 | C | C3'-C2'-C1' | 7.41 | 107.43 | 101.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 83 | DC | 9 | C | P-O5'-C5' | 7.41 | 132.76 | 120.90 |
| 78 | CA | 1086 | A | P-O3'-C3' | -7.41 | 110.81 | 119.70 |
| 81 | DA | 270 | U | O4'-C1'-N1 | 7.41 | 114.13 | 108.20 |
| 81 | DA | 2257 | C | C3'-C2'-C1' | -7.41 | 95.57 | 101.50 |
| 81 | DA | 2463 | G | N9-C1'-C2' | -7.41 | 103.85 | 112.00 |
| 78 | CA | 1136 | U | C3'-C2'-C1' | 7.41 | 107.43 | 101.50 |
| 81 | DA | 2160 | G | C1'-O4'-C4' | -7.41 | 103.97 | 109.90 |
| 81 | DA | 3327 | G | P-O3'-C3' | 7.41 | 128.59 | 119.70 |
| 68 | Bq | 2 | ARG | NE-CZ-NH2 | 7.41 | 124.00 | 120.30 |
| 81 | DA | 3013 | U | C1'-O4'-C4' | -7.41 | 103.97 | 109.90 |
| 3 | AB | 40 | ARG | NE-CZ-NH2 | -7.41 | 116.60 | 120.30 |
| 3 | AB | 152 | PHE | N-CA-CB | 7.41 | 123.93 | 110.60 |
| 32 | BC | 196 | ARG | NE-CZ-NH1 | 7.41 | 124.00 | 120.30 |
| 49 | BV | 21 | TYR | CB-CG-CD1 | 7.41 | 125.44 | 121.00 |
| 78 | CA | 1271 | G | O4'-C1'-N9 | 7.41 | 114.12 | 108.20 |
| 81 | DA | 162 | G | C5'-C4'-O4' | -7.41 | 100.21 | 109.10 |
| 81 | DA | 1488 | G | O4'-C1'-C2' | 7.41 | 114.27 | 107.60 |
| 81 | DA | 2707 | C | C5'-C4'-C3' | -7.41 | 104.15 | 116.00 |
| 15 | AN | 38 | ILE | N-CA-CB | 7.40 | 127.83 | 110.80 |
| 78 | CA | 256 | A | P-O5'-C5' | 7.40 | 132.75 | 120.90 |
| 81 | DA | 1316 | C | C1'-O4'-C4' | -7.40 | 103.98 | 109.90 |
| 81 | DA | 3215 | A | C1'-C2'-O2' | -7.40 | 88.39 | 110.60 |
| 59 | Bh | 44 | ARG | NE-CZ-NH1 | 7.40 | 124.00 | 120.30 |
| 78 | CA | 1213 | G | O4'-C1'-N9 | 7.40 | 114.12 | 108.20 |
| 81 | DA | 1267 | U | O4'-C1'-N1 | 7.40 | 114.12 | 108.20 |
| 81 | DA | 3100 | U | P-O5'-C5' | 7.40 | 132.74 | 120.90 |
| 82 | DB | 91 | C | O4'-C1'-N1 | 7.40 | 114.12 | 108.20 |
| 2 | AA | 185 | ARG | N-CA-CB | 7.40 | 123.92 | 110.60 |
| 17 | AQ | 29 | GLN | N-CA-CB | 7.40 | 123.92 | 110.60 |
| 78 | CA | 1377 | U | O4'-C1'-N1 | 7.40 | 114.12 | 108.20 |
| 81 | DA | 1891 | A | O4'-C1'-N9 | 7.40 | 114.12 | 108.20 |
| 81 | DA | 3337 | G | O4'-C1'-C2' | 7.40 | 114.26 | 107.60 |
| 52 | BY | 90 | VAL | CG1-CB-CG2 | 7.40 | 122.74 | 110.90 |
| 81 | DA | 3131 | U | O4'-C1'-C2' | -7.40 | 98.40 | 105.80 |
| 81 | DA | 266 | A | C5'-C4'-O4' | 7.40 | 117.98 | 109.10 |
| 81 | DA | 2895 | G | C1'-O4'-C4' | -7.40 | 103.98 | 109.90 |
| 78 | CA | 825 | U | O4'-C1'-N1 | 7.40 | 114.12 | 108.20 |
| 8 | AF | 99 | MET | CG-SD-CE | -7.39 | 88.37 | 100.20 |
| 9 | AH | 85 | ASP | CB-CG-OD1 | -7.39 | 111.64 | 118.30 |
| 81 | DA | 676 | G | N9-C1'-C2' | -7.39 | 103.87 | 112.00 |
| 81 | DA | 1087 | G | P-O3'-C3' | -7.39 | 110.83 | 119.70 |
| 1 | Aa | 61 | PHE | CB-CG-CD1 | -7.39 | 115.62 | 120.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 74 | BQ | 123 | GLU | CB-CA-C | -7.39 | 95.61 | 110.40 |
| 78 | CA | 179 | A | O4'-C1'-C2' | -7.39 | 98.41 | 105.80 |
| 78 | CA | 1155 | G | O4'-C1'-N9 | 7.39 | 114.11 | 108.20 |
| 78 | CA | 1222 | C | C4'-C3'-C2' | -7.39 | 95.21 | 102.60 |
| 81 | DA | 1760 | A | O4'-C1'-N9 | 7.39 | 114.11 | 108.20 |
| 81 | DA | 3372 | A | O3'-P-O5' | 7.39 | 118.04 | 104.00 |
| 81 | DA | 720 | A | N9-C1'-C2' | -7.39 | 103.87 | 112.00 |
| 78 | CA | 564 | G | C5-C6-O6 | -7.39 | 124.17 | 128.60 |
| 81 | DA | 268 | A | O4'-C1'-C2' | -7.39 | 98.41 | 105.80 |
| 43 | BP | 42 | PRO | O-C-N | -7.38 | 110.89 | 122.70 |
| 78 | CA | 659 | C | P-O5'-C5' | 7.38 | 132.72 | 120.90 |
| 81 | DA | 139 | G | O4'-C1'-N9 | 7.38 | 114.11 | 108.20 |
| 81 | DA | 1867 | A | N9-C1'-C2' | -7.38 | 103.88 | 112.00 |
| 81 | DA | 2763 | U | P-O5'-C5' | 7.38 | 132.71 | 120.90 |
| 8 | AF | 65 | ARG | NE-CZ-NH2 | -7.38 | 116.61 | 120.30 |
| 31 | BB | 30 | ARG | NE-CZ-NH1 | 7.38 | 123.99 | 120.30 |
| 81 | DA | 2249 | G | O3'-P-O5' | 7.38 | 118.03 | 104.00 |
| 81 | DA | 848 | A | C1'-O4'-C4' | -7.38 | 104.00 | 109.90 |
| 81 | DA | 1342 | C | O4'-C1'-N1 | 7.38 | 114.11 | 108.20 |
| 78 | CA | 903 | U | P-O5'-C5' | -7.38 | 109.09 | 120.90 |
| 17 | AQ | 92 | ASP | N-CA-C | -7.38 | 91.08 | 111.00 |
| 35 | BG | 78 | ARG | NE-CZ-NH1 | 7.38 | 123.99 | 120.30 |
| 59 | Bh | 92 | TYR | CB-CG-CD1 | 7.38 | 125.43 | 121.00 |
| 78 | CA | 44 | U | O4'-C1'-N1 | 7.38 | 114.10 | 108.20 |
| 18 | AP | 119 | VAL | CB-CA-C | 7.38 | 125.41 | 111.40 |
| 35 | BG | 152 | THR | N-CA-C | -7.37 | 91.09 | 111.00 |
| 78 | CA | 402 | C | C3'-C2'-C1' | 7.37 | 107.40 | 101.50 |
| 78 | CA | 1677 | C | O4'-C1'-N1 | 7.37 | 114.10 | 108.20 |
| 81 | DA | 2576 | G | C5-C6-O6 | -7.37 | 124.18 | 128.60 |
| 82 | DB | 72 | A | O3'-P-O5' | -7.37 | 89.99 | 104.00 |
| 33 | BD | 89 | ALA | N-CA-CB | -7.37 | 99.78 | 110.10 |
| 78 | CA | 1751 | C | N1-C1'-C2' | 7.37 | 123.58 | 114.00 |
| 81 | DA | 766 | U | P-O3'-C3' | 7.37 | 128.54 | 119.70 |
| 81 | DA | 1620 | U | C5'-C4'-O4' | -7.37 | 100.25 | 109.10 |
| 81 | DA | 1699 | A | O4'-C4'-C3' | -7.37 | 96.63 | 104.00 |
| 78 | CA | 254 | A | C1'-O4'-C4' | 7.37 | 115.79 | 109.90 |
| 78 | CA | 371 | G | O4'-C1'-N9 | 7.37 | 114.09 | 108.20 |
| 81 | DA | 190 | U | O4'-C1'-N1 | 7.37 | 114.09 | 108.20 |
| 81 | DA | 1743 | G | N9-C1'-C2' | 7.37 | 123.58 | 114.00 |
| 81 | DA | 2783 | U | N1-C1'-C2' | -7.37 | 103.89 | 112.00 |
| 81 | DA | 1250 | G | C4'-C3'-C2' | -7.37 | 95.23 | 102.60 |
| 83 | DC | 55 | A | C3'-C2'-C1' | 7.37 | 107.39 | 101.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 10 | C | C5'-C4'-C3' | 7.37 | 127.78 | 116.00 |
| 81 | DA | 2439 | A | N9-C1'-C2' | 7.37 | 123.58 | 114.00 |
| 81 | DA | 2987 | A | C5'-C4'-C3' | -7.37 | 104.21 | 116.00 |
| 81 | DA | 149 | U | O5'-P-OP1 | 7.36 | 119.54 | 110.70 |
| 3 | AB | 143 | ARG | NE-CZ-NH1 | -7.36 | 116.62 | 120.30 |
| 81 | DA | 238 | A | P-O5'-C5' | 7.36 | 132.68 | 120.90 |
| 81 | DA | 311 | C | C3'-C2'-C1' | 7.36 | 107.39 | 101.50 |
| 81 | DA | 381 | U | O4'-C1'-N1 | 7.36 | 114.09 | 108.20 |
| 81 | DA | 424 | G | C3'-C2'-C1' | 7.36 | 107.39 | 101.50 |
| 81 | DA | 2720 | G | O4'-C1'-N9 | -7.36 | 102.31 | 108.20 |
| 83 | DC | 114 | A | O5'-C5'-C4' | 7.36 | 125.68 | 111.70 |
| 63 | Bm | 37 | TYR | CB-CG-CD1 | -7.36 | 116.59 | 121.00 |
| 81 | DA | 1105 | A | C1'-O4'-C4' | 7.36 | 115.79 | 109.90 |
| 82 | DB | 108 | C | C3'-C2'-C1' | 7.36 | 107.39 | 101.50 |
| 78 | CA | 191 | C | C3'-C2'-C1' | 7.35 | 107.38 | 101.50 |
| 81 | DA | 1570 | U | P-O3'-C3' | 7.35 | 128.52 | 119.70 |
| 81 | DA | 2520 | A | O4'-C1'-C2' | -7.35 | 98.45 | 105.80 |
| 40 | BK | 178 | VAL | CA-C-O | -7.35 | 104.66 | 120.10 |
| 78 | CA | 87 | C | O4'-C1'-C2' | -7.35 | 98.45 | 105.80 |
| 78 | CA | 1228 | G | N9-C1'-C2' | 7.35 | 123.56 | 114.00 |
| 81 | DA | 885 | U | P-O5'-C5' | 7.35 | 132.66 | 120.90 |
| 81 | DA | 1278 | A | P-O3'-C3' | 7.35 | 128.52 | 119.70 |
| 81 | DA | 3382 | U | O3'-P-O5' | -7.35 | 90.03 | 104.00 |
| 81 | DA | 669 | U | O4'-C1'-N1 | 7.35 | 114.08 | 108.20 |
| 59 | Bh | 43 | ARG | NE-CZ-NH2 | -7.35 | 116.62 | 120.30 |
| 78 | CA | 684 | A | C3'-C2'-C1' | 7.35 | 107.38 | 101.50 |
| 80 | CC | 19 | U | C2-N1-C1' | 7.35 | 126.52 | 117.70 |
| 81 | DA | 1422 | G | C3'-C2'-C1' | -7.35 | 95.62 | 101.50 |
| 81 | DA | 2067 | U | O4'-C1'-C2' | -7.35 | 98.45 | 105.80 |
| 81 | DA | 2372 | A | O4'-C1'-C2' | -7.35 | 98.45 | 105.80 |
| 81 | DA | 2450 | G | O3'-P-O5' | -7.35 | 90.04 | 104.00 |
| 78 | CA | 1661 | U | O4'-C1'-N1 | 7.35 | 114.08 | 108.20 |
| 78 | CA | 1497 | U | O4'-C1'-N1 | 7.35 | 114.08 | 108.20 |
| 13 | AL | 40 | SER | N-CA-C | -7.34 | 91.17 | 111.00 |
| 78 | CA | 828 | U | O4'-C1'-N1 | 7.34 | 114.08 | 108.20 |
| 78 | CA | 1280 | C | O4'-C1'-C2' | -7.34 | 98.46 | 105.80 |
| 81 | DA | 1679 | A | O4'-C4'-C3' | -7.34 | 96.66 | 104.00 |
| 81 | DA | 2316 | G | N9-C1'-C2' | 7.34 | 123.55 | 114.00 |
| 82 | DB | 97 | A | OP1-P-O3' | 7.34 | 121.35 | 105.20 |
| 81 | DA | 247 | C | O4'-C1'-C2' | -7.34 | 98.46 | 105.80 |
| 81 | DA | 682 | U | O4'-C1'-C2' | -7.34 | 98.46 | 105.80 |
| 81 | DA | 1438 | U | O4'-C1'-N1 | 7.34 | 114.07 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2275 | A | C1'-O4'-C4' | -7.34 | 104.03 | 109.90 |
| 81 | DA | 2945 | G | O4'-C1'-C2' | 7.34 | 114.21 | 107.60 |
| 49 | BV | 122 | ALA | CB-CA-C | 7.34 | 121.11 | 110.10 |
| 66 | Bo | 41 | ARG | CA-C-N | 7.34 | 133.34 | 117.20 |
| 36 | BF | 31 | ARG | NE-CZ-NH2 | -7.34 | 116.63 | 120.30 |
| 78 | CA | 1245 | G | O4'-C1'-N9 | 7.34 | 114.07 | 108.20 |
| 78 | CA | 1724 | U | O3'-P-O5' | -7.34 | 90.06 | 104.00 |
| 81 | DA | 242 | C | C1'-O4'-C4' | -7.34 | 104.03 | 109.90 |
| 81 | DA | 1379 | G | O4'-C1'-C2' | 7.34 | 114.20 | 107.60 |
| 30 | BA | 54 | LYS | CB-CA-C | 7.33 | 125.07 | 110.40 |
| 34 | BE | 52 | TYR | CD1-CG-CD2 | -7.33 | 109.83 | 117.90 |
| 81 | DA | 1742 | U | C3'-C2'-C1' | 7.33 | 107.37 | 101.50 |
| 81 | DA | 1996 | C | C1'-O4'-C4' | 7.33 | 115.77 | 109.90 |
| 4 | AD | 77 | ARG | NE-CZ-NH1 | 7.33 | 123.97 | 120.30 |
| 78 | CA | 1426 | C | N3-C4-C5 | -7.33 | 118.97 | 121.90 |
| 78 | CA | 47 | A | P-O5'-C5' | 7.33 | 132.63 | 120.90 |
| 78 | CA | 608 | U | O4'-C1'-N1 | 7.33 | 114.06 | 108.20 |
| 81 | DA | 658 | G | C3'-C2'-C1' | -7.33 | 95.64 | 101.50 |
| 78 | CA | 1505 | A | C4-C5-C6 | 7.33 | 120.67 | 117.00 |
| 81 | DA | 1690 | C | O5'-P-OP2 | -7.33 | 99.10 | 105.70 |
| 29 | AU | 72 | PHE | N-CA-C | 7.33 | 130.78 | 111.00 |
| 62 | Bk | 41 | ARG | NE-CZ-NH2 | -7.33 | 116.64 | 120.30 |
| 81 | DA | 1111 | U | O4'-C1'-N1 | 7.33 | 114.06 | 108.20 |
| 81 | DA | 1154 | A | O4'-C1'-N9 | 7.33 | 114.06 | 108.20 |
| 81 | DA | 1162 | U | O3'-P-O5' | -7.33 | 90.08 | 104.00 |
| 9 | AH | 28 | ARG | CD-NE-CZ | 7.33 | 133.86 | 123.60 |
| 81 | DA | 489 | C | N1-C1'-C2' | 7.33 | 123.53 | 114.00 |
| 78 | CA | 26 | A | O4'-C1'-N9 | 7.33 | 114.06 | 108.20 |
| 78 | CA | 127 | G | O4'-C1'-N9 | 7.33 | 114.06 | 108.20 |
| 81 | DA | 2494 | A | P-O5'-C5' | 7.33 | 132.62 | 120.90 |
| 81 | DA | 2646 | C | N1-C1'-C2' | 7.33 | 123.52 | 114.00 |
| 81 | DA | 2667 | A | P-O3'-C3' | -7.33 | 110.91 | 119.70 |
| 81 | DA | 3096 | C | N1-C1'-C2' | 7.33 | 123.52 | 114.00 |
| 78 | CA | 840 | U | P-O5'-C5' | 7.32 | 132.62 | 120.90 |
| 78 | CA | 956 | C | N1-C1'-C2' | 7.32 | 123.52 | 114.00 |
| 81 | DA | 3011 | A | C3'-C2'-C1' | 7.32 | 107.36 | 101.50 |
| 81 | DA | 693 | A | O4'-C1'-C2' | -7.32 | 98.48 | 105.80 |
| 81 | DA | 975 | C | O4'-C1'-N1 | 7.32 | 114.06 | 108.20 |
| 81 | DA | 2211 | U | P-O3'-C3' | 7.32 | 128.49 | 119.70 |
| 78 | CA | 858 | G | N9-C1'-C2' | -7.32 | 103.95 | 112.00 |
| 78 | CA | 1545 | A | O3'-P-O5' | -7.32 | 90.09 | 104.00 |
| 81 | DA | 1126 | G | O4'-C1'-N9 | 7.32 | 114.06 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 309 | U | C5'-C4'-C3' | 7.32 | 127.71 | 116.00 |
| 1 | Aa | 57 | PRO | CB-CA-C | 7.32 | 130.29 | 112.00 |
| 22 | AV | 27 | TRP | N-CA-CB | 7.32 | 123.77 | 110.60 |
| 33 | BD | 353 | ALA | N-CA-C | 7.32 | 130.76 | 111.00 |
| 81 | DA | 43 | A | N9-C1'-C2' | -7.32 | 103.95 | 112.00 |
| 81 | DA | 1219 | C | O4'-C1'-N1 | 7.32 | 114.05 | 108.20 |
| 3 | AB | 117 | ARG | NE-CZ-NH1 | -7.32 | 116.64 | 120.30 |
| 78 | CA | 1246 | C | P-O3'-C3' | 7.32 | 128.48 | 119.70 |
| 81 | DA | 218 | G | N9-C1'-C2' | -7.32 | 103.95 | 112.00 |
| 81 | DA | 1994 | G | O4'-C1'-N9 | 7.32 | 114.05 | 108.20 |
| 81 | DA | 1769 | G | C5-C6-O6 | -7.31 | 124.21 | 128.60 |
| 81 | DA | 3097 | C | P-O3'-C3' | 7.31 | 128.48 | 119.70 |
| 78 | CA | 1433 | G | C3'-C2'-C1' | 7.31 | 107.35 | 101.50 |
| 81 | DA | 607 | A | O4'-C1'-N9 | 7.31 | 114.05 | 108.20 |
| 81 | DA | 686 | G | O4'-C1'-N9 | 7.31 | 114.05 | 108.20 |
| 81 | DA | 3215 | A | P-O3'-C3' | 7.31 | 128.48 | 119.70 |
| 81 | DA | 3281 | U | P-O3'-C3' | 7.31 | 128.47 | 119.70 |
| 78 | CA | 1476 | C | O4'-C4'-C3' | -7.31 | 96.69 | 104.00 |
| 80 | CC | 17 | A | N9-C1'-C2' | 7.31 | 123.50 | 114.00 |
| 81 | DA | 2637 | A | C3'-C2'-C1' | -7.31 | 95.65 | 101.50 |
| 81 | DA | 2709 | C | C3'-C2'-C1' | 7.31 | 107.35 | 101.50 |
| 17 | AQ | 63 | LYS | CB-CA-C | -7.31 | 95.78 | 110.40 |
| 81 | DA | 1206 | G | P-O5'-C5' | 7.31 | 132.59 | 120.90 |
| 81 | DA | 1713 | G | C1'-O4'-C4' | -7.31 | 104.05 | 109.90 |
| 40 | BK | 112 | TYR | CB-CG-CD2 | -7.30 | 116.62 | 121.00 |
| 78 | CA | 1722 | A | C5'-C4'-C3' | 7.30 | 127.69 | 116.00 |
| 81 | DA | 2528 | G | C1'-O4'-C4' | 7.30 | 115.74 | 109.90 |
| 83 | DC | 48 | U | O4'-C1'-C2' | 7.30 | 114.17 | 107.60 |
| 29 | AU | 63 | GLN | CB-CA-C | -7.30 | 95.80 | 110.40 |
| 78 | CA | 908 | U | O4'-C1'-N1 | 7.30 | 114.04 | 108.20 |
| 74 | BQ | 158 | ARG | CA-C-N | 7.30 | 133.26 | 117.20 |
| 78 | CA | 508 | U | P-O3'-C3' | 7.30 | 128.46 | 119.70 |
| 81 | DA | 41 | G | O4'-C1'-N9 | 7.30 | 114.04 | 108.20 |
| 81 | DA | 1535 | A | O3'-P-O5' | -7.30 | 90.13 | 104.00 |
| 81 | DA | 1662 | G | P-O5'-C5' | 7.30 | 132.58 | 120.90 |
| 78 | CA | 582 | U | O4'-C1'-N1 | 7.30 | 114.04 | 108.20 |
| 78 | CA | 1367 | G | O5'-C5'-C4' | 7.30 | 125.57 | 111.70 |
| 78 | CA | 1557 | U | O4'-C1'-N1 | 7.30 | 114.04 | 108.20 |
| 81 | DA | 758 | C | C4'-C3'-C2' | -7.30 | 95.30 | 102.60 |
| 81 | DA | 2351 | U | P-O3'-C3' | -7.30 | 110.94 | 119.70 |
| 81 | DA | 3131 | U | O3'-P-O5' | -7.30 | 90.13 | 104.00 |
| 43 | BP | 51 | LEU | C-N-CA | 7.30 | 137.63 | 122.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 179 | A | P-O3'-C3' | 7.30 | 128.46 | 119.70 |
| 81 | DA | 2723 | U | C3'-C2'-C1' | 7.30 | 107.34 | 101.50 |
| 5 | AC | 157 | ASP | CB-CA-C | -7.30 | 95.81 | 110.40 |
| 38 | Bs | 61 | ARG | NE-CZ-NH2 | -7.30 | 116.65 | 120.30 |
| 81 | DA | 2439 | A | O4'-C1'-N9 | -7.30 | 102.36 | 108.20 |
| 63 | Bm | 6 | LYS | N-CA-CB | 7.29 | 123.73 | 110.60 |
| 4 | AD | 205 | PHE | CB-CG-CD2 | -7.29 | 115.69 | 120.80 |
| 36 | BF | 2 | LYS | N-CA-CB | -7.29 | 97.47 | 110.60 |
| 81 | DA | 601 | U | O4'-C1'-N1 | 7.29 | 114.03 | 108.20 |
| 81 | DA | 1175 | C | P-O3'-C3' | 7.29 | 128.45 | 119.70 |
| 81 | DA | 2872 | A | P-O3'-C3' | -7.29 | 110.95 | 119.70 |
| 81 | DA | 3230 | G | C1'-O4'-C4' | -7.29 | 104.06 | 109.90 |
| 40 | BK | 112 | TYR | CB-CG-CD1 | 7.29 | 125.38 | 121.00 |
| 72 | Bu | 45 | PHE | CB-CG-CD2 | -7.29 | 115.70 | 120.80 |
| 78 | CA | 1095 | U | O4'-C1'-N1 | 7.29 | 114.03 | 108.20 |
| 81 | DA | 2067 | U | C5'-C4'-O4' | 7.29 | 117.85 | 109.10 |
| 81 | DA | 3034 | C | O4'-C1'-N1 | -7.29 | 102.37 | 108.20 |
| 81 | DA | 3126 | C | N1-C1'-C2' | 7.29 | 123.48 | 114.00 |
| 83 | DC | 35 | C | N1-C1'-C2' | 7.29 | 123.48 | 114.00 |
| 78 | CA | 1 | U | O5'-P-OP1 | -7.29 | 99.14 | 105.70 |
| 81 | DA | 2406 | C | P-O5'-C5' | 7.29 | 132.56 | 120.90 |
| 81 | DA | 445 | G | O4'-C1'-N9 | 7.29 | 114.03 | 108.20 |
| 21 | AT | 71 | ARG | NE-CZ-NH2 | 7.29 | 123.94 | 120.30 |
| 78 | CA | 1124 | A | C1'-O4'-C4' | 7.29 | 115.73 | 109.90 |
| 81 | DA | 513 | G | C1'-O4'-C4' | -7.29 | 104.07 | 109.90 |
| 81 | DA | 1624 | G | O5'-C5'-C4' | 7.29 | 125.54 | 111.70 |
| 81 | DA | 2579 | G | C5-C6-O6 | -7.29 | 124.23 | 128.60 |
| 81 | DA | 2988 | C | C4'-C3'-C2' | -7.29 | 95.31 | 102.60 |
| 81 | DA | 3308 | C | N1-C1'-C2' | 7.29 | 123.47 | 114.00 |
| 82 | DB | 102 | U | O4'-C1'-N1 | 7.29 | 114.03 | 108.20 |
| 78 | CA | 565 | C | O4'-C1'-N1 | 7.28 | 114.03 | 108.20 |
| 81 | DA | 2512 | C | C5'-C4'-C3' | -7.28 | 104.35 | 116.00 |
| 81 | DA | 2688 | U | O4'-C1'-C2' | -7.28 | 98.52 | 105.80 |
| 4 | AD | 158 | ASP | CB-CG-OD2 | -7.28 | 111.75 | 118.30 |
| 81 | DA | 525 | C | O4'-C1'-C2' | -7.28 | 98.52 | 105.80 |
| 38 | Bs | 147 | ARG | NE-CZ-NH1 | 7.28 | 123.94 | 120.30 |
| 44 | BO | 20 | GLY | O-C-N | -7.28 | 111.05 | 122.70 |
| 78 | CA | 840 | U | O4'-C1'-N1 | 7.28 | 114.02 | 108.20 |
| 4 | AD | 213 | SER | N-CA-CB | 7.28 | 121.42 | 110.50 |
| 78 | CA | 671 | G | O4'-C1'-N9 | 7.28 | 114.02 | 108.20 |
| 81 | DA | 765 | C | N1-C1'-C2' | 7.28 | 123.46 | 114.00 |
| 81 | DA | 2273 | G | O4'-C1'-N9 | 7.28 | 114.02 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | Be | 223 | PHE | CB-CG-CD1 | -7.28 | 115.71 | 120.80 |
| 78 | CA | 1151 | A | N9-C1'-C2' | -7.28 | 103.99 | 112.00 |
| 83 | DC | 18 | C | O3'-P-O5' | 7.28 | 117.83 | 104.00 |
| 20 | AS | 35 | ASP | CB-CA-C | -7.28 | 95.85 | 110.40 |
| 78 | CA | 519 | C | P-O3'-C3' | 7.28 | 128.43 | 119.70 |
| 78 | CA | 845 | G | C5-C6-O6 | -7.28 | 124.23 | 128.60 |
| 78 | CA | 954 | G | O4'-C1'-N9 | 7.28 | 114.02 | 108.20 |
| 14 | AM | 115 | ARG | NE-CZ-NH2 | -7.27 | 116.66 | 120.30 |
| 81 | DA | 2673 | A | P-O3'-C3' | 7.27 | 128.43 | 119.70 |
| 80 | CC | 13 | A | P-O3'-C3' | 7.27 | 128.43 | 119.70 |
| 57 | Be | 98 | LYS | CA-C-N | -7.27 | 96.74 | 117.10 |
| 4 | AD | 68 | ARG | NH1-CZ-NH2 | 7.27 | 127.40 | 119.40 |
| 29 | AU | 72 | PHE | O-C-N | -7.27 | 110.84 | 123.20 |
| 32 | BC | 162 | VAL | CA-CB-CG1 | 7.27 | 121.80 | 110.90 |
| 76 | BS | 89 | TYR | CG-CD1-CE1 | 7.27 | 127.12 | 121.30 |
| 78 | CA | 1305 | U | O4'-C1'-N1 | 7.27 | 114.02 | 108.20 |
| 81 | DA | 2626 | A | P-O5'-C5' | 7.27 | 132.53 | 120.90 |
| 81 | DA | 3010 | U | C5'-C4'-O4' | -7.27 | 100.38 | 109.10 |
| 2 | AA | 174 | TRP | CB-CG-CD1 | 7.27 | 136.45 | 127.00 |
| 40 | BK | 188 | SER | N-CA-C | 7.27 | 130.62 | 111.00 |
| 81 | DA | 386 | A | P-O3'-C3' | 7.27 | 128.42 | 119.70 |
| 81 | DA | 2031 | U | P-O5'-C5' | 7.27 | 132.53 | 120.90 |
| 81 | DA | 673 | U | C5'-C4'-C3' | -7.26 | 104.38 | 116.00 |
| 81 | DA | 1065 | A | P-O3'-C3' | -7.26 | 110.98 | 119.70 |
| 78 | CA | 1316 | G | C1'-O4'-C4' | -7.26 | 104.09 | 109.90 |
| 81 | DA | 2045 | G | P-O3'-C3' | 7.26 | 128.41 | 119.70 |
| 81 | DA | 2376 | G | N9-C1'-C2' | 7.26 | 123.44 | 114.00 |
| 12 | AK | 126 | THR | N-CA-CB | 7.26 | 124.09 | 110.30 |
| 81 | DA | 427 | C | C3'-C2'-C1' | 7.26 | 107.31 | 101.50 |
| 81 | DA | 2901 | G | N9-C1'-C2' | 7.26 | 123.44 | 114.00 |
| 42 | BM | 66 | LYS | CA-C-N | 7.26 | 137.42 | 117.10 |
| 81 | DA | 1396 | C | O4'-C1'-C2' | -7.26 | 98.54 | 105.80 |
| 81 | DA | 2732 | G | O4'-C1'-N9 | 7.26 | 114.00 | 108.20 |
| 81 | DA | 2950 | G | N9-C1'-C2' | -7.26 | 104.02 | 112.00 |
| 48 | BW | 90 | ARG | N-CA-CB | -7.25 | 97.54 | 110.60 |
| 81 | DA | 2071 | A | O3'-P-O5' | -7.25 | 90.22 | 104.00 |
| 5 | AC | 151 | ASP | CB-CG-OD2 | -7.25 | 111.77 | 118.30 |
| 25 | AY | 57 | MET | N-CA-CB | -7.25 | 97.55 | 110.60 |
| 30 | BA | 191 | VAL | N-CA-CB | 7.25 | 127.46 | 111.50 |
| 78 | CA | 324 | U | O4'-C1'-N1 | 7.25 | 114.00 | 108.20 |
| 81 | DA | 2792 | A | O4'-C1'-N9 | 7.25 | 114.00 | 108.20 |
| 78 | CA | 1354 | G | O4'-C1'-N9 | 7.25 | 114.00 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 1415 | U | N1-C1'-C2' | 7.25 | 123.43 | 114.00 |
| 81 | DA | 1046 | A | O4'-C1'-N9 | 7.25 | 114.00 | 108.20 |
| 81 | DA | 3167 | A | C5'-C4'-C3' | -7.25 | 104.40 | 116.00 |
| 78 | CA | 1723 | U | O4'-C1'-N1 | 7.25 | 114.00 | 108.20 |
| 81 | DA | 2181 | C | P-O5'-C5' | -7.25 | 109.30 | 120.90 |
| 78 | CA | 1164 | G | C3'-C2'-C1' | -7.25 | 95.70 | 101.50 |
| 81 | DA | 804 | C | C3'-C2'-C1' | 7.25 | 107.30 | 101.50 |
| 56 | Bf | 98 | SER | N-CA-CB | 7.25 | 121.37 | 110.50 |
| 81 | DA | 916 | G | C1'-O4'-C4' | 7.25 | 115.70 | 109.90 |
| 81 | DA | 2134 | G | O4'-C1'-N9 | 7.25 | 114.00 | 108.20 |
| 81 | DA | 2175 | U | P-O5'-C5' | 7.25 | 132.49 | 120.90 |
| 78 | CA | 604 | A | C3'-C2'-C1' | 7.25 | 107.30 | 101.50 |
| 2 | AA | 10 | THR | CA-C-O | -7.24 | 104.89 | 120.10 |
| 16 | AO | 124 | ARG | N-CA-CB | -7.24 | 97.56 | 110.60 |
| 35 | BG | 171 | PRO | N-CA-C | -7.24 | 93.27 | 112.10 |
| 49 | BV | 71 | ALA | N-CA-CB | 7.24 | 120.24 | 110.10 |
| 78 | CA | 774 | A | P-O5'-C5' | 7.24 | 132.49 | 120.90 |
| 78 | CA | 1425 | A | P-O3'-C3' | 7.24 | 128.39 | 119.70 |
| 81 | DA | 2136 | C | O4'-C1'-N1 | -7.24 | 102.41 | 108.20 |
| 83 | DC | 57 | C | C1'-O4'-C4' | 7.24 | 115.69 | 109.90 |
| 78 | CA | 635 | A | O4'-C1'-N9 | -7.24 | 102.41 | 108.20 |
| 78 | CA | 1055 | U | P-O3'-C3' | 7.24 | 128.39 | 119.70 |
| 78 | CA | 1728 | A | P-O3'-C3' | 7.24 | 128.39 | 119.70 |
| 81 | DA | 765 | C | C5'-C4'-O4' | 7.24 | 117.79 | 109.10 |
| 81 | DA | 2103 | U | O4'-C1'-N1 | 7.24 | 113.99 | 108.20 |
| 81 | DA | 3047 | U | C4'-C3'-C2' | -7.24 | 95.36 | 102.60 |
| 81 | DA | 3135 | U | P-O3'-C3' | 7.24 | 128.39 | 119.70 |
| 78 | CA | 1274 | C | C6-N1-C1' | -7.24 | 112.11 | 120.80 |
| 78 | CA | 1458 | G | O4'-C1'-N9 | 7.24 | 113.99 | 108.20 |
| 78 | CA | 1705 | C | N1-C1'-C2' | 7.24 | 123.41 | 114.00 |
| 78 | CA | 1746 | A | O4'-C1'-N9 | -7.24 | 102.41 | 108.20 |
| 81 | DA | 1049 | C | N1-C1'-C2' | 7.24 | 123.41 | 114.00 |
| 81 | DA | 1344 | G | C5'-C4'-C3' | 7.24 | 127.58 | 116.00 |
| 81 | DA | 1694 | U | C4'-C3'-C2' | -7.24 | 95.36 | 102.60 |
| 81 | DA | 2750 | U | P-O3'-C3' | -7.24 | 111.01 | 119.70 |
| 81 | DA | 2791 | G | O4'-C1'-C2' | 7.24 | 114.11 | 107.60 |
| 81 | DA | 2673 | A | C3'-C2'-C1' | 7.24 | 107.29 | 101.50 |
| 1 | Aa | 279 | ALA | CB-CA-C | 7.24 | 120.95 | 110.10 |
| 30 | BA | 29 | LEU | CB-CG-CD1 | -7.24 | 98.70 | 111.00 |
| 77 | BI | 154 | ARG | NE-CZ-NH2 | -7.24 | 116.68 | 120.30 |
| 78 | CA | 586 | G | C1'-O4'-C4' | -7.24 | 104.11 | 109.90 |
| 81 | DA | 406 | G | O4'-C1'-C2' | -7.24 | 98.56 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 60 | Bi | 94 | LEU | CB-CA-C | 7.23 | 123.94 | 110.20 |
| 81 | DA | 2152 | A | P-O3'-C3' | -7.23 | 111.02 | 119.70 |
| 36 | BF | 86 | TYR | CB-CG-CD1 | -7.23 | 116.66 | 121.00 |
| 78 | CA | 503 | G | C5-C6-O6 | -7.23 | 124.26 | 128.60 |
| 78 | CA | 942 | G | C3'-C2'-C1' | -7.23 | 95.71 | 101.50 |
| 78 | CA | 1436 | A | C1'-O4'-C4' | -7.23 | 104.12 | 109.90 |
| 78 | CA | 1604 | U | C1'-O4'-C4' | -7.23 | 104.12 | 109.90 |
| 81 | DA | 1975 | C | C1'-O4'-C4' | 7.23 | 115.68 | 109.90 |
| 78 | CA | 156 | A | N9-C1'-C2' | -7.23 | 104.05 | 112.00 |
| 81 | DA | 543 | C | C3'-C2'-C1' | 7.23 | 107.28 | 101.50 |
| 81 | DA | 2438 | A | C5'-C4'-C3' | 7.23 | 127.57 | 116.00 |
| 2 | AA | 81 | PHE | CB-CG-CD1 | 7.23 | 125.86 | 120.80 |
| 43 | BP | 114 | ARG | NE-CZ-NH2 | -7.23 | 116.69 | 120.30 |
| 55 | Bc | 104 | GLN | N-CA-C | -7.23 | 91.49 | 111.00 |
| 66 | Bo | 7 | PHE | C-N-CA | 7.23 | 139.77 | 121.70 |
| 76 | BS | 151 | PHE | C-N-CD | -7.23 | 104.70 | 120.60 |
| 81 | DA | 1085 | A | N9-C1'-C2' | 7.23 | 123.40 | 114.00 |
| 81 | DA | 2928 | C | O4'-C1'-C2' | -7.23 | 98.57 | 105.80 |
| 81 | DA | 1234 | G | O4'-C1'-C2' | 7.23 | 114.10 | 107.60 |
| 3 | AB | 208 | ILE | C-N-CA | -7.22 | 103.64 | 121.70 |
| 29 | AU | 14 | SER | CB-CA-C | 7.22 | 123.83 | 110.10 |
| 76 | BS | 154 | VAL | CA-C-N | 7.22 | 133.09 | 117.20 |
| 78 | CA | 1101 | G | C1'-O4'-C4' | -7.22 | 104.12 | 109.90 |
| 81 | DA | 80 | G | N9-C1'-C2' | 7.22 | 123.39 | 114.00 |
| 81 | DA | 1388 | U | C5'-C4'-C3' | -7.22 | 104.44 | 116.00 |
| 81 | DA | 1427 | U | C3'-C2'-C1' | 7.22 | 107.28 | 101.50 |
| 81 | DA | 2048 | G | C3'-C2'-C1' | 7.22 | 107.28 | 101.50 |
| 81 | DA | 1471 | U | O4'-C1'-N1 | 7.22 | 113.98 | 108.20 |
| 81 | DA | 3037 | U | C5'-C4'-C3' | -7.22 | 104.44 | 116.00 |
| 81 | DA | 3213 | A | P-O3'-C3' | 7.22 | 128.37 | 119.70 |
| 81 | DA | 3358 | U | O4'-C1'-N1 | 7.22 | 113.98 | 108.20 |
| 81 | DA | 510 | G | P-O3'-C3' | 7.22 | 128.37 | 119.70 |
| 69 | Br | 80 | ARG | NE-CZ-NH1 | 7.22 | 123.91 | 120.30 |
| 78 | CA | 480 | G | N1-C6-O6 | 7.22 | 124.23 | 119.90 |
| 78 | CA | 1472 | C | C3'-C2'-C1' | 7.22 | 107.27 | 101.50 |
| 4 | AD | 90 | ILE | C-N-CA | 7.22 | 139.74 | 121.70 |
| 17 | AQ | 26 | LEU | CB-CA-C | 7.22 | 123.91 | 110.20 |
| 81 | DA | 170 | G | O4'-C1'-N9 | 7.22 | 113.97 | 108.20 |
| 78 | CA | 994 | G | N9-C1'-C2' | -7.21 | 104.06 | 112.00 |
| 78 | CA | 1164 | G | N9-C1'-C2' | -7.21 | 104.06 | 112.00 |
| 81 | DA | 748 | U | N1-C1'-C2' | -7.21 | 104.06 | 112.00 |
| 81 | DA | 1716 | U | C3'-C2'-C1' | 7.21 | 107.27 | 101.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2188 | A | C4'-C3'-C2' | -7.21 | 95.39 | 102.60 |
| 81 | DA | 3199 | G | P-O5'-C5' | 7.21 | 132.44 | 120.90 |
| 81 | DA | 1424 | C | C3'-C2'-C1' | 7.21 | 107.27 | 101.50 |
| 81 | DA | 1686 | U | O4'-C4'-C3' | -7.21 | 96.79 | 104.00 |
| 81 | DA | 2443 | A | P-O3'-C3' | 7.21 | 128.36 | 119.70 |
| 78 | CA | 1241 | G | O4'-C1'-N9 | 7.21 | 113.97 | 108.20 |
| 83 | DC | 41 | G | P-O5'-C5' | 7.21 | 132.44 | 120.90 |
| 13 | AL | 39 | LYS | CA-CB-CG | 7.21 | 129.26 | 113.40 |
| 41 | BN | 39 | ILE | CA-CB-CG2 | -7.21 | 96.48 | 110.90 |
| 81 | DA | 1447 | G | O4'-C1'-C2' | -7.21 | 98.59 | 105.80 |
| 81 | DA | 2983 | C | O4'-C1'-C2' | -7.21 | 98.59 | 105.80 |
| 60 | Bi | 77 | GLY | C-N-CA | 7.21 | 137.44 | 122.30 |
| 81 | DA | 55 | G | C1'-O4'-C4' | -7.21 | 104.13 | 109.90 |
| 81 | DA | 692 | A | O4'-C1'-C2' | -7.21 | 98.59 | 105.80 |
| 81 | DA | 2640 | A | O4'-C1'-N9 | 7.21 | 113.97 | 108.20 |
| 37 | BH | 61 | GLN | CA-C-N | 7.21 | 133.06 | 117.20 |
| 43 | BP | 120 | TRP | N-CA-CB | -7.21 | 97.63 | 110.60 |
| 81 | DA | 1689 | U | O3'-P-O5' | 7.21 | 117.69 | 104.00 |
| 81 | DA | 1926 | C | O5'-C5'-C4' | 7.21 | 125.39 | 111.70 |
| 81 | DA | 2333 | C | C3'-C2'-C1' | 7.21 | 107.27 | 101.50 |
| 81 | DA | 2445 | A | C3'-C2'-C1' | 7.21 | 107.27 | 101.50 |
| 81 | DA | 514 | G | C1'-O4'-C4' | -7.21 | 104.14 | 109.90 |
| 81 | DA | 1391 | C | P-O5'-C5' | 7.21 | 132.43 | 120.90 |
| 51 | BZ | 14 | TYR | CB-CG-CD2 | -7.20 | 116.68 | 121.00 |
| 81 | DA | 3309 | G | C5'-C4'-C3' | 7.20 | 127.53 | 116.00 |
| 74 | BQ | 266 | ALA | CB-CA-C | -7.20 | 99.30 | 110.10 |
| 81 | DA | 645 | A | O4'-C1'-C2' | -7.20 | 98.60 | 105.80 |
| 81 | DA | 998 | A | P-O5'-C5' | 7.20 | 132.42 | 120.90 |
| 81 | DA | 2269 | U | P-O3'-C3' | 7.20 | 128.34 | 119.70 |
| 33 | BD | 255 | PHE | CB-CG-CD2 | -7.20 | 115.76 | 120.80 |
| 78 | CA | 597 | G | C3'-C2'-C1' | 7.20 | 107.26 | 101.50 |
| 78 | CA | 1078 | C | C1'-O4'-C4' | -7.20 | 104.14 | 109.90 |
| 79 | CB | 66 | C | P-O3'-C3' | 7.20 | 128.34 | 119.70 |
| 81 | DA | 2633 | U | C4'-C3'-C2' | -7.20 | 95.40 | 102.60 |
| 81 | DA | 3032 | A | O4'-C1'-C2' | -7.20 | 98.60 | 105.80 |
| 12 | AK | 38 | THR | N-CA-CB | 7.20 | 123.98 | 110.30 |
| 78 | CA | 447 | U | O3'-P-O5' | 7.20 | 117.68 | 104.00 |
| 81 | DA | 1059 | G | C1'-O4'-C4' | -7.20 | 104.14 | 109.90 |
| 81 | DA | 1484 | U | P-O3'-C3' | 7.20 | 128.34 | 119.70 |
| 81 | DA | 1933 | A | C1'-O4'-C4' | 7.20 | 115.66 | 109.90 |
| 67 | Bp | 34 | CYS | N-CA-CB | -7.20 | 97.64 | 110.60 |
| 82 | DB | 41 | A | C1'-O4'-C4' | -7.20 | 104.14 | 109.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 46 | BT | 85 | ARG | NE-CZ-NH2 | -7.19 | 116.70 | 120.30 |
| 31 | BB | 89 | TYR | CB-CG-CD2 | 7.19 | 125.31 | 121.00 |
| 78 | CA | 1236 | A | C5'-C4'-C3' | 7.19 | 127.51 | 116.00 |
| 81 | DA | 2718 | U | O4'-C1'-N1 | 7.19 | 113.95 | 108.20 |
| 81 | DA | 3301 | U | P-O3'-C3' | 7.19 | 128.33 | 119.70 |
| 82 | DB | 57 | C | O4'-C1'-N1 | 7.19 | 113.95 | 108.20 |
| 20 | AS | 60 | SER | N-CA-CB | -7.19 | 99.71 | 110.50 |
| 81 | DA | 1189 | C | O4'-C1'-C2' | -7.19 | 98.61 | 105.80 |
| 81 | DA | 1638 | A | O4'-C1'-C2' | 7.19 | 114.07 | 107.60 |
| 11 | AJ | 82 | TYR | CB-CG-CD2 | -7.19 | 116.69 | 121.00 |
| 78 | CA | 219 | A | O4'-C1'-C2' | -7.19 | 98.61 | 105.80 |
| 78 | CA | 1173 | C | P-O5'-C5' | -7.19 | 109.40 | 120.90 |
| 78 | CA | 111 | U | O4'-C1'-N1 | 7.19 | 113.95 | 108.20 |
| 78 | CA | 1397 | U | O4'-C1'-N1 | -7.19 | 102.45 | 108.20 |
| 81 | DA | 1573 | G | O4'-C1'-N9 | 7.18 | 113.95 | 108.20 |
| 81 | DA | 2766 | U | O4'-C1'-N1 | 7.18 | 113.95 | 108.20 |
| 81 | DA | 3287 | U | O4'-C1'-N1 | 7.18 | 113.95 | 108.20 |
| 82 | DB | 93 | U | C1'-O4'-C4' | 7.18 | 115.65 | 109.90 |
| 37 | BH | 98 | ARG | NE-CZ-NH2 | -7.18 | 116.71 | 120.30 |
| 49 | BV | 130 | TYR | CB-CG-CD1 | -7.18 | 116.69 | 121.00 |
| 78 | CA | 932 | U | P-O5'-C5' | -7.18 | 109.41 | 120.90 |
| 80 | CC | 12 | A | C3'-C2'-C1' | -7.18 | 95.75 | 101.50 |
| 81 | DA | 2362 | C | OP2-P-O3' | 7.18 | 121.00 | 105.20 |
| 83 | DC | 54 | A | C1'-O4'-C4' | -7.18 | 104.15 | 109.90 |
| 37 | BH | 222 | PHE | CB-CG-CD2 | 7.18 | 125.83 | 120.80 |
| 41 | BN | 95 | ALA | N-CA-CB | 7.18 | 120.15 | 110.10 |
| 74 | BQ | 21 | ARG | NE-CZ-NH1 | 7.18 | 123.89 | 120.30 |
| 78 | CA | 294 | C | O4'-C1'-C2' | -7.18 | 98.62 | 105.80 |
| 81 | DA | 1770 | G | C5-C6-O6 | -7.18 | 124.29 | 128.60 |
| 29 | AU | 35 | VAL | O-C-N | -7.18 | 111.21 | 122.70 |
| 76 | BS | 75 | LYS | C-N-CA | 7.18 | 139.65 | 121.70 |
| 78 | CA | 323 | A | C1'-O4'-C4' | 7.18 | 115.64 | 109.90 |
| 78 | CA | 1008 | G | O4'-C1'-N9 | 7.18 | 113.94 | 108.20 |
| 78 | CA | 1563 | C | P-O3'-C3' | 7.18 | 128.32 | 119.70 |
| 81 | DA | 696 | C | C3'-C2'-C1' | 7.18 | 107.24 | 101.50 |
| 82 | DB | 89 | A | C3'-C2'-C1' | 7.18 | 107.24 | 101.50 |
| 5 | AC | 18 | PRO | CA-C-O | -7.18 | 102.97 | 120.20 |
| 8 | AF | 76 | ARG | NE-CZ-NH2 | -7.17 | 116.71 | 120.30 |
| 35 | BG | 5 | LYS | N-CA-CB | 7.17 | 123.52 | 110.60 |
| 78 | CA | 1284 | C | P-O5'-C5' | -7.17 | 109.42 | 120.90 |
| 81 | DA | 599 | C | P-O5'-C5' | 7.17 | 132.38 | 120.90 |
| 81 | DA | 1291 | A | N9-C1'-C2' | -7.17 | 104.11 | 112.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1967 | U | P-O3'-C3' | -7.17 | 111.09 | 119.70 |
| 81 | DA | 3215 | A | C3'-C2'-C1' | -7.17 | 95.76 | 101.50 |
| 21 | AT | 9 | VAL | CB-CA-C | 7.17 | 125.03 | 111.40 |
| 81 | DA | 2855 | U | O4'-C1'-N1 | 7.17 | 113.94 | 108.20 |
| 81 | DA | 3369 | G | P-O5'-C5' | 7.17 | 132.38 | 120.90 |
| 14 | AM | 79 | TYR | CB-CG-CD2 | -7.17 | 116.70 | 121.00 |
| 78 | CA | 140 | A | O4'-C1'-N9 | 7.17 | 113.94 | 108.20 |
| 78 | CA | 917 | U | O4'-C1'-N1 | 7.17 | 113.94 | 108.20 |
| 81 | DA | 801 | A | O3'-P-O5' | 7.17 | 117.62 | 104.00 |
| 81 | DA | 2324 | A | O4'-C1'-N9 | 7.17 | 113.94 | 108.20 |
| 34 | BE | 52 | TYR | CB-CG-CD1 | 7.17 | 125.30 | 121.00 |
| 78 | CA | 1610 | G | O4'-C1'-C2' | 7.17 | 114.05 | 107.60 |
| 81 | DA | 153 | U | C5'-C4'-C3' | 7.17 | 127.47 | 116.00 |
| 81 | DA | 1115 | G | O4'-C1'-N9 | -7.17 | 102.47 | 108.20 |
| 81 | DA | 2296 | A | C1'-O4'-C4' | 7.17 | 115.63 | 109.90 |
| 81 | DA | 2504 | U | P-O3'-C3' | -7.17 | 111.10 | 119.70 |
| 20 | AS | 33 | TYR | CB-CG-CD2 | 7.17 | 125.30 | 121.00 |
| 81 | DA | 534 | U | N1-C1'-C2' | -7.17 | 104.12 | 112.00 |
| 31 | BB | 62 | VAL | CB-CA-C | -7.17 | 97.79 | 111.40 |
| 31 | BB | 128 | ARG | NE-CZ-NH1 | -7.17 | 116.72 | 120.30 |
| 61 | Bj | 37 | THR | N-CA-CB | 7.17 | 123.91 | 110.30 |
| 78 | CA | 1470 | C | P-O3'-C3' | 7.17 | 128.30 | 119.70 |
| 2 | AA | 109 | ASN | N-CA-CB | 7.16 | 123.50 | 110.60 |
| 76 | BS | 123 | ILE | CB-CA-C | 7.16 | 125.93 | 111.60 |
| 81 | DA | 1253 | U | P-O3'-C3' | 7.16 | 128.29 | 119.70 |
| 81 | DA | 2897 | A | C3'-C2'-C1' | 7.16 | 107.23 | 101.50 |
| 81 | DA | 3002 | C | O4'-C1'-C2' | -7.16 | 98.64 | 105.80 |
| 82 | DB | 115 | C | C3'-C2'-C1' | 7.16 | 107.23 | 101.50 |
| 44 | BO | 57 | GLY | O-C-N | -7.16 | 111.24 | 122.70 |
| 47 | BU | 63 | VAL | CA-CB-CG2 | -7.16 | 100.16 | 110.90 |
| 78 | CA | 676 | G | O4'-C1'-N9 | 7.16 | 113.93 | 108.20 |
| 81 | DA | 1944 | U | N1-C1'-C2' | 7.16 | 123.31 | 114.00 |
| 78 | CA | 121 | U | O5'-C5'-C4' | 7.16 | 125.30 | 111.70 |
| 78 | CA | 1533 | C | O3'-P-O5' | 7.16 | 117.60 | 104.00 |
| 81 | DA | 2797 | C | P-O3'-C3' | 7.16 | 128.29 | 119.70 |
| 78 | CA | 56 | U | C3'-C2'-C1' | -7.16 | 95.77 | 101.50 |
| 81 | DA | 2112 | U | O4'-C1'-N1 | 7.16 | 113.93 | 108.20 |
| 83 | DC | 59 | G | C3'-C2'-C1' | -7.16 | 95.77 | 101.50 |
| 76 | BS | 73 | THR | N-CA-CB | 7.16 | 123.89 | 110.30 |
| 76 | BS | 161 | PRO | C-N-CA | 7.16 | 139.59 | 121.70 |
| 81 | DA | 434 | U | O4'-C1'-N1 | 7.16 | 113.92 | 108.20 |
| 81 | DA | 2535 | A | C5-C6-N6 | -7.16 | 117.97 | 123.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2653 | C | N1-C1'-C2' | 7.16 | 123.30 | 114.00 |
| 81 | DA | 3147 | G | P-O3'-C3' | 7.16 | 128.28 | 119.70 |
| 81 | DA | 3165 | A | C3'-C2'-C1' | 7.16 | 107.22 | 101.50 |
| 33 | BD | 350 | LYS | C-N-CD | -7.15 | 104.87 | 120.60 |
| 40 | BK | 133 | ARG | NH1-CZ-NH2 | -7.15 | 111.53 | 119.40 |
| 81 | DA | 959 | C | N1-C1'-C2' | 7.15 | 123.30 | 114.00 |
| 81 | DA | 2433 | U | O4'-C1'-N1 | 7.15 | 113.92 | 108.20 |
| 78 | CA | 1156 | C | C3'-C2'-C1' | 7.15 | 107.22 | 101.50 |
| 81 | DA | 2366 | C | N1-C1'-C2' | 7.15 | 123.30 | 114.00 |
| 53 | Ba | 13 | VAL | CG1-CB-CG2 | 7.15 | 122.34 | 110.90 |
| 78 | CA | 1459 | C | C5'-C4'-C3' | 7.15 | 127.44 | 116.00 |
| 78 | CA | 1273 | G | N1-C6-O6 | 7.15 | 124.19 | 119.90 |
| 78 | CA | 1474 | G | N9-C1'-C2' | 7.15 | 123.29 | 114.00 |
| 81 | DA | 2489 | C | C3'-C2'-C1' | 7.15 | 107.22 | 101.50 |
| 81 | DA | 2986 | U | O4'-C1'-N1 | 7.15 | 113.92 | 108.20 |
| 78 | CA | 1181 | U | C1'-O4'-C4' | -7.15 | 104.18 | 109.90 |
| 78 | CA | 10 | G | O4'-C1'-N9 | 7.14 | 113.92 | 108.20 |
| 81 | DA | 166 | C | OP1-P-OP2 | -7.14 | 108.88 | 119.60 |
| 81 | DA | 426 | G | C3'-C2'-C1' | 7.14 | 107.22 | 101.50 |
| 81 | DA | 648 | C | O4'-C1'-C2' | -7.14 | 98.66 | 105.80 |
| 81 | DA | 1237 | G | N9-C1'-C2' | 7.14 | 123.29 | 114.00 |
| 81 | DA | 1853 | U | N1-C1'-C2' | -7.14 | 104.14 | 112.00 |
| 81 | DA | 2438 | A | P-O3'-C3' | 7.14 | 128.27 | 119.70 |
| 42 | BM | 85 | TRP | CE2-CD2-CG | -7.14 | 101.59 | 107.30 |
| 81 | DA | 517 | G | C1'-O4'-C4' | -7.14 | 104.19 | 109.90 |
| 81 | DA | 775 | A | C1'-O4'-C4' | -7.14 | 104.19 | 109.90 |
| 81 | DA | 2486 | A | O4'-C1'-N9 | 7.14 | 113.91 | 108.20 |
| 16 | AO | 65 | VAL | CA-CB-CG1 | -7.14 | 100.19 | 110.90 |
| 78 | CA | 635 | A | N9-C1'-C2' | 7.14 | 123.28 | 114.00 |
| 2 | AA | 5 | ALA | CB-CA-C | -7.14 | 99.39 | 110.10 |
| 81 | DA | 598 | A | C1'-O4'-C4' | -7.14 | 104.19 | 109.90 |
| 81 | DA | 1006 | A | P-O3'-C3' | -7.14 | 111.13 | 119.70 |
| 78 | CA | 483 | A | C4-C5-C6 | 7.14 | 120.57 | 117.00 |
| 78 | CA | 1342 | C | O4'-C1'-N1 | 7.14 | 113.91 | 108.20 |
| 29 | AU | 6 | THR | C-N-CA | 7.13 | 139.54 | 121.70 |
| 81 | DA | 1629 | U | O4'-C1'-N1 | 7.13 | 113.91 | 108.20 |
| 81 | DA | 544 | C | O4'-C1'-N1 | 7.13 | 113.91 | 108.20 |
| 20 | AS | 137 | ALA | CB-CA-C | -7.13 | 99.40 | 110.10 |
| 40 | BK | 132 | GLY | N-CA-C | -7.13 | 95.27 | 113.10 |
| 81 | DA | 1277 | C | N1-C1'-C2' | 7.13 | 123.27 | 114.00 |
| 81 | DA | 1730 | G | C1'-O4'-C4' | 7.13 | 115.61 | 109.90 |
| 33 | BD | 296 | GLN | O-C-N | -7.13 | 111.29 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|---|---|---|---|---|---|---|---|
| 35 | BG | 31 | ARG | NE-CZ-NH2 | -7.13 | 116.74 | 120.30 |
| 37 | BH | 66 | SER | N-CA-CB | 7.13 | 121.19 | 110.50 |
| 81 | DA | 1332 | A | C3'-C2'-C1' | 7.13 | 107.20 | 101.50 |
| 81 | DA | 1742 | U | O4'-C1'-C2' | -7.13 | 98.67 | 105.80 |
| 81 | DA | 1908 | A | N9-C1'-C2' | 7.13 | 123.27 | 114.00 |
| 81 | DA | 2144 | A | O4'-C1'-N9 | 7.13 | 113.90 | 108.20 |
| 81 | DA | 2438 | A | P-O5'-C5' | -7.13 | 109.49 | 120.90 |
| 81 | DA | 3240 | C | N1-C1'-C2' | 7.13 | 123.27 | 114.00 |
| 5 | AC | 142 | ASN | OD1-CG-ND2 | 7.13 | 138.29 | 121.90 |
| 78 | CA | 189 | C | O4'-C1'-N1 | 7.13 | 113.90 | 108.20 |
| 81 | DA | 166 | C | C4'-C3'-C2' | -7.13 | 95.47 | 102.60 |
| 81 | DA | 1884 | A | C3'-C2'-C1' | 7.13 | 107.20 | 101.50 |
| 81 | DA | 110 | G | O4'-C1'-C2' | 7.12 | 114.01 | 107.60 |
| 81 | DA | 227 | G | C3'-C2'-C1' | 7.12 | 107.20 | 101.50 |
| 81 | DA | 1124 | U | P-O3'-C3' | 7.12 | 128.25 | 119.70 |
| 81 | DA | 729 | C | O4'-C1'-N1 | 7.12 | 113.90 | 108.20 |
| 81 | DA | 587 | U | N1-C1'-C2' | 7.12 | 123.26 | 114.00 |
| 46 | BT | 81 | ARG | C-N-CA | 7.12 | 139.50 | 121.70 |
| 81 | DA | 146 | U | O5'-C5'-C4' | 7.12 | 125.23 | 111.70 |
| 81 | DA | 216 | G | O4'-C1'-N9 | 7.12 | 113.90 | 108.20 |
| 81 | DA | 2606 | G | C1'-O4'-C4' | 7.12 | 115.60 | 109.90 |
| 81 | DA | 2702 | A | O4'-C1'-C2' | -7.12 | 98.68 | 105.80 |
| 81 | DA | 386 | A | O4'-C4'-C3' | -7.12 | 96.88 | 104.00 |
| 81 | DA | 1566 | A | O4'-C1'-N9 | 7.12 | 113.89 | 108.20 |
| 81 | DA | 2029 | A | O4'-C1'-N9 | 7.12 | 113.89 | 108.20 |
| 81 | DA | 1477 | A | P-O3'-C3' | 7.12 | 128.24 | 119.70 |
| 13 | AL | 135 | LEU | CA-C-O | 7.12 | 135.04 | 120.10 |
| 46 | BT | 17 | VAL | CG1-CB-CG2 | -7.12 | 99.52 | 110.90 |
| 78 | CA | 120 | U | P-O3'-C3' | -7.12 | 111.16 | 119.70 |
| 78 | CA | 273 | G | C3'-C2'-C1' | 7.12 | 107.19 | 101.50 |
| 78 | CA | 1437 | U | C1'-O4'-C4' | 7.12 | 115.59 | 109.90 |
| 81 | DA | 1378 | U | O3'-P-O5' | -7.12 | 90.48 | 104.00 |
| 81 | DA | 2402 | A | N9-C1'-C2' | -7.12 | 104.17 | 112.00 |
| 81 | DA | 2657 | A | C1'-O4'-C4' | 7.12 | 115.59 | 109.90 |
| 78 | CA | 1478 | G | O5'-C5'-C4' | -7.11 | 98.18 | 111.70 |
| 79 | CB | 56 | A | O4'-C1'-N9 | 7.11 | 113.89 | 108.20 |
| 81 | DA | 1788 | C | C5'-C4'-O4' | -7.11 | 100.56 | 109.10 |
| 81 | DA | 2947 | G | O4'-C1'-N9 | 7.11 | 113.89 | 108.20 |
| 14 | AM | 144 | ARG | NE-CZ-NH2 | 7.11 | 123.86 | 120.30 |
| 78 | CA | 589 | C | P-O3'-C3' | -7.11 | 111.17 | 119.70 |
| 78 | CA | 1585 | U | C1'-O4'-C4' | 7.11 | 115.59 | 109.90 |
| 81 | DA | 875 | G | O4'-C1'-C2' | -7.11 | 98.69 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1077 | U | C3'-C2'-C1' | 7.11 | 107.19 | 101.50 |
| 81 | DA | 1078 | U | O4'-C4'-C3' | -7.11 | 96.89 | 104.00 |
| 81 | DA | 1291 | A | C1'-O4'-C4' | 7.11 | 115.59 | 109.90 |
| 5 | AC | 129 | ILE | CB-CA-C | 7.11 | 125.82 | 111.60 |
| 78 | CA | 1746 | A | O3'-P-O5' | -7.11 | 90.49 | 104.00 |
| 81 | DA | 3337 | G | C3'-C2'-C1' | -7.11 | 95.81 | 101.50 |
| 78 | CA | 217 | A | O4'-C1'-N9 | 7.11 | 113.89 | 108.20 |
| 18 | AP | 109 | VAL | CB-CA-C | -7.11 | 97.90 | 111.40 |
| 65 | Bn | 40 | GLN | N-CA-CB | -7.11 | 97.81 | 110.60 |
| 81 | DA | 3143 | C | P-O3'-C3' | 7.11 | 128.23 | 119.70 |
| 8 | AF | 28 | PRO | N-CA-CB | 7.10 | 111.83 | 103.30 |
| 78 | CA | 93 | A | C1'-O4'-C4' | -7.10 | 104.22 | 109.90 |
| 78 | CA | 1233 | G | C2'-C3'-O3' | 7.10 | 125.13 | 109.50 |
| 81 | DA | 808 | A | N9-C1'-C2' | 7.10 | 123.23 | 114.00 |
| 81 | DA | 1217 | A | C3'-C2'-C1' | 7.10 | 107.18 | 101.50 |
| 6 | AE | 30 | THR | N-CA-C | 7.10 | 130.17 | 111.00 |
| 81 | DA | 1404 | G | O3'-P-O5' | 7.10 | 117.49 | 104.00 |
| 81 | DA | 1427 | U | O4'-C1'-N1 | 7.10 | 113.88 | 108.20 |
| 78 | CA | 773 | C | O3'-P-O5' | -7.10 | 90.51 | 104.00 |
| 81 | DA | 76 | G | N9-C1'-C2' | -7.10 | 104.19 | 112.00 |
| 81 | DA | 1315 | U | P-O5'-C5' | 7.10 | 132.26 | 120.90 |
| 81 | DA | 1901 | A | O4'-C1'-N9 | 7.10 | 113.88 | 108.20 |
| 82 | DB | 103 | G | C1'-O4'-C4' | -7.10 | 104.22 | 109.90 |
| 33 | BD | 194 | TYR | CG-CD2-CE2 | -7.10 | 115.62 | 121.30 |
| 51 | BZ | 51 | TRP | N-CA-CB | 7.10 | 123.38 | 110.60 |
| 81 | DA | 297 | G | N9-C1'-C2' | -7.10 | 104.19 | 112.00 |
| 81 | DA | 1324 | U | O3'-P-O5' | 7.10 | 117.48 | 104.00 |
| 81 | DA | 3303 | G | O4'-C1'-N9 | 7.10 | 113.88 | 108.20 |
| 78 | CA | 471 | A | C3'-C2'-C1' | 7.10 | 107.18 | 101.50 |
| 81 | DA | 548 | G | O4'-C1'-C2' | 7.10 | 113.99 | 107.60 |
| 81 | DA | 1258 | U | C5'-C4'-O4' | 7.10 | 117.61 | 109.10 |
| 34 | BE | 9 | MET | CA-C-N | 7.09 | 132.81 | 117.20 |
| 51 | BZ | 8 | PHE | CB-CG-CD1 | -7.09 | 115.83 | 120.80 |
| 81 | DA | 933 | A | C2'-C3'-O3' | 7.09 | 125.11 | 109.50 |
| 1 | Aa | 121 | MET | CG-SD-CE | -7.09 | 88.85 | 100.20 |
| 81 | DA | 2349 | U | O4'-C1'-N1 | 7.09 | 113.87 | 108.20 |
| 38 | Bs | 58 | MET | CG-SD-CE | -7.09 | 88.85 | 100.20 |
| 78 | CA | 572 | C | O4'-C1'-C2' | -7.09 | 98.71 | 105.80 |
| 78 | CA | 1402 | G | O4'-C1'-N9 | 7.09 | 113.87 | 108.20 |
| 81 | DA | 798 | G | C3'-C2'-C1' | -7.09 | 95.83 | 101.50 |
| 6 | AE | 27 | PRO | O-C-N | 7.09 | 134.04 | 122.70 |
| 81 | DA | 232 | G | O4'-C1'-N9 | 7.09 | 113.87 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 16 | AO | 67 | THR | C-N-CA | -7.09 | 107.42 | 122.30 |
| 78 | CA | 373 | G | P-O5'-C5' | 7.09 | 132.24 | 120.90 |
| 78 | CA | 1680 | G | O3'-P-O5' | -7.09 | 90.54 | 104.00 |
| 81 | DA | 3165 | A | O4'-C1'-C2' | -7.09 | 98.71 | 105.80 |
| 81 | DA | 2146 | C | C5'-C4'-C3' | -7.08 | 104.67 | 116.00 |
| 78 | CA | 307 | G | C1'-O4'-C4' | -7.08 | 104.23 | 109.90 |
| 78 | CA | 444 | C | N1-C1'-C2' | 7.08 | 123.21 | 114.00 |
| 81 | DA | 2026 | A | O4'-C1'-N9 | 7.08 | 113.87 | 108.20 |
| 81 | DA | 2996 | U | O4'-C1'-N1 | 7.08 | 113.87 | 108.20 |
| 81 | DA | 2504 | U | C1'-O4'-C4' | 7.08 | 115.56 | 109.90 |
| 47 | BU | 88 | ARG | NE-CZ-NH2 | -7.08 | 116.76 | 120.30 |
| 81 | DA | 2071 | A | O4'-C1'-C2' | -7.08 | 98.72 | 105.80 |
| 81 | DA | 2837 | A | C1'-O4'-C4' | 7.08 | 115.56 | 109.90 |
| 81 | DA | 1786 | G | N9-C1'-C2' | -7.08 | 104.21 | 112.00 |
| 69 | Br | 34 | SER | N-CA-CB | 7.08 | 121.12 | 110.50 |
| 81 | DA | 725 | G | O4'-C1'-C2' | 7.08 | 113.97 | 107.60 |
| 81 | DA | 2637 | A | C4'-C3'-C2' | -7.08 | 95.52 | 102.60 |
| 78 | CA | 1704 | U | O4'-C1'-N1 | 7.08 | 113.86 | 108.20 |
| 81 | DA | 1950 | U | O4'-C1'-N1 | 7.08 | 113.86 | 108.20 |
| 13 | AL | 99 | ASN | N-CA-CB | 7.07 | 123.33 | 110.60 |
| 15 | AN | 44 | ARG | NE-CZ-NH2 | -7.07 | 116.76 | 120.30 |
| 22 | AV | 32 | MET | CB-CA-C | 7.07 | 124.55 | 110.40 |
| 43 | BP | 121 | VAL | N-CA-C | 7.07 | 130.10 | 111.00 |
| 78 | CA | 895 | G | O4'-C1'-N9 | 7.07 | 113.86 | 108.20 |
| 81 | DA | 1239 | C | P-O5'-C5' | 7.07 | 132.22 | 120.90 |
| 81 | DA | 1579 | C | P-O5'-C5' | 7.07 | 132.22 | 120.90 |
| 81 | DA | 2465 | G | P-O3'-C3' | -7.07 | 111.21 | 119.70 |
| 81 | DA | 1598 | G | P-O5'-C5' | 7.07 | 132.21 | 120.90 |
| 81 | DA | 3214 | U | C1'-O4'-C4' | 7.07 | 115.56 | 109.90 |
| 82 | DB | 35 | C | O4'-C1'-C2' | -7.07 | 98.73 | 105.80 |
| 72 | Bt | 61 | PHE | CB-CA-C | -7.07 | 96.26 | 110.40 |
| 78 | CA | 153 | G | P-O3'-C3' | 7.07 | 128.18 | 119.70 |
| 78 | CA | 205 | U | O4'-C1'-N1 | 7.07 | 113.86 | 108.20 |
| 78 | CA | 855 | A | C4'-C3'-C2' | -7.07 | 95.53 | 102.60 |
| 81 | DA | 1699 | A | P-O3'-C3' | 7.07 | 128.18 | 119.70 |
| 78 | CA | 500 | C | O4'-C1'-N1 | 7.07 | 113.85 | 108.20 |
| 81 | DA | 3081 | C | C3'-C2'-C1' | 7.07 | 107.15 | 101.50 |
| 81 | DA | 3232 | G | N9-C1'-C2' | -7.07 | 104.23 | 112.00 |
| 16 | AO | 64 | ARG | CD-NE-CZ | -7.07 | 113.71 | 123.60 |
| 78 | CA | 577 | G | C5-C6-O6 | -7.07 | 124.36 | 128.60 |
| 81 | DA | 2747 | A | C3'-C2'-C1' | 7.07 | 107.15 | 101.50 |
| 81 | DA | 3069 | G | O4'-C1'-N9 | 7.07 | 113.85 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 33 | BD | 352 | ALA | N-CA-CB | 7.06 | 119.99 | 110.10 |
| 81 | DA | 306 | A | O3'-P-O5' | 7.06 | 117.42 | 104.00 |
| 81 | DA | 524 | U | O4'-C1'-C2' | -7.06 | 98.74 | 105.80 |
| 38 | Bs | 244 | LYS | CB-CA-C | -7.06 | 96.28 | 110.40 |
| 52 | BY | 111 | LEU | C-N-CA | 7.06 | 139.36 | 121.70 |
| 76 | BS | 6 | PHE | N-CA-CB | 7.06 | 123.31 | 110.60 |
| 78 | CA | 197 | A | O4'-C1'-C2' | -7.06 | 98.74 | 105.80 |
| 78 | CA | 1425 | A | O4'-C1'-N9 | 7.06 | 113.85 | 108.20 |
| 81 | DA | 1400 | G | O4'-C4'-C3' | -7.06 | 96.94 | 104.00 |
| 81 | DA | 2981 | U | O4'-C1'-N1 | 7.06 | 113.85 | 108.20 |
| 81 | DA | 1531 | C | C3'-C2'-C1' | 7.06 | 107.15 | 101.50 |
| 81 | DA | 1567 | U | N1-C1'-C2' | 7.06 | 123.18 | 114.00 |
| 81 | DA | 2967 | A | P-O3'-C3' | 7.06 | 128.17 | 119.70 |
| 55 | Bc | 102 | GLU | C-N-CA | 7.06 | 139.35 | 121.70 |
| 35 | BG | 9 | TRP | C-N-CA | 7.06 | 139.34 | 121.70 |
| 74 | BQ | 237 | GLU | N-CA-CB | 7.06 | 123.30 | 110.60 |
| 79 | CB | 74 | C | O4'-C1'-C2' | -7.06 | 98.74 | 105.80 |
| 81 | DA | 1358 | C | P-O5'-C5' | 7.06 | 132.19 | 120.90 |
| 81 | DA | 1826 | C | P-O5'-C5' | 7.06 | 132.19 | 120.90 |
| 81 | DA | 2407 | C | N1-C1'-C2' | 7.06 | 123.18 | 114.00 |
| 82 | DB | 120 | C | O4'-C1'-N1 | 7.06 | 113.85 | 108.20 |
| 37 | BH | 80 | TYR | CG-CD2-CE2 | 7.06 | 126.94 | 121.30 |
| 9 | AH | 78 | ARG | NE-CZ-NH1 | 7.05 | 123.83 | 120.30 |
| 22 | AV | 105 | THR | C-N-CA | -7.05 | 104.06 | 121.70 |
| 79 | CB | 47 | U | N1-C1'-C2' | -7.05 | 104.24 | 112.00 |
| 81 | DA | 700 | C | O4'-C1'-C2' | -7.05 | 98.75 | 105.80 |
| 81 | DA | 1101 | G | P-O3'-C3' | 7.05 | 128.16 | 119.70 |
| 81 | DA | 2210 | G | O4'-C1'-N9 | 7.05 | 113.84 | 108.20 |
| 81 | DA | 2684 | C | P-O5'-C5' | -7.05 | 109.61 | 120.90 |
| 81 | DA | 177 | U | C1'-O4'-C4' | -7.05 | 104.26 | 109.90 |
| 81 | DA | 373 | A | O4'-C4'-C3' | 7.05 | 111.74 | 106.10 |
| 76 | BS | 70 | ASN | CA-CB-CG | 7.05 | 128.91 | 113.40 |
| 78 | CA | 219 | A | C1'-O4'-C4' | 7.05 | 115.54 | 109.90 |
| 78 | CA | 574 | G | C5'-C4'-C3' | 7.05 | 127.28 | 116.00 |
| 65 | Bn | 39 | ARG | NE-CZ-NH2 | -7.05 | 116.78 | 120.30 |
| 81 | DA | 193 | C | C3'-C2'-C1' | 7.05 | 107.14 | 101.50 |
| 80 | CC | 21 | C | O4'-C1'-N1 | 7.05 | 113.84 | 108.20 |
| 81 | DA | 3048 | A | P-O5'-C5' | -7.05 | 109.62 | 120.90 |
| 3 | AB | 214 | GLU | O-C-N | -7.05 | 111.43 | 122.70 |
| 8 | AF | 65 | ARG | NE-CZ-NH1 | 7.05 | 123.82 | 120.30 |
| 48 | BW | 90 | ARG | CB-CA-C | -7.05 | 96.31 | 110.40 |
| 81 | DA | 2080 | C | O4'-C1'-C2' | -7.05 | 98.75 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 857 | G | P-O5'-C5' | 7.04 | 132.17 | 120.90 |
| 81 | DA | 1050 | U | O4'-C1'-C2' | -7.04 | 98.75 | 105.80 |
| 81 | DA | 1640 | G | O4'-C1'-C2' | 7.04 | 113.94 | 107.60 |
| 81 | DA | 1879 | A | O4'-C1'-N9 | -7.04 | 102.56 | 108.20 |
| 44 | BO | 8 | THR | N-CA-C | 7.04 | 130.02 | 111.00 |
| 81 | DA | 835 | G | C3'-C2'-C1' | 7.04 | 107.14 | 101.50 |
| 81 | DA | 2278 | C | P-O3'-C3' | 7.04 | 128.15 | 119.70 |
| 81 | DA | 2606 | G | N9-C1'-C2' | -7.04 | 104.25 | 112.00 |
| 11 | AJ | 81 | THR | CA-C-N | -7.04 | 101.71 | 117.20 |
| 18 | AP | 93 | TYR | CB-CG-CD2 | -7.04 | 116.78 | 121.00 |
| 41 | BN | 5 | SER | CA-C-O | -7.04 | 105.31 | 120.10 |
| 78 | CA | 239 | C | P-O5'-C5' | 7.04 | 132.17 | 120.90 |
| 78 | CA | 662 | U | C3'-C2'-C1' | 7.04 | 107.13 | 101.50 |
| 81 | DA | 3298 | C | C4'-C3'-C2' | 7.04 | 109.64 | 102.60 |
| 3 | AB | 184 | ILE | N-CA-CB | 7.04 | 126.99 | 110.80 |
| 72 | Bt | 61 | PHE | CB-CG-CD2 | -7.04 | 115.87 | 120.80 |
| 74 | BQ | 180 | PHE | CB-CG-CD1 | 7.04 | 125.73 | 120.80 |
| 81 | DA | 1680 | G | P-O3'-C3' | 7.04 | 128.15 | 119.70 |
| 81 | DA | 2972 | G | O4'-C1'-C2' | 7.04 | 113.93 | 107.60 |
| 31 | BB | 70 | ARG | NE-CZ-NH1 | 7.04 | 123.82 | 120.30 |
| 45 | BR | 94 | PHE | C-N-CA | 7.04 | 139.29 | 121.70 |
| 69 | Br | 79 | THR | O-C-N | -7.04 | 111.44 | 122.70 |
| 81 | DA | 255 | A | C1'-O4'-C4' | 7.04 | 115.53 | 109.90 |
| 81 | DA | 871 | U | N1-C1'-C2' | 7.04 | 123.15 | 114.00 |
| 81 | DA | 1840 | U | O4'-C1'-N1 | 7.04 | 113.83 | 108.20 |
| 6 | AE | 27 | PRO | C-N-CA | 7.03 | 139.28 | 121.70 |
| 81 | DA | 302 | U | N1-C1'-C2' | 7.03 | 123.14 | 114.00 |
| 81 | DA | 738 | A | C4-C5-C6 | 7.03 | 120.52 | 117.00 |
| 81 | DA | 1672 | U | O4'-C1'-N1 | 7.03 | 113.83 | 108.20 |
| 78 | CA | 482 | U | C4'-C3'-C2' | -7.03 | 95.57 | 102.60 |
| 81 | DA | 1806 | A | N9-C1'-C2' | 7.03 | 123.14 | 114.00 |
| 81 | DA | 2703 | A | O4'-C1'-N9 | 7.03 | 113.83 | 108.20 |
| 78 | CA | 494 | U | O4'-C1'-N1 | 7.03 | 113.83 | 108.20 |
| 78 | CA | 1300 | A | O4'-C1'-C2' | -7.03 | 98.77 | 105.80 |
| 81 | DA | 994 | G | C3'-C2'-C1' | 7.03 | 107.12 | 101.50 |
| 81 | DA | 1160 | C | C3'-C2'-C1' | 7.03 | 107.12 | 101.50 |
| 82 | DB | 56 | G | P-O3'-C3' | 7.03 | 128.13 | 119.70 |
| 3 | AB | 14 | ASP | CB-CG-OD2 | -7.03 | 111.97 | 118.30 |
| 47 | BU | 136 | ARG | N-CA-CB | 7.03 | 123.25 | 110.60 |
| 52 | BY | 25 | SER | N-CA-CB | -7.03 | 99.96 | 110.50 |
| 78 | CA | 264 | G | P-O3'-C3' | 7.03 | 128.13 | 119.70 |
| 81 | DA | 1568 | U | C3'-C2'-C1' | 7.03 | 107.12 | 101.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1802 | C | C3'-C2'-C1' | 7.03 | 107.12 | 101.50 |
| 81 | DA | 1869 | C | P-O5'-C5' | 7.03 | 132.14 | 120.90 |
| 9 | AH | 101 | TYR | CB-CG-CD2 | 7.03 | 125.22 | 121.00 |
| 43 | BP | 43 | THR | C-N-CA | 7.03 | 139.26 | 121.70 |
| 81 | DA | 1166 | G | O4'-C1'-C2' | -7.03 | 98.78 | 105.80 |
| 81 | DA | 2476 | C | O4'-C1'-C2' | -7.03 | 98.78 | 105.80 |
| 81 | DA | 731 | U | O4'-C1'-N1 | 7.02 | 113.82 | 108.20 |
| 81 | DA | 1359 | C | C1'-O4'-C4' | -7.02 | 104.28 | 109.90 |
| 81 | DA | 1721 | U | N1-C1'-C2' | 7.02 | 123.13 | 114.00 |
| 81 | DA | 2087 | C | OP2-P-O3' | 7.02 | 120.65 | 105.20 |
| 9 | AH | 69 | LEU | N-CA-C | -7.02 | 92.04 | 111.00 |
| 22 | AV | 27 | TRP | CB-CG-CD2 | -7.02 | 117.47 | 126.60 |
| 60 | Bi | 64 | THR | C-N-CA | 7.02 | 139.26 | 121.70 |
| 81 | DA | 1414 | G | N9-C1'-C2' | -7.02 | 104.28 | 112.00 |
| 83 | DC | 97 | C | C3'-C2'-C1' | 7.02 | 107.12 | 101.50 |
| 15 | AN | 12 | ARG | NE-CZ-NH2 | 7.02 | 123.81 | 120.30 |
| 78 | CA | 663 | U | C1'-O4'-C4' | -7.02 | 104.28 | 109.90 |
| 79 | CB | 31 | C | O4'-C1'-N1 | 7.02 | 113.82 | 108.20 |
| 81 | DA | 769 | G | N1-C6-O6 | 7.02 | 124.11 | 119.90 |
| 81 | DA | 1557 | A | P-O3'-C3' | 7.02 | 128.12 | 119.70 |
| 5 | AC | 168 | ARG | CA-CB-CG | 7.02 | 128.84 | 113.40 |
| 32 | BC | 157 | VAL | C-N-CA | 7.02 | 139.25 | 121.70 |
| 45 | BR | 13 | SER | N-CA-CB | -7.02 | 99.97 | 110.50 |
| 78 | CA | 1322 | A | C1'-O4'-C4' | 7.02 | 115.52 | 109.90 |
| 78 | CA | 1386 | G | P-O3'-C3' | 7.02 | 128.12 | 119.70 |
| 81 | DA | 1823 | A | O4'-C1'-N9 | 7.02 | 113.82 | 108.20 |
| 81 | DA | 1951 | C | N1-C1'-C2' | 7.02 | 123.13 | 114.00 |
| 81 | DA | 2462 | A | N9-C1'-C2' | 7.02 | 123.13 | 114.00 |
| 82 | DB | 91 | C | C3'-C2'-C1' | 7.02 | 107.12 | 101.50 |
| 67 | Bp | 46 | ARG | N-CA-C | -7.02 | 92.06 | 111.00 |
| 81 | DA | 1561 | G | O3'-P-O5' | 7.02 | 117.33 | 104.00 |
| 38 | Bs | 73 | PHE | CB-CG-CD1 | -7.02 | 115.89 | 120.80 |
| 81 | DA | 730 | C | N3-C4-C5 | -7.02 | 119.09 | 121.90 |
| 78 | CA | 1094 | G | O4'-C1'-N9 | 7.01 | 113.81 | 108.20 |
| 81 | DA | 43 | A | O4'-C1'-N9 | 7.01 | 113.81 | 108.20 |
| 81 | DA | 2646 | C | C4'-C3'-C2' | 7.01 | 109.61 | 102.60 |
| 82 | DB | 45 | C | O4'-C1'-C2' | -7.01 | 98.78 | 105.80 |
| 83 | DC | 17 | A | C4'-C3'-C2' | 7.01 | 109.61 | 102.60 |
| 45 | BR | 33 | TYR | CB-CG-CD2 | -7.01 | 116.79 | 121.00 |
| 81 | DA | 192 | C | N1-C1'-C2' | 7.01 | 123.12 | 114.00 |
| 81 | DA | 1371 | G | O4'-C1'-N9 | 7.01 | 113.81 | 108.20 |
| 9 | AH | 121 | VAL | CB-CA-C | -7.01 | 98.08 | 111.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | Be | 72 | ALA | N-CA-CB | 7.01 | 119.92 | 110.10 |
| 81 | DA | 321 | C | N1-C1'-C2' | 7.01 | 123.12 | 114.00 |
| 81 | DA | 2067 | U | C4'-C3'-C2' | -7.01 | 95.59 | 102.60 |
| 81 | DA | 2866 | U | C1'-O4'-C4' | 7.01 | 115.51 | 109.90 |
| 55 | Bc | 85 | THR | C-N-CA | 7.01 | 139.22 | 121.70 |
| 78 | CA | 1530 | C | C5'-C4'-C3' | 7.01 | 127.22 | 116.00 |
| 81 | DA | 105 | C | P-O3'-C3' | 7.01 | 128.11 | 119.70 |
| 81 | DA | 320 | G | C1'-O4'-C4' | -7.01 | 104.29 | 109.90 |
| 81 | DA | 1550 | C | C3'-C2'-C1' | 7.01 | 107.11 | 101.50 |
| 81 | DA | 990 | U | P-O3'-C3' | 7.01 | 128.11 | 119.70 |
| 33 | BD | 109 | TRP | N-CA-CB | 7.01 | 123.21 | 110.60 |
| 61 | Bj | 82 | ARG | N-CA-CB | 7.01 | 123.21 | 110.60 |
| 78 | CA | 92 | A | O4'-C4'-C3' | 7.01 | 111.70 | 106.10 |
| 78 | CA | 588 | U | C4'-C3'-C2' | -7.01 | 95.59 | 102.60 |
| 81 | DA | 87 | U | O4'-C1'-N1 | 7.01 | 113.81 | 108.20 |
| 81 | DA | 419 | G | C3'-C2'-C1' | -7.01 | 95.89 | 101.50 |
| 81 | DA | 1261 | G | OP1-P-O3' | 7.01 | 120.61 | 105.20 |
| 81 | DA | 1539 | A | C3'-C2'-C1' | 7.01 | 107.11 | 101.50 |
| 81 | DA | 1692 | U | C5'-C4'-C3' | 7.01 | 127.21 | 116.00 |
| 81 | DA | 2239 | G | O4'-C1'-N9 | 7.01 | 113.81 | 108.20 |
| 83 | DC | 20 | A | C3'-C2'-C1' | -7.01 | 95.90 | 101.50 |
| 53 | Ba | 9 | LYS | CB-CA-C | -7.00 | 96.39 | 110.40 |
| 78 | CA | 487 | G | C5-C6-O6 | -7.00 | 124.40 | 128.60 |
| 4 | AD | 207 | LEU | C-N-CA | 7.00 | 139.21 | 121.70 |
| 31 | BB | 76 | PHE | CB-CG-CD1 | 7.00 | 125.70 | 120.80 |
| 33 | BD | 339 | LEU | CB-CG-CD2 | 7.00 | 122.91 | 111.00 |
| 74 | BQ | 39 | GLN | CA-C-N | 7.00 | 132.61 | 117.20 |
| 78 | CA | 486 | G | O4'-C1'-N9 | 7.00 | 113.80 | 108.20 |
| 78 | CA | 942 | G | C1'-O4'-C4' | -7.00 | 104.30 | 109.90 |
| 78 | CA | 1288 | G | C1'-O4'-C4' | -7.00 | 104.30 | 109.90 |
| 78 | CA | 592 | A | O4'-C1'-N9 | 7.00 | 113.80 | 108.20 |
| 78 | CA | 1745 | G | O4'-C1'-N9 | 7.00 | 113.80 | 108.20 |
| 81 | DA | 2707 | C | C1'-O4'-C4' | -7.00 | 104.30 | 109.90 |
| 81 | DA | 233 | C | C1'-O4'-C4' | 7.00 | 115.50 | 109.90 |
| 78 | CA | 178 | U | C5'-C4'-O4' | -7.00 | 100.70 | 109.10 |
| 81 | DA | 2681 | U | C3'-C2'-C1' | 7.00 | 107.10 | 101.50 |
| 76 | BS | 159 | ARG | CA-C-N | 7.00 | 136.69 | 117.10 |
| 78 | CA | 233 | C | N1-C1'-C2' | 7.00 | 123.10 | 114.00 |
| 81 | DA | 1157 | G | O4'-C1'-N9 | 7.00 | 113.80 | 108.20 |
| 81 | DA | 1295 | G | N9-C1'-C2' | 7.00 | 123.10 | 114.00 |
| 81 | DA | 2130 | G | N9-C1'-C2' | -7.00 | 104.30 | 112.00 |
| 4 | AD | 120 | SER | N-CA-CB | 7.00 | 120.99 | 110.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | AY | 25 | VAL | CG1-CB-CG2 | 7.00 | 122.09 | 110.90 |
| 32 | BC | 104 | THR | N-CA-CB | 6.99 | 123.59 | 110.30 |
| 78 | CA | 970 | A | N9-C1'-C2' | -6.99 | 104.31 | 112.00 |
| 78 | CA | 1546 | G | C1'-C2'-O2' | 6.99 | 131.58 | 110.60 |
| 81 | DA | 2826 | U | O4'-C1'-N1 | 6.99 | 113.80 | 108.20 |
| 78 | CA | 678 | A | O4'-C1'-N9 | 6.99 | 113.79 | 108.20 |
| 83 | DC | 1 | G | C1'-O4'-C4' | 6.99 | 115.49 | 109.90 |
| 63 | Bm | 35 | ALA | N-CA-CB | 6.99 | 119.89 | 110.10 |
| 78 | CA | 1179 | G | N9-C1'-C2' | 6.99 | 123.09 | 114.00 |
| 78 | CA | 1307 | U | O5'-C5'-C4' | 6.99 | 124.98 | 111.70 |
| 78 | CA | 1316 | G | P-O3'-C3' | 6.99 | 128.09 | 119.70 |
| 81 | DA | 1085 | A | P-O3'-C3' | -6.99 | 111.31 | 119.70 |
| 83 | DC | 85 | G | C3'-C2'-C1' | -6.99 | 95.91 | 101.50 |
| 32 | BC | 308 | MET | CA-CB-CG | -6.99 | 101.42 | 113.30 |
| 38 | Bs | 180 | PRO | CA-N-CD | -6.99 | 101.72 | 111.50 |
| 48 | BW | 36 | TYR | CB-CG-CD1 | 6.99 | 125.19 | 121.00 |
| 81 | DA | 1716 | U | O4'-C1'-C2' | -6.99 | 98.81 | 105.80 |
| 81 | DA | 3363 | U | C1'-O4'-C4' | 6.99 | 115.49 | 109.90 |
| 81 | DA | 3110 | C | N1-C1'-C2' | 6.99 | 123.08 | 114.00 |
| 2 | AA | 5 | ALA | O-C-N | -6.99 | 111.52 | 122.70 |
| 81 | DA | 1382 | G | C3'-C2'-C1' | 6.99 | 107.09 | 101.50 |
| 81 | DA | 1665 | C | N1-C1'-C2' | 6.99 | 123.08 | 114.00 |
| 81 | DA | 1824 | U | O4'-C1'-N1 | 6.99 | 113.79 | 108.20 |
| 81 | DA | 2515 | A | N9-C1'-C2' | 6.99 | 123.08 | 114.00 |
| 83 | DC | 99 | A | O4'-C1'-C2' | -6.99 | 98.81 | 105.80 |
| 16 | AO | 76 | LYS | N-CA-CB | 6.98 | 123.17 | 110.60 |
| 78 | CA | 1006 | C | C3'-C2'-C1' | 6.98 | 107.09 | 101.50 |
| 81 | DA | 3042 | U | O4'-C1'-N1 | 6.98 | 113.79 | 108.20 |
| 82 | DB | 91 | C | N1-C1'-C2' | -6.98 | 104.32 | 112.00 |
| 62 | Bk | 70 | ARG | NE-CZ-NH1 | 6.98 | 123.79 | 120.30 |
| 78 | CA | 584 | C | C1'-O4'-C4' | -6.98 | 104.31 | 109.90 |
| 81 | DA | 337 | G | O4'-C1'-N9 | 6.98 | 113.78 | 108.20 |
| 81 | DA | 1000 | C | N1-C1'-C2' | 6.98 | 123.08 | 114.00 |
| 81 | DA | 1968 | G | O4'-C1'-N9 | 6.98 | 113.79 | 108.20 |
| 81 | DA | 2963 | C | C4'-C3'-C2' | -6.98 | 95.62 | 102.60 |
| 64 | Bl | 63 | ARG | NE-CZ-NH1 | 6.98 | 123.79 | 120.30 |
| 78 | CA | 283 | U | C3'-C2'-C1' | 6.98 | 107.08 | 101.50 |
| 78 | CA | 1534 | G | C5'-C4'-C3' | -6.98 | 104.83 | 116.00 |
| 81 | DA | 427 | C | C1'-O4'-C4' | -6.98 | 104.31 | 109.90 |
| 81 | DA | 2538 | U | O4'-C1'-N1 | 6.98 | 113.78 | 108.20 |
| 81 | DA | 2617 | U | O3'-P-O5' | 6.98 | 117.26 | 104.00 |
| 78 | CA | 1498 | G | C5-C6-O6 | -6.98 | 124.41 | 128.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 802 | C | C3'-C2'-C1' | 6.98 | 107.08 | 101.50 |
| 81 | DA | 2479 | C | C5'-C4'-O4' | 6.98 | 117.47 | 109.10 |
| 78 | CA | 1215 | C | N1-C1'-C2' | 6.98 | 123.07 | 114.00 |
| 81 | DA | 3199 | G | C5'-C4'-C3' | 6.98 | 127.16 | 116.00 |
| 81 | DA | 3334 | U | O4'-C1'-C2' | -6.98 | 98.82 | 105.80 |
| 78 | CA | 788 | A | P-O3'-C3' | 6.98 | 128.07 | 119.70 |
| 81 | DA | 969 | C | C5'-C4'-O4' | -6.97 | 100.73 | 109.10 |
| 81 | DA | 2032 | U | O3'-P-O5' | -6.97 | 90.75 | 104.00 |
| 81 | DA | 2685 | C | C1'-O4'-C4' | -6.97 | 104.32 | 109.90 |
| 82 | DB | 49 | G | O3'-P-O5' | -6.97 | 90.75 | 104.00 |
| 53 | Ba | 29 | HIS | CA-CB-CG | 6.97 | 125.45 | 113.60 |
| 61 | Bj | 99 | ARG | NE-CZ-NH2 | -6.97 | 116.81 | 120.30 |
| 78 | CA | 253 | A | O4'-C1'-N9 | 6.97 | 113.78 | 108.20 |
| 78 | CA | 900 | A | C5'-C4'-O4' | -6.97 | 100.73 | 109.10 |
| 81 | DA | 1433 | A | O4'-C1'-N9 | -6.97 | 102.62 | 108.20 |
| 81 | DA | 2597 | U | P-O3'-C3' | 6.97 | 128.07 | 119.70 |
| 81 | DA | 2822 | U | O4'-C1'-N1 | 6.97 | 113.78 | 108.20 |
| 78 | CA | 1037 | C | O4'-C1'-N1 | 6.97 | 113.78 | 108.20 |
| 78 | CA | 1244 | A | O4'-C1'-N9 | 6.97 | 113.78 | 108.20 |
| 44 | BO | 56 | VAL | CB-CA-C | -6.97 | 98.16 | 111.40 |
| 81 | DA | 1705 | U | O4'-C1'-N1 | 6.97 | 113.78 | 108.20 |
| 81 | DA | 523 | A | O4'-C1'-N9 | 6.97 | 113.77 | 108.20 |
| 5 | AC | 107 | ARG | NE-CZ-NH2 | -6.97 | 116.82 | 120.30 |
| 12 | AK | 60 | ALA | CB-CA-C | -6.97 | 99.65 | 110.10 |
| 81 | DA | 571 | U | O4'-C1'-N1 | 6.97 | 113.77 | 108.20 |
| 81 | DA | 1676 | A | O4'-C1'-C2' | -6.97 | 98.83 | 105.80 |
| 81 | DA | 1868 | G | P-O3'-C3' | -6.97 | 111.34 | 119.70 |
| 81 | DA | 2531 | C | O4'-C4'-C3' | -6.97 | 97.03 | 104.00 |
| 78 | CA | 1499 | G | N1-C6-O6 | 6.96 | 124.08 | 119.90 |
| 78 | CA | 1532 | U | O4'-C1'-N1 | 6.96 | 113.77 | 108.20 |
| 81 | DA | 1232 | C | O4'-C1'-C2' | -6.96 | 98.83 | 105.80 |
| 78 | CA | 621 | A | C1'-O4'-C4' | 6.96 | 115.47 | 109.90 |
| 78 | CA | 1181 | U | C3'-C2'-C1' | -6.96 | 95.93 | 101.50 |
| 78 | CA | 641 | G | N9-C1'-C2' | 6.96 | 123.05 | 114.00 |
| 81 | DA | 1365 | G | O4'-C1'-N9 | 6.96 | 113.77 | 108.20 |
| 82 | DB | 20 | U | P-O5'-C5' | 6.96 | 132.04 | 120.90 |
| 3 | AB | 51 | ARG | NE-CZ-NH1 | 6.96 | 123.78 | 120.30 |
| 45 | BR | 31 | LYS | CB-CA-C | 6.96 | 124.32 | 110.40 |
| 78 | CA | 394 | C | C3'-C2'-C1' | 6.96 | 107.07 | 101.50 |
| 81 | DA | 487 | U | O5'-P-OP1 | -6.96 | 99.44 | 105.70 |
| 81 | DA | 1718 | G | C1'-O4'-C4' | -6.96 | 104.33 | 109.90 |
| 10 | AI | 84 | ALA | CB-CA-C | -6.96 | 99.67 | 110.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 968 | U | O4'-C1'-N1 | 6.96 | 113.77 | 108.20 |
| 82 | DB | 44 | A | O3'-P-O5' | -6.96 | 90.78 | 104.00 |
| 40 | BK | 74 | ARG | NE-CZ-NH2 | -6.96 | 116.82 | 120.30 |
| 81 | DA | 1764 | U | O4'-C1'-N1 | 6.96 | 113.76 | 108.20 |
| 81 | DA | 2439 | A | C5'-C4'-O4' | 6.96 | 117.45 | 109.10 |
| 78 | CA | 849 | C | N1-C1'-C2' | 6.95 | 123.04 | 114.00 |
| 81 | DA | 1641 | U | C5'-C4'-C3' | -6.95 | 104.88 | 116.00 |
| 81 | DA | 2687 | G | P-O3'-C3' | 6.95 | 128.04 | 119.70 |
| 81 | DA | 523 | A | N9-C1'-C2' | -6.95 | 104.35 | 112.00 |
| 1 | Aa | 281 | TYR | CB-CG-CD2 | -6.95 | 116.83 | 121.00 |
| 62 | Bk | 28 | TYR | O-C-N | -6.95 | 111.58 | 122.70 |
| 78 | CA | 1321 | A | P-O3'-C3' | -6.95 | 111.36 | 119.70 |
| 78 | CA | 1385 | G | N9-C1'-C2' | -6.95 | 104.36 | 112.00 |
| 81 | DA | 1895 | A | O4'-C1'-C2' | -6.95 | 98.85 | 105.80 |
| 81 | DA | 2529 | A | O4'-C1'-N9 | 6.95 | 113.76 | 108.20 |
| 81 | DA | 2698 | G | C4'-C3'-C2' | -6.95 | 95.65 | 102.60 |
| 81 | DA | 3363 | U | P-O5'-C5' | 6.95 | 132.02 | 120.90 |
| 61 | Bj | 2 | ALA | CA-C-N | 6.95 | 132.49 | 117.20 |
| 81 | DA | 787 | G | P-O3'-C3' | 6.95 | 128.04 | 119.70 |
| 81 | DA | 1297 | C | O4'-C4'-C3' | -6.95 | 97.05 | 104.00 |
| 81 | DA | 1429 | G | C1'-O4'-C4' | -6.95 | 104.34 | 109.90 |
| 81 | DA | 2167 | A | C3'-C2'-C1' | 6.95 | 107.06 | 101.50 |
| 78 | CA | 555 | A | C1'-O4'-C4' | -6.95 | 104.34 | 109.90 |
| 81 | DA | 2013 | C | O4'-C1'-C2' | -6.95 | 98.85 | 105.80 |
| 33 | BD | 140 | HIS | CA-CB-CG | -6.95 | 101.79 | 113.60 |
| 37 | BH | 198 | ALA | N-CA-CB | 6.95 | 119.83 | 110.10 |
| 48 | BW | 91 | ASP | N-CA-CB | 6.95 | 123.10 | 110.60 |
| 74 | BQ | 240 | TYR | CB-CG-CD2 | 6.95 | 125.17 | 121.00 |
| 76 | BS | 165 | LEU | CB-CA-C | -6.95 | 97.00 | 110.20 |
| 81 | DA | 792 | G | P-O3'-C3' | 6.95 | 128.03 | 119.70 |
| 81 | DA | 1582 | C | O4'-C1'-C2' | -6.95 | 98.86 | 105.80 |
| 81 | DA | 2977 | G | O4'-C1'-N9 | 6.95 | 113.76 | 108.20 |
| 3 | AB | 167 | PHE | CB-CG-CD2 | -6.94 | 115.94 | 120.80 |
| 53 | Ba | 60 | LYS | CA-CB-CG | 6.94 | 128.68 | 113.40 |
| 78 | CA | 1426 | C | O4'-C1'-N1 | 6.94 | 113.75 | 108.20 |
| 81 | DA | 277 | G | P-O3'-C3' | 6.94 | 128.03 | 119.70 |
| 78 | CA | 615 | A | N9-C1'-C2' | 6.94 | 123.03 | 114.00 |
| 78 | CA | 1393 | C | O4'-C1'-N1 | 6.94 | 113.75 | 108.20 |
| 81 | DA | 954 | U | O4'-C1'-N1 | 6.94 | 113.75 | 108.20 |
| 81 | DA | 1243 | G | C1'-O4'-C4' | -6.94 | 104.35 | 109.90 |
| 81 | DA | 2175 | U | N1-C1'-C2' | 6.94 | 123.03 | 114.00 |
| 78 | CA | 1700 | C | P-O5'-C5' | 6.94 | 132.01 | 120.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 836 | A | O5'-C5'-C4' | 6.94 | 124.89 | 111.70 |
| 81 | DA | 2390 | A | C3'-C2'-C1' | 6.94 | 107.05 | 101.50 |
| 81 | DA | 3136 | G | C3'-C2'-C1' | -6.94 | 95.95 | 101.50 |
| 44 | BO | 40 | HIS | CB-CA-C | 6.94 | 124.28 | 110.40 |
| 78 | CA | 1301 | U | O4'-C1'-N1 | 6.94 | 113.75 | 108.20 |
| 6 | AE | 24 | ARG | CB-CG-CD | 6.94 | 129.64 | 111.60 |
| 78 | CA | 1411 | A | O4'-C1'-N9 | 6.94 | 113.75 | 108.20 |
| 81 | DA | 851 | C | C3'-C2'-C1' | 6.94 | 107.05 | 101.50 |
| 81 | DA | 996 | A | N9-C1'-C2' | -6.94 | 104.37 | 112.00 |
| 81 | DA | 2697 | A | O4'-C1'-C2' | -6.94 | 98.86 | 105.80 |
| 18 | AP | 41 | GLY | N-CA-C | -6.93 | 95.76 | 113.10 |
| 81 | DA | 429 | U | O4'-C1'-C2' | -6.93 | 98.86 | 105.80 |
| 81 | DA | 1247 | U | N1-C1'-C2' | -6.93 | 104.37 | 112.00 |
| 81 | DA | 1584 | U | O4'-C1'-N1 | 6.93 | 113.75 | 108.20 |
| 81 | DA | 3249 | C | C5'-C4'-O4' | 6.93 | 117.42 | 109.10 |
| 10 | AI | 109 | PHE | CB-CG-CD1 | 6.93 | 125.65 | 120.80 |
| 81 | DA | 1882 | G | C1'-O4'-C4' | -6.93 | 104.36 | 109.90 |
| 78 | CA | 1337 | A | C2'-C3'-O3' | 6.93 | 124.79 | 113.70 |
| 81 | DA | 1172 | G | O4'-C1'-N9 | 6.93 | 113.75 | 108.20 |
| 81 | DA | 1845 | G | O4'-C1'-N9 | 6.93 | 113.75 | 108.20 |
| 81 | DA | 3385 | U | P-O5'-C5' | -6.93 | 109.81 | 120.90 |
| 33 | BD | 347 | THR | C-N-CA | 6.93 | 136.85 | 122.30 |
| 78 | CA | 51 | A | C3'-C2'-C1' | 6.93 | 107.04 | 101.50 |
| 78 | CA | 978 | A | P-O3'-C3' | 6.93 | 128.01 | 119.70 |
| 81 | DA | 1882 | G | O4'-C1'-N9 | 6.93 | 113.74 | 108.20 |
| 81 | DA | 2770 | G | P-O5'-C5' | 6.93 | 131.99 | 120.90 |
| 81 | DA | 3369 | G | C3'-C2'-C1' | 6.93 | 107.04 | 101.50 |
| 74 | BQ | 36 | LEU | CB-CA-C | -6.93 | 97.04 | 110.20 |
| 81 | DA | 1295 | G | C5'-C4'-C3' | -6.93 | 104.92 | 116.00 |
| 62 | Bk | 83 | ALA | CB-CA-C | -6.93 | 99.71 | 110.10 |
| 74 | BQ | 232 | ASP | CB-CG-OD1 | 6.93 | 124.53 | 118.30 |
| 77 | BI | 178 | ARG | NE-CZ-NH1 | 6.93 | 123.76 | 120.30 |
| 78 | CA | 1024 | U | O4'-C1'-N1 | 6.93 | 113.74 | 108.20 |
| 81 | DA | 198 | A | O4'-C1'-N9 | -6.93 | 102.66 | 108.20 |
| 55 | Bc | 110 | ALA | CA-C-N | -6.92 | 101.97 | 117.20 |
| 78 | CA | 830 | U | O4'-C1'-N1 | 6.92 | 113.74 | 108.20 |
| 78 | CA | 967 | A | N9-C1'-C2' | -6.92 | 104.38 | 112.00 |
| 79 | CB | 26 | G | C1'-O4'-C4' | -6.92 | 104.36 | 109.90 |
| 80 | CC | 16 | G | O4'-C1'-C2' | -6.92 | 98.88 | 105.80 |
| 81 | DA | 1413 | G | N9-C1'-C2' | 6.92 | 123.00 | 114.00 |
| 81 | DA | 1599 | G | P-O3'-C3' | 6.92 | 128.01 | 119.70 |
| 32 | BC | 240 | ARG | NE-CZ-NH2 | -6.92 | 116.84 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 49 | BV | 18 | ARG | NE-CZ-NH2 | -6.92 | 116.84 | 120.30 |
| 78 | CA | 465 | G | O4'-C1'-C2' | 6.92 | 113.83 | 107.60 |
| 79 | CB | 26 | G | C3'-C2'-C1' | -6.92 | 95.96 | 101.50 |
| 81 | DA | 946 | U | O4'-C1'-N1 | 6.92 | 113.74 | 108.20 |
| 81 | DA | 2402 | A | O4'-C1'-C2' | -6.92 | 98.88 | 105.80 |
| 81 | DA | 2666 | C | N1-C1'-C2' | 6.92 | 123.00 | 114.00 |
| 34 | BE | 32 | ARG | NE-CZ-NH2 | -6.92 | 116.84 | 120.30 |
| 41 | BN | 19 | ARG | NH1-CZ-NH2 | -6.92 | 111.79 | 119.40 |
| 81 | DA | 2176 | U | O4'-C1'-N1 | 6.92 | 113.73 | 108.20 |
| 81 | DA | 3086 | A | O4'-C1'-C2' | -6.92 | 98.88 | 105.80 |
| 82 | DB | 157 | U | O4'-C1'-N1 | 6.92 | 113.73 | 108.20 |
| 57 | Be | 60 | ARG | NE-CZ-NH2 | -6.92 | 116.84 | 120.30 |
| 78 | CA | 1090 | C | P-O3'-C3' | 6.92 | 128.00 | 119.70 |
| 81 | DA | 485 | A | O4'-C1'-N9 | 6.92 | 113.73 | 108.20 |
| 81 | DA | 1294 | A | C4'-C3'-C2' | -6.92 | 95.68 | 102.60 |
| 82 | DB | 129 | C | O4'-C1'-N1 | 6.92 | 113.73 | 108.20 |
| 40 | BK | 197 | LEU | CB-CA-C | 6.92 | 123.34 | 110.20 |
| 81 | DA | 857 | G | O4'-C1'-N9 | 6.91 | 113.73 | 108.20 |
| 81 | DA | 1980 | C | O4'-C1'-N1 | 6.91 | 113.73 | 108.20 |
| 81 | DA | 2158 | A | O4'-C1'-N9 | 6.91 | 113.73 | 108.20 |
| 15 | AN | 14 | TYR | N-CA-CB | 6.91 | 123.04 | 110.60 |
| 35 | BG | 2 | SER | CA-C-N | -6.91 | 101.99 | 117.20 |
| 81 | DA | 3146 | G | C4'-C3'-C2' | -6.91 | 95.69 | 102.60 |
| 46 | BT | 82 | LYS | N-CA-C | -6.91 | 92.34 | 111.00 |
| 81 | DA | 420 | G | N9-C1'-C2' | -6.91 | 104.40 | 112.00 |
| 81 | DA | 2617 | U | O4'-C1'-N1 | 6.91 | 113.73 | 108.20 |
| 32 | BC | 119 | TYR | CB-CG-CD1 | 6.91 | 125.15 | 121.00 |
| 78 | CA | 1555 | A | C3'-C2'-C1' | 6.91 | 107.03 | 101.50 |
| 78 | CA | 1736 | G | P-O5'-C5' | 6.91 | 131.96 | 120.90 |
| 81 | DA | 103 | G | C1'-O4'-C4' | 6.91 | 115.43 | 109.90 |
| 78 | CA | 836 | U | C3'-C2'-C1' | 6.91 | 107.03 | 101.50 |
| 81 | DA | 595 | G | O4'-C1'-C2' | -6.91 | 98.89 | 105.80 |
| 81 | DA | 1078 | U | P-O3'-C3' | -6.91 | 111.41 | 119.70 |
| 33 | BD | 58 | HIS | CA-CB-CG | 6.91 | 125.34 | 113.60 |
| 38 | Bs | 243 | TYR | CG-CD1-CE1 | -6.91 | 115.78 | 121.30 |
| 81 | DA | 312 | C | P-O5'-C5' | 6.91 | 131.95 | 120.90 |
| 83 | DC | 100 | A | C5'-C4'-C3' | 6.91 | 127.05 | 116.00 |
| 38 | Bs | 180 | PRO | N-CA-C | 6.90 | 130.05 | 112.10 |
| 78 | CA | 307 | G | O4'-C1'-N9 | 6.90 | 113.72 | 108.20 |
| 81 | DA | 1907 | C | P-O3'-C3' | 6.90 | 127.98 | 119.70 |
| 82 | DB | 104 | A | O4'-C1'-N9 | -6.90 | 102.68 | 108.20 |
| 13 | AL | 135 | LEU | N-CA-C | 6.90 | 129.64 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 217 | A | C4'-C3'-C2' | -6.90 | 95.70 | 102.60 |
| 78 | CA | 1477 | G | P-O5'-C5' | 6.90 | 131.94 | 120.90 |
| 81 | DA | 366 | A | C1'-O4'-C4' | -6.90 | 104.38 | 109.90 |
| 81 | DA | 3093 | C | O4'-C1'-N1 | -6.90 | 102.68 | 108.20 |
| 82 | DB | 42 | G | O4'-C1'-N9 | 6.90 | 113.72 | 108.20 |
| 74 | BQ | 180 | PHE | CB-CG-CD2 | -6.90 | 115.97 | 120.80 |
| 78 | CA | 88 | U | C4'-C3'-C2' | -6.90 | 95.70 | 102.60 |
| 81 | DA | 3095 | U | O4'-C1'-N1 | 6.90 | 113.72 | 108.20 |
| 81 | DA | 3295 | A | O3'-P-O5' | 6.90 | 117.10 | 104.00 |
| 81 | DA | 3335 | A | P-O3'-C3' | 6.90 | 127.98 | 119.70 |
| 41 | BN | 62 | GLN | CB-CA-C | 6.90 | 124.19 | 110.40 |
| 40 | BK | 64 | PHE | CB-CG-CD2 | -6.89 | 115.97 | 120.80 |
| 43 | BP | 121 | VAL | CA-C-N | 6.89 | 132.36 | 117.20 |
| 78 | CA | 335 | U | O4'-C1'-N1 | 6.89 | 113.71 | 108.20 |
| 78 | CA | 1375 | A | P-O5'-C5' | 6.89 | 131.93 | 120.90 |
| 78 | CA | 1380 | U | N1-C1'-C2' | 6.89 | 122.96 | 114.00 |
| 81 | DA | 790 | U | O5'-C5'-C4' | 6.89 | 124.80 | 111.70 |
| 74 | BQ | 153 | THR | CA-CB-CG2 | -6.89 | 102.75 | 112.40 |
| 81 | DA | 3235 | C | O4'-C1'-N1 | 6.89 | 113.71 | 108.20 |
| 8 | AF | 123 | VAL | N-CA-CB | -6.89 | 96.34 | 111.50 |
| 35 | BG | 66 | SER | N-CA-CB | 6.89 | 120.83 | 110.50 |
| 37 | BH | 140 | VAL | CA-CB-CG2 | 6.89 | 121.23 | 110.90 |
| 78 | CA | 1569 | A | C1'-O4'-C4' | -6.89 | 104.39 | 109.90 |
| 74 | BQ | 241 | THR | C-N-CA | 6.89 | 138.92 | 121.70 |
| 5 | AC | 168 | ARG | CB-CA-C | -6.89 | 96.62 | 110.40 |
| 78 | CA | 289 | U | C3'-C2'-C1' | 6.89 | 107.01 | 101.50 |
| 81 | DA | 1382 | G | C5'-C4'-C3' | -6.89 | 104.98 | 116.00 |
| 81 | DA | 2966 | G | C1'-O4'-C4' | -6.89 | 104.39 | 109.90 |
| 81 | DA | 422 | A | O4'-C1'-N9 | 6.88 | 113.71 | 108.20 |
| 81 | DA | 3220 | G | C3'-C2'-C1' | 6.88 | 107.01 | 101.50 |
| 5 | AC | 146 | PHE | CB-CG-CD1 | -6.88 | 115.98 | 120.80 |
| 78 | CA | 386 | G | C1'-O4'-C4' | -6.88 | 104.39 | 109.90 |
| 3 | AB | 65 | ARG | NE-CZ-NH1 | 6.88 | 123.74 | 120.30 |
| 44 | BO | 149 | ALA | CB-CA-C | -6.88 | 99.78 | 110.10 |
| 46 | BT | 82 | LYS | N-CA-CB | -6.88 | 98.21 | 110.60 |
| 69 | Br | 100 | LYS | C-N-CA | -6.88 | 107.85 | 122.30 |
| 78 | CA | 897 | C | P-O3'-C3' | 6.88 | 127.96 | 119.70 |
| 81 | DA | 376 | G | O4'-C1'-N9 | 6.88 | 113.70 | 108.20 |
| 81 | DA | 1747 | G | O3'-P-O5' | -6.88 | 90.93 | 104.00 |
| 81 | DA | 1766 | G | P-O5'-C5' | -6.88 | 109.89 | 120.90 |
| 81 | DA | 2757 | U | C2'-C3'-O3' | 6.88 | 124.71 | 113.70 |
| 81 | DA | 3149 | G | O4'-C4'-C3' | -6.88 | 97.12 | 104.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 3071 | U | N1-C1'-C2' | 6.88 | 122.94 | 114.00 |
| 33 | BD | 100 | PHE | CB-CG-CD2 | 6.88 | 125.62 | 120.80 |
| 20 | AS | 59 | ALA | CB-CA-C | -6.88 | 99.78 | 110.10 |
| 83 | DC | 69 | G | O4'-C1'-N9 | 6.88 | 113.70 | 108.20 |
| 78 | CA | 96 | G | O4'-C1'-N9 | 6.88 | 113.70 | 108.20 |
| 81 | DA | 2162 | U | C5'-C4'-C3' | -6.88 | 105.00 | 116.00 |
| 12 | AK | 32 | ASP | CB-CG-OD1 | 6.87 | 124.49 | 118.30 |
| 29 | AU | 29 | HIS | CB-CA-C | -6.87 | 96.65 | 110.40 |
| 43 | BP | 80 | THR | CB-CA-C | -6.87 | 93.04 | 111.60 |
| 81 | DA | 43 | A | C1'-O4'-C4' | -6.87 | 104.40 | 109.90 |
| 81 | DA | 1239 | C | N1-C1'-C2' | 6.87 | 122.94 | 114.00 |
| 81 | DA | 2452 | G | P-O3'-C3' | 6.87 | 127.95 | 119.70 |
| 81 | DA | 3250 | U | P-O5'-C5' | 6.87 | 131.90 | 120.90 |
| 83 | DC | 42 | A | N9-C1'-C2' | 6.87 | 122.94 | 114.00 |
| 81 | DA | 422 | A | N9-C1'-C2' | -6.87 | 104.44 | 112.00 |
| 81 | DA | 1766 | G | N1-C6-O6 | 6.87 | 124.02 | 119.90 |
| 81 | DA | 1826 | C | O4'-C4'-C3' | -6.87 | 97.13 | 104.00 |
| 81 | DA | 2922 | G | C1'-O4'-C4' | -6.87 | 104.40 | 109.90 |
| 81 | DA | 3092 | C | C1'-O4'-C4' | 6.87 | 115.40 | 109.90 |
| 78 | CA | 690 | G | O4'-C1'-N9 | 6.87 | 113.70 | 108.20 |
| 81 | DA | 897 | U | O4'-C1'-N1 | 6.87 | 113.70 | 108.20 |
| 81 | DA | 2381 | G | C5'-C4'-C3' | -6.87 | 105.01 | 116.00 |
| 81 | DA | 2874 | G | C5'-C4'-C3' | -6.87 | 105.01 | 116.00 |
| 20 | AS | 45 | MET | O-C-N | -6.87 | 108.05 | 121.10 |
| 39 | BJ | 123 | ARG | NE-CZ-NH2 | 6.87 | 123.73 | 120.30 |
| 61 | Bj | 39 | GLN | CG-CD-OE1 | 6.87 | 135.34 | 121.60 |
| 78 | CA | 1624 | C | C3'-C2'-C1' | 6.87 | 106.99 | 101.50 |
| 81 | DA | 1180 | A | C2'-C3'-O3' | 6.87 | 124.69 | 113.70 |
| 81 | DA | 1907 | C | C3'-C2'-C1' | 6.87 | 107.00 | 101.50 |
| 81 | DA | 1972 | A | C4'-C3'-C2' | -6.87 | 95.73 | 102.60 |
| 83 | DC | 26 | C | P-O3'-C3' | 6.87 | 127.94 | 119.70 |
| 37 | BH | 221 | ASN | CA-CB-CG | 6.87 | 128.51 | 113.40 |
| 78 | CA | 1657 | U | O4'-C1'-N1 | 6.87 | 113.69 | 108.20 |
| 81 | DA | 3052 | G | C1'-O4'-C4' | -6.87 | 104.41 | 109.90 |
| 26 | AZ | 10 | ARG | NE-CZ-NH1 | -6.87 | 116.87 | 120.30 |
| 81 | DA | 322 | U | O4'-C1'-N1 | 6.87 | 113.69 | 108.20 |
| 81 | DA | 1115 | G | C1'-O4'-C4' | 6.87 | 115.39 | 109.90 |
| 81 | DA | 1366 | A | C3'-C2'-C1' | 6.87 | 106.99 | 101.50 |
| 82 | DB | 21 | C | C3'-C2'-C1' | 6.87 | 106.99 | 101.50 |
| 36 | BF | 91 | ARG | NE-CZ-NH1 | 6.86 | 123.73 | 120.30 |
| 52 | BY | 2 | ALA | CB-CA-C | 6.86 | 120.39 | 110.10 |
| 53 | Ba | 57 | HIS | CA-C-N | -6.86 | 102.47 | 116.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 56 | Bf | 65 | THR | N-CA-CB | 6.86 | 123.34 | 110.30 |
| 78 | CA | 658 | C | O4'-C1'-N1 | -6.86 | 102.71 | 108.20 |
| 78 | CA | 659 | C | O5'-P-OP1 | 6.86 | 118.94 | 110.70 |
| 81 | DA | 172 | G | O5'-P-OP1 | -6.86 | 99.52 | 105.70 |
| 81 | DA | 835 | G | P-O5'-C5' | 6.86 | 131.88 | 120.90 |
| 81 | DA | 1368 | U | O4'-C1'-N1 | 6.86 | 113.69 | 108.20 |
| 81 | DA | 2633 | U | O5'-C5'-C4' | -6.86 | 98.66 | 111.70 |
| 81 | DA | 2962 | U | O4'-C1'-N1 | 6.86 | 113.69 | 108.20 |
| 13 | AL | 120 | VAL | N-CA-C | -6.86 | 92.47 | 111.00 |
| 81 | DA | 70 | A | P-O3'-C3' | 6.86 | 127.94 | 119.70 |
| 81 | DA | 2860 | U | O4'-C1'-C2' | -6.86 | 98.94 | 105.80 |
| 29 | AU | 35 | VAL | CA-C-N | 6.86 | 132.29 | 117.20 |
| 69 | Br | 103 | ALA | N-CA-C | 6.86 | 129.52 | 111.00 |
| 81 | DA | 239 | G | P-O3'-C3' | -6.86 | 111.47 | 119.70 |
| 82 | DB | 3 | A | O4'-C1'-C2' | 6.86 | 113.77 | 107.60 |
| 13 | AL | 86 | PHE | CB-CG-CD1 | -6.86 | 116.00 | 120.80 |
| 78 | CA | 119 | A | C4'-C3'-O3' | 6.86 | 126.72 | 113.00 |
| 81 | DA | 664 | U | P-O3'-C3' | -6.86 | 111.47 | 119.70 |
| 81 | DA | 2055 | U | O4'-C1'-N1 | 6.86 | 113.69 | 108.20 |
| 78 | CA | 1682 | U | P-O5'-C5' | 6.86 | 131.87 | 120.90 |
| 30 | BA | 41 | TYR | CD1-CE1-CZ | 6.86 | 125.97 | 119.80 |
| 78 | CA | 1703 | C | O4'-C1'-C2' | -6.86 | 98.94 | 105.80 |
| 81 | DA | 1181 | U | N1-C1'-C2' | -6.86 | 104.46 | 112.00 |
| 83 | DC | 4 | U | O4'-C1'-C2' | -6.86 | 98.94 | 105.80 |
| 11 | AJ | 114 | VAL | CB-CA-C | -6.85 | 98.38 | 111.40 |
| 43 | BP | 117 | ASN | N-CA-C | 6.85 | 129.50 | 111.00 |
| 78 | CA | 1659 | A | C3'-C2'-C1' | 6.85 | 106.98 | 101.50 |
| 83 | DC | 63 | G | O4'-C1'-N9 | 6.85 | 113.68 | 108.20 |
| 4 | AD | 218 | PHE | N-CA-CB | 6.85 | 122.93 | 110.60 |
| 78 | CA | 318 | U | N1-C1'-C2' | 6.85 | 122.91 | 114.00 |
| 78 | CA | 685 | A | C1'-O4'-C4' | -6.85 | 104.42 | 109.90 |
| 78 | CA | 1535 | U | C5'-C4'-C3' | -6.85 | 105.04 | 116.00 |
| 81 | DA | 687 | U | O4'-C1'-N1 | 6.85 | 113.68 | 108.20 |
| 81 | DA | 733 | G | C5-C6-O6 | -6.85 | 124.49 | 128.60 |
| 81 | DA | 885 | U | O4'-C1'-N1 | 6.85 | 113.68 | 108.20 |
| 81 | DA | 943 | U | O4'-C1'-N1 | 6.85 | 113.68 | 108.20 |
| 33 | BD | 194 | TYR | CB-CG-CD1 | 6.85 | 125.11 | 121.00 |
| 78 | CA | 1424 | A | C5'-C4'-C3' | -6.85 | 105.04 | 116.00 |
| 81 | DA | 949 | C | O4'-C1'-C2' | -6.85 | 98.95 | 105.80 |
| 81 | DA | 3067 | C | P-O5'-C5' | -6.85 | 109.94 | 120.90 |
| 19 | AR | 123 | TYR | CB-CG-CD1 | 6.85 | 125.11 | 121.00 |
| 78 | CA | 295 | A | O5'-C5'-C4' | -6.85 | 98.69 | 111.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 304 | U | O4'-C1'-C2' | -6.85 | 98.95 | 105.80 |
| 78 | CA | 833 | U | C3'-C2'-C1' | -6.85 | 96.02 | 101.50 |
| 78 | CA | 1437 | U | C5'-C4'-C3' | 6.85 | 126.96 | 116.00 |
| 78 | CA | 1632 | C | C3'-C2'-C1' | 6.85 | 106.98 | 101.50 |
| 35 | BG | 79 | VAL | CG1-CB-CG2 | 6.84 | 121.85 | 110.90 |
| 50 | BX | 30 | ALA | N-CA-CB | 6.84 | 119.68 | 110.10 |
| 81 | DA | 912 | G | P-O3'-C3' | 6.84 | 127.91 | 119.70 |
| 81 | DA | 1791 | C | O4'-C1'-N1 | 6.84 | 113.68 | 108.20 |
| 81 | DA | 2707 | C | C4'-C3'-C2' | -6.84 | 95.76 | 102.60 |
| 83 | DC | 29 | C | C5'-C4'-O4' | -6.84 | 100.89 | 109.10 |
| 31 | BB | 1 | MET | CB-CA-C | 6.84 | 124.08 | 110.40 |
| 79 | CB | 22 | G | C1'-O4'-C4' | -6.84 | 104.43 | 109.90 |
| 69 | Br | 64 | THR | N-CA-CB | 6.84 | 123.30 | 110.30 |
| 78 | CA | 294 | C | P-O3'-C3' | 6.84 | 127.91 | 119.70 |
| 78 | CA | 1570 | A | P-O5'-C5' | -6.84 | 109.95 | 120.90 |
| 81 | DA | 847 | A | N9-C1'-C2' | 6.84 | 122.89 | 114.00 |
| 78 | CA | 173 | A | N9-C1'-C2' | -6.84 | 104.48 | 112.00 |
| 78 | CA | 1345 | A | C3'-C2'-C1' | 6.84 | 106.97 | 101.50 |
| 81 | DA | 2100 | A | C1'-O4'-C4' | -6.84 | 104.43 | 109.90 |
| 78 | CA | 326 | G | C5'-C4'-C3' | 6.84 | 126.94 | 116.00 |
| 78 | CA | 1712 | A | N9-C1'-C2' | -6.84 | 104.48 | 112.00 |
| 81 | DA | 1335 | C | O4'-C1'-C2' | -6.84 | 98.96 | 105.80 |
| 74 | BQ | 199 | ILE | N-CA-CB | 6.84 | 126.53 | 110.80 |
| 78 | CA | 1319 | A | O4'-C1'-N9 | 6.84 | 113.67 | 108.20 |
| 81 | DA | 339 | C | C5'-C4'-C3' | -6.84 | 105.06 | 116.00 |
| 81 | DA | 1015 | U | C1'-O4'-C4' | 6.84 | 115.37 | 109.90 |
| 81 | DA | 1427 | U | P-O5'-C5' | -6.83 | 109.96 | 120.90 |
| 81 | DA | 626 | U | C4'-C3'-C2' | -6.83 | 95.77 | 102.60 |
| 81 | DA | 1620 | U | C1'-O4'-C4' | -6.83 | 104.43 | 109.90 |
| 6 | AE | 31 | GLU | CB-CA-C | 6.83 | 124.06 | 110.40 |
| 78 | CA | 491 | C | O4'-C1'-N1 | 6.83 | 113.67 | 108.20 |
| 81 | DA | 846 | A | C3'-C2'-C1' | 6.83 | 106.96 | 101.50 |
| 81 | DA | 1003 | A | N9-C1'-C2' | -6.83 | 104.48 | 112.00 |
| 78 | CA | 1060 | U | O4'-C1'-N1 | 6.83 | 113.66 | 108.20 |
| 81 | DA | 548 | G | C1'-O4'-C4' | -6.83 | 104.44 | 109.90 |
| 81 | DA | 1217 | A | P-O3'-C3' | 6.83 | 127.90 | 119.70 |
| 83 | DC | 54 | A | P-O5'-C5' | 6.83 | 131.83 | 120.90 |
| 5 | AC | 12 | TYR | CB-CG-CD2 | -6.83 | 116.90 | 121.00 |
| 43 | BP | 67 | ARG | N-CA-CB | 6.83 | 122.89 | 110.60 |
| 81 | DA | 2069 | G | O4'-C1'-N9 | 6.83 | 113.66 | 108.20 |
| 8 | AF | 148 | ARG | CG-CD-NE | -6.83 | 97.46 | 111.80 |
| 50 | BX | 138 | ARG | NE-CZ-NH1 | -6.83 | 116.89 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2189 | U | O4'-C1'-N1 | 6.83 | 113.66 | 108.20 |
| 10 | AI | 92 | TYR | CB-CG-CD2 | -6.83 | 116.91 | 121.00 |
| 69 | Br | 62 | ALA | N-CA-C | -6.83 | 92.57 | 111.00 |
| 78 | CA | 437 | A | P-O3'-C3' | 6.83 | 127.89 | 119.70 |
| 10 | AI | 20 | ALA | N-CA-CB | 6.82 | 119.65 | 110.10 |
| 81 | DA | 224 | C | N1-C1'-C2' | 6.82 | 122.87 | 114.00 |
| 82 | DB | 29 | U | N1-C1'-C2' | 6.82 | 122.87 | 114.00 |
| 43 | BP | 96 | ARG | NE-CZ-NH1 | 6.82 | 123.71 | 120.30 |
| 78 | CA | 893 | U | C4'-C3'-C2' | -6.82 | 95.78 | 102.60 |
| 78 | CA | 1312 | A | O4'-C1'-N9 | 6.82 | 113.66 | 108.20 |
| 78 | CA | 1636 | C | O4'-C1'-C2' | -6.82 | 98.98 | 105.80 |
| 81 | DA | 1516 | C | O4'-C1'-N1 | 6.82 | 113.66 | 108.20 |
| 31 | BB | 76 | PHE | CZ-CE2-CD2 | -6.82 | 111.92 | 120.10 |
| 78 | CA | 368 | U | O3'-P-O5' | -6.82 | 91.05 | 104.00 |
| 79 | CB | 75 | A | C1'-O4'-C4' | 6.82 | 115.35 | 109.90 |
| 81 | DA | 181 | U | P-O3'-C3' | 6.82 | 127.88 | 119.70 |
| 81 | DA | 1039 | U | O4'-C1'-N1 | 6.82 | 113.65 | 108.20 |
| 81 | DA | 2335 | G | O4'-C1'-C2' | 6.82 | 113.74 | 107.60 |
| 82 | DB | 96 | A | C1'-O4'-C4' | 6.82 | 115.35 | 109.90 |
| 78 | CA | 925 | G | O4'-C1'-N9 | 6.82 | 113.65 | 108.20 |
| 78 | CA | 1067 | C | C2'-C3'-O3' | 6.82 | 124.61 | 113.70 |
| 44 | BO | 149 | ALA | N-CA-CB | 6.81 | 119.64 | 110.10 |
| 78 | CA | 1063 | U | O4'-C1'-N1 | 6.81 | 113.65 | 108.20 |
| 81 | DA | 2499 | U | C3'-C2'-C1' | 6.81 | 106.95 | 101.50 |
| 81 | DA | 2593 | A | O4'-C1'-N9 | 6.81 | 113.65 | 108.20 |
| 6 | AE | 98 | PHE | CB-CG-CD2 | 6.81 | 125.57 | 120.80 |
| 63 | Bm | 73 | THR | N-CA-CB | 6.81 | 123.25 | 110.30 |
| 78 | CA | 1168 | U | O4'-C1'-N1 | 6.81 | 113.65 | 108.20 |
| 47 | BU | 56 | PHE | CB-CA-C | 6.81 | 124.02 | 110.40 |
| 78 | CA | 29 | U | C5'-C4'-C3' | -6.81 | 105.10 | 116.00 |
| 81 | DA | 1532 | C | O4'-C1'-N1 | 6.81 | 113.65 | 108.20 |
| 50 | BX | 27 | ARG | NE-CZ-NH2 | -6.81 | 116.89 | 120.30 |
| 78 | CA | 636 | A | P-O3'-C3' | 6.81 | 127.87 | 119.70 |
| 79 | CB | 24 | A | P-O3'-C3' | 6.81 | 127.87 | 119.70 |
| 81 | DA | 768 | C | O4'-C4'-C3' | -6.81 | 97.19 | 104.00 |
| 81 | DA | 1827 | C | O4'-C1'-N1 | 6.81 | 113.65 | 108.20 |
| 78 | CA | 253 | A | O4'-C1'-C2' | 6.81 | 113.73 | 107.60 |
| 81 | DA | 400 | G | O4'-C1'-N9 | 6.81 | 113.65 | 108.20 |
| 81 | DA | 2505 | U | O4'-C4'-C3' | -6.81 | 97.19 | 104.00 |
| 81 | DA | 193 | C | N1-C1'-C2' | 6.81 | 122.85 | 114.00 |
| 81 | DA | 2353 | G | C1'-O4'-C4' | -6.81 | 104.45 | 109.90 |
| 17 | AQ | 132 | TYR | CB-CG-CD2 | -6.80 | 116.92 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 29 | AU | 17 | LEU | CB-CA-C | -6.80 | 97.27 | 110.20 |
| 81 | DA | 424 | G | P-O5'-C5' | 6.80 | 131.79 | 120.90 |
| 81 | DA | 2152 | A | C5'-C4'-O4' | -6.80 | 100.94 | 109.10 |
| 81 | DA | 2226 | U | O4'-C1'-N1 | 6.80 | 113.64 | 108.20 |
| 20 | AS | 1 | MET | CB-CA-C | 6.80 | 124.00 | 110.40 |
| 81 | DA | 887 | G | N9-C1'-C2' | 6.80 | 122.84 | 114.00 |
| 81 | DA | 2506 | U | N1-C1'-C2' | 6.80 | 122.84 | 114.00 |
| 60 | Bi | 32 | ALA | N-CA-CB | 6.80 | 119.62 | 110.10 |
| 78 | CA | 1567 | U | O4'-C1'-N1 | 6.80 | 113.64 | 108.20 |
| 81 | DA | 1089 | G | C1'-O4'-C4' | -6.80 | 104.46 | 109.90 |
| 32 | BC | 334 | ARG | NE-CZ-NH1 | 6.80 | 123.70 | 120.30 |
| 81 | DA | 527 | A | O4'-C1'-C2' | -6.80 | 99.00 | 105.80 |
| 81 | DA | 836 | A | C3'-C2'-C1' | 6.80 | 106.94 | 101.50 |
| 13 | AL | 92 | CYS | CA-C-N | -6.80 | 102.25 | 117.20 |
| 78 | CA | 215 | A | O5'-C5'-C4' | -6.80 | 98.78 | 111.70 |
| 81 | DA | 1324 | U | P-O3'-C3' | 6.80 | 127.86 | 119.70 |
| 81 | DA | 2785 | A | C5'-C4'-C3' | -6.80 | 105.12 | 116.00 |
| 81 | DA | 2906 | C | P-O3'-C3' | -6.80 | 111.54 | 119.70 |
| 25 | AY | 48 | VAL | CB-CA-C | 6.80 | 124.31 | 111.40 |
| 78 | CA | 33 | U | O4'-C1'-N1 | 6.80 | 113.64 | 108.20 |
| 78 | CA | 1209 | C | C3'-C2'-C1' | 6.80 | 106.94 | 101.50 |
| 81 | DA | 988 | U | C1'-O4'-C4' | 6.80 | 115.34 | 109.90 |
| 81 | DA | 2295 | A | N9-C1'-C2' | 6.80 | 122.83 | 114.00 |
| 69 | Br | 47 | GLN | CA-C-O | -6.79 | 105.83 | 120.10 |
| 81 | DA | 1484 | U | C3'-C2'-C1' | 6.79 | 106.94 | 101.50 |
| 81 | DA | 1878 | G | O4'-C1'-N9 | 6.79 | 113.64 | 108.20 |
| 19 | AR | 123 | TYR | CB-CG-CD2 | -6.79 | 116.92 | 121.00 |
| 78 | CA | 1290 | U | O4'-C1'-N1 | 6.79 | 113.64 | 108.20 |
| 78 | CA | 1437 | U | O3'-P-O5' | 6.79 | 116.91 | 104.00 |
| 78 | CA | 1690 | G | C5'-C4'-O4' | -6.79 | 100.95 | 109.10 |
| 81 | DA | 45 | A | C4'-C3'-C2' | -6.79 | 95.81 | 102.60 |
| 81 | DA | 1020 | G | O4'-C1'-N9 | 6.79 | 113.64 | 108.20 |
| 81 | DA | 1690 | C | O4'-C4'-C3' | -6.79 | 97.21 | 104.00 |
| 13 | AL | 73 | ARG | NE-CZ-NH1 | 6.79 | 123.70 | 120.30 |
| 78 | CA | 303 | U | O4'-C1'-N1 | 6.79 | 113.63 | 108.20 |
| 78 | CA | 1221 | A | P-O3'-C3' | 6.79 | 127.85 | 119.70 |
| 81 | DA | 984 | G | O4'-C1'-C2' | -6.79 | 99.01 | 105.80 |
| 81 | DA | 1073 | U | P-O3'-C3' | -6.79 | 111.55 | 119.70 |
| 81 | DA | 2369 | G | N9-C1'-C2' | -6.79 | 104.53 | 112.00 |
| 81 | DA | 2542 | U | O4'-C1'-N1 | 6.79 | 113.63 | 108.20 |
| 81 | DA | 2908 | G | C1'-O4'-C4' | -6.79 | 104.47 | 109.90 |
| 81 | DA | 2990 | G | N9-C1'-C2' | -6.79 | 104.53 | 112.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 3321 | C | O4'-C1'-C2' | -6.79 | 99.01 | 105.80 |
| 32 | BC | 97 | ARG | N-CA-CB | 6.79 | 122.82 | 110.60 |
| 81 | DA | 977 | C | N1-C1'-C2' | 6.79 | 122.83 | 114.00 |
| 78 | CA | 947 | U | C3'-C2'-C1' | 6.79 | 106.93 | 101.50 |
| 81 | DA | 3299 | A | N9-C1'-C2' | -6.79 | 104.53 | 112.00 |
| 20 | AS | 91 | TYR | N-CA-C | 6.79 | 129.32 | 111.00 |
| 81 | DA | 345 | G | C1'-O4'-C4' | -6.79 | 104.47 | 109.90 |
| 81 | DA | 577 | C | O4'-C1'-N1 | -6.79 | 102.77 | 108.20 |
| 81 | DA | 2745 | G | P-O5'-C5' | 6.79 | 131.76 | 120.90 |
| 77 | BI | 153 | ARG | NE-CZ-NH1 | 6.79 | 123.69 | 120.30 |
| 78 | CA | 605 | A | C1'-O4'-C4' | -6.79 | 104.47 | 109.90 |
| 78 | CA | 1075 | C | C3'-C2'-C1' | 6.79 | 106.93 | 101.50 |
| 6 | AE | 82 | ASN | N-CA-C | -6.78 | 92.69 | 111.00 |
| 33 | BD | 355 | PHE | CA-C-O | -6.78 | 105.85 | 120.10 |
| 43 | BP | 26 | ARG | NE-CZ-NH2 | -6.78 | 116.91 | 120.30 |
| 78 | CA | 435 | C | C5'-C4'-C3' | -6.78 | 105.15 | 116.00 |
| 78 | CA | 1050 | G | O4'-C1'-N9 | 6.78 | 113.63 | 108.20 |
| 78 | CA | 1564 | U | C3'-C2'-C1' | 6.78 | 106.93 | 101.50 |
| 81 | DA | 2297 | U | C3'-C2'-C1' | 6.78 | 106.93 | 101.50 |
| 81 | DA | 929 | A | O4'-C1'-N9 | 6.78 | 113.63 | 108.20 |
| 81 | DA | 2170 | U | O4'-C1'-C2' | -6.78 | 99.02 | 105.80 |
| 82 | DB | 117 | C | C3'-C2'-C1' | 6.78 | 106.93 | 101.50 |
| 78 | CA | 1645 | G | C1'-O4'-C4' | -6.78 | 104.47 | 109.90 |
| 81 | DA | 2251 | G | N9-C1'-C2' | 6.78 | 122.82 | 114.00 |
| 81 | DA | 2672 | G | O4'-C4'-C3' | -6.78 | 97.22 | 104.00 |
| 81 | DA | 2385 | G | C1'-O4'-C4' | -6.78 | 104.48 | 109.90 |
| 35 | BG | 147 | ALA | C-N-CA | 6.78 | 138.65 | 121.70 |
| 78 | CA | 117 | U | O4'-C1'-C2' | -6.78 | 99.02 | 105.80 |
| 78 | CA | 885 | G | C3'-C2'-C1' | 6.78 | 106.92 | 101.50 |
| 78 | CA | 1324 | G | C5'-C4'-C3' | 6.78 | 126.84 | 116.00 |
| 81 | DA | 491 | C | O4'-C1'-C2' | -6.78 | 99.02 | 105.80 |
| 81 | DA | 514 | G | P-O3'-C3' | 6.78 | 127.83 | 119.70 |
| 81 | DA | 1283 | C | O4'-C1'-C2' | -6.78 | 99.02 | 105.80 |
| 81 | DA | 1617 | G | O4'-C1'-N9 | 6.78 | 113.62 | 108.20 |
| 81 | DA | 2485 | A | O4'-C1'-N9 | 6.78 | 113.62 | 108.20 |
| 81 | DA | 3316 | A | P-O3'-C3' | 6.78 | 127.83 | 119.70 |
| 81 | DA | 1647 | A | C1'-O4'-C4' | 6.77 | 115.32 | 109.90 |
| 81 | DA | 927 | C | N1-C1'-C2' | 6.77 | 122.80 | 114.00 |
| 1 | Aa | 186 | PHE | CB-CG-CD2 | -6.77 | 116.06 | 120.80 |
| 81 | DA | 32 | U | C1'-O4'-C4' | -6.77 | 104.48 | 109.90 |
| 81 | DA | 2049 | A | C1'-O4'-C4' | 6.77 | 115.32 | 109.90 |
| 81 | DA | 2785 | A | N9-C1'-C2' | 6.77 | 122.80 | 114.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 3081 | C | C1'-O4'-C4' | -6.77 | 104.48 | 109.90 |
| 81 | DA | 3365 | U | C3'-C2'-C1' | 6.77 | 106.92 | 101.50 |
| 82 | DB | 43 | A | O5'-P-OP2 | -6.77 | 99.61 | 105.70 |
| 43 | BP | 166 | ALA | N-CA-C | 6.77 | 129.27 | 111.00 |
| 44 | BO | 57 | GLY | C-N-CA | -6.77 | 104.78 | 121.70 |
| 77 | BI | 115 | MET | C-N-CA | 6.77 | 138.62 | 121.70 |
| 78 | CA | 434 | G | N9-C1'-C2' | -6.77 | 104.56 | 112.00 |
| 78 | CA | 1506 | G | P-O5'-C5' | -6.77 | 110.07 | 120.90 |
| 82 | DB | 12 | A | N9-C1'-C2' | -6.77 | 104.56 | 112.00 |
| 26 | AZ | 44 | PHE | N-CA-CB | 6.76 | 122.77 | 110.60 |
| 78 | CA | 868 | G | C1'-O4'-C4' | -6.76 | 104.49 | 109.90 |
| 81 | DA | 104 | G | C5'-C4'-C3' | 6.76 | 126.82 | 116.00 |
| 81 | DA | 776 | U | O4'-C1'-N1 | 6.76 | 113.61 | 108.20 |
| 81 | DA | 2207 | A | N9-C1'-C2' | -6.76 | 104.56 | 112.00 |
| 81 | DA | 2721 | A | C3'-C2'-C1' | 6.76 | 106.91 | 101.50 |
| 81 | DA | 3165 | A | P-O3'-C3' | 6.76 | 127.82 | 119.70 |
| 82 | DB | 92 | A | O4'-C1'-N9 | 6.76 | 113.61 | 108.20 |
| 31 | BB | 70 | ARG | CB-CA-C | -6.76 | 96.87 | 110.40 |
| 81 | DA | 1276 | U | N1-C1'-C2' | 6.76 | 122.79 | 114.00 |
| 81 | DA | 2183 | A | O4'-C1'-N9 | 6.76 | 113.61 | 108.20 |
| 57 | Be | 149 | TYR | CB-CG-CD2 | -6.76 | 116.94 | 121.00 |
| 78 | CA | 574 | G | C5-C6-O6 | -6.76 | 124.54 | 128.60 |
| 81 | DA | 849 | C | O4'-C1'-C2' | -6.76 | 99.04 | 105.80 |
| 81 | DA | 1377 | G | O4'-C1'-N9 | 6.76 | 113.61 | 108.20 |
| 41 | BN | 100 | ALA | N-CA-CB | 6.76 | 119.56 | 110.10 |
| 63 | Bm | 29 | LEU | CB-CA-C | 6.76 | 123.04 | 110.20 |
| 78 | CA | 1199 | G | C1'-O4'-C4' | 6.76 | 115.31 | 109.90 |
| 78 | CA | 1479 | A | C5'-C4'-C3' | 6.76 | 126.81 | 116.00 |
| 81 | DA | 635 | G | P-O3'-C3' | -6.76 | 111.59 | 119.70 |
| 81 | DA | 1320 | C | O4'-C1'-C2' | -6.76 | 99.04 | 105.80 |
| 81 | DA | 1754 | G | C5-C6-O6 | -6.76 | 124.54 | 128.60 |
| 43 | BP | 143 | ARG | NE-CZ-NH2 | -6.76 | 116.92 | 120.30 |
| 78 | CA | 667 | U | C1'-O4'-C4' | 6.76 | 115.31 | 109.90 |
| 78 | CA | 1412 | G | C3'-C2'-C1' | 6.76 | 106.91 | 101.50 |
| 78 | CA | 1752 | U | C1'-O4'-C4' | -6.76 | 104.49 | 109.90 |
| 81 | DA | 2534 | G | P-O3'-C3' | 6.76 | 127.81 | 119.70 |
| 81 | DA | 3141 | A | O5'-C5'-C4' | -6.76 | 98.86 | 111.70 |
| 83 | DC | 53 | U | O3'-P-O5' | 6.76 | 116.84 | 104.00 |
| 32 | BC | 69 | LYS | C-N-CA | 6.76 | 138.59 | 121.70 |
| 37 | BH | 227 | ASP | CB-CG-OD2 | 6.76 | 124.38 | 118.30 |
| 78 | CA | 1141 | G | O4'-C1'-C2' | 6.76 | 113.68 | 107.60 |
| 81 | DA | 106 | A | O4'-C1'-N9 | 6.76 | 113.61 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2668 | U | O4'-C1'-C2' | -6.76 | 99.04 | 105.80 |
| 81 | DA | 2755 | C | O4'-C1'-N1 | 6.76 | 113.61 | 108.20 |
| 81 | DA | 3050 | U | O3'-P-O5' | -6.76 | 91.16 | 104.00 |
| 78 | CA | 1564 | U | N1-C1'-C2' | 6.75 | 122.78 | 114.00 |
| 81 | DA | 230 | U | O4'-C1'-C2' | -6.75 | 99.05 | 105.80 |
| 81 | DA | 1773 | C | C1'-O4'-C4' | -6.75 | 104.50 | 109.90 |
| 81 | DA | 2820 | A | O4'-C1'-N9 | 6.75 | 113.60 | 108.20 |
| 81 | DA | 3093 | C | O4'-C1'-C2' | -6.75 | 99.05 | 105.80 |
| 83 | DC | 30 | G | C3'-C2'-C1' | -6.75 | 96.10 | 101.50 |
| 78 | CA | 37 | U | O4'-C1'-C2' | -6.75 | 99.05 | 105.80 |
| 78 | CA | 174 | U | P-O3'-C3' | 6.75 | 127.81 | 119.70 |
| 81 | DA | 3130 | A | O4'-C1'-C2' | 6.75 | 113.68 | 107.60 |
| 47 | BU | 140 | ILE | CA-C-N | 6.75 | 132.05 | 117.20 |
| 81 | DA | 2394 | G | C1'-O4'-C4' | -6.75 | 104.50 | 109.90 |
| 11 | AJ | 68 | ARG | CB-CA-C | 6.75 | 123.90 | 110.40 |
| 53 | Ba | 15 | ARG | C-N-CA | -6.75 | 108.12 | 122.30 |
| 60 | Bi | 67 | LYS | N-CA-CB | 6.75 | 122.75 | 110.60 |
| 81 | DA | 1050 | U | P-O5'-C5' | 6.75 | 131.70 | 120.90 |
| 78 | CA | 1353 | U | N1-C1'-C2' | 6.75 | 122.77 | 114.00 |
| 78 | CA | 1509 | C | C5-C4-N4 | -6.75 | 115.48 | 120.20 |
| 79 | CB | 12 | U | P-O5'-C5' | -6.75 | 110.10 | 120.90 |
| 81 | DA | 608 | A | C5'-C4'-O4' | 6.75 | 117.20 | 109.10 |
| 81 | DA | 2071 | A | C2'-C3'-O3' | -6.75 | 94.65 | 109.50 |
| 4 | AD | 82 | TYR | N-CA-C | 6.75 | 129.22 | 111.00 |
| 34 | BE | 90 | GLN | N-CA-C | -6.75 | 92.79 | 111.00 |
| 43 | BP | 175 | ASN | CB-CA-C | -6.75 | 96.91 | 110.40 |
| 43 | BP | 181 | ASN | N-CA-CB | 6.75 | 122.74 | 110.60 |
| 63 | Bm | 6 | LYS | CA-CB-CG | 6.75 | 128.24 | 113.40 |
| 78 | CA | 253 | A | C3'-C2'-C1' | -6.75 | 96.10 | 101.50 |
| 78 | CA | 1110 | G | O4'-C1'-N9 | 6.75 | 113.60 | 108.20 |
| 78 | CA | 1197 | C | O4'-C1'-N1 | 6.75 | 113.60 | 108.20 |
| 81 | DA | 274 | G | N9-C1'-C2' | 6.75 | 122.77 | 114.00 |
| 81 | DA | 677 | A | C2'-C3'-O3' | 6.75 | 124.50 | 113.70 |
| 81 | DA | 2123 | G | O4'-C1'-N9 | 6.75 | 113.60 | 108.20 |
| 34 | BE | 61 | ARG | CA-CB-CG | 6.75 | 128.24 | 113.40 |
| 81 | DA | 2115 | G | C1'-O4'-C4' | -6.75 | 104.50 | 109.90 |
| 38 | Bs | 83 | ASN | CB-CA-C | 6.74 | 123.89 | 110.40 |
| 81 | DA | 356 | C | P-O3'-C3' | 6.74 | 127.79 | 119.70 |
| 81 | DA | 1258 | U | O4'-C1'-C2' | -6.74 | 99.06 | 105.80 |
| 81 | DA | 1286 | A | O4'-C1'-C2' | -6.74 | 99.06 | 105.80 |
| 83 | DC | 5 | G | O4'-C1'-N9 | -6.74 | 102.81 | 108.20 |
| 78 | CA | 1337 | A | O4'-C4'-C3' | -6.74 | 97.26 | 104.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 82 | DB | 48 | A | P-O3'-C3' | -6.74 | 111.61 | 119.70 |
| 78 | CA | 492 | A | C5-C6-N6 | -6.74 | 118.31 | 123.70 |
| 78 | CA | 1355 | C | O4'-C1'-N1 | 6.74 | 113.59 | 108.20 |
| 5 | AC | 157 | ASP | CB-CG-OD2 | -6.74 | 112.23 | 118.30 |
| 33 | BD | 203 | ARG | NE-CZ-NH1 | -6.74 | 116.93 | 120.30 |
| 43 | BP | 166 | ALA | N-CA-CB | -6.74 | 100.67 | 110.10 |
| 46 | BT | 114 | LYS | CB-CA-C | 6.74 | 123.88 | 110.40 |
| 78 | CA | 1673 | G | O4'-C1'-N9 | 6.74 | 113.59 | 108.20 |
| 81 | DA | 3161 | C | C3'-C2'-C1' | 6.74 | 106.89 | 101.50 |
| 83 | DC | 29 | C | O4'-C1'-N1 | 6.74 | 113.59 | 108.20 |
| 5 | AC | 78 | ARG | NE-CZ-NH1 | 6.74 | 123.67 | 120.30 |
| 13 | AL | 104 | LEU | CB-CG-CD2 | 6.74 | 122.45 | 111.00 |
| 78 | CA | 474 | A | O4'-C1'-N9 | 6.74 | 113.59 | 108.20 |
| 78 | CA | 1283 | U | O4'-C1'-N1 | 6.74 | 113.59 | 108.20 |
| 81 | DA | 1860 | G | O4'-C1'-N9 | 6.74 | 113.59 | 108.20 |
| 81 | DA | 1876 | U | C4'-C3'-C2' | -6.74 | 95.86 | 102.60 |
| 59 | Bh | 92 | TYR | CB-CG-CD2 | -6.73 | 116.96 | 121.00 |
| 78 | CA | 289 | U | O5'-C5'-C4' | 6.73 | 124.50 | 111.70 |
| 81 | DA | 2782 | U | O4'-C1'-N1 | 6.73 | 113.59 | 108.20 |
| 81 | DA | 3122 | A | O4'-C1'-C2' | -6.73 | 99.07 | 105.80 |
| 81 | DA | 19 | U | O4'-C1'-N1 | 6.73 | 113.59 | 108.20 |
| 81 | DA | 254 | A | O4'-C1'-C2' | -6.73 | 99.07 | 105.80 |
| 81 | DA | 995 | U | C3'-C2'-C1' | 6.73 | 106.89 | 101.50 |
| 82 | DB | 121 | U | O4'-C1'-C2' | -6.73 | 99.07 | 105.80 |
| 83 | DC | 87 | U | N1-C1'-C2' | 6.73 | 122.75 | 114.00 |
| 50 | BX | 106 | ASP | CB-CG-OD2 | -6.73 | 112.24 | 118.30 |
| 78 | CA | 1104 | U | O4'-C1'-N1 | 6.73 | 113.58 | 108.20 |
| 81 | DA | 1297 | C | C4'-C3'-C2' | -6.73 | 95.87 | 102.60 |
| 81 | DA | 1815 | U | O4'-C1'-N1 | 6.73 | 113.58 | 108.20 |
| 82 | DB | 48 | A | C5'-C4'-C3' | -6.73 | 105.23 | 116.00 |
| 78 | CA | 1381 | U | N1-C1'-C2' | -6.73 | 104.60 | 112.00 |
| 78 | CA | 1607 | G | C3'-C2'-C1' | 6.73 | 106.88 | 101.50 |
| 81 | DA | 255 | A | O4'-C1'-C2' | -6.73 | 99.07 | 105.80 |
| 81 | DA | 1258 | U | C1'-O4'-C4' | 6.73 | 115.28 | 109.90 |
| 81 | DA | 2237 | C | O4'-C1'-N1 | 6.73 | 113.58 | 108.20 |
| 32 | BC | 51 | ALA | CB-CA-C | -6.73 | 100.01 | 110.10 |
| 40 | BK | 130 | LYS | N-CA-CB | 6.73 | 122.71 | 110.60 |
| 53 | Ba | 55 | LYS | CA-CB-CG | 6.73 | 128.20 | 113.40 |
| 78 | CA | 173 | A | O4'-C4'-C3' | -6.73 | 97.27 | 104.00 |
| 78 | CA | 385 | A | O4'-C1'-N9 | 6.73 | 113.58 | 108.20 |
| 78 | CA | 853 | G | O4'-C1'-C2' | -6.73 | 99.07 | 105.80 |
| 78 | CA | 890 | C | N1-C1'-C2' | 6.73 | 122.75 | 114.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 1656 | U | C5'-C4'-C3' | 6.73 | 126.77 | 116.00 |
| 81 | DA | 846 | A | O4'-C1'-C2' | -6.73 | 99.07 | 105.80 |
| 81 | DA | 2102 | U | C3'-C2'-C1' | 6.73 | 106.88 | 101.50 |
| 81 | DA | 2392 | C | P-O3'-C3' | 6.73 | 127.77 | 119.70 |
| 42 | BM | 48 | ARG | CB-CA-C | -6.73 | 96.95 | 110.40 |
| 81 | DA | 678 | G | P-O5'-C5' | 6.73 | 131.66 | 120.90 |
| 41 | BN | 115 | PHE | CB-CG-CD1 | 6.72 | 125.51 | 120.80 |
| 74 | BQ | 145 | PHE | CB-CG-CD2 | -6.72 | 116.09 | 120.80 |
| 78 | CA | 314 | C | C1'-O4'-C4' | -6.72 | 104.52 | 109.90 |
| 78 | CA | 1452 | U | C1'-O4'-C4' | -6.72 | 104.52 | 109.90 |
| 78 | CA | 377 | G | O4'-C1'-N9 | 6.72 | 113.58 | 108.20 |
| 81 | DA | 1069 | C | C3'-C2'-C1' | 6.72 | 106.88 | 101.50 |
| 33 | BD | 349 | THR | CB-CA-C | 6.72 | 129.75 | 111.60 |
| 40 | BK | 198 | GLY | N-CA-C | 6.72 | 129.90 | 113.10 |
| 41 | BN | 98 | SER | N-CA-CB | 6.72 | 120.58 | 110.50 |
| 49 | BV | 113 | TYR | CB-CG-CD1 | -6.72 | 116.97 | 121.00 |
| 77 | BI | 106 | ALA | O-C-N | -6.72 | 111.78 | 123.20 |
| 81 | DA | 159 | A | O4'-C1'-C2' | -6.72 | 99.08 | 105.80 |
| 32 | BC | 344 | THR | CA-C-N | 6.72 | 131.98 | 117.20 |
| 78 | CA | 576 | G | C5-C6-O6 | -6.72 | 124.57 | 128.60 |
| 81 | DA | 1475 | A | P-O3'-C3' | 6.72 | 127.76 | 119.70 |
| 78 | CA | 1793 | G | C1'-O4'-C4' | -6.71 | 104.53 | 109.90 |
| 81 | DA | 486 | U | C5'-C4'-C3' | 6.71 | 126.74 | 116.00 |
| 81 | DA | 82 | C | O4'-C1'-N1 | 6.71 | 113.57 | 108.20 |
| 81 | DA | 462 | C | O4'-C1'-C2' | -6.71 | 99.09 | 105.80 |
| 81 | DA | 735 | A | OP2-P-O3' | 6.71 | 119.96 | 105.20 |
| 81 | DA | 2270 | A | O4'-C1'-C2' | -6.71 | 99.09 | 105.80 |
| 74 | BQ | 249 | ALA | CA-C-N | 6.71 | 131.96 | 117.20 |
| 78 | CA | 92 | A | C1'-O4'-C4' | -6.71 | 104.53 | 109.90 |
| 81 | DA | 2504 | U | C4'-C3'-C2' | 6.71 | 109.31 | 102.60 |
| 39 | BJ | 117 | ARG | NE-CZ-NH2 | -6.71 | 116.95 | 120.30 |
| 45 | BR | 38 | ARG | NE-CZ-NH1 | 6.71 | 123.65 | 120.30 |
| 81 | DA | 879 | U | O4'-C1'-N1 | 6.71 | 113.57 | 108.20 |
| 10 | AI | 122 | ARG | NE-CZ-NH2 | -6.71 | 116.95 | 120.30 |
| 78 | CA | 386 | G | P-O3'-C3' | 6.71 | 127.75 | 119.70 |
| 81 | DA | 702 | C | O4'-C1'-C2' | -6.71 | 99.09 | 105.80 |
| 83 | DC | 75 | G | O4'-C1'-N9 | 6.71 | 113.56 | 108.20 |
| 38 | Bs | 55 | LYS | CB-CA-C | -6.71 | 96.99 | 110.40 |
| 78 | CA | 468 | A | N9-C1'-C2' | 6.70 | 122.71 | 114.00 |
| 81 | DA | 143 | G | O4'-C1'-N9 | 6.70 | 113.56 | 108.20 |
| 81 | DA | 647 | A | O4'-C1'-N9 | -6.70 | 102.84 | 108.20 |
| 81 | DA | 1550 | C | O4'-C1'-C2' | -6.70 | 99.10 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 3150 | A | O5'-P-OP1 | 6.70 | 118.75 | 110.70 |
| 81 | DA | 146 | U | O3'-P-O5' | 6.70 | 116.73 | 104.00 |
| 81 | DA | 628 | A | P-O3'-C3' | 6.70 | 127.74 | 119.70 |
| 81 | DA | 1567 | U | C4'-C3'-C2' | -6.70 | 95.90 | 102.60 |
| 81 | DA | 1989 | U | C5'-C4'-C3' | -6.70 | 105.28 | 116.00 |
| 81 | DA | 3246 | G | C5'-C4'-C3' | 6.70 | 126.72 | 116.00 |
| 8 | AF | 27 | THR | N-CA-CB | -6.70 | 97.57 | 110.30 |
| 43 | BP | 120 | TRP | N-CA-C | 6.70 | 129.09 | 111.00 |
| 78 | CA | 433 | C | C3'-C2'-C1' | 6.70 | 106.86 | 101.50 |
| 81 | DA | 3248 | C | C3'-C2'-C1' | 6.70 | 106.86 | 101.50 |
| 10 | AI | 37 | THR | CA-CB-CG2 | -6.70 | 103.02 | 112.40 |
| 11 | AJ | 89 | ARG | N-CA-CB | 6.70 | 122.66 | 110.60 |
| 33 | BD | 148 | ILE | N-CA-C | -6.70 | 92.92 | 111.00 |
| 76 | BS | 66 | ILE | N-CA-C | 6.70 | 129.09 | 111.00 |
| 78 | CA | 343 | C | O4'-C1'-N1 | 6.70 | 113.56 | 108.20 |
| 81 | DA | 1178 | G | P-O5'-C5' | -6.70 | 110.18 | 120.90 |
| 81 | DA | 1206 | G | N9-C1'-C2' | -6.70 | 104.63 | 112.00 |
| 81 | DA | 2509 | U | N1-C1'-C2' | 6.70 | 122.71 | 114.00 |
| 20 | AS | 37 | VAL | N-CA-CB | 6.70 | 126.23 | 111.50 |
| 81 | DA | 2609 | A | C3'-C2'-C1' | 6.70 | 106.86 | 101.50 |
| 6 | AE | 69 | ILE | C-N-CA | 6.70 | 138.44 | 121.70 |
| 78 | CA | 1335 | U | O4'-C1'-N1 | 6.70 | 113.56 | 108.20 |
| 78 | CA | 1682 | U | O4'-C1'-N1 | 6.70 | 113.56 | 108.20 |
| 81 | DA | 1301 | A | N9-C1'-C2' | 6.70 | 122.70 | 114.00 |
| 81 | DA | 2352 | A | C3'-C2'-C1' | 6.70 | 106.86 | 101.50 |
| 81 | DA | 2471 | U | P-O5'-C5' | 6.70 | 131.61 | 120.90 |
| 82 | DB | 11 | C | C3'-C2'-C1' | 6.70 | 106.86 | 101.50 |
| 5 | AC | 18 | PRO | CA-N-CD | -6.69 | 102.13 | 111.50 |
| 66 | Bo | 7 | PHE | CB-CG-CD1 | 6.69 | 125.49 | 120.80 |
| 78 | CA | 1400 | A | C3'-C2'-C1' | 6.69 | 106.86 | 101.50 |
| 78 | CA | 1690 | G | C4'-C3'-C2' | 6.69 | 109.29 | 102.60 |
| 81 | DA | 681 | U | O4'-C1'-N1 | 6.69 | 113.56 | 108.20 |
| 81 | DA | 1784 | G | C4'-C3'-C2' | -6.69 | 95.91 | 102.60 |
| 20 | AS | 68 | ARG | C-N-CA | 6.69 | 138.43 | 121.70 |
| 78 | CA | 569 | C | N3-C4-N4 | 6.69 | 122.69 | 118.00 |
| 81 | DA | 30 | G | P-O3'-C3' | 6.69 | 127.73 | 119.70 |
| 81 | DA | 795 | G | O4'-C1'-N9 | 6.69 | 113.56 | 108.20 |
| 81 | DA | 1597 | C | C3'-C2'-C1' | 6.69 | 106.85 | 101.50 |
| 81 | DA | 2151 | C | O4'-C1'-N1 | 6.69 | 113.55 | 108.20 |
| 81 | DA | 2643 | A | O4'-C1'-N9 | 6.69 | 113.55 | 108.20 |
| 81 | DA | 2897 | A | P-O3'-C3' | 6.69 | 127.73 | 119.70 |
| 41 | BN | 63 | VAL | N-CA-C | -6.69 | 92.93 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 1446 | A | O4'-C1'-C2' | -6.69 | 99.11 | 105.80 |
| 81 | DA | 506 | U | O4'-C1'-C2' | -6.69 | 99.11 | 105.80 |
| 81 | DA | 1776 | G | P-O3'-C3' | -6.69 | 111.67 | 119.70 |
| 81 | DA | 2287 | C | O4'-C1'-C2' | -6.69 | 99.11 | 105.80 |
| 81 | DA | 3253 | G | P-O3'-C3' | 6.69 | 127.73 | 119.70 |
| 81 | DA | 880 | G | O4'-C1'-N9 | 6.69 | 113.55 | 108.20 |
| 81 | DA | 1772 | U | P-O3'-C3' | 6.69 | 127.73 | 119.70 |
| 81 | DA | 2050 | C | N1-C1'-C2' | 6.69 | 122.70 | 114.00 |
| 81 | DA | 3026 | G | O4'-C1'-N9 | 6.69 | 113.55 | 108.20 |
| 44 | BO | 128 | ARG | NE-CZ-NH2 | -6.69 | 116.96 | 120.30 |
| 61 | Bj | 45 | LEU | N-CA-CB | 6.69 | 123.77 | 110.40 |
| 78 | CA | 1277 | G | N9-C1'-C2' | -6.69 | 104.64 | 112.00 |
| 78 | CA | 1339 | C | O4'-C1'-N1 | 6.69 | 113.55 | 108.20 |
| 78 | CA | 1722 | A | P-O3'-C3' | 6.69 | 127.72 | 119.70 |
| 81 | DA | 1084 | A | O4'-C1'-N9 | 6.69 | 113.55 | 108.20 |
| 81 | DA | 2673 | A | O4'-C1'-N9 | -6.69 | 102.85 | 108.20 |
| 81 | DA | 3147 | G | C1'-O4'-C4' | -6.69 | 104.55 | 109.90 |
| 81 | DA | 3149 | G | P-O3'-C3' | -6.69 | 111.67 | 119.70 |
| 81 | DA | 3109 | G | O4'-C1'-N9 | 6.69 | 113.55 | 108.20 |
| 58 | Bg | 25 | PHE | N-CA-CB | 6.68 | 122.63 | 110.60 |
| 78 | CA | 1201 | G | C1'-O4'-C4' | -6.68 | 104.55 | 109.90 |
| 81 | DA | 1789 | G | O3'-P-O5' | 6.68 | 116.70 | 104.00 |
| 38 | Bs | 72 | ASP | N-CA-CB | -6.68 | 98.57 | 110.60 |
| 78 | CA | 288 | A | C5'-C4'-C3' | 6.68 | 126.69 | 116.00 |
| 78 | CA | 850 | A | O4'-C1'-N9 | 6.68 | 113.55 | 108.20 |
| 81 | DA | 720 | A | C1'-O4'-C4' | 6.68 | 115.25 | 109.90 |
| 81 | DA | 2304 | C | N1-C1'-C2' | 6.68 | 122.69 | 114.00 |
| 81 | DA | 113 | C | P-O5'-C5' | 6.68 | 131.59 | 120.90 |
| 81 | DA | 805 | G | O4'-C1'-N9 | 6.68 | 113.54 | 108.20 |
| 81 | DA | 1831 | U | O3'-P-O5' | -6.68 | 91.31 | 104.00 |
| 81 | DA | 2114 | C | C5'-C4'-C3' | -6.68 | 105.31 | 116.00 |
| 81 | DA | 2629 | U | C5'-C4'-C3' | 6.68 | 126.69 | 116.00 |
| 6 | AE | 253 | ARG | NE-CZ-NH1 | 6.68 | 123.64 | 120.30 |
| 40 | BK | 128 | ARG | N-CA-CB | 6.68 | 122.62 | 110.60 |
| 66 | Bo | 1 | MET | CG-SD-CE | -6.68 | 89.52 | 100.20 |
| 78 | CA | 118 | U | O4'-C1'-N1 | 6.68 | 113.54 | 108.20 |
| 81 | DA | 735 | A | P-O3'-C3' | 6.68 | 127.71 | 119.70 |
| 81 | DA | 2087 | C | N1-C1'-C2' | 6.68 | 122.68 | 114.00 |
| 81 | DA | 2319 | U | P-O5'-C5' | 6.68 | 131.58 | 120.90 |
| 81 | DA | 2570 | U | O4'-C1'-N1 | 6.68 | 113.54 | 108.20 |
| 81 | DA | 3079 | U | N1-C1'-C2' | 6.68 | 122.68 | 114.00 |
| 5 | AC | 163 | PRO | N-CA-CB | -6.67 | 95.26 | 102.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 9 | AH | 120 | HIS | N-CA-CB | 6.67 | 122.61 | 110.60 |
| 61 | Bj | 89 | LEU | CA-C-O | -6.67 | 106.08 | 120.10 |
| 81 | DA | 595 | G | O4'-C4'-C3' | -6.67 | 97.33 | 104.00 |
| 81 | DA | 1640 | G | C1'-O4'-C4' | -6.67 | 104.56 | 109.90 |
| 81 | DA | 732 | C | O3'-P-O5' | -6.67 | 91.32 | 104.00 |
| 81 | DA | 1685 | C | C1'-O4'-C4' | -6.67 | 104.56 | 109.90 |
| 81 | DA | 2498 | U | C4'-C3'-C2' | -6.67 | 95.93 | 102.60 |
| 35 | BG | 16 | ALA | N-CA-CB | 6.67 | 119.44 | 110.10 |
| 53 | Ba | 12 | VAL | CB-CA-C | 6.67 | 124.08 | 111.40 |
| 13 | AL | 3 | LYS | N-CA-CB | -6.67 | 98.59 | 110.60 |
| 81 | DA | 2180 | G | O4'-C1'-N9 | 6.67 | 113.54 | 108.20 |
| 81 | DA | 2218 | G | O4'-C1'-N9 | 6.67 | 113.54 | 108.20 |
| 81 | DA | 3248 | C | N1-C1'-C2' | 6.67 | 122.67 | 114.00 |
| 83 | DC | 1 | G | O4'-C1'-N9 | 6.67 | 113.54 | 108.20 |
| 17 | AQ | 135 | ARG | NE-CZ-NH2 | -6.67 | 116.97 | 120.30 |
| 33 | BD | 261 | VAL | N-CA-C | 6.67 | 129.00 | 111.00 |
| 81 | DA | 2665 | U | O4'-C1'-C2' | -6.67 | 99.13 | 105.80 |
| 81 | DA | 3302 | U | O3'-P-O5' | -6.67 | 91.33 | 104.00 |
| 68 | Bq | 6 | ARG | NE-CZ-NH1 | 6.67 | 123.63 | 120.30 |
| 81 | DA | 263 | C | O4'-C1'-C2' | -6.67 | 99.13 | 105.80 |
| 81 | DA | 803 | C | C1'-O4'-C4' | -6.67 | 104.57 | 109.90 |
| 78 | CA | 116 | U | O4'-C1'-N1 | 6.67 | 113.53 | 108.20 |
| 78 | CA | 1415 | U | O4'-C1'-N1 | 6.67 | 113.53 | 108.20 |
| 81 | DA | 699 | A | C5'-C4'-C3' | 6.67 | 126.66 | 116.00 |
| 81 | DA | 1074 | U | O4'-C1'-N1 | 6.67 | 113.53 | 108.20 |
| 81 | DA | 2573 | G | C5-C6-O6 | -6.67 | 124.60 | 128.60 |
| 51 | BZ | 62 | GLY | C-N-CA | 6.66 | 138.36 | 121.70 |
| 78 | CA | 1357 | A | C4'-C3'-C2' | -6.66 | 95.94 | 102.60 |
| 81 | DA | 1842 | A | C1'-O4'-C4' | 6.66 | 115.23 | 109.90 |
| 31 | BB | 133 | TYR | CB-CG-CD2 | -6.66 | 117.00 | 121.00 |
| 78 | CA | 323 | A | O4'-C1'-C2' | -6.66 | 99.14 | 105.80 |
| 42 | BM | 41 | GLY | N-CA-C | 6.66 | 129.75 | 113.10 |
| 78 | CA | 16 | G | C5'-C4'-C3' | 6.66 | 126.66 | 116.00 |
| 13 | AL | 38 | PHE | CD1-CE1-CZ | -6.66 | 112.11 | 120.10 |
| 78 | CA | 663 | U | O4'-C1'-N1 | 6.66 | 113.53 | 108.20 |
| 81 | DA | 152 | U | C5'-C4'-C3' | 6.66 | 126.65 | 116.00 |
| 2 | AA | 11 | PRO | C-N-CA | -6.66 | 105.06 | 121.70 |
| 78 | CA | 30 | G | N9-C1'-C2' | 6.66 | 122.65 | 114.00 |
| 78 | CA | 303 | U | C5'-C4'-C3' | -6.66 | 105.35 | 116.00 |
| 78 | CA | 633 | U | N1-C1'-C2' | 6.66 | 122.65 | 114.00 |
| 81 | DA | 1077 | U | N1-C1'-C2' | 6.66 | 122.65 | 114.00 |
| 81 | DA | 1639 | C | O4'-C1'-C2' | -6.66 | 99.14 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1596 | C | P-O3'-C3' | 6.65 | 127.69 | 119.70 |
| 81 | DA | 2482 | U | C1'-O4'-C4' | -6.65 | 104.58 | 109.90 |
| 81 | DA | 422 | A | O4'-C1'-C2' | -6.65 | 99.15 | 105.80 |
| 81 | DA | 628 | A | N9-C1'-C2' | -6.65 | 104.68 | 112.00 |
| 81 | DA | 1920 | U | O4'-C1'-N1 | 6.65 | 113.52 | 108.20 |
| 81 | DA | 2474 | G | P-O3'-C3' | 6.65 | 127.68 | 119.70 |
| 81 | DA | 3317 | U | O4'-C1'-N1 | 6.65 | 113.52 | 108.20 |
| 35 | BG | 57 | HIS | CB-CA-C | 6.65 | 123.70 | 110.40 |
| 81 | DA | 753 | C | O4'-C1'-N1 | 6.65 | 113.52 | 108.20 |
| 81 | DA | 1496 | C | O3'-P-O5' | -6.65 | 91.36 | 104.00 |
| 81 | DA | 1805 | C | C3'-C2'-C1' | 6.65 | 106.82 | 101.50 |
| 81 | DA | 2663 | G | O3'-P-O5' | 6.65 | 116.64 | 104.00 |
| 81 | DA | 3019 | U | O4'-C1'-C2' | -6.65 | 99.15 | 105.80 |
| 33 | BD | 69 | ARG | NE-CZ-NH2 | -6.65 | 116.98 | 120.30 |
| 81 | DA | 386 | A | C5'-C4'-C3' | 6.65 | 126.64 | 116.00 |
| 83 | DC | 97 | C | N1-C1'-C2' | 6.65 | 122.64 | 114.00 |
| 8 | AF | 102 | ARG | N-CA-CB | 6.65 | 122.57 | 110.60 |
| 45 | BR | 140 | LEU | CB-CA-C | -6.65 | 97.57 | 110.20 |
| 78 | CA | 89 | G | O4'-C1'-N9 | 6.65 | 113.52 | 108.20 |
| 78 | CA | 1090 | C | C1'-O4'-C4' | -6.65 | 104.58 | 109.90 |
| 78 | CA | 1325 | A | O4'-C1'-N9 | 6.65 | 113.52 | 108.20 |
| 81 | DA | 895 | A | O4'-C1'-N9 | 6.65 | 113.52 | 108.20 |
| 81 | DA | 953 | G | O4'-C1'-N9 | 6.65 | 113.52 | 108.20 |
| 81 | DA | 997 | A | C5'-C4'-C3' | 6.65 | 126.64 | 116.00 |
| 81 | DA | 1122 | U | P-O3'-C3' | 6.65 | 127.68 | 119.70 |
| 82 | DB | 154 | C | O4'-C1'-N1 | -6.65 | 102.88 | 108.20 |
| 26 | AZ | 39 | LEU | N-CA-CB | 6.65 | 123.69 | 110.40 |
| 81 | DA | 476 | G | O4'-C1'-N9 | 6.65 | 113.52 | 108.20 |
| 81 | DA | 2765 | C | P-O3'-C3' | -6.65 | 111.72 | 119.70 |
| 82 | DB | 10 | A | N9-C1'-C2' | 6.65 | 122.64 | 114.00 |
| 33 | BD | 323 | VAL | CB-CA-C | 6.64 | 124.02 | 111.40 |
| 81 | DA | 32 | U | P-O5'-C5' | 6.64 | 131.53 | 120.90 |
| 81 | DA | 278 | U | P-O3'-C3' | 6.64 | 127.67 | 119.70 |
| 81 | DA | 1565 | G | C5'-C4'-C3' | 6.64 | 126.63 | 116.00 |
| 81 | DA | 2872 | A | N9-C1'-C2' | -6.64 | 104.69 | 112.00 |
| 54 | Bd | 53 | ALA | N-CA-CB | 6.64 | 119.40 | 110.10 |
| 81 | DA | 2672 | G | C3'-C2'-C1' | -6.64 | 96.19 | 101.50 |
| 81 | DA | 2244 | A | C5'-C4'-O4' | -6.64 | 101.13 | 109.10 |
| 82 | DB | 95 | G | C3'-C2'-C1' | 6.64 | 106.81 | 101.50 |
| 81 | DA | 1292 | C | C3'-C2'-C1' | 6.64 | 106.81 | 101.50 |
| 55 | Bc | 104 | GLN | N-CA-CB | 6.64 | 122.55 | 110.60 |
| 78 | CA | 1088 | A | O4'-C1'-C2' | -6.64 | 99.16 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 1569 | A | C5'-C4'-C3' | -6.64 | 105.38 | 116.00 |
| 78 | CA | 169 | A | C5'-C4'-C3' | 6.64 | 126.62 | 116.00 |
| 78 | CA | 1180 | C | N1-C1'-C2' | 6.64 | 122.63 | 114.00 |
| 81 | DA | 598 | A | C5'-C4'-C3' | -6.64 | 105.38 | 116.00 |
| 81 | DA | 1391 | C | C1'-O4'-C4' | 6.64 | 115.21 | 109.90 |
| 78 | CA | 248 | U | P-O3'-C3' | 6.63 | 127.66 | 119.70 |
| 78 | CA | 896 | U | N1-C1'-C2' | 6.63 | 122.62 | 114.00 |
| 78 | CA | 1381 | U | C5'-C4'-C3' | 6.63 | 126.61 | 116.00 |
| 78 | CA | 1677 | C | O4'-C1'-C2' | -6.63 | 99.17 | 105.80 |
| 81 | DA | 3243 | A | N9-C1'-C2' | 6.63 | 122.62 | 114.00 |
| 81 | DA | 3324 | C | C5'-C4'-O4' | -6.63 | 101.14 | 109.10 |
| 81 | DA | 724 | U | C3'-C2'-C1' | 6.63 | 106.81 | 101.50 |
| 24 | AX | 67 | THR | N-CA-CB | 6.63 | 122.90 | 110.30 |
| 41 | BN | 12 | TRP | CA-CB-CG | 6.63 | 126.30 | 113.70 |
| 78 | CA | 219 | A | N9-C1'-C2' | -6.63 | 104.70 | 112.00 |
| 78 | CA | 288 | A | O4'-C4'-C3' | -6.63 | 97.37 | 104.00 |
| 78 | CA | 479 | C | N3-C4-N4 | 6.63 | 122.64 | 118.00 |
| 78 | CA | 982 | U | O4'-C1'-N1 | 6.63 | 113.51 | 108.20 |
| 82 | DB | 39 | G | N9-C1'-C2' | -6.63 | 104.71 | 112.00 |
| 48 | BW | 83 | TYR | CB-CG-CD2 | -6.63 | 117.02 | 121.00 |
| 78 | CA | 45 | U | O3'-P-O5' | -6.63 | 91.40 | 104.00 |
| 81 | DA | 3383 | G | C3'-C2'-C1' | -6.63 | 96.20 | 101.50 |
| 35 | BG | 129 | GLU | N-CA-CB | 6.63 | 122.53 | 110.60 |
| 74 | BQ | 187 | THR | N-CA-CB | 6.63 | 122.89 | 110.30 |
| 78 | CA | 1000 | C | O4'-C1'-C2' | -6.63 | 99.17 | 105.80 |
| 79 | CB | 35 | U | O4'-C1'-N1 | 6.63 | 113.50 | 108.20 |
| 81 | DA | 1378 | U | O4'-C1'-N1 | 6.63 | 113.50 | 108.20 |
| 81 | DA | 1871 | U | O4'-C4'-C3' | 6.63 | 111.40 | 106.10 |
| 81 | DA | 2987 | A | C3'-C2'-C1' | 6.63 | 106.80 | 101.50 |
| 31 | BB | 152 | SER | CB-CA-C | -6.63 | 97.51 | 110.10 |
| 33 | BD | 352 | ALA | CB-CA-C | -6.63 | 100.16 | 110.10 |
| 60 | Bi | 41 | ARG | CB-CA-C | -6.63 | 97.15 | 110.40 |
| 78 | CA | 162 | A | C3'-C2'-C1' | 6.63 | 106.80 | 101.50 |
| 78 | CA | 573 | C | C3'-C2'-C1' | 6.63 | 106.80 | 101.50 |
| 78 | CA | 853 | G | C1'-O4'-C4' | 6.63 | 115.20 | 109.90 |
| 81 | DA | 1664 | G | O4'-C1'-N9 | 6.63 | 113.50 | 108.20 |
| 81 | DA | 2182 | A | C1'-O4'-C4' | -6.63 | 104.60 | 109.90 |
| 81 | DA | 2505 | U | N1-C1'-C2' | -6.63 | 104.71 | 112.00 |
| 81 | DA | 2619 | G | C1'-O4'-C4' | -6.63 | 104.60 | 109.90 |
| 81 | DA | 3243 | A | C1'-O4'-C4' | -6.63 | 104.60 | 109.90 |
| 81 | DA | 3307 | A | C4'-C3'-C2' | -6.63 | 95.97 | 102.60 |
| 81 | DA | 3341 | U | N1-C1'-C2' | 6.63 | 122.61 | 114.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2757 | U | O4'-C4'-C3' | -6.62 | 97.38 | 104.00 |
| 32 | BC | 266 | ARG | CD-NE-CZ | 6.62 | 132.87 | 123.60 |
| 76 | BS | 156 | ARG | NE-CZ-NH1 | 6.62 | 123.61 | 120.30 |
| 78 | CA | 100 | A | N9-C1'-C2' | -6.62 | 104.71 | 112.00 |
| 78 | CA | 596 | C | O4'-C1'-N1 | 6.62 | 113.50 | 108.20 |
| 81 | DA | 2604 | U | N1-C1'-C2' | 6.62 | 122.61 | 114.00 |
| 57 | Be | 235 | PHE | CB-CG-CD2 | -6.62 | 116.17 | 120.80 |
| 74 | BQ | 250 | ASP | CB-CG-OD1 | -6.62 | 112.34 | 118.30 |
| 78 | CA | 606 | A | C5'-C4'-O4' | 6.62 | 117.05 | 109.10 |
| 81 | DA | 1064 | A | C1'-O4'-C4' | 6.62 | 115.20 | 109.90 |
| 81 | DA | 2781 | U | C3'-C2'-C1' | -6.62 | 96.20 | 101.50 |
| 2 | AA | 5 | ALA | C-N-CA | -6.62 | 105.15 | 121.70 |
| 10 | AI | 86 | ALA | CB-CA-C | -6.62 | 100.17 | 110.10 |
| 57 | Be | 75 | TYR | N-CA-CB | 6.62 | 122.52 | 110.60 |
| 5 | AC | 62 | ARG | NH1-CZ-NH2 | 6.62 | 126.68 | 119.40 |
| 11 | AJ | 102 | ARG | CB-CA-C | -6.62 | 97.16 | 110.40 |
| 32 | BC | 382 | THR | N-CA-C | -6.62 | 93.13 | 111.00 |
| 33 | BD | 313 | LEU | CB-CA-C | -6.62 | 97.62 | 110.20 |
| 45 | BR | 33 | TYR | CB-CG-CD1 | 6.62 | 124.97 | 121.00 |
| 76 | BS | 67 | PHE | C-N-CA | 6.62 | 138.25 | 121.70 |
| 81 | DA | 739 | G | P-O3'-C3' | -6.62 | 111.76 | 119.70 |
| 81 | DA | 1115 | G | P-O3'-C3' | 6.62 | 127.64 | 119.70 |
| 81 | DA | 2303 | A | O4'-C1'-C2' | -6.62 | 99.18 | 105.80 |
| 37 | BH | 129 | PRO | N-CA-CB | 6.62 | 111.24 | 103.30 |
| 81 | DA | 691 | A | C1'-O4'-C4' | 6.62 | 115.19 | 109.90 |
| 81 | DA | 2264 | U | O4'-C4'-C3' | -6.62 | 97.38 | 104.00 |
| 81 | DA | 3299 | A | C1'-O4'-C4' | 6.62 | 115.19 | 109.90 |
| 63 | Bm | 4 | ARG | CB-CA-C | -6.62 | 97.17 | 110.40 |
| 78 | CA | 225 | A | P-O3'-C3' | -6.62 | 111.76 | 119.70 |
| 78 | CA | 892 | A | O4'-C1'-C2' | -6.62 | 99.19 | 105.80 |
| 78 | CA | 1298 | U | C3'-C2'-C1' | 6.62 | 106.79 | 101.50 |
| 16 | AO | 89 | TYR | CB-CG-CD1 | 6.61 | 124.97 | 121.00 |
| 78 | CA | 1279 | C | N1-C1'-C2' | 6.61 | 122.60 | 114.00 |
| 79 | CB | 28 | G | C4'-C3'-C2' | -6.61 | 95.99 | 102.60 |
| 81 | DA | 1086 | C | N1-C1'-C2' | 6.61 | 122.60 | 114.00 |
| 81 | DA | 1226 | G | O4'-C1'-N9 | 6.61 | 113.49 | 108.20 |
| 81 | DA | 519 | A | N9-C1'-C2' | -6.61 | 104.73 | 112.00 |
| 81 | DA | 2181 | C | O3'-P-O5' | 6.61 | 116.56 | 104.00 |
| 50 | BX | 35 | PRO | CA-N-CD | -6.61 | 102.25 | 111.50 |
| 77 | BI | 113 | GLN | N-CA-CB | 6.61 | 122.50 | 110.60 |
| 78 | CA | 435 | C | C3'-C2'-C1' | 6.61 | 106.79 | 101.50 |
| 78 | CA | 658 | C | C4'-C3'-O3' | 6.61 | 126.22 | 113.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 1434 | U | P-O3'-C3' | 6.61 | 127.63 | 119.70 |
| 81 | DA | 35 | A | O4'-C1'-N9 | 6.61 | 113.49 | 108.20 |
| 81 | DA | 49 | A | C1'-O4'-C4' | 6.61 | 115.19 | 109.90 |
| 81 | DA | 337 | G | C1'-O4'-C4' | 6.61 | 115.19 | 109.90 |
| 81 | DA | 3009 | G | C5'-C4'-C3' | 6.61 | 126.58 | 116.00 |
| 81 | DA | 168 | U | O4'-C1'-N1 | 6.61 | 113.49 | 108.20 |
| 78 | CA | 164 | A | O4'-C4'-C3' | 6.61 | 111.39 | 106.10 |
| 78 | CA | 320 | U | C3'-C2'-C1' | 6.61 | 106.78 | 101.50 |
| 81 | DA | 2370 | G | O3'-P-O5' | -6.61 | 91.45 | 104.00 |
| 81 | DA | 2504 | U | C2'-C3'-O3' | 6.61 | 124.27 | 113.70 |
| 81 | DA | 3211 | C | P-O5'-C5' | 6.61 | 131.47 | 120.90 |
| 2 | AA | 113 | ARG | NE-CZ-NH2 | -6.61 | 117.00 | 120.30 |
| 32 | BC | 99 | LEU | CB-CG-CD2 | 6.61 | 122.23 | 111.00 |
| 81 | DA | 290 | G | C1'-O4'-C4' | -6.61 | 104.61 | 109.90 |
| 81 | DA | 873 | C | O4'-C1'-C2' | -6.61 | 99.19 | 105.80 |
| 81 | DA | 1262 | G | N9-C1'-C2' | 6.61 | 122.59 | 114.00 |
| 81 | DA | 3392 | U | O4'-C1'-N1 | 6.61 | 113.48 | 108.20 |
| 33 | BD | 99 | MET | C-N-CA | 6.60 | 138.21 | 121.70 |
| 59 | Bh | 127 | ALA | CB-CA-C | 6.60 | 120.01 | 110.10 |
| 81 | DA | 1001 | G | C1'-O4'-C4' | -6.60 | 104.62 | 109.90 |
| 69 | Br | 42 | ARG | NE-CZ-NH2 | 6.60 | 123.60 | 120.30 |
| 78 | CA | 856 | A | O4'-C1'-C2' | -6.60 | 99.20 | 105.80 |
| 78 | CA | 1789 | G | O4'-C1'-N9 | 6.60 | 113.48 | 108.20 |
| 81 | DA | 180 | C | C3'-C2'-C1' | 6.60 | 106.78 | 101.50 |
| 81 | DA | 1045 | C | C3'-C2'-C1' | -6.60 | 96.22 | 101.50 |
| 81 | DA | 2474 | G | O4'-C1'-N9 | 6.60 | 113.48 | 108.20 |
| 81 | DA | 2756 | C | P-O3'-C3' | 6.60 | 127.62 | 119.70 |
| 81 | DA | 2757 | U | O5'-C5'-C4' | 6.60 | 124.24 | 111.70 |
| 81 | DA | 3081 | C | N1-C1'-C2' | 6.60 | 122.58 | 114.00 |
| 6 | AE | 120 | GLU | N-CA-CB | 6.60 | 122.48 | 110.60 |
| 19 | AR | 61 | ARG | NE-CZ-NH2 | -6.60 | 117.00 | 120.30 |
| 81 | DA | 2338 | C | O4'-C1'-N1 | 6.60 | 113.48 | 108.20 |
| 81 | DA | 2537 | U | O4'-C1'-N1 | 6.60 | 113.48 | 108.20 |
| 39 | BJ | 53 | PHE | CB-CG-CD2 | -6.60 | 116.18 | 120.80 |
| 78 | CA | 465 | G | C3'-C2'-C1' | -6.60 | 96.22 | 101.50 |
| 78 | CA | 1480 | G | C5'-C4'-C3' | -6.60 | 105.44 | 116.00 |
| 81 | DA | 3107 | U | O4'-C4'-C3' | 6.60 | 111.38 | 106.10 |
| 79 | CB | 72 | G | C2'-C3'-O3' | 6.60 | 124.26 | 113.70 |
| 81 | DA | 245 | U | O4'-C1'-N1 | 6.60 | 113.48 | 108.20 |
| 81 | DA | 490 | A | C5'-C4'-C3' | -6.60 | 105.44 | 116.00 |
| 81 | DA | 2251 | G | C1'-O4'-C4' | -6.60 | 104.62 | 109.90 |
| 81 | DA | 3001 | C | O4'-C1'-C2' | -6.60 | 99.20 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 3248 | C | O3'-P-O5' | -6.60 | 91.47 | 104.00 |
| 5 | AC | 54 | ARG | NE-CZ-NH2 | -6.60 | 117.00 | 120.30 |
| 81 | DA | 2728 | G | C1'-O4'-C4' | -6.60 | 104.62 | 109.90 |
| 12 | AK | 125 | SER | N-CA-CB | 6.59 | 120.39 | 110.50 |
| 37 | BH | 177 | TYR | CG-CD1-CE1 | -6.59 | 116.02 | 121.30 |
| 80 | CC | 21 | C | P-O5'-C5' | -6.59 | 110.35 | 120.90 |
| 81 | DA | 2142 | A | C1'-O4'-C4' | 6.59 | 115.18 | 109.90 |
| 25 | AY | 25 | VAL | N-CA-C | -6.59 | 93.20 | 111.00 |
| 47 | BU | 135 | PRO | CA-N-CD | -6.59 | 102.27 | 111.50 |
| 55 | Bc | 81 | ARG | NE-CZ-NH1 | 6.59 | 123.60 | 120.30 |
| 78 | CA | 195 | G | C3'-C2'-C1' | 6.59 | 106.77 | 101.50 |
| 78 | CA | 357 | G | O4'-C1'-N9 | 6.59 | 113.47 | 108.20 |
| 78 | CA | 949 | C | O3'-P-O5' | -6.59 | 91.48 | 104.00 |
| 78 | CA | 1302 | U | O4'-C1'-C2' | -6.59 | 99.21 | 105.80 |
| 78 | CA | 1406 | A | O4'-C1'-C2' | 6.59 | 113.53 | 107.60 |
| 81 | DA | 1697 | A | C3'-C2'-C1' | 6.59 | 106.77 | 101.50 |
| 29 | AU | 19 | ALA | N-CA-CB | 6.59 | 119.33 | 110.10 |
| 31 | BB | 42 | ARG | NE-CZ-NH1 | 6.59 | 123.59 | 120.30 |
| 59 | Bh | 111 | ARG | NE-CZ-NH2 | -6.59 | 117.01 | 120.30 |
| 60 | Bi | 18 | ASN | N-CA-CB | 6.59 | 122.46 | 110.60 |
| 78 | CA | 158 | U | C1'-O4'-C4' | -6.59 | 104.63 | 109.90 |
| 81 | DA | 1248 | C | O4'-C1'-N1 | 6.59 | 113.47 | 108.20 |
| 81 | DA | 2776 | C | P-O3'-C3' | -6.59 | 111.79 | 119.70 |
| 81 | DA | 3246 | G | O3'-P-O5' | -6.59 | 91.48 | 104.00 |
| 3 | AB | 157 | LEU | N-CA-CB | 6.59 | 123.58 | 110.40 |
| 78 | CA | 1429 | G | O4'-C1'-N9 | 6.59 | 113.47 | 108.20 |
| 81 | DA | 578 | A | C3'-C2'-C1' | 6.59 | 106.77 | 101.50 |
| 81 | DA | 2756 | C | O4'-C4'-C3' | -6.59 | 97.41 | 104.00 |
| 81 | DA | 3235 | C | C3'-C2'-C1' | 6.59 | 106.77 | 101.50 |
| 81 | DA | 3356 | G | O4'-C1'-N9 | 6.59 | 113.47 | 108.20 |
| 51 | BZ | 60 | LYS | O-C-N | -6.59 | 112.16 | 122.70 |
| 78 | CA | 358 | U | O4'-C1'-N1 | 6.59 | 113.47 | 108.20 |
| 78 | CA | 1067 | C | O4'-C1'-N1 | 6.59 | 113.47 | 108.20 |
| 81 | DA | 213 | A | O4'-C1'-N9 | 6.59 | 113.47 | 108.20 |
| 81 | DA | 1939 | G | C1'-O4'-C4' | -6.59 | 104.63 | 109.90 |
| 81 | DA | 2536 | A | O4'-C1'-N9 | 6.59 | 113.47 | 108.20 |
| 78 | CA | 237 | C | P-O3'-C3' | 6.58 | 127.60 | 119.70 |
| 55 | Bc | 105 | ARG | C-N-CA | 6.58 | 138.16 | 121.70 |
| 78 | CA | 853 | G | P-O5'-C5' | -6.58 | 110.37 | 120.90 |
| 81 | DA | 1384 | U | P-O3'-C3' | 6.58 | 127.60 | 119.70 |
| 81 | DA | 3361 | G | C3'-C2'-C1' | 6.58 | 106.77 | 101.50 |
| 83 | DC | 1 | G | O3'-P-O5' | -6.58 | 91.49 | 104.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 14 | AM | 122 | HIS | N-CA-CB | 6.58 | 122.44 | 110.60 |
| 35 | BG | 38 | THR | CA-CB-CG2 | -6.58 | 103.19 | 112.40 |
| 76 | BS | 68 | GLU | N-CA-C | 6.58 | 128.77 | 111.00 |
| 78 | CA | 298 | C | O4'-C1'-C2' | -6.58 | 99.22 | 105.80 |
| 78 | CA | 1145 | U | O4'-C1'-N1 | 6.58 | 113.47 | 108.20 |
| 79 | CB | 50 | G | O4'-C1'-C2' | 6.58 | 113.52 | 107.60 |
| 81 | DA | 9 | U | C1'-O4'-C4' | -6.58 | 104.64 | 109.90 |
| 81 | DA | 2651 | G | N9-C1'-C2' | 6.58 | 122.56 | 114.00 |
| 81 | DA | 2799 | A | O4'-C1'-N9 | 6.58 | 113.47 | 108.20 |
| 2 | AA | 31 | VAL | N-CA-CB | 6.58 | 125.98 | 111.50 |
| 52 | BY | 4 | GLN | N-CA-CB | 6.58 | 122.44 | 110.60 |
| 76 | BS | 74 | ILE | CB-CA-C | 6.58 | 124.76 | 111.60 |
| 81 | DA | 2902 | A | O4'-C1'-N9 | 6.58 | 113.46 | 108.20 |
| 81 | DA | 3349 | C | N1-C1'-C2' | 6.58 | 122.55 | 114.00 |
| 46 | BT | 146 | LYS | CB-CA-C | -6.58 | 97.24 | 110.40 |
| 49 | BV | 113 | TYR | CB-CG-CD2 | 6.58 | 124.95 | 121.00 |
| 78 | CA | 447 | U | P-O5'-C5' | 6.58 | 131.43 | 120.90 |
| 78 | CA | 1556 | A | O4'-C1'-C2' | -6.58 | 99.22 | 105.80 |
| 81 | DA | 201 | A | C1'-O4'-C4' | -6.58 | 104.64 | 109.90 |
| 81 | DA | 982 | C | C4'-C3'-C2' | -6.58 | 96.02 | 102.60 |
| 81 | DA | 1002 | A | P-O3'-C3' | 6.58 | 127.59 | 119.70 |
| 74 | BQ | 239 | ILE | N-CA-C | 6.58 | 128.76 | 111.00 |
| 74 | BQ | 282 | ARG | NE-CZ-NH1 | 6.58 | 123.59 | 120.30 |
| 78 | CA | 987 | G | O4'-C1'-N9 | 6.58 | 113.46 | 108.20 |
| 81 | DA | 2346 | C | N1-C1'-C2' | 6.58 | 122.55 | 114.00 |
| 43 | BP | 64 | VAL | CA-CB-CG2 | 6.58 | 120.76 | 110.90 |
| 81 | DA | 2471 | U | N1-C1'-C2' | -6.58 | 104.77 | 112.00 |
| 81 | DA | 3149 | G | OP2-P-O3' | 6.58 | 119.67 | 105.20 |
| 78 | CA | 120 | U | O3'-P-O5' | 6.57 | 116.49 | 104.00 |
| 78 | CA | 424 | C | N1-C1'-C2' | 6.57 | 122.55 | 114.00 |
| 80 | CC | 18 | C | N1-C1'-C2' | 6.57 | 122.55 | 114.00 |
| 20 | AS | 8 | ASP | CB-CG-OD1 | 6.57 | 124.21 | 118.30 |
| 81 | DA | 271 | C | O4'-C1'-C2' | -6.57 | 99.23 | 105.80 |
| 81 | DA | 1054 | A | O4'-C1'-C2' | -6.57 | 99.23 | 105.80 |
| 81 | DA | 1257 | C | OP1-P-O3' | 6.57 | 119.66 | 105.20 |
| 25 | AY | 56 | LEU | CB-CG-CD2 | 6.57 | 122.17 | 111.00 |
| 43 | BP | 188 | ARG | NE-CZ-NH1 | 6.57 | 123.58 | 120.30 |
| 81 | DA | 582 | G | C1'-O4'-C4' | -6.57 | 104.64 | 109.90 |
| 81 | DA | 656 | A | C1'-O4'-C4' | -6.57 | 104.64 | 109.90 |
| 81 | DA | 1505 | C | O4'-C1'-N1 | 6.57 | 113.46 | 108.20 |
| 81 | DA | 2924 | U | O4'-C1'-N1 | 6.57 | 113.46 | 108.20 |
| 81 | DA | 3246 | G | N9-C1'-C2' | 6.57 | 122.54 | 114.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 83 | DC | 25 | G | C3'-C2'-C1' | -6.57 | 96.24 | 101.50 |
| 83 | DC | 81 | U | O4'-C1'-N1 | 6.57 | 113.46 | 108.20 |
| 32 | BC | 321 | PHE | CB-CG-CD1 | 6.57 | 125.40 | 120.80 |
| 74 | BQ | 239 | ILE | CB-CA-C | 6.57 | 124.74 | 111.60 |
| 78 | CA | 100 | A | P-O3'-C3' | 6.57 | 127.58 | 119.70 |
| 81 | DA | 3306 | U | O4'-C1'-C2' | -6.57 | 99.23 | 105.80 |
| 33 | BD | 247 | PHE | CB-CG-CD2 | -6.57 | 116.20 | 120.80 |
| 78 | CA | 299 | A | O4'-C1'-C2' | -6.57 | 99.23 | 105.80 |
| 81 | DA | 1346 | G | C1'-O4'-C4' | 6.57 | 115.15 | 109.90 |
| 81 | DA | 1699 | A | O3'-P-O5' | -6.57 | 91.52 | 104.00 |
| 81 | DA | 3389 | U | O4'-C1'-C2' | -6.57 | 99.23 | 105.80 |
| 35 | BG | 28 | GLN | N-CA-CB | 6.57 | 122.42 | 110.60 |
| 78 | CA | 875 | G | C1'-O4'-C4' | -6.57 | 104.65 | 109.90 |
| 78 | CA | 1455 | G | O5'-P-OP1 | -6.57 | 99.79 | 105.70 |
| 78 | CA | 1691 | A | C5'-C4'-C3' | 6.57 | 126.50 | 116.00 |
| 81 | DA | 9 | U | C5'-C4'-C3' | 6.57 | 126.51 | 116.00 |
| 81 | DA | 1337 | A | O4'-C1'-N9 | 6.57 | 113.45 | 108.20 |
| 18 | AP | 81 | HIS | CA-CB-CG | 6.56 | 124.76 | 113.60 |
| 13 | AL | 84 | THR | N-CA-C | -6.56 | 93.28 | 111.00 |
| 78 | CA | 215 | A | O4'-C1'-C2' | -6.56 | 99.24 | 105.80 |
| 78 | CA | 1095 | U | P-O5'-C5' | 6.56 | 131.40 | 120.90 |
| 79 | CB | 22 | G | O4'-C1'-C2' | 6.56 | 113.51 | 107.60 |
| 81 | DA | 2099 | A | N9-C1'-C2' | 6.56 | 122.53 | 114.00 |
| 81 | DA | 2269 | U | O4'-C1'-N1 | 6.56 | 113.45 | 108.20 |
| 81 | DA | 2790 | A | O4'-C1'-N9 | 6.56 | 113.45 | 108.20 |
| 31 | BB | 26 | ALA | N-CA-CB | 6.56 | 119.28 | 110.10 |
| 81 | DA | 3093 | C | C3'-C2'-C1' | 6.56 | 106.75 | 101.50 |
| 18 | AP | 100 | TYR | CG-CD2-CE2 | -6.56 | 116.05 | 121.30 |
| 46 | BT | 136 | ARG | NE-CZ-NH2 | 6.56 | 123.58 | 120.30 |
| 78 | CA | 672 | U | O4'-C1'-C2' | -6.56 | 99.24 | 105.80 |
| 81 | DA | 702 | C | P-O3'-C3' | 6.56 | 127.57 | 119.70 |
| 81 | DA | 1690 | C | C3'-C2'-C1' | -6.56 | 96.25 | 101.50 |
| 81 | DA | 2994 | A | C1'-O4'-C4' | 6.56 | 115.15 | 109.90 |
| 78 | CA | 1503 | A | O4'-C1'-N9 | 6.56 | 113.45 | 108.20 |
| 79 | CB | 66 | C | C3'-C2'-C1' | 6.56 | 106.75 | 101.50 |
| 81 | DA | 665 | A | C1'-O4'-C4' | -6.56 | 104.65 | 109.90 |
| 81 | DA | 1107 | C | O4'-C1'-N1 | 6.56 | 113.45 | 108.20 |
| 82 | DB | 74 | U | C5'-C4'-C3' | 6.56 | 126.49 | 116.00 |
| 74 | BQ | 55 | PHE | O-C-N | 6.55 | 133.19 | 122.70 |
| 78 | CA | 171 | A | O4'-C1'-N9 | 6.55 | 113.44 | 108.20 |
| 81 | DA | 2626 | A | C5'-C4'-C3' | 6.55 | 126.49 | 116.00 |
| 10 | AI | 79 | TYR | CB-CG-CD2 | -6.55 | 117.07 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 72 | Bu | 61 | PHE | CB-CA-C | -6.55 | 97.29 | 110.40 |
| 81 | DA | 837 | A | C5'-C4'-O4' | -6.55 | 101.24 | 109.10 |
| 81 | DA | 2334 | U | C4'-C3'-C2' | -6.55 | 96.05 | 102.60 |
| 83 | DC | 113 | C | C3'-C2'-C1' | 6.55 | 106.74 | 101.50 |
| 76 | BS | 123 | ILE | CA-CB-CG1 | 6.55 | 123.45 | 111.00 |
| 81 | DA | 1363 | A | N9-C1'-C2' | 6.55 | 122.52 | 114.00 |
| 81 | DA | 1694 | U | C1'-O4'-C4' | 6.55 | 115.14 | 109.90 |
| 81 | DA | 2181 | C | C4'-C3'-C2' | -6.55 | 96.05 | 102.60 |
| 81 | DA | 2844 | C | C3'-C2'-C1' | 6.55 | 106.74 | 101.50 |
| 81 | DA | 2944 | U | C1'-O4'-C4' | 6.55 | 115.14 | 109.90 |
| 55 | Bc | 75 | TYR | CB-CG-CD1 | 6.55 | 124.93 | 121.00 |
| 78 | CA | 972 | G | O4'-C1'-N9 | 6.55 | 113.44 | 108.20 |
| 81 | DA | 622 | A | P-O3'-C3' | 6.55 | 127.56 | 119.70 |
| 81 | DA | 3148 | U | C5'-C4'-C3' | -6.55 | 105.52 | 116.00 |
| 81 | DA | 3229 | G | C1'-O4'-C4' | -6.55 | 104.66 | 109.90 |
| 51 | BZ | 69 | LYS | N-CA-C | 6.55 | 128.68 | 111.00 |
| 81 | DA | 2047 | A | C1'-O4'-C4' | -6.55 | 104.66 | 109.90 |
| 81 | DA | 3253 | G | O4'-C1'-C2' | 6.55 | 113.49 | 107.60 |
| 78 | CA | 295 | A | O4'-C4'-C3' | -6.55 | 97.45 | 104.00 |
| 78 | CA | 880 | C | O4'-C1'-C2' | -6.55 | 99.25 | 105.80 |
| 81 | DA | 1387 | G | P-O3'-C3' | -6.55 | 111.84 | 119.70 |
| 81 | DA | 3031 | G | C1'-O4'-C4' | -6.55 | 104.66 | 109.90 |
| 83 | DC | 6 | C | O4'-C1'-C2' | -6.55 | 99.25 | 105.80 |
| 78 | CA | 490 | C | N3-C4-N4 | 6.54 | 122.58 | 118.00 |
| 78 | CA | 1746 | A | O4'-C1'-C2' | -6.54 | 99.25 | 105.80 |
| 81 | DA | 1238 | C | P-O3'-C3' | 6.54 | 127.55 | 119.70 |
| 81 | DA | 2645 | G | C3'-C2'-C1' | -6.54 | 96.26 | 101.50 |
| 57 | Be | 229 | PHE | CB-CG-CD1 | 6.54 | 125.38 | 120.80 |
| 76 | BS | 161 | PRO | CB-CA-C | 6.54 | 128.36 | 112.00 |
| 78 | CA | 107 | C | C3'-C2'-C1' | 6.54 | 106.73 | 101.50 |
| 81 | DA | 1803 | C | O4'-C1'-N1 | 6.54 | 113.44 | 108.20 |
| 81 | DA | 1849 | C | O4'-C1'-C2' | -6.54 | 99.26 | 105.80 |
| 81 | DA | 2407 | C | C3'-C2'-C1' | 6.54 | 106.73 | 101.50 |
| 48 | BW | 95 | PHE | CB-CG-CD2 | 6.54 | 125.38 | 120.80 |
| 78 | CA | 119 | A | C4'-C3'-C2' | -6.54 | 96.06 | 102.60 |
| 79 | CB | 9 | A | P-O3'-C3' | 6.54 | 127.55 | 119.70 |
| 81 | DA | 94 | G | O4'-C1'-N9 | 6.54 | 113.43 | 108.20 |
| 81 | DA | 1283 | C | O4'-C1'-N1 | 6.54 | 113.43 | 108.20 |
| 47 | BU | 116 | ARG | CB-CA-C | -6.54 | 97.32 | 110.40 |
| 74 | BQ | 129 | TYR | CB-CG-CD1 | 6.54 | 124.92 | 121.00 |
| 81 | DA | 458 | U | N1-C1'-C2' | 6.54 | 122.50 | 114.00 |
| 20 | AS | 123 | ARG | NE-CZ-NH2 | -6.54 | 117.03 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | BG | 99 | GLU | CB-CA-C | -6.54 | 97.32 | 110.40 |
| 41 | BN | 40 | ASP | N-CA-C | -6.54 | 93.34 | 111.00 |
| 78 | CA | 606 | A | O4'-C1'-N9 | -6.54 | 102.97 | 108.20 |
| 81 | DA | 798 | G | O3'-P-O5' | -6.54 | 91.58 | 104.00 |
| 81 | DA | 1101 | G | O3'-P-O5' | -6.54 | 91.58 | 104.00 |
| 81 | DA | 693 | A | C3'-C2'-C1' | 6.54 | 106.73 | 101.50 |
| 81 | DA | 2303 | A | C4'-C3'-C2' | 6.54 | 109.14 | 102.60 |
| 10 | AI | 30 | LYS | N-CA-CB | 6.54 | 122.36 | 110.60 |
| 41 | BN | 106 | ARG | NE-CZ-NH2 | -6.54 | 117.03 | 120.30 |
| 77 | BI | 109 | ASP | CB-CG-OD1 | -6.54 | 112.42 | 118.30 |
| 81 | DA | 64 | G | P-O3'-C3' | 6.54 | 127.54 | 119.70 |
| 81 | DA | 3166 | C | C3'-C2'-C1' | 6.54 | 106.73 | 101.50 |
| 20 | AS | 66 | TYR | CB-CG-CD2 | -6.53 | 117.08 | 121.00 |
| 32 | BC | 369 | ARG | NE-CZ-NH2 | -6.53 | 117.03 | 120.30 |
| 44 | BO | 56 | VAL | CA-C-N | 6.53 | 129.27 | 116.20 |
| 78 | CA | 690 | G | C3'-C2'-C1' | -6.53 | 96.27 | 101.50 |
| 81 | DA | 1151 | U | C3'-C2'-C1' | 6.53 | 106.73 | 101.50 |
| 81 | DA | 2414 | G | O4'-C1'-N9 | 6.53 | 113.43 | 108.20 |
| 81 | DA | 2625 | C | O3'-P-O5' | -6.53 | 91.59 | 104.00 |
| 81 | DA | 3240 | C | O4'-C1'-N1 | 6.53 | 113.43 | 108.20 |
| 34 | BE | 116 | TYR | CB-CG-CD1 | -6.53 | 117.08 | 121.00 |
| 78 | CA | 1501 | C | P-O5'-C5' | 6.53 | 131.35 | 120.90 |
| 59 | Bh | 12 | LYS | N-CA-C | -6.53 | 93.37 | 111.00 |
| 81 | DA | 1347 | U | O4'-C1'-C2' | -6.53 | 99.27 | 105.80 |
| 81 | DA | 3160 | U | O4'-C1'-N1 | 6.53 | 113.42 | 108.20 |
| 78 | CA | 838 | G | C4'-C3'-C2' | -6.53 | 96.07 | 102.60 |
| 81 | DA | 2240 | G | C3'-C2'-C1' | -6.53 | 96.28 | 101.50 |
| 81 | DA | 2876 | C | P-O3'-C3' | -6.53 | 111.86 | 119.70 |
| 81 | DA | 3359 | A | P-O5'-C5' | 6.53 | 131.35 | 120.90 |
| 5 | AC | 146 | PHE | N-CA-CB | 6.53 | 122.35 | 110.60 |
| 20 | AS | 53 | TRP | CA-C-O | 6.53 | 133.81 | 120.10 |
| 32 | BC | 52 | GLY | N-CA-C | -6.53 | 96.78 | 113.10 |
| 37 | BH | 129 | PRO | N-CA-C | -6.53 | 95.13 | 112.10 |
| 78 | CA | 839 | U | O3'-P-O5' | -6.53 | 91.60 | 104.00 |
| 78 | CA | 874 | C | O4'-C1'-C2' | -6.53 | 99.27 | 105.80 |
| 78 | CA | 1065 | A | C5-C6-N1 | -6.53 | 114.44 | 117.70 |
| 78 | CA | 1576 | A | O4'-C1'-C2' | -6.53 | 99.27 | 105.80 |
| 81 | DA | 356 | C | O4'-C1'-C2' | -6.53 | 99.27 | 105.80 |
| 81 | DA | 1896 | A | P-O3'-C3' | 6.53 | 127.53 | 119.70 |
| 78 | CA | 1584 | G | O4'-C1'-N9 | -6.53 | 102.98 | 108.20 |
| 81 | DA | 1314 | C | P-O5'-C5' | 6.53 | 131.34 | 120.90 |
| 81 | DA | 1818 | U | C4'-C3'-C2' | -6.53 | 96.08 | 102.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2478 | C | N1-C1'-C2' | 6.53 | 122.48 | 114.00 |
| 81 | DA | 2752 | U | C3'-C2'-C1' | 6.53 | 106.72 | 101.50 |
| 3 | AB | 107 | PHE | CB-CG-CD2 | 6.52 | 125.37 | 120.80 |
| 2 | AA | 79 | ARG | O-C-N | 6.52 | 133.14 | 122.70 |
| 62 | Bk | 84 | LYS | N-CA-C | 6.52 | 128.61 | 111.00 |
| 69 | Br | 87 | ARG | NE-CZ-NH2 | -6.52 | 117.04 | 120.30 |
| 78 | CA | 1056 | U | O4'-C1'-N1 | 6.52 | 113.42 | 108.20 |
| 78 | CA | 1500 | C | N3-C4-C5 | -6.52 | 119.29 | 121.90 |
| 78 | CA | 1764 | C | N1-C1'-C2' | 6.52 | 122.48 | 114.00 |
| 81 | DA | 2931 | C | P-O3'-C3' | -6.52 | 111.87 | 119.70 |
| 81 | DA | 3211 | C | O4'-C1'-C2' | -6.52 | 99.28 | 105.80 |
| 83 | DC | 93 | U | C4'-C3'-C2' | -6.52 | 96.08 | 102.60 |
| 81 | DA | 51 | A | O4'-C1'-N9 | 6.52 | 113.42 | 108.20 |
| 78 | CA | 141 | U | C4'-C3'-C2' | -6.52 | 96.08 | 102.60 |
| 78 | CA | 1408 | G | O4'-C1'-N9 | 6.52 | 113.42 | 108.20 |
| 81 | DA | 191 | U | O4'-C1'-N1 | 6.52 | 113.42 | 108.20 |
| 81 | DA | 667 | C | O4'-C1'-N1 | 6.52 | 113.42 | 108.20 |
| 81 | DA | 2863 | G | N9-C1'-C2' | 6.52 | 122.48 | 114.00 |
| 81 | DA | 3389 | U | O4'-C4'-C3' | -6.52 | 97.48 | 104.00 |
| 78 | CA | 713 | A | C5'-C4'-C3' | 6.52 | 126.43 | 116.00 |
| 78 | CA | 1066 | C | O4'-C4'-C3' | -6.52 | 97.48 | 104.00 |
| 78 | CA | 1447 | C | C3'-C2'-C1' | 6.52 | 106.72 | 101.50 |
| 81 | DA | 1079 | A | N9-C1'-C2' | -6.52 | 104.83 | 112.00 |
| 81 | DA | 1859 | A | P-O3'-C3' | 6.52 | 127.52 | 119.70 |
| 81 | DA | 3343 | G | O4'-C1'-N9 | 6.52 | 113.41 | 108.20 |
| 78 | CA | 1284 | C | P-O3'-C3' | 6.52 | 127.52 | 119.70 |
| 65 | Bn | 71 | PRO | CA-N-CD | -6.51 | 102.38 | 111.50 |
| 78 | CA | 1237 | G | C3'-C2'-C1' | 6.51 | 106.71 | 101.50 |
| 78 | CA | 1434 | U | N1-C1'-C2' | 6.51 | 122.47 | 114.00 |
| 78 | CA | 1476 | C | P-O5'-C5' | 6.51 | 131.32 | 120.90 |
| 78 | CA | 1553 | G | O4'-C1'-N9 | 6.51 | 113.41 | 108.20 |
| 81 | DA | 110 | G | O4'-C1'-N9 | 6.51 | 113.41 | 108.20 |
| 81 | DA | 1457 | U | N1-C1'-C2' | 6.51 | 122.47 | 114.00 |
| 81 | DA | 1955 | U | O4'-C1'-C2' | -6.51 | 99.29 | 105.80 |
| 3 | AB | 162 | GLN | N-CA-CB | -6.51 | 98.88 | 110.60 |
| 78 | CA | 572 | C | C3'-C2'-C1' | 6.51 | 106.71 | 101.50 |
| 78 | CA | 925 | G | C3'-C2'-C1' | -6.51 | 96.29 | 101.50 |
| 78 | CA | 1202 | A | C3'-C2'-C1' | -6.51 | 96.29 | 101.50 |
| 81 | DA | 1454 | A | C3'-C2'-C1' | 6.51 | 106.71 | 101.50 |
| 81 | DA | 2900 | A | O4'-C1'-N9 | 6.51 | 113.41 | 108.20 |
| 18 | AP | 114 | ALA | N-CA-CB | 6.51 | 119.21 | 110.10 |
| 78 | CA | 1570 | A | C1'-O4'-C4' | 6.51 | 115.11 | 109.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2507 | C | O4'-C1'-C2' | -6.51 | 99.29 | 105.80 |
| 81 | DA | 2934 | A | P-O3'-C3' | 6.51 | 127.51 | 119.70 |
| 78 | CA | 220 | A | C3'-C2'-C1' | 6.51 | 106.71 | 101.50 |
| 78 | CA | 1335 | U | C3'-C2'-C1' | 6.51 | 106.71 | 101.50 |
| 79 | CB | 13 | U | P-O5'-C5' | -6.51 | 110.49 | 120.90 |
| 79 | CB | 56 | A | C5'-C4'-C3' | -6.51 | 105.59 | 116.00 |
| 31 | BB | 227 | ARG | CB-CA-C | -6.51 | 97.39 | 110.40 |
| 45 | BR | 25 | TYR | CD1-CE1-CZ | 6.51 | 125.66 | 119.80 |
| 53 | Ba | 31 | GLU | N-CA-C | -6.51 | 93.43 | 111.00 |
| 64 | Bl | 63 | ARG | C-N-CA | 6.51 | 137.97 | 121.70 |
| 78 | CA | 1188 | G | N9-C1'-C2' | 6.51 | 122.46 | 114.00 |
| 78 | CA | 1315 | U | O4'-C1'-N1 | 6.51 | 113.41 | 108.20 |
| 80 | CC | 12 | A | O4'-C1'-C2' | 6.51 | 113.46 | 107.60 |
| 81 | DA | 520 | U | N1-C1'-C2' | 6.51 | 122.46 | 114.00 |
| 82 | DB | 138 | A | C3'-C2'-C1' | 6.51 | 106.70 | 101.50 |
| 81 | DA | 939 | U | O4'-C1'-N1 | 6.50 | 113.40 | 108.20 |
| 78 | CA | 310 | C | C3'-C2'-C1' | 6.50 | 106.70 | 101.50 |
| 78 | CA | 340 | U | O4'-C1'-N1 | 6.50 | 113.40 | 108.20 |
| 78 | CA | 553 | G | O4'-C1'-N9 | 6.50 | 113.40 | 108.20 |
| 78 | CA | 1018 | U | O4'-C1'-N1 | 6.50 | 113.40 | 108.20 |
| 78 | CA | 1427 | A | C4-C5-C6 | 6.50 | 120.25 | 117.00 |
| 78 | CA | 1429 | G | N1-C6-O6 | 6.50 | 123.80 | 119.90 |
| 79 | CB | 28 | G | C1'-O4'-C4' | -6.50 | 104.70 | 109.90 |
| 81 | DA | 2337 | C | N1-C1'-C2' | 6.50 | 122.45 | 114.00 |
| 40 | BK | 37 | ARG | NE-CZ-NH2 | -6.50 | 117.05 | 120.30 |
| 78 | CA | 465 | G | C1'-O4'-C4' | -6.50 | 104.70 | 109.90 |
| 81 | DA | 239 | G | O4'-C1'-N9 | 6.50 | 113.40 | 108.20 |
| 81 | DA | 263 | C | O3'-P-O5' | 6.50 | 116.35 | 104.00 |
| 81 | DA | 2279 | A | O5'-P-OP1 | 6.50 | 118.50 | 110.70 |
| 83 | DC | 51 | G | O4'-C1'-C2' | 6.50 | 113.45 | 107.60 |
| 4 | AD | 96 | ASN | N-CA-C | -6.50 | 93.45 | 111.00 |
| 45 | BR | 141 | ARG | C-N-CA | 6.50 | 135.95 | 122.30 |
| 41 | BN | 12 | TRP | N-CA-C | -6.50 | 93.45 | 111.00 |
| 81 | DA | 1224 | C | C1'-O4'-C4' | -6.50 | 104.70 | 109.90 |
| 81 | DA | 2991 | A | P-O3'-C3' | 6.50 | 127.50 | 119.70 |
| 4 | AD | 90 | ILE | CA-C-O | -6.50 | 106.46 | 120.10 |
| 18 | AP | 59 | PRO | C-N-CA | 6.50 | 137.94 | 121.70 |
| 78 | CA | 1240 | U | P-O3'-C3' | 6.50 | 127.50 | 119.70 |
| 78 | CA | 1282 | U | C3'-C2'-C1' | 6.50 | 106.70 | 101.50 |
| 81 | DA | 432 | G | O4'-C1'-N9 | 6.50 | 113.40 | 108.20 |
| 59 | Bh | 129 | GLU | CB-CA-C | -6.50 | 97.41 | 110.40 |
| 78 | CA | 1791 | A | O4'-C1'-N9 | -6.50 | 103.00 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 746 | A | P-O3'-C3' | 6.50 | 127.49 | 119.70 |
| 81 | DA | 1691 | U | O4'-C1'-C2' | -6.50 | 99.31 | 105.80 |
| 81 | DA | 1884 | A | O4'-C1'-N9 | 6.50 | 113.40 | 108.20 |
| 78 | CA | 1492 | A | O5'-C5'-C4' | 6.49 | 124.04 | 111.70 |
| 81 | DA | 698 | U | P-O3'-C3' | 6.49 | 127.49 | 119.70 |
| 81 | DA | 1869 | C | N1-C1'-C2' | 6.49 | 122.44 | 114.00 |
| 81 | DA | 3126 | C | C3'-C2'-C1' | 6.49 | 106.69 | 101.50 |
| 22 | AV | 29 | LYS | N-CA-CB | 6.49 | 122.29 | 110.60 |
| 41 | BN | 136 | ALA | CB-CA-C | -6.49 | 100.36 | 110.10 |
| 46 | BT | 84 | THR | CA-CB-CG2 | 6.49 | 121.49 | 112.40 |
| 3 | AB | 141 | LYS | N-CA-CB | 6.49 | 122.28 | 110.60 |
| 13 | AL | 9 | LEU | C-N-CA | 6.49 | 137.93 | 121.70 |
| 39 | BJ | 12 | TYR | O-C-N | -6.49 | 112.31 | 122.70 |
| 60 | Bi | 67 | LYS | CG-CD-CE | 6.49 | 131.37 | 111.90 |
| 78 | CA | 994 | G | C3'-C2'-C1' | -6.49 | 96.31 | 101.50 |
| 78 | CA | 1602 | C | N1-C1'-C2' | 6.49 | 122.44 | 114.00 |
| 81 | DA | 211 | A | C3'-C2'-C1' | 6.49 | 106.69 | 101.50 |
| 81 | DA | 1239 | C | O4'-C1'-N1 | 6.49 | 113.39 | 108.20 |
| 5 | AC | 126 | ARG | N-CA-CB | -6.49 | 98.92 | 110.60 |
| 31 | BB | 200 | ARG | NE-CZ-NH2 | 6.49 | 123.54 | 120.30 |
| 43 | BP | 121 | VAL | CB-CA-C | -6.49 | 99.07 | 111.40 |
| 81 | DA | 1256 | G | O4'-C1'-C2' | 6.49 | 113.44 | 107.60 |
| 31 | BB | 163 | ARG | NE-CZ-NH2 | -6.49 | 117.06 | 120.30 |
| 78 | CA | 1351 | G | O4'-C1'-N9 | 6.49 | 113.39 | 108.20 |
| 18 | AP | 100 | TYR | CB-CG-CD2 | -6.49 | 117.11 | 121.00 |
| 50 | BX | 34 | LEU | CA-C-N | 6.49 | 135.26 | 117.10 |
| 78 | CA | 1067 | C | C5'-C4'-O4' | 6.49 | 116.88 | 109.10 |
| 81 | DA | 1250 | G | C1'-O4'-C4' | 6.49 | 115.09 | 109.90 |
| 81 | DA | 2236 | G | C1'-O4'-C4' | -6.49 | 104.71 | 109.90 |
| 81 | DA | 2316 | G | C3'-C2'-C1' | 6.49 | 106.69 | 101.50 |
| 81 | DA | 2898 | G | O4'-C1'-N9 | -6.49 | 103.01 | 108.20 |
| 81 | DA | 3223 | A | C3'-C2'-C1' | 6.49 | 106.69 | 101.50 |
| 83 | DC | 19 | C | P-O3'-C3' | 6.49 | 127.48 | 119.70 |
| 78 | CA | 169 | A | O4'-C1'-C2' | -6.48 | 99.32 | 105.80 |
| 78 | CA | 1643 | U | C1'-O4'-C4' | 6.48 | 115.09 | 109.90 |
| 78 | CA | 1774 | G | P-O3'-C3' | 6.48 | 127.48 | 119.70 |
| 81 | DA | 1464 | G | O4'-C1'-N9 | 6.48 | 113.39 | 108.20 |
| 9 | AH | 23 | ARG | NH1-CZ-NH2 | 6.48 | 126.53 | 119.40 |
| 37 | BH | 73 | PRO | N-CA-CB | -6.48 | 95.47 | 102.60 |
| 78 | CA | 661 | A | C4'-C3'-C2' | -6.48 | 96.12 | 102.60 |
| 78 | CA | 1676 | U | O3'-P-O5' | 6.48 | 116.32 | 104.00 |
| 81 | DA | 1034 | U | N1-C1'-C2' | 6.48 | 122.43 | 114.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2402 | A | C1'-O4'-C4' | 6.48 | 115.09 | 109.90 |
| 81 | DA | 3354 | U | C1'-O4'-C4' | 6.48 | 115.08 | 109.90 |
| 8 | AF | 29 | ILE | N-CA-C | -6.48 | 93.50 | 111.00 |
| 19 | AR | 61 | ARG | NE-CZ-NH1 | 6.48 | 123.54 | 120.30 |
| 31 | BB | 35 | ALA | N-CA-CB | 6.48 | 119.17 | 110.10 |
| 33 | BD | 260 | GLN | C-N-CA | 6.48 | 137.90 | 121.70 |
| 57 | Be | 203 | TRP | CB-CG-CD2 | -6.48 | 118.17 | 126.60 |
| 78 | CA | 427 | C | C3'-C2'-C1' | 6.48 | 106.69 | 101.50 |
| 81 | DA | 826 | G | O4'-C1'-N9 | 6.48 | 113.38 | 108.20 |
| 81 | DA | 1976 | G | O5'-C5'-C4' | 6.48 | 124.01 | 111.70 |
| 82 | DB | 28 | C | O4'-C1'-C2' | -6.48 | 99.32 | 105.80 |
| 82 | DB | 135 | G | O4'-C1'-N9 | 6.48 | 113.39 | 108.20 |
| 83 | DC | 47 | C | OP2-P-O3' | -6.48 | 90.94 | 105.20 |
| 78 | CA | 1276 | U | O4'-C1'-N1 | 6.48 | 113.38 | 108.20 |
| 81 | DA | 1410 | U | P-O3'-C3' | -6.48 | 111.92 | 119.70 |
| 81 | DA | 3094 | A | O4'-C1'-N9 | -6.48 | 103.02 | 108.20 |
| 9 | AH | 27 | ILE | CB-CA-C | 6.48 | 124.56 | 111.60 |
| 44 | BO | 59 | ARG | N-CA-CB | 6.48 | 122.26 | 110.60 |
| 76 | BS | 70 | ASN | CA-C-O | -6.48 | 106.50 | 120.10 |
| 81 | DA | 6 | A | P-O3'-C3' | 6.48 | 127.47 | 119.70 |
| 81 | DA | 636 | C | O4'-C4'-C3' | -6.48 | 97.52 | 104.00 |
| 81 | DA | 2858 | U | C5'-C4'-C3' | -6.48 | 105.64 | 116.00 |
| 83 | DC | 62 | A | O4'-C1'-N9 | 6.48 | 113.38 | 108.20 |
| 81 | DA | 435 | C | P-O3'-C3' | 6.48 | 127.47 | 119.70 |
| 81 | DA | 2252 | A | C3'-C2'-C1' | 6.48 | 106.68 | 101.50 |
| 81 | DA | 3235 | C | P-O5'-C5' | 6.48 | 131.26 | 120.90 |
| 12 | AK | 58 | TYR | CB-CG-CD1 | 6.47 | 124.89 | 121.00 |
| 20 | AS | 94 | ILE | N-CA-C | -6.47 | 93.52 | 111.00 |
| 40 | BK | 187 | GLU | CA-C-N | 6.47 | 131.44 | 117.20 |
| 78 | CA | 434 | G | C1'-O4'-C4' | 6.47 | 115.08 | 109.90 |
| 78 | CA | 1693 | A | P-O3'-C3' | 6.47 | 127.47 | 119.70 |
| 81 | DA | 2246 | G | C5'-C4'-C3' | -6.47 | 105.64 | 116.00 |
| 82 | DB | 29 | U | P-O5'-C5' | 6.47 | 131.26 | 120.90 |
| 83 | DC | 49 | G | C5'-C4'-O4' | 6.47 | 116.87 | 109.10 |
| 32 | BC | 275 | ARG | NE-CZ-NH2 | -6.47 | 117.06 | 120.30 |
| 44 | BO | 118 | ILE | CA-C-O | -6.47 | 106.51 | 120.10 |
| 44 | BO | 128 | ARG | NE-CZ-NH1 | 6.47 | 123.54 | 120.30 |
| 78 | CA | 579 | A | C4-C5-C6 | 6.47 | 120.24 | 117.00 |
| 81 | DA | 2450 | G | C3'-C2'-C1' | -6.47 | 96.32 | 101.50 |
| 59 | Bh | 23 | ASP | CA-C-N | -6.47 | 102.96 | 117.20 |
| 78 | CA | 1184 | A | O4'-C1'-N9 | 6.47 | 113.38 | 108.20 |
| 83 | DC | 103 | U | O4'-C1'-C2' | -6.47 | 99.33 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|---|---|---|---|---|---|---|---|
| 35 | BG | 59 | GLU | N-CA-C | -6.47 | 93.53 | 111.00 |
| 37 | BH | 65 | LEU | C-N-CA | 6.47 | 137.87 | 121.70 |
| 42 | BM | 70 | ARG | N-CA-CB | 6.47 | 122.25 | 110.60 |
| 81 | DA | 1247 | U | C1'-O4'-C4' | 6.47 | 115.08 | 109.90 |
| 81 | DA | 2497 | U | O4'-C1'-N1 | 6.47 | 113.38 | 108.20 |
| 82 | DB | 115 | C | O4'-C1'-C2' | -6.47 | 99.33 | 105.80 |
| 78 | CA | 642 | G | O4'-C1'-N9 | 6.47 | 113.37 | 108.20 |
| 81 | DA | 1360 | C | O4'-C4'-C3' | 6.47 | 111.28 | 106.10 |
| 81 | DA | 2320 | A | O4'-C1'-N9 | 6.47 | 113.38 | 108.20 |
| 6 | AE | 8 | GLN | N-CA-CB | -6.47 | 98.96 | 110.60 |
| 20 | AS | 45 | MET | CG-SD-CE | -6.47 | 89.86 | 100.20 |
| 69 | Br | 97 | LYS | N-CA-CB | 6.47 | 122.24 | 110.60 |
| 78 | CA | 234 | G | O3'-P-O5' | 6.47 | 116.29 | 104.00 |
| 78 | CA | 839 | U | O4'-C4'-C3' | -6.47 | 97.53 | 104.00 |
| 78 | CA | 1509 | C | O4'-C1'-N1 | 6.47 | 113.37 | 108.20 |
| 81 | DA | 1707 | A | O4'-C1'-C2' | -6.47 | 99.33 | 105.80 |
| 81 | DA | 1925 | U | O4'-C1'-C2' | -6.47 | 99.33 | 105.80 |
| 81 | DA | 1963 | G | P-O5'-C5' | 6.47 | 131.25 | 120.90 |
| 81 | DA | 2511 | A | O4'-C1'-N9 | 6.47 | 113.37 | 108.20 |
| 81 | DA | 2769 | A | C1'-O4'-C4' | -6.47 | 104.73 | 109.90 |
| 78 | CA | 116 | U | C4'-C3'-C2' | -6.46 | 96.14 | 102.60 |
| 78 | CA | 1246 | C | C1'-O4'-C4' | -6.46 | 104.73 | 109.90 |
| 78 | CA | 1708 | U | O4'-C1'-N1 | 6.46 | 113.37 | 108.20 |
| 81 | DA | 1331 | U | O4'-C1'-C2' | -6.46 | 99.34 | 105.80 |
| 81 | DA | 2781 | U | N1-C1'-C2' | -6.46 | 104.89 | 112.00 |
| 81 | DA | 3054 | U | C3'-C2'-C1' | 6.46 | 106.67 | 101.50 |
| 55 | Bc | 70 | TYR | CB-CG-CD2 | -6.46 | 117.12 | 121.00 |
| 81 | DA | 177 | U | O4'-C1'-N1 | 6.46 | 113.37 | 108.20 |
| 81 | DA | 1955 | U | C1'-O4'-C4' | 6.46 | 115.07 | 109.90 |
| 81 | DA | 3314 | A | O5'-P-OP2 | 6.46 | 118.46 | 110.70 |
| 83 | DC | 36 | C | N1-C1'-C2' | 6.46 | 122.40 | 114.00 |
| 78 | CA | 318 | U | C3'-C2'-C1' | 6.46 | 106.67 | 101.50 |
| 81 | DA | 2054 | C | O4'-C1'-N1 | 6.46 | 113.37 | 108.20 |
| 83 | DC | 48 | U | C2'-C3'-O3' | -6.46 | 95.29 | 109.50 |
| 10 | AI | 114 | ARG | NE-CZ-NH2 | -6.46 | 117.07 | 120.30 |
| 81 | DA | 538 | G | P-O3'-C3' | 6.46 | 127.45 | 119.70 |
| 81 | DA | 750 | G | C2'-C3'-O3' | 6.46 | 124.04 | 113.70 |
| 81 | DA | 3122 | A | C3'-C2'-C1' | -6.46 | 96.33 | 101.50 |
| 81 | DA | 3395 | G | C3'-C2'-C1' | 6.46 | 106.67 | 101.50 |
| 81 | DA | 640 | U | C4'-C3'-C2' | -6.46 | 96.14 | 102.60 |
| 32 | BC | 289 | ASP | CB-CA-C | -6.46 | 97.49 | 110.40 |
| 32 | BC | 370 | PHE | O-C-N | -6.46 | 112.37 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 36 | C | C3'-C2'-C1' | 6.46 | 106.67 | 101.50 |
| 78 | CA | 491 | C | N3-C4-C5 | -6.46 | 119.32 | 121.90 |
| 78 | CA | 1062 | A | C4-C5-C6 | 6.46 | 120.23 | 117.00 |
| 81 | DA | 258 | G | N9-C1'-C2' | -6.46 | 104.90 | 112.00 |
| 81 | DA | 931 | C | O4'-C1'-N1 | 6.46 | 113.37 | 108.20 |
| 81 | DA | 1105 | A | O4'-C1'-C2' | -6.46 | 99.34 | 105.80 |
| 78 | CA | 1479 | A | O5'-P-OP2 | -6.46 | 99.89 | 105.70 |
| 81 | DA | 2970 | C | O4'-C1'-C2' | -6.46 | 99.34 | 105.80 |
| 78 | CA | 651 | G | C3'-C2'-C1' | 6.45 | 106.66 | 101.50 |
| 81 | DA | 975 | C | C3'-C2'-C1' | 6.45 | 106.66 | 101.50 |
| 81 | DA | 1186 | G | O4'-C1'-N9 | 6.45 | 113.36 | 108.20 |
| 81 | DA | 1311 | G | O4'-C1'-N9 | 6.45 | 113.36 | 108.20 |
| 81 | DA | 2751 | G | C4'-C3'-C2' | -6.45 | 96.15 | 102.60 |
| 81 | DA | 3022 | G | O4'-C1'-N9 | 6.45 | 113.36 | 108.20 |
| 6 | AE | 6 | ALA | C-N-CA | 6.45 | 137.82 | 121.70 |
| 53 | Ba | 12 | VAL | N-CA-C | -6.45 | 93.58 | 111.00 |
| 46 | BT | 171 | ASP | CB-CG-OD2 | -6.45 | 112.50 | 118.30 |
| 78 | CA | 223 | U | C1'-O4'-C4' | 6.45 | 115.06 | 109.90 |
| 78 | CA | 886 | U | C2'-C3'-O3' | 6.45 | 124.02 | 113.70 |
| 81 | DA | 1382 | G | O3'-P-O5' | 6.45 | 116.25 | 104.00 |
| 81 | DA | 2506 | U | O4'-C1'-C2' | -6.45 | 99.35 | 105.80 |
| 78 | CA | 309 | C | O4'-C1'-C2' | -6.45 | 99.35 | 105.80 |
| 78 | CA | 1504 | G | O4'-C1'-N9 | 6.45 | 113.36 | 108.20 |
| 81 | DA | 1493 | G | C1'-O4'-C4' | -6.45 | 104.74 | 109.90 |
| 81 | DA | 1760 | A | C5-C6-N1 | -6.45 | 114.48 | 117.70 |
| 81 | DA | 2980 | U | O4'-C1'-N1 | 6.45 | 113.36 | 108.20 |
| 42 | BM | 35 | TYR | CB-CA-C | 6.45 | 123.29 | 110.40 |
| 78 | CA | 206 | A | O4'-C1'-C2' | -6.45 | 99.35 | 105.80 |
| 78 | CA | 1654 | G | O4'-C1'-N9 | 6.45 | 113.36 | 108.20 |
| 81 | DA | 265 | A | O5'-C5'-C4' | -6.45 | 99.45 | 111.70 |
| 81 | DA | 727 | G | P-O3'-C3' | 6.45 | 127.44 | 119.70 |
| 81 | DA | 1338 | C | C2'-C3'-O3' | -6.45 | 95.32 | 109.50 |
| 81 | DA | 2576 | G | P-O3'-C3' | -6.45 | 111.96 | 119.70 |
| 31 | BB | 1 | MET | CG-SD-CE | -6.44 | 89.89 | 100.20 |
| 81 | DA | 1542 | G | C1'-O4'-C4' | -6.44 | 104.75 | 109.90 |
| 81 | DA | 2228 | A | C1'-O4'-C4' | 6.44 | 115.06 | 109.90 |
| 9 | AH | 130 | TYR | CB-CG-CD2 | 6.44 | 124.87 | 121.00 |
| 12 | AK | 114 | ARG | NE-CZ-NH1 | 6.44 | 123.52 | 120.30 |
| 36 | BF | 107 | ASP | CB-CG-OD1 | 6.44 | 124.10 | 118.30 |
| 81 | DA | 703 | G | O4'-C1'-N9 | 6.44 | 113.36 | 108.20 |
| 81 | DA | 1223 | A | O4'-C1'-N9 | 6.44 | 113.35 | 108.20 |
| 14 | AM | 99 | HIS | N-CA-C | -6.44 | 93.61 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | Be | 98 | LYS | CB-CA-C | -6.44 | 97.52 | 110.40 |
| 81 | DA | 517 | G | O4'-C1'-N9 | -6.44 | 103.05 | 108.20 |
| 81 | DA | 1114 | U | O4'-C4'-C3' | -6.44 | 97.56 | 104.00 |
| 81 | DA | 2175 | U | O4'-C1'-N1 | 6.44 | 113.35 | 108.20 |
| 81 | DA | 2194 | G | C3'-C2'-C1' | -6.44 | 96.35 | 101.50 |
| 4 | AD | 134 | LYS | CA-C-N | 6.44 | 129.08 | 116.20 |
| 39 | BJ | 90 | ARG | NE-CZ-NH1 | 6.44 | 123.52 | 120.30 |
| 78 | CA | 121 | U | O4'-C1'-N1 | 6.44 | 113.35 | 108.20 |
| 81 | DA | 135 | C | O4'-C1'-C2' | -6.44 | 99.36 | 105.80 |
| 81 | DA | 332 | C | C3'-C2'-C1' | 6.44 | 106.65 | 101.50 |
| 81 | DA | 863 | C | N1-C1'-C2' | 6.44 | 122.37 | 114.00 |
| 81 | DA | 1773 | C | N1-C1'-C2' | -6.44 | 104.92 | 112.00 |
| 81 | DA | 2873 | U | P-O3'-C3' | -6.44 | 111.97 | 119.70 |
| 3 | AB | 173 | ARG | NE-CZ-NH2 | -6.44 | 117.08 | 120.30 |
| 5 | AC | 127 | VAL | CG1-CB-CG2 | 6.44 | 121.20 | 110.90 |
| 19 | AR | 74 | ALA | N-CA-CB | 6.44 | 119.11 | 110.10 |
| 81 | DA | 949 | C | C3'-C2'-C1' | 6.44 | 106.65 | 101.50 |
| 81 | DA | 1297 | C | O4'-C1'-N1 | 6.44 | 113.35 | 108.20 |
| 78 | CA | 1035 | G | O4'-C1'-N9 | 6.43 | 113.35 | 108.20 |
| 81 | DA | 505 | G | O4'-C1'-N9 | 6.43 | 113.35 | 108.20 |
| 81 | DA | 1114 | U | N1-C1'-C2' | 6.43 | 122.37 | 114.00 |
| 81 | DA | 1548 | C | C3'-C2'-C1' | 6.43 | 106.65 | 101.50 |
| 81 | DA | 2013 | C | C5'-C4'-C3' | -6.43 | 105.70 | 116.00 |
| 81 | DA | 2183 | A | C4'-C3'-C2' | -6.43 | 96.17 | 102.60 |
| 81 | DA | 2378 | C | O4'-C1'-C2' | -6.43 | 99.37 | 105.80 |
| 81 | DA | 2515 | A | O3'-P-O5' | -6.43 | 91.77 | 104.00 |
| 81 | DA | 2673 | A | O5'-C5'-C4' | -6.43 | 99.47 | 111.70 |
| 81 | DA | 3163 | A | O4'-C1'-N9 | 6.43 | 113.35 | 108.20 |
| 10 | AI | 87 | LYS | N-CA-C | 6.43 | 128.37 | 111.00 |
| 33 | BD | 319 | LYS | N-CA-CB | 6.43 | 122.18 | 110.60 |
| 45 | BR | 111 | ARG | NE-CZ-NH1 | 6.43 | 123.52 | 120.30 |
| 74 | BQ | 258 | LYS | N-CA-CB | 6.43 | 122.18 | 110.60 |
| 78 | CA | 610 | G | N9-C1'-C2' | -6.43 | 104.92 | 112.00 |
| 78 | CA | 1443 | U | O4'-C1'-N1 | 6.43 | 113.35 | 108.20 |
| 81 | DA | 50 | U | C1'-O4'-C4' | 6.43 | 115.05 | 109.90 |
| 82 | DB | 39 | G | C1'-O4'-C4' | 6.43 | 115.05 | 109.90 |
| 32 | BC | 67 | PHE | CB-CG-CD1 | -6.43 | 116.30 | 120.80 |
| 32 | BC | 349 | LYS | N-CA-CB | 6.43 | 122.18 | 110.60 |
| 83 | DC | 104 | C | O4'-C1'-N1 | 6.43 | 113.34 | 108.20 |
| 1 | Aa | 54 | PHE | CA-C-O | -6.43 | 106.60 | 120.10 |
| 3 | AB | 124 | ARG | NE-CZ-NH2 | -6.43 | 117.08 | 120.30 |
| 78 | CA | 1744 | A | O4'-C1'-N9 | 6.43 | 113.34 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1426 | C | C4'-C3'-O3' | -6.43 | 95.90 | 109.40 |
| 81 | DA | 2256 | A | O4'-C1'-N9 | 6.43 | 113.34 | 108.20 |
| 78 | CA | 1651 | A | O4'-C1'-N9 | 6.43 | 113.34 | 108.20 |
| 78 | CA | 1681 | A | C5'-C4'-C3' | 6.43 | 126.28 | 116.00 |
| 83 | DC | 83 | U | C4'-C3'-C2' | -6.43 | 96.17 | 102.60 |
| 57 | Be | 134 | VAL | N-CA-CB | 6.43 | 125.64 | 111.50 |
| 78 | CA | 1495 | C | N3-C4-C5 | -6.43 | 119.33 | 121.90 |
| 81 | DA | 222 | A | C3'-C2'-C1' | 6.43 | 106.64 | 101.50 |
| 81 | DA | 1285 | G | C1'-O4'-C4' | 6.43 | 115.04 | 109.90 |
| 81 | DA | 1759 | C | N3-C4-C5 | -6.43 | 119.33 | 121.90 |
| 69 | Br | 9 | LYS | N-CA-CB | 6.42 | 122.16 | 110.60 |
| 78 | CA | 1114 | G | C4'-C3'-C2' | -6.42 | 96.18 | 102.60 |
| 81 | DA | 59 | G | N9-C1'-C2' | -6.42 | 104.93 | 112.00 |
| 81 | DA | 344 | A | P-O3'-C3' | -6.42 | 111.99 | 119.70 |
| 81 | DA | 637 | C | N1-C1'-C2' | 6.42 | 122.35 | 114.00 |
| 81 | DA | 1678 | G | C3'-C2'-C1' | -6.42 | 96.36 | 101.50 |
| 81 | DA | 1776 | G | C4'-C3'-C2' | -6.42 | 96.17 | 102.60 |
| 81 | DA | 3090 | U | O4'-C1'-C2' | -6.42 | 99.38 | 105.80 |
| 5 | AC | 161 | THR | CA-CB-CG2 | -6.42 | 103.41 | 112.40 |
| 78 | CA | 575 | C | N3-C4-N4 | 6.42 | 122.50 | 118.00 |
| 78 | CA | 1487 | A | P-O3'-C3' | 6.42 | 127.41 | 119.70 |
| 79 | CB | 70 | G | O4'-C1'-N9 | 6.42 | 113.34 | 108.20 |
| 81 | DA | 643 | U | N1-C1'-C2' | 6.42 | 122.35 | 114.00 |
| 8 | AF | 66 | GLN | N-CA-CB | 6.42 | 122.16 | 110.60 |
| 24 | AX | 38 | PRO | N-CA-CB | 6.42 | 111.01 | 103.30 |
| 37 | BH | 61 | GLN | N-CA-CB | 6.42 | 122.16 | 110.60 |
| 61 | Bj | 56 | SER | N-CA-C | -6.42 | 93.66 | 111.00 |
| 81 | DA | 3085 | G | C1'-O4'-C4' | -6.42 | 104.76 | 109.90 |
| 81 | DA | 208 | C | C3'-C2'-C1' | 6.42 | 106.64 | 101.50 |
| 81 | DA | 2167 | A | N9-C1'-C2' | 6.42 | 122.34 | 114.00 |
| 18 | AP | 108 | PRO | CB-CA-C | -6.42 | 95.95 | 112.00 |
| 31 | BB | 186 | PHE | CB-CG-CD1 | -6.42 | 116.31 | 120.80 |
| 32 | BC | 370 | PHE | C-N-CA | 6.42 | 137.75 | 121.70 |
| 78 | CA | 522 | U | O5'-C5'-C4' | 6.42 | 123.89 | 111.70 |
| 81 | DA | 1625 | A | N9-C1'-C2' | 6.42 | 122.34 | 114.00 |
| 81 | DA | 2393 | G | O5'-C5'-C4' | -6.42 | 99.50 | 111.70 |
| 81 | DA | 3003 | G | C1'-O4'-C4' | -6.42 | 104.77 | 109.90 |
| 81 | DA | 2211 | U | C5'-C4'-C3' | 6.42 | 126.27 | 116.00 |
| 81 | DA | 3364 | C | P-O3'-C3' | 6.42 | 127.40 | 119.70 |
| 33 | BD | 322 | GLN | N-CA-C | 6.42 | 128.32 | 111.00 |
| 81 | DA | 694 | C | P-O3'-C3' | 6.42 | 127.40 | 119.70 |
| 81 | DA | 3330 | A | C4'-C3'-C2' | -6.42 | 96.19 | 102.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 13 | AL | 20 | ARG | NE-CZ-NH2 | -6.41 | 117.09 | 120.30 |
| 78 | CA | 171 | A | C1'-O4'-C4' | 6.41 | 115.03 | 109.90 |
| 78 | CA | 406 | U | N1-C1'-C2' | 6.41 | 122.34 | 114.00 |
| 78 | CA | 948 | G | N9-C1'-C2' | 6.41 | 122.34 | 114.00 |
| 78 | CA | 1158 | C | P-O5'-C5' | 6.41 | 131.16 | 120.90 |
| 78 | CA | 1506 | G | O3'-P-O5' | -6.41 | 91.81 | 104.00 |
| 78 | CA | 1623 | C | N1-C1'-C2' | 6.41 | 122.34 | 114.00 |
| 81 | DA | 1104 | G | C3'-C2'-C1' | -6.41 | 96.37 | 101.50 |
| 81 | DA | 1383 | G | C4'-C3'-C2' | -6.41 | 96.19 | 102.60 |
| 81 | DA | 518 | G | O4'-C1'-C2' | -6.41 | 99.39 | 105.80 |
| 81 | DA | 2729 | U | C3'-C2'-C1' | 6.41 | 106.63 | 101.50 |
| 34 | BE | 82 | ARG | NE-CZ-NH2 | -6.41 | 117.09 | 120.30 |
| 37 | BH | 80 | TYR | CB-CG-CD1 | -6.41 | 117.15 | 121.00 |
| 53 | Ba | 17 | ARG | N-CA-CB | 6.41 | 122.14 | 110.60 |
| 78 | CA | 164 | A | O4'-C1'-N9 | -6.41 | 103.07 | 108.20 |
| 78 | CA | 1501 | C | N3-C4-C5 | -6.41 | 119.34 | 121.90 |
| 78 | CA | 1544 | U | OP1-P-O3' | -6.41 | 91.10 | 105.20 |
| 78 | CA | 1766 | A | P-O3'-C3' | 6.41 | 127.39 | 119.70 |
| 81 | DA | 77 | A | P-O3'-C3' | 6.41 | 127.39 | 119.70 |
| 81 | DA | 1185 | C | O4'-C1'-N1 | 6.41 | 113.33 | 108.20 |
| 81 | DA | 2091 | U | P-O3'-C3' | -6.41 | 112.01 | 119.70 |
| 44 | BO | 68 | PHE | CB-CG-CD2 | -6.41 | 116.31 | 120.80 |
| 62 | Bk | 37 | THR | N-CA-CB | 6.41 | 122.47 | 110.30 |
| 78 | CA | 1500 | C | N3-C4-N4 | 6.41 | 122.49 | 118.00 |
| 81 | DA | 494 | G | O4'-C1'-N9 | 6.41 | 113.33 | 108.20 |
| 81 | DA | 1866 | C | P-O3'-C3' | -6.41 | 112.01 | 119.70 |
| 81 | DA | 2966 | G | O4'-C1'-N9 | -6.41 | 103.07 | 108.20 |
| 81 | DA | 3150 | A | O5'-C5'-C4' | 6.41 | 123.88 | 111.70 |
| 32 | BC | 345 | ASN | CA-C-O | -6.41 | 106.65 | 120.10 |
| 61 | Bj | 48 | ARG | CB-CA-C | -6.41 | 97.59 | 110.40 |
| 78 | CA | 1172 | G | P-O3'-C3' | 6.41 | 127.39 | 119.70 |
| 14 | AM | 10 | SER | N-CA-CB | 6.41 | 120.11 | 110.50 |
| 78 | CA | 1023 | A | P-O3'-C3' | 6.41 | 127.39 | 119.70 |
| 81 | DA | 654 | C | N1-C1'-C2' | 6.41 | 122.33 | 114.00 |
| 81 | DA | 1480 | G | O4'-C1'-C2' | 6.41 | 113.36 | 107.60 |
| 81 | DA | 3166 | C | P-O5'-C5' | 6.41 | 131.15 | 120.90 |
| 17 | AQ | 91 | LEU | N-CA-C | -6.40 | 93.71 | 111.00 |
| 72 | Bt | 60 | ASN | CA-C-O | -6.40 | 106.65 | 120.10 |
| 81 | DA | 1975 | C | C3'-C2'-C1' | 6.40 | 106.62 | 101.50 |
| 81 | DA | 2793 | G | C5'-C4'-C3' | 6.40 | 126.25 | 116.00 |
| 78 | CA | 852 | C | C2'-C3'-O3' | 6.40 | 123.94 | 113.70 |
| 81 | DA | 426 | G | P-O3'-C3' | 6.40 | 127.38 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2237 | C | O3'-P-O5' | 6.40 | 116.16 | 104.00 |
| 81 | DA | 3248 | C | O4'-C1'-N1 | 6.40 | 113.32 | 108.20 |
| 10 | AI | 121 | SER | N-CA-C | -6.40 | 93.72 | 111.00 |
| 25 | AY | 47 | PRO | CA-N-CD | -6.40 | 102.54 | 111.50 |
| 59 | Bh | 46 | PHE | CB-CG-CD1 | -6.40 | 116.32 | 120.80 |
| 60 | Bi | 93 | PHE | CB-CG-CD2 | -6.40 | 116.32 | 120.80 |
| 78 | CA | 500 | C | N3-C4-N4 | 6.40 | 122.48 | 118.00 |
| 78 | CA | 690 | G | C1'-O4'-C4' | -6.40 | 104.78 | 109.90 |
| 78 | CA | 1347 | U | N1-C1'-C2' | -6.40 | 104.96 | 112.00 |
| 81 | DA | 3191 | G | P-O3'-C3' | -6.40 | 112.02 | 119.70 |
| 43 | BP | 180 | PHE | N-CA-C | -6.40 | 93.72 | 111.00 |
| 81 | DA | 2392 | C | C3'-C2'-C1' | 6.40 | 106.62 | 101.50 |
| 16 | AO | 64 | ARG | NE-CZ-NH1 | 6.40 | 123.50 | 120.30 |
| 61 | Bj | 37 | THR | CA-CB-OG1 | 6.40 | 122.44 | 109.00 |
| 81 | DA | 907 | G | O4'-C1'-C2' | 6.40 | 113.36 | 107.60 |
| 81 | DA | 1620 | U | O4'-C1'-C2' | 6.40 | 113.36 | 107.60 |
| 81 | DA | 3111 | U | C1'-O4'-C4' | 6.40 | 115.02 | 109.90 |
| 81 | DA | 3145 | C | O5'-C5'-C4' | -6.40 | 99.55 | 111.70 |
| 81 | DA | 3256 | G | N9-C1'-C2' | 6.40 | 122.32 | 114.00 |
| 31 | BB | 241 | ARG | NE-CZ-NH2 | -6.40 | 117.10 | 120.30 |
| 81 | DA | 1287 | A | C1'-O4'-C4' | 6.40 | 115.02 | 109.90 |
| 31 | BB | 128 | ARG | N-CA-C | -6.39 | 93.73 | 111.00 |
| 36 | BF | 47 | LYS | N-CA-CB | 6.39 | 122.11 | 110.60 |
| 38 | Bs | 222 | SER | N-CA-CB | -6.39 | 100.91 | 110.50 |
| 54 | Bd | 40 | ARG | NE-CZ-NH1 | 6.39 | 123.50 | 120.30 |
| 78 | CA | 4 | C | O4'-C1'-N1 | -6.39 | 103.08 | 108.20 |
| 78 | CA | 1332 | C | N1-C1'-C2' | 6.39 | 122.31 | 114.00 |
| 78 | CA | 1794 | A | N9-C1'-C2' | -6.39 | 104.97 | 112.00 |
| 81 | DA | 74 | G | C5'-C4'-O4' | -6.39 | 101.43 | 109.10 |
| 81 | DA | 1148 | G | O4'-C1'-N9 | 6.39 | 113.31 | 108.20 |
| 81 | DA | 2727 | A | C1'-O4'-C4' | -6.39 | 104.78 | 109.90 |
| 78 | CA | 230 | C | O4'-C1'-C2' | -6.39 | 99.41 | 105.80 |
| 78 | CA | 1479 | A | P-O5'-C5' | -6.39 | 110.67 | 120.90 |
| 81 | DA | 843 | A | P-O5'-C5' | -6.39 | 110.67 | 120.90 |
| 81 | DA | 2027 | C | O4'-C1'-C2' | -6.39 | 99.41 | 105.80 |
| 43 | BP | 150 | TRP | CG-CD2-CE3 | -6.39 | 128.15 | 133.90 |
| 78 | CA | 1065 | A | C4-C5-C6 | 6.39 | 120.19 | 117.00 |
| 57 | Be | 202 | LEU | C-N-CA | -6.39 | 105.72 | 121.70 |
| 81 | DA | 582 | G | C5'-C4'-C3' | -6.39 | 105.78 | 116.00 |
| 81 | DA | 527 | A | O4'-C1'-N9 | 6.39 | 113.31 | 108.20 |
| 81 | DA | 2059 | U | C1'-O4'-C4' | -6.39 | 104.79 | 109.90 |
| 52 | BY | 40 | ARG | NE-CZ-NH2 | -6.39 | 117.11 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 645 | C | C1'-O4'-C4' | 6.39 | 115.01 | 109.90 |
| 78 | CA | 1220 | C | C1'-O4'-C4' | 6.39 | 115.01 | 109.90 |
| 81 | DA | 1177 | G | C1'-O4'-C4' | -6.39 | 104.79 | 109.90 |
| 12 | AK | 107 | ARG | NH1-CZ-NH2 | 6.38 | 126.42 | 119.40 |
| 13 | AL | 87 | VAL | N-CA-C | -6.38 | 93.76 | 111.00 |
| 78 | CA | 351 | C | O4'-C1'-N1 | 6.38 | 113.31 | 108.20 |
| 78 | CA | 595 | G | P-O3'-C3' | 6.38 | 127.36 | 119.70 |
| 78 | CA | 850 | A | C3'-C2'-C1' | 6.38 | 106.61 | 101.50 |
| 79 | CB | 56 | A | N9-C1'-C2' | -6.38 | 104.98 | 112.00 |
| 81 | DA | 2439 | A | O4'-C1'-C2' | -6.38 | 99.42 | 105.80 |
| 81 | DA | 2857 | C | N1-C1'-C2' | 6.38 | 122.30 | 114.00 |
| 46 | BT | 71 | ARG | CA-C-N | 6.38 | 131.24 | 117.20 |
| 78 | CA | 203 | U | O4'-C1'-N1 | 6.38 | 113.31 | 108.20 |
| 78 | CA | 339 | C | C4'-C3'-C2' | -6.38 | 96.22 | 102.60 |
| 81 | DA | 1060 | U | C5'-C4'-C3' | 6.38 | 126.21 | 116.00 |
| 81 | DA | 2226 | U | P-O5'-C5' | 6.38 | 131.11 | 120.90 |
| 81 | DA | 2507 | C | P-O5'-C5' | -6.38 | 110.69 | 120.90 |
| 81 | DA | 2989 | U | OP1-P-OP2 | -6.38 | 110.03 | 119.60 |
| 1 | Aa | 150 | TRP | CA-CB-CG | 6.38 | 125.83 | 113.70 |
| 22 | AV | 63 | SER | CB-CA-C | 6.38 | 122.23 | 110.10 |
| 44 | BO | 62 | HIS | CA-C-O | -6.38 | 106.70 | 120.10 |
| 61 | Bj | 20 | LYS | CB-CA-C | 6.38 | 123.16 | 110.40 |
| 81 | DA | 1447 | G | C4'-C3'-C2' | -6.38 | 96.22 | 102.60 |
| 81 | DA | 1918 | C | C3'-C2'-C1' | 6.38 | 106.61 | 101.50 |
| 45 | BR | 149 | ALA | N-CA-CB | 6.38 | 119.03 | 110.10 |
| 81 | DA | 554 | A | N9-C1'-C2' | 6.38 | 122.29 | 114.00 |
| 81 | DA | 1820 | U | P-O5'-C5' | 6.38 | 131.11 | 120.90 |
| 81 | DA | 1841 | A | O4'-C1'-N9 | 6.38 | 113.30 | 108.20 |
| 83 | DC | 75 | G | C1'-O4'-C4' | -6.38 | 104.80 | 109.90 |
| 78 | CA | 275 | C | O4'-C1'-N1 | 6.38 | 113.30 | 108.20 |
| 81 | DA | 700 | C | P-O3'-C3' | 6.38 | 127.36 | 119.70 |
| 81 | DA | 2535 | A | C4-C5-C6 | 6.38 | 120.19 | 117.00 |
| 81 | DA | 2971 | A | N9-C1'-C2' | -6.38 | 104.98 | 112.00 |
| 33 | BD | 297 | SER | C-N-CA | 6.38 | 137.64 | 121.70 |
| 58 | Bg | 28 | ARG | CG-CD-NE | -6.38 | 98.41 | 111.80 |
| 61 | Bj | 2 | ALA | N-CA-C | 6.38 | 128.22 | 111.00 |
| 78 | CA | 70 | C | C5'-C4'-C3' | 6.38 | 126.20 | 116.00 |
| 33 | BD | 177 | ASP | CB-CG-OD2 | -6.38 | 112.56 | 118.30 |
| 81 | DA | 2708 | C | C3'-C2'-C1' | 6.38 | 106.60 | 101.50 |
| 83 | DC | 14 | U | P-O3'-C3' | -6.38 | 112.05 | 119.70 |
| 5 | AC | 43 | TYR | CG-CD2-CE2 | 6.37 | 126.40 | 121.30 |
| 33 | BD | 108 | LYS | C-N-CA | 6.37 | 137.63 | 121.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | Be | 202 | LEU | N-CA-C | -6.37 | 93.79 | 111.00 |
| 78 | CA | 1310 | U | P-O5'-C5' | 6.37 | 131.10 | 120.90 |
| 78 | CA | 1638 | G | O4'-C1'-N9 | 6.37 | 113.30 | 108.20 |
| 78 | CA | 1786 | G | C3'-C2'-C1' | 6.37 | 106.60 | 101.50 |
| 81 | DA | 319 | A | C1'-O4'-C4' | -6.37 | 104.80 | 109.90 |
| 81 | DA | 662 | U | C2'-C3'-O3' | 6.37 | 123.90 | 113.70 |
| 81 | DA | 776 | U | C1'-O4'-C4' | -6.37 | 104.80 | 109.90 |
| 81 | DA | 1772 | U | C3'-C2'-C1' | 6.37 | 106.60 | 101.50 |
| 81 | DA | 611 | A | P-O3'-C3' | -6.37 | 112.05 | 119.70 |
| 81 | DA | 1245 | A | P-O3'-C3' | 6.37 | 127.35 | 119.70 |
| 81 | DA | 1509 | A | P-O5'-C5' | 6.37 | 131.09 | 120.90 |
| 81 | DA | 3050 | U | C4'-C3'-C2' | -6.37 | 96.23 | 102.60 |
| 82 | DB | 98 | U | C5'-C4'-C3' | -6.37 | 105.81 | 116.00 |
| 34 | BE | 146 | GLY | N-CA-C | -6.37 | 97.17 | 113.10 |
| 43 | BP | 17 | ASP | N-CA-C | 6.37 | 128.20 | 111.00 |
| 81 | DA | 1009 | A | P-O5'-C5' | -6.37 | 110.71 | 120.90 |
| 81 | DA | 1990 | U | O4'-C1'-C2' | -6.37 | 99.43 | 105.80 |
| 81 | DA | 3304 | U | O4'-C1'-N1 | -6.37 | 103.10 | 108.20 |
| 69 | Br | 28 | TYR | CB-CG-CD1 | -6.37 | 117.18 | 121.00 |
| 81 | DA | 2848 | G | O4'-C1'-N9 | 6.37 | 113.30 | 108.20 |
| 83 | DC | 5 | G | C1'-O4'-C4' | -6.37 | 104.81 | 109.90 |
| 39 | BJ | 81 | VAL | CA-CB-CG2 | -6.37 | 101.35 | 110.90 |
| 78 | CA | 975 | C | O4'-C1'-N1 | 6.37 | 113.29 | 108.20 |
| 81 | DA | 203 | G | P-O3'-C3' | -6.37 | 112.06 | 119.70 |
| 81 | DA | 1151 | U | N1-C1'-C2' | 6.37 | 122.28 | 114.00 |
| 81 | DA | 3336 | A | N9-C1'-C2' | -6.37 | 105.00 | 112.00 |
| 4 | AD | 96 | ASN | C-N-CA | 6.36 | 137.61 | 121.70 |
| 13 | AL | 73 | ARG | NE-CZ-NH2 | -6.36 | 117.12 | 120.30 |
| 36 | BF | 83 | THR | CA-CB-CG2 | -6.36 | 103.49 | 112.40 |
| 42 | BM | 66 | LYS | O-C-N | -6.36 | 109.01 | 121.10 |
| 48 | BW | 104 | ARG | NE-CZ-NH2 | -6.36 | 117.12 | 120.30 |
| 81 | DA | 1081 | U | N1-C1'-C2' | 6.36 | 122.27 | 114.00 |
| 81 | DA | 2764 | C | C3'-C2'-C1' | 6.36 | 106.59 | 101.50 |
| 4 | AD | 216 | ASN | C-N-CA | 6.36 | 137.60 | 121.70 |
| 78 | CA | 60 | U | O4'-C1'-N1 | -6.36 | 103.11 | 108.20 |
| 81 | DA | 859 | G | O4'-C1'-C2' | -6.36 | 99.44 | 105.80 |
| 81 | DA | 1632 | A | C5'-C4'-C3' | 6.36 | 126.18 | 116.00 |
| 81 | DA | 2475 | G | P-O3'-C3' | 6.36 | 127.33 | 119.70 |
| 1 | Aa | 85 | TRP | N-CA-CB | 6.36 | 122.05 | 110.60 |
| 43 | BP | 148 | TYR | CB-CG-CD2 | 6.36 | 124.82 | 121.00 |
| 60 | Bi | 43 | LYS | N-CA-C | -6.36 | 93.83 | 111.00 |
| 65 | Bn | 54 | LEU | CB-CG-CD2 | 6.36 | 121.81 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 72 | Bu | 60 | ASN | CA-C-O | -6.36 | 106.75 | 120.10 |
| 78 | CA | 361 | C | N1-C1'-C2' | 6.36 | 122.27 | 114.00 |
| 78 | CA | 423 | G | C4'-C3'-C2' | -6.36 | 96.24 | 102.60 |
| 79 | CB | 14 | A | O4'-C1'-N9 | 6.36 | 113.29 | 108.20 |
| 81 | DA | 375 | A | C3'-C2'-C1' | 6.36 | 106.59 | 101.50 |
| 81 | DA | 2661 | G | O4'-C1'-N9 | 6.36 | 113.29 | 108.20 |
| 82 | DB | 116 | G | P-O5'-C5' | 6.36 | 131.08 | 120.90 |
| 53 | Ba | 31 | GLU | N-CA-CB | 6.36 | 122.05 | 110.60 |
| 64 | Bl | 73 | ARG | NE-CZ-NH2 | 6.36 | 123.48 | 120.30 |
| 78 | CA | 884 | A | O3'-P-O5' | -6.36 | 91.92 | 104.00 |
| 81 | DA | 146 | U | C4'-C3'-O3' | 6.36 | 125.72 | 113.00 |
| 81 | DA | 3372 | A | C4'-C3'-C2' | -6.36 | 96.24 | 102.60 |
| 1 | Aa | 53 | LYS | CA-C-O | -6.36 | 106.75 | 120.10 |
| 33 | BD | 102 | PRO | CA-N-CD | -6.36 | 102.60 | 111.50 |
| 35 | BG | 119 | ALA | CB-CA-C | -6.36 | 100.56 | 110.10 |
| 55 | Bc | 102 | GLU | CA-C-O | -6.36 | 106.75 | 120.10 |
| 78 | CA | 436 | A | O4'-C1'-N9 | 6.36 | 113.29 | 108.20 |
| 78 | CA | 438 | A | N9-C1'-C2' | 6.36 | 122.27 | 114.00 |
| 81 | DA | 816 | A | O4'-C1'-C2' | -6.36 | 99.44 | 105.80 |
| 81 | DA | 839 | C | O4'-C1'-N1 | 6.36 | 113.28 | 108.20 |
| 81 | DA | 911 | C | P-O5'-C5' | 6.36 | 131.07 | 120.90 |
| 81 | DA | 1236 | G | P-O3'-C3' | 6.36 | 127.33 | 119.70 |
| 81 | DA | 1596 | C | O4'-C1'-N1 | 6.36 | 113.29 | 108.20 |
| 81 | DA | 3314 | A | OP1-P-OP2 | -6.36 | 110.06 | 119.60 |
| 81 | DA | 3321 | C | C3'-C2'-C1' | 6.36 | 106.59 | 101.50 |
| 32 | BC | 381 | GLY | N-CA-C | -6.36 | 97.21 | 113.10 |
| 78 | CA | 1372 | U | O4'-C1'-N1 | 6.36 | 113.28 | 108.20 |
| 81 | DA | 1621 | A | O4'-C4'-C3' | -6.36 | 97.64 | 104.00 |
| 81 | DA | 1866 | C | O4'-C1'-C2' | -6.36 | 99.44 | 105.80 |
| 81 | DA | 2100 | A | C5'-C4'-C3' | 6.36 | 126.17 | 116.00 |
| 81 | DA | 2305 | G | O4'-C1'-N9 | 6.36 | 113.28 | 108.20 |
| 81 | DA | 2379 | U | O4'-C1'-N1 | 6.36 | 113.28 | 108.20 |
| 8 | AF | 35 | GLN | C-N-CA | 6.35 | 137.59 | 121.70 |
| 81 | DA | 1771 | C | O4'-C1'-N1 | 6.35 | 113.28 | 108.20 |
| 4 | AD | 109 | PHE | CB-CG-CD1 | -6.35 | 116.35 | 120.80 |
| 74 | BQ | 248 | ARG | NE-CZ-NH2 | -6.35 | 117.12 | 120.30 |
| 78 | CA | 155 | U | C5'-C4'-O4' | 6.35 | 116.72 | 109.10 |
| 78 | CA | 1611 | A | C3'-C2'-C1' | 6.35 | 106.58 | 101.50 |
| 81 | DA | 1972 | A | P-O5'-C5' | -6.35 | 110.74 | 120.90 |
| 81 | DA | 2639 | G | C1'-O4'-C4' | -6.35 | 104.82 | 109.90 |
| 81 | DA | 3243 | A | P-O3'-C3' | 6.35 | 127.32 | 119.70 |
| 37 | BH | 185 | ARG | NE-CZ-NH2 | -6.35 | 117.12 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1842 | A | C5'-C4'-C3' | 6.35 | 126.16 | 116.00 |
| 81 | DA | 2244 | A | C1'-O4'-C4' | 6.35 | 114.98 | 109.90 |
| 78 | CA | 964 | U | C5'-C4'-O4' | 6.35 | 116.72 | 109.10 |
| 78 | CA | 985 | G | O4'-C1'-N9 | 6.35 | 113.28 | 108.20 |
| 81 | DA | 2528 | G | O4'-C1'-N9 | 6.35 | 113.28 | 108.20 |
| 4 | AD | 130 | GLN | C-N-CA | 6.35 | 137.57 | 121.70 |
| 10 | AI | 66 | ARG | NE-CZ-NH1 | 6.35 | 123.47 | 120.30 |
| 18 | AP | 82 | ARG | NE-CZ-NH2 | -6.35 | 117.13 | 120.30 |
| 32 | BC | 272 | TYR | CB-CG-CD2 | -6.35 | 117.19 | 121.00 |
| 69 | Br | 81 | ALA | CB-CA-C | -6.35 | 100.58 | 110.10 |
| 78 | CA | 348 | U | C3'-C2'-C1' | 6.35 | 106.58 | 101.50 |
| 78 | CA | 495 | C | N3-C4-C5 | -6.35 | 119.36 | 121.90 |
| 81 | DA | 84 | U | O4'-C1'-N1 | 6.35 | 113.28 | 108.20 |
| 81 | DA | 485 | A | P-O3'-C3' | 6.35 | 127.32 | 119.70 |
| 81 | DA | 2681 | U | O4'-C4'-C3' | -6.35 | 97.65 | 104.00 |
| 81 | DA | 3015 | G | O4'-C1'-N9 | 6.35 | 113.28 | 108.20 |
| 78 | CA | 1738 | U | O4'-C1'-N1 | 6.35 | 113.28 | 108.20 |
| 31 | BB | 62 | VAL | CA-CB-CG1 | 6.34 | 120.42 | 110.90 |
| 76 | BS | 115 | ARG | NE-CZ-NH2 | -6.34 | 117.13 | 120.30 |
| 78 | CA | 577 | G | O4'-C1'-N9 | 6.34 | 113.28 | 108.20 |
| 78 | CA | 1794 | A | C3'-C2'-C1' | 6.34 | 106.58 | 101.50 |
| 80 | CC | 22 | A | O4'-C1'-N9 | 6.34 | 113.28 | 108.20 |
| 81 | DA | 423 | A | O4'-C1'-N9 | 6.34 | 113.28 | 108.20 |
| 81 | DA | 742 | G | C1'-O4'-C4' | 6.34 | 114.97 | 109.90 |
| 81 | DA | 1334 | U | C3'-C2'-C1' | 6.34 | 106.58 | 101.50 |
| 81 | DA | 2177 | G | P-O3'-C3' | -6.34 | 112.09 | 119.70 |
| 83 | DC | 107 | G | C1'-O4'-C4' | 6.34 | 114.98 | 109.90 |
| 63 | Bm | 64 | VAL | CA-CB-CG2 | 6.34 | 120.41 | 110.90 |
| 78 | CA | 449 | C | C3'-C2'-C1' | 6.34 | 106.57 | 101.50 |
| 81 | DA | 1977 | C | N1-C1'-C2' | 6.34 | 122.25 | 114.00 |
| 81 | DA | 2021 | G | O4'-C1'-N9 | 6.34 | 113.27 | 108.20 |
| 81 | DA | 2061 | G | C3'-C2'-C1' | -6.34 | 96.43 | 101.50 |
| 81 | DA | 3001 | C | C3'-C2'-C1' | 6.34 | 106.57 | 101.50 |
| 43 | BP | 95 | GLN | N-CA-CB | 6.34 | 122.01 | 110.60 |
| 58 | Bg | 101 | ALA | CB-CA-C | -6.34 | 100.59 | 110.10 |
| 81 | DA | 728 | G | O4'-C1'-N9 | 6.34 | 113.27 | 108.20 |
| 81 | DA | 2502 | A | O4'-C1'-C2' | -6.34 | 99.46 | 105.80 |
| 66 | Bo | 34 | THR | N-CA-CB | 6.34 | 122.34 | 110.30 |
| 81 | DA | 384 | A | P-O5'-C5' | 6.34 | 131.04 | 120.90 |
| 81 | DA | 768 | C | N3-C4-C5 | -6.34 | 119.36 | 121.90 |
| 81 | DA | 1526 | U | P-O5'-C5' | -6.34 | 110.76 | 120.90 |
| 81 | DA | 1702 | U | C3'-C2'-C1' | -6.34 | 96.43 | 101.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 31 | BB | 107 | VAL | CG1-CB-CG2 | -6.34 | 100.76 | 110.90 |
| 45 | BR | 18 | ALA | CB-CA-C | -6.34 | 100.59 | 110.10 |
| 78 | CA | 1178 | G | N9-C1'-C2' | 6.34 | 122.24 | 114.00 |
| 81 | DA | 1688 | U | OP1-P-O3' | 6.33 | 119.14 | 105.20 |
| 81 | DA | 1756 | C | N3-C4-N4 | 6.33 | 122.43 | 118.00 |
| 6 | AE | 139 | ILE | N-CA-CB | 6.33 | 125.37 | 110.80 |
| 9 | AH | 90 | THR | CA-CB-CG2 | -6.33 | 103.53 | 112.40 |
| 60 | Bi | 102 | LYS | N-CA-CB | 6.33 | 122.00 | 110.60 |
| 78 | CA | 589 | C | C1'-O4'-C4' | -6.33 | 104.83 | 109.90 |
| 81 | DA | 1882 | G | C3'-C2'-C1' | -6.33 | 96.43 | 101.50 |
| 78 | CA | 268 | C | C3'-C2'-C1' | 6.33 | 106.56 | 101.50 |
| 78 | CA | 1246 | C | N1-C1'-C2' | 6.33 | 122.23 | 114.00 |
| 78 | CA | 1580 | C | P-O3'-C3' | 6.33 | 127.30 | 119.70 |
| 78 | CA | 1591 | C | O4'-C1'-N1 | 6.33 | 113.27 | 108.20 |
| 81 | DA | 1177 | G | P-O3'-C3' | 6.33 | 127.30 | 119.70 |
| 81 | DA | 1771 | C | N3-C4-C5 | -6.33 | 119.37 | 121.90 |
| 42 | BM | 11 | PHE | N-CA-CB | 6.33 | 122.00 | 110.60 |
| 66 | Bo | 14 | ALA | CB-CA-C | -6.33 | 100.61 | 110.10 |
| 81 | DA | 2860 | U | O4'-C1'-N1 | 6.33 | 113.26 | 108.20 |
| 83 | DC | 45 | A | C5'-C4'-C3' | -6.33 | 105.87 | 116.00 |
| 3 | AB | 79 | TYR | CB-CG-CD1 | 6.33 | 124.80 | 121.00 |
| 81 | DA | 1866 | C | O4'-C1'-N1 | -6.33 | 103.14 | 108.20 |
| 81 | DA | 2444 | C | C3'-C2'-C1' | 6.33 | 106.56 | 101.50 |
| 81 | DA | 2637 | A | C1'-O4'-C4' | 6.33 | 114.96 | 109.90 |
| 78 | CA | 1413 | U | O4'-C1'-N1 | -6.33 | 103.14 | 108.20 |
| 81 | DA | 1824 | U | C4'-C3'-C2' | -6.33 | 96.27 | 102.60 |
| 81 | DA | 2375 | G | C1'-O4'-C4' | -6.33 | 104.84 | 109.90 |
| 16 | AO | 57 | ALA | N-CA-CB | 6.33 | 118.96 | 110.10 |
| 32 | BC | 35 | ASP | CB-CG-OD2 | -6.33 | 112.61 | 118.30 |
| 55 | Bc | 110 | ALA | N-CA-C | 6.33 | 128.08 | 111.00 |
| 58 | Bg | 89 | LEU | CB-CG-CD1 | -6.33 | 100.25 | 111.00 |
| 78 | CA | 110 | U | C3'-C2'-C1' | 6.33 | 106.56 | 101.50 |
| 78 | CA | 368 | U | O4'-C4'-C3' | -6.33 | 97.67 | 104.00 |
| 78 | CA | 1537 | C | O4'-C1'-N1 | -6.33 | 103.14 | 108.20 |
| 81 | DA | 2130 | G | C1'-O4'-C4' | 6.33 | 114.96 | 109.90 |
| 81 | DA | 2310 | U | O4'-C1'-N1 | 6.33 | 113.26 | 108.20 |
| 18 | AP | 69 | LYS | CD-CE-NZ | 6.32 | 126.24 | 111.70 |
| 21 | AT | 12 | TYR | CG-CD2-CE2 | 6.32 | 126.36 | 121.30 |
| 81 | DA | 665 | A | C3'-C2'-C1' | 6.32 | 106.56 | 101.50 |
| 81 | DA | 1142 | G | N9-C1'-C2' | 6.32 | 122.22 | 114.00 |
| 81 | DA | 2024 | G | C4'-C3'-C2' | -6.32 | 96.28 | 102.60 |
| 81 | DA | 2443 | A | N9-C1'-C2' | 6.32 | 122.22 | 114.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2963 | C | C1'-O4'-C4' | -6.32 | 104.84 | 109.90 |
| 42 | BM | 37 | ILE | CA-CB-CG1 | 6.32 | 123.01 | 111.00 |
| 55 | Bc | 39 | PRO | C-N-CA | 6.32 | 137.51 | 121.70 |
| 78 | CA | 1239 | U | O4'-C4'-C3' | -6.32 | 97.68 | 104.00 |
| 83 | DC | 66 | C | C3'-C2'-C1' | 6.32 | 106.56 | 101.50 |
| 32 | BC | 382 | THR | N-CA-CB | 6.32 | 122.31 | 110.30 |
| 79 | CB | 52 | G | O4'-C1'-N9 | 6.32 | 113.26 | 108.20 |
| 81 | DA | 63 | A | N9-C1'-C2' | -6.32 | 105.05 | 112.00 |
| 81 | DA | 171 | G | P-O5'-C5' | 6.32 | 131.01 | 120.90 |
| 81 | DA | 339 | C | N1-C1'-C2' | 6.32 | 122.22 | 114.00 |
| 81 | DA | 376 | G | C3'-C2'-C1' | -6.32 | 96.44 | 101.50 |
| 81 | DA | 638 | C | O3'-P-O5' | -6.32 | 91.99 | 104.00 |
| 81 | DA | 2859 | U | N1-C1'-C2' | -6.32 | 105.05 | 112.00 |
| 81 | DA | 3167 | A | O5'-C5'-C4' | 6.32 | 123.71 | 111.70 |
| 82 | DB | 97 | A | O4'-C1'-N9 | 6.32 | 113.25 | 108.20 |
| 5 | AC | 57 | ARG | NE-CZ-NH1 | 6.32 | 123.46 | 120.30 |
| 33 | BD | 221 | ASN | CB-CA-C | -6.32 | 97.77 | 110.40 |
| 37 | BH | 222 | PHE | N-CA-C | -6.32 | 93.94 | 111.00 |
| 69 | Br | 101 | GLY | C-N-CA | -6.32 | 105.91 | 121.70 |
| 74 | BQ | 122 | VAL | N-CA-C | -6.32 | 93.94 | 111.00 |
| 78 | CA | 1254 | U | OP1-P-O3' | 6.32 | 119.10 | 105.20 |
| 81 | DA | 846 | A | O4'-C1'-N9 | -6.32 | 103.15 | 108.20 |
| 81 | DA | 1781 | C | O4'-C1'-C2' | -6.32 | 99.48 | 105.80 |
| 31 | BB | 40 | TYR | CB-CA-C | 6.32 | 123.03 | 110.40 |
| 78 | CA | 408 | C | C3'-C2'-C1' | 6.32 | 106.55 | 101.50 |
| 78 | CA | 888 | U | N1-C1'-C2' | 6.32 | 122.21 | 114.00 |
| 78 | CA | 1437 | U | N1-C1'-C2' | -6.32 | 105.05 | 112.00 |
| 81 | DA | 3009 | G | C3'-C2'-C1' | -6.32 | 96.45 | 101.50 |
| 3 | AB | 77 | PHE | N-CA-C | -6.31 | 93.95 | 111.00 |
| 69 | Br | 87 | ARG | NE-CZ-NH1 | 6.31 | 123.46 | 120.30 |
| 78 | CA | 497 | G | O4'-C1'-N9 | 6.31 | 113.25 | 108.20 |
| 78 | CA | 1120 | U | P-O3'-C3' | -6.31 | 112.12 | 119.70 |
| 81 | DA | 93 | C | O4'-C1'-C2' | -6.31 | 99.49 | 105.80 |
| 81 | DA | 1771 | C | OP1-P-O3' | 6.31 | 119.09 | 105.20 |
| 81 | DA | 2259 | A | O4'-C1'-N9 | 6.31 | 113.25 | 108.20 |
| 81 | DA | 3006 | A | O4'-C1'-N9 | -6.31 | 103.15 | 108.20 |
| 59 | Bh | 24 | ARG | N-CA-CB | -6.31 | 99.24 | 110.60 |
| 81 | DA | 1542 | G | O4'-C1'-C2' | 6.31 | 113.28 | 107.60 |
| 81 | DA | 2146 | C | C3'-C2'-C1' | 6.31 | 106.55 | 101.50 |
| 81 | DA | 3008 | A | O3'-P-O5' | -6.31 | 92.01 | 104.00 |
| 74 | BQ | 238 | ASP | CB-CG-OD2 | -6.31 | 112.62 | 118.30 |
| 81 | DA | 350 | C | O4'-C1'-C2' | -6.31 | 99.49 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 822 | G | O4'-C1'-N9 | 6.31 | 113.25 | 108.20 |
| 81 | DA | 2024 | G | O3'-P-O5' | 6.31 | 115.99 | 104.00 |
| 82 | DB | 18 | U | N1-C1'-C2' | 6.31 | 122.20 | 114.00 |
| 5 | AC | 79 | ARG | NE-CZ-NH2 | -6.31 | 117.15 | 120.30 |
| 57 | Be | 107 | ARG | NE-CZ-NH1 | 6.31 | 123.45 | 120.30 |
| 78 | CA | 905 | A | OP1-P-OP2 | -6.31 | 110.14 | 119.60 |
| 78 | CA | 1461 | C | C3'-C2'-C1' | 6.31 | 106.55 | 101.50 |
| 81 | DA | 1192 | C | P-O3'-C3' | 6.31 | 127.27 | 119.70 |
| 81 | DA | 2171 | G | P-O3'-C3' | -6.31 | 112.13 | 119.70 |
| 38 | Bs | 53 | MET | N-CA-CB | -6.31 | 99.25 | 110.60 |
| 74 | BQ | 286 | VAL | N-CA-C | -6.31 | 93.97 | 111.00 |
| 81 | DA | 3200 | G | P-O3'-C3' | 6.31 | 127.27 | 119.70 |
| 58 | Bg | 10 | ARG | NH1-CZ-NH2 | -6.30 | 112.46 | 119.40 |
| 81 | DA | 679 | U | P-O5'-C5' | 6.30 | 130.99 | 120.90 |
| 81 | DA | 1147 | G | N9-C1'-C2' | -6.30 | 105.07 | 112.00 |
| 81 | DA | 1179 | A | C1'-O4'-C4' | 6.30 | 114.94 | 109.90 |
| 13 | AL | 11 | SER | N-CA-CB | 6.30 | 119.95 | 110.50 |
| 81 | DA | 910 | G | N9-C1'-C2' | 6.30 | 122.19 | 114.00 |
| 81 | DA | 1792 | C | P-O5'-C5' | -6.30 | 110.82 | 120.90 |
| 81 | DA | 2174 | G | C1'-O4'-C4' | 6.30 | 114.94 | 109.90 |
| 81 | DA | 2677 | G | C1'-O4'-C4' | 6.30 | 114.94 | 109.90 |
| 83 | DC | 2 | G | O5'-C5'-C4' | -6.30 | 99.72 | 111.70 |
| 10 | AI | 46 | PHE | CB-CG-CD1 | -6.30 | 116.39 | 120.80 |
| 13 | AL | 87 | VAL | CA-CB-CG1 | -6.30 | 101.45 | 110.90 |
| 55 | Bc | 96 | GLU | CA-C-N | 6.30 | 131.06 | 117.20 |
| 68 | Bq | 21 | ARG | NE-CZ-NH2 | -6.30 | 117.15 | 120.30 |
| 78 | CA | 573 | C | P-O3'-C3' | 6.30 | 127.26 | 119.70 |
| 78 | CA | 1474 | G | C1'-O4'-C4' | -6.30 | 104.86 | 109.90 |
| 81 | DA | 383 | G | O4'-C1'-N9 | 6.30 | 113.24 | 108.20 |
| 81 | DA | 803 | C | P-O3'-C3' | -6.30 | 112.14 | 119.70 |
| 81 | DA | 959 | C | C3'-C2'-C1' | 6.30 | 106.54 | 101.50 |
| 81 | DA | 1522 | U | P-O3'-C3' | 6.30 | 127.26 | 119.70 |
| 82 | DB | 116 | G | P-O3'-C3' | -6.30 | 112.14 | 119.70 |
| 48 | BW | 98 | THR | N-CA-CB | 6.30 | 122.27 | 110.30 |
| 69 | Br | 103 | ALA | C-N-CA | 6.30 | 137.45 | 121.70 |
| 78 | CA | 1053 | G | N3-C2-N2 | 6.30 | 124.31 | 119.90 |
| 81 | DA | 3028 | G | N9-C1'-C2' | 6.30 | 122.19 | 114.00 |
| 81 | DA | 3306 | U | C1'-O4'-C4' | -6.30 | 104.86 | 109.90 |
| 78 | CA | 895 | G | P-O3'-C3' | 6.30 | 127.26 | 119.70 |
| 78 | CA | 1411 | A | C5'-C4'-O4' | -6.30 | 101.54 | 109.10 |
| 78 | CA | 1424 | A | C3'-C2'-C1' | 6.30 | 106.54 | 101.50 |
| 33 | BD | 296 | GLN | CA-C-N | 6.30 | 131.05 | 117.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 44 | BO | 68 | PHE | CB-CG-CD1 | 6.30 | 125.21 | 120.80 |
| 78 | CA | 1064 | G | C5-C6-O6 | -6.30 | 124.82 | 128.60 |
| 81 | DA | 310 | U | O4'-C1'-C2' | -6.30 | 99.50 | 105.80 |
| 81 | DA | 329 | U | O4'-C1'-C2' | 6.29 | 113.27 | 107.60 |
| 81 | DA | 2677 | G | C4'-C3'-C2' | -6.29 | 96.31 | 102.60 |
| 8 | AF | 106 | LYS | CB-CG-CD | 6.29 | 127.96 | 111.60 |
| 15 | AN | 31 | ILE | N-CA-CB | 6.29 | 125.27 | 110.80 |
| 78 | CA | 1506 | G | N1-C6-O6 | 6.29 | 123.68 | 119.90 |
| 78 | CA | 1579 | U | C5'-C4'-C3' | -6.29 | 105.93 | 116.00 |
| 79 | CB | 74 | C | C3'-C2'-C1' | 6.29 | 106.53 | 101.50 |
| 81 | DA | 1178 | G | O4'-C1'-N9 | -6.29 | 103.17 | 108.20 |
| 81 | DA | 3066 | U | N1-C1'-C2' | -6.29 | 105.08 | 112.00 |
| 81 | DA | 3084 | C | O4'-C1'-C2' | -6.29 | 99.51 | 105.80 |
| 17 | AQ | 100 | LEU | CB-CA-C | -6.29 | 98.25 | 110.20 |
| 31 | BB | 249 | SER | C-N-CA | -6.29 | 105.97 | 121.70 |
| 74 | BQ | 185 | PHE | CB-CG-CD1 | 6.29 | 125.20 | 120.80 |
| 78 | CA | 485 | A | C5-C6-N6 | -6.29 | 118.67 | 123.70 |
| 78 | CA | 1269 | U | O4'-C1'-N1 | 6.29 | 113.23 | 108.20 |
| 78 | CA | 1323 | C | C1'-O4'-C4' | -6.29 | 104.87 | 109.90 |
| 81 | DA | 2454 | G | P-O3'-C3' | 6.29 | 127.25 | 119.70 |
| 81 | DA | 2973 | G | O4'-C1'-N9 | 6.29 | 113.23 | 108.20 |
| 5 | AC | 14 | THR | CA-C-N | 6.29 | 134.71 | 117.10 |
| 30 | BA | 86 | SER | N-CA-CB | 6.29 | 119.94 | 110.50 |
| 38 | Bs | 73 | PHE | CB-CG-CD2 | 6.29 | 125.20 | 120.80 |
| 78 | CA | 842 | C | N3-C4-N4 | 6.29 | 122.40 | 118.00 |
| 81 | DA | 614 | C | P-O5'-C5' | 6.29 | 130.96 | 120.90 |
| 81 | DA | 615 | U | N1-C1'-C2' | 6.29 | 122.18 | 114.00 |
| 81 | DA | 1139 | G | N9-C1'-C2' | 6.29 | 122.18 | 114.00 |
| 81 | DA | 2843 | U | O4'-C1'-N1 | 6.29 | 113.23 | 108.20 |
| 21 | AT | 43 | GLY | O-C-N | -6.29 | 112.64 | 122.70 |
| 38 | Bs | 66 | PHE | CB-CG-CD1 | 6.29 | 125.20 | 120.80 |
| 81 | DA | 59 | G | O4'-C1'-N9 | 6.29 | 113.23 | 108.20 |
| 81 | DA | 317 | A | C1'-O4'-C4' | -6.29 | 104.87 | 109.90 |
| 81 | DA | 770 | G | O4'-C1'-N9 | 6.29 | 113.23 | 108.20 |
| 81 | DA | 2581 | U | C5'-C4'-C3' | 6.29 | 126.06 | 116.00 |
| 53 | Ba | 29 | HIS | CB-CA-C | -6.29 | 97.83 | 110.40 |
| 34 | BE | 15 | GLU | CA-CB-CG | 6.29 | 127.23 | 113.40 |
| 47 | BU | 84 | TYR | CG-CD2-CE2 | -6.29 | 116.27 | 121.30 |
| 78 | CA | 99 | C | C3'-C2'-C1' | 6.29 | 106.53 | 101.50 |
| 81 | DA | 541 | U | P-O3'-C3' | -6.29 | 112.16 | 119.70 |
| 81 | DA | 856 | G | P-O5'-C5' | 6.29 | 130.96 | 120.90 |
| 81 | DA | 1478 | C | C1'-O4'-C4' | -6.29 | 104.87 | 109.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1538 | G | O3'-P-O5' | -6.29 | 92.06 | 104.00 |
| 81 | DA | 2576 | G | O4'-C1'-N9 | 6.29 | 113.23 | 108.20 |
| 81 | DA | 3330 | A | C3'-C2'-C1' | 6.29 | 106.53 | 101.50 |
| 83 | DC | 72 | C | C5'-C4'-O4' | -6.29 | 101.56 | 109.10 |
| 43 | BP | 180 | PHE | CA-CB-CG | 6.28 | 128.98 | 113.90 |
| 78 | CA | 672 | U | N1-C1'-C2' | 6.28 | 122.17 | 114.00 |
| 78 | CA | 1132 | A | O4'-C1'-N9 | 6.28 | 113.23 | 108.20 |
| 78 | CA | 1294 | G | C1'-O4'-C4' | -6.28 | 104.87 | 109.90 |
| 82 | DB | 47 | C | P-O3'-C3' | 6.28 | 127.24 | 119.70 |
| 82 | DB | 101 | U | C4'-C3'-C2' | -6.28 | 96.32 | 102.60 |
| 82 | DB | 102 | U | N1-C1'-C2' | 6.28 | 122.17 | 114.00 |
| 4 | AD | 138 | TYR | N-CA-C | -6.28 | 94.04 | 111.00 |
| 77 | BI | 106 | ALA | C-N-CA | 6.28 | 135.49 | 122.30 |
| 78 | CA | 1503 | A | C4-C5-C6 | 6.28 | 120.14 | 117.00 |
| 3 | AB | 18 | TYR | CB-CA-C | 6.28 | 122.96 | 110.40 |
| 78 | CA | 308 | C | C3'-C2'-C1' | 6.28 | 106.53 | 101.50 |
| 78 | CA | 500 | C | N3-C4-C5 | -6.28 | 119.39 | 121.90 |
| 78 | CA | 947 | U | P-O3'-C3' | -6.28 | 112.16 | 119.70 |
| 78 | CA | 1575 | G | C1'-O4'-C4' | -6.28 | 104.88 | 109.90 |
| 81 | DA | 1309 | U | P-O3'-C3' | 6.28 | 127.24 | 119.70 |
| 81 | DA | 1473 | G | O4'-C1'-N9 | 6.28 | 113.22 | 108.20 |
| 81 | DA | 1808 | G | C1'-O4'-C4' | -6.28 | 104.88 | 109.90 |
| 81 | DA | 2746 | A | C1'-O4'-C4' | -6.28 | 104.88 | 109.90 |
| 81 | DA | 2939 | G | O4'-C1'-N9 | 6.28 | 113.22 | 108.20 |
| 81 | DA | 2950 | G | C2'-C3'-O3' | 6.28 | 123.75 | 113.70 |
| 81 | DA | 3012 | A | O4'-C1'-N9 | 6.28 | 113.22 | 108.20 |
| 78 | CA | 528 | U | O3'-P-O5' | -6.28 | 92.07 | 104.00 |
| 81 | DA | 2965 | U | N1-C1'-C2' | 6.28 | 122.16 | 114.00 |
| 81 | DA | 124 | U | O3'-P-O5' | -6.28 | 92.07 | 104.00 |
| 81 | DA | 542 | G | O4'-C1'-N9 | 6.28 | 113.22 | 108.20 |
| 81 | DA | 1899 | G | O4'-C1'-N9 | 6.28 | 113.22 | 108.20 |
| 81 | DA | 2437 | G | P-O5'-C5' | 6.28 | 130.94 | 120.90 |
| 81 | DA | 3112 | G | N9-C1'-C2' | -6.28 | 105.09 | 112.00 |
| 82 | DB | 50 | C | N1-C1'-C2' | -6.28 | 105.09 | 112.00 |
| 4 | AD | 135 | GLY | C-N-CA | 6.28 | 137.39 | 121.70 |
| 56 | Bf | 50 | VAL | CA-CB-CG1 | -6.28 | 101.49 | 110.90 |
| 78 | CA | 377 | G | O4'-C1'-C2' | -6.28 | 99.52 | 105.80 |
| 61 | Bj | 5 | HIS | N-CA-CB | 6.27 | 121.89 | 110.60 |
| 78 | CA | 1111 | G | O4'-C1'-C2' | 6.27 | 113.25 | 107.60 |
| 78 | CA | 1286 | U | C3'-C2'-C1' | 6.27 | 106.52 | 101.50 |
| 78 | CA | 1647 | U | C1'-O4'-C4' | -6.27 | 104.88 | 109.90 |
| 81 | DA | 1105 | A | N9-C1'-C2' | -6.27 | 105.10 | 112.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1379 | G | P-O3'-C3' | 6.27 | 127.23 | 119.70 |
| 81 | DA | 1580 | A | C1'-O4'-C4' | -6.27 | 104.88 | 109.90 |
| 81 | DA | 1956 | A | C1'-O4'-C4' | 6.27 | 114.92 | 109.90 |
| 81 | DA | 136 | G | P-O3'-C3' | 6.27 | 127.23 | 119.70 |
| 81 | DA | 162 | G | C4'-C3'-C2' | -6.27 | 96.33 | 102.60 |
| 81 | DA | 1284 | C | C3'-C2'-C1' | 6.27 | 106.52 | 101.50 |
| 81 | DA | 1963 | G | C3'-C2'-C1' | -6.27 | 96.48 | 101.50 |
| 81 | DA | 3150 | A | C4'-C3'-C2' | -6.27 | 96.33 | 102.60 |
| 78 | CA | 45 | U | C4'-C3'-C2' | 6.27 | 108.87 | 102.60 |
| 78 | CA | 1532 | U | O4'-C1'-C2' | -6.27 | 99.53 | 105.80 |
| 81 | DA | 194 | U | O4'-C1'-N1 | 6.27 | 113.22 | 108.20 |
| 81 | DA | 1632 | A | C4'-C3'-C2' | -6.27 | 96.33 | 102.60 |
| 3 | AB | 18 | TYR | C-N-CA | 6.27 | 137.38 | 121.70 |
| 5 | AC | 88 | GLU | CB-CA-C | 6.27 | 122.94 | 110.40 |
| 59 | Bh | 11 | LYS | C-N-CA | 6.27 | 137.37 | 121.70 |
| 81 | DA | 961 | C | O4'-C1'-C2' | -6.27 | 99.53 | 105.80 |
| 81 | DA | 1647 | A | O4'-C1'-C2' | -6.27 | 99.53 | 105.80 |
| 81 | DA | 1679 | A | C3'-C2'-C1' | 6.27 | 106.52 | 101.50 |
| 81 | DA | 2703 | A | P-O3'-C3' | 6.27 | 127.22 | 119.70 |
| 78 | CA | 138 | A | C3'-C2'-C1' | -6.27 | 96.49 | 101.50 |
| 78 | CA | 402 | C | O4'-C1'-C2' | -6.27 | 99.53 | 105.80 |
| 78 | CA | 1609 | U | N1-C1'-C2' | 6.27 | 122.15 | 114.00 |
| 81 | DA | 983 | A | OP1-P-OP2 | -6.27 | 110.20 | 119.60 |
| 81 | DA | 2105 | G | O4'-C1'-N9 | 6.27 | 113.21 | 108.20 |
| 81 | DA | 2440 | G | P-O3'-C3' | -6.27 | 112.18 | 119.70 |
| 81 | DA | 2787 | G | O4'-C1'-C2' | 6.27 | 113.24 | 107.60 |
| 2 | AA | 241 | GLU | OE1-CD-OE2 | 6.27 | 130.82 | 123.30 |
| 26 | AZ | 57 | ASN | N-CA-C | -6.27 | 94.08 | 111.00 |
| 45 | BR | 14 | GLY | O-C-N | -6.26 | 112.68 | 122.70 |
| 46 | BT | 148 | ASP | CB-CG-OD2 | -6.26 | 112.66 | 118.30 |
| 81 | DA | 982 | C | O4'-C1'-N1 | 6.26 | 113.21 | 108.20 |
| 81 | DA | 1879 | A | C3'-C2'-C1' | 6.26 | 106.51 | 101.50 |
| 81 | DA | 2235 | C | N1-C1'-C2' | 6.26 | 122.14 | 114.00 |
| 81 | DA | 2366 | C | P-O3'-C3' | 6.26 | 127.22 | 119.70 |
| 83 | DC | 72 | C | P-O3'-C3' | 6.26 | 127.22 | 119.70 |
| 48 | BW | 98 | THR | CA-C-N | -6.26 | 103.42 | 117.20 |
| 78 | CA | 234 | G | C5'-C4'-O4' | -6.26 | 101.58 | 109.10 |
| 81 | DA | 2823 | G | N9-C1'-C2' | 6.26 | 122.14 | 114.00 |
| 5 | AC | 83 | VAL | CA-CB-CG2 | -6.26 | 101.51 | 110.90 |
| 81 | DA | 2680 | A | P-O3'-C3' | -6.26 | 112.19 | 119.70 |
| 9 | AH | 28 | ARG | CB-CA-C | -6.26 | 97.88 | 110.40 |
| 18 | AP | 110 | HIS | C-N-CA | 6.26 | 137.35 | 121.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 41 | BN | 10 | SER | N-CA-CB | 6.26 | 119.89 | 110.50 |
| 78 | CA | 146 | U | N1-C1'-C2' | 6.26 | 122.14 | 114.00 |
| 81 | DA | 13 | A | C3'-C2'-C1' | 6.26 | 106.51 | 101.50 |
| 81 | DA | 474 | G | O4'-C1'-N9 | 6.26 | 113.21 | 108.20 |
| 81 | DA | 1756 | C | C3'-C2'-C1' | 6.26 | 106.51 | 101.50 |
| 81 | DA | 2240 | G | C1'-O4'-C4' | -6.26 | 104.89 | 109.90 |
| 81 | DA | 2628 | A | C4'-C3'-C2' | 6.26 | 108.86 | 102.60 |
| 82 | DB | 40 | A | N9-C1'-C2' | 6.26 | 122.14 | 114.00 |
| 82 | DB | 56 | G | C3'-C2'-C1' | 6.26 | 106.51 | 101.50 |
| 83 | DC | 48 | U | C5'-C4'-C3' | -6.26 | 105.98 | 116.00 |
| 51 | BZ | 71 | ARG | CA-C-N | -6.26 | 103.43 | 117.20 |
| 78 | CA | 37 | U | C3'-C2'-C1' | 6.26 | 106.51 | 101.50 |
| 78 | CA | 121 | U | C5'-C4'-C3' | 6.26 | 126.01 | 116.00 |
| 81 | DA | 739 | G | C5-C6-O6 | -6.26 | 124.84 | 128.60 |
| 81 | DA | 873 | C | P-O5'-C5' | -6.26 | 110.89 | 120.90 |
| 81 | DA | 1941 | C | C5'-C4'-C3' | 6.26 | 126.01 | 116.00 |
| 81 | DA | 2278 | C | O4'-C1'-N1 | 6.26 | 113.21 | 108.20 |
| 81 | DA | 2679 | A | O4'-C1'-C2' | 6.26 | 113.23 | 107.60 |
| 83 | DC | 13 | A | N9-C1'-C2' | 6.26 | 122.14 | 114.00 |
| 78 | CA | 345 | U | O4'-C1'-N1 | 6.26 | 113.21 | 108.20 |
| 78 | CA | 1601 | G | C2'-C3'-O3' | 6.26 | 123.71 | 113.70 |
| 81 | DA | 786 | A | C1'-O4'-C4' | 6.26 | 114.91 | 109.90 |
| 81 | DA | 1209 | G | C5'-C4'-C3' | 6.26 | 126.01 | 116.00 |
| 81 | DA | 2735 | U | N1-C1'-C2' | 6.26 | 122.13 | 114.00 |
| 81 | DA | 2829 | U | O3'-P-O5' | -6.26 | 92.11 | 104.00 |
| 3 | AB | 120 | TYR | CB-CG-CD2 | -6.25 | 117.25 | 121.00 |
| 78 | CA | 1659 | A | O4'-C1'-C2' | -6.25 | 99.55 | 105.80 |
| 81 | DA | 229 | G | C1'-O4'-C4' | -6.25 | 104.90 | 109.90 |
| 81 | DA | 2728 | G | N9-C1'-C2' | 6.25 | 122.13 | 114.00 |
| 78 | CA | 1051 | G | C5-C6-O6 | -6.25 | 124.85 | 128.60 |
| 81 | DA | 3250 | U | O4'-C1'-N1 | 6.25 | 113.20 | 108.20 |
| 81 | DA | 3380 | U | O4'-C1'-N1 | 6.25 | 113.20 | 108.20 |
| 48 | BW | 10 | LYS | N-CA-CB | 6.25 | 121.85 | 110.60 |
| 78 | CA | 842 | C | C4'-C3'-C2' | -6.25 | 96.35 | 102.60 |
| 78 | CA | 1580 | C | C1'-O4'-C4' | -6.25 | 104.90 | 109.90 |
| 81 | DA | 636 | C | C5'-C4'-C3' | -6.25 | 106.00 | 116.00 |
| 81 | DA | 1483 | G | N9-C1'-C2' | -6.25 | 105.12 | 112.00 |
| 81 | DA | 3053 | G | O4'-C1'-C2' | 6.25 | 113.23 | 107.60 |
| 78 | CA | 1471 | A | N9-C1'-C2' | -6.25 | 105.12 | 112.00 |
| 78 | CA | 1614 | A | C1'-O4'-C4' | 6.25 | 114.90 | 109.90 |
| 68 | Bq | 14 | LYS | CB-CA-C | 6.25 | 122.90 | 110.40 |
| 78 | CA | 705 | U | P-O5'-C5' | -6.25 | 110.90 | 120.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 992 | A | O4'-C1'-N9 | 6.25 | 113.20 | 108.20 |
| 78 | CA | 1088 | A | C1'-O4'-C4' | 6.25 | 114.90 | 109.90 |
| 81 | DA | 436 | A | N9-C1'-C2' | 6.25 | 122.12 | 114.00 |
| 81 | DA | 1137 | C | O4'-C1'-C2' | -6.25 | 99.55 | 105.80 |
| 81 | DA | 1793 | C | O4'-C1'-C2' | -6.25 | 99.55 | 105.80 |
| 81 | DA | 1947 | G | O3'-P-O5' | -6.25 | 92.13 | 104.00 |
| 81 | DA | 2279 | A | C1'-O4'-C4' | -6.25 | 104.90 | 109.90 |
| 81 | DA | 2424 | A | C3'-C2'-C1' | -6.25 | 96.50 | 101.50 |
| 82 | DB | 25 | G | C3'-C2'-C1' | -6.25 | 96.50 | 101.50 |
| 40 | BK | 187 | GLU | CB-CA-C | 6.25 | 122.89 | 110.40 |
| 81 | DA | 516 | A | O4'-C1'-C2' | -6.25 | 99.55 | 105.80 |
| 81 | DA | 858 | A | O4'-C1'-N9 | 6.25 | 113.20 | 108.20 |
| 81 | DA | 1007 | U | O4'-C1'-C2' | 6.25 | 113.22 | 107.60 |
| 81 | DA | 1061 | A | P-O3'-C3' | -6.25 | 112.20 | 119.70 |
| 81 | DA | 1299 | U | P-O5'-C5' | 6.25 | 130.90 | 120.90 |
| 81 | DA | 1971 | C | N1-C1'-C2' | 6.25 | 122.12 | 114.00 |
| 76 | BS | 23 | HIS | CA-CB-CG | 6.25 | 124.22 | 113.60 |
| 81 | DA | 1668 | G | N9-C1'-C2' | -6.25 | 105.13 | 112.00 |
| 81 | DA | 491 | C | C5'-C4'-O4' | 6.24 | 116.59 | 109.10 |
| 81 | DA | 768 | C | C5'-C4'-C3' | 6.24 | 125.99 | 116.00 |
| 81 | DA | 913 | A | C3'-C2'-C1' | 6.24 | 106.49 | 101.50 |
| 81 | DA | 1329 | U | O4'-C1'-C2' | -6.24 | 99.56 | 105.80 |
| 81 | DA | 1688 | U | O4'-C4'-C3' | -6.24 | 97.76 | 104.00 |
| 81 | DA | 2085 | U | O4'-C1'-C2' | -6.24 | 99.56 | 105.80 |
| 35 | BG | 54 | TYR | CB-CG-CD1 | -6.24 | 117.25 | 121.00 |
| 78 | CA | 1075 | C | O4'-C1'-N1 | -6.24 | 103.21 | 108.20 |
| 13 | AL | 7 | ARG | NE-CZ-NH1 | 6.24 | 123.42 | 120.30 |
| 42 | BM | 80 | ARG | NE-CZ-NH1 | 6.24 | 123.42 | 120.30 |
| 51 | BZ | 31 | PHE | N-CA-CB | 6.24 | 121.83 | 110.60 |
| 81 | DA | 2567 | C | N3-C4-C5 | -6.24 | 119.40 | 121.90 |
| 34 | BE | 115 | LYS | CB-CG-CD | 6.24 | 127.82 | 111.60 |
| 34 | BE | 127 | PHE | N-CA-C | -6.24 | 94.16 | 111.00 |
| 52 | BY | 114 | ASP | N-CA-CB | 6.24 | 121.83 | 110.60 |
| 78 | CA | 305 | C | C5'-C4'-O4' | 6.24 | 116.58 | 109.10 |
| 78 | CA | 574 | G | O4'-C1'-N9 | 6.24 | 113.19 | 108.20 |
| 78 | CA | 1019 | A | O4'-C1'-N9 | 6.24 | 113.19 | 108.20 |
| 81 | DA | 2097 | U | N1-C1'-C2' | 6.24 | 122.11 | 114.00 |
| 81 | DA | 3364 | C | C3'-C2'-C1' | 6.24 | 106.49 | 101.50 |
| 53 | Ba | 85 | TYR | CB-CG-CD1 | 6.24 | 124.74 | 121.00 |
| 1 | Aa | 35 | SER | CB-CA-C | 6.24 | 121.95 | 110.10 |
| 64 | Bl | 1 | MET | CG-SD-CE | -6.24 | 90.22 | 100.20 |
| 81 | DA | 1139 | G | C1'-O4'-C4' | -6.24 | 104.91 | 109.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 3388 | C | P-O3'-C3' | 6.24 | 127.18 | 119.70 |
| 74 | BQ | 158 | ARG | CG-CD-NE | 6.23 | 124.89 | 111.80 |
| 78 | CA | 488 | G | N1-C6-O6 | 6.23 | 123.64 | 119.90 |
| 34 | BE | 143 | ARG | NE-CZ-NH2 | -6.23 | 117.18 | 120.30 |
| 52 | BY | 74 | TYR | CD1-CE1-CZ | -6.23 | 114.19 | 119.80 |
| 81 | DA | 1411 | C | C4'-C3'-C2' | -6.23 | 96.37 | 102.60 |
| 81 | DA | 2309 | A | O4'-C1'-N9 | 6.23 | 113.19 | 108.20 |
| 81 | DA | 3297 | U | C4'-C3'-C2' | -6.23 | 96.37 | 102.60 |
| 83 | DC | 28 | C | N1-C1'-C2' | 6.23 | 122.10 | 114.00 |
| 33 | BD | 320 | ASN | C-N-CA | 6.23 | 137.28 | 121.70 |
| 81 | DA | 3356 | G | P-O3'-C3' | -6.23 | 112.22 | 119.70 |
| 82 | DB | 150 | G | O4'-C1'-N9 | 6.23 | 113.18 | 108.20 |
| 6 | AE | 243 | TYR | N-CA-CB | 6.23 | 121.81 | 110.60 |
| 78 | CA | 255 | U | C5'-C4'-O4' | -6.23 | 101.62 | 109.10 |
| 78 | CA | 1551 | U | O4'-C4'-C3' | 6.23 | 111.08 | 106.10 |
| 81 | DA | 1535 | A | O4'-C1'-C2' | -6.23 | 99.57 | 105.80 |
| 81 | DA | 1655 | G | O4'-C1'-N9 | 6.23 | 113.18 | 108.20 |
| 81 | DA | 3381 | U | O4'-C1'-N1 | 6.23 | 113.18 | 108.20 |
| 78 | CA | 431 | C | C3'-C2'-C1' | 6.23 | 106.48 | 101.50 |
| 78 | CA | 1793 | G | C3'-C2'-C1' | 6.23 | 106.48 | 101.50 |
| 81 | DA | 380 | U | O4'-C1'-N1 | 6.23 | 113.18 | 108.20 |
| 81 | DA | 2784 | G | N9-C1'-C2' | -6.23 | 105.15 | 112.00 |
| 81 | DA | 2213 | A | C3'-C2'-C1' | 6.23 | 106.48 | 101.50 |
| 38 | Bs | 147 | ARG | NE-CZ-NH2 | -6.22 | 117.19 | 120.30 |
| 57 | Be | 33 | ARG | NE-CZ-NH1 | -6.22 | 117.19 | 120.30 |
| 78 | CA | 294 | C | C3'-C2'-C1' | 6.22 | 106.48 | 101.50 |
| 81 | DA | 886 | C | O4'-C1'-N1 | 6.22 | 113.18 | 108.20 |
| 81 | DA | 2464 | U | C1'-O4'-C4' | -6.22 | 104.92 | 109.90 |
| 81 | DA | 2712 | U | C1'-O4'-C4' | 6.22 | 114.88 | 109.90 |
| 33 | BD | 255 | PHE | CB-CG-CD1 | 6.22 | 125.16 | 120.80 |
| 78 | CA | 969 | C | C3'-C2'-C1' | 6.22 | 106.48 | 101.50 |
| 78 | CA | 1511 | U | P-O3'-C3' | -6.22 | 112.23 | 119.70 |
| 81 | DA | 685 | G | C5'-C4'-C3' | -6.22 | 106.05 | 116.00 |
| 81 | DA | 2003 | G | O4'-C1'-N9 | 6.22 | 113.18 | 108.20 |
| 81 | DA | 2039 | C | O4'-C1'-N1 | 6.22 | 113.18 | 108.20 |
| 81 | DA | 2247 | G | C1'-O4'-C4' | -6.22 | 104.92 | 109.90 |
| 81 | DA | 2540 | A | C4-C5-C6 | 6.22 | 120.11 | 117.00 |
| 81 | DA | 3085 | G | C3'-C2'-C1' | -6.22 | 96.52 | 101.50 |
| 81 | DA | 3331 | U | N1-C1'-C2' | -6.22 | 105.16 | 112.00 |
| 78 | CA | 498 | G | O4'-C1'-N9 | 6.22 | 113.18 | 108.20 |
| 78 | CA | 591 | A | O4'-C1'-N9 | -6.22 | 103.22 | 108.20 |
| 32 | BC | 21 | ARG | NE-CZ-NH2 | -6.22 | 117.19 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 38 | Bs | 247 | LEU | C-N-CA | 6.22 | 137.25 | 121.70 |
| 78 | CA | 853 | G | C4'-C3'-C2' | -6.22 | 96.38 | 102.60 |
| 78 | CA | 1149 | G | C1'-O4'-C4' | -6.22 | 104.92 | 109.90 |
| 81 | DA | 632 | G | O4'-C1'-N9 | 6.22 | 113.17 | 108.20 |
| 81 | DA | 815 | G | C1'-O4'-C4' | -6.22 | 104.92 | 109.90 |
| 81 | DA | 1097 | G | P-O3'-C3' | 6.22 | 127.16 | 119.70 |
| 82 | DB | 118 | C | N1-C1'-C2' | 6.22 | 122.08 | 114.00 |
| 6 | AE | 4 | PRO | CB-CA-C | 6.22 | 127.55 | 112.00 |
| 81 | DA | 1773 | C | C5'-C4'-O4' | 6.22 | 116.56 | 109.10 |
| 81 | DA | 2657 | A | O4'-C1'-N9 | -6.22 | 103.22 | 108.20 |
| 10 | AI | 112 | TYR | N-CA-CB | 6.22 | 121.79 | 110.60 |
| 22 | AV | 29 | LYS | O-C-N | -6.22 | 112.75 | 122.70 |
| 78 | CA | 498 | G | P-O3'-C3' | -6.22 | 112.24 | 119.70 |
| 78 | CA | 1000 | C | C1'-O4'-C4' | 6.22 | 114.87 | 109.90 |
| 81 | DA | 767 | U | P-O3'-C3' | -6.22 | 112.24 | 119.70 |
| 81 | DA | 1858 | A | O4'-C1'-N9 | 6.22 | 113.17 | 108.20 |
| 81 | DA | 2181 | C | O5'-C5'-C4' | 6.22 | 123.51 | 111.70 |
| 81 | DA | 3298 | C | O4'-C1'-C2' | -6.22 | 99.58 | 105.80 |
| 83 | DC | 47 | C | O4'-C1'-N1 | 6.22 | 113.17 | 108.20 |
| 20 | AS | 54 | PHE | CB-CG-CD2 | 6.21 | 125.15 | 120.80 |
| 50 | BX | 31 | THR | CA-CB-CG2 | -6.21 | 103.70 | 112.40 |
| 74 | BQ | 111 | GLN | CA-C-O | -6.21 | 107.05 | 120.10 |
| 78 | CA | 1539 | G | O4'-C1'-N9 | 6.21 | 113.17 | 108.20 |
| 78 | CA | 1615 | C | N1-C1'-C2' | 6.21 | 122.08 | 114.00 |
| 81 | DA | 709 | A | C3'-C2'-C1' | 6.21 | 106.47 | 101.50 |
| 81 | DA | 724 | U | O4'-C1'-N1 | 6.21 | 113.17 | 108.20 |
| 81 | DA | 1535 | A | C3'-C2'-C1' | -6.21 | 96.53 | 101.50 |
| 81 | DA | 1689 | U | C5'-C4'-C3' | 6.21 | 125.94 | 116.00 |
| 81 | DA | 2153 | U | C1'-O4'-C4' | -6.21 | 104.93 | 109.90 |
| 81 | DA | 2470 | C | C5'-C4'-C3' | 6.21 | 125.94 | 116.00 |
| 40 | BK | 111 | PRO | N-CA-CB | 6.21 | 110.75 | 103.30 |
| 57 | Be | 67 | ARG | NE-CZ-NH1 | 6.21 | 123.41 | 120.30 |
| 59 | Bh | 25 | TYR | CB-CA-C | -6.21 | 97.98 | 110.40 |
| 81 | DA | 1343 | A | N9-C1'-C2' | 6.21 | 122.08 | 114.00 |
| 83 | DC | 27 | A | N9-C1'-C2' | 6.21 | 122.07 | 114.00 |
| 83 | DC | 58 | U | O4'-C1'-C2' | -6.21 | 99.59 | 105.80 |
| 10 | AI | 119 | ALA | CB-CA-C | 6.21 | 119.42 | 110.10 |
| 81 | DA | 1425 | U | O4'-C1'-N1 | 6.21 | 113.17 | 108.20 |
| 81 | DA | 2864 | A | O3'-P-O5' | -6.21 | 92.20 | 104.00 |
| 25 | AY | 47 | PRO | N-CA-CB | 6.21 | 110.75 | 103.30 |
| 40 | BK | 186 | ALA | CA-C-O | -6.21 | 107.06 | 120.10 |
| 41 | BN | 55 | ARG | NE-CZ-NH2 | -6.21 | 117.20 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 62 | Bk | 53 | TYR | CG-CD1-CE1 | -6.21 | 116.33 | 121.30 |
| 78 | CA | 297 | U | C3'-C2'-C1' | 6.21 | 106.47 | 101.50 |
| 81 | DA | 237 | G | O4'-C4'-C3' | -6.21 | 97.79 | 104.00 |
| 81 | DA | 338 | A | O4'-C1'-N9 | -6.21 | 103.23 | 108.20 |
| 81 | DA | 1240 | A | O4'-C1'-N9 | 6.21 | 113.17 | 108.20 |
| 81 | DA | 1288 | U | O4'-C1'-C2' | -6.21 | 99.59 | 105.80 |
| 81 | DA | 2044 | U | O4'-C1'-C2' | -6.21 | 99.59 | 105.80 |
| 81 | DA | 2144 | A | O4'-C1'-C2' | 6.21 | 113.19 | 107.60 |
| 62 | Bk | 98 | ARG | CB-CA-C | 6.21 | 122.81 | 110.40 |
| 78 | CA | 458 | G | O4'-C1'-C2' | 6.21 | 113.19 | 107.60 |
| 78 | CA | 1373 | C | O4'-C1'-C2' | -6.21 | 99.59 | 105.80 |
| 81 | DA | 133 | U | O4'-C1'-N1 | 6.21 | 113.17 | 108.20 |
| 81 | DA | 136 | G | C5'-C4'-O4' | 6.21 | 116.55 | 109.10 |
| 81 | DA | 2335 | G | C3'-C2'-C1' | -6.21 | 96.53 | 101.50 |
| 81 | DA | 2723 | U | P-O5'-C5' | -6.21 | 110.97 | 120.90 |
| 81 | DA | 820 | A | O4'-C1'-N9 | 6.21 | 113.16 | 108.20 |
| 81 | DA | 1669 | C | C3'-C2'-C1' | 6.21 | 106.46 | 101.50 |
| 8 | AF | 73 | THR | N-CA-CB | 6.20 | 122.09 | 110.30 |
| 78 | CA | 1196 | A | O4'-C1'-C2' | -6.20 | 99.60 | 105.80 |
| 78 | CA | 1507 | G | N1-C6-O6 | 6.20 | 123.62 | 119.90 |
| 78 | CA | 1567 | U | N1-C1'-C2' | 6.20 | 122.06 | 114.00 |
| 78 | CA | 1652 | C | O4'-C1'-C2' | -6.20 | 99.60 | 105.80 |
| 81 | DA | 180 | C | O4'-C1'-C2' | -6.20 | 99.60 | 105.80 |
| 81 | DA | 285 | A | O4'-C1'-C2' | -6.20 | 99.60 | 105.80 |
| 81 | DA | 2292 | U | O4'-C1'-N1 | 6.20 | 113.16 | 108.20 |
| 81 | DA | 360 | G | C3'-C2'-C1' | 6.20 | 106.46 | 101.50 |
| 81 | DA | 2631 | U | O4'-C1'-N1 | 6.20 | 113.16 | 108.20 |
| 83 | DC | 68 | U | O4'-C1'-N1 | 6.20 | 113.16 | 108.20 |
| 40 | BK | 133 | ARG | NE-CZ-NH1 | -6.20 | 117.20 | 120.30 |
| 78 | CA | 1771 | U | N1-C1'-C2' | 6.20 | 122.06 | 114.00 |
| 83 | DC | 98 | G | C3'-C2'-C1' | 6.20 | 106.46 | 101.50 |
| 1 | Aa | 56 | VAL | CA-C-N | 6.20 | 134.46 | 117.10 |
| 67 | Bp | 41 | HIS | N-CA-CB | 6.20 | 121.76 | 110.60 |
| 78 | CA | 284 | G | C4'-C3'-C2' | -6.20 | 96.40 | 102.60 |
| 81 | DA | 251 | G | C3'-C2'-C1' | 6.20 | 106.46 | 101.50 |
| 81 | DA | 488 | U | C5'-C4'-C3' | 6.20 | 125.92 | 116.00 |
| 81 | DA | 514 | G | N9-C1'-C2' | 6.20 | 122.06 | 114.00 |
| 81 | DA | 1820 | U | O4'-C1'-N1 | 6.20 | 113.16 | 108.20 |
| 32 | BC | 256 | HIS | N-CA-C | -6.20 | 94.27 | 111.00 |
| 65 | Bn | 39 | ARG | N-CA-C | 6.20 | 127.73 | 111.00 |
| 78 | CA | 1470 | C | N1-C1'-C2' | 6.20 | 122.06 | 114.00 |
| 81 | DA | 934 | G | O4'-C1'-N9 | 6.20 | 113.16 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2294 | U | O4'-C1'-C2' | -6.20 | 99.60 | 105.80 |
| 9 | AH | 68 | ARG | NE-CZ-NH1 | 6.20 | 123.40 | 120.30 |
| 38 | Bs | 183 | PHE | CB-CG-CD2 | 6.20 | 125.14 | 120.80 |
| 38 | Bs | 229 | TYR | N-CA-CB | 6.20 | 121.75 | 110.60 |
| 41 | BN | 109 | ARG | NE-CZ-NH1 | 6.20 | 123.40 | 120.30 |
| 78 | CA | 1499 | G | O4'-C1'-N9 | 6.20 | 113.16 | 108.20 |
| 81 | DA | 578 | A | O4'-C1'-C2' | -6.20 | 99.60 | 105.80 |
| 81 | DA | 2271 | A | O4'-C1'-N9 | 6.20 | 113.16 | 108.20 |
| 35 | BG | 25 | ALA | N-CA-CB | 6.19 | 118.77 | 110.10 |
| 78 | CA | 460 | A | O5'-C5'-C4' | 6.19 | 123.47 | 111.70 |
| 78 | CA | 1144 | U | C5'-C4'-O4' | 6.19 | 116.53 | 109.10 |
| 81 | DA | 578 | A | P-O5'-C5' | -6.19 | 110.99 | 120.90 |
| 78 | CA | 413 | U | O4'-C1'-N1 | 6.19 | 113.15 | 108.20 |
| 81 | DA | 442 | G | O4'-C1'-N9 | 6.19 | 113.15 | 108.20 |
| 81 | DA | 1166 | G | C3'-C2'-C1' | 6.19 | 106.45 | 101.50 |
| 81 | DA | 1329 | U | P-O3'-C3' | 6.19 | 127.13 | 119.70 |
| 81 | DA | 3351 | U | C1'-O4'-C4' | 6.19 | 114.85 | 109.90 |
| 83 | DC | 83 | U | P-O5'-C5' | 6.19 | 130.81 | 120.90 |
| 78 | CA | 646 | C | O4'-C1'-C2' | 6.19 | 113.17 | 107.60 |
| 81 | DA | 675 | C | C1'-O4'-C4' | 6.19 | 114.85 | 109.90 |
| 81 | DA | 844 | G | P-O3'-C3' | -6.19 | 112.27 | 119.70 |
| 81 | DA | 1933 | A | N9-C1'-C2' | -6.19 | 105.19 | 112.00 |
| 4 | AD | 196 | VAL | CB-CA-C | -6.19 | 99.64 | 111.40 |
| 81 | DA | 2944 | U | O4'-C1'-C2' | -6.19 | 99.61 | 105.80 |
| 3 | AB | 91 | VAL | CG1-CB-CG2 | 6.19 | 120.80 | 110.90 |
| 6 | AE | 23 | ASN | N-CA-CB | 6.19 | 121.74 | 110.60 |
| 43 | BP | 44 | ARG | NH1-CZ-NH2 | -6.19 | 112.59 | 119.40 |
| 78 | CA | 1 | U | P-O5'-C5' | -6.19 | 111.00 | 120.90 |
| 81 | DA | 240 | U | O3'-P-O5' | 6.19 | 115.76 | 104.00 |
| 81 | DA | 1170 | A | O4'-C1'-N9 | 6.19 | 113.15 | 108.20 |
| 81 | DA | 2495 | C | O4'-C1'-C2' | -6.19 | 99.61 | 105.80 |
| 81 | DA | 2873 | U | C5'-C4'-C3' | -6.19 | 106.10 | 116.00 |
| 81 | DA | 3069 | G | C5'-C4'-C3' | 6.19 | 125.90 | 116.00 |
| 10 | AI | 87 | LYS | CB-CA-C | -6.19 | 98.03 | 110.40 |
| 81 | DA | 932 | U | C1'-O4'-C4' | 6.19 | 114.85 | 109.90 |
| 81 | DA | 1625 | A | O4'-C1'-C2' | -6.19 | 99.61 | 105.80 |
| 81 | DA | 2887 | A | C1'-O4'-C4' | -6.19 | 104.95 | 109.90 |
| 13 | AL | 123 | LYS | N-CA-C | 6.18 | 127.70 | 111.00 |
| 34 | BE | 168 | ASP | CB-CG-OD1 | 6.18 | 123.86 | 118.30 |
| 44 | BO | 8 | THR | CA-CB-OG1 | 6.18 | 121.99 | 109.00 |
| 56 | Bf | 23 | TYR | CB-CG-CD1 | -6.18 | 117.29 | 121.00 |
| 57 | Be | 198 | ALA | N-CA-CB | 6.18 | 118.76 | 110.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 503 | G | O4'-C1'-N9 | 6.18 | 113.15 | 108.20 |
| 78 | CA | 1626 | U | O4'-C1'-N1 | 6.18 | 113.15 | 108.20 |
| 81 | DA | 1015 | U | N1-C1'-C2' | -6.18 | 105.20 | 112.00 |
| 81 | DA | 1527 | C | P-O5'-C5' | 6.18 | 130.79 | 120.90 |
| 81 | DA | 1804 | A | P-O3'-C3' | 6.18 | 127.12 | 119.70 |
| 81 | DA | 1804 | A | O4'-C1'-C2' | -6.18 | 99.62 | 105.80 |
| 35 | BG | 94 | GLU | N-CA-CB | 6.18 | 121.73 | 110.60 |
| 76 | BS | 73 | THR | CA-CB-OG1 | 6.18 | 121.98 | 109.00 |
| 78 | CA | 575 | C | O4'-C1'-N1 | 6.18 | 113.15 | 108.20 |
| 81 | DA | 267 | G | O4'-C1'-N9 | -6.18 | 103.25 | 108.20 |
| 33 | BD | 258 | LEU | C-N-CA | 6.18 | 137.15 | 121.70 |
| 35 | BG | 45 | GLY | N-CA-C | -6.18 | 97.65 | 113.10 |
| 14 | AM | 126 | ARG | NE-CZ-NH2 | -6.18 | 117.21 | 120.30 |
| 20 | AS | 69 | LYS | CB-CA-C | 6.18 | 122.76 | 110.40 |
| 41 | BN | 15 | VAL | N-CA-CB | 6.18 | 125.10 | 111.50 |
| 78 | CA | 448 | C | O4'-C1'-N1 | 6.18 | 113.14 | 108.20 |
| 81 | DA | 124 | U | C5'-C4'-O4' | 6.18 | 116.52 | 109.10 |
| 81 | DA | 1806 | A | P-O5'-C5' | 6.18 | 130.79 | 120.90 |
| 81 | DA | 3255 | U | C1'-O4'-C4' | -6.18 | 104.96 | 109.90 |
| 6 | AE | 68 | ILE | N-CA-C | -6.18 | 94.32 | 111.00 |
| 78 | CA | 120 | U | C5'-C4'-C3' | -6.18 | 106.12 | 116.00 |
| 81 | DA | 1774 | C | C5'-C4'-C3' | 6.18 | 125.89 | 116.00 |
| 6 | AE | 28 | ARG | N-CA-CB | 6.18 | 121.72 | 110.60 |
| 61 | Bj | 60 | ARG | N-CA-C | -6.18 | 94.32 | 111.00 |
| 74 | BQ | 289 | LYS | N-CA-C | -6.18 | 94.32 | 111.00 |
| 78 | CA | 1453 | G | C1'-O4'-C4' | 6.18 | 114.84 | 109.90 |
| 78 | CA | 1461 | C | C5'-C4'-O4' | -6.18 | 101.69 | 109.10 |
| 78 | CA | 1604 | U | C5'-C4'-C3' | -6.18 | 106.12 | 116.00 |
| 81 | DA | 232 | G | P-O5'-C5' | -6.18 | 111.02 | 120.90 |
| 81 | DA | 2209 | U | O4'-C4'-C3' | -6.18 | 97.82 | 104.00 |
| 81 | DA | 2245 | C | O4'-C1'-C2' | -6.18 | 99.62 | 105.80 |
| 16 | AO | 123 | HIS | C-N-CA | 6.17 | 137.14 | 121.70 |
| 40 | BK | 68 | ARG | NE-CZ-NH2 | -6.17 | 117.21 | 120.30 |
| 65 | Bn | 78 | LEU | CB-CG-CD2 | 6.17 | 121.50 | 111.00 |
| 77 | BI | 110 | ARG | CA-C-N | 6.17 | 130.79 | 117.20 |
| 78 | CA | 505 | A | C5-C6-N6 | -6.17 | 118.76 | 123.70 |
| 78 | CA | 1721 | A | C3'-C2'-C1' | 6.17 | 106.44 | 101.50 |
| 81 | DA | 173 | G | O4'-C1'-C2' | 6.17 | 113.16 | 107.60 |
| 37 | BH | 233 | TRP | N-CA-C | 6.17 | 127.67 | 111.00 |
| 81 | DA | 147 | U | O5'-P-OP1 | -6.17 | 100.14 | 105.70 |
| 81 | DA | 1916 | U | N1-C1'-C2' | 6.17 | 122.03 | 114.00 |
| 65 | Bn | 52 | TYR | C-N-CA | 6.17 | 137.13 | 121.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 1281 | G | C1'-O4'-C4' | -6.17 | 104.96 | 109.90 |
| 81 | DA | 1035 | G | P-O3'-C3' | -6.17 | 112.29 | 119.70 |
| 81 | DA | 1210 | U | O4'-C1'-C2' | -6.17 | 99.63 | 105.80 |
| 81 | DA | 2148 | U | C3'-C2'-C1' | 6.17 | 106.44 | 101.50 |
| 81 | DA | 2630 | C | O4'-C1'-C2' | -6.17 | 99.63 | 105.80 |
| 81 | DA | 2988 | C | O4'-C1'-N1 | 6.17 | 113.14 | 108.20 |
| 78 | CA | 495 | C | N3-C4-N4 | 6.17 | 122.32 | 118.00 |
| 78 | CA | 1651 | A | O4'-C1'-C2' | -6.17 | 99.63 | 105.80 |
| 81 | DA | 248 | U | C4'-C3'-C2' | -6.17 | 96.43 | 102.60 |
| 33 | BD | 330 | TYR | CB-CG-CD1 | 6.17 | 124.70 | 121.00 |
| 36 | BF | 184 | LYS | N-CA-CB | 6.17 | 121.70 | 110.60 |
| 78 | CA | 276 | C | C3'-C2'-C1' | 6.17 | 106.44 | 101.50 |
| 78 | CA | 404 | G | C1'-O4'-C4' | -6.17 | 104.97 | 109.90 |
| 81 | DA | 1520 | G | O4'-C1'-N9 | 6.17 | 113.13 | 108.20 |
| 6 | AE | 1 | MET | CG-SD-CE | -6.17 | 90.33 | 100.20 |
| 31 | BB | 69 | TYR | CB-CG-CD2 | -6.17 | 117.30 | 121.00 |
| 81 | DA | 1049 | C | O4'-C1'-C2' | -6.17 | 99.63 | 105.80 |
| 81 | DA | 1856 | C | P-O3'-C3' | 6.17 | 127.10 | 119.70 |
| 83 | DC | 11 | A | C1'-O4'-C4' | -6.17 | 104.97 | 109.90 |
| 83 | DC | 32 | U | O4'-C1'-C2' | 6.17 | 113.15 | 107.60 |
| 72 | Bu | 48 | ALA | CB-CA-C | -6.17 | 100.85 | 110.10 |
| 81 | DA | 2101 | C | O4'-C1'-N1 | 6.17 | 113.13 | 108.20 |
| 81 | DA | 3343 | G | C3'-C2'-C1' | -6.17 | 96.57 | 101.50 |
| 5 | AC | 3 | ARG | CA-C-N | 6.16 | 130.76 | 117.20 |
| 10 | AI | 122 | ARG | N-CA-C | -6.16 | 94.36 | 111.00 |
| 42 | BM | 65 | GLY | CA-C-N | 6.16 | 130.76 | 117.20 |
| 64 | Bl | 75 | LYS | N-CA-CB | 6.16 | 121.69 | 110.60 |
| 76 | BS | 89 | TYR | CD1-CE1-CZ | -6.16 | 114.25 | 119.80 |
| 78 | CA | 271 | A | N9-C1'-C2' | 6.16 | 122.01 | 114.00 |
| 78 | CA | 369 | A | C5'-C4'-O4' | 6.16 | 116.50 | 109.10 |
| 78 | CA | 589 | C | C5'-C4'-O4' | 6.16 | 116.50 | 109.10 |
| 81 | DA | 1609 | C | O4'-C1'-N1 | 6.16 | 113.13 | 108.20 |
| 81 | DA | 2958 | A | P-O3'-C3' | -6.16 | 112.30 | 119.70 |
| 81 | DA | 3188 | G | P-O5'-C5' | 6.16 | 130.76 | 120.90 |
| 48 | BW | 95 | PHE | CB-CA-C | 6.16 | 122.72 | 110.40 |
| 81 | DA | 1754 | G | O4'-C1'-N9 | 6.16 | 113.13 | 108.20 |
| 17 | AQ | 6 | THR | N-CA-C | -6.16 | 94.36 | 111.00 |
| 76 | BS | 121 | PRO | N-CA-C | 6.16 | 128.12 | 112.10 |
| 81 | DA | 27 | C | N1-C1'-C2' | 6.16 | 122.01 | 114.00 |
| 81 | DA | 1897 | G | C1'-O4'-C4' | -6.16 | 104.97 | 109.90 |
| 81 | DA | 2916 | U | N1-C1'-C2' | 6.16 | 122.01 | 114.00 |
| 81 | DA | 694 | C | O3'-P-O5' | -6.16 | 92.30 | 104.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 42 | BM | 42 | SER | C-N-CA | 6.16 | 135.23 | 122.30 |
| 42 | BM | 65 | GLY | CA-C-O | -6.16 | 109.52 | 120.60 |
| 58 | Bg | 65 | LYS | N-CA-CB | -6.16 | 99.52 | 110.60 |
| 78 | CA | 1345 | A | O4'-C1'-C2' | -6.16 | 99.64 | 105.80 |
| 81 | DA | 1086 | C | C3'-C2'-C1' | 6.16 | 106.43 | 101.50 |
| 81 | DA | 1314 | C | P-O3'-C3' | -6.16 | 112.31 | 119.70 |
| 74 | BQ | 202 | GLY | N-CA-C | -6.16 | 97.71 | 113.10 |
| 78 | CA | 252 | U | N1-C1'-C2' | -6.16 | 105.23 | 112.00 |
| 78 | CA | 509 | G | P-O3'-C3' | 6.16 | 127.09 | 119.70 |
| 78 | CA | 680 | U | C4'-C3'-C2' | -6.16 | 96.44 | 102.60 |
| 81 | DA | 973 | A | N9-C1'-C2' | -6.16 | 105.23 | 112.00 |
| 81 | DA | 1343 | A | C3'-C2'-C1' | -6.16 | 96.58 | 101.50 |
| 81 | DA | 1409 | G | C1'-O4'-C4' | -6.16 | 104.98 | 109.90 |
| 81 | DA | 2165 | G | O3'-P-O5' | 6.16 | 115.69 | 104.00 |
| 81 | DA | 2250 | G | O4'-C1'-C2' | -6.16 | 99.64 | 105.80 |
| 81 | DA | 2267 | C | O4'-C1'-C2' | -6.16 | 99.64 | 105.80 |
| 81 | DA | 2478 | C | P-O3'-C3' | 6.16 | 127.09 | 119.70 |
| 81 | DA | 2664 | C | C5'-C4'-C3' | 6.16 | 125.85 | 116.00 |
| 81 | DA | 3051 | U | C5'-C4'-O4' | -6.16 | 101.71 | 109.10 |
| 18 | AP | 81 | HIS | N-CA-CB | 6.15 | 121.68 | 110.60 |
| 81 | DA | 3010 | U | C4'-C3'-C2' | -6.15 | 96.45 | 102.60 |
| 78 | CA | 105 | A | C3'-C2'-C1' | 6.15 | 106.42 | 101.50 |
| 78 | CA | 904 | G | C1'-O4'-C4' | -6.15 | 104.98 | 109.90 |
| 78 | CA | 999 | U | O3'-P-O5' | -6.15 | 92.31 | 104.00 |
| 81 | DA | 606 | C | C1'-O4'-C4' | -6.15 | 104.98 | 109.90 |
| 81 | DA | 1384 | U | N1-C1'-C2' | -6.15 | 105.23 | 112.00 |
| 81 | DA | 2127 | U | P-O3'-C3' | -6.15 | 112.32 | 119.70 |
| 11 | AJ | 83 | GLU | C-N-CA | 6.15 | 137.08 | 121.70 |
| 57 | Be | 165 | ASP | CB-CA-C | -6.15 | 98.10 | 110.40 |
| 81 | DA | 900 | G | C1'-O4'-C4' | -6.15 | 104.98 | 109.90 |
| 74 | BQ | 55 | PHE | CA-C-N | -6.15 | 103.67 | 117.20 |
| 81 | DA | 1206 | G | C5'-C4'-O4' | 6.15 | 116.48 | 109.10 |
| 81 | DA | 1700 | G | P-O3'-C3' | 6.15 | 127.08 | 119.70 |
| 9 | AH | 67 | GLY | C-N-CA | -6.15 | 106.33 | 121.70 |
| 78 | CA | 626 | U | N1-C1'-C2' | 6.15 | 121.99 | 114.00 |
| 78 | CA | 1454 | G | C1'-O4'-C4' | -6.15 | 104.98 | 109.90 |
| 81 | DA | 756 | U | N1-C1'-C2' | 6.15 | 121.99 | 114.00 |
| 81 | DA | 1815 | U | P-O3'-C3' | 6.15 | 127.08 | 119.70 |
| 81 | DA | 3107 | U | C5'-C4'-C3' | 6.15 | 125.83 | 116.00 |
| 81 | DA | 3119 | U | O4'-C1'-N1 | 6.15 | 113.12 | 108.20 |
| 10 | AI | 26 | LYS | N-CA-CB | 6.15 | 121.66 | 110.60 |
| 30 | BA | 22 | GLU | N-CA-C | 6.15 | 127.59 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 1370 | U | N1-C1'-C2' | 6.15 | 121.99 | 114.00 |
| 81 | DA | 2411 | U | O4'-C1'-N1 | 6.15 | 113.12 | 108.20 |
| 6 | AE | 56 | ILE | CA-CB-CG2 | -6.14 | 98.61 | 110.90 |
| 31 | BB | 3 | ARG | CB-CA-C | -6.14 | 98.11 | 110.40 |
| 42 | BM | 56 | ASP | CB-CG-OD2 | -6.14 | 112.77 | 118.30 |
| 78 | CA | 1399 | C | C5'-C4'-C3' | 6.14 | 125.83 | 116.00 |
| 81 | DA | 2437 | G | C1'-O4'-C4' | 6.14 | 114.81 | 109.90 |
| 2 | AA | 244 | GLU | OE1-CD-OE2 | 6.14 | 130.67 | 123.30 |
| 20 | AS | 104 | VAL | CA-CB-CG1 | 6.14 | 120.11 | 110.90 |
| 78 | CA | 1596 | C | C3'-C2'-C1' | 6.14 | 106.41 | 101.50 |
| 81 | DA | 608 | A | C1'-O4'-C4' | -6.14 | 104.99 | 109.90 |
| 81 | DA | 812 | G | O3'-P-O5' | -6.14 | 92.33 | 104.00 |
| 81 | DA | 2455 | U | C3'-C2'-C1' | 6.14 | 106.42 | 101.50 |
| 53 | Ba | 70 | PRO | N-CA-CB | 6.14 | 110.67 | 103.30 |
| 78 | CA | 420 | A | O4'-C1'-N9 | 6.14 | 113.11 | 108.20 |
| 78 | CA | 1028 | C | C3'-C2'-C1' | 6.14 | 106.41 | 101.50 |
| 78 | CA | 1387 | G | O4'-C1'-N9 | 6.14 | 113.11 | 108.20 |
| 81 | DA | 1563 | C | O4'-C4'-C3' | -6.14 | 97.86 | 104.00 |
| 81 | DA | 2745 | G | N9-C1'-C2' | -6.14 | 105.25 | 112.00 |
| 13 | AL | 23 | ARG | N-CA-CB | -6.14 | 99.55 | 110.60 |
| 50 | BX | 93 | TYR | N-CA-CB | 6.14 | 121.65 | 110.60 |
| 52 | BY | 51 | ARG | NH1-CZ-NH2 | 6.14 | 126.15 | 119.40 |
| 76 | BS | 150 | LYS | CA-C-N | 6.14 | 130.71 | 117.20 |
| 76 | BS | 159 | ARG | CA-C-O | -6.14 | 107.21 | 120.10 |
| 81 | DA | 418 | A | N9-C1'-C2' | -6.14 | 105.25 | 112.00 |
| 81 | DA | 2572 | C | N3-C4-N4 | 6.14 | 122.30 | 118.00 |
| 81 | DA | 2818 | U | C1'-O4'-C4' | 6.14 | 114.81 | 109.90 |
| 81 | DA | 3062 | G | C3'-C2'-C1' | -6.14 | 96.59 | 101.50 |
| 81 | DA | 3306 | U | C5'-C4'-C3' | -6.14 | 106.18 | 116.00 |
| 83 | DC | 39 | C | C3'-C2'-C1' | 6.14 | 106.41 | 101.50 |
| 22 | AV | 30 | LYS | N-CA-CB | 6.14 | 121.65 | 110.60 |
| 81 | DA | 1284 | C | C1'-O4'-C4' | 6.14 | 114.81 | 109.90 |
| 81 | DA | 1940 | G | C3'-C2'-C1' | 6.14 | 106.41 | 101.50 |
| 13 | AL | 121 | ARG | N-CA-C | -6.14 | 94.43 | 111.00 |
| 64 | Bl | 41 | ALA | N-CA-CB | 6.14 | 118.69 | 110.10 |
| 78 | CA | 471 | A | O4'-C1'-C2' | -6.14 | 99.66 | 105.80 |
| 78 | CA | 963 | A | C3'-C2'-C1' | 6.14 | 106.41 | 101.50 |
| 81 | DA | 39 | A | C3'-C2'-C1' | 6.14 | 106.41 | 101.50 |
| 81 | DA | 1685 | C | O4'-C1'-C2' | -6.14 | 99.66 | 105.80 |
| 81 | DA | 2925 | C | C3'-C2'-C1' | 6.14 | 106.41 | 101.50 |
| 12 | AK | 128 | LYS | C-N-CA | 6.13 | 137.03 | 121.70 |
| 25 | AY | 56 | LEU | N-CA-C | -6.13 | 94.44 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 33 | BD | 74 | ILE | N-CA-C | -6.13 | 94.44 | 111.00 |
| 78 | CA | 505 | A | O4'-C1'-N9 | 6.13 | 113.11 | 108.20 |
| 81 | DA | 45 | A | C3'-C2'-C1' | 6.13 | 106.41 | 101.50 |
| 81 | DA | 2491 | A | O4'-C1'-N9 | 6.13 | 113.11 | 108.20 |
| 13 | AL | 123 | LYS | CA-C-N | 6.13 | 130.69 | 117.20 |
| 78 | CA | 1069 | A | C4-C5-C6 | 6.13 | 120.07 | 117.00 |
| 81 | DA | 746 | A | C1'-O4'-C4' | -6.13 | 104.99 | 109.90 |
| 81 | DA | 1744 | G | C3'-C2'-C1' | -6.13 | 96.59 | 101.50 |
| 4 | AD | 194 | THR | N-CA-CB | 6.13 | 121.95 | 110.30 |
| 35 | BG | 26 | ARG | NE-CZ-NH1 | 6.13 | 123.37 | 120.30 |
| 39 | BJ | 123 | ARG | CB-CA-C | -6.13 | 98.14 | 110.40 |
| 43 | BP | 181 | ASN | N-CA-C | 6.13 | 127.56 | 111.00 |
| 61 | Bj | 39 | GLN | CG-CD-NE2 | -6.13 | 101.98 | 116.70 |
| 81 | DA | 751 | A | C1'-O4'-C4' | -6.13 | 104.99 | 109.90 |
| 14 | AM | 22 | VAL | CA-CB-CG2 | 6.13 | 120.09 | 110.90 |
| 47 | BU | 12 | ARG | NE-CZ-NH2 | -6.13 | 117.23 | 120.30 |
| 81 | DA | 1046 | A | P-O3'-C3' | 6.13 | 127.06 | 119.70 |
| 81 | DA | 1362 | G | C1'-O4'-C4' | -6.13 | 105.00 | 109.90 |
| 81 | DA | 548 | G | N9-C1'-C2' | 6.13 | 121.97 | 114.00 |
| 81 | DA | 739 | G | N3-C2-N2 | 6.13 | 124.19 | 119.90 |
| 81 | DA | 3392 | U | O3'-P-O5' | -6.13 | 92.36 | 104.00 |
| 9 | AH | 37 | PHE | CB-CG-CD2 | 6.13 | 125.09 | 120.80 |
| 15 | AN | 12 | ARG | NE-CZ-NH1 | -6.13 | 117.24 | 120.30 |
| 17 | AQ | 28 | PHE | CB-CG-CD2 | 6.13 | 125.09 | 120.80 |
| 78 | CA | 1558 | U | C5'-C4'-C3' | -6.13 | 106.20 | 116.00 |
| 81 | DA | 1035 | G | O4'-C1'-C2' | -6.13 | 99.67 | 105.80 |
| 81 | DA | 2710 | C | O4'-C1'-C2' | -6.13 | 99.67 | 105.80 |
| 53 | Ba | 43 | VAL | CA-CB-CG2 | -6.12 | 101.71 | 110.90 |
| 78 | CA | 1625 | C | C3'-C2'-C1' | 6.12 | 106.40 | 101.50 |
| 81 | DA | 136 | G | C3'-C2'-C1' | -6.12 | 96.60 | 101.50 |
| 78 | CA | 323 | A | N9-C1'-C2' | -6.12 | 105.27 | 112.00 |
| 78 | CA | 988 | A | O4'-C1'-N9 | -6.12 | 103.30 | 108.20 |
| 78 | CA | 1053 | G | N1-C6-O6 | 6.12 | 123.57 | 119.90 |
| 79 | CB | 65 | U | O4'-C1'-N1 | 6.12 | 113.10 | 108.20 |
| 81 | DA | 43 | A | C4'-C3'-C2' | 6.12 | 108.72 | 102.60 |
| 81 | DA | 519 | A | O3'-P-O5' | 6.12 | 115.63 | 104.00 |
| 81 | DA | 2564 | G | O4'-C1'-N9 | 6.12 | 113.10 | 108.20 |
| 82 | DB | 39 | G | O4'-C1'-N9 | 6.12 | 113.10 | 108.20 |
| 83 | DC | 9 | C | O4'-C4'-C3' | -6.12 | 97.88 | 104.00 |
| 76 | BS | 70 | ASN | CB-CA-C | -6.12 | 98.16 | 110.40 |
| 78 | CA | 1187 | U | O4'-C1'-C2' | -6.12 | 99.68 | 105.80 |
| 81 | DA | 729 | C | N3-C4-C5 | -6.12 | 119.45 | 121.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1046 | A | C1'-O4'-C4' | 6.12 | 114.80 | 109.90 |
| 81 | DA | 1217 | A | C4'-C3'-C2' | -6.12 | 96.48 | 102.60 |
| 81 | DA | 1522 | U | O4'-C1'-N1 | 6.12 | 113.10 | 108.20 |
| 81 | DA | 2257 | C | N1-C1'-C2' | -6.12 | 105.27 | 112.00 |
| 82 | DB | 134 | G | C1'-O4'-C4' | 6.12 | 114.80 | 109.90 |
| 38 | Bs | 30 | VAL | CA-CB-CG1 | 6.12 | 120.08 | 110.90 |
| 81 | DA | 3371 | G | P-O3'-C3' | -6.12 | 112.36 | 119.70 |
| 33 | BD | 156 | LEU | CB-CG-CD2 | 6.12 | 121.40 | 111.00 |
| 35 | BG | 17 | ALA | N-CA-C | 6.12 | 127.52 | 111.00 |
| 46 | BT | 91 | SER | N-CA-CB | 6.12 | 119.68 | 110.50 |
| 47 | BU | 12 | ARG | NE-CZ-NH1 | 6.12 | 123.36 | 120.30 |
| 60 | Bi | 41 | ARG | N-CA-CB | -6.12 | 99.59 | 110.60 |
| 78 | CA | 1194 | A | C3'-C2'-C1' | 6.12 | 106.39 | 101.50 |
| 81 | DA | 738 | A | P-O3'-C3' | 6.12 | 127.04 | 119.70 |
| 81 | DA | 1993 | G | O4'-C1'-N9 | 6.12 | 113.09 | 108.20 |
| 2 | AA | 102 | PHE | CZ-CE2-CD2 | -6.12 | 112.76 | 120.10 |
| 35 | BG | 35 | VAL | CA-CB-CG1 | 6.12 | 120.08 | 110.90 |
| 78 | CA | 56 | U | N1-C1'-C2' | -6.12 | 105.27 | 112.00 |
| 78 | CA | 1042 | G | O4'-C1'-N9 | 6.12 | 113.09 | 108.20 |
| 81 | DA | 595 | G | C1'-O4'-C4' | 6.12 | 114.79 | 109.90 |
| 81 | DA | 871 | U | C1'-O4'-C4' | -6.12 | 105.01 | 109.90 |
| 81 | DA | 2571 | U | O4'-C1'-N1 | 6.12 | 113.09 | 108.20 |
| 29 | AU | 72 | PHE | CA-C-N | 6.12 | 128.43 | 116.20 |
| 33 | BD | 58 | HIS | N-CA-CB | 6.12 | 121.61 | 110.60 |
| 62 | Bk | 53 | TYR | CB-CG-CD2 | -6.12 | 117.33 | 121.00 |
| 78 | CA | 285 | G | C5'-C4'-C3' | -6.12 | 106.22 | 116.00 |
| 81 | DA | 2398 | A | O4'-C1'-C2' | -6.12 | 99.68 | 105.80 |
| 81 | DA | 2568 | C | N3-C4-C5 | -6.12 | 119.45 | 121.90 |
| 2 | AA | 251 | GLU | CB-CA-C | -6.11 | 98.17 | 110.40 |
| 12 | AK | 20 | TYR | N-CA-CB | 6.11 | 121.61 | 110.60 |
| 78 | CA | 858 | G | O4'-C1'-C2' | -6.11 | 99.69 | 105.80 |
| 78 | CA | 1607 | G | C1'-O4'-C4' | -6.11 | 105.01 | 109.90 |
| 81 | DA | 638 | C | O4'-C1'-C2' | -6.11 | 99.69 | 105.80 |
| 81 | DA | 752 | C | C1'-O4'-C4' | -6.11 | 105.01 | 109.90 |
| 81 | DA | 1396 | C | C5'-C4'-C3' | -6.11 | 106.22 | 116.00 |
| 81 | DA | 1423 | C | N1-C1'-C2' | 6.11 | 121.95 | 114.00 |
| 81 | DA | 2499 | U | N1-C1'-C2' | 6.11 | 121.95 | 114.00 |
| 81 | DA | 3327 | G | O4'-C1'-N9 | 6.11 | 113.09 | 108.20 |
| 31 | BB | 84 | THR | N-CA-CB | 6.11 | 121.91 | 110.30 |
| 78 | CA | 1547 | A | P-O5'-C5' | 6.11 | 130.68 | 120.90 |
| 81 | DA | 1586 | G | C1'-O4'-C4' | -6.11 | 105.01 | 109.90 |
| 31 | BB | 145 | LYS | CB-CA-C | -6.11 | 98.18 | 110.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2440 | G | O4'-C4'-C3' | -6.11 | 97.89 | 104.00 |
| 81 | DA | 2464 | U | C5'-C4'-O4' | 6.11 | 116.43 | 109.10 |
| 4 | AD | 230 | GLU | CB-CA-C | -6.11 | 98.18 | 110.40 |
| 81 | DA | 657 | A | O4'-C1'-N9 | 6.11 | 113.09 | 108.20 |
| 53 | Ba | 24 | VAL | C-N-CA | 6.11 | 136.97 | 121.70 |
| 61 | Bj | 20 | LYS | C-N-CA | 6.11 | 136.97 | 121.70 |
| 78 | CA | 1421 | A | C3'-C2'-C1' | -6.11 | 96.61 | 101.50 |
| 81 | DA | 2547 | A | C4-C5-C6 | 6.11 | 120.05 | 117.00 |
| 4 | AD | 240 | LYS | N-CA-CB | 6.11 | 121.59 | 110.60 |
| 29 | AU | 70 | VAL | N-CA-C | -6.11 | 94.52 | 111.00 |
| 78 | CA | 620 | A | O4'-C1'-N9 | 6.11 | 113.08 | 108.20 |
| 78 | CA | 1595 | U | O4'-C1'-N1 | 6.11 | 113.08 | 108.20 |
| 78 | CA | 1754 | A | O4'-C1'-C2' | 6.11 | 113.09 | 107.60 |
| 81 | DA | 1790 | G | O5'-C5'-C4' | -6.11 | 100.10 | 111.70 |
| 81 | DA | 2660 | G | O4'-C1'-N9 | 6.11 | 113.08 | 108.20 |
| 81 | DA | 2776 | C | O4'-C1'-C2' | -6.11 | 99.69 | 105.80 |
| 76 | BS | 15 | GLY | N-CA-C | 6.10 | 128.36 | 113.10 |
| 81 | DA | 306 | A | C1'-O4'-C4' | 6.10 | 114.78 | 109.90 |
| 81 | DA | 1089 | G | O4'-C1'-C2' | 6.10 | 113.09 | 107.60 |
| 81 | DA | 2627 | C | N1-C1'-C2' | 6.10 | 121.94 | 114.00 |
| 83 | DC | 47 | C | O5'-P-OP1 | 6.10 | 118.03 | 110.70 |
| 49 | BV | 166 | VAL | CA-C-N | 6.10 | 130.62 | 117.20 |
| 78 | CA | 680 | U | O4'-C1'-C2' | -6.10 | 99.70 | 105.80 |
| 82 | DB | 44 | A | C1'-O4'-C4' | -6.10 | 105.02 | 109.90 |
| 82 | DB | 56 | G | C1'-O4'-C4' | -6.10 | 105.02 | 109.90 |
| 81 | DA | 2603 | G | O4'-C1'-N9 | 6.10 | 113.08 | 108.20 |
| 2 | AA | 62 | ARG | NE-CZ-NH2 | -6.10 | 117.25 | 120.30 |
| 78 | CA | 1285 | U | O4'-C1'-N1 | 6.10 | 113.08 | 108.20 |
| 81 | DA | 752 | C | O5'-P-OP1 | 6.10 | 118.02 | 110.70 |
| 81 | DA | 799 | G | P-O3'-C3' | 6.10 | 127.02 | 119.70 |
| 81 | DA | 1278 | A | C3'-C2'-C1' | 6.10 | 106.38 | 101.50 |
| 81 | DA | 2236 | G | O4'-C1'-C2' | 6.10 | 113.09 | 107.60 |
| 81 | DA | 2435 | G | P-O5'-C5' | -6.10 | 111.14 | 120.90 |
| 60 | Bi | 36 | LYS | CA-CB-CG | 6.10 | 126.81 | 113.40 |
| 76 | BS | 139 | ASP | CB-CG-OD2 | -6.10 | 112.81 | 118.30 |
| 78 | CA | 418 | G | C1'-O4'-C4' | -6.10 | 105.02 | 109.90 |
| 78 | CA | 827 | C | N3-C4-C5 | -6.10 | 119.46 | 121.90 |
| 81 | DA | 645 | A | O4'-C1'-N9 | 6.10 | 113.08 | 108.20 |
| 81 | DA | 2181 | C | P-O3'-C3' | 6.10 | 127.02 | 119.70 |
| 83 | DC | 89 | A | P-O3'-C3' | 6.10 | 127.02 | 119.70 |
| 78 | CA | 1274 | C | N3-C4-N4 | 6.10 | 122.27 | 118.00 |
| 2 | AA | 231 | GLU | C-N-CA | 6.09 | 136.94 | 121.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | AB | 181 | VAL | N-CA-CB | 6.09 | 124.91 | 111.50 |
| 35 | BG | 111 | LEU | CB-CG-CD2 | 6.09 | 121.36 | 111.00 |
| 38 | Bs | 215 | SER | N-CA-CB | 6.09 | 119.64 | 110.50 |
| 78 | CA | 591 | A | P-O5'-C5' | -6.09 | 111.15 | 120.90 |
| 81 | DA | 701 | G | C3'-C2'-C1' | -6.09 | 96.62 | 101.50 |
| 81 | DA | 832 | G | C3'-C2'-C1' | -6.09 | 96.62 | 101.50 |
| 81 | DA | 2835 | U | N1-C1'-C2' | 6.09 | 121.92 | 114.00 |
| 50 | BX | 37 | THR | N-CA-CB | 6.09 | 121.88 | 110.30 |
| 78 | CA | 901 | G | P-O5'-C5' | 6.09 | 130.65 | 120.90 |
| 81 | DA | 902 | G | O4'-C1'-N9 | 6.09 | 113.07 | 108.20 |
| 39 | BJ | 77 | ALA | CB-CA-C | -6.09 | 100.96 | 110.10 |
| 78 | CA | 1791 | A | C4'-C3'-C2' | -6.09 | 96.51 | 102.60 |
| 81 | DA | 261 | U | O4'-C1'-C2' | 6.09 | 113.08 | 107.60 |
| 81 | DA | 1873 | U | O4'-C1'-N1 | 6.09 | 113.07 | 108.20 |
| 81 | DA | 1928 | G | O4'-C1'-N9 | 6.09 | 113.07 | 108.20 |
| 81 | DA | 2094 | C | O4'-C1'-C2' | -6.09 | 99.71 | 105.80 |
| 81 | DA | 1797 | A | P-O3'-C3' | 6.09 | 127.01 | 119.70 |
| 81 | DA | 2208 | A | C4'-C3'-C2' | -6.09 | 96.51 | 102.60 |
| 33 | BD | 90 | PHE | N-CA-C | -6.09 | 94.57 | 111.00 |
| 46 | BT | 103 | ARG | CD-NE-CZ | -6.09 | 115.08 | 123.60 |
| 81 | DA | 2185 | G | C3'-C2'-C1' | -6.09 | 96.63 | 101.50 |
| 83 | DC | 91 | C | O4'-C1'-N1 | 6.09 | 113.07 | 108.20 |
| 81 | DA | 2390 | A | O4'-C1'-N9 | -6.08 | 103.33 | 108.20 |
| 5 | AC | 168 | ARG | NE-CZ-NH2 | -6.08 | 117.26 | 120.30 |
| 32 | BC | 241 | LYS | N-CA-CB | 6.08 | 121.55 | 110.60 |
| 33 | BD | 355 | PHE | CA-C-N | 6.08 | 130.59 | 117.20 |
| 78 | CA | 1368 | G | P-O5'-C5' | -6.08 | 111.17 | 120.90 |
| 79 | CB | 64 | G | N9-C1'-C2' | 6.08 | 121.91 | 114.00 |
| 81 | DA | 1079 | A | C3'-C2'-C1' | 6.08 | 106.37 | 101.50 |
| 81 | DA | 1478 | C | C5'-C4'-C3' | -6.08 | 106.27 | 116.00 |
| 81 | DA | 2172 | A | O4'-C1'-N9 | 6.08 | 113.07 | 108.20 |
| 81 | DA | 2566 | C | N3-C4-C5 | -6.08 | 119.47 | 121.90 |
| 43 | BP | 14 | LYS | N-CA-CB | -6.08 | 99.65 | 110.60 |
| 78 | CA | 1555 | A | OP1-P-O3' | 6.08 | 118.58 | 105.20 |
| 79 | CB | 47 | U | O4'-C1'-C2' | -6.08 | 99.72 | 105.80 |
| 81 | DA | 3357 | U | N1-C1'-C2' | 6.08 | 121.91 | 114.00 |
| 17 | AQ | 6 | THR | N-CA-CB | 6.08 | 121.85 | 110.30 |
| 20 | AS | 95 | ASP | CA-CB-CG | -6.08 | 100.03 | 113.40 |
| 81 | DA | 434 | U | C4'-C3'-C2' | -6.08 | 96.52 | 102.60 |
| 81 | DA | 1057 | A | C1'-O4'-C4' | 6.08 | 114.76 | 109.90 |
| 81 | DA | 1428 | A | C5'-C4'-O4' | 6.08 | 116.40 | 109.10 |
| 33 | BD | 349 | THR | CA-C-O | -6.08 | 107.33 | 120.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 1352 | G | P-O3'-C3' | 6.08 | 127.00 | 119.70 |
| 81 | DA | 3019 | U | O4'-C1'-N1 | 6.08 | 113.06 | 108.20 |
| 81 | DA | 3344 | A | O4'-C1'-C2' | -6.08 | 99.72 | 105.80 |
| 14 | AM | 111 | ASP | CB-CG-OD2 | -6.08 | 112.83 | 118.30 |
| 81 | DA | 1221 | A | C1'-C2'-O2' | 6.08 | 128.83 | 110.60 |
| 81 | DA | 2061 | G | C5'-C4'-C3' | 6.08 | 125.72 | 116.00 |
| 81 | DA | 2499 | U | P-O3'-C3' | 6.08 | 126.99 | 119.70 |
| 81 | DA | 2650 | U | C3'-C2'-C1' | 6.08 | 106.36 | 101.50 |
| 60 | Bi | 46 | ASP | CB-CG-OD1 | 6.08 | 123.77 | 118.30 |
| 78 | CA | 172 | C | P-O5'-C5' | -6.08 | 111.18 | 120.90 |
| 78 | CA | 588 | U | C5'-C4'-O4' | -6.08 | 101.81 | 109.10 |
| 81 | DA | 226 | C | N1-C1'-C2' | 6.08 | 121.90 | 114.00 |
| 81 | DA | 624 | G | C1'-O4'-C4' | -6.08 | 105.04 | 109.90 |
| 81 | DA | 664 | U | C1'-O4'-C4' | -6.08 | 105.04 | 109.90 |
| 81 | DA | 2916 | U | O3'-P-O5' | -6.08 | 92.45 | 104.00 |
| 83 | DC | 108 | U | C3'-C2'-C1' | 6.08 | 106.36 | 101.50 |
| 58 | Bg | 93 | VAL | CA-CB-CG1 | 6.07 | 120.01 | 110.90 |
| 78 | CA | 457 | G | O4'-C1'-C2' | 6.07 | 113.07 | 107.60 |
| 78 | CA | 484 | C | N3-C4-C5 | -6.07 | 119.47 | 121.90 |
| 78 | CA | 505 | A | C4-C5-C6 | 6.07 | 120.04 | 117.00 |
| 78 | CA | 1349 | G | C1'-O4'-C4' | -6.07 | 105.04 | 109.90 |
| 78 | CA | 1605 | G | C3'-C2'-C1' | -6.07 | 96.64 | 101.50 |
| 81 | DA | 2707 | C | O3'-P-O5' | 6.07 | 115.54 | 104.00 |
| 83 | DC | 18 | C | C5'-C4'-O4' | -6.07 | 101.81 | 109.10 |
| 78 | CA | 1281 | G | N9-C1'-C2' | 6.07 | 121.89 | 114.00 |
| 18 | AP | 60 | PHE | CB-CG-CD1 | 6.07 | 125.05 | 120.80 |
| 57 | Be | 77 | VAL | N-CA-CB | 6.07 | 124.85 | 111.50 |
| 81 | DA | 1422 | G | N9-C1'-C2' | 6.07 | 121.89 | 114.00 |
| 82 | DB | 87 | G | O4'-C1'-N9 | 6.07 | 113.06 | 108.20 |
| 36 | BF | 109 | ALA | N-CA-CB | 6.07 | 118.60 | 110.10 |
| 81 | DA | 3198 | U | P-O3'-C3' | -6.07 | 112.42 | 119.70 |
| 9 | AH | 65 | LEU | N-CA-CB | 6.07 | 122.53 | 110.40 |
| 20 | AS | 58 | ALA | N-CA-CB | -6.07 | 101.61 | 110.10 |
| 39 | BJ | 121 | PHE | N-CA-CB | -6.07 | 99.68 | 110.60 |
| 69 | Br | 58 | PHE | N-CA-CB | 6.07 | 121.52 | 110.60 |
| 78 | CA | 351 | C | O4'-C1'-C2' | -6.07 | 99.73 | 105.80 |
| 78 | CA | 625 | C | O4'-C1'-N1 | 6.07 | 113.05 | 108.20 |
| 81 | DA | 1543 | G | C5'-C4'-O4' | 6.07 | 116.38 | 109.10 |
| 81 | DA | 1757 | A | N1-C6-N6 | 6.07 | 122.24 | 118.60 |
| 81 | DA | 2336 | U | P-O5'-C5' | -6.07 | 111.19 | 120.90 |
| 81 | DA | 2620 | G | C5'-C4'-C3' | 6.07 | 125.71 | 116.00 |
| 81 | DA | 2756 | C | C4'-C3'-C2' | -6.07 | 96.53 | 102.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 3225 | C | P-O3'-C3' | 6.07 | 126.98 | 119.70 |
| 78 | CA | 1391 | A | N9-C1'-C2' | 6.07 | 121.89 | 114.00 |
| 81 | DA | 1154 | A | N9-C1'-C2' | -6.07 | 105.33 | 112.00 |
| 81 | DA | 3078 | U | P-O3'-C3' | 6.07 | 126.98 | 119.70 |
| 81 | DA | 3223 | A | C5'-C4'-C3' | 6.07 | 125.70 | 116.00 |
| 14 | AM | 105 | VAL | CA-CB-CG2 | -6.06 | 101.80 | 110.90 |
| 66 | Bo | 30 | ARG | N-CA-CB | 6.06 | 121.52 | 110.60 |
| 81 | DA | 1549 | U | N1-C1'-C2' | 6.06 | 121.88 | 114.00 |
| 81 | DA | 2155 | G | C1'-O4'-C4' | -6.06 | 105.05 | 109.90 |
| 4 | AD | 95 | THR | N-CA-C | 6.06 | 127.37 | 111.00 |
| 76 | BS | 12 | VAL | CA-CB-CG1 | -6.06 | 101.81 | 110.90 |
| 78 | CA | 1543 | A | O4'-C1'-N9 | -6.06 | 103.35 | 108.20 |
| 81 | DA | 1469 | C | C1'-O4'-C4' | -6.06 | 105.05 | 109.90 |
| 81 | DA | 1946 | A | C1'-O4'-C4' | 6.06 | 114.75 | 109.90 |
| 81 | DA | 2784 | G | O4'-C1'-N9 | 6.06 | 113.05 | 108.20 |
| 32 | BC | 352 | GLU | N-CA-CB | 6.06 | 121.51 | 110.60 |
| 78 | CA | 1393 | C | C3'-C2'-C1' | 6.06 | 106.35 | 101.50 |
| 35 | BG | 54 | TYR | N-CA-CB | 6.06 | 121.51 | 110.60 |
| 74 | BQ | 159 | VAL | CB-CA-C | -6.06 | 99.89 | 111.40 |
| 78 | CA | 575 | C | N3-C4-C5 | -6.06 | 119.48 | 121.90 |
| 81 | DA | 537 | A | O4'-C1'-N9 | 6.06 | 113.05 | 108.20 |
| 81 | DA | 1140 | G | C1'-O4'-C4' | -6.06 | 105.05 | 109.90 |
| 81 | DA | 1915 | A | O4'-C1'-N9 | 6.06 | 113.05 | 108.20 |
| 81 | DA | 2534 | G | O4'-C1'-N9 | 6.06 | 113.05 | 108.20 |
| 19 | AR | 125 | PRO | CB-CA-C | 6.06 | 127.14 | 112.00 |
| 22 | AV | 31 | SER | N-CA-CB | -6.06 | 101.41 | 110.50 |
| 78 | CA | 1226 | A | O3'-P-O5' | -6.06 | 92.49 | 104.00 |
| 81 | DA | 2812 | C | C3'-C2'-C1' | 6.06 | 106.35 | 101.50 |
| 81 | DA | 3068 | U | P-O3'-C3' | 6.06 | 126.97 | 119.70 |
| 81 | DA | 1321 | G | C4'-C3'-C2' | -6.06 | 96.54 | 102.60 |
| 82 | DB | 47 | C | C5'-C4'-O4' | 6.06 | 116.37 | 109.10 |
| 33 | BD | 318 | LEU | N-CA-CB | 6.05 | 122.51 | 110.40 |
| 78 | CA | 115 | G | O4'-C1'-N9 | 6.05 | 113.04 | 108.20 |
| 78 | CA | 229 | U | O4'-C1'-C2' | -6.05 | 99.75 | 105.80 |
| 78 | CA | 1050 | G | C5-C6-O6 | -6.05 | 124.97 | 128.60 |
| 81 | DA | 1693 | C | P-O3'-C3' | -6.05 | 112.44 | 119.70 |
| 81 | DA | 1796 | G | O4'-C1'-N9 | -6.05 | 103.36 | 108.20 |
| 81 | DA | 1944 | U | O4'-C1'-C2' | -6.05 | 99.75 | 105.80 |
| 81 | DA | 2597 | U | O4'-C1'-N1 | 6.05 | 113.04 | 108.20 |
| 78 | CA | 119 | A | O4'-C1'-C2' | -6.05 | 99.75 | 105.80 |
| 78 | CA | 223 | U | O5'-P-OP1 | 6.05 | 117.96 | 110.70 |
| 83 | DC | 20 | A | C1'-O4'-C4' | -6.05 | 105.06 | 109.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 16 | AO | 146 | ALA | C-N-CA | 6.05 | 136.83 | 121.70 |
| 81 | DA | 729 | C | N3-C4-N4 | 6.05 | 122.24 | 118.00 |
| 81 | DA | 1602 | A | OP2-P-O3' | -6.05 | 91.89 | 105.20 |
| 83 | DC | 99 | A | C3'-C2'-C1' | 6.05 | 106.34 | 101.50 |
| 3 | AB | 181 | VAL | CA-CB-CG2 | 6.05 | 119.97 | 110.90 |
| 37 | BH | 89 | GLU | CB-CA-C | 6.05 | 122.50 | 110.40 |
| 48 | BW | 81 | LYS | CA-CB-CG | 6.05 | 126.71 | 113.40 |
| 53 | Ba | 16 | GLY | CA-C-N | 6.05 | 130.51 | 117.20 |
| 78 | CA | 888 | U | C5'-C4'-C3' | 6.05 | 125.68 | 116.00 |
| 81 | DA | 110 | G | C3'-C2'-C1' | -6.05 | 96.66 | 101.50 |
| 81 | DA | 616 | G | C1'-O4'-C4' | -6.05 | 105.06 | 109.90 |
| 81 | DA | 1870 | C | N1-C1'-C2' | 6.05 | 121.86 | 114.00 |
| 81 | DA | 2520 | A | P-O5'-C5' | -6.05 | 111.22 | 120.90 |
| 81 | DA | 2738 | A | C4'-C3'-C2' | -6.05 | 96.55 | 102.60 |
| 35 | BG | 114 | LYS | N-CA-CB | 6.05 | 121.49 | 110.60 |
| 31 | BB | 247 | ARG | C-N-CA | 6.05 | 135.00 | 122.30 |
| 65 | Bn | 29 | LYS | C-N-CA | -6.05 | 106.58 | 121.70 |
| 66 | Bo | 3 | ALA | CB-CA-C | -6.05 | 101.03 | 110.10 |
| 79 | CB | 69 | G | O4'-C1'-N9 | 6.05 | 113.04 | 108.20 |
| 80 | CC | 22 | A | C4-C5-C6 | 6.05 | 120.02 | 117.00 |
| 81 | DA | 369 | A | O4'-C1'-C2' | -6.05 | 99.75 | 105.80 |
| 81 | DA | 2058 | G | O4'-C1'-N9 | 6.05 | 113.04 | 108.20 |
| 8 | AF | 99 | MET | CA-CB-CG | 6.04 | 123.58 | 113.30 |
| 38 | Bs | 42 | ARG | CD-NE-CZ | -6.04 | 115.14 | 123.60 |
| 78 | CA | 171 | A | O3'-P-O5' | 6.04 | 115.49 | 104.00 |
| 78 | CA | 1003 | A | C3'-C2'-C1' | -6.04 | 96.66 | 101.50 |
| 81 | DA | 1007 | U | O4'-C1'-N1 | 6.04 | 113.03 | 108.20 |
| 81 | DA | 1558 | A | P-O3'-C3' | -6.04 | 112.45 | 119.70 |
| 81 | DA | 2972 | G | C1'-O4'-C4' | -6.04 | 105.06 | 109.90 |
| 82 | DB | 54 | A | C3'-C2'-C1' | 6.04 | 106.33 | 101.50 |
| 4 | AD | 81 | THR | C-N-CA | 6.04 | 136.81 | 121.70 |
| 15 | AN | 15 | GLY | C-N-CA | 6.04 | 136.80 | 121.70 |
| 78 | CA | 528 | U | C5'-C4'-C3' | 6.04 | 125.67 | 116.00 |
| 78 | CA | 1226 | A | O4'-C1'-C2' | -6.04 | 99.76 | 105.80 |
| 81 | DA | 1662 | G | O3'-P-O5' | -6.04 | 92.52 | 104.00 |
| 78 | CA | 884 | A | P-O3'-C3' | 6.04 | 126.95 | 119.70 |
| 3 | AB | 199 | PRO | CA-C-O | -6.04 | 105.71 | 120.20 |
| 32 | BC | 49 | TYR | CB-CG-CD2 | -6.04 | 117.38 | 121.00 |
| 33 | BD | 92 | ASN | CB-CA-C | 6.04 | 122.48 | 110.40 |
| 78 | CA | 923 | A | C3'-C2'-C1' | 6.04 | 106.33 | 101.50 |
| 78 | CA | 1086 | A | OP2-P-O3' | 6.04 | 118.48 | 105.20 |
| 81 | DA | 1199 | C | C1'-O4'-C4' | -6.04 | 105.07 | 109.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1446 | A | O3'-P-O5' | -6.04 | 92.53 | 104.00 |
| 81 | DA | 2802 | A | C3'-C2'-C1' | 6.04 | 106.33 | 101.50 |
| 35 | BG | 73 | GLY | N-CA-C | 6.04 | 128.19 | 113.10 |
| 78 | CA | 491 | C | C2-N3-C4 | 6.04 | 122.92 | 119.90 |
| 5 | AC | 146 | PHE | CB-CA-C | 6.04 | 122.47 | 110.40 |
| 78 | CA | 1179 | G | C1'-O4'-C4' | -6.04 | 105.07 | 109.90 |
| 81 | DA | 334 | A | O4'-C1'-N9 | 6.04 | 113.03 | 108.20 |
| 81 | DA | 1333 | C | O4'-C1'-C2' | -6.04 | 99.77 | 105.80 |
| 81 | DA | 1983 | G | O4'-C1'-N9 | 6.04 | 113.03 | 108.20 |
| 81 | DA | 2531 | C | C4'-C3'-C2' | -6.04 | 96.56 | 102.60 |
| 3 | AB | 124 | ARG | NE-CZ-NH1 | 6.03 | 123.32 | 120.30 |
| 13 | AL | 73 | ARG | N-CA-CB | 6.03 | 121.46 | 110.60 |
| 35 | BG | 100 | LYS | CB-CA-C | 6.03 | 122.47 | 110.40 |
| 78 | CA | 203 | U | C3'-C2'-C1' | 6.03 | 106.33 | 101.50 |
| 78 | CA | 1158 | C | O4'-C1'-N1 | -6.03 | 103.37 | 108.20 |
| 79 | CB | 60 | C | O4'-C1'-N1 | 6.03 | 113.03 | 108.20 |
| 81 | DA | 765 | C | C4'-C3'-C2' | -6.03 | 96.57 | 102.60 |
| 81 | DA | 844 | G | O4'-C1'-N9 | 6.03 | 113.03 | 108.20 |
| 81 | DA | 2435 | G | C5'-C4'-C3' | 6.03 | 125.66 | 116.00 |
| 12 | AK | 107 | ARG | NE-CZ-NH1 | -6.03 | 117.28 | 120.30 |
| 29 | AU | 40 | LEU | CB-CG-CD1 | 6.03 | 121.25 | 111.00 |
| 81 | DA | 815 | G | O4'-C1'-N9 | 6.03 | 113.03 | 108.20 |
| 81 | DA | 2423 | U | C5'-C4'-C3' | -6.03 | 106.35 | 116.00 |
| 59 | Bh | 25 | TYR | N-CA-CB | 6.03 | 121.46 | 110.60 |
| 61 | Bj | 75 | HIS | N-CA-C | -6.03 | 94.72 | 111.00 |
| 78 | CA | 1453 | G | C5'-C4'-C3' | -6.03 | 106.35 | 116.00 |
| 81 | DA | 2721 | A | O4'-C1'-C2' | -6.03 | 99.77 | 105.80 |
| 81 | DA | 2993 | G | C3'-C2'-C1' | 6.03 | 106.33 | 101.50 |
| 81 | DA | 3234 | A | O4'-C1'-C2' | -6.03 | 99.77 | 105.80 |
| 74 | BQ | 72 | ASP | CA-CB-CG | -6.03 | 100.14 | 113.40 |
| 81 | DA | 164 | A | C4-C5-C6 | 6.03 | 120.02 | 117.00 |
| 81 | DA | 452 | G | N9-C1'-C2' | 6.03 | 121.84 | 114.00 |
| 20 | AS | 86 | ARG | CD-NE-CZ | -6.03 | 115.16 | 123.60 |
| 26 | AZ | 26 | LYS | C-N-CD | -6.03 | 107.34 | 120.60 |
| 33 | BD | 76 | ARG | NE-CZ-NH1 | 6.03 | 123.31 | 120.30 |
| 47 | BU | 116 | ARG | CG-CD-NE | -6.03 | 99.14 | 111.80 |
| 78 | CA | 587 | C | P-O3'-C3' | -6.03 | 112.47 | 119.70 |
| 78 | CA | 642 | G | N9-C1'-C2' | -6.03 | 105.37 | 112.00 |
| 78 | CA | 840 | U | C1'-O4'-C4' | 6.03 | 114.72 | 109.90 |
| 81 | DA | 252 | U | P-O3'-C3' | 6.03 | 126.93 | 119.70 |
| 81 | DA | 2569 | A | C4-C5-C6 | 6.03 | 120.01 | 117.00 |
| 8 | AF | 27 | THR | CA-CB-OG1 | 6.03 | 121.65 | 109.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | AS | 122 | ARG | NE-CZ-NH1 | 6.03 | 123.31 | 120.30 |
| 41 | BN | 39 | ILE | CB-CG1-CD1 | 6.03 | 130.77 | 113.90 |
| 78 | CA | 479 | C | N3-C4-C5 | -6.03 | 119.49 | 121.90 |
| 78 | CA | 1067 | C | N3-C4-C5 | -6.03 | 119.49 | 121.90 |
| 50 | BX | 30 | ALA | CB-CA-C | -6.02 | 101.06 | 110.10 |
| 81 | DA | 771 | A | C4'-C3'-C2' | -6.02 | 96.58 | 102.60 |
| 81 | DA | 837 | A | C5'-C4'-C3' | 6.02 | 125.64 | 116.00 |
| 81 | DA | 1843 | C | O4'-C1'-N1 | 6.02 | 113.02 | 108.20 |
| 81 | DA | 3360 | C | O4'-C1'-N1 | 6.02 | 113.02 | 108.20 |
| 83 | DC | 17 | A | C5'-C4'-C3' | 6.02 | 125.64 | 116.00 |
| 65 | Bn | 29 | LYS | N-CA-CB | 6.02 | 121.44 | 110.60 |
| 78 | CA | 880 | C | P-O5'-C5' | 6.02 | 130.54 | 120.90 |
| 81 | DA | 79 | U | N1-C1'-C2' | 6.02 | 121.83 | 114.00 |
| 81 | DA | 2284 | C | N1-C1'-C2' | 6.02 | 121.83 | 114.00 |
| 78 | CA | 896 | U | O4'-C1'-N1 | 6.02 | 113.02 | 108.20 |
| 81 | DA | 279 | U | P-O5'-C5' | 6.02 | 130.53 | 120.90 |
| 81 | DA | 593 | C | P-O3'-C3' | 6.02 | 126.92 | 119.70 |
| 78 | CA | 1643 | U | O4'-C1'-C2' | -6.02 | 99.78 | 105.80 |
| 81 | DA | 1042 | U | O4'-C1'-N1 | 6.02 | 113.02 | 108.20 |
| 81 | DA | 2174 | G | O4'-C4'-C3' | -6.02 | 97.98 | 104.00 |
| 81 | DA | 2176 | U | C5'-C4'-O4' | -6.02 | 101.88 | 109.10 |
| 1 | Aa | 317 | THR | N-CA-C | -6.02 | 94.75 | 111.00 |
| 5 | AC | 164 | PHE | CB-CA-C | 6.02 | 122.44 | 110.40 |
| 37 | BH | 228 | GLU | CA-C-O | -6.02 | 107.46 | 120.10 |
| 78 | CA | 493 | U | O4'-C1'-N1 | 6.02 | 113.02 | 108.20 |
| 78 | CA | 897 | C | C3'-C2'-C1' | 6.02 | 106.31 | 101.50 |
| 78 | CA | 924 | A | P-O3'-C3' | 6.02 | 126.92 | 119.70 |
| 81 | DA | 2532 | U | P-O3'-C3' | -6.02 | 112.48 | 119.70 |
| 40 | BK | 147 | TRP | C-N-CA | -6.02 | 106.66 | 121.70 |
| 63 | Bm | 6 | LYS | CB-CA-C | 6.02 | 122.43 | 110.40 |
| 78 | CA | 1580 | C | O5'-C5'-C4' | 6.02 | 123.13 | 111.70 |
| 81 | DA | 2323 | G | C1'-O4'-C4' | 6.02 | 114.71 | 109.90 |
| 50 | BX | 60 | TYR | CD1-CE1-CZ | 6.01 | 125.21 | 119.80 |
| 74 | BQ | 185 | PHE | CB-CG-CD2 | -6.01 | 116.59 | 120.80 |
| 78 | CA | 482 | U | P-O5'-C5' | -6.01 | 111.28 | 120.90 |
| 78 | CA | 966 | A | O4'-C1'-N9 | 6.01 | 113.01 | 108.20 |
| 78 | CA | 1016 | C | N1-C1'-C2' | 6.01 | 121.82 | 114.00 |
| 78 | CA | 1433 | G | C1'-O4'-C4' | 6.01 | 114.71 | 109.90 |
| 81 | DA | 815 | G | C3'-C2'-C1' | -6.01 | 96.69 | 101.50 |
| 81 | DA | 1826 | C | O5'-C5'-C4' | 6.01 | 123.13 | 111.70 |
| 81 | DA | 2480 | A | C5'-C4'-C3' | 6.01 | 125.62 | 116.00 |
| 57 | Be | 107 | ARG | N-CA-CB | 6.01 | 121.42 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 63 | Bm | 24 | ARG | NE-CZ-NH1 | -6.01 | 117.29 | 120.30 |
| 74 | BQ | 237 | GLU | CB-CA-C | 6.01 | 122.43 | 110.40 |
| 78 | CA | 178 | U | N1-C1'-C2' | -6.01 | 105.39 | 112.00 |
| 78 | CA | 1476 | C | O5'-C5'-C4' | -6.01 | 100.28 | 111.70 |
| 62 | Bk | 82 | ARG | CA-C-N | 6.01 | 130.43 | 117.20 |
| 81 | DA | 839 | C | C5'-C4'-C3' | 6.01 | 125.62 | 116.00 |
| 81 | DA | 1058 | U | O4'-C1'-N1 | 6.01 | 113.01 | 108.20 |
| 81 | DA | 2648 | G | C4'-C3'-C2' | -6.01 | 96.59 | 102.60 |
| 81 | DA | 3235 | C | O5'-C5'-C4' | 6.01 | 123.12 | 111.70 |
| 82 | DB | 12 | A | C1'-O4'-C4' | 6.01 | 114.71 | 109.90 |
| 83 | DC | 35 | C | O4'-C1'-C2' | -6.01 | 99.79 | 105.80 |
| 32 | BC | 365 | PHE | CA-CB-CG | 6.01 | 128.32 | 113.90 |
| 33 | BD | 354 | VAL | CB-CA-C | -6.01 | 99.98 | 111.40 |
| 81 | DA | 1972 | A | O5'-C5'-C4' | 6.01 | 123.12 | 111.70 |
| 44 | BO | 20 | GLY | C-N-CA | 6.01 | 136.72 | 121.70 |
| 32 | BC | 266 | ARG | CG-CD-NE | 6.01 | 124.41 | 111.80 |
| 81 | DA | 1844 | C | P-O3'-C3' | 6.01 | 126.91 | 119.70 |
| 12 | AK | 99 | GLN | CB-CA-C | -6.00 | 98.39 | 110.40 |
| 17 | AQ | 132 | TYR | N-CA-C | -6.00 | 94.79 | 111.00 |
| 18 | AP | 115 | PHE | CB-CG-CD1 | 6.00 | 125.00 | 120.80 |
| 35 | BG | 22 | ARG | N-CA-CB | 6.00 | 121.41 | 110.60 |
| 38 | Bs | 244 | LYS | N-CA-CB | 6.00 | 121.41 | 110.60 |
| 78 | CA | 1651 | A | C3'-C2'-C1' | 6.00 | 106.30 | 101.50 |
| 31 | BB | 30 | ARG | NE-CZ-NH2 | -6.00 | 117.30 | 120.30 |
| 40 | BK | 196 | ALA | N-CA-CB | 6.00 | 118.50 | 110.10 |
| 42 | BM | 10 | LYS | N-CA-CB | 6.00 | 121.41 | 110.60 |
| 48 | BW | 46 | ALA | N-CA-CB | 6.00 | 118.51 | 110.10 |
| 81 | DA | 105 | C | O3'-P-O5' | -6.00 | 92.59 | 104.00 |
| 81 | DA | 433 | A | C3'-C2'-C1' | 6.00 | 106.30 | 101.50 |
| 81 | DA | 1418 | A | O4'-C1'-N9 | 6.00 | 113.00 | 108.20 |
| 81 | DA | 2753 | G | P-O3'-C3' | 6.00 | 126.90 | 119.70 |
| 62 | Bk | 25 | LYS | CB-CA-C | 6.00 | 122.40 | 110.40 |
| 76 | BS | 29 | MET | N-CA-CB | 6.00 | 121.40 | 110.60 |
| 78 | CA | 485 | A | C4-C5-C6 | 6.00 | 120.00 | 117.00 |
| 78 | CA | 1696 | G | O4'-C1'-N9 | 6.00 | 113.00 | 108.20 |
| 81 | DA | 1072 | G | C1'-O4'-C4' | -6.00 | 105.10 | 109.90 |
| 81 | DA | 1130 | A | C3'-C2'-C1' | 6.00 | 106.30 | 101.50 |
| 81 | DA | 1412 | G | N9-C1'-C2' | -6.00 | 105.40 | 112.00 |
| 81 | DA | 2654 | C | O4'-C1'-N1 | 6.00 | 113.00 | 108.20 |
| 83 | DC | 102 | C | P-O3'-C3' | 6.00 | 126.90 | 119.70 |
| 35 | BG | 98 | VAL | CG1-CB-CG2 | -6.00 | 101.30 | 110.90 |
| 65 | Bn | 72 | THR | N-CA-C | -6.00 | 94.80 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 336 | G | C4'-C3'-C2' | -6.00 | 96.60 | 102.60 |
| 1 | Aa | 181 | TRP | CD1-CG-CD2 | 6.00 | 111.10 | 106.30 |
| 6 | AE | 95 | ARG | NE-CZ-NH1 | 6.00 | 123.30 | 120.30 |
| 33 | BD | 356 | THR | N-CA-C | 6.00 | 127.19 | 111.00 |
| 78 | CA | 637 | C | O4'-C1'-C2' | -6.00 | 99.80 | 105.80 |
| 78 | CA | 831 | U | P-O3'-C3' | 6.00 | 126.90 | 119.70 |
| 79 | CB | 57 | A | O4'-C1'-N9 | 6.00 | 113.00 | 108.20 |
| 81 | DA | 205 | C | O4'-C1'-N1 | 6.00 | 113.00 | 108.20 |
| 81 | DA | 3346 | U | P-O5'-C5' | 6.00 | 130.50 | 120.90 |
| 29 | AU | 63 | GLN | CB-CG-CD | 6.00 | 127.19 | 111.60 |
| 48 | BW | 90 | ARG | CA-CB-CG | 6.00 | 126.59 | 113.40 |
| 50 | BX | 24 | LEU | CB-CA-C | 6.00 | 121.59 | 110.20 |
| 81 | DA | 1974 | A | O4'-C1'-N9 | 6.00 | 113.00 | 108.20 |
| 46 | BT | 173 | ARG | NE-CZ-NH1 | 6.00 | 123.30 | 120.30 |
| 74 | BQ | 243 | ALA | C-N-CA | 6.00 | 136.69 | 121.70 |
| 78 | CA | 1607 | G | N9-C1'-C2' | 6.00 | 121.79 | 114.00 |
| 2 | AA | 10 | THR | CA-CB-CG2 | -5.99 | 104.01 | 112.40 |
| 32 | BC | 127 | LYS | N-CA-CB | 5.99 | 121.39 | 110.60 |
| 55 | Bc | 40 | SER | N-CA-CB | -5.99 | 101.51 | 110.50 |
| 79 | CB | 21 | A | O4'-C1'-N9 | 5.99 | 113.00 | 108.20 |
| 81 | DA | 2653 | C | O4'-C1'-C2' | -5.99 | 99.81 | 105.80 |
| 81 | DA | 2767 | U | N1-C1'-C2' | 5.99 | 121.79 | 114.00 |
| 81 | DA | 3035 | A | C5'-C4'-C3' | -5.99 | 106.41 | 116.00 |
| 43 | BP | 108 | ARG | NE-CZ-NH2 | -5.99 | 117.30 | 120.30 |
| 44 | BO | 8 | THR | CB-CA-C | -5.99 | 95.42 | 111.60 |
| 81 | DA | 2 | U | P-O3'-C3' | -5.99 | 112.51 | 119.70 |
| 2 | AA | 67 | ILE | CA-C-N | 5.99 | 133.88 | 117.10 |
| 78 | CA | 171 | A | O4'-C1'-C2' | -5.99 | 99.81 | 105.80 |
| 78 | CA | 498 | G | C5-C6-O6 | -5.99 | 125.01 | 128.60 |
| 78 | CA | 644 | C | C4'-C3'-C2' | -5.99 | 96.61 | 102.60 |
| 78 | CA | 651 | G | O4'-C1'-N9 | -5.99 | 103.41 | 108.20 |
| 78 | CA | 1336 | A | O4'-C1'-N9 | -5.99 | 103.41 | 108.20 |
| 78 | CA | 1456 | C | C3'-C2'-C1' | 5.99 | 106.29 | 101.50 |
| 81 | DA | 183 | G | C3'-C2'-C1' | -5.99 | 96.71 | 101.50 |
| 81 | DA | 420 | G | P-O3'-C3' | 5.99 | 126.89 | 119.70 |
| 81 | DA | 1748 | G | N9-C1'-C2' | -5.99 | 105.41 | 112.00 |
| 81 | DA | 2190 | U | C4'-C3'-C2' | -5.99 | 96.61 | 102.60 |
| 18 | AP | 60 | PHE | CB-CA-C | -5.99 | 98.42 | 110.40 |
| 81 | DA | 199 | A | N9-C1'-C2' | -5.99 | 105.41 | 112.00 |
| 81 | DA | 249 | U | C5'-C4'-C3' | 5.99 | 125.58 | 116.00 |
| 81 | DA | 701 | G | O3'-P-O5' | -5.99 | 92.62 | 104.00 |
| 81 | DA | 2190 | U | O4'-C1'-C2' | -5.99 | 99.81 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2879 | C | O4'-C1'-N1 | 5.99 | 112.99 | 108.20 |
| 81 | DA | 3236 | U | P-O5'-C5' | 5.99 | 130.48 | 120.90 |
| 4 | AD | 130 | GLN | CA-C-O | 5.99 | 132.67 | 120.10 |
| 31 | BB | 230 | VAL | CG1-CB-CG2 | -5.99 | 101.32 | 110.90 |
| 81 | DA | 674 | G | C3'-C2'-C1' | 5.99 | 106.29 | 101.50 |
| 81 | DA | 2626 | A | O4'-C1'-C2' | 5.99 | 112.99 | 107.60 |
| 1 | Aa | 269 | TYR | CB-CG-CD1 | -5.99 | 117.41 | 121.00 |
| 41 | BN | 63 | VAL | N-CA-CB | 5.99 | 124.67 | 111.50 |
| 81 | DA | 877 | C | C3'-C2'-C1' | 5.99 | 106.29 | 101.50 |
| 81 | DA | 1235 | U | N1-C1'-C2' | 5.99 | 121.78 | 114.00 |
| 81 | DA | 2503 | G | O4'-C4'-C3' | -5.99 | 98.02 | 104.00 |
| 81 | DA | 3371 | G | C1'-O4'-C4' | -5.99 | 105.11 | 109.90 |
| 82 | DB | 136 | G | O4'-C1'-N9 | 5.99 | 112.99 | 108.20 |
| 18 | AP | 55 | ASP | O-C-N | -5.98 | 113.13 | 122.70 |
| 33 | BD | 342 | LYS | CA-C-O | -5.98 | 107.53 | 120.10 |
| 45 | BR | 153 | PHE | CB-CG-CD1 | 5.98 | 124.99 | 120.80 |
| 46 | BT | 94 | VAL | CA-CB-CG2 | -5.98 | 101.92 | 110.90 |
| 74 | BQ | 129 | TYR | CA-C-N | 5.98 | 130.37 | 117.20 |
| 78 | CA | 1763 | A | P-O3'-C3' | 5.98 | 126.88 | 119.70 |
| 81 | DA | 838 | G | P-O5'-C5' | -5.98 | 111.33 | 120.90 |
| 81 | DA | 1968 | G | C5'-C4'-C3' | 5.98 | 125.57 | 116.00 |
| 81 | DA | 2211 | U | N1-C1'-C2' | -5.98 | 105.42 | 112.00 |
| 33 | BD | 56 | ALA | CB-CA-C | 5.98 | 119.07 | 110.10 |
| 78 | CA | 1353 | U | P-O3'-C3' | 5.98 | 126.88 | 119.70 |
| 81 | DA | 2061 | G | P-O3'-C3' | -5.98 | 112.52 | 119.70 |
| 81 | DA | 2531 | C | N3-C4-N4 | 5.98 | 122.19 | 118.00 |
| 82 | DB | 146 | U | O4'-C1'-N1 | 5.98 | 112.99 | 108.20 |
| 83 | DC | 12 | U | N1-C1'-C2' | 5.98 | 121.78 | 114.00 |
| 5 | AC | 15 | PRO | C-N-CA | -5.98 | 106.75 | 121.70 |
| 5 | AC | 81 | VAL | CA-CB-CG2 | -5.98 | 101.93 | 110.90 |
| 78 | CA | 588 | U | O4'-C1'-N1 | 5.98 | 112.98 | 108.20 |
| 78 | CA | 1745 | G | C5'-C4'-O4' | 5.98 | 116.28 | 109.10 |
| 81 | DA | 69 | C | O4'-C1'-N1 | 5.98 | 112.98 | 108.20 |
| 81 | DA | 1561 | G | C3'-C2'-C1' | -5.98 | 96.72 | 101.50 |
| 81 | DA | 1622 | U | O4'-C4'-C3' | -5.98 | 98.02 | 104.00 |
| 81 | DA | 2788 | C | O4'-C1'-N1 | -5.98 | 103.42 | 108.20 |
| 78 | CA | 1722 | A | O4'-C1'-N9 | 5.98 | 112.98 | 108.20 |
| 81 | DA | 1219 | C | C1'-O4'-C4' | 5.98 | 114.68 | 109.90 |
| 81 | DA | 3042 | U | C3'-C2'-C1' | 5.98 | 106.28 | 101.50 |
| 34 | BE | 16 | LYS | N-CA-CB | 5.98 | 121.36 | 110.60 |
| 46 | BT | 22 | VAL | CB-CA-C | -5.98 | 100.04 | 111.40 |
| 59 | Bh | 102 | ALA | CB-CA-C | -5.98 | 101.13 | 110.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 1144 | U | C3'-C2'-C1' | 5.98 | 106.28 | 101.50 |
| 81 | DA | 2030 | C | O4'-C1'-C2' | -5.98 | 99.82 | 105.80 |
| 81 | DA | 2904 | U | O4'-C1'-C2' | -5.98 | 99.82 | 105.80 |
| 82 | DB | 11 | C | O4'-C1'-C2' | -5.98 | 99.82 | 105.80 |
| 82 | DB | 154 | C | O4'-C1'-C2' | -5.98 | 99.82 | 105.80 |
| 8 | AF | 135 | ASP | CB-CG-OD2 | -5.98 | 112.92 | 118.30 |
| 78 | CA | 629 | U | C5'-C4'-O4' | 5.98 | 116.27 | 109.10 |
| 78 | CA | 1304 | G | O4'-C1'-N9 | 5.98 | 112.98 | 108.20 |
| 78 | CA | 1570 | A | P-O3'-C3' | 5.98 | 126.87 | 119.70 |
| 81 | DA | 172 | G | O4'-C4'-C3' | -5.98 | 98.02 | 104.00 |
| 83 | DC | 38 | U | C5'-C4'-C3' | 5.98 | 125.56 | 116.00 |
| 1 | Aa | 59 | ARG | NE-CZ-NH2 | -5.97 | 117.31 | 120.30 |
| 81 | DA | 998 | A | C5'-C4'-C3' | 5.97 | 125.56 | 116.00 |
| 81 | DA | 1474 | A | C5'-C4'-C3' | -5.97 | 106.44 | 116.00 |
| 81 | DA | 1790 | G | C5'-C4'-C3' | -5.97 | 106.44 | 116.00 |
| 81 | DA | 2718 | U | P-O3'-C3' | 5.97 | 126.87 | 119.70 |
| 81 | DA | 2916 | U | O5'-C5'-C4' | 5.97 | 123.05 | 111.70 |
| 82 | DB | 22 | U | O4'-C1'-N1 | 5.97 | 112.98 | 108.20 |
| 2 | AA | 175 | TYR | N-CA-CB | 5.97 | 121.35 | 110.60 |
| 51 | BZ | 30 | ARG | NE-CZ-NH1 | 5.97 | 123.29 | 120.30 |
| 61 | Bj | 85 | PHE | C-N-CA | 5.97 | 136.63 | 121.70 |
| 81 | DA | 2961 | G | C1'-O4'-C4' | -5.97 | 105.12 | 109.90 |
| 52 | BY | 11 | ASP | CB-CG-OD2 | 5.97 | 123.67 | 118.30 |
| 60 | Bi | 108 | GLN | CB-CA-C | -5.97 | 98.46 | 110.40 |
| 78 | CA | 164 | A | C4'-C3'-C2' | -5.97 | 96.63 | 102.60 |
| 21 | AT | 32 | VAL | CA-C-N | -5.97 | 104.07 | 117.20 |
| 78 | CA | 579 | A | O4'-C1'-N9 | 5.97 | 112.97 | 108.20 |
| 81 | DA | 683 | U | O4'-C1'-C2' | -5.97 | 99.83 | 105.80 |
| 81 | DA | 1263 | A | O4'-C1'-N9 | -5.97 | 103.42 | 108.20 |
| 81 | DA | 1996 | C | C3'-C2'-C1' | 5.97 | 106.28 | 101.50 |
| 81 | DA | 2503 | G | O4'-C1'-N9 | 5.97 | 112.98 | 108.20 |
| 81 | DA | 2792 | A | N9-C1'-C2' | -5.97 | 105.43 | 112.00 |
| 83 | DC | 51 | G | C5'-C4'-C3' | -5.97 | 106.45 | 116.00 |
| 58 | Bg | 35 | GLU | N-CA-CB | 5.97 | 121.34 | 110.60 |
| 81 | DA | 627 | U | C3'-C2'-C1' | 5.97 | 106.27 | 101.50 |
| 81 | DA | 676 | G | O4'-C1'-C2' | -5.97 | 99.83 | 105.80 |
| 33 | BD | 138 | ARG | NE-CZ-NH1 | -5.97 | 117.32 | 120.30 |
| 79 | CB | 25 | U | C1'-O4'-C4' | -5.97 | 105.13 | 109.90 |
| 81 | DA | 455 | C | N1-C1'-C2' | 5.97 | 121.76 | 114.00 |
| 81 | DA | 1819 | U | O4'-C1'-C2' | -5.97 | 99.83 | 105.80 |
| 81 | DA | 2053 | C | O4'-C1'-N1 | 5.97 | 112.97 | 108.20 |
| 81 | DA | 2328 | U | O4'-C1'-N1 | 5.97 | 112.97 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | AA | 15 | GLN | N-CA-CB | 5.96 | 121.34 | 110.60 |
| 2 | AA | 81 | PHE | N-CA-CB | 5.96 | 121.33 | 110.60 |
| 32 | BC | 61 | ASP | N-CA-CB | 5.96 | 121.34 | 110.60 |
| 36 | BF | 47 | LYS | CB-CA-C | -5.96 | 98.47 | 110.40 |
| 69 | Br | 102 | GLN | N-CA-C | -5.96 | 94.90 | 111.00 |
| 78 | CA | 1635 | A | C4-C5-C6 | 5.96 | 119.98 | 117.00 |
| 78 | CA | 1756 | A | P-O3'-C3' | 5.96 | 126.86 | 119.70 |
| 81 | DA | 1338 | C | P-O3'-C3' | -5.96 | 112.54 | 119.70 |
| 81 | DA | 1412 | G | P-O5'-C5' | -5.96 | 111.36 | 120.90 |
| 81 | DA | 1537 | A | P-O3'-C3' | 5.96 | 126.86 | 119.70 |
| 81 | DA | 2235 | C | C5'-C4'-C3' | 5.96 | 125.54 | 116.00 |
| 19 | AR | 80 | MET | CG-SD-CE | -5.96 | 90.66 | 100.20 |
| 78 | CA | 468 | A | P-O3'-C3' | 5.96 | 126.86 | 119.70 |
| 78 | CA | 1666 | U | C5'-C4'-O4' | 5.96 | 116.25 | 109.10 |
| 78 | CA | 1753 | A | C4'-C3'-C2' | -5.96 | 96.64 | 102.60 |
| 81 | DA | 737 | G | N3-C2-N2 | 5.96 | 124.07 | 119.90 |
| 31 | BB | 245 | LEU | O-C-N | -5.96 | 113.16 | 122.70 |
| 78 | CA | 500 | C | O3'-P-O5' | 5.96 | 115.33 | 104.00 |
| 78 | CA | 648 | G | C3'-C2'-C1' | 5.96 | 106.27 | 101.50 |
| 78 | CA | 934 | C | O4'-C1'-C2' | -5.96 | 99.84 | 105.80 |
| 79 | CB | 13 | U | C5'-C4'-C3' | -5.96 | 106.46 | 116.00 |
| 81 | DA | 723 | U | C5'-C4'-O4' | -5.96 | 101.95 | 109.10 |
| 81 | DA | 1746 | U | P-O3'-C3' | 5.96 | 126.85 | 119.70 |
| 81 | DA | 2072 | G | O3'-P-O5' | 5.96 | 115.33 | 104.00 |
| 81 | DA | 2619 | G | C5'-C4'-C3' | 5.96 | 125.54 | 116.00 |
| 81 | DA | 2938 | G | O4'-C1'-C2' | -5.96 | 99.84 | 105.80 |
| 17 | AQ | 89 | SER | N-CA-CB | 5.96 | 119.44 | 110.50 |
| 35 | BG | 9 | TRP | N-CA-CB | -5.96 | 99.87 | 110.60 |
| 63 | Bm | 41 | PHE | CB-CG-CD1 | 5.96 | 124.97 | 120.80 |
| 81 | DA | 2020 | A | C3'-C2'-C1' | 5.96 | 106.27 | 101.50 |
| 81 | DA | 2216 | G | O4'-C1'-N9 | 5.96 | 112.97 | 108.20 |
| 82 | DB | 4 | C | C3'-C2'-C1' | -5.96 | 96.73 | 101.50 |
| 10 | AI | 86 | ALA | N-CA-C | 5.96 | 127.09 | 111.00 |
| 42 | BM | 124 | ASP | CB-CG-OD2 | -5.96 | 112.94 | 118.30 |
| 57 | Be | 30 | ARG | NE-CZ-NH1 | 5.96 | 123.28 | 120.30 |
| 74 | BQ | 54 | ARG | N-CA-C | 5.96 | 127.09 | 111.00 |
| 76 | BS | 26 | ILE | CB-CA-C | 5.96 | 123.52 | 111.60 |
| 78 | CA | 223 | U | C5'-C4'-O4' | -5.96 | 101.95 | 109.10 |
| 78 | CA | 911 | U | O4'-C1'-N1 | 5.96 | 112.97 | 108.20 |
| 81 | DA | 243 | G | N9-C1'-C2' | -5.96 | 105.44 | 112.00 |
| 81 | DA | 735 | A | C4-C5-C6 | 5.96 | 119.98 | 117.00 |
| 81 | DA | 1243 | G | O4'-C1'-N9 | 5.96 | 112.97 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2277 | C | O4'-C1'-N1 | 5.96 | 112.97 | 108.20 |
| 81 | DA | 2569 | A | O4'-C1'-N9 | 5.96 | 112.97 | 108.20 |
| 57 | Be | 23 | ALA | C-N-CA | 5.96 | 136.59 | 121.70 |
| 78 | CA | 836 | U | C1'-O4'-C4' | 5.96 | 114.67 | 109.90 |
| 78 | CA | 1118 | G | O4'-C1'-N9 | 5.96 | 112.96 | 108.20 |
| 81 | DA | 92 | G | C5'-C4'-O4' | 5.96 | 116.25 | 109.10 |
| 81 | DA | 506 | U | O4'-C1'-N1 | 5.96 | 112.97 | 108.20 |
| 81 | DA | 1578 | C | C3'-C2'-C1' | 5.96 | 106.27 | 101.50 |
| 81 | DA | 2956 | A | O3'-P-O5' | 5.96 | 115.32 | 104.00 |
| 81 | DA | 3013 | U | N1-C1'-C2' | 5.96 | 121.74 | 114.00 |
| 82 | DB | 121 | U | C1'-O4'-C4' | 5.96 | 114.67 | 109.90 |
| 83 | DC | 76 | U | C3'-C2'-C1' | 5.96 | 106.27 | 101.50 |
| 81 | DA | 246 | U | C4'-C3'-C2' | -5.96 | 96.64 | 102.60 |
| 81 | DA | 1791 | C | OP1-P-O3' | 5.96 | 118.30 | 105.20 |
| 6 | AE | 153 | SER | N-CA-CB | 5.95 | 119.43 | 110.50 |
| 33 | BD | 318 | LEU | O-C-N | -5.95 | 113.18 | 122.70 |
| 62 | Bk | 70 | ARG | NE-CZ-NH2 | -5.95 | 117.32 | 120.30 |
| 78 | CA | 672 | U | C3'-C2'-C1' | 5.95 | 106.26 | 101.50 |
| 78 | CA | 1394 | G | C1'-O4'-C4' | -5.95 | 105.14 | 109.90 |
| 78 | CA | 1666 | U | N1-C1'-C2' | -5.95 | 105.45 | 112.00 |
| 81 | DA | 241 | G | C5'-C4'-O4' | -5.95 | 101.96 | 109.10 |
| 81 | DA | 2374 | C | C5'-C4'-C3' | -5.95 | 106.47 | 116.00 |
| 81 | DA | 2688 | U | P-O3'-C3' | 5.95 | 126.84 | 119.70 |
| 81 | DA | 2682 | C | P-O5'-C5' | 5.95 | 130.42 | 120.90 |
| 40 | BK | 128 | ARG | N-CA-C | 5.95 | 127.07 | 111.00 |
| 41 | BN | 62 | GLN | CG-CD-OE1 | -5.95 | 109.70 | 121.60 |
| 78 | CA | 338 | C | P-O5'-C5' | -5.95 | 111.38 | 120.90 |
| 78 | CA | 1326 | A | C3'-C2'-C1' | 5.95 | 106.26 | 101.50 |
| 78 | CA | 1709 | C | C3'-C2'-C1' | 5.95 | 106.26 | 101.50 |
| 81 | DA | 1399 | A | P-O3'-C3' | -5.95 | 112.56 | 119.70 |
| 81 | DA | 1981 | G | P-O3'-C3' | -5.95 | 112.56 | 119.70 |
| 81 | DA | 2729 | U | P-O5'-C5' | -5.95 | 111.38 | 120.90 |
| 5 | AC | 16 | LYS | CB-CA-C | -5.95 | 98.50 | 110.40 |
| 9 | AH | 108 | ALA | N-CA-C | -5.95 | 94.94 | 111.00 |
| 78 | CA | 1039 | A | O4'-C1'-N9 | 5.95 | 112.96 | 108.20 |
| 78 | CA | 1303 | U | C5'-C4'-O4' | 5.95 | 116.24 | 109.10 |
| 81 | DA | 2229 | A | C1'-O4'-C4' | 5.95 | 114.66 | 109.90 |
| 81 | DA | 2443 | A | C4'-C3'-C2' | -5.95 | 96.65 | 102.60 |
| 81 | DA | 2827 | U | O4'-C1'-C2' | -5.95 | 99.85 | 105.80 |
| 81 | DA | 3257 | C | C5'-C4'-O4' | 5.95 | 116.24 | 109.10 |
| 81 | DA | 3389 | U | P-O5'-C5' | 5.95 | 130.42 | 120.90 |
| 78 | CA | 1425 | A | C5-C6-N1 | -5.95 | 114.73 | 117.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 671 | U | N1-C1'-C2' | -5.95 | 105.46 | 112.00 |
| 81 | DA | 680 | G | N9-C1'-C2' | -5.95 | 105.46 | 112.00 |
| 81 | DA | 2592 | G | C3'-C2'-C1' | 5.95 | 106.26 | 101.50 |
| 36 | BF | 88 | TYR | CB-CG-CD2 | -5.95 | 117.43 | 121.00 |
| 62 | Bk | 55 | ARG | NH1-CZ-NH2 | -5.95 | 112.86 | 119.40 |
| 76 | BS | 32 | TRP | CA-CB-CG | 5.95 | 125.00 | 113.70 |
| 81 | DA | 2027 | C | O4'-C1'-N1 | 5.95 | 112.96 | 108.20 |
| 81 | DA | 2122 | G | O4'-C1'-N9 | 5.95 | 112.96 | 108.20 |
| 78 | CA | 460 | A | C1'-O4'-C4' | -5.94 | 105.14 | 109.90 |
| 78 | CA | 1091 | A | P-O3'-C3' | -5.94 | 112.57 | 119.70 |
| 81 | DA | 1823 | A | C5'-C4'-C3' | -5.94 | 106.49 | 116.00 |
| 81 | DA | 2238 | G | P-O5'-C5' | -5.94 | 111.39 | 120.90 |
| 81 | DA | 2709 | C | O4'-C1'-C2' | -5.94 | 99.86 | 105.80 |
| 81 | DA | 3050 | U | C2'-C3'-O3' | 5.94 | 123.21 | 113.70 |
| 83 | DC | 47 | C | C4'-C3'-O3' | -5.94 | 96.92 | 109.40 |
| 4 | AD | 240 | LYS | N-CA-C | -5.94 | 94.95 | 111.00 |
| 33 | BD | 145 | ILE | CA-CB-CG2 | 5.94 | 122.78 | 110.90 |
| 46 | BT | 8 | LYS | CB-CA-C | -5.94 | 98.52 | 110.40 |
| 81 | DA | 1227 | C | O4'-C1'-N1 | 5.94 | 112.95 | 108.20 |
| 81 | DA | 2274 | U | O4'-C1'-N1 | 5.94 | 112.95 | 108.20 |
| 78 | CA | 966 | A | N9-C1'-C2' | -5.94 | 105.47 | 112.00 |
| 81 | DA | 131 | C | C3'-C2'-C1' | 5.94 | 106.25 | 101.50 |
| 81 | DA | 244 | G | C1'-O4'-C4' | -5.94 | 105.15 | 109.90 |
| 81 | DA | 799 | G | C1'-O4'-C4' | 5.94 | 114.65 | 109.90 |
| 81 | DA | 1292 | C | O4'-C1'-C2' | -5.94 | 99.86 | 105.80 |
| 81 | DA | 2350 | C | O4'-C1'-C2' | -5.94 | 99.86 | 105.80 |
| 81 | DA | 2665 | U | C3'-C2'-C1' | -5.94 | 96.75 | 101.50 |
| 81 | DA | 2882 | U | C5'-C4'-C3' | 5.94 | 125.50 | 116.00 |
| 78 | CA | 488 | G | P-O3'-C3' | 5.94 | 126.83 | 119.70 |
| 78 | CA | 1131 | A | P-O3'-C3' | 5.94 | 126.83 | 119.70 |
| 6 | AE | 174 | ARG | O-C-N | -5.94 | 113.11 | 123.20 |
| 78 | CA | 507 | U | O3'-P-O5' | -5.94 | 92.72 | 104.00 |
| 78 | CA | 569 | C | N3-C4-C5 | -5.94 | 119.53 | 121.90 |
| 78 | CA | 1645 | G | O4'-C1'-N9 | 5.94 | 112.95 | 108.20 |
| 81 | DA | 785 | G | C1'-O4'-C4' | 5.94 | 114.65 | 109.90 |
| 81 | DA | 808 | A | O3'-P-O5' | -5.94 | 92.72 | 104.00 |
| 78 | CA | 1339 | C | C4'-C3'-C2' | -5.94 | 96.66 | 102.60 |
| 35 | BG | 151 | LYS | N-CA-CB | 5.93 | 121.28 | 110.60 |
| 43 | BP | 77 | LYS | N-CA-CB | 5.93 | 121.28 | 110.60 |
| 48 | BW | 78 | TYR | CB-CG-CD1 | -5.93 | 117.44 | 121.00 |
| 55 | Bc | 116 | TYR | CG-CD2-CE2 | -5.93 | 116.55 | 121.30 |
| 74 | BQ | 240 | TYR | CB-CG-CD1 | -5.93 | 117.44 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 297 | U | C5'-C4'-C3' | 5.93 | 125.49 | 116.00 |
| 81 | DA | 646 | A | N9-C1'-C2' | 5.93 | 121.71 | 114.00 |
| 81 | DA | 916 | G | N9-C1'-C2' | -5.93 | 105.47 | 112.00 |
| 81 | DA | 2500 | A | O3'-P-O5' | -5.93 | 92.72 | 104.00 |
| 83 | DC | 29 | C | N1-C1'-C2' | 5.93 | 121.72 | 114.00 |
| 5 | AC | 149 | ARG | NH1-CZ-NH2 | -5.93 | 112.88 | 119.40 |
| 46 | BT | 124 | TYR | CG-CD1-CE1 | -5.93 | 116.55 | 121.30 |
| 64 | Bl | 72 | ARG | NE-CZ-NH2 | -5.93 | 117.33 | 120.30 |
| 81 | DA | 617 | G | O4'-C1'-N9 | 5.93 | 112.94 | 108.20 |
| 81 | DA | 1768 | U | N3-C4-O4 | 5.93 | 123.55 | 119.40 |
| 5 | AC | 17 | ARG | C-N-CD | -5.93 | 107.55 | 120.60 |
| 33 | BD | 302 | ALA | CB-CA-C | -5.93 | 101.20 | 110.10 |
| 81 | DA | 1290 | A | N9-C1'-C2' | -5.93 | 105.48 | 112.00 |
| 31 | BB | 40 | TYR | CB-CG-CD2 | -5.93 | 117.44 | 121.00 |
| 31 | BB | 63 | PHE | CB-CG-CD1 | -5.93 | 116.65 | 120.80 |
| 41 | BN | 5 | SER | N-CA-CB | 5.93 | 119.39 | 110.50 |
| 45 | BR | 102 | ALA | N-CA-CB | 5.93 | 118.40 | 110.10 |
| 55 | Bc | 41 | LEU | CA-CB-CG | -5.93 | 101.66 | 115.30 |
| 78 | CA | 1653 | C | C3'-C2'-C1' | 5.93 | 106.24 | 101.50 |
| 81 | DA | 1193 | A | P-O3'-C3' | -5.93 | 112.58 | 119.70 |
| 81 | DA | 1262 | G | OP1-P-OP2 | -5.93 | 110.70 | 119.60 |
| 81 | DA | 1653 | G | N9-C1'-C2' | 5.93 | 121.71 | 114.00 |
| 81 | DA | 2270 | A | C3'-C2'-C1' | 5.93 | 106.24 | 101.50 |
| 81 | DA | 2317 | A | C3'-C2'-C1' | 5.93 | 106.24 | 101.50 |
| 61 | Bj | 86 | ARG | NE-CZ-NH1 | 5.93 | 123.26 | 120.30 |
| 81 | DA | 243 | G | O4'-C1'-C2' | 5.93 | 112.94 | 107.60 |
| 81 | DA | 699 | A | C5'-C4'-O4' | 5.93 | 116.21 | 109.10 |
| 81 | DA | 727 | G | C3'-C2'-C1' | 5.93 | 106.24 | 101.50 |
| 81 | DA | 2146 | C | N1-C1'-C2' | 5.93 | 121.71 | 114.00 |
| 81 | DA | 3080 | G | C3'-C2'-C1' | 5.93 | 106.24 | 101.50 |
| 78 | CA | 1719 | A | C5'-C4'-C3' | 5.93 | 125.48 | 116.00 |
| 81 | DA | 544 | C | O4'-C1'-C2' | -5.93 | 99.87 | 105.80 |
| 81 | DA | 2546 | C | N3-C4-C5 | -5.93 | 119.53 | 121.90 |
| 81 | DA | 2711 | C | C3'-C2'-C1' | 5.93 | 106.24 | 101.50 |
| 81 | DA | 3289 | G | O4'-C1'-N9 | 5.93 | 112.94 | 108.20 |
| 55 | Bc | 96 | GLU | N-CA-CB | 5.92 | 121.26 | 110.60 |
| 78 | CA | 1637 | C | C2-N1-C1' | 5.92 | 125.32 | 118.80 |
| 81 | DA | 1932 | A | O4'-C1'-N9 | 5.92 | 112.94 | 108.20 |
| 81 | DA | 2534 | G | C5-C6-O6 | -5.92 | 125.05 | 128.60 |
| 81 | DA | 3298 | C | N1-C1'-C2' | 5.92 | 121.70 | 114.00 |
| 9 | AH | 97 | ARG | NE-CZ-NH1 | 5.92 | 123.26 | 120.30 |
| 24 | AX | 75 | GLU | N-CA-C | -5.92 | 95.01 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 979 | A | C3'-C2'-C1' | 5.92 | 106.24 | 101.50 |
| 78 | CA | 1401 | A | O4'-C1'-N9 | 5.92 | 112.94 | 108.20 |
| 81 | DA | 2129 | U | O4'-C1'-N1 | 5.92 | 112.94 | 108.20 |
| 81 | DA | 3303 | G | O4'-C1'-C2' | 5.92 | 112.93 | 107.60 |
| 30 | BA | 24 | LYS | CB-CA-C | 5.92 | 122.24 | 110.40 |
| 34 | BE | 168 | ASP | CB-CG-OD2 | -5.92 | 112.97 | 118.30 |
| 81 | DA | 253 | A | N9-C1'-C2' | -5.92 | 105.49 | 112.00 |
| 10 | AI | 120 | ASP | N-CA-CB | 5.92 | 121.25 | 110.60 |
| 40 | BK | 87 | MET | CG-SD-CE | -5.92 | 90.73 | 100.20 |
| 49 | BV | 165 | VAL | CA-C-N | 5.92 | 130.22 | 117.20 |
| 76 | BS | 9 | TYR | CB-CG-CD2 | -5.92 | 117.45 | 121.00 |
| 81 | DA | 281 | G | O4'-C1'-N9 | 5.92 | 112.94 | 108.20 |
| 81 | DA | 1886 | A | C3'-C2'-C1' | 5.92 | 106.23 | 101.50 |
| 81 | DA | 2455 | U | O3'-P-O5' | -5.92 | 92.75 | 104.00 |
| 81 | DA | 3117 | C | N1-C1'-C2' | 5.92 | 121.69 | 114.00 |
| 35 | BG | 176 | PHE | CB-CG-CD1 | 5.92 | 124.94 | 120.80 |
| 78 | CA | 257 | A | C5'-C4'-C3' | 5.92 | 125.47 | 116.00 |
| 78 | CA | 313 | U | N1-C1'-C2' | -5.92 | 105.49 | 112.00 |
| 81 | DA | 942 | U | O4'-C1'-N1 | 5.92 | 112.93 | 108.20 |
| 81 | DA | 1234 | G | P-O5'-C5' | -5.92 | 111.43 | 120.90 |
| 81 | DA | 1956 | A | O4'-C1'-C2' | -5.92 | 99.88 | 105.80 |
| 81 | DA | 2147 | A | P-O3'-C3' | -5.92 | 112.60 | 119.70 |
| 81 | DA | 2633 | U | O3'-P-O5' | 5.92 | 115.24 | 104.00 |
| 5 | AC | 189 | ASP | C-N-CA | 5.92 | 136.49 | 121.70 |
| 13 | AL | 110 | LYS | N-CA-C | -5.92 | 95.03 | 111.00 |
| 14 | AM | 99 | HIS | N-CA-CB | -5.92 | 99.95 | 110.60 |
| 43 | BP | 179 | LYS | CB-CA-C | 5.92 | 122.23 | 110.40 |
| 78 | CA | 1069 | A | C5-C6-N1 | -5.92 | 114.74 | 117.70 |
| 53 | Ba | 57 | HIS | CB-CG-CD2 | -5.91 | 112.47 | 130.80 |
| 65 | Bn | 17 | ARG | NE-CZ-NH1 | 5.91 | 123.26 | 120.30 |
| 62 | Bk | 28 | TYR | CB-CG-CD2 | 5.91 | 124.55 | 121.00 |
| 78 | CA | 1600 | A | N9-C1'-C2' | -5.91 | 105.50 | 112.00 |
| 81 | DA | 2369 | G | O4'-C1'-C2' | -5.91 | 99.89 | 105.80 |
| 17 | AQ | 21 | TYR | CB-CG-CD1 | 5.91 | 124.55 | 121.00 |
| 20 | AS | 87 | GLY | C-N-CA | 5.91 | 136.48 | 121.70 |
| 21 | AT | 44 | ARG | CA-CB-CG | 5.91 | 126.40 | 113.40 |
| 32 | BC | 346 | THR | N-CA-CB | 5.91 | 121.53 | 110.30 |
| 78 | CA | 948 | G | C3'-C2'-C1' | -5.91 | 96.77 | 101.50 |
| 81 | DA | 214 | G | C1'-O4'-C4' | 5.91 | 114.63 | 109.90 |
| 81 | DA | 1017 | C | N1-C1'-C2' | 5.91 | 121.69 | 114.00 |
| 81 | DA | 1269 | U | P-O3'-C3' | 5.91 | 126.79 | 119.70 |
| 81 | DA | 2037 | G | O4'-C1'-N9 | 5.91 | 112.93 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 3042 | U | C5'-C4'-O4' | 5.91 | 116.19 | 109.10 |
| 20 | AS | 11 | ALA | CB-CA-C | -5.91 | 101.24 | 110.10 |
| 48 | BW | 100 | THR | N-CA-C | -5.91 | 95.05 | 111.00 |
| 55 | Bc | 95 | PHE | CB-CG-CD2 | 5.91 | 124.94 | 120.80 |
| 78 | CA | 783 | G | C5'-C4'-C3' | 5.91 | 125.45 | 116.00 |
| 78 | CA | 846 | G | P-O5'-C5' | -5.91 | 111.44 | 120.90 |
| 78 | CA | 1104 | U | N1-C1'-C2' | 5.91 | 121.68 | 114.00 |
| 78 | CA | 1356 | U | N1-C1'-C2' | 5.91 | 121.68 | 114.00 |
| 78 | CA | 1400 | A | C1'-O4'-C4' | -5.91 | 105.17 | 109.90 |
| 78 | CA | 1721 | A | C1'-O4'-C4' | 5.91 | 114.63 | 109.90 |
| 81 | DA | 539 | C | O4'-C1'-N1 | 5.91 | 112.93 | 108.20 |
| 81 | DA | 1016 | C | C3'-C2'-C1' | 5.91 | 106.23 | 101.50 |
| 81 | DA | 3002 | C | O4'-C4'-C3' | -5.91 | 98.09 | 104.00 |
| 81 | DA | 3047 | U | O4'-C1'-C2' | -5.91 | 99.89 | 105.80 |
| 82 | DB | 59 | A | N9-C1'-C2' | 5.91 | 121.68 | 114.00 |
| 77 | BI | 119 | TRP | CB-CA-C | -5.91 | 98.58 | 110.40 |
| 81 | DA | 1368 | U | O4'-C1'-C2' | -5.91 | 99.89 | 105.80 |
| 57 | Be | 138 | TYR | CB-CG-CD1 | 5.91 | 124.54 | 121.00 |
| 81 | DA | 728 | G | P-O5'-C5' | -5.91 | 111.45 | 120.90 |
| 81 | DA | 1323 | G | C3'-C2'-C1' | -5.91 | 96.78 | 101.50 |
| 81 | DA | 1602 | A | P-O3'-C3' | 5.91 | 126.79 | 119.70 |
| 81 | DA | 2563 | G | C5-C6-O6 | -5.91 | 125.06 | 128.60 |
| 81 | DA | 2691 | A | C5'-C4'-C3' | 5.91 | 125.45 | 116.00 |
| 81 | DA | 2697 | A | C5'-C4'-C3' | -5.91 | 106.55 | 116.00 |
| 78 | CA | 637 | C | O4'-C1'-N1 | 5.90 | 112.92 | 108.20 |
| 78 | CA | 1635 | A | C5-C6-N6 | -5.90 | 118.98 | 123.70 |
| 81 | DA | 1293 | U | O3'-P-O5' | -5.90 | 92.78 | 104.00 |
| 81 | DA | 1814 | A | C3'-C2'-C1' | -5.90 | 96.78 | 101.50 |
| 81 | DA | 2535 | A | O4'-C4'-C3' | -5.90 | 98.10 | 104.00 |
| 82 | DB | 62 | C | O4'-C1'-C2' | 5.90 | 112.91 | 107.60 |
| 18 | AP | 40 | LEU | N-CA-C | -5.90 | 95.06 | 111.00 |
| 30 | BA | 107 | TYR | CB-CG-CD1 | 5.90 | 124.54 | 121.00 |
| 35 | BG | 92 | SER | C-N-CA | 5.90 | 136.46 | 121.70 |
| 49 | BV | 126 | ARG | NE-CZ-NH1 | 5.90 | 123.25 | 120.30 |
| 63 | Bm | 4 | ARG | NE-CZ-NH2 | -5.90 | 117.35 | 120.30 |
| 81 | DA | 2479 | C | P-O3'-C3' | -5.90 | 112.62 | 119.70 |
| 39 | BJ | 76 | SER | CA-CB-OG | 5.90 | 127.13 | 111.20 |
| 51 | BZ | 68 | ALA | N-CA-CB | 5.90 | 118.36 | 110.10 |
| 78 | CA | 417 | A | O4'-C1'-N9 | -5.90 | 103.48 | 108.20 |
| 78 | CA | 1635 | A | O4'-C1'-N9 | 5.90 | 112.92 | 108.20 |
| 81 | DA | 2214 | A | O4'-C1'-N9 | 5.90 | 112.92 | 108.20 |
| 81 | DA | 2293 | C | C3'-C2'-C1' | 5.90 | 106.22 | 101.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 29 | AU | 49 | LYS | N-CA-C | -5.90 | 95.07 | 111.00 |
| 81 | DA | 1407 | A | C3'-C2'-C1' | 5.90 | 106.22 | 101.50 |
| 81 | DA | 1784 | G | O4'-C4'-C3' | -5.90 | 98.10 | 104.00 |
| 78 | CA | 152 | U | P-O3'-C3' | -5.90 | 112.62 | 119.70 |
| 78 | CA | 1673 | G | O3'-P-O5' | -5.90 | 92.79 | 104.00 |
| 81 | DA | 1871 | U | C1'-O4'-C4' | -5.90 | 105.18 | 109.90 |
| 16 | AO | 110 | ASP | CB-CG-OD1 | 5.90 | 123.61 | 118.30 |
| 72 | Bu | 60 | ASN | C-N-CA | -5.90 | 106.96 | 121.70 |
| 79 | CB | 29 | C | O4'-C1'-N1 | 5.90 | 112.92 | 108.20 |
| 81 | DA | 1144 | U | C2'-C3'-O3' | 5.90 | 123.13 | 113.70 |
| 78 | CA | 189 | C | N1-C1'-C2' | -5.89 | 105.52 | 112.00 |
| 78 | CA | 1157 | A | C3'-C2'-C1' | 5.89 | 106.22 | 101.50 |
| 81 | DA | 63 | A | P-O5'-C5' | -5.89 | 111.47 | 120.90 |
| 81 | DA | 252 | U | C5'-C4'-C3' | 5.89 | 125.43 | 116.00 |
| 81 | DA | 276 | U | P-O3'-C3' | -5.89 | 112.63 | 119.70 |
| 81 | DA | 1478 | C | C4'-C3'-C2' | -5.89 | 96.71 | 102.60 |
| 81 | DA | 2345 | A | O4'-C1'-C2' | 5.89 | 112.91 | 107.60 |
| 81 | DA | 3245 | A | C3'-C2'-C1' | -5.89 | 96.78 | 101.50 |
| 82 | DB | 143 | U | O4'-C1'-N1 | 5.89 | 112.92 | 108.20 |
| 83 | DC | 89 | A | O4'-C1'-C2' | -5.89 | 99.91 | 105.80 |
| 31 | BB | 83 | HIS | CB-CA-C | -5.89 | 98.61 | 110.40 |
| 37 | BH | 229 | VAL | CB-CA-C | -5.89 | 100.20 | 111.40 |
| 40 | BK | 127 | LEU | N-CA-CB | 5.89 | 122.19 | 110.40 |
| 78 | CA | 30 | G | O3'-P-O5' | -5.89 | 92.81 | 104.00 |
| 78 | CA | 560 | U | O3'-P-O5' | -5.89 | 92.81 | 104.00 |
| 81 | DA | 1263 | A | C1'-O4'-C4' | -5.89 | 105.19 | 109.90 |
| 81 | DA | 1534 | A | N9-C1'-C2' | -5.89 | 105.52 | 112.00 |
| 37 | BH | 88 | ALA | N-CA-CB | 5.89 | 118.35 | 110.10 |
| 78 | CA | 150 | U | C2'-C3'-O3' | 5.89 | 123.13 | 113.70 |
| 78 | CA | 1640 | C | N3-C4-N4 | 5.89 | 122.12 | 118.00 |
| 81 | DA | 2617 | U | O4'-C1'-C2' | -5.89 | 99.91 | 105.80 |
| 81 | DA | 3099 | C | C5'-C4'-O4' | -5.89 | 102.03 | 109.10 |
| 81 | DA | 3335 | A | N9-C1'-C2' | 5.89 | 121.66 | 114.00 |
| 42 | BM | 85 | TRP | CB-CG-CD2 | -5.89 | 118.94 | 126.60 |
| 78 | CA | 1534 | G | C5'-C4'-O4' | 5.89 | 116.17 | 109.10 |
| 81 | DA | 1907 | C | N1-C1'-C2' | 5.89 | 121.66 | 114.00 |
| 81 | DA | 2449 | A | O4'-C1'-C2' | -5.89 | 99.91 | 105.80 |
| 8 | AF | 76 | ARG | NE-CZ-NH1 | 5.89 | 123.24 | 120.30 |
| 14 | AM | 53 | ASP | CB-CG-OD1 | -5.89 | 113.00 | 118.30 |
| 74 | BQ | 12 | TYR | CD1-CE1-CZ | -5.89 | 114.50 | 119.80 |
| 78 | CA | 1428 | G | C5-C6-O6 | -5.89 | 125.07 | 128.60 |
| 81 | DA | 751 | A | O3'-P-O5' | -5.89 | 92.81 | 104.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2798 | C | C3'-C2'-C1' | 5.89 | 106.21 | 101.50 |
| 81 | DA | 3212 | C | O5'-C5'-C4' | 5.89 | 122.88 | 111.70 |
| 83 | DC | 34 | C | O4'-C1'-N1 | 5.89 | 112.91 | 108.20 |
| 6 | AE | 196 | VAL | CA-CB-CG1 | -5.88 | 102.07 | 110.90 |
| 12 | AK | 37 | GLU | N-CA-CB | 5.88 | 121.19 | 110.60 |
| 29 | AU | 89 | TYR | CA-CB-CG | 5.88 | 124.58 | 113.40 |
| 53 | Ba | 91 | ALA | CB-CA-C | -5.88 | 101.27 | 110.10 |
| 74 | BQ | 260 | PHE | CB-CG-CD1 | -5.88 | 116.68 | 120.80 |
| 81 | DA | 1706 | C | C3'-C2'-C1' | 5.88 | 106.21 | 101.50 |
| 81 | DA | 1943 | C | C3'-C2'-C1' | 5.88 | 106.21 | 101.50 |
| 81 | DA | 2477 | G | C5'-C4'-O4' | 5.88 | 116.16 | 109.10 |
| 81 | DA | 2774 | C | N1-C1'-C2' | 5.88 | 121.65 | 114.00 |
| 81 | DA | 2837 | A | O4'-C1'-C2' | -5.88 | 99.92 | 105.80 |
| 83 | DC | 103 | U | C3'-C2'-C1' | 5.88 | 106.21 | 101.50 |
| 40 | BK | 162 | VAL | CG1-CB-CG2 | 5.88 | 120.31 | 110.90 |
| 49 | BV | 113 | TYR | CA-CB-CG | 5.88 | 124.58 | 113.40 |
| 78 | CA | 483 | A | C5-C6-N6 | -5.88 | 118.99 | 123.70 |
| 81 | DA | 275 | U | C3'-C2'-C1' | 5.88 | 106.21 | 101.50 |
| 81 | DA | 2074 | C | N1-C1'-C2' | 5.88 | 121.65 | 114.00 |
| 81 | DA | 2296 | A | O4'-C1'-N9 | 5.88 | 112.91 | 108.20 |
| 17 | AQ | 81 | LYS | CB-CA-C | -5.88 | 98.64 | 110.40 |
| 32 | BC | 118 | PHE | CA-CB-CG | 5.88 | 128.01 | 113.90 |
| 37 | BH | 61 | GLN | O-C-N | -5.88 | 113.29 | 122.70 |
| 43 | BP | 193 | ARG | NE-CZ-NH2 | -5.88 | 117.36 | 120.30 |
| 79 | CB | 10 | G | C5'-C4'-C3' | -5.88 | 106.59 | 116.00 |
| 81 | DA | 820 | A | P-O3'-C3' | -5.88 | 112.64 | 119.70 |
| 81 | DA | 1518 | U | O4'-C1'-N1 | 5.88 | 112.91 | 108.20 |
| 81 | DA | 1622 | U | O4'-C1'-C2' | -5.88 | 99.92 | 105.80 |
| 81 | DA | 1883 | A | O4'-C1'-C2' | -5.88 | 99.92 | 105.80 |
| 81 | DA | 2599 | U | O4'-C1'-N1 | 5.88 | 112.91 | 108.20 |
| 81 | DA | 2704 | A | C1'-O4'-C4' | 5.88 | 114.61 | 109.90 |
| 82 | DB | 130 | C | P-O5'-C5' | 5.88 | 130.31 | 120.90 |
| 78 | CA | 854 | U | C5'-C4'-O4' | 5.88 | 116.16 | 109.10 |
| 79 | CB | 6 | G | N9-C1'-C2' | 5.88 | 121.64 | 114.00 |
| 81 | DA | 1018 | G | O4'-C1'-N9 | 5.88 | 112.90 | 108.20 |
| 81 | DA | 2124 | G | C3'-C2'-C1' | -5.88 | 96.80 | 101.50 |
| 24 | AX | 53 | ALA | N-CA-CB | 5.88 | 118.33 | 110.10 |
| 63 | Bm | 17 | ARG | N-CA-CB | -5.88 | 100.02 | 110.60 |
| 69 | Br | 26 | THR | CA-CB-CG2 | -5.88 | 104.17 | 112.40 |
| 81 | DA | 715 | A | C3'-C2'-C1' | -5.88 | 96.80 | 101.50 |
| 81 | DA | 1716 | U | C1'-O4'-C4' | 5.88 | 114.60 | 109.90 |
| 81 | DA | 2210 | G | C5'-C4'-C3' | 5.88 | 125.40 | 116.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 82 | DB | 60 | U | N1-C1'-C2' | -5.88 | 105.54 | 112.00 |
| 82 | DB | 134 | G | P-O5'-C5' | -5.88 | 111.50 | 120.90 |
| 37 | BH | 62 | LYS | N-CA-C | -5.88 | 95.14 | 111.00 |
| 78 | CA | 226 | A | P-O5'-C5' | 5.88 | 130.30 | 120.90 |
| 78 | CA | 571 | G | C3'-C2'-C1' | 5.88 | 106.20 | 101.50 |
| 78 | CA | 1070 | C | N3-C4-C5 | -5.88 | 119.55 | 121.90 |
| 81 | DA | 2313 | A | P-O5'-C5' | -5.88 | 111.50 | 120.90 |
| 81 | DA | 2356 | A | O4'-C1'-N9 | 5.88 | 112.90 | 108.20 |
| 9 | AH | 69 | LEU | CA-CB-CG | 5.87 | 128.81 | 115.30 |
| 20 | AS | 69 | LYS | N-CA-CB | 5.87 | 121.17 | 110.60 |
| 76 | BS | 92 | MET | CG-SD-CE | -5.87 | 90.80 | 100.20 |
| 78 | CA | 1201 | G | N9-C1'-C2' | 5.87 | 121.64 | 114.00 |
| 81 | DA | 1477 | A | C5'-C4'-C3' | -5.87 | 106.60 | 116.00 |
| 17 | AQ | 58 | MET | CG-SD-CE | -5.87 | 90.80 | 100.20 |
| 29 | AU | 71 | GLY | C-N-CA | 5.87 | 136.38 | 121.70 |
| 78 | CA | 567 | A | C4-C5-C6 | 5.87 | 119.94 | 117.00 |
| 78 | CA | 1438 | G | O4'-C1'-N9 | 5.87 | 112.90 | 108.20 |
| 81 | DA | 178 | U | O4'-C1'-C2' | -5.87 | 99.93 | 105.80 |
| 81 | DA | 500 | C | O4'-C1'-N1 | 5.87 | 112.90 | 108.20 |
| 81 | DA | 2443 | A | C3'-C2'-C1' | 5.87 | 106.20 | 101.50 |
| 81 | DA | 736 | A | C4-C5-C6 | 5.87 | 119.94 | 117.00 |
| 81 | DA | 2047 | A | P-O3'-C3' | 5.87 | 126.75 | 119.70 |
| 82 | DB | 86 | U | C1'-O4'-C4' | 5.87 | 114.60 | 109.90 |
| 6 | AE | 100 | ALA | N-CA-CB | 5.87 | 118.31 | 110.10 |
| 55 | Bc | 95 | PHE | CB-CG-CD1 | -5.87 | 116.69 | 120.80 |
| 78 | CA | 204 | G | P-O3'-C3' | -5.87 | 112.66 | 119.70 |
| 78 | CA | 213 | A | C5-C6-N1 | -5.87 | 114.77 | 117.70 |
| 81 | DA | 329 | U | C1'-O4'-C4' | -5.87 | 105.20 | 109.90 |
| 81 | DA | 838 | G | C5'-C4'-O4' | -5.87 | 102.06 | 109.10 |
| 81 | DA | 3094 | A | C1'-O4'-C4' | -5.87 | 105.21 | 109.90 |
| 78 | CA | 385 | A | P-O3'-C3' | -5.87 | 112.66 | 119.70 |
| 81 | DA | 2839 | G | O4'-C1'-N9 | 5.87 | 112.89 | 108.20 |
| 22 | AV | 59 | TYR | N-CA-CB | 5.87 | 121.16 | 110.60 |
| 43 | BP | 71 | ARG | NE-CZ-NH2 | 5.87 | 123.23 | 120.30 |
| 47 | BU | 159 | PHE | CB-CG-CD2 | -5.87 | 116.69 | 120.80 |
| 62 | Bk | 81 | THR | C-N-CA | -5.87 | 107.04 | 121.70 |
| 76 | BS | 120 | PHE | CA-C-O | -5.87 | 107.78 | 120.10 |
| 78 | CA | 225 | A | OP1-P-OP2 | -5.87 | 110.80 | 119.60 |
| 81 | DA | 313 | A | N9-C1'-C2' | -5.87 | 105.55 | 112.00 |
| 81 | DA | 528 | U | P-O3'-C3' | -5.87 | 112.66 | 119.70 |
| 32 | BC | 9 | PRO | N-CD-CG | 5.86 | 111.99 | 103.20 |
| 32 | BC | 18 | PRO | N-CD-CG | -5.86 | 94.41 | 103.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 51 | BZ | 60 | LYS | N-CA-C | -5.86 | 95.17 | 111.00 |
| 81 | DA | 63 | A | C3'-C2'-C1' | -5.86 | 96.81 | 101.50 |
| 81 | DA | 524 | U | C4'-C3'-C2' | -5.86 | 96.74 | 102.60 |
| 81 | DA | 599 | C | O4'-C1'-C2' | -5.86 | 99.94 | 105.80 |
| 81 | DA | 697 | A | C3'-C2'-C1' | 5.86 | 106.19 | 101.50 |
| 81 | DA | 3391 | A | O3'-P-O5' | -5.86 | 92.86 | 104.00 |
| 81 | DA | 164 | A | C5-C6-N1 | -5.86 | 114.77 | 117.70 |
| 81 | DA | 1416 | C | C3'-C2'-C1' | 5.86 | 106.19 | 101.50 |
| 81 | DA | 1633 | C | C5'-C4'-O4' | 5.86 | 116.13 | 109.10 |
| 14 | AM | 93 | THR | N-CA-CB | 5.86 | 121.44 | 110.30 |
| 61 | Bj | 33 | GLU | OE1-CD-OE2 | 5.86 | 130.33 | 123.30 |
| 78 | CA | 1408 | G | C2'-C3'-O3' | 5.86 | 123.08 | 113.70 |
| 81 | DA | 1817 | G | C5'-C4'-O4' | 5.86 | 116.13 | 109.10 |
| 81 | DA | 2281 | A | O4'-C1'-N9 | 5.86 | 112.89 | 108.20 |
| 81 | DA | 2742 | C | P-O5'-C5' | 5.86 | 130.28 | 120.90 |
| 81 | DA | 3232 | G | P-O3'-C3' | -5.86 | 112.67 | 119.70 |
| 5 | AC | 39 | LYS | N-CA-CB | 5.86 | 121.15 | 110.60 |
| 62 | Bk | 56 | ARG | NE-CZ-NH1 | -5.86 | 117.37 | 120.30 |
| 81 | DA | 682 | U | N1-C1'-C2' | 5.86 | 121.62 | 114.00 |
| 81 | DA | 2190 | U | O4'-C1'-N1 | 5.86 | 112.89 | 108.20 |
| 33 | BD | 326 | ARG | NE-CZ-NH2 | -5.86 | 117.37 | 120.30 |
| 78 | CA | 206 | A | C3'-C2'-C1' | 5.86 | 106.19 | 101.50 |
| 78 | CA | 535 | A | O5'-C5'-C4' | 5.86 | 122.83 | 111.70 |
| 78 | CA | 1389 | C | N1-C1'-C2' | 5.86 | 121.61 | 114.00 |
| 81 | DA | 163 | C | C5'-C4'-C3' | -5.86 | 106.63 | 116.00 |
| 81 | DA | 1059 | G | N9-C1'-C2' | 5.86 | 121.62 | 114.00 |
| 81 | DA | 2407 | C | P-O5'-C5' | 5.86 | 130.27 | 120.90 |
| 81 | DA | 2514 | U | N1-C1'-C2' | -5.86 | 105.56 | 112.00 |
| 81 | DA | 2622 | C | C1'-O4'-C4' | -5.86 | 105.21 | 109.90 |
| 83 | DC | 82 | A | O4'-C1'-N9 | 5.86 | 112.89 | 108.20 |
| 5 | AC | 3 | ARG | O-C-N | -5.86 | 113.33 | 122.70 |
| 48 | BW | 91 | ASP | C-N-CA | 5.86 | 136.34 | 121.70 |
| 78 | CA | 409 | C | O4'-C1'-N1 | 5.86 | 112.88 | 108.20 |
| 81 | DA | 162 | G | P-O5'-C5' | 5.86 | 130.27 | 120.90 |
| 81 | DA | 700 | C | C1'-O4'-C4' | 5.86 | 114.58 | 109.90 |
| 81 | DA | 1244 | A | P-O3'-C3' | 5.86 | 126.73 | 119.70 |
| 81 | DA | 2417 | U | N1-C1'-C2' | 5.86 | 121.61 | 114.00 |
| 81 | DA | 2579 | G | OP2-P-O3' | 5.86 | 118.08 | 105.20 |
| 83 | DC | 117 | C | O4'-C1'-N1 | 5.86 | 112.88 | 108.20 |
| 57 | Be | 85 | PHE | CB-CG-CD2 | -5.85 | 116.70 | 120.80 |
| 78 | CA | 386 | G | C3'-C2'-C1' | 5.85 | 106.18 | 101.50 |
| 78 | CA | 522 | U | P-O5'-C5' | -5.85 | 111.53 | 120.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2190 | U | P-O3'-C3' | 5.85 | 126.72 | 119.70 |
| 81 | DA | 2495 | C | O4'-C1'-N1 | 5.85 | 112.88 | 108.20 |
| 25 | AY | 20 | GLY | N-CA-C | -5.85 | 98.47 | 113.10 |
| 55 | Bc | 96 | GLU | CA-C-O | -5.85 | 107.81 | 120.10 |
| 79 | CB | 13 | U | C2'-C3'-O3' | 5.85 | 123.06 | 113.70 |
| 81 | DA | 68 | C | C1'-O4'-C4' | -5.85 | 105.22 | 109.90 |
| 43 | BP | 131 | GLU | N-CA-CB | 5.85 | 121.13 | 110.60 |
| 76 | BS | 156 | ARG | N-CA-CB | 5.85 | 121.13 | 110.60 |
| 78 | CA | 681 | U | P-O3'-C3' | 5.85 | 126.72 | 119.70 |
| 81 | DA | 2 | U | O4'-C1'-C2' | -5.85 | 99.95 | 105.80 |
| 81 | DA | 72 | C | C5'-C4'-C3' | -5.85 | 106.64 | 116.00 |
| 81 | DA | 677 | A | C5'-C4'-O4' | 5.85 | 116.12 | 109.10 |
| 81 | DA | 1514 | G | O4'-C1'-N9 | 5.85 | 112.88 | 108.20 |
| 78 | CA | 1289 | U | O4'-C1'-N1 | 5.85 | 112.88 | 108.20 |
| 81 | DA | 2545 | C | N3-C4-C5 | -5.85 | 119.56 | 121.90 |
| 4 | AD | 240 | LYS | O-C-N | -5.85 | 113.26 | 123.20 |
| 5 | AC | 15 | PRO | N-CA-CB | 5.85 | 110.32 | 103.30 |
| 13 | AL | 123 | LYS | O-C-N | -5.85 | 113.34 | 122.70 |
| 43 | BP | 74 | PRO | CA-N-CD | 5.85 | 119.89 | 111.70 |
| 43 | BP | 134 | LEU | N-CA-CB | 5.85 | 122.09 | 110.40 |
| 81 | DA | 458 | U | O4'-C1'-N1 | 5.85 | 112.88 | 108.20 |
| 81 | DA | 967 | A | O4'-C1'-C2' | -5.85 | 99.95 | 105.80 |
| 81 | DA | 1171 | G | O4'-C1'-N9 | 5.85 | 112.88 | 108.20 |
| 81 | DA | 1769 | G | O4'-C1'-N9 | 5.85 | 112.88 | 108.20 |
| 81 | DA | 1824 | U | P-O5'-C5' | 5.85 | 130.25 | 120.90 |
| 81 | DA | 2218 | G | O4'-C1'-C2' | 5.85 | 112.86 | 107.60 |
| 81 | DA | 3372 | A | C3'-C2'-C1' | 5.85 | 106.18 | 101.50 |
| 4 | AD | 218 | PHE | CG-CD2-CE2 | 5.85 | 127.23 | 120.80 |
| 78 | CA | 151 | G | O4'-C1'-N9 | 5.85 | 112.88 | 108.20 |
| 78 | CA | 304 | U | C1'-O4'-C4' | 5.85 | 114.58 | 109.90 |
| 81 | DA | 2527 | G | O4'-C1'-C2' | 5.85 | 112.86 | 107.60 |
| 76 | BS | 67 | PHE | CB-CA-C | -5.84 | 98.71 | 110.40 |
| 81 | DA | 603 | A | C3'-C2'-C1' | 5.84 | 106.17 | 101.50 |
| 81 | DA | 726 | G | N9-C1'-C2' | 5.84 | 121.60 | 114.00 |
| 81 | DA | 1211 | U | C1'-O4'-C4' | -5.84 | 105.22 | 109.90 |
| 81 | DA | 2046 | U | C3'-C2'-C1' | -5.84 | 96.82 | 101.50 |
| 81 | DA | 3019 | U | C3'-C2'-C1' | 5.84 | 106.18 | 101.50 |
| 78 | CA | 872 | G | P-O3'-C3' | 5.84 | 126.71 | 119.70 |
| 79 | CB | 8 | U | C1'-O4'-C4' | 5.84 | 114.57 | 109.90 |
| 81 | DA | 839 | C | O4'-C1'-C2' | -5.84 | 99.96 | 105.80 |
| 81 | DA | 1427 | U | O3'-P-O5' | 5.84 | 115.10 | 104.00 |
| 32 | BC | 4 | ARG | N-CA-C | -5.84 | 95.22 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 53 | Ba | 76 | ASN | N-CA-CB | 5.84 | 121.11 | 110.60 |
| 59 | Bh | 104 | ASN | CA-CB-CG | -5.84 | 100.55 | 113.40 |
| 78 | CA | 1237 | G | O4'-C1'-C2' | -5.84 | 99.96 | 105.80 |
| 81 | DA | 720 | A | O4'-C1'-C2' | -5.84 | 99.96 | 105.80 |
| 81 | DA | 1072 | G | O4'-C1'-C2' | 5.84 | 112.86 | 107.60 |
| 81 | DA | 1894 | U | O3'-P-O5' | -5.84 | 92.90 | 104.00 |
| 81 | DA | 2452 | G | C3'-C2'-C1' | 5.84 | 106.17 | 101.50 |
| 64 | Bl | 64 | MET | CG-SD-CE | -5.84 | 90.86 | 100.20 |
| 78 | CA | 98 | U | O4'-C1'-N1 | 5.84 | 112.87 | 108.20 |
| 78 | CA | 1154 | G | P-O3'-C3' | 5.84 | 126.71 | 119.70 |
| 78 | CA | 1291 | G | N9-C1'-C2' | 5.84 | 121.59 | 114.00 |
| 78 | CA | 1566 | U | C5'-C4'-C3' | 5.84 | 125.34 | 116.00 |
| 81 | DA | 732 | C | N3-C4-C5 | -5.84 | 119.56 | 121.90 |
| 81 | DA | 738 | A | C5-C6-N6 | -5.84 | 119.03 | 123.70 |
| 81 | DA | 801 | A | O5'-P-OP1 | -5.84 | 100.44 | 105.70 |
| 81 | DA | 3060 | C | P-O3'-C3' | -5.84 | 112.69 | 119.70 |
| 38 | Bs | 101 | VAL | CA-CB-CG2 | -5.84 | 102.14 | 110.90 |
| 74 | BQ | 60 | ILE | CA-CB-CG1 | 5.84 | 122.09 | 111.00 |
| 81 | DA | 1376 | C | N1-C1'-C2' | 5.84 | 121.59 | 114.00 |
| 81 | DA | 1777 | U | P-O5'-C5' | 5.84 | 130.24 | 120.90 |
| 81 | DA | 3083 | G | O4'-C1'-N9 | 5.84 | 112.87 | 108.20 |
| 9 | AH | 8 | ALA | N-CA-CB | 5.84 | 118.27 | 110.10 |
| 31 | BB | 76 | PHE | CB-CG-CD2 | -5.84 | 116.71 | 120.80 |
| 32 | BC | 130 | PHE | CB-CG-CD1 | 5.84 | 124.89 | 120.80 |
| 78 | CA | 229 | U | P-O5'-C5' | -5.84 | 111.56 | 120.90 |
| 78 | CA | 401 | A | P-O3'-C3' | 5.84 | 126.70 | 119.70 |
| 78 | CA | 1562 | G | P-O3'-C3' | -5.84 | 112.70 | 119.70 |
| 81 | DA | 269 | G | P-O3'-C3' | 5.84 | 126.70 | 119.70 |
| 82 | DB | 134 | G | C4'-C3'-C2' | -5.84 | 96.76 | 102.60 |
| 32 | BC | 298 | PHE | CB-CA-C | -5.83 | 98.73 | 110.40 |
| 16 | AO | 117 | LEU | N-CA-CB | 5.83 | 122.07 | 110.40 |
| 16 | AO | 118 | ILE | CB-CA-C | 5.83 | 123.27 | 111.60 |
| 32 | BC | 281 | LYS | CA-CB-CG | 5.83 | 126.23 | 113.40 |
| 47 | BU | 8 | ARG | CB-CA-C | -5.83 | 98.73 | 110.40 |
| 81 | DA | 373 | A | C3'-C2'-C1' | 5.83 | 106.17 | 101.50 |
| 81 | DA | 1001 | G | O4'-C1'-C2' | 5.83 | 112.85 | 107.60 |
| 81 | DA | 2376 | G | O5'-P-OP2 | -5.83 | 100.45 | 105.70 |
| 81 | DA | 2577 | C | N3-C4-C5 | -5.83 | 119.57 | 121.90 |
| 81 | DA | 2621 | G | P-O3'-C3' | 5.83 | 126.70 | 119.70 |
| 5 | AC | 16 | LYS | O-C-N | -5.83 | 113.37 | 122.70 |
| 78 | CA | 1005 | A | O4'-C1'-N9 | -5.83 | 103.53 | 108.20 |
| 81 | DA | 2354 | C | C5'-C4'-C3' | -5.83 | 106.67 | 116.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 3296 | A | P-O5'-C5' | 5.83 | 130.23 | 120.90 |
| 78 | CA | 232 | U | P-O3'-C3' | -5.83 | 112.70 | 119.70 |
| 78 | CA | 642 | G | O4'-C1'-C2' | -5.83 | 99.97 | 105.80 |
| 81 | DA | 263 | C | C3'-C2'-C1' | 5.83 | 106.16 | 101.50 |
| 81 | DA | 626 | U | P-O3'-C3' | -5.83 | 112.70 | 119.70 |
| 81 | DA | 869 | G | O3'-P-O5' | -5.83 | 92.92 | 104.00 |
| 81 | DA | 2020 | A | O4'-C1'-N9 | 5.83 | 112.86 | 108.20 |
| 81 | DA | 2632 | G | C3'-C2'-C1' | -5.83 | 96.84 | 101.50 |
| 81 | DA | 3078 | U | O4'-C1'-N1 | -5.83 | 103.54 | 108.20 |
| 78 | CA | 1341 | A | C4'-C3'-C2' | -5.83 | 96.77 | 102.60 |
| 81 | DA | 523 | A | O4'-C1'-C2' | -5.83 | 99.97 | 105.80 |
| 81 | DA | 662 | U | O3'-P-O5' | -5.83 | 92.93 | 104.00 |
| 81 | DA | 1257 | C | C1'-O4'-C4' | -5.83 | 105.24 | 109.90 |
| 81 | DA | 1374 | G | O4'-C1'-N9 | 5.83 | 112.86 | 108.20 |
| 81 | DA | 1677 | G | C1'-O4'-C4' | -5.83 | 105.24 | 109.90 |
| 19 | AR | 130 | ARG | NE-CZ-NH1 | 5.83 | 123.21 | 120.30 |
| 78 | CA | 506 | A | P-O3'-C3' | 5.83 | 126.69 | 119.70 |
| 81 | DA | 1260 | A | OP1-P-OP2 | -5.83 | 110.86 | 119.60 |
| 81 | DA | 3311 | C | C1'-O4'-C4' | -5.83 | 105.24 | 109.90 |
| 11 | AJ | 23 | ARG | NH1-CZ-NH2 | 5.83 | 125.81 | 119.40 |
| 65 | Bn | 75 | VAL | N-CA-CB | 5.83 | 124.32 | 111.50 |
| 81 | DA | 1728 | G | C3'-C2'-C1' | -5.83 | 96.84 | 101.50 |
| 81 | DA | 2880 | U | O4'-C1'-N1 | -5.83 | 103.54 | 108.20 |
| 1 | Aa | 31 | ASN | N-CA-C | -5.82 | 95.28 | 111.00 |
| 6 | AE | 143 | TYR | CB-CG-CD2 | 5.82 | 124.49 | 121.00 |
| 42 | BM | 128 | ARG | NE-CZ-NH2 | 5.82 | 123.21 | 120.30 |
| 53 | Ba | 74 | VAL | CA-CB-CG1 | -5.82 | 102.16 | 110.90 |
| 61 | Bj | 99 | ARG | NE-CZ-NH1 | 5.82 | 123.21 | 120.30 |
| 81 | DA | 843 | A | C1'-O4'-C4' | 5.82 | 114.56 | 109.90 |
| 78 | CA | 205 | U | C4'-C3'-C2' | -5.82 | 96.78 | 102.60 |
| 78 | CA | 342 | C | O4'-C1'-C2' | -5.82 | 99.98 | 105.80 |
| 78 | CA | 867 | G | N9-C1'-C2' | -5.82 | 105.60 | 112.00 |
| 78 | CA | 1073 | G | O4'-C1'-N9 | 5.82 | 112.86 | 108.20 |
| 78 | CA | 1775 | U | O3'-P-O5' | 5.82 | 115.06 | 104.00 |
| 81 | DA | 2647 | A | O3'-P-O5' | -5.82 | 92.94 | 104.00 |
| 4 | AD | 132 | GLY | C-N-CA | 5.82 | 136.25 | 121.70 |
| 17 | AQ | 28 | PHE | CB-CG-CD1 | -5.82 | 116.72 | 120.80 |
| 57 | Be | 203 | TRP | CB-CG-CD1 | 5.82 | 134.57 | 127.00 |
| 59 | Bh | 20 | HIS | CA-CB-CG | 5.82 | 123.50 | 113.60 |
| 78 | CA | 1639 | C | N3-C4-N4 | 5.82 | 122.07 | 118.00 |
| 81 | DA | 2174 | G | C5'-C4'-O4' | -5.82 | 102.12 | 109.10 |
| 82 | DB | 27 | U | P-O3'-C3' | 5.82 | 126.69 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2377 | G | C4'-C3'-C2' | 5.82 | 108.42 | 102.60 |
| 53 | Ba | 96 | VAL | CA-CB-CG1 | 5.82 | 119.63 | 110.90 |
| 56 | Bf | 59 | TYR | CB-CG-CD2 | -5.82 | 117.51 | 121.00 |
| 78 | CA | 891 | A | C4'-C3'-C2' | -5.82 | 96.78 | 102.60 |
| 78 | CA | 1113 | A | C3'-C2'-C1' | -5.82 | 96.85 | 101.50 |
| 81 | DA | 1058 | U | O4'-C1'-C2' | -5.82 | 99.98 | 105.80 |
| 81 | DA | 1537 | A | C3'-C2'-C1' | 5.82 | 106.15 | 101.50 |
| 81 | DA | 1923 | C | O4'-C1'-N1 | 5.82 | 112.85 | 108.20 |
| 81 | DA | 3075 | G | O4'-C1'-N9 | 5.82 | 112.86 | 108.20 |
| 12 | AK | 106 | ALA | N-CA-CB | 5.82 | 118.24 | 110.10 |
| 22 | AV | 30 | LYS | CA-CB-CG | 5.82 | 126.19 | 113.40 |
| 43 | BP | 16 | SER | N-CA-CB | -5.82 | 101.78 | 110.50 |
| 64 | Bl | 3 | LYS | N-CA-C | -5.82 | 95.30 | 111.00 |
| 78 | CA | 254 | A | O4'-C1'-C2' | -5.82 | 99.98 | 105.80 |
| 78 | CA | 1294 | G | O4'-C1'-N9 | 5.82 | 112.85 | 108.20 |
| 78 | CA | 1644 | C | O4'-C1'-C2' | -5.82 | 99.98 | 105.80 |
| 81 | DA | 467 | U | O4'-C1'-N1 | 5.82 | 112.85 | 108.20 |
| 81 | DA | 1206 | G | O5'-C5'-C4' | -5.82 | 100.65 | 111.70 |
| 81 | DA | 1627 | U | P-O3'-C3' | -5.82 | 112.72 | 119.70 |
| 81 | DA | 2039 | C | O4'-C1'-C2' | -5.82 | 99.98 | 105.80 |
| 81 | DA | 2240 | G | P-O3'-C3' | -5.82 | 112.72 | 119.70 |
| 81 | DA | 2327 | U | O4'-C1'-N1 | 5.82 | 112.85 | 108.20 |
| 81 | DA | 3143 | C | O4'-C1'-C2' | -5.82 | 99.98 | 105.80 |
| 20 | AS | 66 | TYR | CG-CD1-CE1 | -5.81 | 116.65 | 121.30 |
| 78 | CA | 1655 | A | P-O3'-C3' | -5.81 | 112.72 | 119.70 |
| 81 | DA | 645 | A | C1'-O4'-C4' | 5.81 | 114.55 | 109.90 |
| 81 | DA | 1783 | U | C4'-C3'-O3' | 5.81 | 124.63 | 113.00 |
| 38 | Bs | 26 | PHE | N-CA-CB | 5.81 | 121.06 | 110.60 |
| 67 | Bp | 46 | ARG | NE-CZ-NH2 | -5.81 | 117.39 | 120.30 |
| 73 | Bv | 17 | PRO | CA-N-CD | -5.81 | 103.36 | 111.50 |
| 78 | CA | 255 | U | O4'-C1'-C2' | -5.81 | 99.99 | 105.80 |
| 78 | CA | 842 | C | N3-C4-C5 | -5.81 | 119.58 | 121.90 |
| 81 | DA | 2535 | A | O3'-P-O5' | -5.81 | 92.96 | 104.00 |
| 81 | DA | 2885 | C | N1-C1'-C2' | 5.81 | 121.56 | 114.00 |
| 81 | DA | 3130 | A | C3'-C2'-C1' | -5.81 | 96.85 | 101.50 |
| 2 | AA | 110 | TYR | CG-CD2-CE2 | -5.81 | 116.65 | 121.30 |
| 5 | AC | 15 | PRO | N-CA-C | 5.81 | 127.21 | 112.10 |
| 5 | AC | 167 | ALA | N-CA-CB | 5.81 | 118.23 | 110.10 |
| 33 | BD | 313 | LEU | CB-CG-CD1 | -5.81 | 101.12 | 111.00 |
| 81 | DA | 640 | U | O4'-C1'-C2' | -5.81 | 99.99 | 105.80 |
| 81 | DA | 2437 | G | O4'-C1'-C2' | -5.81 | 99.99 | 105.80 |
| 81 | DA | 3383 | G | C5'-C4'-C3' | 5.81 | 125.30 | 116.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 82 | DB | 38 | U | O4'-C1'-C2' | -5.81 | 99.99 | 105.80 |
| 78 | CA | 296 | U | N1-C1'-C2' | 5.81 | 121.55 | 114.00 |
| 78 | CA | 560 | U | N1-C1'-C2' | 5.81 | 121.55 | 114.00 |
| 78 | CA | 1657 | U | O3'-P-O5' | -5.81 | 92.96 | 104.00 |
| 81 | DA | 1152 | G | C2'-C3'-O3' | 5.81 | 123.00 | 113.70 |
| 81 | DA | 1691 | U | P-O3'-C3' | -5.81 | 112.73 | 119.70 |
| 81 | DA | 1717 | U | C5'-C4'-C3' | 5.81 | 125.30 | 116.00 |
| 81 | DA | 2577 | C | C4'-C3'-C2' | -5.81 | 96.79 | 102.60 |
| 5 | AC | 153 | GLU | N-CA-CB | 5.81 | 121.05 | 110.60 |
| 64 | Bl | 85 | LYS | N-CA-C | -5.81 | 95.32 | 111.00 |
| 78 | CA | 145 | A | P-O3'-C3' | 5.81 | 126.67 | 119.70 |
| 78 | CA | 496 | G | O4'-C1'-N9 | 5.81 | 112.85 | 108.20 |
| 78 | CA | 845 | G | O4'-C1'-N9 | 5.81 | 112.85 | 108.20 |
| 78 | CA | 892 | A | O4'-C1'-N9 | 5.81 | 112.84 | 108.20 |
| 81 | DA | 1152 | G | O4'-C1'-C2' | 5.81 | 112.83 | 107.60 |
| 6 | AE | 11 | ARG | NE-CZ-NH2 | -5.81 | 117.40 | 120.30 |
| 8 | AF | 43 | PHE | N-CA-CB | 5.81 | 121.05 | 110.60 |
| 78 | CA | 1615 | C | O3'-P-O5' | -5.81 | 92.97 | 104.00 |
| 81 | DA | 1748 | G | C3'-C2'-C1' | -5.81 | 96.86 | 101.50 |
| 81 | DA | 2511 | A | C5'-C4'-C3' | -5.81 | 106.71 | 116.00 |
| 2 | AA | 229 | LYS | N-CA-CB | -5.80 | 100.15 | 110.60 |
| 14 | AM | 125 | ILE | N-CA-CB | 5.80 | 124.15 | 110.80 |
| 78 | CA | 164 | A | P-O3'-C3' | 5.80 | 126.67 | 119.70 |
| 78 | CA | 224 | C | C3'-C2'-C1' | 5.80 | 106.14 | 101.50 |
| 78 | CA | 1472 | C | C1'-O4'-C4' | 5.80 | 114.54 | 109.90 |
| 81 | DA | 1536 | G | C3'-C2'-C1' | 5.80 | 106.14 | 101.50 |
| 81 | DA | 2663 | G | N9-C1'-C2' | -5.80 | 105.62 | 112.00 |
| 82 | DB | 73 | U | C5'-C4'-C3' | -5.80 | 106.71 | 116.00 |
| 83 | DC | 2 | G | O4'-C1'-N9 | 5.80 | 112.84 | 108.20 |
| 78 | CA | 190 | C | N1-C1'-C2' | 5.80 | 121.54 | 114.00 |
| 81 | DA | 1755 | C | N3-C4-N4 | 5.80 | 122.06 | 118.00 |
| 34 | BE | 90 | GLN | N-CA-CB | 5.80 | 121.04 | 110.60 |
| 78 | CA | 1061 | A | C5-C6-N1 | -5.80 | 114.80 | 117.70 |
| 81 | DA | 1102 | A | C3'-C2'-C1' | 5.80 | 106.14 | 101.50 |
| 81 | DA | 1799 | A | P-O3'-C3' | 5.80 | 126.66 | 119.70 |
| 81 | DA | 2536 | A | C5-C6-N1 | -5.80 | 114.80 | 117.70 |
| 81 | DA | 3125 | U | C4'-C3'-C2' | -5.80 | 96.80 | 102.60 |
| 4 | AD | 151 | ASP | N-CA-CB | 5.80 | 121.04 | 110.60 |
| 36 | BF | 56 | ALA | CB-CA-C | -5.80 | 101.40 | 110.10 |
| 53 | Ba | 44 | ALA | CB-CA-C | -5.80 | 101.40 | 110.10 |
| 78 | CA | 965 | U | C5'-C4'-O4' | 5.80 | 116.06 | 109.10 |
| 78 | CA | 1616 | G | N9-C1'-C2' | 5.80 | 121.54 | 114.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1009 | A | O4'-C1'-N9 | 5.80 | 112.84 | 108.20 |
| 81 | DA | 2228 | A | P-O5'-C5' | 5.80 | 130.18 | 120.90 |
| 4 | AD | 47 | PHE | CG-CD1-CE1 | -5.80 | 114.42 | 120.80 |
| 47 | BU | 1 | MET | C-N-CA | 5.80 | 134.48 | 122.30 |
| 78 | CA | 670 | U | C1'-O4'-C4' | -5.80 | 105.26 | 109.90 |
| 81 | DA | 1183 | C | O4'-C1'-N1 | 5.80 | 112.84 | 108.20 |
| 81 | DA | 1701 | C | P-O3'-C3' | -5.80 | 112.74 | 119.70 |
| 14 | AM | 129 | TRP | CZ3-CH2-CZ2 | -5.80 | 114.64 | 121.60 |
| 33 | BD | 313 | LEU | CD1-CG-CD2 | 5.80 | 127.89 | 110.50 |
| 51 | BZ | 51 | TRP | CA-CB-CG | 5.80 | 124.71 | 113.70 |
| 76 | BS | 108 | MET | N-CA-CB | 5.80 | 121.03 | 110.60 |
| 78 | CA | 1144 | U | N1-C1'-C2' | 5.80 | 121.54 | 114.00 |
| 81 | DA | 2796 | G | C1'-O4'-C4' | 5.80 | 114.54 | 109.90 |
| 81 | DA | 328 | U | N1-C1'-C2' | -5.79 | 105.63 | 112.00 |
| 81 | DA | 1967 | U | O4'-C1'-C2' | -5.79 | 100.00 | 105.80 |
| 81 | DA | 2618 | G | C2'-C3'-O3' | 5.79 | 122.97 | 113.70 |
| 25 | AY | 48 | VAL | N-CA-C | -5.79 | 95.36 | 111.00 |
| 78 | CA | 1123 | C | O4'-C1'-C2' | -5.79 | 100.01 | 105.80 |
| 78 | CA | 1603 | U | N1-C1'-C2' | -5.79 | 105.63 | 112.00 |
| 81 | DA | 225 | C | O4'-C1'-N1 | 5.79 | 112.83 | 108.20 |
| 81 | DA | 1343 | A | O3'-P-O5' | 5.79 | 115.01 | 104.00 |
| 81 | DA | 1440 | G | O4'-C1'-N9 | 5.79 | 112.83 | 108.20 |
| 81 | DA | 1513 | G | C3'-C2'-C1' | -5.79 | 96.87 | 101.50 |
| 81 | DA | 1578 | C | O4'-C1'-N1 | 5.79 | 112.83 | 108.20 |
| 81 | DA | 1972 | A | O3'-P-O5' | 5.79 | 115.01 | 104.00 |
| 81 | DA | 3111 | U | O4'-C1'-C2' | -5.79 | 100.01 | 105.80 |
| 82 | DB | 124 | G | P-O5'-C5' | 5.79 | 130.17 | 120.90 |
| 25 | AY | 22 | ARG | C-N-CA | -5.79 | 110.14 | 122.30 |
| 57 | Be | 119 | VAL | CB-CA-C | -5.79 | 100.40 | 111.40 |
| 81 | DA | 573 | C | C5'-C4'-O4' | 5.79 | 116.05 | 109.10 |
| 81 | DA | 3221 | C | N1-C1'-C2' | 5.79 | 121.53 | 114.00 |
| 81 | DA | 3248 | C | O4'-C4'-C3' | -5.79 | 98.21 | 104.00 |
| 3 | AB | 120 | TYR | CB-CG-CD1 | 5.79 | 124.47 | 121.00 |
| 78 | CA | 1633 | A | C4-C5-C6 | 5.79 | 119.89 | 117.00 |
| 81 | DA | 1673 | G | C1'-O4'-C4' | -5.79 | 105.27 | 109.90 |
| 65 | Bn | 77 | ARG | N-CA-CB | 5.79 | 121.02 | 110.60 |
| 72 | Bt | 61 | PHE | N-CA-CB | 5.79 | 121.02 | 110.60 |
| 78 | CA | 142 | G | O4'-C1'-C2' | -5.79 | 100.01 | 105.80 |
| 78 | CA | 1638 | G | C5-C6-O6 | -5.79 | 125.13 | 128.60 |
| 79 | CB | 19 | U | P-O5'-C5' | 5.79 | 130.16 | 120.90 |
| 81 | DA | 657 | A | C4'-C3'-C2' | -5.79 | 96.81 | 102.60 |
| 81 | DA | 1000 | C | P-O3'-C3' | -5.79 | 112.75 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2572 | C | N3-C4-C5 | -5.79 | 119.58 | 121.90 |
| 81 | DA | 2705 | A | C3'-C2'-C1' | -5.79 | 96.87 | 101.50 |
| 81 | DA | 2775 | U | C1'-O4'-C4' | 5.79 | 114.53 | 109.90 |
| 2 | AA | 194 | PRO | C-N-CA | 5.79 | 136.17 | 121.70 |
| 17 | AQ | 85 | VAL | CA-CB-CG1 | 5.79 | 119.58 | 110.90 |
| 41 | BN | 51 | ALA | N-CA-CB | 5.79 | 118.20 | 110.10 |
| 66 | Bo | 8 | ARG | NE-CZ-NH1 | 5.79 | 123.19 | 120.30 |
| 78 | CA | 1711 | C | O4'-C1'-N1 | 5.79 | 112.83 | 108.20 |
| 81 | DA | 882 | A | C3'-C2'-C1' | 5.79 | 106.13 | 101.50 |
| 83 | DC | 31 | U | P-O5'-C5' | 5.79 | 130.16 | 120.90 |
| 35 | BG | 48 | ARG | CG-CD-NE | -5.79 | 99.65 | 111.80 |
| 48 | BW | 15 | PHE | CB-CG-CD2 | 5.79 | 124.85 | 120.80 |
| 78 | CA | 27 | U | C4'-C3'-C2' | -5.79 | 96.81 | 102.60 |
| 78 | CA | 492 | A | C4-C5-C6 | 5.79 | 119.89 | 117.00 |
| 81 | DA | 2506 | U | C5'-C4'-C3' | -5.79 | 106.74 | 116.00 |
| 81 | DA | 2989 | U | O4'-C4'-C3' | -5.79 | 98.22 | 104.00 |
| 33 | BD | 102 | PRO | N-CA-C | 5.78 | 127.14 | 112.10 |
| 58 | Bg | 28 | ARG | CD-NE-CZ | -5.78 | 115.50 | 123.60 |
| 61 | Bj | 5 | HIS | C-N-CA | 5.78 | 136.16 | 121.70 |
| 61 | Bj | 45 | LEU | C-N-CA | 5.78 | 134.45 | 122.30 |
| 78 | CA | 1101 | G | C4'-C3'-C2' | -5.78 | 96.82 | 102.60 |
| 78 | CA | 1306 | C | O5'-C5'-C4' | 5.78 | 122.69 | 111.70 |
| 78 | CA | 1412 | G | N9-C1'-C2' | 5.78 | 121.52 | 114.00 |
| 81 | DA | 173 | G | C1'-O4'-C4' | -5.78 | 105.27 | 109.90 |
| 81 | DA | 353 | G | N9-C1'-C2' | -5.78 | 105.64 | 112.00 |
| 81 | DA | 798 | G | O4'-C4'-C3' | 5.78 | 110.73 | 106.10 |
| 81 | DA | 954 | U | O4'-C1'-C2' | -5.78 | 100.02 | 105.80 |
| 81 | DA | 1192 | C | C3'-C2'-C1' | 5.78 | 106.13 | 101.50 |
| 81 | DA | 2953 | U | O4'-C1'-N1 | 5.78 | 112.83 | 108.20 |
| 46 | BT | 143 | ILE | CA-CB-CG1 | 5.78 | 121.99 | 111.00 |
| 78 | CA | 1053 | G | O4'-C1'-N9 | 5.78 | 112.83 | 108.20 |
| 78 | CA | 1425 | A | C5'-C4'-C3' | 5.78 | 125.25 | 116.00 |
| 81 | DA | 779 | G | C1'-O4'-C4' | -5.78 | 105.27 | 109.90 |
| 81 | DA | 2208 | A | C4'-C3'-O3' | 5.78 | 124.56 | 113.00 |
| 1 | Aa | 58 | VAL | CG1-CB-CG2 | 5.78 | 120.15 | 110.90 |
| 6 | AE | 197 | TYR | CA-CB-CG | -5.78 | 102.42 | 113.40 |
| 9 | AH | 120 | HIS | CB-CA-C | 5.78 | 121.96 | 110.40 |
| 45 | BR | 78 | ASN | N-CA-CB | 5.78 | 121.00 | 110.60 |
| 78 | CA | 81 | G | O4'-C4'-C3' | 5.78 | 110.72 | 106.10 |
| 78 | CA | 993 | A | C3'-C2'-C1' | 5.78 | 106.12 | 101.50 |
| 78 | CA | 1419 | G | O4'-C4'-C3' | -5.78 | 98.22 | 104.00 |
| 80 | CC | 21 | C | O5'-P-OP2 | -5.78 | 100.50 | 105.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 563 | U | O4'-C1'-N1 | 5.78 | 112.82 | 108.20 |
| 81 | DA | 677 | A | O3'-P-O5' | 5.78 | 114.98 | 104.00 |
| 81 | DA | 1786 | G | C4'-C3'-C2' | -5.78 | 96.82 | 102.60 |
| 81 | DA | 2109 | U | O4'-C1'-N1 | 5.78 | 112.83 | 108.20 |
| 33 | BD | 342 | LYS | CB-CA-C | 5.78 | 121.96 | 110.40 |
| 49 | BV | 167 | ARG | O-C-N | -5.78 | 113.45 | 122.70 |
| 78 | CA | 941 | A | P-O3'-C3' | 5.78 | 126.64 | 119.70 |
| 14 | AM | 145 | ARG | NE-CZ-NH2 | -5.78 | 117.41 | 120.30 |
| 32 | BC | 240 | ARG | N-CA-CB | 5.78 | 121.00 | 110.60 |
| 78 | CA | 975 | C | P-O5'-C5' | -5.78 | 111.66 | 120.90 |
| 81 | DA | 3332 | U | N1-C1'-C2' | -5.78 | 105.64 | 112.00 |
| 81 | DA | 3356 | G | C5'-C4'-C3' | 5.78 | 125.25 | 116.00 |
| 1 | Aa | 58 | VAL | CA-CB-CG2 | -5.78 | 102.24 | 110.90 |
| 3 | AB | 163 | PRO | N-CD-CG | 5.78 | 111.86 | 103.20 |
| 35 | BG | 143 | LYS | CB-CA-C | -5.78 | 98.85 | 110.40 |
| 41 | BN | 131 | VAL | CA-CB-CG2 | 5.78 | 119.56 | 110.90 |
| 68 | Bq | 17 | ARG | NE-CZ-NH2 | -5.78 | 117.41 | 120.30 |
| 78 | CA | 1437 | U | O4'-C4'-C3' | -5.78 | 98.22 | 104.00 |
| 81 | DA | 282 | G | O4'-C1'-N9 | 5.78 | 112.82 | 108.20 |
| 81 | DA | 769 | G | C5-C6-O6 | -5.78 | 125.13 | 128.60 |
| 81 | DA | 2484 | A | C3'-C2'-C1' | -5.78 | 96.88 | 101.50 |
| 74 | BQ | 112 | ARG | NE-CZ-NH2 | -5.77 | 117.41 | 120.30 |
| 78 | CA | 302 | U | C4'-C3'-C2' | -5.77 | 96.83 | 102.60 |
| 78 | CA | 1351 | G | P-O5'-C5' | -5.77 | 111.66 | 120.90 |
| 78 | CA | 1695 | G | O4'-C1'-N9 | 5.77 | 112.82 | 108.20 |
| 81 | DA | 978 | G | P-O5'-C5' | 5.77 | 130.14 | 120.90 |
| 33 | BD | 85 | SER | N-CA-CB | -5.77 | 101.84 | 110.50 |
| 78 | CA | 448 | C | P-O5'-C5' | 5.77 | 130.13 | 120.90 |
| 78 | CA | 1724 | U | C1'-O4'-C4' | 5.77 | 114.52 | 109.90 |
| 81 | DA | 170 | G | P-O3'-C3' | -5.77 | 112.77 | 119.70 |
| 81 | DA | 376 | G | C1'-O4'-C4' | -5.77 | 105.28 | 109.90 |
| 81 | DA | 1739 | U | P-O5'-C5' | 5.77 | 130.14 | 120.90 |
| 81 | DA | 3146 | G | C3'-C2'-C1' | 5.77 | 106.12 | 101.50 |
| 15 | AN | 22 | ARG | CB-CA-C | 5.77 | 121.94 | 110.40 |
| 57 | Be | 20 | GLN | N-CA-CB | 5.77 | 120.99 | 110.60 |
| 37 | BH | 63 | LYS | C-N-CA | -5.77 | 107.28 | 121.70 |
| 41 | BN | 137 | LYS | N-CA-CB | 5.77 | 120.99 | 110.60 |
| 48 | BW | 107 | PHE | N-CA-C | 5.77 | 126.58 | 111.00 |
| 78 | CA | 1769 | U | O4'-C1'-N1 | 5.77 | 112.81 | 108.20 |
| 81 | DA | 974 | G | C5'-C4'-O4' | -5.77 | 102.18 | 109.10 |
| 81 | DA | 2271 | A | O4'-C1'-C2' | -5.77 | 100.03 | 105.80 |
| 81 | DA | 2540 | A | C5-C6-N6 | -5.77 | 119.08 | 123.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 3365 | U | C5'-C4'-C3' | -5.77 | 106.77 | 116.00 |
| 12 | AK | 121 | VAL | CA-C-N | 5.77 | 133.25 | 117.10 |
| 17 | AQ | 73 | LEU | N-CA-C | -5.77 | 95.43 | 111.00 |
| 25 | AY | 60 | GLU | N-CA-C | -5.77 | 95.43 | 111.00 |
| 78 | CA | 1220 | C | C3'-C2'-C1' | 5.77 | 106.11 | 101.50 |
| 81 | DA | 1458 | U | O4'-C1'-N1 | 5.77 | 112.81 | 108.20 |
| 81 | DA | 1873 | U | P-O5'-C5' | 5.77 | 130.13 | 120.90 |
| 81 | DA | 2574 | G | C5-C6-O6 | -5.77 | 125.14 | 128.60 |
| 51 | BZ | 65 | GLU | CB-CA-C | 5.77 | 121.93 | 110.40 |
| 78 | CA | 1338 | C | O4'-C1'-N1 | 5.77 | 112.81 | 108.20 |
| 32 | BC | 344 | THR | CA-CB-CG2 | -5.76 | 104.33 | 112.40 |
| 78 | CA | 1719 | A | P-O3'-C3' | 5.76 | 126.62 | 119.70 |
| 81 | DA | 1608 | C | C1'-O4'-C4' | -5.76 | 105.29 | 109.90 |
| 78 | CA | 146 | U | C1'-O4'-C4' | -5.76 | 105.29 | 109.90 |
| 81 | DA | 1638 | A | C1'-O4'-C4' | -5.76 | 105.29 | 109.90 |
| 26 | AZ | 21 | VAL | C-N-CA | 5.76 | 136.10 | 121.70 |
| 78 | CA | 29 | U | C5'-C4'-O4' | 5.76 | 116.01 | 109.10 |
| 78 | CA | 1007 | C | N1-C1'-C2' | 5.76 | 121.49 | 114.00 |
| 78 | CA | 1148 | C | P-O3'-C3' | -5.76 | 112.79 | 119.70 |
| 78 | CA | 1711 | C | O4'-C1'-C2' | -5.76 | 100.04 | 105.80 |
| 81 | DA | 212 | G | O4'-C1'-C2' | -5.76 | 100.04 | 105.80 |
| 81 | DA | 2603 | G | P-O3'-C3' | -5.76 | 112.78 | 119.70 |
| 32 | BC | 17 | LEU | N-CA-CB | 5.76 | 121.92 | 110.40 |
| 78 | CA | 918 | U | P-O5'-C5' | 5.76 | 130.12 | 120.90 |
| 78 | CA | 1068 | C | C4'-C3'-C2' | -5.76 | 96.84 | 102.60 |
| 81 | DA | 2587 | U | P-O5'-C5' | -5.76 | 111.69 | 120.90 |
| 60 | Bi | 76 | TYR | CB-CG-CD1 | 5.76 | 124.45 | 121.00 |
| 78 | CA | 489 | C | N3-C4-C5 | -5.76 | 119.60 | 121.90 |
| 78 | CA | 1772 | C | C3'-C2'-C1' | 5.76 | 106.11 | 101.50 |
| 81 | DA | 664 | U | N1-C1'-C2' | 5.76 | 121.49 | 114.00 |
| 81 | DA | 1984 | C | C3'-C2'-C1' | 5.76 | 106.11 | 101.50 |
| 81 | DA | 2147 | A | O4'-C1'-N9 | 5.76 | 112.81 | 108.20 |
| 81 | DA | 2151 | C | P-O3'-C3' | -5.76 | 112.79 | 119.70 |
| 81 | DA | 2306 | C | N1-C1'-C2' | 5.76 | 121.48 | 114.00 |
| 81 | DA | 2446 | U | C5'-C4'-O4' | 5.76 | 116.01 | 109.10 |
| 35 | BG | 164 | SER | N-CA-CB | 5.76 | 119.14 | 110.50 |
| 43 | BP | 140 | LYS | N-CA-CB | 5.76 | 120.96 | 110.60 |
| 77 | BI | 174 | THR | N-CA-CB | 5.76 | 121.24 | 110.30 |
| 78 | CA | 337 | G | O4'-C1'-N9 | 5.76 | 112.80 | 108.20 |
| 78 | CA | 448 | C | C3'-C2'-C1' | 5.76 | 106.11 | 101.50 |
| 78 | CA | 728 | U | P-O5'-C5' | -5.76 | 111.69 | 120.90 |
| 78 | CA | 1203 | A | C1'-O4'-C4' | -5.76 | 105.29 | 109.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 1707 | A | O4'-C1'-N9 | 5.76 | 112.81 | 108.20 |
| 81 | DA | 1234 | G | C3'-C2'-C1' | -5.76 | 96.89 | 101.50 |
| 81 | DA | 2591 | A | O3'-P-O5' | -5.76 | 93.06 | 104.00 |
| 81 | DA | 3389 | U | C1'-O4'-C4' | 5.76 | 114.50 | 109.90 |
| 6 | AE | 174 | ARG | CA-CB-CG | 5.75 | 126.06 | 113.40 |
| 78 | CA | 1762 | A | C3'-C2'-C1' | 5.75 | 106.10 | 101.50 |
| 81 | DA | 1976 | G | C5'-C4'-O4' | -5.75 | 102.19 | 109.10 |
| 81 | DA | 2625 | C | C5'-C4'-C3' | -5.75 | 106.79 | 116.00 |
| 65 | Bn | 68 | SER | O-C-N | 5.75 | 131.91 | 122.70 |
| 78 | CA | 168 | A | O4'-C1'-N9 | 5.75 | 112.80 | 108.20 |
| 78 | CA | 257 | A | O3'-P-O5' | 5.75 | 114.93 | 104.00 |
| 78 | CA | 619 | A | P-O3'-C3' | 5.75 | 126.60 | 119.70 |
| 78 | CA | 1527 | C | O3'-P-O5' | -5.75 | 93.07 | 104.00 |
| 82 | DB | 149 | A | O4'-C1'-N9 | 5.75 | 112.80 | 108.20 |
| 14 | AM | 98 | TYR | CZ-CE2-CD2 | 5.75 | 124.98 | 119.80 |
| 17 | AQ | 70 | SER | N-CA-CB | 5.75 | 119.13 | 110.50 |
| 78 | CA | 235 | G | C5'-C4'-C3' | -5.75 | 106.80 | 116.00 |
| 79 | CB | 74 | C | C1'-O4'-C4' | 5.75 | 114.50 | 109.90 |
| 81 | DA | 1897 | G | O4'-C1'-N9 | 5.75 | 112.80 | 108.20 |
| 81 | DA | 2217 | U | P-O3'-C3' | -5.75 | 112.80 | 119.70 |
| 81 | DA | 2963 | C | C3'-C2'-C1' | 5.75 | 106.10 | 101.50 |
| 83 | DC | 47 | C | P-O5'-C5' | 5.75 | 130.10 | 120.90 |
| 76 | BS | 37 | VAL | CB-CA-C | -5.75 | 100.47 | 111.40 |
| 81 | DA | 163 | C | O4'-C1'-N1 | 5.75 | 112.80 | 108.20 |
| 81 | DA | 173 | G | N9-C1'-C2' | 5.75 | 121.47 | 114.00 |
| 81 | DA | 1552 | G | O4'-C1'-N9 | -5.75 | 103.60 | 108.20 |
| 81 | DA | 2391 | G | P-O3'-C3' | 5.75 | 126.60 | 119.70 |
| 81 | DA | 3222 | U | C5'-C4'-C3' | 5.75 | 125.20 | 116.00 |
| 12 | AK | 62 | LEU | N-CA-CB | 5.75 | 121.90 | 110.40 |
| 78 | CA | 907 | A | O4'-C1'-N9 | 5.75 | 112.80 | 108.20 |
| 81 | DA | 352 | A | C1'-O4'-C4' | 5.75 | 114.50 | 109.90 |
| 81 | DA | 2141 | U | N1-C1'-C2' | 5.75 | 121.47 | 114.00 |
| 81 | DA | 3328 | G | N9-C1'-C2' | -5.75 | 105.68 | 112.00 |
| 1 | Aa | 92 | TRP | CB-CG-CD2 | -5.75 | 119.13 | 126.60 |
| 25 | AY | 57 | MET | N-CA-C | 5.75 | 126.52 | 111.00 |
| 32 | BC | 16 | PHE | CB-CA-C | 5.75 | 121.89 | 110.40 |
| 32 | BC | 241 | LYS | C-N-CA | -5.75 | 107.33 | 121.70 |
| 39 | BJ | 73 | VAL | N-CA-C | -5.75 | 95.49 | 111.00 |
| 43 | BP | 78 | GLY | N-CA-C | -5.75 | 98.73 | 113.10 |
| 78 | CA | 1676 | U | O4'-C1'-N1 | 5.75 | 112.80 | 108.20 |
| 81 | DA | 1477 | A | C3'-C2'-C1' | 5.75 | 106.10 | 101.50 |
| 6 | AE | 74 | PRO | N-CA-C | 5.75 | 127.04 | 112.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | BH | 189 | LEU | N-CA-CB | 5.75 | 121.89 | 110.40 |
| 43 | BP | 73 | ARG | NE-CZ-NH2 | 5.75 | 123.17 | 120.30 |
| 78 | CA | 48 | G | C3'-C2'-C1' | 5.75 | 106.10 | 101.50 |
| 81 | DA | 185 | C | N1-C1'-C2' | 5.75 | 121.47 | 114.00 |
| 81 | DA | 668 | G | C1'-O4'-C4' | -5.75 | 105.30 | 109.90 |
| 25 | AY | 25 | VAL | C-N-CA | 5.74 | 136.06 | 121.70 |
| 78 | CA | 662 | U | N1-C1'-C2' | 5.74 | 121.47 | 114.00 |
| 78 | CA | 1189 | A | OP1-P-O3' | 5.74 | 117.83 | 105.20 |
| 78 | CA | 1419 | G | C1'-O4'-C4' | -5.74 | 105.31 | 109.90 |
| 81 | DA | 855 | U | C1'-O4'-C4' | -5.74 | 105.31 | 109.90 |
| 81 | DA | 881 | C | N1-C1'-C2' | 5.74 | 121.47 | 114.00 |
| 81 | DA | 3012 | A | O4'-C4'-C3' | -5.74 | 98.26 | 104.00 |
| 33 | BD | 89 | ALA | N-CA-C | -5.74 | 95.50 | 111.00 |
| 78 | CA | 1621 | U | P-O3'-C3' | -5.74 | 112.81 | 119.70 |
| 81 | DA | 1675 | G | C3'-C2'-C1' | -5.74 | 96.91 | 101.50 |
| 81 | DA | 1731 | A | O4'-C1'-N9 | 5.74 | 112.79 | 108.20 |
| 81 | DA | 2160 | G | O4'-C1'-C2' | 5.74 | 112.77 | 107.60 |
| 2 | AA | 46 | HIS | N-CA-C | -5.74 | 95.50 | 111.00 |
| 2 | AA | 119 | ARG | CD-NE-CZ | 5.74 | 131.64 | 123.60 |
| 30 | BA | 107 | TYR | CB-CG-CD2 | -5.74 | 117.56 | 121.00 |
| 76 | BS | 155 | TYR | CB-CG-CD2 | -5.74 | 117.56 | 121.00 |
| 78 | CA | 1149 | G | O4'-C1'-N9 | -5.74 | 103.61 | 108.20 |
| 78 | CA | 1633 | A | C5-C6-N6 | -5.74 | 119.11 | 123.70 |
| 81 | DA | 77 | A | C1'-O4'-C4' | -5.74 | 105.31 | 109.90 |
| 81 | DA | 543 | C | N1-C1'-C2' | 5.74 | 121.46 | 114.00 |
| 81 | DA | 2743 | A | P-O3'-C3' | 5.74 | 126.59 | 119.70 |
| 1 | Aa | 154 | VAL | N-CA-C | -5.74 | 95.50 | 111.00 |
| 38 | Bs | 22 | TYR | CB-CG-CD2 | 5.74 | 124.44 | 121.00 |
| 78 | CA | 1333 | C | C3'-C2'-C1' | 5.74 | 106.09 | 101.50 |
| 81 | DA | 424 | G | O3'-P-O5' | -5.74 | 93.10 | 104.00 |
| 81 | DA | 635 | G | C5'-C4'-O4' | 5.74 | 115.99 | 109.10 |
| 81 | DA | 671 | U | OP2-P-O3' | 5.74 | 117.82 | 105.20 |
| 81 | DA | 767 | U | C1'-O4'-C4' | 5.74 | 114.49 | 109.90 |
| 81 | DA | 2718 | U | O3'-P-O5' | -5.74 | 93.10 | 104.00 |
| 82 | DB | 46 | G | P-O3'-C3' | 5.74 | 126.59 | 119.70 |
| 83 | DC | 89 | A | O4'-C1'-N9 | 5.74 | 112.79 | 108.20 |
| 2 | AA | 208 | GLU | N-CA-C | -5.74 | 95.51 | 111.00 |
| 61 | Bj | 21 | ARG | N-CA-CB | 5.74 | 120.93 | 110.60 |
| 74 | BQ | 39 | GLN | C-N-CA | 5.74 | 136.04 | 121.70 |
| 81 | DA | 2032 | U | O4'-C1'-N1 | 5.74 | 112.79 | 108.20 |
| 81 | DA | 2190 | U | C3'-C2'-C1' | 5.74 | 106.09 | 101.50 |
| 18 | AP | 109 | VAL | CA-CB-CG2 | -5.74 | 102.30 | 110.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 32 | BC | 240 | ARG | N-CA-C | -5.74 | 95.51 | 111.00 |
| 52 | BY | 50 | ILE | CA-CB-CG1 | 5.74 | 121.90 | 111.00 |
| 81 | DA | 550 | A | O4'-C1'-C2' | -5.74 | 100.06 | 105.80 |
| 81 | DA | 1145 | G | C1'-O4'-C4' | -5.74 | 105.31 | 109.90 |
| 81 | DA | 2634 | U | C5'-C4'-O4' | 5.74 | 115.98 | 109.10 |
| 81 | DA | 2700 | G | O4'-C1'-C2' | 5.74 | 112.76 | 107.60 |
| 81 | DA | 2756 | C | C1'-O4'-C4' | -5.74 | 105.31 | 109.90 |
| 81 | DA | 2928 | C | O3'-P-O5' | 5.74 | 114.90 | 104.00 |
| 33 | BD | 346 | LYS | O-C-N | -5.73 | 113.53 | 122.70 |
| 76 | BS | 100 | THR | N-CA-CB | 5.73 | 121.19 | 110.30 |
| 81 | DA | 1137 | C | C3'-C2'-C1' | 5.73 | 106.09 | 101.50 |
| 81 | DA | 1189 | C | O4'-C1'-N1 | 5.73 | 112.79 | 108.20 |
| 81 | DA | 2536 | A | P-O3'-C3' | -5.73 | 112.82 | 119.70 |
| 81 | DA | 2671 | A | O3'-P-O5' | -5.73 | 93.11 | 104.00 |
| 30 | BA | 48 | ARG | NE-CZ-NH2 | -5.73 | 117.43 | 120.30 |
| 78 | CA | 10 | G | P-O3'-C3' | -5.73 | 112.82 | 119.70 |
| 81 | DA | 428 | A | C1'-O4'-C4' | -5.73 | 105.31 | 109.90 |
| 81 | DA | 1200 | A | C3'-C2'-C1' | 5.73 | 106.09 | 101.50 |
| 81 | DA | 3323 | A | O4'-C1'-N9 | 5.73 | 112.79 | 108.20 |
| 47 | BU | 8 | ARG | NE-CZ-NH1 | 5.73 | 123.17 | 120.30 |
| 78 | CA | 153 | G | C5'-C4'-C3' | 5.73 | 125.17 | 116.00 |
| 78 | CA | 485 | A | O4'-C1'-N9 | 5.73 | 112.78 | 108.20 |
| 81 | DA | 760 | G | O4'-C1'-C2' | 5.73 | 112.76 | 107.60 |
| 81 | DA | 2650 | U | P-O3'-C3' | 5.73 | 126.58 | 119.70 |
| 81 | DA | 2823 | G | P-O3'-C3' | -5.73 | 112.82 | 119.70 |
| 82 | DB | 98 | U | O4'-C4'-C3' | -5.73 | 98.27 | 104.00 |
| 20 | AS | 30 | VAL | CA-C-N | 5.73 | 133.14 | 117.10 |
| 61 | Bj | 93 | THR | N-CA-CB | 5.73 | 121.18 | 110.30 |
| 81 | DA | 2518 | C | C3'-C2'-C1' | 5.73 | 106.08 | 101.50 |
| 38 | Bs | 191 | TYR | CG-CD1-CE1 | -5.73 | 116.72 | 121.30 |
| 78 | CA | 568 | G | N3-C2-N2 | 5.73 | 123.91 | 119.90 |
| 78 | CA | 829 | A | O4'-C1'-N9 | 5.73 | 112.78 | 108.20 |
| 81 | DA | 2 | U | C1'-O4'-C4' | 5.73 | 114.48 | 109.90 |
| 81 | DA | 296 | A | C3'-C2'-C1' | 5.73 | 106.08 | 101.50 |
| 81 | DA | 771 | A | C3'-C2'-C1' | 5.73 | 106.08 | 101.50 |
| 81 | DA | 1741 | A | O4'-C1'-N9 | 5.73 | 112.78 | 108.20 |
| 81 | DA | 2159 | U | N1-C1'-C2' | -5.73 | 105.70 | 112.00 |
| 81 | DA | 3121 | U | C5'-C4'-C3' | 5.73 | 125.16 | 116.00 |
| 81 | DA | 3143 | C | C3'-C2'-C1' | 5.73 | 106.08 | 101.50 |
| 82 | DB | 85 | G | N9-C1'-C2' | -5.73 | 105.70 | 112.00 |
| 12 | AK | 62 | LEU | CB-CG-CD1 | 5.73 | 120.73 | 111.00 |
| 78 | CA | 264 | G | P-O5'-C5' | -5.73 | 111.74 | 120.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 333 | G | O4'-C1'-N9 | 5.73 | 112.78 | 108.20 |
| 81 | DA | 513 | G | N9-C1'-C2' | 5.73 | 121.44 | 114.00 |
| 81 | DA | 1684 | U | C3'-C2'-C1' | 5.73 | 106.08 | 101.50 |
| 81 | DA | 1786 | G | O4'-C1'-C2' | 5.73 | 112.75 | 107.60 |
| 6 | AE | 126 | ARG | N-CA-CB | -5.72 | 100.30 | 110.60 |
| 14 | AM | 119 | ILE | CB-CA-C | -5.72 | 100.15 | 111.60 |
| 78 | CA | 1462 | G | C4'-C3'-C2' | -5.72 | 96.88 | 102.60 |
| 81 | DA | 1528 | G | N9-C1'-C2' | -5.72 | 105.70 | 112.00 |
| 81 | DA | 1651 | U | O4'-C1'-C2' | -5.72 | 100.08 | 105.80 |
| 81 | DA | 1864 | A | O4'-C1'-C2' | -5.72 | 100.08 | 105.80 |
| 3 | AB | 99 | VAL | CA-CB-CG2 | 5.72 | 119.48 | 110.90 |
| 30 | BA | 188 | ASN | O-C-N | 5.72 | 131.86 | 122.70 |
| 78 | CA | 88 | U | C5'-C4'-C3' | -5.72 | 106.84 | 116.00 |
| 78 | CA | 1612 | U | C1'-O4'-C4' | 5.72 | 114.48 | 109.90 |
| 78 | CA | 1758 | U | O4'-C1'-N1 | 5.72 | 112.78 | 108.20 |
| 81 | DA | 796 | U | N1-C1'-C2' | 5.72 | 121.44 | 114.00 |
| 81 | DA | 1077 | U | O4'-C1'-C2' | -5.72 | 100.08 | 105.80 |
| 78 | CA | 232 | U | O5'-P-OP2 | -5.72 | 100.55 | 105.70 |
| 78 | CA | 1642 | G | C1'-O4'-C4' | 5.72 | 114.48 | 109.90 |
| 78 | CA | 1736 | G | O4'-C4'-C3' | -5.72 | 98.28 | 104.00 |
| 81 | DA | 320 | G | O4'-C1'-C2' | 5.72 | 112.75 | 107.60 |
| 81 | DA | 862 | U | N1-C1'-C2' | 5.72 | 121.44 | 114.00 |
| 81 | DA | 3057 | U | O4'-C1'-N1 | 5.72 | 112.78 | 108.20 |
| 83 | DC | 1 | G | C5'-C4'-C3' | 5.72 | 125.15 | 116.00 |
| 1 | Aa | 127 | ARG | NE-CZ-NH2 | -5.72 | 117.44 | 120.30 |
| 5 | AC | 158 | PHE | N-CA-CB | 5.72 | 120.89 | 110.60 |
| 22 | AV | 36 | ALA | N-CA-CB | 5.72 | 118.11 | 110.10 |
| 65 | Bn | 39 | ARG | C-N-CA | -5.72 | 107.40 | 121.70 |
| 77 | BI | 108 | ALA | N-CA-C | 5.72 | 126.44 | 111.00 |
| 81 | DA | 126 | U | C1'-O4'-C4' | 5.72 | 114.47 | 109.90 |
| 81 | DA | 623 | U | C2'-C3'-O3' | 5.72 | 122.85 | 113.70 |
| 81 | DA | 1193 | A | O4'-C1'-C2' | -5.72 | 100.08 | 105.80 |
| 81 | DA | 1244 | A | O4'-C1'-N9 | 5.72 | 112.78 | 108.20 |
| 81 | DA | 3354 | U | P-O3'-C3' | 5.72 | 126.56 | 119.70 |
| 82 | DB | 92 | A | C1'-O4'-C4' | -5.72 | 105.33 | 109.90 |
| 3 | AB | 199 | PRO | O-C-N | -5.72 | 113.55 | 122.70 |
| 81 | DA | 599 | C | C5'-C4'-O4' | 5.72 | 115.96 | 109.10 |
| 81 | DA | 2338 | C | C5'-C4'-C3' | 5.72 | 125.15 | 116.00 |
| 5 | AC | 116 | LEU | CB-CG-CD2 | 5.72 | 120.72 | 111.00 |
| 6 | AE | 213 | ALA | N-CA-CB | 5.72 | 118.10 | 110.10 |
| 74 | BQ | 208 | MET | CG-SD-CE | -5.72 | 91.06 | 100.20 |
| 76 | BS | 167 | THR | N-CA-CB | 5.72 | 121.16 | 110.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 229 | U | N1-C1'-C2' | 5.72 | 121.43 | 114.00 |
| 78 | CA | 774 | A | O5'-C5'-C4' | 5.72 | 122.56 | 111.70 |
| 81 | DA | 26 | A | N9-C1'-C2' | -5.72 | 105.71 | 112.00 |
| 81 | DA | 775 | A | O4'-C1'-C2' | 5.72 | 112.74 | 107.60 |
| 81 | DA | 1752 | A | P-O5'-C5' | -5.72 | 111.75 | 120.90 |
| 81 | DA | 3124 | G | O4'-C1'-N9 | 5.72 | 112.77 | 108.20 |
| 81 | DA | 3330 | A | C1'-O4'-C4' | -5.72 | 105.33 | 109.90 |
| 83 | DC | 50 | U | O3'-P-O5' | 5.72 | 114.86 | 104.00 |
| 20 | AS | 83 | ALA | N-CA-CB | 5.71 | 118.10 | 110.10 |
| 37 | BH | 236 | GLY | O-C-N | 5.71 | 131.84 | 122.70 |
| 46 | BT | 167 | ARG | NE-CZ-NH2 | 5.71 | 123.16 | 120.30 |
| 81 | DA | 17 | G | O4'-C1'-N9 | 5.71 | 112.77 | 108.20 |
| 81 | DA | 3002 | C | C5'-C4'-C3' | -5.71 | 106.86 | 116.00 |
| 2 | AA | 6 | THR | CA-C-N | 5.71 | 129.77 | 117.20 |
| 13 | AL | 105 | ALA | CB-CA-C | -5.71 | 101.53 | 110.10 |
| 49 | BV | 69 | ARG | NE-CZ-NH2 | -5.71 | 117.44 | 120.30 |
| 51 | BZ | 31 | PHE | CB-CG-CD2 | -5.71 | 116.80 | 120.80 |
| 65 | Bn | 52 | TYR | CB-CG-CD1 | 5.71 | 124.43 | 121.00 |
| 78 | CA | 9 | U | O4'-C1'-N1 | 5.71 | 112.77 | 108.20 |
| 78 | CA | 1340 | U | O4'-C1'-C2' | -5.71 | 100.09 | 105.80 |
| 78 | CA | 1341 | A | C1'-O4'-C4' | 5.71 | 114.47 | 109.90 |
| 81 | DA | 2418 | G | P-O3'-C3' | -5.71 | 112.84 | 119.70 |
| 13 | AL | 92 | CYS | O-C-N | 5.71 | 131.84 | 122.70 |
| 14 | AM | 120 | ARG | NE-CZ-NH2 | -5.71 | 117.44 | 120.30 |
| 16 | AO | 76 | LYS | CB-CA-C | -5.71 | 98.98 | 110.40 |
| 32 | BC | 183 | LEU | N-CA-CB | 5.71 | 121.82 | 110.40 |
| 42 | BM | 61 | THR | CA-CB-CG2 | -5.71 | 104.40 | 112.40 |
| 47 | BU | 24 | ALA | N-CA-CB | 5.71 | 118.10 | 110.10 |
| 74 | BQ | 289 | LYS | N-CA-CB | 5.71 | 120.88 | 110.60 |
| 76 | BS | 151 | PHE | CB-CG-CD1 | 5.71 | 124.80 | 120.80 |
| 81 | DA | 2575 | G | O4'-C1'-N9 | 5.71 | 112.77 | 108.20 |
| 81 | DA | 3313 | U | O5'-P-OP2 | -5.71 | 100.56 | 105.70 |
| 6 | AE | 175 | GLY | N-CA-C | -5.71 | 98.82 | 113.10 |
| 76 | BS | 72 | THR | CA-C-N | 5.71 | 129.76 | 117.20 |
| 78 | CA | 122 | U | N1-C1'-C2' | -5.71 | 105.72 | 112.00 |
| 81 | DA | 1565 | G | P-O5'-C5' | 5.71 | 130.04 | 120.90 |
| 81 | DA | 1819 | U | C5'-C4'-O4' | -5.71 | 102.25 | 109.10 |
| 81 | DA | 2486 | A | O4'-C1'-C2' | -5.71 | 100.09 | 105.80 |
| 81 | DA | 2858 | U | C1'-O4'-C4' | -5.71 | 105.33 | 109.90 |
| 81 | DA | 3043 | C | O4'-C1'-N1 | 5.71 | 112.77 | 108.20 |
| 33 | BD | 300 | ARG | NH1-CZ-NH2 | 5.71 | 125.68 | 119.40 |
| 81 | DA | 486 | U | P-O3'-C3' | -5.71 | 112.85 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 682 | U | O4'-C1'-N1 | 5.71 | 112.77 | 108.20 |
| 81 | DA | 848 | A | N9-C1'-C2' | 5.71 | 121.42 | 114.00 |
| 81 | DA | 2082 | U | O4'-C1'-N1 | 5.71 | 112.77 | 108.20 |
| 36 | BF | 104 | VAL | CA-CB-CG2 | -5.71 | 102.34 | 110.90 |
| 76 | BS | 69 | LYS | CA-C-N | 5.71 | 129.75 | 117.20 |
| 78 | CA | 1581 | C | C1'-O4'-C4' | -5.71 | 105.33 | 109.90 |
| 81 | DA | 1626 | U | N1-C1'-C2' | 5.71 | 121.42 | 114.00 |
| 81 | DA | 1895 | A | P-O3'-C3' | 5.71 | 126.55 | 119.70 |
| 81 | DA | 2938 | G | C3'-C2'-C1' | 5.71 | 106.07 | 101.50 |
| 50 | BX | 90 | ALA | N-CA-CB | 5.71 | 118.09 | 110.10 |
| 81 | DA | 329 | U | O5'-C5'-C4' | 5.71 | 122.54 | 111.70 |
| 8 | AF | 161 | ASP | CB-CA-C | -5.70 | 98.99 | 110.40 |
| 9 | AH | 80 | ASN | C-N-CA | 5.70 | 135.96 | 121.70 |
| 55 | Bc | 99 | GLN | N-CA-CB | 5.70 | 120.87 | 110.60 |
| 78 | CA | 1032 | G | C5'-C4'-C3' | 5.70 | 125.13 | 116.00 |
| 81 | DA | 1499 | C | C3'-C2'-C1' | 5.70 | 106.06 | 101.50 |
| 81 | DA | 2087 | C | P-O3'-C3' | -5.70 | 112.86 | 119.70 |
| 81 | DA | 2431 | C | O4'-C1'-C2' | -5.70 | 100.10 | 105.80 |
| 81 | DA | 2444 | C | O3'-P-O5' | 5.70 | 114.84 | 104.00 |
| 78 | CA | 648 | G | C1'-O4'-C4' | -5.70 | 105.34 | 109.90 |
| 78 | CA | 1745 | G | P-O3'-C3' | 5.70 | 126.54 | 119.70 |
| 81 | DA | 371 | G | O4'-C1'-N9 | 5.70 | 112.76 | 108.20 |
| 1 | Aa | 123 | ILE | N-CA-C | -5.70 | 95.61 | 111.00 |
| 14 | AM | 145 | ARG | NE-CZ-NH1 | 5.70 | 123.15 | 120.30 |
| 22 | AV | 90 | LYS | O-C-N | -5.70 | 110.27 | 121.10 |
| 42 | BM | 122 | CYS | CB-CA-C | -5.70 | 99.00 | 110.40 |
| 78 | CA | 956 | C | C3'-C2'-C1' | 5.70 | 106.06 | 101.50 |
| 81 | DA | 614 | C | O4'-C1'-N1 | 5.70 | 112.76 | 108.20 |
| 81 | DA | 2769 | A | C5'-C4'-C3' | -5.70 | 106.88 | 116.00 |
| 50 | BX | 111 | ASN | CA-CB-CG | -5.70 | 100.86 | 113.40 |
| 81 | DA | 1176 | C | O4'-C1'-N1 | 5.70 | 112.76 | 108.20 |
| 81 | DA | 1712 | G | C1'-O4'-C4' | -5.70 | 105.34 | 109.90 |
| 81 | DA | 2568 | C | O4'-C1'-N1 | 5.70 | 112.76 | 108.20 |
| 81 | DA | 2701 | U | O4'-C1'-N1 | 5.70 | 112.76 | 108.20 |
| 81 | DA | 3027 | A | C3'-C2'-C1' | 5.70 | 106.06 | 101.50 |
| 81 | DA | 1305 | U | O4'-C1'-N1 | 5.70 | 112.76 | 108.20 |
| 81 | DA | 2974 | U | O4'-C1'-N1 | 5.70 | 112.76 | 108.20 |
| 35 | BG | 82 | ARG | NE-CZ-NH2 | 5.70 | 123.15 | 120.30 |
| 78 | CA | 223 | U | C3'-C2'-C1' | 5.70 | 106.06 | 101.50 |
| 78 | CA | 1208 | A | O4'-C1'-C2' | 5.70 | 112.73 | 107.60 |
| 78 | CA | 1677 | C | O3'-P-O5' | 5.70 | 114.82 | 104.00 |
| 79 | CB | 12 | U | C5'-C4'-C3' | -5.70 | 106.89 | 116.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1061 | A | OP1-P-OP2 | -5.70 | 111.06 | 119.60 |
| 81 | DA | 1174 | G | N9-C1'-C2' | 5.70 | 121.41 | 114.00 |
| 78 | CA | 1566 | U | N1-C1'-C2' | -5.69 | 105.74 | 112.00 |
| 78 | CA | 1576 | A | N9-C1'-C2' | -5.69 | 105.74 | 112.00 |
| 81 | DA | 737 | G | C5'-C4'-C3' | 5.69 | 125.11 | 116.00 |
| 29 | AU | 88 | THR | N-CA-CB | 5.69 | 121.12 | 110.30 |
| 74 | BQ | 46 | THR | N-CA-C | -5.69 | 95.63 | 111.00 |
| 78 | CA | 585 | A | C3'-C2'-C1' | 5.69 | 106.05 | 101.50 |
| 78 | CA | 1500 | C | P-O3'-C3' | -5.69 | 112.87 | 119.70 |
| 81 | DA | 2683 | U | C4'-C3'-C2' | -5.69 | 96.91 | 102.60 |
| 82 | DB | 147 | U | O4'-C1'-N1 | 5.69 | 112.75 | 108.20 |
| 78 | CA | 1173 | C | O5'-C5'-C4' | 5.69 | 122.51 | 111.70 |
| 78 | CA | 1378 | U | C3'-C2'-C1' | 5.69 | 106.05 | 101.50 |
| 81 | DA | 894 | G | N9-C1'-C2' | -5.69 | 105.74 | 112.00 |
| 81 | DA | 1804 | A | O4'-C1'-N9 | 5.69 | 112.75 | 108.20 |
| 81 | DA | 2507 | C | O4'-C1'-N1 | 5.69 | 112.75 | 108.20 |
| 81 | DA | 2562 | A | C5-C6-N6 | -5.69 | 119.15 | 123.70 |
| 83 | DC | 36 | C | O4'-C1'-N1 | 5.69 | 112.75 | 108.20 |
| 9 | AH | 54 | ASP | CB-CG-OD2 | -5.69 | 113.18 | 118.30 |
| 11 | AJ | 26 | LEU | CB-CA-C | -5.69 | 99.39 | 110.20 |
| 35 | BG | 96 | VAL | CG1-CB-CG2 | 5.69 | 120.00 | 110.90 |
| 39 | BJ | 116 | MET | CG-SD-CE | 5.69 | 109.30 | 100.20 |
| 78 | CA | 1702 | A | C5'-C4'-O4' | -5.69 | 102.27 | 109.10 |
| 81 | DA | 166 | C | C5'-C4'-O4' | 5.69 | 115.93 | 109.10 |
| 81 | DA | 376 | G | N9-C1'-C2' | -5.69 | 105.74 | 112.00 |
| 81 | DA | 630 | A | P-O5'-C5' | 5.69 | 130.00 | 120.90 |
| 81 | DA | 1622 | U | OP1-P-O3' | 5.69 | 117.72 | 105.20 |
| 81 | DA | 2471 | U | O4'-C1'-C2' | -5.69 | 100.11 | 105.80 |
| 33 | BD | 351 | PRO | CA-N-CD | -5.69 | 103.54 | 111.50 |
| 45 | BR | 16 | ARG | NE-CZ-NH1 | 5.69 | 123.14 | 120.30 |
| 78 | CA | 592 | A | N9-C1'-C2' | -5.69 | 105.74 | 112.00 |
| 78 | CA | 1544 | U | C1'-O4'-C4' | -5.69 | 105.35 | 109.90 |
| 81 | DA | 160 | G | C5'-C4'-O4' | 5.69 | 115.93 | 109.10 |
| 81 | DA | 733 | G | O4'-C1'-N9 | 5.69 | 112.75 | 108.20 |
| 81 | DA | 964 | G | C1'-O4'-C4' | -5.69 | 105.35 | 109.90 |
| 81 | DA | 1574 | C | C3'-C2'-C1' | 5.69 | 106.05 | 101.50 |
| 81 | DA | 1739 | U | C3'-C2'-C1' | 5.69 | 106.05 | 101.50 |
| 81 | DA | 1794 | G | P-O5'-C5' | -5.69 | 111.80 | 120.90 |
| 81 | DA | 2638 | C | C3'-C2'-C1' | 5.69 | 106.05 | 101.50 |
| 81 | DA | 2659 | G | O4'-C1'-N9 | 5.69 | 112.75 | 108.20 |
| 81 | DA | 278 | U | O4'-C1'-C2' | -5.69 | 100.11 | 105.80 |
| 81 | DA | 2510 | U | C5'-C4'-O4' | 5.69 | 115.92 | 109.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 15 | AN | 47 | ALA | CA-C-N | 5.68 | 129.71 | 117.20 |
| 38 | Bs | 5 | ARG | NE-CZ-NH2 | -5.68 | 117.46 | 120.30 |
| 44 | BO | 62 | HIS | CB-CA-C | 5.68 | 121.77 | 110.40 |
| 48 | BW | 35 | LYS | N-CA-CB | 5.68 | 120.83 | 110.60 |
| 57 | Be | 71 | ALA | CB-CA-C | -5.68 | 101.57 | 110.10 |
| 62 | Bk | 82 | ARG | CB-CA-C | -5.68 | 99.03 | 110.40 |
| 78 | CA | 221 | A | O4'-C1'-C2' | -5.68 | 100.12 | 105.80 |
| 78 | CA | 927 | C | C3'-C2'-C1' | 5.68 | 106.05 | 101.50 |
| 78 | CA | 1640 | C | N3-C4-C5 | -5.68 | 119.63 | 121.90 |
| 78 | CA | 1784 | C | C3'-C2'-C1' | 5.68 | 106.05 | 101.50 |
| 81 | DA | 483 | G | O4'-C1'-N9 | 5.68 | 112.75 | 108.20 |
| 81 | DA | 762 | U | O4'-C1'-N1 | 5.68 | 112.75 | 108.20 |
| 81 | DA | 1689 | U | N1-C1'-C2' | -5.68 | 105.75 | 112.00 |
| 81 | DA | 1894 | U | O4'-C1'-C2' | -5.68 | 100.11 | 105.80 |
| 5 | AC | 12 | TYR | CB-CG-CD1 | 5.68 | 124.41 | 121.00 |
| 34 | BE | 164 | LYS | N-CA-CB | 5.68 | 120.83 | 110.60 |
| 35 | BG | 79 | VAL | CB-CA-C | -5.68 | 100.61 | 111.40 |
| 60 | Bi | 106 | LYS | C-N-CA | 5.68 | 135.91 | 121.70 |
| 78 | CA | 475 | A | C5'-C4'-C3' | -5.68 | 106.91 | 116.00 |
| 78 | CA | 1004 | U | O4'-C1'-N1 | 5.68 | 112.75 | 108.20 |
| 31 | BB | 97 | ASN | N-CA-C | -5.68 | 95.66 | 111.00 |
| 36 | BF | 184 | LYS | CB-CA-C | -5.68 | 99.04 | 110.40 |
| 3 | AB | 70 | THR | C-N-CA | 5.68 | 135.90 | 121.70 |
| 4 | AD | 103 | TYR | C-N-CA | 5.68 | 135.90 | 121.70 |
| 8 | AF | 30 | PRO | N-CA-C | 5.68 | 126.87 | 112.10 |
| 9 | AH | 106 | THR | CA-CB-CG2 | 5.68 | 120.35 | 112.40 |
| 34 | BE | 5 | ALA | N-CA-CB | 5.68 | 118.05 | 110.10 |
| 41 | BN | 13 | ARG | C-N-CA | 5.68 | 135.90 | 121.70 |
| 51 | BZ | 26 | SER | N-CA-CB | 5.68 | 119.02 | 110.50 |
| 76 | BS | 122 | CYS | CB-CA-C | -5.68 | 99.04 | 110.40 |
| 78 | CA | 616 | G | N9-C1'-C2' | 5.68 | 121.38 | 114.00 |
| 78 | CA | 821 | U | O4'-C1'-N1 | 5.68 | 112.74 | 108.20 |
| 78 | CA | 1150 | G | O4'-C1'-N9 | 5.68 | 112.74 | 108.20 |
| 81 | DA | 343 | U | O4'-C1'-N1 | 5.68 | 112.74 | 108.20 |
| 81 | DA | 638 | C | C4'-C3'-C2' | 5.68 | 108.28 | 102.60 |
| 81 | DA | 1704 | A | N9-C1'-C2' | -5.68 | 105.75 | 112.00 |
| 81 | DA | 2303 | A | P-O3'-C3' | -5.68 | 112.88 | 119.70 |
| 81 | DA | 2479 | C | O4'-C1'-C2' | 5.68 | 112.71 | 107.60 |
| 81 | DA | 2927 | C | P-O3'-C3' | -5.68 | 112.88 | 119.70 |
| 83 | DC | 68 | U | C3'-C2'-C1' | -5.68 | 96.96 | 101.50 |
| 2 | AA | 87 | LEU | CB-CA-C | -5.68 | 99.41 | 110.20 |
| 2 | AA | 250 | VAL | CA-CB-CG1 | -5.68 | 102.38 | 110.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 76 | BS | 123 | ILE | C-N-CA | 5.68 | 135.90 | 121.70 |
| 78 | CA | 162 | A | N9-C1'-C2' | 5.68 | 121.38 | 114.00 |
| 78 | CA | 901 | G | O4'-C1'-N9 | 5.68 | 112.74 | 108.20 |
| 81 | DA | 1755 | C | P-O5'-C5' | 5.68 | 129.98 | 120.90 |
| 81 | DA | 2316 | G | C4'-C3'-C2' | -5.68 | 96.92 | 102.60 |
| 26 | AZ | 46 | ASN | N-CA-CB | 5.68 | 120.82 | 110.60 |
| 53 | Ba | 20 | GLY | N-CA-C | 5.68 | 127.29 | 113.10 |
| 78 | CA | 169 | A | C5'-C4'-O4' | -5.68 | 102.29 | 109.10 |
| 78 | CA | 629 | U | C1'-O4'-C4' | -5.68 | 105.36 | 109.90 |
| 78 | CA | 1454 | G | C5'-C4'-O4' | 5.68 | 115.91 | 109.10 |
| 81 | DA | 1808 | G | C3'-C2'-C1' | 5.68 | 106.04 | 101.50 |
| 81 | DA | 2206 | G | O4'-C1'-N9 | 5.68 | 112.74 | 108.20 |
| 1 | Aa | 236 | ALA | N-CA-CB | 5.67 | 118.05 | 110.10 |
| 53 | Ba | 14 | VAL | N-CA-CB | 5.67 | 123.99 | 111.50 |
| 55 | Bc | 109 | ILE | N-CA-C | -5.67 | 95.68 | 111.00 |
| 73 | Bv | 7 | TYR | CB-CA-C | -5.67 | 99.05 | 110.40 |
| 78 | CA | 37 | U | C4'-C3'-C2' | -5.67 | 96.92 | 102.60 |
| 78 | CA | 1634 | C | N3-C4-C5 | -5.67 | 119.63 | 121.90 |
| 81 | DA | 529 | A | P-O3'-C3' | 5.67 | 126.51 | 119.70 |
| 81 | DA | 2494 | A | O4'-C4'-C3' | -5.67 | 98.33 | 104.00 |
| 82 | DB | 148 | G | P-O3'-C3' | 5.67 | 126.51 | 119.70 |
| 5 | AC | 17 | ARG | N-CA-C | -5.67 | 95.68 | 111.00 |
| 76 | BS | 81 | LEU | CA-CB-CG | 5.67 | 128.35 | 115.30 |
| 78 | CA | 441 | A | P-O3'-C3' | 5.67 | 126.51 | 119.70 |
| 16 | AO | 128 | TYR | CB-CG-CD2 | 5.67 | 124.40 | 121.00 |
| 32 | BC | 21 | ARG | N-CA-CB | 5.67 | 120.81 | 110.60 |
| 81 | DA | 990 | U | C3'-C2'-C1' | -5.67 | 96.96 | 101.50 |
| 81 | DA | 1564 | U | O3'-P-O5' | -5.67 | 93.22 | 104.00 |
| 81 | DA | 1639 | C | C3'-C2'-C1' | 5.67 | 106.04 | 101.50 |
| 81 | DA | 3346 | U | O3'-P-O5' | 5.67 | 114.78 | 104.00 |
| 10 | AI | 84 | ALA | C-N-CA | 5.67 | 135.88 | 121.70 |
| 78 | CA | 158 | U | N1-C1'-C2' | 5.67 | 121.37 | 114.00 |
| 78 | CA | 1197 | C | C3'-C2'-C1' | 5.67 | 106.04 | 101.50 |
| 83 | DC | 5 | G | C5'-C4'-O4' | 5.67 | 115.90 | 109.10 |
| 10 | AI | 124 | PRO | N-CA-CB | -5.67 | 96.36 | 102.60 |
| 11 | AJ | 15 | GLN | N-CA-C | -5.67 | 95.70 | 111.00 |
| 12 | AK | 121 | VAL | CA-C-O | -5.67 | 108.20 | 120.10 |
| 35 | BG | 146 | ILE | CA-CB-CG1 | 5.67 | 121.77 | 111.00 |
| 44 | BO | 58 | MET | CB-CA-C | -5.67 | 99.06 | 110.40 |
| 78 | CA | 153 | G | C3'-C2'-C1' | 5.67 | 106.03 | 101.50 |
| 78 | CA | 683 | C | P-O3'-C3' | -5.67 | 112.90 | 119.70 |
| 78 | CA | 1532 | U | P-O3'-C3' | -5.67 | 112.90 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 840 | C | P-O3'-C3' | 5.67 | 126.50 | 119.70 |
| 81 | DA | 1054 | A | C4'-C3'-C2' | -5.67 | 96.93 | 102.60 |
| 81 | DA | 1665 | C | C1'-O4'-C4' | -5.67 | 105.36 | 109.90 |
| 81 | DA | 2394 | G | O4'-C1'-N9 | 5.67 | 112.73 | 108.20 |
| 81 | DA | 2439 | A | C4'-C3'-C2' | -5.67 | 96.93 | 102.60 |
| 45 | BR | 157 | PRO | N-CA-CB | 5.67 | 110.10 | 103.30 |
| 58 | Bg | 69 | TYR | CB-CG-CD2 | 5.67 | 124.40 | 121.00 |
| 79 | CB | 8 | U | O4'-C1'-N1 | 5.67 | 112.73 | 108.20 |
| 81 | DA | 174 | C | O4'-C1'-N1 | 5.67 | 112.73 | 108.20 |
| 82 | DB | 30 | C | O4'-C1'-N1 | 5.67 | 112.73 | 108.20 |
| 31 | BB | 19 | HIS | CB-CA-C | 5.67 | 121.73 | 110.40 |
| 32 | BC | 272 | TYR | CB-CG-CD1 | 5.67 | 124.40 | 121.00 |
| 78 | CA | 1061 | A | C4-C5-C6 | 5.67 | 119.83 | 117.00 |
| 78 | CA | 1462 | G | N9-C1'-C2' | -5.67 | 105.77 | 112.00 |
| 81 | DA | 523 | A | C1'-O4'-C4' | 5.67 | 114.43 | 109.90 |
| 16 | AO | 41 | ALA | N-CA-C | -5.66 | 95.71 | 111.00 |
| 18 | AP | 108 | PRO | CA-N-CD | -5.66 | 103.57 | 111.50 |
| 20 | AS | 79 | LEU | C-N-CA | 5.66 | 135.86 | 121.70 |
| 37 | BH | 177 | TYR | CB-CG-CD2 | -5.66 | 117.60 | 121.00 |
| 78 | CA | 1273 | G | O4'-C1'-N9 | 5.66 | 112.73 | 108.20 |
| 81 | DA | 158 | G | P-O5'-C5' | -5.66 | 111.84 | 120.90 |
| 81 | DA | 1823 | A | O3'-P-O5' | -5.66 | 93.24 | 104.00 |
| 81 | DA | 3116 | G | O4'-C1'-N9 | 5.66 | 112.73 | 108.20 |
| 82 | DB | 33 | A | O3'-P-O5' | -5.66 | 93.24 | 104.00 |
| 41 | BN | 3 | THR | CA-CB-CG2 | 5.66 | 120.33 | 112.40 |
| 3 | AB | 212 | LYS | C-N-CA | -5.66 | 107.55 | 121.70 |
| 14 | AM | 91 | ASP | CB-CG-OD2 | 5.66 | 123.39 | 118.30 |
| 29 | AU | 87 | PRO | C-N-CA | 5.66 | 135.85 | 121.70 |
| 50 | BX | 111 | ASN | CB-CA-C | -5.66 | 99.08 | 110.40 |
| 53 | Ba | 9 | LYS | CA-C-N | 5.66 | 129.65 | 117.20 |
| 78 | CA | 288 | A | C3'-C2'-C1' | 5.66 | 106.03 | 101.50 |
| 81 | DA | 676 | G | O4'-C1'-N9 | 5.66 | 112.73 | 108.20 |
| 81 | DA | 2307 | G | N9-C1'-C2' | -5.66 | 105.77 | 112.00 |
| 81 | DA | 2647 | A | P-O5'-C5' | -5.66 | 111.84 | 120.90 |
| 40 | BK | 5 | PRO | CA-N-CD | -5.66 | 103.58 | 111.50 |
| 47 | BU | 18 | ASP | CB-CG-OD2 | -5.66 | 113.21 | 118.30 |
| 78 | CA | 100 | A | O4'-C1'-C2' | -5.66 | 100.14 | 105.80 |
| 78 | CA | 384 | G | O4'-C1'-N9 | 5.66 | 112.73 | 108.20 |
| 78 | CA | 652 | G | C5'-C4'-C3' | 5.66 | 125.05 | 116.00 |
| 78 | CA | 1441 | C | C3'-C2'-C1' | 5.66 | 106.03 | 101.50 |
| 81 | DA | 341 | G | C2'-C3'-O3' | 5.66 | 122.75 | 113.70 |
| 81 | DA | 1667 | A | P-O3'-C3' | 5.66 | 126.49 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2468 | A | C2'-C3'-O3' | 5.66 | 122.75 | 113.70 |
| 81 | DA | 3039 | C | N1-C1'-C2' | 5.66 | 121.36 | 114.00 |
| 12 | AK | 25 | ASP | CB-CG-OD1 | 5.66 | 123.39 | 118.30 |
| 42 | BM | 62 | VAL | CA-CB-CG1 | -5.66 | 102.42 | 110.90 |
| 81 | DA | 131 | C | O4'-C1'-C2' | -5.66 | 100.14 | 105.80 |
| 81 | DA | 912 | G | O4'-C1'-C2' | 5.66 | 112.69 | 107.60 |
| 10 | AI | 142 | TYR | CA-CB-CG | 5.66 | 124.14 | 113.40 |
| 78 | CA | 39 | A | C1'-O4'-C4' | -5.66 | 105.38 | 109.90 |
| 78 | CA | 272 | U | C4'-C3'-C2' | -5.66 | 96.94 | 102.60 |
| 78 | CA | 407 | A | N9-C1'-C2' | -5.66 | 105.78 | 112.00 |
| 79 | CB | 72 | G | C1'-O4'-C4' | 5.66 | 114.42 | 109.90 |
| 81 | DA | 861 | C | O4'-C1'-N1 | 5.66 | 112.72 | 108.20 |
| 81 | DA | 1664 | G | C3'-C2'-C1' | -5.66 | 96.98 | 101.50 |
| 81 | DA | 2101 | C | C1'-O4'-C4' | -5.66 | 105.38 | 109.90 |
| 83 | DC | 52 | U | C4'-C3'-C2' | -5.66 | 96.94 | 102.60 |
| 74 | BQ | 23 | ARG | NE-CZ-NH2 | 5.65 | 123.13 | 120.30 |
| 78 | CA | 152 | U | C4'-C3'-C2' | -5.65 | 96.95 | 102.60 |
| 81 | DA | 240 | U | O4'-C1'-C2' | -5.65 | 100.15 | 105.80 |
| 81 | DA | 248 | U | P-O3'-C3' | 5.65 | 126.48 | 119.70 |
| 1 | Aa | 226 | ALA | CB-CA-C | -5.65 | 101.62 | 110.10 |
| 34 | BE | 110 | ILE | CA-CB-CG1 | 5.65 | 121.74 | 111.00 |
| 40 | BK | 18 | ARG | NE-CZ-NH2 | 5.65 | 123.13 | 120.30 |
| 78 | CA | 943 | C | C1'-O4'-C4' | -5.65 | 105.38 | 109.90 |
| 81 | DA | 462 | C | P-O5'-C5' | 5.65 | 129.94 | 120.90 |
| 81 | DA | 638 | C | O5'-C5'-C4' | 5.65 | 122.44 | 111.70 |
| 81 | DA | 3211 | C | P-O3'-C3' | 5.65 | 126.48 | 119.70 |
| 13 | AL | 22 | ASN | N-CA-CB | 5.65 | 120.77 | 110.60 |
| 24 | AX | 52 | THR | CA-CB-CG2 | -5.65 | 104.49 | 112.40 |
| 39 | BJ | 80 | LEU | N-CA-CB | 5.65 | 121.70 | 110.40 |
| 46 | BT | 111 | ASP | CB-CG-OD2 | -5.65 | 113.22 | 118.30 |
| 50 | BX | 34 | LEU | CA-C-O | -5.65 | 108.23 | 120.10 |
| 53 | Ba | 15 | ARG | N-CA-CB | 5.65 | 120.77 | 110.60 |
| 62 | Bk | 36 | ARG | NE-CZ-NH2 | -5.65 | 117.47 | 120.30 |
| 76 | BS | 67 | PHE | CB-CG-CD2 | -5.65 | 116.84 | 120.80 |
| 78 | CA | 1332 | C | C3'-C2'-C1' | 5.65 | 106.02 | 101.50 |
| 81 | DA | 2737 | C | O4'-C1'-C2' | -5.65 | 100.15 | 105.80 |
| 81 | DA | 3354 | U | O4'-C1'-C2' | -5.65 | 100.15 | 105.80 |
| 30 | BA | 84 | ALA | N-CA-CB | 5.65 | 118.01 | 110.10 |
| 81 | DA | 2828 | G | P-O3'-C3' | -5.65 | 112.92 | 119.70 |
| 77 | BI | 98 | ARG | NE-CZ-NH2 | -5.65 | 117.48 | 120.30 |
| 78 | CA | 223 | U | C5'-C4'-C3' | 5.65 | 125.04 | 116.00 |
| 78 | CA | 1062 | A | C5-C6-N6 | -5.65 | 119.18 | 123.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 797 | U | O3'-P-O5' | -5.65 | 93.27 | 104.00 |
| 81 | DA | 912 | G | C1'-O4'-C4' | -5.65 | 105.38 | 109.90 |
| 81 | DA | 1662 | G | O4'-C1'-N9 | 5.65 | 112.72 | 108.20 |
| 81 | DA | 2084 | C | O4'-C1'-C2' | -5.65 | 100.15 | 105.80 |
| 81 | DA | 2193 | U | P-O3'-C3' | -5.65 | 112.92 | 119.70 |
| 33 | BD | 329 | PRO | C-N-CA | 5.65 | 135.82 | 121.70 |
| 81 | DA | 363 | G | C3'-C2'-C1' | -5.65 | 96.98 | 101.50 |
| 81 | DA | 430 | U | O4'-C1'-N1 | 5.65 | 112.72 | 108.20 |
| 81 | DA | 570 | A | P-O3'-C3' | 5.65 | 126.47 | 119.70 |
| 81 | DA | 2447 | A | O4'-C1'-N9 | 5.65 | 112.72 | 108.20 |
| 81 | DA | 2639 | G | O4'-C1'-N9 | 5.65 | 112.72 | 108.20 |
| 81 | DA | 3081 | C | C4'-C3'-C2' | -5.65 | 96.95 | 102.60 |
| 81 | DA | 3382 | U | C1'-O4'-C4' | -5.65 | 105.38 | 109.90 |
| 82 | DB | 86 | U | O4'-C1'-C2' | -5.65 | 100.15 | 105.80 |
| 26 | AZ | 43 | ARG | NE-CZ-NH2 | -5.64 | 117.48 | 120.30 |
| 37 | BH | 123 | GLN | N-CA-C | 5.64 | 126.24 | 111.00 |
| 40 | BK | 130 | LYS | C-N-CA | -5.64 | 98.30 | 122.00 |
| 81 | DA | 183 | G | O4'-C1'-N9 | 5.64 | 112.72 | 108.20 |
| 81 | DA | 460 | C | C3'-C2'-C1' | 5.64 | 106.02 | 101.50 |
| 81 | DA | 1872 | C | C5'-C4'-C3' | 5.64 | 125.03 | 116.00 |
| 5 | AC | 184 | SER | N-CA-CB | 5.64 | 118.96 | 110.50 |
| 12 | AK | 58 | TYR | C-N-CA | 5.64 | 135.81 | 121.70 |
| 31 | BB | 242 | ARG | NE-CZ-NH1 | 5.64 | 123.12 | 120.30 |
| 76 | BS | 51 | LYS | C-N-CA | 5.64 | 135.81 | 121.70 |
| 78 | CA | 1359 | C | O4'-C1'-C2' | -5.64 | 100.16 | 105.80 |
| 81 | DA | 1746 | U | O3'-P-O5' | -5.64 | 93.28 | 104.00 |
| 81 | DA | 2098 | C | O4'-C1'-N1 | 5.64 | 112.71 | 108.20 |
| 81 | DA | 2162 | U | P-O5'-C5' | 5.64 | 129.93 | 120.90 |
| 35 | BG | 10 | TYR | CB-CG-CD1 | -5.64 | 117.61 | 121.00 |
| 78 | CA | 439 | U | O4'-C1'-C2' | -5.64 | 100.16 | 105.80 |
| 78 | CA | 838 | G | N9-C1'-C2' | -5.64 | 105.80 | 112.00 |
| 78 | CA | 1732 | A | O4'-C1'-N9 | 5.64 | 112.71 | 108.20 |
| 22 | AV | 81 | ARG | NE-CZ-NH1 | 5.64 | 123.12 | 120.30 |
| 46 | BT | 181 | ARG | NE-CZ-NH1 | 5.64 | 123.12 | 120.30 |
| 69 | Br | 43 | TYR | CB-CG-CD1 | 5.64 | 124.38 | 121.00 |
| 78 | CA | 1598 | U | O4'-C1'-N1 | -5.64 | 103.69 | 108.20 |
| 81 | DA | 1040 | A | O4'-C1'-C2' | -5.64 | 100.16 | 105.80 |
| 81 | DA | 1205 | A | P-O3'-C3' | 5.64 | 126.47 | 119.70 |
| 81 | DA | 1544 | G | O4'-C1'-N9 | 5.64 | 112.71 | 108.20 |
| 81 | DA | 2994 | A | N9-C1'-C2' | -5.64 | 105.80 | 112.00 |
| 81 | DA | 3248 | C | O4'-C1'-C2' | -5.64 | 100.16 | 105.80 |
| 81 | DA | 1127 | G | C3'-C2'-C1' | -5.64 | 96.99 | 101.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1168 | U | O4'-C1'-C2' | -5.64 | 100.16 | 105.80 |
| 81 | DA | 1392 | G | P-O5'-C5' | -5.64 | 111.88 | 120.90 |
| 81 | DA | 2331 | C | N1-C1'-C2' | 5.64 | 121.33 | 114.00 |
| 1 | Aa | 178 | VAL | N-CA-C | -5.64 | 95.78 | 111.00 |
| 31 | BB | 193 | ARG | NE-CZ-NH2 | -5.64 | 117.48 | 120.30 |
| 37 | BH | 123 | GLN | C-N-CA | 5.64 | 135.79 | 121.70 |
| 49 | BV | 78 | VAL | N-CA-C | -5.64 | 95.78 | 111.00 |
| 78 | CA | 565 | C | P-O3'-C3' | 5.64 | 126.46 | 119.70 |
| 81 | DA | 329 | U | C2'-C3'-O3' | 5.64 | 122.72 | 113.70 |
| 81 | DA | 1108 | U | O4'-C1'-N1 | 5.64 | 112.71 | 108.20 |
| 81 | DA | 2033 | G | O4'-C1'-N9 | 5.64 | 112.71 | 108.20 |
| 10 | AI | 57 | LEU | C-N-CA | 5.63 | 135.79 | 121.70 |
| 43 | BP | 101 | THR | CA-CB-CG2 | -5.63 | 104.51 | 112.40 |
| 44 | BO | 60 | TYR | CG-CD1-CE1 | -5.63 | 116.79 | 121.30 |
| 78 | CA | 367 | A | O3'-P-O5' | 5.63 | 114.71 | 104.00 |
| 78 | CA | 1586 | A | OP1-P-O3' | -5.63 | 92.80 | 105.20 |
| 81 | DA | 711 | A | O4'-C1'-N9 | 5.63 | 112.71 | 108.20 |
| 81 | DA | 964 | G | C3'-C2'-C1' | -5.63 | 96.99 | 101.50 |
| 81 | DA | 1592 | G | C1'-O4'-C4' | -5.63 | 105.39 | 109.90 |
| 81 | DA | 1637 | A | N9-C1'-C2' | 5.63 | 121.33 | 114.00 |
| 81 | DA | 2620 | G | P-O5'-C5' | 5.63 | 129.91 | 120.90 |
| 3 | AB | 27 | ARG | NE-CZ-NH2 | 5.63 | 123.12 | 120.30 |
| 10 | AI | 107 | LYS | N-CA-C | -5.63 | 95.79 | 111.00 |
| 13 | AL | 119 | GLY | N-CA-C | -5.63 | 99.02 | 113.10 |
| 81 | DA | 420 | G | C1'-O4'-C4' | 5.63 | 114.41 | 109.90 |
| 81 | DA | 1211 | U | N1-C1'-C2' | 5.63 | 121.32 | 114.00 |
| 81 | DA | 1693 | C | O4'-C4'-C3' | -5.63 | 98.37 | 104.00 |
| 81 | DA | 1754 | G | C5'-C4'-O4' | -5.63 | 102.34 | 109.10 |
| 81 | DA | 2072 | G | N9-C1'-C2' | -5.63 | 105.80 | 112.00 |
| 11 | AJ | 28 | SER | N-CA-CB | 5.63 | 118.95 | 110.50 |
| 36 | BF | 97 | PHE | CB-CG-CD2 | -5.63 | 116.86 | 120.80 |
| 78 | CA | 679 | U | O4'-C1'-C2' | -5.63 | 100.17 | 105.80 |
| 45 | BR | 153 | PHE | CB-CG-CD2 | -5.63 | 116.86 | 120.80 |
| 78 | CA | 979 | A | O4'-C1'-C2' | -5.63 | 100.17 | 105.80 |
| 81 | DA | 836 | A | P-O3'-C3' | -5.63 | 112.94 | 119.70 |
| 81 | DA | 1571 | A | O3'-P-O5' | 5.63 | 114.70 | 104.00 |
| 81 | DA | 1590 | G | N9-C1'-C2' | 5.63 | 121.32 | 114.00 |
| 81 | DA | 3054 | U | O4'-C1'-N1 | 5.63 | 112.70 | 108.20 |
| 35 | BG | 1 | MET | C-N-CA | 5.63 | 135.77 | 121.70 |
| 78 | CA | 282 | C | C3'-C2'-C1' | 5.63 | 106.00 | 101.50 |
| 78 | CA | 296 | U | P-O5'-C5' | -5.63 | 111.89 | 120.90 |
| 81 | DA | 981 | U | P-O3'-C3' | -5.63 | 112.95 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1525 | G | C3'-C2'-C1' | 5.63 | 106.00 | 101.50 |
| 81 | DA | 1585 | C | C3'-C2'-C1' | 5.63 | 106.00 | 101.50 |
| 81 | DA | 2716 | U | O4'-C1'-N1 | 5.63 | 112.70 | 108.20 |
| 81 | DA | 3115 | C | C3'-C2'-C1' | 5.63 | 106.00 | 101.50 |
| 21 | AT | 58 | TYR | CB-CA-C | 5.63 | 121.65 | 110.40 |
| 78 | CA | 1677 | C | C4'-C3'-C2' | -5.63 | 96.97 | 102.60 |
| 81 | DA | 171 | G | O4'-C4'-C3' | -5.63 | 98.37 | 104.00 |
| 81 | DA | 386 | A | O4'-C1'-C2' | -5.63 | 100.17 | 105.80 |
| 81 | DA | 2138 | A | N9-C1'-C2' | -5.63 | 105.81 | 112.00 |
| 26 | AZ | 10 | ARG | NE-CZ-NH2 | -5.62 | 117.49 | 120.30 |
| 33 | BD | 322 | GLN | CA-C-N | 5.62 | 129.58 | 117.20 |
| 78 | CA | 723 | G | P-O3'-C3' | -5.62 | 112.95 | 119.70 |
| 78 | CA | 1215 | C | C3'-C2'-C1' | 5.62 | 106.00 | 101.50 |
| 78 | CA | 1250 | U | P-O5'-C5' | -5.62 | 111.90 | 120.90 |
| 81 | DA | 1733 | G | O4'-C1'-N9 | 5.62 | 112.70 | 108.20 |
| 81 | DA | 3285 | C | P-O3'-C3' | -5.62 | 112.95 | 119.70 |
| 1 | Aa | 246 | SER | CB-CA-C | 5.62 | 120.78 | 110.10 |
| 4 | AD | 136 | VAL | CG1-CB-CG2 | 5.62 | 119.90 | 110.90 |
| 6 | AE | 81 | MET | CA-CB-CG | 5.62 | 122.86 | 113.30 |
| 31 | BB | 21 | ARG | NE-CZ-NH2 | -5.62 | 117.49 | 120.30 |
| 33 | BD | 348 | GLY | N-CA-C | 5.62 | 127.16 | 113.10 |
| 44 | BO | 95 | SER | N-CA-CB | 5.62 | 118.93 | 110.50 |
| 53 | Ba | 82 | PRO | CA-N-CD | -5.62 | 103.63 | 111.50 |
| 72 | Bu | 61 | PHE | N-CA-CB | 5.62 | 120.72 | 110.60 |
| 78 | CA | 506 | A | O4'-C1'-N9 | 5.62 | 112.70 | 108.20 |
| 78 | CA | 588 | U | OP1-P-OP2 | 5.62 | 128.04 | 119.60 |
| 81 | DA | 184 | U | O4'-C1'-N1 | 5.62 | 112.70 | 108.20 |
| 81 | DA | 1559 | A | P-O3'-C3' | 5.62 | 126.45 | 119.70 |
| 81 | DA | 1718 | G | N9-C1'-C2' | 5.62 | 121.31 | 114.00 |
| 81 | DA | 1770 | G | N3-C2-N2 | 5.62 | 123.84 | 119.90 |
| 81 | DA | 2182 | A | N9-C1'-C2' | 5.62 | 121.31 | 114.00 |
| 81 | DA | 2523 | A | C5'-C4'-C3' | -5.62 | 107.00 | 116.00 |
| 81 | DA | 3086 | A | O4'-C1'-N9 | 5.62 | 112.70 | 108.20 |
| 11 | AJ | 102 | ARG | NE-CZ-NH2 | -5.62 | 117.49 | 120.30 |
| 15 | AN | 45 | GLU | C-N-CA | 5.62 | 135.75 | 121.70 |
| 33 | BD | 351 | PRO | C-N-CA | -5.62 | 107.64 | 121.70 |
| 62 | Bk | 53 | TYR | CB-CA-C | 5.62 | 121.64 | 110.40 |
| 78 | CA | 364 | G | C1'-O4'-C4' | -5.62 | 105.40 | 109.90 |
| 81 | DA | 231 | G | P-O5'-C5' | 5.62 | 129.90 | 120.90 |
| 81 | DA | 1101 | G | C5'-C4'-O4' | 5.62 | 115.85 | 109.10 |
| 81 | DA | 2066 | C | O4'-C1'-N1 | 5.62 | 112.70 | 108.20 |
| 81 | DA | 2131 | A | N9-C1'-C2' | 5.62 | 121.31 | 114.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2296 | A | N9-C1'-C2' | -5.62 | 105.82 | 112.00 |
| 81 | DA | 2762 | A | O4'-C1'-N9 | 5.62 | 112.70 | 108.20 |
| 78 | CA | 1419 | G | N9-C1'-C2' | 5.62 | 121.31 | 114.00 |
| 1 | Aa | 142 | ALA | N-CA-CB | 5.62 | 117.97 | 110.10 |
| 35 | BG | 48 | ARG | NE-CZ-NH1 | 5.62 | 123.11 | 120.30 |
| 39 | BJ | 17 | ALA | N-CA-CB | 5.62 | 117.97 | 110.10 |
| 52 | BY | 75 | ARG | NE-CZ-NH1 | 5.62 | 123.11 | 120.30 |
| 68 | Bq | 18 | ARG | N-CA-CB | -5.62 | 100.49 | 110.60 |
| 81 | DA | 1327 | C | N1-C1'-C2' | 5.62 | 121.30 | 114.00 |
| 81 | DA | 1831 | U | C3'-C2'-C1' | 5.62 | 105.99 | 101.50 |
| 81 | DA | 1896 | A | C1'-O4'-C4' | -5.62 | 105.41 | 109.90 |
| 81 | DA | 3052 | G | C3'-C2'-C1' | 5.62 | 105.99 | 101.50 |
| 81 | DA | 3120 | C | O4'-C1'-C2' | -5.62 | 100.18 | 105.80 |
| 83 | DC | 30 | G | C1'-O4'-C4' | -5.62 | 105.41 | 109.90 |
| 33 | BD | 325 | LEU | C-N-CA | 5.62 | 135.74 | 121.70 |
| 78 | CA | 1409 | G | C3'-C2'-C1' | 5.62 | 105.99 | 101.50 |
| 81 | DA | 735 | A | O4'-C1'-N9 | 5.62 | 112.69 | 108.20 |
| 81 | DA | 2674 | A | C3'-C2'-C1' | -5.62 | 97.01 | 101.50 |
| 37 | BH | 226 | TYR | CB-CG-CD2 | 5.62 | 124.37 | 121.00 |
| 53 | Ba | 49 | TYR | CA-C-N | 5.62 | 132.83 | 117.10 |
| 81 | DA | 2196 | C | C5'-C4'-C3' | -5.62 | 107.02 | 116.00 |
| 81 | DA | 2759 | U | C3'-C2'-C1' | 5.62 | 105.99 | 101.50 |
| 9 | AH | 28 | ARG | NE-CZ-NH1 | 5.61 | 123.11 | 120.30 |
| 14 | AM | 132 | ARG | N-CA-CB | 5.61 | 120.70 | 110.60 |
| 21 | AT | 59 | VAL | O-C-N | -5.61 | 113.72 | 122.70 |
| 55 | Bc | 108 | GLN | CA-C-N | 5.61 | 129.55 | 117.20 |
| 78 | CA | 1478 | G | O5'-P-OP2 | 5.61 | 117.44 | 110.70 |
| 81 | DA | 730 | C | N3-C4-N4 | 5.61 | 121.93 | 118.00 |
| 81 | DA | 1756 | C | N3-C4-C5 | -5.61 | 119.66 | 121.90 |
| 81 | DA | 2563 | G | O4'-C4'-C3' | -5.61 | 98.39 | 104.00 |
| 35 | BG | 169 | ASP | CB-CG-OD1 | -5.61 | 113.25 | 118.30 |
| 81 | DA | 1201 | C | N1-C1'-C2' | 5.61 | 121.30 | 114.00 |
| 73 | Bw | 7 | TYR | CB-CA-C | -5.61 | 99.18 | 110.40 |
| 78 | CA | 1290 | U | P-O3'-C3' | 5.61 | 126.43 | 119.70 |
| 81 | DA | 2206 | G | C2'-C3'-O3' | 5.61 | 122.68 | 113.70 |
| 81 | DA | 2908 | G | O4'-C1'-C2' | 5.61 | 112.65 | 107.60 |
| 81 | DA | 2925 | C | N1-C1'-C2' | 5.61 | 121.29 | 114.00 |
| 35 | BG | 145 | LEU | N-CA-CB | 5.61 | 121.62 | 110.40 |
| 47 | BU | 17 | ARG | NE-CZ-NH1 | -5.61 | 117.50 | 120.30 |
| 78 | CA | 102 | U | O4'-C1'-N1 | 5.61 | 112.69 | 108.20 |
| 78 | CA | 634 | G | C3'-C2'-C1' | -5.61 | 97.01 | 101.50 |
| 81 | DA | 1163 | A | O4'-C1'-N9 | 5.61 | 112.69 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1297 | C | O3'-P-O5' | -5.61 | 93.34 | 104.00 |
| 81 | DA | 1883 | A | C1'-O4'-C4' | 5.61 | 114.39 | 109.90 |
| 16 | AO | 135 | LEU | CA-C-N | 5.61 | 132.80 | 117.10 |
| 64 | Bl | 39 | TYR | CB-CA-C | 5.61 | 121.61 | 110.40 |
| 78 | CA | 1225 | U | O4'-C1'-C2' | -5.61 | 100.19 | 105.80 |
| 78 | CA | 1244 | A | C1'-O4'-C4' | -5.61 | 105.41 | 109.90 |
| 78 | CA | 1440 | C | C5'-C4'-C3' | -5.61 | 107.03 | 116.00 |
| 78 | CA | 1700 | C | O4'-C1'-C2' | -5.61 | 100.19 | 105.80 |
| 81 | DA | 1227 | C | C3'-C2'-C1' | 5.61 | 105.99 | 101.50 |
| 81 | DA | 2781 | U | O3'-P-O5' | 5.61 | 114.65 | 104.00 |
| 5 | AC | 161 | THR | N-CA-C | -5.61 | 95.87 | 111.00 |
| 5 | AC | 191 | ALA | N-CA-C | 5.61 | 126.14 | 111.00 |
| 19 | AR | 62 | ALA | C-N-CA | 5.61 | 135.72 | 121.70 |
| 81 | DA | 527 | A | C3'-C2'-C1' | 5.61 | 105.98 | 101.50 |
| 81 | DA | 803 | C | C5'-C4'-O4' | -5.61 | 102.37 | 109.10 |
| 81 | DA | 3312 | U | C5'-C4'-O4' | 5.61 | 115.83 | 109.10 |
| 78 | CA | 1408 | G | O4'-C4'-C3' | 5.60 | 110.58 | 106.10 |
| 81 | DA | 1847 | A | C1'-O4'-C4' | 5.60 | 114.38 | 109.90 |
| 82 | DB | 46 | G | O4'-C1'-C2' | 5.60 | 112.64 | 107.60 |
| 58 | Bg | 95 | PRO | CA-N-CD | -5.60 | 103.66 | 111.50 |
| 77 | BI | 154 | ARG | NE-CZ-NH1 | 5.60 | 123.10 | 120.30 |
| 78 | CA | 994 | G | O4'-C1'-C2' | 5.60 | 112.64 | 107.60 |
| 78 | CA | 1409 | G | P-O5'-C5' | 5.60 | 129.87 | 120.90 |
| 81 | DA | 1297 | C | C3'-C2'-C1' | 5.60 | 105.98 | 101.50 |
| 81 | DA | 2034 | C | O4'-C1'-N1 | 5.60 | 112.68 | 108.20 |
| 81 | DA | 2629 | U | C5'-C4'-O4' | -5.60 | 102.38 | 109.10 |
| 81 | DA | 3098 | G | P-O5'-C5' | -5.60 | 111.94 | 120.90 |
| 83 | DC | 82 | A | C5'-C4'-C3' | -5.60 | 107.04 | 116.00 |
| 35 | BG | 58 | LEU | CB-CG-CD1 | 5.60 | 120.52 | 111.00 |
| 46 | BT | 64 | ARG | CB-CA-C | -5.60 | 99.20 | 110.40 |
| 53 | Ba | 65 | ARG | CB-CA-C | -5.60 | 99.20 | 110.40 |
| 61 | Bj | 85 | PHE | O-C-N | 5.60 | 131.66 | 122.70 |
| 78 | CA | 435 | C | O3'-P-O5' | 5.60 | 114.64 | 104.00 |
| 78 | CA | 487 | G | O4'-C1'-N9 | 5.60 | 112.68 | 108.20 |
| 78 | CA | 1447 | C | C1'-O4'-C4' | 5.60 | 114.38 | 109.90 |
| 78 | CA | 1505 | A | O4'-C1'-N9 | 5.60 | 112.68 | 108.20 |
| 78 | CA | 1639 | C | N3-C4-C5 | -5.60 | 119.66 | 121.90 |
| 81 | DA | 338 | A | C5'-C4'-C3' | -5.60 | 107.04 | 116.00 |
| 81 | DA | 740 | G | N1-C2-N3 | -5.60 | 120.54 | 123.90 |
| 81 | DA | 1408 | G | C4'-C3'-C2' | -5.60 | 97.00 | 102.60 |
| 81 | DA | 1458 | U | P-O3'-C3' | -5.60 | 112.98 | 119.70 |
| 81 | DA | 2319 | U | C5'-C4'-C3' | 5.60 | 124.96 | 116.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 3324 | C | P-O3'-C3' | 5.60 | 126.42 | 119.70 |
| 6 | AE | 128 | GLY | N-CA-C | -5.60 | 99.11 | 113.10 |
| 64 | Bl | 78 | PHE | CB-CG-CD1 | 5.60 | 124.72 | 120.80 |
| 78 | CA | 922 | G | N9-C1'-C2' | 5.60 | 121.28 | 114.00 |
| 78 | CA | 1507 | G | N1-C2-N3 | -5.60 | 120.54 | 123.90 |
| 79 | CB | 64 | G | C1'-O4'-C4' | -5.60 | 105.42 | 109.90 |
| 64 | Bl | 67 | LEU | C-N-CA | 5.60 | 135.69 | 121.70 |
| 72 | Bt | 60 | ASN | C-N-CA | -5.60 | 107.71 | 121.70 |
| 78 | CA | 1390 | U | C5'-C4'-C3' | 5.60 | 124.95 | 116.00 |
| 81 | DA | 3359 | A | O4'-C1'-N9 | 5.60 | 112.68 | 108.20 |
| 53 | Ba | 10 | VAL | CG1-CB-CG2 | -5.59 | 101.95 | 110.90 |
| 55 | Bc | 49 | LYS | CB-CA-C | -5.59 | 99.21 | 110.40 |
| 78 | CA | 164 | A | C5'-C4'-C3' | -5.59 | 107.05 | 116.00 |
| 78 | CA | 1380 | U | O4'-C1'-N1 | 5.59 | 112.68 | 108.20 |
| 78 | CA | 1633 | A | O4'-C1'-N9 | 5.59 | 112.68 | 108.20 |
| 81 | DA | 262 | U | C4'-C3'-C2' | -5.59 | 97.00 | 102.60 |
| 81 | DA | 685 | G | O4'-C1'-N9 | 5.59 | 112.68 | 108.20 |
| 81 | DA | 1050 | U | N1-C1'-C2' | -5.59 | 105.85 | 112.00 |
| 81 | DA | 2188 | A | O4'-C1'-N9 | 5.59 | 112.67 | 108.20 |
| 81 | DA | 2508 | U | C1'-O4'-C4' | 5.59 | 114.38 | 109.90 |
| 32 | BC | 26 | ARG | CD-NE-CZ | -5.59 | 115.77 | 123.60 |
| 8 | AF | 70 | VAL | N-CA-C | -5.59 | 95.90 | 111.00 |
| 32 | BC | 137 | TYR | CZ-CE2-CD2 | 5.59 | 124.83 | 119.80 |
| 34 | BE | 51 | ARG | CA-C-N | -5.59 | 104.90 | 117.20 |
| 78 | CA | 112 | A | C3'-C2'-C1' | 5.59 | 105.97 | 101.50 |
| 81 | DA | 677 | A | OP2-P-O3' | -5.59 | 92.90 | 105.20 |
| 81 | DA | 1267 | U | C1'-O4'-C4' | 5.59 | 114.37 | 109.90 |
| 81 | DA | 1894 | U | O4'-C1'-N1 | 5.59 | 112.67 | 108.20 |
| 81 | DA | 2459 | A | C1'-O4'-C4' | -5.59 | 105.43 | 109.90 |
| 81 | DA | 3298 | C | O4'-C4'-C3' | -5.59 | 98.41 | 104.00 |
| 82 | DB | 149 | A | C5'-C4'-C3' | 5.59 | 124.95 | 116.00 |
| 83 | DC | 25 | G | C4'-C3'-C2' | -5.59 | 97.01 | 102.60 |
| 32 | BC | 311 | PHE | N-CA-CB | 5.59 | 120.66 | 110.60 |
| 35 | BG | 111 | LEU | O-C-N | -5.59 | 113.76 | 122.70 |
| 46 | BT | 130 | ASN | N-CA-CB | 5.59 | 120.66 | 110.60 |
| 56 | Bf | 85 | PHE | CA-CB-CG | 5.59 | 127.31 | 113.90 |
| 78 | CA | 101 | U | N1-C1'-C2' | 5.59 | 121.27 | 114.00 |
| 81 | DA | 1971 | C | O4'-C4'-C3' | -5.59 | 98.41 | 104.00 |
| 81 | DA | 2794 | G | C1'-O4'-C4' | -5.59 | 105.43 | 109.90 |
| 81 | DA | 3244 | A | P-O5'-C5' | -5.59 | 111.96 | 120.90 |
| 43 | BP | 41 | ARG | NE-CZ-NH1 | 5.59 | 123.09 | 120.30 |
| 52 | BY | 114 | ASP | CB-CA-C | 5.59 | 121.58 | 110.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 415 | C | O4'-C1'-C2' | -5.59 | 100.21 | 105.80 |
| 78 | CA | 1724 | U | C2'-C3'-O3' | -5.59 | 97.21 | 109.50 |
| 81 | DA | 2623 | G | P-O3'-C3' | 5.59 | 126.41 | 119.70 |
| 81 | DA | 2788 | C | O4'-C1'-C2' | -5.59 | 100.21 | 105.80 |
| 81 | DA | 3223 | A | O4'-C1'-C2' | -5.59 | 100.21 | 105.80 |
| 32 | BC | 347 | SER | N-CA-CB | 5.59 | 118.88 | 110.50 |
| 45 | BR | 32 | LEU | CB-CG-CD2 | 5.59 | 120.50 | 111.00 |
| 60 | Bi | 68 | THR | N-CA-C | 5.59 | 126.08 | 111.00 |
| 78 | CA | 179 | A | N9-C1'-C2' | -5.59 | 105.86 | 112.00 |
| 81 | DA | 1093 | A | O4'-C1'-N9 | 5.59 | 112.67 | 108.20 |
| 81 | DA | 1357 | G | O3'-P-O5' | 5.59 | 114.61 | 104.00 |
| 81 | DA | 1500 | G | C4'-C3'-C2' | -5.59 | 97.01 | 102.60 |
| 81 | DA | 109 | A | C1'-O4'-C4' | -5.58 | 105.43 | 109.90 |
| 81 | DA | 2629 | U | C4'-C3'-C2' | -5.58 | 97.02 | 102.60 |
| 77 | BI | 106 | ALA | N-CA-CB | -5.58 | 102.28 | 110.10 |
| 78 | CA | 1238 | A | O4'-C1'-C2' | -5.58 | 100.22 | 105.80 |
| 81 | DA | 1924 | U | C3'-C2'-C1' | 5.58 | 105.97 | 101.50 |
| 81 | DA | 2311 | G | C3'-C2'-C1' | 5.58 | 105.97 | 101.50 |
| 81 | DA | 2315 | G | N9-C1'-C2' | 5.58 | 121.26 | 114.00 |
| 81 | DA | 2960 | C | N1-C1'-C2' | 5.58 | 121.26 | 114.00 |
| 32 | BC | 131 | THR | CB-CA-C | 5.58 | 126.67 | 111.60 |
| 55 | Bc | 10 | ARG | NE-CZ-NH1 | 5.58 | 123.09 | 120.30 |
| 74 | BQ | 24 | ARG | NE-CZ-NH1 | -5.58 | 117.51 | 120.30 |
| 81 | DA | 533 | A | N9-C1'-C2' | -5.58 | 105.86 | 112.00 |
| 81 | DA | 1180 | A | P-O5'-C5' | -5.58 | 111.97 | 120.90 |
| 81 | DA | 1268 | G | N9-C1'-C2' | 5.58 | 121.26 | 114.00 |
| 81 | DA | 1758 | G | C2'-C3'-O3' | 5.58 | 122.63 | 113.70 |
| 81 | DA | 1800 | A | N9-C1'-C2' | -5.58 | 105.86 | 112.00 |
| 81 | DA | 2127 | U | O4'-C1'-N1 | 5.58 | 112.67 | 108.20 |
| 81 | DA | 2539 | C | N3-C4-N4 | 5.58 | 121.91 | 118.00 |
| 83 | DC | 107 | G | P-O3'-C3' | -5.58 | 113.00 | 119.70 |
| 38 | Bs | 64 | ARG | NE-CZ-NH1 | 5.58 | 123.09 | 120.30 |
| 78 | CA | 930 | A | P-O3'-C3' | -5.58 | 113.00 | 119.70 |
| 81 | DA | 1597 | C | O4'-C1'-C2' | -5.58 | 100.22 | 105.80 |
| 81 | DA | 1711 | C | C1'-O4'-C4' | -5.58 | 105.44 | 109.90 |
| 81 | DA | 3333 | G | N9-C1'-C2' | 5.58 | 121.25 | 114.00 |
| 34 | BE | 61 | ARG | NE-CZ-NH2 | -5.58 | 117.51 | 120.30 |
| 45 | BR | 16 | ARG | NE-CZ-NH2 | -5.58 | 117.51 | 120.30 |
| 78 | CA | 687 | G | O4'-C1'-C2' | -5.58 | 100.22 | 105.80 |
| 78 | CA | 769 | A | P-O3'-C3' | 5.58 | 126.39 | 119.70 |
| 78 | CA | 1022 | C | O4'-C1'-N1 | -5.58 | 103.74 | 108.20 |
| 78 | CA | 1545 | A | C5'-C4'-C3' | -5.58 | 107.08 | 116.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 520 | U | O4'-C4'-C3' | -5.58 | 98.42 | 104.00 |
| 81 | DA | 582 | G | C5'-C4'-O4' | 5.58 | 115.80 | 109.10 |
| 81 | DA | 730 | C | C6-N1-C2 | -5.58 | 118.07 | 120.30 |
| 81 | DA | 1597 | C | O3'-P-O5' | 5.58 | 114.60 | 104.00 |
| 38 | Bs | 33 | VAL | CB-CA-C | -5.58 | 100.80 | 111.40 |
| 53 | Ba | 19 | ALA | C-N-CA | 5.58 | 134.01 | 122.30 |
| 78 | CA | 251 | A | P-O3'-C3' | 5.58 | 126.39 | 119.70 |
| 16 | AO | 124 | ARG | CD-NE-CZ | 5.58 | 131.41 | 123.60 |
| 35 | BG | 65 | ILE | N-CA-CB | -5.58 | 97.98 | 110.80 |
| 41 | BN | 70 | PHE | N-CA-CB | 5.58 | 120.64 | 110.60 |
| 78 | CA | 1554 | U | C1'-O4'-C4' | 5.58 | 114.36 | 109.90 |
| 80 | CC | 19 | U | O4'-C1'-N1 | 5.58 | 112.66 | 108.20 |
| 81 | DA | 693 | A | N9-C1'-C2' | -5.58 | 105.87 | 112.00 |
| 81 | DA | 1962 | G | O3'-P-O5' | 5.58 | 114.59 | 104.00 |
| 81 | DA | 2844 | C | P-O3'-C3' | 5.58 | 126.39 | 119.70 |
| 81 | DA | 2951 | G | O4'-C1'-C2' | -5.58 | 100.22 | 105.80 |
| 82 | DB | 111 | A | P-O3'-C3' | -5.58 | 113.01 | 119.70 |
| 22 | AV | 59 | TYR | CB-CG-CD1 | -5.57 | 117.66 | 121.00 |
| 31 | BB | 34 | TYR | N-CA-CB | 5.57 | 120.63 | 110.60 |
| 44 | BO | 10 | LYS | N-CA-C | 5.57 | 126.05 | 111.00 |
| 78 | CA | 57 | G | C3'-C2'-C1' | -5.57 | 97.04 | 101.50 |
| 78 | CA | 960 | U | C3'-C2'-C1' | 5.57 | 105.96 | 101.50 |
| 78 | CA | 992 | A | C5'-C4'-C3' | -5.57 | 107.08 | 116.00 |
| 78 | CA | 1337 | A | O4'-C1'-C2' | -5.57 | 100.23 | 105.80 |
| 81 | DA | 1931 | U | O4'-C1'-N1 | 5.57 | 112.66 | 108.20 |
| 81 | DA | 2114 | C | C3'-C2'-C1' | -5.57 | 97.04 | 101.50 |
| 78 | CA | 182 | A | C4'-C3'-C2' | -5.57 | 97.03 | 102.60 |
| 78 | CA | 1549 | C | N1-C1'-C2' | 5.57 | 121.24 | 114.00 |
| 78 | CA | 1558 | U | O5'-C5'-C4' | 5.57 | 122.29 | 111.70 |
| 81 | DA | 2266 | U | O4'-C1'-N1 | 5.57 | 112.66 | 108.20 |
| 81 | DA | 2857 | C | C1'-O4'-C4' | -5.57 | 105.44 | 109.90 |
| 81 | DA | 2972 | G | O4'-C1'-N9 | 5.57 | 112.66 | 108.20 |
| 2 | AA | 4 | PRO | O-C-N | -5.57 | 113.79 | 122.70 |
| 18 | AP | 99 | ARG | CB-CA-C | 5.57 | 121.54 | 110.40 |
| 24 | AX | 66 | PRO | CA-C-N | 5.57 | 129.46 | 117.20 |
| 35 | BG | 140 | VAL | C-N-CA | 5.57 | 135.63 | 121.70 |
| 38 | Bs | 28 | VAL | C-N-CA | 5.57 | 134.00 | 122.30 |
| 40 | BK | 47 | PHE | CG-CD1-CE1 | -5.57 | 114.67 | 120.80 |
| 41 | BN | 117 | ARG | NE-CZ-NH2 | -5.57 | 117.51 | 120.30 |
| 81 | DA | 306 | A | C4'-C3'-C2' | -5.57 | 97.03 | 102.60 |
| 81 | DA | 3010 | U | O3'-P-O5' | 5.57 | 114.58 | 104.00 |
| 78 | CA | 178 | U | C1'-O4'-C4' | 5.57 | 114.36 | 109.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 50 | BX | 45 | LYS | CB-CA-C | -5.57 | 99.26 | 110.40 |
| 76 | BS | 52 | LYS | N-CA-CB | -5.57 | 100.58 | 110.60 |
| 81 | DA | 639 | G | C4'-C3'-C2' | -5.57 | 97.03 | 102.60 |
| 81 | DA | 750 | G | O4'-C4'-C3' | -5.57 | 98.43 | 104.00 |
| 81 | DA | 1582 | C | O3'-P-O5' | -5.57 | 93.42 | 104.00 |
| 78 | CA | 419 | G | N9-C1'-C2' | -5.57 | 105.88 | 112.00 |
| 81 | DA | 320 | G | C3'-C2'-C1' | -5.57 | 97.05 | 101.50 |
| 81 | DA | 1144 | U | O4'-C1'-N1 | -5.57 | 103.75 | 108.20 |
| 81 | DA | 1175 | C | O3'-P-O5' | 5.57 | 114.57 | 104.00 |
| 81 | DA | 1674 | G | O4'-C4'-C3' | -5.57 | 98.44 | 104.00 |
| 81 | DA | 2342 | U | O4'-C1'-N1 | 5.57 | 112.65 | 108.20 |
| 81 | DA | 2698 | G | O3'-P-O5' | 5.57 | 114.57 | 104.00 |
| 26 | AZ | 29 | LYS | N-CA-CB | 5.56 | 120.62 | 110.60 |
| 74 | BQ | 10 | SER | N-CA-CB | 5.56 | 118.85 | 110.50 |
| 74 | BQ | 142 | PHE | C-N-CA | 5.56 | 135.61 | 121.70 |
| 78 | CA | 1595 | U | O4'-C4'-C3' | 5.56 | 110.55 | 106.10 |
| 81 | DA | 2840 | C | C1'-O4'-C4' | 5.56 | 114.35 | 109.90 |
| 82 | DB | 19 | C | O4'-C1'-N1 | 5.56 | 112.65 | 108.20 |
| 82 | DB | 129 | C | O4'-C1'-C2' | -5.56 | 100.24 | 105.80 |
| 83 | DC | 59 | G | O4'-C1'-N9 | 5.56 | 112.65 | 108.20 |
| 1 | Aa | 47 | LEU | CB-CA-C | -5.56 | 99.63 | 110.20 |
| 1 | Aa | 245 | PHE | CB-CG-CD2 | -5.56 | 116.91 | 120.80 |
| 21 | AT | 85 | TYR | CG-CD2-CE2 | -5.56 | 116.85 | 121.30 |
| 78 | CA | 310 | C | N1-C1'-C2' | 5.56 | 121.23 | 114.00 |
| 78 | CA | 1226 | A | O4'-C1'-N9 | 5.56 | 112.65 | 108.20 |
| 78 | CA | 1609 | U | C5'-C4'-C3' | -5.56 | 107.10 | 116.00 |
| 79 | CB | 49 | G | O4'-C1'-N9 | 5.56 | 112.65 | 108.20 |
| 81 | DA | 1863 | G | C3'-C2'-C1' | 5.56 | 105.95 | 101.50 |
| 21 | AT | 12 | TYR | N-CA-CB | -5.56 | 100.59 | 110.60 |
| 59 | Bh | 71 | HIS | CB-CA-C | -5.56 | 99.28 | 110.40 |
| 78 | CA | 306 | U | C5'-C4'-C3' | -5.56 | 107.10 | 116.00 |
| 81 | DA | 552 | G | C5'-C4'-O4' | 5.56 | 115.77 | 109.10 |
| 81 | DA | 1013 | G | P-O3'-C3' | -5.56 | 113.03 | 119.70 |
| 81 | DA | 1382 | G | P-O5'-C5' | 5.56 | 129.79 | 120.90 |
| 81 | DA | 2332 | A | N9-C1'-C2' | 5.56 | 121.23 | 114.00 |
| 81 | DA | 2528 | G | O4'-C4'-C3' | -5.56 | 98.44 | 104.00 |
| 82 | DB | 127 | U | O4'-C1'-N1 | 5.56 | 112.65 | 108.20 |
| 83 | DC | 61 | U | C1'-O4'-C4' | 5.56 | 114.35 | 109.90 |
| 2 | AA | 242 | TRP | CE2-CD2-CG | -5.56 | 102.85 | 107.30 |
| 13 | AL | 39 | LYS | CG-CD-CE | 5.56 | 128.57 | 111.90 |
| 32 | BC | 290 | ASP | N-CA-C | -5.56 | 95.99 | 111.00 |
| 57 | Be | 224 | ILE | CG1-CB-CG2 | 5.56 | 123.63 | 111.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 73 | Bv | 16 | THR | CB-CA-C | -5.56 | 96.59 | 111.60 |
| 78 | CA | 242 | U | P-O3'-C3' | 5.56 | 126.37 | 119.70 |
| 81 | DA | 1145 | G | N9-C1'-C2' | 5.56 | 121.23 | 114.00 |
| 81 | DA | 1331 | U | C3'-C2'-C1' | 5.56 | 105.94 | 101.50 |
| 81 | DA | 1623 | G | N9-C1'-C2' | 5.56 | 121.22 | 114.00 |
| 81 | DA | 1941 | C | O3'-P-O5' | -5.56 | 93.44 | 104.00 |
| 81 | DA | 1973 | G | O5'-C5'-C4' | 5.56 | 122.26 | 111.70 |
| 81 | DA | 2422 | C | C5'-C4'-C3' | -5.56 | 107.11 | 116.00 |
| 81 | DA | 2427 | U | O4'-C1'-N1 | 5.56 | 112.64 | 108.20 |
| 62 | Bk | 97 | SER | N-CA-CB | 5.56 | 118.83 | 110.50 |
| 67 | Bp | 27 | LEU | CB-CA-C | 5.56 | 120.76 | 110.20 |
| 78 | CA | 1669 | U | P-O3'-C3' | 5.56 | 126.37 | 119.70 |
| 81 | DA | 599 | C | P-O3'-C3' | 5.56 | 126.37 | 119.70 |
| 12 | AK | 58 | TYR | CB-CG-CD2 | -5.55 | 117.67 | 121.00 |
| 16 | AO | 140 | LYS | N-CA-CB | 5.55 | 120.60 | 110.60 |
| 31 | BB | 50 | HIS | CA-CB-CG | -5.55 | 104.16 | 113.60 |
| 60 | Bi | 46 | ASP | N-CA-C | 5.55 | 126.00 | 111.00 |
| 81 | DA | 173 | G | O4'-C4'-C3' | -5.55 | 98.44 | 104.00 |
| 81 | DA | 1039 | U | C1'-O4'-C4' | 5.55 | 114.34 | 109.90 |
| 81 | DA | 2244 | A | C3'-C2'-C1' | -5.55 | 97.06 | 101.50 |
| 81 | DA | 980 | A | P-O3'-C3' | -5.55 | 113.04 | 119.70 |
| 81 | DA | 1415 | U | N1-C1'-C2' | 5.55 | 121.22 | 114.00 |
| 41 | BN | 43 | LYS | CB-CA-C | 5.55 | 121.50 | 110.40 |
| 56 | Bf | 94 | GLU | OE1-CD-OE2 | 5.55 | 129.96 | 123.30 |
| 76 | BS | 45 | TYR | CG-CD2-CE2 | 5.55 | 125.74 | 121.30 |
| 78 | CA | 1136 | U | N1-C1'-C2' | -5.55 | 105.89 | 112.00 |
| 81 | DA | 547 | G | P-O5'-C5' | -5.55 | 112.02 | 120.90 |
| 81 | DA | 1409 | G | P-O3'-C3' | 5.55 | 126.36 | 119.70 |
| 81 | DA | 1787 | A | C3'-C2'-C1' | 5.55 | 105.94 | 101.50 |
| 81 | DA | 2777 | G | C3'-C2'-C1' | 5.55 | 105.94 | 101.50 |
| 81 | DA | 2898 | G | P-O5'-C5' | 5.55 | 129.78 | 120.90 |
| 19 | AR | 120 | SER | N-CA-CB | 5.55 | 118.83 | 110.50 |
| 53 | Ba | 75 | VAL | CA-CB-CG1 | -5.55 | 102.58 | 110.90 |
| 81 | DA | 713 | U | N1-C1'-C2' | 5.55 | 121.21 | 114.00 |
| 81 | DA | 3018 | C | N1-C1'-C2' | 5.55 | 121.21 | 114.00 |
| 81 | DA | 3252 | G | O3'-P-O5' | -5.55 | 93.45 | 104.00 |
| 45 | BR | 16 | ARG | CA-CB-CG | 5.55 | 125.61 | 113.40 |
| 50 | BX | 63 | ILE | N-CA-C | -5.55 | 96.02 | 111.00 |
| 78 | CA | 844 | A | C4-C5-C6 | 5.55 | 119.77 | 117.00 |
| 78 | CA | 1239 | U | P-O3'-C3' | 5.55 | 126.36 | 119.70 |
| 81 | DA | 2063 | U | O4'-C1'-N1 | 5.55 | 112.64 | 108.20 |
| 18 | AP | 74 | THR | OG1-CB-CG2 | 5.55 | 122.76 | 110.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | AX | 70 | LYS | CB-CA-C | -5.55 | 99.31 | 110.40 |
| 52 | BY | 73 | VAL | N-CA-C | -5.55 | 96.02 | 111.00 |
| 61 | Bj | 5 | HIS | N-CA-C | -5.55 | 96.03 | 111.00 |
| 78 | CA | 340 | U | C5'-C4'-O4' | 5.55 | 115.76 | 109.10 |
| 78 | CA | 1274 | C | N3-C4-C5 | -5.55 | 119.68 | 121.90 |
| 78 | CA | 1463 | C | O3'-P-O5' | -5.55 | 93.46 | 104.00 |
| 81 | DA | 176 | G | O4'-C1'-N9 | 5.55 | 112.64 | 108.20 |
| 81 | DA | 216 | G | O4'-C1'-C2' | 5.55 | 112.59 | 107.60 |
| 81 | DA | 230 | U | O3'-P-O5' | 5.55 | 114.54 | 104.00 |
| 81 | DA | 1478 | C | N1-C1'-C2' | 5.55 | 121.21 | 114.00 |
| 81 | DA | 2153 | U | P-O3'-C3' | 5.55 | 126.36 | 119.70 |
| 81 | DA | 3257 | C | C3'-C2'-C1' | 5.55 | 105.94 | 101.50 |
| 78 | CA | 600 | U | P-O3'-C3' | 5.54 | 126.35 | 119.70 |
| 81 | DA | 648 | C | C3'-C2'-C1' | 5.54 | 105.94 | 101.50 |
| 14 | AM | 53 | ASP | CB-CG-OD2 | 5.54 | 123.29 | 118.30 |
| 76 | BS | 138 | ARG | C-N-CA | -5.54 | 107.84 | 121.70 |
| 78 | CA | 1047 | G | P-O3'-C3' | 5.54 | 126.35 | 119.70 |
| 78 | CA | 1284 | C | O5'-P-OP2 | -5.54 | 100.71 | 105.70 |
| 81 | DA | 635 | G | O3'-P-O5' | 5.54 | 114.53 | 104.00 |
| 81 | DA | 938 | C | O3'-P-O5' | -5.54 | 93.47 | 104.00 |
| 81 | DA | 1381 | A | P-O3'-C3' | -5.54 | 113.05 | 119.70 |
| 81 | DA | 1990 | U | O4'-C1'-N1 | 5.54 | 112.64 | 108.20 |
| 1 | Aa | 61 | PHE | CB-CA-C | -5.54 | 99.32 | 110.40 |
| 39 | BJ | 88 | PRO | CA-C-N | 5.54 | 132.61 | 117.10 |
| 47 | BU | 38 | ASP | CB-CG-OD2 | -5.54 | 113.31 | 118.30 |
| 78 | CA | 256 | A | C3'-C2'-C1' | 5.54 | 105.93 | 101.50 |
| 78 | CA | 913 | G | C5'-C4'-O4' | -5.54 | 102.45 | 109.10 |
| 81 | DA | 182 | U | C3'-C2'-C1' | -5.54 | 97.07 | 101.50 |
| 81 | DA | 1478 | C | C3'-C2'-C1' | 5.54 | 105.93 | 101.50 |
| 81 | DA | 3344 | A | P-O3'-C3' | 5.54 | 126.35 | 119.70 |
| 82 | DB | 65 | A | N9-C1'-C2' | 5.54 | 121.20 | 114.00 |
| 4 | AD | 96 | ASN | CB-CA-C | 5.54 | 121.47 | 110.40 |
| 4 | AD | 147 | ILE | N-CA-C | -5.54 | 96.05 | 111.00 |
| 42 | BM | 97 | ASP | N-CA-CB | 5.54 | 120.57 | 110.60 |
| 47 | BU | 154 | VAL | CA-CB-CG2 | -5.54 | 102.59 | 110.90 |
| 69 | Br | 89 | LYS | N-CA-C | -5.54 | 96.05 | 111.00 |
| 78 | CA | 483 | A | C8-N9-C4 | -5.54 | 103.58 | 105.80 |
| 78 | CA | 568 | G | C5-C6-O6 | -5.54 | 125.28 | 128.60 |
| 79 | CB | 27 | G | C4'-C3'-C2' | -5.54 | 97.06 | 102.60 |
| 81 | DA | 564 | G | O4'-C1'-N9 | 5.54 | 112.63 | 108.20 |
| 81 | DA | 2235 | C | O4'-C1'-C2' | -5.54 | 100.26 | 105.80 |
| 81 | DA | 2367 | A | O4'-C1'-N9 | 5.54 | 112.63 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 68 | Bq | 11 | ARG | NE-CZ-NH1 | 5.54 | 123.07 | 120.30 |
| 78 | CA | 1637 | C | N3-C4-C5 | -5.54 | 119.69 | 121.90 |
| 81 | DA | 2513 | U | C2'-C3'-O3' | 5.54 | 122.56 | 113.70 |
| 32 | BC | 59 | ASP | CB-CG-OD2 | -5.54 | 113.32 | 118.30 |
| 35 | BG | 46 | ARG | C-N-CA | 5.54 | 135.54 | 121.70 |
| 63 | Bm | 55 | TRP | CB-CG-CD2 | -5.54 | 119.40 | 126.60 |
| 78 | CA | 114 | C | O4'-C1'-C2' | -5.54 | 100.26 | 105.80 |
| 78 | CA | 880 | C | O4'-C4'-C3' | 5.54 | 110.53 | 106.10 |
| 78 | CA | 1236 | A | P-O3'-C3' | -5.54 | 113.06 | 119.70 |
| 81 | DA | 1666 | G | O4'-C1'-N9 | 5.54 | 112.63 | 108.20 |
| 81 | DA | 2170 | U | C1'-O4'-C4' | 5.54 | 114.33 | 109.90 |
| 82 | DB | 98 | U | O4'-C1'-C2' | 5.54 | 112.58 | 107.60 |
| 26 | AZ | 37 | ARG | NE-CZ-NH2 | -5.53 | 117.53 | 120.30 |
| 29 | AU | 36 | SER | N-CA-C | 5.53 | 125.94 | 111.00 |
| 78 | CA | 490 | C | N3-C4-C5 | -5.53 | 119.69 | 121.90 |
| 81 | DA | 638 | C | C1'-O4'-C4' | -5.53 | 105.47 | 109.90 |
| 81 | DA | 1853 | U | C1'-O4'-C4' | 5.53 | 114.33 | 109.90 |
| 83 | DC | 26 | C | C4'-C3'-C2' | -5.53 | 97.07 | 102.60 |
| 15 | AN | 40 | ARG | NE-CZ-NH1 | -5.53 | 117.53 | 120.30 |
| 25 | AY | 49 | ARG | N-CA-C | -5.53 | 96.06 | 111.00 |
| 5 | AC | 145 | SER | N-CA-CB | 5.53 | 118.80 | 110.50 |
| 8 | AF | 112 | ARG | NE-CZ-NH1 | 5.53 | 123.07 | 120.30 |
| 34 | BE | 29 | ARG | CB-CG-CD | 5.53 | 125.98 | 111.60 |
| 43 | BP | 75 | VAL | N-CA-C | -5.53 | 96.06 | 111.00 |
| 78 | CA | 412 | A | N9-C1'-C2' | -5.53 | 105.92 | 112.00 |
| 78 | CA | 1080 | U | C5'-C4'-O4' | 5.53 | 115.74 | 109.10 |
| 81 | DA | 1916 | U | C3'-C2'-C1' | 5.53 | 105.92 | 101.50 |
| 81 | DA | 2770 | G | C5'-C4'-C3' | -5.53 | 107.15 | 116.00 |
| 81 | DA | 3140 | G | C1'-O4'-C4' | 5.53 | 114.33 | 109.90 |
| 81 | DA | 583 | G | O4'-C4'-C3' | -5.53 | 98.47 | 104.00 |
| 81 | DA | 618 | C | O4'-C1'-C2' | -5.53 | 100.27 | 105.80 |
| 81 | DA | 2100 | A | O5'-C5'-C4' | -5.53 | 101.19 | 111.70 |
| 81 | DA | 2747 | A | O4'-C1'-N9 | 5.53 | 112.62 | 108.20 |
| 81 | DA | 3100 | U | O4'-C1'-N1 | 5.53 | 112.62 | 108.20 |
| 18 | AP | 111 | VAL | N-CA-CB | 5.53 | 123.66 | 111.50 |
| 30 | BA | 72 | PHE | CB-CG-CD1 | -5.53 | 116.93 | 120.80 |
| 32 | BC | 364 | LYS | CA-CB-CG | 5.53 | 125.56 | 113.40 |
| 33 | BD | 29 | PRO | CA-C-N | 5.53 | 129.36 | 117.20 |
| 78 | CA | 661 | A | C3'-C2'-C1' | 5.53 | 105.92 | 101.50 |
| 78 | CA | 933 | A | O4'-C1'-N9 | 5.53 | 112.62 | 108.20 |
| 81 | DA | 629 | U | O4'-C1'-N1 | 5.53 | 112.62 | 108.20 |
| 81 | DA | 1166 | G | N9-C1'-C2' | -5.53 | 105.92 | 112.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1419 | A | P-O3'-C3' | -5.53 | 113.07 | 119.70 |
| 81 | DA | 2904 | U | N1-C1'-C2' | 5.53 | 121.19 | 114.00 |
| 81 | DA | 3285 | C | C3'-C2'-C1' | 5.53 | 105.92 | 101.50 |
| 3 | AB | 122 | VAL | CA-CB-CG2 | -5.53 | 102.61 | 110.90 |
| 17 | AQ | 53 | TYR | CG-CD1-CE1 | -5.53 | 116.88 | 121.30 |
| 44 | BO | 39 | HIS | C-N-CA | 5.53 | 135.51 | 121.70 |
| 78 | CA | 67 | A | P-O3'-C3' | 5.53 | 126.33 | 119.70 |
| 78 | CA | 576 | G | O4'-C1'-N9 | 5.53 | 112.62 | 108.20 |
| 78 | CA | 1466 | G | N9-C1'-C2' | 5.53 | 121.18 | 114.00 |
| 81 | DA | 185 | C | C5'-C4'-O4' | -5.53 | 102.47 | 109.10 |
| 81 | DA | 1105 | A | O4'-C1'-N9 | 5.53 | 112.62 | 108.20 |
| 81 | DA | 1612 | A | C1'-O4'-C4' | 5.53 | 114.32 | 109.90 |
| 81 | DA | 2294 | U | C1'-O4'-C4' | 5.53 | 114.32 | 109.90 |
| 81 | DA | 2630 | C | O5'-C5'-C4' | 5.53 | 122.20 | 111.70 |
| 35 | BG | 61 | ASN | CB-CA-C | -5.52 | 99.35 | 110.40 |
| 78 | CA | 1206 | U | N1-C1'-C2' | 5.52 | 121.18 | 114.00 |
| 78 | CA | 1491 | U | O3'-P-O5' | -5.52 | 93.50 | 104.00 |
| 81 | DA | 1515 | A | N9-C1'-C2' | 5.52 | 121.18 | 114.00 |
| 81 | DA | 1657 | C | C3'-C2'-C1' | 5.52 | 105.92 | 101.50 |
| 10 | AI | 85 | ILE | C-N-CA | 5.52 | 135.50 | 121.70 |
| 10 | AI | 122 | ARG | C-N-CA | 5.52 | 135.50 | 121.70 |
| 78 | CA | 1045 | C | C1'-O4'-C4' | -5.52 | 105.48 | 109.90 |
| 78 | CA | 1427 | A | C1'-O4'-C4' | 5.52 | 114.32 | 109.90 |
| 79 | CB | 36 | C | C1'-O4'-C4' | -5.52 | 105.48 | 109.90 |
| 81 | DA | 124 | U | O4'-C1'-N1 | -5.52 | 103.78 | 108.20 |
| 81 | DA | 1230 | G | N9-C1'-C2' | -5.52 | 105.92 | 112.00 |
| 81 | DA | 1329 | U | N1-C1'-C2' | 5.52 | 121.18 | 114.00 |
| 81 | DA | 1717 | U | C1'-O4'-C4' | 5.52 | 114.32 | 109.90 |
| 81 | DA | 1754 | G | N3-C2-N2 | 5.52 | 123.77 | 119.90 |
| 81 | DA | 1770 | G | O4'-C1'-N9 | 5.52 | 112.62 | 108.20 |
| 81 | DA | 1958 | U | O4'-C1'-C2' | -5.52 | 100.28 | 105.80 |
| 81 | DA | 2061 | G | O4'-C4'-C3' | -5.52 | 98.48 | 104.00 |
| 81 | DA | 2251 | G | C5'-C4'-C3' | 5.52 | 124.84 | 116.00 |
| 81 | DA | 2439 | A | C1'-O4'-C4' | -5.52 | 105.48 | 109.90 |
| 81 | DA | 2467 | G | P-O5'-C5' | -5.52 | 112.06 | 120.90 |
| 81 | DA | 2965 | U | C3'-C2'-C1' | 5.52 | 105.92 | 101.50 |
| 83 | DC | 30 | G | C4'-C3'-C2' | -5.52 | 97.08 | 102.60 |
| 62 | Bk | 28 | TYR | N-CA-CB | -5.52 | 100.66 | 110.60 |
| 81 | DA | 2410 | U | C5'-C4'-C3' | -5.52 | 107.17 | 116.00 |
| 21 | AT | 82 | VAL | N-CA-C | -5.52 | 96.10 | 111.00 |
| 60 | Bi | 50 | ALA | CB-CA-C | 5.52 | 118.38 | 110.10 |
| 78 | CA | 567 | A | C5-C6-N6 | -5.52 | 119.28 | 123.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 1107 | G | P-O3'-C3' | 5.52 | 126.32 | 119.70 |
| 81 | DA | 144 | A | P-O3'-C3' | 5.52 | 126.32 | 119.70 |
| 81 | DA | 1614 | C | P-O3'-C3' | -5.52 | 113.08 | 119.70 |
| 81 | DA | 2281 | A | C2'-C3'-O3' | 5.52 | 122.53 | 113.70 |
| 81 | DA | 2423 | U | C4'-C3'-C2' | -5.52 | 97.08 | 102.60 |
| 78 | CA | 243 | G | P-O3'-C3' | 5.52 | 126.32 | 119.70 |
| 78 | CA | 412 | A | O4'-C1'-N9 | 5.52 | 112.61 | 108.20 |
| 78 | CA | 615 | A | C3'-C2'-C1' | 5.52 | 105.91 | 101.50 |
| 78 | CA | 1084 | A | P-O5'-C5' | -5.52 | 112.07 | 120.90 |
| 79 | CB | 12 | U | C3'-C2'-C1' | 5.52 | 105.91 | 101.50 |
| 79 | CB | 47 | U | C1'-O4'-C4' | 5.52 | 114.31 | 109.90 |
| 81 | DA | 1429 | G | O4'-C1'-C2' | 5.52 | 112.57 | 107.60 |
| 81 | DA | 1622 | U | C1'-O4'-C4' | 5.52 | 114.31 | 109.90 |
| 81 | DA | 1770 | G | P-O5'-C5' | 5.52 | 129.73 | 120.90 |
| 81 | DA | 2645 | G | C5'-C4'-C3' | -5.52 | 107.17 | 116.00 |
| 41 | BN | 62 | GLN | C-N-CA | 5.52 | 135.49 | 121.70 |
| 78 | CA | 1209 | C | C1'-O4'-C4' | -5.52 | 105.49 | 109.90 |
| 78 | CA | 1319 | A | C1'-O4'-C4' | 5.52 | 114.31 | 109.90 |
| 3 | AB | 19 | ALA | N-CA-CB | 5.51 | 117.82 | 110.10 |
| 5 | AC | 174 | ARG | NE-CZ-NH2 | -5.51 | 117.54 | 120.30 |
| 22 | AV | 105 | THR | O-C-N | -5.51 | 113.88 | 122.70 |
| 24 | AX | 63 | LEU | N-CA-C | -5.51 | 96.11 | 111.00 |
| 31 | BB | 72 | ARG | C-N-CA | 5.51 | 135.49 | 121.70 |
| 47 | BU | 13 | TYR | CG-CD1-CE1 | 5.51 | 125.71 | 121.30 |
| 53 | Ba | 27 | LYS | CA-CB-CG | 5.51 | 125.53 | 113.40 |
| 78 | CA | 1172 | G | O4'-C1'-N9 | 5.51 | 112.61 | 108.20 |
| 81 | DA | 3224 | G | O4'-C1'-C2' | 5.51 | 112.56 | 107.60 |
| 78 | CA | 1108 | G | C3'-C2'-C1' | -5.51 | 97.09 | 101.50 |
| 79 | CB | 25 | U | C4'-C3'-C2' | -5.51 | 97.09 | 102.60 |
| 81 | DA | 2486 | A | O4'-C4'-C3' | -5.51 | 98.49 | 104.00 |
| 81 | DA | 2764 | C | N1-C1'-C2' | 5.51 | 121.17 | 114.00 |
| 3 | AB | 169 | ASP | CB-CG-OD2 | -5.51 | 113.34 | 118.30 |
| 10 | AI | 137 | ARG | CB-CA-C | -5.51 | 99.38 | 110.40 |
| 33 | BD | 313 | LEU | N-CA-C | 5.51 | 125.88 | 111.00 |
| 33 | BD | 346 | LYS | CA-CB-CG | 5.51 | 125.52 | 113.40 |
| 50 | BX | 34 | LEU | C-N-CD | -5.51 | 108.47 | 120.60 |
| 78 | CA | 173 | A | C5'-C4'-C3' | 5.51 | 124.82 | 116.00 |
| 78 | CA | 999 | U | O4'-C1'-N1 | -5.51 | 103.79 | 108.20 |
| 81 | DA | 39 | A | O4'-C1'-C2' | -5.51 | 100.29 | 105.80 |
| 81 | DA | 108 | A | P-O3'-C3' | 5.51 | 126.31 | 119.70 |
| 81 | DA | 2638 | C | C5'-C4'-C3' | 5.51 | 124.82 | 116.00 |
| 9 | AH | 52 | TYR | CG-CD1-CE1 | -5.51 | 116.89 | 121.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 13 | AL | 1 | MET | CG-SD-CE | -5.51 | 91.39 | 100.20 |
| 59 | Bh | 32 | TRP | CG-CD2-CE3 | -5.51 | 128.94 | 133.90 |
| 78 | CA | 253 | A | C1'-O4'-C4' | -5.51 | 105.49 | 109.90 |
| 78 | CA | 1437 | U | O4'-C1'-C2' | -5.51 | 100.29 | 105.80 |
| 78 | CA | 1637 | C | N3-C4-N4 | 5.51 | 121.86 | 118.00 |
| 78 | CA | 1762 | A | O4'-C1'-C2' | -5.51 | 100.29 | 105.80 |
| 81 | DA | 126 | U | O4'-C1'-C2' | -5.51 | 100.29 | 105.80 |
| 81 | DA | 229 | G | N9-C1'-C2' | 5.51 | 121.16 | 114.00 |
| 81 | DA | 822 | G | P-O3'-C3' | 5.51 | 126.31 | 119.70 |
| 81 | DA | 2130 | G | O3'-P-O5' | 5.51 | 114.47 | 104.00 |
| 53 | Ba | 22 | LYS | CB-CA-C | 5.51 | 121.42 | 110.40 |
| 64 | Bl | 63 | ARG | CD-NE-CZ | 5.51 | 131.31 | 123.60 |
| 81 | DA | 1497 | C | O4'-C1'-N1 | 5.51 | 112.61 | 108.20 |
| 81 | DA | 2172 | A | O4'-C4'-C3' | -5.51 | 98.49 | 104.00 |
| 81 | DA | 2684 | C | N1-C1'-C2' | 5.51 | 121.16 | 114.00 |
| 18 | AP | 74 | THR | CA-CB-CG2 | -5.51 | 104.69 | 112.40 |
| 33 | BD | 146 | PRO | CA-N-CD | -5.51 | 103.79 | 111.50 |
| 78 | CA | 143 | G | N9-C1'-C2' | 5.51 | 121.16 | 114.00 |
| 78 | CA | 1051 | G | O4'-C1'-N9 | 5.51 | 112.61 | 108.20 |
| 81 | DA | 467 | U | P-O3'-C3' | 5.51 | 126.31 | 119.70 |
| 81 | DA | 790 | U | P-O5'-C5' | 5.51 | 129.71 | 120.90 |
| 81 | DA | 1104 | G | P-O3'-C3' | 5.51 | 126.31 | 119.70 |
| 81 | DA | 2861 | U | N1-C1'-C2' | 5.51 | 121.16 | 114.00 |
| 82 | DB | 94 | C | N1-C1'-C2' | 5.51 | 121.16 | 114.00 |
| 43 | BP | 123 | GLN | CA-C-N | 5.50 | 129.31 | 117.20 |
| 50 | BX | 36 | LYS | CB-CA-C | -5.50 | 99.39 | 110.40 |
| 81 | DA | 3218 | A | P-O3'-C3' | 5.50 | 126.31 | 119.70 |
| 74 | BQ | 201 | GLY | N-CA-C | 5.50 | 126.86 | 113.10 |
| 76 | BS | 152 | PRO | CA-N-CD | -5.50 | 103.80 | 111.50 |
| 78 | CA | 56 | U | C2'-C3'-O3' | 5.50 | 122.51 | 113.70 |
| 78 | CA | 1055 | U | O4'-C1'-N1 | 5.50 | 112.60 | 108.20 |
| 81 | DA | 749 | C | O4'-C1'-N1 | 5.50 | 112.60 | 108.20 |
| 81 | DA | 976 | U | N1-C1'-C2' | -5.50 | 105.95 | 112.00 |
| 81 | DA | 1047 | A | O4'-C1'-N9 | 5.50 | 112.60 | 108.20 |
| 81 | DA | 2205 | U | O4'-C1'-N1 | 5.50 | 112.60 | 108.20 |
| 81 | DA | 2249 | G | C4'-C3'-C2' | -5.50 | 97.10 | 102.60 |
| 81 | DA | 2689 | A | O4'-C1'-N9 | -5.50 | 103.80 | 108.20 |
| 81 | DA | 2763 | U | P-O3'-C3' | 5.50 | 126.31 | 119.70 |
| 81 | DA | 2969 | A | O3'-P-O5' | 5.50 | 114.46 | 104.00 |
| 82 | DB | 11 | C | C4'-C3'-C2' | -5.50 | 97.10 | 102.60 |
| 82 | DB | 61 | A | C1'-O4'-C4' | -5.50 | 105.50 | 109.90 |
| 3 | AB | 17 | PHE | CB-CG-CD2 | -5.50 | 116.95 | 120.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 43 | BP | 176 | LYS | N-CA-C | -5.50 | 96.15 | 111.00 |
| 57 | Be | 76 | TYR | CB-CG-CD1 | -5.50 | 117.70 | 121.00 |
| 78 | CA | 174 | U | O4'-C1'-N1 | -5.50 | 103.80 | 108.20 |
| 78 | CA | 563 | U | C3'-C2'-C1' | 5.50 | 105.90 | 101.50 |
| 78 | CA | 1092 | A | P-O5'-C5' | 5.50 | 129.70 | 120.90 |
| 81 | DA | 1018 | G | C1'-O4'-C4' | 5.50 | 114.30 | 109.90 |
| 81 | DA | 1273 | A | C3'-C2'-C1' | 5.50 | 105.90 | 101.50 |
| 82 | DB | 100 | U | C5'-C4'-C3' | -5.50 | 107.20 | 116.00 |
| 13 | AL | 97 | ASP | N-CA-CB | 5.50 | 120.50 | 110.60 |
| 57 | Be | 31 | ALA | CB-CA-C | -5.50 | 101.85 | 110.10 |
| 65 | Bn | 56 | ILE | C-N-CA | 5.50 | 135.45 | 121.70 |
| 76 | BS | 27 | TYR | CB-CG-CD1 | -5.50 | 117.70 | 121.00 |
| 78 | CA | 1391 | A | C5'-C4'-O4' | 5.50 | 115.70 | 109.10 |
| 81 | DA | 1218 | U | O4'-C1'-N1 | 5.50 | 112.60 | 108.20 |
| 81 | DA | 2385 | G | O4'-C1'-N9 | 5.50 | 112.60 | 108.20 |
| 81 | DA | 2912 | G | O4'-C1'-N9 | 5.50 | 112.60 | 108.20 |
| 1 | Aa | 240 | VAL | C-N-CA | 5.50 | 135.45 | 121.70 |
| 2 | AA | 31 | VAL | CA-CB-CG1 | 5.50 | 119.15 | 110.90 |
| 18 | AP | 93 | TYR | CB-CG-CD1 | -5.50 | 117.70 | 121.00 |
| 30 | BA | 54 | LYS | CB-CG-CD | 5.50 | 125.90 | 111.60 |
| 67 | Bp | 44 | GLN | N-CA-C | -5.50 | 96.15 | 111.00 |
| 78 | CA | 1307 | U | P-O5'-C5' | -5.50 | 112.10 | 120.90 |
| 81 | DA | 1233 | G | N9-C1'-C2' | -5.50 | 105.95 | 112.00 |
| 13 | AL | 2 | GLY | CA-C-N | -5.50 | 105.11 | 117.20 |
| 31 | BB | 40 | TYR | N-CA-CB | 5.50 | 120.49 | 110.60 |
| 58 | Bg | 50 | ARG | N-CA-CB | 5.50 | 120.50 | 110.60 |
| 58 | Bg | 87 | ASN | CB-CA-C | 5.50 | 121.39 | 110.40 |
| 78 | CA | 396 | G | O4'-C1'-N9 | 5.50 | 112.60 | 108.20 |
| 78 | CA | 1061 | A | P-O3'-C3' | 5.50 | 126.30 | 119.70 |
| 81 | DA | 363 | G | O4'-C1'-C2' | 5.50 | 112.55 | 107.60 |
| 81 | DA | 735 | A | C5-C6-N6 | -5.50 | 119.30 | 123.70 |
| 81 | DA | 1290 | A | O4'-C4'-C3' | -5.50 | 98.50 | 104.00 |
| 81 | DA | 2137 | U | P-O5'-C5' | -5.50 | 112.11 | 120.90 |
| 81 | DA | 2153 | U | C4'-C3'-C2' | -5.50 | 97.10 | 102.60 |
| 81 | DA | 2265 | C | C5'-C4'-C3' | 5.50 | 124.79 | 116.00 |
| 6 | AE | 197 | TYR | N-CA-CB | 5.50 | 120.49 | 110.60 |
| 37 | BH | 150 | LEU | CB-CG-CD2 | -5.50 | 101.66 | 111.00 |
| 43 | BP | 110 | ALA | N-CA-CB | 5.50 | 117.79 | 110.10 |
| 74 | BQ | 141 | PRO | N-CA-C | 5.50 | 126.39 | 112.10 |
| 78 | CA | 293 | U | O4'-C1'-N1 | 5.50 | 112.60 | 108.20 |
| 14 | AM | 80 | LYS | N-CA-CB | 5.49 | 120.49 | 110.60 |
| 21 | AT | 72 | LEU | CB-CG-CD1 | 5.49 | 120.34 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 31 | BB | 4 | VAL | CA-CB-CG2 | -5.49 | 102.66 | 110.90 |
| 41 | BN | 109 | ARG | NE-CZ-NH2 | -5.49 | 117.55 | 120.30 |
| 59 | Bh | 6 | HIS | CA-CB-CG | 5.49 | 122.94 | 113.60 |
| 67 | Bp | 34 | CYS | C-N-CA | -5.49 | 107.97 | 121.70 |
| 78 | CA | 1010 | C | P-O5'-C5' | -5.49 | 112.11 | 120.90 |
| 81 | DA | 1162 | U | P-O3'-C3' | 5.49 | 126.29 | 119.70 |
| 81 | DA | 2834 | G | O4'-C1'-N9 | 5.49 | 112.59 | 108.20 |
| 83 | DC | 92 | A | O4'-C1'-N9 | 5.49 | 112.59 | 108.20 |
| 78 | CA | 1257 | U | O4'-C1'-N1 | 5.49 | 112.59 | 108.20 |
| 81 | DA | 2072 | G | P-O5'-C5' | 5.49 | 129.69 | 120.90 |
| 81 | DA | 2471 | U | C4'-C3'-C2' | -5.49 | 97.11 | 102.60 |
| 81 | DA | 2734 | A | C4'-C3'-C2' | -5.49 | 97.11 | 102.60 |
| 81 | DA | 2967 | A | O3'-P-O5' | -5.49 | 93.57 | 104.00 |
| 81 | DA | 3151 | U | N1-C1'-C2' | -5.49 | 105.96 | 112.00 |
| 20 | AS | 12 | GLN | CG-CD-NE2 | -5.49 | 103.52 | 116.70 |
| 41 | BN | 43 | LYS | CA-CB-CG | 5.49 | 125.48 | 113.40 |
| 63 | Bm | 4 | ARG | NE-CZ-NH1 | 5.49 | 123.05 | 120.30 |
| 78 | CA | 448 | C | C1'-O4'-C4' | -5.49 | 105.51 | 109.90 |
| 78 | CA | 586 | G | O4'-C4'-C3' | 5.49 | 110.49 | 106.10 |
| 81 | DA | 264 | G | P-O5'-C5' | 5.49 | 129.68 | 120.90 |
| 81 | DA | 1752 | A | N9-C1'-C2' | 5.49 | 121.14 | 114.00 |
| 81 | DA | 2087 | C | P-O5'-C5' | 5.49 | 129.69 | 120.90 |
| 83 | DC | 45 | A | P-O5'-C5' | 5.49 | 129.69 | 120.90 |
| 17 | AQ | 107 | SER | CB-CA-C | 5.49 | 120.53 | 110.10 |
| 32 | BC | 371 | GLN | N-CA-CB | 5.49 | 120.48 | 110.60 |
| 33 | BD | 103 | THR | N-CA-C | -5.49 | 96.18 | 111.00 |
| 64 | Bl | 8 | PHE | CB-CG-CD1 | -5.49 | 116.96 | 120.80 |
| 67 | Bp | 34 | CYS | N-CA-C | 5.49 | 125.82 | 111.00 |
| 81 | DA | 2176 | U | O3'-P-O5' | -5.49 | 93.57 | 104.00 |
| 81 | DA | 2269 | U | C1'-O4'-C4' | 5.49 | 114.29 | 109.90 |
| 81 | DA | 2700 | G | C4'-C3'-C2' | -5.49 | 97.11 | 102.60 |
| 81 | DA | 3242 | G | O4'-C4'-C3' | -5.49 | 98.51 | 104.00 |
| 4 | AD | 103 | TYR | CB-CA-C | -5.49 | 99.42 | 110.40 |
| 62 | Bk | 48 | ALA | C-N-CA | 5.49 | 133.82 | 122.30 |
| 78 | CA | 1492 | A | P-O3'-C3' | 5.49 | 126.28 | 119.70 |
| 81 | DA | 1277 | C | C5'-C4'-O4' | -5.49 | 102.52 | 109.10 |
| 81 | DA | 1699 | A | N9-C1'-C2' | -5.49 | 105.97 | 112.00 |
| 81 | DA | 2674 | A | O4'-C1'-C2' | 5.49 | 112.54 | 107.60 |
| 2 | AA | 72 | ASP | CB-CG-OD1 | -5.49 | 113.36 | 118.30 |
| 5 | AC | 14 | THR | CA-C-O | -5.49 | 108.58 | 120.10 |
| 32 | BC | 241 | LYS | CB-CA-C | 5.49 | 121.37 | 110.40 |
| 76 | BS | 71 | PRO | C-N-CA | 5.49 | 135.41 | 121.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 1324 | G | C5'-C4'-O4' | 5.49 | 115.68 | 109.10 |
| 81 | DA | 969 | C | O3'-P-O5' | -5.49 | 93.58 | 104.00 |
| 81 | DA | 1119 | C | N1-C1'-C2' | 5.49 | 121.13 | 114.00 |
| 81 | DA | 2363 | A | C4'-C3'-C2' | -5.49 | 97.11 | 102.60 |
| 81 | DA | 2462 | A | O4'-C1'-C2' | -5.49 | 100.31 | 105.80 |
| 81 | DA | 2887 | A | C3'-C2'-C1' | 5.49 | 105.89 | 101.50 |
| 83 | DC | 7 | G | O4'-C1'-N9 | 5.49 | 112.59 | 108.20 |
| 78 | CA | 964 | U | O4'-C1'-C2' | -5.48 | 100.32 | 105.80 |
| 78 | CA | 1068 | C | N3-C4-C5 | -5.48 | 119.71 | 121.90 |
| 78 | CA | 1301 | U | P-O5'-C5' | -5.48 | 112.13 | 120.90 |
| 81 | DA | 2885 | C | C1'-O4'-C4' | -5.48 | 105.51 | 109.90 |
| 81 | DA | 3085 | G | C5'-C4'-C3' | 5.48 | 124.77 | 116.00 |
| 81 | DA | 3345 | G | C3'-C2'-C1' | -5.48 | 97.11 | 101.50 |
| 13 | AL | 122 | PHE | N-CA-C | 5.48 | 125.80 | 111.00 |
| 33 | BD | 358 | THR | C-N-CA | 5.48 | 135.41 | 121.70 |
| 78 | CA | 14 | C | C1'-O4'-C4' | -5.48 | 105.52 | 109.90 |
| 78 | CA | 150 | U | O4'-C1'-N1 | 5.48 | 112.59 | 108.20 |
| 81 | DA | 623 | U | O4'-C1'-C2' | -5.48 | 100.32 | 105.80 |
| 81 | DA | 1578 | C | O4'-C1'-C2' | -5.48 | 100.32 | 105.80 |
| 81 | DA | 1697 | A | O4'-C1'-C2' | -5.48 | 100.32 | 105.80 |
| 81 | DA | 2035 | G | C1'-O4'-C4' | -5.48 | 105.52 | 109.90 |
| 81 | DA | 3000 | A | P-O5'-C5' | 5.48 | 129.67 | 120.90 |
| 82 | DB | 101 | U | O4'-C1'-N1 | 5.48 | 112.59 | 108.20 |
| 83 | DC | 87 | U | O4'-C1'-N1 | 5.48 | 112.59 | 108.20 |
| 48 | BW | 83 | TYR | CB-CG-CD1 | 5.48 | 124.29 | 121.00 |
| 78 | CA | 295 | A | C5'-C4'-O4' | -5.48 | 102.52 | 109.10 |
| 78 | CA | 1264 | G | O4'-C1'-C2' | -5.48 | 100.32 | 105.80 |
| 81 | DA | 2207 | A | C1'-O4'-C4' | 5.48 | 114.28 | 109.90 |
| 81 | DA | 2646 | C | O3'-P-O5' | -5.48 | 93.59 | 104.00 |
| 81 | DA | 2706 | G | P-O3'-C3' | 5.48 | 126.28 | 119.70 |
| 81 | DA | 3385 | U | C4'-C3'-C2' | -5.48 | 97.12 | 102.60 |
| 82 | DB | 62 | C | C1'-O4'-C4' | -5.48 | 105.52 | 109.90 |
| 37 | BH | 104 | GLU | OE1-CD-OE2 | 5.48 | 129.88 | 123.30 |
| 78 | CA | 320 | U | N1-C1'-C2' | 5.48 | 121.12 | 114.00 |
| 81 | DA | 596 | C | O5'-C5'-C4' | -5.48 | 101.29 | 111.70 |
| 81 | DA | 837 | A | O5'-C5'-C4' | 5.48 | 122.11 | 111.70 |
| 81 | DA | 993 | G | P-O3'-C3' | 5.48 | 126.28 | 119.70 |
| 13 | AL | 2 | GLY | N-CA-C | -5.48 | 99.41 | 113.10 |
| 33 | BD | 209 | TYR | CB-CG-CD1 | -5.48 | 117.71 | 121.00 |
| 78 | CA | 1092 | A | C3'-C2'-C1' | 5.48 | 105.88 | 101.50 |
| 81 | DA | 36 | C | P-O3'-C3' | 5.48 | 126.27 | 119.70 |
| 81 | DA | 71 | A | C1'-O4'-C4' | -5.48 | 105.52 | 109.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1585 | C | C5'-C4'-O4' | 5.48 | 115.67 | 109.10 |
| 81 | DA | 1833 | G | O4'-C4'-C3' | -5.48 | 98.52 | 104.00 |
| 81 | DA | 1914 | G | C1'-O4'-C4' | -5.48 | 105.52 | 109.90 |
| 81 | DA | 2007 | G | O4'-C1'-N9 | 5.48 | 112.58 | 108.20 |
| 81 | DA | 2661 | G | C4'-C3'-C2' | -5.48 | 97.12 | 102.60 |
| 81 | DA | 3149 | G | O3'-P-O5' | -5.48 | 93.59 | 104.00 |
| 81 | DA | 3250 | U | N1-C1'-C2' | 5.48 | 121.12 | 114.00 |
| 82 | DB | 152 | G | C4'-C3'-C2' | -5.48 | 97.12 | 102.60 |
| 43 | BP | 20 | ARG | O-C-N | -5.48 | 113.94 | 122.70 |
| 78 | CA | 1207 | C | O4'-C1'-C2' | -5.48 | 100.32 | 105.80 |
| 78 | CA | 1545 | A | O5'-P-OP1 | 5.48 | 117.27 | 110.70 |
| 81 | DA | 273 | A | C5'-C4'-C3' | 5.48 | 124.76 | 116.00 |
| 81 | DA | 878 | G | N9-C1'-C2' | 5.48 | 121.12 | 114.00 |
| 81 | DA | 2705 | A | O4'-C1'-C2' | 5.48 | 112.53 | 107.60 |
| 81 | DA | 3257 | C | P-O3'-C3' | -5.48 | 113.13 | 119.70 |
| 43 | BP | 150 | TRP | CE2-CD2-CE3 | 5.47 | 125.27 | 118.70 |
| 76 | BS | 32 | TRP | CB-CG-CD2 | -5.47 | 119.48 | 126.60 |
| 78 | CA | 394 | C | N1-C1'-C2' | 5.47 | 121.12 | 114.00 |
| 81 | DA | 319 | A | P-O3'-C3' | -5.47 | 113.13 | 119.70 |
| 81 | DA | 533 | A | O4'-C1'-C2' | -5.47 | 100.33 | 105.80 |
| 81 | DA | 2047 | A | C2'-C3'-O3' | 5.47 | 122.46 | 113.70 |
| 81 | DA | 2457 | G | P-O3'-C3' | 5.47 | 126.27 | 119.70 |
| 81 | DA | 2536 | A | C4-C5-C6 | 5.47 | 119.74 | 117.00 |
| 13 | AL | 22 | ASN | CA-C-O | -5.47 | 108.61 | 120.10 |
| 20 | AS | 12 | GLN | OE1-CD-NE2 | 5.47 | 134.49 | 121.90 |
| 44 | BO | 60 | TYR | N-CA-C | -5.47 | 96.22 | 111.00 |
| 78 | CA | 553 | G | O4'-C1'-C2' | 5.47 | 112.53 | 107.60 |
| 78 | CA | 918 | U | C3'-C2'-C1' | 5.47 | 105.88 | 101.50 |
| 78 | CA | 978 | A | C2'-C3'-O3' | 5.47 | 122.46 | 113.70 |
| 81 | DA | 454 | C | C3'-C2'-C1' | 5.47 | 105.88 | 101.50 |
| 81 | DA | 790 | U | C5'-C4'-C3' | -5.47 | 107.24 | 116.00 |
| 81 | DA | 2337 | C | O4'-C1'-C2' | -5.47 | 100.33 | 105.80 |
| 81 | DA | 2345 | A | C5'-C4'-C3' | -5.47 | 107.24 | 116.00 |
| 81 | DA | 2369 | G | C4'-C3'-C2' | -5.47 | 97.13 | 102.60 |
| 81 | DA | 3336 | A | P-O3'-C3' | 5.47 | 126.27 | 119.70 |
| 19 | AR | 130 | ARG | NE-CZ-NH2 | -5.47 | 117.56 | 120.30 |
| 78 | CA | 660 | G | O4'-C1'-C2' | -5.47 | 100.33 | 105.80 |
| 78 | CA | 1220 | C | O4'-C1'-C2' | -5.47 | 100.33 | 105.80 |
| 81 | DA | 503 | C | O4'-C1'-N1 | 5.47 | 112.58 | 108.20 |
| 81 | DA | 1006 | A | O3'-P-O5' | -5.47 | 93.61 | 104.00 |
| 81 | DA | 1767 | C | N3-C4-N4 | 5.47 | 121.83 | 118.00 |
| 81 | DA | 3006 | A | O4'-C1'-C2' | 5.47 | 112.52 | 107.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 79 | CB | 45 | G | C3'-C2'-C1' | 5.47 | 105.87 | 101.50 |
| 81 | DA | 1823 | A | C4'-C3'-C2' | -5.47 | 97.13 | 102.60 |
| 35 | BG | 169 | ASP | O-C-N | 5.47 | 131.44 | 122.70 |
| 78 | CA | 122 | U | P-O3'-C3' | 5.47 | 126.26 | 119.70 |
| 78 | CA | 566 | C | N3-C4-C5 | -5.47 | 119.71 | 121.90 |
| 78 | CA | 648 | G | N9-C1'-C2' | 5.47 | 121.11 | 114.00 |
| 80 | CC | 20 | U | O3'-P-O5' | 5.47 | 114.39 | 104.00 |
| 81 | DA | 109 | A | P-O3'-C3' | 5.47 | 126.26 | 119.70 |
| 81 | DA | 293 | C | O4'-C1'-N1 | 5.47 | 112.57 | 108.20 |
| 81 | DA | 672 | A | OP1-P-O3' | 5.47 | 117.23 | 105.20 |
| 81 | DA | 1050 | U | P-O3'-C3' | 5.47 | 126.26 | 119.70 |
| 81 | DA | 2528 | G | P-O5'-C5' | -5.47 | 112.15 | 120.90 |
| 81 | DA | 2547 | A | C5-C6-N1 | -5.47 | 114.97 | 117.70 |
| 81 | DA | 2778 | G | C3'-C2'-C1' | 5.47 | 105.87 | 101.50 |
| 32 | BC | 284 | ARG | NE-CZ-NH1 | 5.46 | 123.03 | 120.30 |
| 61 | Bj | 45 | LEU | CA-C-N | -5.46 | 105.27 | 116.20 |
| 78 | CA | 927 | C | P-O3'-C3' | 5.46 | 126.26 | 119.70 |
| 78 | CA | 1202 | A | P-O3'-C3' | 5.46 | 126.26 | 119.70 |
| 81 | DA | 192 | C | C3'-C2'-C1' | 5.46 | 105.87 | 101.50 |
| 81 | DA | 1239 | C | C3'-C2'-C1' | 5.46 | 105.87 | 101.50 |
| 81 | DA | 1453 | A | P-O3'-C3' | 5.46 | 126.26 | 119.70 |
| 81 | DA | 1762 | C | N3-C4-N4 | 5.46 | 121.83 | 118.00 |
| 83 | DC | 4 | U | C1'-O4'-C4' | 5.46 | 114.27 | 109.90 |
| 83 | DC | 82 | A | O4'-C1'-C2' | -5.46 | 100.34 | 105.80 |
| 58 | Bg | 72 | ARG | NE-CZ-NH2 | 5.46 | 123.03 | 120.30 |
| 78 | CA | 287 | G | C1'-O4'-C4' | -5.46 | 105.53 | 109.90 |
| 78 | CA | 1278 | G | O4'-C1'-N9 | 5.46 | 112.57 | 108.20 |
| 81 | DA | 1259 | A | N9-C1'-C2' | -5.46 | 105.99 | 112.00 |
| 81 | DA | 1293 | U | O4'-C4'-C3' | -5.46 | 98.54 | 104.00 |
| 81 | DA | 1792 | C | C3'-C2'-C1' | 5.46 | 105.87 | 101.50 |
| 81 | DA | 2415 | C | O4'-C1'-N1 | 5.46 | 112.57 | 108.20 |
| 33 | BD | 242 | ALA | CB-CA-C | -5.46 | 101.91 | 110.10 |
| 78 | CA | 346 | G | O3'-P-O5' | -5.46 | 93.62 | 104.00 |
| 78 | CA | 1189 | A | O3'-P-O5' | -5.46 | 93.62 | 104.00 |
| 81 | DA | 636 | C | C4'-C3'-O3' | 5.46 | 123.92 | 113.00 |
| 81 | DA | 737 | G | C5-C6-O6 | -5.46 | 125.32 | 128.60 |
| 81 | DA | 787 | G | C1'-O4'-C4' | -5.46 | 105.53 | 109.90 |
| 81 | DA | 2738 | A | C1'-O4'-C4' | -5.46 | 105.53 | 109.90 |
| 81 | DA | 3054 | U | P-O5'-C5' | 5.46 | 129.64 | 120.90 |
| 9 | AH | 6 | VAL | CA-CB-CG1 | -5.46 | 102.71 | 110.90 |
| 14 | AM | 93 | THR | CA-CB-CG2 | 5.46 | 120.04 | 112.40 |
| 56 | Bf | 68 | TYR | CB-CG-CD1 | 5.46 | 124.28 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 61 | Bj | 39 | GLN | CB-CA-C | -5.46 | 99.48 | 110.40 |
| 78 | CA | 596 | C | O4'-C1'-C2' | -5.46 | 100.34 | 105.80 |
| 81 | DA | 184 | U | OP2-P-O3' | 5.46 | 117.21 | 105.20 |
| 81 | DA | 1404 | G | P-O5'-C5' | -5.46 | 112.16 | 120.90 |
| 81 | DA | 2297 | U | N1-C1'-C2' | 5.46 | 121.10 | 114.00 |
| 82 | DB | 142 | C | N1-C1'-C2' | 5.46 | 121.10 | 114.00 |
| 6 | AE | 178 | ILE | CA-CB-CG1 | 5.46 | 121.37 | 111.00 |
| 78 | CA | 255 | U | C3'-C2'-C1' | 5.46 | 105.87 | 101.50 |
| 78 | CA | 852 | C | C1'-O4'-C4' | 5.46 | 114.27 | 109.90 |
| 78 | CA | 952 | A | O4'-C1'-N9 | 5.46 | 112.57 | 108.20 |
| 78 | CA | 1746 | A | C4'-C3'-C2' | 5.46 | 108.06 | 102.60 |
| 81 | DA | 547 | G | C1'-O4'-C4' | -5.46 | 105.53 | 109.90 |
| 81 | DA | 1755 | C | N3-C4-C5 | -5.46 | 119.72 | 121.90 |
| 81 | DA | 1782 | U | C3'-C2'-C1' | 5.46 | 105.87 | 101.50 |
| 18 | AP | 111 | VAL | N-CA-C | -5.46 | 96.27 | 111.00 |
| 20 | AS | 3 | GLY | CA-C-N | -5.46 | 105.19 | 117.20 |
| 44 | BO | 139 | ARG | NE-CZ-NH2 | -5.46 | 117.57 | 120.30 |
| 78 | CA | 1209 | C | N1-C1'-C2' | 5.46 | 121.09 | 114.00 |
| 78 | CA | 1292 | G | C3'-C2'-C1' | -5.46 | 97.13 | 101.50 |
| 78 | CA | 1685 | G | O4'-C1'-N9 | 5.46 | 112.57 | 108.20 |
| 79 | CB | 73 | C | C3'-C2'-C1' | 5.46 | 105.86 | 101.50 |
| 81 | DA | 640 | U | C5'-C4'-C3' | -5.46 | 107.27 | 116.00 |
| 81 | DA | 761 | A | C1'-O4'-C4' | -5.46 | 105.53 | 109.90 |
| 81 | DA | 934 | G | N9-C1'-C2' | 5.46 | 121.09 | 114.00 |
| 81 | DA | 2283 | G | C4'-C3'-C2' | 5.46 | 108.06 | 102.60 |
| 81 | DA | 2412 | G | O4'-C1'-N9 | 5.46 | 112.56 | 108.20 |
| 81 | DA | 2999 | U | C4'-C3'-C2' | -5.46 | 97.14 | 102.60 |
| 81 | DA | 3009 | G | C5'-C4'-O4' | -5.46 | 102.55 | 109.10 |
| 18 | AP | 75 | VAL | CA-CB-CG1 | 5.46 | 119.08 | 110.90 |
| 30 | BA | 120 | VAL | CA-CB-CG2 | 5.46 | 119.08 | 110.90 |
| 81 | DA | 559 | A | O4'-C4'-C3' | -5.46 | 98.55 | 104.00 |
| 82 | DB | 24 | G | O4'-C1'-N9 | 5.46 | 112.56 | 108.20 |
| 83 | DC | 107 | G | O3'-P-O5' | 5.46 | 114.36 | 104.00 |
| 4 | AD | 219 | VAL | CA-CB-CG1 | 5.45 | 119.08 | 110.90 |
| 5 | AC | 71 | PHE | CB-CG-CD1 | 5.45 | 124.62 | 120.80 |
| 53 | Ba | 13 | VAL | C-N-CA | -5.45 | 108.07 | 121.70 |
| 59 | Bh | 46 | PHE | CB-CG-CD2 | 5.45 | 124.62 | 120.80 |
| 78 | CA | 407 | A | C1'-O4'-C4' | 5.45 | 114.26 | 109.90 |
| 78 | CA | 469 | C | O4'-C1'-N1 | -5.45 | 103.84 | 108.20 |
| 78 | CA | 1656 | U | O5'-C5'-C4' | 5.45 | 122.06 | 111.70 |
| 81 | DA | 908 | G | C3'-C2'-C1' | 5.45 | 105.86 | 101.50 |
| 81 | DA | 1549 | U | O3'-P-O5' | -5.45 | 93.64 | 104.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2146 | C | O4'-C1'-C2' | -5.45 | 100.35 | 105.80 |
| 81 | DA | 3361 | G | C1'-O4'-C4' | -5.45 | 105.54 | 109.90 |
| 82 | DB | 141 | C | O4'-C1'-N1 | 5.45 | 112.56 | 108.20 |
| 5 | AC | 127 | VAL | CA-CB-CG1 | -5.45 | 102.72 | 110.90 |
| 81 | DA | 84 | U | N1-C1'-C2' | 5.45 | 121.09 | 114.00 |
| 81 | DA | 1859 | A | C1'-O4'-C4' | 5.45 | 114.26 | 109.90 |
| 81 | DA | 2736 | A | C5'-C4'-C3' | 5.45 | 124.72 | 116.00 |
| 82 | DB | 123 | G | O4'-C1'-N9 | 5.45 | 112.56 | 108.20 |
| 13 | AL | 86 | PHE | CA-CB-CG | 5.45 | 126.98 | 113.90 |
| 22 | AV | 105 | THR | CA-CB-OG1 | 5.45 | 120.45 | 109.00 |
| 78 | CA | 172 | C | C1'-O4'-C4' | -5.45 | 105.54 | 109.90 |
| 78 | CA | 499 | U | C4'-C3'-C2' | -5.45 | 97.15 | 102.60 |
| 78 | CA | 1409 | G | C4'-C3'-C2' | 5.45 | 108.05 | 102.60 |
| 81 | DA | 396 | A | P-O3'-C3' | 5.45 | 126.24 | 119.70 |
| 81 | DA | 838 | G | C3'-C2'-C1' | -5.45 | 97.14 | 101.50 |
| 81 | DA | 1046 | A | O4'-C1'-C2' | -5.45 | 100.35 | 105.80 |
| 81 | DA | 1148 | G | C3'-C2'-C1' | -5.45 | 97.14 | 101.50 |
| 81 | DA | 1396 | C | P-O5'-C5' | 5.45 | 129.62 | 120.90 |
| 81 | DA | 3301 | U | C4'-C3'-C2' | -5.45 | 97.15 | 102.60 |
| 13 | AL | 109 | ARG | NH1-CZ-NH2 | 5.45 | 125.39 | 119.40 |
| 21 | AT | 81 | ASN | C-N-CA | 5.45 | 135.32 | 121.70 |
| 68 | Bq | 15 | ARG | N-CA-CB | 5.45 | 120.41 | 110.60 |
| 78 | CA | 480 | G | C5-C6-O6 | -5.45 | 125.33 | 128.60 |
| 78 | CA | 1090 | C | O3'-P-O5' | -5.45 | 93.65 | 104.00 |
| 81 | DA | 9 | U | O4'-C4'-C3' | -5.45 | 98.55 | 104.00 |
| 81 | DA | 598 | A | P-O5'-C5' | 5.45 | 129.62 | 120.90 |
| 81 | DA | 2041 | U | C4'-C3'-C2' | -5.45 | 97.15 | 102.60 |
| 29 | AU | 61 | ARG | C-N-CA | 5.45 | 135.32 | 121.70 |
| 51 | BZ | 31 | PHE | CB-CG-CD1 | 5.45 | 124.61 | 120.80 |
| 78 | CA | 1637 | C | O4'-C1'-N1 | 5.45 | 112.56 | 108.20 |
| 81 | DA | 754 | G | C1'-O4'-C4' | -5.45 | 105.54 | 109.90 |
| 81 | DA | 983 | A | O4'-C4'-C3' | -5.45 | 98.55 | 104.00 |
| 81 | DA | 2436 | U | P-O3'-C3' | 5.45 | 126.24 | 119.70 |
| 81 | DA | 2722 | U | C2'-C3'-O3' | 5.45 | 122.42 | 113.70 |
| 81 | DA | 2994 | A | O4'-C1'-C2' | -5.45 | 100.35 | 105.80 |
| 81 | DA | 3026 | G | C4'-C3'-C2' | -5.45 | 97.15 | 102.60 |
| 31 | BB | 126 | LEU | CB-CA-C | -5.45 | 99.85 | 110.20 |
| 37 | BH | 207 | ASP | N-CA-C | -5.45 | 96.30 | 111.00 |
| 63 | Bm | 85 | ARG | NE-CZ-NH1 | 5.45 | 123.02 | 120.30 |
| 78 | CA | 1173 | C | OP1-P-OP2 | -5.45 | 111.43 | 119.60 |
| 78 | CA | 1506 | G | N3-C2-N2 | 5.45 | 123.71 | 119.90 |
| 81 | DA | 31 | C | O4'-C1'-C2' | -5.45 | 100.36 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1488 | G | C1'-O4'-C4' | -5.45 | 105.54 | 109.90 |
| 81 | DA | 1810 | A | O4'-C1'-N9 | 5.45 | 112.56 | 108.20 |
| 81 | DA | 2272 | G | C1'-O4'-C4' | 5.45 | 114.26 | 109.90 |
| 81 | DA | 2940 | A | O3'-P-O5' | 5.45 | 114.35 | 104.00 |
| 81 | DA | 3213 | A | C1'-O4'-C4' | 5.45 | 114.26 | 109.90 |
| 81 | DA | 837 | A | P-O5'-C5' | -5.44 | 112.19 | 120.90 |
| 81 | DA | 2110 | G | O4'-C1'-N9 | 5.44 | 112.56 | 108.20 |
| 18 | AP | 109 | VAL | CG1-CB-CG2 | 5.44 | 119.61 | 110.90 |
| 33 | BD | 65 | TRP | CH2-CZ2-CE2 | -5.44 | 111.96 | 117.40 |
| 44 | BO | 73 | LEU | C-N-CA | 5.44 | 135.31 | 121.70 |
| 48 | BW | 71 | PHE | CB-CG-CD1 | -5.44 | 116.99 | 120.80 |
| 77 | BI | 107 | GLY | CA-C-N | -5.44 | 105.23 | 117.20 |
| 81 | DA | 2126 | A | P-O3'-C3' | -5.44 | 113.17 | 119.70 |
| 81 | DA | 2280 | A | C3'-C2'-C1' | 5.44 | 105.86 | 101.50 |
| 81 | DA | 2622 | C | O4'-C1'-N1 | -5.44 | 103.85 | 108.20 |
| 81 | DA | 3034 | C | C2'-C3'-O3' | 5.44 | 122.41 | 113.70 |
| 20 | AS | 18 | TYR | CB-CG-CD2 | -5.44 | 117.74 | 121.00 |
| 42 | BM | 44 | SER | C-N-CA | 5.44 | 135.30 | 121.70 |
| 61 | Bj | 27 | VAL | CA-CB-CG2 | -5.44 | 102.74 | 110.90 |
| 78 | CA | 1134 | C | C1'-O4'-C4' | -5.44 | 105.55 | 109.90 |
| 81 | DA | 2034 | C | O4'-C1'-C2' | -5.44 | 100.36 | 105.80 |
| 81 | DA | 2162 | U | C5'-C4'-O4' | 5.44 | 115.63 | 109.10 |
| 35 | BG | 43 | LEU | CB-CA-C | -5.44 | 99.87 | 110.20 |
| 39 | BJ | 129 | THR | CA-CB-CG2 | -5.44 | 104.78 | 112.40 |
| 74 | BQ | 53 | VAL | C-N-CA | 5.44 | 135.30 | 121.70 |
| 78 | CA | 1459 | C | C1'-O4'-C4' | 5.44 | 114.25 | 109.90 |
| 81 | DA | 910 | G | C5'-C4'-O4' | 5.44 | 115.63 | 109.10 |
| 81 | DA | 1336 | U | O3'-P-O5' | -5.44 | 93.67 | 104.00 |
| 81 | DA | 1339 | C | P-O3'-C3' | 5.44 | 126.23 | 119.70 |
| 11 | AJ | 81 | THR | C-N-CA | 5.44 | 135.29 | 121.70 |
| 13 | AL | 2 | GLY | CA-C-O | 5.44 | 130.39 | 120.60 |
| 30 | BA | 148 | VAL | CA-CB-CG1 | -5.44 | 102.74 | 110.90 |
| 35 | BG | 29 | LYS | N-CA-CB | 5.44 | 120.39 | 110.60 |
| 37 | BH | 90 | THR | N-CA-CB | 5.44 | 120.63 | 110.30 |
| 47 | BU | 18 | ASP | CB-CG-OD1 | 5.44 | 123.19 | 118.30 |
| 62 | Bk | 82 | ARG | NE-CZ-NH1 | -5.44 | 117.58 | 120.30 |
| 78 | CA | 386 | G | O3'-P-O5' | 5.44 | 114.33 | 104.00 |
| 81 | DA | 977 | C | O4'-C1'-C2' | -5.44 | 100.36 | 105.80 |
| 81 | DA | 990 | U | O3'-P-O5' | -5.44 | 93.67 | 104.00 |
| 81 | DA | 1411 | C | O4'-C1'-N1 | 5.44 | 112.55 | 108.20 |
| 81 | DA | 1591 | G | N9-C1'-C2' | 5.44 | 121.07 | 114.00 |
| 81 | DA | 2540 | A | O4'-C1'-N9 | 5.44 | 112.55 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2708 | C | C1'-O4'-C4' | -5.44 | 105.55 | 109.90 |
| 82 | DB | 104 | A | P-O3'-C3' | 5.44 | 126.23 | 119.70 |
| 78 | CA | 461 | G | O3'-P-O5' | -5.44 | 93.67 | 104.00 |
| 78 | CA | 1439 | C | O4'-C1'-N1 | 5.44 | 112.55 | 108.20 |
| 78 | CA | 1760 | G | P-O5'-C5' | -5.44 | 112.20 | 120.90 |
| 81 | DA | 3010 | U | O4'-C4'-C3' | -5.44 | 98.56 | 104.00 |
| 81 | DA | 3144 | G | O4'-C1'-N9 | 5.44 | 112.55 | 108.20 |
| 81 | DA | 3322 | A | C3'-C2'-C1' | 5.44 | 105.85 | 101.50 |
| 11 | AJ | 79 | TRP | N-CA-CB | 5.43 | 120.38 | 110.60 |
| 30 | BA | 205 | VAL | CA-CB-CG1 | 5.43 | 119.05 | 110.90 |
| 78 | CA | 304 | U | C4'-C3'-C2' | -5.43 | 97.17 | 102.60 |
| 78 | CA | 1085 | G | C1'-O4'-C4' | -5.43 | 105.55 | 109.90 |
| 78 | CA | 1379 | C | OP2-P-O3' | 5.43 | 117.15 | 105.20 |
| 81 | DA | 307 | A | N9-C1'-C2' | -5.43 | 106.02 | 112.00 |
| 81 | DA | 1231 | A | O4'-C1'-N9 | 5.43 | 112.55 | 108.20 |
| 81 | DA | 1850 | A | O4'-C1'-C2' | -5.43 | 100.37 | 105.80 |
| 1 | Aa | 38 | ARG | CD-NE-CZ | 5.43 | 131.21 | 123.60 |
| 6 | AE | 177 | GLY | O-C-N | -5.43 | 114.01 | 122.70 |
| 29 | AU | 59 | GLY | N-CA-C | -5.43 | 99.52 | 113.10 |
| 74 | BQ | 249 | ALA | CA-C-O | -5.43 | 108.69 | 120.10 |
| 78 | CA | 530 | C | P-O5'-C5' | -5.43 | 112.21 | 120.90 |
| 78 | CA | 846 | G | C1'-O4'-C4' | -5.43 | 105.55 | 109.90 |
| 78 | CA | 1392 | U | P-O5'-C5' | 5.43 | 129.59 | 120.90 |
| 81 | DA | 1057 | A | C2'-C3'-O3' | 5.43 | 122.39 | 113.70 |
| 81 | DA | 2540 | A | C5-C6-N1 | -5.43 | 114.98 | 117.70 |
| 81 | DA | 2633 | U | N1-C1'-C2' | 5.43 | 121.06 | 114.00 |
| 76 | BS | 53 | VAL | N-CA-C | 5.43 | 125.67 | 111.00 |
| 77 | BI | 24 | ARG | NE-CZ-NH1 | 5.43 | 123.02 | 120.30 |
| 78 | CA | 189 | C | C1'-O4'-C4' | 5.43 | 114.25 | 109.90 |
| 81 | DA | 216 | G | C1'-O4'-C4' | -5.43 | 105.56 | 109.90 |
| 81 | DA | 498 | A | P-O5'-C5' | 5.43 | 129.59 | 120.90 |
| 81 | DA | 2196 | C | O4'-C1'-N1 | 5.43 | 112.55 | 108.20 |
| 81 | DA | 3284 | G | N9-C1'-C2' | 5.43 | 121.06 | 114.00 |
| 20 | AS | 90 | PRO | N-CD-CG | 5.43 | 111.34 | 103.20 |
| 38 | Bs | 230 | PRO | CA-C-N | 5.43 | 129.14 | 117.20 |
| 42 | BM | 88 | ARG | NE-CZ-NH2 | -5.43 | 117.59 | 120.30 |
| 48 | BW | 91 | ASP | CA-C-N | -5.43 | 105.25 | 117.20 |
| 51 | BZ | 62 | GLY | O-C-N | -5.43 | 114.01 | 122.70 |
| 55 | Bc | 112 | PRO | N-CA-C | 5.43 | 126.21 | 112.10 |
| 78 | CA | 1412 | G | C5'-C4'-C3' | 5.43 | 124.69 | 116.00 |
| 78 | CA | 1656 | U | C3'-C2'-C1' | 5.43 | 105.84 | 101.50 |
| 80 | CC | 22 | A | C5-C6-N6 | -5.43 | 119.36 | 123.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 969 | C | P-O3'-C3' | 5.43 | 126.22 | 119.70 |
| 81 | DA | 1796 | G | C3'-C2'-C1' | 5.43 | 105.84 | 101.50 |
| 81 | DA | 2370 | G | P-O3'-C3' | 5.43 | 126.22 | 119.70 |
| 81 | DA | 2382 | G | O4'-C1'-C2' | 5.43 | 112.49 | 107.60 |
| 81 | DA | 3212 | C | O4'-C1'-N1 | -5.43 | 103.86 | 108.20 |
| 81 | DA | 3219 | G | C1'-O4'-C4' | 5.43 | 114.24 | 109.90 |
| 82 | DB | 40 | A | O4'-C1'-C2' | 5.43 | 112.49 | 107.60 |
| 32 | BC | 249 | VAL | N-CA-CB | -5.43 | 99.56 | 111.50 |
| 81 | DA | 248 | U | P-O5'-C5' | 5.43 | 129.59 | 120.90 |
| 82 | DB | 8 | C | O4'-C1'-N1 | 5.43 | 112.54 | 108.20 |
| 62 | Bk | 52 | PRO | CA-N-CD | -5.43 | 103.90 | 111.50 |
| 72 | Bu | 46 | ALA | CB-CA-C | -5.43 | 101.96 | 110.10 |
| 78 | CA | 393 | C | O4'-C1'-N1 | -5.43 | 103.86 | 108.20 |
| 81 | DA | 1714 | A | O4'-C1'-N9 | 5.43 | 112.54 | 108.20 |
| 81 | DA | 1853 | U | O4'-C1'-C2' | -5.43 | 100.37 | 105.80 |
| 81 | DA | 2797 | C | O4'-C1'-N1 | 5.43 | 112.54 | 108.20 |
| 69 | Br | 57 | VAL | C-N-CA | 5.42 | 135.26 | 121.70 |
| 78 | CA | 1210 | C | C1'-O4'-C4' | -5.42 | 105.56 | 109.90 |
| 79 | CB | 19 | U | P-O3'-C3' | 5.42 | 126.21 | 119.70 |
| 81 | DA | 309 | U | O4'-C1'-N1 | 5.42 | 112.54 | 108.20 |
| 81 | DA | 736 | A | O3'-P-O5' | -5.42 | 93.69 | 104.00 |
| 81 | DA | 1298 | C | O4'-C1'-C2' | -5.42 | 100.38 | 105.80 |
| 81 | DA | 1419 | A | N9-C1'-C2' | -5.42 | 106.03 | 112.00 |
| 81 | DA | 1462 | A | O4'-C1'-N9 | 5.42 | 112.54 | 108.20 |
| 81 | DA | 2022 | G | O4'-C1'-N9 | 5.42 | 112.54 | 108.20 |
| 81 | DA | 2194 | G | P-O5'-C5' | -5.42 | 112.22 | 120.90 |
| 41 | BN | 106 | ARG | NE-CZ-NH1 | 5.42 | 123.01 | 120.30 |
| 78 | CA | 216 | U | C3'-C2'-C1' | 5.42 | 105.84 | 101.50 |
| 81 | DA | 220 | G | C5'-C4'-O4' | -5.42 | 102.59 | 109.10 |
| 81 | DA | 736 | A | C4'-C3'-O3' | 5.42 | 123.85 | 113.00 |
| 81 | DA | 2100 | A | P-O5'-C5' | 5.42 | 129.58 | 120.90 |
| 81 | DA | 2481 | G | O4'-C1'-C2' | -5.42 | 100.38 | 105.80 |
| 3 | AB | 167 | PHE | CB-CG-CD1 | 5.42 | 124.60 | 120.80 |
| 5 | AC | 114 | TYR | CG-CD1-CE1 | -5.42 | 116.96 | 121.30 |
| 9 | AH | 38 | LEU | CB-CA-C | -5.42 | 99.90 | 110.20 |
| 14 | AM | 12 | GLN | N-CA-C | -5.42 | 96.36 | 111.00 |
| 20 | AS | 8 | ASP | CA-CB-CG | 5.42 | 125.33 | 113.40 |
| 34 | BE | 53 | THR | C-N-CA | 5.42 | 135.25 | 121.70 |
| 78 | CA | 153 | G | N9-C1'-C2' | 5.42 | 121.05 | 114.00 |
| 78 | CA | 1234 | A | C5'-C4'-O4' | 5.42 | 115.61 | 109.10 |
| 81 | DA | 1301 | A | C1'-O4'-C4' | -5.42 | 105.56 | 109.90 |
| 81 | DA | 1964 | C | O4'-C1'-N1 | 5.42 | 112.54 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 83 | DC | 17 | A | O5'-C5'-C4' | 5.42 | 122.00 | 111.70 |
| 44 | BO | 129 | PHE | CB-CG-CD2 | -5.42 | 117.01 | 120.80 |
| 78 | CA | 519 | C | P-O5'-C5' | 5.42 | 129.57 | 120.90 |
| 78 | CA | 1482 | C | O5'-P-OP2 | -5.42 | 100.82 | 105.70 |
| 81 | DA | 260 | C | C5'-C4'-O4' | 5.42 | 115.60 | 109.10 |
| 81 | DA | 1179 | A | N9-C1'-C2' | -5.42 | 106.04 | 112.00 |
| 5 | AC | 47 | PHE | CB-CG-CD2 | -5.42 | 117.01 | 120.80 |
| 16 | AO | 111 | ALA | C-N-CA | 5.42 | 135.25 | 121.70 |
| 63 | Bm | 41 | PHE | N-CA-CB | -5.42 | 100.84 | 110.60 |
| 74 | BQ | 116 | ASP | N-CA-C | 5.42 | 125.63 | 111.00 |
| 78 | CA | 1503 | A | C5-C6-N1 | -5.42 | 114.99 | 117.70 |
| 81 | DA | 62 | A | C2'-C3'-O3' | 5.42 | 122.37 | 113.70 |
| 81 | DA | 275 | U | C5'-C4'-C3' | -5.42 | 107.33 | 116.00 |
| 81 | DA | 1220 | U | C2'-C3'-O3' | 5.42 | 122.37 | 113.70 |
| 81 | DA | 1868 | G | O4'-C1'-N9 | 5.42 | 112.53 | 108.20 |
| 81 | DA | 2787 | G | C1'-O4'-C4' | -5.42 | 105.56 | 109.90 |
| 81 | DA | 2909 | U | O4'-C1'-N1 | 5.42 | 112.54 | 108.20 |
| 6 | AE | 99 | LYS | N-CA-CB | 5.42 | 120.35 | 110.60 |
| 22 | AV | 67 | ASP | CB-CG-OD2 | -5.42 | 113.42 | 118.30 |
| 33 | BD | 353 | ALA | CB-CA-C | -5.42 | 101.97 | 110.10 |
| 35 | BG | 106 | PHE | N-CA-C | 5.42 | 125.62 | 111.00 |
| 58 | Bg | 26 | LYS | N-CA-CB | 5.42 | 120.35 | 110.60 |
| 73 | Bw | 16 | THR | C-N-CD | -5.42 | 108.69 | 120.60 |
| 78 | CA | 565 | C | N3-C4-C5 | -5.42 | 119.73 | 121.90 |
| 78 | CA | 824 | G | N1-C2-N3 | -5.42 | 120.65 | 123.90 |
| 81 | DA | 384 | A | C3'-C2'-C1' | 5.42 | 105.83 | 101.50 |
| 81 | DA | 2080 | C | O5'-P-OP2 | -5.42 | 100.83 | 105.70 |
| 81 | DA | 2164 | A | P-O5'-C5' | 5.42 | 129.57 | 120.90 |
| 81 | DA | 2821 | C | N1-C1'-C2' | 5.42 | 121.04 | 114.00 |
| 81 | DA | 3236 | U | O3'-P-O5' | -5.42 | 93.71 | 104.00 |
| 83 | DC | 92 | A | O3'-P-O5' | 5.42 | 114.29 | 104.00 |
| 81 | DA | 1706 | C | O4'-C1'-C2' | -5.42 | 100.39 | 105.80 |
| 29 | AU | 18 | LEU | N-CA-C | -5.41 | 96.38 | 111.00 |
| 33 | BD | 78 | GLY | N-CA-C | -5.41 | 99.56 | 113.10 |
| 53 | Ba | 21 | LYS | N-CA-C | -5.41 | 96.38 | 111.00 |
| 65 | Bn | 11 | PHE | CG-CD1-CE1 | -5.41 | 114.85 | 120.80 |
| 81 | DA | 75 | G | O4'-C1'-N9 | 5.41 | 112.53 | 108.20 |
| 81 | DA | 2547 | A | O4'-C1'-N9 | 5.41 | 112.53 | 108.20 |
| 81 | DA | 3122 | A | O4'-C4'-C3' | -5.41 | 98.59 | 104.00 |
| 83 | DC | 34 | C | C3'-C2'-C1' | 5.41 | 105.83 | 101.50 |
| 34 | BE | 59 | ILE | C-N-CA | 5.41 | 135.23 | 121.70 |
| 78 | CA | 49 | C | O4'-C1'-C2' | -5.41 | 100.39 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2706 | G | C5'-C4'-C3' | -5.41 | 107.34 | 116.00 |
| 82 | DB | 28 | C | O4'-C1'-N1 | 5.41 | 112.53 | 108.20 |
| 30 | BA | 208 | SER | CB-CA-C | 5.41 | 120.38 | 110.10 |
| 33 | BD | 309 | ARG | NE-CZ-NH1 | 5.41 | 123.01 | 120.30 |
| 35 | BG | 124 | GLU | N-CA-CB | 5.41 | 120.34 | 110.60 |
| 78 | CA | 483 | A | C5-C6-N1 | -5.41 | 115.00 | 117.70 |
| 78 | CA | 521 | A | C5'-C4'-C3' | 5.41 | 124.66 | 116.00 |
| 78 | CA | 840 | U | N1-C1'-C2' | -5.41 | 106.05 | 112.00 |
| 78 | CA | 1578 | U | C3'-C2'-C1' | -5.41 | 97.17 | 101.50 |
| 81 | DA | 627 | U | N1-C1'-C2' | 5.41 | 121.03 | 114.00 |
| 83 | DC | 48 | U | O5'-C5'-C4' | 5.41 | 121.98 | 111.70 |
| 53 | Ba | 28 | PRO | CB-CA-C | -5.41 | 98.48 | 112.00 |
| 78 | CA | 773 | C | C5'-C4'-C3' | 5.41 | 124.66 | 116.00 |
| 81 | DA | 281 | G | N9-C1'-C2' | 5.41 | 121.03 | 114.00 |
| 81 | DA | 1064 | A | C5'-C4'-C3' | 5.41 | 124.65 | 116.00 |
| 78 | CA | 110 | U | N1-C1'-C2' | 5.41 | 121.03 | 114.00 |
| 78 | CA | 868 | G | O3'-P-O5' | -5.41 | 93.73 | 104.00 |
| 81 | DA | 519 | A | C4'-C3'-C2' | -5.41 | 97.19 | 102.60 |
| 81 | DA | 922 | U | C5'-C4'-O4' | 5.41 | 115.59 | 109.10 |
| 81 | DA | 1820 | U | C5'-C4'-C3' | 5.41 | 124.65 | 116.00 |
| 81 | DA | 1953 | G | P-O5'-C5' | -5.41 | 112.25 | 120.90 |
| 81 | DA | 2032 | U | P-O5'-C5' | 5.41 | 129.55 | 120.90 |
| 78 | CA | 1306 | C | OP2-P-O3' | 5.41 | 117.09 | 105.20 |
| 78 | CA | 1648 | A | C3'-C2'-C1' | 5.41 | 105.82 | 101.50 |
| 81 | DA | 213 | A | C1'-O4'-C4' | 5.41 | 114.22 | 109.90 |
| 81 | DA | 1681 | U | O4'-C1'-C2' | -5.41 | 100.39 | 105.80 |
| 81 | DA | 2751 | G | C5'-C4'-O4' | 5.41 | 115.59 | 109.10 |
| 81 | DA | 3097 | C | O3'-P-O5' | 5.41 | 114.27 | 104.00 |
| 81 | DA | 3367 | C | C3'-C2'-C1' | 5.41 | 105.83 | 101.50 |
| 18 | AP | 55 | ASP | C-N-CA | -5.40 | 108.19 | 121.70 |
| 34 | BE | 136 | ALA | CB-CA-C | -5.40 | 101.99 | 110.10 |
| 35 | BG | 153 | PRO | CA-N-CD | 5.40 | 119.27 | 111.70 |
| 81 | DA | 1519 | G | O4'-C1'-N9 | 5.40 | 112.52 | 108.20 |
| 5 | AC | 62 | ARG | CA-CB-CG | 5.40 | 125.28 | 113.40 |
| 6 | AE | 242 | ILE | N-CA-C | -5.40 | 96.41 | 111.00 |
| 77 | BI | 88 | ARG | NE-CZ-NH2 | -5.40 | 117.60 | 120.30 |
| 78 | CA | 446 | A | N9-C1'-C2' | -5.40 | 106.06 | 112.00 |
| 78 | CA | 1427 | A | C5'-C4'-O4' | -5.40 | 102.62 | 109.10 |
| 79 | CB | 66 | C | O4'-C1'-C2' | -5.40 | 100.40 | 105.80 |
| 81 | DA | 583 | G | N9-C1'-C2' | -5.40 | 106.06 | 112.00 |
| 81 | DA | 1326 | A | O4'-C1'-N9 | 5.40 | 112.52 | 108.20 |
| 81 | DA | 1854 | C | P-O3'-C3' | -5.40 | 113.22 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1946 | A | O3'-P-O5' | -5.40 | 93.74 | 104.00 |
| 81 | DA | 2547 | A | C5-C6-N6 | -5.40 | 119.38 | 123.70 |
| 83 | DC | 107 | G | C3'-C2'-C1' | -5.40 | 97.18 | 101.50 |
| 50 | BX | 35 | PRO | N-CD-CG | 5.40 | 111.30 | 103.20 |
| 81 | DA | 1058 | U | N1-C1'-C2' | 5.40 | 121.02 | 114.00 |
| 81 | DA | 2041 | U | P-O5'-C5' | -5.40 | 112.26 | 120.90 |
| 81 | DA | 2394 | G | P-O5'-C5' | -5.40 | 112.26 | 120.90 |
| 81 | DA | 3040 | A | O4'-C1'-N9 | 5.40 | 112.52 | 108.20 |
| 81 | DA | 3046 | A | O4'-C1'-N9 | 5.40 | 112.52 | 108.20 |
| 82 | DB | 134 | G | O4'-C1'-C2' | -5.40 | 100.40 | 105.80 |
| 81 | DA | 3094 | A | O3'-P-O5' | -5.40 | 93.74 | 104.00 |
| 3 | AB | 185 | LYS | CB-CA-C | -5.40 | 99.61 | 110.40 |
| 40 | BK | 72 | HIS | N-CA-CB | 5.40 | 120.31 | 110.60 |
| 47 | BU | 114 | ALA | N-CA-CB | 5.40 | 117.66 | 110.10 |
| 78 | CA | 319 | U | O4'-C1'-N1 | 5.40 | 112.52 | 108.20 |
| 78 | CA | 667 | U | O4'-C1'-C2' | -5.40 | 100.40 | 105.80 |
| 78 | CA | 1720 | G | N9-C1'-C2' | -5.40 | 106.06 | 112.00 |
| 81 | DA | 230 | U | C1'-O4'-C4' | 5.40 | 114.22 | 109.90 |
| 81 | DA | 413 | U | O4'-C1'-C2' | -5.40 | 100.40 | 105.80 |
| 81 | DA | 462 | C | C3'-C2'-C1' | 5.40 | 105.82 | 101.50 |
| 81 | DA | 1308 | A | O4'-C1'-N9 | 5.40 | 112.52 | 108.20 |
| 81 | DA | 2270 | A | P-O3'-C3' | 5.40 | 126.18 | 119.70 |
| 81 | DA | 2653 | C | C3'-C2'-C1' | 5.40 | 105.82 | 101.50 |
| 64 | Bl | 66 | TYR | CB-CG-CD2 | -5.40 | 117.76 | 121.00 |
| 78 | CA | 554 | C | C3'-C2'-C1' | 5.40 | 105.82 | 101.50 |
| 81 | DA | 10 | C | O4'-C1'-N1 | 5.40 | 112.52 | 108.20 |
| 81 | DA | 466 | G | C1'-O4'-C4' | -5.40 | 105.58 | 109.90 |
| 81 | DA | 699 | A | N9-C1'-C2' | -5.40 | 106.06 | 112.00 |
| 81 | DA | 2438 | A | O4'-C4'-C3' | -5.40 | 98.60 | 104.00 |
| 81 | DA | 3325 | G | P-O3'-C3' | -5.40 | 113.22 | 119.70 |
| 16 | AO | 112 | LYS | CA-CB-CG | 5.39 | 125.27 | 113.40 |
| 31 | BB | 22 | LEU | CB-CA-C | -5.39 | 99.95 | 110.20 |
| 38 | Bs | 55 | LYS | N-CA-CB | 5.39 | 120.31 | 110.60 |
| 57 | Be | 183 | ASP | CB-CG-OD1 | 5.39 | 123.16 | 118.30 |
| 76 | BS | 45 | TYR | CD1-CG-CD2 | -5.39 | 111.97 | 117.90 |
| 78 | CA | 1066 | C | N3-C4-C5 | -5.39 | 119.74 | 121.90 |
| 81 | DA | 278 | U | C4'-C3'-C2' | -5.39 | 97.20 | 102.60 |
| 81 | DA | 858 | A | N9-C1'-C2' | -5.39 | 106.07 | 112.00 |
| 29 | AU | 10 | ARG | N-CA-CB | 5.39 | 120.31 | 110.60 |
| 29 | AU | 89 | TYR | CB-CG-CD2 | 5.39 | 124.24 | 121.00 |
| 44 | BO | 7 | LYS | N-CA-C | 5.39 | 125.56 | 111.00 |
| 52 | BY | 56 | VAL | N-CA-C | -5.39 | 96.44 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 60 | Bi | 74 | ARG | CD-NE-CZ | 5.39 | 131.15 | 123.60 |
| 73 | Bw | 16 | THR | CB-CA-C | -5.39 | 97.04 | 111.60 |
| 74 | BQ | 158 | ARG | N-CA-CB | 5.39 | 120.31 | 110.60 |
| 78 | CA | 50 | C | C4'-C3'-C2' | -5.39 | 97.21 | 102.60 |
| 78 | CA | 730 | G | P-O5'-C5' | 5.39 | 129.53 | 120.90 |
| 78 | CA | 1195 | C | C3'-C2'-C1' | 5.39 | 105.81 | 101.50 |
| 81 | DA | 928 | C | C1'-O4'-C4' | -5.39 | 105.59 | 109.90 |
| 81 | DA | 2201 | G | O4'-C1'-N9 | 5.39 | 112.52 | 108.20 |
| 81 | DA | 2871 | G | C3'-C2'-C1' | 5.39 | 105.81 | 101.50 |
| 83 | DC | 17 | A | O4'-C1'-C2' | -5.39 | 100.41 | 105.80 |
| 2 | AA | 41 | ARG | NE-CZ-NH2 | -5.39 | 117.61 | 120.30 |
| 53 | Ba | 21 | LYS | CB-CA-C | -5.39 | 99.62 | 110.40 |
| 81 | DA | 310 | U | C5'-C4'-O4' | -5.39 | 102.63 | 109.10 |
| 18 | AP | 122 | ILE | N-CA-C | -5.39 | 96.45 | 111.00 |
| 22 | AV | 78 | ILE | CA-CB-CG1 | -5.39 | 100.76 | 111.00 |
| 69 | Br | 47 | GLN | CB-CA-C | -5.39 | 99.62 | 110.40 |
| 78 | CA | 373 | G | C3'-C2'-C1' | -5.39 | 97.19 | 101.50 |
| 78 | CA | 1784 | C | O4'-C1'-N1 | 5.39 | 112.51 | 108.20 |
| 81 | DA | 59 | G | O4'-C1'-C2' | -5.39 | 100.41 | 105.80 |
| 81 | DA | 1876 | U | O4'-C1'-C2' | -5.39 | 100.41 | 105.80 |
| 81 | DA | 2410 | U | O4'-C1'-N1 | 5.39 | 112.51 | 108.20 |
| 78 | CA | 492 | A | O4'-C1'-N9 | 5.39 | 112.51 | 108.20 |
| 81 | DA | 1791 | C | C1'-O4'-C4' | -5.39 | 105.59 | 109.90 |
| 81 | DA | 3100 | U | O4'-C1'-C2' | -5.39 | 100.41 | 105.80 |
| 44 | BO | 125 | VAL | N-CA-C | -5.39 | 96.46 | 111.00 |
| 48 | BW | 22 | PRO | N-CD-CG | 5.39 | 111.28 | 103.20 |
| 78 | CA | 1677 | C | C3'-C2'-C1' | 5.39 | 105.81 | 101.50 |
| 78 | CA | 1703 | C | O4'-C1'-N1 | 5.39 | 112.51 | 108.20 |
| 81 | DA | 1572 | U | O4'-C1'-N1 | -5.39 | 103.89 | 108.20 |
| 22 | AV | 37 | GLN | N-CA-CB | 5.38 | 120.29 | 110.60 |
| 29 | AU | 58 | PHE | CB-CG-CD2 | -5.38 | 117.03 | 120.80 |
| 39 | BJ | 79 | SER | N-CA-CB | 5.38 | 118.58 | 110.50 |
| 78 | CA | 411 | C | O4'-C1'-C2' | -5.38 | 100.42 | 105.80 |
| 78 | CA | 1282 | U | C1'-O4'-C4' | -5.38 | 105.59 | 109.90 |
| 78 | CA | 1359 | C | O4'-C1'-N1 | 5.38 | 112.51 | 108.20 |
| 81 | DA | 222 | A | O3'-P-O5' | 5.38 | 114.23 | 104.00 |
| 81 | DA | 265 | A | P-O3'-C3' | 5.38 | 126.16 | 119.70 |
| 81 | DA | 1173 | U | O4'-C1'-N1 | 5.38 | 112.51 | 108.20 |
| 81 | DA | 2174 | G | O4'-C1'-N9 | 5.38 | 112.51 | 108.20 |
| 81 | DA | 340 | C | C3'-C2'-C1' | 5.38 | 105.81 | 101.50 |
| 81 | DA | 450 | G | C2'-C3'-O3' | 5.38 | 122.31 | 113.70 |
| 81 | DA | 804 | C | C4'-C3'-C2' | -5.38 | 97.22 | 102.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2607 | G | O4'-C4'-C3' | -5.38 | 98.62 | 104.00 |
| 81 | DA | 3088 | G | P-O3'-C3' | 5.38 | 126.16 | 119.70 |
| 1 | Aa | 285 | ALA | N-CA-CB | 5.38 | 117.63 | 110.10 |
| 4 | AD | 218 | PHE | N-CA-C | -5.38 | 96.47 | 111.00 |
| 20 | AS | 45 | MET | N-CA-CB | -5.38 | 100.91 | 110.60 |
| 49 | BV | 139 | TYR | N-CA-C | -5.38 | 96.47 | 111.00 |
| 64 | Bl | 24 | ARG | NE-CZ-NH2 | -5.38 | 117.61 | 120.30 |
| 81 | DA | 113 | C | O4'-C1'-C2' | -5.38 | 100.42 | 105.80 |
| 81 | DA | 158 | G | OP1-P-OP2 | -5.38 | 111.53 | 119.60 |
| 81 | DA | 985 | U | C5'-C4'-O4' | -5.38 | 102.64 | 109.10 |
| 83 | DC | 46 | A | P-O5'-C5' | 5.38 | 129.51 | 120.90 |
| 24 | AX | 47 | PHE | CB-CG-CD1 | 5.38 | 124.57 | 120.80 |
| 31 | BB | 67 | TYR | N-CA-C | 5.38 | 125.53 | 111.00 |
| 49 | BV | 13 | LYS | CB-CA-C | 5.38 | 121.16 | 110.40 |
| 79 | CB | 61 | C | C3'-C2'-C1' | 5.38 | 105.80 | 101.50 |
| 83 | DC | 16 | U | C4'-C3'-C2' | -5.38 | 97.22 | 102.60 |
| 32 | BC | 249 | VAL | O-C-N | -5.38 | 114.09 | 122.70 |
| 46 | BT | 55 | VAL | CB-CA-C | 5.38 | 121.62 | 111.40 |
| 63 | Bm | 33 | GLN | CB-CA-C | -5.38 | 99.64 | 110.40 |
| 78 | CA | 671 | G | O3'-P-O5' | -5.38 | 93.78 | 104.00 |
| 81 | DA | 1211 | U | O4'-C1'-N1 | 5.38 | 112.50 | 108.20 |
| 81 | DA | 1319 | G | P-O5'-C5' | 5.38 | 129.50 | 120.90 |
| 81 | DA | 1564 | U | O4'-C1'-N1 | 5.38 | 112.50 | 108.20 |
| 81 | DA | 2517 | U | C3'-C2'-C1' | 5.38 | 105.80 | 101.50 |
| 20 | AS | 90 | PRO | N-CA-CB | 5.38 | 109.75 | 103.30 |
| 35 | BG | 16 | ALA | CA-C-N | -5.38 | 105.37 | 117.20 |
| 48 | BW | 104 | ARG | NE-CZ-NH1 | 5.38 | 122.99 | 120.30 |
| 59 | Bh | 45 | ARG | CD-NE-CZ | 5.38 | 131.13 | 123.60 |
| 78 | CA | 167 | U | O4'-C1'-N1 | 5.38 | 112.50 | 108.20 |
| 78 | CA | 1680 | G | O4'-C1'-N9 | 5.38 | 112.50 | 108.20 |
| 81 | DA | 2593 | A | C1'-O4'-C4' | 5.38 | 114.20 | 109.90 |
| 2 | AA | 229 | LYS | CB-CA-C | -5.38 | 99.65 | 110.40 |
| 40 | BK | 178 | VAL | C-N-CA | -5.38 | 108.26 | 121.70 |
| 81 | DA | 1666 | G | C4'-C3'-C2' | -5.38 | 97.22 | 102.60 |
| 81 | DA | 2725 | U | O4'-C1'-N1 | 5.38 | 112.50 | 108.20 |
| 6 | AE | 43 | ARG | N-CA-C | 5.37 | 125.51 | 111.00 |
| 55 | Bc | 86 | ARG | N-CA-C | 5.37 | 125.51 | 111.00 |
| 60 | Bi | 17 | SER | N-CA-CB | 5.37 | 118.56 | 110.50 |
| 78 | CA | 342 | C | C3'-C2'-C1' | 5.37 | 105.80 | 101.50 |
| 81 | DA | 2569 | A | C5-C6-N1 | -5.37 | 115.01 | 117.70 |
| 81 | DA | 2633 | U | C3'-C2'-C1' | 5.37 | 105.80 | 101.50 |
| 10 | AI | 65 | ILE | CB-CA-C | -5.37 | 100.86 | 111.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 207 | U | C4'-C3'-C2' | -5.37 | 97.23 | 102.60 |
| 78 | CA | 580 | A | C5-C6-N6 | -5.37 | 119.40 | 123.70 |
| 78 | CA | 645 | C | C5'-C4'-O4' | -5.37 | 102.65 | 109.10 |
| 78 | CA | 905 | A | P-O5'-C5' | 5.37 | 129.50 | 120.90 |
| 78 | CA | 1692 | G | O4'-C1'-N9 | 5.37 | 112.50 | 108.20 |
| 81 | DA | 1132 | C | N1-C1'-C2' | 5.37 | 120.98 | 114.00 |
| 81 | DA | 1663 | C | C3'-C2'-C1' | 5.37 | 105.80 | 101.50 |
| 81 | DA | 2206 | G | C3'-C2'-C1' | 5.37 | 105.80 | 101.50 |
| 81 | DA | 2423 | U | N1-C1'-C2' | 5.37 | 120.98 | 114.00 |
| 81 | DA | 2636 | A | N9-C1'-C2' | 5.37 | 120.98 | 114.00 |
| 42 | BM | 65 | GLY | O-C-N | -5.37 | 114.11 | 122.70 |
| 44 | BO | 60 | TYR | CD1-CE1-CZ | 5.37 | 124.63 | 119.80 |
| 81 | DA | 1091 | A | O4'-C1'-N9 | 5.37 | 112.50 | 108.20 |
| 81 | DA | 2161 | G | O4'-C1'-N9 | 5.37 | 112.50 | 108.20 |
| 81 | DA | 2907 | G | C3'-C2'-C1' | -5.37 | 97.20 | 101.50 |
| 1 | Aa | 206 | PRO | N-CD-CG | 5.37 | 111.25 | 103.20 |
| 26 | AZ | 18 | THR | CA-C-N | 5.37 | 132.13 | 117.10 |
| 33 | BD | 98 | ARG | NE-CZ-NH2 | -5.37 | 117.62 | 120.30 |
| 33 | BD | 145 | ILE | CA-C-N | 5.37 | 132.13 | 117.10 |
| 46 | BT | 139 | VAL | CB-CA-C | 5.37 | 121.60 | 111.40 |
| 59 | Bh | 33 | ARG | NE-CZ-NH2 | -5.37 | 117.62 | 120.30 |
| 78 | CA | 889 | U | N1-C1'-C2' | 5.37 | 120.98 | 114.00 |
| 81 | DA | 295 | A | O4'-C1'-C2' | -5.37 | 100.43 | 105.80 |
| 81 | DA | 541 | U | O4'-C1'-C2' | -5.37 | 100.43 | 105.80 |
| 81 | DA | 645 | A | O3'-P-O5' | -5.37 | 93.80 | 104.00 |
| 81 | DA | 1483 | G | C1'-O4'-C4' | 5.37 | 114.19 | 109.90 |
| 81 | DA | 1918 | C | C4'-C3'-C2' | -5.37 | 97.23 | 102.60 |
| 81 | DA | 1940 | G | O4'-C1'-C2' | -5.37 | 100.43 | 105.80 |
| 81 | DA | 2216 | G | C3'-C2'-C1' | 5.37 | 105.79 | 101.50 |
| 81 | DA | 3246 | G | C5'-C4'-O4' | 5.37 | 115.54 | 109.10 |
| 83 | DC | 47 | C | O4'-C4'-C3' | -5.37 | 98.63 | 104.00 |
| 1 | Aa | 316 | MET | N-CA-CB | 5.37 | 120.26 | 110.60 |
| 22 | AV | 77 | ARG | CD-NE-CZ | -5.37 | 116.09 | 123.60 |
| 78 | CA | 934 | C | N1-C1'-C2' | -5.37 | 106.10 | 112.00 |
| 78 | CA | 1239 | U | P-O5'-C5' | 5.37 | 129.49 | 120.90 |
| 81 | DA | 2184 | U | C5'-C4'-C3' | 5.37 | 124.58 | 116.00 |
| 81 | DA | 2689 | A | C1'-O4'-C4' | -5.37 | 105.61 | 109.90 |
| 81 | DA | 2870 | C | C5'-C4'-C3' | -5.37 | 107.42 | 116.00 |
| 81 | DA | 3072 | C | C1'-O4'-C4' | -5.37 | 105.61 | 109.90 |
| 2 | AA | 182 | LEU | CB-CG-CD1 | -5.36 | 101.88 | 111.00 |
| 38 | Bs | 244 | LYS | O-C-N | 5.36 | 131.28 | 122.70 |
| 50 | BX | 94 | GLN | N-CA-CB | 5.36 | 120.25 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 59 | Bh | 23 | ASP | N-CA-C | 5.36 | 125.48 | 111.00 |
| 59 | Bh | 24 | ARG | NH1-CZ-NH2 | 5.36 | 125.30 | 119.40 |
| 81 | DA | 103 | G | C3'-C2'-C1' | 5.36 | 105.79 | 101.50 |
| 81 | DA | 1220 | U | C3'-C2'-C1' | 5.36 | 105.79 | 101.50 |
| 81 | DA | 1501 | U | O4'-C1'-N1 | 5.36 | 112.49 | 108.20 |
| 81 | DA | 1871 | U | C4'-C3'-C2' | -5.36 | 97.24 | 102.60 |
| 81 | DA | 2569 | A | C5-C6-N6 | -5.36 | 119.41 | 123.70 |
| 81 | DA | 2634 | U | P-O5'-C5' | 5.36 | 129.48 | 120.90 |
| 81 | DA | 3347 | A | C3'-C2'-C1' | 5.36 | 105.79 | 101.50 |
| 78 | CA | 1101 | G | O5'-C5'-C4' | 5.36 | 121.89 | 111.70 |
| 17 | AQ | 61 | ILE | CB-CA-C | 5.36 | 122.32 | 111.60 |
| 37 | BH | 89 | GLU | N-CA-C | -5.36 | 96.53 | 111.00 |
| 41 | BN | 6 | ILE | N-CA-C | 5.36 | 125.47 | 111.00 |
| 64 | Bl | 65 | ARG | CB-CA-C | -5.36 | 99.68 | 110.40 |
| 78 | CA | 1587 | A | P-O5'-C5' | 5.36 | 129.48 | 120.90 |
| 78 | CA | 1699 | G | O4'-C1'-N9 | 5.36 | 112.49 | 108.20 |
| 79 | CB | 71 | A | C3'-C2'-C1' | 5.36 | 105.79 | 101.50 |
| 81 | DA | 186 | U | O4'-C1'-C2' | -5.36 | 100.44 | 105.80 |
| 81 | DA | 1692 | U | O4'-C1'-C2' | 5.36 | 112.42 | 107.60 |
| 81 | DA | 2138 | A | C1'-O4'-C4' | 5.36 | 114.19 | 109.90 |
| 81 | DA | 3296 | A | C5'-C4'-O4' | 5.36 | 115.53 | 109.10 |
| 81 | DA | 3348 | G | N9-C1'-C2' | -5.36 | 106.10 | 112.00 |
| 81 | DA | 3387 | U | C4'-C3'-C2' | -5.36 | 97.24 | 102.60 |
| 31 | BB | 156 | LYS | CB-CA-C | -5.36 | 99.68 | 110.40 |
| 48 | BW | 90 | ARG | NE-CZ-NH2 | 5.36 | 122.98 | 120.30 |
| 78 | CA | 1645 | G | C3'-C2'-C1' | -5.36 | 97.21 | 101.50 |
| 81 | DA | 487 | U | OP1-P-OP2 | -5.36 | 111.56 | 119.60 |
| 81 | DA | 2626 | A | C3'-C2'-C1' | -5.36 | 97.21 | 101.50 |
| 81 | DA | 3131 | U | C3'-C2'-C1' | 5.36 | 105.79 | 101.50 |
| 46 | BT | 72 | GLU | C-N-CA | 5.36 | 133.55 | 122.30 |
| 78 | CA | 107 | C | O4'-C1'-C2' | -5.36 | 100.44 | 105.80 |
| 78 | CA | 1298 | U | O4'-C1'-N1 | -5.36 | 103.91 | 108.20 |
| 81 | DA | 1476 | G | C1'-O4'-C4' | -5.36 | 105.61 | 109.90 |
| 81 | DA | 1999 | C | O4'-C1'-C2' | -5.36 | 100.44 | 105.80 |
| 3 | AB | 76 | ARG | CA-CB-CG | 5.36 | 125.18 | 113.40 |
| 3 | AB | 125 | TYR | CB-CG-CD2 | -5.36 | 117.79 | 121.00 |
| 6 | AE | 108 | ASN | CB-CG-OD1 | -5.36 | 110.89 | 121.60 |
| 10 | AI | 142 | TYR | CB-CG-CD1 | -5.36 | 117.79 | 121.00 |
| 81 | DA | 734 | C | N3-C4-N4 | 5.36 | 121.75 | 118.00 |
| 81 | DA | 938 | C | P-O3'-C3' | 5.36 | 126.13 | 119.70 |
| 3 | AB | 201 | ALA | N-CA-C | -5.35 | 96.55 | 111.00 |
| 79 | CB | 28 | G | O3'-P-O5' | 5.35 | 114.17 | 104.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 32 | U | N1-C1'-C2' | 5.35 | 120.96 | 114.00 |
| 81 | DA | 1816 | A | P-O3'-C3' | 5.35 | 126.12 | 119.70 |
| 32 | BC | 37 | ARG | NE-CZ-NH1 | -5.35 | 117.62 | 120.30 |
| 32 | BC | 130 | PHE | CB-CG-CD2 | -5.35 | 117.05 | 120.80 |
| 43 | BP | 66 | VAL | CA-CB-CG2 | -5.35 | 102.87 | 110.90 |
| 55 | Bc | 48 | ARG | NE-CZ-NH1 | 5.35 | 122.98 | 120.30 |
| 78 | CA | 468 | A | C5'-C4'-C3' | -5.35 | 107.44 | 116.00 |
| 78 | CA | 1213 | G | C4'-C3'-C2' | -5.35 | 97.25 | 102.60 |
| 78 | CA | 1765 | A | O4'-C1'-C2' | -5.35 | 100.45 | 105.80 |
| 80 | CC | 21 | C | N3-C4-C5 | -5.35 | 119.76 | 121.90 |
| 81 | DA | 435 | C | C5'-C4'-O4' | 5.35 | 115.52 | 109.10 |
| 81 | DA | 1006 | A | O4'-C4'-C3' | -5.35 | 98.65 | 104.00 |
| 81 | DA | 1382 | G | C1'-O4'-C4' | -5.35 | 105.62 | 109.90 |
| 6 | AE | 49 | LYS | CA-CB-CG | 5.35 | 125.17 | 113.40 |
| 11 | AJ | 119 | ALA | C-N-CA | -5.35 | 108.32 | 121.70 |
| 74 | BQ | 252 | ALA | N-CA-CB | 5.35 | 117.59 | 110.10 |
| 78 | CA | 1617 | U | O4'-C4'-C3' | 5.35 | 110.38 | 106.10 |
| 81 | DA | 1238 | C | O4'-C1'-C2' | -5.35 | 100.45 | 105.80 |
| 81 | DA | 1583 | A | C3'-C2'-C1' | 5.35 | 105.78 | 101.50 |
| 81 | DA | 2684 | C | C4'-C3'-C2' | -5.35 | 97.25 | 102.60 |
| 81 | DA | 3232 | G | C4'-C3'-C2' | -5.35 | 97.25 | 102.60 |
| 38 | Bs | 177 | ASN | N-CA-CB | 5.35 | 120.23 | 110.60 |
| 40 | BK | 188 | SER | C-N-CA | 5.35 | 135.07 | 121.70 |
| 69 | Br | 44 | ASP | CB-CG-OD1 | 5.35 | 123.11 | 118.30 |
| 78 | CA | 1560 | U | P-O5'-C5' | -5.35 | 112.34 | 120.90 |
| 78 | CA | 219 | A | C5'-C4'-C3' | -5.35 | 107.44 | 116.00 |
| 81 | DA | 253 | A | O4'-C1'-C2' | -5.35 | 100.45 | 105.80 |
| 81 | DA | 862 | U | C1'-O4'-C4' | -5.35 | 105.62 | 109.90 |
| 81 | DA | 1005 | G | O4'-C4'-C3' | -5.35 | 98.65 | 104.00 |
| 81 | DA | 1411 | C | C3'-C2'-C1' | 5.35 | 105.78 | 101.50 |
| 81 | DA | 1897 | G | O4'-C1'-C2' | 5.35 | 112.41 | 107.60 |
| 81 | DA | 2195 | C | O4'-C1'-N1 | 5.35 | 112.48 | 108.20 |
| 81 | DA | 3338 | C | N1-C1'-C2' | 5.35 | 120.95 | 114.00 |
| 11 | AJ | 119 | ALA | N-CA-C | -5.35 | 96.57 | 111.00 |
| 78 | CA | 1550 | A | C5'-C4'-O4' | 5.35 | 115.52 | 109.10 |
| 81 | DA | 241 | G | C1'-O4'-C4' | -5.35 | 105.62 | 109.90 |
| 81 | DA | 2809 | C | N1-C1'-C2' | 5.35 | 120.95 | 114.00 |
| 82 | DB | 150 | G | P-O5'-C5' | -5.35 | 112.35 | 120.90 |
| 2 | AA | 74 | VAL | CA-CB-CG2 | -5.34 | 102.88 | 110.90 |
| 16 | AO | 55 | ARG | NE-CZ-NH1 | -5.34 | 117.63 | 120.30 |
| 32 | BC | 259 | HIS | CA-CB-CG | 5.34 | 122.68 | 113.60 |
| 33 | BD | 323 | VAL | CA-CB-CG2 | -5.34 | 102.88 | 110.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 61 | Bj | 26 | ASN | N-CA-CB | 5.34 | 120.22 | 110.60 |
| 64 | Bl | 5 | THR | N-CA-CB | 5.34 | 120.45 | 110.30 |
| 68 | Bq | 22 | ALA | N-CA-CB | -5.34 | 102.62 | 110.10 |
| 78 | CA | 174 | U | C1'-O4'-C4' | -5.34 | 105.62 | 109.90 |
| 78 | CA | 1260 | U | C1'-O4'-C4' | 5.34 | 114.18 | 109.90 |
| 81 | DA | 1796 | G | C5'-C4'-C3' | 5.34 | 124.55 | 116.00 |
| 81 | DA | 2410 | U | C4'-C3'-C2' | -5.34 | 97.26 | 102.60 |
| 32 | BC | 62 | ARG | NE-CZ-NH2 | 5.34 | 122.97 | 120.30 |
| 81 | DA | 270 | U | O4'-C1'-C2' | -5.34 | 100.46 | 105.80 |
| 1 | Aa | 92 | TRP | CB-CG-CD1 | 5.34 | 133.94 | 127.00 |
| 32 | BC | 119 | TYR | C-N-CA | 5.34 | 135.05 | 121.70 |
| 38 | Bs | 255 | TYR | CD1-CE1-CZ | 5.34 | 124.61 | 119.80 |
| 78 | CA | 1207 | C | N1-C1'-C2' | 5.34 | 120.94 | 114.00 |
| 81 | DA | 1737 | U | C5'-C4'-O4' | 5.34 | 115.51 | 109.10 |
| 81 | DA | 2086 | A | O4'-C1'-N9 | 5.34 | 112.47 | 108.20 |
| 29 | AU | 58 | PHE | N-CA-CB | -5.34 | 100.99 | 110.60 |
| 37 | BH | 63 | LYS | CB-CA-C | 5.34 | 121.08 | 110.40 |
| 76 | BS | 115 | ARG | CD-NE-CZ | -5.34 | 116.12 | 123.60 |
| 81 | DA | 674 | G | C4'-C3'-C2' | -5.34 | 97.26 | 102.60 |
| 81 | DA | 677 | A | N9-C1'-C2' | -5.34 | 106.13 | 112.00 |
| 81 | DA | 1324 | U | C5'-C4'-C3' | -5.34 | 107.46 | 116.00 |
| 81 | DA | 1883 | A | N9-C1'-C2' | -5.34 | 106.13 | 112.00 |
| 81 | DA | 2662 | G | C1'-O4'-C4' | -5.34 | 105.63 | 109.90 |
| 78 | CA | 1543 | A | N9-C1'-C2' | -5.34 | 106.13 | 112.00 |
| 81 | DA | 399 | A | C5'-C4'-C3' | -5.34 | 107.46 | 116.00 |
| 81 | DA | 1015 | U | O4'-C1'-C2' | -5.34 | 100.46 | 105.80 |
| 81 | DA | 1404 | G | C5'-C4'-C3' | -5.34 | 107.46 | 116.00 |
| 62 | Bk | 25 | LYS | N-CA-C | -5.34 | 96.59 | 111.00 |
| 78 | CA | 138 | A | O4'-C1'-C2' | 5.34 | 112.40 | 107.60 |
| 78 | CA | 283 | U | C1'-O4'-C4' | 5.34 | 114.17 | 109.90 |
| 81 | DA | 1262 | G | C5'-C4'-C3' | -5.34 | 107.46 | 116.00 |
| 32 | BC | 47 | LEU | N-CA-CB | 5.33 | 121.07 | 110.40 |
| 78 | CA | 888 | U | O4'-C1'-N1 | 5.33 | 112.47 | 108.20 |
| 78 | CA | 1070 | C | N3-C4-N4 | 5.33 | 121.73 | 118.00 |
| 81 | DA | 1929 | G | O4'-C1'-N9 | 5.33 | 112.47 | 108.20 |
| 64 | Bl | 5 | THR | CA-C-N | 5.33 | 132.03 | 117.10 |
| 78 | CA | 1647 | U | N1-C1'-C2' | 5.33 | 120.93 | 114.00 |
| 81 | DA | 1762 | C | N3-C4-C5 | -5.33 | 119.77 | 121.90 |
| 81 | DA | 1892 | G | O3'-P-O5' | -5.33 | 93.87 | 104.00 |
| 81 | DA | 2829 | U | N1-C1'-C2' | 5.33 | 120.93 | 114.00 |
| 5 | AC | 157 | ASP | C-N-CA | 5.33 | 135.03 | 121.70 |
| 31 | BB | 245 | LEU | C-N-CA | -5.33 | 108.37 | 121.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 41 | BN | 2 | SER | C-N-CA | -5.33 | 108.37 | 121.70 |
| 81 | DA | 666 | A | C3'-C2'-C1' | -5.33 | 97.23 | 101.50 |
| 81 | DA | 913 | A | C5'-C4'-O4' | 5.33 | 115.50 | 109.10 |
| 81 | DA | 2918 | G | C1'-O4'-C4' | -5.33 | 105.64 | 109.90 |
| 81 | DA | 3365 | U | N1-C1'-C2' | 5.33 | 120.93 | 114.00 |
| 83 | DC | 71 | C | C3'-C2'-C1' | 5.33 | 105.77 | 101.50 |
| 34 | BE | 30 | LEU | CB-CG-CD2 | 5.33 | 120.06 | 111.00 |
| 41 | BN | 5 | SER | N-CA-C | 5.33 | 125.39 | 111.00 |
| 78 | CA | 1283 | U | O4'-C1'-C2' | -5.33 | 100.47 | 105.80 |
| 81 | DA | 1887 | A | C3'-C2'-C1' | 5.33 | 105.76 | 101.50 |
| 81 | DA | 2630 | C | P-O5'-C5' | -5.33 | 112.37 | 120.90 |
| 81 | DA | 2635 | A | P-O3'-C3' | 5.33 | 126.10 | 119.70 |
| 81 | DA | 2966 | G | C3'-C2'-C1' | 5.33 | 105.76 | 101.50 |
| 81 | DA | 3086 | A | C3'-C2'-C1' | 5.33 | 105.76 | 101.50 |
| 36 | BF | 107 | ASP | CB-CG-OD2 | -5.33 | 113.50 | 118.30 |
| 78 | CA | 1655 | A | O4'-C1'-C2' | -5.33 | 100.47 | 105.80 |
| 81 | DA | 549 | U | O4'-C1'-N1 | 5.33 | 112.46 | 108.20 |
| 81 | DA | 2645 | G | O4'-C1'-C2' | 5.33 | 112.40 | 107.60 |
| 81 | DA | 3325 | G | O4'-C4'-C3' | -5.33 | 98.67 | 104.00 |
| 4 | AD | 218 | PHE | CZ-CE2-CD2 | -5.33 | 113.71 | 120.10 |
| 8 | AF | 68 | ILE | N-CA-C | -5.33 | 96.62 | 111.00 |
| 13 | AL | 16 | ARG | NE-CZ-NH2 | -5.33 | 117.64 | 120.30 |
| 35 | BG | 27 | PRO | N-CA-C | -5.33 | 98.25 | 112.10 |
| 43 | BP | 119 | TYR | CG-CD1-CE1 | -5.33 | 117.04 | 121.30 |
| 78 | CA | 154 | G | O3'-P-O5' | 5.33 | 114.12 | 104.00 |
| 78 | CA | 372 | G | C4'-C3'-C2' | -5.33 | 97.27 | 102.60 |
| 81 | DA | 1760 | A | C4-C5-C6 | 5.33 | 119.66 | 117.00 |
| 81 | DA | 2177 | G | O4'-C1'-C2' | -5.33 | 100.47 | 105.80 |
| 29 | AU | 18 | LEU | N-CA-CB | 5.33 | 121.05 | 110.40 |
| 42 | BM | 14 | SER | N-CA-CB | 5.33 | 118.49 | 110.50 |
| 50 | BX | 82 | LEU | CB-CG-CD2 | 5.33 | 120.05 | 111.00 |
| 51 | BZ | 48 | ARG | C-N-CA | 5.33 | 135.01 | 121.70 |
| 78 | CA | 1669 | U | O4'-C1'-N1 | 5.33 | 112.46 | 108.20 |
| 81 | DA | 2312 | A | C3'-C2'-C1' | 5.33 | 105.76 | 101.50 |
| 81 | DA | 2496 | C | C4'-C3'-C2' | 5.33 | 107.93 | 102.60 |
| 82 | DB | 147 | U | O4'-C1'-C2' | -5.33 | 100.47 | 105.80 |
| 18 | AP | 107 | VAL | CG1-CB-CG2 | 5.32 | 119.42 | 110.90 |
| 22 | AV | 79 | ALA | N-CA-CB | 5.32 | 117.55 | 110.10 |
| 34 | BE | 154 | THR | CA-CB-CG2 | -5.32 | 104.95 | 112.40 |
| 78 | CA | 1746 | A | N9-C1'-C2' | -5.32 | 106.14 | 112.00 |
| 81 | DA | 166 | C | C3'-C2'-C1' | 5.32 | 105.76 | 101.50 |
| 81 | DA | 1298 | C | C2'-C3'-O3' | 5.32 | 122.22 | 113.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2884 | C | C3'-C2'-C1' | 5.32 | 105.76 | 101.50 |
| 83 | DC | 10 | C | C5'-C4'-O4' | 5.32 | 115.49 | 109.10 |
| 8 | AF | 106 | LYS | N-CA-CB | 5.32 | 120.18 | 110.60 |
| 33 | BD | 241 | GLY | C-N-CA | 5.32 | 135.00 | 121.70 |
| 61 | Bj | 68 | TRP | CG-CD2-CE3 | -5.32 | 129.11 | 133.90 |
| 78 | CA | 406 | U | C1'-O4'-C4' | -5.32 | 105.64 | 109.90 |
| 81 | DA | 1073 | U | C4'-C3'-C2' | -5.32 | 97.28 | 102.60 |
| 81 | DA | 1795 | U | P-O3'-C3' | 5.32 | 126.09 | 119.70 |
| 48 | BW | 78 | TYR | CA-CB-CG | 5.32 | 123.51 | 113.40 |
| 49 | BV | 3 | ARG | CG-CD-NE | 5.32 | 122.97 | 111.80 |
| 78 | CA | 333 | A | N9-C1'-C2' | 5.32 | 120.92 | 114.00 |
| 78 | CA | 584 | C | P-O3'-C3' | -5.32 | 113.31 | 119.70 |
| 78 | CA | 650 | U | O5'-C5'-C4' | 5.32 | 121.81 | 111.70 |
| 78 | CA | 1062 | A | O4'-C1'-N9 | 5.32 | 112.46 | 108.20 |
| 78 | CA | 1535 | U | O5'-C5'-C4' | -5.32 | 101.59 | 111.70 |
| 81 | DA | 44 | U | O4'-C1'-N1 | 5.32 | 112.46 | 108.20 |
| 81 | DA | 691 | A | O4'-C1'-C2' | -5.32 | 100.48 | 105.80 |
| 81 | DA | 1102 | A | C1'-O4'-C4' | 5.32 | 114.16 | 109.90 |
| 81 | DA | 1293 | U | C4'-C3'-C2' | -5.32 | 97.28 | 102.60 |
| 81 | DA | 1754 | G | O5'-C5'-C4' | 5.32 | 121.81 | 111.70 |
| 81 | DA | 2437 | G | C2'-C3'-O3' | 5.32 | 122.21 | 113.70 |
| 81 | DA | 2491 | A | O3'-P-O5' | -5.32 | 93.89 | 104.00 |
| 35 | BG | 8 | LYS | N-CA-CB | 5.32 | 120.17 | 110.60 |
| 61 | Bj | 73 | ARG | O-C-N | -5.32 | 114.19 | 122.70 |
| 78 | CA | 1633 | A | C5-C6-N1 | -5.32 | 115.04 | 117.70 |
| 79 | CB | 56 | A | C5'-C4'-O4' | 5.32 | 115.48 | 109.10 |
| 81 | DA | 764 | U | OP1-P-O3' | 5.32 | 116.90 | 105.20 |
| 81 | DA | 2579 | G | C4-N9-C1' | -5.32 | 119.59 | 126.50 |
| 81 | DA | 2668 | U | C4'-C3'-C2' | -5.32 | 97.28 | 102.60 |
| 5 | AC | 37 | LYS | CB-CG-CD | 5.32 | 125.43 | 111.60 |
| 6 | AE | 24 | ARG | NE-CZ-NH1 | -5.32 | 117.64 | 120.30 |
| 40 | BK | 131 | PRO | CA-N-CD | -5.32 | 104.06 | 111.50 |
| 81 | DA | 413 | U | O4'-C1'-N1 | 5.32 | 112.45 | 108.20 |
| 81 | DA | 742 | G | O4'-C1'-C2' | -5.32 | 100.48 | 105.80 |
| 81 | DA | 836 | A | C1'-O4'-C4' | 5.32 | 114.15 | 109.90 |
| 81 | DA | 1889 | G | N9-C1'-C2' | 5.32 | 120.91 | 114.00 |
| 81 | DA | 2985 | C | O4'-C1'-N1 | 5.32 | 112.45 | 108.20 |
| 1 | Aa | 258 | THR | CA-CB-CG2 | 5.32 | 119.84 | 112.40 |
| 10 | AI | 48 | VAL | CG1-CB-CG2 | -5.32 | 102.39 | 110.90 |
| 32 | BC | 42 | ALA | N-CA-CB | 5.32 | 117.54 | 110.10 |
| 38 | Bs | 12 | PHE | CB-CG-CD2 | 5.32 | 124.52 | 120.80 |
| 40 | BK | 135 | TYR | N-CA-C | -5.32 | 96.65 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 53 | Ba | 71 | PHE | CB-CG-CD2 | -5.32 | 117.08 | 120.80 |
| 57 | Be | 220 | PHE | CD1-CG-CD2 | 5.32 | 125.21 | 118.30 |
| 78 | CA | 931 | C | OP1-P-OP2 | -5.32 | 111.63 | 119.60 |
| 81 | DA | 282 | G | C2'-C3'-O3' | 5.32 | 122.20 | 113.70 |
| 81 | DA | 288 | C | O4'-C1'-N1 | 5.32 | 112.45 | 108.20 |
| 81 | DA | 1285 | G | C4'-C3'-O3' | 5.32 | 123.63 | 113.00 |
| 81 | DA | 3053 | G | C1'-O4'-C4' | -5.32 | 105.65 | 109.90 |
| 33 | BD | 351 | PRO | N-CA-CB | 5.31 | 109.68 | 103.30 |
| 48 | BW | 93 | ILE | CA-CB-CG2 | 5.31 | 121.53 | 110.90 |
| 78 | CA | 1635 | A | C5-C6-N1 | -5.31 | 115.04 | 117.70 |
| 81 | DA | 1800 | A | C3'-C2'-C1' | 5.31 | 105.75 | 101.50 |
| 81 | DA | 1912 | U | C1'-O4'-C4' | -5.31 | 105.65 | 109.90 |
| 81 | DA | 2533 | G | C5-C6-O6 | -5.31 | 125.41 | 128.60 |
| 81 | DA | 2758 | A | C1'-O4'-C4' | 5.31 | 114.15 | 109.90 |
| 82 | DB | 85 | G | C3'-C2'-C1' | 5.31 | 105.75 | 101.50 |
| 1 | Aa | 166 | SER | N-CA-CB | 5.31 | 118.47 | 110.50 |
| 35 | BG | 52 | VAL | CG1-CB-CG2 | 5.31 | 119.40 | 110.90 |
| 55 | Bc | 110 | ALA | CB-CA-C | -5.31 | 102.13 | 110.10 |
| 62 | Bk | 76 | ARG | NH1-CZ-NH2 | -5.31 | 113.56 | 119.40 |
| 78 | CA | 367 | A | C4'-C3'-C2' | -5.31 | 97.29 | 102.60 |
| 78 | CA | 591 | A | C1'-O4'-C4' | -5.31 | 105.65 | 109.90 |
| 78 | CA | 821 | U | C3'-C2'-C1' | 5.31 | 105.75 | 101.50 |
| 78 | CA | 962 | C | C3'-C2'-C1' | 5.31 | 105.75 | 101.50 |
| 78 | CA | 1275 | A | C4-C5-C6 | 5.31 | 119.66 | 117.00 |
| 81 | DA | 69 | C | C5'-C4'-C3' | 5.31 | 124.50 | 116.00 |
| 81 | DA | 657 | A | O3'-P-O5' | 5.31 | 114.09 | 104.00 |
| 81 | DA | 862 | U | O4'-C1'-N1 | 5.31 | 112.45 | 108.20 |
| 81 | DA | 1912 | U | O4'-C1'-N1 | 5.31 | 112.45 | 108.20 |
| 12 | AK | 103 | ARG | NE-CZ-NH1 | -5.31 | 117.64 | 120.30 |
| 25 | AY | 31 | GLU | N-CA-CB | 5.31 | 120.16 | 110.60 |
| 31 | BB | 246 | LEU | C-N-CA | 5.31 | 134.98 | 121.70 |
| 34 | BE | 108 | GLU | CB-CA-C | -5.31 | 99.78 | 110.40 |
| 81 | DA | 1793 | C | O4'-C1'-N1 | 5.31 | 112.45 | 108.20 |
| 6 | AE | 95 | ARG | NE-CZ-NH2 | -5.31 | 117.64 | 120.30 |
| 18 | AP | 58 | CYS | CA-C-N | 5.31 | 131.97 | 117.10 |
| 32 | BC | 283 | TYR | CZ-CE2-CD2 | 5.31 | 124.58 | 119.80 |
| 35 | BG | 99 | GLU | C-N-CA | 5.31 | 134.97 | 121.70 |
| 50 | BX | 56 | ARG | NE-CZ-NH2 | -5.31 | 117.64 | 120.30 |
| 78 | CA | 423 | G | O4'-C4'-C3' | 5.31 | 110.35 | 106.10 |
| 78 | CA | 485 | A | C5-C6-N1 | -5.31 | 115.05 | 117.70 |
| 78 | CA | 547 | U | C4'-C3'-C2' | -5.31 | 97.29 | 102.60 |
| 81 | DA | 890 | C | O4'-C1'-N1 | 5.31 | 112.45 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2209 | U | C5'-C4'-O4' | -5.31 | 102.73 | 109.10 |
| 81 | DA | 2564 | G | C5-C6-O6 | -5.31 | 125.41 | 128.60 |
| 81 | DA | 3389 | U | C3'-C2'-C1' | -5.31 | 97.25 | 101.50 |
| 35 | BG | 77 | ARG | NH1-CZ-NH2 | 5.31 | 125.24 | 119.40 |
| 38 | Bs | 77 | LEU | N-CA-C | -5.31 | 96.67 | 111.00 |
| 46 | BT | 47 | ASN | CA-CB-CG | -5.31 | 101.72 | 113.40 |
| 65 | Bn | 71 | PRO | CB-CA-C | 5.31 | 125.27 | 112.00 |
| 73 | Bv | 16 | THR | C-N-CD | -5.31 | 108.92 | 120.60 |
| 78 | CA | 1037 | C | N1-C1'-C2' | 5.31 | 120.90 | 114.00 |
| 78 | CA | 1220 | C | OP2-P-O3' | 5.31 | 116.88 | 105.20 |
| 78 | CA | 1317 | C | C3'-C2'-C1' | 5.31 | 105.75 | 101.50 |
| 81 | DA | 705 | A | P-O5'-C5' | -5.31 | 112.41 | 120.90 |
| 81 | DA | 1146 | C | O4'-C1'-C2' | -5.31 | 100.49 | 105.80 |
| 81 | DA | 2197 | C | C1'-O4'-C4' | 5.31 | 114.15 | 109.90 |
| 81 | DA | 2564 | G | N3-C2-N2 | 5.31 | 123.61 | 119.90 |
| 78 | CA | 851 | U | C3'-C2'-C1' | 5.31 | 105.74 | 101.50 |
| 78 | CA | 1705 | C | C3'-C2'-C1' | 5.31 | 105.74 | 101.50 |
| 81 | DA | 3297 | U | O4'-C1'-C2' | -5.31 | 100.49 | 105.80 |
| 81 | DA | 178 | U | C2'-C3'-O3' | 5.30 | 122.19 | 113.70 |
| 81 | DA | 1154 | A | O4'-C1'-C2' | -5.30 | 100.50 | 105.80 |
| 81 | DA | 1627 | U | O4'-C4'-C3' | -5.30 | 98.70 | 104.00 |
| 81 | DA | 1691 | U | O4'-C1'-N1 | 5.30 | 112.44 | 108.20 |
| 81 | DA | 2420 | C | P-O5'-C5' | -5.30 | 112.41 | 120.90 |
| 81 | DA | 3295 | A | N9-C1'-C2' | 5.30 | 120.90 | 114.00 |
| 82 | DB | 100 | U | O4'-C1'-N1 | 5.30 | 112.44 | 108.20 |
| 78 | CA | 161 | U | O3'-P-O5' | 5.30 | 114.08 | 104.00 |
| 78 | CA | 1167 | G | N9-C1'-C2' | -5.30 | 106.17 | 112.00 |
| 34 | BE | 2 | SER | CA-CB-OG | -5.30 | 96.89 | 111.20 |
| 78 | CA | 565 | C | N3-C4-N4 | 5.30 | 121.71 | 118.00 |
| 78 | CA | 1471 | A | O4'-C1'-N9 | 5.30 | 112.44 | 108.20 |
| 81 | DA | 2080 | C | C1'-O4'-C4' | 5.30 | 114.14 | 109.90 |
| 81 | DA | 2789 | U | P-O5'-C5' | 5.30 | 129.38 | 120.90 |
| 43 | BP | 14 | LYS | N-CA-C | 5.30 | 125.31 | 111.00 |
| 64 | Bl | 20 | ASN | CB-CA-C | -5.30 | 99.80 | 110.40 |
| 78 | CA | 36 | C | N1-C1'-C2' | 5.30 | 120.89 | 114.00 |
| 81 | DA | 164 | A | C5-C6-N6 | -5.30 | 119.46 | 123.70 |
| 81 | DA | 170 | G | N9-C1'-C2' | -5.30 | 106.17 | 112.00 |
| 81 | DA | 688 | G | N9-C1'-C2' | -5.30 | 106.17 | 112.00 |
| 81 | DA | 1008 | U | O4'-C1'-C2' | -5.30 | 100.50 | 105.80 |
| 81 | DA | 2165 | G | C5'-C4'-C3' | 5.30 | 124.48 | 116.00 |
| 83 | DC | 23 | A | O4'-C1'-N9 | 5.30 | 112.44 | 108.20 |
| 17 | AQ | 129 | ASP | C-N-CA | -5.30 | 108.45 | 121.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 48 | BW | 33 | TYR | CB-CG-CD1 | -5.30 | 117.82 | 121.00 |
| 81 | DA | 2099 | A | C4'-C3'-O3' | -5.30 | 98.27 | 109.40 |
| 81 | DA | 2602 | G | O4'-C1'-C2' | 5.30 | 112.37 | 107.60 |
| 44 | BO | 59 | ARG | NE-CZ-NH1 | 5.30 | 122.95 | 120.30 |
| 76 | BS | 32 | TRP | CB-CG-CD1 | 5.30 | 133.89 | 127.00 |
| 78 | CA | 100 | A | O4'-C1'-N9 | 5.30 | 112.44 | 108.20 |
| 78 | CA | 506 | A | C4-C5-C6 | 5.30 | 119.65 | 117.00 |
| 81 | DA | 1252 | A | C3'-C2'-C1' | 5.30 | 105.74 | 101.50 |
| 81 | DA | 2958 | A | C5'-C4'-C3' | 5.30 | 124.47 | 116.00 |
| 81 | DA | 3256 | G | P-O5'-C5' | 5.30 | 129.37 | 120.90 |
| 37 | BH | 103 | ALA | CB-CA-C | -5.29 | 102.16 | 110.10 |
| 40 | BK | 186 | ALA | O-C-N | 5.29 | 131.17 | 122.70 |
| 78 | CA | 339 | C | O4'-C1'-C2' | -5.29 | 100.50 | 105.80 |
| 78 | CA | 1597 | A | C1'-O4'-C4' | -5.29 | 105.66 | 109.90 |
| 78 | CA | 1608 | U | OP1-P-O3' | 5.29 | 116.85 | 105.20 |
| 81 | DA | 498 | A | O4'-C1'-C2' | -5.29 | 100.50 | 105.80 |
| 81 | DA | 2455 | U | O4'-C1'-N1 | 5.29 | 112.44 | 108.20 |
| 82 | DB | 34 | U | C3'-C2'-C1' | 5.29 | 105.74 | 101.50 |
| 1 | Aa | 250 | TYR | CB-CG-CD1 | -5.29 | 117.82 | 121.00 |
| 26 | AZ | 40 | TYR | CB-CA-C | 5.29 | 120.99 | 110.40 |
| 37 | BH | 74 | THR | N-CA-CB | 5.29 | 120.36 | 110.30 |
| 43 | BP | 176 | LYS | N-CA-CB | -5.29 | 101.07 | 110.60 |
| 78 | CA | 405 | C | C3'-C2'-C1' | 5.29 | 105.73 | 101.50 |
| 78 | CA | 1275 | A | C5-C6-N1 | -5.29 | 115.05 | 117.70 |
| 81 | DA | 36 | C | C3'-C2'-C1' | 5.29 | 105.73 | 101.50 |
| 81 | DA | 524 | U | P-O3'-C3' | 5.29 | 126.05 | 119.70 |
| 81 | DA | 2479 | C | C5'-C4'-C3' | 5.29 | 124.47 | 116.00 |
| 81 | DA | 3246 | G | P-O5'-C5' | 5.29 | 129.37 | 120.90 |
| 33 | BD | 142 | VAL | CA-CB-CG2 | 5.29 | 118.84 | 110.90 |
| 43 | BP | 13 | LYS | O-C-N | -5.29 | 114.23 | 122.70 |
| 72 | Bu | 43 | ASP | N-CA-CB | 5.29 | 120.12 | 110.60 |
| 78 | CA | 218 | A | O4'-C1'-N9 | -5.29 | 103.97 | 108.20 |
| 81 | DA | 779 | G | C5'-C4'-C3' | -5.29 | 107.53 | 116.00 |
| 81 | DA | 2367 | A | O3'-P-O5' | 5.29 | 114.05 | 104.00 |
| 82 | DB | 4 | C | C1'-O4'-C4' | -5.29 | 105.67 | 109.90 |
| 5 | AC | 164 | PHE | CA-C-O | -5.29 | 108.99 | 120.10 |
| 34 | BE | 52 | TYR | O-C-N | -5.29 | 114.23 | 122.70 |
| 50 | BX | 40 | LEU | CB-CG-CD2 | 5.29 | 119.99 | 111.00 |
| 78 | CA | 514 | G | C5'-C4'-C3' | -5.29 | 107.54 | 116.00 |
| 81 | DA | 1982 | G | O4'-C1'-N9 | 5.29 | 112.43 | 108.20 |
| 81 | DA | 2787 | G | O4'-C1'-N9 | 5.29 | 112.43 | 108.20 |
| 16 | AO | 113 | PHE | CB-CG-CD1 | -5.29 | 117.10 | 120.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 466 | U | C5'-C4'-C3' | -5.29 | 107.54 | 116.00 |
| 78 | CA | 669 | G | C5'-C4'-C3' | -5.29 | 107.54 | 116.00 |
| 79 | CB | 3 | C | O4'-C1'-N1 | 5.29 | 112.43 | 108.20 |
| 81 | DA | 502 | U | O4'-C1'-C2' | -5.29 | 100.51 | 105.80 |
| 81 | DA | 1272 | C | P-O5'-C5' | -5.29 | 112.44 | 120.90 |
| 81 | DA | 1847 | A | O4'-C1'-C2' | -5.29 | 100.51 | 105.80 |
| 81 | DA | 2201 | G | C4'-C3'-C2' | -5.29 | 97.31 | 102.60 |
| 78 | CA | 314 | C | N1-C1'-C2' | 5.29 | 120.87 | 114.00 |
| 79 | CB | 21 | A | P-O5'-C5' | 5.29 | 129.36 | 120.90 |
| 81 | DA | 2533 | G | O4'-C1'-N9 | 5.29 | 112.43 | 108.20 |
| 81 | DA | 2578 | U | O3'-P-O5' | -5.29 | 93.95 | 104.00 |
| 62 | Bk | 96 | ALA | CB-CA-C | -5.29 | 102.17 | 110.10 |
| 78 | CA | 960 | U | C4'-C3'-C2' | -5.29 | 97.31 | 102.60 |
| 78 | CA | 1264 | G | C5'-C4'-O4' | -5.29 | 102.76 | 109.10 |
| 78 | CA | 1267 | G | C1'-O4'-C4' | -5.29 | 105.67 | 109.90 |
| 81 | DA | 33 | G | C1'-O4'-C4' | -5.29 | 105.67 | 109.90 |
| 81 | DA | 42 | C | C5'-C4'-C3' | -5.29 | 107.54 | 116.00 |
| 81 | DA | 734 | C | N3-C4-C5 | -5.29 | 119.79 | 121.90 |
| 81 | DA | 1388 | U | C4'-C3'-C2' | -5.29 | 97.31 | 102.60 |
| 81 | DA | 1683 | A | P-O3'-C3' | 5.29 | 126.04 | 119.70 |
| 81 | DA | 1696 | A | C1'-O4'-C4' | -5.29 | 105.67 | 109.90 |
| 81 | DA | 2854 | U | C4'-C3'-C2' | -5.29 | 97.31 | 102.60 |
| 81 | DA | 3124 | G | P-O3'-C3' | -5.29 | 113.36 | 119.70 |
| 14 | AM | 88 | ARG | CA-C-N | 5.28 | 128.82 | 117.20 |
| 37 | BH | 108 | ARG | N-CA-CB | 5.28 | 120.11 | 110.60 |
| 40 | BK | 129 | LEU | N-CA-CB | 5.28 | 120.97 | 110.40 |
| 45 | BR | 13 | SER | CA-C-N | -5.28 | 105.63 | 116.20 |
| 53 | Ba | 95 | VAL | CG1-CB-CG2 | -5.28 | 102.45 | 110.90 |
| 59 | Bh | 26 | HIS | C-N-CA | 5.28 | 134.91 | 121.70 |
| 78 | CA | 833 | U | C5'-C4'-O4' | 5.28 | 115.44 | 109.10 |
| 81 | DA | 1230 | G | C4'-C3'-C2' | 5.28 | 107.88 | 102.60 |
| 81 | DA | 1807 | G | O3'-P-O5' | 5.28 | 114.04 | 104.00 |
| 81 | DA | 1876 | U | C3'-C2'-C1' | 5.28 | 105.73 | 101.50 |
| 81 | DA | 2205 | U | C3'-C2'-C1' | 5.28 | 105.73 | 101.50 |
| 81 | DA | 2312 | A | P-O3'-C3' | 5.28 | 126.04 | 119.70 |
| 81 | DA | 3034 | C | C5'-C4'-C3' | -5.28 | 107.55 | 116.00 |
| 83 | DC | 106 | G | O4'-C1'-N9 | 5.28 | 112.43 | 108.20 |
| 13 | AL | 6 | PRO | N-CA-CB | 5.28 | 109.64 | 103.30 |
| 16 | AO | 109 | LYS | N-CA-C | 5.28 | 125.26 | 111.00 |
| 81 | DA | 2264 | U | P-O3'-C3' | -5.28 | 113.36 | 119.70 |
| 47 | BU | 137 | GLU | N-CA-C | -5.28 | 96.74 | 111.00 |
| 52 | BY | 20 | PHE | N-CA-CB | 5.28 | 120.11 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 396 | A | C3'-C2'-C1' | 5.28 | 105.72 | 101.50 |
| 81 | DA | 415 | G | N9-C1'-C2' | 5.28 | 120.86 | 114.00 |
| 81 | DA | 724 | U | O4'-C1'-C2' | -5.28 | 100.52 | 105.80 |
| 81 | DA | 1473 | G | C1'-O4'-C4' | -5.28 | 105.68 | 109.90 |
| 81 | DA | 1885 | U | C5'-C4'-O4' | -5.28 | 102.76 | 109.10 |
| 5 | AC | 18 | PRO | N-CA-CB | 5.28 | 109.64 | 103.30 |
| 6 | AE | 84 | LYS | N-CA-CB | 5.28 | 120.10 | 110.60 |
| 78 | CA | 1664 | C | O4'-C1'-N1 | 5.28 | 112.42 | 108.20 |
| 81 | DA | 561 | C | N1-C1'-C2' | 5.28 | 120.86 | 114.00 |
| 81 | DA | 736 | A | C5-C6-N1 | -5.28 | 115.06 | 117.70 |
| 81 | DA | 840 | C | O4'-C1'-N1 | 5.28 | 112.42 | 108.20 |
| 81 | DA | 1141 | C | C3'-C2'-C1' | 5.28 | 105.72 | 101.50 |
| 81 | DA | 2830 | G | O4'-C4'-C3' | -5.28 | 98.72 | 104.00 |
| 9 | AH | 96 | ALA | N-CA-CB | 5.28 | 117.49 | 110.10 |
| 78 | CA | 1323 | C | N1-C1'-C2' | 5.28 | 120.86 | 114.00 |
| 78 | CA | 1777 | G | O4'-C1'-N9 | 5.28 | 112.42 | 108.20 |
| 81 | DA | 2075 | C | C3'-C2'-C1' | 5.28 | 105.72 | 101.50 |
| 81 | DA | 2200 | U | N1-C1'-C2' | 5.28 | 120.86 | 114.00 |
| 81 | DA | 2900 | A | P-O5'-C5' | 5.28 | 129.34 | 120.90 |
| 82 | DB | 93 | U | O4'-C1'-C2' | -5.28 | 100.52 | 105.80 |
| 83 | DC | 107 | G | C4'-C3'-C2' | -5.28 | 97.32 | 102.60 |
| 31 | BB | 25 | GLY | C-N-CA | 5.28 | 134.89 | 121.70 |
| 37 | BH | 62 | LYS | C-N-CA | 5.28 | 134.89 | 121.70 |
| 43 | BP | 181 | ASN | CB-CA-C | -5.28 | 99.85 | 110.40 |
| 76 | BS | 26 | ILE | N-CA-CB | -5.28 | 98.67 | 110.80 |
| 78 | CA | 122 | U | C5'-C4'-O4' | 5.28 | 115.43 | 109.10 |
| 81 | DA | 724 | U | N1-C1'-C2' | 5.28 | 120.86 | 114.00 |
| 81 | DA | 1703 | U | C1'-O4'-C4' | 5.28 | 114.12 | 109.90 |
| 81 | DA | 3233 | C | C3'-C2'-C1' | 5.28 | 105.72 | 101.50 |
| 81 | DA | 3258 | U | C5'-C4'-C3' | 5.28 | 124.44 | 116.00 |
| 9 | AH | 98 | GLN | O-C-N | 5.27 | 131.14 | 122.70 |
| 11 | AJ | 60 | THR | N-CA-CB | 5.27 | 120.32 | 110.30 |
| 76 | BS | 66 | ILE | C-N-CA | -5.27 | 108.52 | 121.70 |
| 78 | CA | 1197 | C | C5'-C4'-O4' | 5.27 | 115.43 | 109.10 |
| 81 | DA | 1581 | C | O4'-C1'-C2' | -5.27 | 100.53 | 105.80 |
| 22 | AV | 29 | LYS | CA-C-O | -5.27 | 109.03 | 120.10 |
| 41 | BN | 100 | ALA | C-N-CA | 5.27 | 134.88 | 121.70 |
| 78 | CA | 1595 | U | P-O3'-C3' | 5.27 | 126.03 | 119.70 |
| 81 | DA | 136 | G | C1'-O4'-C4' | -5.27 | 105.68 | 109.90 |
| 81 | DA | 198 | A | C1'-O4'-C4' | 5.27 | 114.12 | 109.90 |
| 81 | DA | 215 | G | O4'-C1'-N9 | 5.27 | 112.42 | 108.20 |
| 81 | DA | 1738 | C | P-O3'-C3' | -5.27 | 113.37 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 83 | DC | 67 | C | O4'-C1'-C2' | -5.27 | 100.53 | 105.80 |
| 78 | CA | 284 | G | C1'-O4'-C4' | 5.27 | 114.12 | 109.90 |
| 81 | DA | 1490 | A | O4'-C1'-N9 | 5.27 | 112.42 | 108.20 |
| 81 | DA | 1826 | C | C5'-C4'-C3' | 5.27 | 124.43 | 116.00 |
| 81 | DA | 2065 | U | N1-C1'-C2' | 5.27 | 120.85 | 114.00 |
| 3 | AB | 190 | ARG | NE-CZ-NH2 | -5.27 | 117.67 | 120.30 |
| 4 | AD | 47 | PHE | CB-CG-CD2 | -5.27 | 117.11 | 120.80 |
| 37 | BH | 61 | GLN | CA-C-O | -5.27 | 109.03 | 120.10 |
| 45 | BR | 80 | THR | N-CA-CB | 5.27 | 120.31 | 110.30 |
| 52 | BY | 74 | TYR | N-CA-C | -5.27 | 96.77 | 111.00 |
| 78 | CA | 846 | G | O4'-C1'-N9 | 5.27 | 112.42 | 108.20 |
| 81 | DA | 627 | U | C5'-C4'-C3' | 5.27 | 124.43 | 116.00 |
| 81 | DA | 1107 | C | P-O5'-C5' | 5.27 | 129.33 | 120.90 |
| 81 | DA | 2758 | A | N9-C1'-C2' | -5.27 | 106.20 | 112.00 |
| 83 | DC | 76 | U | C1'-O4'-C4' | 5.27 | 114.11 | 109.90 |
| 4 | AD | 138 | TYR | CB-CG-CD1 | -5.27 | 117.84 | 121.00 |
| 16 | AO | 80 | LEU | C-N-CA | 5.27 | 134.87 | 121.70 |
| 30 | BA | 168 | ALA | N-CA-CB | 5.27 | 117.47 | 110.10 |
| 42 | BM | 46 | LEU | C-N-CA | 5.27 | 134.87 | 121.70 |
| 46 | BT | 55 | VAL | N-CA-CB | 5.27 | 123.09 | 111.50 |
| 63 | Bm | 41 | PHE | CB-CG-CD2 | -5.27 | 117.11 | 120.80 |
| 74 | BQ | 237 | GLU | N-CA-C | -5.27 | 96.78 | 111.00 |
| 78 | CA | 348 | U | C4'-C3'-C2' | -5.27 | 97.33 | 102.60 |
| 78 | CA | 590 | C | C3'-C2'-C1' | 5.27 | 105.71 | 101.50 |
| 78 | CA | 842 | C | C5-C6-N1 | 5.27 | 123.63 | 121.00 |
| 78 | CA | 1085 | G | P-O3'-C3' | -5.27 | 113.38 | 119.70 |
| 81 | DA | 841 | A | N9-C1'-C2' | 5.27 | 120.85 | 114.00 |
| 81 | DA | 1109 | U | O4'-C1'-C2' | -5.27 | 100.53 | 105.80 |
| 81 | DA | 3327 | G | C4'-C3'-C2' | -5.27 | 97.33 | 102.60 |
| 3 | AB | 152 | PHE | CB-CG-CD2 | 5.27 | 124.49 | 120.80 |
| 47 | BU | 84 | TYR | CD1-CG-CD2 | 5.27 | 123.69 | 117.90 |
| 81 | DA | 3007 | U | O4'-C1'-N1 | 5.27 | 112.41 | 108.20 |
| 16 | AO | 65 | VAL | N-CA-CB | 5.26 | 123.08 | 111.50 |
| 29 | AU | 31 | ASN | N-CA-CB | 5.26 | 120.08 | 110.60 |
| 30 | BA | 53 | LEU | CB-CG-CD1 | -5.26 | 102.05 | 111.00 |
| 64 | Bl | 11 | ARG | O-C-N | -5.26 | 114.28 | 122.70 |
| 74 | BQ | 239 | ILE | N-CA-CB | -5.26 | 98.69 | 110.80 |
| 78 | CA | 1471 | A | C5'-C4'-C3' | -5.26 | 107.58 | 116.00 |
| 81 | DA | 1598 | G | O5'-C5'-C4' | 5.26 | 121.70 | 111.70 |
| 81 | DA | 1767 | C | C4'-C3'-C2' | -5.26 | 97.34 | 102.60 |
| 81 | DA | 2119 | A | C5'-C4'-O4' | 5.26 | 115.42 | 109.10 |
| 81 | DA | 2286 | U | O4'-C1'-N1 | 5.26 | 112.41 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2621 | G | N9-C1'-C2' | 5.26 | 120.84 | 114.00 |
| 15 | AN | 20 | GLN | O-C-N | -5.26 | 114.28 | 122.70 |
| 53 | Ba | 66 | THR | CA-CB-CG2 | -5.26 | 105.03 | 112.40 |
| 81 | DA | 820 | A | O4'-C1'-C2' | -5.26 | 100.54 | 105.80 |
| 47 | BU | 48 | ILE | C-N-CA | 5.26 | 134.85 | 121.70 |
| 62 | Bk | 83 | ALA | N-CA-C | 5.26 | 125.20 | 111.00 |
| 78 | CA | 1117 | U | C5'-C4'-C3' | 5.26 | 124.42 | 116.00 |
| 78 | CA | 1294 | G | P-O3'-C3' | -5.26 | 113.39 | 119.70 |
| 78 | CA | 1571 | C | P-O5'-C5' | -5.26 | 112.48 | 120.90 |
| 81 | DA | 32 | U | C5'-C4'-C3' | 5.26 | 124.42 | 116.00 |
| 81 | DA | 285 | A | P-O3'-C3' | -5.26 | 113.39 | 119.70 |
| 81 | DA | 1335 | C | C4'-C3'-C2' | -5.26 | 97.34 | 102.60 |
| 22 | AV | 71 | ILE | N-CA-C | -5.26 | 96.80 | 111.00 |
| 32 | BC | 10 | ARG | NE-CZ-NH2 | -5.26 | 117.67 | 120.30 |
| 32 | BC | 369 | ARG | NE-CZ-NH1 | 5.26 | 122.93 | 120.30 |
| 41 | BN | 108 | ARG | CA-C-O | 5.26 | 131.14 | 120.10 |
| 62 | Bk | 57 | LEU | CB-CG-CD2 | 5.26 | 119.94 | 111.00 |
| 78 | CA | 1235 | C | C5'-C4'-C3' | 5.26 | 124.42 | 116.00 |
| 78 | CA | 1476 | C | O4'-C1'-N1 | 5.26 | 112.41 | 108.20 |
| 81 | DA | 560 | G | C1'-O4'-C4' | 5.26 | 114.11 | 109.90 |
| 81 | DA | 984 | G | C5'-C4'-C3' | 5.26 | 124.42 | 116.00 |
| 81 | DA | 127 | G | C1'-O4'-C4' | -5.26 | 105.69 | 109.90 |
| 81 | DA | 2114 | C | C4'-C3'-O3' | 5.26 | 123.52 | 113.00 |
| 82 | DB | 73 | U | P-O5'-C5' | 5.26 | 129.31 | 120.90 |
| 6 | AE | 197 | TYR | CG-CD1-CE1 | -5.26 | 117.09 | 121.30 |
| 20 | AS | 57 | ARG | NE-CZ-NH1 | 5.26 | 122.93 | 120.30 |
| 60 | Bi | 42 | PRO | CA-C-N | 5.26 | 128.76 | 117.20 |
| 78 | CA | 889 | U | C3'-C2'-C1' | 5.26 | 105.70 | 101.50 |
| 78 | CA | 1420 | C | N1-C1'-C2' | 5.26 | 120.83 | 114.00 |
| 78 | CA | 1529 | C | C1'-O4'-C4' | -5.26 | 105.69 | 109.90 |
| 81 | DA | 606 | C | O4'-C1'-N1 | 5.26 | 112.41 | 108.20 |
| 81 | DA | 808 | A | P-O3'-C3' | 5.26 | 126.01 | 119.70 |
| 81 | DA | 2839 | G | C1'-O4'-C4' | -5.26 | 105.69 | 109.90 |
| 81 | DA | 2916 | U | O4'-C1'-C2' | -5.26 | 100.54 | 105.80 |
| 83 | DC | 30 | G | O4'-C1'-C2' | 5.26 | 112.33 | 107.60 |
| 5 | AC | 57 | ARG | NE-CZ-NH2 | -5.25 | 117.67 | 120.30 |
| 20 | AS | 91 | TYR | CA-C-N | -5.25 | 105.64 | 117.20 |
| 40 | BK | 147 | TRP | CB-CA-C | -5.25 | 99.89 | 110.40 |
| 78 | CA | 1577 | A | O4'-C1'-C2' | -5.25 | 100.55 | 105.80 |
| 10 | AI | 140 | LYS | CB-CA-C | -5.25 | 99.89 | 110.40 |
| 20 | AS | 30 | VAL | CA-C-O | -5.25 | 109.07 | 120.10 |
| 35 | BG | 2 | SER | CB-CA-C | 5.25 | 120.08 | 110.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 868 | G | P-O5'-C5' | -5.25 | 112.49 | 120.90 |
| 81 | DA | 448 | U | C5'-C4'-C3' | -5.25 | 107.59 | 116.00 |
| 81 | DA | 1491 | A | O4'-C1'-N9 | 5.25 | 112.40 | 108.20 |
| 81 | DA | 2464 | U | O4'-C1'-N1 | 5.25 | 112.40 | 108.20 |
| 81 | DA | 2760 | C | C4'-C3'-O3' | 5.25 | 123.51 | 113.00 |
| 81 | DA | 2773 | C | O4'-C1'-N1 | 5.25 | 112.40 | 108.20 |
| 11 | AJ | 64 | LYS | N-CA-CB | 5.25 | 120.05 | 110.60 |
| 30 | BA | 161 | LYS | N-CA-CB | 5.25 | 120.05 | 110.60 |
| 69 | Br | 99 | GLN | N-CA-C | -5.25 | 96.82 | 111.00 |
| 78 | CA | 308 | C | O4'-C1'-C2' | -5.25 | 100.55 | 105.80 |
| 78 | CA | 1476 | C | O3'-P-O5' | 5.25 | 113.98 | 104.00 |
| 81 | DA | 637 | C | C4'-C3'-O3' | 5.25 | 123.50 | 113.00 |
| 81 | DA | 1003 | A | C5'-C4'-O4' | 5.25 | 115.40 | 109.10 |
| 81 | DA | 2151 | C | O4'-C1'-C2' | -5.25 | 100.55 | 105.80 |
| 81 | DA | 2221 | G | C5'-C4'-O4' | -5.25 | 102.80 | 109.10 |
| 81 | DA | 2272 | G | N9-C1'-C2' | -5.25 | 106.22 | 112.00 |
| 8 | AF | 215 | ASP | CB-CG-OD2 | -5.25 | 113.58 | 118.30 |
| 15 | AN | 9 | SER | CB-CA-C | 5.25 | 120.08 | 110.10 |
| 54 | Bd | 52 | LYS | CB-CG-CD | 5.25 | 125.25 | 111.60 |
| 78 | CA | 1648 | A | C1'-O4'-C4' | -5.25 | 105.70 | 109.90 |
| 81 | DA | 1975 | C | C5'-C4'-C3' | 5.25 | 124.40 | 116.00 |
| 82 | DB | 32 | C | O4'-C1'-C2' | -5.25 | 100.55 | 105.80 |
| 1 | Aa | 302 | PHE | CB-CG-CD1 | -5.25 | 117.13 | 120.80 |
| 37 | BH | 232 | HIS | CA-C-N | 5.25 | 128.75 | 117.20 |
| 72 | Bt | 56 | ASP | CB-CG-OD2 | 5.25 | 123.02 | 118.30 |
| 78 | CA | 1051 | G | N1-C2-N3 | -5.25 | 120.75 | 123.90 |
| 78 | CA | 1393 | C | C4'-C3'-O3' | 5.25 | 123.50 | 113.00 |
| 78 | CA | 1416 | G | O4'-C1'-N9 | 5.25 | 112.40 | 108.20 |
| 78 | CA | 1475 | A | O4'-C4'-C3' | -5.25 | 98.75 | 104.00 |
| 81 | DA | 57 | A | O4'-C1'-N9 | 5.25 | 112.40 | 108.20 |
| 81 | DA | 1761 | C | N3-C4-N4 | 5.25 | 121.67 | 118.00 |
| 81 | DA | 2321 | A | O4'-C1'-N9 | 5.25 | 112.40 | 108.20 |
| 3 | AB | 215 | GLU | N-CA-C | -5.25 | 96.83 | 111.00 |
| 51 | BZ | 66 | GLU | N-CA-CB | 5.25 | 120.04 | 110.60 |
| 69 | Br | 59 | HIS | CA-CB-CG | -5.25 | 104.68 | 113.60 |
| 78 | CA | 214 | G | O4'-C1'-N9 | 5.25 | 112.40 | 108.20 |
| 78 | CA | 216 | U | P-O3'-C3' | 5.25 | 126.00 | 119.70 |
| 78 | CA | 578 | U | O4'-C1'-N1 | 5.25 | 112.40 | 108.20 |
| 78 | CA | 1436 | A | C2'-C3'-O3' | 5.25 | 122.09 | 113.70 |
| 81 | DA | 1647 | A | P-O3'-C3' | 5.25 | 126.00 | 119.70 |
| 81 | DA | 1933 | A | O4'-C1'-C2' | -5.25 | 100.55 | 105.80 |
| 81 | DA | 2933 | A | C3'-C2'-C1' | 5.25 | 105.70 | 101.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 82 | DB | 92 | A | P-O5'-C5' | 5.25 | 129.30 | 120.90 |
| 1 | Aa | 75 | ALA | CB-CA-C | -5.25 | 102.23 | 110.10 |
| 2 | AA | 45 | VAL | CG1-CB-CG2 | 5.25 | 119.29 | 110.90 |
| 43 | BP | 179 | LYS | CA-C-O | -5.25 | 109.09 | 120.10 |
| 72 | Bt | 58 | LEU | CB-CA-C | -5.25 | 100.23 | 110.20 |
| 81 | DA | 61 | A | O4'-C1'-N9 | 5.25 | 112.40 | 108.20 |
| 81 | DA | 1096 | U | P-O3'-C3' | 5.25 | 125.99 | 119.70 |
| 81 | DA | 2360 | C | C1'-O4'-C4' | -5.25 | 105.70 | 109.90 |
| 81 | DA | 2904 | U | C3'-C2'-C1' | 5.25 | 105.70 | 101.50 |
| 81 | DA | 2964 | G | C4'-C3'-C2' | -5.25 | 97.36 | 102.60 |
| 83 | DC | 38 | U | C3'-C2'-C1' | -5.25 | 97.30 | 101.50 |
| 35 | BG | 142 | ASP | N-CA-C | -5.24 | 96.84 | 111.00 |
| 78 | CA | 1728 | A | O4'-C1'-N9 | 5.24 | 112.39 | 108.20 |
| 81 | DA | 444 | U | N1-C1'-C2' | 5.24 | 120.82 | 114.00 |
| 81 | DA | 1668 | G | O3'-P-O5' | 5.24 | 113.96 | 104.00 |
| 17 | AQ | 45 | ARG | NE-CZ-NH1 | 5.24 | 122.92 | 120.30 |
| 36 | BF | 129 | ARG | NE-CZ-NH2 | -5.24 | 117.68 | 120.30 |
| 81 | DA | 1250 | G | O4'-C1'-C2' | -5.24 | 100.56 | 105.80 |
| 4 | AD | 54 | TYR | CD1-CE1-CZ | 5.24 | 124.52 | 119.80 |
| 5 | AC | 118 | LEU | CB-CA-C | 5.24 | 120.16 | 110.20 |
| 11 | AJ | 84 | MET | N-CA-CB | 5.24 | 120.03 | 110.60 |
| 14 | AM | 88 | ARG | C-N-CA | 5.24 | 134.80 | 121.70 |
| 21 | AT | 46 | ILE | N-CA-C | -5.24 | 96.85 | 111.00 |
| 32 | BC | 60 | LEU | CB-CA-C | 5.24 | 120.16 | 110.20 |
| 39 | BJ | 51 | LYS | N-CA-CB | 5.24 | 120.03 | 110.60 |
| 57 | Be | 151 | ARG | CD-NE-CZ | -5.24 | 116.27 | 123.60 |
| 76 | BS | 118 | VAL | CA-CB-CG1 | 5.24 | 118.76 | 110.90 |
| 78 | CA | 1681 | A | O3'-P-O5' | -5.24 | 94.04 | 104.00 |
| 81 | DA | 102 | C | N1-C1'-C2' | 5.24 | 120.81 | 114.00 |
| 81 | DA | 721 | G | C1'-O4'-C4' | 5.24 | 114.09 | 109.90 |
| 81 | DA | 1338 | C | O4'-C1'-C2' | -5.24 | 100.56 | 105.80 |
| 81 | DA | 1616 | U | N1-C1'-C2' | 5.24 | 120.81 | 114.00 |
| 81 | DA | 1902 | G | O4'-C1'-C2' | 5.24 | 112.32 | 107.60 |
| 81 | DA | 2870 | C | O4'-C1'-C2' | -5.24 | 100.56 | 105.80 |
| 82 | DB | 28 | C | C3'-C2'-C1' | 5.24 | 105.69 | 101.50 |
| 5 | AC | 127 | VAL | CB-CA-C | 5.24 | 121.35 | 111.40 |
| 69 | Br | 79 | THR | N-CA-C | -5.24 | 96.86 | 111.00 |
| 74 | BQ | 31 | TYR | CB-CG-CD1 | 5.24 | 124.14 | 121.00 |
| 78 | CA | 1547 | A | C4'-C3'-C2' | -5.24 | 97.36 | 102.60 |
| 81 | DA | 1131 | G | C4'-C3'-C2' | 5.24 | 107.84 | 102.60 |
| 81 | DA | 1171 | G | O3'-P-O5' | 5.24 | 113.95 | 104.00 |
| 81 | DA | 2565 | U | C4'-C3'-C2' | -5.24 | 97.36 | 102.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2745 | G | C1'-O4'-C4' | 5.24 | 114.09 | 109.90 |
| 78 | CA | 856 | A | C3'-C2'-C1' | -5.24 | 97.31 | 101.50 |
| 78 | CA | 1498 | G | O4'-C1'-N9 | 5.24 | 112.39 | 108.20 |
| 81 | DA | 838 | G | C5'-C4'-C3' | 5.24 | 124.38 | 116.00 |
| 33 | BD | 352 | ALA | C-N-CA | -5.24 | 108.61 | 121.70 |
| 44 | BO | 14 | HIS | N-CA-CB | 5.24 | 120.02 | 110.60 |
| 44 | BO | 60 | TYR | CB-CG-CD2 | -5.24 | 117.86 | 121.00 |
| 78 | CA | 618 | U | C3'-C2'-C1' | 5.24 | 105.69 | 101.50 |
| 78 | CA | 1339 | C | C5'-C4'-C3' | -5.24 | 107.62 | 116.00 |
| 79 | CB | 41 | G | P-O3'-C3' | 5.24 | 125.98 | 119.70 |
| 79 | CB | 69 | G | C1'-O4'-C4' | -5.24 | 105.71 | 109.90 |
| 81 | DA | 239 | G | C3'-C2'-C1' | -5.24 | 97.31 | 101.50 |
| 81 | DA | 513 | G | C5'-C4'-O4' | 5.24 | 115.38 | 109.10 |
| 81 | DA | 2176 | U | C5'-C4'-C3' | 5.24 | 124.38 | 116.00 |
| 81 | DA | 2539 | C | N3-C4-C5 | -5.24 | 119.81 | 121.90 |
| 81 | DA | 2627 | C | O4'-C1'-C2' | -5.24 | 100.56 | 105.80 |
| 81 | DA | 2868 | U | O4'-C1'-N1 | 5.24 | 112.39 | 108.20 |
| 81 | DA | 3350 | C | O4'-C4'-C3' | -5.24 | 98.77 | 104.00 |
| 83 | DC | 28 | C | C5'-C4'-C3' | -5.24 | 107.62 | 116.00 |
| 83 | DC | 112 | G | P-O5'-C5' | 5.24 | 129.28 | 120.90 |
| 20 | AS | 45 | MET | N-CA-C | 5.23 | 125.13 | 111.00 |
| 43 | BP | 116 | LEU | C-N-CA | 5.23 | 134.78 | 121.70 |
| 81 | DA | 2256 | A | N9-C1'-C2' | -5.23 | 106.24 | 112.00 |
| 81 | DA | 2687 | G | O4'-C1'-N9 | 5.23 | 112.39 | 108.20 |
| 81 | DA | 3037 | U | P-O3'-C3' | -5.23 | 113.42 | 119.70 |
| 39 | BJ | 121 | PHE | CB-CG-CD1 | -5.23 | 117.14 | 120.80 |
| 45 | BR | 144 | ARG | N-CA-C | 5.23 | 125.12 | 111.00 |
| 64 | Bl | 3 | LYS | N-CA-CB | 5.23 | 120.02 | 110.60 |
| 78 | CA | 579 | A | C5-C6-N1 | -5.23 | 115.08 | 117.70 |
| 78 | CA | 1314 | U | C1'-O4'-C4' | -5.23 | 105.71 | 109.90 |
| 78 | CA | 1502 | G | O4'-C1'-N9 | 5.23 | 112.39 | 108.20 |
| 81 | DA | 736 | A | C5'-C4'-O4' | 5.23 | 115.38 | 109.10 |
| 81 | DA | 1635 | G | N9-C1'-C2' | 5.23 | 120.80 | 114.00 |
| 81 | DA | 3149 | G | P-O5'-C5' | 5.23 | 129.27 | 120.90 |
| 81 | DA | 3167 | A | N9-C1'-C2' | -5.23 | 106.24 | 112.00 |
| 9 | AH | 111 | MET | N-CA-CB | 5.23 | 120.01 | 110.60 |
| 39 | BJ | 71 | ALA | N-CA-CB | 5.23 | 117.42 | 110.10 |
| 41 | BN | 5 | SER | C-N-CA | -5.23 | 108.62 | 121.70 |
| 51 | BZ | 25 | ASP | N-CA-CB | 5.23 | 120.02 | 110.60 |
| 81 | DA | 2487 | U | O3'-P-O5' | 5.23 | 113.94 | 104.00 |
| 82 | DB | 22 | U | O4'-C1'-C2' | -5.23 | 100.57 | 105.80 |
| 83 | DC | 99 | A | P-O3'-C3' | -5.23 | 113.42 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 47 | A | N9-C1'-C2' | -5.23 | 106.25 | 112.00 |
| 81 | DA | 223 | U | O4'-C1'-N1 | 5.23 | 112.38 | 108.20 |
| 81 | DA | 869 | G | P-O3'-C3' | 5.23 | 125.97 | 119.70 |
| 81 | DA | 3254 | G | C5'-C4'-O4' | 5.23 | 115.38 | 109.10 |
| 4 | AD | 216 | ASN | CA-C-N | -5.23 | 105.70 | 117.20 |
| 6 | AE | 35 | TRP | CB-CG-CD2 | -5.23 | 119.81 | 126.60 |
| 8 | AF | 35 | GLN | CB-CA-C | -5.23 | 99.95 | 110.40 |
| 32 | BC | 163 | HIS | N-CA-CB | 5.23 | 120.01 | 110.60 |
| 34 | BE | 123 | PHE | CB-CG-CD1 | 5.23 | 124.46 | 120.80 |
| 49 | BV | 161 | ALA | C-N-CA | 5.23 | 134.77 | 121.70 |
| 65 | Bn | 40 | GLN | C-N-CA | 5.23 | 134.77 | 121.70 |
| 78 | CA | 648 | G | C5'-C4'-O4' | -5.23 | 102.83 | 109.10 |
| 78 | CA | 1398 | U | C5'-C4'-C3' | 5.23 | 124.36 | 116.00 |
| 78 | CA | 1440 | C | C4'-C3'-C2' | -5.23 | 97.37 | 102.60 |
| 78 | CA | 1596 | C | N1-C1'-C2' | -5.23 | 106.25 | 112.00 |
| 81 | DA | 2564 | G | P-O3'-C3' | -5.23 | 113.43 | 119.70 |
| 81 | DA | 2650 | U | O4'-C1'-C2' | -5.23 | 100.57 | 105.80 |
| 81 | DA | 2669 | G | C1'-O4'-C4' | -5.23 | 105.72 | 109.90 |
| 81 | DA | 3072 | C | N1-C1'-C2' | 5.23 | 120.80 | 114.00 |
| 83 | DC | 49 | G | C1'-O4'-C4' | 5.23 | 114.08 | 109.90 |
| 49 | BV | 76 | PHE | CB-CG-CD2 | -5.23 | 117.14 | 120.80 |
| 81 | DA | 526 | C | C1'-O4'-C4' | -5.23 | 105.72 | 109.90 |
| 81 | DA | 1139 | G | O4'-C1'-C2' | 5.23 | 112.30 | 107.60 |
| 53 | Ba | 44 | ALA | N-CA-CB | 5.22 | 117.41 | 110.10 |
| 76 | BS | 80 | TRP | CB-CG-CD1 | 5.22 | 133.79 | 127.00 |
| 78 | CA | 203 | U | O4'-C4'-C3' | -5.22 | 98.78 | 104.00 |
| 78 | CA | 481 | A | C5'-C4'-C3' | 5.22 | 124.36 | 116.00 |
| 78 | CA | 1235 | C | P-O3'-C3' | -5.22 | 113.43 | 119.70 |
| 81 | DA | 11 | A | C3'-C2'-C1' | 5.22 | 105.68 | 101.50 |
| 81 | DA | 222 | A | O4'-C1'-C2' | -5.22 | 100.58 | 105.80 |
| 81 | DA | 226 | C | C1'-O4'-C4' | -5.22 | 105.72 | 109.90 |
| 81 | DA | 384 | A | C1'-O4'-C4' | -5.22 | 105.72 | 109.90 |
| 81 | DA | 1269 | U | C5'-C4'-C3' | 5.22 | 124.36 | 116.00 |
| 81 | DA | 1330 | A | O4'-C1'-N9 | 5.22 | 112.38 | 108.20 |
| 81 | DA | 1641 | U | C5'-C4'-O4' | 5.22 | 115.37 | 109.10 |
| 81 | DA | 1790 | G | C4'-C3'-C2' | -5.22 | 97.38 | 102.60 |
| 81 | DA | 1897 | G | C4'-C3'-C2' | -5.22 | 97.38 | 102.60 |
| 81 | DA | 2723 | U | O4'-C1'-N1 | 5.22 | 112.38 | 108.20 |
| 81 | DA | 2724 | U | O4'-C1'-N1 | 5.22 | 112.38 | 108.20 |
| 81 | DA | 2844 | C | C1'-O4'-C4' | -5.22 | 105.72 | 109.90 |
| 81 | DA | 3221 | C | O3'-P-O5' | 5.22 | 113.92 | 104.00 |
| 4 | AD | 106 | LYS | CB-CA-C | -5.22 | 99.96 | 110.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 910 | G | C1'-O4'-C4' | -5.22 | 105.72 | 109.90 |
| 81 | DA | 1392 | G | C1'-O4'-C4' | -5.22 | 105.72 | 109.90 |
| 81 | DA | 1564 | U | C5'-C4'-C3' | 5.22 | 124.36 | 116.00 |
| 81 | DA | 1610 | G | O4'-C1'-N9 | 5.22 | 112.38 | 108.20 |
| 81 | DA | 2261 | G | O4'-C1'-N9 | 5.22 | 112.38 | 108.20 |
| 81 | DA | 2754 | G | C2'-C3'-O3' | 5.22 | 122.06 | 113.70 |
| 81 | DA | 3235 | C | C5'-C4'-O4' | 5.22 | 115.37 | 109.10 |
| 2 | AA | 59 | LEU | N-CA-CB | 5.22 | 120.84 | 110.40 |
| 3 | AB | 207 | THR | C-N-CA | 5.22 | 134.75 | 121.70 |
| 13 | AL | 87 | VAL | C-N-CD | -5.22 | 109.11 | 120.60 |
| 49 | BV | 77 | GLY | N-CA-C | -5.22 | 100.05 | 113.10 |
| 72 | Bt | 37 | ASP | CB-CG-OD2 | 5.22 | 123.00 | 118.30 |
| 78 | CA | 295 | A | P-O5'-C5' | 5.22 | 129.25 | 120.90 |
| 78 | CA | 1304 | G | C1'-O4'-C4' | -5.22 | 105.72 | 109.90 |
| 81 | DA | 1435 | A | C3'-C2'-C1' | 5.22 | 105.68 | 101.50 |
| 81 | DA | 1523 | U | C1'-O4'-C4' | 5.22 | 114.08 | 109.90 |
| 81 | DA | 1708 | C | O4'-C1'-C2' | -5.22 | 100.58 | 105.80 |
| 12 | AK | 57 | PRO | C-N-CA | 5.22 | 134.75 | 121.70 |
| 78 | CA | 190 | C | O4'-C1'-C2' | -5.22 | 100.58 | 105.80 |
| 78 | CA | 980 | G | N9-C1'-C2' | 5.22 | 120.79 | 114.00 |
| 81 | DA | 1198 | C | C4'-C3'-C2' | -5.22 | 97.38 | 102.60 |
| 81 | DA | 1912 | U | N1-C1'-C2' | 5.22 | 120.78 | 114.00 |
| 81 | DA | 2753 | G | C5'-C4'-C3' | 5.22 | 124.35 | 116.00 |
| 8 | AF | 31 | GLU | N-CA-CB | 5.22 | 119.99 | 110.60 |
| 81 | DA | 891 | G | O4'-C1'-N9 | 5.22 | 112.37 | 108.20 |
| 81 | DA | 1995 | A | O4'-C1'-C2' | -5.22 | 100.58 | 105.80 |
| 50 | BX | 35 | PRO | N-CA-CB | 5.22 | 109.56 | 103.30 |
| 78 | CA | 93 | A | N9-C1'-C2' | 5.22 | 120.78 | 114.00 |
| 78 | CA | 610 | G | O3'-P-O5' | -5.22 | 94.09 | 104.00 |
| 81 | DA | 1344 | G | P-O5'-C5' | 5.22 | 129.25 | 120.90 |
| 81 | DA | 1488 | G | O4'-C1'-N9 | 5.22 | 112.37 | 108.20 |
| 81 | DA | 1892 | G | O4'-C1'-C2' | 5.22 | 112.29 | 107.60 |
| 81 | DA | 2575 | G | N3-C2-N2 | 5.22 | 123.55 | 119.90 |
| 81 | DA | 3340 | G | P-O3'-C3' | 5.22 | 125.96 | 119.70 |
| 82 | DB | 72 | A | C5'-C4'-C3' | -5.22 | 107.65 | 116.00 |
| 22 | AV | 105 | THR | N-CA-C | 5.21 | 125.08 | 111.00 |
| 37 | BH | 119 | GLY | N-CA-C | 5.21 | 126.14 | 113.10 |
| 38 | Bs | 55 | LYS | CB-CG-CD | 5.21 | 125.16 | 111.60 |
| 46 | BT | 136 | ARG | NH1-CZ-NH2 | -5.21 | 113.66 | 119.40 |
| 53 | Ba | 9 | LYS | O-C-N | -5.21 | 114.36 | 122.70 |
| 72 | Bt | 50 | ASP | CB-CG-OD2 | 5.21 | 122.99 | 118.30 |
| 74 | BQ | 119 | TYR | CB-CG-CD2 | 5.21 | 124.13 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 248 | U | O3'-P-O5' | -5.21 | 94.09 | 104.00 |
| 81 | DA | 249 | U | P-O5'-C5' | -5.21 | 112.56 | 120.90 |
| 81 | DA | 805 | G | P-O3'-C3' | -5.21 | 113.44 | 119.70 |
| 81 | DA | 1493 | G | O4'-C1'-C2' | -5.21 | 100.58 | 105.80 |
| 81 | DA | 2931 | C | N1-C1'-C2' | 5.21 | 120.78 | 114.00 |
| 15 | AN | 25 | SER | N-CA-CB | 5.21 | 118.32 | 110.50 |
| 51 | BZ | 51 | TRP | CB-CG-CD2 | 5.21 | 133.38 | 126.60 |
| 78 | CA | 1418 | G | C3'-C2'-C1' | 5.21 | 105.67 | 101.50 |
| 78 | CA | 1607 | G | C5'-C4'-O4' | 5.21 | 115.36 | 109.10 |
| 81 | DA | 2202 | C | N1-C1'-C2' | 5.21 | 120.78 | 114.00 |
| 82 | DB | 84 | C | C3'-C2'-C1' | -5.21 | 97.33 | 101.50 |
| 12 | AK | 84 | ARG | N-CA-CB | 5.21 | 119.98 | 110.60 |
| 21 | AT | 58 | TYR | CG-CD1-CE1 | -5.21 | 117.13 | 121.30 |
| 37 | BH | 190 | VAL | CA-CB-CG1 | -5.21 | 103.08 | 110.90 |
| 46 | BT | 39 | ASN | CB-CA-C | -5.21 | 99.98 | 110.40 |
| 72 | Bt | 16 | ASP | CB-CG-OD2 | 5.21 | 122.99 | 118.30 |
| 78 | CA | 279 | G | C5'-C4'-C3' | 5.21 | 124.34 | 116.00 |
| 78 | CA | 1227 | A | C5'-C4'-C3' | 5.21 | 124.34 | 116.00 |
| 81 | DA | 782 | U | O4'-C1'-C2' | -5.21 | 100.59 | 105.80 |
| 81 | DA | 991 | G | C3'-C2'-C1' | 5.21 | 105.67 | 101.50 |
| 81 | DA | 1272 | C | C4'-C3'-C2' | -5.21 | 97.39 | 102.60 |
| 81 | DA | 2791 | G | O3'-P-O5' | 5.21 | 113.90 | 104.00 |
| 4 | AD | 233 | LYS | CA-C-N | 5.21 | 131.69 | 117.10 |
| 35 | BG | 75 | PRO | C-N-CA | -5.21 | 108.68 | 121.70 |
| 78 | CA | 1771 | U | C1'-O4'-C4' | -5.21 | 105.73 | 109.90 |
| 78 | CA | 1791 | A | P-O5'-C5' | 5.21 | 129.24 | 120.90 |
| 81 | DA | 688 | G | O3'-P-O5' | -5.21 | 94.10 | 104.00 |
| 81 | DA | 2198 | A | C3'-C2'-C1' | 5.21 | 105.67 | 101.50 |
| 5 | AC | 95 | TYR | CB-CG-CD1 | 5.21 | 124.12 | 121.00 |
| 57 | Be | 223 | PHE | O-C-N | -5.21 | 114.37 | 122.70 |
| 78 | CA | 638 | U | C3'-C2'-C1' | 5.21 | 105.67 | 101.50 |
| 78 | CA | 918 | U | C5'-C4'-O4' | -5.21 | 102.85 | 109.10 |
| 78 | CA | 1460 | A | P-O5'-C5' | -5.21 | 112.57 | 120.90 |
| 81 | DA | 403 | C | C3'-C2'-C1' | 5.21 | 105.67 | 101.50 |
| 81 | DA | 1336 | U | O4'-C1'-N1 | 5.21 | 112.37 | 108.20 |
| 81 | DA | 2631 | U | C4'-C3'-C2' | -5.21 | 97.39 | 102.60 |
| 14 | AM | 7 | GLU | C-N-CA | 5.21 | 134.72 | 121.70 |
| 32 | BC | 290 | ASP | CB-CA-C | 5.21 | 120.81 | 110.40 |
| 43 | BP | 28 | TRP | CB-CG-CD1 | 5.21 | 133.77 | 127.00 |
| 44 | BO | 68 | PHE | N-CA-CB | 5.21 | 119.97 | 110.60 |
| 49 | BV | 130 | TYR | CB-CG-CD2 | 5.21 | 124.12 | 121.00 |
| 63 | Bm | 87 | ARG | NE-CZ-NH2 | -5.21 | 117.70 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 72 | Bt | 43 | ASP | CB-CG-OD2 | 5.21 | 122.99 | 118.30 |
| 76 | BS | 165 | LEU | N-CA-CB | 5.21 | 120.81 | 110.40 |
| 78 | CA | 232 | U | O4'-C1'-N1 | 5.21 | 112.36 | 108.20 |
| 78 | CA | 1226 | A | C5'-C4'-C3' | 5.21 | 124.33 | 116.00 |
| 81 | DA | 1549 | U | P-O3'-C3' | -5.21 | 113.45 | 119.70 |
| 81 | DA | 3145 | C | C1'-O4'-C4' | -5.21 | 105.73 | 109.90 |
| 81 | DA | 3349 | C | C3'-C2'-C1' | 5.21 | 105.66 | 101.50 |
| 1 | Aa | 162 | ALA | N-CA-CB | 5.20 | 117.39 | 110.10 |
| 1 | Aa | 167 | VAL | CA-CB-CG2 | -5.20 | 103.09 | 110.90 |
| 78 | CA | 1439 | C | N1-C1'-C2' | 5.20 | 120.77 | 114.00 |
| 78 | CA | 1544 | U | O5'-P-OP1 | 5.20 | 116.94 | 110.70 |
| 78 | CA | 1768 | G | C3'-C2'-C1' | 5.20 | 105.66 | 101.50 |
| 81 | DA | 2458 | A | P-O3'-C3' | 5.20 | 125.94 | 119.70 |
| 81 | DA | 2579 | G | N1-C2-N3 | -5.20 | 120.78 | 123.90 |
| 83 | DC | 49 | G | C5'-C4'-C3' | -5.20 | 107.67 | 116.00 |
| 33 | BD | 152 | VAL | CG1-CB-CG2 | 5.20 | 119.22 | 110.90 |
| 78 | CA | 116 | U | OP2-P-O3' | 5.20 | 116.64 | 105.20 |
| 81 | DA | 596 | C | P-O5'-C5' | -5.20 | 112.58 | 120.90 |
| 3 | AB | 162 | GLN | CB-CA-C | 5.20 | 120.80 | 110.40 |
| 4 | AD | 240 | LYS | CB-CA-C | 5.20 | 120.80 | 110.40 |
| 9 | AH | 22 | LYS | CB-CA-C | -5.20 | 100.00 | 110.40 |
| 55 | Bc | 10 | ARG | NE-CZ-NH2 | -5.20 | 117.70 | 120.30 |
| 59 | Bh | 101 | SER | CB-CA-C | -5.20 | 100.22 | 110.10 |
| 72 | Bu | 16 | ASP | CB-CG-OD2 | 5.20 | 122.98 | 118.30 |
| 78 | CA | 567 | A | C5-C6-N1 | -5.20 | 115.10 | 117.70 |
| 81 | DA | 279 | U | O4'-C1'-N1 | 5.20 | 112.36 | 108.20 |
| 81 | DA | 1019 | G | O4'-C1'-N9 | 5.20 | 112.36 | 108.20 |
| 81 | DA | 1639 | C | N1-C1'-C2' | 5.20 | 120.76 | 114.00 |
| 83 | DC | 13 | A | O3'-P-O5' | 5.20 | 113.88 | 104.00 |
| 44 | BO | 96 | LYS | C-N-CA | 5.20 | 134.70 | 121.70 |
| 72 | Bu | 50 | ASP | CB-CG-OD2 | 5.20 | 122.98 | 118.30 |
| 74 | BQ | 33 | ARG | CD-NE-CZ | -5.20 | 116.32 | 123.60 |
| 78 | CA | 117 | U | C5'-C4'-C3' | 5.20 | 124.32 | 116.00 |
| 81 | DA | 90 | C | N1-C1'-C2' | 5.20 | 120.76 | 114.00 |
| 81 | DA | 697 | A | O4'-C1'-C2' | -5.20 | 100.60 | 105.80 |
| 81 | DA | 759 | U | P-O5'-C5' | -5.20 | 112.58 | 120.90 |
| 81 | DA | 804 | C | O4'-C1'-C2' | -5.20 | 100.60 | 105.80 |
| 81 | DA | 2743 | A | O3'-P-O5' | -5.20 | 94.12 | 104.00 |
| 83 | DC | 60 | G | P-O3'-C3' | 5.20 | 125.94 | 119.70 |
| 58 | Bg | 23 | VAL | C-N-CA | 5.20 | 134.69 | 121.70 |
| 81 | DA | 2409 | G | O4'-C1'-N9 | 5.20 | 112.36 | 108.20 |
| 81 | DA | 2416 | U | C3'-C2'-C1' | -5.20 | 97.34 | 101.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 3258 | U | O4'-C1'-C2' | -5.20 | 100.60 | 105.80 |
| 1 | Aa | 269 | TYR | N-CA-CB | 5.20 | 119.95 | 110.60 |
| 44 | BO | 48 | TYR | CB-CG-CD1 | -5.20 | 117.88 | 121.00 |
| 55 | Bc | 116 | TYR | CB-CG-CD1 | -5.20 | 117.88 | 121.00 |
| 72 | Bu | 37 | ASP | CB-CG-OD2 | 5.20 | 122.98 | 118.30 |
| 77 | BI | 176 | LEU | C-N-CA | 5.20 | 134.69 | 121.70 |
| 78 | CA | 1309 | C | P-O3'-C3' | -5.20 | 113.47 | 119.70 |
| 78 | CA | 1433 | G | C4'-C3'-C2' | -5.20 | 97.40 | 102.60 |
| 81 | DA | 2189 | U | P-O3'-C3' | 5.20 | 125.93 | 119.70 |
| 81 | DA | 2419 | A | P-O5'-C5' | -5.20 | 112.59 | 120.90 |
| 81 | DA | 2633 | U | C5'-C4'-C3' | 5.20 | 124.31 | 116.00 |
| 83 | DC | 115 | A | C3'-C2'-C1' | -5.20 | 97.34 | 101.50 |
| 17 | AQ | 11 | ARG | NE-CZ-NH2 | -5.19 | 117.70 | 120.30 |
| 45 | BR | 98 | LYS | CA-CB-CG | -5.19 | 101.97 | 113.40 |
| 66 | Bo | 24 | PRO | N-CA-C | -5.19 | 98.60 | 112.10 |
| 78 | CA | 369 | A | P-O5'-C5' | 5.19 | 129.21 | 120.90 |
| 78 | CA | 1087 | A | O4'-C1'-N9 | 5.19 | 112.36 | 108.20 |
| 79 | CB | 68 | C | P-O5'-C5' | 5.19 | 129.21 | 120.90 |
| 81 | DA | 1017 | C | C3'-C2'-C1' | 5.19 | 105.66 | 101.50 |
| 47 | BU | 131 | GLN | CA-C-O | -5.19 | 109.19 | 120.10 |
| 60 | Bi | 16 | ARG | C-N-CA | 5.19 | 134.68 | 121.70 |
| 69 | Br | 98 | LYS | N-CA-C | -5.19 | 96.98 | 111.00 |
| 72 | Bu | 56 | ASP | CB-CG-OD2 | 5.19 | 122.97 | 118.30 |
| 78 | CA | 611 | U | N1-C1'-C2' | 5.19 | 120.75 | 114.00 |
| 78 | CA | 644 | C | O4'-C1'-C2' | -5.19 | 100.61 | 105.80 |
| 78 | CA | 989 | U | C3'-C2'-C1' | -5.19 | 97.35 | 101.50 |
| 78 | CA | 1480 | G | C3'-C2'-C1' | -5.19 | 97.34 | 101.50 |
| 78 | CA | 1553 | G | N9-C1'-C2' | 5.19 | 120.75 | 114.00 |
| 81 | DA | 1562 | C | O3'-P-O5' | 5.19 | 113.87 | 104.00 |
| 81 | DA | 2867 | C | O4'-C1'-N1 | 5.19 | 112.35 | 108.20 |
| 81 | DA | 3106 | A | OP2-P-O3' | 5.19 | 116.62 | 105.20 |
| 50 | BX | 23 | ALA | C-N-CA | 5.19 | 134.68 | 121.70 |
| 78 | CA | 191 | C | C1'-O4'-C4' | 5.19 | 114.05 | 109.90 |
| 78 | CA | 990 | C | O4'-C1'-N1 | -5.19 | 104.05 | 108.20 |
| 79 | CB | 8 | U | O4'-C1'-C2' | -5.19 | 100.61 | 105.80 |
| 81 | DA | 1690 | C | C5'-C4'-C3' | 5.19 | 124.31 | 116.00 |
| 81 | DA | 1756 | C | P-O3'-C3' | 5.19 | 125.93 | 119.70 |
| 81 | DA | 1873 | U | C1'-O4'-C4' | -5.19 | 105.75 | 109.90 |
| 11 | AJ | 9 | VAL | C-N-CA | 5.19 | 134.67 | 121.70 |
| 81 | DA | 957 | C | O4'-C1'-C2' | -5.19 | 100.61 | 105.80 |
| 81 | DA | 1086 | C | O3'-P-O5' | -5.19 | 94.14 | 104.00 |
| 81 | DA | 1435 | A | C5'-C4'-C3' | -5.19 | 107.70 | 116.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | AY | 29 | ARG | NE-CZ-NH1 | 5.19 | 122.89 | 120.30 |
| 43 | BP | 177 | GLY | CA-C-N | 5.19 | 128.61 | 117.20 |
| 81 | DA | 293 | C | C3'-C2'-C1' | 5.19 | 105.65 | 101.50 |
| 81 | DA | 1180 | A | P-O3'-C3' | 5.19 | 125.92 | 119.70 |
| 81 | DA | 1272 | C | O4'-C1'-C2' | -5.19 | 100.61 | 105.80 |
| 81 | DA | 1568 | U | P-O5'-C5' | 5.19 | 129.20 | 120.90 |
| 81 | DA | 2756 | C | O4'-C1'-C2' | -5.19 | 100.61 | 105.80 |
| 81 | DA | 2942 | C | O4'-C1'-N1 | -5.19 | 104.05 | 108.20 |
| 5 | AC | 132 | ARG | NE-CZ-NH2 | -5.19 | 117.71 | 120.30 |
| 37 | BH | 233 | TRP | O-C-N | -5.19 | 114.38 | 123.20 |
| 61 | Bj | 83 | ALA | N-CA-CB | 5.19 | 117.36 | 110.10 |
| 78 | CA | 1449 | U | O4'-C1'-C2' | -5.19 | 100.61 | 105.80 |
| 79 | CB | 48 | C | C3'-C2'-C1' | 5.19 | 105.65 | 101.50 |
| 81 | DA | 173 | G | C4'-C3'-C2' | -5.19 | 97.41 | 102.60 |
| 81 | DA | 756 | U | P-O3'-C3' | 5.19 | 125.92 | 119.70 |
| 81 | DA | 2227 | C | O4'-C1'-C2' | -5.19 | 100.61 | 105.80 |
| 81 | DA | 2274 | U | N1-C1'-C2' | 5.19 | 120.74 | 114.00 |
| 37 | BH | 151 | VAL | CA-CB-CG1 | -5.18 | 103.12 | 110.90 |
| 37 | BH | 232 | HIS | CB-CA-C | -5.18 | 100.03 | 110.40 |
| 46 | BT | 88 | ARG | NH1-CZ-NH2 | 5.18 | 125.10 | 119.40 |
| 49 | BV | 147 | GLU | CB-CA-C | 5.18 | 120.77 | 110.40 |
| 81 | DA | 149 | U | O5'-C5'-C4' | 5.18 | 121.55 | 111.70 |
| 81 | DA | 704 | U | O3'-P-O5' | -5.18 | 94.15 | 104.00 |
| 82 | DB | 133 | G | C5'-C4'-O4' | 5.18 | 115.32 | 109.10 |
| 16 | AO | 110 | ASP | C-N-CA | 5.18 | 134.66 | 121.70 |
| 78 | CA | 220 | A | O4'-C1'-C2' | -5.18 | 100.62 | 105.80 |
| 78 | CA | 267 | U | O5'-C5'-C4' | -5.18 | 101.85 | 111.70 |
| 78 | CA | 717 | C | C5'-C4'-C3' | 5.18 | 124.29 | 116.00 |
| 78 | CA | 1442 | U | O4'-C1'-N1 | 5.18 | 112.35 | 108.20 |
| 78 | CA | 1734 | U | O4'-C1'-N1 | 5.18 | 112.35 | 108.20 |
| 81 | DA | 1399 | A | O3'-P-O5' | -5.18 | 94.15 | 104.00 |
| 81 | DA | 1773 | C | C3'-C2'-C1' | 5.18 | 105.65 | 101.50 |
| 80 | CC | 22 | A | C5-C6-N1 | -5.18 | 115.11 | 117.70 |
| 81 | DA | 961 | C | O4'-C1'-N1 | -5.18 | 104.06 | 108.20 |
| 1 | Aa | 192 | PHE | CB-CG-CD1 | -5.18 | 117.17 | 120.80 |
| 14 | AM | 100 | THR | N-CA-CB | 5.18 | 120.14 | 110.30 |
| 14 | AM | 101 | LEU | CD1-CG-CD2 | 5.18 | 126.04 | 110.50 |
| 17 | AQ | 134 | LYS | C-N-CA | 5.18 | 134.65 | 121.70 |
| 49 | BV | 152 | GLU | N-CA-C | 5.18 | 124.98 | 111.00 |
| 57 | Be | 220 | PHE | CE1-CZ-CE2 | 5.18 | 129.32 | 120.00 |
| 78 | CA | 152 | U | O4'-C1'-C2' | -5.18 | 100.62 | 105.80 |
| 78 | CA | 172 | C | O5'-C5'-C4' | 5.18 | 121.54 | 111.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 635 | A | P-O3'-C3' | -5.18 | 113.48 | 119.70 |
| 78 | CA | 1751 | C | C3'-C2'-C1' | 5.18 | 105.64 | 101.50 |
| 81 | DA | 188 | U | C1'-O4'-C4' | 5.18 | 114.04 | 109.90 |
| 81 | DA | 626 | U | O4'-C1'-C2' | -5.18 | 100.62 | 105.80 |
| 81 | DA | 1892 | G | C3'-C2'-C1' | -5.18 | 97.36 | 101.50 |
| 81 | DA | 1935 | G | O4'-C1'-N9 | 5.18 | 112.34 | 108.20 |
| 81 | DA | 1942 | U | C3'-C2'-C1' | 5.18 | 105.64 | 101.50 |
| 81 | DA | 2043 | U | O4'-C1'-C2' | -5.18 | 100.62 | 105.80 |
| 81 | DA | 2193 | U | OP1-P-O3' | 5.18 | 116.60 | 105.20 |
| 81 | DA | 2878 | G | P-O3'-C3' | -5.18 | 113.48 | 119.70 |
| 26 | AZ | 18 | THR | N-CA-C | -5.18 | 97.02 | 111.00 |
| 40 | BK | 7 | VAL | N-CA-C | -5.18 | 97.02 | 111.00 |
| 78 | CA | 1407 | U | O4'-C1'-N1 | 5.18 | 112.34 | 108.20 |
| 81 | DA | 713 | U | C3'-C2'-C1' | 5.18 | 105.64 | 101.50 |
| 49 | BV | 165 | VAL | C-N-CA | -5.18 | 108.76 | 121.70 |
| 76 | BS | 155 | TYR | CG-CD1-CE1 | -5.18 | 117.16 | 121.30 |
| 78 | CA | 447 | U | N1-C1'-C2' | 5.18 | 120.73 | 114.00 |
| 78 | CA | 1604 | U | C3'-C2'-C1' | -5.18 | 97.36 | 101.50 |
| 81 | DA | 1296 | C | O4'-C4'-C3' | -5.18 | 98.82 | 104.00 |
| 81 | DA | 2675 | C | O4'-C1'-C2' | -5.18 | 100.62 | 105.80 |
| 81 | DA | 3358 | U | C4'-C3'-C2' | -5.18 | 97.42 | 102.60 |
| 83 | DC | 77 | A | C1'-O4'-C4' | 5.18 | 114.04 | 109.90 |
| 2 | AA | 244 | GLU | CB-CA-C | 5.17 | 120.75 | 110.40 |
| 12 | AK | 89 | THR | N-CA-CB | 5.17 | 120.13 | 110.30 |
| 43 | BP | 177 | GLY | CA-C-O | -5.17 | 111.28 | 120.60 |
| 46 | BT | 81 | ARG | NE-CZ-NH2 | -5.17 | 117.71 | 120.30 |
| 48 | BW | 96 | VAL | C-N-CA | 5.17 | 134.64 | 121.70 |
| 78 | CA | 877 | G | N9-C1'-C2' | 5.17 | 120.73 | 114.00 |
| 78 | CA | 1500 | C | C6-N1-C2 | -5.17 | 118.23 | 120.30 |
| 81 | DA | 281 | G | C1'-O4'-C4' | -5.17 | 105.76 | 109.90 |
| 81 | DA | 1978 | A | C3'-C2'-C1' | 5.17 | 105.64 | 101.50 |
| 82 | DB | 34 | U | O4'-C1'-N1 | 5.17 | 112.34 | 108.20 |
| 83 | DC | 115 | A | O5'-C5'-C4' | 5.17 | 121.53 | 111.70 |
| 13 | AL | 40 | SER | CA-CB-OG | 5.17 | 125.17 | 111.20 |
| 32 | BC | 209 | PHE | CB-CG-CD1 | 5.17 | 124.42 | 120.80 |
| 32 | BC | 240 | ARG | CA-C-O | 5.17 | 130.96 | 120.10 |
| 43 | BP | 12 | ARG | NE-CZ-NH1 | 5.17 | 122.89 | 120.30 |
| 78 | CA | 1064 | G | N3-C2-N2 | 5.17 | 123.52 | 119.90 |
| 81 | DA | 2610 | G | C3'-C2'-C1' | 5.17 | 105.64 | 101.50 |
| 2 | AA | 232 | VAL | N-CA-CB | 5.17 | 122.88 | 111.50 |
| 6 | AE | 92 | ALA | N-CA-CB | -5.17 | 102.86 | 110.10 |
| 78 | CA | 1433 | G | N9-C1'-C2' | -5.17 | 106.31 | 112.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 164 | A | O4'-C1'-N9 | 5.17 | 112.34 | 108.20 |
| 81 | DA | 706 | A | P-O5'-C5' | -5.17 | 112.63 | 120.90 |
| 81 | DA | 1007 | U | O3'-P-O5' | -5.17 | 94.17 | 104.00 |
| 81 | DA | 2752 | U | O5'-C5'-C4' | 5.17 | 121.53 | 111.70 |
| 82 | DB | 137 | C | O4'-C1'-N1 | 5.17 | 112.34 | 108.20 |
| 2 | AA | 6 | THR | N-CA-CB | 5.17 | 120.12 | 110.30 |
| 78 | CA | 470 | A | C3'-C2'-C1' | 5.17 | 105.64 | 101.50 |
| 78 | CA | 574 | G | N1-C2-N3 | -5.17 | 120.80 | 123.90 |
| 81 | DA | 633 | C | O4'-C1'-N1 | 5.17 | 112.34 | 108.20 |
| 81 | DA | 872 | U | N1-C1'-C2' | 5.17 | 120.72 | 114.00 |
| 81 | DA | 1975 | C | O4'-C4'-C3' | -5.17 | 98.83 | 104.00 |
| 81 | DA | 3238 | G | C4'-C3'-C2' | -5.17 | 97.43 | 102.60 |
| 1 | Aa | 48 | THR | CA-C-N | 5.17 | 126.54 | 116.20 |
| 31 | BB | 245 | LEU | N-CA-C | -5.17 | 97.05 | 111.00 |
| 35 | BG | 152 | THR | CA-CB-OG1 | 5.17 | 119.85 | 109.00 |
| 45 | BR | 99 | THR | N-CA-CB | 5.17 | 120.12 | 110.30 |
| 51 | BZ | 2 | LYS | C-N-CA | 5.17 | 134.62 | 121.70 |
| 62 | Bk | 70 | ARG | C-N-CA | 5.17 | 134.62 | 121.70 |
| 78 | CA | 391 | A | O4'-C1'-N9 | 5.17 | 112.33 | 108.20 |
| 78 | CA | 1067 | C | N3-C4-N4 | 5.17 | 121.62 | 118.00 |
| 78 | CA | 1322 | A | O4'-C1'-N9 | 5.17 | 112.33 | 108.20 |
| 78 | CA | 1396 | U | O4'-C1'-N1 | 5.17 | 112.33 | 108.20 |
| 81 | DA | 298 | U | O4'-C1'-C2' | -5.17 | 100.63 | 105.80 |
| 81 | DA | 1827 | C | O4'-C1'-C2' | -5.17 | 100.63 | 105.80 |
| 81 | DA | 2113 | A | O4'-C1'-N9 | 5.17 | 112.33 | 108.20 |
| 81 | DA | 2362 | C | O4'-C4'-C3' | -5.17 | 98.83 | 104.00 |
| 82 | DB | 16 | G | N9-C1'-C2' | -5.17 | 106.31 | 112.00 |
| 83 | DC | 17 | A | O4'-C4'-C3' | -5.17 | 98.83 | 104.00 |
| 44 | BO | 62 | HIS | C-N-CA | 5.17 | 134.61 | 121.70 |
| 48 | BW | 92 | TRP | N-CA-C | -5.17 | 97.05 | 111.00 |
| 74 | BQ | 250 | ASP | CB-CG-OD2 | 5.17 | 122.95 | 118.30 |
| 78 | CA | 204 | G | O4'-C1'-C2' | 5.17 | 112.25 | 107.60 |
| 78 | CA | 367 | A | C5'-C4'-C3' | 5.17 | 124.27 | 116.00 |
| 78 | CA | 846 | G | C5'-C4'-O4' | 5.17 | 115.30 | 109.10 |
| 78 | CA | 1612 | U | P-O5'-C5' | -5.17 | 112.63 | 120.90 |
| 81 | DA | 264 | G | C4'-C3'-C2' | -5.17 | 97.43 | 102.60 |
| 81 | DA | 427 | C | O4'-C1'-N1 | -5.17 | 104.07 | 108.20 |
| 81 | DA | 1405 | U | P-O3'-C3' | -5.17 | 113.50 | 119.70 |
| 81 | DA | 1674 | G | C3'-C2'-C1' | -5.17 | 97.37 | 101.50 |
| 81 | DA | 1761 | C | N3-C4-C5 | -5.17 | 119.83 | 121.90 |
| 81 | DA | 2264 | U | C5'-C4'-C3' | 5.17 | 124.27 | 116.00 |
| 81 | DA | 2346 | C | O4'-C1'-C2' | -5.17 | 100.63 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2950 | G | C1'-O4'-C4' | 5.17 | 114.03 | 109.90 |
| 21 | AT | 70 | ASN | C-N-CA | 5.17 | 134.61 | 121.70 |
| 81 | DA | 2393 | G | C5'-C4'-C3' | 5.17 | 124.26 | 116.00 |
| 81 | DA | 2631 | U | C2'-C3'-O3' | 5.17 | 121.97 | 113.70 |
| 81 | DA | 2775 | U | C3'-C2'-C1' | 5.17 | 105.63 | 101.50 |
| 82 | DB | 35 | C | C3'-C2'-C1' | 5.17 | 105.63 | 101.50 |
| 31 | BB | 47 | GLN | CB-CA-C | -5.16 | 100.07 | 110.40 |
| 45 | BR | 39 | ARG | CB-CA-C | 5.16 | 120.73 | 110.40 |
| 47 | BU | 54 | HIS | CA-CB-CG | -5.16 | 104.82 | 113.60 |
| 74 | BQ | 55 | PHE | N-CA-CB | 5.16 | 119.90 | 110.60 |
| 78 | CA | 579 | A | C5-C6-N6 | -5.16 | 119.57 | 123.70 |
| 78 | CA | 614 | C | C3'-C2'-C1' | 5.16 | 105.63 | 101.50 |
| 78 | CA | 1029 | U | O4'-C1'-C2' | -5.16 | 100.64 | 105.80 |
| 78 | CA | 1345 | A | O4'-C1'-N9 | 5.16 | 112.33 | 108.20 |
| 78 | CA | 1500 | C | C5-C6-N1 | 5.16 | 123.58 | 121.00 |
| 81 | DA | 787 | G | C5'-C4'-O4' | 5.16 | 115.30 | 109.10 |
| 81 | DA | 968 | G | OP1-P-O3' | 5.16 | 116.56 | 105.20 |
| 81 | DA | 1396 | C | C3'-C2'-C1' | 5.16 | 105.63 | 101.50 |
| 81 | DA | 2740 | A | P-O3'-C3' | -5.16 | 113.50 | 119.70 |
| 81 | DA | 2760 | C | C4'-C3'-C2' | 5.16 | 107.76 | 102.60 |
| 81 | DA | 3213 | A | O3'-P-O5' | -5.16 | 94.19 | 104.00 |
| 83 | DC | 98 | G | O4'-C1'-N9 | -5.16 | 104.07 | 108.20 |
| 9 | AH | 67 | GLY | CA-C-O | -5.16 | 111.31 | 120.60 |
| 78 | CA | 270 | C | N1-C1'-C2' | 5.16 | 120.71 | 114.00 |
| 78 | CA | 835 | U | P-O5'-C5' | 5.16 | 129.16 | 120.90 |
| 81 | DA | 735 | A | C5-C6-N1 | -5.16 | 115.12 | 117.70 |
| 81 | DA | 1963 | G | O4'-C1'-C2' | 5.16 | 112.25 | 107.60 |
| 81 | DA | 1966 | U | C2'-C3'-O3' | 5.16 | 121.96 | 113.70 |
| 37 | BH | 119 | GLY | C-N-CA | 5.16 | 134.60 | 121.70 |
| 42 | BM | 11 | PHE | CB-CG-CD1 | -5.16 | 117.19 | 120.80 |
| 78 | CA | 328 | A | O4'-C1'-N9 | 5.16 | 112.33 | 108.20 |
| 78 | CA | 1503 | A | C5-C6-N6 | -5.16 | 119.57 | 123.70 |
| 78 | CA | 1596 | C | O4'-C1'-C2' | -5.16 | 100.64 | 105.80 |
| 81 | DA | 550 | A | N9-C1'-C2' | -5.16 | 106.32 | 112.00 |
| 81 | DA | 812 | G | C5'-C4'-C3' | 5.16 | 124.26 | 116.00 |
| 81 | DA | 1082 | U | C1'-O4'-C4' | 5.16 | 114.03 | 109.90 |
| 81 | DA | 1791 | C | O4'-C4'-C3' | -5.16 | 98.84 | 104.00 |
| 81 | DA | 2510 | U | N1-C1'-C2' | -5.16 | 106.32 | 112.00 |
| 81 | DA | 2724 | U | C1'-O4'-C4' | -5.16 | 105.77 | 109.90 |
| 2 | AA | 185 | ARG | NE-CZ-NH1 | 5.16 | 122.88 | 120.30 |
| 9 | AH | 84 | GLY | N-CA-C | 5.16 | 125.99 | 113.10 |
| 32 | BC | 16 | PHE | N-CA-C | -5.16 | 97.07 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 40 | BK | 141 | LEU | CB-CG-CD1 | -5.16 | 102.23 | 111.00 |
| 48 | BW | 57 | THR | CA-CB-CG2 | -5.16 | 105.18 | 112.40 |
| 78 | CA | 163 | G | N9-C1'-C2' | -5.16 | 106.33 | 112.00 |
| 81 | DA | 1985 | G | C1'-O4'-C4' | -5.16 | 105.77 | 109.90 |
| 81 | DA | 3051 | U | O3'-P-O5' | 5.16 | 113.80 | 104.00 |
| 81 | DA | 3233 | C | O4'-C1'-N1 | 5.16 | 112.33 | 108.20 |
| 48 | BW | 83 | TYR | CZ-CE2-CD2 | 5.16 | 124.44 | 119.80 |
| 57 | Be | 132 | PRO | CB-CA-C | -5.16 | 99.11 | 112.00 |
| 81 | DA | 80 | G | O4'-C1'-C2' | 5.16 | 112.24 | 107.60 |
| 81 | DA | 490 | A | P-O3'-C3' | -5.16 | 113.51 | 119.70 |
| 81 | DA | 835 | G | O3'-P-O5' | 5.16 | 113.80 | 104.00 |
| 81 | DA | 2489 | C | C1'-O4'-C4' | -5.16 | 105.78 | 109.90 |
| 1 | Aa | 19 | TRP | N-CA-CB | -5.15 | 101.32 | 110.60 |
| 16 | AO | 72 | MET | CG-SD-CE | 5.15 | 108.45 | 100.20 |
| 17 | AQ | 85 | VAL | CB-CA-C | -5.15 | 101.61 | 111.40 |
| 32 | BC | 100 | ARG | NH1-CZ-NH2 | 5.15 | 125.07 | 119.40 |
| 62 | Bk | 68 | ARG | CD-NE-CZ | -5.15 | 116.38 | 123.60 |
| 69 | Br | 28 | TYR | CG-CD2-CE2 | -5.15 | 117.18 | 121.30 |
| 78 | CA | 1536 | G | P-O3'-C3' | -5.15 | 113.52 | 119.70 |
| 81 | DA | 109 | A | O4'-C1'-N9 | -5.15 | 104.08 | 108.20 |
| 81 | DA | 556 | U | C1'-O4'-C4' | -5.15 | 105.78 | 109.90 |
| 82 | DB | 52 | A | O4'-C1'-N9 | -5.15 | 104.08 | 108.20 |
| 32 | BC | 8 | ALA | CB-CA-C | -5.15 | 102.37 | 110.10 |
| 32 | BC | 308 | MET | CG-SD-CE | -5.15 | 91.96 | 100.20 |
| 40 | BK | 131 | PRO | CB-CA-C | -5.15 | 99.12 | 112.00 |
| 44 | BO | 91 | LEU | C-N-CA | 5.15 | 134.58 | 121.70 |
| 49 | BV | 164 | LYS | N-CA-C | 5.15 | 124.91 | 111.00 |
| 78 | CA | 19 | A | O4'-C1'-N9 | -5.15 | 104.08 | 108.20 |
| 78 | CA | 50 | C | C5'-C4'-C3' | -5.15 | 107.75 | 116.00 |
| 78 | CA | 644 | C | P-O3'-C3' | -5.15 | 113.52 | 119.70 |
| 78 | CA | 903 | U | C3'-C2'-C1' | 5.15 | 105.62 | 101.50 |
| 78 | CA | 1028 | C | O4'-C1'-C2' | -5.15 | 100.65 | 105.80 |
| 78 | CA | 1345 | A | C1'-O4'-C4' | 5.15 | 114.02 | 109.90 |
| 78 | CA | 1783 | C | P-O5'-C5' | -5.15 | 112.65 | 120.90 |
| 81 | DA | 327 | A | N9-C1'-C2' | 5.15 | 120.70 | 114.00 |
| 81 | DA | 1101 | G | C4'-C3'-C2' | 5.15 | 107.75 | 102.60 |
| 81 | DA | 1290 | A | C1'-O4'-C4' | 5.15 | 114.02 | 109.90 |
| 81 | DA | 1552 | G | C1'-O4'-C4' | -5.15 | 105.78 | 109.90 |
| 81 | DA | 3228 | C | P-O3'-C3' | -5.15 | 113.52 | 119.70 |
| 83 | DC | 104 | C | C4'-C3'-C2' | -5.15 | 97.45 | 102.60 |
| 1 | Aa | 149 | ASP | N-CA-CB | 5.15 | 119.87 | 110.60 |
| 18 | AP | 102 | LYS | N-CA-C | -5.15 | 97.10 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 32 | BC | 100 | ARG | N-CA-CB | 5.15 | 119.87 | 110.60 |
| 35 | BG | 52 | VAL | CB-CA-C | -5.15 | 101.61 | 111.40 |
| 42 | BM | 102 | ILE | C-N-CA | 5.15 | 134.57 | 121.70 |
| 74 | BQ | 52 | VAL | O-C-N | -5.15 | 114.46 | 122.70 |
| 78 | CA | 1240 | U | P-O5'-C5' | 5.15 | 129.14 | 120.90 |
| 81 | DA | 159 | A | C1'-O4'-C4' | 5.15 | 114.02 | 109.90 |
| 81 | DA | 1034 | U | O4'-C1'-N1 | 5.15 | 112.32 | 108.20 |
| 81 | DA | 1273 | A | O3'-P-O5' | -5.15 | 94.21 | 104.00 |
| 81 | DA | 2294 | U | N1-C1'-C2' | -5.15 | 106.33 | 112.00 |
| 81 | DA | 3069 | G | P-O3'-C3' | -5.15 | 113.52 | 119.70 |
| 17 | AQ | 20 | TYR | CD1-CE1-CZ | 5.15 | 124.43 | 119.80 |
| 78 | CA | 438 | A | C2'-C3'-O3' | 5.15 | 121.94 | 113.70 |
| 81 | DA | 2648 | G | C3'-C2'-C1' | -5.15 | 97.38 | 101.50 |
| 8 | AF | 36 | ALA | N-CA-C | 5.15 | 124.90 | 111.00 |
| 76 | BS | 119 | ARG | N-CA-C | -5.15 | 97.10 | 111.00 |
| 78 | CA | 13 | C | C1'-O4'-C4' | -5.15 | 105.78 | 109.90 |
| 78 | CA | 505 | A | C5-C6-N1 | -5.15 | 115.13 | 117.70 |
| 78 | CA | 892 | A | C4'-C3'-C2' | -5.15 | 97.45 | 102.60 |
| 78 | CA | 1436 | A | OP1-P-O3' | 5.15 | 116.52 | 105.20 |
| 81 | DA | 1704 | A | P-O5'-C5' | 5.15 | 129.14 | 120.90 |
| 81 | DA | 2031 | U | N1-C1'-C2' | 5.15 | 120.69 | 114.00 |
| 81 | DA | 2457 | G | O4'-C1'-N9 | 5.15 | 112.32 | 108.20 |
| 81 | DA | 2545 | C | N3-C4-N4 | 5.15 | 121.60 | 118.00 |
| 81 | DA | 2580 | A | P-O5'-C5' | 5.15 | 129.14 | 120.90 |
| 81 | DA | 2606 | G | C3'-C2'-C1' | -5.15 | 97.38 | 101.50 |
| 81 | DA | 3375 | A | O4'-C1'-C2' | -5.15 | 100.65 | 105.80 |
| 3 | AB | 139 | SER | N-CA-CB | -5.15 | 102.78 | 110.50 |
| 29 | AU | 72 | PHE | C-N-CA | 5.15 | 133.11 | 122.30 |
| 45 | BR | 13 | SER | CB-CA-C | -5.15 | 100.32 | 110.10 |
| 48 | BW | 84 | LEU | CB-CA-C | -5.15 | 100.42 | 110.20 |
| 78 | CA | 388 | G | C3'-C2'-C1' | -5.15 | 97.38 | 101.50 |
| 78 | CA | 1086 | A | C3'-C2'-C1' | 5.15 | 105.62 | 101.50 |
| 78 | CA | 1616 | G | C1'-O4'-C4' | -5.15 | 105.78 | 109.90 |
| 81 | DA | 251 | G | C4'-C3'-C2' | -5.15 | 97.45 | 102.60 |
| 81 | DA | 540 | U | P-O5'-C5' | 5.15 | 129.13 | 120.90 |
| 81 | DA | 1261 | G | C4'-C3'-C2' | -5.15 | 97.45 | 102.60 |
| 81 | DA | 2948 | C | C3'-C2'-C1' | 5.15 | 105.62 | 101.50 |
| 78 | CA | 554 | C | N1-C1'-C2' | 5.14 | 120.69 | 114.00 |
| 78 | CA | 1425 | A | C4-C5-C6 | 5.14 | 119.57 | 117.00 |
| 78 | CA | 1634 | C | N3-C4-N4 | 5.14 | 121.60 | 118.00 |
| 81 | DA | 515 | C | C3'-C2'-C1' | 5.14 | 105.61 | 101.50 |
| 81 | DA | 1047 | A | P-O3'-C3' | 5.14 | 125.87 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 67 | Bp | 51 | LEU | CB-CA-C | 5.14 | 119.97 | 110.20 |
| 81 | DA | 91 | G | O4'-C1'-N9 | 5.14 | 112.31 | 108.20 |
| 1 | Aa | 7 | LEU | N-CA-CB | 5.14 | 120.68 | 110.40 |
| 41 | BN | 123 | LEU | N-CA-CB | 5.14 | 120.68 | 110.40 |
| 78 | CA | 157 | A | O4'-C1'-C2' | -5.14 | 100.66 | 105.80 |
| 78 | CA | 1424 | A | O4'-C1'-N9 | 5.14 | 112.31 | 108.20 |
| 78 | CA | 1547 | A | C5'-C4'-O4' | -5.14 | 102.93 | 109.10 |
| 81 | DA | 515 | C | C5'-C4'-C3' | -5.14 | 107.78 | 116.00 |
| 81 | DA | 694 | C | N1-C1'-C2' | 5.14 | 120.68 | 114.00 |
| 83 | DC | 101 | A | C4'-C3'-C2' | -5.14 | 97.46 | 102.60 |
| 19 | AR | 128 | HIS | C-N-CA | 5.14 | 133.09 | 122.30 |
| 31 | BB | 1 | MET | O-C-N | -5.14 | 114.46 | 123.20 |
| 38 | Bs | 42 | ARG | NE-CZ-NH2 | -5.14 | 117.73 | 120.30 |
| 43 | BP | 24 | ARG | NE-CZ-NH2 | -5.14 | 117.73 | 120.30 |
| 77 | BI | 106 | ALA | CB-CA-C | -5.14 | 102.39 | 110.10 |
| 78 | CA | 158 | U | C5'-C4'-C3' | 5.14 | 124.22 | 116.00 |
| 78 | CA | 852 | C | P-O5'-C5' | -5.14 | 112.68 | 120.90 |
| 78 | CA | 1588 | G | O4'-C1'-N9 | 5.14 | 112.31 | 108.20 |
| 79 | CB | 9 | A | O4'-C1'-N9 | 5.14 | 112.31 | 108.20 |
| 81 | DA | 1500 | G | C1'-O4'-C4' | -5.14 | 105.79 | 109.90 |
| 81 | DA | 3018 | C | C5'-C4'-C3' | 5.14 | 124.22 | 116.00 |
| 20 | AS | 55 | TYR | CG-CD1-CE1 | 5.14 | 125.41 | 121.30 |
| 33 | BD | 222 | VAL | CA-CB-CG1 | 5.14 | 118.61 | 110.90 |
| 69 | Br | 61 | LYS | C-N-CA | 5.14 | 134.55 | 121.70 |
| 78 | CA | 158 | U | P-O3'-C3' | 5.14 | 125.87 | 119.70 |
| 78 | CA | 831 | U | O4'-C1'-C2' | -5.14 | 100.66 | 105.80 |
| 81 | DA | 2757 | U | C3'-C2'-C1' | 5.14 | 105.61 | 101.50 |
| 6 | AE | 226 | THR | CA-CB-CG2 | -5.14 | 105.21 | 112.40 |
| 74 | BQ | 46 | THR | N-CA-CB | 5.14 | 120.06 | 110.30 |
| 78 | CA | 554 | C | C1'-O4'-C4' | -5.14 | 105.79 | 109.90 |
| 78 | CA | 638 | U | C5'-C4'-C3' | 5.14 | 124.22 | 116.00 |
| 78 | CA | 1062 | A | C5-C6-N1 | -5.14 | 115.13 | 117.70 |
| 81 | DA | 948 | C | O4'-C1'-C2' | -5.14 | 100.66 | 105.80 |
| 81 | DA | 1151 | U | P-O3'-C3' | 5.14 | 125.86 | 119.70 |
| 81 | DA | 1372 | C | O4'-C1'-N1 | 5.14 | 112.31 | 108.20 |
| 81 | DA | 2491 | A | C3'-C2'-C1' | -5.14 | 97.39 | 101.50 |
| 81 | DA | 2641 | U | C5'-C4'-C3' | -5.14 | 107.78 | 116.00 |
| 81 | DA | 2879 | C | P-O3'-C3' | 5.14 | 125.86 | 119.70 |
| 82 | DB | 10 | A | C3'-C2'-C1' | 5.14 | 105.61 | 101.50 |
| 1 | Aa | 75 | ALA | N-CA-CB | 5.13 | 117.29 | 110.10 |
| 37 | BH | 200 | LEU | N-CA-CB | 5.13 | 120.67 | 110.40 |
| 69 | Br | 58 | PHE | CB-CA-C | 5.13 | 120.67 | 110.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 76 | BS | 65 | GLU | C-N-CA | 5.13 | 134.54 | 121.70 |
| 78 | CA | 368 | U | C5'-C4'-C3' | 5.13 | 124.22 | 116.00 |
| 78 | CA | 1143 | A | O4'-C1'-N9 | 5.13 | 112.31 | 108.20 |
| 81 | DA | 1647 | A | N9-C1'-C2' | -5.13 | 106.35 | 112.00 |
| 81 | DA | 2032 | U | P-O3'-C3' | -5.13 | 113.54 | 119.70 |
| 81 | DA | 2046 | U | OP2-P-O3' | 5.13 | 116.50 | 105.20 |
| 81 | DA | 2250 | G | O4'-C1'-N9 | 5.13 | 112.31 | 108.20 |
| 81 | DA | 2279 | A | N9-C1'-C2' | 5.13 | 120.67 | 114.00 |
| 59 | Bh | 77 | ALA | CB-CA-C | -5.13 | 102.40 | 110.10 |
| 78 | CA | 90 | C | N1-C1'-C2' | 5.13 | 120.67 | 114.00 |
| 78 | CA | 568 | G | O4'-C1'-N9 | 5.13 | 112.31 | 108.20 |
| 78 | CA | 586 | G | OP1-P-OP2 | -5.13 | 111.90 | 119.60 |
| 78 | CA | 1724 | U | C3'-C2'-C1' | 5.13 | 105.61 | 101.50 |
| 81 | DA | 55 | G | N9-C1'-C2' | 5.13 | 120.67 | 114.00 |
| 81 | DA | 1864 | A | N9-C1'-C2' | -5.13 | 106.35 | 112.00 |
| 81 | DA | 3314 | A | P-O5'-C5' | -5.13 | 112.69 | 120.90 |
| 61 | Bj | 44 | TYR | CG-CD1-CE1 | -5.13 | 117.19 | 121.30 |
| 78 | CA | 1534 | G | O5'-C5'-C4' | 5.13 | 121.45 | 111.70 |
| 81 | DA | 223 | U | N1-C1'-C2' | 5.13 | 120.67 | 114.00 |
| 81 | DA | 847 | A | C3'-C2'-C1' | 5.13 | 105.60 | 101.50 |
| 81 | DA | 1313 | G | O4'-C1'-N9 | 5.13 | 112.30 | 108.20 |
| 81 | DA | 3235 | C | C4'-C3'-C2' | -5.13 | 97.47 | 102.60 |
| 81 | DA | 3325 | G | C3'-C2'-C1' | -5.13 | 97.39 | 101.50 |
| 53 | Ba | 27 | LYS | CB-CG-CD | 5.13 | 124.94 | 111.60 |
| 67 | Bp | 51 | LEU | N-CA-CB | 5.13 | 120.66 | 110.40 |
| 81 | DA | 482 | C | O4'-C1'-C2' | -5.13 | 100.67 | 105.80 |
| 81 | DA | 695 | C | O4'-C1'-N1 | 5.13 | 112.30 | 108.20 |
| 81 | DA | 1257 | C | C5'-C4'-O4' | -5.13 | 102.94 | 109.10 |
| 81 | DA | 1261 | G | C5'-C4'-C3' | 5.13 | 124.21 | 116.00 |
| 34 | BE | 167 | TYR | N-CA-C | 5.13 | 124.85 | 111.00 |
| 78 | CA | 1590 | G | O4'-C1'-N9 | 5.13 | 112.30 | 108.20 |
| 81 | DA | 1534 | A | C2'-C3'-O3' | 5.13 | 121.91 | 113.70 |
| 81 | DA | 2173 | U | O4'-C4'-C3' | -5.13 | 98.87 | 104.00 |
| 81 | DA | 2572 | C | O4'-C1'-N1 | 5.13 | 112.30 | 108.20 |
| 81 | DA | 2691 | A | C3'-C2'-C1' | 5.13 | 105.60 | 101.50 |
| 81 | DA | 3166 | C | O5'-C5'-C4' | 5.13 | 121.44 | 111.70 |
| 1 | Aa | 51 | ASP | N-CA-CB | 5.13 | 119.83 | 110.60 |
| 15 | AN | 33 | LYS | C-N-CA | 5.13 | 134.52 | 121.70 |
| 17 | AQ | 53 | TYR | CD1-CG-CD2 | 5.13 | 123.54 | 117.90 |
| 73 | Bw | 17 | PRO | CA-N-CD | -5.13 | 104.32 | 111.50 |
| 78 | CA | 70 | C | O4'-C1'-C2' | -5.13 | 100.67 | 105.80 |
| 78 | CA | 818 | C | C3'-C2'-C1' | 5.13 | 105.60 | 101.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 823 | G | C5-C6-O6 | -5.13 | 125.53 | 128.60 |
| 78 | CA | 1627 | U | N1-C1'-C2' | 5.13 | 120.66 | 114.00 |
| 81 | DA | 70 | A | C1'-O4'-C4' | -5.13 | 105.80 | 109.90 |
| 81 | DA | 337 | G | P-O3'-C3' | 5.13 | 125.85 | 119.70 |
| 81 | DA | 2293 | C | O4'-C1'-C2' | -5.13 | 100.67 | 105.80 |
| 19 | AR | 89 | MET | CA-CB-CG | 5.12 | 122.01 | 113.30 |
| 46 | BT | 167 | ARG | NE-CZ-NH1 | -5.12 | 117.74 | 120.30 |
| 65 | Bn | 76 | ASN | C-N-CA | 5.12 | 134.51 | 121.70 |
| 77 | BI | 110 | ARG | O-C-N | -5.12 | 114.50 | 122.70 |
| 81 | DA | 274 | G | C1'-O4'-C4' | -5.12 | 105.80 | 109.90 |
| 81 | DA | 1232 | C | C1'-O4'-C4' | 5.12 | 114.00 | 109.90 |
| 1 | Aa | 131 | ILE | CB-CA-C | 5.12 | 121.85 | 111.60 |
| 6 | AE | 30 | THR | N-CA-CB | 5.12 | 120.03 | 110.30 |
| 32 | BC | 28 | ARG | NE-CZ-NH2 | -5.12 | 117.74 | 120.30 |
| 33 | BD | 330 | TYR | N-CA-C | 5.12 | 124.83 | 111.00 |
| 78 | CA | 1594 | G | O4'-C1'-N9 | 5.12 | 112.30 | 108.20 |
| 81 | DA | 820 | A | C3'-C2'-C1' | 5.12 | 105.60 | 101.50 |
| 81 | DA | 1548 | C | O4'-C1'-C2' | -5.12 | 100.68 | 105.80 |
| 3 | AB | 181 | VAL | CB-CA-C | -5.12 | 101.67 | 111.40 |
| 33 | BD | 138 | ARG | NE-CZ-NH2 | 5.12 | 122.86 | 120.30 |
| 39 | BJ | 85 | LEU | O-C-N | 5.12 | 130.90 | 122.70 |
| 45 | BR | 20 | LYS | CA-CB-CG | 5.12 | 124.67 | 113.40 |
| 61 | Bj | 86 | ARG | NE-CZ-NH2 | -5.12 | 117.74 | 120.30 |
| 78 | CA | 664 | U | O4'-C1'-N1 | 5.12 | 112.30 | 108.20 |
| 78 | CA | 665 | U | O4'-C1'-N1 | -5.12 | 104.10 | 108.20 |
| 81 | DA | 646 | A | C5'-C4'-C3' | 5.12 | 124.19 | 116.00 |
| 81 | DA | 704 | U | P-O5'-C5' | 5.12 | 129.10 | 120.90 |
| 81 | DA | 2044 | U | C3'-C2'-C1' | 5.12 | 105.60 | 101.50 |
| 81 | DA | 3088 | G | C3'-C2'-C1' | 5.12 | 105.60 | 101.50 |
| 83 | DC | 83 | U | O3'-P-O5' | 5.12 | 113.73 | 104.00 |
| 11 | AJ | 74 | GLU | N-CA-CB | -5.12 | 101.39 | 110.60 |
| 32 | BC | 72 | VAL | CA-CB-CG2 | -5.12 | 103.22 | 110.90 |
| 45 | BR | 25 | TYR | CB-CG-CD2 | 5.12 | 124.07 | 121.00 |
| 80 | CC | 19 | U | C6-N1-C1' | -5.12 | 114.03 | 121.20 |
| 81 | DA | 2174 | G | N9-C1'-C2' | 5.12 | 120.66 | 114.00 |
| 81 | DA | 2472 | U | O4'-C1'-N1 | 5.12 | 112.30 | 108.20 |
| 13 | AL | 93 | LEU | O-C-N | -5.12 | 114.51 | 122.70 |
| 29 | AU | 33 | ALA | N-CA-C | 5.12 | 124.82 | 111.00 |
| 32 | BC | 126 | LYS | C-N-CA | 5.12 | 134.50 | 121.70 |
| 32 | BC | 172 | ALA | N-CA-CB | 5.12 | 117.27 | 110.10 |
| 58 | Bg | 95 | PRO | N-CD-CG | 5.12 | 110.88 | 103.20 |
| 78 | CA | 645 | C | P-O3'-C3' | -5.12 | 113.56 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 829 | A | C4-C5-C6 | 5.12 | 119.56 | 117.00 |
| 81 | DA | 15 | C | P-O3'-C3' | -5.12 | 113.56 | 119.70 |
| 81 | DA | 241 | G | O3'-P-O5' | 5.12 | 113.73 | 104.00 |
| 81 | DA | 1190 | A | N9-C1'-C2' | 5.12 | 120.66 | 114.00 |
| 81 | DA | 1774 | C | O4'-C1'-C2' | -5.12 | 100.68 | 105.80 |
| 81 | DA | 1876 | U | N1-C1'-C2' | -5.12 | 106.37 | 112.00 |
| 81 | DA | 2088 | A | O5'-C5'-C4' | 5.12 | 121.43 | 111.70 |
| 81 | DA | 2952 | G | N9-C1'-C2' | 5.12 | 120.65 | 114.00 |
| 81 | DA | 3136 | G | C4'-C3'-C2' | -5.12 | 97.48 | 102.60 |
| 1 | Aa | 145 | LEU | CB-CG-CD2 | 5.12 | 119.70 | 111.00 |
| 8 | AF | 27 | THR | CA-CB-CG2 | -5.12 | 105.24 | 112.40 |
| 78 | CA | 473 | A | O4'-C1'-N9 | 5.12 | 112.29 | 108.20 |
| 78 | CA | 922 | G | C1'-O4'-C4' | -5.12 | 105.81 | 109.90 |
| 78 | CA | 1086 | A | C1'-O4'-C4' | -5.12 | 105.81 | 109.90 |
| 81 | DA | 2467 | G | C5'-C4'-C3' | 5.12 | 124.19 | 116.00 |
| 81 | DA | 2856 | G | N9-C1'-C2' | 5.12 | 120.65 | 114.00 |
| 22 | AV | 55 | PRO | N-CD-CG | 5.12 | 110.87 | 103.20 |
| 52 | BY | 113 | LYS | CA-CB-CG | 5.12 | 124.65 | 113.40 |
| 81 | DA | 161 | G | C5'-C4'-O4' | 5.12 | 115.24 | 109.10 |
| 81 | DA | 1592 | G | P-O3'-C3' | 5.12 | 125.84 | 119.70 |
| 81 | DA | 1717 | U | C4'-C3'-C2' | 5.12 | 107.72 | 102.60 |
| 81 | DA | 3038 | U | C4'-C3'-C2' | -5.12 | 97.48 | 102.60 |
| 30 | BA | 145 | TYR | CB-CG-CD1 | -5.11 | 117.93 | 121.00 |
| 57 | Be | 51 | TYR | CZ-CE2-CD2 | -5.11 | 115.20 | 119.80 |
| 81 | DA | 538 | G | N9-C1'-C2' | 5.11 | 120.65 | 114.00 |
| 81 | DA | 1477 | A | O3'-P-O5' | 5.11 | 113.72 | 104.00 |
| 81 | DA | 2575 | G | C5-C6-O6 | -5.11 | 125.53 | 128.60 |
| 81 | DA | 2984 | C | O4'-C1'-C2' | -5.11 | 100.69 | 105.80 |
| 81 | DA | 3164 | C | O4'-C1'-C2' | -5.11 | 100.69 | 105.80 |
| 21 | AT | 12 | TYR | CZ-CE2-CD2 | -5.11 | 115.20 | 119.80 |
| 78 | CA | 1136 | U | C4'-C3'-C2' | 5.11 | 107.71 | 102.60 |
| 81 | DA | 311 | C | C1'-O4'-C4' | 5.11 | 113.99 | 109.90 |
| 81 | DA | 359 | U | N1-C1'-C2' | 5.11 | 120.65 | 114.00 |
| 81 | DA | 2343 | C | C3'-C2'-C1' | 5.11 | 105.59 | 101.50 |
| 81 | DA | 3247 | G | N9-C1'-C2' | -5.11 | 106.38 | 112.00 |
| 43 | BP | 121 | VAL | O-C-N | -5.11 | 114.52 | 122.70 |
| 45 | BR | 36 | LEU | CB-CA-C | 5.11 | 119.91 | 110.20 |
| 78 | CA | 309 | C | C4'-C3'-C2' | -5.11 | 97.49 | 102.60 |
| 78 | CA | 489 | C | C4'-C3'-C2' | -5.11 | 97.49 | 102.60 |
| 78 | CA | 1537 | C | N1-C1'-C2' | 5.11 | 120.64 | 114.00 |
| 81 | DA | 202 | G | C1'-O4'-C4' | -5.11 | 105.81 | 109.90 |
| 81 | DA | 843 | A | O4'-C1'-C2' | -5.11 | 100.69 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1550 | C | C4'-C3'-C2' | -5.11 | 97.49 | 102.60 |
| 81 | DA | 2498 | U | O3'-P-O5' | 5.11 | 113.71 | 104.00 |
| 81 | DA | 3128 | G | O4'-C1'-N9 | 5.11 | 112.29 | 108.20 |
| 41 | BN | 26 | GLY | C-N-CA | 5.11 | 134.47 | 121.70 |
| 78 | CA | 641 | G | O4'-C1'-N9 | 5.11 | 112.29 | 108.20 |
| 78 | CA | 1260 | U | O4'-C1'-C2' | -5.11 | 100.69 | 105.80 |
| 81 | DA | 1454 | A | O4'-C1'-C2' | -5.11 | 100.69 | 105.80 |
| 81 | DA | 2476 | C | C5'-C4'-O4' | -5.11 | 102.97 | 109.10 |
| 4 | AD | 209 | HIS | N-CA-CB | 5.11 | 119.79 | 110.60 |
| 13 | AL | 38 | PHE | O-C-N | -5.11 | 114.53 | 122.70 |
| 18 | AP | 65 | SER | N-CA-CB | 5.11 | 118.16 | 110.50 |
| 59 | Bh | 21 | HIS | CB-CG-ND1 | 5.11 | 135.97 | 123.20 |
| 78 | CA | 267 | U | C4'-C3'-C2' | -5.11 | 97.49 | 102.60 |
| 78 | CA | 1546 | G | P-O5'-C5' | 5.11 | 129.07 | 120.90 |
| 81 | DA | 299 | G | O4'-C1'-C2' | 5.11 | 112.20 | 107.60 |
| 81 | DA | 436 | A | O4'-C1'-N9 | -5.11 | 104.11 | 108.20 |
| 81 | DA | 673 | U | C1'-O4'-C4' | -5.11 | 105.81 | 109.90 |
| 81 | DA | 2218 | G | C3'-C2'-C1' | -5.11 | 97.41 | 101.50 |
| 53 | Ba | 44 | ALA | N-CA-C | -5.11 | 97.21 | 111.00 |
| 78 | CA | 257 | A | P-O3'-C3' | 5.11 | 125.83 | 119.70 |
| 78 | CA | 1300 | A | N9-C1'-C2' | -5.11 | 106.38 | 112.00 |
| 81 | DA | 1364 | C | O4'-C1'-C2' | -5.11 | 100.69 | 105.80 |
| 81 | DA | 2398 | A | C5'-C4'-C3' | -5.11 | 107.83 | 116.00 |
| 81 | DA | 3289 | G | C1'-O4'-C4' | -5.11 | 105.82 | 109.90 |
| 78 | CA | 1083 | G | O4'-C1'-N9 | 5.10 | 112.28 | 108.20 |
| 78 | CA | 1381 | U | C1'-O4'-C4' | 5.10 | 113.98 | 109.90 |
| 2 | AA | 191 | ARG | NE-CZ-NH2 | -5.10 | 117.75 | 120.30 |
| 4 | AD | 140 | VAL | N-CA-C | -5.10 | 97.22 | 111.00 |
| 5 | AC | 63 | ASP | O-C-N | -5.10 | 114.53 | 122.70 |
| 13 | AL | 124 | VAL | O-C-N | -5.10 | 114.53 | 122.70 |
| 69 | Br | 71 | ARG | NE-CZ-NH1 | 5.10 | 122.85 | 120.30 |
| 77 | BI | 178 | ARG | CA-C-N | 5.10 | 131.39 | 117.10 |
| 78 | CA | 344 | A | P-O3'-C3' | 5.10 | 125.82 | 119.70 |
| 78 | CA | 1395 | G | O3'-P-O5' | 5.10 | 113.69 | 104.00 |
| 81 | DA | 283 | G | C1'-O4'-C4' | -5.10 | 105.82 | 109.90 |
| 81 | DA | 902 | G | C1'-O4'-C4' | -5.10 | 105.82 | 109.90 |
| 81 | DA | 1198 | C | O4'-C1'-N1 | 5.10 | 112.28 | 108.20 |
| 81 | DA | 1679 | A | P-O3'-C3' | 5.10 | 125.82 | 119.70 |
| 81 | DA | 1881 | A | O4'-C1'-C2' | -5.10 | 100.70 | 105.80 |
| 81 | DA | 2178 | A | C1'-O4'-C4' | -5.10 | 105.82 | 109.90 |
| 81 | DA | 2700 | G | N9-C1'-C2' | 5.10 | 120.63 | 114.00 |
| 81 | DA | 2876 | C | C1'-O4'-C4' | -5.10 | 105.82 | 109.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 66 | Bo | 32 | ASN | N-CA-CB | 5.10 | 119.78 | 110.60 |
| 81 | DA | 790 | U | O4'-C1'-N1 | 5.10 | 112.28 | 108.20 |
| 81 | DA | 1004 | U | O4'-C1'-N1 | 5.10 | 112.28 | 108.20 |
| 81 | DA | 1209 | G | C4'-C3'-C2' | -5.10 | 97.50 | 102.60 |
| 2 | AA | 54 | TRP | CD1-CG-CD2 | -5.10 | 102.22 | 106.30 |
| 13 | AL | 1 | MET | CA-CB-CG | 5.10 | 121.97 | 113.30 |
| 38 | Bs | 124 | VAL | CB-CA-C | 5.10 | 121.09 | 111.40 |
| 51 | BZ | 11 | ALA | N-CA-CB | 5.10 | 117.24 | 110.10 |
| 57 | Be | 179 | LEU | CB-CA-C | -5.10 | 100.51 | 110.20 |
| 78 | CA | 246 | G | P-O3'-C3' | -5.10 | 113.58 | 119.70 |
| 78 | CA | 542 | A | C5'-C4'-C3' | 5.10 | 124.16 | 116.00 |
| 80 | CC | 21 | C | N3-C4-N4 | 5.10 | 121.57 | 118.00 |
| 81 | DA | 793 | C | C3'-C2'-C1' | 5.10 | 105.58 | 101.50 |
| 16 | AO | 107 | LYS | N-CA-CB | 5.10 | 119.78 | 110.60 |
| 17 | AQ | 60 | ARG | CB-CA-C | -5.10 | 100.21 | 110.40 |
| 78 | CA | 117 | U | C4'-C3'-C2' | -5.10 | 97.50 | 102.60 |
| 78 | CA | 847 | A | O4'-C1'-C2' | 5.10 | 112.19 | 107.60 |
| 78 | CA | 1505 | A | C8-N9-C4 | -5.10 | 103.76 | 105.80 |
| 78 | CA | 1566 | U | O4'-C4'-C3' | 5.10 | 110.18 | 106.10 |
| 81 | DA | 1673 | G | N9-C1'-C2' | 5.10 | 120.63 | 114.00 |
| 81 | DA | 1774 | C | C4'-C3'-C2' | -5.10 | 97.50 | 102.60 |
| 81 | DA | 1865 | A | O4'-C1'-C2' | -5.10 | 100.70 | 105.80 |
| 81 | DA | 2305 | G | O4'-C1'-C2' | 5.10 | 112.19 | 107.60 |
| 78 | CA | 1193 | A | O4'-C1'-C2' | -5.10 | 100.70 | 105.80 |
| 81 | DA | 2599 | U | C3'-C2'-C1' | 5.10 | 105.58 | 101.50 |
| 81 | DA | 3140 | G | O3'-P-O5' | -5.10 | 94.32 | 104.00 |
| 26 | AZ | 44 | PHE | N-CA-C | -5.09 | 97.25 | 111.00 |
| 65 | Bn | 11 | PHE | CB-CG-CD2 | -5.09 | 117.23 | 120.80 |
| 78 | CA | 487 | G | N3-C2-N2 | 5.09 | 123.47 | 119.90 |
| 78 | CA | 490 | C | C5'-C4'-O4' | 5.09 | 115.21 | 109.10 |
| 78 | CA | 629 | U | O4'-C1'-C2' | -5.09 | 100.71 | 105.80 |
| 78 | CA | 1279 | C | C3'-C2'-C1' | 5.09 | 105.58 | 101.50 |
| 81 | DA | 1445 | U | N1-C1'-C2' | 5.09 | 120.62 | 114.00 |
| 81 | DA | 1753 | G | O4'-C1'-C2' | -5.09 | 100.70 | 105.80 |
| 81 | DA | 2318 | U | O3'-P-O5' | -5.09 | 94.32 | 104.00 |
| 82 | DB | 137 | C | O4'-C1'-C2' | -5.09 | 100.71 | 105.80 |
| 2 | AA | 243 | ALA | CB-CA-C | -5.09 | 102.46 | 110.10 |
| 20 | AS | 48 | GLN | O-C-N | -5.09 | 114.55 | 122.70 |
| 78 | CA | 546 | U | O3'-P-O5' | 5.09 | 113.68 | 104.00 |
| 81 | DA | 182 | U | C4'-C3'-C2' | 5.09 | 107.69 | 102.60 |
| 81 | DA | 308 | A | P-O3'-C3' | 5.09 | 125.81 | 119.70 |
| 10 | AI | 28 | LEU | CB-CA-C | 5.09 | 119.87 | 110.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 74 | BQ | 243 | ALA | CA-C-O | -5.09 | 109.41 | 120.10 |
| 78 | CA | 1221 | A | C4'-C3'-C2' | -5.09 | 97.51 | 102.60 |
| 81 | DA | 275 | U | O3'-P-O5' | 5.09 | 113.67 | 104.00 |
| 81 | DA | 883 | A | P-O3'-C3' | 5.09 | 125.81 | 119.70 |
| 81 | DA | 1826 | C | C1'-O4'-C4' | -5.09 | 105.83 | 109.90 |
| 81 | DA | 2750 | U | N1-C1'-C2' | 5.09 | 120.62 | 114.00 |
| 81 | DA | 3213 | A | C5'-C4'-C3' | 5.09 | 124.15 | 116.00 |
| 13 | AL | 97 | ASP | CB-CG-OD2 | -5.09 | 113.72 | 118.30 |
| 31 | BB | 54 | ARG | CB-CA-C | -5.09 | 100.22 | 110.40 |
| 78 | CA | 339 | C | O4'-C1'-N1 | 5.09 | 112.27 | 108.20 |
| 81 | DA | 480 | C | P-O3'-C3' | 5.09 | 125.81 | 119.70 |
| 81 | DA | 1425 | U | C3'-C2'-C1' | 5.09 | 105.57 | 101.50 |
| 81 | DA | 2625 | C | P-O5'-C5' | 5.09 | 129.04 | 120.90 |
| 76 | BS | 29 | MET | CG-SD-CE | -5.09 | 92.06 | 100.20 |
| 20 | AS | 44 | GLU | CA-C-N | -5.09 | 106.01 | 117.20 |
| 32 | BC | 240 | ARG | CA-C-N | -5.09 | 106.01 | 117.20 |
| 38 | Bs | 155 | ASP | CB-CG-OD2 | -5.09 | 113.72 | 118.30 |
| 46 | BT | 71 | ARG | NE-CZ-NH2 | -5.09 | 117.76 | 120.30 |
| 78 | CA | 1398 | U | O4'-C1'-N1 | 5.09 | 112.27 | 108.20 |
| 81 | DA | 492 | U | O4'-C1'-C2' | -5.09 | 100.71 | 105.80 |
| 81 | DA | 1728 | G | P-O5'-C5' | 5.09 | 129.04 | 120.90 |
| 81 | DA | 1741 | A | P-O5'-C5' | -5.09 | 112.76 | 120.90 |
| 81 | DA | 1848 | G | C3'-C2'-C1' | 5.09 | 105.57 | 101.50 |
| 81 | DA | 1852 | G | N9-C1'-C2' | 5.09 | 120.61 | 114.00 |
| 81 | DA | 2400 | G | N9-C1'-C2' | 5.09 | 120.61 | 114.00 |
| 81 | DA | 3392 | U | P-O3'-C3' | 5.09 | 125.81 | 119.70 |
| 1 | Aa | 212 | ALA | CB-CA-C | -5.08 | 102.47 | 110.10 |
| 19 | AR | 50 | THR | N-CA-C | -5.08 | 97.27 | 111.00 |
| 31 | BB | 67 | TYR | CB-CA-C | 5.08 | 120.57 | 110.40 |
| 37 | BH | 185 | ARG | CB-CA-C | -5.08 | 100.23 | 110.40 |
| 64 | Bl | 73 | ARG | NE-CZ-NH1 | -5.08 | 117.76 | 120.30 |
| 81 | DA | 328 | U | C4'-C3'-C2' | 5.08 | 107.69 | 102.60 |
| 81 | DA | 1562 | C | O4'-C1'-C2' | -5.08 | 100.72 | 105.80 |
| 81 | DA | 2726 | C | O4'-C1'-C2' | -5.08 | 100.72 | 105.80 |
| 9 | AH | 69 | LEU | CB-CG-CD1 | 5.08 | 119.64 | 111.00 |
| 20 | AS | 116 | ILE | CA-CB-CG1 | 5.08 | 120.66 | 111.00 |
| 25 | AY | 20 | GLY | CA-C-O | -5.08 | 111.45 | 120.60 |
| 81 | DA | 24 | G | N9-C1'-C2' | -5.08 | 106.41 | 112.00 |
| 81 | DA | 1254 | C | C3'-C2'-C1' | 5.08 | 105.57 | 101.50 |
| 81 | DA | 3002 | C | OP2-P-O3' | -5.08 | 94.02 | 105.20 |
| 81 | DA | 3030 | G | C5'-C4'-C3' | 5.08 | 124.13 | 116.00 |
| 81 | DA | 3141 | A | C3'-C2'-C1' | 5.08 | 105.57 | 101.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 82 | DB | 100 | U | C1'-O4'-C4' | -5.08 | 105.83 | 109.90 |
| 83 | DC | 49 | G | P-O3'-C3' | 5.08 | 125.80 | 119.70 |
| 83 | DC | 85 | G | O4'-C1'-C2' | 5.08 | 112.17 | 107.60 |
| 4 | AD | 136 | VAL | N-CA-C | -5.08 | 97.28 | 111.00 |
| 8 | AF | 28 | PRO | CA-C-N | -5.08 | 106.02 | 117.20 |
| 17 | AQ | 94 | SER | N-CA-C | -5.08 | 97.28 | 111.00 |
| 38 | Bs | 244 | LYS | C-N-CA | 5.08 | 134.40 | 121.70 |
| 49 | BV | 69 | ARG | NE-CZ-NH1 | 5.08 | 122.84 | 120.30 |
| 51 | BZ | 69 | LYS | CA-C-N | -5.08 | 106.02 | 117.20 |
| 76 | BS | 72 | THR | N-CA-C | -5.08 | 97.28 | 111.00 |
| 78 | CA | 912 | U | C5'-C4'-C3' | -5.08 | 107.87 | 116.00 |
| 78 | CA | 1205 | C | N1-C1'-C2' | 5.08 | 120.61 | 114.00 |
| 78 | CA | 1246 | C | O4'-C1'-N1 | 5.08 | 112.27 | 108.20 |
| 81 | DA | 125 | C | O4'-C1'-N1 | 5.08 | 112.27 | 108.20 |
| 81 | DA | 243 | G | C5'-C4'-C3' | 5.08 | 124.13 | 116.00 |
| 81 | DA | 983 | A | O5'-P-OP1 | 5.08 | 116.80 | 110.70 |
| 81 | DA | 1587 | A | C1'-O4'-C4' | 5.08 | 113.97 | 109.90 |
| 81 | DA | 2658 | G | O4'-C1'-N9 | 5.08 | 112.26 | 108.20 |
| 81 | DA | 2684 | C | O4'-C1'-C2' | -5.08 | 100.72 | 105.80 |
| 81 | DA | 3324 | C | O4'-C1'-N1 | 5.08 | 112.27 | 108.20 |
| 82 | DB | 85 | G | P-O3'-C3' | -5.08 | 113.60 | 119.70 |
| 42 | BM | 85 | TRP | NE1-CE2-CD2 | 5.08 | 112.38 | 107.30 |
| 78 | CA | 1775 | U | C4'-C3'-C2' | -5.08 | 97.52 | 102.60 |
| 81 | DA | 2416 | U | O3'-P-O5' | 5.08 | 113.65 | 104.00 |
| 6 | AE | 236 | PRO | C-N-CA | 5.08 | 134.40 | 121.70 |
| 8 | AF | 28 | PRO | CA-N-CD | -5.08 | 104.39 | 111.50 |
| 39 | BJ | 73 | VAL | CA-CB-CG1 | 5.08 | 118.52 | 110.90 |
| 44 | BO | 107 | ALA | N-CA-CB | 5.08 | 117.21 | 110.10 |
| 53 | Ba | 77 | TYR | CB-CG-CD1 | -5.08 | 117.95 | 121.00 |
| 81 | DA | 2354 | C | P-O5'-C5' | 5.08 | 129.02 | 120.90 |
| 81 | DA | 3222 | U | O4'-C4'-C3' | -5.08 | 98.92 | 104.00 |
| 81 | DA | 3313 | U | OP1-P-O3' | 5.08 | 116.38 | 105.20 |
| 15 | AN | 13 | ARG | NE-CZ-NH1 | 5.08 | 122.84 | 120.30 |
| 21 | AT | 29 | HIS | C-N-CA | 5.08 | 134.39 | 121.70 |
| 76 | BS | 157 | LYS | N-CA-C | 5.08 | 124.71 | 111.00 |
| 78 | CA | 850 | A | OP1-P-OP2 | -5.08 | 111.98 | 119.60 |
| 81 | DA | 1190 | A | O4'-C1'-N9 | -5.08 | 104.14 | 108.20 |
| 4 | AD | 224 | ASN | CA-CB-CG | -5.08 | 102.23 | 113.40 |
| 11 | AJ | 76 | SER | N-CA-C | -5.08 | 97.30 | 111.00 |
| 32 | BC | 295 | ALA | CB-CA-C | -5.08 | 102.49 | 110.10 |
| 38 | Bs | 104 | ARG | NE-CZ-NH1 | 5.08 | 122.84 | 120.30 |
| 43 | BP | 119 | TYR | C-N-CA | 5.08 | 134.39 | 121.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 1404 | C | N1-C1'-C2' | 5.08 | 120.60 | 114.00 |
| 78 | CA | 1611 | A | O4'-C1'-C2' | -5.08 | 100.72 | 105.80 |
| 81 | DA | 245 | U | C1'-O4'-C4' | -5.08 | 105.84 | 109.90 |
| 81 | DA | 440 | A | P-O3'-C3' | 5.08 | 125.79 | 119.70 |
| 81 | DA | 1013 | G | C5'-C4'-C3' | 5.08 | 124.12 | 116.00 |
| 81 | DA | 1322 | U | O4'-C1'-N1 | 5.08 | 112.26 | 108.20 |
| 81 | DA | 1591 | G | C3'-C2'-C1' | -5.08 | 97.44 | 101.50 |
| 81 | DA | 3025 | C | P-O3'-C3' | -5.08 | 113.61 | 119.70 |
| 81 | DA | 3105 | U | O4'-C1'-N1 | 5.08 | 112.26 | 108.20 |
| 16 | AO | 75 | LEU | O-C-N | -5.07 | 114.58 | 122.70 |
| 32 | BC | 367 | LYS | C-N-CA | 5.07 | 132.96 | 122.30 |
| 35 | BG | 52 | VAL | CA-CB-CG1 | -5.07 | 103.29 | 110.90 |
| 37 | BH | 150 | LEU | CB-CG-CD1 | 5.07 | 119.62 | 111.00 |
| 38 | Bs | 184 | GLY | N-CA-C | -5.07 | 100.42 | 113.10 |
| 45 | BR | 58 | ASN | N-CA-CB | 5.07 | 119.73 | 110.60 |
| 78 | CA | 305 | C | P-O3'-C3' | -5.07 | 113.61 | 119.70 |
| 78 | CA | 588 | U | C5'-C4'-C3' | 5.07 | 124.12 | 116.00 |
| 78 | CA | 1612 | U | O4'-C1'-C2' | -5.07 | 100.73 | 105.80 |
| 81 | DA | 975 | C | C1'-O4'-C4' | 5.07 | 113.96 | 109.90 |
| 81 | DA | 1160 | C | N1-C1'-C2' | 5.07 | 120.59 | 114.00 |
| 81 | DA | 2963 | C | O3'-P-O5' | 5.07 | 113.64 | 104.00 |
| 1 | Aa | 317 | THR | N-CA-CB | 5.07 | 119.94 | 110.30 |
| 8 | AF | 184 | PHE | CG-CD1-CE1 | -5.07 | 115.22 | 120.80 |
| 78 | CA | 1120 | U | N1-C1'-C2' | 5.07 | 120.59 | 114.00 |
| 35 | BG | 150 | LYS | N-CA-C | -5.07 | 97.31 | 111.00 |
| 57 | Be | 107 | ARG | NE-CZ-NH2 | -5.07 | 117.77 | 120.30 |
| 78 | CA | 483 | A | O4'-C1'-N9 | 5.07 | 112.26 | 108.20 |
| 78 | CA | 702 | G | C5'-C4'-C3' | 5.07 | 124.11 | 116.00 |
| 78 | CA | 1316 | G | C4'-C3'-C2' | -5.07 | 97.53 | 102.60 |
| 78 | CA | 1502 | G | N3-C2-N2 | 5.07 | 123.45 | 119.90 |
| 79 | CB | 17 | G | C5'-C4'-C3' | -5.07 | 107.89 | 116.00 |
| 81 | DA | 329 | U | P-O5'-C5' | -5.07 | 112.79 | 120.90 |
| 8 | AF | 82 | PHE | CB-CG-CD1 | 5.07 | 124.35 | 120.80 |
| 44 | BO | 3 | SER | C-N-CA | 5.07 | 134.37 | 121.70 |
| 81 | DA | 1758 | G | C5'-C4'-O4' | 5.07 | 115.18 | 109.10 |
| 81 | DA | 2010 | U | P-O3'-C3' | -5.07 | 113.62 | 119.70 |
| 81 | DA | 3301 | U | C1'-O4'-C4' | -5.07 | 105.84 | 109.90 |
| 9 | AH | 50 | PHE | N-CA-CB | 5.07 | 119.72 | 110.60 |
| 41 | BN | 112 | LEU | N-CA-CB | 5.07 | 120.53 | 110.40 |
| 44 | BO | 97 | GLU | N-CA-CB | 5.07 | 119.72 | 110.60 |
| 50 | BX | 127 | THR | CA-CB-CG2 | -5.07 | 105.31 | 112.40 |
| 67 | Bp | 15 | CYS | N-CA-C | 5.07 | 124.68 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | CA | 179 | A | O5'-C5'-C4' | -5.07 | 102.07 | 111.70 |
| 78 | CA | 335 | U | C2'-C3'-O3' | 5.07 | 121.81 | 113.70 |
| 78 | CA | 686 | C | N1-C1'-C2' | 5.07 | 120.59 | 114.00 |
| 78 | CA | 1694 | A | O4'-C1'-N9 | 5.07 | 112.25 | 108.20 |
| 81 | DA | 1295 | G | C5'-C4'-O4' | 5.07 | 115.18 | 109.10 |
| 81 | DA | 2351 | U | C1'-O4'-C4' | -5.07 | 105.85 | 109.90 |
| 81 | DA | 2686 | A | O4'-C1'-N9 | 5.07 | 112.25 | 108.20 |
| 81 | DA | 2834 | G | C1'-O4'-C4' | -5.07 | 105.85 | 109.90 |
| 81 | DA | 3324 | C | N1-C1'-C2' | 5.07 | 120.59 | 114.00 |
| 6 | AE | 143 | TYR | CB-CG-CD1 | -5.07 | 117.96 | 121.00 |
| 8 | AF | 225 | ARG | NH1-CZ-NH2 | -5.07 | 113.83 | 119.40 |
| 78 | CA | 270 | C | P-O5'-C5' | -5.07 | 112.80 | 120.90 |
| 81 | DA | 1681 | U | N1-C1'-C2' | 5.07 | 120.58 | 114.00 |
| 81 | DA | 2447 | A | C1'-O4'-C4' | -5.07 | 105.85 | 109.90 |
| 81 | DA | 2996 | U | P-O3'-C3' | 5.07 | 125.78 | 119.70 |
| 81 | DA | 3363 | U | O3'-P-O5' | -5.07 | 94.38 | 104.00 |
| 35 | BG | 92 | SER | N-CA-CB | 5.06 | 118.10 | 110.50 |
| 78 | CA | 50 | C | N1-C1'-C2' | 5.06 | 120.58 | 114.00 |
| 78 | CA | 1691 | A | O5'-C5'-C4' | 5.06 | 121.32 | 111.70 |
| 81 | DA | 1757 | A | P-O5'-C5' | 5.06 | 129.00 | 120.90 |
| 81 | DA | 77 | A | C3'-C2'-C1' | -5.06 | 97.45 | 101.50 |
| 81 | DA | 623 | U | C5'-C4'-O4' | 5.06 | 115.17 | 109.10 |
| 81 | DA | 964 | G | N9-C1'-C2' | 5.06 | 120.58 | 114.00 |
| 81 | DA | 1198 | C | C5'-C4'-C3' | -5.06 | 107.90 | 116.00 |
| 29 | AU | 35 | VAL | C-N-CA | -5.06 | 109.05 | 121.70 |
| 33 | BD | 34 | ILE | N-CA-CB | 5.06 | 122.44 | 110.80 |
| 43 | BP | 28 | TRP | CB-CA-C | -5.06 | 100.28 | 110.40 |
| 47 | BU | 56 | PHE | C-N-CA | 5.06 | 134.35 | 121.70 |
| 81 | DA | 77 | A | N9-C1'-C2' | 5.06 | 120.58 | 114.00 |
| 81 | DA | 1419 | A | O4'-C1'-N9 | 5.06 | 112.25 | 108.20 |
| 81 | DA | 1574 | C | P-O3'-C3' | 5.06 | 125.77 | 119.70 |
| 81 | DA | 2700 | G | O4'-C1'-N9 | 5.06 | 112.25 | 108.20 |
| 81 | DA | 2859 | U | C1'-O4'-C4' | 5.06 | 113.95 | 109.90 |
| 20 | AS | 69 | LYS | CA-CB-CG | 5.06 | 124.53 | 113.40 |
| 32 | BC | 266 | ARG | CB-CA-C | -5.06 | 100.28 | 110.40 |
| 42 | BM | 45 | ARG | N-CA-CB | -5.06 | 101.49 | 110.60 |
| 43 | BP | 67 | ARG | NE-CZ-NH1 | 5.06 | 122.83 | 120.30 |
| 78 | CA | 344 | A | N9-C1'-C2' | 5.06 | 120.58 | 114.00 |
| 78 | CA | 544 | A | O3'-P-O5' | 5.06 | 113.61 | 104.00 |
| 78 | CA | 1210 | C | O4'-C1'-N1 | 5.06 | 112.25 | 108.20 |
| 81 | DA | 358 | G | O4'-C1'-N9 | 5.06 | 112.25 | 108.20 |
| 81 | DA | 1668 | G | P-O5'-C5' | 5.06 | 129.00 | 120.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2192 | C | O4'-C1'-N1 | 5.06 | 112.25 | 108.20 |
| 81 | DA | 3023 | U | O4'-C1'-C2' | -5.06 | 100.74 | 105.80 |
| 46 | BT | 85 | ARG | NE-CZ-NH1 | 5.06 | 122.83 | 120.30 |
| 64 | Bl | 66 | TYR | CB-CG-CD1 | 5.06 | 124.03 | 121.00 |
| 78 | CA | 284 | G | P-O3'-C3' | -5.06 | 113.63 | 119.70 |
| 78 | CA | 337 | G | O4'-C4'-C3' | 5.06 | 110.15 | 106.10 |
| 78 | CA | 1389 | C | C1'-O4'-C4' | 5.06 | 113.95 | 109.90 |
| 79 | CB | 11 | U | C1'-O4'-C4' | 5.06 | 113.95 | 109.90 |
| 81 | DA | 66 | A | C1'-O4'-C4' | 5.06 | 113.94 | 109.90 |
| 81 | DA | 327 | A | C3'-C2'-C1' | 5.06 | 105.55 | 101.50 |
| 81 | DA | 743 | C | C1'-O4'-C4' | -5.06 | 105.85 | 109.90 |
| 81 | DA | 777 | U | O4'-C1'-C2' | 5.06 | 112.15 | 107.60 |
| 81 | DA | 2191 | U | N1-C1'-C2' | 5.06 | 120.58 | 114.00 |
| 81 | DA | 2492 | C | C2'-C3'-O3' | 5.06 | 121.79 | 113.70 |
| 81 | DA | 2618 | G | O5'-P-OP2 | -5.06 | 101.15 | 105.70 |
| 81 | DA | 1615 | C | C1'-O4'-C4' | -5.06 | 105.86 | 109.90 |
| 8 | AF | 202 | ALA | CB-CA-C | -5.05 | 102.52 | 110.10 |
| 21 | AT | 34 | ILE | N-CA-CB | 5.05 | 122.42 | 110.80 |
| 33 | BD | 260 | GLN | N-CA-CB | 5.05 | 119.70 | 110.60 |
| 46 | BT | 89 | LEU | N-CA-C | -5.05 | 97.35 | 111.00 |
| 58 | Bg | 65 | LYS | N-CA-C | 5.05 | 124.65 | 111.00 |
| 59 | Bh | 15 | LYS | C-N-CA | 5.05 | 134.34 | 121.70 |
| 78 | CA | 140 | A | C3'-C2'-C1' | 5.05 | 105.54 | 101.50 |
| 78 | CA | 1336 | A | O4'-C1'-C2' | -5.05 | 100.75 | 105.80 |
| 79 | CB | 9 | A | O4'-C1'-C2' | -5.05 | 100.75 | 105.80 |
| 81 | DA | 39 | A | O4'-C1'-N9 | 5.05 | 112.24 | 108.20 |
| 81 | DA | 102 | C | C3'-C2'-C1' | 5.05 | 105.54 | 101.50 |
| 81 | DA | 202 | G | C3'-C2'-C1' | 5.05 | 105.54 | 101.50 |
| 81 | DA | 393 | U | C1'-O4'-C4' | -5.05 | 105.86 | 109.90 |
| 81 | DA | 888 | A | O4'-C1'-C2' | -5.05 | 100.75 | 105.80 |
| 81 | DA | 970 | A | O4'-C1'-N9 | 5.05 | 112.24 | 108.20 |
| 81 | DA | 1359 | C | N1-C1'-C2' | 5.05 | 120.57 | 114.00 |
| 81 | DA | 1702 | U | O5'-C5'-C4' | 5.05 | 121.30 | 111.70 |
| 81 | DA | 1704 | A | C2'-C3'-O3' | 5.05 | 121.79 | 113.70 |
| 81 | DA | 2375 | G | C5'-C4'-C3' | 5.05 | 124.09 | 116.00 |
| 81 | DA | 2757 | U | O3'-P-O5' | -5.05 | 94.39 | 104.00 |
| 81 | DA | 3147 | G | C3'-C2'-C1' | 5.05 | 105.54 | 101.50 |
| 81 | DA | 3325 | G | C4'-C3'-O3' | 5.05 | 123.11 | 113.00 |
| 2 | AA | 71 | GLU | N-CA-CB | 5.05 | 119.69 | 110.60 |
| 8 | AF | 218 | GLU | N-CA-CB | 5.05 | 119.70 | 110.60 |
| 54 | Bd | 56 | ALA | N-CA-C | 5.05 | 124.64 | 111.00 |
| 1 | Aa | 6 | VAL | N-CA-C | -5.05 | 97.36 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 16 | AO | 127 | ARG | N-CA-CB | 5.05 | 119.69 | 110.60 |
| 20 | AS | 37 | VAL | N-CA-C | -5.05 | 97.36 | 111.00 |
| 49 | BV | 90 | PHE | CB-CG-CD2 | 5.05 | 124.34 | 120.80 |
| 59 | Bh | 28 | VAL | CA-CB-CG2 | -5.05 | 103.32 | 110.90 |
| 78 | CA | 566 | C | N3-C4-N4 | 5.05 | 121.54 | 118.00 |
| 78 | CA | 1135 | U | N1-C1'-C2' | 5.05 | 120.57 | 114.00 |
| 79 | CB | 37 | G | C1'-O4'-C4' | -5.05 | 105.86 | 109.90 |
| 81 | DA | 584 | G | N9-C1'-C2' | 5.05 | 120.57 | 114.00 |
| 81 | DA | 678 | G | O4'-C1'-N9 | 5.05 | 112.24 | 108.20 |
| 81 | DA | 2526 | C | C2'-C3'-O3' | 5.05 | 121.78 | 113.70 |
| 8 | AF | 148 | ARG | CB-CA-C | -5.05 | 100.30 | 110.40 |
| 19 | AR | 105 | VAL | N-CA-CB | 5.05 | 122.61 | 111.50 |
| 32 | BC | 380 | MET | CB-CA-C | 5.05 | 120.50 | 110.40 |
| 42 | BM | 68 | GLU | CB-CA-C | 5.05 | 120.50 | 110.40 |
| 53 | Ba | 14 | VAL | CA-CB-CG1 | 5.05 | 118.47 | 110.90 |
| 59 | Bh | 17 | PHE | N-CA-CB | 5.05 | 119.69 | 110.60 |
| 78 | CA | 412 | A | O4'-C1'-C2' | -5.05 | 100.75 | 105.80 |
| 78 | CA | 718 | U | O3'-P-O5' | -5.05 | 94.41 | 104.00 |
| 78 | CA | 1109 | G | O4'-C1'-N9 | 5.05 | 112.24 | 108.20 |
| 78 | CA | 1126 | G | C5'-C4'-O4' | 5.05 | 115.16 | 109.10 |
| 78 | CA | 1452 | U | OP1-P-O3' | 5.05 | 116.31 | 105.20 |
| 78 | CA | 1550 | A | O4'-C4'-C3' | 5.05 | 110.14 | 106.10 |
| 81 | DA | 1383 | G | C1'-O4'-C4' | -5.05 | 105.86 | 109.90 |
| 81 | DA | 2104 | A | C3'-C2'-C1' | 5.05 | 105.54 | 101.50 |
| 81 | DA | 3035 | A | N9-C1'-C2' | 5.05 | 120.56 | 114.00 |
| 35 | BG | 99 | GLU | CA-C-O | 5.05 | 130.70 | 120.10 |
| 46 | BT | 52 | LYS | CA-CB-CG | -5.05 | 102.29 | 113.40 |
| 50 | BX | 84 | PHE | N-CA-CB | 5.05 | 119.68 | 110.60 |
| 78 | CA | 193 | U | O4'-C1'-N1 | 5.05 | 112.24 | 108.20 |
| 78 | CA | 205 | U | P-O5'-C5' | 5.05 | 128.97 | 120.90 |
| 78 | CA | 1129 | U | C1'-O4'-C4' | 5.05 | 113.94 | 109.90 |
| 78 | CA | 1554 | U | C3'-C2'-C1' | 5.05 | 105.54 | 101.50 |
| 81 | DA | 8 | C | N1-C1'-C2' | 5.05 | 120.56 | 114.00 |
| 81 | DA | 715 | A | O4'-C1'-C2' | 5.05 | 112.14 | 107.60 |
| 81 | DA | 738 | A | C5-C6-N1 | -5.05 | 115.18 | 117.70 |
| 81 | DA | 2171 | G | C3'-C2'-C1' | 5.05 | 105.54 | 101.50 |
| 81 | DA | 2631 | U | P-O5'-C5' | -5.05 | 112.83 | 120.90 |
| 33 | BD | 104 | LYS | N-CA-CB | 5.04 | 119.68 | 110.60 |
| 74 | BQ | 293 | LEU | N-CA-CB | 5.04 | 120.49 | 110.40 |
| 78 | CA | 122 | U | C4'-C3'-C2' | -5.04 | 97.56 | 102.60 |
| 78 | CA | 644 | C | O4'-C1'-N1 | 5.04 | 112.24 | 108.20 |
| 78 | CA | 1586 | A | N9-C1'-C2' | 5.04 | 120.56 | 114.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2145 | A | C3'-C2'-C1' | 5.04 | 105.54 | 101.50 |
| 5 | AC | 62 | ARG | NE-CZ-NH1 | -5.04 | 117.78 | 120.30 |
| 6 | AE | 21 | ARG | CA-C-N | 5.04 | 131.22 | 117.10 |
| 30 | BA | 17 | LEU | CB-CG-CD2 | 5.04 | 119.58 | 111.00 |
| 32 | BC | 105 | VAL | N-CA-C | -5.04 | 97.38 | 111.00 |
| 33 | BD | 220 | ARG | NE-CZ-NH1 | 5.04 | 122.82 | 120.30 |
| 58 | Bg | 94 | GLU | N-CA-C | -5.04 | 97.38 | 111.00 |
| 78 | CA | 658 | C | O3'-P-O5' | -5.04 | 94.42 | 104.00 |
| 81 | DA | 944 | C | O4'-C1'-N1 | 5.04 | 112.24 | 108.20 |
| 81 | DA | 1011 | A | C3'-C2'-C1' | 5.04 | 105.53 | 101.50 |
| 81 | DA | 1568 | U | O4'-C1'-C2' | -5.04 | 100.76 | 105.80 |
| 10 | AI | 73 | GLY | N-CA-C | -5.04 | 100.50 | 113.10 |
| 49 | BV | 162 | GLU | CA-C-N | 5.04 | 128.29 | 117.20 |
| 60 | Bi | 1 | MET | CG-SD-CE | 5.04 | 108.27 | 100.20 |
| 60 | Bi | 9 | ARG | NE-CZ-NH1 | 5.04 | 122.82 | 120.30 |
| 78 | CA | 887 | A | C4'-C3'-C2' | -5.04 | 97.56 | 102.60 |
| 78 | CA | 1646 | C | O4'-C1'-N1 | 5.04 | 112.23 | 108.20 |
| 81 | DA | 271 | C | O4'-C1'-N1 | 5.04 | 112.23 | 108.20 |
| 81 | DA | 856 | G | C3'-C2'-C1' | 5.04 | 105.53 | 101.50 |
| 81 | DA | 1400 | G | C4'-C3'-O3' | 5.04 | 123.08 | 113.00 |
| 81 | DA | 1998 | G | N9-C1'-C2' | -5.04 | 106.45 | 112.00 |
| 81 | DA | 2625 | C | C2'-C3'-O3' | 5.04 | 121.77 | 113.70 |
| 6 | AE | 240 | LEU | N-CA-CB | 5.04 | 120.48 | 110.40 |
| 9 | AH | 97 | ARG | CB-CA-C | 5.04 | 120.48 | 110.40 |
| 31 | BB | 242 | ARG | NE-CZ-NH2 | -5.04 | 117.78 | 120.30 |
| 44 | BO | 56 | VAL | CA-CB-CG1 | -5.04 | 103.34 | 110.90 |
| 76 | BS | 66 | ILE | CB-CA-C | -5.04 | 101.52 | 111.60 |
| 78 | CA | 1568 | C | N1-C1'-C2' | -5.04 | 106.46 | 112.00 |
| 81 | DA | 901 | G | C1'-O4'-C4' | -5.04 | 105.87 | 109.90 |
| 81 | DA | 1630 | U | P-O5'-C5' | 5.04 | 128.96 | 120.90 |
| 1 | Aa | 47 | LEU | N-CA-CB | 5.04 | 120.48 | 110.40 |
| 2 | AA | 230 | GLU | N-CA-C | 5.04 | 124.61 | 111.00 |
| 4 | AD | 184 | THR | CA-CB-CG2 | -5.04 | 105.34 | 112.40 |
| 34 | BE | 52 | TYR | CG-CD2-CE2 | 5.04 | 125.33 | 121.30 |
| 60 | Bi | 7 | PHE | CB-CG-CD1 | -5.04 | 117.27 | 120.80 |
| 61 | Bj | 73 | ARG | CA-C-O | 5.04 | 130.68 | 120.10 |
| 78 | CA | 661 | A | O4'-C1'-C2' | -5.04 | 100.76 | 105.80 |
| 78 | CA | 1158 | C | C5'-C4'-C3' | -5.04 | 107.94 | 116.00 |
| 78 | CA | 1366 | U | O3'-P-O5' | 5.04 | 113.57 | 104.00 |
| 78 | CA | 1793 | G | N9-C1'-C2' | 5.04 | 120.55 | 114.00 |
| 81 | DA | 696 | C | C4'-C3'-C2' | -5.04 | 97.56 | 102.60 |
| 81 | DA | 1319 | G | O3'-P-O5' | -5.04 | 94.42 | 104.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2230 | C | N1-C1'-C2' | 5.04 | 120.55 | 114.00 |
| 35 | BG | 55 | LEU | CB-CA-C | 5.04 | 119.77 | 110.20 |
| 78 | CA | 1347 | U | C1'-O4'-C4' | 5.04 | 113.93 | 109.90 |
| 78 | CA | 1638 | G | N3-C2-N2 | 5.04 | 123.43 | 119.90 |
| 81 | DA | 319 | A | C4'-C3'-C2' | -5.04 | 97.56 | 102.60 |
| 81 | DA | 2735 | U | C5'-C4'-C3' | -5.04 | 107.94 | 116.00 |
| 2 | AA | 242 | TRP | CB-CG-CD2 | -5.04 | 120.05 | 126.60 |
| 11 | AJ | 77 | LYS | CA-CB-CG | 5.04 | 124.48 | 113.40 |
| 14 | AM | 79 | TYR | CB-CG-CD1 | 5.04 | 124.02 | 121.00 |
| 21 | AT | 22 | ARG | NE-CZ-NH2 | 5.04 | 122.82 | 120.30 |
| 42 | BM | 85 | TRP | CE2-CD2-CE3 | 5.04 | 124.74 | 118.70 |
| 43 | BP | 180 | PHE | C-N-CA | -5.04 | 109.11 | 121.70 |
| 51 | BZ | 70 | LYS | O-C-N | 5.04 | 130.75 | 122.70 |
| 64 | Bl | 73 | ARG | CD-NE-CZ | -5.04 | 116.55 | 123.60 |
| 78 | CA | 1424 | A | C4'-C3'-C2' | -5.04 | 97.56 | 102.60 |
| 81 | DA | 567 | G | C1'-O4'-C4' | -5.04 | 105.87 | 109.90 |
| 81 | DA | 749 | C | OP1-P-OP2 | -5.04 | 112.05 | 119.60 |
| 81 | DA | 1360 | C | C2'-C3'-O3' | 5.04 | 121.76 | 113.70 |
| 81 | DA | 2155 | G | O4'-C1'-C2' | 5.04 | 112.13 | 107.60 |
| 81 | DA | 2341 | A | C3'-C2'-C1' | 5.04 | 105.53 | 101.50 |
| 81 | DA | 3384 | U | C5'-C4'-O4' | -5.04 | 103.06 | 109.10 |
| 8 | AF | 71 | ALA | N-CA-CB | 5.03 | 117.15 | 110.10 |
| 13 | AL | 124 | VAL | N-CA-C | 5.03 | 124.59 | 111.00 |
| 21 | AT | 1 | MET | CG-SD-CE | -5.03 | 92.15 | 100.20 |
| 25 | AY | 57 | MET | CA-CB-CG | 5.03 | 121.86 | 113.30 |
| 44 | BO | 117 | ARG | N-CA-CB | 5.03 | 119.66 | 110.60 |
| 47 | BU | 156 | TYR | CD1-CG-CD2 | -5.03 | 112.36 | 117.90 |
| 64 | Bl | 80 | THR | N-CA-CB | 5.03 | 119.86 | 110.30 |
| 78 | CA | 587 | C | N1-C1'-C2' | 5.03 | 120.54 | 114.00 |
| 78 | CA | 1427 | A | P-O3'-C3' | 5.03 | 125.74 | 119.70 |
| 81 | DA | 1082 | U | C2'-C3'-O3' | 5.03 | 121.75 | 113.70 |
| 81 | DA | 1392 | G | N9-C1'-C2' | 5.03 | 120.54 | 114.00 |
| 81 | DA | 1618 | G | P-O5'-C5' | 5.03 | 128.95 | 120.90 |
| 81 | DA | 2336 | U | P-O3'-C3' | -5.03 | 113.66 | 119.70 |
| 81 | DA | 2903 | A | O4'-C4'-C3' | 5.03 | 110.13 | 106.10 |
| 82 | DB | 105 | A | O4'-C1'-N9 | -5.03 | 104.17 | 108.20 |
| 76 | BS | 110 | THR | CA-CB-CG2 | 5.03 | 119.44 | 112.40 |
| 78 | CA | 276 | C | O4'-C1'-C2' | -5.03 | 100.77 | 105.80 |
| 78 | CA | 433 | C | N1-C1'-C2' | 5.03 | 120.54 | 114.00 |
| 78 | CA | 442 | C | N1-C1'-C2' | 5.03 | 120.54 | 114.00 |
| 81 | DA | 103 | G | P-O3'-C3' | -5.03 | 113.66 | 119.70 |
| 81 | DA | 2528 | G | C3'-C2'-C1' | -5.03 | 97.47 | 101.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|---|---|---|---|---|---|---|---|
| 12 | AK | 29 | HIS | C-N-CA | 5.03 | 134.27 | 121.70 |
| 31 | BB | 127 | ALA | CA-C-N | 5.03 | 128.27 | 117.20 |
| 32 | BC | 118 | PHE | CB-CG-CD2 | -5.03 | 117.28 | 120.80 |
| 54 | Bd | 58 | LYS | N-CA-CB | 5.03 | 119.66 | 110.60 |
| 74 | BQ | 23 | ARG | N-CA-CB | 5.03 | 119.66 | 110.60 |
| 74 | BQ | 129 | TYR | CB-CA-C | 5.03 | 120.46 | 110.40 |
| 78 | CA | 107 | C | P-O3'-C3' | 5.03 | 125.74 | 119.70 |
| 78 | CA | 300 | A | O4'-C1'-C2' | -5.03 | 100.77 | 105.80 |
| 78 | CA | 1288 | G | P-O5'-C5' | 5.03 | 128.95 | 120.90 |
| 78 | CA | 1722 | A | O3'-P-O5' | -5.03 | 94.44 | 104.00 |
| 81 | DA | 306 | A | C5'-C4'-C3' | -5.03 | 107.95 | 116.00 |
| 81 | DA | 935 | U | C1'-O4'-C4' | -5.03 | 105.88 | 109.90 |
| 81 | DA | 1193 | A | C5'-C4'-O4' | 5.03 | 115.14 | 109.10 |
| 81 | DA | 1222 | G | O4'-C1'-C2' | -5.03 | 100.77 | 105.80 |
| 81 | DA | 1251 | A | O4'-C1'-N9 | 5.03 | 112.22 | 108.20 |
| 81 | DA | 1687 | U | O5'-C5'-C4' | -5.03 | 102.14 | 111.70 |
| 32 | BC | 4 | ARG | N-CA-CB | 5.03 | 119.65 | 110.60 |
| 37 | BH | 232 | HIS | CA-C-O | -5.03 | 109.54 | 120.10 |
| 46 | BT | 29 | THR | CA-CB-CG2 | -5.03 | 105.36 | 112.40 |
| 74 | BQ | 16 | PHE | CD1-CE1-CZ | -5.03 | 114.06 | 120.10 |
| 79 | CB | 59 | U | C1'-O4'-C4' | 5.03 | 113.92 | 109.90 |
| 81 | DA | 25 | U | C5'-C4'-O4' | -5.03 | 103.06 | 109.10 |
| 81 | DA | 958 | C | C1'-O4'-C4' | 5.03 | 113.92 | 109.90 |
| 81 | DA | 2931 | C | OP1-P-O3' | 5.03 | 116.27 | 105.20 |
| 41 | BN | 71 | ALA | CB-CA-C | -5.03 | 102.56 | 110.10 |
| 52 | BY | 78 | PHE | CB-CG-CD2 | -5.03 | 117.28 | 120.80 |
| 76 | BS | 35 | ASN | N-CA-CB | 5.03 | 119.65 | 110.60 |
| 78 | CA | 271 | A | C1'-O4'-C4' | -5.03 | 105.88 | 109.90 |
| 78 | CA | 428 | A | O4'-C1'-N9 | 5.03 | 112.22 | 108.20 |
| 78 | CA | 455 | C | O4'-C1'-C2' | -5.03 | 100.77 | 105.80 |
| 78 | CA | 1255 | G | OP2-P-O3' | 5.03 | 116.26 | 105.20 |
| 81 | DA | 1320 | C | O4'-C4'-C3' | -5.03 | 98.97 | 104.00 |
| 81 | DA | 2154 | U | C3'-C2'-C1' | 5.03 | 105.52 | 101.50 |
| 81 | DA | 2814 | G | O4'-C1'-N9 | 5.03 | 112.22 | 108.20 |
| 81 | DA | 3025 | C | C3'-C2'-C1' | 5.03 | 105.52 | 101.50 |
| 81 | DA | 3149 | G | C5'-C4'-O4' | 5.03 | 115.13 | 109.10 |
| 5 | AC | 34 | PHE | N-CA-CB | 5.03 | 119.65 | 110.60 |
| 39 | BJ | 80 | LEU | CB-CG-CD2 | 5.03 | 119.55 | 111.00 |
| 48 | BW | 13 | LYS | N-CA-C | -5.03 | 97.43 | 111.00 |
| 61 | Bj | 66 | VAL | CA-CB-CG1 | 5.03 | 118.44 | 110.90 |
| 74 | BQ | 139 | PRO | N-CA-C | 5.03 | 125.16 | 112.10 |
| 78 | CA | 1753 | A | C1'-O4'-C4' | -5.03 | 105.88 | 109.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 79 | CB | 37 | G | N9-C1'-C2' | 5.03 | 120.53 | 114.00 |
| 81 | DA | 178 | U | C1'-O4'-C4' | 5.03 | 113.92 | 109.90 |
| 81 | DA | 636 | C | O3'-P-O5' | -5.03 | 94.45 | 104.00 |
| 81 | DA | 1062 | A | N9-C1'-C2' | -5.03 | 106.47 | 112.00 |
| 81 | DA | 1124 | U | O4'-C1'-C2' | -5.03 | 100.77 | 105.80 |
| 81 | DA | 1680 | G | O3'-P-O5' | 5.03 | 113.55 | 104.00 |
| 81 | DA | 1833 | G | C5'-C4'-C3' | 5.03 | 124.04 | 116.00 |
| 81 | DA | 2238 | G | C2'-C3'-O3' | -5.03 | 98.44 | 109.50 |
| 81 | DA | 2288 | G | P-O3'-C3' | 5.03 | 125.73 | 119.70 |
| 81 | DA | 2673 | A | C5'-C4'-O4' | 5.03 | 115.13 | 109.10 |
| 81 | DA | 3055 | U | N1-C1'-C2' | -5.03 | 106.47 | 112.00 |
| 33 | BD | 109 | TRP | CA-CB-CG | 5.02 | 123.25 | 113.70 |
| 78 | CA | 336 | G | C1'-O4'-C4' | -5.02 | 105.88 | 109.90 |
| 78 | CA | 389 | G | O4'-C1'-N9 | 5.02 | 112.22 | 108.20 |
| 81 | DA | 2100 | A | O4'-C1'-N9 | -5.02 | 104.18 | 108.20 |
| 3 | AB | 213 | GLU | C-N-CA | 5.02 | 134.25 | 121.70 |
| 4 | AD | 238 | LEU | C-N-CA | 5.02 | 143.10 | 122.00 |
| 5 | AC | 46 | SER | N-CA-CB | 5.02 | 118.03 | 110.50 |
| 34 | BE | 59 | ILE | CB-CA-C | -5.02 | 101.55 | 111.60 |
| 37 | BH | 234 | GLY | N-CA-C | -5.02 | 100.54 | 113.10 |
| 40 | BK | 117 | ARG | NE-CZ-NH2 | 5.02 | 122.81 | 120.30 |
| 45 | BR | 44 | PHE | CB-CA-C | -5.02 | 100.35 | 110.40 |
| 67 | Bp | 48 | LYS | CB-CA-C | -5.02 | 100.36 | 110.40 |
| 78 | CA | 390 | G | O4'-C1'-N9 | 5.02 | 112.22 | 108.20 |
| 78 | CA | 1294 | G | C4'-C3'-C2' | -5.02 | 97.58 | 102.60 |
| 4 | AD | 51 | ARG | NE-CZ-NH1 | -5.02 | 117.79 | 120.30 |
| 37 | BH | 238 | LEU | CB-CA-C | 5.02 | 119.74 | 110.20 |
| 38 | Bs | 86 | PHE | CB-CG-CD1 | -5.02 | 117.28 | 120.80 |
| 61 | Bj | 86 | ARG | N-CA-CB | -5.02 | 101.56 | 110.60 |
| 81 | DA | 3099 | C | C4'-C3'-C2' | 5.02 | 107.62 | 102.60 |
| 2 | AA | 174 | TRP | CB-CA-C | 5.02 | 120.44 | 110.40 |
| 32 | BC | 220 | VAL | CG1-CB-CG2 | 5.02 | 118.93 | 110.90 |
| 41 | BN | 114 | ASP | N-CA-CB | 5.02 | 119.64 | 110.60 |
| 43 | BP | 44 | ARG | CA-C-N | 5.02 | 131.16 | 117.10 |
| 47 | BU | 159 | PHE | CA-C-N | -5.02 | 106.16 | 117.20 |
| 55 | Bc | 4 | VAL | CA-CB-CG1 | 5.02 | 118.43 | 110.90 |
| 61 | Bj | 2 | ALA | C-N-CA | -5.02 | 109.15 | 121.70 |
| 72 | Bu | 58 | LEU | CB-CA-C | -5.02 | 100.66 | 110.20 |
| 81 | DA | 95 | A | O4'-C1'-N9 | 5.02 | 112.22 | 108.20 |
| 81 | DA | 507 | U | P-O3'-C3' | 5.02 | 125.72 | 119.70 |
| 81 | DA | 1396 | C | O3'-P-O5' | 5.02 | 113.54 | 104.00 |
| 81 | DA | 2166 | A | P-O5'-C5' | -5.02 | 112.87 | 120.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2849 | C | O4'-C1'-N1 | 5.02 | 112.22 | 108.20 |
| 81 | DA | 3161 | C | O4'-C1'-N1 | 5.02 | 112.22 | 108.20 |
| 81 | DA | 3218 | A | C2'-C3'-O3' | 5.02 | 121.73 | 113.70 |
| 13 | AL | 72 | VAL | CA-CB-CG2 | -5.02 | 103.37 | 110.90 |
| 32 | BC | 97 | ARG | CA-CB-CG | 5.02 | 124.44 | 113.40 |
| 78 | CA | 103 | A | C1'-O4'-C4' | 5.02 | 113.91 | 109.90 |
| 78 | CA | 1700 | C | O4'-C1'-N1 | 5.02 | 112.21 | 108.20 |
| 81 | DA | 977 | C | C5'-C4'-C3' | 5.02 | 124.03 | 116.00 |
| 81 | DA | 2599 | U | O4'-C1'-C2' | -5.02 | 100.78 | 105.80 |
| 81 | DA | 3164 | C | N1-C1'-C2' | -5.02 | 106.48 | 112.00 |
| 82 | DB | 30 | C | C4'-C3'-C2' | -5.02 | 97.58 | 102.60 |
| 31 | BB | 74 | GLU | N-CA-CB | 5.02 | 119.63 | 110.60 |
| 74 | BQ | 248 | ARG | CA-CB-CG | 5.02 | 124.44 | 113.40 |
| 78 | CA | 826 | U | P-O3'-C3' | 5.02 | 125.72 | 119.70 |
| 81 | DA | 2148 | U | O4'-C1'-C2' | -5.02 | 100.78 | 105.80 |
| 82 | DB | 98 | U | O4'-C1'-N1 | 5.02 | 112.21 | 108.20 |
| 5 | AC | 152 | SER | N-CA-CB | 5.01 | 118.02 | 110.50 |
| 32 | BC | 298 | PHE | N-CA-CB | -5.01 | 101.57 | 110.60 |
| 63 | Bm | 7 | LYS | C-N-CA | 5.01 | 134.24 | 121.70 |
| 78 | CA | 433 | C | O4'-C1'-C2' | -5.01 | 100.79 | 105.80 |
| 79 | CB | 38 | C | O4'-C1'-N1 | 5.01 | 112.21 | 108.20 |
| 81 | DA | 1165 | A | C3'-C2'-C1' | 5.01 | 105.51 | 101.50 |
| 81 | DA | 2188 | A | O4'-C1'-C2' | -5.01 | 100.78 | 105.80 |
| 81 | DA | 2460 | U | O4'-C1'-N1 | 5.01 | 112.21 | 108.20 |
| 81 | DA | 3220 | G | C4'-C3'-C2' | -5.01 | 97.59 | 102.60 |
| 16 | AO | 113 | PHE | CA-CB-CG | 5.01 | 125.93 | 113.90 |
| 47 | BU | 156 | TYR | N-CA-C | -5.01 | 97.47 | 111.00 |
| 78 | CA | 310 | C | O4'-C1'-C2' | -5.01 | 100.79 | 105.80 |
| 81 | DA | 255 | A | C4'-C3'-C2' | -5.01 | 97.59 | 102.60 |
| 81 | DA | 1340 | G | C1'-O4'-C4' | -5.01 | 105.89 | 109.90 |
| 81 | DA | 2080 | C | C3'-C2'-C1' | 5.01 | 105.51 | 101.50 |
| 1 | Aa | 214 | ALA | N-CA-CB | 5.01 | 117.12 | 110.10 |
| 46 | BT | 14 | VAL | CA-CB-CG2 | -5.01 | 103.38 | 110.90 |
| 46 | BT | 62 | ARG | NE-CZ-NH1 | -5.01 | 117.79 | 120.30 |
| 48 | BW | 94 | ARG | N-CA-C | -5.01 | 97.47 | 111.00 |
| 56 | Bf | 48 | THR | CA-CB-CG2 | -5.01 | 105.38 | 112.40 |
| 78 | CA | 1501 | C | C2-N3-C4 | 5.01 | 122.41 | 119.90 |
| 81 | DA | 3091 | A | O4'-C4'-C3' | -5.01 | 98.99 | 104.00 |
| 60 | Bi | 73 | SER | N-CA-C | -5.01 | 97.48 | 111.00 |
| 78 | CA | 165 | G | P-O3'-C3' | 5.01 | 125.71 | 119.70 |
| 78 | CA | 293 | U | C3'-C2'-C1' | 5.01 | 105.51 | 101.50 |
| 81 | DA | 1075 | A | C3'-C2'-C1' | 5.01 | 105.51 | 101.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 1160 | C | C1'-O4'-C4' | -5.01 | 105.89 | 109.90 |
| 81 | DA | 1397 | C | O4'-C1'-N1 | -5.01 | 104.19 | 108.20 |
| 81 | DA | 1399 | A | O4'-C1'-N9 | 5.01 | 112.21 | 108.20 |
| 81 | DA | 1730 | G | O4'-C1'-C2' | -5.01 | 100.79 | 105.80 |
| 81 | DA | 2118 | C | P-O3'-C3' | 5.01 | 125.71 | 119.70 |
| 81 | DA | 2142 | A | N9-C1'-C2' | -5.01 | 106.49 | 112.00 |
| 81 | DA | 2453 | U | C3'-C2'-C1' | 5.01 | 105.51 | 101.50 |
| 81 | DA | 3345 | G | O4'-C4'-C3' | -5.01 | 98.99 | 104.00 |
| 17 | AQ | 10 | LYS | N-CA-CB | 5.01 | 119.61 | 110.60 |
| 1 | Aa | 201 | THR | CA-CB-CG2 | 5.01 | 119.41 | 112.40 |
| 4 | AD | 90 | ILE | CB-CA-C | -5.01 | 101.59 | 111.60 |
| 4 | AD | 133 | LYS | CB-CA-C | 5.01 | 120.41 | 110.40 |
| 57 | Be | 142 | SER | N-CA-C | 5.01 | 124.52 | 111.00 |
| 78 | CA | 1273 | G | C5-C6-O6 | -5.01 | 125.60 | 128.60 |
| 78 | CA | 1637 | C | C6-N1-C1' | -5.01 | 114.79 | 120.80 |
| 81 | DA | 337 | G | O3'-P-O5' | -5.01 | 94.49 | 104.00 |
| 81 | DA | 560 | G | C5'-C4'-O4' | 5.01 | 115.11 | 109.10 |
| 81 | DA | 678 | G | N9-C1'-C2' | -5.01 | 106.49 | 112.00 |
| 81 | DA | 2422 | C | C4'-C3'-O3' | -5.01 | 98.88 | 109.40 |
| 81 | DA | 3367 | C | P-O3'-C3' | 5.01 | 125.71 | 119.70 |
| 83 | DC | 47 | C | O5'-C5'-C4' | -5.01 | 102.19 | 111.70 |
| 17 | AQ | 71 | PHE | C-N-CA | 5.00 | 134.21 | 121.70 |
| 47 | BU | 44 | ALA | N-CA-CB | 5.00 | 117.11 | 110.10 |
| 65 | Bn | 46 | ARG | NE-CZ-NH2 | -5.00 | 117.80 | 120.30 |
| 78 | CA | 1752 | U | P-O3'-C3' | -5.00 | 113.69 | 119.70 |
| 81 | DA | 1502 | C | O4'-C1'-C2' | -5.00 | 100.80 | 105.80 |
| 81 | DA | 1824 | U | O4'-C1'-C2' | -5.00 | 100.80 | 105.80 |
| 81 | DA | 3343 | G | C1'-O4'-C4' | -5.00 | 105.90 | 109.90 |
| 83 | DC | 6 | C | O4'-C1'-N1 | 5.00 | 112.20 | 108.20 |
| 31 | BB | 112 | ILE | CB-CA-C | 5.00 | 121.61 | 111.60 |
| 39 | BJ | 123 | ARG | N-CA-CB | 5.00 | 119.61 | 110.60 |
| 78 | CA | 339 | C | C5'-C4'-C3' | -5.00 | 108.00 | 116.00 |
| 78 | CA | 1235 | C | P-O5'-C5' | 5.00 | 128.91 | 120.90 |
| 78 | CA | 1396 | U | C2'-C3'-O3' | 5.00 | 121.70 | 113.70 |
| 78 | CA | 1710 | U | O4'-C1'-N1 | 5.00 | 112.20 | 108.20 |
| 81 | DA | 50 | U | O4'-C1'-N1 | 5.00 | 112.20 | 108.20 |
| 81 | DA | 311 | C | P-O5'-C5' | -5.00 | 112.89 | 120.90 |
| 81 | DA | 835 | G | C4'-C3'-C2' | -5.00 | 97.60 | 102.60 |
| 81 | DA | 1002 | A | O3'-P-O5' | 5.00 | 113.51 | 104.00 |
| 81 | DA | 1263 | A | C4'-C3'-C2' | 5.00 | 107.60 | 102.60 |
| 81 | DA | 1361 | U | O3'-P-O5' | -5.00 | 94.49 | 104.00 |
| 81 | DA | 2512 | C | C3'-C2'-C1' | 5.00 | 105.50 | 101.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 81 | DA | 2864 | A | C3'-C2'-C1' | -5.00 | 97.50 | 101.50 |
| 81 | DA | 3188 | G | C5'-C4'-C3' | 5.00 | 124.00 | 116.00 |
| 20 | AS | 7 | ARG | NE-CZ-NH2 | -5.00 | 117.80 | 120.30 |
| 30 | BA | 174 | MET | CG-SD-CE | 5.00 | 108.20 | 100.20 |
| 35 | BG | 155 | LEU | CB-CA-C | -5.00 | 100.70 | 110.20 |
| 57 | Be | 60 | ARG | CB-CG-CD | 5.00 | 124.60 | 111.60 |
| 78 | CA | 257 | A | C3'-C2'-C1' | 5.00 | 105.50 | 101.50 |
| 78 | CA | 1657 | U | C5'-C4'-C3' | 5.00 | 124.00 | 116.00 |
| 78 | CA | 1767 | G | C3'-C2'-C1' | 5.00 | 105.50 | 101.50 |
| 81 | DA | 242 | C | O4'-C1'-N1 | -5.00 | 104.20 | 108.20 |
| 81 | DA | 434 | U | O3'-P-O5' | 5.00 | 113.50 | 104.00 |
| 81 | DA | 1062 | A | P-O3'-C3' | 5.00 | 125.70 | 119.70 |
| 81 | DA | 1204 | A | O4'-C1'-C2' | 5.00 | 112.10 | 107.60 |
| 81 | DA | 1741 | A | C1'-O4'-C4' | -5.00 | 105.90 | 109.90 |
| 81 | DA | 2125 | A | O4'-C1'-N9 | 5.00 | 112.20 | 108.20 |
| 81 | DA | 3046 | A | P-O3'-C3' | 5.00 | 125.70 | 119.70 |
| 81 | DA | 3358 | U | O4'-C1'-C2' | -5.00 | 100.80 | 105.80 |

All (85) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 2 | AA | 241 | GLU | CA |
| 5 | AC | 129 | ILE | CA |
| 5 | AC | 162 | SER | CA |
| 6 | AE | 28 | ARG | CA |
| 6 | AE | 30 | THR | CA |
| 6 | AE | 31 | GLU | CA |
| 12 | AK | 67 | VAL | CA |
| 16 | AO | 67 | THR | CA |
| 16 | AO | 118 | ILE | CA |
| 29 | AU | 5 | VAL | CA |
| 29 | AU | 62 | THR | CA |
| 31 | BB | 40 | TYR | CA |
| 31 | BB | 67 | TYR | CA |
| 32 | BC | 241 | LYS | CA |
| 32 | BC | 344 | THR | CA |
| 33 | BD | 261 | VAL | CA |
| 33 | BD | 296 | GLN | CA |
| 34 | BE | 52 | TYR | CA |
| 34 | BE | 55 | ARG | CA |
| 35 | BG | 8 | LYS | CA |
| 35 | BG | 75 | PRO | CA |

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| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 39 | BJ | 14 | TYR | CA |
| 41 | BN | 62 | GLN | CA |
| 43 | BP | 13 | LYS | CA |
| 43 | BP | 44 | ARG | CA |
| 43 | BP | 122 | ASN | CA |
| 43 | BP | 123 | GLN | CA |
| 44 | BO | 7 | LYS | CA |
| 47 | BU | 126 | VAL | CA |
| 57 | Be | 98 | LYS | CA |
| 61 | Bj | 21 | ARG | CA |
| 62 | Bk | 27 | SER | CA |
| 63 | Bm | 29 | LEU | CA |
| 76 | BS | 66 | ILE | CA |
| 77 | BI | 13 | LYS | CA |
| 77 | BI | 90 | ARG | CA |
| 78 | CA | 558 | U | C3' |
| 78 | CA | 963 | A | C3' |
| 78 | CA | 1337 | A | C3' |
| 78 | CA | 1434 | U | C3' |
| 78 | CA | 1444 | A | C2' |
| 78 | CA | 1459 | C | C2' |
| 78 | CA | 1546 | G | C1' |
| 78 | CA | 1601 | G | C1' |
| 78 | CA | 1700 | C | C2' |
| 78 | CA | 1735 | U | C4' |
| 79 | CB | 55 | C | C1' |
| 80 | CC | 20 | U | C4' |
| 81 | DA | 476 | G | C3' |
| 81 | DA | 527 | A | C3' |
| 81 | DA | 609 | G | C3' |
| 81 | DA | 637 | C | C3' |
| 81 | DA | 699 | A | C4' |
| 81 | DA | 702 | C | C3' |
| 81 | DA | 782 | U | C2' |
| 81 | DA | 975 | C | C3' |
| 81 | DA | 1047 | A | C3' |
| 81 | DA | 1209 | G | C3' |
| 81 | DA | 1221 | A | C1' |
| 81 | DA | 1251 | A | C1' |
| 81 | DA | 1384 | U | C3' |
| 81 | DA | 1537 | A | C3' |
| 81 | DA | 1701 | C | C3' |

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| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 81 | DA | 1754 | G | C3' |
| 81 | DA | 1771 | C | C4',C2',C3' |
| 81 | DA | 1856 | C | C3' |
| 81 | DA | 2067 | U | C4' |
| 81 | DA | 2137 | U | C3' |
| 81 | DA | 2211 | U | C3' |
| 81 | DA | 2362 | C | C3' |
| 81 | DA | 2384 | A | C3' |
| 81 | DA | 2757 | U | C2' |
| 81 | DA | 2760 | C | C3' |
| 81 | DA | 2970 | C | C3' |
| 81 | DA | 3044 | G | C3' |
| 81 | DA | 3092 | C | C3' |
| 81 | DA | 3215 | A | C2',C1' |
| 82 | DB | 51 | G | C3' |
| 82 | DB | 94 | C | C3' |
| 82 | DB | 120 | C | C3' |
| 82 | DB | 132 | G | C3' |
| 82 | DB | 138 | A | C3' |

All (1514) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 2 | AA | 10 | THR | Peptide,Mainchain |
| 2 | AA | 101 | ARG | Sidechain |
| 2 | AA | 104 | PRO | Peptide |
| 2 | AA | 11 | PRO | Peptide,Mainchain |
| 2 | AA | 110 | TYR | Sidechain |
| 2 | AA | 13 | ASP | Peptide |
| 2 | AA | 175 | TYR | Sidechain |
| 2 | AA | 194 | PRO | Peptide |
| 2 | AA | 195 | TRP | Peptide,Mainchain |
| 2 | AA | 197 | ILE | Peptide |
| 2 | AA | 229 | LYS | Peptide,Mainchain |
| 2 | AA | 230 | GLU | Peptide |
| 2 | AA | 232 | VAL | Peptide |
| 2 | AA | 250 | VAL | Peptide,Mainchain |
| 2 | AA | 251 | GLU | Peptide,Mainchain |
| 2 | AA | 36 | TYR | Sidechain |
| 2 | AA | 4 | PRO | Peptide,Mainchain |
| 2 | AA | 5 | ALA | Peptide |
| 2 | AA | 6 | THR | Peptide,Mainchain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 2 | AA | 82 | GLY | Peptide |
| 2 | AA | 84 | ARG | Sidechain |
| 2 | AA | 9 | LEU | Peptide |
| 3 | AB | 116 | ARG | Sidechain |
| 3 | AB | 117 | ARG | Sidechain |
| 3 | AB | 120 | TYR | Sidechain |
| 3 | AB | 125 | TYR | Sidechain |
| 3 | AB | 17 | PHE | Sidechain |
| 3 | AB | 18 | TYR | Sidechain |
| 3 | AB | 192 | PRO | Peptide |
| 3 | AB | 198 | GLY | Peptide |
| 3 | AB | 199 | PRO | Peptide,Mainchain |
| 3 | AB | 201 | ALA | Peptide |
| 3 | AB | 202 | LEU | Peptide |
| 3 | AB | 205 | ALA | Peptide,Mainchain |
| 3 | AB | 206 | VAL | Peptide |
| 3 | AB | 208 | ILE | Peptide |
| 3 | AB | 209 | ILE | Peptide,Mainchain |
| 3 | AB | 210 | GLU | Peptide |
| 3 | AB | 212 | LYS | Peptide,Mainchain |
| 3 | AB | 214 | GLU | Peptide,Mainchain |
| 3 | AB | 64 | ARG | Sidechain |
| 3 | AB | 72 | LEU | Mainchain |
| 3 | AB | 78 | LYS | Peptide,Mainchain |
| 3 | AB | 79 | TYR | Peptide |
| 3 | AB | 87 | TYR | Sidechain |
| 5 | AC | 104 | PHE | Sidechain |
| 5 | AC | 117 | GLY | Peptide |
| 5 | AC | 118 | LEU | Peptide |
| 5 | AC | 126 | ARG | Sidechain |
| 5 | AC | 133 | HIS | Sidechain |
| 5 | AC | 14 | THR | Peptide |
| 5 | AC | 142 | ASN | Sidechain |
| 5 | AC | 148 | VAL | Peptide |
| 5 | AC | 15 | PRO | Mainchain |
| 5 | AC | 151 | ASP | Peptide |
| 5 | AC | 157 | ASP | Peptide,Mainchain |
| 5 | AC | 158 | PHE | Peptide,Sidechain |
| 5 | AC | 16 | LYS | Peptide |
| 5 | AC | 160 | PRO | Peptide |
| 5 | AC | 162 | SER | Peptide,Mainchain |
| 5 | AC | 163 | PRO | Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 5 | AC | 164 | PHE | Peptide,Mainchain |
| 5 | AC | 168 | ARG | Peptide,Mainchain |
| 5 | AC | 18 | PRO | Peptide,Mainchain |
| 5 | AC | 182 | GLU | Peptide |
| 5 | AC | 183 | ALA | Peptide |
| 5 | AC | 184 | SER | Peptide |
| 5 | AC | 186 | GLU | Peptide |
| 5 | AC | 187 | ALA | Peptide |
| 5 | AC | 188 | ALA | Peptide |
| 5 | AC | 19 | TYR | Peptide |
| 5 | AC | 190 | GLU | Peptide |
| 5 | AC | 191 | ALA | Peptide |
| 5 | AC | 193 | GLU | Peptide |
| 5 | AC | 2 | PRO | Peptide |
| 5 | AC | 21 | SER | Peptide |
| 5 | AC | 3 | ARG | Peptide |
| 5 | AC | 57 | ARG | Sidechain |
| 5 | AC | 6 | ARG | Sidechain |
| 4 | AD | 103 | TYR | Sidechain |
| 4 | AD | 108 | ARG | Sidechain |
| 4 | AD | 131 | LEU | Peptide |
| 4 | AD | 134 | LYS | Peptide |
| 4 | AD | 142 | HIS | Sidechain |
| 4 | AD | 149 | TYR | Sidechain |
| 4 | AD | 150 | PRO | Peptide |
| 4 | AD | 153 | ASN | Peptide,Mainchain |
| 4 | AD | 182 | TYR | Sidechain |
| 4 | AD | 187 | ARG | Sidechain |
| 4 | AD | 211 | LYS | Peptide |
| 4 | AD | 212 | ASP | Peptide |
| 4 | AD | 218 | PHE | Mainchain |
| 4 | AD | 230 | GLU | Peptide |
| 4 | AD | 231 | GLN | Peptide |
| 4 | AD | 234 | PRO | Peptide |
| 4 | AD | 235 | TYR | Mainchain |
| 4 | AD | 238 | LEU | Peptide |
| 4 | AD | 239 | PRO | Peptide |
| 4 | AD | 240 | LYS | Peptide,Mainchain |
| 4 | AD | 51 | ARG | Sidechain |
| 4 | AD | 54 | TYR | Peptide |
| 4 | AD | 55 | ALA | Peptide |
| 4 | AD | 57 | ASN | Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 4 | AD | 82 | TYR | Sidechain |
| 4 | AD | 90 | ILE | Peptide,Mainchain |
| 4 | AD | 93 | ASP | Peptide,Mainchain |
| 4 | AD | 94 | ALA | Peptide,Mainchain |
| 4 | AD | 95 | THR | Peptide |
| 4 | AD | 96 | ASN | Mainchain |
| 4 | AD | 99 | PHE | Sidechain |
| 6 | AE | 109 | GLY | Peptide |
| 6 | AE | 110 | HIS | Sidechain |
| 6 | AE | 126 | ARG | Sidechain |
| 6 | AE | 137 | ILE | Peptide |
| 6 | AE | 168 | ARG | Sidechain |
| 6 | AE | 174 | ARG | Peptide,Mainchain |
| 6 | AE | 205 | ARG | Sidechain |
| 6 | AE | 225 | LEU | Peptide |
| 6 | AE | 239 | PRO | Peptide |
| 6 | AE | 24 | ARG | Sidechain |
| 6 | AE | 243 | TYR | Mainchain |
| 6 | AE | 25 | ARG | Peptide |
| 6 | AE | 28 | ARG | Peptide |
| 6 | AE | 30 | THR | Peptide |
| 6 | AE | 31 | GLU | Peptide |
| 6 | AE | 4 | PRO | Peptide,Mainchain |
| 6 | AE | 67 | GLN | Peptide |
| 6 | AE | 69 | ILE | Peptide |
| 6 | AE | 7 | GLN | Peptide,Mainchain |
| 6 | AE | 70 | ASP | Mainchain |
| 6 | AE | 71 | THR | Peptide |
| 6 | AE | 81 | MET | Peptide,Mainchain |
| 6 | AE | 92 | ALA | Peptide,Mainchain |
| 6 | AE | 95 | ARG | Sidechain |
| 8 | AF | 101 | GLY | Peptide |
| 8 | AF | 103 | ASN | Peptide |
| 8 | AF | 116 | HIS | Sidechain |
| 8 | AF | 157 | ARG | Sidechain |
| 8 | AF | 209 | TYR | Sidechain |
| 8 | AF | 28 | PRO | Peptide |
| 8 | AF | 35 | GLN | Peptide,Mainchain |
| 8 | AF | 36 | ALA | Peptide |
| 8 | AF | 37 | GLN | Peptide |
| 8 | AF | 61 | TYR | Sidechain |
| 8 | AF | 65 | ARG | Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 8 | AF | 79 | ASN | Peptide |
| 8 | AF | 92 | ARG | Sidechain |
| 7 | AG | 10 | UNK | Peptide,Mainchain |
| 7 | AG | 100 | UNK | Peptide,Mainchain |
| 7 | AG | 101 | UNK | Peptide,Mainchain |
| 7 | AG | 103 | UNK | Peptide,Mainchain |
| 7 | AG | 104 | UNK | Peptide,Mainchain |
| 7 | AG | 107 | UNK | Peptide,Mainchain |
| 7 | AG | 11 | UNK | Peptide |
| 7 | AG | 127 | UNK | Peptide,Mainchain |
| 7 | AG | 128 | UNK | Peptide |
| 7 | AG | 131 | UNK | Peptide |
| 7 | AG | 21 | UNK | Peptide,Mainchain |
| 7 | AG | 35 | UNK | Peptide,Mainchain |
| 7 | AG | 37 | UNK | Peptide,Mainchain |
| 7 | AG | 38 | UNK | Peptide,Mainchain |
| 7 | AG | 52 | UNK | Peptide,Mainchain |
| 7 | AG | 53 | UNK | Peptide |
| 7 | AG | 55 | UNK | Peptide,Mainchain |
| 7 | AG | 56 | UNK | Peptide |
| 7 | AG | 68 | UNK | Mainchain |
| 7 | AG | 69 | UNK | Peptide |
| 7 | AG | 71 | UNK | Peptide,Mainchain |
| 7 | AG | 75 | UNK | Peptide,Mainchain |
| 7 | AG | 79 | UNK | Peptide |
| 7 | AG | 81 | UNK | Peptide,Mainchain |
| 7 | AG | 83 | UNK | Peptide,Mainchain |
| 7 | AG | 86 | UNK | Peptide,Mainchain |
| 7 | AG | 87 | UNK | Peptide,Mainchain |
| 7 | AG | 9 | UNK | Peptide,Mainchain |
| 7 | AG | 96 | UNK | Peptide,Mainchain |
| 7 | AG | 97 | UNK | Peptide,Mainchain |
| 9 | AH | 101 | TYR | Sidechain |
| 9 | AH | 121 | VAL | Peptide |
| 9 | AH | 3 | ARG | Sidechain |
| 9 | AH | 41 | MET | Peptide |
| 9 | AH | 52 | TYR | Sidechain |
| 9 | AH | 57 | ARG | Sidechain |
| 9 | AH | 64 | GLN | Peptide |
| 9 | AH | 65 | LEU | Peptide |
| 9 | AH | 66 | ASN | Peptide,Mainchain |
| 9 | AH | 67 | GLY | Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 9 | AH | 79 | PHE | Peptide,Sidechain |
| 9 | AH | 80 | ASN | Peptide |
| 9 | AH | 83 | ILE | Peptide |
| 10 | AI | 119 | ALA | Peptide,Mainchain |
| 10 | AI | 123 | ARG | Peptide,Sidechain |
| 10 | AI | 125 | GLU | Peptide |
| 10 | AI | 126 | PRO | Peptide |
| 10 | AI | 140 | LYS | Peptide,Mainchain |
| 10 | AI | 27 | GLY | Peptide |
| 10 | AI | 49 | TYR | Sidechain |
| 10 | AI | 54 | LEU | Peptide,Mainchain |
| 10 | AI | 83 | GLN | Peptide |
| 10 | AI | 85 | ILE | Peptide |
| 11 | AJ | 119 | ALA | Peptide,Mainchain |
| 11 | AJ | 21 | LYS | Peptide |
| 11 | AJ | 57 | ARG | Sidechain |
| 11 | AJ | 61 | LYS | Peptide |
| 11 | AJ | 64 | LYS | Peptide |
| 11 | AJ | 68 | ARG | Sidechain |
| 11 | AJ | 71 | PRO | Peptide |
| 11 | AJ | 73 | GLY | Peptide |
| 11 | AJ | 74 | GLU | Peptide |
| 11 | AJ | 78 | THR | Peptide |
| 11 | AJ | 81 | THR | Peptide,Mainchain |
| 11 | AJ | 82 | TYR | Peptide |
| 11 | AJ | 86 | ILE | Peptide |
| 11 | AJ | 87 | HIS | Peptide |
| 11 | AJ | 90 | TYR | Sidechain |
| 12 | AK | 107 | ARG | Sidechain |
| 12 | AK | 111 | ARG | Sidechain |
| 12 | AK | 114 | ARG | Sidechain |
| 12 | AK | 119 | THR | Peptide |
| 12 | AK | 123 | SER | Peptide,Mainchain |
| 12 | AK | 136 | ARG | Peptide |
| 12 | AK | 21 | ALA | Peptide |
| 12 | AK | 22 | SER | Peptide,Mainchain |
| 12 | AK | 30 | VAL | Peptide |
| 12 | AK | 59 | ALA | Peptide,Mainchain |
| 12 | AK | 60 | ALA | Peptide,Mainchain |
| 13 | AL | 10 | ASN | Mainchain |
| 13 | AL | 124 | VAL | Peptide |
| 13 | AL | 13 | ARG | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 13 | AL | 134 | ALA | Peptide,Mainchain |
| 13 | AL | 22 | ASN | Peptide,Mainchain |
| 13 | AL | 34 | LEU | Peptide,Mainchain |
| 13 | AL | 38 | PHE | Peptide,Sidechain |
| 13 | AL | 87 | VAL | Mainchain |
| 13 | AL | 93 | LEU | Mainchain |
| 13 | AL | 98 | GLU | Peptide |
| 14 | AM | 10 | SER | Peptide |
| 14 | AM | 11 | PHE | Sidechain |
| 14 | AM | 110 | ARG | Sidechain |
| 14 | AM | 134 | ARG | Sidechain |
| 14 | AM | 140 | THR | Peptide |
| 14 | AM | 145 | ARG | Sidechain |
| 14 | AM | 22 | VAL | Peptide |
| 14 | AM | 87 | ASN | Peptide |
| 14 | AM | 88 | ARG | Peptide |
| 14 | AM | 90 | ASN | Peptide |
| 14 | AM | 99 | HIS | Peptide,Mainchain |
| 15 | AN | 10 | HIS | Peptide,Sidechain |
| 15 | AN | 37 | ASN | Peptide |
| 15 | AN | 44 | ARG | Sidechain |
| 15 | AN | 46 | LYS | Peptide,Mainchain |
| 15 | AN | 47 | ALA | Mainchain |
| 15 | AN | 52 | PHE | Mainchain |
| 15 | AN | 53 | ASN | Peptide,Mainchain |
| 15 | AN | 54 | LYS | Peptide,Mainchain |
| 16 | AO | 104 | ARG | Sidechain |
| 16 | AO | 106 | ARG | Sidechain |
| 16 | AO | 114 | ARG | Sidechain |
| 16 | AO | 127 | ARG | Sidechain |
| 16 | AO | 128 | TYR | Sidechain |
| 16 | AO | 129 | TYR | Sidechain |
| 16 | AO | 40 | TYR | Peptide,Sidechain |
| 16 | AO | 41 | ALA | Peptide |
| 16 | AO | 63 | ALA | Mainchain |
| 16 | AO | 64 | ARG | Sidechain |
| 16 | AO | 67 | THR | Peptide,Mainchain |
| 16 | AO | 89 | TYR | Sidechain |
| 16 | AO | 90 | TYR | Sidechain |
| 18 | AP | 100 | TYR | Sidechain |
| 18 | AP | 109 | VAL | Peptide |
| 18 | AP | 110 | HIS | Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 18 | AP | 122 | ILE | Peptide,Mainchain |
| 18 | AP | 40 | LEU | Peptide,Mainchain |
| 18 | AP | 53 | TYR | Mainchain |
| 18 | AP | 54 | ILE | Peptide |
| 18 | AP | 55 | ASP | Peptide,Mainchain |
| 18 | AP | 57 | LYS | Mainchain |
| 18 | AP | 59 | PRO | Peptide |
| 18 | AP | 60 | PHE | Sidechain |
| 18 | AP | 93 | TYR | Sidechain |
| 17 | AQ | 101 | ASN | Peptide |
| 17 | AQ | 128 | ARG | Peptide |
| 17 | AQ | 129 | ASP | Peptide,Mainchain |
| 17 | AQ | 131 | ARG | Peptide,Sidechain |
| 17 | AQ | 132 | TYR | Sidechain |
| 17 | AQ | 133 | ARG | Sidechain |
| 17 | AQ | 134 | LYS | Peptide |
| 17 | AQ | 19 | ARG | Sidechain |
| 17 | AQ | 20 | TYR | Sidechain |
| 17 | AQ | 26 | LEU | Peptide,Mainchain |
| 17 | AQ | 5 | ARG | Peptide,Sidechain |
| 17 | AQ | 60 | ARG | Sidechain |
| 17 | AQ | 63 | LYS | Mainchain |
| 17 | AQ | 71 | PHE | Sidechain |
| 17 | AQ | 81 | LYS | Peptide,Mainchain |
| 17 | AQ | 82 | ASP | Peptide,Mainchain |
| 17 | AQ | 85 | VAL | Peptide,Mainchain |
| 17 | AQ | 87 | GLU | Peptide |
| 17 | AQ | 93 | LEU | Peptide |
| 17 | AQ | 94 | SER | Peptide |
| 17 | AQ | 95 | ARG | Sidechain |
| 17 | AQ | 99 | VAL | Peptide |
| 19 | AR | 108 | ARG | Sidechain |
| 19 | AR | 125 | PRO | Peptide |
| 19 | AR | 127 | ARG | Sidechain |
| 19 | AR | 131 | ALA | Peptide |
| 19 | AR | 134 | THR | Peptide |
| 19 | AR | 52 | LYS | Peptide |
| 19 | AR | 77 | ARG | Sidechain |
| 19 | AR | 97 | TYR | Sidechain |
| 20 | AS | 122 | ARG | Sidechain |
| 20 | AS | 130 | ARG | Sidechain |
| 20 | AS | 30 | VAL | Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 20 | AS | 43 | ASN | Peptide |
| 20 | AS | 60 | SER | Mainchain |
| 20 | AS | 68 | ARG | Sidechain |
| 20 | AS | 69 | LYS | Peptide |
| 20 | AS | 7 | ARG | Sidechain |
| 20 | AS | 70 | GLN | Peptide |
| 20 | AS | 78 | LYS | Peptide |
| 20 | AS | 80 | TYR | Sidechain |
| 20 | AS | 87 | GLY | Peptide |
| 20 | AS | 90 | PRO | Peptide,Mainchain |
| 20 | AS | 91 | TYR | Peptide |
| 20 | AS | 95 | ASP | Peptide,Mainchain |
| 20 | AS | 96 | ALA | Peptide,Mainchain |
| 21 | AT | 27 | ASP | Peptide |
| 21 | AT | 43 | GLY | Peptide,Mainchain |
| 21 | AT | 44 | ARG | Peptide,Mainchain |
| 21 | AT | 53 | TYR | Peptide |
| 21 | AT | 54 | ALA | Peptide,Mainchain |
| 21 | AT | 58 | TYR | Sidechain |
| 21 | AT | 68 | SER | Peptide |
| 21 | AT | 8 | LEU | Peptide |
| 21 | AT | 85 | TYR | Peptide,Sidechain |
| 21 | AT | 9 | VAL | Peptide,Mainchain |
| 29 | AU | 27 | VAL | Peptide |
| 29 | AU | 35 | VAL | Peptide |
| 29 | AU | 36 | SER | Peptide,Mainchain |
| 29 | AU | 37 | LYS | Peptide |
| 29 | AU | 52 | LYS | Peptide |
| 29 | AU | 58 | PHE | Sidechain |
| 29 | AU | 62 | THR | Mainchain |
| 29 | AU | 66 | GLY | Peptide |
| 29 | AU | 70 | VAL | Mainchain |
| 29 | AU | 72 | PHE | Peptide |
| 29 | AU | 89 | TYR | Sidechain |
| 22 | AV | 103 | ARG | Peptide,Sidechain |
| 22 | AV | 104 | ALA | Mainchain |
| 22 | AV | 105 | THR | Mainchain |
| 22 | AV | 106 | ALA | Peptide |
| 22 | AV | 26 | LYS | Peptide,Mainchain |
| 22 | AV | 28 | SER | Peptide |
| 22 | AV | 29 | LYS | Peptide |
| 22 | AV | 43 | ASP | Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 22 | AV | 47 | TYR | Sidechain |
| 22 | AV | 77 | ARG | Sidechain |
| 23 | AW | 117 | UNK | Peptide |
| 23 | AW | 15 | UNK | Peptide,Mainchain |
| 23 | AW | 60 | UNK | Peptide |
| 23 | AW | 61 | UNK | Peptide |
| 23 | AW | 62 | UNK | Peptide |
| 23 | AW | 63 | UNK | Peptide |
| 23 | AW | 64 | UNK | Peptide |
| 23 | AW | 66 | UNK | Peptide |
| 23 | AW | 67 | UNK | Peptide |
| 23 | AW | 69 | UNK | Peptide |
| 23 | AW | 70 | UNK | Peptide |
| 23 | AW | 72 | UNK | Peptide |
| 23 | AW | 73 | UNK | Peptide |
| 23 | AW | 75 | UNK | Peptide |
| 23 | AW | 77 | UNK | Peptide |
| 23 | AW | 91 | UNK | Peptide |
| 23 | AW | 92 | UNK | Peptide |
| 23 | AW | 93 | UNK | Peptide |
| 23 | AW | 94 | UNK | Peptide |
| 24 | AX | 47 | PHE | Sidechain |
| 24 | AX | 58 | SER | Peptide |
| 25 | AY | 20 | GLY | Peptide |
| 25 | AY | 21 | SER | Peptide |
| 25 | AY | 22 | ARG | Peptide |
| 25 | AY | 23 | GLY | Peptide |
| 26 | AZ | 10 | ARG | Sidechain |
| 26 | AZ | 18 | THR | Peptide,Mainchain |
| 26 | AZ | 19 | PRO | Peptide |
| 26 | AZ | 21 | VAL | Peptide |
| 26 | AZ | 22 | GLU | Peptide |
| 26 | AZ | 24 | THR | Peptide |
| 26 | AZ | 26 | LYS | Peptide |
| 26 | AZ | 35 | TYR | Sidechain |
| 26 | AZ | 39 | LEU | Peptide,Mainchain |
| 26 | AZ | 40 | TYR | Peptide,Mainchain |
| 26 | AZ | 41 | THR | Peptide |
| 26 | AZ | 42 | ARG | Sidechain |
| 26 | AZ | 43 | ARG | Sidechain |
| 26 | AZ | 44 | PHE | Peptide,Mainchain |
| 26 | AZ | 46 | ASN | Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 26 | AZ | 54 | ARG | Peptide |
| 26 | AZ | 55 | ARG | Peptide |
| 26 | AZ | 57 | ASN | Peptide |
| 26 | AZ | 58 | PRO | Peptide |
| 26 | AZ | 59 | GLY | Peptide |
| 26 | AZ | 61 | SER | Peptide |
| 1 | Aa | 10 | ARG | Sidechain |
| 1 | Aa | 192 | PHE | Sidechain |
| 1 | Aa | 232 | TYR | Sidechain |
| 1 | Aa | 240 | VAL | Peptide |
| 1 | Aa | 280 | GLY | Peptide |
| 1 | Aa | 302 | PHE | Sidechain |
| 1 | Aa | 305 | TYR | Sidechain |
| 1 | Aa | 48 | THR | Peptide |
| 1 | Aa | 49 | GLY | Peptide |
| 1 | Aa | 53 | LYS | Peptide,Mainchain |
| 1 | Aa | 54 | PHE | Peptide,Mainchain |
| 1 | Aa | 58 | VAL | Peptide |
| 1 | Aa | 59 | ARG | Peptide,Mainchain |
| 1 | Aa | 60 | SER | Peptide |
| 1 | Aa | 78 | ALA | Peptide |
| 27 | Ab | 1 | UNK | Mainchain |
| 27 | Ab | 27 | UNK | Mainchain |
| 27 | Ab | 29 | UNK | Mainchain |
| 28 | Ac | 3 | UNK | Peptide |
| 30 | BA | 107 | TYR | Sidechain |
| 30 | BA | 122 | ARG | Sidechain |
| 30 | BA | 19 | TYR | Peptide |
| 30 | BA | 208 | SER | Mainchain |
| 30 | BA | 210 | MET | Peptide |
| 30 | BA | 214 | PHE | Sidechain |
| 30 | BA | 41 | TYR | Sidechain |
| 30 | BA | 68 | PHE | Sidechain |
| 31 | BB | 1 | MET | Mainchain |
| 31 | BB | 127 | ALA | Peptide,Mainchain |
| 31 | BB | 128 | ARG | Sidechain |
| 31 | BB | 140 | ASN | Peptide |
| 31 | BB | 19 | HIS | Sidechain |
| 31 | BB | 193 | ARG | Sidechain |
| 31 | BB | 196 | TRP | Peptide,Mainchain |
| 31 | BB | 2 | GLY | Peptide |
| 31 | BB | 239 | ALA | Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 31 | BB | 241 | ARG | Sidechain |
| 31 | BB | 242 | ARG | Sidechain |
| 31 | BB | 243 | THR | Peptide |
| 31 | BB | 244 | GLY | Peptide,Mainchain |
| 31 | BB | 245 | LEU | Mainchain |
| 31 | BB | 249 | SER | Peptide,Mainchain |
| 31 | BB | 252 | THR | Peptide,Mainchain |
| 31 | BB | 26 | ALA | Peptide |
| 31 | BB | 27 | ALA | Peptide |
| 31 | BB | 30 | ARG | Sidechain |
| 31 | BB | 34 | TYR | Sidechain |
| 31 | BB | 37 | ARG | Mainchain |
| 31 | BB | 39 | GLY | Peptide |
| 31 | BB | 40 | TYR | Peptide,Sidechain |
| 31 | BB | 42 | ARG | Sidechain |
| 31 | BB | 50 | HIS | Sidechain |
| 31 | BB | 54 | ARG | Sidechain |
| 31 | BB | 6 | ARG | Sidechain |
| 31 | BB | 62 | VAL | Peptide,Mainchain |
| 31 | BB | 67 | TYR | Sidechain |
| 31 | BB | 68 | LYS | Peptide |
| 31 | BB | 69 | TYR | Sidechain |
| 31 | BB | 70 | ARG | Peptide |
| 31 | BB | 73 | GLU | Peptide,Mainchain |
| 31 | BB | 83 | HIS | Sidechain |
| 31 | BB | 84 | THR | Mainchain |
| 31 | BB | 89 | TYR | Sidechain |
| 31 | BB | 9 | ARG | Sidechain |
| 32 | BC | 10 | ARG | Sidechain |
| 32 | BC | 100 | ARG | Sidechain |
| 32 | BC | 101 | SER | Mainchain |
| 32 | BC | 103 | THR | Peptide |
| 32 | BC | 109 | HIS | Peptide |
| 32 | BC | 117 | ARG | Sidechain |
| 32 | BC | 119 | TYR | Sidechain |
| 32 | BC | 121 | ASN | Peptide |
| 32 | BC | 129 | ALA | Peptide |
| 32 | BC | 130 | PHE | Peptide,Mainchain |
| 32 | BC | 154 | TYR | Peptide |
| 32 | BC | 155 | ALA | Peptide |
| 32 | BC | 169 | THR | Peptide |
| 32 | BC | 17 | LEU | Peptide,Mainchain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 32 | BC | 19 | ARG | Sidechain |
| 32 | BC | 247 | ARG | Sidechain |
| 32 | BC | 256 | HIS | Peptide,Mainchain |
| 32 | BC | 28 | ARG | Sidechain |
| 32 | BC | 283 | TYR | Sidechain |
| 32 | BC | 288 | GLY | Peptide |
| 32 | BC | 289 | ASP | Peptide,Mainchain |
| 32 | BC | 297 | SER | Peptide,Mainchain |
| 32 | BC | 298 | PHE | Peptide,Mainchain |
| 32 | BC | 3 | HIS | Peptide,Mainchain |
| 32 | BC | 314 | TYR | Sidechain |
| 32 | BC | 334 | ARG | Sidechain |
| 32 | BC | 339 | ARG | Sidechain |
| 32 | BC | 344 | THR | Mainchain |
| 32 | BC | 345 | ASN | Peptide,Mainchain |
| 32 | BC | 353 | GLU | Peptide |
| 32 | BC | 360 | ASP | Peptide,Mainchain |
| 32 | BC | 362 | ALA | Peptide,Mainchain |
| 32 | BC | 365 | PHE | Sidechain |
| 32 | BC | 368 | GLY | Peptide,Mainchain |
| 32 | BC | 371 | GLN | Mainchain |
| 32 | BC | 381 | GLY | Peptide,Mainchain |
| 32 | BC | 386 | ASP | Peptide,Mainchain |
| 32 | BC | 49 | TYR | Sidechain |
| 32 | BC | 5 | LYS | Peptide,Mainchain |
| 32 | BC | 6 | TYR | Sidechain |
| 32 | BC | 70 | ARG | Sidechain |
| 32 | BC | 92 | TYR | Mainchain |
| 33 | BD | 105 | THR | Peptide |
| 33 | BD | 107 | ARG | Sidechain |
| 33 | BD | 108 | LYS | Peptide |
| 33 | BD | 12 | THR | Peptide,Mainchain |
| 33 | BD | 143 | GLU | Peptide |
| 33 | BD | 145 | ILE | Peptide,Mainchain |
| 33 | BD | 146 | PRO | Peptide |
| 33 | BD | 148 | ILE | Peptide,Mainchain |
| 33 | BD | 195 | ARG | Sidechain |
| 33 | BD | 197 | ARG | Sidechain |
| 33 | BD | 209 | TYR | Sidechain |
| 33 | BD | 220 | ARG | Sidechain |
| 33 | BD | 258 | LEU | Peptide |
| 33 | BD | 260 | GLN | Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 33 | BD | 295 | ILE | Peptide |
| 33 | BD | 314 | LYS | Peptide |
| 33 | BD | 318 | LEU | Peptide,Mainchain |
| 33 | BD | 319 | LYS | Peptide |
| 33 | BD | 320 | ASN | Peptide |
| 33 | BD | 321 | LYS | Peptide,Mainchain |
| 33 | BD | 323 | VAL | Peptide,Mainchain |
| 33 | BD | 326 | ARG | Sidechain |
| 33 | BD | 330 | TYR | Peptide,Sidechain |
| 33 | BD | 331 | ALA | Peptide,Mainchain |
| 33 | BD | 334 | PHE | Sidechain |
| 33 | BD | 346 | LYS | Mainchain |
| 33 | BD | 348 | GLY | Peptide |
| 33 | BD | 349 | THR | Peptide,Mainchain |
| 33 | BD | 350 | LYS | Peptide |
| 33 | BD | 351 | PRO | Peptide,Mainchain |
| 33 | BD | 353 | ALA | Peptide |
| 33 | BD | 354 | VAL | Mainchain |
| 33 | BD | 355 | PHE | Peptide |
| 33 | BD | 47 | ARG | Sidechain |
| 33 | BD | 73 | ARG | Sidechain |
| 33 | BD | 76 | ARG | Sidechain |
| 33 | BD | 78 | GLY | Peptide,Mainchain |
| 33 | BD | 84 | ARG | Peptide,Mainchain |
| 33 | BD | 88 | GLY | Peptide |
| 33 | BD | 89 | ALA | Peptide,Mainchain |
| 34 | BE | 116 | TYR | Sidechain |
| 34 | BE | 121 | GLY | Peptide |
| 34 | BE | 123 | PHE | Peptide,Mainchain |
| 34 | BE | 124 | GLY | Peptide |
| 34 | BE | 127 | PHE | Sidechain |
| 34 | BE | 128 | TYR | Sidechain |
| 34 | BE | 2 | SER | Peptide |
| 34 | BE | 51 | ARG | Mainchain |
| 34 | BE | 52 | TYR | Peptide,Sidechain |
| 34 | BE | 53 | THR | Peptide,Mainchain |
| 34 | BE | 54 | VAL | Peptide,Mainchain |
| 34 | BE | 55 | ARG | Peptide,Mainchain |
| 34 | BE | 58 | GLY | Mainchain |
| 34 | BE | 60 | ARG | Mainchain |
| 34 | BE | 72 | ARG | Sidechain |
| 34 | BE | 89 | TYR | Peptide,Mainchain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 34 | BE | 9 | MET | Peptide,Mainchain |
| 34 | BE | 94 | ARG | Sidechain |
| 36 | BF | 184 | LYS | Peptide |
| 36 | BF | 185 | GLY | Peptide |
| 36 | BF | 2 | LYS | Peptide,Mainchain |
| 36 | BF | 23 | ARG | Sidechain |
| 36 | BF | 3 | TYR | Sidechain |
| 36 | BF | 44 | THR | Peptide |
| 36 | BF | 45 | PHE | Mainchain |
| 36 | BF | 62 | ARG | Sidechain |
| 36 | BF | 96 | HIS | Peptide |
| 35 | BG | 10 | TYR | Peptide,Mainchain |
| 35 | BG | 102 | ASN | Peptide |
| 35 | BG | 105 | TYR | Mainchain |
| 35 | BG | 11 | PRO | Peptide |
| 35 | BG | 12 | SER | Peptide |
| 35 | BG | 128 | LYS | Peptide |
| 35 | BG | 129 | GLU | Peptide |
| 35 | BG | 134 | ARG | Sidechain |
| 35 | BG | 14 | ASP | Peptide |
| 35 | BG | 141 | VAL | Peptide |
| 35 | BG | 142 | ASP | Peptide,Mainchain |
| 35 | BG | 148 | GLU | Peptide,Mainchain |
| 35 | BG | 15 | VAL | Peptide,Mainchain |
| 35 | BG | 150 | LYS | Peptide |
| 35 | BG | 152 | THR | Peptide,Mainchain |
| 35 | BG | 154 | LEU | Peptide |
| 35 | BG | 16 | ALA | Peptide,Mainchain |
| 35 | BG | 169 | ASP | Peptide |
| 35 | BG | 17 | ALA | Peptide |
| 35 | BG | 2 | SER | Peptide,Mainchain |
| 35 | BG | 22 | ARG | Sidechain |
| 35 | BG | 25 | ALA | Peptide |
| 35 | BG | 27 | PRO | Peptide,Mainchain |
| 35 | BG | 3 | ALA | Peptide,Mainchain |
| 35 | BG | 34 | LEU | Peptide |
| 35 | BG | 38 | THR | Peptide,Mainchain |
| 35 | BG | 44 | ALA | Peptide |
| 35 | BG | 46 | ARG | Sidechain |
| 35 | BG | 47 | PHE | Sidechain |
| 35 | BG | 49 | GLY | Peptide,Mainchain |
| 35 | BG | 5 | LYS | Peptide,Mainchain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 35 | BG | 54 | TYR | Sidechain |
| 35 | BG | 56 | LYS | Peptide |
| 35 | BG | 57 | HIS | Peptide |
| 35 | BG | 75 | PRO | Peptide,Mainchain |
| 35 | BG | 77 | ARG | Peptide,Sidechain |
| 35 | BG | 8 | LYS | Peptide,Mainchain |
| 35 | BG | 81 | ALA | Peptide |
| 35 | BG | 93 | VAL | Peptide |
| 35 | BG | 94 | GLU | Peptide |
| 35 | BG | 96 | VAL | Peptide |
| 35 | BG | 99 | GLU | Mainchain |
| 37 | BH | 108 | ARG | Sidechain |
| 37 | BH | 117 | ALA | Peptide |
| 37 | BH | 119 | GLY | Mainchain |
| 37 | BH | 120 | LYS | Peptide |
| 37 | BH | 122 | LYS | Peptide |
| 37 | BH | 123 | GLN | Peptide |
| 37 | BH | 125 | ALA | Peptide |
| 37 | BH | 128 | LYS | Peptide |
| 37 | BH | 130 | TYR | Peptide |
| 37 | BH | 134 | TYR | Sidechain |
| 37 | BH | 138 | HIS | Sidechain |
| 37 | BH | 158 | ASP | Peptide,Mainchain |
| 37 | BH | 226 | TYR | Peptide |
| 37 | BH | 228 | GLU | Peptide,Mainchain |
| 37 | BH | 232 | HIS | Sidechain,Mainchain |
| 37 | BH | 236 | GLY | Peptide,Mainchain |
| 37 | BH | 60 | ARG | Sidechain |
| 37 | BH | 61 | GLN | Mainchain |
| 37 | BH | 62 | LYS | Peptide |
| 37 | BH | 63 | LYS | Peptide,Mainchain |
| 37 | BH | 64 | ILE | Peptide |
| 37 | BH | 68 | ARG | Sidechain |
| 37 | BH | 70 | LYS | Peptide |
| 37 | BH | 73 | PRO | Peptide,Mainchain |
| 37 | BH | 84 | ARG | Sidechain |
| 37 | BH | 89 | GLU | Peptide,Sidechain,Mainchain |
| 37 | BH | 98 | ARG | Peptide,Sidechain |
| 77 | BI | 10 | ARG | Sidechain |
| 77 | BI | 106 | ALA | Peptide |
| 77 | BI | 108 | ALA | Peptide |
| 77 | BI | 109 | ASP | Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 77 | BI | 110 | ARG | Sidechain |
| 77 | BI | 111 | LEU | Peptide |
| 77 | BI | 114 | GLY | Peptide |
| 77 | BI | 116 | ARG | Peptide |
| 77 | BI | 128 | ARG | Sidechain |
| 77 | BI | 13 | LYS | Peptide |
| 77 | BI | 139 | ARG | Sidechain |
| 77 | BI | 154 | ARG | Sidechain |
| 77 | BI | 156 | ARG | Sidechain |
| 77 | BI | 17 | TYR | Peptide |
| 77 | BI | 170 | LYS | Peptide |
| 77 | BI | 21 | ARG | Peptide |
| 77 | BI | 24 | ARG | Sidechain |
| 77 | BI | 3 | ARG | Sidechain |
| 77 | BI | 4 | ARG | Peptide,Sidechain |
| 77 | BI | 69 | ARG | Sidechain |
| 77 | BI | 7 | ARG | Sidechain |
| 77 | BI | 82 | ARG | Sidechain |
| 77 | BI | 88 | ARG | Sidechain |
| 39 | BJ | 121 | PHE | Peptide |
| 39 | BJ | 123 | ARG | Sidechain |
| 39 | BJ | 14 | TYR | Sidechain |
| 39 | BJ | 59 | THR | Peptide |
| 39 | BJ | 74 | VAL | Peptide |
| 39 | BJ | 75 | PRO | Peptide,Mainchain |
| 39 | BJ | 76 | SER | Peptide,Mainchain |
| 39 | BJ | 92 | ARG | Sidechain |
| 40 | BK | 1 | MET | Peptide |
| 40 | BK | 110 | PRO | Peptide |
| 40 | BK | 120 | VAL | Peptide |
| 40 | BK | 125 | ARG | Peptide |
| 40 | BK | 128 | ARG | Mainchain |
| 40 | BK | 129 | LEU | Peptide |
| 40 | BK | 130 | LYS | Peptide |
| 40 | BK | 131 | PRO | Peptide |
| 40 | BK | 133 | ARG | Peptide |
| 40 | BK | 147 | TRP | Peptide,Mainchain |
| 40 | BK | 168 | TYR | Sidechain |
| 40 | BK | 178 | VAL | Mainchain |
| 40 | BK | 180 | SER | Peptide,Mainchain |
| 40 | BK | 181 | ALA | Peptide |
| 40 | BK | 182 | ASN | Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 40 | BK | 184 | THR | Peptide,Mainchain |
| 40 | BK | 187 | GLU | Mainchain |
| 40 | BK | 4 | GLU | Peptide |
| 40 | BK | 6 | VAL | Peptide |
| 40 | BK | 63 | ALA | Peptide,Mainchain |
| 40 | BK | 64 | PHE | Sidechain |
| 40 | BK | 69 | GLY | Peptide,Mainchain |
| 40 | BK | 74 | ARG | Peptide |
| 40 | BK | 90 | HIS | Sidechain |
| 75 | BL | 122 | UNK | Peptide |
| 75 | BL | 145 | UNK | Peptide |
| 75 | BL | 149 | UNK | Peptide |
| 75 | BL | 52 | UNK | Peptide |
| 75 | BL | 82 | UNK | Peptide |
| 42 | BM | 109 | MET | Peptide |
| 42 | BM | 11 | PHE | Sidechain |
| 42 | BM | 12 | ARG | Sidechain |
| 42 | BM | 35 | TYR | Sidechain |
| 42 | BM | 40 | LYS | Mainchain |
| 42 | BM | 45 | ARG | Sidechain |
| 42 | BM | 48 | ARG | Mainchain |
| 42 | BM | 64 | LYS | Mainchain |
| 42 | BM | 65 | GLY | Mainchain |
| 42 | BM | 75 | PRO | Mainchain |
| 42 | BM | 80 | ARG | Sidechain |
| 41 | BN | 10 | SER | Peptide |
| 41 | BN | 115 | PHE | Sidechain |
| 41 | BN | 124 | ARG | Sidechain |
| 41 | BN | 129 | TYR | Sidechain |
| 41 | BN | 19 | ARG | Sidechain |
| 41 | BN | 2 | SER | Peptide,Mainchain |
| 41 | BN | 3 | THR | Mainchain |
| 41 | BN | 5 | SER | Peptide,Mainchain |
| 41 | BN | 52 | GLY | Peptide |
| 41 | BN | 61 | GLY | Peptide |
| 41 | BN | 9 | ALA | Peptide |
| 44 | BO | 117 | ARG | Sidechain |
| 44 | BO | 128 | ARG | Sidechain |
| 44 | BO | 139 | ARG | Sidechain |
| 44 | BO | 14 | HIS | Sidechain |
| 44 | BO | 142 | GLY | Peptide,Mainchain |
| 44 | BO | 27 | LYS | Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 44 | BO | 29 | PRO | Peptide |
| 44 | BO | 3 | SER | Mainchain |
| 44 | BO | 32 | ARG | Sidechain |
| 44 | BO | 40 | HIS | Mainchain |
| 44 | BO | 48 | TYR | Sidechain |
| 44 | BO | 5 | PHE | Sidechain |
| 44 | BO | 56 | VAL | Mainchain |
| 44 | BO | 57 | GLY | Mainchain |
| 44 | BO | 59 | ARG | Sidechain |
| 44 | BO | 6 | THR | Peptide |
| 44 | BO | 61 | PHE | Sidechain |
| 44 | BO | 62 | HIS | Peptide,Mainchain |
| 44 | BO | 7 | LYS | Peptide,Mainchain |
| 44 | BO | 8 | THR | Peptide,Mainchain |
| 44 | BO | 87 | ARG | Sidechain |
| 44 | BO | 90 | TYR | Peptide,Sidechain |
| 44 | BO | 98 | THR | Peptide |
| 43 | BP | 114 | ARG | Sidechain |
| 43 | BP | 116 | LEU | Peptide,Mainchain |
| 43 | BP | 12 | ARG | Sidechain |
| 43 | BP | 120 | TRP | Peptide |
| 43 | BP | 121 | VAL | Peptide |
| 43 | BP | 123 | GLN | Peptide |
| 43 | BP | 127 | TYR | Sidechain |
| 43 | BP | 129 | TYR | Sidechain |
| 43 | BP | 13 | LYS | Peptide,Mainchain |
| 43 | BP | 137 | PRO | Peptide |
| 43 | BP | 147 | ARG | Sidechain |
| 43 | BP | 159 | ARG | Sidechain |
| 43 | BP | 16 | SER | Peptide,Mainchain |
| 43 | BP | 162 | ARG | Sidechain |
| 43 | BP | 165 | THR | Mainchain |
| 43 | BP | 175 | ASN | Peptide,Mainchain |
| 43 | BP | 176 | LYS | Peptide |
| 43 | BP | 177 | GLY | Peptide,Mainchain |
| 43 | BP | 179 | LYS | Peptide,Mainchain |
| 43 | BP | 180 | PHE | Peptide |
| 43 | BP | 185 | ALA | Peptide |
| 43 | BP | 187 | ARG | Sidechain |
| 43 | BP | 2 | GLY | Peptide,Mainchain |
| 43 | BP | 20 | ARG | Sidechain |
| 43 | BP | 4 | TYR | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 43 | BP | 42 | PRO | Mainchain |
| 43 | BP | 50 | ARG | Sidechain |
| 43 | BP | 51 | LEU | Peptide |
| 43 | BP | 62 | TYR | Sidechain |
| 43 | BP | 67 | ARG | Sidechain |
| 43 | BP | 68 | ARG | Sidechain |
| 43 | BP | 74 | PRO | Peptide,Mainchain |
| 43 | BP | 80 | THR | Peptide,Mainchain |
| 43 | BP | 81 | TYR | Sidechain |
| 43 | BP | 96 | ARG | Sidechain |
| 74 | BQ | 111 | GLN | Peptide,Mainchain |
| 74 | BQ | 115 | LEU | Peptide,Mainchain |
| 74 | BQ | 119 | TYR | Sidechain |
| 74 | BQ | 121 | GLY | Peptide,Mainchain |
| 74 | BQ | 123 | GLU | Mainchain |
| 74 | BQ | 128 | GLU | Peptide,Mainchain |
| 74 | BQ | 129 | TYR | Peptide,Mainchain |
| 74 | BQ | 136 | GLU | Peptide |
| 74 | BQ | 145 | PHE | Sidechain |
| 74 | BQ | 158 | ARG | Sidechain,Mainchain |
| 74 | BQ | 172 | TYR | Sidechain |
| 74 | BQ | 180 | PHE | Peptide |
| 74 | BQ | 189 | GLU | Peptide |
| 74 | BQ | 190 | ILE | Peptide,Mainchain |
| 74 | BQ | 197 | SER | Peptide,Mainchain |
| 74 | BQ | 2 | ALA | Peptide |
| 74 | BQ | 201 | GLY | Peptide,Mainchain |
| 74 | BQ | 203 | HIS | Sidechain |
| 74 | BQ | 21 | ARG | Sidechain |
| 74 | BQ | 223 | PHE | Sidechain |
| 74 | BQ | 237 | GLU | Peptide,Mainchain |
| 74 | BQ | 238 | ASP | Peptide,Mainchain |
| 74 | BQ | 239 | ILE | Peptide |
| 74 | BQ | 240 | TYR | Peptide |
| 74 | BQ | 242 | SER | Mainchain |
| 74 | BQ | 243 | ALA | Mainchain |
| 74 | BQ | 248 | ARG | Peptide |
| 74 | BQ | 249 | ALA | Peptide |
| 74 | BQ | 258 | LYS | Peptide |
| 74 | BQ | 265 | TYR | Sidechain |
| 74 | BQ | 27 | LYS | Peptide |
| 74 | BQ | 272 | TYR | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 74 | BQ | 33 | ARG | Sidechain |
| 74 | BQ | 51 | LEU | Peptide |
| 74 | BQ | 52 | VAL | Peptide |
| 74 | BQ | 54 | ARG | Sidechain |
| 74 | BQ | 55 | PHE | Peptide |
| 45 | BR | 1 | MET | Peptide |
| 45 | BR | 11 | LYS | Peptide |
| 45 | BR | 111 | ARG | Sidechain |
| 45 | BR | 13 | SER | Peptide,Mainchain |
| 45 | BR | 131 | ALA | Peptide |
| 45 | BR | 14 | GLY | Mainchain |
| 45 | BR | 140 | LEU | Peptide,Mainchain |
| 45 | BR | 142 | GLY | Peptide,Mainchain |
| 45 | BR | 143 | PRO | Peptide,Mainchain |
| 45 | BR | 15 | HIS | Peptide |
| 45 | BR | 156 | GLY | Peptide |
| 45 | BR | 157 | PRO | Peptide,Mainchain |
| 45 | BR | 159 | LYS | Peptide |
| 45 | BR | 17 | THR | Peptide |
| 45 | BR | 2 | GLY | Peptide |
| 45 | BR | 3 | ILE | Peptide,Mainchain |
| 45 | BR | 38 | ARG | Sidechain |
| 45 | BR | 39 | ARG | Sidechain |
| 45 | BR | 53 | PHE | Sidechain |
| 45 | BR | 75 | GLY | Peptide |
| 45 | BR | 95 | GLU | Peptide,Mainchain |
| 45 | BR | 96 | PHE | Sidechain |
| 45 | BR | 98 | LYS | Peptide,Mainchain |
| 76 | BS | 115 | ARG | Sidechain |
| 76 | BS | 117 | ARG | Sidechain |
| 76 | BS | 119 | ARG | Sidechain |
| 76 | BS | 120 | PHE | Mainchain |
| 76 | BS | 122 | CYS | Peptide,Mainchain |
| 76 | BS | 123 | ILE | Peptide,Mainchain |
| 76 | BS | 124 | GLN | Peptide |
| 76 | BS | 138 | ARG | Peptide,Sidechain |
| 76 | BS | 14 | ARG | Peptide |
| 76 | BS | 144 | PHE | Sidechain |
| 76 | BS | 15 | GLY | Peptide,Mainchain |
| 76 | BS | 150 | LYS | Peptide |
| 76 | BS | 151 | PHE | Peptide,Sidechain |
| 76 | BS | 152 | PRO | Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 76 | BS | 153 | LEU | Peptide |
| 76 | BS | 156 | ARG | Peptide,Mainchain |
| 76 | BS | 157 | LYS | Peptide |
| 76 | BS | 159 | ARG | Peptide,Sidechain |
| 76 | BS | 161 | PRO | Peptide |
| 76 | BS | 18 | THR | Peptide |
| 76 | BS | 25 | LYS | Peptide |
| 76 | BS | 28 | ARG | Peptide |
| 76 | BS | 43 | PHE | Sidechain |
| 76 | BS | 52 | LYS | Peptide |
| 76 | BS | 53 | VAL | Peptide |
| 76 | BS | 54 | LYS | Peptide |
| 76 | BS | 69 | LYS | Peptide |
| 76 | BS | 70 | ASN | Peptide,Mainchain |
| 76 | BS | 72 | THR | Peptide |
| 76 | BS | 73 | THR | Peptide,Mainchain |
| 76 | BS | 74 | ILE | Peptide |
| 76 | BS | 96 | TYR | Sidechain |
| 46 | BT | 103 | ARG | Sidechain |
| 46 | BT | 114 | LYS | Peptide |
| 46 | BT | 151 | ARG | Sidechain |
| 46 | BT | 162 | ARG | Sidechain |
| 46 | BT | 163 | ARG | Sidechain |
| 46 | BT | 173 | ARG | Sidechain |
| 46 | BT | 38 | ARG | Sidechain |
| 46 | BT | 56 | THR | Peptide |
| 46 | BT | 58 | HIS | Sidechain |
| 46 | BT | 62 | ARG | Sidechain |
| 46 | BT | 71 | ARG | Peptide,Mainchain |
| 46 | BT | 78 | TYR | Sidechain |
| 46 | BT | 82 | LYS | Peptide,Mainchain |
| 46 | BT | 83 | GLY | Peptide |
| 46 | BT | 88 | ARG | Sidechain |
| 47 | BU | 10 | ARG | Sidechain |
| 47 | BU | 102 | ARG | Sidechain |
| 47 | BU | 108 | ARG | Sidechain |
| 47 | BU | 126 | VAL | Peptide,Mainchain |
| 47 | BU | 136 | ARG | Peptide |
| 47 | BU | 137 | GLU | Peptide |
| 47 | BU | 138 | SER | Peptide |
| 47 | BU | 140 | ILE | Peptide,Mainchain |
| 47 | BU | 141 | VAL | Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 47 | BU | 20 | ARG | Sidechain |
| 47 | BU | 5 | HIS | Peptide |
| 47 | BU | 8 | ARG | Sidechain |
| 47 | BU | 84 | TYR | Sidechain |
| 47 | BU | 88 | ARG | Sidechain |
| 49 | BV | 113 | TYR | Sidechain |
| 49 | BV | 122 | ALA | Peptide |
| 49 | BV | 130 | TYR | Sidechain |
| 49 | BV | 139 | TYR | Sidechain |
| 49 | BV | 152 | GLU | Peptide,Mainchain |
| 49 | BV | 162 | GLU | Peptide,Mainchain |
| 49 | BV | 165 | VAL | Peptide,Mainchain |
| 49 | BV | 167 | ARG | Peptide,Mainchain |
| 49 | BV | 2 | ALA | Peptide |
| 49 | BV | 3 | ARG | Peptide |
| 49 | BV | 47 | TYR | Sidechain |
| 49 | BV | 56 | ARG | Sidechain |
| 49 | BV | 63 | PHE | Peptide |
| 49 | BV | 69 | ARG | Peptide,Sidechain |
| 49 | BV | 90 | PHE | Sidechain |
| 48 | BW | 106 | ALA | Peptide |
| 48 | BW | 107 | PHE | Peptide |
| 48 | BW | 109 | GLN | Peptide |
| 48 | BW | 19 | VAL | Peptide |
| 48 | BW | 20 | SER | Peptide |
| 48 | BW | 28 | PHE | Sidechain |
| 48 | BW | 29 | ASP | Peptide |
| 48 | BW | 7 | ARG | Peptide |
| 48 | BW | 78 | TYR | Sidechain |
| 48 | BW | 90 | ARG | Peptide,Mainchain |
| 48 | BW | 93 | ILE | Mainchain |
| 50 | BX | 123 | TYR | Sidechain |
| 50 | BX | 130 | TYR | Sidechain |
| 50 | BX | 138 | ARG | Sidechain |
| 50 | BX | 22 | LYS | Peptide |
| 50 | BX | 34 | LEU | Peptide |
| 50 | BX | 36 | LYS | Peptide |
| 50 | BX | 37 | THR | Peptide |
| 50 | BX | 39 | LYS | Peptide |
| 50 | BX | 43 | ALA | Peptide |
| 50 | BX | 46 | TYR | Peptide |
| 50 | BX | 54 | TYR | Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 50 | BX | 56 | ARG | Sidechain |
| 50 | BX | 60 | TYR | Sidechain |
| 52 | BY | 10 | SER | Peptide |
| 52 | BY | 13 | ARG | Sidechain |
| 52 | BY | 27 | ARG | Sidechain |
| 52 | BY | 51 | ARG | Sidechain |
| 52 | BY | 60 | ARG | Peptide |
| 52 | BY | 74 | TYR | Sidechain |
| 52 | BY | 78 | PHE | Sidechain |
| 52 | BY | 9 | SER | Peptide |
| 51 | BZ | 14 | TYR | Sidechain |
| 51 | BZ | 51 | TRP | Peptide,Mainchain |
| 51 | BZ | 56 | ARG | Sidechain |
| 51 | BZ | 57 | LYS | Peptide |
| 51 | BZ | 58 | HIS | Peptide |
| 51 | BZ | 59 | HIS | Peptide |
| 51 | BZ | 60 | LYS | Peptide,Mainchain |
| 51 | BZ | 62 | GLY | Peptide |
| 51 | BZ | 63 | ILE | Peptide |
| 51 | BZ | 65 | GLU | Peptide |
| 51 | BZ | 67 | VAL | Mainchain |
| 51 | BZ | 68 | ALA | Peptide |
| 51 | BZ | 69 | LYS | Peptide |
| 51 | BZ | 70 | LYS | Peptide,Mainchain |
| 51 | BZ | 71 | ARG | Peptide |
| 53 | Ba | 11 | ALA | Peptide |
| 53 | Ba | 12 | VAL | Peptide |
| 53 | Ba | 13 | VAL | Peptide,Mainchain |
| 53 | Ba | 15 | ARG | Peptide,Mainchain |
| 53 | Ba | 16 | GLY | Peptide,Mainchain |
| 53 | Ba | 20 | GLY | Mainchain |
| 53 | Ba | 36 | HIS | Peptide |
| 53 | Ba | 41 | ALA | Peptide |
| 53 | Ba | 44 | ALA | Peptide |
| 53 | Ba | 46 | ILE | Peptide |
| 53 | Ba | 53 | VAL | Peptide |
| 53 | Ba | 55 | LYS | Peptide |
| 53 | Ba | 56 | LYS | Peptide |
| 53 | Ba | 57 | HIS | Peptide,Sidechain |
| 53 | Ba | 59 | ALA | Peptide |
| 53 | Ba | 60 | LYS | Peptide,Mainchain |
| 53 | Ba | 64 | LYS | Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 53 | Ba | 8 | GLY | Peptide,Mainchain |
| 53 | Ba | 9 | LYS | Peptide |
| 55 | Bc | 102 | GLU | Peptide,Mainchain |
| 55 | Bc | 104 | GLN | Peptide,Mainchain |
| 55 | Bc | 108 | GLN | Mainchain |
| 55 | Bc | 110 | ALA | Peptide |
| 55 | Bc | 112 | PRO | Peptide,Mainchain |
| 55 | Bc | 119 | LYS | Peptide |
| 55 | Bc | 70 | TYR | Sidechain |
| 55 | Bc | 76 | GLN | Peptide |
| 55 | Bc | 81 | ARG | Sidechain |
| 55 | Bc | 86 | ARG | Peptide |
| 55 | Bc | 94 | LYS | Peptide,Mainchain |
| 55 | Bc | 96 | GLU | Mainchain |
| 54 | Bd | 41 | ARG | Sidechain |
| 57 | Be | 107 | ARG | Sidechain |
| 57 | Be | 132 | PRO | Peptide,Mainchain |
| 57 | Be | 133 | TYR | Peptide,Sidechain |
| 57 | Be | 134 | VAL | Peptide |
| 57 | Be | 141 | TYR | Sidechain |
| 57 | Be | 151 | ARG | Sidechain |
| 57 | Be | 164 | SER | Peptide |
| 57 | Be | 202 | LEU | Peptide,Mainchain |
| 57 | Be | 220 | PHE | Sidechain |
| 57 | Be | 55 | TYR | Sidechain |
| 57 | Be | 97 | PRO | Peptide |
| 56 | Bf | 3 | PRO | Peptide |
| 56 | Bf | 35 | ARG | Sidechain |
| 56 | Bf | 5 | LYS | Peptide |
| 56 | Bf | 52 | ARG | Sidechain |
| 56 | Bf | 64 | LYS | Peptide |
| 56 | Bf | 85 | PHE | Sidechain |
| 58 | Bg | 107 | VAL | Peptide,Mainchain |
| 58 | Bg | 12 | TYR | Sidechain |
| 58 | Bg | 28 | ARG | Sidechain |
| 58 | Bg | 31 | ARG | Sidechain |
| 58 | Bg | 4 | LEU | Peptide |
| 58 | Bg | 63 | GLY | Peptide |
| 58 | Bg | 64 | VAL | Peptide |
| 58 | Bg | 69 | TYR | Sidechain |
| 58 | Bg | 72 | ARG | Sidechain |
| 58 | Bg | 90 | PHE | Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 58 | Bg | 92 | TYR | Peptide |
| 58 | Bg | 94 | GLU | Peptide |
| 59 | Bh | 12 | LYS | Peptide,Mainchain |
| 59 | Bh | 125 | ARG | Sidechain |
| 59 | Bh | 13 | HIS | Peptide |
| 59 | Bh | 18 | LYS | Peptide |
| 59 | Bh | 20 | HIS | Peptide,Mainchain |
| 59 | Bh | 23 | ASP | Mainchain |
| 59 | Bh | 24 | ARG | Sidechain |
| 59 | Bh | 25 | TYR | Sidechain |
| 59 | Bh | 26 | HIS | Sidechain |
| 59 | Bh | 43 | ARG | Sidechain |
| 59 | Bh | 46 | PHE | Sidechain |
| 59 | Bh | 47 | ARG | Sidechain |
| 60 | Bi | 108 | GLN | Peptide,Mainchain |
| 60 | Bi | 110 | GLU | Peptide |
| 60 | Bi | 16 | ARG | Mainchain |
| 60 | Bi | 19 | LYS | Peptide |
| 60 | Bi | 34 | HIS | Sidechain |
| 60 | Bi | 41 | ARG | Peptide,Mainchain |
| 60 | Bi | 42 | PRO | Peptide,Mainchain |
| 60 | Bi | 43 | LYS | Peptide |
| 60 | Bi | 55 | SER | Peptide,Mainchain |
| 60 | Bi | 58 | ARG | Peptide |
| 60 | Bi | 60 | ARG | Peptide |
| 60 | Bi | 62 | TYR | Sidechain |
| 60 | Bi | 67 | LYS | Peptide |
| 60 | Bi | 68 | THR | Peptide,Mainchain |
| 60 | Bi | 77 | GLY | Mainchain |
| 60 | Bi | 78 | GLY | Peptide,Mainchain |
| 60 | Bi | 79 | SER | Peptide,Mainchain |
| 60 | Bi | 88 | ARG | Sidechain |
| 61 | Bj | 18 | ARG | Sidechain |
| 61 | Bj | 2 | ALA | Peptide,Mainchain |
| 61 | Bj | 20 | LYS | Peptide,Mainchain |
| 61 | Bj | 35 | VAL | Peptide |
| 61 | Bj | 36 | ALA | Peptide |
| 61 | Bj | 37 | THR | Peptide,Mainchain |
| 61 | Bj | 4 | SER | Peptide |
| 61 | Bj | 43 | PHE | Peptide |
| 61 | Bj | 44 | TYR | Peptide,Sidechain |
| 61 | Bj | 51 | TYR | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 61 | Bj | 56 | SER | Peptide |
| 61 | Bj | 57 | LYS | Peptide |
| 61 | Bj | 58 | GLU | Peptide |
| 61 | Bj | 65 | ARG | Sidechain |
| 61 | Bj | 8 | TYR | Peptide,Sidechain,Mainchain |
| 61 | Bj | 86 | ARG | Sidechain |
| 61 | Bj | 89 | LEU | Mainchain |
| 61 | Bj | 90 | PRO | Peptide |
| 61 | Bj | 98 | VAL | Peptide |
| 61 | Bj | 99 | ARG | Peptide |
| 62 | Bk | 25 | LYS | Peptide,Mainchain |
| 62 | Bk | 27 | SER | Mainchain |
| 62 | Bk | 28 | TYR | Mainchain |
| 62 | Bk | 45 | ARG | Sidechain |
| 62 | Bk | 54 | GLU | Peptide |
| 62 | Bk | 55 | ARG | Peptide |
| 62 | Bk | 62 | ARG | Sidechain |
| 62 | Bk | 81 | THR | Peptide,Mainchain |
| 62 | Bk | 82 | ARG | Peptide,Mainchain |
| 62 | Bk | 83 | ALA | Peptide,Mainchain |
| 62 | Bk | 98 | ARG | Mainchain |
| 64 | Bl | 11 | ARG | Peptide,Sidechain |
| 64 | Bl | 25 | ARG | Sidechain |
| 64 | Bl | 39 | TYR | Peptide,Mainchain |
| 64 | Bl | 56 | ARG | Sidechain |
| 64 | Bl | 64 | MET | Peptide |
| 64 | Bl | 65 | ARG | Peptide,Sidechain |
| 64 | Bl | 73 | ARG | Sidechain |
| 64 | Bl | 74 | PHE | Sidechain |
| 64 | Bl | 83 | ALA | Peptide |
| 64 | Bl | 84 | SER | Peptide |
| 63 | Bm | 1 | MET | Peptide |
| 63 | Bm | 14 | TYR | Sidechain |
| 63 | Bm | 37 | TYR | Sidechain |
| 63 | Bm | 41 | PHE | Sidechain |
| 63 | Bm | 80 | ARG | Sidechain |
| 65 | Bn | 11 | PHE | Sidechain |
| 65 | Bn | 26 | LYS | Peptide |
| 65 | Bn | 29 | LYS | Peptide |
| 65 | Bn | 34 | ALA | Peptide,Mainchain |
| 65 | Bn | 35 | GLY | Peptide,Mainchain |
| 65 | Bn | 36 | LYS | Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 65 | Bn | 39 | ARG | Peptide |
| 65 | Bn | 46 | ARG | Sidechain |
| 65 | Bn | 51 | LEU | Peptide |
| 65 | Bn | 52 | TYR | Peptide |
| 65 | Bn | 71 | PRO | Peptide,Mainchain |
| 65 | Bn | 72 | THR | Peptide |
| 66 | Bo | 1 | MET | Peptide |
| 66 | Bo | 2 | ALA | Peptide |
| 66 | Bo | 28 | ARG | Sidechain |
| 66 | Bo | 3 | ALA | Peptide |
| 66 | Bo | 30 | ARG | Peptide |
| 66 | Bo | 34 | THR | Peptide |
| 66 | Bo | 4 | GLN | Peptide |
| 66 | Bo | 40 | LYS | Peptide |
| 66 | Bo | 42 | ARG | Peptide |
| 66 | Bo | 45 | ARG | Peptide,Sidechain |
| 66 | Bo | 46 | ARG | Peptide |
| 66 | Bo | 49 | MET | Peptide |
| 66 | Bo | 6 | SER | Peptide |
| 66 | Bo | 8 | ARG | Sidechain |
| 67 | Bp | 13 | TYR | Peptide |
| 67 | Bp | 14 | ASN | Peptide |
| 67 | Bp | 34 | CYS | Mainchain |
| 67 | Bp | 37 | ARG | Sidechain |
| 67 | Bp | 41 | HIS | Sidechain |
| 67 | Bp | 46 | ARG | Sidechain |
| 67 | Bp | 49 | LYS | Peptide |
| 67 | Bp | 50 | LYS | Peptide |
| 68 | Bq | 12 | ARG | Sidechain |
| 68 | Bq | 21 | ARG | Sidechain |
| 68 | Bq | 23 | ARG | Peptide |
| 68 | Bq | 24 | SER | Peptide |
| 69 | Br | 100 | LYS | Peptide |
| 69 | Br | 101 | GLY | Peptide,Mainchain |
| 69 | Br | 102 | GLN | Peptide |
| 69 | Br | 103 | ALA | Peptide,Mainchain |
| 69 | Br | 104 | LEU | Mainchain |
| 69 | Br | 28 | TYR | Sidechain |
| 69 | Br | 31 | GLY | Peptide |
| 69 | Br | 36 | PHE | Sidechain |
| 69 | Br | 43 | TYR | Sidechain |
| 69 | Br | 46 | LYS | Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 69 | Br | 47 | GLN | Peptide,Mainchain |
| 69 | Br | 49 | GLY | Peptide |
| 69 | Br | 56 | PRO | Peptide |
| 69 | Br | 58 | PHE | Peptide,Mainchain |
| 69 | Br | 59 | HIS | Sidechain |
| 69 | Br | 62 | ALA | Mainchain |
| 69 | Br | 89 | LYS | Peptide,Mainchain |
| 69 | Br | 99 | GLN | Peptide |
| 38 | Bs | 202 | LEU | Peptide |
| 38 | Bs | 203 | ASP | Peptide |
| 38 | Bs | 243 | TYR | Sidechain |
| 38 | Bs | 254 | SER | Peptide |
| 38 | Bs | 257 | TYR | Sidechain |
| 38 | Bs | 26 | PHE | Sidechain |
| 38 | Bs | 30 | VAL | Peptide |
| 38 | Bs | 42 | ARG | Sidechain |
| 38 | Bs | 46 | ARG | Sidechain |
| 38 | Bs | 49 | ALA | Peptide |
| 38 | Bs | 5 | ARG | Peptide,Mainchain |
| 38 | Bs | 52 | LEU | Peptide |
| 38 | Bs | 55 | LYS | Peptide |
| 38 | Bs | 60 | ARG | Sidechain |
| 38 | Bs | 64 | ARG | Sidechain |
| 38 | Bs | 72 | ASP | Peptide,Mainchain |
| 72 | Bt | 52 | GLN | Peptide |
| 72 | Bt | 60 | ASN | Mainchain |
| 72 | Bt | 61 | PHE | Sidechain |
| 72 | Bu | 52 | GLN | Peptide |
| 72 | Bu | 60 | ASN | Mainchain |
| 72 | Bu | 61 | PHE | Sidechain |
| 73 | Bv | 55 | THR | Peptide |
| 73 | Bw | 55 | THR | Peptide |
| 70 | Bx | 1 | UNK | Peptide |
| 70 | Bx | 3 | UNK | Peptide,Mainchain |
| 70 | Bx | 6 | UNK | Peptide,Mainchain |
| 70 | Bx | 8 | UNK | Peptide,Mainchain |
| 71 | Bz | 2 | UNK | Peptide |
| 78 | CA | 1057 | U | Sidechain |
| 78 | CA | 1058 | U | Sidechain |
| 78 | CA | 1064 | G | Sidechain |
| 78 | CA | 1275 | A | Sidechain |
| 78 | CA | 1427 | A | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 78 | CA | 1428 | G | Sidechain |
| 78 | CA | 1499 | G | Sidechain |
| 78 | CA | 1502 | G | Sidechain |
| 78 | CA | 1506 | G | Sidechain |
| 78 | CA | 1634 | C | Sidechain |
| 78 | CA | 1761 | U | Sidechain |
| 78 | CA | 479 | C | Sidechain |
| 78 | CA | 488 | G | Sidechain |
| 78 | CA | 489 | C | Sidechain |
| 78 | CA | 496 | G | Sidechain |
| 78 | CA | 507 | U | Sidechain |
| 78 | CA | 567 | A | Sidechain |
| 78 | CA | 577 | G | Sidechain |
| 78 | CA | 824 | G | Sidechain |
| 78 | CA | 829 | A | Sidechain |
| 78 | CA | 841 | U | Sidechain |
| 78 | CA | 842 | C | Sidechain |
| 81 | DA | 164 | A | Sidechain |
| 81 | DA | 1756 | C | Sidechain |
| 81 | DA | 1766 | G | Sidechain |
| 81 | DA | 1768 | U | Sidechain |
| 81 | DA | 1771 | C | Sidechain |
| 81 | DA | 2531 | C | Sidechain |
| 81 | DA | 2534 | G | Sidechain |
| 81 | DA | 2562 | A | Sidechain |
| 81 | DA | 2564 | G | Sidechain |
| 81 | DA | 2576 | G | Sidechain |
| 81 | DA | 2579 | G | Sidechain |
| 81 | DA | 731 | U | Sidechain |
| 81 | DA | 733 | G | Sidechain |
| 81 | DA | 737 | G | Sidechain |
| 81 | DA | 769 | G | Sidechain |

## 5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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 | Aa | 317/319 (99%) | 274 (86%) | 23 (7%) | 20 (6%) | 1 17 |
| 2 | AA | 250/252 (99%) | 199 (80%) | 21 (8%) | 30 (12%) | 0 6 |
| 3 | AB | 202/240 (84%) | 137 (68%) | 30 (15%) | 35 (17%) | 0 3 |
| 4 | AD | 198/261 (76%) | 160 (81%) | 17 (9%) | 21 (11%) | 0 8 |
| 5 | AC | 192/197 (98%) | 136 (71%) | 28 (15%) | 28 (15%) | 0 4 |
| 6 | AE | 252/254 (99%) | 176 (70%) | 36 (14%) | 40 (16%) | 0 3 |
| 8 | AF | 197/225 (88%) | 170 (86%) | 9 (5%) | 18 (9%) | 1 11 |
| 9 | AH | 128/130 (98%) | 95 (74%) | 17 (13%) | 16 (12%) | 0 5 |
| 10 | AI | 124/143 (87%) | 84 (68%) | 16 (13%) | 24 (19%) | 0 2 |
| 11 | AJ | 108/121 (89%) | 92 (85%) | 8 (7%) | 8 (7%) | 1 14 |
| 12 | AK | 117/137 (85%) | 81 (69%) | 9 (8%) | 27 (23%) | 0 1 |
| 13 | AL | 143/145 (99%) | 100 (70%) | 22 (15%) | 21 (15%) | 0 4 |
| 14 | AM | 138/146 (94%) | 107 (78%) | 21 (15%) | 10 (7%) | 1 14 |
| 15 | AN | 46/56 (82%) | 31 (67%) | 2 (4%) | 13 (28%) | 0 0 |
| 16 | AO | 119/151 (79%) | 95 (80%) | 12 (10%) | 12 (10%) | 0 9 |
| 17 | AQ | 134/136 (98%) | 90 (67%) | 22 (16%) | 22 (16%) | 0 3 |
| 18 | AP | 83/156 (53%) | 65 (78%) | 12 (14%) | 6 (7%) | 1 14 |
| 19 | AR | 86/142 (61%) | 64 (74%) | 10 (12%) | 12 (14%) | 0 4 |
| 20 | AS | 142/144 (99%) | 118 (83%) | 8 (6%) | 16 (11%) | 0 7 |
| 21 | AT | 85/87 (98%) | 66 (78%) | 10 (12%) | 9 (11%) | 0 8 |
| 22 | AV | 83/108 (77%) | 66 (80%) | 7 (8%) | 10 (12%) | 0 6 |
| 24 | AX | 48/82 (58%) | 37 (77%) | 7 (15%) | 4 (8%) | 1 12 |
| 25 | AY | 58/67 (87%) | 46 (79%) | 7 (12%) | 5 (9%) | 1 12 |
| 26 | AZ | 61/63 (97%) | 41 (67%) | 6 (10%) | 14 (23%) | 0 1 |
| 29 | AU | 94/135 (70%) | 62 (66%) | 14 (15%) | 18 (19%) | 0 2 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 30 | BA | 215/217 (99%) | 194 (90%) | 11 (5%) | 10 (5%) | 2 | 21 |
| 31 | BB | 252/254 (99%) | 208 (82%) | 18 (7%) | 26 (10%) | 0 | 8 |
| 32 | BC | 386/388 (100%) | 316 (82%) | 33 (8%) | 37 (10%) | 0 | 10 |
| 33 | BD | 325/362 (90%) | 250 (77%) | 34 (10%) | 41 (13%) | 0 | 5 |
| 34 | BE | 166/174 (95%) | 136 (82%) | 11 (7%) | 19 (11%) | 0 | 7 |
| 35 | BG | 174/176 (99%) | 108 (62%) | 15 (9%) | 51 (29%) | 0 | 0 |
| 36 | BF | 189/191 (99%) | 173 (92%) | 13 (7%) | 3 (2%) | 9 | 44 |
| 37 | BH | 195/256 (76%) | 156 (80%) | 18 (9%) | 21 (11%) | 0 | 8 |
| 38 | Bs | 255/312 (82%) | 224 (88%) | 16 (6%) | 15 (6%) | 1 | 17 |
| 39 | BJ | 125/165 (76%) | 107 (86%) | 11 (9%) | 7 (6%) | 2 | 19 |
| 40 | BK | 197/199 (99%) | 161 (82%) | 15 (8%) | 21 (11%) | 0 | 8 |
| 41 | BN | 136/138 (99%) | 104 (76%) | 14 (10%) | 18 (13%) | 0 | 5 |
| 42 | BM | 129/137 (94%) | 124 (96%) | 5 (4%) | 0 | 100 | 100 |
| 43 | BP | 191/204 (94%) | 168 (88%) | 14 (7%) | 9 (5%) | 2 | 21 |
| 44 | BO | 147/149 (99%) | 100 (68%) | 24 (16%) | 23 (16%) | 0 | 3 |
| 45 | BR | 159/186 (86%) | 116 (73%) | 22 (14%) | 21 (13%) | 0 | 5 |
| 46 | BT | 187/189 (99%) | 163 (87%) | 14 (8%) | 10 (5%) | 2 | 19 |
| 47 | BU | 158/160 (99%) | 144 (91%) | 7 (4%) | 7 (4%) | 2 | 22 |
| 48 | BW | 103/121 (85%) | 79 (77%) | 15 (15%) | 9 (9%) | 1 | 11 |
| 49 | BV | 168/170 (99%) | 135 (80%) | 20 (12%) | 13 (8%) | 1 | 13 |
| 50 | BX | 120/142 (84%) | 95 (79%) | 11 (9%) | 14 (12%) | 0 | 6 |
| 51 | BZ | 71/155 (46%) | 48 (68%) | 13 (18%) | 10 (14%) | 0 | 4 |
| 52 | BY | 121/123 (98%) | 115 (95%) | 2 (2%) | 4 (3%) | 4 | 26 |
| 53 | Ba | 93/136 (68%) | 62 (67%) | 15 (16%) | 16 (17%) | 0 | 3 |
| 54 | Bd | 20/59 (34%) | 19 (95%) | 1 (5%) | 0 | 100 | 100 |
| 55 | Bc | 116/120 (97%) | 92 (79%) | 11 (10%) | 13 (11%) | 0 | 7 |
| 56 | Bf | 103/105 (98%) | 91 (88%) | 7 (7%) | 5 (5%) | 2 | 20 |
| 57 | Be | 237/244 (97%) | 213 (90%) | 14 (6%) | 10 (4%) | 3 | 22 |
| 58 | Bg | 108/113 (96%) | 95 (88%) | 4 (4%) | 9 (8%) | 1 | 12 |
| 59 | Bh | 128/130 (98%) | 115 (90%) | 7 (6%) | 6 (5%) | 2 | 21 |
| 60 | Bi | 116/118 (98%) | 76 (66%) | 13 (11%) | 27 (23%) | 0 | 1 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 61 | Bj | 98/107 (92%) | 66 (67%) | 15 (15%) | 17 (17%) | 0 3 |
| 62 | Bk | 75/100 (75%) | 61 (81%) | 6 (8%) | 8 (11%) | 0 8 |
| 63 | Bm | 90/92 (98%) | 78 (87%) | 10 (11%) | 2 (2%) | 6 35 |
| 64 | Bl | 86/88 (98%) | 65 (76%) | 14 (16%) | 7 (8%) | 1 12 |
| 65 | Bn | 76/78 (97%) | 56 (74%) | 10 (13%) | 10 (13%) | 0 5 |
| 66 | Bo | 49/51 (96%) | 38 (78%) | 3 (6%) | 8 (16%) | 0 3 |
| 67 | Bp | 38/52 (73%) | 28 (74%) | 7 (18%) | 3 (8%) | 1 13 |
| 68 | Bq | 23/25 (92%) | 21 (91%) | 1 (4%) | 1 (4%) | 2 22 |
| 69 | Br | 104/106 (98%) | 71 (68%) | 14 (14%) | 19 (18%) | 0 3 |
| 72 | Bt | 56/106 (53%) | 53 (95%) | 0 | 3 (5%) | 2 19 |
| 72 | Bu | 56/106 (53%) | 53 (95%) | 0 | 3 (5%) | 2 19 |
| 73 | Bv | 56/106 (53%) | 53 (95%) | 1 (2%) | 2 (4%) | 3 25 |
| 73 | Bw | 56/106 (53%) | 53 (95%) | 1 (2%) | 2 (4%) | 3 25 |
| 74 | BQ | 295/297 (99%) | 232 (79%) | 27 (9%) | 36 (12%) | 0 6 |
| 76 | BS | 165/167 (99%) | 116 (70%) | 15 (9%) | 34 (21%) | 0 2 |
| 77 | BI | 179/221 (81%) | 135 (75%) | 23 (13%) | 21 (12%) | 0 6 |
| All | All | 9997/11298 (88%) | 7958 (80%) | 949 (10%) | 1090 (11%) | 1 8 |

All (1090) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | Aa | 29 | GLN |
| 1 | Aa | 51 | ASP |
| 1 | Aa | 55 | GLY |
| 1 | Aa | 57 | PRO |
| 1 | Aa | 84 | SER |
| 1 | Aa | 129 | LYS |
| 1 | Aa | 160 | GLU |
| 1 | Aa | 246 | SER |
| 1 | Aa | 281 | TYR |
| 1 | Aa | 285 | ALA |
| 2 | AA | 4 | PRO |
| 2 | AA | 6 | THR |
| 2 | AA | 10 | THR |
| 2 | AA | 11 | PRO |
| 2 | AA | 43 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | AA | 97 | PRO |
| 2 | AA | 195 | TRP |
| 2 | AA | 201 | LEU |
| 2 | AA | 232 | VAL |
| 2 | AA | 250 | VAL |
| 3 | AB | 30 | ALA |
| 3 | AB | 32 | GLU |
| 3 | AB | 36 | GLY |
| 3 | AB | 62 | ASN |
| 3 | AB | 78 | LYS |
| 3 | AB | 113 | LEU |
| 3 | AB | 141 | LYS |
| 3 | AB | 152 | PHE |
| 3 | AB | 156 | PHE |
| 3 | AB | 184 | ILE |
| 3 | AB | 189 | MET |
| 3 | AB | 190 | ARG |
| 3 | AB | 199 | PRO |
| 3 | AB | 209 | ILE |
| 3 | AB | 211 | PRO |
| 3 | AB | 213 | GLU |
| 3 | AB | 214 | GLU |
| 4 | AD | 53 | LYS |
| 4 | AD | 96 | ASN |
| 4 | AD | 133 | LYS |
| 4 | AD | 137 | PRO |
| 4 | AD | 149 | TYR |
| 4 | AD | 151 | ASP |
| 4 | AD | 154 | ILE |
| 4 | AD | 215 | ASP |
| 4 | AD | 233 | LYS |
| 4 | AD | 234 | PRO |
| 4 | AD | 236 | ILE |
| 4 | AD | 239 | PRO |
| 5 | AC | 15 | PRO |
| 5 | AC | 17 | ARG |
| 5 | AC | 18 | PRO |
| 5 | AC | 39 | LYS |
| 5 | AC | 56 | ALA |
| 5 | AC | 145 | SER |
| 5 | AC | 148 | VAL |
| 5 | AC | 152 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | AC | 159 | ALA |
| 5 | AC | 168 | ARG |
| 5 | AC | 170 | GLY |
| 5 | AC | 184 | SER |
| 5 | AC | 186 | GLU |
| 5 | AC | 187 | ALA |
| 5 | AC | 188 | ALA |
| 5 | AC | 189 | ASP |
| 5 | AC | 192 | ASP |
| 6 | AE | 4 | PRO |
| 6 | AE | 7 | GLN |
| 6 | AE | 13 | GLY |
| 6 | AE | 14 | PHE |
| 6 | AE | 43 | ARG |
| 6 | AE | 50 | ILE |
| 6 | AE | 51 | THR |
| 6 | AE | 67 | GLN |
| 6 | AE | 68 | ILE |
| 6 | AE | 70 | ASP |
| 6 | AE | 72 | LEU |
| 6 | AE | 84 | LYS |
| 6 | AE | 99 | LYS |
| 6 | AE | 108 | ASN |
| 6 | AE | 120 | GLU |
| 6 | AE | 125 | ILE |
| 6 | AE | 224 | PHE |
| 6 | AE | 242 | ILE |
| 6 | AE | 243 | TYR |
| 6 | AE | 244 | SER |
| 6 | AE | 251 | LYS |
| 8 | AF | 29 | ILE |
| 8 | AF | 30 | PRO |
| 8 | AF | 36 | ALA |
| 8 | AF | 37 | GLN |
| 8 | AF | 66 | GLN |
| 8 | AF | 68 | ILE |
| 8 | AF | 71 | ALA |
| 8 | AF | 161 | ASP |
| 8 | AF | 163 | SER |
| 9 | AH | 43 | LYS |
| 9 | AH | 53 | ILE |
| 9 | AH | 65 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 9 | AH | 66 | ASN |
| 9 | AH | 81 | VAL |
| 9 | AH | 84 | GLY |
| 9 | AH | 108 | ALA |
| 10 | AI | 30 | LYS |
| 10 | AI | 39 | VAL |
| 10 | AI | 55 | VAL |
| 10 | AI | 70 | THR |
| 10 | AI | 84 | ALA |
| 10 | AI | 85 | ILE |
| 10 | AI | 86 | ALA |
| 10 | AI | 87 | LYS |
| 10 | AI | 108 | ALA |
| 10 | AI | 118 | ILE |
| 10 | AI | 121 | SER |
| 10 | AI | 122 | ARG |
| 10 | AI | 123 | ARG |
| 10 | AI | 136 | SER |
| 10 | AI | 138 | PHE |
| 11 | AJ | 51 | VAL |
| 11 | AJ | 96 | PRO |
| 12 | AK | 22 | SER |
| 12 | AK | 39 | ILE |
| 12 | AK | 40 | ALA |
| 12 | AK | 53 | ASP |
| 12 | AK | 59 | ALA |
| 12 | AK | 60 | ALA |
| 12 | AK | 62 | LEU |
| 12 | AK | 80 | HIS |
| 12 | AK | 81 | VAL |
| 12 | AK | 84 | ARG |
| 12 | AK | 121 | VAL |
| 12 | AK | 122 | PRO |
| 12 | AK | 127 | ARG |
| 12 | AK | 128 | LYS |
| 12 | AK | 129 | LYS |
| 13 | AL | 9 | LEU |
| 13 | AL | 37 | ALA |
| 13 | AL | 81 | LYS |
| 13 | AL | 87 | VAL |
| 13 | AL | 99 | ASN |
| 13 | AL | 116 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 13 | AL | 121 | ARG |
| 13 | AL | 123 | LYS |
| 13 | AL | 132 | LEU |
| 13 | AL | 134 | ALA |
| 14 | AM | 8 | GLN |
| 14 | AM | 93 | THR |
| 14 | AM | 102 | ALA |
| 14 | AM | 141 | THR |
| 15 | AN | 10 | HIS |
| 15 | AN | 11 | PRO |
| 15 | AN | 14 | TYR |
| 15 | AN | 34 | TYR |
| 15 | AN | 47 | ALA |
| 15 | AN | 52 | PHE |
| 16 | AO | 43 | LYS |
| 16 | AO | 58 | HIS |
| 16 | AO | 81 | ALA |
| 17 | AQ | 4 | VAL |
| 17 | AQ | 27 | ASP |
| 17 | AQ | 71 | PHE |
| 17 | AQ | 74 | GLN |
| 17 | AQ | 78 | ARG |
| 17 | AQ | 88 | VAL |
| 17 | AQ | 117 | LEU |
| 17 | AQ | 133 | ARG |
| 17 | AQ | 135 | ARG |
| 18 | AP | 55 | ASP |
| 18 | AP | 119 | VAL |
| 19 | AR | 62 | ALA |
| 19 | AR | 79 | HIS |
| 19 | AR | 107 | ILE |
| 19 | AR | 134 | THR |
| 20 | AS | 27 | LYS |
| 20 | AS | 37 | VAL |
| 20 | AS | 69 | LYS |
| 20 | AS | 79 | LEU |
| 20 | AS | 83 | ALA |
| 20 | AS | 88 | VAL |
| 20 | AS | 90 | PRO |
| 20 | AS | 91 | TYR |
| 20 | AS | 96 | ALA |
| 21 | AT | 29 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 21 | AT | 34 | ILE |
| 21 | AT | 45 | ALA |
| 21 | AT | 55 | LEU |
| 21 | AT | 68 | SER |
| 22 | AV | 26 | LYS |
| 22 | AV | 30 | LYS |
| 22 | AV | 31 | SER |
| 22 | AV | 105 | THR |
| 22 | AV | 106 | ALA |
| 24 | AX | 66 | PRO |
| 24 | AX | 67 | THR |
| 24 | AX | 77 | THR |
| 25 | AY | 18 | ARG |
| 25 | AY | 26 | THR |
| 26 | AZ | 18 | THR |
| 26 | AZ | 27 | PRO |
| 26 | AZ | 46 | ASN |
| 26 | AZ | 57 | ASN |
| 26 | AZ | 58 | PRO |
| 26 | AZ | 60 | PRO |
| 26 | AZ | 61 | SER |
| 29 | AU | 5 | VAL |
| 29 | AU | 6 | THR |
| 29 | AU | 19 | ALA |
| 29 | AU | 32 | ARG |
| 29 | AU | 49 | LYS |
| 29 | AU | 52 | LYS |
| 29 | AU | 63 | GLN |
| 29 | AU | 94 | TYR |
| 30 | BA | 21 | ASN |
| 30 | BA | 74 | VAL |
| 30 | BA | 135 | PRO |
| 30 | BA | 151 | VAL |
| 31 | BB | 27 | ALA |
| 31 | BB | 63 | PHE |
| 31 | BB | 67 | TYR |
| 31 | BB | 68 | LYS |
| 31 | BB | 71 | LEU |
| 31 | BB | 73 | GLU |
| 31 | BB | 128 | ARG |
| 31 | BB | 227 | ARG |
| 31 | BB | 241 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 31 | BB | 244 | GLY |
| 31 | BB | 246 | LEU |
| 31 | BB | 247 | ARG |
| 31 | BB | 249 | SER |
| 31 | BB | 253 | GLN |
| 32 | BC | 5 | LYS |
| 32 | BC | 60 | LEU |
| 32 | BC | 61 | ASP |
| 32 | BC | 127 | LYS |
| 32 | BC | 137 | TYR |
| 32 | BC | 158 | VAL |
| 32 | BC | 259 | HIS |
| 32 | BC | 292 | ALA |
| 32 | BC | 296 | THR |
| 32 | BC | 345 | ASN |
| 32 | BC | 349 | LYS |
| 32 | BC | 352 | GLU |
| 32 | BC | 355 | SER |
| 32 | BC | 371 | GLN |
| 33 | BD | 11 | LEU |
| 33 | BD | 15 | ALA |
| 33 | BD | 49 | ALA |
| 33 | BD | 84 | ARG |
| 33 | BD | 89 | ALA |
| 33 | BD | 100 | PHE |
| 33 | BD | 102 | PRO |
| 33 | BD | 103 | THR |
| 33 | BD | 104 | LYS |
| 33 | BD | 106 | TRP |
| 33 | BD | 109 | TRP |
| 33 | BD | 142 | VAL |
| 33 | BD | 144 | LYS |
| 33 | BD | 146 | PRO |
| 33 | BD | 173 | GLY |
| 33 | BD | 196 | ASN |
| 33 | BD | 298 | ALA |
| 33 | BD | 300 | ARG |
| 33 | BD | 315 | LYS |
| 33 | BD | 317 | PRO |
| 33 | BD | 319 | LYS |
| 33 | BD | 321 | LYS |
| 33 | BD | 323 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 33 | BD | 329 | PRO |
| 33 | BD | 330 | TYR |
| 33 | BD | 350 | LYS |
| 33 | BD | 351 | PRO |
| 33 | BD | 354 | VAL |
| 33 | BD | 355 | PHE |
| 33 | BD | 356 | THR |
| 34 | BE | 5 | ALA |
| 34 | BE | 9 | MET |
| 34 | BE | 25 | GLU |
| 34 | BE | 52 | TYR |
| 34 | BE | 53 | THR |
| 34 | BE | 54 | VAL |
| 34 | BE | 59 | ILE |
| 34 | BE | 61 | ARG |
| 34 | BE | 89 | TYR |
| 34 | BE | 111 | ASP |
| 34 | BE | 122 | ILE |
| 35 | BG | 2 | SER |
| 35 | BG | 4 | GLN |
| 35 | BG | 10 | TYR |
| 35 | BG | 11 | PRO |
| 35 | BG | 15 | VAL |
| 35 | BG | 18 | LEU |
| 35 | BG | 27 | PRO |
| 35 | BG | 35 | VAL |
| 35 | BG | 61 | ASN |
| 35 | BG | 69 | PHE |
| 35 | BG | 75 | PRO |
| 35 | BG | 76 | LEU |
| 35 | BG | 81 | ALA |
| 35 | BG | 88 | SER |
| 35 | BG | 98 | VAL |
| 35 | BG | 99 | GLU |
| 35 | BG | 103 | VAL |
| 35 | BG | 139 | LYS |
| 35 | BG | 140 | VAL |
| 35 | BG | 141 | VAL |
| 35 | BG | 143 | LYS |
| 35 | BG | 145 | LEU |
| 35 | BG | 151 | LYS |
| 35 | BG | 152 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 35 | BG | 153 | PRO |
| 35 | BG | 155 | LEU |
| 35 | BG | 171 | PRO |
| 36 | BF | 141 | LYS |
| 37 | BH | 62 | LYS |
| 37 | BH | 63 | LYS |
| 37 | BH | 65 | LEU |
| 37 | BH | 73 | PRO |
| 37 | BH | 88 | ALA |
| 37 | BH | 89 | GLU |
| 37 | BH | 96 | LYS |
| 37 | BH | 123 | GLN |
| 37 | BH | 124 | ASP |
| 37 | BH | 126 | SER |
| 37 | BH | 129 | PRO |
| 37 | BH | 232 | HIS |
| 37 | BH | 233 | TRP |
| 37 | BH | 237 | ILE |
| 38 | Bs | 60 | ARG |
| 38 | Bs | 70 | LEU |
| 38 | Bs | 71 | PRO |
| 38 | Bs | 73 | PHE |
| 38 | Bs | 83 | ASN |
| 38 | Bs | 124 | VAL |
| 38 | Bs | 179 | SER |
| 38 | Bs | 180 | PRO |
| 38 | Bs | 231 | THR |
| 39 | BJ | 37 | LEU |
| 39 | BJ | 51 | LYS |
| 39 | BJ | 75 | PRO |
| 39 | BJ | 76 | SER |
| 40 | BK | 5 | PRO |
| 40 | BK | 66 | LYS |
| 40 | BK | 70 | PRO |
| 40 | BK | 121 | PRO |
| 40 | BK | 127 | LEU |
| 40 | BK | 129 | LEU |
| 40 | BK | 130 | LYS |
| 40 | BK | 131 | PRO |
| 40 | BK | 185 | ALA |
| 40 | BK | 188 | SER |
| 40 | BK | 189 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | BK | 198 | GLY |
| 41 | BN | 6 | ILE |
| 41 | BN | 14 | LEU |
| 41 | BN | 27 | GLN |
| 41 | BN | 29 | ALA |
| 41 | BN | 51 | ALA |
| 41 | BN | 63 | VAL |
| 41 | BN | 72 | LEU |
| 41 | BN | 73 | PRO |
| 41 | BN | 90 | VAL |
| 41 | BN | 98 | SER |
| 41 | BN | 101 | LYS |
| 41 | BN | 112 | LEU |
| 41 | BN | 137 | LYS |
| 43 | BP | 14 | LYS |
| 43 | BP | 44 | ARG |
| 43 | BP | 51 | LEU |
| 43 | BP | 52 | GLY |
| 43 | BP | 120 | TRP |
| 43 | BP | 123 | GLN |
| 44 | BO | 2 | PRO |
| 44 | BO | 15 | VAL |
| 44 | BO | 22 | ILE |
| 44 | BO | 58 | MET |
| 44 | BO | 92 | LYS |
| 44 | BO | 95 | SER |
| 44 | BO | 97 | GLU |
| 44 | BO | 99 | ALA |
| 44 | BO | 101 | VAL |
| 45 | BR | 4 | ASP |
| 45 | BR | 15 | HIS |
| 45 | BR | 16 | ARG |
| 45 | BR | 20 | LYS |
| 45 | BR | 78 | ASN |
| 45 | BR | 95 | GLU |
| 45 | BR | 122 | ILE |
| 45 | BR | 141 | ARG |
| 45 | BR | 144 | ARG |
| 45 | BR | 149 | ALA |
| 45 | BR | 155 | MET |
| 46 | BT | 55 | VAL |
| 46 | BT | 59 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 46 | BT | 74 | ARG |
| 46 | BT | 82 | LYS |
| 46 | BT | 91 | SER |
| 46 | BT | 115 | ILE |
| 47 | BU | 4 | SER |
| 47 | BU | 69 | LYS |
| 47 | BU | 137 | GLU |
| 47 | BU | 140 | ILE |
| 47 | BU | 142 | SER |
| 48 | BW | 23 | THR |
| 48 | BW | 46 | ALA |
| 49 | BV | 70 | THR |
| 49 | BV | 111 | LYS |
| 49 | BV | 122 | ALA |
| 49 | BV | 163 | LYS |
| 49 | BV | 164 | LYS |
| 49 | BV | 166 | VAL |
| 50 | BX | 24 | LEU |
| 50 | BX | 42 | ARG |
| 50 | BX | 50 | ALA |
| 51 | BZ | 49 | ILE |
| 51 | BZ | 55 | PHE |
| 51 | BZ | 59 | HIS |
| 51 | BZ | 60 | LYS |
| 51 | BZ | 63 | ILE |
| 51 | BZ | 67 | VAL |
| 51 | BZ | 70 | LYS |
| 51 | BZ | 72 | SER |
| 52 | BY | 9 | SER |
| 52 | BY | 11 | ASP |
| 52 | BY | 22 | ALA |
| 53 | Ba | 10 | VAL |
| 53 | Ba | 11 | ALA |
| 53 | Ba | 13 | VAL |
| 53 | Ba | 17 | ARG |
| 53 | Ba | 20 | GLY |
| 53 | Ba | 27 | LYS |
| 53 | Ba | 28 | PRO |
| 53 | Ba | 31 | GLU |
| 53 | Ba | 35 | SER |
| 53 | Ba | 37 | PRO |
| 53 | Ba | 54 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 55 | Bc | 38 | ARG |
| 55 | Bc | 39 | PRO |
| 55 | Bc | 40 | SER |
| 55 | Bc | 102 | GLU |
| 55 | Bc | 103 | LYS |
| 55 | Bc | 104 | GLN |
| 55 | Bc | 107 | LYS |
| 55 | Bc | 109 | ILE |
| 55 | Bc | 112 | PRO |
| 56 | Bf | 4 | VAL |
| 56 | Bf | 98 | SER |
| 57 | Be | 82 | LYS |
| 57 | Be | 98 | LYS |
| 57 | Be | 134 | VAL |
| 57 | Be | 172 | ASN |
| 58 | Bg | 2 | ALA |
| 58 | Bg | 64 | VAL |
| 58 | Bg | 65 | LYS |
| 58 | Bg | 79 | ARG |
| 58 | Bg | 91 | SER |
| 58 | Bg | 107 | VAL |
| 60 | Bi | 11 | ASN |
| 60 | Bi | 12 | PRO |
| 60 | Bi | 18 | ASN |
| 60 | Bi | 19 | LYS |
| 60 | Bi | 37 | LYS |
| 60 | Bi | 42 | PRO |
| 60 | Bi | 43 | LYS |
| 60 | Bi | 44 | CYS |
| 60 | Bi | 57 | LEU |
| 60 | Bi | 65 | VAL |
| 60 | Bi | 67 | LYS |
| 60 | Bi | 68 | THR |
| 60 | Bi | 79 | SER |
| 60 | Bi | 80 | ARG |
| 60 | Bi | 102 | LYS |
| 60 | Bi | 107 | GLU |
| 61 | Bj | 2 | ALA |
| 61 | Bj | 3 | GLU |
| 61 | Bj | 4 | SER |
| 61 | Bj | 6 | ARG |
| 61 | Bj | 9 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 61 | Bj | 21 | ARG |
| 61 | Bj | 25 | PRO |
| 61 | Bj | 35 | VAL |
| 61 | Bj | 38 | PRO |
| 61 | Bj | 57 | LYS |
| 61 | Bj | 87 | ASN |
| 61 | Bj | 96 | ALA |
| 62 | Bk | 26 | ILE |
| 62 | Bk | 51 | SER |
| 62 | Bk | 52 | PRO |
| 62 | Bk | 54 | GLU |
| 63 | Bm | 6 | LYS |
| 63 | Bm | 17 | ARG |
| 64 | Bl | 11 | ARG |
| 64 | Bl | 12 | HIS |
| 64 | Bl | 63 | ARG |
| 64 | Bl | 84 | SER |
| 64 | Bl | 85 | LYS |
| 64 | Bl | 86 | ALA |
| 65 | Bn | 29 | LYS |
| 65 | Bn | 34 | ALA |
| 65 | Bn | 36 | LYS |
| 65 | Bn | 50 | SER |
| 65 | Bn | 53 | THR |
| 65 | Bn | 72 | THR |
| 66 | Bo | 2 | ALA |
| 66 | Bo | 34 | THR |
| 66 | Bo | 35 | ILE |
| 66 | Bo | 38 | ASN |
| 67 | Bp | 51 | LEU |
| 69 | Br | 33 | ALA |
| 69 | Br | 34 | SER |
| 69 | Br | 48 | SER |
| 69 | Br | 56 | PRO |
| 69 | Br | 58 | PHE |
| 69 | Br | 59 | HIS |
| 69 | Br | 62 | ALA |
| 69 | Br | 64 | THR |
| 69 | Br | 96 | GLU |
| 69 | Br | 97 | LYS |
| 69 | Br | 102 | GLN |
| 72 | Bt | 61 | PHE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 72 | Bu | 61 | PHE |
| 73 | Bv | 17 | PRO |
| 73 | Bw | 17 | PRO |
| 74 | BQ | 10 | SER |
| 74 | BQ | 54 | ARG |
| 74 | BQ | 88 | ILE |
| 74 | BQ | 116 | ASP |
| 74 | BQ | 118 | THR |
| 74 | BQ | 144 | VAL |
| 74 | BQ | 159 | VAL |
| 74 | BQ | 198 | TYR |
| 74 | BQ | 199 | ILE |
| 74 | BQ | 218 | ARG |
| 74 | BQ | 236 | LEU |
| 74 | BQ | 238 | ASP |
| 74 | BQ | 239 | ILE |
| 74 | BQ | 242 | SER |
| 74 | BQ | 243 | ALA |
| 74 | BQ | 245 | GLU |
| 74 | BQ | 258 | LYS |
| 74 | BQ | 285 | ARG |
| 74 | BQ | 286 | VAL |
| 74 | BQ | 289 | LYS |
| 74 | BQ | 293 | LEU |
| 76 | BS | 4 | PHE |
| 76 | BS | 6 | PHE |
| 76 | BS | 17 | PRO |
| 76 | BS | 19 | PRO |
| 76 | BS | 23 | HIS |
| 76 | BS | 35 | ASN |
| 76 | BS | 54 | LYS |
| 76 | BS | 68 | GLU |
| 76 | BS | 71 | PRO |
| 76 | BS | 72 | THR |
| 76 | BS | 73 | THR |
| 76 | BS | 87 | THR |
| 76 | BS | 120 | PHE |
| 76 | BS | 121 | PRO |
| 76 | BS | 123 | ILE |
| 76 | BS | 124 | GLN |
| 76 | BS | 138 | ARG |
| 76 | BS | 151 | PHE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 76 | BS | 152 | PRO |
| 76 | BS | 156 | ARG |
| 76 | BS | 157 | LYS |
| 76 | BS | 158 | VAL |
| 76 | BS | 159 | ARG |
| 77 | BI | 4 | ARG |
| 77 | BI | 5 | PRO |
| 77 | BI | 18 | PRO |
| 77 | BI | 108 | ALA |
| 77 | BI | 109 | ASP |
| 77 | BI | 112 | GLN |
| 77 | BI | 113 | GLN |
| 77 | BI | 115 | MET |
| 1 | Aa | 58 | VAL |
| 1 | Aa | 240 | VAL |
| 1 | Aa | 283 | LYS |
| 2 | AA | 13 | ASP |
| 2 | AA | 15 | GLN |
| 2 | AA | 16 | LEU |
| 2 | AA | 21 | ASN |
| 2 | AA | 210 | VAL |
| 2 | AA | 230 | GLU |
| 3 | AB | 48 | VAL |
| 3 | AB | 63 | GLY |
| 3 | AB | 173 | ARG |
| 3 | AB | 183 | GLY |
| 3 | AB | 208 | ILE |
| 4 | AD | 94 | ALA |
| 4 | AD | 189 | LEU |
| 4 | AD | 213 | SER |
| 5 | AC | 14 | THR |
| 5 | AC | 19 | TYR |
| 5 | AC | 84 | GLY |
| 5 | AC | 116 | LEU |
| 5 | AC | 154 | LYS |
| 5 | AC | 165 | GLY |
| 6 | AE | 28 | ARG |
| 6 | AE | 42 | GLY |
| 6 | AE | 83 | ILE |
| 6 | AE | 100 | ALA |
| 6 | AE | 110 | HIS |
| 6 | AE | 178 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 8 | AF | 67 | PRO |
| 8 | AF | 72 | HIS |
| 8 | AF | 79 | ASN |
| 9 | AH | 67 | GLY |
| 9 | AH | 99 | PHE |
| 9 | AH | 121 | VAL |
| 10 | AI | 75 | VAL |
| 11 | AJ | 59 | PRO |
| 11 | AJ | 73 | GLY |
| 11 | AJ | 79 | TRP |
| 12 | AK | 63 | ALA |
| 12 | AK | 75 | GLY |
| 12 | AK | 76 | ILE |
| 12 | AK | 120 | PRO |
| 12 | AK | 124 | ASP |
| 12 | AK | 126 | THR |
| 12 | AK | 131 | GLY |
| 13 | AL | 28 | ASN |
| 13 | AL | 30 | LYS |
| 13 | AL | 34 | LEU |
| 13 | AL | 88 | PRO |
| 13 | AL | 102 | VAL |
| 13 | AL | 120 | VAL |
| 13 | AL | 130 | VAL |
| 14 | AM | 85 | PHE |
| 15 | AN | 13 | ARG |
| 15 | AN | 33 | LYS |
| 15 | AN | 38 | ILE |
| 15 | AN | 48 | ASN |
| 15 | AN | 55 | PHE |
| 16 | AO | 80 | LEU |
| 16 | AO | 112 | LYS |
| 16 | AO | 147 | SER |
| 17 | AQ | 6 | THR |
| 17 | AQ | 62 | GLN |
| 17 | AQ | 67 | ARG |
| 17 | AQ | 72 | LYS |
| 17 | AQ | 73 | LEU |
| 17 | AQ | 82 | ASP |
| 17 | AQ | 94 | SER |
| 17 | AQ | 121 | VAL |
| 17 | AQ | 127 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 18 | AP | 75 | VAL |
| 18 | AP | 108 | PRO |
| 19 | AR | 65 | LEU |
| 19 | AR | 66 | ALA |
| 20 | AS | 71 | VAL |
| 22 | AV | 42 | LEU |
| 22 | AV | 99 | ALA |
| 26 | AZ | 16 | SER |
| 26 | AZ | 62 | VAL |
| 29 | AU | 18 | LEU |
| 29 | AU | 31 | ASN |
| 29 | AU | 54 | ALA |
| 30 | BA | 99 | LEU |
| 30 | BA | 168 | ALA |
| 30 | BA | 198 | TRP |
| 30 | BA | 199 | GLN |
| 31 | BB | 11 | GLY |
| 31 | BB | 30 | ARG |
| 31 | BB | 35 | ALA |
| 31 | BB | 74 | GLU |
| 31 | BB | 140 | ASN |
| 32 | BC | 70 | ARG |
| 32 | BC | 97 | ARG |
| 32 | BC | 124 | LYS |
| 32 | BC | 138 | ALA |
| 32 | BC | 139 | GLN |
| 32 | BC | 344 | THR |
| 32 | BC | 346 | THR |
| 32 | BC | 367 | LYS |
| 32 | BC | 381 | GLY |
| 33 | BD | 12 | THR |
| 33 | BD | 53 | SER |
| 33 | BD | 78 | GLY |
| 33 | BD | 172 | VAL |
| 33 | BD | 326 | ARG |
| 33 | BD | 339 | LEU |
| 33 | BD | 352 | ALA |
| 34 | BE | 56 | THR |
| 35 | BG | 7 | PRO |
| 35 | BG | 13 | GLU |
| 35 | BG | 14 | ASP |
| 35 | BG | 19 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 35 | BG | 36 | PRO |
| 35 | BG | 71 | VAL |
| 35 | BG | 82 | ARG |
| 35 | BG | 97 | ASN |
| 35 | BG | 142 | ASP |
| 35 | BG | 146 | ILE |
| 35 | BG | 154 | LEU |
| 37 | BH | 66 | SER |
| 37 | BH | 238 | LEU |
| 38 | Bs | 49 | ALA |
| 38 | Bs | 206 | ASP |
| 38 | Bs | 253 | ALA |
| 39 | BJ | 32 | ILE |
| 39 | BJ | 77 | ALA |
| 40 | BK | 3 | VAL |
| 40 | BK | 68 | ARG |
| 40 | BK | 184 | THR |
| 43 | BP | 166 | ALA |
| 44 | BO | 7 | LYS |
| 44 | BO | 8 | THR |
| 44 | BO | 61 | PHE |
| 44 | BO | 63 | LYS |
| 44 | BO | 68 | PHE |
| 44 | BO | 105 | LEU |
| 44 | BO | 106 | ALA |
| 45 | BR | 3 | ILE |
| 45 | BR | 11 | LYS |
| 45 | BR | 75 | GLY |
| 45 | BR | 123 | THR |
| 45 | BR | 124 | LEU |
| 45 | BR | 146 | SER |
| 47 | BU | 80 | VAL |
| 48 | BW | 86 | LYS |
| 48 | BW | 96 | VAL |
| 49 | BV | 38 | GLY |
| 49 | BV | 169 | THR |
| 50 | BX | 36 | LYS |
| 50 | BX | 37 | THR |
| 50 | BX | 45 | LYS |
| 50 | BX | 52 | PRO |
| 50 | BX | 57 | LEU |
| 50 | BX | 58 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 51 | BZ | 66 | GLU |
| 53 | Ba | 15 | ARG |
| 53 | Ba | 16 | GLY |
| 53 | Ba | 19 | ALA |
| 55 | Bc | 94 | LYS |
| 56 | Bf | 6 | SER |
| 56 | Bf | 65 | THR |
| 57 | Be | 75 | TYR |
| 57 | Be | 77 | VAL |
| 57 | Be | 107 | ARG |
| 58 | Bg | 92 | TYR |
| 59 | Bh | 19 | ARG |
| 60 | Bi | 34 | HIS |
| 60 | Bi | 35 | VAL |
| 60 | Bi | 55 | SER |
| 60 | Bi | 69 | HIS |
| 60 | Bi | 106 | LYS |
| 61 | Bj | 99 | ARG |
| 62 | Bk | 30 | LYS |
| 62 | Bk | 68 | ARG |
| 65 | Bn | 57 | ASN |
| 66 | Bo | 39 | ALA |
| 66 | Bo | 47 | THR |
| 67 | Bp | 15 | CYS |
| 69 | Br | 29 | LYS |
| 69 | Br | 63 | LYS |
| 69 | Br | 89 | LYS |
| 72 | Bt | 18 | GLU |
| 72 | Bt | 34 | ASN |
| 72 | Bu | 18 | GLU |
| 72 | Bu | 34 | ASN |
| 73 | Bv | 18 | ASP |
| 73 | Bw | 18 | ASP |
| 74 | BQ | 112 | ARG |
| 74 | BQ | 122 | VAL |
| 74 | BQ | 129 | TYR |
| 74 | BQ | 130 | GLU |
| 74 | BQ | 200 | PHE |
| 74 | BQ | 234 | ASP |
| 76 | BS | 3 | ALA |
| 76 | BS | 22 | GLU |
| 76 | BS | 52 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 76 | BS | 86 | ARG |
| 76 | BS | 125 | ILE |
| 76 | BS | 165 | LEU |
| 76 | BS | 166 | LYS |
| 77 | BI | 28 | ASP |
| 77 | BI | 103 | LEU |
| 77 | BI | 106 | ALA |
| 77 | BI | 107 | GLY |
| 77 | BI | 117 | GLY |
| 1 | Aa | 31 | ASN |
| 1 | Aa | 95 | ALA |
| 1 | Aa | 236 | ALA |
| 1 | Aa | 317 | THR |
| 2 | AA | 9 | LEU |
| 2 | AA | 67 | ILE |
| 2 | AA | 185 | ARG |
| 2 | AA | 196 | SER |
| 2 | AA | 212 | GLN |
| 2 | AA | 231 | GLU |
| 3 | AB | 64 | ARG |
| 3 | AB | 98 | ALA |
| 3 | AB | 157 | LEU |
| 4 | AD | 95 | THR |
| 5 | AC | 37 | LYS |
| 5 | AC | 151 | ASP |
| 5 | AC | 195 | ASP |
| 6 | AE | 10 | LYS |
| 6 | AE | 238 | SER |
| 6 | AE | 241 | ASP |
| 9 | AH | 18 | GLU |
| 9 | AH | 80 | ASN |
| 9 | AH | 97 | ARG |
| 10 | AI | 26 | LYS |
| 10 | AI | 35 | PRO |
| 10 | AI | 58 | ASP |
| 10 | AI | 124 | PRO |
| 10 | AI | 126 | PRO |
| 10 | AI | 140 | LYS |
| 11 | AJ | 18 | GLN |
| 11 | AJ | 23 | ARG |
| 11 | AJ | 71 | PRO |
| 12 | AK | 96 | PRO |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 13 | AL | 70 | LYS |
| 15 | AN | 16 | LYS |
| 16 | AO | 67 | THR |
| 16 | AO | 79 | GLY |
| 16 | AO | 86 | GLU |
| 17 | AQ | 26 | LEU |
| 17 | AQ | 68 | GLY |
| 17 | AQ | 102 | VAL |
| 18 | AP | 59 | PRO |
| 19 | AR | 54 | ALA |
| 19 | AR | 61 | ARG |
| 19 | AR | 63 | ALA |
| 21 | AT | 54 | ALA |
| 21 | AT | 82 | VAL |
| 22 | AV | 27 | TRP |
| 25 | AY | 19 | THR |
| 26 | AZ | 19 | PRO |
| 26 | AZ | 24 | THR |
| 26 | AZ | 47 | VAL |
| 29 | AU | 17 | LEU |
| 29 | AU | 34 | ASN |
| 30 | BA | 137 | PRO |
| 31 | BB | 32 | LEU |
| 31 | BB | 38 | HIS |
| 32 | BC | 130 | PHE |
| 32 | BC | 169 | THR |
| 32 | BC | 319 | ASN |
| 32 | BC | 354 | VAL |
| 32 | BC | 370 | PHE |
| 33 | BD | 18 | ASN |
| 34 | BE | 30 | LEU |
| 34 | BE | 88 | GLU |
| 35 | BG | 12 | SER |
| 35 | BG | 34 | LEU |
| 35 | BG | 47 | PHE |
| 35 | BG | 84 | VAL |
| 35 | BG | 96 | VAL |
| 35 | BG | 129 | GLU |
| 35 | BG | 150 | LYS |
| 35 | BG | 172 | HIS |
| 37 | BH | 130 | TYR |
| 38 | Bs | 6 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | BK | 186 | ALA |
| 40 | BK | 187 | GLU |
| 41 | BN | 4 | ASP |
| 41 | BN | 10 | SER |
| 41 | BN | 89 | ALA |
| 43 | BP | 125 | SER |
| 44 | BO | 28 | HIS |
| 44 | BO | 96 | LYS |
| 45 | BR | 151 | ARG |
| 45 | BR | 159 | LYS |
| 47 | BU | 78 | LYS |
| 49 | BV | 74 | LYS |
| 49 | BV | 153 | LYS |
| 50 | BX | 35 | PRO |
| 51 | BZ | 58 | HIS |
| 53 | Ba | 59 | ALA |
| 55 | Bc | 37 | SER |
| 55 | Bc | 85 | THR |
| 55 | Bc | 92 | LEU |
| 59 | Bh | 50 | ILE |
| 60 | Bi | 59 | PRO |
| 61 | Bj | 5 | HIS |
| 61 | Bj | 46 | GLY |
| 62 | Bk | 53 | TYR |
| 62 | Bk | 55 | ARG |
| 66 | Bo | 40 | LYS |
| 69 | Br | 57 | VAL |
| 69 | Br | 90 | HIS |
| 69 | Br | 99 | GLN |
| 74 | BQ | 4 | GLN |
| 74 | BQ | 111 | GLN |
| 74 | BQ | 141 | PRO |
| 74 | BQ | 158 | ARG |
| 74 | BQ | 188 | GLU |
| 76 | BS | 70 | ASN |
| 76 | BS | 130 | THR |
| 77 | BI | 14 | ASN |
| 77 | BI | 23 | ASN |
| 77 | BI | 84 | ALA |
| 77 | BI | 93 | PRO |
| 77 | BI | 104 | SER |
| 77 | BI | 174 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | AA | 28 | ASN |
| 2 | AA | 208 | GLU |
| 3 | AB | 93 | ASP |
| 3 | AB | 99 | VAL |
| 3 | AB | 149 | ALA |
| 3 | AB | 192 | PRO |
| 3 | AB | 197 | THR |
| 4 | AD | 163 | ASP |
| 4 | AD | 231 | GLN |
| 5 | AC | 38 | ASN |
| 5 | AC | 160 | PRO |
| 6 | AE | 17 | ARG |
| 6 | AE | 41 | LEU |
| 6 | AE | 82 | ASN |
| 6 | AE | 109 | GLY |
| 6 | AE | 140 | ARG |
| 6 | AE | 253 | ARG |
| 8 | AF | 88 | PRO |
| 8 | AF | 99 | MET |
| 9 | AH | 50 | PHE |
| 9 | AH | 111 | MET |
| 9 | AH | 120 | HIS |
| 10 | AI | 25 | GLY |
| 10 | AI | 132 | LYS |
| 12 | AK | 20 | TYR |
| 12 | AK | 94 | PRO |
| 12 | AK | 123 | SER |
| 13 | AL | 57 | LEU |
| 14 | AM | 76 | PRO |
| 14 | AM | 82 | PRO |
| 14 | AM | 97 | ASP |
| 16 | AO | 109 | LYS |
| 19 | AR | 64 | LYS |
| 20 | AS | 30 | VAL |
| 20 | AS | 31 | PRO |
| 20 | AS | 68 | ARG |
| 22 | AV | 94 | LYS |
| 25 | AY | 9 | LEU |
| 26 | AZ | 40 | TYR |
| 29 | AU | 2 | SER |
| 31 | BB | 34 | TYR |
| 31 | BB | 36 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 31 | BB | 66 | PRO |
| 32 | BC | 40 | PRO |
| 32 | BC | 95 | THR |
| 32 | BC | 129 | ALA |
| 32 | BC | 347 | SER |
| 32 | BC | 385 | LYS |
| 32 | BC | 387 | LEU |
| 33 | BD | 17 | ALA |
| 34 | BE | 23 | VAL |
| 34 | BE | 106 | ILE |
| 34 | BE | 143 | ARG |
| 35 | BG | 74 | VAL |
| 35 | BG | 102 | ASN |
| 36 | BF | 51 | GLN |
| 37 | BH | 203 | VAL |
| 37 | BH | 224 | ASP |
| 38 | Bs | 233 | PRO |
| 40 | BK | 134 | LYS |
| 40 | BK | 135 | TYR |
| 41 | BN | 99 | TRP |
| 43 | BP | 181 | ASN |
| 44 | BO | 35 | ALA |
| 44 | BO | 100 | PRO |
| 44 | BO | 111 | LYS |
| 46 | BT | 71 | ARG |
| 46 | BT | 130 | ASN |
| 48 | BW | 9 | GLN |
| 48 | BW | 88 | GLN |
| 48 | BW | 101 | ASN |
| 49 | BV | 8 | SER |
| 50 | BX | 44 | PRO |
| 52 | BY | 10 | SER |
| 57 | Be | 71 | ALA |
| 59 | Bh | 12 | LYS |
| 59 | Bh | 16 | LYS |
| 59 | Bh | 89 | THR |
| 60 | Bi | 76 | TYR |
| 61 | Bj | 15 | SER |
| 64 | Bl | 76 | ASN |
| 67 | Bp | 14 | ASN |
| 74 | BQ | 248 | ARG |
| 77 | BI | 160 | PRO |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | Aa | 79 | TYR |
| 1 | Aa | 284 | ALA |
| 2 | AA | 124 | THR |
| 2 | AA | 167 | LYS |
| 2 | AA | 207 | PRO |
| 2 | AA | 213 | GLN |
| 3 | AB | 61 | GLU |
| 3 | AB | 110 | LEU |
| 3 | AB | 205 | ALA |
| 3 | AB | 207 | THR |
| 6 | AE | 126 | ARG |
| 8 | AF | 33 | VAL |
| 8 | AF | 77 | TYR |
| 13 | AL | 118 | PRO |
| 14 | AM | 100 | THR |
| 16 | AO | 57 | ALA |
| 16 | AO | 150 | VAL |
| 18 | AP | 58 | CYS |
| 19 | AR | 81 | ARG |
| 20 | AS | 40 | SER |
| 20 | AS | 92 | LYS |
| 21 | AT | 83 | TRP |
| 24 | AX | 60 | SER |
| 29 | AU | 95 | GLY |
| 31 | BB | 127 | ALA |
| 32 | BC | 62 | ARG |
| 32 | BC | 136 | LYS |
| 33 | BD | 29 | PRO |
| 33 | BD | 327 | LEU |
| 34 | BE | 87 | LYS |
| 35 | BG | 16 | ALA |
| 36 | BF | 186 | PHE |
| 37 | BH | 61 | GLN |
| 37 | BH | 117 | ALA |
| 39 | BJ | 95 | ASP |
| 40 | BK | 126 | VAL |
| 48 | BW | 7 | ARG |
| 49 | BV | 63 | PHE |
| 49 | BV | 167 | ARG |
| 50 | BX | 104 | GLU |
| 53 | Ba | 55 | LYS |
| 59 | Bh | 11 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 60 | Bi | 13 | TYR |
| 65 | Bn | 28 | ASN |
| 69 | Br | 50 | PHE |
| 74 | BQ | 190 | ILE |
| 76 | BS | 117 | ARG |
| 2 | AA | 46 | HIS |
| 3 | AB | 80 | ALA |
| 4 | AD | 241 | GLY |
| 8 | AF | 103 | ASN |
| 8 | AF | 159 | ALA |
| 17 | AQ | 85 | VAL |
| 20 | AS | 32 | GLY |
| 22 | AV | 92 | ILE |
| 26 | AZ | 26 | LYS |
| 30 | BA | 134 | PHE |
| 31 | BB | 226 | SER |
| 32 | BC | 96 | PRO |
| 35 | BG | 130 | ILE |
| 41 | BN | 7 | VAL |
| 44 | BO | 10 | LYS |
| 44 | BO | 56 | VAL |
| 45 | BR | 131 | ALA |
| 50 | BX | 38 | LEU |
| 57 | Be | 173 | LEU |
| 58 | Bg | 93 | VAL |
| 60 | Bi | 54 | ILE |
| 68 | Bq | 4 | LYS |
| 69 | Br | 105 | GLN |
| 74 | BQ | 52 | VAL |
| 1 | Aa | 193 | ILE |
| 6 | AE | 74 | PRO |
| 13 | AL | 52 | ILE |
| 15 | AN | 15 | GLY |
| 29 | AU | 16 | PRO |
| 34 | BE | 24 | GLY |
| 46 | BT | 83 | GLY |
| 48 | BW | 22 | PRO |
| 56 | Bf | 3 | PRO |
| 57 | Be | 204 | PRO |
| 58 | Bg | 94 | GLU |
| 65 | Bn | 35 | GLY |
| 14 | AM | 135 | GLY |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 21 | AT | 32 | VAL |
| 29 | AU | 29 | HIS |
| 46 | BT | 57 | VAL |
| 76 | BS | 74 | ILE |
| 77 | BI | 178 | ARG |
| 2 | AA | 70 | PRO |
| 6 | AE | 16 | GLY |
| 12 | AK | 79 | VAL |
| 25 | AY | 6 | PRO |
| 50 | BX | 51 | VAL |
| 60 | Bi | 101 | VAL |
| 65 | Bn | 75 | VAL |
| 74 | BQ | 192 | PRO |
| 4 | AD | 135 | GLY |
| 4 | AD | 150 | PRO |
| 29 | AU | 7 | ILE |
| 35 | BG | 68 | PRO |
| 38 | Bs | 228 | GLY |
| 40 | BK | 111 | PRO |
| 45 | BR | 14 | GLY |
| 60 | Bi | 58 | ARG |
| 61 | Bj | 90 | PRO |
| 66 | Bo | 24 | PRO |
| 6 | AE | 101 | VAL |
| 19 | AR | 132 | GLY |

### 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 | Aa | 259/262 (99%) | 238 (92%) | 21 (8%) | 11 35 |
| 2 | AA | 198/210 (94%) | 180 (91%) | 18 (9%) | 9 29 |
| 3 | AB | 148/195 (76%) | 136 (92%) | 12 (8%) | 11 35 |
| 4 | AD | 173/222 (78%) | 158 (91%) | 15 (9%) | 10 31 |
| 5 | AC | 153/166 (92%) | 132 (86%) | 21 (14%) | 3 17 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 6 | AE | 205/205 (100%) | 188 (92%) | 17 (8%) | 11 | 34 |
| 8 | AF | 163/191 (85%) | 144 (88%) | 19 (12%) | 5 | 21 |
| 9 | AH | 111/111 (100%) | 98 (88%) | 13 (12%) | 5 | 21 |
| 10 | AI | 105/119 (88%) | 93 (89%) | 12 (11%) | 5 | 21 |
| 11 | AJ | 93/114 (82%) | 88 (95%) | 5 (5%) | 22 | 47 |
| 12 | AK | 82/105 (78%) | 77 (94%) | 5 (6%) | 18 | 44 |
| 13 | AL | 87/120 (72%) | 75 (86%) | 12 (14%) | 3 | 17 |
| 14 | AM | 123/129 (95%) | 104 (85%) | 19 (15%) | 2 | 14 |
| 15 | AN | 34/49 (69%) | 30 (88%) | 4 (12%) | 5 | 20 |
| 16 | AO | 105/128 (82%) | 91 (87%) | 14 (13%) | 4 | 18 |
| 17 | AQ | 122/124 (98%) | 109 (89%) | 13 (11%) | 6 | 23 |
| 18 | AP | 63/137 (46%) | 56 (89%) | 7 (11%) | 6 | 22 |
| 19 | AR | 71/118 (60%) | 62 (87%) | 9 (13%) | 4 | 18 |
| 20 | AS | 115/116 (99%) | 100 (87%) | 15 (13%) | 4 | 18 |
| 21 | AT | 74/74 (100%) | 67 (90%) | 7 (10%) | 8 | 27 |
| 22 | AV | 74/89 (83%) | 67 (90%) | 7 (10%) | 8 | 27 |
| 24 | AX | 43/71 (61%) | 33 (77%) | 10 (23%) | 1 | 4 |
| 25 | AY | 50/60 (83%) | 47 (94%) | 3 (6%) | 19 | 44 |
| 26 | AZ | 51/54 (94%) | 47 (92%) | 4 (8%) | 12 | 36 |
| 29 | AU | 72/113 (64%) | 62 (86%) | 10 (14%) | 3 | 17 |
| 30 | BA | 198/198 (100%) | 184 (93%) | 14 (7%) | 14 | 39 |
| 31 | BB | 189/196 (96%) | 177 (94%) | 12 (6%) | 18 | 43 |
| 32 | BC | 315/323 (98%) | 265 (84%) | 50 (16%) | 2 | 13 |
| 33 | BD | 253/289 (88%) | 222 (88%) | 31 (12%) | 4 | 19 |
| 34 | BE | 145/150 (97%) | 118 (81%) | 27 (19%) | 1 | 9 |
| 35 | BG | 153/153 (100%) | 124 (81%) | 29 (19%) | 1 | 8 |
| 36 | BF | 170/171 (99%) | 152 (89%) | 18 (11%) | 6 | 24 |
| 37 | BH | 154/208 (74%) | 136 (88%) | 18 (12%) | 5 | 21 |
| 38 | Bs | 216/254 (85%) | 209 (97%) | 7 (3%) | 39 | 61 |
| 39 | BJ | 102/136 (75%) | 94 (92%) | 8 (8%) | 12 | 36 |
| 40 | BK | 162/162 (100%) | 143 (88%) | 19 (12%) | 5 | 21 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 41 | BN | 109/109 (100%) | 96 (88%) | 13 (12%) | 5 | 20 |
| 42 | BM | 101/105 (96%) | 85 (84%) | 16 (16%) | 2 | 13 |
| 43 | BP | 165/176 (94%) | 141 (86%) | 24 (14%) | 3 | 15 |
| 44 | BO | 119/119 (100%) | 100 (84%) | 19 (16%) | 2 | 13 |
| 45 | BR | 131/151 (87%) | 106 (81%) | 25 (19%) | 1 | 8 |
| 46 | BT | 154/154 (100%) | 144 (94%) | 10 (6%) | 17 | 42 |
| 47 | BU | 132/137 (96%) | 113 (86%) | 19 (14%) | 3 | 16 |
| 48 | BW | 90/107 (84%) | 77 (86%) | 13 (14%) | 3 | 16 |
| 49 | BV | 131/137 (96%) | 117 (89%) | 14 (11%) | 6 | 23 |
| 50 | BX | 106/118 (90%) | 99 (93%) | 7 (7%) | 16 | 41 |
| 51 | BZ | 59/129 (46%) | 51 (86%) | 8 (14%) | 3 | 17 |
| 52 | BY | 107/107 (100%) | 93 (87%) | 14 (13%) | 4 | 18 |
| 53 | Ba | 73/116 (63%) | 63 (86%) | 10 (14%) | 3 | 17 |
| 54 | Bd | 15/47 (32%) | 13 (87%) | 2 (13%) | 4 | 18 |
| 55 | Bc | 104/105 (99%) | 88 (85%) | 16 (15%) | 2 | 14 |
| 56 | Bf | 83/88 (94%) | 75 (90%) | 8 (10%) | 8 | 27 |
| 57 | Be | 202/205 (98%) | 182 (90%) | 20 (10%) | 8 | 26 |
| 58 | Bg | 90/97 (93%) | 79 (88%) | 11 (12%) | 5 | 20 |
| 59 | Bh | 111/111 (100%) | 95 (86%) | 16 (14%) | 3 | 16 |
| 60 | Bi | 99/101 (98%) | 87 (88%) | 12 (12%) | 5 | 20 |
| 61 | Bj | 71/91 (78%) | 63 (89%) | 8 (11%) | 6 | 21 |
| 62 | Bk | 64/82 (78%) | 58 (91%) | 6 (9%) | 8 | 28 |
| 63 | Bm | 72/72 (100%) | 67 (93%) | 5 (7%) | 15 | 40 |
| 64 | Bl | 68/71 (96%) | 61 (90%) | 7 (10%) | 7 | 25 |
| 65 | Bn | 66/69 (96%) | 53 (80%) | 13 (20%) | 1 | 8 |
| 66 | Bo | 46/46 (100%) | 38 (83%) | 8 (17%) | 2 | 11 |
| 67 | Bp | 37/47 (79%) | 35 (95%) | 2 (5%) | 22 | 47 |
| 68 | Bq | 23/23 (100%) | 21 (91%) | 2 (9%) | 10 | 31 |
| 69 | Br | 87/91 (96%) | 76 (87%) | 11 (13%) | 4 | 19 |
| 72 | Bt | 48/76 (63%) | 48 (100%) | 0 | 100 | 100 |
| 72 | Bu | 48/76 (63%) | 48 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 73 | Bv | 47/74 (64%) | 45 (96%) | 2 (4%) | 29 53 |
| 73 | Bw | 47/74 (64%) | 46 (98%) | 1 (2%) | 53 72 |
| 74 | BQ | 238/245 (97%) | 196 (82%) | 42 (18%) | 2 11 |
| 76 | BS | 153/153 (100%) | 116 (76%) | 37 (24%) | 0 4 |
| 77 | BI | 151/187 (81%) | 133 (88%) | 18 (12%) | 5 20 |
| All | All | 8278/9418 (88%) | 7314 (88%) | 964 (12%) | 9 21 |

All (964) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | Aa | 9 | LEU |
| 1 | Aa | 16 | HIS |
| 1 | Aa | 35 | SER |
| 1 | Aa | 47 | LEU |
| 1 | Aa | 54 | PHE |
| 1 | Aa | 59 | ARG |
| 1 | Aa | 64 | HIS |
| 1 | Aa | 67 | ILE |
| 1 | Aa | 71 | CYS |
| 1 | Aa | 82 | SER |
| 1 | Aa | 86 | ASP |
| 1 | Aa | 92 | TRP |
| 1 | Aa | 145 | LEU |
| 1 | Aa | 150 | TRP |
| 1 | Aa | 188 | ILE |
| 1 | Aa | 201 | THR |
| 1 | Aa | 211 | ILE |
| 1 | Aa | 229 | LYS |
| 1 | Aa | 258 | THR |
| 1 | Aa | 306 | THR |
| 1 | Aa | 308 | ASN |
| 2 | AA | 9 | LEU |
| 2 | AA | 11 | PRO |
| 2 | AA | 23 | HIS |
| 2 | AA | 58 | VAL |
| 2 | AA | 71 | GLU |
| 2 | AA | 108 | THR |
| 2 | AA | 110 | TYR |
| 2 | AA | 120 | LEU |
| 2 | AA | 139 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | AA | 157 | ASP |
| 2 | AA | 165 | ARG |
| 2 | AA | 193 | GLN |
| 2 | AA | 208 | GLU |
| 2 | AA | 217 | GLU |
| 2 | AA | 231 | GLU |
| 2 | AA | 234 | GLU |
| 2 | AA | 240 | THR |
| 2 | AA | 250 | VAL |
| 3 | AB | 18 | TYR |
| 3 | AB | 22 | ASN |
| 3 | AB | 67 | ASN |
| 3 | AB | 71 | LEU |
| 3 | AB | 75 | LYS |
| 3 | AB | 78 | LYS |
| 3 | AB | 84 | ILE |
| 3 | AB | 86 | LEU |
| 3 | AB | 91 | VAL |
| 3 | AB | 115 | ILE |
| 3 | AB | 176 | LEU |
| 3 | AB | 191 | ASP |
| 4 | AD | 56 | LEU |
| 4 | AD | 73 | ASP |
| 4 | AD | 102 | VAL |
| 4 | AD | 118 | GLU |
| 4 | AD | 123 | LEU |
| 4 | AD | 136 | VAL |
| 4 | AD | 137 | PRO |
| 4 | AD | 146 | THR |
| 4 | AD | 154 | ILE |
| 4 | AD | 182 | TYR |
| 4 | AD | 189 | LEU |
| 4 | AD | 192 | ILE |
| 4 | AD | 207 | LEU |
| 4 | AD | 220 | THR |
| 4 | AD | 239 | PRO |
| 5 | AC | 10 | LYS |
| 5 | AC | 15 | PRO |
| 5 | AC | 16 | LYS |
| 5 | AC | 24 | LEU |
| 5 | AC | 38 | ASN |
| 5 | AC | 47 | PHE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | AC | 51 | LYS |
| 5 | AC | 61 | THR |
| 5 | AC | 65 | LYS |
| 5 | AC | 67 | PRO |
| 5 | AC | 87 | SER |
| 5 | AC | 91 | LYS |
| 5 | AC | 95 | TYR |
| 5 | AC | 103 | ASP |
| 5 | AC | 118 | LEU |
| 5 | AC | 143 | ILE |
| 5 | AC | 146 | PHE |
| 5 | AC | 153 | GLU |
| 5 | AC | 158 | PHE |
| 5 | AC | 168 | ARG |
| 5 | AC | 174 | ARG |
| 6 | AE | 29 | ASN |
| 6 | AE | 30 | THR |
| 6 | AE | 39 | THR |
| 6 | AE | 51 | THR |
| 6 | AE | 69 | ILE |
| 6 | AE | 71 | THR |
| 6 | AE | 83 | ILE |
| 6 | AE | 96 | THR |
| 6 | AE | 139 | ILE |
| 6 | AE | 141 | ARG |
| 6 | AE | 185 | LYS |
| 6 | AE | 196 | VAL |
| 6 | AE | 224 | PHE |
| 6 | AE | 225 | LEU |
| 6 | AE | 235 | LEU |
| 6 | AE | 241 | ASP |
| 6 | AE | 245 | ASP |
| 8 | AF | 27 | THR |
| 8 | AF | 30 | PRO |
| 8 | AF | 31 | GLU |
| 8 | AF | 42 | LEU |
| 8 | AF | 58 | LEU |
| 8 | AF | 73 | THR |
| 8 | AF | 80 | LYS |
| 8 | AF | 81 | ARG |
| 8 | AF | 84 | LYS |
| 8 | AF | 106 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 8 | AF | 108 | LEU |
| 8 | AF | 160 | VAL |
| 8 | AF | 161 | ASP |
| 8 | AF | 180 | ARG |
| 8 | AF | 184 | PHE |
| 8 | AF | 189 | THR |
| 8 | AF | 203 | LYS |
| 8 | AF | 217 | LEU |
| 8 | AF | 222 | LYS |
| 9 | AH | 27 | ILE |
| 9 | AH | 28 | ARG |
| 9 | AH | 40 | VAL |
| 9 | AH | 65 | LEU |
| 9 | AH | 68 | ARG |
| 9 | AH | 69 | LEU |
| 9 | AH | 79 | PHE |
| 9 | AH | 89 | TRP |
| 9 | AH | 94 | LEU |
| 9 | AH | 97 | ARG |
| 9 | AH | 113 | HIS |
| 9 | AH | 122 | SER |
| 9 | AH | 130 | TYR |
| 10 | AI | 36 | ILE |
| 10 | AI | 37 | THR |
| 10 | AI | 39 | VAL |
| 10 | AI | 57 | LEU |
| 10 | AI | 70 | THR |
| 10 | AI | 85 | ILE |
| 10 | AI | 93 | HIS |
| 10 | AI | 94 | GLN |
| 10 | AI | 118 | ILE |
| 10 | AI | 132 | LYS |
| 10 | AI | 138 | PHE |
| 10 | AI | 142 | TYR |
| 11 | AJ | 25 | THR |
| 11 | AJ | 56 | VAL |
| 11 | AJ | 71 | PRO |
| 11 | AJ | 78 | THR |
| 11 | AJ | 79 | TRP |
| 12 | AK | 24 | ASN |
| 12 | AK | 46 | MET |
| 12 | AK | 49 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 12 | AK | 51 | ASP |
| 12 | AK | 107 | ARG |
| 13 | AL | 6 | PRO |
| 13 | AL | 9 | LEU |
| 13 | AL | 13 | ARG |
| 13 | AL | 22 | ASN |
| 13 | AL | 38 | PHE |
| 13 | AL | 53 | VAL |
| 13 | AL | 78 | LYS |
| 13 | AL | 82 | LYS |
| 13 | AL | 86 | PHE |
| 13 | AL | 87 | VAL |
| 13 | AL | 96 | VAL |
| 13 | AL | 114 | LYS |
| 14 | AM | 13 | HIS |
| 14 | AM | 18 | LEU |
| 14 | AM | 20 | THR |
| 14 | AM | 25 | ASN |
| 14 | AM | 27 | LYS |
| 14 | AM | 40 | ARG |
| 14 | AM | 51 | ASP |
| 14 | AM | 60 | GLU |
| 14 | AM | 66 | LEU |
| 14 | AM | 76 | PRO |
| 14 | AM | 80 | LYS |
| 14 | AM | 81 | ILE |
| 14 | AM | 87 | ASN |
| 14 | AM | 92 | ILE |
| 14 | AM | 93 | THR |
| 14 | AM | 106 | GLU |
| 14 | AM | 137 | HIS |
| 14 | AM | 139 | LYS |
| 14 | AM | 144 | ARG |
| 15 | AN | 9 | SER |
| 15 | AN | 12 | ARG |
| 15 | AN | 20 | GLN |
| 15 | AN | 37 | ASN |
| 16 | AO | 40 | TYR |
| 16 | AO | 46 | THR |
| 16 | AO | 55 | ARG |
| 16 | AO | 64 | ARG |
| 16 | AO | 65 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 16 | AO | 70 | LYS |
| 16 | AO | 83 | GLU |
| 16 | AO | 92 | ILE |
| 16 | AO | 112 | LYS |
| 16 | AO | 113 | PHE |
| 16 | AO | 118 | ILE |
| 16 | AO | 120 | SER |
| 16 | AO | 124 | ARG |
| 16 | AO | 145 | THR |
| 17 | AQ | 14 | LYS |
| 17 | AQ | 28 | PHE |
| 17 | AQ | 29 | GLN |
| 17 | AQ | 50 | ILE |
| 17 | AQ | 95 | ARG |
| 17 | AQ | 96 | SER |
| 17 | AQ | 97 | ASN |
| 17 | AQ | 99 | VAL |
| 17 | AQ | 102 | VAL |
| 17 | AQ | 119 | LEU |
| 17 | AQ | 125 | SER |
| 17 | AQ | 132 | TYR |
| 17 | AQ | 135 | ARG |
| 18 | AP | 63 | LEU |
| 18 | AP | 78 | THR |
| 18 | AP | 97 | TYR |
| 18 | AP | 99 | ARG |
| 18 | AP | 101 | GLU |
| 18 | AP | 115 | PHE |
| 18 | AP | 119 | VAL |
| 19 | AR | 49 | MET |
| 19 | AR | 52 | LYS |
| 19 | AR | 60 | LEU |
| 19 | AR | 72 | LYS |
| 19 | AR | 80 | MET |
| 19 | AR | 88 | GLU |
| 19 | AR | 106 | GLU |
| 19 | AR | 107 | ILE |
| 19 | AR | 130 | ARG |
| 20 | AS | 4 | VAL |
| 20 | AS | 7 | ARG |
| 20 | AS | 15 | ILE |
| 20 | AS | 38 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 20 | AS | 46 | PRO |
| 20 | AS | 56 | LYS |
| 20 | AS | 63 | ARG |
| 20 | AS | 75 | LYS |
| 20 | AS | 84 | LYS |
| 20 | AS | 89 | ARG |
| 20 | AS | 90 | PRO |
| 20 | AS | 100 | ILE |
| 20 | AS | 101 | ASN |
| 20 | AS | 116 | ILE |
| 20 | AS | 122 | ARG |
| 21 | AT | 33 | GLN |
| 21 | AT | 44 | ARG |
| 21 | AT | 46 | ILE |
| 21 | AT | 55 | LEU |
| 21 | AT | 68 | SER |
| 21 | AT | 71 | ARG |
| 21 | AT | 72 | LEU |
| 22 | AV | 24 | LYS |
| 22 | AV | 27 | TRP |
| 22 | AV | 54 | VAL |
| 22 | AV | 59 | TYR |
| 22 | AV | 60 | VAL |
| 22 | AV | 96 | SER |
| 22 | AV | 105 | THR |
| 24 | AX | 32 | PHE |
| 24 | AX | 35 | VAL |
| 24 | AX | 42 | ASN |
| 24 | AX | 43 | ILE |
| 24 | AX | 44 | THR |
| 24 | AX | 47 | PHE |
| 24 | AX | 56 | CYS |
| 24 | AX | 61 | THR |
| 24 | AX | 73 | LEU |
| 24 | AX | 77 | THR |
| 25 | AY | 4 | LYS |
| 25 | AY | 7 | VAL |
| 25 | AY | 36 | THR |
| 26 | AZ | 18 | THR |
| 26 | AZ | 30 | PRO |
| 26 | AZ | 42 | ARG |
| 26 | AZ | 58 | PRO |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 29 | AU | 2 | SER |
| 29 | AU | 3 | ASP |
| 29 | AU | 20 | ARG |
| 29 | AU | 25 | VAL |
| 29 | AU | 30 | PRO |
| 29 | AU | 32 | ARG |
| 29 | AU | 60 | PHE |
| 29 | AU | 63 | GLN |
| 29 | AU | 72 | PHE |
| 29 | AU | 86 | GLU |
| 30 | BA | 49 | PHE |
| 30 | BA | 93 | LEU |
| 30 | BA | 103 | LEU |
| 30 | BA | 105 | LYS |
| 30 | BA | 108 | ASN |
| 30 | BA | 135 | PRO |
| 30 | BA | 136 | THR |
| 30 | BA | 149 | THR |
| 30 | BA | 155 | ILE |
| 30 | BA | 160 | LYS |
| 30 | BA | 178 | VAL |
| 30 | BA | 181 | ASN |
| 30 | BA | 190 | PHE |
| 30 | BA | 191 | VAL |
| 31 | BB | 15 | ILE |
| 31 | BB | 61 | VAL |
| 31 | BB | 66 | PRO |
| 31 | BB | 67 | TYR |
| 31 | BB | 83 | HIS |
| 31 | BB | 102 | LEU |
| 31 | BB | 134 | VAL |
| 31 | BB | 142 | ASP |
| 31 | BB | 155 | LYS |
| 31 | BB | 186 | PHE |
| 31 | BB | 199 | THR |
| 31 | BB | 242 | ARG |
| 32 | BC | 1 | MET |
| 32 | BC | 2 | SER |
| 32 | BC | 3 | HIS |
| 32 | BC | 6 | TYR |
| 32 | BC | 39 | LYS |
| 32 | BC | 40 | PRO |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 32 | BC | 43 | LEU |
| 32 | BC | 45 | SER |
| 32 | BC | 55 | THR |
| 32 | BC | 60 | LEU |
| 32 | BC | 66 | LYS |
| 32 | BC | 68 | HIS |
| 32 | BC | 72 | VAL |
| 32 | BC | 78 | VAL |
| 32 | BC | 84 | VAL |
| 32 | BC | 95 | THR |
| 32 | BC | 100 | ARG |
| 32 | BC | 118 | PHE |
| 32 | BC | 120 | LYS |
| 32 | BC | 130 | PHE |
| 32 | BC | 154 | TYR |
| 32 | BC | 164 | THR |
| 32 | BC | 174 | LYS |
| 32 | BC | 175 | LYS |
| 32 | BC | 183 | LEU |
| 32 | BC | 196 | ARG |
| 32 | BC | 212 | ASN |
| 32 | BC | 241 | LYS |
| 32 | BC | 248 | LYS |
| 32 | BC | 251 | CYS |
| 32 | BC | 252 | ILE |
| 32 | BC | 261 | MET |
| 32 | BC | 262 | TRP |
| 32 | BC | 264 | VAL |
| 32 | BC | 266 | ARG |
| 32 | BC | 270 | ARG |
| 32 | BC | 300 | ARG |
| 32 | BC | 318 | LYS |
| 32 | BC | 321 | PHE |
| 32 | BC | 323 | MET |
| 32 | BC | 324 | VAL |
| 32 | BC | 331 | ASN |
| 32 | BC | 332 | ARG |
| 32 | BC | 335 | ILE |
| 32 | BC | 346 | THR |
| 32 | BC | 348 | ARG |
| 32 | BC | 354 | VAL |
| 32 | BC | 361 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 32 | BC | 364 | LYS |
| 32 | BC | 370 | PHE |
| 33 | BD | 1 | MET |
| 33 | BD | 5 | GLN |
| 33 | BD | 6 | VAL |
| 33 | BD | 8 | VAL |
| 33 | BD | 25 | VAL |
| 33 | BD | 29 | PRO |
| 33 | BD | 30 | ILE |
| 33 | BD | 33 | ASP |
| 33 | BD | 47 | ARG |
| 33 | BD | 100 | PHE |
| 33 | BD | 102 | PRO |
| 33 | BD | 109 | TRP |
| 33 | BD | 122 | THR |
| 33 | BD | 131 | VAL |
| 33 | BD | 140 | HIS |
| 33 | BD | 142 | VAL |
| 33 | BD | 143 | GLU |
| 33 | BD | 145 | ILE |
| 33 | BD | 156 | LEU |
| 33 | BD | 219 | LEU |
| 33 | BD | 244 | LEU |
| 33 | BD | 256 | THR |
| 33 | BD | 259 | ASP |
| 33 | BD | 260 | GLN |
| 33 | BD | 295 | ILE |
| 33 | BD | 312 | VAL |
| 33 | BD | 318 | LEU |
| 33 | BD | 324 | LEU |
| 33 | BD | 333 | VAL |
| 33 | BD | 341 | SER |
| 33 | BD | 349 | THR |
| 34 | BE | 4 | LYS |
| 34 | BE | 10 | ARG |
| 34 | BE | 17 | LEU |
| 34 | BE | 25 | GLU |
| 34 | BE | 29 | ARG |
| 34 | BE | 32 | ARG |
| 34 | BE | 36 | VAL |
| 34 | BE | 53 | THR |
| 34 | BE | 55 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 34 | BE | 57 | PHE |
| 34 | BE | 59 | ILE |
| 34 | BE | 60 | ARG |
| 34 | BE | 64 | LYS |
| 34 | BE | 67 | VAL |
| 34 | BE | 89 | TYR |
| 34 | BE | 94 | ARG |
| 34 | BE | 101 | ASN |
| 34 | BE | 110 | ILE |
| 34 | BE | 115 | LYS |
| 34 | BE | 117 | ASP |
| 34 | BE | 125 | MET |
| 34 | BE | 131 | MET |
| 34 | BE | 143 | ARG |
| 34 | BE | 147 | THR |
| 34 | BE | 152 | HIS |
| 34 | BE | 156 | LYS |
| 34 | BE | 166 | LYS |
| 35 | BG | 4 | GLN |
| 35 | BG | 5 | LYS |
| 35 | BG | 11 | PRO |
| 35 | BG | 18 | LEU |
| 35 | BG | 22 | ARG |
| 35 | BG | 27 | PRO |
| 35 | BG | 42 | LEU |
| 35 | BG | 46 | ARG |
| 35 | BG | 50 | LYS |
| 35 | BG | 52 | VAL |
| 35 | BG | 56 | LYS |
| 35 | BG | 57 | HIS |
| 35 | BG | 62 | THR |
| 35 | BG | 64 | LEU |
| 35 | BG | 65 | ILE |
| 35 | BG | 74 | VAL |
| 35 | BG | 75 | PRO |
| 35 | BG | 79 | VAL |
| 35 | BG | 84 | VAL |
| 35 | BG | 85 | ILE |
| 35 | BG | 93 | VAL |
| 35 | BG | 99 | GLU |
| 35 | BG | 102 | ASN |
| 35 | BG | 111 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 35 | BG | 114 | LYS |
| 35 | BG | 146 | ILE |
| 35 | BG | 151 | LYS |
| 35 | BG | 154 | LEU |
| 35 | BG | 160 | SER |
| 36 | BF | 2 | LYS |
| 36 | BF | 3 | TYR |
| 36 | BF | 4 | ILE |
| 36 | BF | 31 | ARG |
| 36 | BF | 36 | LYS |
| 36 | BF | 39 | LYS |
| 36 | BF | 41 | ILE |
| 36 | BF | 44 | THR |
| 36 | BF | 47 | LYS |
| 36 | BF | 53 | ILE |
| 36 | BF | 54 | LYS |
| 36 | BF | 62 | ARG |
| 36 | BF | 69 | ARG |
| 36 | BF | 103 | ILE |
| 36 | BF | 106 | LYS |
| 36 | BF | 141 | LYS |
| 36 | BF | 149 | ASN |
| 36 | BF | 174 | LYS |
| 37 | BH | 66 | SER |
| 37 | BH | 70 | LYS |
| 37 | BH | 73 | PRO |
| 37 | BH | 78 | PHE |
| 37 | BH | 92 | LYS |
| 37 | BH | 110 | THR |
| 37 | BH | 128 | LYS |
| 37 | BH | 136 | LEU |
| 37 | BH | 152 | LEU |
| 37 | BH | 158 | ASP |
| 37 | BH | 165 | PHE |
| 37 | BH | 173 | MET |
| 37 | BH | 181 | LYS |
| 37 | BH | 193 | LYS |
| 37 | BH | 218 | ILE |
| 37 | BH | 221 | ASN |
| 37 | BH | 225 | LYS |
| 37 | BH | 229 | VAL |
| 38 | Bs | 36 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 38 | Bs | 53 | MET |
| 38 | Bs | 58 | MET |
| 38 | Bs | 60 | ARG |
| 38 | Bs | 73 | PHE |
| 38 | Bs | 89 | THR |
| 38 | Bs | 230 | PRO |
| 39 | BJ | 13 | LEU |
| 39 | BJ | 14 | TYR |
| 39 | BJ | 37 | LEU |
| 39 | BJ | 41 | LYS |
| 39 | BJ | 90 | ARG |
| 39 | BJ | 94 | LYS |
| 39 | BJ | 96 | LYS |
| 39 | BJ | 98 | VAL |
| 40 | BK | 26 | GLN |
| 40 | BK | 32 | LYS |
| 40 | BK | 39 | GLU |
| 40 | BK | 43 | ILE |
| 40 | BK | 49 | ARG |
| 40 | BK | 59 | ARG |
| 40 | BK | 60 | LYS |
| 40 | BK | 62 | THR |
| 40 | BK | 64 | PHE |
| 40 | BK | 84 | LEU |
| 40 | BK | 117 | ARG |
| 40 | BK | 121 | PRO |
| 40 | BK | 126 | VAL |
| 40 | BK | 129 | LEU |
| 40 | BK | 133 | ARG |
| 40 | BK | 153 | VAL |
| 40 | BK | 155 | LYS |
| 40 | BK | 162 | VAL |
| 40 | BK | 197 | LEU |
| 41 | BN | 6 | ILE |
| 41 | BN | 8 | LYS |
| 41 | BN | 10 | SER |
| 41 | BN | 22 | LEU |
| 41 | BN | 36 | VAL |
| 41 | BN | 39 | ILE |
| 41 | BN | 43 | LYS |
| 41 | BN | 65 | LEU |
| 41 | BN | 66 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | BN | 72 | LEU |
| 41 | BN | 85 | TRP |
| 41 | BN | 99 | TRP |
| 41 | BN | 129 | TYR |
| 42 | BM | 12 | ARG |
| 42 | BM | 22 | ILE |
| 42 | BM | 45 | ARG |
| 42 | BM | 49 | LEU |
| 42 | BM | 53 | SER |
| 42 | BM | 54 | LEU |
| 42 | BM | 56 | ASP |
| 42 | BM | 59 | MET |
| 42 | BM | 61 | THR |
| 42 | BM | 62 | VAL |
| 42 | BM | 71 | LYS |
| 42 | BM | 75 | PRO |
| 42 | BM | 78 | VAL |
| 42 | BM | 101 | VAL |
| 42 | BM | 110 | LYS |
| 42 | BM | 125 | LEU |
| 43 | BP | 1 | MET |
| 43 | BP | 14 | LYS |
| 43 | BP | 21 | PHE |
| 43 | BP | 22 | LEU |
| 43 | BP | 25 | VAL |
| 43 | BP | 50 | ARG |
| 43 | BP | 73 | ARG |
| 43 | BP | 84 | PRO |
| 43 | BP | 86 | ASN |
| 43 | BP | 87 | GLN |
| 43 | BP | 95 | GLN |
| 43 | BP | 98 | LEU |
| 43 | BP | 116 | LEU |
| 43 | BP | 120 | TRP |
| 43 | BP | 125 | SER |
| 43 | BP | 138 | GLN |
| 43 | BP | 143 | ARG |
| 43 | BP | 144 | ARG |
| 43 | BP | 160 | GLU |
| 43 | BP | 174 | ILE |
| 43 | BP | 176 | LYS |
| 43 | BP | 180 | PHE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 43 | BP | 184 | LYS |
| 43 | BP | 192 | LYS |
| 44 | BO | 4 | ARG |
| 44 | BO | 8 | THR |
| 44 | BO | 19 | LYS |
| 44 | BO | 39 | HIS |
| 44 | BO | 46 | ASP |
| 44 | BO | 47 | LYS |
| 44 | BO | 60 | TYR |
| 44 | BO | 61 | PHE |
| 44 | BO | 62 | HIS |
| 44 | BO | 72 | VAL |
| 44 | BO | 75 | LEU |
| 44 | BO | 80 | THR |
| 44 | BO | 84 | GLU |
| 44 | BO | 89 | GLN |
| 44 | BO | 101 | VAL |
| 44 | BO | 117 | ARG |
| 44 | BO | 122 | PRO |
| 44 | BO | 123 | VAL |
| 44 | BO | 128 | ARG |
| 45 | BR | 3 | ILE |
| 45 | BR | 4 | ASP |
| 45 | BR | 10 | HIS |
| 45 | BR | 11 | LYS |
| 45 | BR | 12 | ARG |
| 45 | BR | 13 | SER |
| 45 | BR | 15 | HIS |
| 45 | BR | 17 | THR |
| 45 | BR | 22 | ASP |
| 45 | BR | 24 | VAL |
| 45 | BR | 28 | LEU |
| 45 | BR | 32 | LEU |
| 45 | BR | 35 | PHE |
| 45 | BR | 36 | LEU |
| 45 | BR | 39 | ARG |
| 45 | BR | 49 | LEU |
| 45 | BR | 54 | LEU |
| 45 | BR | 89 | ASP |
| 45 | BR | 92 | ARG |
| 45 | BR | 93 | ILE |
| 45 | BR | 95 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 45 | BR | 100 | THR |
| 45 | BR | 147 | ARG |
| 45 | BR | 148 | GLU |
| 45 | BR | 155 | MET |
| 46 | BT | 14 | VAL |
| 46 | BT | 17 | VAL |
| 46 | BT | 20 | ARG |
| 46 | BT | 57 | VAL |
| 46 | BT | 80 | LYS |
| 46 | BT | 82 | LYS |
| 46 | BT | 96 | ILE |
| 46 | BT | 124 | TYR |
| 46 | BT | 130 | ASN |
| 46 | BT | 143 | ILE |
| 47 | BU | 7 | TYR |
| 47 | BU | 8 | ARG |
| 47 | BU | 10 | ARG |
| 47 | BU | 15 | PHE |
| 47 | BU | 20 | ARG |
| 47 | BU | 25 | VAL |
| 47 | BU | 26 | HIS |
| 47 | BU | 27 | LEU |
| 47 | BU | 31 | LEU |
| 47 | BU | 42 | ILE |
| 47 | BU | 56 | PHE |
| 47 | BU | 69 | LYS |
| 47 | BU | 89 | LEU |
| 47 | BU | 91 | LEU |
| 47 | BU | 96 | ILE |
| 47 | BU | 134 | GLN |
| 47 | BU | 141 | VAL |
| 47 | BU | 151 | LEU |
| 47 | BU | 160 | ILE |
| 48 | BW | 8 | LYS |
| 48 | BW | 11 | ILE |
| 48 | BW | 13 | LYS |
| 48 | BW | 24 | GLU |
| 48 | BW | 29 | ASP |
| 48 | BW | 42 | LYS |
| 48 | BW | 81 | LYS |
| 48 | BW | 90 | ARG |
| 48 | BW | 92 | TRP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 48 | BW | 95 | PHE |
| 48 | BW | 97 | SER |
| 48 | BW | 98 | THR |
| 48 | BW | 99 | LYS |
| 49 | BV | 4 | TYR |
| 49 | BV | 18 | ARG |
| 49 | BV | 22 | LEU |
| 49 | BV | 30 | ARG |
| 49 | BV | 47 | TYR |
| 49 | BV | 69 | ARG |
| 49 | BV | 70 | THR |
| 49 | BV | 74 | LYS |
| 49 | BV | 78 | VAL |
| 49 | BV | 79 | THR |
| 49 | BV | 83 | TRP |
| 49 | BV | 143 | PRO |
| 49 | BV | 145 | HIS |
| 49 | BV | 169 | THR |
| 50 | BX | 28 | THR |
| 50 | BX | 36 | LYS |
| 50 | BX | 40 | LEU |
| 50 | BX | 48 | SER |
| 50 | BX | 93 | TYR |
| 50 | BX | 113 | LEU |
| 50 | BX | 141 | TYR |
| 51 | BZ | 5 | ILE |
| 51 | BZ | 27 | LYS |
| 51 | BZ | 30 | ARG |
| 51 | BZ | 49 | ILE |
| 51 | BZ | 51 | TRP |
| 51 | BZ | 56 | ARG |
| 51 | BZ | 67 | VAL |
| 51 | BZ | 69 | LYS |
| 52 | BY | 3 | LYS |
| 52 | BY | 16 | ARG |
| 52 | BY | 21 | THR |
| 52 | BY | 46 | LYS |
| 52 | BY | 48 | LEU |
| 52 | BY | 51 | ARG |
| 52 | BY | 70 | ILE |
| 52 | BY | 74 | TYR |
| 52 | BY | 80 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 52 | BY | 91 | ASN |
| 52 | BY | 106 | ILE |
| 52 | BY | 110 | HIS |
| 52 | BY | 118 | LEU |
| 52 | BY | 121 | ARG |
| 53 | Ba | 10 | VAL |
| 53 | Ba | 21 | LYS |
| 53 | Ba | 27 | LYS |
| 53 | Ba | 29 | HIS |
| 53 | Ba | 37 | PRO |
| 53 | Ba | 42 | LEU |
| 53 | Ba | 55 | LYS |
| 53 | Ba | 56 | LYS |
| 53 | Ba | 61 | LYS |
| 53 | Ba | 82 | PRO |
| 54 | Bd | 44 | LYS |
| 54 | Bd | 52 | LYS |
| 55 | Bc | 14 | LYS |
| 55 | Bc | 20 | GLN |
| 55 | Bc | 28 | LEU |
| 55 | Bc | 32 | LYS |
| 55 | Bc | 36 | LEU |
| 55 | Bc | 38 | ARG |
| 55 | Bc | 39 | PRO |
| 55 | Bc | 48 | ARG |
| 55 | Bc | 71 | LYS |
| 55 | Bc | 75 | TYR |
| 55 | Bc | 88 | LEU |
| 55 | Bc | 93 | THR |
| 55 | Bc | 94 | LYS |
| 55 | Bc | 95 | PHE |
| 55 | Bc | 109 | ILE |
| 55 | Bc | 118 | ILE |
| 56 | Bf | 13 | LYS |
| 56 | Bf | 14 | LEU |
| 56 | Bf | 18 | ILE |
| 56 | Bf | 50 | VAL |
| 56 | Bf | 51 | LEU |
| 56 | Bf | 64 | LYS |
| 56 | Bf | 65 | THR |
| 56 | Bf | 77 | LEU |
| 57 | Be | 17 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 57 | Be | 22 | THR |
| 57 | Be | 60 | ARG |
| 57 | Be | 70 | LYS |
| 57 | Be | 82 | LYS |
| 57 | Be | 95 | ILE |
| 57 | Be | 105 | LEU |
| 57 | Be | 107 | ARG |
| 57 | Be | 142 | SER |
| 57 | Be | 160 | ARG |
| 57 | Be | 162 | PRO |
| 57 | Be | 163 | LEU |
| 57 | Be | 165 | ASP |
| 57 | Be | 180 | SER |
| 57 | Be | 181 | ILE |
| 57 | Be | 199 | ASN |
| 57 | Be | 200 | ASN |
| 57 | Be | 224 | ILE |
| 57 | Be | 229 | PHE |
| 57 | Be | 242 | SER |
| 58 | Bg | 1 | MET |
| 58 | Bg | 7 | VAL |
| 58 | Bg | 10 | ARG |
| 58 | Bg | 11 | GLU |
| 58 | Bg | 23 | VAL |
| 58 | Bg | 25 | PHE |
| 58 | Bg | 65 | LYS |
| 58 | Bg | 71 | LEU |
| 58 | Bg | 72 | ARG |
| 58 | Bg | 77 | ARG |
| 58 | Bg | 100 | SER |
| 59 | Bh | 9 | ILE |
| 59 | Bh | 24 | ARG |
| 59 | Bh | 25 | TYR |
| 59 | Bh | 30 | GLU |
| 59 | Bh | 35 | GLN |
| 59 | Bh | 36 | LYS |
| 59 | Bh | 41 | VAL |
| 59 | Bh | 43 | ARG |
| 59 | Bh | 45 | ARG |
| 59 | Bh | 46 | PHE |
| 59 | Bh | 50 | ILE |
| 59 | Bh | 57 | TYR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 59 | Bh | 60 | ASN |
| 59 | Bh | 75 | LEU |
| 59 | Bh | 76 | VAL |
| 59 | Bh | 89 | THR |
| 60 | Bi | 3 | GLN |
| 60 | Bi | 9 | ARG |
| 60 | Bi | 10 | ARG |
| 60 | Bi | 12 | PRO |
| 60 | Bi | 29 | ILE |
| 60 | Bi | 36 | LYS |
| 60 | Bi | 38 | LEU |
| 60 | Bi | 55 | SER |
| 60 | Bi | 57 | LEU |
| 60 | Bi | 58 | ARG |
| 60 | Bi | 74 | ARG |
| 60 | Bi | 80 | ARG |
| 61 | Bj | 7 | LEU |
| 61 | Bj | 18 | ARG |
| 61 | Bj | 19 | SER |
| 61 | Bj | 37 | THR |
| 61 | Bj | 51 | TYR |
| 61 | Bj | 80 | VAL |
| 61 | Bj | 86 | ARG |
| 61 | Bj | 90 | PRO |
| 62 | Bk | 26 | ILE |
| 62 | Bk | 27 | SER |
| 62 | Bk | 28 | TYR |
| 62 | Bk | 56 | ARG |
| 62 | Bk | 57 | LEU |
| 62 | Bk | 63 | ASN |
| 63 | Bm | 3 | LYS |
| 63 | Bm | 6 | LYS |
| 63 | Bm | 17 | ARG |
| 63 | Bm | 29 | LEU |
| 63 | Bm | 61 | LYS |
| 64 | Bl | 1 | MET |
| 64 | Bl | 7 | SER |
| 64 | Bl | 12 | HIS |
| 64 | Bl | 63 | ARG |
| 64 | Bl | 67 | LEU |
| 64 | Bl | 76 | ASN |
| 64 | Bl | 79 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 65 | Bn | 15 | THR |
| 65 | Bn | 16 | ARG |
| 65 | Bn | 17 | ARG |
| 65 | Bn | 20 | VAL |
| 65 | Bn | 31 | LEU |
| 65 | Bn | 33 | LYS |
| 65 | Bn | 40 | GLN |
| 65 | Bn | 46 | ARG |
| 65 | Bn | 52 | TYR |
| 65 | Bn | 54 | LEU |
| 65 | Bn | 57 | ASN |
| 65 | Bn | 72 | THR |
| 65 | Bn | 73 | LEU |
| 66 | Bo | 1 | MET |
| 66 | Bo | 5 | LYS |
| 66 | Bo | 6 | SER |
| 66 | Bo | 7 | PHE |
| 66 | Bo | 8 | ARG |
| 66 | Bo | 30 | ARG |
| 66 | Bo | 34 | THR |
| 66 | Bo | 45 | ARG |
| 67 | Bp | 35 | ARG |
| 67 | Bp | 51 | LEU |
| 68 | Bq | 11 | ARG |
| 68 | Bq | 24 | SER |
| 69 | Br | 17 | CYS |
| 69 | Br | 18 | ARG |
| 69 | Br | 32 | LYS |
| 69 | Br | 45 | ARG |
| 69 | Br | 47 | GLN |
| 69 | Br | 50 | PHE |
| 69 | Br | 55 | LYS |
| 69 | Br | 56 | PRO |
| 69 | Br | 61 | LYS |
| 69 | Br | 75 | VAL |
| 69 | Br | 86 | LYS |
| 73 | Bv | 17 | PRO |
| 73 | Bv | 20 | THR |
| 73 | Bw | 20 | THR |
| 74 | BQ | 3 | PHE |
| 74 | BQ | 9 | SER |
| 74 | BQ | 18 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 74 | BQ | 20 | PHE |
| 74 | BQ | 23 | ARG |
| 74 | BQ | 34 | LYS |
| 74 | BQ | 36 | LEU |
| 74 | BQ | 46 | THR |
| 74 | BQ | 49 | TYR |
| 74 | BQ | 50 | ARG |
| 74 | BQ | 53 | VAL |
| 74 | BQ | 55 | PHE |
| 74 | BQ | 74 | VAL |
| 74 | BQ | 79 | TYR |
| 74 | BQ | 88 | ILE |
| 74 | BQ | 107 | ARG |
| 74 | BQ | 113 | LEU |
| 74 | BQ | 120 | LYS |
| 74 | BQ | 129 | TYR |
| 74 | BQ | 131 | LEU |
| 74 | BQ | 142 | PHE |
| 74 | BQ | 148 | ILE |
| 74 | BQ | 151 | GLN |
| 74 | BQ | 159 | VAL |
| 74 | BQ | 167 | SER |
| 74 | BQ | 179 | ARG |
| 74 | BQ | 196 | ARG |
| 74 | BQ | 200 | PHE |
| 74 | BQ | 208 | MET |
| 74 | BQ | 216 | GLU |
| 74 | BQ | 219 | PHE |
| 74 | BQ | 224 | LYS |
| 74 | BQ | 227 | LEU |
| 74 | BQ | 239 | ILE |
| 74 | BQ | 240 | TYR |
| 74 | BQ | 248 | ARG |
| 74 | BQ | 251 | PRO |
| 74 | BQ | 259 | LYS |
| 74 | BQ | 260 | PHE |
| 74 | BQ | 273 | ARG |
| 74 | BQ | 289 | LYS |
| 74 | BQ | 293 | LEU |
| 76 | BS | 5 | ARG |
| 76 | BS | 7 | HIS |
| 76 | BS | 16 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 76 | BS | 19 | PRO |
| 76 | BS | 23 | HIS |
| 76 | BS | 25 | LYS |
| 76 | BS | 31 | LEU |
| 76 | BS | 32 | TRP |
| 76 | BS | 43 | PHE |
| 76 | BS | 51 | LYS |
| 76 | BS | 52 | LYS |
| 76 | BS | 53 | VAL |
| 76 | BS | 55 | LYS |
| 76 | BS | 66 | ILE |
| 76 | BS | 68 | GLU |
| 76 | BS | 69 | LYS |
| 76 | BS | 73 | THR |
| 76 | BS | 74 | ILE |
| 76 | BS | 75 | LYS |
| 76 | BS | 79 | ILE |
| 76 | BS | 92 | MET |
| 76 | BS | 94 | LYS |
| 76 | BS | 97 | ARG |
| 76 | BS | 98 | ASP |
| 76 | BS | 105 | VAL |
| 76 | BS | 114 | SER |
| 76 | BS | 115 | ARG |
| 76 | BS | 118 | VAL |
| 76 | BS | 119 | ARG |
| 76 | BS | 123 | ILE |
| 76 | BS | 132 | HIS |
| 76 | BS | 142 | LYS |
| 76 | BS | 152 | PRO |
| 76 | BS | 157 | LYS |
| 76 | BS | 158 | VAL |
| 76 | BS | 159 | ARG |
| 76 | BS | 163 | ARG |
| 77 | BI | 4 | ARG |
| 77 | BI | 5 | PRO |
| 77 | BI | 12 | GLN |
| 77 | BI | 13 | LYS |
| 77 | BI | 17 | TYR |
| 77 | BI | 20 | SER |
| 77 | BI | 23 | ASN |
| 77 | BI | 28 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 77 | BI | 30 | LYS |
| 77 | BI | 63 | GLU |
| 77 | BI | 65 | LEU |
| 77 | BI | 90 | ARG |
| 77 | BI | 95 | HIS |
| 77 | BI | 110 | ARG |
| 77 | BI | 144 | ASN |
| 77 | BI | 146 | ASP |
| 77 | BI | 156 | ARG |
| 77 | BI | 177 | ASP |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (133) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | Aa | 64 | HIS |
| 1 | Aa | 159 | ASN |
| 1 | Aa | 182 | ASN |
| 1 | Aa | 185 | GLN |
| 1 | Aa | 187 | GLN |
| 1 | Aa | 195 | HIS |
| 1 | Aa | 288 | HIS |
| 1 | Aa | 314 | GLN |
| 2 | AA | 23 | HIS |
| 2 | AA | 46 | HIS |
| 2 | AA | 109 | ASN |
| 2 | AA | 164 | ASN |
| 3 | AB | 165 | ASN |
| 4 | AD | 142 | HIS |
| 4 | AD | 153 | ASN |
| 4 | AD | 201 | HIS |
| 5 | AC | 48 | GLN |
| 5 | AC | 124 | HIS |
| 6 | AE | 29 | ASN |
| 6 | AE | 67 | GLN |
| 6 | AE | 110 | HIS |
| 8 | AF | 44 | ASN |
| 8 | AF | 116 | HIS |
| 8 | AF | 128 | ASN |
| 9 | AH | 113 | HIS |
| 10 | AI | 32 | ASN |
| 10 | AI | 74 | HIS |
| 10 | AI | 93 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 11 | AJ | 44 | ASN |
| 13 | AL | 18 | HIS |
| 13 | AL | 22 | ASN |
| 13 | AL | 99 | ASN |
| 14 | AM | 122 | HIS |
| 16 | AO | 58 | HIS |
| 16 | AO | 123 | HIS |
| 17 | AQ | 62 | GLN |
| 18 | AP | 104 | HIS |
| 20 | AS | 70 | GLN |
| 20 | AS | 129 | GLN |
| 24 | AX | 49 | HIS |
| 29 | AU | 29 | HIS |
| 30 | BA | 40 | ASN |
| 30 | BA | 158 | GLN |
| 30 | BA | 199 | GLN |
| 31 | BB | 38 | HIS |
| 31 | BB | 50 | HIS |
| 31 | BB | 187 | HIS |
| 31 | BB | 205 | ASN |
| 31 | BB | 216 | HIS |
| 32 | BC | 68 | HIS |
| 32 | BC | 121 | ASN |
| 32 | BC | 163 | HIS |
| 32 | BC | 182 | GLN |
| 33 | BD | 48 | GLN |
| 33 | BD | 320 | ASN |
| 33 | BD | 322 | GLN |
| 33 | BD | 361 | HIS |
| 34 | BE | 7 | ASN |
| 34 | BE | 101 | ASN |
| 35 | BG | 28 | GLN |
| 35 | BG | 125 | GLN |
| 35 | BG | 138 | GLN |
| 36 | BF | 58 | HIS |
| 36 | BF | 64 | HIS |
| 37 | BH | 138 | HIS |
| 37 | BH | 155 | ASN |
| 37 | BH | 232 | HIS |
| 37 | BH | 243 | GLN |
| 38 | Bs | 37 | GLN |
| 38 | Bs | 189 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 39 | BJ | 61 | GLN |
| 39 | BJ | 100 | HIS |
| 40 | BK | 90 | HIS |
| 41 | BN | 126 | GLN |
| 42 | BM | 47 | ASN |
| 43 | BP | 37 | HIS |
| 43 | BP | 86 | ASN |
| 43 | BP | 112 | ASN |
| 43 | BP | 149 | ASN |
| 44 | BO | 11 | HIS |
| 44 | BO | 14 | HIS |
| 44 | BO | 49 | HIS |
| 44 | BO | 62 | HIS |
| 44 | BO | 89 | GLN |
| 45 | BR | 45 | ASN |
| 45 | BR | 58 | ASN |
| 46 | BT | 58 | HIS |
| 46 | BT | 75 | HIS |
| 47 | BU | 16 | GLN |
| 47 | BU | 26 | HIS |
| 47 | BU | 58 | GLN |
| 49 | BV | 54 | HIS |
| 49 | BV | 72 | GLN |
| 49 | BV | 97 | ASN |
| 49 | BV | 101 | ASN |
| 49 | BV | 116 | HIS |
| 49 | BV | 118 | GLN |
| 52 | BY | 66 | GLN |
| 52 | BY | 98 | ASN |
| 52 | BY | 120 | GLN |
| 53 | Ba | 36 | HIS |
| 53 | Ba | 57 | HIS |
| 54 | Bd | 48 | HIS |
| 55 | Bc | 99 | GLN |
| 56 | Bf | 75 | ASN |
| 57 | Be | 80 | GLN |
| 57 | Be | 159 | GLN |
| 57 | Be | 194 | HIS |
| 57 | Be | 222 | HIS |
| 57 | Be | 225 | GLN |
| 59 | Bh | 13 | HIS |
| 59 | Bh | 21 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 59 | Bh | 71 | HIS |
| 60 | Bi | 18 | ASN |
| 60 | Bi | 34 | HIS |
| 60 | Bi | 52 | GLN |
| 60 | Bi | 61 | GLN |
| 60 | Bi | 69 | HIS |
| 60 | Bi | 98 | GLN |
| 61 | Bj | 13 | HIS |
| 61 | Bj | 88 | ASN |
| 64 | Bl | 76 | ASN |
| 67 | Bp | 43 | ASN |
| 69 | Br | 20 | HIS |
| 74 | BQ | 32 | GLN |
| 74 | BQ | 45 | ASN |
| 74 | BQ | 151 | GLN |
| 74 | BQ | 203 | HIS |
| 76 | BS | 7 | HIS |
| 76 | BS | 76 | ASN |
| 76 | BS | 124 | GLN |
| 76 | BS | 145 | HIS |
| 77 | BI | 112 | GLN |

### 5.3.3 RNA (i)

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 78 | CA | 1485/1800 (82%) | 521 (35%) | 209 (14%) |
| 79 | CB | 74/75 (98%) | 26 (35%) | 10 (13%) |
| 80 | CC | 10/11 (90%) | 7 (70%) | 1 (10%) |
| 81 | DA | 3156/3396 (92%) | 1246 (39%) | 607 (19%) |
| 82 | DB | 142/158 (89%) | 65 (45%) | 36 (25%) |
| 83 | DC | 117/118 (99%) | 60 (51%) | 26 (22%) |
| All | All | 4984/5558 (89%) | 1925 (38%) | 889 (17%) |

All (1925) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 78 | CA | 3 | U |
| 78 | CA | 4 | C |
| 78 | CA | 5 | U |
| 78 | CA | 10 | G |
| 78 | CA | 11 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 78 | CA | 16 | G |
| 78 | CA | 26 | A |
| 78 | CA | 28 | A |
| 78 | CA | 29 | U |
| 78 | CA | 30 | G |
| 78 | CA | 31 | C |
| 78 | CA | 34 | G |
| 78 | CA | 37 | U |
| 78 | CA | 42 | G |
| 78 | CA | 45 | U |
| 78 | CA | 46 | A |
| 78 | CA | 47 | A |
| 78 | CA | 49 | C |
| 78 | CA | 50 | C |
| 78 | CA | 51 | A |
| 78 | CA | 55 | A |
| 78 | CA | 57 | G |
| 78 | CA | 58 | U |
| 78 | CA | 59 | C |
| 78 | CA | 60 | U |
| 78 | CA | 61 | A |
| 78 | CA | 65 | A |
| 78 | CA | 68 | A |
| 78 | CA | 70 | C |
| 78 | CA | 84 | A |
| 78 | CA | 87 | C |
| 78 | CA | 89 | G |
| 78 | CA | 93 | A |
| 78 | CA | 100 | A |
| 78 | CA | 101 | U |
| 78 | CA | 104 | A |
| 78 | CA | 105 | A |
| 78 | CA | 114 | C |
| 78 | CA | 115 | G |
| 78 | CA | 116 | U |
| 78 | CA | 117 | U |
| 78 | CA | 118 | U |
| 78 | CA | 119 | A |
| 78 | CA | 120 | U |
| 78 | CA | 123 | G |
| 78 | CA | 140 | A |
| 78 | CA | 141 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 78 | CA | 142 | G |
| 78 | CA | 146 | U |
| 78 | CA | 149 | C |
| 78 | CA | 151 | G |
| 78 | CA | 153 | G |
| 78 | CA | 156 | A |
| 78 | CA | 157 | A |
| 78 | CA | 158 | U |
| 78 | CA | 162 | A |
| 78 | CA | 163 | G |
| 78 | CA | 164 | A |
| 78 | CA | 169 | A |
| 78 | CA | 170 | U |
| 78 | CA | 172 | C |
| 78 | CA | 173 | A |
| 78 | CA | 174 | U |
| 78 | CA | 175 | G |
| 78 | CA | 178 | U |
| 78 | CA | 179 | A |
| 78 | CA | 180 | A |
| 78 | CA | 183 | U |
| 78 | CA | 184 | C |
| 78 | CA | 185 | U |
| 78 | CA | 189 | C |
| 78 | CA | 191 | C |
| 78 | CA | 192 | U |
| 78 | CA | 195 | G |
| 78 | CA | 196 | G |
| 78 | CA | 202 | A |
| 78 | CA | 206 | A |
| 78 | CA | 219 | A |
| 78 | CA | 220 | A |
| 78 | CA | 221 | A |
| 78 | CA | 222 | A |
| 78 | CA | 223 | U |
| 78 | CA | 229 | U |
| 78 | CA | 231 | U |
| 78 | CA | 235 | G |
| 78 | CA | 236 | A |
| 78 | CA | 252 | U |
| 78 | CA | 255 | U |
| 78 | CA | 256 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 78 | CA | 267 | U |
| 78 | CA | 271 | A |
| 78 | CA | 276 | C |
| 78 | CA | 279 | G |
| 78 | CA | 282 | C |
| 78 | CA | 288 | A |
| 78 | CA | 289 | U |
| 78 | CA | 294 | C |
| 78 | CA | 295 | A |
| 78 | CA | 298 | C |
| 78 | CA | 304 | U |
| 78 | CA | 305 | C |
| 78 | CA | 309 | C |
| 78 | CA | 310 | C |
| 78 | CA | 313 | U |
| 78 | CA | 316 | A |
| 78 | CA | 319 | U |
| 78 | CA | 320 | U |
| 78 | CA | 324 | U |
| 78 | CA | 335 | U |
| 78 | CA | 337 | G |
| 78 | CA | 338 | C |
| 78 | CA | 345 | U |
| 78 | CA | 348 | U |
| 78 | CA | 352 | A |
| 78 | CA | 354 | C |
| 78 | CA | 359 | A |
| 78 | CA | 361 | C |
| 78 | CA | 369 | A |
| 78 | CA | 373 | G |
| 78 | CA | 378 | A |
| 78 | CA | 387 | A |
| 78 | CA | 393 | C |
| 78 | CA | 394 | C |
| 78 | CA | 400 | A |
| 78 | CA | 401 | A |
| 78 | CA | 404 | G |
| 78 | CA | 413 | U |
| 78 | CA | 418 | G |
| 78 | CA | 421 | A |
| 78 | CA | 423 | G |
| 78 | CA | 424 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 78 | CA | 425 | A |
| 78 | CA | 426 | G |
| 78 | CA | 435 | C |
| 78 | CA | 438 | A |
| 78 | CA | 439 | U |
| 78 | CA | 444 | C |
| 78 | CA | 445 | A |
| 78 | CA | 449 | C |
| 78 | CA | 452 | A |
| 78 | CA | 453 | U |
| 78 | CA | 454 | U |
| 78 | CA | 455 | C |
| 78 | CA | 456 | A |
| 78 | CA | 459 | G |
| 78 | CA | 460 | A |
| 78 | CA | 461 | G |
| 78 | CA | 463 | U |
| 78 | CA | 468 | A |
| 78 | CA | 477 | A |
| 78 | CA | 478 | A |
| 78 | CA | 479 | C |
| 78 | CA | 481 | A |
| 78 | CA | 482 | U |
| 78 | CA | 483 | A |
| 78 | CA | 484 | C |
| 78 | CA | 486 | G |
| 78 | CA | 487 | G |
| 78 | CA | 489 | C |
| 78 | CA | 490 | C |
| 78 | CA | 491 | C |
| 78 | CA | 492 | A |
| 78 | CA | 493 | U |
| 78 | CA | 494 | U |
| 78 | CA | 496 | G |
| 78 | CA | 497 | G |
| 78 | CA | 498 | G |
| 78 | CA | 499 | U |
| 78 | CA | 500 | C |
| 78 | CA | 501 | U |
| 78 | CA | 502 | U |
| 78 | CA | 504 | U |
| 78 | CA | 505 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 78 | CA | 506 | A |
| 78 | CA | 508 | U |
| 78 | CA | 548 | G |
| 78 | CA | 551 | G |
| 78 | CA | 554 | C |
| 78 | CA | 555 | A |
| 78 | CA | 556 | A |
| 78 | CA | 558 | U |
| 78 | CA | 559 | C |
| 78 | CA | 565 | C |
| 78 | CA | 566 | C |
| 78 | CA | 571 | G |
| 78 | CA | 574 | G |
| 78 | CA | 577 | G |
| 78 | CA | 578 | U |
| 78 | CA | 579 | A |
| 78 | CA | 580 | A |
| 78 | CA | 581 | U |
| 78 | CA | 582 | U |
| 78 | CA | 586 | G |
| 78 | CA | 589 | C |
| 78 | CA | 591 | A |
| 78 | CA | 594 | A |
| 78 | CA | 597 | G |
| 78 | CA | 598 | U |
| 78 | CA | 604 | A |
| 78 | CA | 606 | A |
| 78 | CA | 607 | G |
| 78 | CA | 608 | U |
| 78 | CA | 611 | U |
| 78 | CA | 613 | G |
| 78 | CA | 618 | U |
| 78 | CA | 619 | A |
| 78 | CA | 620 | A |
| 78 | CA | 623 | A |
| 78 | CA | 624 | G |
| 78 | CA | 627 | C |
| 78 | CA | 629 | U |
| 78 | CA | 630 | A |
| 78 | CA | 631 | G |
| 78 | CA | 634 | G |
| 78 | CA | 635 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 78 | CA | 636 | A |
| 78 | CA | 637 | C |
| 78 | CA | 638 | U |
| 78 | CA | 645 | C |
| 78 | CA | 647 | G |
| 78 | CA | 650 | U |
| 78 | CA | 651 | G |
| 78 | CA | 652 | G |
| 78 | CA | 662 | U |
| 78 | CA | 671 | G |
| 78 | CA | 677 | G |
| 78 | CA | 678 | A |
| 78 | CA | 685 | A |
| 78 | CA | 690 | G |
| 78 | CA | 823 | G |
| 78 | CA | 825 | U |
| 78 | CA | 826 | U |
| 78 | CA | 830 | U |
| 78 | CA | 831 | U |
| 78 | CA | 832 | U |
| 78 | CA | 833 | U |
| 78 | CA | 838 | G |
| 78 | CA | 840 | U |
| 78 | CA | 841 | U |
| 78 | CA | 842 | C |
| 78 | CA | 843 | U |
| 78 | CA | 849 | C |
| 78 | CA | 853 | G |
| 78 | CA | 855 | A |
| 78 | CA | 857 | U |
| 78 | CA | 876 | G |
| 78 | CA | 886 | U |
| 78 | CA | 887 | A |
| 78 | CA | 888 | U |
| 78 | CA | 892 | A |
| 78 | CA | 893 | U |
| 78 | CA | 898 | A |
| 78 | CA | 899 | G |
| 78 | CA | 912 | U |
| 78 | CA | 913 | G |
| 78 | CA | 914 | G |
| 78 | CA | 921 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 78 | CA | 925 | G |
| 78 | CA | 926 | A |
| 78 | CA | 930 | A |
| 78 | CA | 934 | C |
| 78 | CA | 935 | U |
| 78 | CA | 942 | G |
| 78 | CA | 944 | A |
| 78 | CA | 945 | U |
| 78 | CA | 960 | U |
| 78 | CA | 963 | A |
| 78 | CA | 964 | U |
| 78 | CA | 966 | A |
| 78 | CA | 979 | A |
| 78 | CA | 1004 | U |
| 78 | CA | 1026 | A |
| 78 | CA | 1027 | A |
| 78 | CA | 1028 | C |
| 78 | CA | 1032 | G |
| 78 | CA | 1039 | A |
| 78 | CA | 1044 | U |
| 78 | CA | 1050 | G |
| 78 | CA | 1056 | U |
| 78 | CA | 1057 | U |
| 78 | CA | 1058 | U |
| 78 | CA | 1059 | U |
| 78 | CA | 1060 | U |
| 78 | CA | 1061 | A |
| 78 | CA | 1064 | G |
| 78 | CA | 1066 | C |
| 78 | CA | 1067 | C |
| 78 | CA | 1068 | C |
| 78 | CA | 1069 | A |
| 78 | CA | 1076 | A |
| 78 | CA | 1080 | U |
| 78 | CA | 1081 | A |
| 78 | CA | 1091 | A |
| 78 | CA | 1092 | A |
| 78 | CA | 1096 | C |
| 78 | CA | 1101 | G |
| 78 | CA | 1108 | G |
| 78 | CA | 1109 | G |
| 78 | CA | 1118 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 78 | CA | 1132 | A |
| 78 | CA | 1138 | A |
| 78 | CA | 1144 | U |
| 78 | CA | 1151 | A |
| 78 | CA | 1155 | G |
| 78 | CA | 1158 | C |
| 78 | CA | 1160 | A |
| 78 | CA | 1173 | C |
| 78 | CA | 1174 | C |
| 78 | CA | 1185 | U |
| 78 | CA | 1190 | C |
| 78 | CA | 1191 | U |
| 78 | CA | 1194 | A |
| 78 | CA | 1196 | A |
| 78 | CA | 1197 | C |
| 78 | CA | 1199 | G |
| 78 | CA | 1200 | G |
| 78 | CA | 1202 | A |
| 78 | CA | 1209 | C |
| 78 | CA | 1214 | U |
| 78 | CA | 1221 | A |
| 78 | CA | 1222 | C |
| 78 | CA | 1223 | A |
| 78 | CA | 1226 | A |
| 78 | CA | 1228 | G |
| 78 | CA | 1234 | A |
| 78 | CA | 1237 | G |
| 78 | CA | 1239 | U |
| 78 | CA | 1242 | A |
| 78 | CA | 1243 | G |
| 78 | CA | 1246 | C |
| 78 | CA | 1258 | U |
| 78 | CA | 1262 | U |
| 78 | CA | 1263 | G |
| 78 | CA | 1265 | G |
| 78 | CA | 1268 | G |
| 78 | CA | 1270 | G |
| 78 | CA | 1274 | C |
| 78 | CA | 1275 | A |
| 78 | CA | 1281 | G |
| 78 | CA | 1282 | U |
| 78 | CA | 1285 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 78 | CA | 1286 | U |
| 78 | CA | 1289 | U |
| 78 | CA | 1290 | U |
| 78 | CA | 1291 | G |
| 78 | CA | 1301 | U |
| 78 | CA | 1303 | U |
| 78 | CA | 1305 | U |
| 78 | CA | 1306 | C |
| 78 | CA | 1310 | U |
| 78 | CA | 1312 | A |
| 78 | CA | 1314 | U |
| 78 | CA | 1321 | A |
| 78 | CA | 1324 | G |
| 78 | CA | 1325 | A |
| 78 | CA | 1327 | C |
| 78 | CA | 1337 | A |
| 78 | CA | 1338 | C |
| 78 | CA | 1339 | C |
| 78 | CA | 1340 | U |
| 78 | CA | 1341 | A |
| 78 | CA | 1342 | C |
| 78 | CA | 1343 | U |
| 78 | CA | 1344 | A |
| 78 | CA | 1349 | G |
| 78 | CA | 1352 | G |
| 78 | CA | 1353 | U |
| 78 | CA | 1354 | G |
| 78 | CA | 1355 | C |
| 78 | CA | 1356 | U |
| 78 | CA | 1357 | A |
| 78 | CA | 1358 | G |
| 78 | CA | 1364 | G |
| 78 | CA | 1365 | C |
| 78 | CA | 1366 | U |
| 78 | CA | 1367 | G |
| 78 | CA | 1368 | G |
| 78 | CA | 1375 | A |
| 78 | CA | 1376 | C |
| 78 | CA | 1377 | U |
| 78 | CA | 1382 | A |
| 78 | CA | 1387 | G |
| 78 | CA | 1388 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 78 | CA | 1389 | C |
| 78 | CA | 1391 | A |
| 78 | CA | 1392 | U |
| 78 | CA | 1394 | G |
| 78 | CA | 1396 | U |
| 78 | CA | 1397 | U |
| 78 | CA | 1401 | A |
| 78 | CA | 1402 | G |
| 78 | CA | 1405 | G |
| 78 | CA | 1410 | A |
| 78 | CA | 1418 | G |
| 78 | CA | 1419 | G |
| 78 | CA | 1420 | C |
| 78 | CA | 1425 | A |
| 78 | CA | 1426 | C |
| 78 | CA | 1427 | A |
| 78 | CA | 1428 | G |
| 78 | CA | 1432 | U |
| 78 | CA | 1433 | G |
| 78 | CA | 1434 | U |
| 78 | CA | 1436 | A |
| 78 | CA | 1437 | U |
| 78 | CA | 1438 | G |
| 78 | CA | 1440 | C |
| 78 | CA | 1441 | C |
| 78 | CA | 1442 | U |
| 78 | CA | 1444 | A |
| 78 | CA | 1448 | G |
| 78 | CA | 1451 | C |
| 78 | CA | 1453 | G |
| 78 | CA | 1454 | G |
| 78 | CA | 1455 | G |
| 78 | CA | 1456 | C |
| 78 | CA | 1459 | C |
| 78 | CA | 1460 | A |
| 78 | CA | 1461 | C |
| 78 | CA | 1462 | G |
| 78 | CA | 1463 | C |
| 78 | CA | 1467 | C |
| 78 | CA | 1471 | A |
| 78 | CA | 1472 | C |
| 78 | CA | 1473 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 78 | CA | 1477 | G |
| 78 | CA | 1478 | G |
| 78 | CA | 1479 | A |
| 78 | CA | 1497 | U |
| 78 | CA | 1499 | G |
| 78 | CA | 1502 | G |
| 78 | CA | 1503 | A |
| 78 | CA | 1505 | A |
| 78 | CA | 1506 | G |
| 78 | CA | 1507 | G |
| 78 | CA | 1508 | U |
| 78 | CA | 1509 | C |
| 78 | CA | 1528 | U |
| 78 | CA | 1529 | C |
| 78 | CA | 1530 | C |
| 78 | CA | 1534 | G |
| 78 | CA | 1535 | U |
| 78 | CA | 1537 | C |
| 78 | CA | 1538 | U |
| 78 | CA | 1542 | G |
| 78 | CA | 1548 | G |
| 78 | CA | 1549 | C |
| 78 | CA | 1550 | A |
| 78 | CA | 1557 | U |
| 78 | CA | 1558 | U |
| 78 | CA | 1568 | C |
| 78 | CA | 1571 | C |
| 78 | CA | 1573 | A |
| 78 | CA | 1575 | G |
| 78 | CA | 1578 | U |
| 78 | CA | 1580 | C |
| 78 | CA | 1583 | A |
| 78 | CA | 1584 | G |
| 78 | CA | 1590 | G |
| 78 | CA | 1601 | G |
| 78 | CA | 1602 | C |
| 78 | CA | 1603 | U |
| 78 | CA | 1614 | A |
| 78 | CA | 1615 | C |
| 78 | CA | 1617 | U |
| 78 | CA | 1618 | C |
| 78 | CA | 1629 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 78 | CA | 1636 | C |
| 78 | CA | 1645 | G |
| 78 | CA | 1648 | A |
| 78 | CA | 1649 | G |
| 78 | CA | 1650 | U |
| 78 | CA | 1654 | G |
| 78 | CA | 1656 | U |
| 78 | CA | 1659 | A |
| 78 | CA | 1665 | U |
| 78 | CA | 1666 | U |
| 78 | CA | 1670 | G |
| 78 | CA | 1673 | G |
| 78 | CA | 1674 | C |
| 78 | CA | 1677 | C |
| 78 | CA | 1678 | A |
| 78 | CA | 1680 | G |
| 78 | CA | 1690 | G |
| 78 | CA | 1691 | A |
| 78 | CA | 1694 | A |
| 78 | CA | 1699 | G |
| 78 | CA | 1700 | C |
| 78 | CA | 1701 | A |
| 78 | CA | 1702 | A |
| 78 | CA | 1703 | C |
| 78 | CA | 1708 | U |
| 78 | CA | 1721 | A |
| 78 | CA | 1724 | U |
| 78 | CA | 1725 | U |
| 78 | CA | 1729 | C |
| 78 | CA | 1732 | A |
| 78 | CA | 1735 | U |
| 78 | CA | 1736 | G |
| 78 | CA | 1737 | G |
| 78 | CA | 1744 | A |
| 78 | CA | 1745 | G |
| 78 | CA | 1749 | A |
| 78 | CA | 1750 | A |
| 78 | CA | 1751 | C |
| 78 | CA | 1754 | A |
| 78 | CA | 1755 | A |
| 78 | CA | 1756 | A |
| 78 | CA | 1757 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 78 | CA | 1761 | U |
| 78 | CA | 1762 | A |
| 78 | CA | 1764 | C |
| 78 | CA | 1765 | A |
| 78 | CA | 1766 | A |
| 78 | CA | 1767 | G |
| 78 | CA | 1768 | G |
| 78 | CA | 1771 | U |
| 78 | CA | 1775 | U |
| 78 | CA | 1783 | C |
| 78 | CA | 1786 | G |
| 78 | CA | 1793 | G |
| 79 | CB | 8 | U |
| 79 | CB | 12 | U |
| 79 | CB | 13 | U |
| 79 | CB | 14 | A |
| 79 | CB | 17 | G |
| 79 | CB | 18 | G |
| 79 | CB | 19 | U |
| 79 | CB | 20 | C |
| 79 | CB | 21 | A |
| 79 | CB | 22 | G |
| 79 | CB | 26 | G |
| 79 | CB | 28 | G |
| 79 | CB | 32 | U |
| 79 | CB | 33 | U |
| 79 | CB | 37 | G |
| 79 | CB | 38 | C |
| 79 | CB | 42 | C |
| 79 | CB | 45 | G |
| 79 | CB | 47 | U |
| 79 | CB | 51 | G |
| 79 | CB | 60 | C |
| 79 | CB | 65 | U |
| 79 | CB | 68 | C |
| 79 | CB | 73 | C |
| 79 | CB | 74 | C |
| 79 | CB | 75 | A |
| 80 | CC | 13 | A |
| 80 | CC | 14 | A |
| 80 | CC | 18 | C |
| 80 | CC | 19 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 80 | CC | 20 | U |
| 80 | CC | 21 | C |
| 80 | CC | 22 | A |
| 81 | DA | 2 | U |
| 81 | DA | 3 | U |
| 81 | DA | 7 | C |
| 81 | DA | 8 | C |
| 81 | DA | 9 | U |
| 81 | DA | 21 | G |
| 81 | DA | 31 | C |
| 81 | DA | 32 | U |
| 81 | DA | 33 | G |
| 81 | DA | 37 | U |
| 81 | DA | 40 | A |
| 81 | DA | 43 | A |
| 81 | DA | 44 | U |
| 81 | DA | 50 | U |
| 81 | DA | 60 | A |
| 81 | DA | 61 | A |
| 81 | DA | 63 | A |
| 81 | DA | 64 | G |
| 81 | DA | 66 | A |
| 81 | DA | 72 | C |
| 81 | DA | 73 | C |
| 81 | DA | 74 | G |
| 81 | DA | 77 | A |
| 81 | DA | 92 | G |
| 81 | DA | 93 | C |
| 81 | DA | 105 | C |
| 81 | DA | 109 | A |
| 81 | DA | 110 | G |
| 81 | DA | 114 | A |
| 81 | DA | 134 | U |
| 81 | DA | 135 | C |
| 81 | DA | 136 | G |
| 81 | DA | 137 | G |
| 81 | DA | 160 | G |
| 81 | DA | 162 | G |
| 81 | DA | 167 | U |
| 81 | DA | 170 | G |
| 81 | DA | 171 | G |
| 81 | DA | 179 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 81 | DA | 186 | U |
| 81 | DA | 187 | A |
| 81 | DA | 190 | U |
| 81 | DA | 191 | U |
| 81 | DA | 210 | U |
| 81 | DA | 211 | A |
| 81 | DA | 212 | G |
| 81 | DA | 218 | G |
| 81 | DA | 219 | A |
| 81 | DA | 228 | U |
| 81 | DA | 229 | G |
| 81 | DA | 230 | U |
| 81 | DA | 231 | G |
| 81 | DA | 249 | U |
| 81 | DA | 250 | U |
| 81 | DA | 251 | G |
| 81 | DA | 261 | U |
| 81 | DA | 264 | G |
| 81 | DA | 265 | A |
| 81 | DA | 266 | A |
| 81 | DA | 267 | G |
| 81 | DA | 269 | G |
| 81 | DA | 281 | G |
| 81 | DA | 283 | G |
| 81 | DA | 285 | A |
| 81 | DA | 286 | U |
| 81 | DA | 295 | A |
| 81 | DA | 298 | U |
| 81 | DA | 299 | G |
| 81 | DA | 304 | G |
| 81 | DA | 305 | U |
| 81 | DA | 308 | A |
| 81 | DA | 311 | C |
| 81 | DA | 312 | C |
| 81 | DA | 327 | A |
| 81 | DA | 329 | U |
| 81 | DA | 330 | G |
| 81 | DA | 339 | C |
| 81 | DA | 342 | A |
| 81 | DA | 346 | C |
| 81 | DA | 350 | C |
| 81 | DA | 351 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 81 | DA | 367 | A |
| 81 | DA | 370 | U |
| 81 | DA | 374 | A |
| 81 | DA | 375 | A |
| 81 | DA | 376 | G |
| 81 | DA | 384 | A |
| 81 | DA | 385 | A |
| 81 | DA | 386 | A |
| 81 | DA | 387 | A |
| 81 | DA | 391 | A |
| 81 | DA | 398 | A |
| 81 | DA | 399 | A |
| 81 | DA | 400 | G |
| 81 | DA | 402 | A |
| 81 | DA | 403 | C |
| 81 | DA | 409 | A |
| 81 | DA | 420 | G |
| 81 | DA | 425 | G |
| 81 | DA | 426 | G |
| 81 | DA | 427 | C |
| 81 | DA | 430 | U |
| 81 | DA | 433 | A |
| 81 | DA | 434 | U |
| 81 | DA | 435 | C |
| 81 | DA | 436 | A |
| 81 | DA | 440 | A |
| 81 | DA | 441 | U |
| 81 | DA | 443 | G |
| 81 | DA | 444 | U |
| 81 | DA | 451 | U |
| 81 | DA | 453 | C |
| 81 | DA | 456 | U |
| 81 | DA | 457 | C |
| 81 | DA | 458 | U |
| 81 | DA | 460 | C |
| 81 | DA | 462 | C |
| 81 | DA | 463 | C |
| 81 | DA | 466 | G |
| 81 | DA | 467 | U |
| 81 | DA | 468 | G |
| 81 | DA | 469 | G |
| 81 | DA | 470 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 81 | DA | 471 | U |
| 81 | DA | 473 | G |
| 81 | DA | 474 | G |
| 81 | DA | 475 | G |
| 81 | DA | 476 | G |
| 81 | DA | 481 | U |
| 81 | DA | 482 | C |
| 81 | DA | 483 | G |
| 81 | DA | 484 | C |
| 81 | DA | 485 | A |
| 81 | DA | 489 | C |
| 81 | DA | 490 | A |
| 81 | DA | 491 | C |
| 81 | DA | 492 | U |
| 81 | DA | 493 | G |
| 81 | DA | 494 | G |
| 81 | DA | 495 | G |
| 81 | DA | 496 | C |
| 81 | DA | 497 | C |
| 81 | DA | 498 | A |
| 81 | DA | 500 | C |
| 81 | DA | 501 | A |
| 81 | DA | 502 | U |
| 81 | DA | 506 | U |
| 81 | DA | 507 | U |
| 81 | DA | 508 | U |
| 81 | DA | 510 | G |
| 81 | DA | 511 | G |
| 81 | DA | 512 | U |
| 81 | DA | 513 | G |
| 81 | DA | 516 | A |
| 81 | DA | 517 | G |
| 81 | DA | 518 | G |
| 81 | DA | 519 | A |
| 81 | DA | 520 | U |
| 81 | DA | 521 | A |
| 81 | DA | 523 | A |
| 81 | DA | 524 | U |
| 81 | DA | 525 | C |
| 81 | DA | 527 | A |
| 81 | DA | 528 | U |
| 81 | DA | 530 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 81 | DA | 532 | A |
| 81 | DA | 533 | A |
| 81 | DA | 534 | U |
| 81 | DA | 535 | G |
| 81 | DA | 536 | U |
| 81 | DA | 537 | A |
| 81 | DA | 538 | G |
| 81 | DA | 539 | C |
| 81 | DA | 540 | U |
| 81 | DA | 541 | U |
| 81 | DA | 544 | C |
| 81 | DA | 545 | U |
| 81 | DA | 547 | G |
| 81 | DA | 548 | G |
| 81 | DA | 549 | U |
| 81 | DA | 551 | A |
| 81 | DA | 552 | G |
| 81 | DA | 553 | U |
| 81 | DA | 555 | U |
| 81 | DA | 556 | U |
| 81 | DA | 557 | A |
| 81 | DA | 558 | U |
| 81 | DA | 559 | A |
| 81 | DA | 560 | G |
| 81 | DA | 561 | C |
| 81 | DA | 562 | C |
| 81 | DA | 563 | U |
| 81 | DA | 565 | U |
| 81 | DA | 567 | G |
| 81 | DA | 569 | A |
| 81 | DA | 570 | A |
| 81 | DA | 571 | U |
| 81 | DA | 573 | C |
| 81 | DA | 577 | C |
| 81 | DA | 578 | A |
| 81 | DA | 579 | G |
| 81 | DA | 581 | U |
| 81 | DA | 582 | G |
| 81 | DA | 583 | G |
| 81 | DA | 585 | A |
| 81 | DA | 586 | C |
| 81 | DA | 587 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 81 | DA | 593 | C |
| 81 | DA | 594 | U |
| 81 | DA | 595 | G |
| 81 | DA | 597 | G |
| 81 | DA | 599 | C |
| 81 | DA | 600 | G |
| 81 | DA | 601 | U |
| 81 | DA | 602 | A |
| 81 | DA | 603 | A |
| 81 | DA | 604 | G |
| 81 | DA | 606 | C |
| 81 | DA | 607 | A |
| 81 | DA | 608 | A |
| 81 | DA | 609 | G |
| 81 | DA | 612 | U |
| 81 | DA | 614 | C |
| 81 | DA | 616 | G |
| 81 | DA | 617 | G |
| 81 | DA | 623 | U |
| 81 | DA | 624 | G |
| 81 | DA | 626 | U |
| 81 | DA | 628 | A |
| 81 | DA | 629 | U |
| 81 | DA | 634 | C |
| 81 | DA | 635 | G |
| 81 | DA | 636 | C |
| 81 | DA | 637 | C |
| 81 | DA | 638 | C |
| 81 | DA | 639 | G |
| 81 | DA | 640 | U |
| 81 | DA | 641 | C |
| 81 | DA | 647 | A |
| 81 | DA | 648 | C |
| 81 | DA | 649 | A |
| 81 | DA | 652 | G |
| 81 | DA | 656 | A |
| 81 | DA | 662 | U |
| 81 | DA | 663 | C |
| 81 | DA | 671 | U |
| 81 | DA | 672 | A |
| 81 | DA | 673 | U |
| 81 | DA | 674 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 81 | DA | 675 | C |
| 81 | DA | 676 | G |
| 81 | DA | 677 | A |
| 81 | DA | 678 | G |
| 81 | DA | 679 | U |
| 81 | DA | 681 | U |
| 81 | DA | 682 | U |
| 81 | DA | 688 | G |
| 81 | DA | 689 | U |
| 81 | DA | 690 | A |
| 81 | DA | 691 | A |
| 81 | DA | 698 | U |
| 81 | DA | 699 | A |
| 81 | DA | 700 | C |
| 81 | DA | 701 | G |
| 81 | DA | 702 | C |
| 81 | DA | 703 | G |
| 81 | DA | 704 | U |
| 81 | DA | 705 | A |
| 81 | DA | 706 | A |
| 81 | DA | 709 | A |
| 81 | DA | 710 | A |
| 81 | DA | 714 | G |
| 81 | DA | 715 | A |
| 81 | DA | 723 | U |
| 81 | DA | 729 | C |
| 81 | DA | 730 | C |
| 81 | DA | 732 | C |
| 81 | DA | 733 | G |
| 81 | DA | 735 | A |
| 81 | DA | 736 | A |
| 81 | DA | 737 | G |
| 81 | DA | 740 | G |
| 81 | DA | 741 | U |
| 81 | DA | 742 | G |
| 81 | DA | 745 | C |
| 81 | DA | 751 | A |
| 81 | DA | 753 | C |
| 81 | DA | 763 | G |
| 81 | DA | 764 | U |
| 81 | DA | 765 | C |
| 81 | DA | 767 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 81 | DA | 768 | C |
| 81 | DA | 769 | G |
| 81 | DA | 770 | G |
| 81 | DA | 773 | G |
| 81 | DA | 781 | G |
| 81 | DA | 782 | U |
| 81 | DA | 783 | A |
| 81 | DA | 784 | A |
| 81 | DA | 785 | G |
| 81 | DA | 786 | A |
| 81 | DA | 787 | G |
| 81 | DA | 788 | C |
| 81 | DA | 789 | A |
| 81 | DA | 792 | G |
| 81 | DA | 793 | C |
| 81 | DA | 799 | G |
| 81 | DA | 800 | G |
| 81 | DA | 808 | A |
| 81 | DA | 813 | G |
| 81 | DA | 814 | U |
| 81 | DA | 817 | A |
| 81 | DA | 835 | G |
| 81 | DA | 837 | A |
| 81 | DA | 838 | G |
| 81 | DA | 839 | C |
| 81 | DA | 840 | C |
| 81 | DA | 843 | A |
| 81 | DA | 849 | C |
| 81 | DA | 852 | U |
| 81 | DA | 856 | G |
| 81 | DA | 857 | G |
| 81 | DA | 858 | A |
| 81 | DA | 859 | G |
| 81 | DA | 861 | C |
| 81 | DA | 862 | U |
| 81 | DA | 864 | G |
| 81 | DA | 865 | U |
| 81 | DA | 874 | U |
| 81 | DA | 879 | U |
| 81 | DA | 884 | A |
| 81 | DA | 888 | A |
| 81 | DA | 895 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 81 | DA | 896 | A |
| 81 | DA | 897 | U |
| 81 | DA | 900 | G |
| 81 | DA | 903 | U |
| 81 | DA | 907 | G |
| 81 | DA | 908 | G |
| 81 | DA | 914 | A |
| 81 | DA | 916 | G |
| 81 | DA | 917 | A |
| 81 | DA | 921 | A |
| 81 | DA | 924 | G |
| 81 | DA | 928 | C |
| 81 | DA | 933 | A |
| 81 | DA | 934 | G |
| 81 | DA | 937 | G |
| 81 | DA | 944 | C |
| 81 | DA | 948 | C |
| 81 | DA | 960 | U |
| 81 | DA | 962 | A |
| 81 | DA | 966 | U |
| 81 | DA | 969 | C |
| 81 | DA | 970 | A |
| 81 | DA | 975 | C |
| 81 | DA | 976 | U |
| 81 | DA | 977 | C |
| 81 | DA | 983 | A |
| 81 | DA | 985 | U |
| 81 | DA | 987 | U |
| 81 | DA | 991 | G |
| 81 | DA | 993 | G |
| 81 | DA | 994 | G |
| 81 | DA | 995 | U |
| 81 | DA | 996 | A |
| 81 | DA | 997 | A |
| 81 | DA | 1002 | A |
| 81 | DA | 1003 | A |
| 81 | DA | 1005 | G |
| 81 | DA | 1006 | A |
| 81 | DA | 1009 | A |
| 81 | DA | 1011 | A |
| 81 | DA | 1014 | U |
| 81 | DA | 1018 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 81 | DA | 1021 | G |
| 81 | DA | 1035 | G |
| 81 | DA | 1038 | C |
| 81 | DA | 1040 | A |
| 81 | DA | 1042 | U |
| 81 | DA | 1044 | U |
| 81 | DA | 1047 | A |
| 81 | DA | 1048 | A |
| 81 | DA | 1049 | C |
| 81 | DA | 1050 | U |
| 81 | DA | 1055 | A |
| 81 | DA | 1056 | U |
| 81 | DA | 1058 | U |
| 81 | DA | 1061 | A |
| 81 | DA | 1062 | A |
| 81 | DA | 1063 | G |
| 81 | DA | 1064 | A |
| 81 | DA | 1067 | U |
| 81 | DA | 1077 | U |
| 81 | DA | 1079 | A |
| 81 | DA | 1080 | A |
| 81 | DA | 1085 | A |
| 81 | DA | 1088 | U |
| 81 | DA | 1089 | G |
| 81 | DA | 1094 | U |
| 81 | DA | 1100 | U |
| 81 | DA | 1102 | A |
| 81 | DA | 1105 | A |
| 81 | DA | 1114 | U |
| 81 | DA | 1115 | G |
| 81 | DA | 1116 | G |
| 81 | DA | 1117 | G |
| 81 | DA | 1125 | U |
| 81 | DA | 1130 | A |
| 81 | DA | 1131 | G |
| 81 | DA | 1132 | C |
| 81 | DA | 1137 | C |
| 81 | DA | 1143 | A |
| 81 | DA | 1144 | U |
| 81 | DA | 1145 | G |
| 81 | DA | 1152 | G |
| 81 | DA | 1153 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 81 | DA | 1159 | A |
| 81 | DA | 1160 | C |
| 81 | DA | 1161 | G |
| 81 | DA | 1165 | A |
| 81 | DA | 1172 | G |
| 81 | DA | 1178 | G |
| 81 | DA | 1179 | A |
| 81 | DA | 1181 | U |
| 81 | DA | 1182 | A |
| 81 | DA | 1186 | G |
| 81 | DA | 1191 | U |
| 81 | DA | 1193 | A |
| 81 | DA | 1194 | G |
| 81 | DA | 1195 | A |
| 81 | DA | 1196 | C |
| 81 | DA | 1199 | C |
| 81 | DA | 1200 | A |
| 81 | DA | 1201 | C |
| 81 | DA | 1206 | G |
| 81 | DA | 1207 | G |
| 81 | DA | 1208 | U |
| 81 | DA | 1209 | G |
| 81 | DA | 1210 | U |
| 81 | DA | 1215 | U |
| 81 | DA | 1216 | C |
| 81 | DA | 1217 | A |
| 81 | DA | 1219 | C |
| 81 | DA | 1220 | U |
| 81 | DA | 1221 | A |
| 81 | DA | 1227 | C |
| 81 | DA | 1231 | A |
| 81 | DA | 1232 | C |
| 81 | DA | 1233 | G |
| 81 | DA | 1234 | G |
| 81 | DA | 1235 | U |
| 81 | DA | 1236 | G |
| 81 | DA | 1237 | G |
| 81 | DA | 1242 | G |
| 81 | DA | 1243 | G |
| 81 | DA | 1244 | A |
| 81 | DA | 1245 | A |
| 81 | DA | 1246 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 81 | DA | 1248 | C |
| 81 | DA | 1251 | A |
| 81 | DA | 1252 | A |
| 81 | DA | 1256 | G |
| 81 | DA | 1258 | U |
| 81 | DA | 1259 | A |
| 81 | DA | 1260 | A |
| 81 | DA | 1262 | G |
| 81 | DA | 1263 | A |
| 81 | DA | 1265 | U |
| 81 | DA | 1269 | U |
| 81 | DA | 1270 | A |
| 81 | DA | 1274 | A |
| 81 | DA | 1278 | A |
| 81 | DA | 1279 | C |
| 81 | DA | 1283 | C |
| 81 | DA | 1286 | A |
| 81 | DA | 1287 | A |
| 81 | DA | 1289 | G |
| 81 | DA | 1290 | A |
| 81 | DA | 1291 | A |
| 81 | DA | 1292 | C |
| 81 | DA | 1293 | U |
| 81 | DA | 1294 | A |
| 81 | DA | 1296 | C |
| 81 | DA | 1297 | C |
| 81 | DA | 1298 | C |
| 81 | DA | 1299 | U |
| 81 | DA | 1301 | A |
| 81 | DA | 1307 | G |
| 81 | DA | 1308 | A |
| 81 | DA | 1309 | U |
| 81 | DA | 1310 | G |
| 81 | DA | 1313 | G |
| 81 | DA | 1314 | C |
| 81 | DA | 1321 | G |
| 81 | DA | 1322 | U |
| 81 | DA | 1334 | U |
| 81 | DA | 1336 | U |
| 81 | DA | 1339 | C |
| 81 | DA | 1344 | G |
| 81 | DA | 1361 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 81 | DA | 1366 | A |
| 81 | DA | 1379 | G |
| 81 | DA | 1384 | U |
| 81 | DA | 1385 | C |
| 81 | DA | 1391 | C |
| 81 | DA | 1392 | G |
| 81 | DA | 1394 | A |
| 81 | DA | 1397 | C |
| 81 | DA | 1401 | A |
| 81 | DA | 1404 | G |
| 81 | DA | 1407 | A |
| 81 | DA | 1408 | G |
| 81 | DA | 1409 | G |
| 81 | DA | 1412 | G |
| 81 | DA | 1414 | G |
| 81 | DA | 1417 | G |
| 81 | DA | 1418 | A |
| 81 | DA | 1419 | A |
| 81 | DA | 1421 | G |
| 81 | DA | 1428 | A |
| 81 | DA | 1430 | U |
| 81 | DA | 1432 | C |
| 81 | DA | 1434 | G |
| 81 | DA | 1436 | U |
| 81 | DA | 1437 | C |
| 81 | DA | 1446 | A |
| 81 | DA | 1447 | G |
| 81 | DA | 1454 | A |
| 81 | DA | 1456 | A |
| 81 | DA | 1479 | U |
| 81 | DA | 1480 | G |
| 81 | DA | 1481 | A |
| 81 | DA | 1482 | A |
| 81 | DA | 1483 | G |
| 81 | DA | 1484 | U |
| 81 | DA | 1485 | G |
| 81 | DA | 1493 | G |
| 81 | DA | 1500 | G |
| 81 | DA | 1501 | U |
| 81 | DA | 1506 | A |
| 81 | DA | 1507 | G |
| 81 | DA | 1514 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 81 | DA | 1515 | A |
| 81 | DA | 1518 | U |
| 81 | DA | 1525 | G |
| 81 | DA | 1526 | U |
| 81 | DA | 1527 | C |
| 81 | DA | 1528 | G |
| 81 | DA | 1529 | A |
| 81 | DA | 1531 | C |
| 81 | DA | 1534 | A |
| 81 | DA | 1535 | A |
| 81 | DA | 1536 | G |
| 81 | DA | 1537 | A |
| 81 | DA | 1538 | G |
| 81 | DA | 1539 | A |
| 81 | DA | 1540 | U |
| 81 | DA | 1541 | G |
| 81 | DA | 1542 | G |
| 81 | DA | 1543 | G |
| 81 | DA | 1547 | G |
| 81 | DA | 1551 | C |
| 81 | DA | 1552 | G |
| 81 | DA | 1561 | G |
| 81 | DA | 1563 | C |
| 81 | DA | 1564 | U |
| 81 | DA | 1565 | G |
| 81 | DA | 1566 | A |
| 81 | DA | 1568 | U |
| 81 | DA | 1570 | U |
| 81 | DA | 1571 | A |
| 81 | DA | 1572 | U |
| 81 | DA | 1573 | G |
| 81 | DA | 1575 | A |
| 81 | DA | 1576 | G |
| 81 | DA | 1579 | C |
| 81 | DA | 1580 | A |
| 81 | DA | 1581 | C |
| 81 | DA | 1583 | A |
| 81 | DA | 1584 | U |
| 81 | DA | 1585 | C |
| 81 | DA | 1586 | G |
| 81 | DA | 1587 | A |
| 81 | DA | 1588 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 81 | DA | 1589 | A |
| 81 | DA | 1590 | G |
| 81 | DA | 1593 | A |
| 81 | DA | 1598 | G |
| 81 | DA | 1603 | A |
| 81 | DA | 1607 | U |
| 81 | DA | 1608 | C |
| 81 | DA | 1609 | C |
| 81 | DA | 1610 | G |
| 81 | DA | 1616 | U |
| 81 | DA | 1618 | G |
| 81 | DA | 1621 | A |
| 81 | DA | 1622 | U |
| 81 | DA | 1623 | G |
| 81 | DA | 1624 | G |
| 81 | DA | 1625 | A |
| 81 | DA | 1626 | U |
| 81 | DA | 1629 | U |
| 81 | DA | 1630 | U |
| 81 | DA | 1631 | C |
| 81 | DA | 1633 | C |
| 81 | DA | 1634 | G |
| 81 | DA | 1635 | G |
| 81 | DA | 1638 | A |
| 81 | DA | 1639 | C |
| 81 | DA | 1640 | G |
| 81 | DA | 1641 | U |
| 81 | DA | 1645 | U |
| 81 | DA | 1648 | A |
| 81 | DA | 1649 | U |
| 81 | DA | 1653 | G |
| 81 | DA | 1657 | C |
| 81 | DA | 1658 | G |
| 81 | DA | 1662 | G |
| 81 | DA | 1666 | G |
| 81 | DA | 1667 | A |
| 81 | DA | 1668 | G |
| 81 | DA | 1674 | G |
| 81 | DA | 1676 | A |
| 81 | DA | 1679 | A |
| 81 | DA | 1683 | A |
| 81 | DA | 1684 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 81 | DA | 1685 | C |
| 81 | DA | 1686 | U |
| 81 | DA | 1687 | U |
| 81 | DA | 1688 | U |
| 81 | DA | 1690 | C |
| 81 | DA | 1691 | U |
| 81 | DA | 1692 | U |
| 81 | DA | 1693 | C |
| 81 | DA | 1694 | U |
| 81 | DA | 1695 | U |
| 81 | DA | 1696 | A |
| 81 | DA | 1698 | C |
| 81 | DA | 1699 | A |
| 81 | DA | 1701 | C |
| 81 | DA | 1702 | U |
| 81 | DA | 1703 | U |
| 81 | DA | 1704 | A |
| 81 | DA | 1705 | U |
| 81 | DA | 1707 | A |
| 81 | DA | 1709 | C |
| 81 | DA | 1710 | C |
| 81 | DA | 1711 | C |
| 81 | DA | 1713 | G |
| 81 | DA | 1717 | U |
| 81 | DA | 1718 | G |
| 81 | DA | 1728 | G |
| 81 | DA | 1729 | A |
| 81 | DA | 1730 | G |
| 81 | DA | 1731 | A |
| 81 | DA | 1734 | G |
| 81 | DA | 1742 | U |
| 81 | DA | 1743 | G |
| 81 | DA | 1745 | C |
| 81 | DA | 1747 | G |
| 81 | DA | 1749 | A |
| 81 | DA | 1750 | A |
| 81 | DA | 1751 | G |
| 81 | DA | 1752 | A |
| 81 | DA | 1754 | G |
| 81 | DA | 1755 | C |
| 81 | DA | 1756 | C |
| 81 | DA | 1757 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 81 | DA | 1758 | G |
| 81 | DA | 1767 | C |
| 81 | DA | 1768 | U |
| 81 | DA | 1769 | G |
| 81 | DA | 1771 | C |
| 81 | DA | 1772 | U |
| 81 | DA | 1773 | C |
| 81 | DA | 1774 | C |
| 81 | DA | 1775 | G |
| 81 | DA | 1777 | U |
| 81 | DA | 1778 | G |
| 81 | DA | 1779 | C |
| 81 | DA | 1781 | C |
| 81 | DA | 1782 | U |
| 81 | DA | 1784 | G |
| 81 | DA | 1789 | G |
| 81 | DA | 1792 | C |
| 81 | DA | 1794 | G |
| 81 | DA | 1802 | C |
| 81 | DA | 1806 | A |
| 81 | DA | 1807 | G |
| 81 | DA | 1809 | A |
| 81 | DA | 1810 | A |
| 81 | DA | 1811 | G |
| 81 | DA | 1814 | A |
| 81 | DA | 1815 | U |
| 81 | DA | 1816 | A |
| 81 | DA | 1817 | G |
| 81 | DA | 1818 | U |
| 81 | DA | 1819 | U |
| 81 | DA | 1820 | U |
| 81 | DA | 1821 | U |
| 81 | DA | 1824 | U |
| 81 | DA | 1826 | C |
| 81 | DA | 1827 | C |
| 81 | DA | 1829 | G |
| 81 | DA | 1830 | G |
| 81 | DA | 1831 | U |
| 81 | DA | 1832 | C |
| 81 | DA | 1833 | G |
| 81 | DA | 1839 | A |
| 81 | DA | 1840 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 81 | DA | 1841 | A |
| 81 | DA | 1842 | A |
| 81 | DA | 1847 | A |
| 81 | DA | 1848 | G |
| 81 | DA | 1849 | C |
| 81 | DA | 1850 | A |
| 81 | DA | 1856 | C |
| 81 | DA | 1857 | C |
| 81 | DA | 1858 | A |
| 81 | DA | 1860 | G |
| 81 | DA | 1864 | A |
| 81 | DA | 1865 | A |
| 81 | DA | 1869 | C |
| 81 | DA | 1871 | U |
| 81 | DA | 1872 | C |
| 81 | DA | 1873 | U |
| 81 | DA | 1877 | U |
| 81 | DA | 1878 | G |
| 81 | DA | 1879 | A |
| 81 | DA | 1880 | U |
| 81 | DA | 1886 | A |
| 81 | DA | 1896 | A |
| 81 | DA | 1897 | G |
| 81 | DA | 1898 | G |
| 81 | DA | 1904 | C |
| 81 | DA | 1906 | G |
| 81 | DA | 1907 | C |
| 81 | DA | 1908 | A |
| 81 | DA | 1928 | G |
| 81 | DA | 1932 | A |
| 81 | DA | 1940 | G |
| 81 | DA | 1943 | C |
| 81 | DA | 1944 | U |
| 81 | DA | 1948 | G |
| 81 | DA | 1949 | G |
| 81 | DA | 1954 | G |
| 81 | DA | 1966 | U |
| 81 | DA | 1967 | U |
| 81 | DA | 1973 | G |
| 81 | DA | 1975 | C |
| 81 | DA | 1976 | G |
| 81 | DA | 1989 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 81 | DA | 1990 | U |
| 81 | DA | 1995 | A |
| 81 | DA | 2010 | U |
| 81 | DA | 2011 | U |
| 81 | DA | 2013 | C |
| 81 | DA | 2031 | U |
| 81 | DA | 2032 | U |
| 81 | DA | 2041 | U |
| 81 | DA | 2042 | G |
| 81 | DA | 2044 | U |
| 81 | DA | 2047 | A |
| 81 | DA | 2048 | G |
| 81 | DA | 2067 | U |
| 81 | DA | 2068 | U |
| 81 | DA | 2071 | A |
| 81 | DA | 2072 | G |
| 81 | DA | 2073 | A |
| 81 | DA | 2080 | C |
| 81 | DA | 2081 | U |
| 81 | DA | 2087 | C |
| 81 | DA | 2099 | A |
| 81 | DA | 2100 | A |
| 81 | DA | 2102 | U |
| 81 | DA | 2108 | C |
| 81 | DA | 2115 | G |
| 81 | DA | 2116 | G |
| 81 | DA | 2119 | A |
| 81 | DA | 2120 | A |
| 81 | DA | 2121 | G |
| 81 | DA | 2122 | G |
| 81 | DA | 2131 | A |
| 81 | DA | 2137 | U |
| 81 | DA | 2138 | A |
| 81 | DA | 2149 | A |
| 81 | DA | 2157 | G |
| 81 | DA | 2158 | A |
| 81 | DA | 2170 | U |
| 81 | DA | 2174 | G |
| 81 | DA | 2175 | U |
| 81 | DA | 2177 | G |
| 81 | DA | 2178 | A |
| 81 | DA | 2179 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 81 | DA | 2180 | G |
| 81 | DA | 2181 | C |
| 81 | DA | 2182 | A |
| 81 | DA | 2187 | G |
| 81 | DA | 2188 | A |
| 81 | DA | 2189 | U |
| 81 | DA | 2190 | U |
| 81 | DA | 2194 | G |
| 81 | DA | 2207 | A |
| 81 | DA | 2208 | A |
| 81 | DA | 2209 | U |
| 81 | DA | 2210 | G |
| 81 | DA | 2211 | U |
| 81 | DA | 2212 | C |
| 81 | DA | 2216 | G |
| 81 | DA | 2225 | U |
| 81 | DA | 2229 | A |
| 81 | DA | 2230 | C |
| 81 | DA | 2236 | G |
| 81 | DA | 2237 | C |
| 81 | DA | 2239 | G |
| 81 | DA | 2244 | A |
| 81 | DA | 2245 | C |
| 81 | DA | 2251 | G |
| 81 | DA | 2258 | U |
| 81 | DA | 2259 | A |
| 81 | DA | 2266 | U |
| 81 | DA | 2267 | C |
| 81 | DA | 2268 | U |
| 81 | DA | 2270 | A |
| 81 | DA | 2273 | G |
| 81 | DA | 2275 | A |
| 81 | DA | 2280 | A |
| 81 | DA | 2281 | A |
| 81 | DA | 2282 | U |
| 81 | DA | 2283 | G |
| 81 | DA | 2284 | C |
| 81 | DA | 2287 | C |
| 81 | DA | 2298 | U |
| 81 | DA | 2305 | G |
| 81 | DA | 2306 | C |
| 81 | DA | 2308 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 81 | DA | 2310 | U |
| 81 | DA | 2313 | A |
| 81 | DA | 2314 | U |
| 81 | DA | 2315 | G |
| 81 | DA | 2316 | G |
| 81 | DA | 2323 | G |
| 81 | DA | 2335 | G |
| 81 | DA | 2336 | U |
| 81 | DA | 2339 | C |
| 81 | DA | 2340 | U |
| 81 | DA | 2351 | U |
| 81 | DA | 2355 | G |
| 81 | DA | 2362 | C |
| 81 | DA | 2363 | A |
| 81 | DA | 2364 | G |
| 81 | DA | 2365 | C |
| 81 | DA | 2368 | A |
| 81 | DA | 2369 | G |
| 81 | DA | 2370 | G |
| 81 | DA | 2373 | A |
| 81 | DA | 2374 | C |
| 81 | DA | 2375 | G |
| 81 | DA | 2376 | G |
| 81 | DA | 2377 | G |
| 81 | DA | 2378 | C |
| 81 | DA | 2384 | A |
| 81 | DA | 2385 | G |
| 81 | DA | 2387 | A |
| 81 | DA | 2392 | C |
| 81 | DA | 2394 | G |
| 81 | DA | 2397 | A |
| 81 | DA | 2402 | A |
| 81 | DA | 2403 | G |
| 81 | DA | 2406 | C |
| 81 | DA | 2407 | C |
| 81 | DA | 2411 | U |
| 81 | DA | 2419 | A |
| 81 | DA | 2421 | U |
| 81 | DA | 2422 | C |
| 81 | DA | 2424 | A |
| 81 | DA | 2435 | G |
| 81 | DA | 2436 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 81 | DA | 2438 | A |
| 81 | DA | 2439 | A |
| 81 | DA | 2440 | G |
| 81 | DA | 2441 | A |
| 81 | DA | 2443 | A |
| 81 | DA | 2444 | C |
| 81 | DA | 2445 | A |
| 81 | DA | 2446 | U |
| 81 | DA | 2447 | A |
| 81 | DA | 2448 | G |
| 81 | DA | 2451 | G |
| 81 | DA | 2452 | G |
| 81 | DA | 2453 | U |
| 81 | DA | 2454 | G |
| 81 | DA | 2455 | U |
| 81 | DA | 2458 | A |
| 81 | DA | 2459 | A |
| 81 | DA | 2461 | A |
| 81 | DA | 2463 | G |
| 81 | DA | 2464 | U |
| 81 | DA | 2467 | G |
| 81 | DA | 2468 | A |
| 81 | DA | 2469 | G |
| 81 | DA | 2470 | C |
| 81 | DA | 2471 | U |
| 81 | DA | 2472 | U |
| 81 | DA | 2473 | C |
| 81 | DA | 2474 | G |
| 81 | DA | 2475 | G |
| 81 | DA | 2477 | G |
| 81 | DA | 2478 | C |
| 81 | DA | 2479 | C |
| 81 | DA | 2480 | A |
| 81 | DA | 2481 | G |
| 81 | DA | 2482 | U |
| 81 | DA | 2484 | A |
| 81 | DA | 2485 | A |
| 81 | DA | 2487 | U |
| 81 | DA | 2488 | A |
| 81 | DA | 2489 | C |
| 81 | DA | 2490 | C |
| 81 | DA | 2491 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 81 | DA | 2492 | C |
| 81 | DA | 2493 | U |
| 81 | DA | 2494 | A |
| 81 | DA | 2495 | C |
| 81 | DA | 2496 | C |
| 81 | DA | 2498 | U |
| 81 | DA | 2499 | U |
| 81 | DA | 2501 | U |
| 81 | DA | 2502 | A |
| 81 | DA | 2503 | G |
| 81 | DA | 2504 | U |
| 81 | DA | 2505 | U |
| 81 | DA | 2506 | U |
| 81 | DA | 2507 | C |
| 81 | DA | 2508 | U |
| 81 | DA | 2509 | U |
| 81 | DA | 2510 | U |
| 81 | DA | 2511 | A |
| 81 | DA | 2514 | U |
| 81 | DA | 2526 | C |
| 81 | DA | 2530 | G |
| 81 | DA | 2545 | C |
| 81 | DA | 2547 | A |
| 81 | DA | 2563 | G |
| 81 | DA | 2567 | C |
| 81 | DA | 2569 | A |
| 81 | DA | 2571 | U |
| 81 | DA | 2573 | G |
| 81 | DA | 2579 | G |
| 81 | DA | 2580 | A |
| 81 | DA | 2581 | U |
| 81 | DA | 2587 | U |
| 81 | DA | 2592 | G |
| 81 | DA | 2593 | A |
| 81 | DA | 2594 | C |
| 81 | DA | 2596 | U |
| 81 | DA | 2597 | U |
| 81 | DA | 2606 | G |
| 81 | DA | 2607 | G |
| 81 | DA | 2614 | G |
| 81 | DA | 2615 | G |
| 81 | DA | 2617 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 81 | DA | 2618 | G |
| 81 | DA | 2619 | G |
| 81 | DA | 2620 | G |
| 81 | DA | 2621 | G |
| 81 | DA | 2622 | C |
| 81 | DA | 2625 | C |
| 81 | DA | 2626 | A |
| 81 | DA | 2627 | C |
| 81 | DA | 2629 | U |
| 81 | DA | 2630 | C |
| 81 | DA | 2632 | G |
| 81 | DA | 2633 | U |
| 81 | DA | 2636 | A |
| 81 | DA | 2637 | A |
| 81 | DA | 2638 | C |
| 81 | DA | 2640 | A |
| 81 | DA | 2649 | A |
| 81 | DA | 2651 | G |
| 81 | DA | 2652 | U |
| 81 | DA | 2656 | A |
| 81 | DA | 2657 | A |
| 81 | DA | 2658 | G |
| 81 | DA | 2665 | U |
| 81 | DA | 2667 | A |
| 81 | DA | 2669 | G |
| 81 | DA | 2673 | A |
| 81 | DA | 2674 | A |
| 81 | DA | 2675 | C |
| 81 | DA | 2676 | A |
| 81 | DA | 2677 | G |
| 81 | DA | 2678 | A |
| 81 | DA | 2680 | A |
| 81 | DA | 2681 | U |
| 81 | DA | 2682 | C |
| 81 | DA | 2683 | U |
| 81 | DA | 2684 | C |
| 81 | DA | 2686 | A |
| 81 | DA | 2688 | U |
| 81 | DA | 2689 | A |
| 81 | DA | 2690 | G |
| 81 | DA | 2694 | A |
| 81 | DA | 2696 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 81 | DA | 2699 | G |
| 81 | DA | 2702 | A |
| 81 | DA | 2703 | A |
| 81 | DA | 2704 | A |
| 81 | DA | 2706 | G |
| 81 | DA | 2709 | C |
| 81 | DA | 2711 | C |
| 81 | DA | 2713 | U |
| 81 | DA | 2714 | G |
| 81 | DA | 2715 | A |
| 81 | DA | 2717 | U |
| 81 | DA | 2718 | U |
| 81 | DA | 2721 | A |
| 81 | DA | 2723 | U |
| 81 | DA | 2724 | U |
| 81 | DA | 2727 | A |
| 81 | DA | 2728 | G |
| 81 | DA | 2729 | U |
| 81 | DA | 2735 | U |
| 81 | DA | 2736 | A |
| 81 | DA | 2737 | C |
| 81 | DA | 2738 | A |
| 81 | DA | 2747 | A |
| 81 | DA | 2752 | U |
| 81 | DA | 2755 | C |
| 81 | DA | 2756 | C |
| 81 | DA | 2757 | U |
| 81 | DA | 2758 | A |
| 81 | DA | 2759 | U |
| 81 | DA | 2760 | C |
| 81 | DA | 2761 | G |
| 81 | DA | 2763 | U |
| 81 | DA | 2764 | C |
| 81 | DA | 2777 | G |
| 81 | DA | 2780 | A |
| 81 | DA | 2784 | G |
| 81 | DA | 2785 | A |
| 81 | DA | 2788 | C |
| 81 | DA | 2795 | U |
| 81 | DA | 2796 | G |
| 81 | DA | 2797 | C |
| 81 | DA | 2798 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 81 | DA | 2799 | A |
| 81 | DA | 2800 | G |
| 81 | DA | 2801 | A |
| 81 | DA | 2802 | A |
| 81 | DA | 2803 | A |
| 81 | DA | 2810 | C |
| 81 | DA | 2816 | G |
| 81 | DA | 2817 | A |
| 81 | DA | 2825 | C |
| 81 | DA | 2830 | G |
| 81 | DA | 2841 | G |
| 81 | DA | 2845 | A |
| 81 | DA | 2859 | U |
| 81 | DA | 2860 | U |
| 81 | DA | 2861 | U |
| 81 | DA | 2864 | A |
| 81 | DA | 2866 | U |
| 81 | DA | 2867 | C |
| 81 | DA | 2871 | G |
| 81 | DA | 2872 | A |
| 81 | DA | 2873 | U |
| 81 | DA | 2875 | U |
| 81 | DA | 2887 | A |
| 81 | DA | 2890 | A |
| 81 | DA | 2898 | G |
| 81 | DA | 2899 | C |
| 81 | DA | 2900 | A |
| 81 | DA | 2904 | U |
| 81 | DA | 2912 | G |
| 81 | DA | 2916 | U |
| 81 | DA | 2923 | U |
| 81 | DA | 2929 | C |
| 81 | DA | 2935 | U |
| 81 | DA | 2936 | A |
| 81 | DA | 2941 | A |
| 81 | DA | 2942 | C |
| 81 | DA | 2947 | G |
| 81 | DA | 2951 | G |
| 81 | DA | 2954 | U |
| 81 | DA | 2957 | G |
| 81 | DA | 2964 | G |
| 81 | DA | 2968 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 81 | DA | 2970 | C |
| 81 | DA | 2971 | A |
| 81 | DA | 2972 | G |
| 81 | DA | 2983 | C |
| 81 | DA | 2989 | U |
| 81 | DA | 2993 | G |
| 81 | DA | 2994 | A |
| 81 | DA | 2997 | G |
| 81 | DA | 2998 | U |
| 81 | DA | 2999 | U |
| 81 | DA | 3000 | A |
| 81 | DA | 3001 | C |
| 81 | DA | 3002 | C |
| 81 | DA | 3003 | G |
| 81 | DA | 3011 | A |
| 81 | DA | 3012 | A |
| 81 | DA | 3013 | U |
| 81 | DA | 3035 | A |
| 81 | DA | 3041 | U |
| 81 | DA | 3042 | U |
| 81 | DA | 3044 | G |
| 81 | DA | 3045 | G |
| 81 | DA | 3048 | A |
| 81 | DA | 3051 | U |
| 81 | DA | 3052 | G |
| 81 | DA | 3056 | U |
| 81 | DA | 3063 | C |
| 81 | DA | 3071 | U |
| 81 | DA | 3072 | C |
| 81 | DA | 3079 | U |
| 81 | DA | 3081 | C |
| 81 | DA | 3087 | A |
| 81 | DA | 3090 | U |
| 81 | DA | 3091 | A |
| 81 | DA | 3092 | C |
| 81 | DA | 3093 | C |
| 81 | DA | 3094 | A |
| 81 | DA | 3098 | G |
| 81 | DA | 3099 | C |
| 81 | DA | 3100 | U |
| 81 | DA | 3107 | U |
| 81 | DA | 3108 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 81 | DA | 3113 | A |
| 81 | DA | 3116 | G |
| 81 | DA | 3122 | A |
| 81 | DA | 3130 | A |
| 81 | DA | 3131 | U |
| 81 | DA | 3136 | G |
| 81 | DA | 3137 | C |
| 81 | DA | 3138 | U |
| 81 | DA | 3139 | A |
| 81 | DA | 3141 | A |
| 81 | DA | 3142 | A |
| 81 | DA | 3143 | C |
| 81 | DA | 3144 | G |
| 81 | DA | 3145 | C |
| 81 | DA | 3146 | G |
| 81 | DA | 3150 | A |
| 81 | DA | 3151 | U |
| 81 | DA | 3163 | A |
| 81 | DA | 3164 | C |
| 81 | DA | 3165 | A |
| 81 | DA | 3166 | C |
| 81 | DA | 3167 | A |
| 81 | DA | 3168 | A |
| 81 | DA | 3212 | C |
| 81 | DA | 3215 | A |
| 81 | DA | 3216 | G |
| 81 | DA | 3217 | C |
| 81 | DA | 3218 | A |
| 81 | DA | 3219 | G |
| 81 | DA | 3220 | G |
| 81 | DA | 3221 | C |
| 81 | DA | 3222 | U |
| 81 | DA | 3223 | A |
| 81 | DA | 3229 | G |
| 81 | DA | 3230 | G |
| 81 | DA | 3231 | U |
| 81 | DA | 3232 | G |
| 81 | DA | 3234 | A |
| 81 | DA | 3235 | C |
| 81 | DA | 3237 | U |
| 81 | DA | 3239 | G |
| 81 | DA | 3240 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 81 | DA | 3241 | G |
| 81 | DA | 3242 | G |
| 81 | DA | 3243 | A |
| 81 | DA | 3244 | A |
| 81 | DA | 3246 | G |
| 81 | DA | 3247 | G |
| 81 | DA | 3248 | C |
| 81 | DA | 3249 | C |
| 81 | DA | 3250 | U |
| 81 | DA | 3251 | U |
| 81 | DA | 3252 | G |
| 81 | DA | 3253 | G |
| 81 | DA | 3254 | G |
| 81 | DA | 3256 | G |
| 81 | DA | 3257 | C |
| 81 | DA | 3258 | U |
| 81 | DA | 3282 | U |
| 81 | DA | 3283 | U |
| 81 | DA | 3284 | G |
| 81 | DA | 3285 | C |
| 81 | DA | 3288 | G |
| 81 | DA | 3289 | G |
| 81 | DA | 3290 | G |
| 81 | DA | 3296 | A |
| 81 | DA | 3297 | U |
| 81 | DA | 3299 | A |
| 81 | DA | 3300 | U |
| 81 | DA | 3301 | U |
| 81 | DA | 3304 | U |
| 81 | DA | 3305 | A |
| 81 | DA | 3306 | U |
| 81 | DA | 3308 | C |
| 81 | DA | 3312 | U |
| 81 | DA | 3314 | A |
| 81 | DA | 3316 | A |
| 81 | DA | 3317 | U |
| 81 | DA | 3318 | G |
| 81 | DA | 3319 | U |
| 81 | DA | 3320 | A |
| 81 | DA | 3321 | C |
| 81 | DA | 3325 | G |
| 81 | DA | 3326 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 81 | DA | 3328 | G |
| 81 | DA | 3334 | U |
| 81 | DA | 3336 | A |
| 81 | DA | 3337 | G |
| 81 | DA | 3342 | A |
| 81 | DA | 3343 | G |
| 81 | DA | 3344 | A |
| 81 | DA | 3346 | U |
| 81 | DA | 3361 | G |
| 81 | DA | 3362 | A |
| 81 | DA | 3363 | U |
| 81 | DA | 3364 | C |
| 81 | DA | 3365 | U |
| 81 | DA | 3368 | U |
| 81 | DA | 3369 | G |
| 81 | DA | 3370 | A |
| 81 | DA | 3371 | G |
| 81 | DA | 3373 | U |
| 81 | DA | 3374 | U |
| 81 | DA | 3375 | A |
| 81 | DA | 3382 | U |
| 81 | DA | 3383 | G |
| 81 | DA | 3384 | U |
| 81 | DA | 3385 | U |
| 81 | DA | 3386 | G |
| 81 | DA | 3387 | U |
| 81 | DA | 3388 | C |
| 81 | DA | 3389 | U |
| 81 | DA | 3394 | U |
| 81 | DA | 3395 | G |
| 81 | DA | 3396 | U |
| 82 | DB | 3 | A |
| 82 | DB | 4 | C |
| 82 | DB | 20 | U |
| 82 | DB | 21 | C |
| 82 | DB | 23 | U |
| 82 | DB | 29 | U |
| 82 | DB | 34 | U |
| 82 | DB | 36 | G |
| 82 | DB | 37 | A |
| 82 | DB | 38 | U |
| 82 | DB | 39 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 82 | DB | 45 | C |
| 82 | DB | 47 | C |
| 82 | DB | 48 | A |
| 82 | DB | 49 | G |
| 82 | DB | 51 | G |
| 82 | DB | 52 | A |
| 82 | DB | 59 | A |
| 82 | DB | 60 | U |
| 82 | DB | 61 | A |
| 82 | DB | 62 | C |
| 82 | DB | 64 | U |
| 82 | DB | 66 | A |
| 82 | DB | 83 | C |
| 82 | DB | 84 | C |
| 82 | DB | 85 | G |
| 82 | DB | 86 | U |
| 82 | DB | 88 | A |
| 82 | DB | 89 | A |
| 82 | DB | 90 | U |
| 82 | DB | 91 | C |
| 82 | DB | 92 | A |
| 82 | DB | 94 | C |
| 82 | DB | 95 | G |
| 82 | DB | 96 | A |
| 82 | DB | 97 | A |
| 82 | DB | 98 | U |
| 82 | DB | 100 | U |
| 82 | DB | 104 | A |
| 82 | DB | 105 | A |
| 82 | DB | 106 | C |
| 82 | DB | 107 | G |
| 82 | DB | 111 | A |
| 82 | DB | 112 | U |
| 82 | DB | 120 | C |
| 82 | DB | 121 | U |
| 82 | DB | 122 | U |
| 82 | DB | 125 | U |
| 82 | DB | 126 | A |
| 82 | DB | 127 | U |
| 82 | DB | 128 | U |
| 82 | DB | 129 | C |
| 82 | DB | 132 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 82 | DB | 133 | G |
| 82 | DB | 134 | G |
| 82 | DB | 135 | G |
| 82 | DB | 138 | A |
| 82 | DB | 139 | U |
| 82 | DB | 145 | U |
| 82 | DB | 150 | G |
| 82 | DB | 151 | C |
| 82 | DB | 152 | G |
| 82 | DB | 154 | C |
| 82 | DB | 157 | U |
| 82 | DB | 158 | U |
| 83 | DC | 4 | U |
| 83 | DC | 9 | C |
| 83 | DC | 11 | A |
| 83 | DC | 13 | A |
| 83 | DC | 15 | C |
| 83 | DC | 16 | U |
| 83 | DC | 18 | C |
| 83 | DC | 19 | C |
| 83 | DC | 21 | G |
| 83 | DC | 22 | A |
| 83 | DC | 23 | A |
| 83 | DC | 24 | A |
| 83 | DC | 25 | G |
| 83 | DC | 26 | C |
| 83 | DC | 27 | A |
| 83 | DC | 28 | C |
| 83 | DC | 29 | C |
| 83 | DC | 30 | G |
| 83 | DC | 31 | U |
| 83 | DC | 32 | U |
| 83 | DC | 38 | U |
| 83 | DC | 39 | C |
| 83 | DC | 41 | G |
| 83 | DC | 42 | A |
| 83 | DC | 45 | A |
| 83 | DC | 46 | A |
| 83 | DC | 47 | C |
| 83 | DC | 48 | U |
| 83 | DC | 49 | G |
| 83 | DC | 50 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 83 | DC | 51 | G |
| 83 | DC | 52 | U |
| 83 | DC | 54 | A |
| 83 | DC | 55 | A |
| 83 | DC | 56 | G |
| 83 | DC | 58 | U |
| 83 | DC | 61 | U |
| 83 | DC | 62 | A |
| 83 | DC | 63 | G |
| 83 | DC | 64 | A |
| 83 | DC | 70 | A |
| 83 | DC | 71 | C |
| 83 | DC | 73 | G |
| 83 | DC | 74 | A |
| 83 | DC | 75 | G |
| 83 | DC | 76 | U |
| 83 | DC | 84 | G |
| 83 | DC | 86 | G |
| 83 | DC | 90 | C |
| 83 | DC | 93 | U |
| 83 | DC | 95 | C |
| 83 | DC | 99 | A |
| 83 | DC | 101 | A |
| 83 | DC | 102 | C |
| 83 | DC | 105 | A |
| 83 | DC | 108 | U |
| 83 | DC | 109 | G |
| 83 | DC | 114 | A |
| 83 | DC | 115 | A |
| 83 | DC | 116 | U |

All (889) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 78 | CA | 4 | C |
| 78 | CA | 10 | G |
| 78 | CA | 16 | G |
| 78 | CA | 25 | C |
| 78 | CA | 29 | U |
| 78 | CA | 36 | C |
| 78 | CA | 44 | U |
| 78 | CA | 45 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 78 | CA | 46 | A |
| 78 | CA | 49 | C |
| 78 | CA | 50 | C |
| 78 | CA | 56 | U |
| 78 | CA | 69 | G |
| 78 | CA | 70 | C |
| 78 | CA | 86 | A |
| 78 | CA | 88 | U |
| 78 | CA | 92 | A |
| 78 | CA | 103 | A |
| 78 | CA | 104 | A |
| 78 | CA | 117 | U |
| 78 | CA | 118 | U |
| 78 | CA | 120 | U |
| 78 | CA | 139 | C |
| 78 | CA | 140 | A |
| 78 | CA | 141 | U |
| 78 | CA | 150 | U |
| 78 | CA | 161 | U |
| 78 | CA | 163 | G |
| 78 | CA | 169 | A |
| 78 | CA | 172 | C |
| 78 | CA | 174 | U |
| 78 | CA | 177 | U |
| 78 | CA | 179 | A |
| 78 | CA | 183 | U |
| 78 | CA | 191 | C |
| 78 | CA | 194 | U |
| 78 | CA | 195 | G |
| 78 | CA | 205 | U |
| 78 | CA | 219 | A |
| 78 | CA | 220 | A |
| 78 | CA | 222 | A |
| 78 | CA | 228 | G |
| 78 | CA | 234 | G |
| 78 | CA | 275 | C |
| 78 | CA | 278 | U |
| 78 | CA | 281 | G |
| 78 | CA | 287 | G |
| 78 | CA | 288 | A |
| 78 | CA | 289 | U |
| 78 | CA | 293 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 78 | CA | 294 | C |
| 78 | CA | 303 | U |
| 78 | CA | 304 | U |
| 78 | CA | 305 | C |
| 78 | CA | 306 | U |
| 78 | CA | 309 | C |
| 78 | CA | 312 | A |
| 78 | CA | 315 | A |
| 78 | CA | 337 | G |
| 78 | CA | 392 | G |
| 78 | CA | 400 | A |
| 78 | CA | 434 | G |
| 78 | CA | 438 | A |
| 78 | CA | 448 | C |
| 78 | CA | 462 | G |
| 78 | CA | 474 | A |
| 78 | CA | 478 | A |
| 78 | CA | 481 | A |
| 78 | CA | 485 | A |
| 78 | CA | 488 | G |
| 78 | CA | 489 | C |
| 78 | CA | 490 | C |
| 78 | CA | 500 | C |
| 78 | CA | 501 | U |
| 78 | CA | 504 | U |
| 78 | CA | 555 | A |
| 78 | CA | 558 | U |
| 78 | CA | 565 | C |
| 78 | CA | 577 | G |
| 78 | CA | 580 | A |
| 78 | CA | 588 | U |
| 78 | CA | 590 | C |
| 78 | CA | 606 | A |
| 78 | CA | 607 | G |
| 78 | CA | 613 | G |
| 78 | CA | 622 | A |
| 78 | CA | 626 | U |
| 78 | CA | 629 | U |
| 78 | CA | 630 | A |
| 78 | CA | 631 | G |
| 78 | CA | 636 | A |
| 78 | CA | 637 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 78 | CA | 646 | C |
| 78 | CA | 650 | U |
| 78 | CA | 658 | C |
| 78 | CA | 661 | A |
| 78 | CA | 670 | U |
| 78 | CA | 689 | G |
| 78 | CA | 824 | G |
| 78 | CA | 825 | U |
| 78 | CA | 837 | G |
| 78 | CA | 838 | G |
| 78 | CA | 842 | C |
| 78 | CA | 852 | C |
| 78 | CA | 886 | U |
| 78 | CA | 891 | A |
| 78 | CA | 898 | A |
| 78 | CA | 924 | A |
| 78 | CA | 955 | A |
| 78 | CA | 959 | U |
| 78 | CA | 960 | U |
| 78 | CA | 963 | A |
| 78 | CA | 978 | A |
| 78 | CA | 1057 | U |
| 78 | CA | 1058 | U |
| 78 | CA | 1063 | U |
| 78 | CA | 1066 | C |
| 78 | CA | 1067 | C |
| 78 | CA | 1068 | C |
| 78 | CA | 1080 | U |
| 78 | CA | 1090 | C |
| 78 | CA | 1096 | C |
| 78 | CA | 1108 | G |
| 78 | CA | 1137 | A |
| 78 | CA | 1173 | C |
| 78 | CA | 1190 | C |
| 78 | CA | 1196 | A |
| 78 | CA | 1220 | C |
| 78 | CA | 1221 | A |
| 78 | CA | 1222 | C |
| 78 | CA | 1233 | G |
| 78 | CA | 1281 | G |
| 78 | CA | 1284 | C |
| 78 | CA | 1285 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 78 | CA | 1302 | U |
| 78 | CA | 1324 | G |
| 78 | CA | 1338 | C |
| 78 | CA | 1339 | C |
| 78 | CA | 1340 | U |
| 78 | CA | 1342 | C |
| 78 | CA | 1351 | G |
| 78 | CA | 1355 | C |
| 78 | CA | 1356 | U |
| 78 | CA | 1357 | A |
| 78 | CA | 1359 | C |
| 78 | CA | 1364 | G |
| 78 | CA | 1381 | U |
| 78 | CA | 1388 | A |
| 78 | CA | 1389 | C |
| 78 | CA | 1393 | C |
| 78 | CA | 1394 | G |
| 78 | CA | 1396 | U |
| 78 | CA | 1398 | U |
| 78 | CA | 1401 | A |
| 78 | CA | 1409 | G |
| 78 | CA | 1419 | G |
| 78 | CA | 1425 | A |
| 78 | CA | 1427 | A |
| 78 | CA | 1432 | U |
| 78 | CA | 1434 | U |
| 78 | CA | 1436 | A |
| 78 | CA | 1437 | U |
| 78 | CA | 1441 | C |
| 78 | CA | 1452 | U |
| 78 | CA | 1459 | C |
| 78 | CA | 1460 | A |
| 78 | CA | 1461 | C |
| 78 | CA | 1462 | G |
| 78 | CA | 1472 | C |
| 78 | CA | 1476 | C |
| 78 | CA | 1501 | C |
| 78 | CA | 1507 | G |
| 78 | CA | 1508 | U |
| 78 | CA | 1529 | C |
| 78 | CA | 1533 | C |
| 78 | CA | 1537 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 78 | CA | 1539 | G |
| 78 | CA | 1547 | A |
| 78 | CA | 1548 | G |
| 78 | CA | 1585 | U |
| 78 | CA | 1601 | G |
| 78 | CA | 1617 | U |
| 78 | CA | 1647 | U |
| 78 | CA | 1649 | G |
| 78 | CA | 1658 | G |
| 78 | CA | 1666 | U |
| 78 | CA | 1672 | G |
| 78 | CA | 1677 | C |
| 78 | CA | 1691 | A |
| 78 | CA | 1698 | G |
| 78 | CA | 1700 | C |
| 78 | CA | 1701 | A |
| 78 | CA | 1702 | A |
| 78 | CA | 1720 | G |
| 78 | CA | 1724 | U |
| 78 | CA | 1731 | A |
| 78 | CA | 1735 | U |
| 78 | CA | 1736 | G |
| 78 | CA | 1743 | U |
| 78 | CA | 1744 | A |
| 78 | CA | 1746 | A |
| 78 | CA | 1748 | G |
| 78 | CA | 1753 | A |
| 78 | CA | 1755 | A |
| 78 | CA | 1761 | U |
| 78 | CA | 1765 | A |
| 78 | CA | 1767 | G |
| 78 | CA | 1785 | U |
| 78 | CA | 1792 | G |
| 79 | CB | 11 | U |
| 79 | CB | 12 | U |
| 79 | CB | 13 | U |
| 79 | CB | 25 | U |
| 79 | CB | 32 | U |
| 79 | CB | 37 | G |
| 79 | CB | 44 | A |
| 79 | CB | 64 | G |
| 79 | CB | 72 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 79 | CB | 73 | C |
| 80 | CC | 20 | U |
| 81 | DA | 1 | G |
| 81 | DA | 8 | C |
| 81 | DA | 20 | A |
| 81 | DA | 21 | G |
| 81 | DA | 31 | C |
| 81 | DA | 32 | U |
| 81 | DA | 43 | A |
| 81 | DA | 49 | A |
| 81 | DA | 62 | A |
| 81 | DA | 63 | A |
| 81 | DA | 65 | A |
| 81 | DA | 71 | A |
| 81 | DA | 72 | C |
| 81 | DA | 73 | C |
| 81 | DA | 104 | G |
| 81 | DA | 124 | U |
| 81 | DA | 136 | G |
| 81 | DA | 166 | C |
| 81 | DA | 178 | U |
| 81 | DA | 185 | C |
| 81 | DA | 186 | U |
| 81 | DA | 209 | A |
| 81 | DA | 210 | U |
| 81 | DA | 211 | A |
| 81 | DA | 228 | U |
| 81 | DA | 229 | G |
| 81 | DA | 248 | U |
| 81 | DA | 249 | U |
| 81 | DA | 250 | U |
| 81 | DA | 263 | C |
| 81 | DA | 266 | A |
| 81 | DA | 282 | G |
| 81 | DA | 298 | U |
| 81 | DA | 310 | U |
| 81 | DA | 326 | U |
| 81 | DA | 331 | G |
| 81 | DA | 338 | A |
| 81 | DA | 341 | G |
| 81 | DA | 369 | A |
| 81 | DA | 374 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 81 | DA | 384 | A |
| 81 | DA | 385 | A |
| 81 | DA | 402 | A |
| 81 | DA | 406 | G |
| 81 | DA | 408 | A |
| 81 | DA | 419 | G |
| 81 | DA | 425 | G |
| 81 | DA | 432 | G |
| 81 | DA | 434 | U |
| 81 | DA | 442 | G |
| 81 | DA | 450 | G |
| 81 | DA | 466 | G |
| 81 | DA | 468 | G |
| 81 | DA | 472 | A |
| 81 | DA | 474 | G |
| 81 | DA | 476 | G |
| 81 | DA | 485 | A |
| 81 | DA | 491 | C |
| 81 | DA | 512 | U |
| 81 | DA | 521 | A |
| 81 | DA | 523 | A |
| 81 | DA | 527 | A |
| 81 | DA | 534 | U |
| 81 | DA | 535 | G |
| 81 | DA | 537 | A |
| 81 | DA | 538 | G |
| 81 | DA | 540 | U |
| 81 | DA | 556 | U |
| 81 | DA | 562 | C |
| 81 | DA | 566 | G |
| 81 | DA | 568 | G |
| 81 | DA | 572 | A |
| 81 | DA | 586 | C |
| 81 | DA | 588 | G |
| 81 | DA | 594 | U |
| 81 | DA | 596 | C |
| 81 | DA | 599 | C |
| 81 | DA | 602 | A |
| 81 | DA | 606 | C |
| 81 | DA | 607 | A |
| 81 | DA | 608 | A |
| 81 | DA | 609 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 81 | DA | 618 | C |
| 81 | DA | 623 | U |
| 81 | DA | 637 | C |
| 81 | DA | 638 | C |
| 81 | DA | 640 | U |
| 81 | DA | 647 | A |
| 81 | DA | 651 | G |
| 81 | DA | 655 | C |
| 81 | DA | 663 | C |
| 81 | DA | 670 | C |
| 81 | DA | 671 | U |
| 81 | DA | 672 | A |
| 81 | DA | 673 | U |
| 81 | DA | 674 | G |
| 81 | DA | 676 | G |
| 81 | DA | 677 | A |
| 81 | DA | 678 | G |
| 81 | DA | 681 | U |
| 81 | DA | 690 | A |
| 81 | DA | 699 | A |
| 81 | DA | 701 | G |
| 81 | DA | 702 | C |
| 81 | DA | 704 | U |
| 81 | DA | 708 | G |
| 81 | DA | 714 | G |
| 81 | DA | 720 | A |
| 81 | DA | 728 | G |
| 81 | DA | 734 | C |
| 81 | DA | 735 | A |
| 81 | DA | 736 | A |
| 81 | DA | 740 | G |
| 81 | DA | 741 | U |
| 81 | DA | 744 | A |
| 81 | DA | 750 | G |
| 81 | DA | 752 | C |
| 81 | DA | 764 | U |
| 81 | DA | 768 | C |
| 81 | DA | 769 | G |
| 81 | DA | 783 | A |
| 81 | DA | 786 | A |
| 81 | DA | 798 | G |
| 81 | DA | 807 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 81 | DA | 813 | G |
| 81 | DA | 834 | U |
| 81 | DA | 837 | A |
| 81 | DA | 838 | G |
| 81 | DA | 839 | C |
| 81 | DA | 842 | G |
| 81 | DA | 851 | C |
| 81 | DA | 855 | U |
| 81 | DA | 858 | A |
| 81 | DA | 861 | C |
| 81 | DA | 873 | C |
| 81 | DA | 887 | G |
| 81 | DA | 894 | G |
| 81 | DA | 896 | A |
| 81 | DA | 899 | U |
| 81 | DA | 916 | G |
| 81 | DA | 932 | U |
| 81 | DA | 933 | A |
| 81 | DA | 959 | C |
| 81 | DA | 968 | G |
| 81 | DA | 969 | C |
| 81 | DA | 975 | C |
| 81 | DA | 984 | G |
| 81 | DA | 986 | U |
| 81 | DA | 992 | A |
| 81 | DA | 995 | U |
| 81 | DA | 996 | A |
| 81 | DA | 1001 | G |
| 81 | DA | 1006 | A |
| 81 | DA | 1008 | U |
| 81 | DA | 1017 | C |
| 81 | DA | 1020 | G |
| 81 | DA | 1021 | G |
| 81 | DA | 1039 | U |
| 81 | DA | 1046 | A |
| 81 | DA | 1047 | A |
| 81 | DA | 1050 | U |
| 81 | DA | 1054 | A |
| 81 | DA | 1055 | A |
| 81 | DA | 1057 | A |
| 81 | DA | 1061 | A |
| 81 | DA | 1063 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 81 | DA | 1064 | A |
| 81 | DA | 1079 | A |
| 81 | DA | 1084 | A |
| 81 | DA | 1088 | U |
| 81 | DA | 1114 | U |
| 81 | DA | 1115 | G |
| 81 | DA | 1116 | G |
| 81 | DA | 1131 | G |
| 81 | DA | 1144 | U |
| 81 | DA | 1152 | G |
| 81 | DA | 1160 | C |
| 81 | DA | 1164 | G |
| 81 | DA | 1178 | G |
| 81 | DA | 1180 | A |
| 81 | DA | 1185 | C |
| 81 | DA | 1193 | A |
| 81 | DA | 1194 | G |
| 81 | DA | 1198 | C |
| 81 | DA | 1206 | G |
| 81 | DA | 1208 | U |
| 81 | DA | 1209 | G |
| 81 | DA | 1214 | U |
| 81 | DA | 1215 | U |
| 81 | DA | 1220 | U |
| 81 | DA | 1221 | A |
| 81 | DA | 1226 | G |
| 81 | DA | 1232 | C |
| 81 | DA | 1233 | G |
| 81 | DA | 1241 | U |
| 81 | DA | 1242 | G |
| 81 | DA | 1243 | G |
| 81 | DA | 1244 | A |
| 81 | DA | 1251 | A |
| 81 | DA | 1258 | U |
| 81 | DA | 1259 | A |
| 81 | DA | 1261 | G |
| 81 | DA | 1263 | A |
| 81 | DA | 1268 | G |
| 81 | DA | 1277 | C |
| 81 | DA | 1282 | G |
| 81 | DA | 1285 | G |
| 81 | DA | 1288 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 81 | DA | 1289 | G |
| 81 | DA | 1290 | A |
| 81 | DA | 1291 | A |
| 81 | DA | 1292 | C |
| 81 | DA | 1293 | U |
| 81 | DA | 1296 | C |
| 81 | DA | 1297 | C |
| 81 | DA | 1298 | C |
| 81 | DA | 1301 | A |
| 81 | DA | 1303 | A |
| 81 | DA | 1317 | A |
| 81 | DA | 1320 | C |
| 81 | DA | 1333 | C |
| 81 | DA | 1338 | C |
| 81 | DA | 1344 | G |
| 81 | DA | 1366 | A |
| 81 | DA | 1378 | U |
| 81 | DA | 1384 | U |
| 81 | DA | 1390 | A |
| 81 | DA | 1391 | C |
| 81 | DA | 1406 | A |
| 81 | DA | 1408 | G |
| 81 | DA | 1413 | G |
| 81 | DA | 1427 | U |
| 81 | DA | 1429 | G |
| 81 | DA | 1435 | A |
| 81 | DA | 1454 | A |
| 81 | DA | 1455 | U |
| 81 | DA | 1481 | A |
| 81 | DA | 1482 | A |
| 81 | DA | 1483 | G |
| 81 | DA | 1484 | U |
| 81 | DA | 1500 | G |
| 81 | DA | 1505 | C |
| 81 | DA | 1524 | A |
| 81 | DA | 1526 | U |
| 81 | DA | 1527 | C |
| 81 | DA | 1528 | G |
| 81 | DA | 1534 | A |
| 81 | DA | 1535 | A |
| 81 | DA | 1536 | G |
| 81 | DA | 1537 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 81 | DA | 1539 | A |
| 81 | DA | 1542 | G |
| 81 | DA | 1543 | G |
| 81 | DA | 1560 | G |
| 81 | DA | 1562 | C |
| 81 | DA | 1563 | C |
| 81 | DA | 1567 | U |
| 81 | DA | 1569 | U |
| 81 | DA | 1571 | A |
| 81 | DA | 1572 | U |
| 81 | DA | 1576 | G |
| 81 | DA | 1578 | C |
| 81 | DA | 1579 | C |
| 81 | DA | 1583 | A |
| 81 | DA | 1588 | A |
| 81 | DA | 1602 | A |
| 81 | DA | 1605 | A |
| 81 | DA | 1609 | C |
| 81 | DA | 1615 | C |
| 81 | DA | 1617 | G |
| 81 | DA | 1621 | A |
| 81 | DA | 1622 | U |
| 81 | DA | 1623 | G |
| 81 | DA | 1624 | G |
| 81 | DA | 1632 | A |
| 81 | DA | 1633 | C |
| 81 | DA | 1637 | A |
| 81 | DA | 1639 | C |
| 81 | DA | 1648 | A |
| 81 | DA | 1656 | A |
| 81 | DA | 1657 | C |
| 81 | DA | 1661 | G |
| 81 | DA | 1666 | G |
| 81 | DA | 1667 | A |
| 81 | DA | 1675 | G |
| 81 | DA | 1678 | G |
| 81 | DA | 1682 | U |
| 81 | DA | 1684 | U |
| 81 | DA | 1685 | C |
| 81 | DA | 1687 | U |
| 81 | DA | 1689 | U |
| 81 | DA | 1692 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 81 | DA | 1698 | C |
| 81 | DA | 1699 | A |
| 81 | DA | 1701 | C |
| 81 | DA | 1704 | A |
| 81 | DA | 1709 | C |
| 81 | DA | 1712 | G |
| 81 | DA | 1730 | G |
| 81 | DA | 1741 | A |
| 81 | DA | 1744 | G |
| 81 | DA | 1745 | C |
| 81 | DA | 1746 | U |
| 81 | DA | 1748 | G |
| 81 | DA | 1750 | A |
| 81 | DA | 1753 | G |
| 81 | DA | 1755 | C |
| 81 | DA | 1756 | C |
| 81 | DA | 1766 | G |
| 81 | DA | 1767 | C |
| 81 | DA | 1770 | G |
| 81 | DA | 1771 | C |
| 81 | DA | 1772 | U |
| 81 | DA | 1773 | C |
| 81 | DA | 1774 | C |
| 81 | DA | 1777 | U |
| 81 | DA | 1778 | G |
| 81 | DA | 1781 | C |
| 81 | DA | 1783 | U |
| 81 | DA | 1788 | C |
| 81 | DA | 1801 | U |
| 81 | DA | 1806 | A |
| 81 | DA | 1810 | A |
| 81 | DA | 1814 | A |
| 81 | DA | 1818 | U |
| 81 | DA | 1819 | U |
| 81 | DA | 1820 | U |
| 81 | DA | 1823 | A |
| 81 | DA | 1824 | U |
| 81 | DA | 1825 | G |
| 81 | DA | 1826 | C |
| 81 | DA | 1828 | A |
| 81 | DA | 1831 | U |
| 81 | DA | 1832 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 81 | DA | 1840 | U |
| 81 | DA | 1841 | A |
| 81 | DA | 1847 | A |
| 81 | DA | 1856 | C |
| 81 | DA | 1870 | C |
| 81 | DA | 1872 | C |
| 81 | DA | 1876 | U |
| 81 | DA | 1877 | U |
| 81 | DA | 1883 | A |
| 81 | DA | 1884 | A |
| 81 | DA | 1939 | G |
| 81 | DA | 1942 | U |
| 81 | DA | 1943 | C |
| 81 | DA | 1948 | G |
| 81 | DA | 1965 | C |
| 81 | DA | 1966 | U |
| 81 | DA | 1972 | A |
| 81 | DA | 1974 | A |
| 81 | DA | 2030 | C |
| 81 | DA | 2031 | U |
| 81 | DA | 2041 | U |
| 81 | DA | 2043 | U |
| 81 | DA | 2046 | U |
| 81 | DA | 2047 | A |
| 81 | DA | 2067 | U |
| 81 | DA | 2070 | U |
| 81 | DA | 2071 | A |
| 81 | DA | 2072 | G |
| 81 | DA | 2080 | C |
| 81 | DA | 2086 | A |
| 81 | DA | 2100 | A |
| 81 | DA | 2107 | A |
| 81 | DA | 2114 | C |
| 81 | DA | 2130 | G |
| 81 | DA | 2137 | U |
| 81 | DA | 2148 | U |
| 81 | DA | 2157 | G |
| 81 | DA | 2174 | G |
| 81 | DA | 2177 | G |
| 81 | DA | 2178 | A |
| 81 | DA | 2179 | C |
| 81 | DA | 2186 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 81 | DA | 2187 | G |
| 81 | DA | 2208 | A |
| 81 | DA | 2209 | U |
| 81 | DA | 2211 | U |
| 81 | DA | 2224 | A |
| 81 | DA | 2228 | A |
| 81 | DA | 2236 | G |
| 81 | DA | 2238 | G |
| 81 | DA | 2244 | A |
| 81 | DA | 2254 | U |
| 81 | DA | 2266 | U |
| 81 | DA | 2267 | C |
| 81 | DA | 2269 | U |
| 81 | DA | 2279 | A |
| 81 | DA | 2280 | A |
| 81 | DA | 2281 | A |
| 81 | DA | 2283 | G |
| 81 | DA | 2286 | U |
| 81 | DA | 2304 | C |
| 81 | DA | 2307 | G |
| 81 | DA | 2313 | A |
| 81 | DA | 2315 | G |
| 81 | DA | 2322 | C |
| 81 | DA | 2334 | U |
| 81 | DA | 2339 | C |
| 81 | DA | 2362 | C |
| 81 | DA | 2363 | A |
| 81 | DA | 2364 | G |
| 81 | DA | 2369 | G |
| 81 | DA | 2375 | G |
| 81 | DA | 2376 | G |
| 81 | DA | 2377 | G |
| 81 | DA | 2384 | A |
| 81 | DA | 2391 | G |
| 81 | DA | 2405 | C |
| 81 | DA | 2406 | C |
| 81 | DA | 2410 | U |
| 81 | DA | 2423 | U |
| 81 | DA | 2434 | U |
| 81 | DA | 2437 | G |
| 81 | DA | 2439 | A |
| 81 | DA | 2445 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 81 | DA | 2446 | U |
| 81 | DA | 2447 | A |
| 81 | DA | 2450 | G |
| 81 | DA | 2462 | A |
| 81 | DA | 2463 | G |
| 81 | DA | 2468 | A |
| 81 | DA | 2469 | G |
| 81 | DA | 2479 | C |
| 81 | DA | 2480 | A |
| 81 | DA | 2483 | G |
| 81 | DA | 2486 | A |
| 81 | DA | 2487 | U |
| 81 | DA | 2489 | C |
| 81 | DA | 2492 | C |
| 81 | DA | 2493 | U |
| 81 | DA | 2494 | A |
| 81 | DA | 2495 | C |
| 81 | DA | 2497 | U |
| 81 | DA | 2500 | A |
| 81 | DA | 2501 | U |
| 81 | DA | 2502 | A |
| 81 | DA | 2503 | G |
| 81 | DA | 2504 | U |
| 81 | DA | 2506 | U |
| 81 | DA | 2507 | C |
| 81 | DA | 2508 | U |
| 81 | DA | 2509 | U |
| 81 | DA | 2510 | U |
| 81 | DA | 2513 | U |
| 81 | DA | 2529 | A |
| 81 | DA | 2544 | U |
| 81 | DA | 2546 | C |
| 81 | DA | 2562 | A |
| 81 | DA | 2566 | C |
| 81 | DA | 2570 | U |
| 81 | DA | 2571 | U |
| 81 | DA | 2578 | U |
| 81 | DA | 2579 | G |
| 81 | DA | 2591 | A |
| 81 | DA | 2593 | A |
| 81 | DA | 2596 | U |
| 81 | DA | 2613 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 81 | DA | 2614 | G |
| 81 | DA | 2617 | U |
| 81 | DA | 2618 | G |
| 81 | DA | 2619 | G |
| 81 | DA | 2625 | C |
| 81 | DA | 2626 | A |
| 81 | DA | 2631 | U |
| 81 | DA | 2637 | A |
| 81 | DA | 2640 | A |
| 81 | DA | 2648 | G |
| 81 | DA | 2651 | G |
| 81 | DA | 2655 | U |
| 81 | DA | 2666 | C |
| 81 | DA | 2668 | U |
| 81 | DA | 2672 | G |
| 81 | DA | 2676 | A |
| 81 | DA | 2681 | U |
| 81 | DA | 2682 | C |
| 81 | DA | 2683 | U |
| 81 | DA | 2688 | U |
| 81 | DA | 2698 | G |
| 81 | DA | 2703 | A |
| 81 | DA | 2705 | A |
| 81 | DA | 2708 | C |
| 81 | DA | 2710 | C |
| 81 | DA | 2712 | U |
| 81 | DA | 2714 | G |
| 81 | DA | 2715 | A |
| 81 | DA | 2722 | U |
| 81 | DA | 2723 | U |
| 81 | DA | 2734 | A |
| 81 | DA | 2735 | U |
| 81 | DA | 2736 | A |
| 81 | DA | 2748 | A |
| 81 | DA | 2754 | G |
| 81 | DA | 2755 | C |
| 81 | DA | 2756 | C |
| 81 | DA | 2757 | U |
| 81 | DA | 2758 | A |
| 81 | DA | 2760 | C |
| 81 | DA | 2762 | A |
| 81 | DA | 2763 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 81 | DA | 2779 | A |
| 81 | DA | 2783 | U |
| 81 | DA | 2784 | G |
| 81 | DA | 2787 | G |
| 81 | DA | 2794 | G |
| 81 | DA | 2797 | C |
| 81 | DA | 2799 | A |
| 81 | DA | 2801 | A |
| 81 | DA | 2802 | A |
| 81 | DA | 2816 | G |
| 81 | DA | 2829 | U |
| 81 | DA | 2840 | C |
| 81 | DA | 2860 | U |
| 81 | DA | 2865 | U |
| 81 | DA | 2870 | C |
| 81 | DA | 2872 | A |
| 81 | DA | 2889 | C |
| 81 | DA | 2916 | U |
| 81 | DA | 2928 | C |
| 81 | DA | 2934 | A |
| 81 | DA | 2941 | A |
| 81 | DA | 2950 | G |
| 81 | DA | 2970 | C |
| 81 | DA | 2971 | A |
| 81 | DA | 2988 | C |
| 81 | DA | 2992 | U |
| 81 | DA | 2993 | G |
| 81 | DA | 2997 | G |
| 81 | DA | 2998 | U |
| 81 | DA | 2999 | U |
| 81 | DA | 3001 | C |
| 81 | DA | 3002 | C |
| 81 | DA | 3010 | U |
| 81 | DA | 3034 | C |
| 81 | DA | 3041 | U |
| 81 | DA | 3044 | G |
| 81 | DA | 3047 | U |
| 81 | DA | 3050 | U |
| 81 | DA | 3051 | U |
| 81 | DA | 3062 | G |
| 81 | DA | 3078 | U |
| 81 | DA | 3080 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 81 | DA | 3086 | A |
| 81 | DA | 3090 | U |
| 81 | DA | 3092 | C |
| 81 | DA | 3093 | C |
| 81 | DA | 3107 | U |
| 81 | DA | 3121 | U |
| 81 | DA | 3136 | G |
| 81 | DA | 3137 | C |
| 81 | DA | 3141 | A |
| 81 | DA | 3142 | A |
| 81 | DA | 3143 | C |
| 81 | DA | 3144 | G |
| 81 | DA | 3145 | C |
| 81 | DA | 3151 | U |
| 81 | DA | 3167 | A |
| 81 | DA | 3169 | U |
| 81 | DA | 3214 | U |
| 81 | DA | 3215 | A |
| 81 | DA | 3217 | C |
| 81 | DA | 3218 | A |
| 81 | DA | 3219 | G |
| 81 | DA | 3220 | G |
| 81 | DA | 3221 | C |
| 81 | DA | 3222 | U |
| 81 | DA | 3224 | G |
| 81 | DA | 3231 | U |
| 81 | DA | 3236 | U |
| 81 | DA | 3240 | C |
| 81 | DA | 3243 | A |
| 81 | DA | 3245 | A |
| 81 | DA | 3246 | G |
| 81 | DA | 3247 | G |
| 81 | DA | 3248 | C |
| 81 | DA | 3252 | G |
| 81 | DA | 3255 | U |
| 81 | DA | 3258 | U |
| 81 | DA | 3288 | G |
| 81 | DA | 3296 | A |
| 81 | DA | 3299 | A |
| 81 | DA | 3300 | U |
| 81 | DA | 3303 | G |
| 81 | DA | 3304 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 81 | DA | 3305 | A |
| 81 | DA | 3311 | C |
| 81 | DA | 3313 | U |
| 81 | DA | 3316 | A |
| 81 | DA | 3319 | U |
| 81 | DA | 3320 | A |
| 81 | DA | 3341 | U |
| 81 | DA | 3344 | A |
| 81 | DA | 3345 | G |
| 81 | DA | 3361 | G |
| 81 | DA | 3368 | U |
| 81 | DA | 3373 | U |
| 81 | DA | 3381 | U |
| 81 | DA | 3382 | U |
| 81 | DA | 3383 | G |
| 81 | DA | 3384 | U |
| 81 | DA | 3385 | U |
| 81 | DA | 3386 | G |
| 81 | DA | 3387 | U |
| 81 | DA | 3394 | U |
| 81 | DA | 3395 | G |
| 82 | DB | 2 | A |
| 82 | DB | 20 | U |
| 82 | DB | 38 | U |
| 82 | DB | 39 | G |
| 82 | DB | 44 | A |
| 82 | DB | 47 | C |
| 82 | DB | 51 | G |
| 82 | DB | 63 | G |
| 82 | DB | 65 | A |
| 82 | DB | 83 | C |
| 82 | DB | 87 | G |
| 82 | DB | 88 | A |
| 82 | DB | 89 | A |
| 82 | DB | 90 | U |
| 82 | DB | 93 | U |
| 82 | DB | 94 | C |
| 82 | DB | 95 | G |
| 82 | DB | 96 | A |
| 82 | DB | 97 | A |
| 82 | DB | 106 | C |
| 82 | DB | 120 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 82 | DB | 121 | U |
| 82 | DB | 124 | G |
| 82 | DB | 126 | A |
| 82 | DB | 128 | U |
| 82 | DB | 131 | A |
| 82 | DB | 132 | G |
| 82 | DB | 134 | G |
| 82 | DB | 137 | C |
| 82 | DB | 138 | A |
| 82 | DB | 144 | G |
| 82 | DB | 149 | A |
| 82 | DB | 150 | G |
| 82 | DB | 151 | C |
| 82 | DB | 153 | U |
| 82 | DB | 156 | U |
| 83 | DC | 2 | G |
| 83 | DC | 3 | U |
| 83 | DC | 8 | G |
| 83 | DC | 12 | U |
| 83 | DC | 15 | C |
| 83 | DC | 18 | C |
| 83 | DC | 22 | A |
| 83 | DC | 23 | A |
| 83 | DC | 24 | A |
| 83 | DC | 26 | C |
| 83 | DC | 28 | C |
| 83 | DC | 29 | C |
| 83 | DC | 30 | G |
| 83 | DC | 31 | U |
| 83 | DC | 32 | U |
| 83 | DC | 41 | G |
| 83 | DC | 44 | C |
| 83 | DC | 46 | A |
| 83 | DC | 48 | U |
| 83 | DC | 49 | G |
| 83 | DC | 51 | G |
| 83 | DC | 53 | U |
| 83 | DC | 72 | C |
| 83 | DC | 75 | G |
| 83 | DC | 83 | U |
| 83 | DC | 100 | A |

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

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

## 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)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|---|---|---|
| 78 | CA | 4 |
| 44 | BO | 3 |
| 23 | AW | 1 |
| 80 | CC | 1 |
| 74 | BQ | 1 |
| 76 | BS | 1 |
| 20 | AS | 1 |
| 7 | AG | 1 |
| 14 | AM | 1 |
| 34 | BE | 1 |
| 32 | BC | 1 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|---|---|---|---|---|---|---|
| 1 | AW | 31:UNK | C | 59:UNK | N | 10.96 |
| 1 | CC | 18:C | O3' | 19:U | P | 2.07 |
| 1 | CA | 1255:G | O3' | 1256:A | P | 1.94 |
| 1 | BQ | 39:GLN | C | 40:HIS | N | 1.90 |
| 1 | CA | 1254:U | O3' | 1255:G | P | 1.83 |
| 1 | BO | 21:ARG | C | 22:ILE | N | 1.82 |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|---|---|---|---|---|---|---|
| 1 | CA | 1189:A | O3' | 1190:C | P | 1.81 |
| 1 | CA | 120:U | O3' | 121:U | P | 1.78 |
| 1 | BS | 84:GLN | C | 85:SER | N | 1.20 |
| 1 | AS | 53:TRP | C | 54:PHE | N | 1.18 |
| 1 | AG | 106:UNK | C | 107:UNK | N | 1.17 |
| 1 | AM | 12:GLN | C | 13:HIS | N | 1.17 |
| 1 | BE | 54:VAL | C | 55:ARG | N | 1.16 |
| 1 | BC | 371:GLN | C | 372:THR | N | 1.14 |
| 1 | BO | 73:LEU | C | 74:ASN | N | 1.03 |
| 1 | BO | 20:GLY | C | 21:ARG | N | 0.61 |

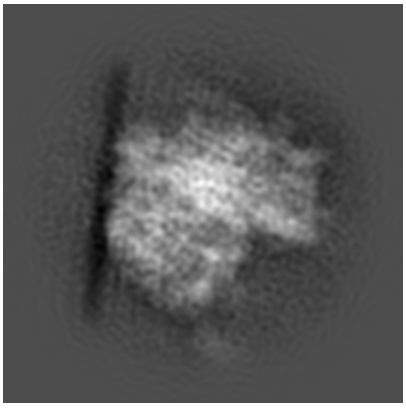
# 6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-1669. These allow visual inspection of the internal detail of the map and identification of artifacts.

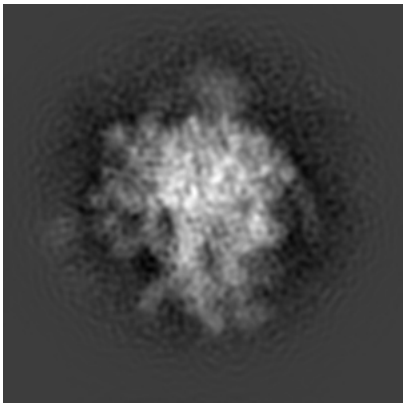
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

## 6.1 Orthogonal projections (i)

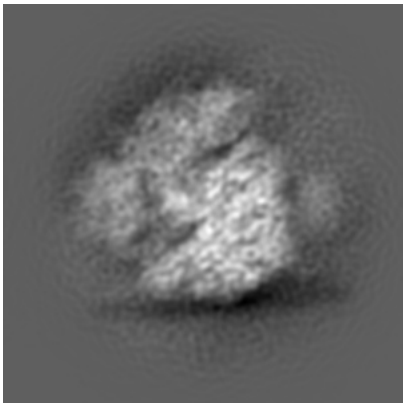
### 6.1.1 Primary map



X



Y

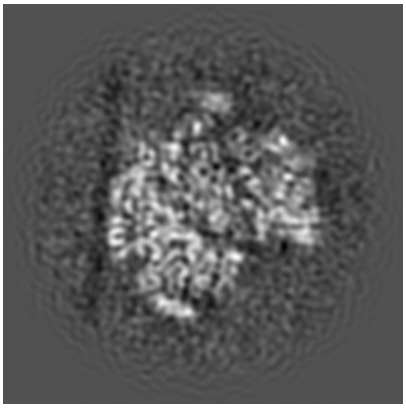


Z

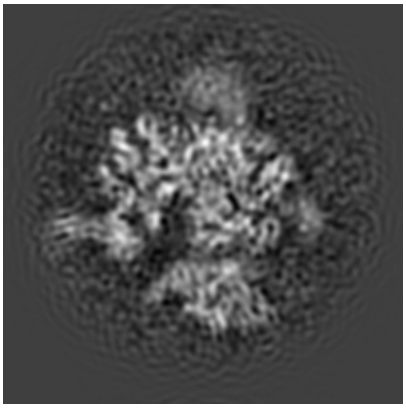
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

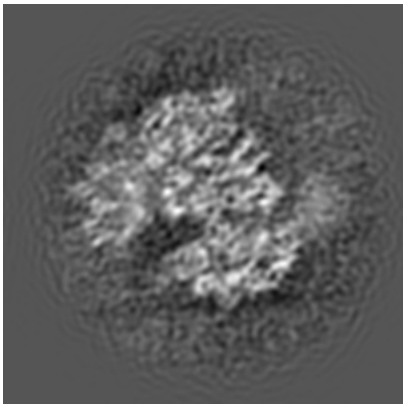
### 6.2.1 Primary map



X Index: 184



Y Index: 184

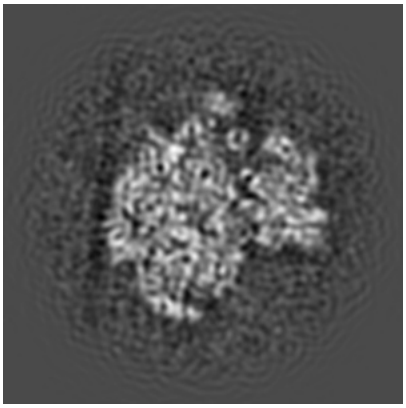


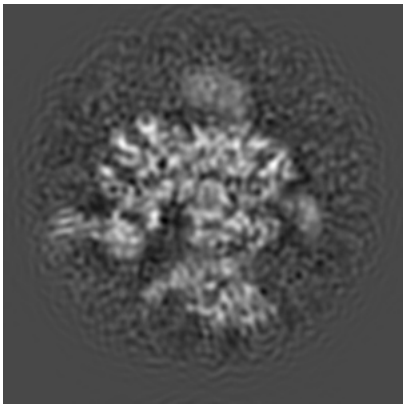
Z Index: 184

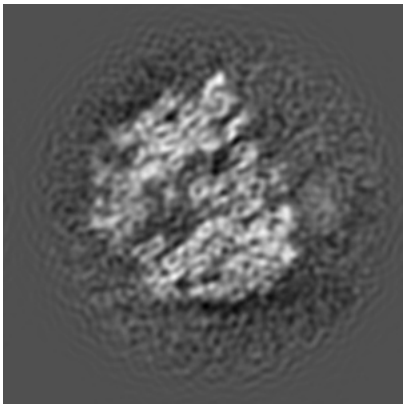
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

### 6.3.1 Primary map


X Index: 188

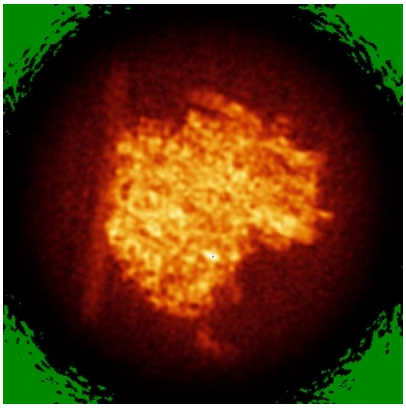

Y Index: 187

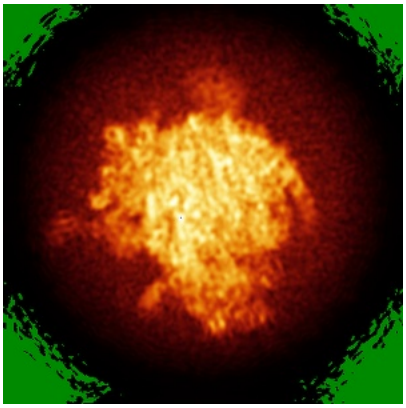

Z Index: 172

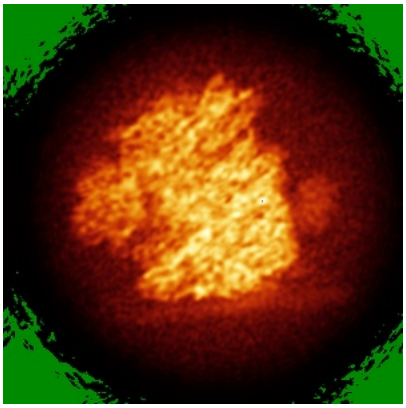
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map


X

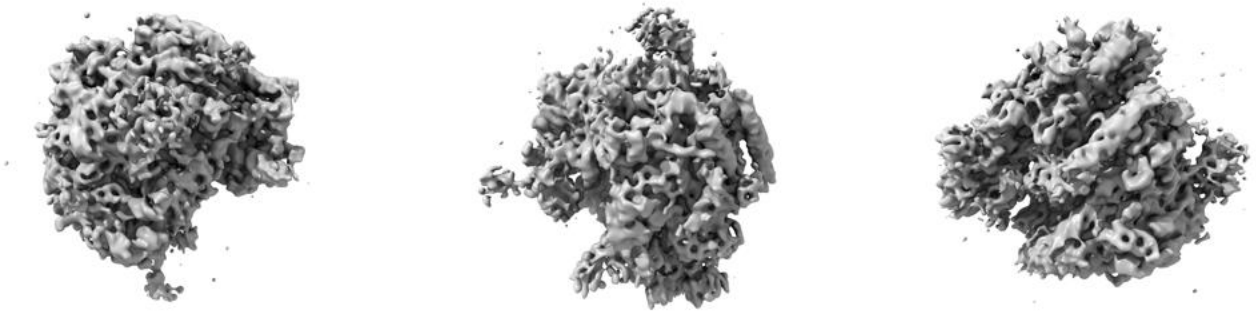

Y


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 1.75. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

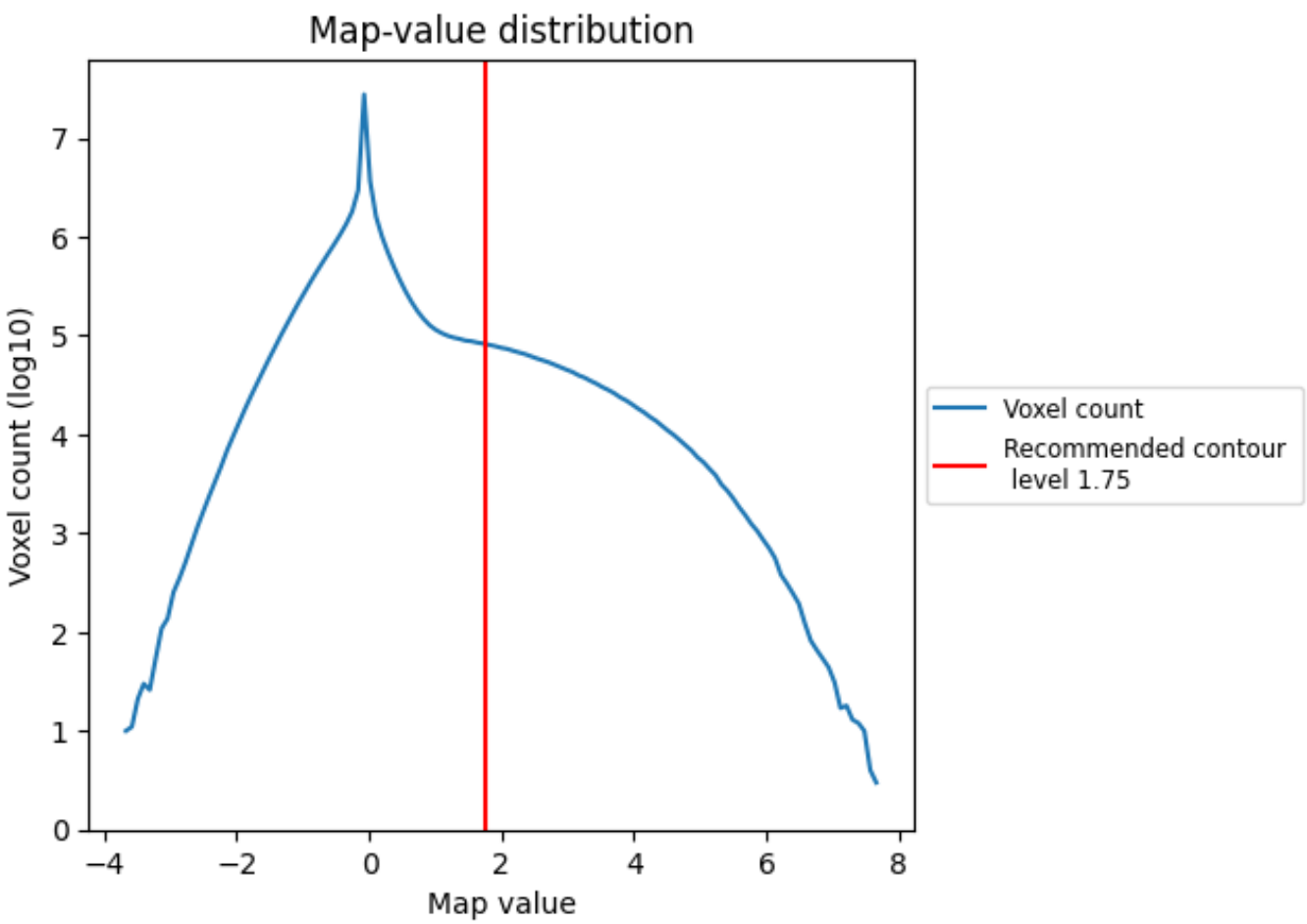
## 6.6 Mask visualisation (i)

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

# 7 Map analysis (i)

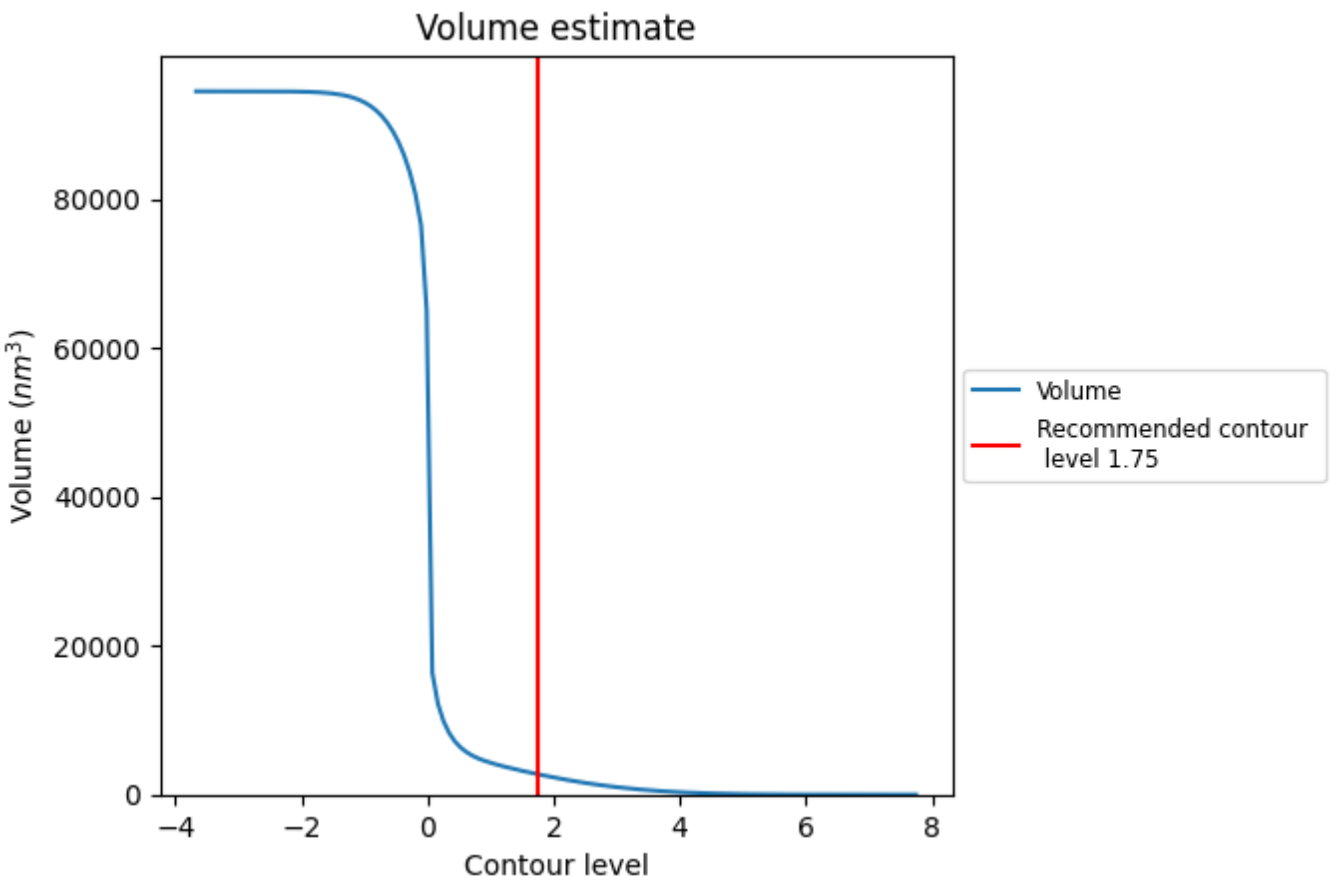
This section contains the results of statistical analysis of the map.

## 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.

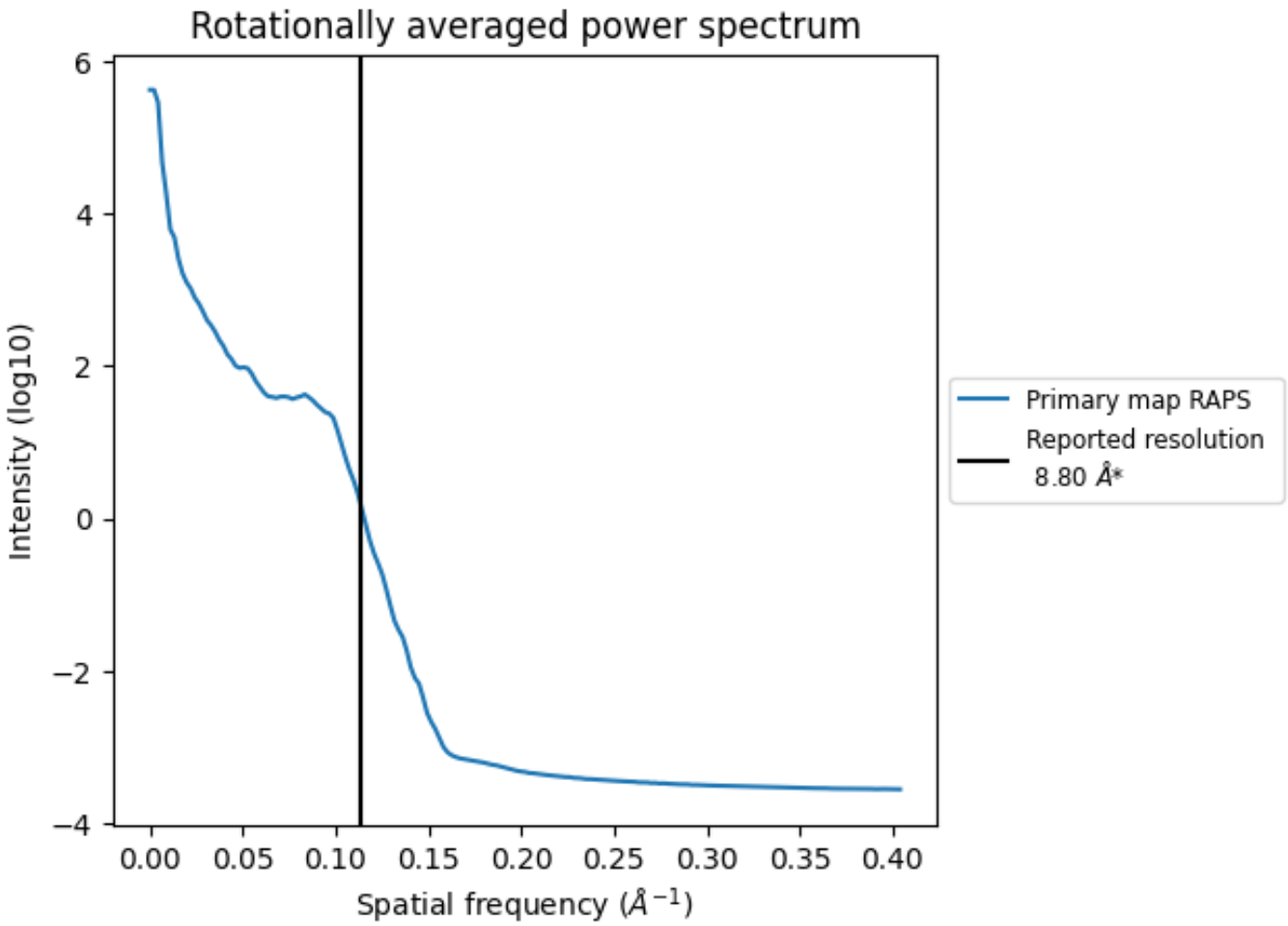
## 7.2 Volume estimate (i)




The volume at the recommended contour level is 2728 $nm^3$; this corresponds to an approximate mass of 2464 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 0.114 Å$^{-1}$

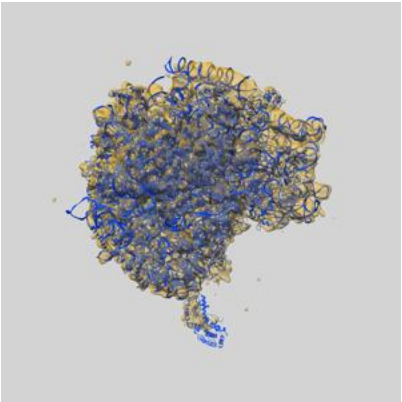
# 8 Fourier-Shell correlation (i)

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

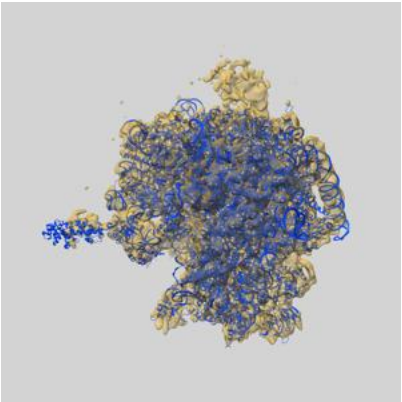
# 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-1669 and PDB model 4V6I. Per-residue inclusion information can be found in section 3 on page 20.

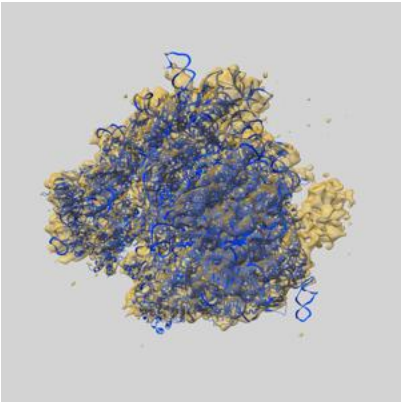
## 9.1 Map-model overlay (i)



X



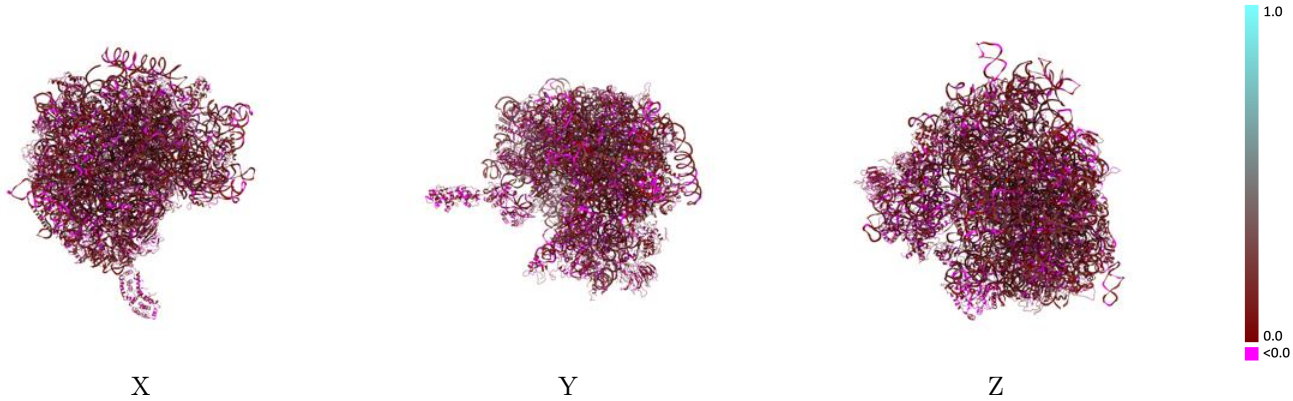
Y



Z

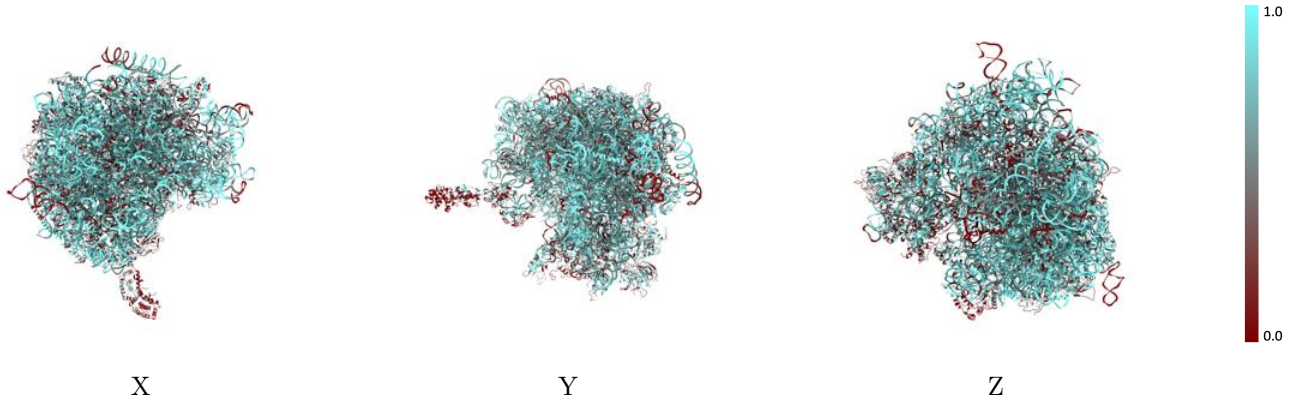
The images above show the 3D surface view of the map at the recommended contour level 1.75 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



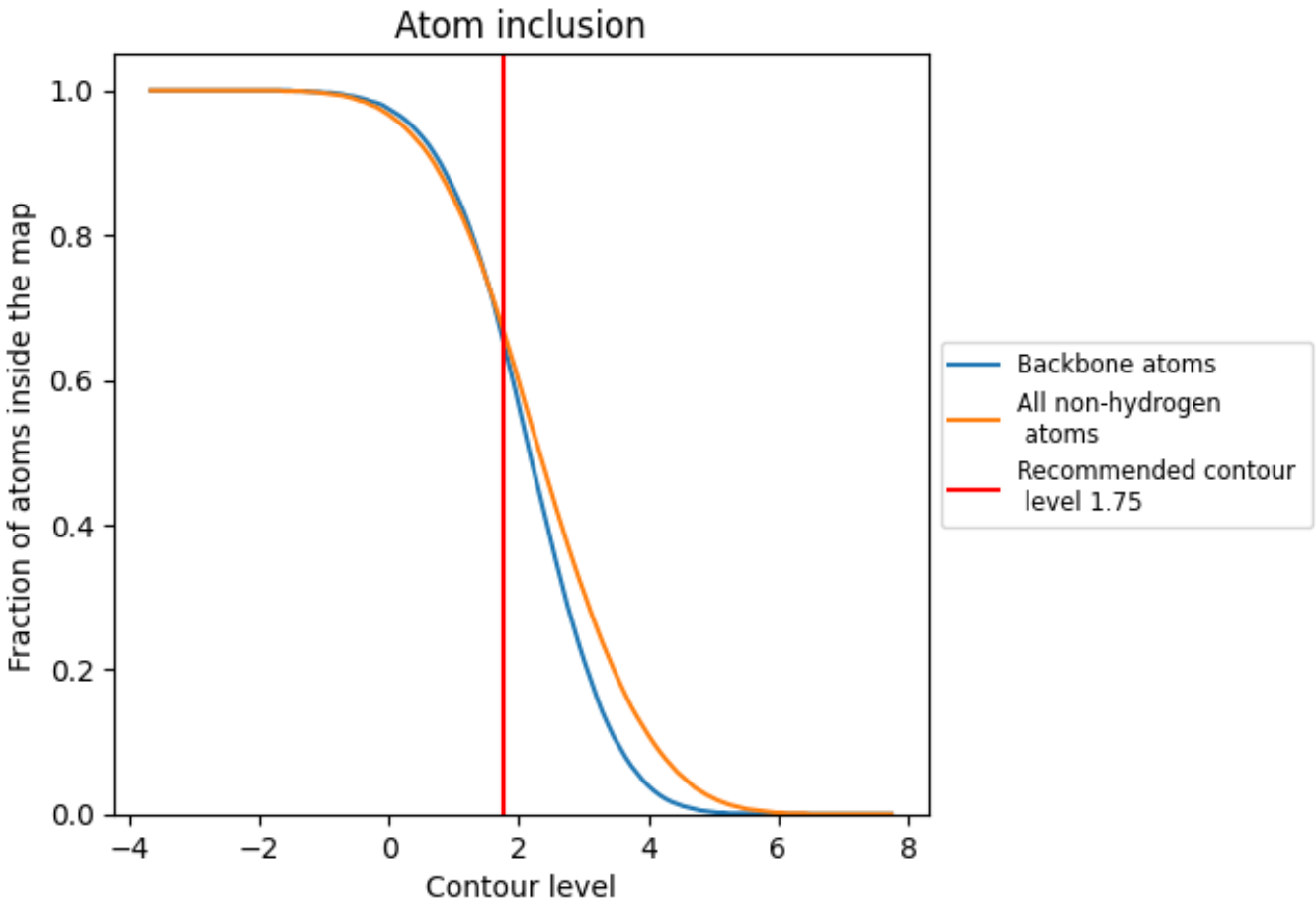

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.75).

## 9.4 Atom inclusion (i)




At the recommended contour level, 66% of all backbone atoms, 67% 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 (1.75) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.6720 | 0.0940 |
| AA | 0.6070 | 0.1010 |
| AB | 0.4530 | 0.0770 |
| AC | 0.5850 | 0.0770 |
| AD | 0.5780 | 0.0860 |
| AE | 0.5530 | 0.0920 |
| AF | 0.5030 | 0.0710 |
| AG | 0.6840 | 0.1610 |
| AH | 0.5130 | 0.0870 |
| AI | 0.5430 | 0.0530 |
| AJ | 0.5000 | 0.0680 |
| AK | 0.5770 | 0.0700 |
| AL | 0.6540 | 0.0570 |
| AM | 0.2950 | 0.0500 |
| AN | 0.3770 | 0.0420 |
| AO | 0.4520 | 0.0830 |
| AP | 0.4140 | 0.0750 |
| AQ | 0.3000 | 0.0670 |
| AR | 0.3300 | 0.0730 |
| AS | 0.5260 | 0.0540 |
| AT | 0.4160 | 0.1050 |
| AU | 0.5370 | 0.0730 |
| AV | 0.3770 | 0.0800 |
| AW | 0.7200 | 0.1670 |
| AX | 0.4820 | 0.0650 |
| AY | 0.3320 | 0.0120 |
| AZ | 0.4960 | 0.0540 |
| Aa | 0.4650 | 0.0690 |
| Ab | 0.8670 | 0.2310 |
| Ac | 0.6350 | 0.2370 |
| BA | 0.2180 | 0.0010 |
| BB | 0.4620 | 0.0460 |
| BC | 0.5830 | 0.0580 |
| BD | 0.5840 | 0.0660 |
| BE | 0.5590 | 0.0870 |

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| Chain | Atom inclusion | Q-score |
|---|---|---|
| BF | 0.5300 | 0.0860 |
| BG | 0.5860 | 0.0780 |
| BH | 0.6210 | 0.0830 |
| BI | 0.6600 | 0.0620 |
| BJ | 0.3380 | 0.0300 |
| BK | 0.5740 | 0.0870 |
| BL | 0.7800 | 0.1700 |
| BM | 0.2620 | 0.0860 |
| BN | 0.6400 | 0.0980 |
| BO | 0.4910 | 0.0400 |
| BP | 0.5560 | 0.0370 |
| BQ | 0.7450 | 0.0620 |
| BR | 0.5520 | 0.1000 |
| BS | 0.5020 | 0.0650 |
| BT | 0.4790 | 0.0960 |
| BU | 0.6290 | 0.0650 |
| BV | 0.5070 | 0.0570 |
| BW | 0.6070 | 0.0800 |
| BX | 0.5130 | 0.0770 |
| BY | 0.6950 | 0.0860 |
| BZ | 0.3940 | 0.0600 |
| Ba | 0.4830 | 0.0350 |
| Bc | 0.7380 | 0.1170 |
| Bd | 0.6180 | 0.0590 |
| Be | 0.5650 | 0.0900 |
| Bf | 0.4790 | 0.1190 |
| Bg | 0.5580 | 0.0760 |
| Bh | 0.4620 | 0.0730 |
| Bi | 0.4370 | 0.0580 |
| Bj | 0.4450 | 0.0490 |
| Bk | 0.6900 | 0.0950 |
| Bl | 0.6730 | 0.0500 |
| Bm | 0.3920 | 0.0810 |
| Bn | 0.5630 | 0.0860 |
| Bo | 0.4720 | 0.0500 |
| Bp | 0.4370 | -0.0300 |
| Bq | 0.4880 | 0.1170 |
| Br | 0.4650 | 0.0650 |
| Bs | 0.2770 | 0.0350 |
| Bt | 0.3560 | 0.0260 |
| Bu | 0.0000 | 0.0530 |
| Bv | 0.2740 | 0.0480 |

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| Chain | Atom inclusion | Q-score |
|---|---|---|
| Bw | 0.0370 | 0.0100 |
| Bx | 0.7900 | 0.1580 |
| By | 0.9100 | 0.2380 |
| Bz | 0.6140 | 0.2150 |
| CA | 0.7890 | 0.1050 |
| CB | 0.0690 | 0.0440 |
| CC | 0.1440 | -0.0370 |
| DA | 0.7960 | 0.1160 |
| DB | 0.8120 | 0.1140 |
| DC | 0.9130 | 0.1250 |