# Full wwPDB EM Validation Report ⓘ

Feb 12, 2024 – 04:59 PM EST

| | | |
|---|---|---|
| PDB ID | : | 3JBP |
| EMDB ID | : | EMD-6454 |
| Title | : | Cryo-electron microscopy reconstruction of the Plasmodium falciparum 80S ribosome bound to E-tRNA |
| Authors | : | Sun, M.; Li, W.; Blomqvist, K.; Das, S.; Hashem, Y.; Dvorin, J.D.; Frank, J. |
| Deposited on | : | 2015-09-16 |
| Resolution | : | 6.70 Å(reported) |
| Based on initial models | : | 3J7A, 3J79 |

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 ⓘ 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 ⓘ) were used in the production of this report:

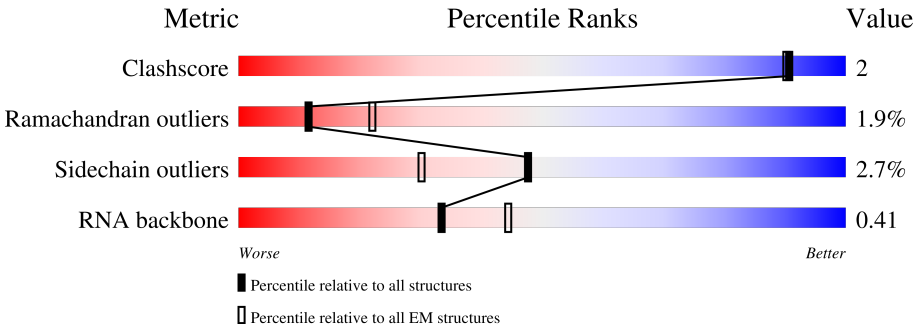
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev70 |
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | FAILED |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA)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

# 1 Overall quality at a glance

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

The reported resolution of this entry is 6.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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%

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 1608 | 29% 44% 22% 5% |
| 2 | 7 | 74 | 9% 41% 38% 12% |
| 3 | D | 209 | 70% · · 25% |
| 4 | E | 185 | 88% 11% · |
| 5 | G | 224 | 93% 7% |
| 6 | I | 189 | 87% 5% · 5% |
| 7 | K | 129 | 90% 5% · · |

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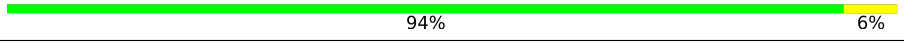
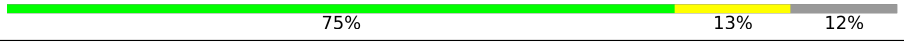
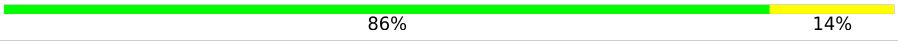
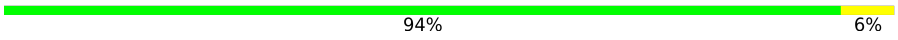
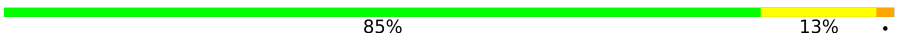
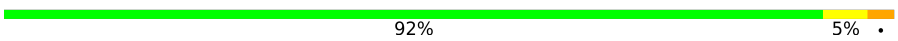
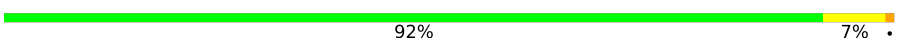
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 8 | M | 138 |   |
| 9 | W | 108 |   |
| 10 | R | 114 |   |
| 11 | O | 79 |   |
| 12 | Y | 154 |   |
| 13 | Z | 72 |   |
| 14 | 1 | 120 |   |
| 15 | 2 | 68 |   |
| 16 | 3 | 95 |   |
| 17 | 4 | 76 |   |
| 18 | 5 | 65 |   |
| 19 | 6 | 43 |   |
| 20 | B | 210 |   |
| 21 | F | 257 |   |
| 22 | H | 214 |   |
| 23 | J | 188 |   |
| 24 | L | 214 |   |
| 25 | N | 98 |   |
| 26 | P | 127 |   |
| 27 | Q | 144 |   |
| 28 | S | 128 |   |
| 29 | T | 48 |   |
| 30 | U | 149 |   |
| 31 | V | 156 |   |
| 32 | X | 103 |   |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 33 | C | 195 | 89% 10% |
| 34 | AA | 3193 | 25% 43% 24% 8% |
| 35 | AC | 151 | 24% 51% 23% |
| 36 | AB | 118 | 29% 52% 13% 7% |
| 37 | AL | 211 | 92% 7% |
| 38 | A1 | 145 | 89% 8% |
| 39 | A2 | 118 | 82% 6% 12% |
| 40 | A4 | 66 | 86% 8% 5% |
| 41 | A6 | 98 | 90% 8% |
| 42 | A7 | 102 | 86% 8% 6% |
| 43 | AN | 146 | 90% 8% |
| 44 | A8 | 125 | 88% 10% |
| 45 | A9 | 103 | 88% 9% |
| 46 | Aa | 106 | 83% 16% |
| 47 | Ab | 105 | 87% 10% |
| 48 | Ad | 76 | 91% 5% |
| 49 | Ae | 50 | 68% 14% 14% |
| 50 | Af | 51 | 94% |
| 51 | AP | 204 | 84% 15% |
| 52 | Ah | 85 | 95% |
| 53 | Ai | 95 | 91% 8% |
| 54 | AI | 213 | 91% 6% |
| 55 | AJ | 244 | 87% 9% |
| 56 | Ac | 89 | 82% 16% |
| 57 | AK | 201 | 90% 9% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 58 | AM | 132 | 93% 5% |
| 59 | AS | 186 | 86% 12% |
| 60 | AO | 147 | 89% 10% |
| 61 | AQ | 205 | 80% 11% 8% |
| 62 | AR | 289 | 77% 9% 13% |
| 63 | AW | 170 | 88% 9% |
| 64 | AY | 101 | 94% 5% |
| 65 | AT | 181 | 91% 8% |
| 66 | AZ | 121 | 93% 5% |
| 67 | A3 | 119 | 92% 8% |
| 68 | A5 | 223 | 86% 11% |
| 69 | AD | 247 | 89% 9% |
| 70 | AE | 380 | 89% 10% |
| 71 | AF | 390 | 92% 7% |
| 72 | AG | 159 | 70% 6% 22% |
| 73 | AU | 180 | 88% 7% |
| 74 | AH | 185 | 91% 8% |
| 75 | AV | 155 | 89% 10% |
| 76 | Ag | 37 | 76% 16% 8% |
| 77 | AX | 97 | 94% 6% |
| 78 | A0 | 62 | 92% 6% |

# 2 Entry composition

There are 78 unique types of molecules in this entry. The entry contains 193012 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 RNA chain called 18S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 1 | A | 1608 | 34207 | 15346 | 6106 | 11169 | 1586 | 0 | 0 |

- Molecule 2 is a RNA chain called E-tRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 2 | 7 | 74 | 1571 | 702 | 275 | 521 | 73 | 0 | 0 |

- Molecule 3 is a protein called 40S ribosomal protein uS3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 3 | D | 157 | 1229 | 782 | 225 | 215 | 7 | 0 | 0 |

- Molecule 4 is a protein called 40S ribosomal protein uS4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 4 | E | 185 | 1515 | 962 | 290 | 261 | 2 | 0 | 0 |

- Molecule 5 is a protein called 40S ribosomal protein uS5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 5 | G | 224 | 1758 | 1132 | 307 | 310 | 9 | 0 | 0 |

- Molecule 6 is a protein called 40S ribosomal protein uS7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 6 | I | 180 | 1424 | 893 | 263 | 258 | 10 | 0 | 0 |

- Molecule 7 is a protein called 40S ribosomal protein uS8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 7 | K | 129 | Total | C | N | O | S | 0 | 0 |
| | | | 1037 | 665 | 189 | 178 | 5 | | |

- Molecule 8 is a protein called 40S ribosomal protein uS9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 8 | M | 138 | Total | C | N | O | S | 0 | 0 |
| | | | 1099 | 704 | 200 | 194 | 1 | | |

- Molecule 9 is a protein called 40S ribosomal protein eS17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 9 | W | 95 | Total | C | N | O | S | 0 | 0 |
| | | | 786 | 498 | 149 | 136 | 3 | | |

- Molecule 10 is a protein called 40S ribosomal protein eS12.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 10 | R | 98 | Total | C | N | O | S | 0 | 0 |
| | | | 747 | 474 | 123 | 146 | 4 | | |

- Molecule 11 is a protein called 40S ribosomal protein eS10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 11 | O | 79 | Total | C | N | O | S | 0 | 0 |
| | | | 687 | 450 | 116 | 119 | 2 | | |

- Molecule 12 is a protein called 40S ribosomal protein eS19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 12 | Y | 154 | Total | C | N | O | S | 0 | 0 |
| | | | 1267 | 811 | 239 | 215 | 2 | | |

- Molecule 13 is a protein called 40S ribosomal protein eS21.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 13 | Z | 72 | Total | C | N | O | S | 0 | 0 |
| | | | 557 | 346 | 102 | 105 | 4 | | |

- Molecule 14 is a protein called 40S ribosomal protein eS24.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 14 | 1 | 120 | Total | C | N | O | S | 0 | 0 |
| | | | 986 | 632 | 189 | 163 | 2 | | |

- Molecule 15 is a protein called 40S ribosomal protein eS25.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 15 | 2 | 41 | Total | C | N | O | 0 | 0 |
| | | | 321 | 208 | 56 | 57 | | |

- Molecule 16 is a protein called 40S ribosomal protein eS26.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 16 | 3 | 95 | Total | C | N | O | S | 0 | 0 |
| | | | 782 | 478 | 169 | 129 | 6 | | |

- Molecule 17 is a protein called 40S ribosomal protein eS27.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 17 | 4 | 76 | Total | C | N | O | S | 0 | 0 |
| | | | 586 | 368 | 102 | 107 | 9 | | |

- Molecule 18 is a protein called 40S ribosomal protein eS28.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 18 | 5 | 58 | Total | C | N | O | 0 | 0 |
| | | | 458 | 285 | 93 | 80 | | |

- Molecule 19 is a protein called 40S ribosomal protein eS30.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 19 | 6 | 43 | Total | C | N | O | 0 | 0 |
| | | | 346 | 213 | 75 | 58 | | |

- Molecule 20 is a protein called 40S ribosomal protein eS1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 20 | B | 210 | Total | C | N | O | S | 0 | 0 |
| | | | 1714 | 1097 | 301 | 304 | 12 | | |

- Molecule 21 is a protein called 40S ribosomal protein eS4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 21 | F | 257 | Total | C | N | O | S | 0 | 0 |
| | | | 2062 | 1320 | 377 | 357 | 8 | | |

- Molecule 22 is a protein called 40S ribosomal protein eS6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 22 | H | 204 | Total | C | N | O | S | 0 | 0 |
| | | | 1648 | 1045 | 313 | 284 | 6 | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| H | 158 | ILE | - | insertion | UNP Q8IDR9 |
| H | 195 | ASP | GLU | conflict | UNP Q8IDR9 |

- Molecule 23 is a protein called 40S ribosomal protein eS7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 23 | J | 188 | Total | C | N | O | S | 0 | 0 |
| | | | 1529 | 982 | 264 | 279 | 4 | | |

- Molecule 24 is a protein called 40S ribosomal protein eS8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 24 | L | 171 | Total | C | N | O | S | 0 | 0 |
| | | | 1383 | 872 | 264 | 243 | 4 | | |

- Molecule 25 is a protein called 40S ribosomal protein uS10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 25 | N | 98 | Total | C | N | O | S | 0 | 0 |
| | | | 772 | 484 | 135 | 148 | 5 | | |

- Molecule 26 is a protein called 40S ribosomal protein uS11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 26 | P | 127 | Total | C | N | O | S | 0 | 0 |
| | | | 954 | 591 | 184 | 176 | 3 | | |

- Molecule 27 is a protein called 40S ribosomal protein uS12.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 27 | Q | 144 | Total | C | N | O | S | 0 | 0 |
| | | | 1129 | 712 | 222 | 193 | 2 | | |

- Molecule 28 is a protein called 40S ribosomal protein uS13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 28 | S | 128 | Total | C | N | O | S | 0 | 0 |
| | | | 1047 | 657 | 205 | 181 | 4 | | |

- Molecule 29 is a protein called 40S ribosomal protein uS14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 29 | T | 48 | Total | C | N | O | S | 0 | 0 |
| | | | 405 | 252 | 85 | 64 | 4 | | |

- Molecule 30 is a protein called 40S ribosomal protein uS15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 30 | U | 149 | Total | C | N | O | S | 0 | 0 |
| | | | 1202 | 769 | 220 | 210 | 3 | | |

- Molecule 31 is a protein called 40S ribosomal protein uS17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 31 | V | 146 | Total | C | N | O | S | 0 | 0 |
| | | | 1206 | 772 | 227 | 200 | 7 | | |

- Molecule 32 is a protein called 40S ribosomal protein uS19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 32 | X | 96 | Total | C | N | O | S | 0 | 0 |
| | | | 777 | 497 | 137 | 139 | 4 | | |

- Molecule 33 is a protein called 40S ribosomal protein uS2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 33 | C | 195 | Total | C | N | O | S | 0 | 0 |
| | | | 1539 | 990 | 266 | 274 | 9 | | |

- Molecule 34 is a RNA chain called 28S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 34 | AA | 3193 | Total | C | N | O | P | 0 | 0 |
| | | | 67884 | 30446 | 12054 | 22223 | 3161 | | |

- Molecule 35 is a RNA chain called 5.8S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 35 | AC | 151 | Total | C | N | O | P | 0 | 0 |
| | | | 3215 | 1444 | 589 | 1034 | 148 | | |

- Molecule 36 is a RNA chain called 5S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 36 | AB | 118 | Total | C | N | O | P | 0 | 0 |
| | | | 2522 | 1128 | 461 | 816 | 117 | | |

- Molecule 37 is a protein called 60S ribosomal protein eL13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 37 | AL | 211 | Total | C | N | O | S | 0 | 0 |
| | | | 1757 | 1116 | 346 | 291 | 4 | | |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| AL | 19 | HIS | ARG | conflict | UNP Q8IAX6 |
| AL | 20 | ARG | HIS | conflict | UNP Q8IAX6 |
| AL | 201 | CYS | ARG | conflict | UNP Q8IAX6 |

- Molecule 38 is a protein called 60S ribosomal protein eL27.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 38 | A1 | 140 | Total | C | N | O | S | 0 | 0 |
| | | | 1134 | 736 | 204 | 191 | 3 | | |

- Molecule 39 is a protein called 60S ribosomal protein eL28.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 39 | A2 | 104 | Total | C | N | O | S | 0 | 0 |
| | | | 831 | 529 | 151 | 148 | 3 | | |

- Molecule 40 is a protein called 60S ribosomal protein eL29.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 40 | A4 | 66 | Total | C | N | O | S | 0 | 0 |
| | | | 555 | 347 | 116 | 90 | 2 | | |

- Molecule 41 is a protein called 60S ribosomal protein eL30.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 41 | A6 | 98 | Total | C | N | O | S | 0 | 0 |
| | | | 741 | 462 | 132 | 140 | 7 | | |

- Molecule 42 is a protein called 60S ribosomal protein eL31.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 42 | A7 | 96 | Total | C | N | O | S | 0 | 0 |
| | | | 794 | 508 | 151 | 130 | 5 | | |

- Molecule 43 is a protein called 60S ribosomal protein eL14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 43 | AN | 146 | Total | C | N | O | S | 0 | 0 |
| | | | 1202 | 781 | 210 | 205 | 6 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| AN | ? | - | LYS | deletion | UNP Q8ILE8 |

- Molecule 44 is a protein called 60S ribosomal protein eL32.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 44 | A8 | 125 | Total | C | N | O | S | 0 | 0 |
| | | | 1037 | 660 | 206 | 164 | 7 | | |

- Molecule 45 is a protein called 60S ribosomal protein eL33.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 45 | A9 | 103 | Total | C | N | O | S | 0 | 0 |
| | | | 845 | 543 | 163 | 136 | 3 | | |

- Molecule 46 is a protein called 60S ribosomal protein eL34.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 46 | Aa | 106 | Total | C | N | O | S | 0 | 0 |
| | | | 859 | 530 | 184 | 139 | 6 | | |

- Molecule 47 is a protein called 60S ribosomal protein eL36.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 47 | Ab | 95 | Total | C | N | O | 0 | 0 |
| | | | 757 | 477 | 150 | 130 | | |

- Molecule 48 is a protein called 60S ribosomal protein eL38.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 48 | Ad | 72 | Total | C | N | O | S | 0 | 0 |
| | | | 604 | 395 | 107 | 100 | 2 | | |

- Molecule 49 is a protein called 60S ribosomal protein eL39.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 49 | Ae | 43 | Total | C | N | O | S | 0 | 0 |
| | | | 388 | 243 | 92 | 52 | 1 | | |

- Molecule 50 is a protein called 60S ribosomal protein eL40.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 50 | Af | 51 | Total | C | N | O | S | 0 | 0 |
| | | | 414 | 255 | 87 | 67 | 5 | | |

- Molecule 51 is a protein called 60S ribosomal protein eL15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 51 | AP | 204 | Total | C | N | O | S | 0 | 0 |
| | | | 1697 | 1075 | 351 | 267 | 4 | | |

- Molecule 52 is a protein called 60S ribosomal protein eL43.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 52 | Ah | 85 | Total | C | N | O | S | 0 | 0 |
| | | | 659 | 417 | 127 | 108 | 7 | | |

- Molecule 53 is a protein called 60S ribosomal protein eL44.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 53 | Ai | 95 | Total | C | N | O | S | 0 | 0 |
| | | | 779 | 490 | 152 | 128 | 9 | | |

- Molecule 54 is a protein called 60S ribosomal protein eL6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 54 | AI | 207 | Total | C | N | O | S | 0 | 0 |
| | | | 1685 | 1096 | 298 | 286 | 5 | | |

- Molecule 55 is a protein called 60S ribosomal protein eL8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 55 | AJ | 222 | Total | C | N | O | S | 0 | 0 |
| | | | 1813 | 1174 | 323 | 309 | 7 | | |

- Molecule 56 is a protein called 60S ribosomal protein eL37.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 56 | Ac | 89 | Total | C | N | O | S | 0 | 0 |
| | | | 710 | 441 | 150 | 114 | 5 | | |

- Molecule 57 is a protein called 60S ribosomal protein uL13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 57 | AK | 201 | Total | C | N | O | S | 0 | 0 |
| | | | 1660 | 1064 | 311 | 277 | 8 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| AK | 109 | ALA | TYR | conflict | UNP Q8IJZ7 |

- Molecule 58 is a protein called 60S ribosomal protein uL14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 58 | AM | 132 | Total | C | N | O | S | 0 | 0 |
| | | | 996 | 631 | 179 | 178 | 8 | | |

- Molecule 59 is a protein called 60S ribosomal protein eL18.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 59 | AS | 186 | Total | C | N | O | S | 0 | 0 |
| | | | 1503 | 958 | 299 | 241 | 5 | | |

- Molecule 60 is a protein called 60S ribosomal protein uL15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 60 | AO | 147 | Total | C | N | O | S | 0 | 0 |
| | | | 1172 | 747 | 232 | 189 | 4 | | |

- Molecule 61 is a protein called 60S ribosomal protein uL16.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 61 | AQ | 189 | Total | C | N | O | S | 0 | 0 |
| | | | 1545 | 984 | 291 | 262 | 8 | | |

- Molecule 62 is a protein called 60S ribosomal protein uL18.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 62 | AR | 252 | Total | C | N | O | S | 0 | 0 |
| | | | 2050 | 1300 | 385 | 359 | 6 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| AR | ? | - | LYS | deletion | UNP Q8ILL3 |

- Molecule 63 is a protein called 60S ribosomal protein uL22.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 63 | AW | 170 | Total | C | N | O | S | 0 | 0 |
| | | | 1319 | 824 | 266 | 222 | 7 | | |

- Molecule 64 is a protein called 60S ribosomal protein uL23.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 64 | AY | 101 | Total | C | N | O | S | 0 | 0 |
| | | | 797 | 502 | 144 | 145 | 6 | | |

- Molecule 65 is a protein called 60S ribosomal protein eL19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 65 | AT | 181 | Total | C | N | O | S | 0 | 0 |
| | | | 1509 | 952 | 309 | 244 | 4 | | |

- Molecule 66 is a protein called 60S ribosomal protein uL24.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 66 | AZ | 121 | Total | C | N | O | S | 0 | 0 |
| | | | 1001 | 626 | 206 | 166 | 3 | | |

- Molecule 67 is a protein called 60S ribosomal protein uL29.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 67 | A3 | 119 | Total | C | N | O | S | 0 | 0 |
| | | | 995 | 635 | 194 | 164 | 2 | | |

- Molecule 68 is a protein called 60S ribosomal protein uL30.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 68 | A5 | 223 | Total | C | N | O | S | 0 | 0 |
| | | | 1879 | 1211 | 357 | 306 | 5 | | |

- Molecule 69 is a protein called 60S ribosomal protein uL2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 69 | AD | 247 | Total | C | N | O | S | 0 | 0 |
| | | | 1867 | 1166 | 374 | 318 | 9 | | |

- Molecule 70 is a protein called 60S ribosomal protein uL3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 70 | AE | 380 | Total | C | N | O | S | 0 | 0 |
| | | | 3062 | 1948 | 575 | 522 | 17 | | |

- Molecule 71 is a protein called 60S ribosomal protein uL4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 71 | AF | 390 | Total | C | N | O | S | 0 | 0 |
| | | | 3095 | 1962 | 594 | 528 | 11 | | |

- Molecule 72 is a protein called 60S ribosomal protein uL5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 72 | AG | 124 | Total | C | N | O | S | 0 | 0 |
| | | | 1011 | 636 | 197 | 172 | 6 | | |

- Molecule 73 is a protein called 60S ribosomal protein eL20.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 73 | AU | 180 | Total | C | N | O | S | 0 | 0 |
| | | | 1497 | 946 | 289 | 255 | 7 | | |

- Molecule 74 is a protein called 60S ribosomal protein uL6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 74 | AH | 185 | Total | C | N | O | S | 0 | 0 |
| | | | 1476 | 950 | 264 | 256 | 6 | | |

- Molecule 75 is a protein called 60S ribosomal protein eL21.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 75 | AV | 155 | Total | C | N | O | S | 0 | 0 |
| | | | 1276 | 814 | 241 | 215 | 6 | | |

- Molecule 76 is a protein called 60S ribosomal protein eL41.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 76 | Ag | 37 | Total | C | N | O | S | 0 | 0 |
| | | | 343 | 210 | 86 | 45 | 2 | | |

- Molecule 77 is a protein called 60S ribosomal protein eL22.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 77 | AX | 97 | Total | C | N | O | S | 0 | 0 |
| | | | 825 | 548 | 135 | 140 | 2 | | |

- Molecule 78 is a protein called 60S ribosomal protein eL24.

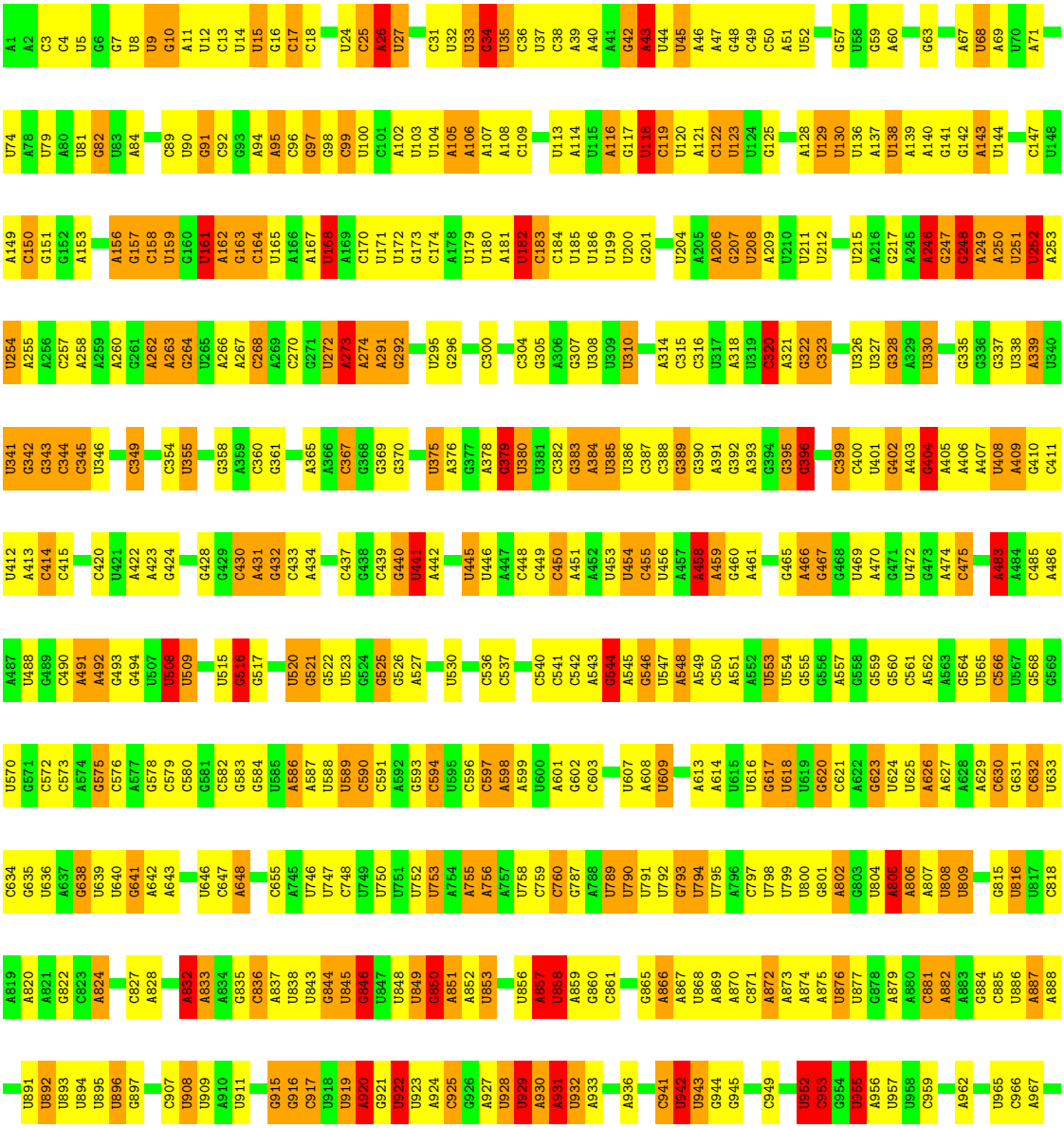
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 78 | A0 | 62 | Total | C | N | O | S | 0 | 0 |
| | | | 522 | 336 | 97 | 88 | 1 | | |

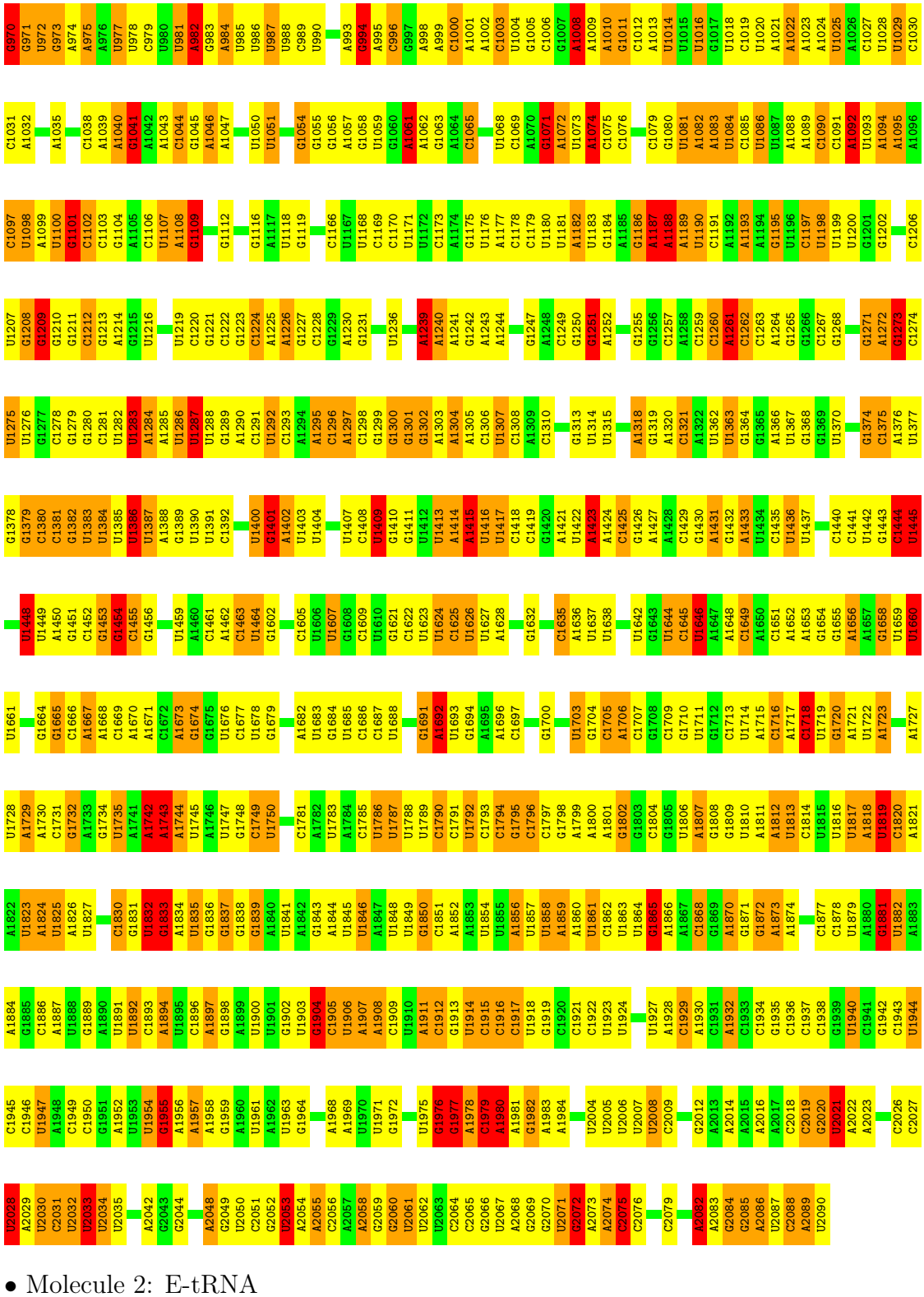
# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: 18S ribosomal RNA

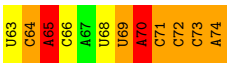
Chain A: 29% 44% 22% 5%





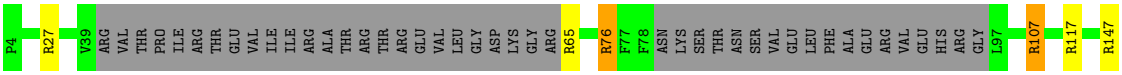
• Molecule 2: E-tRNA

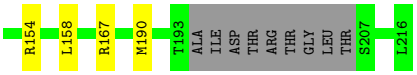
Chain 7:


• Molecule 3: 40S ribosomal protein uS3

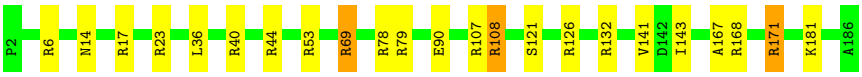
Chain D:

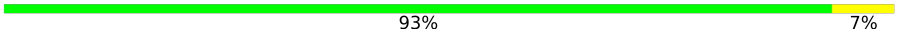

• Molecule 4: 40S ribosomal protein uS4

Chain E:


• Molecule 5: 40S ribosomal protein uS5

Chain G:





• Molecule 6: 40S ribosomal protein uS7

Chain I:



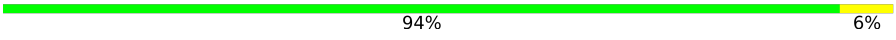
• Molecule 7: 40S ribosomal protein uS8

Chain K:



• Molecule 8: 40S ribosomal protein uS9

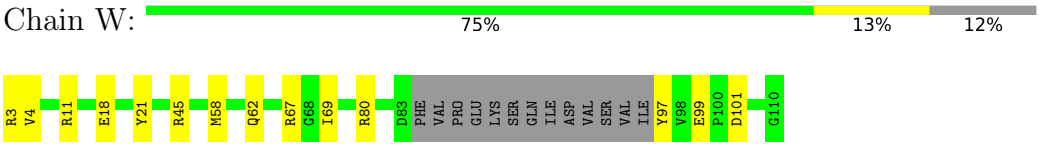
Chain M:





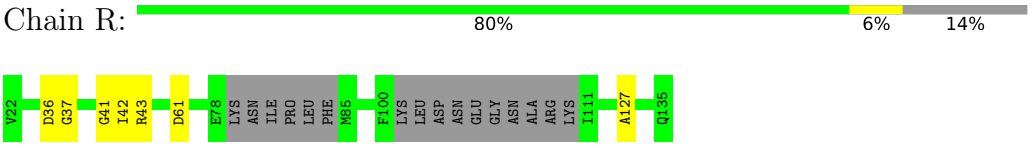
• Molecule 9: 40S ribosomal protein eS17

Chain W:



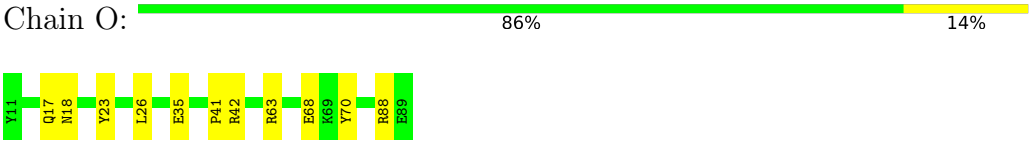

• Molecule 10: 40S ribosomal protein eS12

Chain R:



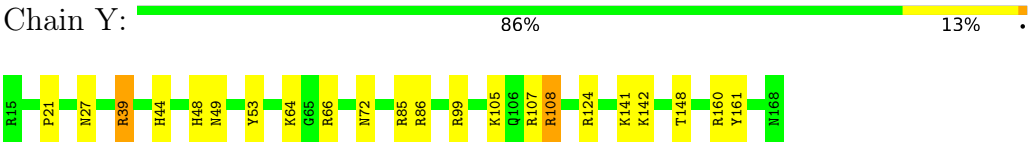

• Molecule 11: 40S ribosomal protein eS10

Chain O:



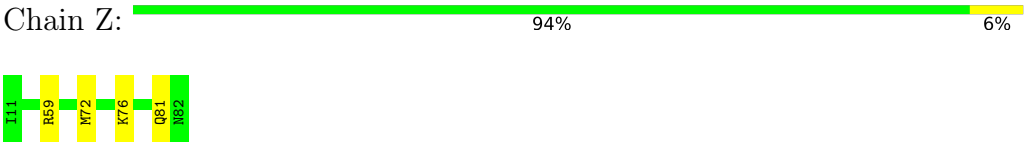

• Molecule 12: 40S ribosomal protein eS19

Chain Y:



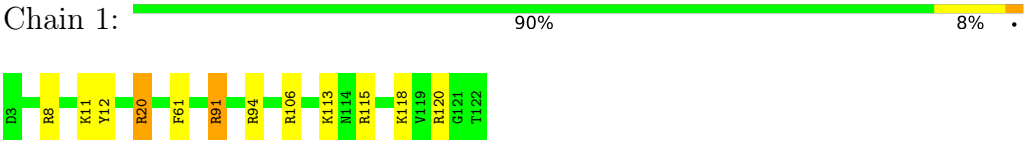

• Molecule 13: 40S ribosomal protein eS21

Chain Z:



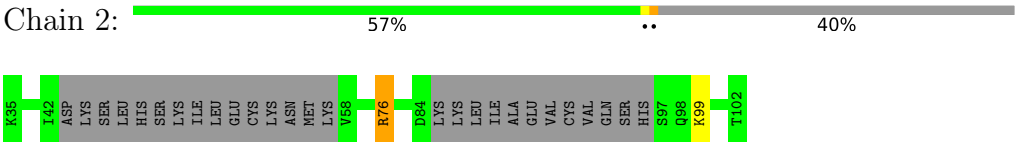

• Molecule 14: 40S ribosomal protein eS24

Chain 1:




• Molecule 15: 40S ribosomal protein eS25

Chain 2:



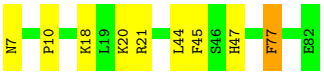

• Molecule 16: 40S ribosomal protein eS26

Chain 3:



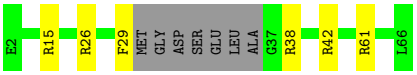
• Molecule 17: 40S ribosomal protein eS27

Chain 4:


• Molecule 18: 40S ribosomal protein eS28

Chain 5:


• Molecule 19: 40S ribosomal protein eS30

Chain 6:



• Molecule 20: 40S ribosomal protein eS1

Chain B:



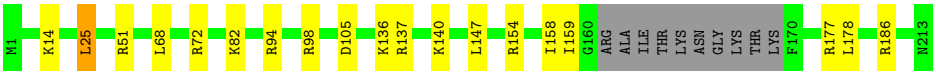
• Molecule 21: 40S ribosomal protein eS4

Chain F:



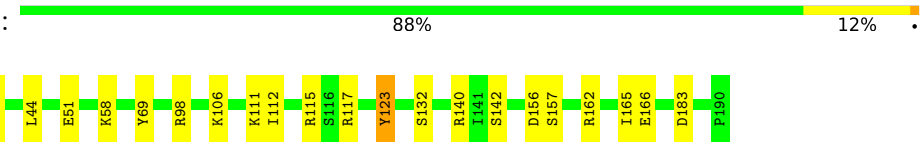
• Molecule 22: 40S ribosomal protein eS6

Chain H:

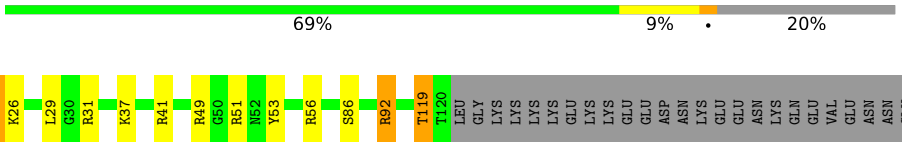

• Molecule 23: 40S ribosomal protein eS7

Chain J:



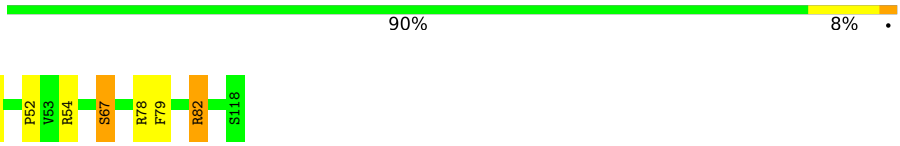

• Molecule 24: 40S ribosomal protein eS8

Chain L:



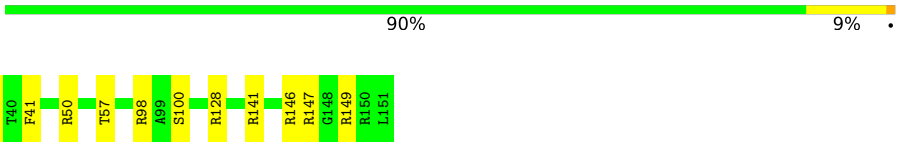

• Molecule 25: 40S ribosomal protein uS10

Chain N:



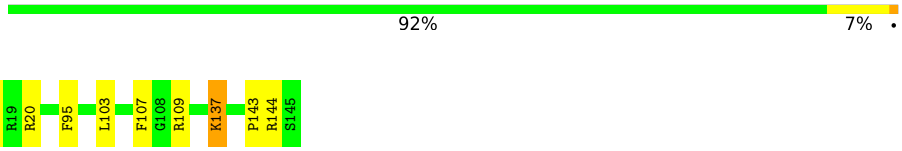

• Molecule 26: 40S ribosomal protein uS11

Chain P:



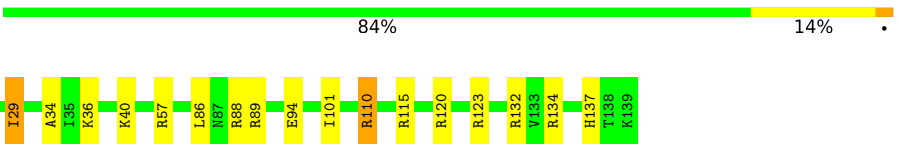

• Molecule 27: 40S ribosomal protein uS12

Chain Q:



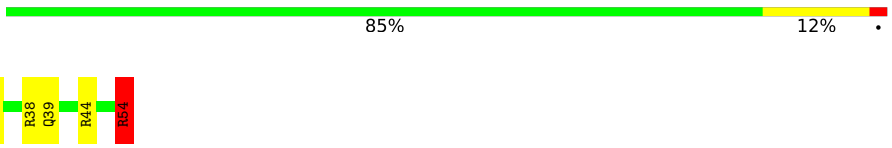

• Molecule 28: 40S ribosomal protein uS13

Chain S:



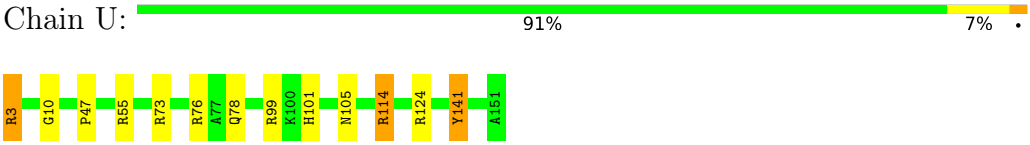

• Molecule 29: 40S ribosomal protein uS14

Chain T:



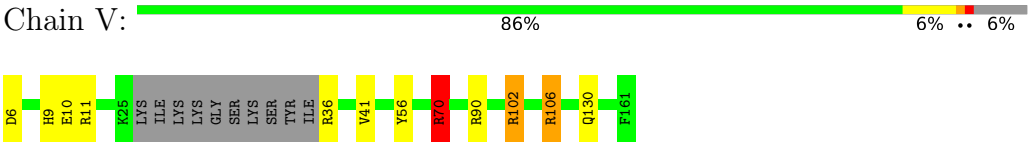
• Molecule 30: 40S ribosomal protein uS15

Chain U:



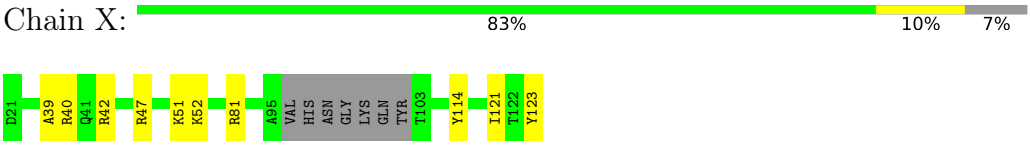

• Molecule 31: 40S ribosomal protein uS17

Chain V:



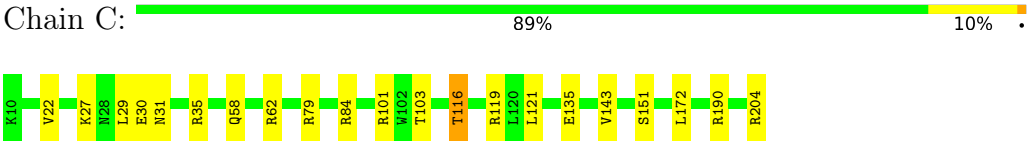

• Molecule 32: 40S ribosomal protein uS19

Chain X:



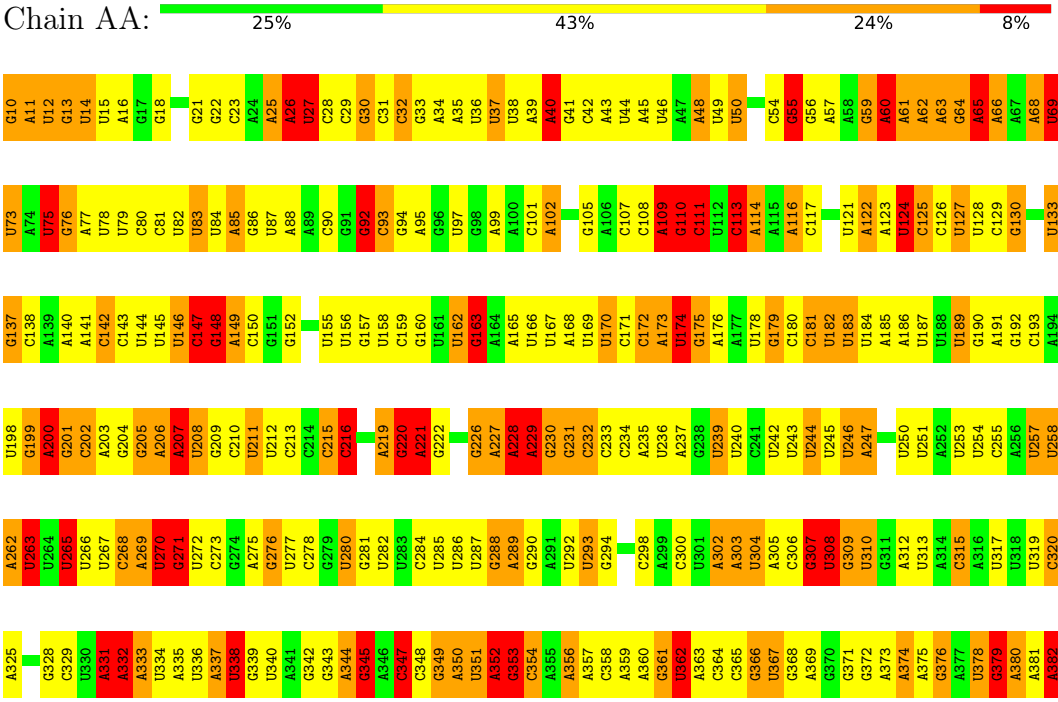

• Molecule 33: 40S ribosomal protein uS2

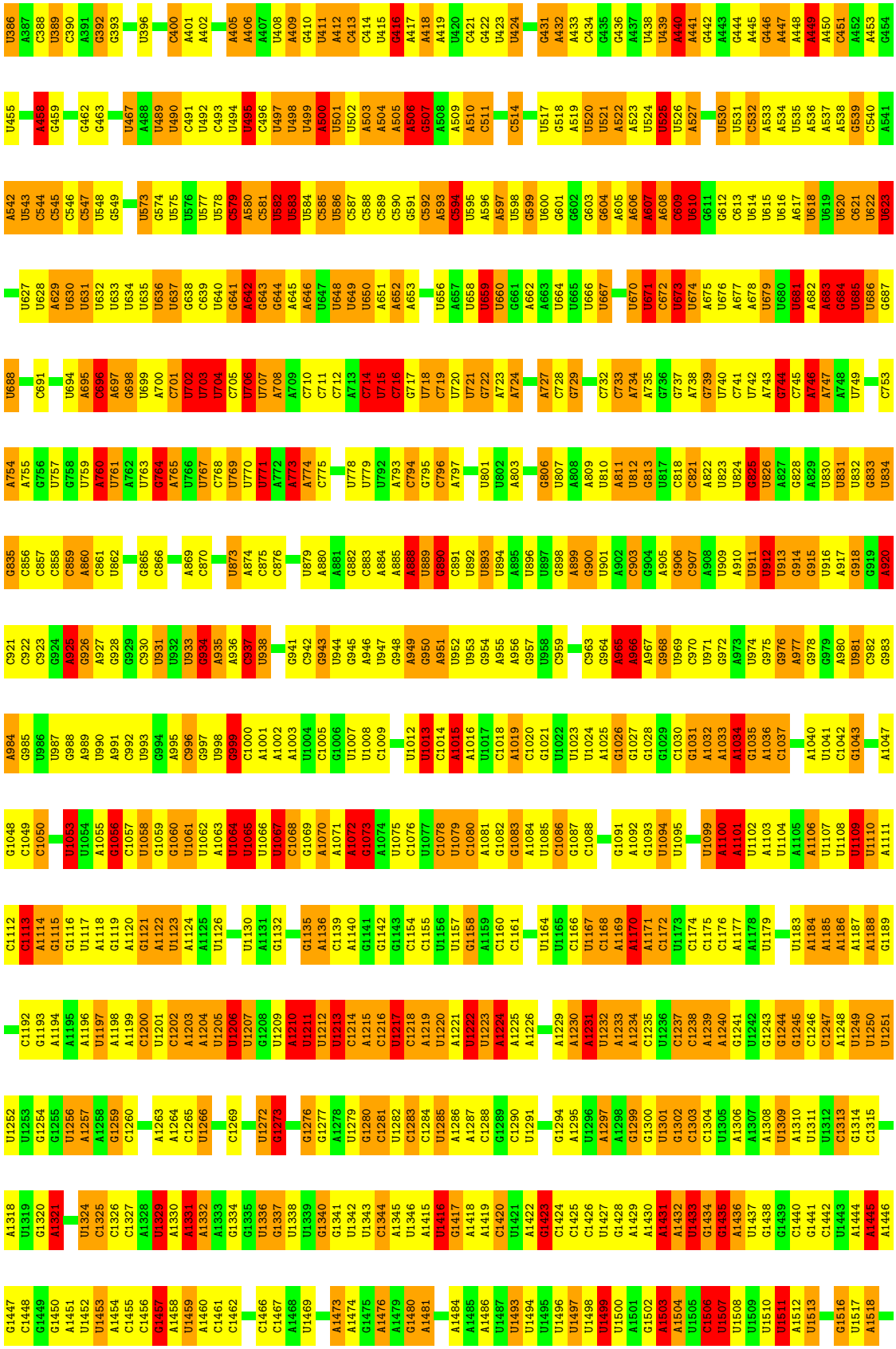
Chain C:

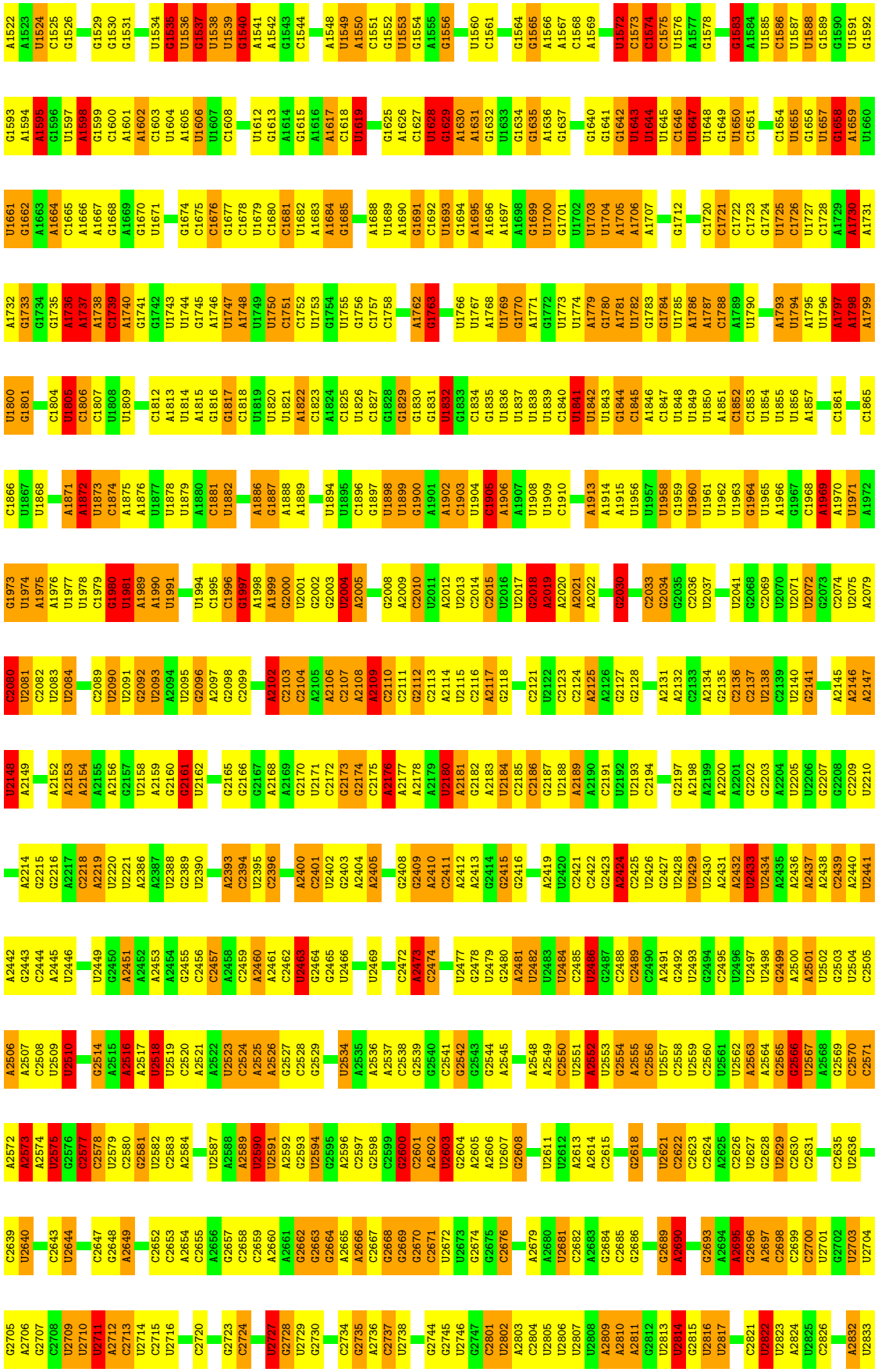


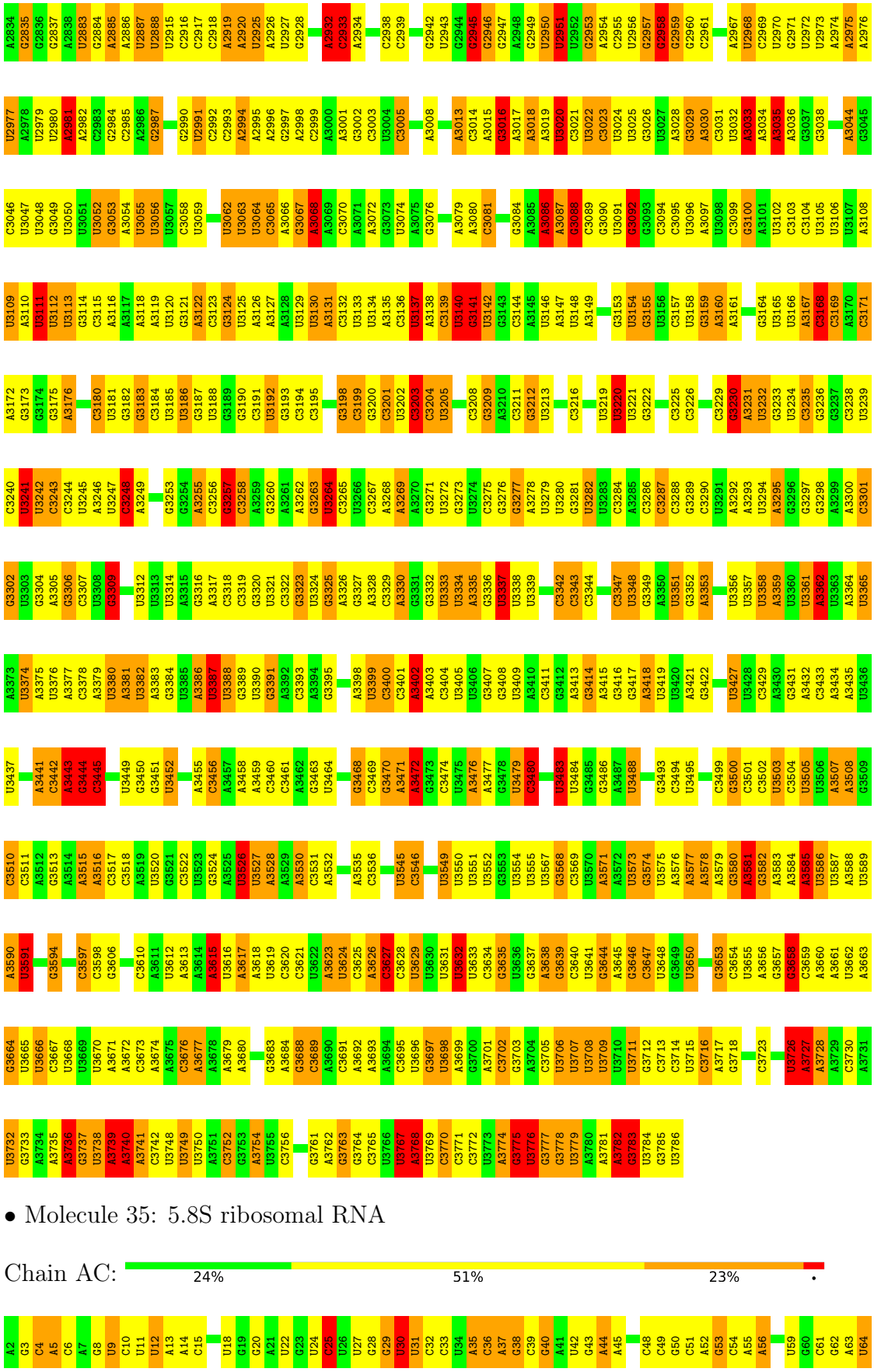

• Molecule 34: 28S ribosomal RNA

Chain AA:



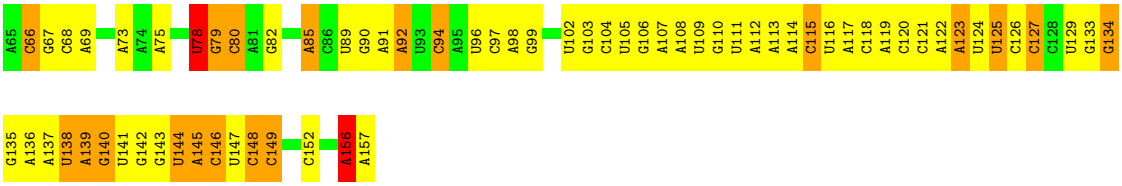






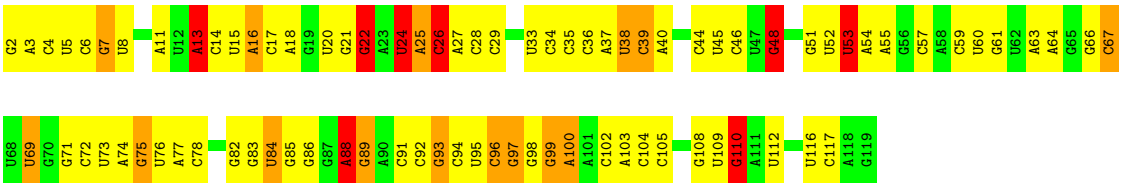
• Molecule 35: 5.8S ribosomal RNA

Chain AC:



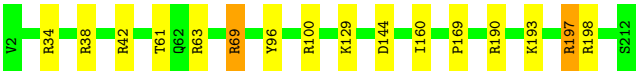

• Molecule 36: 5S ribosomal RNA

Chain AB:

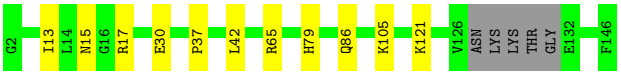

• Molecule 37: 60S ribosomal protein eL13

Chain AL:

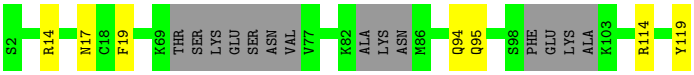

• Molecule 38: 60S ribosomal protein eL27

Chain A1:

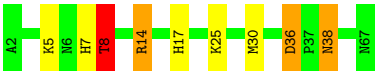

• Molecule 39: 60S ribosomal protein eL28

Chain A2:


• Molecule 40: 60S ribosomal protein eL29

Chain A4:

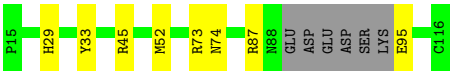




• Molecule 41: 60S ribosomal protein eL30

Chain A6:

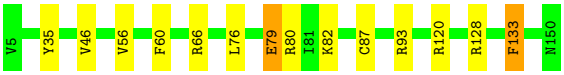

• Molecule 42: 60S ribosomal protein eL31

Chain A7:

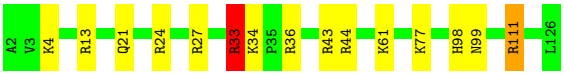

• Molecule 43: 60S ribosomal protein eL14

Chain AN:

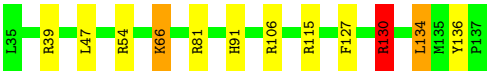

• Molecule 44: 60S ribosomal protein eL32

Chain A8:


• Molecule 45: 60S ribosomal protein eL33

Chain A9:


• Molecule 46: 60S ribosomal protein eL34

Chain Aa:



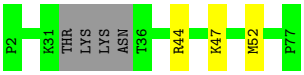
• Molecule 47: 60S ribosomal protein eL36

Chain Ab:



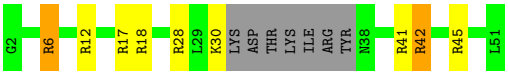
• Molecule 48: 60S ribosomal protein eL38

Chain Ad:



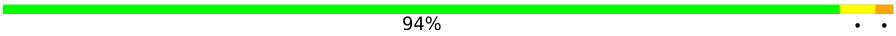

• Molecule 49: 60S ribosomal protein eL39

Chain Ae:


• Molecule 50: 60S ribosomal protein eL40

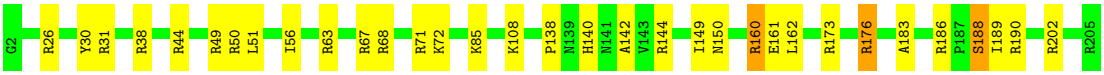
Chain Af:





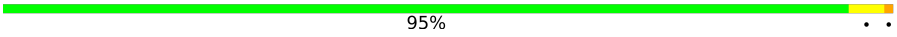
• Molecule 51: 60S ribosomal protein eL15

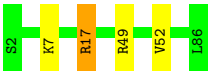
Chain AP:


• Molecule 52: 60S ribosomal protein eL43

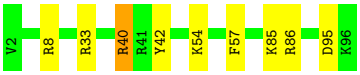
Chain Ah:



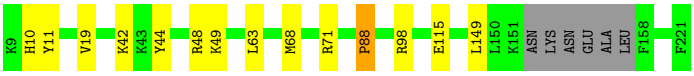

• Molecule 53: 60S ribosomal protein eL44

Chain Ai:


• Molecule 54: 60S ribosomal protein eL6

Chain AI:


• Molecule 55: 60S ribosomal protein eL8

Chain AJ:

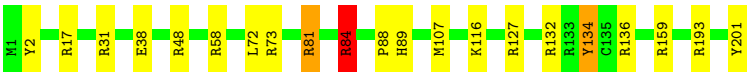

• Molecule 56: 60S ribosomal protein eL37

Chain Ac:



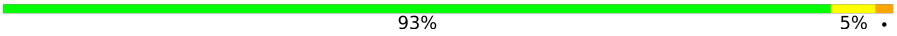
• Molecule 57: 60S ribosomal protein uL13

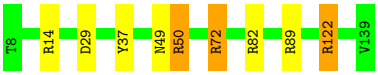
Chain AK:


• Molecule 58: 60S ribosomal protein uL14

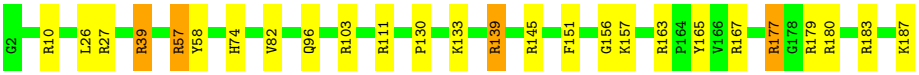
Chain AM:



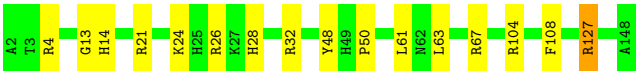

• Molecule 59: 60S ribosomal protein eL18

Chain AS:

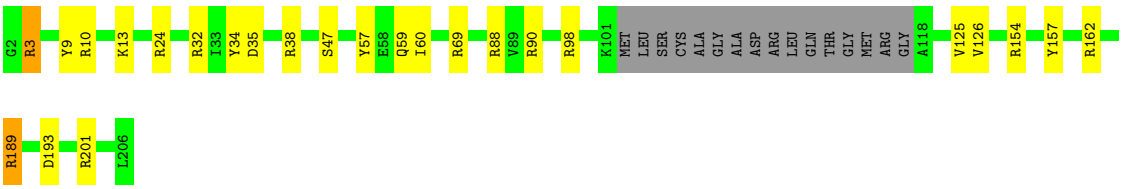

• Molecule 60: 60S ribosomal protein uL15

Chain AO:

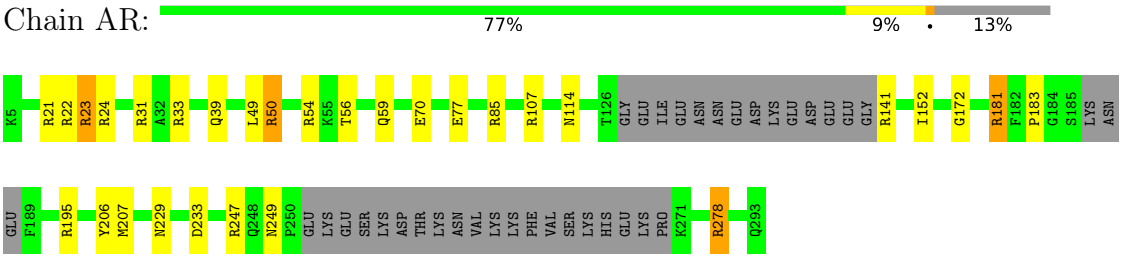

• Molecule 61: 60S ribosomal protein uL16

Chain AQ:

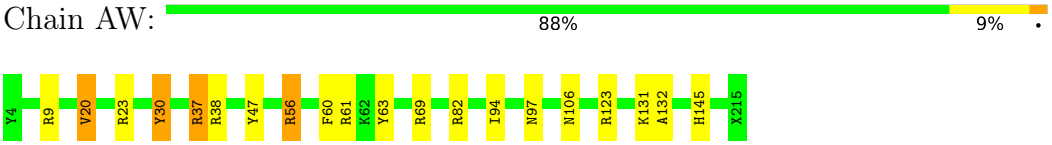

• Molecule 62: 60S ribosomal protein uL18

Chain AR:



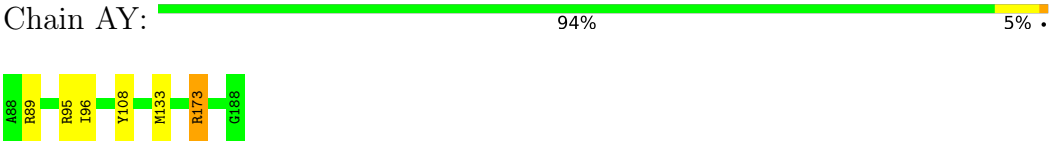

- Molecule 63: 60S ribosomal protein uL22

Chain AW:



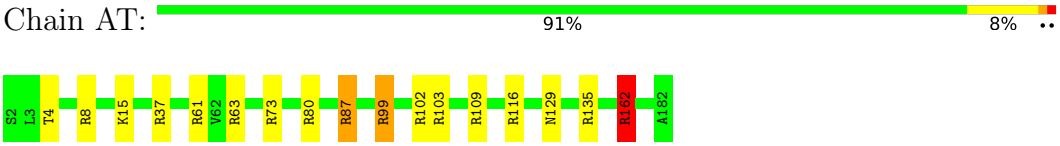

- Molecule 64: 60S ribosomal protein uL23

Chain AY:



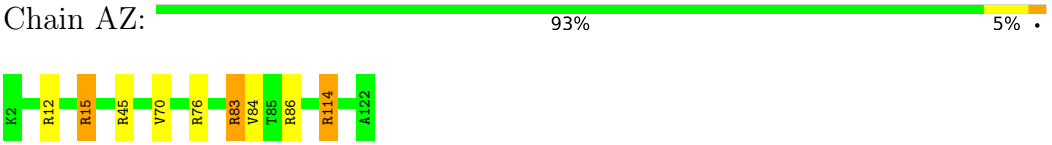

- Molecule 65: 60S ribosomal protein eL19

Chain AT:



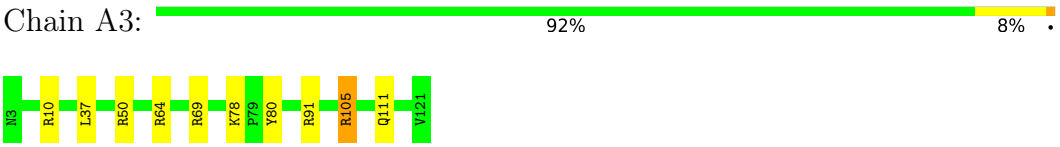

- Molecule 66: 60S ribosomal protein uL24

Chain AZ:



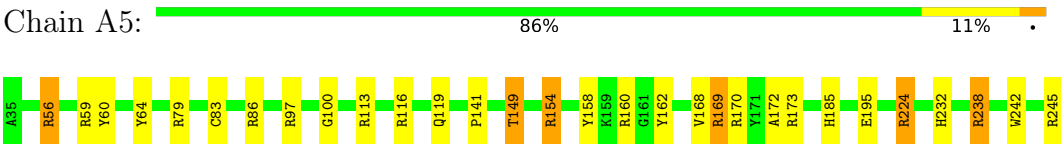

- Molecule 67: 60S ribosomal protein uL29

Chain A3:




- Molecule 68: 60S ribosomal protein uL30

Chain A5:



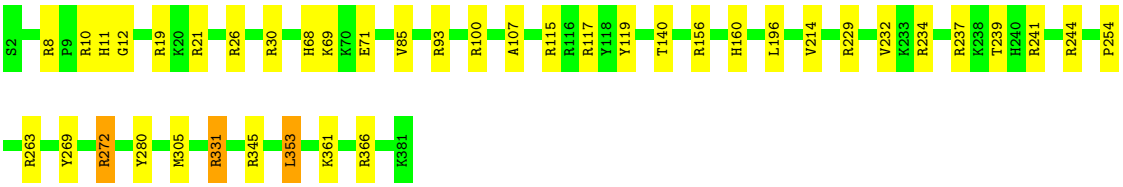

• Molecule 69: 60S ribosomal protein uL2

Chain AD:



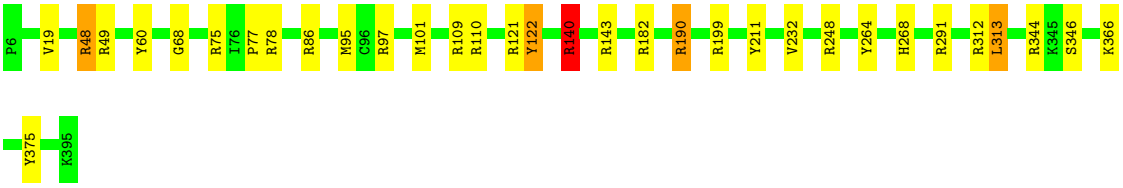
• Molecule 70: 60S ribosomal protein uL3

Chain AE:

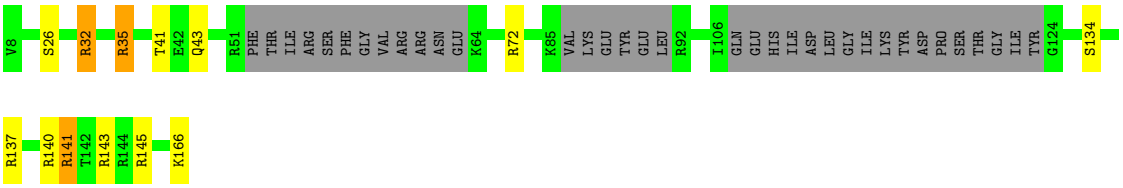

• Molecule 71: 60S ribosomal protein uL4

Chain AF:

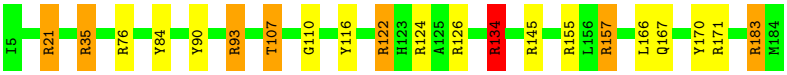

• Molecule 72: 60S ribosomal protein uL5

Chain AG:

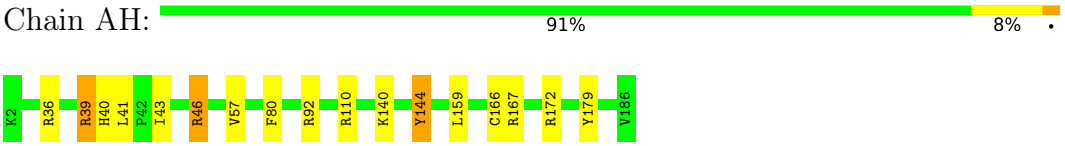

• Molecule 73: 60S ribosomal protein eL20

Chain AU:

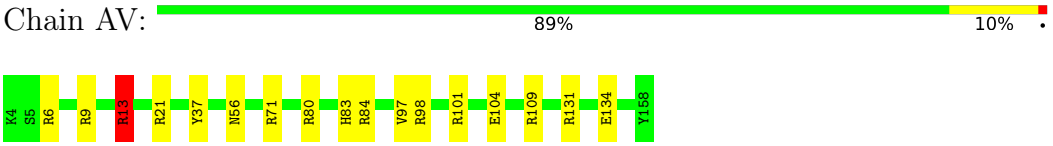

• Molecule 74: 60S ribosomal protein uL6

Chain AH:



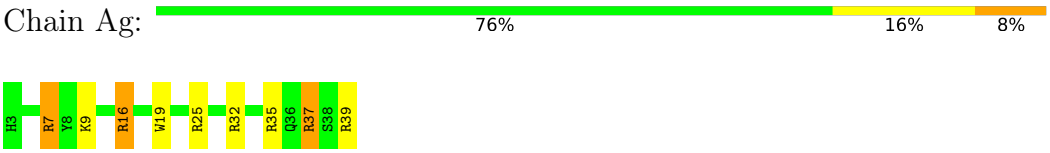

• Molecule 75: 60S ribosomal protein eL21

Chain AV:



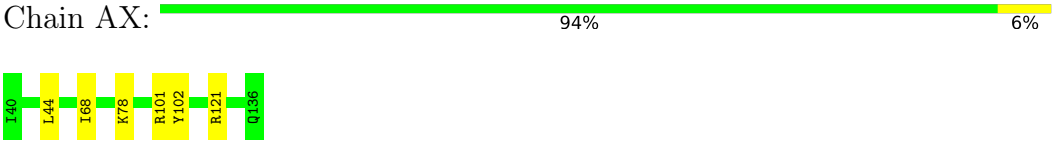

• Molecule 76: 60S ribosomal protein eL41

Chain Ag:



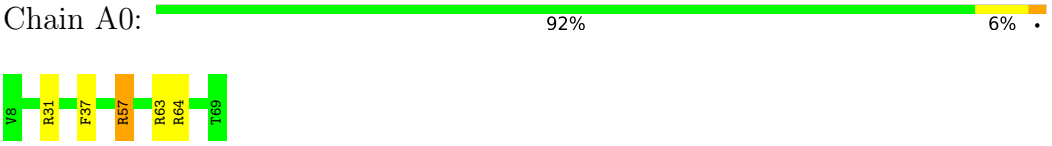

• Molecule 77: 60S ribosomal protein eL22

Chain AX:




• Molecule 78: 60S ribosomal protein eL24

Chain A0:



# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of particles used | 96732 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | Each micrograph | Depositor |
| Microscope | FEI POLARA 300 | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 25 | Depositor |
| Minimum defocus (nm) | 1500 | Depositor |
| Maximum defocus (nm) | 3500 | Depositor |
| Magnification | 30120 | Depositor |
| Image detector | GATAN K2 (4k x 4k) | 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 | A | 1.23 | 26/38275 (0.1%) | 1.58 | 870/59596 (1.5%) |
| 2 | 7 | 1.23 | 4/1754 (0.2%) | 1.79 | 69/2732 (2.5%) |
| 3 | D | 0.75 | 0/1241 | 1.13 | 10/1652 (0.6%) |
| 4 | E | 0.70 | 0/1539 | 1.16 | 13/2055 (0.6%) |
| 5 | G | 0.70 | 0/1800 | 1.01 | 5/2429 (0.2%) |
| 6 | I | 0.69 | 0/1443 | 1.22 | 15/1936 (0.8%) |
| 7 | K | 0.70 | 0/1054 | 1.15 | 10/1411 (0.7%) |
| 8 | M | 0.71 | 0/1114 | 1.12 | 4/1487 (0.3%) |
| 9 | W | 0.71 | 0/793 | 1.18 | 4/1053 (0.4%) |
| 10 | R | 0.74 | 0/755 | 1.06 | 0/1013 |
| 11 | O | 0.72 | 0/706 | 1.03 | 3/950 (0.3%) |
| 12 | Y | 0.70 | 0/1295 | 1.18 | 9/1742 (0.5%) |
| 13 | Z | 0.70 | 0/565 | 1.08 | 2/758 (0.3%) |
| 14 | 1 | 0.70 | 0/999 | 1.17 | 11/1321 (0.8%) |
| 15 | 2 | 0.75 | 0/324 | 0.98 | 1/435 (0.2%) |
| 16 | 3 | 0.71 | 0/794 | 1.24 | 10/1055 (0.9%) |
| 17 | 4 | 0.68 | 0/597 | 1.09 | 0/801 |
| 18 | 5 | 0.75 | 0/459 | 1.33 | 9/606 (1.5%) |
| 19 | 6 | 0.73 | 0/349 | 1.24 | 3/458 (0.7%) |
| 20 | B | 0.65 | 0/1738 | 1.11 | 9/2321 (0.4%) |
| 21 | F | 0.67 | 0/2098 | 1.14 | 11/2819 (0.4%) |
| 22 | H | 0.67 | 0/1665 | 1.10 | 5/2210 (0.2%) |
| 23 | J | 0.68 | 0/1545 | 1.07 | 7/2064 (0.3%) |
| 24 | L | 0.71 | 0/1407 | 1.23 | 16/1879 (0.9%) |
| 25 | N | 0.70 | 0/780 | 1.24 | 7/1053 (0.7%) |
| 26 | P | 0.70 | 0/966 | 1.23 | 8/1295 (0.6%) |
| 27 | Q | 0.69 | 0/1149 | 1.25 | 11/1532 (0.7%) |
| 28 | S | 0.65 | 0/1063 | 1.27 | 11/1425 (0.8%) |
| 29 | T | 0.73 | 0/412 | 1.25 | 6/544 (1.1%) |
| 30 | U | 0.67 | 0/1223 | 1.14 | 9/1634 (0.6%) |
| 31 | V | 0.71 | 0/1233 | 1.10 | 4/1645 (0.2%) |
| 32 | X | 0.71 | 0/788 | 1.18 | 7/1050 (0.7%) |
| 33 | C | 0.67 | 0/1570 | 1.08 | 4/2129 (0.2%) |
| 34 | AA | 1.30 | 70/75947 (0.1%) | 1.59 | 1892/118255 (1.6%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 35 | AC | 1.30 | 7/3599 (0.2%) | 1.55 | 88/5603 (1.6%) |
| 36 | AB | 1.27 | 2/2823 (0.1%) | 1.52 | 57/4400 (1.3%) |
| 37 | AL | 0.67 | 0/1789 | 1.14 | 9/2381 (0.4%) |
| 38 | A1 | 0.68 | 0/1151 | 1.02 | 1/1531 (0.1%) |
| 39 | A2 | 0.72 | 0/840 | 1.01 | 3/1114 (0.3%) |
| 40 | A4 | 0.66 | 0/564 | 1.01 | 3/737 (0.4%) |
| 41 | A6 | 0.69 | 0/749 | 0.99 | 2/1001 (0.2%) |
| 42 | A7 | 0.70 | 0/806 | 1.14 | 3/1073 (0.3%) |
| 43 | AN | 0.69 | 0/1218 | 1.12 | 6/1621 (0.4%) |
| 44 | A8 | 0.70 | 0/1054 | 1.24 | 10/1399 (0.7%) |
| 45 | A9 | 0.72 | 0/865 | 1.20 | 7/1160 (0.6%) |
| 46 | Aa | 0.68 | 0/872 | 1.26 | 11/1161 (0.9%) |
| 47 | Ab | 0.71 | 0/763 | 1.13 | 5/1008 (0.5%) |
| 48 | Ad | 0.72 | 0/612 | 1.09 | 2/812 (0.2%) |
| 49 | Ae | 0.75 | 0/396 | 1.41 | 6/521 (1.2%) |
| 50 | Af | 0.67 | 0/419 | 1.16 | 3/556 (0.5%) |
| 51 | AP | 0.69 | 0/1735 | 1.31 | 21/2320 (0.9%) |
| 52 | Ah | 0.68 | 0/668 | 1.13 | 2/887 (0.2%) |
| 53 | Ai | 0.67 | 0/789 | 1.16 | 6/1032 (0.6%) |
| 54 | AI | 0.66 | 0/1708 | 1.04 | 6/2274 (0.3%) |
| 55 | AJ | 0.67 | 0/1840 | 1.03 | 3/2456 (0.1%) |
| 56 | Ac | 0.72 | 0/723 | 1.29 | 8/951 (0.8%) |
| 57 | AK | 0.67 | 0/1690 | 1.15 | 13/2260 (0.6%) |
| 58 | AM | 0.68 | 0/1012 | 1.15 | 5/1363 (0.4%) |
| 59 | AS | 0.69 | 0/1531 | 1.24 | 17/2040 (0.8%) |
| 60 | AO | 0.66 | 0/1199 | 1.18 | 10/1597 (0.6%) |
| 61 | AQ | 0.73 | 0/1580 | 1.21 | 16/2113 (0.8%) |
| 62 | AR | 0.68 | 0/2079 | 1.16 | 20/2777 (0.7%) |
| 63 | AW | 0.68 | 0/1244 | 1.22 | 12/1663 (0.7%) |
| 64 | AY | 0.67 | 0/806 | 1.15 | 5/1074 (0.5%) |
| 65 | AT | 0.66 | 0/1525 | 1.17 | 15/2016 (0.7%) |
| 66 | AZ | 0.68 | 0/1013 | 1.17 | 9/1339 (0.7%) |
| 67 | A3 | 0.65 | 0/1005 | 1.09 | 8/1329 (0.6%) |
| 68 | A5 | 0.70 | 0/1917 | 1.25 | 22/2562 (0.9%) |
| 69 | AD | 0.68 | 0/1902 | 1.19 | 17/2544 (0.7%) |
| 70 | AE | 0.68 | 0/3130 | 1.16 | 25/4195 (0.6%) |
| 71 | AF | 0.68 | 0/3145 | 1.16 | 23/4205 (0.5%) |
| 72 | AG | 0.73 | 0/1021 | 1.19 | 9/1349 (0.7%) |
| 73 | AU | 0.70 | 0/1527 | 1.18 | 15/2043 (0.7%) |
| 74 | AH | 0.69 | 0/1501 | 1.17 | 10/2025 (0.5%) |
| 75 | AV | 0.68 | 0/1301 | 1.20 | 11/1732 (0.6%) |
| 76 | Ag | 0.74 | 0/348 | 1.57 | 8/448 (1.8%) |
| 77 | AX | 0.72 | 0/842 | 1.06 | 3/1125 (0.3%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 78 | A0 | 0.73 | 0/534 | 1.12 | 4/711 (0.6%) |
| All | All | 1.07 | 109/207275 (0.1%) | 1.44 | 3594/303853 (1.2%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 1 | A | 0 | 231 |
| 2 | 7 | 0 | 18 |
| 3 | D | 0 | 1 |
| 4 | E | 0 | 6 |
| 5 | G | 0 | 4 |
| 6 | I | 0 | 4 |
| 7 | K | 0 | 2 |
| 8 | M | 0 | 1 |
| 9 | W | 0 | 3 |
| 11 | O | 0 | 1 |
| 12 | Y | 0 | 6 |
| 14 | 1 | 0 | 2 |
| 15 | 2 | 0 | 1 |
| 16 | 3 | 0 | 2 |
| 17 | 4 | 0 | 3 |
| 19 | 6 | 0 | 2 |
| 20 | B | 0 | 4 |
| 21 | F | 0 | 5 |
| 22 | H | 0 | 3 |
| 23 | J | 0 | 5 |
| 24 | L | 0 | 3 |
| 25 | N | 0 | 1 |
| 26 | P | 0 | 3 |
| 27 | Q | 0 | 2 |
| 29 | T | 0 | 1 |
| 30 | U | 0 | 2 |
| 31 | V | 0 | 6 |
| 32 | X | 0 | 1 |
| 33 | C | 0 | 6 |
| 34 | AA | 1 | 546 |
| 35 | AC | 0 | 19 |
| 36 | AB | 0 | 14 |
| 37 | AL | 0 | 5 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 38 | A1 | 0 | 1 |
| 39 | A2 | 0 | 1 |
| 40 | A4 | 0 | 2 |
| 41 | A6 | 0 | 4 |
| 42 | A7 | 0 | 1 |
| 43 | AN | 0 | 3 |
| 44 | A8 | 0 | 2 |
| 45 | A9 | 0 | 2 |
| 46 | Aa | 0 | 4 |
| 47 | Ab | 0 | 1 |
| 49 | Ae | 0 | 5 |
| 50 | Af | 0 | 2 |
| 51 | AP | 0 | 6 |
| 52 | Ah | 0 | 2 |
| 53 | Ai | 0 | 3 |
| 54 | AI | 0 | 2 |
| 55 | AJ | 0 | 2 |
| 56 | Ac | 0 | 3 |
| 57 | AK | 0 | 5 |
| 58 | AM | 0 | 5 |
| 59 | AS | 0 | 8 |
| 60 | AO | 0 | 3 |
| 61 | AQ | 0 | 4 |
| 62 | AR | 0 | 4 |
| 63 | AW | 0 | 6 |
| 64 | AY | 0 | 1 |
| 65 | AT | 0 | 6 |
| 66 | AZ | 0 | 4 |
| 67 | A3 | 0 | 1 |
| 68 | A5 | 0 | 7 |
| 69 | AD | 0 | 6 |
| 70 | AE | 0 | 4 |
| 71 | AF | 0 | 6 |
| 72 | AG | 0 | 3 |
| 73 | AU | 0 | 7 |
| 74 | AH | 0 | 3 |
| 75 | AV | 0 | 5 |
| 76 | Ag | 0 | 2 |
| 77 | AX | 0 | 1 |
| 78 | A0 | 0 | 2 |
| All | All | 1 | 1052 |

All (109) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 34 | AA | 2552 | A | N9-C4 | -8.94 | 1.32 | 1.37 |
| 2 | 7 | 74 | A | C4'-C3' | 8.62 | 1.62 | 1.53 |
| 34 | AA | 275 | A | O3'-P | -7.93 | 1.51 | 1.61 |
| 34 | AA | 3122 | A | N9-C4 | -7.49 | 1.33 | 1.37 |
| 1 | A | 2055 | A | N9-C4 | -7.09 | 1.33 | 1.37 |
| 34 | AA | 2451 | A | N9-C4 | -7.05 | 1.33 | 1.37 |
| 34 | AA | 440 | A | N9-C4 | -6.91 | 1.33 | 1.37 |
| 34 | AA | 3160 | A | N9-C4 | -6.66 | 1.33 | 1.37 |
| 34 | AA | 629 | A | N9-C4 | -6.61 | 1.33 | 1.37 |
| 34 | AA | 1871 | A | N9-C4 | -6.52 | 1.33 | 1.37 |
| 1 | A | 2066 | G | P-O5' | -6.41 | 1.53 | 1.59 |
| 1 | A | 2082 | A | O3'-P | -6.24 | 1.53 | 1.61 |
| 34 | AA | 236 | U | O3'-P | -6.24 | 1.53 | 1.61 |
| 34 | AA | 2481 | A | N9-C4 | -6.24 | 1.34 | 1.37 |
| 34 | AA | 1184 | A | N9-C4 | -6.21 | 1.34 | 1.37 |
| 2 | 7 | 74 | A | C5'-C4' | 6.19 | 1.58 | 1.51 |
| 34 | AA | 3735 | A | N9-C4 | -6.16 | 1.34 | 1.37 |
| 34 | AA | 1500 | U | O3'-P | -6.11 | 1.53 | 1.61 |
| 34 | AA | 73 | U | O3'-P | -6.06 | 1.53 | 1.61 |
| 34 | AA | 3441 | A | N9-C4 | -6.02 | 1.34 | 1.37 |
| 34 | AA | 2516 | A | O3'-P | -6.01 | 1.53 | 1.61 |
| 34 | AA | 1540 | G | O3'-P | -5.97 | 1.53 | 1.61 |
| 34 | AA | 1574 | C | C2'-C1' | -5.96 | 1.46 | 1.53 |
| 2 | 7 | 38 | A | N9-C4 | -5.90 | 1.34 | 1.37 |
| 34 | AA | 1445 | A | N9-C4 | -5.89 | 1.34 | 1.37 |
| 34 | AA | 1575 | C | O3'-P | -5.88 | 1.54 | 1.61 |
| 1 | A | 1827 | U | P-O5' | -5.85 | 1.53 | 1.59 |
| 1 | A | 1957 | A | N9-C4 | -5.83 | 1.34 | 1.37 |
| 1 | A | 1819 | U | C5'-C4' | 5.78 | 1.58 | 1.51 |
| 34 | AA | 1594 | A | N9-C4 | -5.76 | 1.34 | 1.37 |
| 35 | AC | 127 | C | O3'-P | -5.71 | 1.54 | 1.61 |
| 34 | AA | 1576 | U | O3'-P | -5.70 | 1.54 | 1.61 |
| 34 | AA | 2166 | G | N9-C4 | -5.66 | 1.33 | 1.38 |
| 34 | AA | 1231 | A | O3'-P | -5.64 | 1.54 | 1.61 |
| 34 | AA | 2424 | A | N9-C4 | -5.62 | 1.34 | 1.37 |
| 34 | AA | 2998 | A | N9-C4 | -5.62 | 1.34 | 1.37 |
| 34 | AA | 2109 | A | N9-C4 | -5.58 | 1.34 | 1.37 |
| 34 | AA | 1015 | A | N9-C4 | -5.58 | 1.34 | 1.37 |
| 34 | AA | 1185 | A | N9-C4 | -5.54 | 1.34 | 1.37 |
| 34 | AA | 3632 | U | C5'-C4' | 5.53 | 1.57 | 1.51 |
| 34 | AA | 1071 | A | O3'-P | -5.53 | 1.54 | 1.61 |
| 35 | AC | 123 | A | N9-C4 | -5.52 | 1.34 | 1.37 |
| 34 | AA | 3067 | G | O3'-P | -5.51 | 1.54 | 1.61 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | A | 321 | A | N9-C4 | -5.49 | 1.34 | 1.37 |
| 34 | AA | 183 | U | C5'-C4' | 5.45 | 1.57 | 1.51 |
| 34 | AA | 765 | A | N9-C4 | -5.45 | 1.34 | 1.37 |
| 34 | AA | 3337 | U | C5'-C4' | 5.44 | 1.57 | 1.51 |
| 1 | A | 320 | C | C5'-C4' | 5.42 | 1.57 | 1.51 |
| 1 | A | 981 | U | O3'-P | -5.41 | 1.54 | 1.61 |
| 1 | A | 339 | A | P-O5' | -5.41 | 1.54 | 1.59 |
| 34 | AA | 3584 | A | O3'-P | -5.41 | 1.54 | 1.61 |
| 35 | AC | 145 | A | O3'-P | -5.41 | 1.54 | 1.61 |
| 34 | AA | 1480 | G | O3'-P | -5.41 | 1.54 | 1.61 |
| 1 | A | 802 | A | O3'-P | -5.39 | 1.54 | 1.61 |
| 35 | AC | 113 | A | O3'-P | -5.39 | 1.54 | 1.61 |
| 1 | A | 337 | G | O3'-P | -5.38 | 1.54 | 1.61 |
| 34 | AA | 2156 | A | N9-C4 | -5.38 | 1.34 | 1.37 |
| 34 | AA | 61 | A | O3'-P | -5.38 | 1.54 | 1.61 |
| 34 | AA | 406 | A | N9-C4 | -5.37 | 1.34 | 1.37 |
| 34 | AA | 2431 | A | N9-C4 | -5.37 | 1.34 | 1.37 |
| 34 | AA | 2152 | A | O3'-P | -5.37 | 1.54 | 1.61 |
| 35 | AC | 49 | C | O3'-P | -5.34 | 1.54 | 1.61 |
| 34 | AA | 1595 | A | N9-C4 | -5.34 | 1.34 | 1.37 |
| 34 | AA | 2706 | A | N9-C4 | -5.33 | 1.34 | 1.37 |
| 34 | AA | 48 | A | N9-C4 | -5.32 | 1.34 | 1.37 |
| 34 | AA | 2974 | A | N9-C4 | -5.32 | 1.34 | 1.37 |
| 35 | AC | 92 | A | N9-C4 | -5.31 | 1.34 | 1.37 |
| 34 | AA | 1508 | U | O3'-P | -5.30 | 1.54 | 1.61 |
| 1 | A | 314 | A | N9-C4 | -5.30 | 1.34 | 1.37 |
| 34 | AA | 3062 | U | O3'-P | -5.29 | 1.54 | 1.61 |
| 1 | A | 338 | U | O3'-P | -5.29 | 1.54 | 1.61 |
| 34 | AA | 3063 | U | P-O5' | -5.29 | 1.54 | 1.59 |
| 34 | AA | 3255 | A | N9-C4 | -5.28 | 1.34 | 1.37 |
| 34 | AA | 1642 | G | O3'-P | -5.27 | 1.54 | 1.61 |
| 1 | A | 617 | G | O3'-P | -5.26 | 1.54 | 1.61 |
| 34 | AA | 674 | U | O3'-P | -5.25 | 1.54 | 1.61 |
| 34 | AA | 3632 | U | P-O5' | -5.25 | 1.54 | 1.59 |
| 34 | AA | 3587 | U | P-O5' | -5.25 | 1.54 | 1.59 |
| 34 | AA | 2605 | A | N9-C4 | -5.24 | 1.34 | 1.37 |
| 34 | AA | 369 | A | N9-C4 | -5.24 | 1.34 | 1.37 |
| 34 | AA | 1526 | G | N9-C4 | -5.23 | 1.33 | 1.38 |
| 1 | A | 618 | U | P-O5' | -5.23 | 1.54 | 1.59 |
| 34 | AA | 1297 | A | N3-C4 | -5.23 | 1.31 | 1.34 |
| 1 | A | 824 | A | N9-C4 | -5.21 | 1.34 | 1.37 |
| 34 | AA | 925 | A | C2'-C1' | -5.20 | 1.47 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 34 | AA | 345 | G | N9-C4 | -5.20 | 1.33 | 1.38 |
| 34 | AA | 1072 | A | N9-C4 | -5.17 | 1.34 | 1.37 |
| 1 | A | 920 | A | C5'-C4' | 5.14 | 1.57 | 1.51 |
| 34 | AA | 1340 | G | O3'-P | -5.14 | 1.54 | 1.61 |
| 34 | AA | 1746 | A | N9-C4 | -5.13 | 1.34 | 1.37 |
| 34 | AA | 1743 | U | O3'-P | -5.13 | 1.54 | 1.61 |
| 2 | 7 | 65 | A | N9-C4 | -5.12 | 1.34 | 1.37 |
| 1 | A | 982 | A | N9-C4 | -5.12 | 1.34 | 1.37 |
| 1 | A | 1800 | A | O3'-P | -5.11 | 1.55 | 1.61 |
| 1 | A | 391 | A | N9-C4 | -5.11 | 1.34 | 1.37 |
| 34 | AA | 2674 | G | O3'-P | -5.10 | 1.55 | 1.61 |
| 1 | A | 2050 | U | O3'-P | -5.09 | 1.55 | 1.61 |
| 1 | A | 915 | G | C5'-C4' | 5.09 | 1.57 | 1.51 |
| 34 | AA | 2885 | A | O3'-P | -5.09 | 1.55 | 1.61 |
| 36 | AB | 103 | A | N9-C4 | -5.08 | 1.34 | 1.37 |
| 35 | AC | 140 | G | C5'-C4' | 5.08 | 1.57 | 1.51 |
| 34 | AA | 898 | G | O3'-P | -5.07 | 1.55 | 1.61 |
| 1 | A | 1039 | A | N7-C5 | -5.07 | 1.36 | 1.39 |
| 34 | AA | 3708 | U | O3'-P | -5.07 | 1.55 | 1.61 |
| 34 | AA | 206 | A | O3'-P | -5.05 | 1.55 | 1.61 |
| 1 | A | 404 | G | O3'-P | -5.05 | 1.55 | 1.61 |
| 34 | AA | 1069 | G | O3'-P | -5.04 | 1.55 | 1.61 |
| 36 | AB | 6 | C | O3'-P | -5.01 | 1.55 | 1.61 |
| 1 | A | 1071 | G | O3'-P | -5.01 | 1.55 | 1.61 |

All (3594) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 34 | AA | 3632 | U | P-O5'-C5' | 19.68 | 152.39 | 120.90 |
| 34 | AA | 257 | U | P-O3'-C3' | 18.75 | 142.20 | 119.70 |
| 34 | AA | 181 | C | P-O3'-C3' | 15.57 | 138.38 | 119.70 |
| 34 | AA | 3018 | A | P-O3'-C3' | 15.30 | 138.06 | 119.70 |
| 2 | 7 | 74 | A | C5'-C4'-O4' | -14.85 | 91.28 | 109.10 |
| 1 | A | 981 | U | P-O3'-C3' | 14.75 | 137.41 | 119.70 |
| 6 | I | 195 | ARG | NE-CZ-NH1 | 14.75 | 127.67 | 120.30 |
| 34 | AA | 859 | C | P-O3'-C3' | 14.02 | 136.52 | 119.70 |
| 1 | A | 1912 | C | P-O3'-C3' | 13.96 | 136.46 | 119.70 |
| 34 | AA | 1574 | C | O4'-C1'-N1 | 13.26 | 118.81 | 108.20 |
| 34 | AA | 621 | C | P-O3'-C3' | 13.08 | 135.40 | 119.70 |
| 34 | AA | 162 | U | P-O3'-C3' | 12.59 | 134.81 | 119.70 |
| 34 | AA | 101 | C | O4'-C1'-N1 | 12.50 | 118.20 | 108.20 |
| 35 | AC | 37 | A | P-O3'-C3' | 12.21 | 134.36 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 34 | AA | 1205 | U | P-O3'-C3' | 12.16 | 134.29 | 119.70 |
| 1 | A | 1413 | U | P-O3'-C3' | 12.00 | 134.10 | 119.70 |
| 64 | AY | 173 | ARG | NE-CZ-NH2 | -11.98 | 114.31 | 120.30 |
| 1 | A | 1448 | U | P-O3'-C3' | 11.96 | 134.05 | 119.70 |
| 1 | A | 250 | A | P-O3'-C3' | 11.94 | 134.03 | 119.70 |
| 1 | A | 1897 | A | P-O3'-C3' | 11.86 | 133.94 | 119.70 |
| 34 | AA | 1574 | C | P-O3'-C3' | 11.81 | 133.87 | 119.70 |
| 34 | AA | 289 | A | P-O3'-C3' | 11.81 | 133.87 | 119.70 |
| 34 | AA | 674 | U | P-O3'-C3' | 11.80 | 133.87 | 119.70 |
| 34 | AA | 270 | U | P-O3'-C3' | 11.73 | 133.78 | 119.70 |
| 34 | AA | 1230 | A | O4'-C1'-N9 | 11.63 | 117.51 | 108.20 |
| 34 | AA | 2696 | G | P-O3'-C3' | 11.58 | 133.59 | 119.70 |
| 34 | AA | 1989 | A | P-O3'-C3' | 11.53 | 133.54 | 119.70 |
| 1 | A | 291 | A | P-O3'-C3' | 11.50 | 133.50 | 119.70 |
| 2 | 7 | 74 | A | C5'-C4'-C3' | 11.46 | 134.34 | 116.00 |
| 34 | AA | 769 | U | O4'-C1'-N1 | 11.45 | 117.36 | 108.20 |
| 34 | AA | 803 | A | O4'-C1'-N9 | 11.25 | 117.20 | 108.20 |
| 71 | AF | 182 | ARG | NE-CZ-NH2 | -11.21 | 114.69 | 120.30 |
| 34 | AA | 2180 | U | P-O3'-C3' | 11.15 | 133.08 | 119.70 |
| 34 | AA | 697 | A | P-O3'-C3' | 11.12 | 133.04 | 119.70 |
| 59 | AS | 145 | ARG | NE-CZ-NH2 | 11.06 | 125.83 | 120.30 |
| 21 | F | 145 | ARG | NE-CZ-NH1 | 11.03 | 125.81 | 120.30 |
| 34 | AA | 2883 | U | P-O3'-C3' | 10.99 | 132.88 | 119.70 |
| 27 | Q | 144 | ARG | NE-CZ-NH1 | 10.98 | 125.79 | 120.30 |
| 34 | AA | 1435 | G | P-O3'-C3' | 10.96 | 132.86 | 119.70 |
| 34 | AA | 2822 | U | P-O3'-C3' | 10.95 | 132.84 | 119.70 |
| 2 | 7 | 74 | A | O4'-C4'-C3' | -10.90 | 93.10 | 104.00 |
| 34 | AA | 179 | G | P-O3'-C3' | 10.89 | 132.77 | 119.70 |
| 34 | AA | 411 | U | P-O3'-C3' | 10.82 | 132.68 | 119.70 |
| 4 | E | 126 | ARG | NE-CZ-NH1 | 10.75 | 125.68 | 120.30 |
| 34 | AA | 580 | A | P-O3'-C3' | 10.75 | 132.60 | 119.70 |
| 34 | AA | 702 | U | O4'-C1'-N1 | 10.75 | 116.80 | 108.20 |
| 1 | A | 1865 | G | P-O3'-C3' | 10.75 | 132.60 | 119.70 |
| 51 | AP | 176 | ARG | NE-CZ-NH1 | 10.71 | 125.66 | 120.30 |
| 1 | A | 156 | A | P-O3'-C3' | 10.68 | 132.51 | 119.70 |
| 1 | A | 1673 | A | P-O3'-C3' | 10.68 | 132.51 | 119.70 |
| 57 | AK | 136 | ARG | NE-CZ-NH1 | 10.67 | 125.64 | 120.30 |
| 68 | A5 | 158 | TYR | CB-CG-CD2 | -10.52 | 114.69 | 121.00 |
| 1 | A | 1832 | U | P-O3'-C3' | 10.49 | 132.29 | 119.70 |
| 70 | AE | 30 | ARG | NE-CZ-NH2 | -10.47 | 115.06 | 120.30 |
| 42 | A7 | 73 | ARG | NE-CZ-NH1 | 10.46 | 125.53 | 120.30 |
| 34 | AA | 860 | A | P-O5'-C5' | 10.46 | 137.63 | 120.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 1381 | C | P-O3'-C3' | 10.45 | 132.24 | 119.70 |
| 1 | A | 1645 | C | P-O3'-C3' | 10.41 | 132.19 | 119.70 |
| 1 | A | 1448 | U | O4'-C1'-N1 | 10.38 | 116.51 | 108.20 |
| 29 | T | 54 | ARG | NE-CZ-NH1 | -10.38 | 115.11 | 120.30 |
| 37 | AL | 69 | ARG | NE-CZ-NH1 | 10.37 | 125.49 | 120.30 |
| 34 | AA | 2919 | A | P-O3'-C3' | 10.31 | 132.07 | 119.70 |
| 31 | V | 102 | ARG | NE-CZ-NH2 | -10.30 | 115.15 | 120.30 |
| 75 | AV | 84 | ARG | NE-CZ-NH1 | -10.29 | 115.16 | 120.30 |
| 1 | A | 1071 | G | P-O3'-C3' | 10.27 | 132.02 | 119.70 |
| 71 | AF | 182 | ARG | NE-CZ-NH1 | 10.26 | 125.43 | 120.30 |
| 1 | A | 1069 | C | O4'-C1'-N1 | 10.20 | 116.36 | 108.20 |
| 34 | AA | 673 | U | O4'-C1'-N1 | 10.19 | 116.35 | 108.20 |
| 34 | AA | 2695 | A | P-O5'-C5' | 10.14 | 137.12 | 120.90 |
| 1 | A | 544 | G | P-O3'-C3' | 10.13 | 131.86 | 119.70 |
| 1 | A | 1621 | G | C5-C6-O6 | -10.11 | 122.53 | 128.60 |
| 58 | AM | 14 | ARG | NE-CZ-NH1 | 10.07 | 125.33 | 120.30 |
| 34 | AA | 2004 | U | O4'-C1'-N1 | 10.06 | 116.25 | 108.20 |
| 58 | AM | 89 | ARG | NE-CZ-NH1 | 10.06 | 125.33 | 120.30 |
| 34 | AA | 949 | A | O4'-C1'-N9 | 10.01 | 116.21 | 108.20 |
| 73 | AU | 171 | ARG | NE-CZ-NH1 | 9.99 | 125.30 | 120.30 |
| 62 | AR | 54 | ARG | NE-CZ-NH1 | 9.96 | 125.28 | 120.30 |
| 73 | AU | 122 | ARG | NE-CZ-NH1 | -9.93 | 115.33 | 120.30 |
| 1 | A | 1414 | A | P-O3'-C3' | 9.91 | 131.60 | 119.70 |
| 28 | S | 88 | ARG | NE-CZ-NH2 | 9.89 | 125.25 | 120.30 |
| 34 | AA | 858 | C | O4'-C1'-N1 | 9.89 | 116.11 | 108.20 |
| 1 | A | 248 | G | P-O3'-C3' | 9.86 | 131.53 | 119.70 |
| 60 | AO | 26 | ARG | NE-CZ-NH1 | 9.86 | 125.23 | 120.30 |
| 30 | U | 55 | ARG | NE-CZ-NH1 | -9.84 | 115.38 | 120.30 |
| 34 | AA | 500 | A | P-O3'-C3' | 9.80 | 131.46 | 119.70 |
| 1 | A | 647 | C | C2-N1-C1' | 9.79 | 129.57 | 118.80 |
| 24 | L | 217 | ARG | NE-CZ-NH1 | -9.77 | 115.42 | 120.30 |
| 34 | AA | 579 | C | P-O3'-C3' | 9.76 | 131.41 | 119.70 |
| 1 | A | 1857 | U | O4'-C1'-N1 | 9.76 | 116.00 | 108.20 |
| 1 | A | 1788 | U | O4'-C1'-N1 | 9.75 | 116.00 | 108.20 |
| 34 | AA | 3230 | G | P-O3'-C3' | 9.75 | 131.40 | 119.70 |
| 59 | AS | 145 | ARG | NE-CZ-NH1 | -9.72 | 115.44 | 120.30 |
| 34 | AA | 432 | A | P-O3'-C3' | 9.72 | 131.37 | 119.70 |
| 34 | AA | 594 | C | C2-N1-C1' | 9.72 | 129.49 | 118.80 |
| 6 | I | 62 | ARG | NE-CZ-NH2 | 9.70 | 125.15 | 120.30 |
| 73 | AU | 122 | ARG | NE-CZ-NH2 | 9.70 | 125.15 | 120.30 |
| 68 | A5 | 224 | ARG | NE-CZ-NH1 | 9.68 | 125.14 | 120.30 |
| 34 | AA | 1881 | C | O4'-C1'-N1 | 9.68 | 115.94 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 34 | AA | 3507 | A | O4'-C1'-N9 | 9.64 | 115.92 | 108.20 |
| 1 | A | 161 | U | O4'-C1'-N1 | 9.60 | 115.88 | 108.20 |
| 1 | A | 1069 | C | C2-N1-C1' | 9.60 | 129.36 | 118.80 |
| 34 | AA | 1207 | U | O4'-C1'-N1 | 9.58 | 115.87 | 108.20 |
| 34 | AA | 607 | A | P-O3'-C3' | 9.58 | 131.20 | 119.70 |
| 1 | A | 1283 | U | P-O3'-C3' | 9.53 | 131.13 | 119.70 |
| 34 | AA | 581 | C | P-O3'-C3' | 9.52 | 131.13 | 119.70 |
| 34 | AA | 2394 | C | P-O3'-C3' | 9.52 | 131.12 | 119.70 |
| 34 | AA | 3205 | U | O4'-C1'-N1 | 9.49 | 115.80 | 108.20 |
| 1 | A | 1799 | A | O4'-C1'-N9 | 9.49 | 115.79 | 108.20 |
| 34 | AA | 702 | U | C2-N1-C1' | 9.47 | 129.07 | 117.70 |
| 1 | A | 789 | U | P-O3'-C3' | 9.47 | 131.06 | 119.70 |
| 1 | A | 1455 | C | P-O3'-C3' | 9.46 | 131.05 | 119.70 |
| 34 | AA | 501 | U | O4'-C1'-N1 | 9.46 | 115.77 | 108.20 |
| 34 | AA | 934 | G | C5-C6-O6 | -9.46 | 122.92 | 128.60 |
| 62 | AR | 33 | ARG | NE-CZ-NH1 | 9.43 | 125.01 | 120.30 |
| 35 | AC | 35 | A | P-O3'-C3' | 9.41 | 131.00 | 119.70 |
| 1 | A | 460 | G | O4'-C1'-N9 | 9.41 | 115.72 | 108.20 |
| 34 | AA | 3167 | A | O4'-C1'-N9 | 9.40 | 115.72 | 108.20 |
| 1 | A | 1182 | A | P-O3'-C3' | 9.40 | 130.98 | 119.70 |
| 59 | AS | 57 | ARG | NE-CZ-NH1 | -9.39 | 115.60 | 120.30 |
| 30 | U | 76 | ARG | NE-CZ-NH1 | 9.38 | 124.99 | 120.30 |
| 34 | AA | 122 | A | O4'-C1'-N9 | 9.38 | 115.70 | 108.20 |
| 34 | AA | 3754 | A | O4'-C1'-N9 | 9.35 | 115.68 | 108.20 |
| 34 | AA | 926 | G | O4'-C1'-N9 | 9.34 | 115.67 | 108.20 |
| 1 | A | 253 | A | O4'-C1'-N9 | 9.33 | 115.67 | 108.20 |
| 34 | AA | 1805 | U | P-O3'-C3' | 9.33 | 130.90 | 119.70 |
| 68 | A5 | 158 | TYR | CB-CG-CD1 | 9.30 | 126.58 | 121.00 |
| 49 | Ae | 42 | ARG | NE-CZ-NH1 | 9.29 | 124.95 | 120.30 |
| 34 | AA | 504 | A | P-O3'-C3' | 9.27 | 130.83 | 119.70 |
| 44 | A8 | 27 | ARG | NE-CZ-NH1 | 9.25 | 124.93 | 120.30 |
| 34 | AA | 698 | G | P-O3'-C3' | 9.22 | 130.77 | 119.70 |
| 1 | A | 546 | G | O4'-C1'-N9 | 9.21 | 115.57 | 108.20 |
| 34 | AA | 3658 | G | P-O3'-C3' | 9.21 | 130.75 | 119.70 |
| 69 | AD | 30 | ARG | NE-CZ-NH1 | 9.20 | 124.90 | 120.30 |
| 34 | AA | 888 | A | P-O3'-C3' | 9.19 | 130.73 | 119.70 |
| 59 | AS | 180 | ARG | NE-CZ-NH1 | 9.19 | 124.89 | 120.30 |
| 26 | P | 98 | ARG | NE-CZ-NH1 | 9.18 | 124.89 | 120.30 |
| 12 | Y | 124 | ARG | NE-CZ-NH2 | 9.18 | 124.89 | 120.30 |
| 68 | A5 | 56 | ARG | NE-CZ-NH2 | -9.17 | 115.71 | 120.30 |
| 34 | AA | 1502 | G | O4'-C1'-N9 | 9.17 | 115.53 | 108.20 |
| 1 | A | 1732 | G | O4'-C1'-N9 | 9.16 | 115.53 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 34 | AA | 2885 | A | P-O3'-C3' | 9.15 | 130.68 | 119.70 |
| 25 | N | 78 | ARG | NE-CZ-NH1 | -9.12 | 115.74 | 120.30 |
| 1 | A | 483 | A | O4'-C1'-N9 | 9.11 | 115.49 | 108.20 |
| 34 | AA | 101 | C | C2-N1-C1' | 9.09 | 128.80 | 118.80 |
| 51 | AP | 50 | ARG | NE-CZ-NH1 | 9.08 | 124.84 | 120.30 |
| 68 | A5 | 245 | ARG | NE-CZ-NH2 | 9.06 | 124.83 | 120.30 |
| 1 | A | 1209 | G | C5-C6-O6 | -9.05 | 123.17 | 128.60 |
| 75 | AV | 6 | ARG | NE-CZ-NH1 | 9.03 | 124.82 | 120.30 |
| 34 | AA | 228 | A | O4'-C1'-N9 | 9.03 | 115.42 | 108.20 |
| 34 | AA | 3476 | A | P-O3'-C3' | 9.02 | 130.53 | 119.70 |
| 34 | AA | 1990 | A | P-O3'-C3' | 9.02 | 130.52 | 119.70 |
| 2 | 7 | 42 | C | O4'-C1'-N1 | 9.01 | 115.41 | 108.20 |
| 34 | AA | 3528 | A | O4'-C1'-N9 | 9.00 | 115.40 | 108.20 |
| 34 | AA | 1269 | C | O4'-C1'-N1 | 8.99 | 115.39 | 108.20 |
| 34 | AA | 1474 | A | O4'-C1'-N9 | 8.99 | 115.39 | 108.20 |
| 34 | AA | 2393 | A | O4'-C1'-N9 | 8.98 | 115.39 | 108.20 |
| 34 | AA | 2925 | U | O4'-C1'-N1 | 8.98 | 115.39 | 108.20 |
| 1 | A | 1786 | U | P-O3'-C3' | 8.98 | 130.47 | 119.70 |
| 34 | AA | 2816 | U | P-O3'-C3' | 8.98 | 130.47 | 119.70 |
| 34 | AA | 2801 | C | O4'-C1'-N1 | 8.97 | 115.38 | 108.20 |
| 28 | S | 134 | ARG | NE-CZ-NH1 | 8.95 | 124.77 | 120.30 |
| 1 | A | 251 | U | P-O3'-C3' | 8.91 | 130.39 | 119.70 |
| 1 | A | 1231 | G | C5-C6-O6 | -8.91 | 123.26 | 128.60 |
| 1 | A | 833 | A | O4'-C1'-N9 | 8.90 | 115.32 | 108.20 |
| 34 | AA | 2033 | C | P-O3'-C3' | 8.90 | 130.38 | 119.70 |
| 34 | AA | 2682 | C | O4'-C1'-N1 | 8.90 | 115.32 | 108.20 |
| 34 | AA | 1630 | A | P-O3'-C3' | -8.89 | 109.03 | 119.70 |
| 34 | AA | 3590 | A | P-O3'-C3' | 8.89 | 130.36 | 119.70 |
| 34 | AA | 2727 | U | O4'-C1'-N1 | 8.86 | 115.28 | 108.20 |
| 34 | AA | 1100 | A | O4'-C1'-N9 | 8.85 | 115.28 | 108.20 |
| 34 | AA | 1504 | A | O4'-C1'-N9 | 8.85 | 115.28 | 108.20 |
| 34 | AA | 3502 | C | O4'-C1'-N1 | 8.85 | 115.28 | 108.20 |
| 1 | A | 1224 | C | O4'-C1'-N1 | 8.84 | 115.27 | 108.20 |
| 51 | AP | 31 | ARG | NE-CZ-NH1 | 8.81 | 124.70 | 120.30 |
| 34 | AA | 2572 | A | O4'-C1'-N9 | 8.80 | 115.24 | 108.20 |
| 1 | A | 1976 | G | P-O3'-C3' | 8.79 | 130.25 | 119.70 |
| 34 | AA | 2577 | C | O4'-C1'-N1 | 8.79 | 115.23 | 108.20 |
| 34 | AA | 3342 | C | O4'-C1'-N1 | 8.77 | 115.22 | 108.20 |
| 51 | AP | 38 | ARG | NE-CZ-NH2 | 8.76 | 124.68 | 120.30 |
| 34 | AA | 1758 | C | O4'-C1'-N1 | 8.75 | 115.20 | 108.20 |
| 34 | AA | 2437 | A | O4'-C1'-N9 | 8.74 | 115.19 | 108.20 |
| 34 | AA | 1481 | A | P-O3'-C3' | 8.74 | 130.19 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 8 | M | 83 | ARG | NE-CZ-NH1 | 8.73 | 124.67 | 120.30 |
| 34 | AA | 745 | C | O4'-C1'-N1 | 8.73 | 115.18 | 108.20 |
| 51 | AP | 202 | ARG | NE-CZ-NH2 | -8.72 | 115.94 | 120.30 |
| 1 | A | 1621 | G | N1-C6-O6 | 8.72 | 125.13 | 119.90 |
| 27 | Q | 20 | ARG | NE-CZ-NH1 | 8.72 | 124.66 | 120.30 |
| 34 | AA | 1739 | C | O4'-C1'-N1 | 8.71 | 115.17 | 108.20 |
| 34 | AA | 1281 | C | O4'-C1'-N1 | 8.71 | 115.17 | 108.20 |
| 34 | AA | 1480 | G | O4'-C1'-N9 | 8.70 | 115.16 | 108.20 |
| 34 | AA | 2591 | U | O4'-C1'-N1 | 8.70 | 115.16 | 108.20 |
| 34 | AA | 2499 | G | C4-N9-C1' | 8.69 | 137.80 | 126.50 |
| 34 | AA | 1681 | C | O4'-C1'-N1 | 8.69 | 115.15 | 108.20 |
| 34 | AA | 1794 | U | C1'-O4'-C4' | -8.69 | 102.95 | 109.90 |
| 34 | AA | 116 | A | O4'-C1'-N9 | 8.69 | 115.15 | 108.20 |
| 34 | AA | 1035 | G | P-O3'-C3' | 8.68 | 130.11 | 119.70 |
| 1 | A | 206 | A | P-O3'-C3' | 8.66 | 130.10 | 119.70 |
| 34 | AA | 643 | G | O4'-C1'-N9 | 8.66 | 115.13 | 108.20 |
| 34 | AA | 3526 | U | O4'-C1'-N1 | 8.66 | 115.12 | 108.20 |
| 62 | AR | 278 | ARG | NE-CZ-NH2 | -8.65 | 115.97 | 120.30 |
| 34 | AA | 2501 | A | O4'-C1'-N9 | 8.64 | 115.11 | 108.20 |
| 75 | AV | 101 | ARG | NE-CZ-NH2 | -8.62 | 115.99 | 120.30 |
| 34 | AA | 1224 | A | P-O3'-C3' | 8.62 | 130.04 | 119.70 |
| 1 | A | 647 | C | O4'-C1'-N1 | 8.60 | 115.08 | 108.20 |
| 14 | 1 | 91 | ARG | NE-CZ-NH1 | -8.59 | 116.00 | 120.30 |
| 68 | A5 | 56 | ARG | NE-CZ-NH1 | 8.59 | 124.60 | 120.30 |
| 1 | A | 383 | G | P-O3'-C3' | 8.59 | 130.01 | 119.70 |
| 1 | A | 25 | C | O4'-C1'-N1 | 8.58 | 115.06 | 108.20 |
| 34 | AA | 2608 | G | O4'-C1'-N9 | 8.58 | 115.06 | 108.20 |
| 35 | AC | 115 | C | O4'-C1'-N1 | 8.58 | 115.06 | 108.20 |
| 34 | AA | 3711 | U | O4'-C1'-N1 | 8.57 | 115.06 | 108.20 |
| 34 | AA | 239 | U | O4'-C1'-N1 | 8.57 | 115.05 | 108.20 |
| 1 | A | 2071 | U | P-O3'-C3' | 8.56 | 129.97 | 119.70 |
| 34 | AA | 61 | A | P-O3'-C3' | 8.56 | 129.97 | 119.70 |
| 34 | AA | 544 | C | O4'-C1'-N1 | 8.54 | 115.03 | 108.20 |
| 34 | AA | 2015 | C | O4'-C1'-N1 | 8.52 | 115.02 | 108.20 |
| 34 | AA | 532 | C | O4'-C1'-N1 | 8.52 | 115.02 | 108.20 |
| 1 | A | 1231 | G | N1-C6-O6 | 8.51 | 125.00 | 119.90 |
| 25 | N | 78 | ARG | NE-CZ-NH2 | 8.51 | 124.55 | 120.30 |
| 34 | AA | 1705 | A | P-O3'-C3' | 8.50 | 129.90 | 119.70 |
| 47 | Ab | 106 | ARG | NE-CZ-NH2 | -8.50 | 116.05 | 120.30 |
| 36 | AB | 39 | C | P-O3'-C3' | 8.49 | 129.89 | 119.70 |
| 24 | L | 217 | ARG | NE-CZ-NH2 | 8.49 | 124.55 | 120.30 |
| 26 | P | 128 | ARG | NE-CZ-NH2 | 8.48 | 124.54 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 36 | AB | 102 | C | O4'-C1'-N1 | 8.48 | 114.98 | 108.20 |
| 2 | 7 | 28 | C | O4'-C1'-N1 | 8.47 | 114.98 | 108.20 |
| 1 | A | 970 | G | O4'-C1'-N9 | 8.46 | 114.97 | 108.20 |
| 76 | Ag | 37 | ARG | NE-CZ-NH1 | 8.46 | 124.53 | 120.30 |
| 1 | A | 485 | C | O4'-C1'-N1 | 8.46 | 114.97 | 108.20 |
| 34 | AA | 101 | C | C6-N1-C1' | -8.46 | 110.64 | 120.80 |
| 34 | AA | 1913 | A | P-O3'-C3' | 8.46 | 129.85 | 119.70 |
| 71 | AF | 122 | TYR | CB-CG-CD2 | -8.46 | 115.92 | 121.00 |
| 65 | AT | 162 | ARG | NE-CZ-NH1 | 8.46 | 124.53 | 120.30 |
| 34 | AA | 3067 | G | C1'-O4'-C4' | -8.45 | 103.14 | 109.90 |
| 66 | AZ | 15 | ARG | NE-CZ-NH2 | -8.45 | 116.08 | 120.30 |
| 34 | AA | 347 | C | O4'-C1'-N1 | 8.43 | 114.95 | 108.20 |
| 65 | AT | 87 | ARG | NE-CZ-NH2 | -8.43 | 116.08 | 120.30 |
| 1 | A | 1660 | U | O4'-C1'-N1 | 8.43 | 114.94 | 108.20 |
| 19 | 6 | 33 | ARG | NE-CZ-NH2 | 8.43 | 124.52 | 120.30 |
| 30 | U | 124 | ARG | NE-CZ-NH1 | -8.43 | 116.08 | 120.30 |
| 34 | AA | 621 | C | O4'-C1'-N1 | 8.42 | 114.94 | 108.20 |
| 74 | AH | 144 | TYR | CB-CG-CD2 | -8.42 | 115.95 | 121.00 |
| 16 | 3 | 6 | ARG | NE-CZ-NH2 | 8.42 | 124.51 | 120.30 |
| 37 | AL | 190 | ARG | NE-CZ-NH2 | -8.41 | 116.09 | 120.30 |
| 34 | AA | 10 | G | P-O3'-C3' | 8.40 | 129.78 | 119.70 |
| 24 | L | 92 | ARG | NE-CZ-NH2 | -8.40 | 116.10 | 120.30 |
| 1 | A | 1386 | U | P-O3'-C3' | 8.39 | 129.76 | 119.70 |
| 51 | AP | 173 | ARG | NE-CZ-NH1 | 8.39 | 124.49 | 120.30 |
| 34 | AA | 2439 | C | O4'-C1'-N1 | 8.38 | 114.91 | 108.20 |
| 68 | A5 | 169 | ARG | NE-CZ-NH1 | 8.38 | 124.49 | 120.30 |
| 61 | AQ | 98 | ARG | NE-CZ-NH1 | -8.36 | 116.12 | 120.30 |
| 12 | Y | 39 | ARG | NE-CZ-NH1 | 8.36 | 124.48 | 120.30 |
| 34 | AA | 737 | G | C5-C6-O6 | -8.36 | 123.58 | 128.60 |
| 34 | AA | 1841 | U | P-O3'-C3' | 8.34 | 129.71 | 119.70 |
| 34 | AA | 62 | A | P-O3'-C3' | 8.34 | 129.70 | 119.70 |
| 34 | AA | 3627 | C | O4'-C1'-N1 | 8.34 | 114.87 | 108.20 |
| 34 | AA | 620 | U | P-O3'-C3' | 8.33 | 129.70 | 119.70 |
| 34 | AA | 1553 | U | O4'-C1'-N1 | 8.33 | 114.86 | 108.20 |
| 34 | AA | 306 | C | C2-N1-C1' | 8.30 | 127.94 | 118.80 |
| 1 | A | 994 | G | C5-C6-O6 | -8.30 | 123.62 | 128.60 |
| 34 | AA | 889 | U | P-O3'-C3' | 8.30 | 129.66 | 119.70 |
| 34 | AA | 2658 | C | O4'-C1'-N1 | 8.30 | 114.84 | 108.20 |
| 1 | A | 2084 | G | P-O3'-C3' | 8.28 | 129.64 | 119.70 |
| 6 | I | 155 | ARG | NE-CZ-NH2 | 8.28 | 124.44 | 120.30 |
| 34 | AA | 1235 | C | O4'-C1'-N1 | 8.28 | 114.82 | 108.20 |
| 34 | AA | 1073 | G | O4'-C1'-N9 | 8.28 | 114.82 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 63 | AW | 123 | ARG | NE-CZ-NH2 | -8.28 | 116.16 | 120.30 |
| 34 | AA | 3443 | A | O4'-C1'-N9 | 8.27 | 114.82 | 108.20 |
| 46 | Aa | 21 | ARG | NE-CZ-NH1 | 8.27 | 124.44 | 120.30 |
| 34 | AA | 1704 | U | O4'-C1'-N1 | 8.27 | 114.81 | 108.20 |
| 1 | A | 1856 | A | O4'-C1'-N9 | 8.26 | 114.81 | 108.20 |
| 34 | AA | 80 | C | O4'-C1'-N1 | 8.26 | 114.81 | 108.20 |
| 12 | Y | 39 | ARG | NE-CZ-NH2 | -8.25 | 116.17 | 120.30 |
| 34 | AA | 2421 | C | O4'-C1'-N1 | 8.25 | 114.80 | 108.20 |
| 34 | AA | 2957 | G | O4'-C1'-N9 | 8.25 | 114.80 | 108.20 |
| 34 | AA | 858 | C | P-O3'-C3' | 8.24 | 129.59 | 119.70 |
| 64 | AY | 108 | TYR | CB-CG-CD2 | -8.24 | 116.06 | 121.00 |
| 60 | AO | 67 | ARG | NE-CZ-NH1 | 8.23 | 124.42 | 120.30 |
| 36 | AB | 39 | C | O4'-C1'-N1 | 8.23 | 114.79 | 108.20 |
| 34 | AA | 1101 | A | P-O3'-C3' | 8.23 | 129.58 | 119.70 |
| 1 | A | 1731 | C | O4'-C1'-N1 | 8.23 | 114.78 | 108.20 |
| 34 | AA | 345 | G | C5-C6-O6 | -8.22 | 123.67 | 128.60 |
| 34 | AA | 3241 | U | O4'-C1'-N1 | 8.22 | 114.78 | 108.20 |
| 69 | AD | 9 | ARG | NE-CZ-NH1 | 8.22 | 124.41 | 120.30 |
| 18 | 5 | 42 | ARG | NE-CZ-NH2 | -8.22 | 116.19 | 120.30 |
| 34 | AA | 372 | G | C5-C6-O6 | -8.21 | 123.67 | 128.60 |
| 34 | AA | 69 | U | O4'-C1'-N1 | 8.21 | 114.77 | 108.20 |
| 34 | AA | 930 | C | O4'-C1'-N1 | 8.21 | 114.76 | 108.20 |
| 1 | A | 1109 | G | P-O5'-C5' | 8.20 | 134.02 | 120.90 |
| 34 | AA | 1996 | C | P-O3'-C3' | 8.20 | 129.54 | 119.70 |
| 34 | AA | 1503 | A | P-O3'-C3' | 8.20 | 129.53 | 119.70 |
| 34 | AA | 2107 | C | P-O3'-C3' | 8.20 | 129.53 | 119.70 |
| 34 | AA | 2655 | C | O4'-C1'-N1 | 8.19 | 114.75 | 108.20 |
| 3 | D | 167 | ARG | NE-CZ-NH2 | -8.19 | 116.21 | 120.30 |
| 34 | AA | 136 | U | C2-N1-C1' | 8.19 | 127.53 | 117.70 |
| 34 | AA | 288 | G | O4'-C1'-N9 | 8.19 | 114.75 | 108.20 |
| 34 | AA | 1798 | A | O4'-C1'-N9 | 8.19 | 114.75 | 108.20 |
| 1 | A | 857 | A | O4'-C1'-N9 | 8.18 | 114.75 | 108.20 |
| 2 | 7 | 49 | C | O4'-C1'-N1 | 8.18 | 114.74 | 108.20 |
| 34 | AA | 2933 | C | O4'-C1'-N1 | 8.17 | 114.73 | 108.20 |
| 63 | AW | 82 | ARG | NE-CZ-NH1 | 8.17 | 124.38 | 120.30 |
| 60 | AO | 67 | ARG | NE-CZ-NH2 | -8.15 | 116.22 | 120.30 |
| 61 | AQ | 162 | ARG | NE-CZ-NH1 | 8.15 | 124.38 | 120.30 |
| 34 | AA | 2154 | A | O4'-C1'-N9 | 8.15 | 114.72 | 108.20 |
| 2 | 7 | 57 | C | O4'-C1'-N1 | 8.13 | 114.70 | 108.20 |
| 43 | AN | 128 | ARG | NE-CZ-NH1 | 8.13 | 124.36 | 120.30 |
| 34 | AA | 866 | C | O4'-C1'-N1 | 8.13 | 114.70 | 108.20 |
| 34 | AA | 2959 | G | P-O3'-C3' | 8.13 | 129.45 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 68 | A5 | 224 | ARG | NE-CZ-NH2 | -8.13 | 116.24 | 120.30 |
| 34 | AA | 449 | A | O4'-C1'-N9 | 8.12 | 114.70 | 108.20 |
| 1 | A | 1845 | U | O4'-C1'-N1 | 8.12 | 114.70 | 108.20 |
| 34 | AA | 3199 | C | O4'-C1'-N1 | 8.12 | 114.70 | 108.20 |
| 69 | AD | 163 | ARG | NE-CZ-NH1 | -8.12 | 116.24 | 120.30 |
| 34 | AA | 963 | C | O4'-C1'-N1 | 8.09 | 114.67 | 108.20 |
| 34 | AA | 3621 | C | O4'-C1'-N1 | 8.08 | 114.67 | 108.20 |
| 34 | AA | 1572 | U | O4'-C1'-N1 | 8.07 | 114.66 | 108.20 |
| 34 | AA | 966 | A | N1-C6-N6 | 8.07 | 123.44 | 118.60 |
| 63 | AW | 56 | ARG | NE-CZ-NH2 | -8.06 | 116.27 | 120.30 |
| 34 | AA | 3111 | U | O4'-C1'-N1 | 8.06 | 114.65 | 108.20 |
| 53 | Ai | 40 | ARG | NE-CZ-NH2 | -8.06 | 116.27 | 120.30 |
| 1 | A | 844 | G | P-O3'-C3' | 8.05 | 129.36 | 119.70 |
| 34 | AA | 2604 | G | C5-C6-O6 | -8.05 | 123.77 | 128.60 |
| 76 | Ag | 39 | ARG | NE-CZ-NH2 | 8.05 | 124.32 | 120.30 |
| 75 | AV | 13 | ARG | NE-CZ-NH2 | 8.04 | 124.32 | 120.30 |
| 1 | A | 161 | U | C5'-C4'-O4' | 8.04 | 118.75 | 109.10 |
| 1 | A | 759 | C | O4'-C1'-N1 | 8.04 | 114.63 | 108.20 |
| 20 | B | 213 | ARG | NE-CZ-NH2 | -8.04 | 116.28 | 120.30 |
| 34 | AA | 3248 | C | O4'-C1'-N1 | 8.04 | 114.63 | 108.20 |
| 30 | U | 55 | ARG | NE-CZ-NH2 | 8.03 | 124.31 | 120.30 |
| 34 | AA | 137 | G | O4'-C1'-N9 | 8.02 | 114.62 | 108.20 |
| 1 | A | 1832 | U | O4'-C1'-N1 | 8.02 | 114.62 | 108.20 |
| 34 | AA | 1980 | G | O4'-C1'-N9 | 8.02 | 114.61 | 108.20 |
| 34 | AA | 3585 | A | O4'-C1'-N9 | 8.02 | 114.61 | 108.20 |
| 34 | AA | 2004 | U | C2-N1-C1' | 8.01 | 127.32 | 117.70 |
| 34 | AA | 830 | U | O4'-C1'-N1 | 8.01 | 114.61 | 108.20 |
| 51 | AP | 71 | ARG | NE-CZ-NH1 | 8.01 | 124.30 | 120.30 |
| 1 | A | 2072 | G | O4'-C1'-N9 | 8.00 | 114.60 | 108.20 |
| 4 | E | 79 | ARG | NE-CZ-NH2 | 8.00 | 124.30 | 120.30 |
| 34 | AA | 1078 | C | O4'-C1'-N1 | 7.99 | 114.59 | 108.20 |
| 71 | AF | 122 | TYR | CB-CG-CD1 | 7.98 | 125.79 | 121.00 |
| 34 | AA | 2932 | A | P-O3'-C3' | 7.98 | 129.27 | 119.70 |
| 34 | AA | 1999 | A | P-O3'-C3' | 7.97 | 129.27 | 119.70 |
| 34 | AA | 2734 | C | O4'-C1'-N1 | 7.97 | 114.58 | 108.20 |
| 76 | Ag | 32 | ARG | NE-CZ-NH1 | 7.97 | 124.28 | 120.30 |
| 36 | AB | 78 | C | O4'-C1'-N1 | 7.96 | 114.57 | 108.20 |
| 66 | AZ | 76 | ARG | NE-CZ-NH1 | 7.94 | 124.27 | 120.30 |
| 34 | AA | 812 | U | O4'-C1'-N1 | 7.94 | 114.55 | 108.20 |
| 1 | A | 876 | U | P-O3'-C3' | 7.92 | 129.21 | 119.70 |
| 1 | A | 2051 | C | O4'-C1'-N1 | 7.92 | 114.54 | 108.20 |
| 34 | AA | 3289 | G | O4'-C1'-N9 | 7.92 | 114.54 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 69 | AD | 200 | ARG | NE-CZ-NH2 | 7.92 | 124.26 | 120.30 |
| 34 | AA | 3765 | C | O4'-C1'-N1 | 7.90 | 114.52 | 108.20 |
| 51 | AP | 190 | ARG | NE-CZ-NH1 | 7.90 | 124.25 | 120.30 |
| 75 | AV | 84 | ARG | NE-CZ-NH2 | 7.90 | 124.25 | 120.30 |
| 34 | AA | 1325 | C | O4'-C1'-N1 | 7.89 | 114.51 | 108.20 |
| 35 | AC | 78 | U | O4'-C1'-N1 | 7.89 | 114.51 | 108.20 |
| 65 | AT | 135 | ARG | NE-CZ-NH2 | -7.89 | 116.36 | 120.30 |
| 51 | AP | 67 | ARG | NE-CZ-NH2 | 7.88 | 124.24 | 120.30 |
| 34 | AA | 711 | C | O4'-C1'-N1 | 7.88 | 114.51 | 108.20 |
| 34 | AA | 715 | U | P-O3'-C3' | 7.88 | 129.15 | 119.70 |
| 44 | A8 | 44 | ARG | NE-CZ-NH2 | -7.88 | 116.36 | 120.30 |
| 34 | AA | 2969 | C | O4'-C1'-N1 | 7.87 | 114.50 | 108.20 |
| 1 | A | 2026 | C | O4'-C1'-N1 | 7.87 | 114.50 | 108.20 |
| 21 | F | 49 | ARG | NE-CZ-NH1 | 7.87 | 124.23 | 120.30 |
| 1 | A | 1079 | C | O4'-C1'-N1 | 7.86 | 114.49 | 108.20 |
| 34 | AA | 540 | C | O4'-C1'-N1 | 7.86 | 114.49 | 108.20 |
| 34 | AA | 1026 | G | P-O3'-C3' | 7.86 | 129.13 | 119.70 |
| 34 | AA | 830 | U | C2-N1-C1' | 7.85 | 127.12 | 117.70 |
| 1 | A | 760 | C | O4'-C1'-N1 | 7.85 | 114.48 | 108.20 |
| 1 | A | 2048 | A | O4'-C1'-N9 | 7.85 | 114.48 | 108.20 |
| 1 | A | 647 | C | C6-N1-C1' | -7.85 | 111.38 | 120.80 |
| 7 | K | 97 | ARG | NE-CZ-NH2 | -7.85 | 116.38 | 120.30 |
| 34 | AA | 329 | C | O4'-C1'-N1 | 7.85 | 114.48 | 108.20 |
| 34 | AA | 2623 | C | O4'-C1'-N1 | 7.84 | 114.47 | 108.20 |
| 34 | AA | 2034 | G | P-O5'-C5' | 7.84 | 133.44 | 120.90 |
| 34 | AA | 1540 | G | O4'-C1'-N9 | 7.83 | 114.47 | 108.20 |
| 34 | AA | 2089 | C | P-O3'-C3' | 7.83 | 129.10 | 119.70 |
| 34 | AA | 883 | C | O4'-C1'-N1 | 7.83 | 114.46 | 108.20 |
| 68 | A5 | 173 | ARG | NE-CZ-NH1 | -7.83 | 116.39 | 120.30 |
| 61 | AQ | 3 | ARG | NE-CZ-NH1 | -7.83 | 116.39 | 120.30 |
| 1 | A | 1800 | A | P-O3'-C3' | 7.82 | 129.09 | 119.70 |
| 34 | AA | 706 | U | O4'-C1'-N1 | 7.82 | 114.46 | 108.20 |
| 34 | AA | 3763 | G | C5-C6-O6 | -7.82 | 123.91 | 128.60 |
| 65 | AT | 162 | ARG | NE-CZ-NH2 | -7.82 | 116.39 | 120.30 |
| 1 | A | 1030 | C | O4'-C1'-N1 | 7.82 | 114.46 | 108.20 |
| 69 | AD | 174 | ARG | NE-CZ-NH1 | 7.82 | 124.21 | 120.30 |
| 34 | AA | 1003 | A | P-O3'-C3' | 7.82 | 129.08 | 119.70 |
| 69 | AD | 12 | ARG | NE-CZ-NH1 | 7.82 | 124.21 | 120.30 |
| 2 | 7 | 17 | U | P-O3'-C3' | 7.81 | 129.07 | 119.70 |
| 34 | AA | 921 | C | O4'-C1'-N1 | 7.80 | 114.44 | 108.20 |
| 57 | AK | 193 | ARG | NE-CZ-NH2 | 7.80 | 124.20 | 120.30 |
| 34 | AA | 2219 | A | C2'-C3'-O3' | 7.79 | 126.64 | 109.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 34 | AA | 1222 | U | P-O3'-C3' | 7.79 | 129.05 | 119.70 |
| 34 | AA | 1525 | C | O4'-C1'-N1 | 7.79 | 114.43 | 108.20 |
| 34 | AA | 3140 | U | P-O3'-C3' | 7.79 | 129.05 | 119.70 |
| 44 | A8 | 24 | ARG | NE-CZ-NH1 | 7.78 | 124.19 | 120.30 |
| 69 | AD | 163 | ARG | NE-CZ-NH2 | 7.77 | 124.19 | 120.30 |
| 35 | AC | 145 | A | P-O3'-C3' | 7.76 | 129.01 | 119.70 |
| 68 | A5 | 160 | ARG | NE-CZ-NH2 | 7.76 | 124.18 | 120.30 |
| 1 | A | 2033 | U | O4'-C1'-N1 | 7.76 | 114.41 | 108.20 |
| 34 | AA | 3302 | G | P-O5'-C5' | 7.76 | 133.31 | 120.90 |
| 1 | A | 1945 | C | O4'-C1'-N1 | 7.75 | 114.40 | 108.20 |
| 57 | AK | 201 | TYR | CB-CG-CD2 | -7.75 | 116.35 | 121.00 |
| 34 | AA | 959 | C | O4'-C1'-N1 | 7.75 | 114.40 | 108.20 |
| 34 | AA | 1168 | C | O4'-C1'-N1 | 7.74 | 114.39 | 108.20 |
| 34 | AA | 2727 | U | C2-N1-C1' | 7.74 | 126.99 | 117.70 |
| 37 | AL | 69 | ARG | NE-CZ-NH2 | -7.73 | 116.43 | 120.30 |
| 34 | AA | 3549 | U | O4'-C1'-N1 | 7.73 | 114.38 | 108.20 |
| 69 | AD | 241 | ARG | NE-CZ-NH1 | 7.72 | 124.16 | 120.30 |
| 70 | AE | 234 | ARG | NE-CZ-NH2 | 7.72 | 124.16 | 120.30 |
| 34 | AA | 2662 | G | O4'-C1'-N9 | 7.72 | 114.38 | 108.20 |
| 21 | F | 100 | ARG | NE-CZ-NH2 | -7.72 | 116.44 | 120.30 |
| 34 | AA | 345 | G | N1-C6-O6 | 7.72 | 124.53 | 119.90 |
| 34 | AA | 2107 | C | O4'-C1'-N1 | 7.72 | 114.37 | 108.20 |
| 1 | A | 1452 | C | O4'-C1'-N1 | 7.71 | 114.37 | 108.20 |
| 34 | AA | 3442 | C | O4'-C1'-N1 | 7.71 | 114.37 | 108.20 |
| 54 | AI | 71 | ARG | NE-CZ-NH2 | -7.71 | 116.45 | 120.30 |
| 1 | A | 161 | U | C2-N1-C1' | 7.71 | 126.95 | 117.70 |
| 1 | A | 1281 | C | O4'-C1'-N1 | 7.71 | 114.37 | 108.20 |
| 1 | A | 1431 | A | P-O3'-C3' | 7.70 | 128.94 | 119.70 |
| 34 | AA | 136 | U | O4'-C1'-N1 | 7.70 | 114.36 | 108.20 |
| 34 | AA | 107 | C | O4'-C1'-N1 | 7.70 | 114.36 | 108.20 |
| 34 | AA | 3191 | C | O4'-C1'-N1 | 7.70 | 114.36 | 108.20 |
| 36 | AB | 72 | C | O4'-C1'-N1 | 7.69 | 114.35 | 108.20 |
| 57 | AK | 73 | ARG | NE-CZ-NH1 | 7.69 | 124.14 | 120.30 |
| 34 | AA | 1866 | C | O4'-C1'-N1 | 7.69 | 114.35 | 108.20 |
| 34 | AA | 2104 | C | O4'-C1'-N1 | 7.69 | 114.35 | 108.20 |
| 34 | AA | 2074 | C | O4'-C1'-N1 | 7.69 | 114.35 | 108.20 |
| 14 | 1 | 106 | ARG | NE-CZ-NH2 | 7.68 | 124.14 | 120.30 |
| 34 | AA | 1537 | G | P-O3'-C3' | -7.68 | 110.48 | 119.70 |
| 18 | 5 | 26 | ARG | NE-CZ-NH2 | -7.67 | 116.47 | 120.30 |
| 34 | AA | 372 | G | N1-C6-O6 | 7.67 | 124.50 | 119.90 |
| 34 | AA | 2804 | C | O4'-C1'-N1 | 7.66 | 114.33 | 108.20 |
| 34 | AA | 2437 | A | C1'-O4'-C4' | -7.66 | 103.77 | 109.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 34 | AA | 3494 | C | O4'-C1'-N1 | 7.65 | 114.32 | 108.20 |
| 1 | A | 630 | C | C2-N1-C1' | 7.65 | 127.22 | 118.80 |
| 34 | AA | 1260 | C | O4'-C1'-N1 | 7.65 | 114.32 | 108.20 |
| 34 | AA | 2175 | C | O4'-C1'-N1 | 7.65 | 114.32 | 108.20 |
| 62 | AR | 23 | ARG | NE-CZ-NH2 | -7.65 | 116.47 | 120.30 |
| 35 | AC | 134 | G | P-O3'-C3' | 7.65 | 128.88 | 119.70 |
| 61 | AQ | 90 | ARG | NE-CZ-NH2 | -7.64 | 116.48 | 120.30 |
| 34 | AA | 542 | A | N1-C6-N6 | 7.64 | 123.19 | 118.60 |
| 1 | A | 941 | C | O4'-C1'-N1 | 7.64 | 114.31 | 108.20 |
| 59 | AS | 179 | ARG | NE-CZ-NH1 | 7.64 | 124.12 | 120.30 |
| 34 | AA | 934 | G | N1-C6-O6 | 7.64 | 124.48 | 119.90 |
| 34 | AA | 3723 | C | O4'-C1'-N1 | 7.63 | 114.31 | 108.20 |
| 34 | AA | 1493 | U | O4'-C1'-N1 | 7.63 | 114.31 | 108.20 |
| 49 | Ae | 6 | ARG | NE-CZ-NH2 | -7.63 | 116.49 | 120.30 |
| 52 | Ah | 17 | ARG | NE-CZ-NH1 | 7.63 | 124.11 | 120.30 |
| 34 | AA | 2191 | C | O4'-C1'-N1 | 7.62 | 114.29 | 108.20 |
| 1 | A | 1872 | G | O4'-C1'-N9 | 7.62 | 114.29 | 108.20 |
| 45 | A9 | 130 | ARG | NE-CZ-NH2 | -7.61 | 116.49 | 120.30 |
| 1 | A | 525 | G | P-O3'-C3' | 7.61 | 128.83 | 119.70 |
| 24 | L | 56 | ARG | NE-CZ-NH1 | 7.61 | 124.10 | 120.30 |
| 2 | 7 | 71 | C | O4'-C1'-N1 | 7.60 | 114.28 | 108.20 |
| 34 | AA | 501 | U | P-O3'-C3' | 7.60 | 128.82 | 119.70 |
| 34 | AA | 1853 | C | O4'-C1'-N1 | 7.60 | 114.28 | 108.20 |
| 34 | AA | 278 | C | O4'-C1'-N1 | 7.59 | 114.27 | 108.20 |
| 34 | AA | 1654 | C | O4'-C1'-N1 | 7.59 | 114.27 | 108.20 |
| 1 | A | 246 | A | P-O3'-C3' | 7.59 | 128.81 | 119.70 |
| 36 | AB | 17 | C | O4'-C1'-N1 | 7.59 | 114.27 | 108.20 |
| 1 | A | 315 | C | O4'-C1'-N1 | 7.58 | 114.27 | 108.20 |
| 1 | A | 375 | U | O4'-C1'-N1 | 7.58 | 114.27 | 108.20 |
| 1 | A | 1069 | C | C6-N1-C1' | -7.58 | 111.70 | 120.80 |
| 34 | AA | 257 | U | O4'-C1'-N1 | 7.58 | 114.27 | 108.20 |
| 34 | AA | 255 | C | O4'-C1'-N1 | 7.58 | 114.26 | 108.20 |
| 76 | Ag | 7 | ARG | NE-CZ-NH1 | 7.58 | 124.09 | 120.30 |
| 34 | AA | 453 | A | N1-C6-N6 | -7.57 | 114.06 | 118.60 |
| 55 | AJ | 73 | ARG | NE-CZ-NH2 | -7.57 | 116.51 | 120.30 |
| 1 | A | 843 | U | O4'-C1'-N1 | 7.57 | 114.25 | 108.20 |
| 71 | AF | 78 | ARG | NE-CZ-NH1 | 7.56 | 124.08 | 120.30 |
| 71 | AF | 190 | ARG | NE-CZ-NH2 | 7.56 | 124.08 | 120.30 |
| 34 | AA | 650 | U | O4'-C1'-N1 | 7.56 | 114.25 | 108.20 |
| 34 | AA | 200 | A | N1-C6-N6 | 7.56 | 123.14 | 118.60 |
| 34 | AA | 594 | C | C6-N1-C1' | -7.55 | 111.73 | 120.80 |
| 34 | AA | 1780 | G | P-O5'-C5' | 7.55 | 132.99 | 120.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 34 | AA | 1905 | C | O4'-C1'-N1 | 7.55 | 114.24 | 108.20 |
| 34 | AA | 2821 | C | O4'-C1'-N1 | 7.55 | 114.24 | 108.20 |
| 65 | AT | 73 | ARG | NE-CZ-NH1 | 7.55 | 124.08 | 120.30 |
| 34 | AA | 739 | G | O4'-C1'-N9 | 7.55 | 114.24 | 108.20 |
| 59 | AS | 10 | ARG | NE-CZ-NH1 | 7.55 | 124.07 | 120.30 |
| 34 | AA | 2499 | G | C8-N9-C1' | -7.55 | 117.19 | 127.00 |
| 34 | AA | 215 | C | P-O3'-C3' | 7.54 | 128.75 | 119.70 |
| 34 | AA | 2697 | A | O4'-C1'-N9 | 7.53 | 114.23 | 108.20 |
| 36 | AB | 35 | C | O4'-C1'-N1 | 7.53 | 114.23 | 108.20 |
| 1 | A | 1819 | U | O4'-C1'-N1 | 7.53 | 114.22 | 108.20 |
| 34 | AA | 284 | C | O4'-C1'-N1 | 7.53 | 114.22 | 108.20 |
| 34 | AA | 3664 | G | P-O3'-C3' | 7.53 | 128.73 | 119.70 |
| 75 | AV | 101 | ARG | NE-CZ-NH1 | 7.53 | 124.06 | 120.30 |
| 14 | 1 | 20 | ARG | NE-CZ-NH2 | 7.52 | 124.06 | 120.30 |
| 34 | AA | 400 | C | O4'-C1'-N1 | 7.52 | 114.22 | 108.20 |
| 45 | A9 | 130 | ARG | NE-CZ-NH1 | 7.52 | 124.06 | 120.30 |
| 2 | 7 | 73 | C | O4'-C1'-N1 | 7.52 | 114.22 | 108.20 |
| 1 | A | 1785 | C | O4'-C1'-N1 | 7.51 | 114.21 | 108.20 |
| 1 | A | 1908 | A | O4'-C1'-N9 | 7.51 | 114.21 | 108.20 |
| 8 | M | 43 | TYR | CB-CG-CD2 | -7.51 | 116.49 | 121.00 |
| 34 | AA | 93 | C | O4'-C1'-N1 | 7.51 | 114.21 | 108.20 |
| 34 | AA | 90 | C | O4'-C1'-N1 | 7.51 | 114.20 | 108.20 |
| 34 | AA | 309 | G | O4'-C1'-N9 | 7.50 | 114.20 | 108.20 |
| 34 | AA | 236 | U | P-O3'-C3' | 7.50 | 128.70 | 119.70 |
| 1 | A | 885 | C | O4'-C1'-N1 | 7.50 | 114.20 | 108.20 |
| 1 | A | 1286 | U | O4'-C1'-N1 | 7.50 | 114.20 | 108.20 |
| 34 | AA | 2401 | C | O4'-C1'-N1 | 7.49 | 114.19 | 108.20 |
| 34 | AA | 3181 | U | O4'-C1'-N1 | 7.49 | 114.19 | 108.20 |
| 34 | AA | 773 | A | O4'-C1'-N9 | 7.49 | 114.19 | 108.20 |
| 2 | 7 | 21 | U | O4'-C1'-N1 | 7.48 | 114.19 | 108.20 |
| 34 | AA | 715 | U | O4'-C1'-N1 | 7.48 | 114.19 | 108.20 |
| 1 | A | 630 | C | O4'-C1'-N1 | 7.48 | 114.19 | 108.20 |
| 1 | A | 1716 | C | O4'-C1'-N1 | 7.48 | 114.19 | 108.20 |
| 34 | AA | 833 | G | P-O3'-C3' | 7.47 | 128.67 | 119.70 |
| 34 | AA | 1680 | C | O4'-C1'-N1 | 7.47 | 114.18 | 108.20 |
| 1 | A | 871 | C | O4'-C1'-N1 | 7.47 | 114.18 | 108.20 |
| 34 | AA | 3065 | C | O4'-C1'-N1 | 7.47 | 114.18 | 108.20 |
| 64 | AY | 173 | ARG | NE-CZ-NH1 | 7.47 | 124.03 | 120.30 |
| 1 | A | 1014 | U | O4'-C1'-N1 | 7.47 | 114.17 | 108.20 |
| 34 | AA | 1326 | C | O4'-C1'-N1 | 7.46 | 114.17 | 108.20 |
| 6 | I | 195 | ARG | NE-CZ-NH2 | -7.46 | 116.57 | 120.30 |
| 34 | AA | 672 | C | O4'-C1'-N1 | 7.46 | 114.17 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 34 | AA | 3483 | U | O4'-C1'-N1 | 7.45 | 114.16 | 108.20 |
| 67 | A3 | 91 | ARG | NE-CZ-NH1 | 7.45 | 124.03 | 120.30 |
| 36 | AB | 29 | C | O4'-C1'-N1 | 7.45 | 114.16 | 108.20 |
| 34 | AA | 3613 | A | O4'-C1'-N9 | 7.44 | 114.15 | 108.20 |
| 34 | AA | 1960 | U | O4'-C1'-N1 | 7.43 | 114.15 | 108.20 |
| 65 | AT | 102 | ARG | NE-CZ-NH1 | 7.43 | 124.02 | 120.30 |
| 34 | AA | 1166 | C | O4'-C1'-N1 | 7.43 | 114.14 | 108.20 |
| 62 | AR | 206 | TYR | CB-CG-CD2 | -7.43 | 116.54 | 121.00 |
| 34 | AA | 320 | C | O4'-C1'-N1 | 7.43 | 114.14 | 108.20 |
| 34 | AA | 2095 | U | P-O3'-C3' | 7.43 | 128.61 | 119.70 |
| 1 | A | 367 | C | O4'-C1'-N1 | 7.42 | 114.14 | 108.20 |
| 34 | AA | 1431 | A | O4'-C1'-N9 | 7.42 | 114.14 | 108.20 |
| 71 | AF | 97 | ARG | NE-CZ-NH1 | -7.42 | 116.59 | 120.30 |
| 2 | 7 | 73 | C | C2-N1-C1' | 7.42 | 126.96 | 118.80 |
| 4 | E | 107 | ARG | NE-CZ-NH1 | 7.42 | 124.01 | 120.30 |
| 3 | D | 147 | ARG | NE-CZ-NH2 | -7.42 | 116.59 | 120.30 |
| 34 | AA | 737 | G | N1-C6-O6 | 7.41 | 124.35 | 119.90 |
| 28 | S | 110 | ARG | NE-CZ-NH1 | 7.41 | 124.00 | 120.30 |
| 34 | AA | 10 | G | N1-C6-O6 | 7.41 | 124.34 | 119.90 |
| 34 | AA | 2958 | G | P-O3'-C3' | 7.40 | 128.59 | 119.70 |
| 34 | AA | 3628 | C | O4'-C1'-N1 | 7.40 | 114.12 | 108.20 |
| 34 | AA | 150 | C | O4'-C1'-N1 | 7.40 | 114.12 | 108.20 |
| 35 | AC | 25 | C | C6-N1-C2 | -7.40 | 117.34 | 120.30 |
| 1 | A | 1707 | C | O4'-C1'-N1 | 7.39 | 114.11 | 108.20 |
| 34 | AA | 1873 | U | P-O3'-C3' | 7.39 | 128.57 | 119.70 |
| 1 | A | 1790 | C | O4'-C1'-N1 | 7.39 | 114.11 | 108.20 |
| 34 | AA | 1321 | A | O4'-C1'-N9 | 7.39 | 114.11 | 108.20 |
| 1 | A | 1419 | C | O4'-C1'-N1 | 7.39 | 114.11 | 108.20 |
| 61 | AQ | 88 | ARG | NE-CZ-NH1 | 7.38 | 123.99 | 120.30 |
| 34 | AA | 125 | C | O4'-C1'-N1 | 7.38 | 114.11 | 108.20 |
| 34 | AA | 3632 | U | O4'-C1'-N1 | 7.38 | 114.11 | 108.20 |
| 24 | L | 31 | ARG | NE-CZ-NH2 | -7.38 | 116.61 | 120.30 |
| 34 | AA | 1752 | C | O4'-C1'-N1 | 7.38 | 114.10 | 108.20 |
| 34 | AA | 2713 | C | O4'-C1'-N1 | 7.38 | 114.10 | 108.20 |
| 34 | AA | 3691 | C | O4'-C1'-N1 | 7.38 | 114.10 | 108.20 |
| 66 | AZ | 114 | ARG | NE-CZ-NH1 | 7.38 | 123.99 | 120.30 |
| 34 | AA | 3195 | C | C2-N1-C1' | 7.37 | 126.91 | 118.80 |
| 1 | A | 1917 | C | O4'-C1'-N1 | 7.37 | 114.09 | 108.20 |
| 1 | A | 1856 | A | C1'-O4'-C4' | -7.37 | 104.01 | 109.90 |
| 34 | AA | 702 | U | C6-N1-C1' | -7.37 | 110.89 | 121.20 |
| 21 | F | 113 | ARG | NE-CZ-NH1 | 7.36 | 123.98 | 120.30 |
| 34 | AA | 1217 | U | P-O3'-C3' | 7.36 | 128.53 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | L | 188 | ARG | NE-CZ-NH2 | -7.36 | 116.62 | 120.30 |
| 34 | AA | 607 | A | N1-C6-N6 | 7.36 | 123.02 | 118.60 |
| 34 | AA | 3235 | C | O4'-C1'-N1 | 7.36 | 114.09 | 108.20 |
| 1 | A | 832 | A | O4'-C1'-N9 | 7.36 | 114.08 | 108.20 |
| 31 | V | 102 | ARG | NE-CZ-NH1 | 7.35 | 123.97 | 120.30 |
| 34 | AA | 438 | U | O4'-C1'-N1 | 7.35 | 114.08 | 108.20 |
| 1 | A | 1441 | C | O4'-C1'-N1 | 7.35 | 114.08 | 108.20 |
| 71 | AF | 97 | ARG | NE-CZ-NH2 | 7.35 | 123.97 | 120.30 |
| 34 | AA | 315 | C | O4'-C1'-N1 | 7.34 | 114.08 | 108.20 |
| 34 | AA | 1971 | U | O4'-C1'-N1 | 7.34 | 114.08 | 108.20 |
| 34 | AA | 1874 | C | O4'-C1'-N1 | 7.34 | 114.07 | 108.20 |
| 34 | AA | 732 | C | O4'-C1'-N1 | 7.34 | 114.07 | 108.20 |
| 1 | A | 1820 | C | O4'-C1'-N1 | 7.34 | 114.07 | 108.20 |
| 34 | AA | 172 | C | O4'-C1'-N1 | 7.34 | 114.07 | 108.20 |
| 34 | AA | 3031 | C | O4'-C1'-N1 | 7.33 | 114.07 | 108.20 |
| 34 | AA | 3400 | C | O4'-C1'-N1 | 7.33 | 114.06 | 108.20 |
| 34 | AA | 771 | U | O4'-C1'-N1 | 7.33 | 114.06 | 108.20 |
| 34 | AA | 2172 | C | O4'-C1'-N1 | 7.33 | 114.06 | 108.20 |
| 34 | AA | 2103 | C | O4'-C1'-N1 | 7.33 | 114.06 | 108.20 |
| 34 | AA | 1313 | C | O4'-C1'-N1 | 7.33 | 114.06 | 108.20 |
| 66 | AZ | 12 | ARG | NE-CZ-NH2 | -7.32 | 116.64 | 120.30 |
| 71 | AF | 75 | ARG | NE-CZ-NH1 | 7.32 | 123.96 | 120.30 |
| 1 | A | 1813 | U | O4'-C1'-N1 | 7.32 | 114.05 | 108.20 |
| 34 | AA | 3282 | U | P-O5'-C5' | -7.32 | 109.20 | 120.90 |
| 1 | A | 49 | C | O4'-C1'-N1 | 7.31 | 114.05 | 108.20 |
| 34 | AA | 431 | G | O4'-C1'-N9 | 7.31 | 114.05 | 108.20 |
| 1 | A | 1297 | A | O4'-C1'-N9 | 7.30 | 114.04 | 108.20 |
| 34 | AA | 197 | G | O4'-C1'-N9 | 7.30 | 114.04 | 108.20 |
| 47 | Ab | 94 | ARG | NE-CZ-NH1 | -7.30 | 116.65 | 120.30 |
| 28 | S | 132 | ARG | NE-CZ-NH1 | 7.30 | 123.95 | 120.30 |
| 34 | AA | 2456 | C | O4'-C1'-N1 | 7.30 | 114.04 | 108.20 |
| 34 | AA | 3344 | C | O4'-C1'-N1 | 7.30 | 114.04 | 108.20 |
| 34 | AA | 147 | C | O4'-C1'-N1 | 7.30 | 114.04 | 108.20 |
| 1 | A | 955 | U | O4'-C1'-N1 | 7.29 | 114.03 | 108.20 |
| 34 | AA | 3258 | C | C2-N1-C1' | 7.29 | 126.82 | 118.80 |
| 25 | N | 54 | ARG | NE-CZ-NH1 | 7.29 | 123.94 | 120.30 |
| 35 | AC | 40 | G | C5-C6-O6 | -7.29 | 124.23 | 128.60 |
| 34 | AA | 1112 | C | O4'-C1'-N1 | 7.29 | 114.03 | 108.20 |
| 34 | AA | 3307 | C | O4'-C1'-N1 | 7.29 | 114.03 | 108.20 |
| 34 | AA | 3567 | U | O4'-C1'-N1 | 7.28 | 114.03 | 108.20 |
| 1 | A | 320 | C | O4'-C1'-N1 | 7.28 | 114.03 | 108.20 |
| 64 | AY | 108 | TYR | CB-CG-CD1 | 7.28 | 125.37 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 1624 | U | P-O3'-C3' | 7.28 | 128.44 | 119.70 |
| 34 | AA | 2652 | C | O4'-C1'-N1 | 7.28 | 114.02 | 108.20 |
| 43 | AN | 60 | PHE | CB-CG-CD2 | 7.28 | 125.90 | 120.80 |
| 34 | AA | 349 | G | C5-C6-O6 | -7.28 | 124.23 | 128.60 |
| 34 | AA | 2626 | C | O4'-C1'-N1 | 7.28 | 114.02 | 108.20 |
| 34 | AA | 2604 | G | N1-C6-O6 | 7.28 | 124.27 | 119.90 |
| 15 | 2 | 76 | ARG | NE-CZ-NH1 | 7.27 | 123.94 | 120.30 |
| 34 | AA | 1290 | C | O4'-C1'-N1 | 7.27 | 114.02 | 108.20 |
| 34 | AA | 1231 | A | P-O5'-C5' | 7.26 | 132.52 | 120.90 |
| 56 | Ac | 48 | ARG | NE-CZ-NH2 | -7.26 | 116.67 | 120.30 |
| 34 | AA | 3620 | C | O4'-C1'-N1 | 7.26 | 114.01 | 108.20 |
| 69 | AD | 6 | ARG | NE-CZ-NH1 | 7.26 | 123.93 | 120.30 |
| 62 | AR | 181 | ARG | NE-CZ-NH2 | -7.25 | 116.67 | 120.30 |
| 1 | A | 32 | U | O4'-C1'-N1 | 7.25 | 114.00 | 108.20 |
| 1 | A | 1896 | C | O4'-C1'-N1 | 7.25 | 114.00 | 108.20 |
| 34 | AA | 577 | U | P-O5'-C5' | 7.25 | 132.50 | 120.90 |
| 34 | AA | 2647 | C | O4'-C1'-N1 | 7.25 | 114.00 | 108.20 |
| 34 | AA | 251 | U | O4'-C1'-N1 | 7.25 | 114.00 | 108.20 |
| 34 | AA | 3460 | C | O4'-C1'-N1 | 7.25 | 114.00 | 108.20 |
| 1 | A | 590 | C | O4'-C1'-N1 | 7.24 | 114.00 | 108.20 |
| 34 | AA | 2615 | C | O4'-C1'-N1 | 7.24 | 114.00 | 108.20 |
| 1 | A | 1907 | A | C4'-C3'-C2' | -7.24 | 95.36 | 102.60 |
| 34 | AA | 353 | G | P-O3'-C3' | 7.24 | 128.39 | 119.70 |
| 34 | AA | 922 | C | O4'-C1'-N1 | 7.24 | 113.99 | 108.20 |
| 34 | AA | 870 | C | O4'-C1'-N1 | 7.24 | 113.99 | 108.20 |
| 34 | AA | 1796 | U | O4'-C1'-N1 | 7.24 | 113.99 | 108.20 |
| 34 | AA | 2590 | U | C2-N1-C1' | 7.24 | 126.39 | 117.70 |
| 34 | AA | 1573 | C | O4'-C1'-N1 | 7.24 | 113.99 | 108.20 |
| 34 | AA | 1991 | U | O4'-C1'-N1 | 7.23 | 113.99 | 108.20 |
| 1 | A | 1444 | C | O4'-C1'-N1 | 7.23 | 113.98 | 108.20 |
| 34 | AA | 1852 | C | O4'-C1'-N1 | 7.23 | 113.98 | 108.20 |
| 1 | A | 158 | C | O4'-C1'-N1 | 7.23 | 113.98 | 108.20 |
| 1 | A | 1409 | U | O4'-C1'-N1 | 7.23 | 113.98 | 108.20 |
| 32 | X | 114 | TYR | CB-CG-CD2 | -7.23 | 116.66 | 121.00 |
| 34 | AA | 216 | C | O4'-C1'-N1 | 7.23 | 113.98 | 108.20 |
| 1 | A | 793 | G | O4'-C1'-N9 | 7.23 | 113.98 | 108.20 |
| 34 | AA | 3634 | C | O4'-C1'-N1 | 7.23 | 113.98 | 108.20 |
| 1 | A | 548 | A | P-O3'-C3' | -7.22 | 111.03 | 119.70 |
| 70 | AE | 280 | TYR | CB-CG-CD2 | -7.22 | 116.67 | 121.00 |
| 37 | AL | 190 | ARG | NE-CZ-NH1 | 7.22 | 123.91 | 120.30 |
| 34 | AA | 1726 | C | O4'-C1'-N1 | 7.22 | 113.97 | 108.20 |
| 1 | A | 1943 | C | O4'-C1'-N1 | 7.21 | 113.97 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 34 | AA | 705 | C | O4'-C1'-N1 | 7.21 | 113.96 | 108.20 |
| 34 | AA | 293 | U | O4'-C1'-N1 | 7.20 | 113.96 | 108.20 |
| 78 | A0 | 31 | ARG | NE-CZ-NH2 | -7.20 | 116.70 | 120.30 |
| 1 | A | 494 | G | O4'-C1'-N9 | 7.20 | 113.96 | 108.20 |
| 34 | AA | 3029 | G | O4'-C1'-N9 | 7.20 | 113.96 | 108.20 |
| 70 | AE | 156 | ARG | NE-CZ-NH1 | 7.20 | 123.90 | 120.30 |
| 34 | AA | 2425 | C | O4'-C1'-N1 | 7.20 | 113.96 | 108.20 |
| 46 | Aa | 67 | ARG | NE-CZ-NH2 | -7.20 | 116.70 | 120.30 |
| 1 | A | 1750 | U | O4'-C1'-N1 | 7.20 | 113.96 | 108.20 |
| 34 | AA | 1266 | U | O4'-C1'-N1 | 7.19 | 113.95 | 108.20 |
| 34 | AA | 2146 | A | C1'-O4'-C4' | -7.19 | 104.15 | 109.90 |
| 34 | AA | 1575 | C | C6-N1-C2 | -7.19 | 117.42 | 120.30 |
| 34 | AA | 1818 | C | O4'-C1'-N1 | 7.19 | 113.95 | 108.20 |
| 1 | A | 1408 | C | O4'-C1'-N1 | 7.19 | 113.95 | 108.20 |
| 4 | E | 132 | ARG | NE-CZ-NH1 | -7.19 | 116.71 | 120.30 |
| 11 | O | 23 | TYR | CB-CG-CD2 | -7.18 | 116.69 | 121.00 |
| 76 | Ag | 16 | ARG | NE-CZ-NH1 | 7.18 | 123.89 | 120.30 |
| 1 | A | 167 | A | P-O3'-C3' | 7.18 | 128.32 | 119.70 |
| 1 | A | 1375 | C | O4'-C1'-N1 | 7.18 | 113.95 | 108.20 |
| 34 | AA | 200 | A | C5-C6-N6 | -7.18 | 117.95 | 123.70 |
| 35 | AC | 49 | C | O4'-C1'-N1 | 7.18 | 113.95 | 108.20 |
| 34 | AA | 944 | U | O4'-C1'-N1 | 7.18 | 113.94 | 108.20 |
| 34 | AA | 3319 | C | O4'-C1'-N1 | 7.17 | 113.94 | 108.20 |
| 70 | AE | 10 | ARG | NE-CZ-NH1 | 7.17 | 123.88 | 120.30 |
| 12 | Y | 108 | ARG | NE-CZ-NH1 | 7.17 | 123.88 | 120.30 |
| 34 | AA | 1845 | C | O4'-C1'-N1 | 7.17 | 113.93 | 108.20 |
| 35 | AC | 146 | C | O4'-C1'-N1 | 7.17 | 113.93 | 108.20 |
| 18 | 5 | 42 | ARG | NE-CZ-NH1 | 7.16 | 123.88 | 120.30 |
| 34 | AA | 1058 | U | O4'-C1'-N1 | 7.16 | 113.93 | 108.20 |
| 2 | 7 | 33 | C | P-O3'-C3' | -7.16 | 111.11 | 119.70 |
| 34 | AA | 597 | A | P-O3'-C3' | 7.16 | 128.29 | 119.70 |
| 59 | AS | 39 | ARG | NE-CZ-NH1 | 7.16 | 123.88 | 120.30 |
| 62 | AR | 107 | ARG | NE-CZ-NH1 | 7.16 | 123.88 | 120.30 |
| 34 | AA | 1722 | C | O4'-C1'-N1 | 7.16 | 113.93 | 108.20 |
| 34 | AA | 1806 | C | O4'-C1'-N1 | 7.16 | 113.93 | 108.20 |
| 58 | AM | 50 | ARG | NE-CZ-NH2 | 7.16 | 123.88 | 120.30 |
| 1 | A | 566 | C | O4'-C1'-N1 | 7.15 | 113.92 | 108.20 |
| 34 | AA | 1175 | C | O4'-C1'-N1 | 7.15 | 113.92 | 108.20 |
| 34 | AA | 3433 | C | O4'-C1'-N1 | 7.15 | 113.92 | 108.20 |
| 36 | AB | 93 | G | O4'-C1'-N9 | 7.15 | 113.92 | 108.20 |
| 34 | AA | 451 | C | O4'-C1'-N1 | 7.15 | 113.92 | 108.20 |
| 34 | AA | 992 | C | O4'-C1'-N1 | 7.15 | 113.92 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 34 | AA | 3157 | C | O4'-C1'-N1 | 7.15 | 113.92 | 108.20 |
| 34 | AA | 2985 | C | O4'-C1'-N1 | 7.15 | 113.92 | 108.20 |
| 2 | 7 | 66 | C | O4'-C1'-N1 | 7.15 | 113.92 | 108.20 |
| 34 | AA | 3240 | C | O4'-C1'-N1 | 7.14 | 113.92 | 108.20 |
| 34 | AA | 2570 | C | O4'-C1'-N1 | 7.14 | 113.91 | 108.20 |
| 1 | A | 1979 | C | O4'-C1'-N1 | 7.14 | 113.91 | 108.20 |
| 34 | AA | 683 | A | P-O3'-C3' | 7.14 | 128.27 | 119.70 |
| 29 | T | 54 | ARG | NE-CZ-NH2 | 7.13 | 123.87 | 120.30 |
| 34 | AA | 591 | G | O4'-C1'-N9 | 7.13 | 113.91 | 108.20 |
| 34 | AA | 875 | C | O4'-C1'-N1 | 7.13 | 113.91 | 108.20 |
| 34 | AA | 1431 | A | C1'-O4'-C4' | -7.13 | 104.19 | 109.90 |
| 34 | AA | 2479 | U | O4'-C1'-N1 | 7.13 | 113.90 | 108.20 |
| 34 | AA | 233 | C | O4'-C1'-N1 | 7.13 | 113.90 | 108.20 |
| 34 | AA | 1076 | C | O4'-C1'-N1 | 7.13 | 113.90 | 108.20 |
| 34 | AA | 1644 | U | C2-N3-C4 | -7.13 | 122.72 | 127.00 |
| 34 | AA | 2034 | G | O4'-C1'-N9 | 7.13 | 113.90 | 108.20 |
| 70 | AE | 19 | ARG | NE-CZ-NH1 | 7.13 | 123.86 | 120.30 |
| 1 | A | 1877 | C | O4'-C1'-N1 | 7.12 | 113.90 | 108.20 |
| 2 | 7 | 24 | C | O4'-C1'-N1 | 7.12 | 113.90 | 108.20 |
| 1 | A | 874 | A | P-O3'-C3' | 7.12 | 128.24 | 119.70 |
| 34 | AA | 32 | C | O4'-C1'-N1 | 7.12 | 113.89 | 108.20 |
| 72 | AG | 137 | ARG | NE-CZ-NH2 | 7.12 | 123.86 | 120.30 |
| 21 | F | 108 | ARG | NE-CZ-NH1 | 7.12 | 123.86 | 120.30 |
| 34 | AA | 733 | C | O4'-C1'-N1 | 7.11 | 113.89 | 108.20 |
| 34 | AA | 3205 | U | C2-N1-C1' | 7.11 | 126.24 | 117.70 |
| 34 | AA | 2116 | C | O4'-C1'-N1 | 7.11 | 113.89 | 108.20 |
| 1 | A | 95 | A | O4'-C1'-N9 | 7.11 | 113.89 | 108.20 |
| 34 | AA | 2916 | C | O4'-C1'-N1 | 7.11 | 113.88 | 108.20 |
| 34 | AA | 28 | C | O4'-C1'-N1 | 7.10 | 113.88 | 108.20 |
| 34 | AA | 2961 | C | O4'-C1'-N1 | 7.10 | 113.88 | 108.20 |
| 34 | AA | 3220 | U | O4'-C1'-N1 | 7.10 | 113.88 | 108.20 |
| 34 | AA | 2037 | U | O4'-C1'-N1 | 7.10 | 113.88 | 108.20 |
| 34 | AA | 1788 | C | O4'-C1'-N1 | 7.10 | 113.88 | 108.20 |
| 70 | AE | 244 | ARG | NE-CZ-NH1 | 7.10 | 123.85 | 120.30 |
| 34 | AA | 3216 | C | O4'-C1'-N1 | 7.09 | 113.88 | 108.20 |
| 2 | 7 | 41 | C | O4'-C1'-N1 | 7.09 | 113.87 | 108.20 |
| 34 | AA | 542 | A | C5-C6-N6 | -7.09 | 118.03 | 123.70 |
| 34 | AA | 3013 | A | P-O5'-C5' | 7.09 | 132.24 | 120.90 |
| 2 | 7 | 14 | A | O4'-C1'-N9 | 7.08 | 113.87 | 108.20 |
| 34 | AA | 728 | C | O4'-C1'-N1 | 7.08 | 113.87 | 108.20 |
| 34 | AA | 1656 | G | O4'-C1'-N9 | 7.08 | 113.87 | 108.20 |
| 34 | AA | 489 | U | P-O3'-C3' | 7.08 | 128.19 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 31 | C | O4'-C1'-N1 | 7.08 | 113.86 | 108.20 |
| 34 | AA | 2455 | G | C5-C6-O6 | -7.08 | 124.35 | 128.60 |
| 63 | AW | 69 | ARG | NE-CZ-NH1 | 7.07 | 123.84 | 120.30 |
| 34 | AA | 990 | U | O4'-C1'-N1 | 7.07 | 113.86 | 108.20 |
| 34 | AA | 2010 | C | O4'-C1'-N1 | 7.07 | 113.86 | 108.20 |
| 34 | AA | 414 | C | O4'-C1'-N1 | 7.07 | 113.86 | 108.20 |
| 1 | A | 1980 | A | O4'-C1'-N9 | 7.07 | 113.85 | 108.20 |
| 34 | AA | 1769 | U | O4'-C1'-N1 | 7.06 | 113.85 | 108.20 |
| 1 | A | 437 | C | O4'-C1'-N1 | 7.06 | 113.85 | 108.20 |
| 1 | A | 1404 | U | O4'-C1'-N1 | 7.06 | 113.85 | 108.20 |
| 1 | A | 1416 | U | O4'-C1'-N1 | 7.06 | 113.85 | 108.20 |
| 51 | AP | 31 | ARG | NE-CZ-NH2 | -7.06 | 116.77 | 120.30 |
| 1 | A | 1909 | C | C6-N1-C2 | -7.06 | 117.48 | 120.30 |
| 34 | AA | 1155 | C | O4'-C1'-N1 | 7.06 | 113.85 | 108.20 |
| 77 | AX | 121 | ARG | NE-CZ-NH2 | 7.05 | 123.83 | 120.30 |
| 1 | A | 638 | G | C5-C6-O6 | -7.05 | 124.37 | 128.60 |
| 65 | AT | 61 | ARG | NE-CZ-NH1 | 7.05 | 123.83 | 120.30 |
| 1 | A | 1440 | C | O4'-C1'-N1 | 7.05 | 113.84 | 108.20 |
| 34 | AA | 1020 | C | O4'-C1'-N1 | 7.05 | 113.84 | 108.20 |
| 27 | Q | 20 | ARG | NE-CZ-NH2 | -7.04 | 116.78 | 120.30 |
| 34 | AA | 83 | U | O4'-C1'-N1 | 7.04 | 113.84 | 108.20 |
| 34 | AA | 3511 | C | O4'-C1'-N1 | 7.04 | 113.83 | 108.20 |
| 68 | A5 | 173 | ARG | NE-CZ-NH2 | 7.04 | 123.82 | 120.30 |
| 61 | AQ | 98 | ARG | NE-CZ-NH2 | 7.04 | 123.82 | 120.30 |
| 1 | A | 1729 | A | O4'-C1'-N9 | 7.04 | 113.83 | 108.20 |
| 34 | AA | 3168 | C | O4'-C1'-N1 | 7.04 | 113.83 | 108.20 |
| 1 | A | 1209 | G | N1-C6-O6 | 7.04 | 124.12 | 119.90 |
| 27 | Q | 18 | ARG | NE-CZ-NH1 | 7.04 | 123.82 | 120.30 |
| 35 | AC | 152 | C | O4'-C1'-N1 | 7.03 | 113.83 | 108.20 |
| 34 | AA | 719 | C | O4'-C1'-N1 | 7.03 | 113.83 | 108.20 |
| 28 | S | 89 | ARG | NE-CZ-NH2 | 7.03 | 123.81 | 120.30 |
| 28 | S | 115 | ARG | NE-CZ-NH1 | -7.03 | 116.79 | 120.30 |
| 1 | A | 17 | C | O4'-C1'-N1 | 7.03 | 113.82 | 108.20 |
| 1 | A | 586 | A | C1'-O4'-C4' | -7.03 | 104.28 | 109.90 |
| 1 | A | 150 | C | O4'-C1'-N1 | 7.02 | 113.82 | 108.20 |
| 1 | A | 2079 | C | O4'-C1'-N1 | 7.02 | 113.82 | 108.20 |
| 34 | AA | 10 | G | C5-C6-O6 | -7.02 | 124.39 | 128.60 |
| 57 | AK | 81 | ARG | NE-CZ-NH2 | 7.02 | 123.81 | 120.30 |
| 67 | A3 | 64 | ARG | NE-CZ-NH1 | 7.02 | 123.81 | 120.30 |
| 1 | A | 1936 | C | O4'-C1'-N1 | 7.02 | 113.81 | 108.20 |
| 34 | AA | 3171 | C | O4'-C1'-N1 | 7.02 | 113.81 | 108.20 |
| 34 | AA | 674 | U | O4'-C1'-N1 | 7.01 | 113.81 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 36 | AB | 67 | C | O4'-C1'-N1 | 7.01 | 113.81 | 108.20 |
| 65 | AT | 99 | ARG | NE-CZ-NH2 | -7.00 | 116.80 | 120.30 |
| 2 | 7 | 74 | A | O4'-C1'-N9 | 7.00 | 113.80 | 108.20 |
| 34 | AA | 1440 | C | O4'-C1'-N1 | 7.00 | 113.80 | 108.20 |
| 34 | AA | 3695 | C | O4'-C1'-N1 | 7.00 | 113.80 | 108.20 |
| 1 | A | 1812 | A | O4'-C1'-N9 | 7.00 | 113.80 | 108.20 |
| 2 | 7 | 74 | A | C4'-C3'-C2' | -7.00 | 95.60 | 102.60 |
| 6 | I | 189 | ARG | NE-CZ-NH1 | 7.00 | 123.80 | 120.30 |
| 34 | AA | 82 | U | O4'-C1'-N1 | 7.00 | 113.80 | 108.20 |
| 34 | AA | 1827 | C | O4'-C1'-N1 | 7.00 | 113.80 | 108.20 |
| 36 | AB | 93 | G | C5-C6-O6 | -7.00 | 124.40 | 128.60 |
| 59 | AS | 103 | ARG | NE-CZ-NH1 | 7.00 | 123.80 | 120.30 |
| 34 | AA | 1720 | C | O4'-C1'-N1 | 7.00 | 113.80 | 108.20 |
| 1 | A | 414 | C | O4'-C1'-N1 | 6.99 | 113.79 | 108.20 |
| 34 | AA | 234 | C | O4'-C1'-N1 | 6.99 | 113.80 | 108.20 |
| 1 | A | 586 | A | O4'-C1'-N9 | 6.99 | 113.79 | 108.20 |
| 1 | A | 2062 | U | O4'-C1'-N1 | 6.99 | 113.79 | 108.20 |
| 1 | A | 1267 | C | O4'-C1'-N1 | 6.99 | 113.79 | 108.20 |
| 34 | AA | 1430 | A | O4'-C1'-N9 | 6.99 | 113.79 | 108.20 |
| 34 | AA | 2955 | C | O4'-C1'-N1 | 6.99 | 113.79 | 108.20 |
| 34 | AA | 3131 | A | O4'-C1'-N9 | 6.99 | 113.79 | 108.20 |
| 34 | AA | 124 | U | O4'-C1'-N1 | 6.98 | 113.78 | 108.20 |
| 34 | AA | 2004 | U | C2-N3-C4 | -6.98 | 122.81 | 127.00 |
| 34 | AA | 2099 | C | O4'-C1'-N1 | 6.98 | 113.79 | 108.20 |
| 34 | AA | 2444 | C | O4'-C1'-N1 | 6.98 | 113.79 | 108.20 |
| 34 | AA | 3070 | C | O4'-C1'-N1 | 6.98 | 113.79 | 108.20 |
| 34 | AA | 1452 | U | O4'-C1'-N1 | 6.98 | 113.78 | 108.20 |
| 34 | AA | 3782 | A | P-O3'-C3' | 6.98 | 128.07 | 119.70 |
| 34 | AA | 1026 | G | C5-C6-O6 | -6.97 | 124.42 | 128.60 |
| 34 | AA | 1265 | C | O4'-C1'-N1 | 6.97 | 113.78 | 108.20 |
| 63 | AW | 56 | ARG | NE-CZ-NH1 | 6.97 | 123.79 | 120.30 |
| 1 | A | 1886 | C | O4'-C1'-N1 | 6.97 | 113.77 | 108.20 |
| 34 | AA | 1797 | A | N1-C6-N6 | 6.97 | 122.78 | 118.60 |
| 34 | AA | 138 | C | O4'-C1'-N1 | 6.97 | 113.77 | 108.20 |
| 61 | AQ | 3 | ARG | NE-CZ-NH2 | 6.96 | 123.78 | 120.30 |
| 34 | AA | 3461 | C | O4'-C1'-N1 | 6.95 | 113.76 | 108.20 |
| 34 | AA | 1442 | C | O4'-C1'-N1 | 6.95 | 113.76 | 108.20 |
| 34 | AA | 3633 | U | O4'-C1'-N1 | 6.95 | 113.76 | 108.20 |
| 7 | K | 121 | THR | N-CA-CB | 6.95 | 123.51 | 110.30 |
| 1 | A | 439 | C | O4'-C1'-N1 | 6.95 | 113.76 | 108.20 |
| 34 | AA | 3702 | C | O4'-C1'-N1 | 6.94 | 113.75 | 108.20 |
| 32 | X | 47 | ARG | NE-CZ-NH2 | 6.94 | 123.77 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 34 | AA | 3323 | G | C5-C6-O6 | -6.94 | 124.43 | 128.60 |
| 34 | AA | 3714 | C | O4'-C1'-N1 | 6.94 | 113.75 | 108.20 |
| 34 | AA | 1249 | U | O4'-C1'-N1 | 6.94 | 113.75 | 108.20 |
| 1 | A | 932 | U | O4'-C1'-N1 | 6.94 | 113.75 | 108.20 |
| 1 | A | 1839 | G | O4'-C1'-N9 | 6.94 | 113.75 | 108.20 |
| 45 | A9 | 106 | ARG | NE-CZ-NH1 | 6.94 | 123.77 | 120.30 |
| 34 | AA | 1825 | C | O4'-C1'-N1 | 6.93 | 113.75 | 108.20 |
| 1 | A | 1298 | C | O4'-C1'-N1 | 6.93 | 113.75 | 108.20 |
| 34 | AA | 213 | C | O4'-C1'-N1 | 6.93 | 113.75 | 108.20 |
| 6 | I | 51 | ARG | NE-CZ-NH1 | 6.93 | 123.77 | 120.30 |
| 34 | AA | 937 | C | O4'-C1'-N1 | 6.93 | 113.74 | 108.20 |
| 1 | A | 170 | C | O4'-C1'-N1 | 6.92 | 113.74 | 108.20 |
| 28 | S | 134 | ARG | NE-CZ-NH2 | -6.92 | 116.84 | 120.30 |
| 34 | AA | 210 | C | O4'-C1'-N1 | 6.92 | 113.74 | 108.20 |
| 34 | AA | 741 | C | O4'-C1'-N1 | 6.92 | 113.74 | 108.20 |
| 34 | AA | 1665 | C | O4'-C1'-N1 | 6.92 | 113.74 | 108.20 |
| 1 | A | 1865 | G | O4'-C1'-N9 | 6.92 | 113.74 | 108.20 |
| 34 | AA | 2553 | U | O4'-C1'-N1 | 6.92 | 113.74 | 108.20 |
| 70 | AE | 30 | ARG | NE-CZ-NH1 | 6.92 | 123.76 | 120.30 |
| 1 | A | 300 | C | O4'-C1'-N1 | 6.92 | 113.73 | 108.20 |
| 34 | AA | 2624 | C | O4'-C1'-N1 | 6.92 | 113.73 | 108.20 |
| 34 | AA | 3005 | C | O4'-C1'-N1 | 6.92 | 113.73 | 108.20 |
| 70 | AE | 366 | ARG | NE-CZ-NH1 | 6.92 | 123.76 | 120.30 |
| 2 | 7 | 16 | U | O4'-C1'-N1 | 6.92 | 113.73 | 108.20 |
| 21 | F | 100 | ARG | NE-CZ-NH1 | 6.91 | 123.76 | 120.30 |
| 34 | AA | 589 | C | O4'-C1'-N1 | 6.91 | 113.73 | 108.20 |
| 34 | AA | 202 | C | O4'-C1'-N1 | 6.91 | 113.73 | 108.20 |
| 34 | AA | 2622 | C | O4'-C1'-N1 | 6.91 | 113.73 | 108.20 |
| 1 | A | 1198 | U | O4'-C1'-N1 | 6.91 | 113.73 | 108.20 |
| 34 | AA | 1035 | G | C5-C6-O6 | -6.91 | 124.45 | 128.60 |
| 34 | AA | 1088 | C | O4'-C1'-N1 | 6.91 | 113.73 | 108.20 |
| 34 | AA | 1979 | C | O4'-C1'-N1 | 6.91 | 113.73 | 108.20 |
| 34 | AA | 306 | C | O4'-C1'-N1 | 6.91 | 113.73 | 108.20 |
| 34 | AA | 3324 | U | O4'-C1'-N1 | 6.91 | 113.73 | 108.20 |
| 36 | AB | 44 | C | O4'-C1'-N1 | 6.90 | 113.72 | 108.20 |
| 1 | A | 408 | U | O4'-C1'-N1 | 6.90 | 113.72 | 108.20 |
| 34 | AA | 175 | G | O4'-C1'-N9 | 6.90 | 113.72 | 108.20 |
| 34 | AA | 2558 | C | O4'-C1'-N1 | 6.90 | 113.72 | 108.20 |
| 34 | AA | 2591 | U | C2-N1-C1' | 6.90 | 125.98 | 117.70 |
| 34 | AA | 3732 | U | O4'-C1'-N1 | 6.90 | 113.72 | 108.20 |
| 34 | AA | 3204 | C | O4'-C1'-N1 | 6.90 | 113.72 | 108.20 |
| 1 | A | 845 | U | P-O3'-C3' | 6.89 | 127.97 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 895 | U | O4'-C1'-N1 | 6.89 | 113.72 | 108.20 |
| 34 | AA | 3469 | C | O4'-C1'-N1 | 6.89 | 113.72 | 108.20 |
| 34 | AA | 3081 | C | O4'-C1'-N1 | 6.89 | 113.71 | 108.20 |
| 68 | A5 | 86 | ARG | NE-CZ-NH2 | -6.89 | 116.85 | 120.30 |
| 34 | AA | 1026 | G | N1-C6-O6 | 6.89 | 124.03 | 119.90 |
| 34 | AA | 1823 | C | O4'-C1'-N1 | 6.89 | 113.71 | 108.20 |
| 34 | AA | 2689 | G | O4'-C1'-N9 | 6.89 | 113.71 | 108.20 |
| 34 | AA | 3381 | A | P-O3'-C3' | 6.89 | 127.96 | 119.70 |
| 1 | A | 1463 | C | O4'-C1'-N1 | 6.88 | 113.71 | 108.20 |
| 24 | L | 49 | ARG | NE-CZ-NH2 | -6.88 | 116.86 | 120.30 |
| 34 | AA | 701 | C | O4'-C1'-N1 | 6.88 | 113.70 | 108.20 |
| 34 | AA | 1200 | C | O4'-C1'-N1 | 6.88 | 113.70 | 108.20 |
| 51 | AP | 26 | ARG | NE-CZ-NH1 | 6.88 | 123.74 | 120.30 |
| 1 | A | 1817 | U | P-O3'-C3' | 6.88 | 127.95 | 119.70 |
| 34 | AA | 3770 | C | O4'-C1'-N1 | 6.88 | 113.70 | 108.20 |
| 34 | AA | 710 | C | O4'-C1'-N1 | 6.87 | 113.70 | 108.20 |
| 73 | AU | 21 | ARG | NE-CZ-NH1 | -6.87 | 116.86 | 120.30 |
| 74 | AH | 144 | TYR | CB-CG-CD1 | 6.87 | 125.12 | 121.00 |
| 1 | A | 818 | C | O4'-C1'-N1 | 6.87 | 113.70 | 108.20 |
| 1 | A | 1296 | C | O4'-C1'-N1 | 6.87 | 113.70 | 108.20 |
| 35 | AC | 104 | C | O4'-C1'-N1 | 6.87 | 113.70 | 108.20 |
| 34 | AA | 2036 | C | O4'-C1'-N1 | 6.87 | 113.69 | 108.20 |
| 34 | AA | 1794 | U | O4'-C1'-N1 | 6.87 | 113.69 | 108.20 |
| 34 | AA | 3517 | C | O4'-C1'-N1 | 6.87 | 113.69 | 108.20 |
| 1 | A | 2064 | C | O4'-C1'-N1 | 6.86 | 113.69 | 108.20 |
| 34 | AA | 1457 | G | C5-C6-O6 | -6.86 | 124.48 | 128.60 |
| 34 | AA | 1646 | C | O4'-C1'-N1 | 6.86 | 113.69 | 108.20 |
| 34 | AA | 3065 | C | C2-N1-C1' | 6.86 | 126.35 | 118.80 |
| 1 | A | 379 | G | C5-C6-O6 | -6.86 | 124.49 | 128.60 |
| 1 | A | 2053 | U | P-O3'-C3' | 6.86 | 127.93 | 119.70 |
| 57 | AK | 201 | TYR | CB-CG-CD1 | 6.85 | 125.11 | 121.00 |
| 34 | AA | 718 | U | O4'-C1'-N1 | 6.85 | 113.68 | 108.20 |
| 1 | A | 979 | C | O4'-C1'-N1 | 6.85 | 113.68 | 108.20 |
| 1 | A | 907 | C | O4'-C1'-N1 | 6.85 | 113.68 | 108.20 |
| 34 | AA | 3139 | C | C2-N1-C1' | 6.85 | 126.33 | 118.80 |
| 34 | AA | 1725 | U | O4'-C1'-N1 | 6.84 | 113.67 | 108.20 |
| 34 | AA | 525 | U | O4'-C1'-N1 | 6.84 | 113.67 | 108.20 |
| 34 | AA | 1679 | U | O4'-C1'-N1 | 6.84 | 113.67 | 108.20 |
| 1 | A | 2023 | A | N1-C6-N6 | 6.84 | 122.70 | 118.60 |
| 20 | B | 220 | ARG | NE-CZ-NH2 | 6.83 | 123.72 | 120.30 |
| 1 | A | 415 | C | O4'-C1'-N1 | 6.83 | 113.67 | 108.20 |
| 3 | D | 167 | ARG | NE-CZ-NH1 | 6.83 | 123.72 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 31 | V | 70 | ARG | NE-CZ-NH1 | 6.83 | 123.72 | 120.30 |
| 34 | AA | 1031 | G | N3-C2-N2 | 6.83 | 124.68 | 119.90 |
| 34 | AA | 3739 | A | O4'-C1'-N9 | 6.83 | 113.66 | 108.20 |
| 34 | AA | 1575 | C | C5'-C4'-O4' | 6.83 | 117.29 | 109.10 |
| 34 | AA | 1757 | C | O4'-C1'-N1 | 6.82 | 113.66 | 108.20 |
| 34 | AA | 3258 | C | O4'-C1'-N1 | 6.82 | 113.66 | 108.20 |
| 34 | AA | 3352 | G | C5-C6-O6 | -6.82 | 124.50 | 128.60 |
| 34 | AA | 3053 | G | O4'-C1'-N9 | 6.82 | 113.66 | 108.20 |
| 1 | A | 1635 | C | C2-N1-C1' | 6.82 | 126.30 | 118.80 |
| 34 | AA | 1506 | C | O4'-C1'-N1 | 6.82 | 113.66 | 108.20 |
| 1 | A | 1956 | A | N1-C6-N6 | 6.82 | 122.69 | 118.60 |
| 34 | AA | 2934 | A | O4'-C1'-N9 | 6.82 | 113.65 | 108.20 |
| 1 | A | 953 | C | O4'-C1'-N1 | 6.82 | 113.65 | 108.20 |
| 34 | AA | 1301 | U | O4'-C1'-N1 | 6.82 | 113.65 | 108.20 |
| 34 | AA | 3209 | G | C5-C6-O6 | -6.82 | 124.51 | 128.60 |
| 1 | A | 621 | C | O4'-C1'-N1 | 6.81 | 113.65 | 108.20 |
| 3 | D | 76 | ARG | NE-CZ-NH1 | 6.81 | 123.71 | 120.30 |
| 34 | AA | 1502 | G | C5'-C4'-O4' | 6.81 | 117.28 | 109.10 |
| 34 | AA | 1539 | U | O4'-C1'-N1 | 6.81 | 113.65 | 108.20 |
| 1 | A | 1377 | U | O4'-C1'-N1 | 6.81 | 113.65 | 108.20 |
| 25 | N | 79 | PHE | CB-CG-CD1 | 6.81 | 125.56 | 120.80 |
| 26 | P | 128 | ARG | NE-CZ-NH1 | -6.81 | 116.90 | 120.30 |
| 70 | AE | 272 | ARG | NE-CZ-NH1 | -6.81 | 116.90 | 120.30 |
| 34 | AA | 577 | U | O4'-C1'-N1 | 6.80 | 113.64 | 108.20 |
| 34 | AA | 3783 | G | C5'-C4'-O4' | 6.80 | 117.26 | 109.10 |
| 34 | AA | 3020 | U | O4'-C1'-N1 | 6.80 | 113.64 | 108.20 |
| 35 | AC | 148 | C | O4'-C1'-N1 | 6.80 | 113.64 | 108.20 |
| 34 | AA | 982 | C | O4'-C1'-N1 | 6.80 | 113.64 | 108.20 |
| 1 | A | 323 | C | O4'-C1'-N1 | 6.79 | 113.63 | 108.20 |
| 35 | AC | 61 | C | O4'-C1'-N1 | 6.79 | 113.63 | 108.20 |
| 46 | Aa | 58 | ARG | NE-CZ-NH1 | -6.79 | 116.90 | 120.30 |
| 34 | AA | 92 | G | C5-C6-O6 | -6.79 | 124.53 | 128.60 |
| 34 | AA | 146 | U | O4'-C1'-N1 | 6.79 | 113.63 | 108.20 |
| 34 | AA | 3414 | G | P-O3'-C3' | 6.79 | 127.85 | 119.70 |
| 34 | AA | 127 | U | O4'-C1'-N1 | 6.79 | 113.63 | 108.20 |
| 34 | AA | 349 | G | N1-C6-O6 | 6.79 | 123.97 | 119.90 |
| 34 | AA | 2810 | A | P-O3'-C3' | 6.79 | 127.84 | 119.70 |
| 2 | 7 | 73 | C | C6-N1-C1' | -6.78 | 112.66 | 120.80 |
| 34 | AA | 3160 | A | O4'-C1'-N9 | 6.78 | 113.63 | 108.20 |
| 56 | Ac | 48 | ARG | NE-CZ-NH1 | 6.78 | 123.69 | 120.30 |
| 34 | AA | 2635 | C | O4'-C1'-N1 | 6.78 | 113.62 | 108.20 |
| 34 | AA | 1086 | C | O4'-C1'-N1 | 6.78 | 113.62 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 34 | AA | 1631 | A | C5'-C4'-O4' | 6.78 | 117.24 | 109.10 |
| 34 | AA | 873 | U | P-O3'-C3' | 6.78 | 127.83 | 119.70 |
| 32 | X | 42 | ARG | NE-CZ-NH1 | 6.78 | 123.69 | 120.30 |
| 34 | AA | 231 | G | O4'-C1'-N9 | 6.78 | 113.62 | 108.20 |
| 34 | AA | 3738 | U | O4'-C1'-N1 | 6.78 | 113.62 | 108.20 |
| 2 | 7 | 32 | U | P-O3'-C3' | 6.77 | 127.83 | 119.70 |
| 34 | AA | 3257 | G | C5-C6-O6 | -6.77 | 124.54 | 128.60 |
| 34 | AA | 467 | U | O4'-C1'-N1 | 6.77 | 113.62 | 108.20 |
| 34 | AA | 623 | U | O4'-C1'-N1 | 6.77 | 113.62 | 108.20 |
| 34 | AA | 1849 | U | O4'-C1'-N1 | 6.77 | 113.62 | 108.20 |
| 34 | AA | 3301 | C | P-O3'-C3' | -6.77 | 111.58 | 119.70 |
| 1 | A | 1835 | U | O4'-C1'-N1 | 6.77 | 113.61 | 108.20 |
| 49 | Ae | 42 | ARG | NE-CZ-NH2 | -6.77 | 116.92 | 120.30 |
| 1 | A | 360 | C | O4'-C1'-N1 | 6.77 | 113.61 | 108.20 |
| 34 | AA | 1336 | U | P-O3'-C3' | -6.77 | 111.58 | 119.70 |
| 1 | A | 1687 | C | O4'-C1'-N1 | 6.76 | 113.61 | 108.20 |
| 63 | AW | 23 | ARG | NE-CZ-NH1 | 6.76 | 123.68 | 120.30 |
| 16 | 3 | 93 | ARG | NE-CZ-NH2 | 6.76 | 123.68 | 120.30 |
| 34 | AA | 857 | C | O4'-C1'-N1 | 6.76 | 113.61 | 108.20 |
| 1 | A | 868 | U | P-O3'-C3' | 6.76 | 127.81 | 119.70 |
| 53 | Ai | 40 | ARG | NE-CZ-NH1 | 6.76 | 123.68 | 120.30 |
| 1 | A | 1061 | A | O4'-C1'-N9 | 6.76 | 113.61 | 108.20 |
| 1 | A | 1916 | C | O4'-C1'-N1 | 6.76 | 113.61 | 108.20 |
| 7 | K | 97 | ARG | NE-CZ-NH1 | 6.76 | 123.68 | 120.30 |
| 34 | AA | 306 | C | C6-N1-C1' | -6.76 | 112.69 | 120.80 |
| 46 | Aa | 67 | ARG | NE-CZ-NH1 | 6.76 | 123.68 | 120.30 |
| 1 | A | 344 | C | O4'-C1'-N1 | 6.76 | 113.61 | 108.20 |
| 34 | AA | 3456 | C | O4'-C1'-N1 | 6.76 | 113.61 | 108.20 |
| 34 | AA | 3545 | U | O4'-C1'-N1 | 6.76 | 113.61 | 108.20 |
| 35 | AC | 15 | C | O4'-C1'-N1 | 6.76 | 113.61 | 108.20 |
| 34 | AA | 3265 | C | O4'-C1'-N1 | 6.75 | 113.60 | 108.20 |
| 22 | H | 186 | ARG | NE-CZ-NH1 | 6.75 | 123.68 | 120.30 |
| 34 | AA | 1840 | C | O4'-C1'-N1 | 6.75 | 113.60 | 108.20 |
| 34 | AA | 2993 | C | O4'-C1'-N1 | 6.75 | 113.60 | 108.20 |
| 2 | 7 | 26 | C | O4'-C1'-N1 | 6.75 | 113.60 | 108.20 |
| 35 | AC | 68 | C | O4'-C1'-N1 | 6.75 | 113.60 | 108.20 |
| 1 | A | 1310 | C | O4'-C1'-N1 | 6.75 | 113.60 | 108.20 |
| 43 | AN | 60 | PHE | CB-CG-CD1 | -6.75 | 116.08 | 120.80 |
| 1 | A | 270 | C | O4'-C1'-N1 | 6.75 | 113.60 | 108.20 |
| 49 | Ae | 41 | ARG | NE-CZ-NH1 | 6.75 | 123.67 | 120.30 |
| 1 | A | 909 | U | O4'-C1'-N1 | 6.75 | 113.60 | 108.20 |
| 34 | AA | 1117 | U | O4'-C1'-N1 | 6.74 | 113.59 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 34 | AA | 2700 | C | O4'-C1'-N1 | 6.74 | 113.60 | 108.20 |
| 2 | 7 | 45 | A | P-O3'-C3' | 6.74 | 127.79 | 119.70 |
| 34 | AA | 1572 | U | C2-N1-C1' | 6.74 | 125.79 | 117.70 |
| 1 | A | 1012 | C | O4'-C1'-N1 | 6.74 | 113.59 | 108.20 |
| 34 | AA | 2498 | U | O4'-C1'-N1 | 6.74 | 113.59 | 108.20 |
| 34 | AA | 348 | C | O4'-C1'-N1 | 6.74 | 113.59 | 108.20 |
| 7 | K | 57 | ARG | NE-CZ-NH1 | 6.73 | 123.67 | 120.30 |
| 36 | AB | 57 | C | O4'-C1'-N1 | 6.73 | 113.59 | 108.20 |
| 1 | A | 553 | U | O4'-C1'-N1 | 6.73 | 113.58 | 108.20 |
| 35 | AC | 121 | C | O4'-C1'-N1 | 6.73 | 113.59 | 108.20 |
| 1 | A | 1922 | C | O4'-C1'-N1 | 6.73 | 113.58 | 108.20 |
| 35 | AC | 103 | G | C5-C6-O6 | -6.73 | 124.56 | 128.60 |
| 34 | AA | 1167 | U | O4'-C1'-N1 | 6.73 | 113.58 | 108.20 |
| 34 | AA | 1692 | C | O4'-C1'-N1 | 6.73 | 113.58 | 108.20 |
| 1 | A | 1686 | C | O4'-C1'-N1 | 6.72 | 113.58 | 108.20 |
| 34 | AA | 1000 | C | O4'-C1'-N1 | 6.72 | 113.58 | 108.20 |
| 34 | AA | 3275 | C | O4'-C1'-N1 | 6.72 | 113.58 | 108.20 |
| 34 | AA | 182 | U | O4'-C1'-N1 | 6.72 | 113.58 | 108.20 |
| 36 | AB | 46 | C | O4'-C1'-N1 | 6.72 | 113.58 | 108.20 |
| 1 | A | 2005 | U | O4'-C1'-N1 | 6.72 | 113.58 | 108.20 |
| 34 | AA | 39 | A | O4'-C1'-N9 | 6.72 | 113.58 | 108.20 |
| 71 | AF | 248 | ARG | NE-CZ-NH1 | 6.72 | 123.66 | 120.30 |
| 34 | AA | 667 | U | C2-N1-C1' | 6.72 | 125.76 | 117.70 |
| 34 | AA | 1139 | C | O4'-C1'-N1 | 6.72 | 113.57 | 108.20 |
| 1 | A | 458 | A | O4'-C1'-N9 | 6.71 | 113.57 | 108.20 |
| 1 | A | 1362 | U | O4'-C1'-N1 | 6.71 | 113.57 | 108.20 |
| 34 | AA | 109 | A | P-O3'-C3' | 6.71 | 127.76 | 119.70 |
| 34 | AA | 999 | G | O4'-C1'-N9 | 6.71 | 113.57 | 108.20 |
| 34 | AA | 2396 | C | C6-N1-C2 | -6.71 | 117.61 | 120.30 |
| 1 | A | 540 | C | O4'-C1'-N1 | 6.71 | 113.56 | 108.20 |
| 34 | AA | 966 | A | C5-C6-N6 | -6.71 | 118.34 | 123.70 |
| 34 | AA | 3021 | C | O4'-C1'-N1 | 6.71 | 113.56 | 108.20 |
| 1 | A | 396 | G | O4'-C1'-N9 | 6.70 | 113.56 | 108.20 |
| 34 | AA | 1657 | U | O4'-C1'-N1 | 6.70 | 113.56 | 108.20 |
| 34 | AA | 3419 | U | O4'-C1'-N1 | 6.70 | 113.56 | 108.20 |
| 1 | A | 475 | C | O4'-C1'-N1 | 6.70 | 113.56 | 108.20 |
| 1 | A | 1169 | C | O4'-C1'-N1 | 6.70 | 113.56 | 108.20 |
| 34 | AA | 1661 | U | O4'-C1'-N1 | 6.70 | 113.56 | 108.20 |
| 34 | AA | 3023 | C | O4'-C1'-N1 | 6.70 | 113.56 | 108.20 |
| 1 | A | 433 | C | O4'-C1'-N1 | 6.70 | 113.56 | 108.20 |
| 1 | A | 1845 | U | C5'-C4'-C3' | -6.70 | 105.29 | 116.00 |
| 35 | AC | 141 | U | O4'-C1'-N1 | 6.70 | 113.56 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 34 | AA | 3619 | U | O4'-C1'-N1 | 6.69 | 113.55 | 108.20 |
| 1 | A | 15 | U | O4'-C1'-N1 | 6.69 | 113.55 | 108.20 |
| 1 | A | 1644 | U | O4'-C1'-N1 | 6.69 | 113.55 | 108.20 |
| 1 | A | 1749 | C | O4'-C1'-N1 | 6.69 | 113.55 | 108.20 |
| 34 | AA | 3046 | C | O4'-C1'-N1 | 6.69 | 113.55 | 108.20 |
| 1 | A | 200 | U | O4'-C1'-N1 | 6.69 | 113.55 | 108.20 |
| 34 | AA | 2171 | U | O4'-C1'-N1 | 6.69 | 113.55 | 108.20 |
| 1 | A | 2085 | G | P-O3'-C3' | -6.69 | 111.68 | 119.70 |
| 34 | AA | 1480 | G | C5-C6-O6 | -6.69 | 124.59 | 128.60 |
| 34 | AA | 2542 | G | O4'-C1'-N9 | 6.69 | 113.55 | 108.20 |
| 1 | A | 536 | C | O4'-C1'-N1 | 6.68 | 113.54 | 108.20 |
| 69 | AD | 242 | ARG | NE-CZ-NH2 | 6.68 | 123.64 | 120.30 |
| 13 | Z | 72 | MET | CG-SD-CE | -6.67 | 89.52 | 100.20 |
| 45 | A9 | 127 | PHE | CB-CG-CD1 | 6.67 | 125.47 | 120.80 |
| 1 | A | 572 | C | O4'-C1'-N1 | 6.67 | 113.54 | 108.20 |
| 34 | AA | 2409 | G | O4'-C1'-N9 | 6.67 | 113.54 | 108.20 |
| 34 | AA | 3139 | C | C5'-C4'-O4' | 6.67 | 117.11 | 109.10 |
| 51 | AP | 144 | ARG | NE-CZ-NH1 | 6.67 | 123.64 | 120.30 |
| 34 | AA | 3407 | G | N1-C6-O6 | 6.67 | 123.90 | 119.90 |
| 1 | A | 1781 | C | O4'-C1'-N1 | 6.67 | 113.53 | 108.20 |
| 34 | AA | 796 | C | O4'-C1'-N1 | 6.67 | 113.53 | 108.20 |
| 70 | AE | 280 | TYR | CB-CG-CD1 | 6.67 | 125.00 | 121.00 |
| 1 | A | 597 | C | O4'-C1'-N1 | 6.66 | 113.53 | 108.20 |
| 1 | A | 2085 | G | C5-C6-O6 | -6.66 | 124.60 | 128.60 |
| 34 | AA | 1618 | C | P-O3'-C3' | -6.66 | 111.70 | 119.70 |
| 1 | A | 1300 | G | O4'-C1'-N9 | 6.66 | 113.53 | 108.20 |
| 34 | AA | 1041 | U | C2-N1-C1' | 6.66 | 125.69 | 117.70 |
| 34 | AA | 2402 | U | O4'-C1'-N1 | 6.66 | 113.53 | 108.20 |
| 34 | AA | 2495 | C | O4'-C1'-N1 | 6.66 | 113.53 | 108.20 |
| 69 | AD | 242 | ARG | NE-CZ-NH1 | -6.65 | 116.97 | 120.30 |
| 34 | AA | 1751 | C | C6-N1-C2 | -6.65 | 117.64 | 120.30 |
| 34 | AA | 3673 | C | O4'-C1'-N1 | 6.65 | 113.52 | 108.20 |
| 28 | S | 115 | ARG | NE-CZ-NH2 | 6.65 | 123.63 | 120.30 |
| 1 | A | 2084 | G | O4'-C1'-N9 | 6.65 | 113.52 | 108.20 |
| 34 | AA | 2883 | U | O4'-C1'-N1 | 6.65 | 113.52 | 108.20 |
| 34 | AA | 2972 | U | O4'-C1'-N1 | 6.65 | 113.52 | 108.20 |
| 34 | AA | 3640 | C | O4'-C1'-N1 | 6.65 | 113.52 | 108.20 |
| 1 | A | 1425 | C | O4'-C1'-N1 | 6.65 | 113.52 | 108.20 |
| 34 | AA | 957 | G | C5-C6-O6 | -6.65 | 124.61 | 128.60 |
| 34 | AA | 3437 | U | O4'-C1'-N1 | 6.64 | 113.52 | 108.20 |
| 1 | A | 836 | C | O4'-C1'-N1 | 6.64 | 113.51 | 108.20 |
| 76 | Ag | 35 | ARG | NE-CZ-NH1 | 6.64 | 123.62 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 34 | AA | 3226 | C | O4'-C1'-N1 | 6.64 | 113.51 | 108.20 |
| 35 | AC | 113 | A | P-O3'-C3' | 6.64 | 127.66 | 119.70 |
| 34 | AA | 1537 | G | C5'-C4'-C3' | -6.63 | 105.38 | 116.00 |
| 71 | AF | 291 | ARG | NE-CZ-NH2 | -6.63 | 116.98 | 120.30 |
| 34 | AA | 1480 | G | C4-N9-C1' | 6.63 | 135.12 | 126.50 |
| 34 | AA | 3407 | G | C5-C6-O6 | -6.63 | 124.62 | 128.60 |
| 34 | AA | 821 | C | O4'-C1'-N1 | 6.63 | 113.50 | 108.20 |
| 56 | Ac | 24 | ARG | NE-CZ-NH2 | 6.63 | 123.61 | 120.30 |
| 63 | AW | 82 | ARG | NE-CZ-NH2 | -6.63 | 116.98 | 120.30 |
| 1 | A | 179 | U | O4'-C1'-N1 | 6.63 | 113.50 | 108.20 |
| 1 | A | 1019 | C | O4'-C1'-N1 | 6.63 | 113.50 | 108.20 |
| 11 | O | 23 | TYR | CB-CG-CD1 | 6.63 | 124.98 | 121.00 |
| 36 | AB | 24 | U | O4'-C1'-N1 | 6.63 | 113.50 | 108.20 |
| 1 | A | 25 | C | P-O3'-C3' | 6.63 | 127.65 | 119.70 |
| 34 | AA | 1995 | C | O4'-C1'-N1 | 6.62 | 113.50 | 108.20 |
| 1 | A | 1906 | U | O4'-C1'-N1 | 6.62 | 113.50 | 108.20 |
| 34 | AA | 660 | U | O4'-C1'-N1 | 6.62 | 113.50 | 108.20 |
| 2 | 7 | 7 | U | P-O3'-C3' | 6.62 | 127.65 | 119.70 |
| 75 | AV | 37 | TYR | CB-CG-CD2 | -6.62 | 117.03 | 121.00 |
| 1 | A | 570 | U | O4'-C1'-N1 | 6.62 | 113.49 | 108.20 |
| 1 | A | 2027 | C | O4'-C1'-N1 | 6.62 | 113.49 | 108.20 |
| 2 | 7 | 40 | U | O4'-C1'-N1 | 6.62 | 113.49 | 108.20 |
| 1 | A | 551 | A | P-O3'-C3' | 6.61 | 127.64 | 119.70 |
| 34 | AA | 29 | C | O4'-C1'-N1 | 6.61 | 113.49 | 108.20 |
| 36 | AB | 36 | C | O4'-C1'-N1 | 6.61 | 113.49 | 108.20 |
| 34 | AA | 3095 | C | O4'-C1'-N1 | 6.61 | 113.49 | 108.20 |
| 34 | AA | 3115 | C | O4'-C1'-N1 | 6.61 | 113.49 | 108.20 |
| 34 | AA | 3632 | U | C2-N3-C4 | -6.61 | 123.03 | 127.00 |
| 1 | A | 1893 | C | O4'-C1'-N1 | 6.61 | 113.48 | 108.20 |
| 36 | AB | 92 | C | O4'-C1'-N1 | 6.60 | 113.48 | 108.20 |
| 34 | AA | 3288 | C | O4'-C1'-N1 | 6.60 | 113.48 | 108.20 |
| 35 | AC | 78 | U | C2-N1-C1' | 6.60 | 125.62 | 117.70 |
| 1 | A | 420 | C | O4'-C1'-N1 | 6.60 | 113.48 | 108.20 |
| 34 | AA | 3186 | U | O4'-C1'-N1 | 6.60 | 113.48 | 108.20 |
| 34 | AA | 1002 | A | P-O3'-C3' | -6.59 | 111.79 | 119.70 |
| 34 | AA | 2991 | U | O4'-C1'-N1 | 6.59 | 113.47 | 108.20 |
| 27 | Q | 13 | ARG | NE-CZ-NH1 | -6.59 | 117.00 | 120.30 |
| 34 | AA | 3159 | G | C5-C6-O6 | -6.59 | 124.64 | 128.60 |
| 1 | A | 522 | G | C5-C6-O6 | -6.59 | 124.65 | 128.60 |
| 35 | AC | 32 | C | O4'-C1'-N1 | 6.59 | 113.47 | 108.20 |
| 34 | AA | 1302 | G | O4'-C1'-N9 | 6.58 | 113.47 | 108.20 |
| 1 | A | 1796 | C | C5'-C4'-C3' | -6.58 | 105.47 | 116.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | E | 40 | ARG | NE-CZ-NH1 | 6.58 | 123.59 | 120.30 |
| 34 | AA | 941 | G | O4'-C1'-N9 | 6.58 | 113.47 | 108.20 |
| 34 | AA | 1430 | A | P-O3'-C3' | -6.58 | 111.80 | 119.70 |
| 34 | AA | 3404 | C | O4'-C1'-N1 | 6.58 | 113.46 | 108.20 |
| 34 | AA | 298 | C | O4'-C1'-N1 | 6.58 | 113.46 | 108.20 |
| 1 | A | 1313 | G | O4'-C1'-N9 | 6.58 | 113.46 | 108.20 |
| 34 | AA | 860 | A | O4'-C1'-N9 | 6.58 | 113.46 | 108.20 |
| 34 | AA | 2216 | G | C5-C6-O6 | -6.58 | 124.65 | 128.60 |
| 1 | A | 1461 | C | O4'-C1'-N1 | 6.57 | 113.46 | 108.20 |
| 34 | AA | 573 | U | O4'-C1'-N1 | 6.57 | 113.46 | 108.20 |
| 34 | AA | 3774 | A | O4'-C1'-N9 | 6.57 | 113.46 | 108.20 |
| 61 | AQ | 69 | ARG | NE-CZ-NH1 | 6.57 | 123.59 | 120.30 |
| 1 | A | 1851 | C | O4'-C1'-N1 | 6.57 | 113.46 | 108.20 |
| 8 | M | 43 | TYR | CB-CG-CD1 | 6.57 | 124.94 | 121.00 |
| 34 | AA | 3401 | C | O4'-C1'-N1 | 6.57 | 113.45 | 108.20 |
| 72 | AG | 143 | ARG | NE-CZ-NH1 | 6.57 | 123.58 | 120.30 |
| 35 | AC | 138 | U | P-O3'-C3' | 6.57 | 127.58 | 119.70 |
| 50 | Af | 35 | ARG | NE-CZ-NH1 | 6.57 | 123.58 | 120.30 |
| 27 | Q | 16 | ARG | NE-CZ-NH2 | 6.57 | 123.58 | 120.30 |
| 34 | AA | 434 | C | O4'-C1'-N1 | 6.57 | 113.45 | 108.20 |
| 34 | AA | 1013 | U | O4'-C1'-N1 | 6.57 | 113.45 | 108.20 |
| 30 | U | 3 | ARG | NE-CZ-NH1 | 6.56 | 123.58 | 120.30 |
| 32 | X | 114 | TYR | CB-CG-CD1 | 6.56 | 124.94 | 121.00 |
| 34 | AA | 3144 | C | O4'-C1'-N1 | 6.56 | 113.45 | 108.20 |
| 34 | AA | 2727 | U | C6-N1-C1' | -6.56 | 112.01 | 121.20 |
| 53 | Ai | 33 | ARG | NE-CZ-NH2 | -6.56 | 117.02 | 120.30 |
| 34 | AA | 1241 | G | C5-C6-O6 | -6.56 | 124.67 | 128.60 |
| 1 | A | 1900 | U | O4'-C1'-N1 | 6.55 | 113.44 | 108.20 |
| 34 | AA | 2703 | U | O4'-C1'-N1 | 6.55 | 113.44 | 108.20 |
| 34 | AA | 1689 | U | O4'-C1'-N1 | 6.55 | 113.44 | 108.20 |
| 34 | AA | 2528 | C | O4'-C1'-N1 | 6.55 | 113.44 | 108.20 |
| 34 | AA | 1049 | C | O4'-C1'-N1 | 6.55 | 113.44 | 108.20 |
| 35 | AC | 51 | C | O4'-C1'-N1 | 6.55 | 113.44 | 108.20 |
| 65 | AT | 135 | ARG | NE-CZ-NH1 | 6.55 | 123.57 | 120.30 |
| 1 | A | 908 | U | O4'-C1'-N1 | 6.55 | 113.44 | 108.20 |
| 34 | AA | 126 | C | O4'-C1'-N1 | 6.55 | 113.44 | 108.20 |
| 2 | 7 | 62 | C | O4'-C1'-N1 | 6.55 | 113.44 | 108.20 |
| 33 | C | 35 | ARG | NE-CZ-NH2 | 6.55 | 123.57 | 120.30 |
| 34 | AA | 136 | U | C6-N1-C1' | -6.54 | 112.04 | 121.20 |
| 34 | AA | 686 | U | O4'-C1'-N1 | 6.54 | 113.43 | 108.20 |
| 45 | A9 | 127 | PHE | CB-CG-CD2 | -6.54 | 116.22 | 120.80 |
| 67 | A3 | 69 | ARG | NE-CZ-NH1 | 6.54 | 123.57 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 1706 | A | O4'-C1'-N9 | 6.54 | 113.43 | 108.20 |
| 4 | E | 132 | ARG | NE-CZ-NH2 | 6.54 | 123.57 | 120.30 |
| 14 | 1 | 8 | ARG | NE-CZ-NH1 | 6.54 | 123.57 | 120.30 |
| 1 | A | 379 | G | O4'-C1'-N9 | 6.54 | 113.43 | 108.20 |
| 37 | AL | 38 | ARG | NE-CZ-NH1 | 6.53 | 123.57 | 120.30 |
| 34 | AA | 3105 | U | O4'-C1'-N1 | 6.53 | 113.42 | 108.20 |
| 36 | AB | 105 | C | O4'-C1'-N1 | 6.53 | 113.42 | 108.20 |
| 1 | A | 449 | C | O4'-C1'-N1 | 6.53 | 113.42 | 108.20 |
| 1 | A | 1791 | C | O4'-C1'-N1 | 6.53 | 113.42 | 108.20 |
| 34 | AA | 2209 | C | O4'-C1'-N1 | 6.53 | 113.42 | 108.20 |
| 34 | AA | 3399 | U | O4'-C1'-N1 | 6.53 | 113.42 | 108.20 |
| 65 | AT | 63 | ARG | NE-CZ-NH1 | 6.53 | 123.56 | 120.30 |
| 63 | AW | 69 | ARG | NE-CZ-NH2 | -6.52 | 117.04 | 120.30 |
| 18 | 5 | 26 | ARG | NE-CZ-NH1 | 6.52 | 123.56 | 120.30 |
| 34 | AA | 1961 | U | O4'-C1'-N1 | 6.52 | 113.42 | 108.20 |
| 1 | A | 1044 | C | O4'-C1'-N1 | 6.52 | 113.42 | 108.20 |
| 34 | AA | 11 | A | O4'-C1'-N9 | 6.52 | 113.42 | 108.20 |
| 34 | AA | 31 | C | C6-N1-C2 | -6.52 | 117.69 | 120.30 |
| 34 | AA | 600 | U | O4'-C1'-N1 | 6.52 | 113.42 | 108.20 |
| 34 | AA | 3653 | G | O4'-C1'-N9 | 6.52 | 113.42 | 108.20 |
| 34 | AA | 590 | C | O4'-C1'-N1 | 6.52 | 113.42 | 108.20 |
| 34 | AA | 2480 | G | C5'-C4'-O4' | 6.52 | 116.92 | 109.10 |
| 34 | AA | 833 | G | P-O5'-C5' | 6.51 | 131.32 | 120.90 |
| 34 | AA | 2685 | C | O4'-C1'-N1 | 6.51 | 113.41 | 108.20 |
| 34 | AA | 3429 | C | O4'-C1'-N1 | 6.51 | 113.41 | 108.20 |
| 70 | AE | 26 | ARG | NE-CZ-NH1 | 6.51 | 123.56 | 120.30 |
| 1 | A | 36 | C | O4'-C1'-N1 | 6.51 | 113.41 | 108.20 |
| 34 | AA | 312 | A | O4'-C1'-N9 | 6.51 | 113.41 | 108.20 |
| 34 | AA | 616 | U | O4'-C1'-N1 | 6.51 | 113.41 | 108.20 |
| 71 | AF | 109 | ARG | NE-CZ-NH2 | 6.51 | 123.56 | 120.30 |
| 71 | AF | 121 | ARG | NE-CZ-NH2 | -6.51 | 117.05 | 120.30 |
| 34 | AA | 493 | C | O4'-C1'-N1 | 6.51 | 113.41 | 108.20 |
| 35 | AC | 120 | C | O4'-C1'-N1 | 6.51 | 113.41 | 108.20 |
| 1 | A | 268 | C | O4'-C1'-N1 | 6.50 | 113.40 | 108.20 |
| 1 | A | 12 | U | O4'-C1'-N1 | 6.50 | 113.40 | 108.20 |
| 66 | AZ | 45 | ARG | NE-CZ-NH1 | 6.50 | 123.55 | 120.30 |
| 71 | AF | 110 | ARG | NE-CZ-NH1 | 6.50 | 123.55 | 120.30 |
| 1 | A | 994 | G | N1-C6-O6 | 6.50 | 123.80 | 119.90 |
| 34 | AA | 2092 | G | C5-C6-O6 | -6.50 | 124.70 | 128.60 |
| 37 | AL | 100 | ARG | NE-CZ-NH2 | 6.50 | 123.55 | 120.30 |
| 1 | A | 118 | U | O4'-C1'-N1 | 6.50 | 113.40 | 108.20 |
| 1 | A | 1018 | U | O4'-C1'-N1 | 6.50 | 113.40 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 1911 | A | O4'-C1'-N9 | 6.50 | 113.40 | 108.20 |
| 34 | AA | 1615 | G | C5-C6-O6 | -6.50 | 124.70 | 128.60 |
| 70 | AE | 117 | ARG | NE-CZ-NH2 | 6.50 | 123.55 | 120.30 |
| 35 | AC | 40 | G | N1-C6-O6 | 6.50 | 123.80 | 119.90 |
| 2 | 7 | 11 | C | O4'-C1'-N1 | 6.49 | 113.39 | 108.20 |
| 34 | AA | 3343 | C | O4'-C1'-N1 | 6.49 | 113.39 | 108.20 |
| 34 | AA | 3417 | G | C5-C6-O6 | -6.49 | 124.70 | 128.60 |
| 36 | AB | 96 | C | O4'-C1'-N1 | 6.49 | 113.39 | 108.20 |
| 1 | A | 1645 | C | C2-N1-C1' | 6.49 | 125.94 | 118.80 |
| 34 | AA | 2603 | U | O4'-C1'-N1 | 6.49 | 113.39 | 108.20 |
| 34 | AA | 3623 | A | O4'-C1'-N9 | 6.49 | 113.39 | 108.20 |
| 1 | A | 588 | U | O4'-C1'-N1 | 6.49 | 113.39 | 108.20 |
| 34 | AA | 1497 | U | P-O3'-C3' | 6.48 | 127.48 | 119.70 |
| 34 | AA | 2970 | U | O4'-C1'-N1 | 6.48 | 113.39 | 108.20 |
| 34 | AA | 3536 | C | O4'-C1'-N1 | 6.48 | 113.39 | 108.20 |
| 1 | A | 576 | C | O4'-C1'-N1 | 6.48 | 113.38 | 108.20 |
| 34 | AA | 1161 | C | C6-N1-C2 | -6.48 | 117.71 | 120.30 |
| 36 | AB | 28 | C | O4'-C1'-N1 | 6.48 | 113.38 | 108.20 |
| 34 | AA | 3587 | U | C5'-C4'-C3' | 6.48 | 126.36 | 116.00 |
| 44 | A8 | 36 | ARG | NE-CZ-NH1 | 6.48 | 123.54 | 120.30 |
| 34 | AA | 695 | A | N1-C6-N6 | -6.48 | 114.71 | 118.60 |
| 34 | AA | 1461 | C | O4'-C1'-N1 | 6.48 | 113.38 | 108.20 |
| 34 | AA | 2154 | A | C1'-O4'-C4' | -6.48 | 104.72 | 109.90 |
| 34 | AA | 3527 | U | O4'-C1'-N1 | 6.47 | 113.38 | 108.20 |
| 1 | A | 1318 | A | O4'-C1'-N9 | 6.47 | 113.38 | 108.20 |
| 13 | Z | 59 | ARG | NE-CZ-NH1 | 6.47 | 123.54 | 120.30 |
| 60 | AO | 108 | PHE | CB-CG-CD1 | 6.47 | 125.33 | 120.80 |
| 1 | A | 1709 | C | O4'-C1'-N1 | 6.47 | 113.38 | 108.20 |
| 34 | AA | 390 | C | O4'-C1'-N1 | 6.47 | 113.38 | 108.20 |
| 34 | AA | 3358 | U | O4'-C1'-N1 | 6.47 | 113.38 | 108.20 |
| 35 | AC | 126 | C | O4'-C1'-N1 | 6.47 | 113.38 | 108.20 |
| 1 | A | 1166 | C | O4'-C1'-N1 | 6.47 | 113.37 | 108.20 |
| 34 | AA | 2525 | A | O4'-C1'-N9 | 6.47 | 113.37 | 108.20 |
| 34 | AA | 3696 | U | O4'-C1'-N1 | 6.47 | 113.37 | 108.20 |
| 34 | AA | 113 | C | O4'-C1'-N1 | 6.46 | 113.37 | 108.20 |
| 34 | AA | 2124 | C | O4'-C1'-N1 | 6.46 | 113.37 | 108.20 |
| 18 | 5 | 15 | ARG | NE-CZ-NH1 | -6.46 | 117.07 | 120.30 |
| 34 | AA | 1009 | C | O4'-C1'-N1 | 6.46 | 113.37 | 108.20 |
| 34 | AA | 3232 | U | O4'-C1'-N1 | 6.46 | 113.37 | 108.20 |
| 34 | AA | 3768 | A | P-O3'-C3' | -6.46 | 111.95 | 119.70 |
| 34 | AA | 2104 | C | C6-N1-C2 | -6.46 | 117.72 | 120.30 |
| 1 | A | 122 | C | O4'-C1'-N1 | 6.45 | 113.36 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 34 | AA | 609 | C | O4'-C1'-N1 | 6.45 | 113.36 | 108.20 |
| 34 | AA | 1618 | C | O4'-C1'-N1 | 6.45 | 113.36 | 108.20 |
| 39 | A2 | 14 | ARG | NE-CZ-NH2 | -6.45 | 117.08 | 120.30 |
| 46 | Aa | 9 | ARG | NE-CZ-NH1 | 6.45 | 123.53 | 120.30 |
| 34 | AA | 599 | G | O4'-C1'-N9 | 6.45 | 113.36 | 108.20 |
| 34 | AA | 859 | C | O4'-C1'-N1 | 6.45 | 113.36 | 108.20 |
| 70 | AE | 331 | ARG | NE-CZ-NH2 | -6.45 | 117.08 | 120.30 |
| 34 | AA | 587 | C | O4'-C1'-N1 | 6.45 | 113.36 | 108.20 |
| 34 | AA | 3148 | U | O4'-C1'-N1 | 6.45 | 113.36 | 108.20 |
| 34 | AA | 3474 | C | C6-N1-C2 | -6.45 | 117.72 | 120.30 |
| 20 | B | 64 | ARG | NE-CZ-NH1 | 6.44 | 123.52 | 120.30 |
| 24 | L | 8 | ARG | NE-CZ-NH1 | 6.44 | 123.52 | 120.30 |
| 34 | AA | 588 | C | O4'-C1'-N1 | 6.44 | 113.35 | 108.20 |
| 34 | AA | 3055 | U | O4'-C1'-N1 | 6.44 | 113.35 | 108.20 |
| 1 | A | 573 | C | O4'-C1'-N1 | 6.44 | 113.35 | 108.20 |
| 1 | A | 1797 | C | O4'-C1'-N1 | 6.44 | 113.35 | 108.20 |
| 1 | A | 1863 | U | C5'-C4'-O4' | 6.44 | 116.83 | 109.10 |
| 33 | C | 101 | ARG | NE-CZ-NH2 | 6.44 | 123.52 | 120.30 |
| 34 | AA | 3067 | G | O4'-C1'-N9 | 6.44 | 113.35 | 108.20 |
| 34 | AA | 1996 | C | O4'-C1'-N1 | 6.44 | 113.35 | 108.20 |
| 34 | AA | 2411 | C | O4'-C1'-N1 | 6.44 | 113.35 | 108.20 |
| 34 | AA | 2556 | C | C5'-C4'-O4' | 6.44 | 116.83 | 109.10 |
| 1 | A | 1415 | A | O4'-C1'-N9 | 6.44 | 113.35 | 108.20 |
| 34 | AA | 3657 | G | O4'-C1'-N9 | 6.43 | 113.35 | 108.20 |
| 1 | A | 257 | C | O4'-C1'-N1 | 6.43 | 113.35 | 108.20 |
| 1 | A | 1713 | C | O4'-C1'-N1 | 6.43 | 113.35 | 108.20 |
| 2 | 7 | 23 | G | O4'-C1'-N9 | 6.43 | 113.35 | 108.20 |
| 34 | AA | 1466 | C | O4'-C1'-N1 | 6.43 | 113.35 | 108.20 |
| 25 | N | 79 | PHE | CB-CG-CD2 | -6.43 | 116.30 | 120.80 |
| 34 | AA | 3631 | U | O4'-C1'-N1 | 6.43 | 113.34 | 108.20 |
| 34 | AA | 271 | G | O4'-C1'-N9 | 6.43 | 113.34 | 108.20 |
| 34 | AA | 1154 | C | C2-N1-C1' | 6.43 | 125.87 | 118.80 |
| 34 | AA | 1257 | A | O4'-C1'-N9 | 6.43 | 113.34 | 108.20 |
| 34 | AA | 2080 | C | O4'-C1'-N1 | 6.43 | 113.34 | 108.20 |
| 34 | AA | 2168 | A | N1-C6-N6 | -6.43 | 114.74 | 118.60 |
| 34 | AA | 2668 | G | O4'-C1'-N9 | 6.43 | 113.34 | 108.20 |
| 1 | A | 925 | C | O4'-C1'-N1 | 6.42 | 113.34 | 108.20 |
| 1 | A | 1090 | C | O4'-C1'-N1 | 6.42 | 113.34 | 108.20 |
| 34 | AA | 635 | U | O4'-C1'-N1 | 6.42 | 113.34 | 108.20 |
| 34 | AA | 3405 | U | O4'-C1'-N1 | 6.42 | 113.34 | 108.20 |
| 28 | S | 57 | ARG | NE-CZ-NH1 | 6.42 | 123.51 | 120.30 |
| 34 | AA | 159 | C | O4'-C1'-N1 | 6.42 | 113.34 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 34 | AA | 2162 | U | O4'-C1'-N1 | 6.42 | 113.34 | 108.20 |
| 1 | A | 1263 | C | O4'-C1'-N1 | 6.42 | 113.33 | 108.20 |
| 4 | E | 108 | ARG | NE-CZ-NH1 | 6.42 | 123.51 | 120.30 |
| 34 | AA | 865 | G | O4'-C1'-N9 | 6.42 | 113.33 | 108.20 |
| 1 | A | 1423 | A | C1'-O4'-C4' | -6.42 | 104.77 | 109.90 |
| 35 | AC | 6 | C | O4'-C1'-N1 | 6.42 | 113.33 | 108.20 |
| 1 | A | 183 | C | O4'-C1'-N1 | 6.41 | 113.33 | 108.20 |
| 30 | U | 114 | ARG | NE-CZ-NH1 | 6.41 | 123.50 | 120.30 |
| 34 | AA | 1428 | G | C5-C6-O6 | -6.41 | 124.75 | 128.60 |
| 34 | AA | 2422 | C | O4'-C1'-N1 | 6.41 | 113.33 | 108.20 |
| 34 | AA | 3550 | U | O4'-C1'-N1 | 6.41 | 113.33 | 108.20 |
| 34 | AA | 3679 | A | P-O3'-C3' | 6.41 | 127.39 | 119.70 |
| 34 | AA | 3192 | U | O4'-C1'-N1 | 6.41 | 113.33 | 108.20 |
| 1 | A | 915 | G | C5-C6-O6 | -6.41 | 124.76 | 128.60 |
| 34 | AA | 2945 | G | O4'-C1'-N9 | 6.41 | 113.33 | 108.20 |
| 34 | AA | 3382 | U | O4'-C1'-N1 | 6.41 | 113.33 | 108.20 |
| 34 | AA | 769 | U | C2-N1-C1' | 6.41 | 125.39 | 117.70 |
| 1 | A | 185 | U | O4'-C1'-N1 | 6.40 | 113.32 | 108.20 |
| 1 | A | 758 | U | O4'-C1'-N1 | 6.40 | 113.32 | 108.20 |
| 34 | AA | 1467 | C | O4'-C1'-N1 | 6.40 | 113.32 | 108.20 |
| 74 | AH | 172 | ARG | NE-CZ-NH1 | 6.40 | 123.50 | 120.30 |
| 1 | A | 1946 | C | O4'-C1'-N1 | 6.40 | 113.32 | 108.20 |
| 34 | AA | 901 | U | O4'-C1'-N1 | 6.40 | 113.32 | 108.20 |
| 1 | A | 2018 | C | O4'-C1'-N1 | 6.40 | 113.32 | 108.20 |
| 34 | AA | 1160 | C | O4'-C1'-N1 | 6.40 | 113.32 | 108.20 |
| 73 | AU | 35 | ARG | NE-CZ-NH2 | 6.40 | 123.50 | 120.30 |
| 1 | A | 448 | C | O4'-C1'-N1 | 6.39 | 113.31 | 108.20 |
| 34 | AA | 1285 | U | O4'-C1'-N1 | 6.39 | 113.31 | 108.20 |
| 34 | AA | 3244 | C | O4'-C1'-N1 | 6.39 | 113.32 | 108.20 |
| 34 | AA | 2485 | C | O4'-C1'-N1 | 6.39 | 113.31 | 108.20 |
| 42 | A7 | 45 | ARG | NE-CZ-NH1 | 6.39 | 123.50 | 120.30 |
| 60 | AO | 21 | ARG | NE-CZ-NH2 | 6.39 | 123.50 | 120.30 |
| 34 | AA | 2033 | C | O4'-C1'-N1 | 6.39 | 113.31 | 108.20 |
| 1 | A | 996 | C | O4'-C1'-N1 | 6.39 | 113.31 | 108.20 |
| 34 | AA | 806 | G | O4'-C1'-N9 | 6.39 | 113.31 | 108.20 |
| 1 | A | 917 | C | O4'-C1'-N1 | 6.38 | 113.31 | 108.20 |
| 7 | K | 20 | ARG | NE-CZ-NH1 | 6.38 | 123.49 | 120.30 |
| 34 | AA | 775 | C | O4'-C1'-N1 | 6.38 | 113.31 | 108.20 |
| 34 | AA | 3284 | C | O4'-C1'-N1 | 6.38 | 113.31 | 108.20 |
| 1 | A | 130 | U | O4'-C1'-N1 | 6.38 | 113.31 | 108.20 |
| 1 | A | 981 | U | O4'-C1'-N1 | 6.38 | 113.31 | 108.20 |
| 34 | AA | 3333 | U | O4'-C1'-N1 | 6.38 | 113.31 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 61 | AQ | 32 | ARG | NE-CZ-NH2 | 6.38 | 123.49 | 120.30 |
| 1 | A | 630 | C | C6-N1-C1' | -6.38 | 113.14 | 120.80 |
| 34 | AA | 1172 | C | O4'-C1'-N1 | 6.38 | 113.31 | 108.20 |
| 34 | AA | 1861 | C | O4'-C1'-N1 | 6.38 | 113.31 | 108.20 |
| 34 | AA | 3211 | C | O4'-C1'-N1 | 6.38 | 113.31 | 108.20 |
| 57 | AK | 48 | ARG | NE-CZ-NH1 | 6.38 | 123.49 | 120.30 |
| 61 | AQ | 189 | ARG | NE-CZ-NH1 | 6.38 | 123.49 | 120.30 |
| 1 | A | 1710 | G | C5-C6-O6 | -6.38 | 124.77 | 128.60 |
| 34 | AA | 673 | U | C1'-O4'-C4' | -6.38 | 104.80 | 109.90 |
| 35 | AC | 38 | G | C4'-C3'-C2' | -6.38 | 96.22 | 102.60 |
| 1 | A | 972 | U | P-O5'-C5' | -6.38 | 110.69 | 120.90 |
| 1 | A | 1949 | C | O4'-C1'-N1 | 6.38 | 113.30 | 108.20 |
| 34 | AA | 3647 | C | O4'-C1'-N1 | 6.38 | 113.30 | 108.20 |
| 69 | AD | 200 | ARG | NE-CZ-NH1 | -6.38 | 117.11 | 120.30 |
| 3 | D | 154 | ARG | NE-CZ-NH2 | 6.37 | 123.49 | 120.30 |
| 34 | AA | 1627 | C | O4'-C1'-N1 | 6.37 | 113.30 | 108.20 |
| 34 | AA | 1873 | U | C2'-C3'-O3' | 6.37 | 123.89 | 113.70 |
| 1 | A | 1794 | C | O4'-C1'-N1 | 6.37 | 113.30 | 108.20 |
| 71 | AF | 143 | ARG | NE-CZ-NH1 | 6.37 | 123.48 | 120.30 |
| 78 | A0 | 31 | ARG | NE-CZ-NH1 | 6.37 | 123.48 | 120.30 |
| 34 | AA | 1561 | C | O4'-C1'-N1 | 6.37 | 113.29 | 108.20 |
| 34 | AA | 1662 | G | O4'-C1'-N9 | 6.37 | 113.29 | 108.20 |
| 34 | AA | 3706 | U | O4'-C1'-N1 | 6.37 | 113.29 | 108.20 |
| 68 | A5 | 79 | ARG | NE-CZ-NH1 | 6.36 | 123.48 | 120.30 |
| 1 | A | 1814 | C | O4'-C1'-N1 | 6.36 | 113.29 | 108.20 |
| 35 | AC | 59 | U | O4'-C1'-N1 | 6.36 | 113.29 | 108.20 |
| 23 | J | 123 | TYR | CB-CG-CD2 | -6.36 | 117.19 | 121.00 |
| 18 | 5 | 38 | ARG | NE-CZ-NH1 | -6.36 | 117.12 | 120.30 |
| 34 | AA | 2428 | U | O4'-C1'-N1 | 6.36 | 113.29 | 108.20 |
| 71 | AF | 140 | ARG | NE-CZ-NH2 | -6.36 | 117.12 | 120.30 |
| 34 | AA | 696 | C | O4'-C1'-N1 | 6.35 | 113.28 | 108.20 |
| 34 | AA | 1031 | G | N1-C2-N2 | -6.35 | 110.48 | 116.20 |
| 1 | A | 1178 | C | O4'-C1'-N1 | 6.35 | 113.28 | 108.20 |
| 1 | A | 1187 | A | P-O3'-C3' | 6.35 | 127.32 | 119.70 |
| 34 | AA | 1706 | A | O4'-C1'-N9 | 6.35 | 113.28 | 108.20 |
| 36 | AB | 26 | C | O4'-C1'-N1 | 6.35 | 113.28 | 108.20 |
| 34 | AA | 3531 | C | O4'-C1'-N1 | 6.34 | 113.28 | 108.20 |
| 36 | AB | 117 | C | O4'-C1'-N1 | 6.34 | 113.28 | 108.20 |
| 1 | A | 582 | C | O4'-C1'-N1 | 6.34 | 113.27 | 108.20 |
| 1 | A | 1031 | C | O4'-C1'-N1 | 6.34 | 113.27 | 108.20 |
| 1 | A | 1098 | U | P-O3'-C3' | 6.34 | 127.31 | 119.70 |
| 34 | AA | 2013 | U | O4'-C1'-N1 | 6.34 | 113.27 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 34 | AA | 2185 | C | O4'-C1'-N1 | 6.34 | 113.27 | 108.20 |
| 1 | A | 996 | C | C6-N1-C2 | -6.34 | 117.76 | 120.30 |
| 34 | AA | 1724 | G | O4'-C1'-N9 | 6.34 | 113.27 | 108.20 |
| 57 | AK | 132 | ARG | NE-CZ-NH1 | 6.34 | 123.47 | 120.30 |
| 34 | AA | 1720 | C | C6-N1-C2 | -6.34 | 117.77 | 120.30 |
| 46 | Aa | 64 | ARG | NE-CZ-NH1 | 6.34 | 123.47 | 120.30 |
| 1 | A | 1059 | U | O4'-C1'-N1 | 6.33 | 113.27 | 108.20 |
| 12 | Y | 85 | ARG | NE-CZ-NH1 | 6.33 | 123.47 | 120.30 |
| 35 | AC | 147 | U | O4'-C1'-N1 | 6.33 | 113.27 | 108.20 |
| 1 | A | 1278 | C | O4'-C1'-N1 | 6.33 | 113.27 | 108.20 |
| 34 | AA | 3615 | A | P-O3'-C3' | -6.33 | 112.10 | 119.70 |
| 34 | AA | 2202 | G | O4'-C1'-N9 | 6.33 | 113.26 | 108.20 |
| 34 | AA | 1529 | G | O4'-C1'-N9 | 6.33 | 113.26 | 108.20 |
| 34 | AA | 3705 | C | O4'-C1'-N1 | 6.33 | 113.26 | 108.20 |
| 35 | AC | 133 | G | O4'-C1'-N9 | 6.33 | 113.26 | 108.20 |
| 71 | AF | 375 | TYR | CB-CG-CD2 | -6.33 | 117.20 | 121.00 |
| 1 | A | 1841 | U | O4'-C1'-N1 | 6.32 | 113.26 | 108.20 |
| 2 | 7 | 30 | G | O4'-C1'-N9 | 6.32 | 113.26 | 108.20 |
| 34 | AA | 2188 | U | O4'-C1'-N1 | 6.32 | 113.26 | 108.20 |
| 34 | AA | 2601 | C | O4'-C1'-N1 | 6.32 | 113.26 | 108.20 |
| 34 | AA | 3030 | A | O4'-C1'-N9 | 6.32 | 113.26 | 108.20 |
| 35 | AC | 48 | C | O4'-C1'-N1 | 6.32 | 113.26 | 108.20 |
| 34 | AA | 1247 | C | O4'-C1'-N1 | 6.32 | 113.26 | 108.20 |
| 34 | AA | 2502 | U | O4'-C1'-N1 | 6.32 | 113.26 | 108.20 |
| 1 | A | 1222 | C | O4'-C1'-N1 | 6.32 | 113.26 | 108.20 |
| 1 | A | 1823 | U | O4'-C1'-N1 | 6.32 | 113.26 | 108.20 |
| 16 | 3 | 51 | ARG | NE-CZ-NH2 | 6.32 | 123.46 | 120.30 |
| 34 | AA | 721 | U | O4'-C1'-N1 | 6.32 | 113.25 | 108.20 |
| 4 | E | 23 | ARG | NE-CZ-NH1 | 6.31 | 123.46 | 120.30 |
| 1 | A | 920 | A | O4'-C1'-N9 | 6.31 | 113.25 | 108.20 |
| 34 | AA | 768 | C | C2-N1-C1' | 6.31 | 125.74 | 118.80 |
| 34 | AA | 2538 | C | O4'-C1'-N1 | 6.31 | 113.25 | 108.20 |
| 22 | H | 94 | ARG | NE-CZ-NH1 | 6.31 | 123.45 | 120.30 |
| 34 | AA | 382 | A | N1-C6-N6 | -6.31 | 114.81 | 118.60 |
| 34 | AA | 328 | G | C5-C6-O6 | -6.31 | 124.81 | 128.60 |
| 48 | Ad | 44 | ARG | NE-CZ-NH2 | 6.31 | 123.45 | 120.30 |
| 61 | AQ | 90 | ARG | NE-CZ-NH1 | 6.31 | 123.45 | 120.30 |
| 1 | A | 43 | A | N1-C6-N6 | 6.30 | 122.38 | 118.60 |
| 34 | AA | 859 | C | P-O5'-C5' | 6.30 | 130.99 | 120.90 |
| 34 | AA | 1136 | A | N1-C6-N6 | 6.30 | 122.38 | 118.60 |
| 36 | AB | 34 | C | O4'-C1'-N1 | 6.30 | 113.24 | 108.20 |
| 1 | A | 157 | G | O4'-C1'-N9 | 6.30 | 113.24 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 60 | AO | 21 | ARG | NE-CZ-NH1 | -6.30 | 117.15 | 120.30 |
| 1 | A | 2072 | G | C5-C6-O6 | -6.30 | 124.82 | 128.60 |
| 34 | AA | 1030 | C | O4'-C1'-N1 | 6.30 | 113.24 | 108.20 |
| 34 | AA | 1678 | C | O4'-C1'-N1 | 6.29 | 113.23 | 108.20 |
| 34 | AA | 3329 | C | O4'-C1'-N1 | 6.29 | 113.23 | 108.20 |
| 1 | A | 1228 | C | O4'-C1'-N1 | 6.29 | 113.23 | 108.20 |
| 34 | AA | 83 | U | C5'-C4'-O4' | 6.29 | 116.65 | 109.10 |
| 34 | AA | 2090 | U | O4'-C1'-N1 | 6.29 | 113.23 | 108.20 |
| 1 | A | 18 | C | O4'-C1'-N1 | 6.29 | 113.23 | 108.20 |
| 1 | A | 915 | G | N1-C6-O6 | 6.29 | 123.67 | 119.90 |
| 35 | AC | 124 | U | O4'-C1'-N1 | 6.29 | 113.23 | 108.20 |
| 34 | AA | 3431 | G | O4'-C1'-N9 | 6.29 | 113.23 | 108.20 |
| 1 | A | 982 | A | O4'-C1'-N9 | 6.28 | 113.23 | 108.20 |
| 34 | AA | 764 | G | O4'-C1'-N9 | 6.28 | 113.23 | 108.20 |
| 34 | AA | 3390 | U | O4'-C1'-N1 | 6.28 | 113.23 | 108.20 |
| 1 | A | 409 | A | N1-C6-N6 | 6.28 | 122.37 | 118.60 |
| 1 | A | 1870 | A | P-O3'-C3' | 6.28 | 127.24 | 119.70 |
| 34 | AA | 3180 | C | O4'-C1'-N1 | 6.28 | 113.23 | 108.20 |
| 34 | AA | 1179 | U | O4'-C1'-N1 | 6.28 | 113.22 | 108.20 |
| 34 | AA | 3125 | U | O4'-C1'-N1 | 6.28 | 113.22 | 108.20 |
| 34 | AA | 2618 | G | C5'-C4'-O4' | 6.28 | 116.63 | 109.10 |
| 35 | AC | 30 | U | O4'-C1'-N1 | 6.28 | 113.22 | 108.20 |
| 1 | A | 1212 | C | O4'-C1'-N1 | 6.27 | 113.22 | 108.20 |
| 28 | S | 89 | ARG | NE-CZ-NH1 | -6.27 | 117.16 | 120.30 |
| 34 | AA | 1480 | G | C8-N9-C1' | -6.27 | 118.85 | 127.00 |
| 34 | AA | 2002 | G | O4'-C1'-N9 | 6.27 | 113.22 | 108.20 |
| 34 | AA | 3580 | G | O4'-C1'-N9 | 6.27 | 113.22 | 108.20 |
| 71 | AF | 48 | ARG | NE-CZ-NH2 | 6.27 | 123.44 | 120.30 |
| 34 | AA | 3024 | U | O4'-C1'-N1 | 6.27 | 113.22 | 108.20 |
| 1 | A | 273 | A | O4'-C1'-N9 | 6.27 | 113.22 | 108.20 |
| 1 | A | 1649 | C | O4'-C1'-N1 | 6.27 | 113.21 | 108.20 |
| 34 | AA | 1997 | G | O4'-C1'-N9 | 6.27 | 113.21 | 108.20 |
| 34 | AA | 2689 | G | C5-C6-O6 | -6.26 | 124.84 | 128.60 |
| 34 | AA | 1216 | C | O4'-C1'-N1 | 6.26 | 113.21 | 108.20 |
| 1 | A | 1381 | C | C2'-C3'-O3' | 6.26 | 123.72 | 113.70 |
| 34 | AA | 2690 | A | O4'-C1'-N9 | 6.26 | 113.21 | 108.20 |
| 1 | A | 1818 | A | O4'-C1'-N9 | 6.26 | 113.21 | 108.20 |
| 34 | AA | 613 | C | O4'-C1'-N1 | 6.26 | 113.21 | 108.20 |
| 34 | AA | 764 | G | P-O3'-C3' | 6.26 | 127.21 | 119.70 |
| 34 | AA | 3598 | C | O4'-C1'-N1 | 6.26 | 113.21 | 108.20 |
| 34 | AA | 3610 | C | O4'-C1'-N1 | 6.26 | 113.20 | 108.20 |
| 36 | AB | 104 | C | O4'-C1'-N1 | 6.26 | 113.20 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 580 | C | O4'-C1'-N1 | 6.25 | 113.20 | 108.20 |
| 34 | AA | 2698 | C | O4'-C1'-N1 | 6.25 | 113.20 | 108.20 |
| 7 | K | 118 | ARG | NE-CZ-NH1 | 6.25 | 123.42 | 120.30 |
| 34 | AA | 143 | C | O4'-C1'-N1 | 6.25 | 113.20 | 108.20 |
| 34 | AA | 716 | C | C6-N1-C2 | -6.25 | 117.80 | 120.30 |
| 34 | AA | 1212 | U | O4'-C1'-N1 | 6.25 | 113.20 | 108.20 |
| 66 | AZ | 15 | ARG | NE-CZ-NH1 | 6.25 | 123.43 | 120.30 |
| 34 | AA | 2951 | U | O4'-C1'-N1 | 6.25 | 113.20 | 108.20 |
| 34 | AA | 1728 | C | O4'-C1'-N1 | 6.25 | 113.20 | 108.20 |
| 35 | AC | 118 | C | O4'-C1'-N1 | 6.25 | 113.20 | 108.20 |
| 1 | A | 1818 | A | C1'-O4'-C4' | -6.25 | 104.90 | 109.90 |
| 34 | AA | 670 | U | O4'-C1'-N1 | 6.25 | 113.20 | 108.20 |
| 34 | AA | 1126 | U | O4'-C1'-N1 | 6.25 | 113.20 | 108.20 |
| 1 | A | 147 | C | O4'-C1'-N1 | 6.24 | 113.19 | 108.20 |
| 1 | A | 411 | C | O4'-C1'-N1 | 6.24 | 113.19 | 108.20 |
| 34 | AA | 3713 | C | O4'-C1'-N1 | 6.24 | 113.19 | 108.20 |
| 1 | A | 1284 | A | P-O3'-C3' | 6.24 | 127.19 | 119.70 |
| 4 | E | 17 | ARG | NE-CZ-NH2 | 6.24 | 123.42 | 120.30 |
| 34 | AA | 1750 | U | P-O3'-C3' | 6.24 | 127.19 | 119.70 |
| 59 | AS | 163 | ARG | NE-CZ-NH2 | -6.24 | 117.18 | 120.30 |
| 16 | 3 | 92 | ARG | NE-CZ-NH2 | 6.24 | 123.42 | 120.30 |
| 18 | 5 | 15 | ARG | NE-CZ-NH2 | 6.24 | 123.42 | 120.30 |
| 34 | AA | 1057 | C | O4'-C1'-N1 | 6.24 | 113.19 | 108.20 |
| 1 | A | 516 | G | O4'-C1'-N9 | 6.24 | 113.19 | 108.20 |
| 34 | AA | 2524 | C | C2-N1-C1' | 6.23 | 125.66 | 118.80 |
| 34 | AA | 931 | U | O4'-C1'-N1 | 6.23 | 113.19 | 108.20 |
| 1 | A | 1029 | U | O4'-C1'-N1 | 6.23 | 113.18 | 108.20 |
| 1 | A | 1669 | C | O4'-C1'-N1 | 6.23 | 113.18 | 108.20 |
| 34 | AA | 912 | U | O4'-C1'-N1 | 6.23 | 113.18 | 108.20 |
| 34 | AA | 2580 | C | O4'-C1'-N1 | 6.23 | 113.19 | 108.20 |
| 34 | AA | 2887 | U | O4'-C1'-N1 | 6.23 | 113.18 | 108.20 |
| 1 | A | 919 | U | O4'-C1'-N1 | 6.23 | 113.18 | 108.20 |
| 1 | A | 1705 | C | C5'-C4'-O4' | 6.23 | 116.57 | 109.10 |
| 34 | AA | 1804 | C | O4'-C1'-N1 | 6.23 | 113.18 | 108.20 |
| 34 | AA | 1973 | G | C5-C6-O6 | -6.23 | 124.86 | 128.60 |
| 34 | AA | 1516 | G | C5-C6-O6 | -6.23 | 124.86 | 128.60 |
| 1 | A | 1956 | A | C5-C6-N6 | -6.23 | 118.72 | 123.70 |
| 1 | A | 876 | U | O4'-C1'-N1 | 6.22 | 113.18 | 108.20 |
| 1 | A | 1934 | C | O4'-C1'-N1 | 6.22 | 113.18 | 108.20 |
| 34 | AA | 312 | A | P-O3'-C3' | -6.22 | 112.23 | 119.70 |
| 34 | AA | 334 | U | O4'-C1'-N1 | 6.22 | 113.18 | 108.20 |
| 34 | AA | 884 | A | O4'-C1'-N9 | 6.22 | 113.18 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 72 | AG | 35 | ARG | NE-CZ-NH1 | -6.22 | 117.19 | 120.30 |
| 1 | A | 1455 | C | O4'-C1'-N1 | 6.22 | 113.18 | 108.20 |
| 34 | AA | 583 | U | O4'-C1'-N1 | 6.22 | 113.18 | 108.20 |
| 34 | AA | 1793 | A | O4'-C1'-N9 | 6.22 | 113.18 | 108.20 |
| 34 | AA | 1896 | C | O4'-C1'-N1 | 6.22 | 113.18 | 108.20 |
| 34 | AA | 2630 | C | O4'-C1'-N1 | 6.22 | 113.18 | 108.20 |
| 34 | AA | 200 | A | O4'-C1'-N9 | 6.22 | 113.17 | 108.20 |
| 34 | AA | 1572 | U | C6-N1-C1' | -6.22 | 112.50 | 121.20 |
| 34 | AA | 3480 | C | O4'-C1'-N1 | 6.22 | 113.17 | 108.20 |
| 1 | A | 401 | U | O4'-C1'-N1 | 6.22 | 113.17 | 108.20 |
| 34 | AA | 2041 | U | O4'-C1'-N1 | 6.21 | 113.17 | 108.20 |
| 51 | AP | 63 | ARG | NE-CZ-NH1 | 6.21 | 123.41 | 120.30 |
| 34 | AA | 354 | C | O4'-C1'-N1 | 6.21 | 113.17 | 108.20 |
| 1 | A | 1418 | C | O4'-C1'-N1 | 6.21 | 113.17 | 108.20 |
| 34 | AA | 2590 | U | C6-N1-C1' | -6.21 | 112.51 | 121.20 |
| 34 | AA | 3730 | C | O4'-C1'-N1 | 6.21 | 113.17 | 108.20 |
| 34 | AA | 2541 | C | O4'-C1'-N1 | 6.21 | 113.17 | 108.20 |
| 34 | AA | 3230 | G | O4'-C1'-N9 | 6.21 | 113.17 | 108.20 |
| 36 | AB | 59 | C | O4'-C1'-N1 | 6.21 | 113.17 | 108.20 |
| 1 | A | 455 | C | O4'-C1'-N1 | 6.21 | 113.16 | 108.20 |
| 1 | A | 2076 | C | O4'-C1'-N1 | 6.21 | 113.17 | 108.20 |
| 1 | A | 341 | U | O4'-C1'-N1 | 6.20 | 113.16 | 108.20 |
| 1 | A | 578 | G | O4'-C1'-N9 | 6.20 | 113.16 | 108.20 |
| 24 | L | 25 | ARG | NE-CZ-NH1 | 6.20 | 123.40 | 120.30 |
| 34 | AA | 942 | C | O4'-C1'-N1 | 6.20 | 113.16 | 108.20 |
| 1 | A | 466 | A | N1-C6-N6 | -6.20 | 114.88 | 118.60 |
| 1 | A | 1293 | C | O4'-C1'-N1 | 6.20 | 113.16 | 108.20 |
| 1 | A | 2029 | A | C5'-C4'-C3' | 6.20 | 125.92 | 116.00 |
| 34 | AA | 367 | U | O4'-C1'-N1 | 6.20 | 113.16 | 108.20 |
| 34 | AA | 2174 | G | C5-C6-O6 | -6.20 | 124.88 | 128.60 |
| 34 | AA | 3130 | U | P-O3'-C3' | 6.20 | 127.14 | 119.70 |
| 34 | AA | 3221 | U | O4'-C1'-N1 | 6.20 | 113.16 | 108.20 |
| 1 | A | 1180 | U | O4'-C1'-N1 | 6.20 | 113.16 | 108.20 |
| 1 | A | 1714 | U | O4'-C1'-N1 | 6.20 | 113.16 | 108.20 |
| 34 | AA | 199 | G | C5-C6-O6 | -6.20 | 124.88 | 128.60 |
| 34 | AA | 3258 | C | C6-N1-C1' | -6.20 | 113.36 | 120.80 |
| 44 | A8 | 33 | ARG | NE-CZ-NH2 | -6.20 | 117.20 | 120.30 |
| 1 | A | 949 | C | O4'-C1'-N1 | 6.19 | 113.16 | 108.20 |
| 34 | AA | 2557 | U | O4'-C1'-N1 | 6.19 | 113.15 | 108.20 |
| 34 | AA | 3756 | C | O4'-C1'-N1 | 6.19 | 113.15 | 108.20 |
| 34 | AA | 1035 | G | N1-C6-O6 | 6.19 | 123.61 | 119.90 |
| 34 | AA | 953 | U | O4'-C1'-N1 | 6.19 | 113.15 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 34 | AA | 59 | G | C5-C6-O6 | -6.19 | 124.89 | 128.60 |
| 34 | AA | 1969 | A | O4'-C1'-N9 | 6.19 | 113.15 | 108.20 |
| 34 | AA | 2459 | C | O4'-C1'-N1 | 6.19 | 113.15 | 108.20 |
| 34 | AA | 3501 | C | O4'-C1'-N1 | 6.19 | 113.15 | 108.20 |
| 21 | F | 214 | ARG | NE-CZ-NH1 | 6.19 | 123.39 | 120.30 |
| 1 | A | 881 | C | C5'-C4'-O4' | 6.18 | 116.52 | 109.10 |
| 34 | AA | 447 | A | N1-C6-N6 | 6.18 | 122.31 | 118.60 |
| 34 | AA | 1454 | A | O4'-C1'-N9 | 6.18 | 113.15 | 108.20 |
| 34 | AA | 1704 | U | P-O3'-C3' | -6.18 | 112.28 | 119.70 |
| 34 | AA | 3003 | C | O4'-C1'-N1 | 6.18 | 113.15 | 108.20 |
| 34 | AA | 3242 | U | O4'-C1'-N1 | 6.18 | 113.15 | 108.20 |
| 1 | A | 787 | G | O4'-C1'-N9 | 6.18 | 113.15 | 108.20 |
| 34 | AA | 388 | C | O4'-C1'-N1 | 6.18 | 113.14 | 108.20 |
| 34 | AA | 3409 | U | O4'-C1'-N1 | 6.18 | 113.15 | 108.20 |
| 1 | A | 1830 | C | O4'-C1'-N1 | 6.18 | 113.14 | 108.20 |
| 1 | A | 2044 | G | O3'-P-O5' | -6.18 | 92.26 | 104.00 |
| 34 | AA | 3058 | C | O4'-C1'-N1 | 6.18 | 113.14 | 108.20 |
| 34 | AA | 361 | G | C5-C6-O6 | -6.18 | 124.89 | 128.60 |
| 34 | AA | 3518 | C | O4'-C1'-N1 | 6.18 | 113.14 | 108.20 |
| 1 | A | 1671 | A | C5'-C4'-C3' | -6.18 | 106.12 | 116.00 |
| 34 | AA | 1216 | C | C6-N1-C2 | -6.18 | 117.83 | 120.30 |
| 34 | AA | 3290 | C | O4'-C1'-N1 | 6.18 | 113.14 | 108.20 |
| 34 | AA | 3458 | A | P-O3'-C3' | 6.18 | 127.11 | 119.70 |
| 54 | AI | 71 | ARG | NE-CZ-NH1 | 6.18 | 123.39 | 120.30 |
| 1 | A | 45 | U | O4'-C1'-N1 | 6.17 | 113.14 | 108.20 |
| 1 | A | 1275 | U | O4'-C1'-N1 | 6.17 | 113.14 | 108.20 |
| 34 | AA | 891 | C | O4'-C1'-N1 | 6.17 | 113.14 | 108.20 |
| 34 | AA | 2508 | C | O4'-C1'-N1 | 6.17 | 113.14 | 108.20 |
| 34 | AA | 2631 | C | O4'-C1'-N1 | 6.17 | 113.14 | 108.20 |
| 36 | AB | 91 | C | O4'-C1'-N1 | 6.17 | 113.14 | 108.20 |
| 1 | A | 1651 | C | O4'-C1'-N1 | 6.17 | 113.14 | 108.20 |
| 34 | AA | 861 | C | O4'-C1'-N1 | 6.17 | 113.14 | 108.20 |
| 1 | A | 1074 | A | O4'-C1'-N9 | 6.17 | 113.14 | 108.20 |
| 3 | D | 76 | ARG | NE-CZ-NH2 | -6.17 | 117.22 | 120.30 |
| 1 | A | 1321 | C | C5'-C4'-C3' | -6.17 | 106.13 | 116.00 |
| 34 | AA | 2949 | G | O4'-C1'-N9 | 6.17 | 113.14 | 108.20 |
| 36 | AB | 45 | U | O4'-C1'-N1 | 6.17 | 113.14 | 108.20 |
| 34 | AA | 603 | G | O4'-C1'-N9 | 6.17 | 113.13 | 108.20 |
| 34 | AA | 1763 | G | N1-C6-O6 | 6.17 | 123.60 | 119.90 |
| 34 | AA | 1799 | A | O4'-C1'-N9 | 6.17 | 113.13 | 108.20 |
| 34 | AA | 2478 | G | O4'-C1'-N9 | 6.17 | 113.13 | 108.20 |
| 34 | AA | 3323 | G | N1-C6-O6 | 6.17 | 123.60 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | B | 213 | ARG | NE-CZ-NH1 | 6.16 | 123.38 | 120.30 |
| 34 | AA | 147 | C | C6-N1-C2 | -6.16 | 117.83 | 120.30 |
| 34 | AA | 753 | C | O4'-C1'-N1 | 6.16 | 113.13 | 108.20 |
| 34 | AA | 65 | A | P-O3'-C3' | 6.16 | 127.09 | 119.70 |
| 34 | AA | 2197 | G | C5-C6-O6 | -6.16 | 124.90 | 128.60 |
| 1 | A | 1793 | C | O4'-C1'-N1 | 6.16 | 113.13 | 108.20 |
| 34 | AA | 2394 | C | O4'-C1'-N1 | 6.16 | 113.13 | 108.20 |
| 61 | AQ | 157 | TYR | CB-CG-CD2 | -6.16 | 117.30 | 121.00 |
| 67 | A3 | 80 | TYR | CB-CG-CD1 | -6.16 | 117.30 | 121.00 |
| 1 | A | 9 | U | O4'-C1'-N1 | 6.16 | 113.13 | 108.20 |
| 34 | AA | 1438 | G | O4'-C1'-N9 | 6.16 | 113.13 | 108.20 |
| 63 | AW | 30 | TYR | CB-CG-CD2 | -6.16 | 117.31 | 121.00 |
| 2 | 7 | 51 | U | C5'-C4'-C3' | 6.16 | 125.85 | 116.00 |
| 62 | AR | 206 | TYR | CB-CG-CD1 | 6.16 | 124.69 | 121.00 |
| 34 | AA | 2671 | C | O4'-C1'-N1 | 6.15 | 113.12 | 108.20 |
| 28 | S | 123 | ARG | NE-CZ-NH2 | 6.15 | 123.38 | 120.30 |
| 34 | AA | 1544 | C | O4'-C1'-N1 | 6.15 | 113.12 | 108.20 |
| 34 | AA | 1730 | A | P-O3'-C3' | -6.15 | 112.32 | 119.70 |
| 1 | A | 1429 | C | O4'-C1'-N1 | 6.15 | 113.12 | 108.20 |
| 34 | AA | 3631 | U | O3'-P-O5' | -6.15 | 92.31 | 104.00 |
| 34 | AA | 3771 | C | O4'-C1'-N1 | 6.15 | 113.12 | 108.20 |
| 1 | A | 1220 | C | O4'-C1'-N1 | 6.15 | 113.12 | 108.20 |
| 1 | A | 105 | A | P-O3'-C3' | 6.15 | 127.08 | 119.70 |
| 1 | A | 493 | G | O4'-C1'-N9 | 6.15 | 113.12 | 108.20 |
| 34 | AA | 129 | C | O4'-C1'-N1 | 6.15 | 113.12 | 108.20 |
| 34 | AA | 952 | U | O4'-C1'-N1 | 6.15 | 113.12 | 108.20 |
| 54 | AI | 44 | TYR | CB-CG-CD1 | -6.15 | 117.31 | 121.00 |
| 69 | AD | 3 | ARG | NE-CZ-NH1 | 6.15 | 123.37 | 120.30 |
| 1 | A | 1609 | C | O4'-C1'-N1 | 6.15 | 113.12 | 108.20 |
| 1 | A | 989 | C | O4'-C1'-N1 | 6.14 | 113.12 | 108.20 |
| 1 | A | 1625 | C | O4'-C1'-N1 | 6.14 | 113.12 | 108.20 |
| 65 | AT | 80 | ARG | NE-CZ-NH1 | 6.14 | 123.37 | 120.30 |
| 1 | A | 1249 | C | O4'-C1'-N1 | 6.14 | 113.11 | 108.20 |
| 34 | AA | 691 | C | O4'-C1'-N1 | 6.14 | 113.11 | 108.20 |
| 34 | AA | 911 | U | O4'-C1'-N1 | 6.14 | 113.11 | 108.20 |
| 34 | AA | 923 | C | O4'-C1'-N1 | 6.14 | 113.11 | 108.20 |
| 70 | AE | 229 | ARG | NE-CZ-NH1 | 6.14 | 123.37 | 120.30 |
| 34 | AA | 2550 | C | O4'-C1'-N1 | 6.14 | 113.11 | 108.20 |
| 1 | A | 328 | G | C5-C6-O6 | -6.14 | 124.92 | 128.60 |
| 1 | A | 891 | U | O4'-C1'-N1 | 6.14 | 113.11 | 108.20 |
| 1 | A | 929 | U | O4'-C1'-N1 | 6.14 | 113.11 | 108.20 |
| 1 | A | 1670 | A | O4'-C1'-N9 | 6.14 | 113.11 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 7 | K | 117 | ARG | NE-CZ-NH1 | 6.14 | 123.37 | 120.30 |
| 34 | AA | 1826 | U | O4'-C1'-N1 | 6.14 | 113.11 | 108.20 |
| 1 | A | 184 | C | O4'-C1'-N1 | 6.13 | 113.11 | 108.20 |
| 34 | AA | 2578 | C | O4'-C1'-N1 | 6.13 | 113.11 | 108.20 |
| 34 | AA | 3053 | G | C5'-C4'-O4' | 6.13 | 116.46 | 109.10 |
| 51 | AP | 30 | TYR | CB-CG-CD2 | -6.13 | 117.32 | 121.00 |
| 34 | AA | 81 | C | O4'-C1'-N1 | 6.13 | 113.11 | 108.20 |
| 34 | AA | 412 | A | O4'-C1'-N9 | 6.13 | 113.11 | 108.20 |
| 34 | AA | 1834 | C | O4'-C1'-N1 | 6.13 | 113.11 | 108.20 |
| 1 | A | 856 | U | O4'-C1'-N1 | 6.13 | 113.10 | 108.20 |
| 1 | A | 2031 | C | O4'-C1'-N1 | 6.13 | 113.10 | 108.20 |
| 1 | A | 525 | G | O4'-C1'-N9 | 6.13 | 113.10 | 108.20 |
| 34 | AA | 547 | C | O4'-C1'-N1 | 6.13 | 113.10 | 108.20 |
| 34 | AA | 1251 | U | O4'-C1'-N1 | 6.13 | 113.10 | 108.20 |
| 23 | J | 7 | ARG | NE-CZ-NH1 | 6.12 | 123.36 | 120.30 |
| 34 | AA | 1452 | U | P-O3'-C3' | 6.12 | 127.05 | 119.70 |
| 34 | AA | 3581 | A | O4'-C1'-N9 | 6.12 | 113.10 | 108.20 |
| 1 | A | 382 | C | O4'-C1'-N1 | 6.12 | 113.10 | 108.20 |
| 34 | AA | 1865 | C | O4'-C1'-N1 | 6.12 | 113.10 | 108.20 |
| 34 | AA | 3201 | C | O4'-C1'-N1 | 6.12 | 113.10 | 108.20 |
| 35 | AC | 62 | G | C5-C6-O6 | -6.12 | 124.93 | 128.60 |
| 34 | AA | 3134 | U | O4'-C1'-N1 | 6.12 | 113.09 | 108.20 |
| 1 | A | 1697 | C | O4'-C1'-N1 | 6.12 | 113.09 | 108.20 |
| 61 | AQ | 38 | ARG | NE-CZ-NH1 | 6.12 | 123.36 | 120.30 |
| 34 | AA | 1703 | U | O4'-C1'-N1 | 6.12 | 113.09 | 108.20 |
| 34 | AA | 3500 | G | O4'-C1'-N9 | 6.12 | 113.09 | 108.20 |
| 34 | AA | 3737 | G | C5-C6-O6 | -6.12 | 124.93 | 128.60 |
| 35 | AC | 10 | C | O4'-C1'-N1 | 6.12 | 113.09 | 108.20 |
| 34 | AA | 1797 | A | C5-C6-N6 | -6.11 | 118.81 | 123.70 |
| 34 | AA | 1113 | C | O4'-C1'-N1 | 6.11 | 113.09 | 108.20 |
| 44 | A8 | 33 | ARG | NE-CZ-NH1 | 6.11 | 123.36 | 120.30 |
| 21 | F | 255 | ARG | NE-CZ-NH1 | 6.11 | 123.36 | 120.30 |
| 34 | AA | 1556 | G | C5-C6-O6 | -6.11 | 124.93 | 128.60 |
| 34 | AA | 1606 | U | O4'-C1'-N1 | 6.11 | 113.09 | 108.20 |
| 34 | AA | 2737 | C | O4'-C1'-N1 | 6.11 | 113.09 | 108.20 |
| 34 | AA | 3606 | G | O4'-C1'-N9 | 6.11 | 113.09 | 108.20 |
| 34 | AA | 142 | C | O4'-C1'-N1 | 6.11 | 113.09 | 108.20 |
| 34 | AA | 3387 | U | O4'-C1'-N1 | 6.11 | 113.09 | 108.20 |
| 24 | L | 56 | ARG | NE-CZ-NH2 | -6.11 | 117.25 | 120.30 |
| 1 | A | 617 | G | C8-N9-C1' | -6.11 | 119.06 | 127.00 |
| 1 | A | 1403 | U | O4'-C1'-N1 | 6.11 | 113.08 | 108.20 |
| 24 | L | 92 | ARG | NE-CZ-NH1 | 6.11 | 123.35 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 881 | C | O4'-C1'-N1 | 6.10 | 113.08 | 108.20 |
| 34 | AA | 312 | A | C5'-C4'-C3' | -6.10 | 106.23 | 116.00 |
| 34 | AA | 876 | C | O4'-C1'-N1 | 6.10 | 113.08 | 108.20 |
| 1 | A | 89 | C | O4'-C1'-N1 | 6.10 | 113.08 | 108.20 |
| 1 | A | 2056 | C | O4'-C1'-N1 | 6.10 | 113.08 | 108.20 |
| 34 | AA | 2429 | U | O4'-C1'-N1 | 6.10 | 113.08 | 108.20 |
| 35 | AC | 33 | C | O4'-C1'-N1 | 6.09 | 113.08 | 108.20 |
| 34 | AA | 3417 | G | N1-C6-O6 | 6.09 | 123.56 | 119.90 |
| 71 | AF | 312 | ARG | NE-CZ-NH1 | 6.09 | 123.35 | 120.30 |
| 46 | Aa | 66 | ARG | NE-CZ-NH2 | 6.09 | 123.35 | 120.30 |
| 1 | A | 2053 | U | O4'-C1'-N1 | 6.09 | 113.07 | 108.20 |
| 23 | J | 117 | ARG | NE-CZ-NH1 | 6.09 | 123.34 | 120.30 |
| 34 | AA | 3650 | U | P-O5'-C5' | 6.09 | 130.64 | 120.90 |
| 35 | AC | 54 | C | O4'-C1'-N1 | 6.09 | 113.07 | 108.20 |
| 34 | AA | 411 | U | O4'-C1'-N1 | 6.09 | 113.07 | 108.20 |
| 34 | AA | 630 | U | O4'-C1'-N1 | 6.09 | 113.07 | 108.20 |
| 74 | AH | 39 | ARG | NE-CZ-NH2 | 6.09 | 123.34 | 120.30 |
| 71 | AF | 121 | ARG | NE-CZ-NH1 | 6.09 | 123.34 | 120.30 |
| 34 | AA | 3632 | U | N1-C2-N3 | 6.08 | 118.55 | 114.90 |
| 56 | Ac | 66 | ARG | NE-CZ-NH1 | 6.08 | 123.34 | 120.30 |
| 1 | A | 400 | C | O4'-C1'-N1 | 6.08 | 113.07 | 108.20 |
| 1 | A | 1786 | U | O4'-C1'-N1 | 6.08 | 113.07 | 108.20 |
| 1 | A | 1868 | C | O4'-C1'-N1 | 6.08 | 113.07 | 108.20 |
| 14 | 1 | 115 | ARG | NE-CZ-NH1 | 6.08 | 123.34 | 120.30 |
| 34 | AA | 2221 | U | O4'-C1'-N1 | 6.08 | 113.07 | 108.20 |
| 35 | AC | 22 | U | O4'-C1'-N1 | 6.08 | 113.07 | 108.20 |
| 34 | AA | 1612 | U | O4'-C1'-N1 | 6.08 | 113.06 | 108.20 |
| 34 | AA | 2917 | C | O4'-C1'-N1 | 6.08 | 113.06 | 108.20 |
| 1 | A | 827 | C | O4'-C1'-N1 | 6.08 | 113.06 | 108.20 |
| 14 | 1 | 61 | PHE | CB-CG-CD2 | -6.08 | 116.54 | 120.80 |
| 34 | AA | 574 | G | O4'-C1'-N9 | 6.08 | 113.06 | 108.20 |
| 34 | AA | 54 | C | O4'-C1'-N1 | 6.08 | 113.06 | 108.20 |
| 34 | AA | 2973 | U | O4'-C1'-N1 | 6.08 | 113.06 | 108.20 |
| 1 | A | 1627 | U | O4'-C1'-N1 | 6.08 | 113.06 | 108.20 |
| 34 | AA | 1615 | G | N1-C6-O6 | 6.08 | 123.55 | 119.90 |
| 76 | Ag | 39 | ARG | NE-CZ-NH1 | -6.08 | 117.26 | 120.30 |
| 1 | A | 1658 | G | P-O3'-C3' | -6.07 | 112.41 | 119.70 |
| 1 | A | 894 | U | O4'-C1'-N1 | 6.07 | 113.06 | 108.20 |
| 34 | AA | 744 | G | C5-C6-O6 | -6.07 | 124.96 | 128.60 |
| 34 | AA | 3468 | G | C5-C6-O6 | -6.07 | 124.96 | 128.60 |
| 34 | AA | 1283 | C | O4'-C1'-N1 | 6.07 | 113.06 | 108.20 |
| 34 | AA | 3709 | U | P-O3'-C3' | 6.07 | 126.98 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 537 | C | O4'-C1'-N1 | 6.07 | 113.05 | 108.20 |
| 34 | AA | 1809 | U | O4'-C1'-N1 | 6.07 | 113.05 | 108.20 |
| 1 | A | 1423 | A | O4'-C1'-N9 | 6.07 | 113.05 | 108.20 |
| 1 | A | 1674 | G | O4'-C1'-N9 | 6.07 | 113.05 | 108.20 |
| 34 | AA | 2529 | G | O4'-C1'-N9 | 6.07 | 113.05 | 108.20 |
| 1 | A | 2075 | C | O4'-C1'-N1 | 6.06 | 113.05 | 108.20 |
| 34 | AA | 1065 | U | O4'-C1'-N1 | 6.06 | 113.05 | 108.20 |
| 76 | Ag | 25 | ARG | NE-CZ-NH1 | 6.06 | 123.33 | 120.30 |
| 1 | A | 977 | U | O4'-C1'-N1 | 6.06 | 113.05 | 108.20 |
| 36 | AB | 20 | U | O4'-C1'-N1 | 6.06 | 113.05 | 108.20 |
| 1 | A | 1824 | A | O4'-C1'-N9 | 6.06 | 113.05 | 108.20 |
| 34 | AA | 3026 | G | N1-C6-O6 | 6.06 | 123.54 | 119.90 |
| 34 | AA | 1237 | C | O4'-C1'-N1 | 6.06 | 113.05 | 108.20 |
| 1 | A | 1862 | C | O4'-C1'-N1 | 6.06 | 113.05 | 108.20 |
| 16 | 3 | 10 | ARG | NE-CZ-NH1 | 6.06 | 123.33 | 120.30 |
| 34 | AA | 3776 | U | O4'-C1'-N1 | 6.06 | 113.05 | 108.20 |
| 34 | AA | 212 | U | O4'-C1'-N1 | 6.05 | 113.04 | 108.20 |
| 34 | AA | 1747 | U | C2-N1-C1' | 6.05 | 124.96 | 117.70 |
| 1 | A | 1301 | G | O4'-C1'-N9 | 6.05 | 113.04 | 108.20 |
| 34 | AA | 1658 | G | C5-C6-O6 | -6.05 | 124.97 | 128.60 |
| 34 | AA | 1962 | U | O4'-C1'-N1 | 6.05 | 113.04 | 108.20 |
| 34 | AA | 1784 | G | N3-C2-N2 | 6.05 | 124.14 | 119.90 |
| 34 | AA | 3309 | G | O4'-C1'-N9 | 6.05 | 113.04 | 108.20 |
| 51 | AP | 202 | ARG | NE-CZ-NH1 | 6.05 | 123.32 | 120.30 |
| 34 | AA | 294 | G | O4'-C1'-N9 | 6.05 | 113.04 | 108.20 |
| 34 | AA | 947 | U | O4'-C1'-N1 | 6.05 | 113.04 | 108.20 |
| 1 | A | 181 | A | O4'-C1'-N9 | 6.04 | 113.03 | 108.20 |
| 1 | A | 292 | G | O4'-C1'-N9 | 6.04 | 113.03 | 108.20 |
| 34 | AA | 1455 | C | O4'-C1'-N1 | 6.04 | 113.03 | 108.20 |
| 1 | A | 1191 | C | O4'-C1'-N1 | 6.04 | 113.03 | 108.20 |
| 34 | AA | 2918 | C | O4'-C1'-N1 | 6.04 | 113.03 | 108.20 |
| 34 | AA | 496 | C | O4'-C1'-N1 | 6.04 | 113.03 | 108.20 |
| 34 | AA | 92 | G | N1-C6-O6 | 6.04 | 123.52 | 119.90 |
| 34 | AA | 1123 | U | O4'-C1'-N1 | 6.04 | 113.03 | 108.20 |
| 34 | AA | 1694 | G | C5-C6-O6 | -6.04 | 124.98 | 128.60 |
| 36 | AB | 16 | A | O4'-C1'-N9 | 6.04 | 113.03 | 108.20 |
| 72 | AG | 140 | ARG | NE-CZ-NH1 | 6.04 | 123.32 | 120.30 |
| 1 | A | 522 | G | N1-C6-O6 | 6.04 | 123.52 | 119.90 |
| 3 | D | 27 | ARG | NE-CZ-NH1 | 6.04 | 123.32 | 120.30 |
| 34 | AA | 78 | U | O4'-C1'-N1 | 6.04 | 113.03 | 108.20 |
| 34 | AA | 3113 | U | O4'-C1'-N1 | 6.04 | 113.03 | 108.20 |
| 34 | AA | 3306 | G | O4'-C1'-N9 | 6.04 | 113.03 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 1025 | U | O4'-C1'-N1 | 6.03 | 113.03 | 108.20 |
| 29 | T | 44 | ARG | NE-CZ-NH1 | 6.03 | 123.32 | 120.30 |
| 34 | AA | 36 | U | O4'-C1'-N1 | 6.03 | 113.03 | 108.20 |
| 34 | AA | 1053 | U | O4'-C1'-N1 | 6.03 | 113.03 | 108.20 |
| 34 | AA | 3185 | U | O4'-C1'-N1 | 6.03 | 113.03 | 108.20 |
| 34 | AA | 2445 | A | O4'-C1'-N9 | 6.03 | 113.02 | 108.20 |
| 1 | A | 985 | U | O4'-C1'-N1 | 6.03 | 113.02 | 108.20 |
| 1 | A | 1321 | C | O4'-C1'-N1 | 6.03 | 113.02 | 108.20 |
| 34 | AA | 698 | G | O4'-C1'-N9 | 6.03 | 113.02 | 108.20 |
| 34 | AA | 3749 | U | O4'-C1'-N1 | 6.03 | 113.02 | 108.20 |
| 1 | A | 316 | C | O4'-C1'-N1 | 6.02 | 113.02 | 108.20 |
| 1 | A | 1720 | G | C5-C6-O6 | -6.02 | 124.99 | 128.60 |
| 21 | F | 145 | ARG | NE-CZ-NH2 | -6.02 | 117.29 | 120.30 |
| 34 | AA | 158 | U | O4'-C1'-N1 | 6.02 | 113.02 | 108.20 |
| 34 | AA | 3393 | C | O4'-C1'-N1 | 6.02 | 113.02 | 108.20 |
| 34 | AA | 3154 | U | P-O3'-C3' | -6.02 | 112.48 | 119.70 |
| 1 | A | 971 | G | C5-C6-O6 | -6.01 | 124.99 | 128.60 |
| 1 | A | 1804 | C | O4'-C1'-N1 | 6.01 | 113.01 | 108.20 |
| 34 | AA | 3195 | C | C6-N1-C1' | -6.01 | 113.58 | 120.80 |
| 36 | AB | 38 | U | O4'-C1'-N1 | 6.01 | 113.01 | 108.20 |
| 66 | AZ | 12 | ARG | NE-CZ-NH1 | 6.01 | 123.31 | 120.30 |
| 5 | G | 103 | ARG | NE-CZ-NH2 | -6.01 | 117.30 | 120.30 |
| 34 | AA | 1246 | C | O4'-C1'-N1 | 6.01 | 113.01 | 108.20 |
| 9 | W | 80 | ARG | NE-CZ-NH1 | 6.01 | 123.30 | 120.30 |
| 29 | T | 38 | ARG | NE-CZ-NH2 | 6.01 | 123.30 | 120.30 |
| 34 | AA | 3065 | C | C6-N1-C1' | -6.01 | 113.59 | 120.80 |
| 36 | AB | 15 | U | O4'-C1'-N1 | 6.01 | 113.00 | 108.20 |
| 1 | A | 1622 | C | O4'-C1'-N1 | 6.00 | 113.00 | 108.20 |
| 34 | AA | 2974 | A | N1-C6-N6 | 6.00 | 122.20 | 118.60 |
| 34 | AA | 130 | G | N1-C6-O6 | 6.00 | 123.50 | 119.90 |
| 34 | AA | 2457 | C | P-O3'-C3' | -6.00 | 112.50 | 119.70 |
| 34 | AA | 3203 | C | O4'-C1'-N1 | 6.00 | 113.00 | 108.20 |
| 3 | D | 147 | ARG | NE-CZ-NH1 | 6.00 | 123.30 | 120.30 |
| 34 | AA | 1329 | U | O4'-C1'-N1 | 6.00 | 113.00 | 108.20 |
| 34 | AA | 2590 | U | C2-N3-C4 | -6.00 | 123.40 | 127.00 |
| 1 | A | 632 | C | O4'-C1'-N1 | 6.00 | 113.00 | 108.20 |
| 1 | A | 1959 | G | O4'-C1'-N9 | 6.00 | 113.00 | 108.20 |
| 1 | A | 186 | U | O4'-C1'-N1 | 5.99 | 112.99 | 108.20 |
| 1 | A | 1179 | C | O4'-C1'-N1 | 5.99 | 113.00 | 108.20 |
| 19 | 6 | 33 | ARG | NE-CZ-NH1 | -5.99 | 117.30 | 120.30 |
| 1 | A | 1833 | G | O4'-C1'-N9 | 5.99 | 112.99 | 108.20 |
| 70 | AE | 263 | ARG | NE-CZ-NH1 | 5.99 | 123.30 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 34 | AA | 759 | U | P-O3'-C3' | -5.99 | 112.51 | 119.70 |
| 34 | AA | 2822 | U | O4'-C1'-N1 | 5.99 | 112.99 | 108.20 |
| 1 | A | 349 | C | O4'-C1'-N1 | 5.99 | 112.99 | 108.20 |
| 12 | Y | 86 | ARG | NE-CZ-NH1 | 5.99 | 123.30 | 120.30 |
| 34 | AA | 1064 | U | O4'-C1'-N1 | 5.99 | 112.99 | 108.20 |
| 34 | AA | 1573 | C | C2-N1-C1' | 5.99 | 125.39 | 118.80 |
| 34 | AA | 2390 | U | O4'-C1'-N1 | 5.99 | 112.99 | 108.20 |
| 34 | AA | 1311 | U | O4'-C1'-N1 | 5.99 | 112.99 | 108.20 |
| 34 | AA | 1974 | U | O4'-C1'-N1 | 5.99 | 112.99 | 108.20 |
| 34 | AA | 2161 | G | C5-C6-O6 | -5.99 | 125.01 | 128.60 |
| 34 | AA | 3286 | C | O4'-C1'-N1 | 5.99 | 112.99 | 108.20 |
| 34 | AA | 2992 | C | O4'-C1'-N1 | 5.98 | 112.99 | 108.20 |
| 34 | AA | 996 | C | O4'-C1'-N1 | 5.98 | 112.98 | 108.20 |
| 34 | AA | 2621 | U | O4'-C1'-N1 | 5.98 | 112.98 | 108.20 |
| 1 | A | 204 | U | O4'-C1'-N1 | 5.98 | 112.98 | 108.20 |
| 1 | A | 1282 | U | O4'-C1'-N1 | 5.98 | 112.98 | 108.20 |
| 34 | AA | 3154 | U | C4'-C3'-C2' | 5.98 | 108.58 | 102.60 |
| 1 | A | 2032 | U | O4'-C1'-N1 | 5.97 | 112.98 | 108.20 |
| 34 | AA | 410 | G | C5-C6-O6 | -5.97 | 125.02 | 128.60 |
| 34 | AA | 2524 | C | O4'-C1'-N1 | 5.97 | 112.98 | 108.20 |
| 73 | AU | 155 | ARG | NE-CZ-NH1 | 5.97 | 123.29 | 120.30 |
| 16 | 3 | 39 | PHE | CB-CG-CD1 | 5.97 | 124.98 | 120.80 |
| 32 | X | 42 | ARG | NE-CZ-NH2 | -5.97 | 117.31 | 120.30 |
| 34 | AA | 171 | C | O4'-C1'-N1 | 5.97 | 112.98 | 108.20 |
| 34 | AA | 1805 | U | C2'-C3'-O3' | 5.97 | 123.26 | 113.70 |
| 1 | A | 2019 | C | O4'-C1'-N1 | 5.97 | 112.98 | 108.20 |
| 34 | AA | 2957 | G | P-O5'-C5' | 5.97 | 130.45 | 120.90 |
| 34 | AA | 3348 | U | O4'-C1'-N1 | 5.97 | 112.97 | 108.20 |
| 34 | AA | 3205 | U | C6-N1-C1' | -5.97 | 112.84 | 121.20 |
| 1 | A | 17 | C | C6-N1-C2 | -5.97 | 117.91 | 120.30 |
| 34 | AA | 416 | G | O4'-C1'-N9 | 5.97 | 112.97 | 108.20 |
| 34 | AA | 2523 | U | P-O3'-C3' | 5.97 | 126.86 | 119.70 |
| 68 | A5 | 60 | TYR | CB-CG-CD2 | -5.97 | 117.42 | 121.00 |
| 1 | A | 789 | U | O4'-C1'-N1 | 5.96 | 112.97 | 108.20 |
| 34 | AA | 1801 | G | O4'-C1'-N9 | 5.96 | 112.97 | 108.20 |
| 34 | AA | 3089 | C | O4'-C1'-N1 | 5.96 | 112.97 | 108.20 |
| 35 | AC | 156 | A | O4'-C1'-N9 | 5.96 | 112.97 | 108.20 |
| 1 | A | 942 | U | C2-N3-C4 | -5.96 | 123.42 | 127.00 |
| 34 | AA | 64 | G | C5-C6-O6 | -5.96 | 125.02 | 128.60 |
| 34 | AA | 1109 | U | O4'-C1'-N1 | 5.96 | 112.97 | 108.20 |
| 34 | AA | 720 | U | O4'-C1'-N1 | 5.96 | 112.97 | 108.20 |
| 34 | AA | 975 | G | C5-C6-O6 | -5.96 | 125.02 | 128.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 34 | AA | 1095 | U | O4'-C1'-N1 | 5.96 | 112.97 | 108.20 |
| 34 | AA | 1415 | A | O4'-C1'-N9 | 5.96 | 112.97 | 108.20 |
| 34 | AA | 546 | C | O4'-C1'-N1 | 5.96 | 112.97 | 108.20 |
| 34 | AA | 1176 | C | O4'-C1'-N1 | 5.96 | 112.97 | 108.20 |
| 34 | AA | 1691 | G | C5-C6-O6 | -5.96 | 125.02 | 128.60 |
| 34 | AA | 2938 | C | O4'-C1'-N1 | 5.96 | 112.97 | 108.20 |
| 1 | A | 1750 | U | P-O5'-C5' | 5.96 | 130.43 | 120.90 |
| 34 | AA | 676 | U | O4'-C1'-N1 | 5.96 | 112.96 | 108.20 |
| 34 | AA | 1101 | A | O4'-C1'-N9 | 5.96 | 112.96 | 108.20 |
| 74 | AH | 36 | ARG | NE-CZ-NH1 | 5.96 | 123.28 | 120.30 |
| 34 | AA | 232 | C | O4'-C1'-N1 | 5.95 | 112.96 | 108.20 |
| 34 | AA | 797 | A | O4'-C1'-N9 | 5.95 | 112.96 | 108.20 |
| 34 | AA | 1007 | U | O4'-C1'-N1 | 5.95 | 112.96 | 108.20 |
| 34 | AA | 1157 | U | O4'-C1'-N1 | 5.95 | 112.96 | 108.20 |
| 1 | A | 1787 | U | C2-N1-C1' | 5.95 | 124.84 | 117.70 |
| 1 | A | 1092 | A | P-O3'-C3' | 5.95 | 126.84 | 119.70 |
| 72 | AG | 32 | ARG | NE-CZ-NH2 | -5.95 | 117.33 | 120.30 |
| 1 | A | 1802 | G | O4'-C1'-N9 | 5.95 | 112.96 | 108.20 |
| 35 | AC | 105 | U | O4'-C1'-N1 | 5.95 | 112.96 | 108.20 |
| 1 | A | 748 | C | O4'-C1'-N1 | 5.94 | 112.95 | 108.20 |
| 34 | AA | 3271 | G | C5-C6-O6 | -5.94 | 125.03 | 128.60 |
| 67 | A3 | 105 | ARG | NE-CZ-NH2 | 5.94 | 123.27 | 120.30 |
| 34 | AA | 3772 | C | O4'-C1'-N1 | 5.94 | 112.95 | 108.20 |
| 20 | B | 136 | ARG | NE-CZ-NH1 | -5.94 | 117.33 | 120.30 |
| 34 | AA | 1522 | A | O4'-C1'-N9 | 5.94 | 112.95 | 108.20 |
| 34 | AA | 3364 | A | O4'-C1'-N9 | 5.94 | 112.95 | 108.20 |
| 34 | AA | 3273 | G | O4'-C1'-N9 | 5.94 | 112.95 | 108.20 |
| 1 | A | 399 | C | O4'-C1'-N1 | 5.94 | 112.95 | 108.20 |
| 1 | A | 1291 | C | O4'-C1'-N1 | 5.94 | 112.95 | 108.20 |
| 1 | A | 1796 | C | O4'-C1'-N1 | 5.94 | 112.95 | 108.20 |
| 34 | AA | 999 | G | C1'-O4'-C4' | -5.94 | 105.15 | 109.90 |
| 34 | AA | 1670 | G | C5-C6-O6 | -5.94 | 125.04 | 128.60 |
| 34 | AA | 1068 | C | O4'-C1'-N1 | 5.94 | 112.95 | 108.20 |
| 34 | AA | 2186 | C | O4'-C1'-N1 | 5.94 | 112.95 | 108.20 |
| 34 | AA | 1516 | G | N1-C6-O6 | 5.93 | 123.46 | 119.90 |
| 56 | Ac | 59 | ARG | NE-CZ-NH1 | 5.93 | 123.27 | 120.30 |
| 61 | AQ | 9 | TYR | CB-CG-CD2 | -5.93 | 117.44 | 121.00 |
| 34 | AA | 1540 | G | C3'-C2'-C1' | -5.93 | 96.75 | 101.50 |
| 34 | AA | 3112 | U | O4'-C1'-N1 | 5.93 | 112.94 | 108.20 |
| 34 | AA | 1817 | G | O4'-C1'-N9 | 5.93 | 112.94 | 108.20 |
| 34 | AA | 2701 | U | O4'-C1'-N1 | 5.93 | 112.94 | 108.20 |
| 1 | A | 1102 | C | O4'-C1'-N1 | 5.93 | 112.94 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 1666 | C | O4'-C1'-N1 | 5.93 | 112.94 | 108.20 |
| 30 | U | 73 | ARG | NE-CZ-NH2 | 5.93 | 123.26 | 120.30 |
| 34 | AA | 1202 | C | O4'-C1'-N1 | 5.92 | 112.94 | 108.20 |
| 39 | A2 | 14 | ARG | NE-CZ-NH1 | 5.92 | 123.26 | 120.30 |
| 1 | A | 1952 | A | N1-C6-N6 | 5.92 | 122.15 | 118.60 |
| 34 | AA | 1763 | G | C5-C6-O6 | -5.92 | 125.05 | 128.60 |
| 34 | AA | 2949 | G | C5-C6-O6 | -5.92 | 125.05 | 128.60 |
| 34 | AA | 3524 | G | O4'-C1'-N9 | 5.92 | 112.94 | 108.20 |
| 34 | AA | 2816 | U | O4'-C1'-N1 | 5.92 | 112.94 | 108.20 |
| 1 | A | 623 | G | O4'-C1'-N9 | 5.92 | 112.94 | 108.20 |
| 34 | AA | 1847 | C | O4'-C1'-N1 | 5.92 | 112.94 | 108.20 |
| 34 | AA | 3298 | G | O4'-C1'-N9 | 5.92 | 112.94 | 108.20 |
| 1 | A | 1076 | C | O4'-C1'-N1 | 5.92 | 112.93 | 108.20 |
| 34 | AA | 2173 | G | O4'-C1'-N9 | 5.92 | 112.93 | 108.20 |
| 34 | AA | 3260 | G | C5-C6-O6 | -5.92 | 125.05 | 128.60 |
| 34 | AA | 3486 | G | O4'-C1'-N9 | 5.92 | 112.93 | 108.20 |
| 34 | AA | 2699 | C | O4'-C1'-N1 | 5.92 | 112.93 | 108.20 |
| 1 | A | 99 | C | O4'-C1'-N1 | 5.91 | 112.93 | 108.20 |
| 34 | AA | 1909 | U | O4'-C1'-N1 | 5.91 | 112.93 | 108.20 |
| 34 | AA | 3301 | C | O4'-C1'-N1 | 5.91 | 112.93 | 108.20 |
| 34 | AA | 491 | C | O4'-C1'-N1 | 5.91 | 112.93 | 108.20 |
| 34 | AA | 376 | G | C5-C6-O6 | -5.91 | 125.05 | 128.60 |
| 34 | AA | 505 | A | P-O3'-C3' | 5.91 | 126.79 | 119.70 |
| 35 | AC | 35 | A | O4'-C1'-N9 | 5.91 | 112.93 | 108.20 |
| 1 | A | 805 | A | O4'-C1'-N9 | 5.91 | 112.93 | 108.20 |
| 36 | AB | 60 | U | O4'-C1'-N1 | 5.91 | 112.93 | 108.20 |
| 34 | AA | 3365 | U | O4'-C1'-N1 | 5.91 | 112.93 | 108.20 |
| 1 | A | 2050 | U | O4'-C1'-N1 | 5.91 | 112.92 | 108.20 |
| 34 | AA | 950 | G | O4'-C1'-N9 | 5.91 | 112.92 | 108.20 |
| 22 | H | 177 | ARG | NE-CZ-NH1 | 5.90 | 123.25 | 120.30 |
| 34 | AA | 548 | U | O4'-C1'-N1 | 5.90 | 112.92 | 108.20 |
| 34 | AA | 580 | A | C5'-C4'-C3' | 5.90 | 125.44 | 116.00 |
| 34 | AA | 3676 | C | O4'-C1'-N1 | 5.90 | 112.92 | 108.20 |
| 44 | A8 | 13 | ARG | NE-CZ-NH1 | 5.90 | 123.25 | 120.30 |
| 59 | AS | 167 | ARG | NE-CZ-NH2 | -5.90 | 117.35 | 120.30 |
| 1 | A | 1893 | C | C2-N1-C1' | 5.90 | 125.29 | 118.80 |
| 34 | AA | 307 | G | C5-C6-O6 | -5.90 | 125.06 | 128.60 |
| 1 | A | 1168 | U | O4'-C1'-N1 | 5.89 | 112.92 | 108.20 |
| 34 | AA | 1197 | U | O4'-C1'-N1 | 5.89 | 112.92 | 108.20 |
| 34 | AA | 3552 | U | O4'-C1'-N1 | 5.89 | 112.92 | 108.20 |
| 65 | AT | 103 | ARG | NE-CZ-NH1 | 5.89 | 123.25 | 120.30 |
| 4 | E | 44 | ARG | NE-CZ-NH1 | 5.89 | 123.25 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 34 | AA | 2693 | G | N1-C6-O6 | 5.89 | 123.44 | 119.90 |
| 34 | AA | 3411 | C | O4'-C1'-N1 | 5.89 | 112.91 | 108.20 |
| 26 | P | 141 | ARG | NE-CZ-NH2 | 5.89 | 123.25 | 120.30 |
| 34 | AA | 1910 | C | O4'-C1'-N1 | 5.89 | 112.91 | 108.20 |
| 34 | AA | 749 | U | O4'-C1'-N1 | 5.89 | 112.91 | 108.20 |
| 34 | AA | 1425 | C | O4'-C1'-N1 | 5.89 | 112.91 | 108.20 |
| 34 | AA | 2643 | C | O4'-C1'-N1 | 5.89 | 112.91 | 108.20 |
| 34 | AA | 3086 | A | O4'-C1'-N9 | 5.89 | 112.91 | 108.20 |
| 34 | AA | 268 | C | O4'-C1'-N1 | 5.89 | 112.91 | 108.20 |
| 34 | AA | 2520 | C | O4'-C1'-N1 | 5.89 | 112.91 | 108.20 |
| 34 | AA | 3654 | C | O4'-C1'-N1 | 5.89 | 112.91 | 108.20 |
| 1 | A | 1685 | U | O4'-C1'-N1 | 5.89 | 112.91 | 108.20 |
| 34 | AA | 2021 | A | O4'-C1'-N9 | 5.89 | 112.91 | 108.20 |
| 36 | AB | 110 | G | O4'-C1'-N9 | 5.89 | 112.91 | 108.20 |
| 1 | A | 1006 | C | O4'-C1'-N1 | 5.88 | 112.91 | 108.20 |
| 34 | AA | 1568 | C | O4'-C1'-N1 | 5.88 | 112.91 | 108.20 |
| 35 | AC | 103 | G | N1-C6-O6 | 5.88 | 123.43 | 119.90 |
| 36 | AB | 99 | G | C5-C6-O6 | -5.88 | 125.07 | 128.60 |
| 1 | A | 345 | C | O4'-C1'-N1 | 5.88 | 112.91 | 108.20 |
| 34 | AA | 1192 | C | O4'-C1'-N1 | 5.88 | 112.91 | 108.20 |
| 34 | AA | 1224 | A | P-O5'-C5' | 5.88 | 130.31 | 120.90 |
| 68 | A5 | 255 | ARG | NE-CZ-NH2 | -5.88 | 117.36 | 120.30 |
| 19 | 6 | 29 | ARG | NE-CZ-NH1 | 5.88 | 123.24 | 120.30 |
| 1 | A | 1299 | G | O4'-C1'-N9 | 5.88 | 112.90 | 108.20 |
| 1 | A | 1795 | G | O4'-C1'-N9 | 5.88 | 112.90 | 108.20 |
| 2 | 7 | 51 | U | O4'-C1'-N1 | 5.88 | 112.90 | 108.20 |
| 34 | AA | 3646 | G | C5-C6-O6 | -5.88 | 125.07 | 128.60 |
| 65 | AT | 63 | ARG | NE-CZ-NH2 | -5.88 | 117.36 | 120.30 |
| 1 | A | 942 | U | O4'-C1'-N1 | 5.88 | 112.90 | 108.20 |
| 34 | AA | 1183 | U | O4'-C1'-N1 | 5.88 | 112.90 | 108.20 |
| 34 | AA | 1667 | A | O4'-C1'-N9 | 5.88 | 112.90 | 108.20 |
| 34 | AA | 2648 | G | C5-C6-O6 | -5.88 | 125.07 | 128.60 |
| 1 | A | 509 | U | O4'-C1'-N1 | 5.88 | 112.90 | 108.20 |
| 34 | AA | 1586 | C | O4'-C1'-N1 | 5.88 | 112.90 | 108.20 |
| 34 | AA | 2835 | G | O4'-C1'-N9 | 5.88 | 112.90 | 108.20 |
| 1 | A | 1207 | U | O4'-C1'-N1 | 5.87 | 112.90 | 108.20 |
| 1 | A | 1386 | U | C2'-C3'-O3' | 5.87 | 123.10 | 113.70 |
| 1 | A | 1947 | U | O4'-C1'-N1 | 5.87 | 112.90 | 108.20 |
| 61 | AQ | 10 | ARG | NE-CZ-NH1 | 5.87 | 123.24 | 120.30 |
| 1 | A | 1978 | A | O4'-C1'-N9 | 5.87 | 112.90 | 108.20 |
| 34 | AA | 801 | U | O4'-C1'-N1 | 5.87 | 112.90 | 108.20 |
| 34 | AA | 1647 | U | O4'-C1'-N1 | 5.87 | 112.90 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 1667 | A | P-O3'-C3' | 5.87 | 126.74 | 119.70 |
| 34 | AA | 1256 | U | O4'-C1'-N1 | 5.87 | 112.90 | 108.20 |
| 2 | 7 | 54 | G | C5'-C4'-O4' | 5.87 | 116.14 | 109.10 |
| 34 | AA | 966 | A | O4'-C1'-N9 | 5.87 | 112.89 | 108.20 |
| 34 | AA | 2571 | C | O4'-C1'-N1 | 5.87 | 112.89 | 108.20 |
| 34 | AA | 3100 | G | C5-C6-O6 | -5.87 | 125.08 | 128.60 |
| 23 | J | 123 | TYR | CB-CG-CD1 | 5.86 | 124.52 | 121.00 |
| 34 | AA | 1416 | U | O4'-C1'-N1 | 5.86 | 112.89 | 108.20 |
| 34 | AA | 3198 | G | C5-C6-O6 | -5.86 | 125.08 | 128.60 |
| 34 | AA | 3302 | G | O4'-C1'-N9 | 5.86 | 112.89 | 108.20 |
| 43 | AN | 133 | PHE | CB-CG-CD1 | 5.86 | 124.91 | 120.80 |
| 57 | AK | 127 | ARG | NE-CZ-NH1 | 5.86 | 123.23 | 120.30 |
| 34 | AA | 1303 | C | O4'-C1'-N1 | 5.86 | 112.89 | 108.20 |
| 34 | AA | 3092 | G | O4'-C1'-N9 | 5.86 | 112.89 | 108.20 |
| 1 | A | 897 | G | O4'-C1'-N9 | 5.86 | 112.89 | 108.20 |
| 1 | A | 1298 | C | P-O3'-C3' | -5.86 | 112.67 | 119.70 |
| 1 | A | 380 | U | O4'-C1'-N1 | 5.86 | 112.89 | 108.20 |
| 2 | 7 | 3 | G | O4'-C1'-N9 | 5.86 | 112.89 | 108.20 |
| 1 | A | 1181 | U | O4'-C1'-N1 | 5.86 | 112.89 | 108.20 |
| 5 | G | 222 | PHE | CB-CG-CD2 | -5.86 | 116.70 | 120.80 |
| 34 | AA | 37 | U | O4'-C1'-N1 | 5.86 | 112.89 | 108.20 |
| 34 | AA | 1753 | U | O4'-C1'-N1 | 5.86 | 112.89 | 108.20 |
| 34 | AA | 2205 | U | O4'-C1'-N1 | 5.86 | 112.89 | 108.20 |
| 34 | AA | 2724 | C | O4'-C1'-N1 | 5.86 | 112.89 | 108.20 |
| 1 | A | 96 | C | O4'-C1'-N1 | 5.86 | 112.89 | 108.20 |
| 1 | A | 746 | U | O4'-C1'-N1 | 5.86 | 112.89 | 108.20 |
| 1 | A | 1980 | A | C4'-C3'-C2' | -5.86 | 96.74 | 102.60 |
| 3 | D | 65 | ARG | NE-CZ-NH1 | 5.86 | 123.23 | 120.30 |
| 34 | AA | 627 | U | O4'-C1'-N1 | 5.86 | 112.88 | 108.20 |
| 34 | AA | 1603 | C | O4'-C1'-N1 | 5.86 | 112.88 | 108.20 |
| 34 | AA | 1013 | U | C1'-O4'-C4' | -5.85 | 105.22 | 109.90 |
| 1 | A | 430 | C | O4'-C1'-N1 | 5.85 | 112.88 | 108.20 |
| 34 | AA | 239 | U | C2-N1-C1' | 5.85 | 124.72 | 117.70 |
| 34 | AA | 1280 | G | O4'-C1'-N9 | 5.85 | 112.88 | 108.20 |
| 34 | AA | 2510 | U | O4'-C1'-N1 | 5.85 | 112.88 | 108.20 |
| 34 | AA | 3656 | A | O4'-C1'-N9 | 5.85 | 112.88 | 108.20 |
| 1 | A | 1954 | U | O4'-C1'-N1 | 5.85 | 112.88 | 108.20 |
| 34 | AA | 1282 | U | O4'-C1'-N1 | 5.85 | 112.88 | 108.20 |
| 34 | AA | 2123 | C | O4'-C1'-N1 | 5.85 | 112.88 | 108.20 |
| 73 | AU | 183 | ARG | NE-CZ-NH1 | 5.85 | 123.22 | 120.30 |
| 1 | A | 1170 | C | O4'-C1'-N1 | 5.85 | 112.88 | 108.20 |
| 4 | E | 171 | ARG | NE-CZ-NH2 | 5.85 | 123.22 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 34 | AA | 1234 | A | N1-C6-N6 | 5.85 | 122.11 | 118.60 |
| 34 | AA | 3522 | C | O4'-C1'-N1 | 5.85 | 112.88 | 108.20 |
| 1 | A | 492 | A | P-O5'-C5' | 5.85 | 130.25 | 120.90 |
| 34 | AA | 2486 | U | P-O3'-C3' | 5.85 | 126.72 | 119.70 |
| 34 | AA | 2943 | U | O4'-C1'-N1 | 5.85 | 112.88 | 108.20 |
| 34 | AA | 2140 | U | O4'-C1'-N1 | 5.84 | 112.88 | 108.20 |
| 34 | AA | 3427 | U | O4'-C1'-N1 | 5.84 | 112.88 | 108.20 |
| 34 | AA | 1750 | U | O4'-C1'-N1 | 5.84 | 112.87 | 108.20 |
| 34 | AA | 3736 | A | C1'-O4'-C4' | -5.84 | 105.22 | 109.90 |
| 24 | L | 31 | ARG | NE-CZ-NH1 | 5.84 | 123.22 | 120.30 |
| 34 | AA | 811 | A | O4'-C1'-N9 | 5.84 | 112.87 | 108.20 |
| 1 | A | 402 | G | O4'-C1'-N9 | 5.84 | 112.87 | 108.20 |
| 1 | A | 824 | A | O4'-C1'-N9 | 5.84 | 112.87 | 108.20 |
| 1 | A | 747 | U | O4'-C1'-N1 | 5.84 | 112.87 | 108.20 |
| 34 | AA | 581 | C | O4'-C1'-N1 | 5.84 | 112.87 | 108.20 |
| 34 | AA | 2607 | U | O4'-C1'-N1 | 5.84 | 112.87 | 108.20 |
| 34 | AA | 3142 | U | O4'-C1'-N1 | 5.84 | 112.87 | 108.20 |
| 34 | AA | 2216 | G | N1-C6-O6 | 5.83 | 123.40 | 119.90 |
| 34 | AA | 3703 | G | O4'-C1'-N9 | 5.83 | 112.87 | 108.20 |
| 34 | AA | 108 | C | O4'-C1'-N1 | 5.83 | 112.86 | 108.20 |
| 34 | AA | 2714 | U | O4'-C1'-N1 | 5.83 | 112.86 | 108.20 |
| 34 | AA | 1157 | U | P-O3'-C3' | 5.83 | 126.70 | 119.70 |
| 34 | AA | 1206 | U | P-O3'-C3' | 5.83 | 126.70 | 119.70 |
| 56 | Ac | 75 | ARG | NE-CZ-NH1 | 5.83 | 123.22 | 120.30 |
| 34 | AA | 1676 | C | O4'-C1'-N1 | 5.83 | 112.86 | 108.20 |
| 34 | AA | 2802 | U | O4'-C1'-N1 | 5.83 | 112.86 | 108.20 |
| 1 | A | 34 | G | O4'-C1'-N9 | 5.83 | 112.86 | 108.20 |
| 6 | I | 51 | ARG | NE-CZ-NH2 | -5.83 | 117.39 | 120.30 |
| 34 | AA | 594 | C | O4'-C1'-N1 | 5.83 | 112.86 | 108.20 |
| 1 | A | 1287 | U | O4'-C1'-N1 | 5.82 | 112.86 | 108.20 |
| 34 | AA | 3257 | G | N1-C6-O6 | 5.82 | 123.39 | 119.90 |
| 35 | AC | 28 | G | O4'-C1'-N9 | 5.82 | 112.86 | 108.20 |
| 62 | AR | 195 | ARG | NE-CZ-NH1 | -5.82 | 117.39 | 120.30 |
| 1 | A | 42 | G | O4'-C1'-N9 | 5.82 | 112.86 | 108.20 |
| 34 | AA | 2956 | U | O4'-C1'-N1 | 5.82 | 112.86 | 108.20 |
| 34 | AA | 3617 | A | O4'-C1'-N9 | 5.82 | 112.86 | 108.20 |
| 59 | AS | 27 | ARG | NE-CZ-NH1 | 5.82 | 123.21 | 120.30 |
| 1 | A | 1918 | U | O4'-C1'-N1 | 5.82 | 112.86 | 108.20 |
| 1 | A | 544 | G | C4'-C3'-C2' | -5.82 | 96.78 | 102.60 |
| 34 | AA | 861 | C | C6-N1-C2 | -5.82 | 117.97 | 120.30 |
| 34 | AA | 907 | C | O4'-C1'-N1 | 5.82 | 112.85 | 108.20 |
| 34 | AA | 3022 | U | O4'-C1'-N1 | 5.82 | 112.85 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 34 | AA | 1448 | C | O4'-C1'-N1 | 5.82 | 112.85 | 108.20 |
| 34 | AA | 2071 | U | O4'-C1'-N1 | 5.82 | 112.85 | 108.20 |
| 34 | AA | 3775 | G | O4'-C1'-N9 | 5.82 | 112.85 | 108.20 |
| 35 | AC | 80 | C | O4'-C1'-N1 | 5.82 | 112.85 | 108.20 |
| 35 | AC | 94 | C | O4'-C1'-N1 | 5.82 | 112.85 | 108.20 |
| 1 | A | 550 | C | O4'-C1'-N1 | 5.81 | 112.85 | 108.20 |
| 34 | AA | 3625 | C | O4'-C1'-N1 | 5.81 | 112.85 | 108.20 |
| 42 | A7 | 33 | TYR | CB-CG-CD2 | -5.81 | 117.51 | 121.00 |
| 2 | 7 | 13 | C | O4'-C1'-N1 | 5.81 | 112.85 | 108.20 |
| 14 | 1 | 91 | ARG | NE-CZ-NH2 | 5.81 | 123.20 | 120.30 |
| 34 | AA | 1233 | A | P-O5'-C5' | 5.81 | 130.19 | 120.90 |
| 34 | AA | 1536 | U | P-O3'-C3' | 5.81 | 126.67 | 119.70 |
| 34 | AA | 2693 | G | C5-C6-O6 | -5.81 | 125.11 | 128.60 |
| 34 | AA | 3637 | G | C5-C6-O6 | -5.81 | 125.11 | 128.60 |
| 34 | AA | 3781 | A | P-O3'-C3' | 5.81 | 126.67 | 119.70 |
| 1 | A | 1108 | A | P-O3'-C3' | 5.81 | 126.67 | 119.70 |
| 34 | AA | 2953 | G | O4'-C1'-N9 | 5.81 | 112.85 | 108.20 |
| 1 | A | 1808 | G | O4'-C1'-N9 | 5.81 | 112.84 | 108.20 |
| 34 | AA | 240 | U | O4'-C1'-N1 | 5.81 | 112.84 | 108.20 |
| 26 | P | 147 | ARG | NE-CZ-NH2 | 5.80 | 123.20 | 120.30 |
| 1 | A | 579 | C | O4'-C1'-N1 | 5.80 | 112.84 | 108.20 |
| 34 | AA | 1290 | C | P-O3'-C3' | 5.80 | 126.66 | 119.70 |
| 34 | AA | 1721 | C | O4'-C1'-N1 | 5.80 | 112.84 | 108.20 |
| 71 | AF | 48 | ARG | NE-CZ-NH1 | -5.80 | 117.40 | 120.30 |
| 34 | AA | 1457 | G | N1-C6-O6 | 5.80 | 123.38 | 119.90 |
| 34 | AA | 2426 | U | O4'-C1'-N1 | 5.80 | 112.84 | 108.20 |
| 36 | AB | 85 | G | O4'-C1'-N9 | 5.80 | 112.84 | 108.20 |
| 1 | A | 1718 | C | P-O3'-C3' | -5.80 | 112.74 | 119.70 |
| 1 | A | 454 | U | O4'-C1'-N1 | 5.80 | 112.84 | 108.20 |
| 27 | Q | 95 | PHE | CB-CG-CD1 | -5.80 | 116.74 | 120.80 |
| 34 | AA | 769 | U | C6-N1-C1' | -5.80 | 113.09 | 121.20 |
| 35 | AC | 145 | A | C2'-C3'-O3' | 5.80 | 122.97 | 113.70 |
| 34 | AA | 122 | A | C5'-C4'-O4' | 5.79 | 116.05 | 109.10 |
| 34 | AA | 1343 | U | O4'-C1'-N1 | 5.79 | 112.84 | 108.20 |
| 1 | A | 1392 | C | O4'-C1'-N1 | 5.79 | 112.83 | 108.20 |
| 34 | AA | 3664 | G | C5-C6-O6 | -5.79 | 125.12 | 128.60 |
| 34 | AA | 2643 | C | P-O3'-C3' | -5.79 | 112.75 | 119.70 |
| 35 | AC | 149 | C | O4'-C1'-N1 | 5.79 | 112.83 | 108.20 |
| 1 | A | 1905 | C | O4'-C1'-N1 | 5.79 | 112.83 | 108.20 |
| 34 | AA | 3716 | C | O4'-C1'-N1 | 5.79 | 112.83 | 108.20 |
| 1 | A | 753 | U | P-O3'-C3' | 5.79 | 126.64 | 119.70 |
| 1 | A | 1626 | U | O4'-C1'-N1 | 5.79 | 112.83 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 1628 | A | O4'-C1'-N9 | 5.79 | 112.83 | 108.20 |
| 34 | AA | 3711 | U | C1'-O4'-C4' | -5.79 | 105.27 | 109.90 |
| 1 | A | 167 | A | O4'-C1'-N9 | 5.78 | 112.83 | 108.20 |
| 1 | A | 596 | C | O4'-C1'-N1 | 5.78 | 112.83 | 108.20 |
| 1 | A | 971 | G | N1-C6-O6 | 5.78 | 123.37 | 119.90 |
| 34 | AA | 607 | A | C5-C6-N6 | -5.78 | 119.07 | 123.70 |
| 34 | AA | 716 | C | O4'-C1'-N1 | 5.78 | 112.83 | 108.20 |
| 34 | AA | 2098 | G | C5-C6-O6 | -5.78 | 125.13 | 128.60 |
| 34 | AA | 3013 | A | O4'-C1'-N9 | 5.78 | 112.83 | 108.20 |
| 34 | AA | 3573 | U | O4'-C1'-N1 | 5.78 | 112.83 | 108.20 |
| 34 | AA | 1736 | A | P-O3'-C3' | 5.78 | 126.64 | 119.70 |
| 34 | AA | 2888 | U | O4'-C1'-N1 | 5.78 | 112.83 | 108.20 |
| 34 | AA | 3689 | C | O4'-C1'-N1 | 5.78 | 112.83 | 108.20 |
| 1 | A | 617 | G | C4-N9-C1' | 5.78 | 134.01 | 126.50 |
| 34 | AA | 421 | C | O4'-C1'-N1 | 5.78 | 112.82 | 108.20 |
| 34 | AA | 1797 | A | P-O5'-C5' | 5.78 | 130.15 | 120.90 |
| 1 | A | 1085 | C | O4'-C1'-N1 | 5.78 | 112.82 | 108.20 |
| 1 | A | 1433 | A | C5'-C4'-O4' | 5.78 | 116.03 | 109.10 |
| 34 | AA | 1604 | U | O4'-C1'-N1 | 5.78 | 112.82 | 108.20 |
| 1 | A | 975 | A | C5'-C4'-O4' | 5.78 | 116.03 | 109.10 |
| 1 | A | 1942 | G | C5'-C4'-C3' | -5.78 | 106.76 | 116.00 |
| 34 | AA | 3639 | G | C5-C6-O6 | -5.78 | 125.13 | 128.60 |
| 1 | A | 1635 | C | O4'-C1'-N1 | 5.77 | 112.82 | 108.20 |
| 20 | B | 94 | ARG | NE-CZ-NH1 | 5.77 | 123.19 | 120.30 |
| 34 | AA | 652 | A | P-O3'-C3' | 5.77 | 126.63 | 119.70 |
| 34 | AA | 2463 | U | O4'-C1'-N1 | 5.77 | 112.82 | 108.20 |
| 34 | AA | 1494 | U | O4'-C1'-N1 | 5.77 | 112.82 | 108.20 |
| 34 | AA | 2640 | U | O4'-C1'-N1 | 5.77 | 112.82 | 108.20 |
| 1 | A | 594 | C | O4'-C1'-N1 | 5.77 | 112.82 | 108.20 |
| 34 | AA | 543 | U | O4'-C1'-N1 | 5.77 | 112.81 | 108.20 |
| 34 | AA | 1135 | G | P-O3'-C3' | 5.77 | 126.62 | 119.70 |
| 2 | 7 | 31 | G | O4'-C1'-N9 | 5.76 | 112.81 | 108.20 |
| 34 | AA | 265 | U | O4'-C1'-N1 | 5.76 | 112.81 | 108.20 |
| 36 | AB | 84 | U | P-O3'-C3' | -5.76 | 112.78 | 119.70 |
| 22 | H | 98 | ARG | NE-CZ-NH1 | 5.76 | 123.18 | 120.30 |
| 35 | AC | 24 | U | O4'-C1'-N1 | 5.76 | 112.81 | 108.20 |
| 26 | P | 146 | ARG | NE-CZ-NH2 | 5.76 | 123.18 | 120.30 |
| 1 | A | 38 | C | O4'-C1'-N1 | 5.76 | 112.81 | 108.20 |
| 1 | A | 207 | G | C5-C6-O6 | -5.76 | 125.14 | 128.60 |
| 1 | A | 388 | C | O4'-C1'-N1 | 5.76 | 112.81 | 108.20 |
| 34 | AA | 300 | C | O4'-C1'-N1 | 5.76 | 112.81 | 108.20 |
| 1 | A | 102 | A | N1-C6-N6 | -5.76 | 115.14 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 18 | 5 | 38 | ARG | NE-CZ-NH2 | 5.76 | 123.18 | 120.30 |
| 34 | AA | 3052 | U | P-O3'-C3' | -5.76 | 112.79 | 119.70 |
| 34 | AA | 652 | A | C2'-C3'-O3' | 5.76 | 122.91 | 113.70 |
| 34 | AA | 1210 | A | O4'-C1'-N9 | 5.76 | 112.80 | 108.20 |
| 34 | AA | 3445 | C | O4'-C1'-N1 | 5.76 | 112.81 | 108.20 |
| 1 | A | 1660 | U | P-O3'-C3' | -5.75 | 112.80 | 119.70 |
| 34 | AA | 1583 | G | C5-C6-O6 | -5.75 | 125.15 | 128.60 |
| 36 | AB | 93 | G | N1-C6-O6 | 5.75 | 123.35 | 119.90 |
| 34 | AA | 975 | G | O4'-C1'-N9 | 5.75 | 112.80 | 108.20 |
| 34 | AA | 2141 | G | O4'-C1'-N9 | 5.75 | 112.80 | 108.20 |
| 34 | AA | 2526 | A | O4'-C1'-N9 | 5.75 | 112.80 | 108.20 |
| 46 | Aa | 58 | ARG | NE-CZ-NH2 | 5.75 | 123.18 | 120.30 |
| 77 | AX | 102 | TYR | CB-CG-CD2 | -5.75 | 117.55 | 121.00 |
| 34 | AA | 3742 | C | O4'-C1'-N1 | 5.75 | 112.80 | 108.20 |
| 34 | AA | 2092 | G | N1-C6-O6 | 5.75 | 123.35 | 119.90 |
| 34 | AA | 2396 | C | O4'-C1'-N1 | 5.75 | 112.80 | 108.20 |
| 34 | AA | 2560 | C | O4'-C1'-N1 | 5.75 | 112.80 | 108.20 |
| 34 | AA | 2566 | G | N1-C6-O6 | 5.75 | 123.35 | 119.90 |
| 1 | A | 295 | U | O4'-C1'-N1 | 5.74 | 112.80 | 108.20 |
| 1 | A | 1171 | U | O4'-C1'-N1 | 5.74 | 112.80 | 108.20 |
| 1 | A | 1929 | C | O4'-C1'-N1 | 5.74 | 112.80 | 108.20 |
| 34 | AA | 2121 | C | O4'-C1'-N1 | 5.74 | 112.79 | 108.20 |
| 34 | AA | 2659 | C | O4'-C1'-N1 | 5.74 | 112.80 | 108.20 |
| 34 | AA | 3096 | U | O4'-C1'-N1 | 5.74 | 112.80 | 108.20 |
| 34 | AA | 3674 | A | O4'-C1'-N9 | 5.74 | 112.79 | 108.20 |
| 1 | A | 307 | G | P-O3'-C3' | 5.74 | 126.59 | 119.70 |
| 34 | AA | 892 | U | P-O3'-C3' | -5.74 | 112.81 | 119.70 |
| 34 | AA | 2015 | C | C1'-O4'-C4' | -5.74 | 105.31 | 109.90 |
| 34 | AA | 3256 | C | O4'-C1'-N1 | 5.74 | 112.79 | 108.20 |
| 36 | AB | 2 | G | C5-C6-O6 | -5.74 | 125.16 | 128.60 |
| 55 | AJ | 73 | ARG | NE-CZ-NH1 | 5.74 | 123.17 | 120.30 |
| 1 | A | 988 | U | O4'-C1'-N1 | 5.74 | 112.79 | 108.20 |
| 34 | AA | 3551 | U | O4'-C1'-N1 | 5.74 | 112.79 | 108.20 |
| 71 | AF | 375 | TYR | CB-CG-CD1 | 5.74 | 124.44 | 121.00 |
| 34 | AA | 1705 | A | P-O5'-C5' | 5.74 | 130.08 | 120.90 |
| 44 | A8 | 27 | ARG | NH1-CZ-NH2 | -5.74 | 113.09 | 119.40 |
| 56 | Ac | 14 | ARG | NE-CZ-NH2 | 5.74 | 123.17 | 120.30 |
| 1 | A | 201 | G | C5-C6-O6 | -5.74 | 125.16 | 128.60 |
| 1 | A | 1251 | G | O4'-C1'-N9 | 5.74 | 112.79 | 108.20 |
| 1 | A | 1368 | G | O4'-C1'-N9 | 5.74 | 112.79 | 108.20 |
| 34 | AA | 1629 | G | O4'-C1'-N9 | 5.74 | 112.79 | 108.20 |
| 35 | AC | 110 | G | C5-C6-O6 | -5.73 | 125.16 | 128.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 34 | AA | 1881 | C | C2'-C3'-O3' | 5.73 | 122.87 | 113.70 |
| 36 | AB | 7 | G | O4'-C1'-N9 | 5.73 | 112.79 | 108.20 |
| 62 | AR | 247 | ARG | NE-CZ-NH1 | 5.73 | 123.17 | 120.30 |
| 1 | A | 26 | A | P-O3'-C3' | 5.73 | 126.58 | 119.70 |
| 34 | AA | 2696 | G | O4'-C1'-N9 | 5.73 | 112.78 | 108.20 |
| 34 | AA | 2089 | C | O4'-C1'-N1 | 5.73 | 112.78 | 108.20 |
| 34 | AA | 3645 | A | N1-C6-N6 | -5.73 | 115.16 | 118.60 |
| 34 | AA | 1587 | U | O4'-C1'-N1 | 5.73 | 112.78 | 108.20 |
| 34 | AA | 2566 | G | C5-C6-O6 | -5.73 | 125.16 | 128.60 |
| 34 | AA | 2806 | U | O4'-C1'-N1 | 5.73 | 112.78 | 108.20 |
| 1 | A | 1786 | U | P-O5'-C5' | 5.72 | 130.06 | 120.90 |
| 34 | AA | 659 | U | C5'-C4'-O4' | 5.72 | 115.97 | 109.10 |
| 34 | AA | 2597 | C | O4'-C1'-N1 | 5.72 | 112.78 | 108.20 |
| 34 | AA | 3014 | C | O4'-C1'-N1 | 5.72 | 112.78 | 108.20 |
| 1 | A | 655 | C | O4'-C1'-N1 | 5.72 | 112.78 | 108.20 |
| 1 | A | 1321 | C | C6-N1-C2 | -5.72 | 118.01 | 120.30 |
| 62 | AR | 141 | ARG | NE-CZ-NH1 | -5.72 | 117.44 | 120.30 |
| 34 | AA | 3026 | G | C5-C6-O6 | -5.72 | 125.17 | 128.60 |
| 1 | A | 648 | A | P-O5'-C5' | 5.72 | 130.05 | 120.90 |
| 1 | A | 1106 | C | O4'-C1'-N1 | 5.72 | 112.77 | 108.20 |
| 1 | A | 1262 | C | O4'-C1'-N1 | 5.72 | 112.77 | 108.20 |
| 1 | A | 2006 | U | O4'-C1'-N1 | 5.72 | 112.77 | 108.20 |
| 34 | AA | 253 | U | O4'-C1'-N1 | 5.72 | 112.77 | 108.20 |
| 34 | AA | 276 | G | O4'-C1'-N9 | 5.72 | 112.77 | 108.20 |
| 34 | AA | 1130 | U | O4'-C1'-N1 | 5.72 | 112.77 | 108.20 |
| 1 | A | 163 | G | O4'-C1'-N9 | 5.71 | 112.77 | 108.20 |
| 1 | A | 1197 | C | O4'-C1'-N1 | 5.71 | 112.77 | 108.20 |
| 34 | AA | 1535 | G | P-O5'-C5' | 5.71 | 130.04 | 120.90 |
| 1 | A | 1001 | A | O4'-C1'-N9 | 5.71 | 112.77 | 108.20 |
| 1 | A | 1825 | U | O4'-C1'-N1 | 5.71 | 112.77 | 108.20 |
| 34 | AA | 1829 | G | O4'-C1'-N9 | 5.71 | 112.77 | 108.20 |
| 2 | 7 | 43 | C | O4'-C1'-N1 | 5.71 | 112.77 | 108.20 |
| 32 | X | 81 | ARG | NE-CZ-NH2 | -5.71 | 117.44 | 120.30 |
| 1 | A | 48 | G | O4'-C1'-N9 | 5.71 | 112.77 | 108.20 |
| 34 | AA | 1804 | C | P-O3'-C3' | 5.71 | 126.55 | 119.70 |
| 34 | AA | 3121 | G | O4'-C1'-N9 | 5.71 | 112.77 | 108.20 |
| 35 | AC | 140 | G | P-O5'-C5' | 5.71 | 130.03 | 120.90 |
| 51 | AP | 188 | SER | N-CA-CB | 5.71 | 119.06 | 110.50 |
| 1 | A | 199 | U | O4'-C1'-N1 | 5.71 | 112.77 | 108.20 |
| 34 | AA | 621 | C | C4'-C3'-C2' | -5.71 | 96.89 | 102.60 |
| 60 | AO | 127 | ARG | NE-CZ-NH1 | 5.71 | 123.15 | 120.30 |
| 67 | A3 | 80 | TYR | CB-CG-CD2 | 5.71 | 124.42 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 34 | AA | 3209 | G | N1-C6-O6 | 5.70 | 123.32 | 119.90 |
| 1 | A | 109 | C | O4'-C1'-N1 | 5.70 | 112.76 | 108.20 |
| 34 | AA | 642 | A | P-O3'-C3' | 5.70 | 126.54 | 119.70 |
| 34 | AA | 1958 | U | O4'-C1'-N1 | 5.70 | 112.76 | 108.20 |
| 34 | AA | 2197 | G | N1-C6-O6 | 5.70 | 123.32 | 119.90 |
| 1 | A | 520 | U | O4'-C1'-N1 | 5.70 | 112.76 | 108.20 |
| 34 | AA | 1634 | G | O4'-C1'-N9 | 5.70 | 112.76 | 108.20 |
| 1 | A | 1637 | U | O4'-C1'-N1 | 5.70 | 112.76 | 108.20 |
| 34 | AA | 1881 | C | P-O3'-C3' | 5.70 | 126.54 | 119.70 |
| 1 | A | 607 | U | O4'-C1'-N1 | 5.70 | 112.76 | 108.20 |
| 34 | AA | 3263 | G | O4'-C1'-N9 | 5.69 | 112.75 | 108.20 |
| 34 | AA | 3677 | A | O4'-C1'-N9 | 5.69 | 112.75 | 108.20 |
| 47 | Ab | 106 | ARG | NE-CZ-NH1 | 5.69 | 123.15 | 120.30 |
| 2 | 7 | 34 | U | O4'-C1'-N1 | 5.69 | 112.75 | 108.20 |
| 34 | AA | 648 | U | O4'-C1'-N1 | 5.69 | 112.75 | 108.20 |
| 34 | AA | 2136 | C | O4'-C1'-N1 | 5.69 | 112.75 | 108.20 |
| 34 | AA | 972 | G | O4'-C1'-N9 | 5.69 | 112.75 | 108.20 |
| 34 | AA | 2639 | C | O4'-C1'-N1 | 5.69 | 112.75 | 108.20 |
| 34 | AA | 3136 | C | O4'-C1'-N1 | 5.69 | 112.75 | 108.20 |
| 34 | AA | 1712 | G | O4'-C1'-N9 | 5.69 | 112.75 | 108.20 |
| 34 | AA | 111 | C | O4'-C1'-N1 | 5.69 | 112.75 | 108.20 |
| 34 | AA | 409 | A | O4'-C1'-N9 | 5.69 | 112.75 | 108.20 |
| 34 | AA | 3361 | U | P-O3'-C3' | 5.69 | 126.53 | 119.70 |
| 61 | AQ | 201 | ARG | NE-CZ-NH1 | 5.69 | 123.14 | 120.30 |
| 34 | AA | 3137 | U | P-O3'-C3' | 5.69 | 126.52 | 119.70 |
| 62 | AR | 85 | ARG | NE-CZ-NH2 | 5.69 | 123.14 | 120.30 |
| 21 | F | 132 | ARG | NE-CZ-NH2 | 5.68 | 123.14 | 120.30 |
| 34 | AA | 684 | G | P-O3'-C3' | 5.68 | 126.52 | 119.70 |
| 34 | AA | 2669 | G | O4'-C1'-N9 | 5.68 | 112.75 | 108.20 |
| 34 | AA | 364 | C | O4'-C1'-N1 | 5.68 | 112.74 | 108.20 |
| 34 | AA | 511 | C | O4'-C1'-N1 | 5.68 | 112.74 | 108.20 |
| 34 | AA | 1548 | A | O4'-C1'-N9 | 5.68 | 112.74 | 108.20 |
| 34 | AA | 3503 | U | O4'-C1'-N1 | 5.68 | 112.74 | 108.20 |
| 1 | A | 1306 | C | O4'-C1'-N1 | 5.68 | 112.74 | 108.20 |
| 34 | AA | 1841 | U | O4'-C1'-N1 | 5.68 | 112.74 | 108.20 |
| 34 | AA | 3287 | C | O4'-C1'-N1 | 5.68 | 112.74 | 108.20 |
| 2 | 7 | 4 | U | O4'-C1'-N1 | 5.68 | 112.74 | 108.20 |
| 1 | A | 523 | U | O4'-C1'-N1 | 5.67 | 112.74 | 108.20 |
| 1 | A | 1288 | U | O4'-C1'-N1 | 5.67 | 112.74 | 108.20 |
| 34 | AA | 1230 | A | C1'-O4'-C4' | -5.67 | 105.36 | 109.90 |
| 34 | AA | 1763 | G | O4'-C1'-N9 | 5.67 | 112.74 | 108.20 |
| 34 | AA | 2813 | U | O4'-C1'-N1 | 5.67 | 112.74 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 34 | AA | 882 | G | O4'-C1'-N9 | 5.67 | 112.74 | 108.20 |
| 2 | 7 | 37 | U | P-O3'-C3' | 5.67 | 126.50 | 119.70 |
| 34 | AA | 1887 | G | O4'-C1'-N9 | 5.67 | 112.74 | 108.20 |
| 34 | AA | 3752 | C | O4'-C1'-N1 | 5.67 | 112.74 | 108.20 |
| 2 | 7 | 54 | G | O4'-C1'-N9 | 5.67 | 112.74 | 108.20 |
| 34 | AA | 3574 | G | O4'-C1'-N9 | 5.67 | 112.74 | 108.20 |
| 1 | A | 1881 | G | C5-C6-O6 | -5.67 | 125.20 | 128.60 |
| 34 | AA | 1655 | U | O4'-C1'-N1 | 5.67 | 112.73 | 108.20 |
| 34 | AA | 2388 | U | O4'-C1'-N1 | 5.67 | 112.73 | 108.20 |
| 34 | AA | 2484 | U | O4'-C1'-N1 | 5.67 | 112.73 | 108.20 |
| 34 | AA | 3767 | U | O4'-C1'-N1 | 5.67 | 112.73 | 108.20 |
| 36 | AB | 13 | A | C4'-C3'-C2' | -5.67 | 96.93 | 102.60 |
| 62 | AR | 31 | ARG | NE-CZ-NH1 | 5.67 | 123.13 | 120.30 |
| 1 | A | 1955 | G | C5-C6-O6 | -5.67 | 125.20 | 128.60 |
| 2 | 7 | 55 | U | O4'-C1'-N1 | 5.67 | 112.73 | 108.20 |
| 35 | AC | 37 | A | C2'-C3'-O3' | 5.67 | 122.77 | 113.70 |
| 1 | A | 370 | G | O4'-C1'-N9 | 5.67 | 112.73 | 108.20 |
| 1 | A | 1206 | C | O4'-C1'-N1 | 5.66 | 112.73 | 108.20 |
| 34 | AA | 189 | U | O4'-C1'-N1 | 5.66 | 112.73 | 108.20 |
| 34 | AA | 2019 | A | O4'-C1'-N9 | 5.66 | 112.73 | 108.20 |
| 34 | AA | 3314 | U | O4'-C1'-N1 | 5.66 | 112.73 | 108.20 |
| 34 | AA | 130 | G | C5-C6-O6 | -5.66 | 125.20 | 128.60 |
| 34 | AA | 328 | G | N1-C6-O6 | 5.66 | 123.30 | 119.90 |
| 34 | AA | 622 | U | O4'-C1'-N1 | 5.66 | 112.73 | 108.20 |
| 34 | AA | 1511 | U | O4'-C1'-N1 | 5.66 | 112.73 | 108.20 |
| 34 | AA | 3267 | C | O4'-C1'-N1 | 5.66 | 112.73 | 108.20 |
| 68 | A5 | 255 | ARG | NE-CZ-NH1 | 5.66 | 123.13 | 120.30 |
| 34 | AA | 133 | U | O4'-C1'-N1 | 5.66 | 112.73 | 108.20 |
| 34 | AA | 1690 | A | N1-C6-N6 | -5.66 | 115.20 | 118.60 |
| 34 | AA | 1738 | A | O4'-C1'-N9 | 5.66 | 112.73 | 108.20 |
| 34 | AA | 3629 | U | O4'-C1'-N1 | 5.66 | 112.73 | 108.20 |
| 52 | Ah | 49 | ARG | NE-CZ-NH2 | 5.66 | 123.13 | 120.30 |
| 34 | AA | 893 | U | O4'-C1'-N1 | 5.66 | 112.72 | 108.20 |
| 1 | A | 1909 | C | O4'-C1'-N1 | 5.66 | 112.72 | 108.20 |
| 34 | AA | 794 | C | O4'-C1'-N1 | 5.66 | 112.72 | 108.20 |
| 34 | AA | 1104 | U | O4'-C1'-N1 | 5.66 | 112.72 | 108.20 |
| 34 | AA | 2817 | U | O4'-C1'-N1 | 5.66 | 112.72 | 108.20 |
| 35 | AC | 97 | C | O4'-C1'-N1 | 5.66 | 112.72 | 108.20 |
| 34 | AA | 1608 | C | O4'-C1'-N1 | 5.65 | 112.72 | 108.20 |
| 34 | AA | 2519 | U | O4'-C1'-N1 | 5.65 | 112.72 | 108.20 |
| 1 | A | 171 | U | O4'-C1'-N1 | 5.65 | 112.72 | 108.20 |
| 1 | A | 793 | G | C4'-C3'-C2' | 5.65 | 108.25 | 102.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 34 | AA | 352 | A | O4'-C1'-N9 | 5.65 | 112.72 | 108.20 |
| 59 | AS | 139 | ARG | NE-CZ-NH1 | 5.65 | 123.12 | 120.30 |
| 58 | AM | 72 | ARG | NE-CZ-NH1 | 5.65 | 123.12 | 120.30 |
| 1 | A | 1091 | C | O4'-C1'-N1 | 5.65 | 112.72 | 108.20 |
| 1 | A | 1260 | C | O4'-C1'-N1 | 5.65 | 112.72 | 108.20 |
| 34 | AA | 704 | U | O4'-C1'-N1 | 5.65 | 112.72 | 108.20 |
| 34 | AA | 3650 | U | O4'-C1'-N1 | 5.65 | 112.72 | 108.20 |
| 36 | AB | 112 | U | O4'-C1'-N1 | 5.65 | 112.72 | 108.20 |
| 62 | AR | 278 | ARG | NE-CZ-NH1 | 5.65 | 123.12 | 120.30 |
| 1 | A | 1435 | C | O4'-C1'-N1 | 5.64 | 112.72 | 108.20 |
| 34 | AA | 521 | U | C4'-C3'-C2' | -5.64 | 96.96 | 102.60 |
| 34 | AA | 1158 | G | C5-C6-O6 | -5.64 | 125.21 | 128.60 |
| 34 | AA | 3727 | A | O4'-C1'-N9 | 5.64 | 112.72 | 108.20 |
| 34 | AA | 3777 | G | O4'-C1'-N9 | 5.64 | 112.71 | 108.20 |
| 1 | A | 1798 | G | C5-C6-O6 | -5.64 | 125.22 | 128.60 |
| 34 | AA | 1037 | C | O4'-C1'-N1 | 5.64 | 112.71 | 108.20 |
| 1 | A | 1065 | C | C6-N1-C2 | -5.64 | 118.05 | 120.30 |
| 22 | H | 72 | ARG | NE-CZ-NH1 | 5.64 | 123.12 | 120.30 |
| 27 | Q | 107 | PHE | CB-CG-CD2 | -5.64 | 116.85 | 120.80 |
| 34 | AA | 1428 | G | N1-C6-O6 | 5.64 | 123.28 | 119.90 |
| 34 | AA | 2096 | G | O4'-C1'-N9 | 5.64 | 112.71 | 108.20 |
| 1 | A | 893 | U | O4'-C1'-N1 | 5.64 | 112.71 | 108.20 |
| 1 | A | 2089 | A | O4'-C1'-N9 | 5.64 | 112.71 | 108.20 |
| 1 | A | 1314 | U | O4'-C1'-N1 | 5.64 | 112.71 | 108.20 |
| 34 | AA | 592 | C | O4'-C1'-N1 | 5.64 | 112.71 | 108.20 |
| 34 | AA | 987 | U | O4'-C1'-N1 | 5.64 | 112.71 | 108.20 |
| 36 | AB | 4 | C | O4'-C1'-N1 | 5.64 | 112.71 | 108.20 |
| 34 | AA | 215 | C | C2'-C3'-O3' | 5.63 | 122.72 | 113.70 |
| 34 | AA | 3233 | G | O4'-C1'-N9 | 5.63 | 112.71 | 108.20 |
| 35 | AC | 102 | U | O4'-C1'-N1 | 5.63 | 112.71 | 108.20 |
| 14 | 1 | 120 | ARG | NE-CZ-NH2 | -5.63 | 117.48 | 120.30 |
| 34 | AA | 122 | A | C1'-O4'-C4' | -5.63 | 105.39 | 109.90 |
| 34 | AA | 243 | U | O4'-C1'-N1 | 5.63 | 112.70 | 108.20 |
| 34 | AA | 1727 | U | O4'-C1'-N1 | 5.63 | 112.70 | 108.20 |
| 1 | A | 1963 | U | O4'-C1'-N1 | 5.63 | 112.70 | 108.20 |
| 1 | A | 1937 | C | O4'-C1'-N1 | 5.63 | 112.70 | 108.20 |
| 34 | AA | 350 | A | O4'-C1'-N9 | 5.63 | 112.70 | 108.20 |
| 34 | AA | 1994 | U | O4'-C1'-N1 | 5.63 | 112.70 | 108.20 |
| 34 | AA | 2112 | G | O4'-C1'-N9 | 5.63 | 112.70 | 108.20 |
| 34 | AA | 2554 | G | C5-C6-O6 | -5.63 | 125.22 | 128.60 |
| 1 | A | 162 | A | O4'-C1'-N9 | 5.63 | 112.70 | 108.20 |
| 1 | A | 1050 | U | O4'-C1'-N1 | 5.63 | 112.70 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 34 | AA | 1658 | G | N1-C6-O6 | 5.63 | 123.28 | 119.90 |
| 73 | AU | 35 | ARG | NE-CZ-NH1 | -5.62 | 117.49 | 120.30 |
| 30 | U | 99 | ARG | NE-CZ-NH1 | 5.62 | 123.11 | 120.30 |
| 34 | AA | 1879 | U | O4'-C1'-N1 | 5.62 | 112.70 | 108.20 |
| 34 | AA | 3750 | U | O4'-C1'-N1 | 5.62 | 112.70 | 108.20 |
| 35 | AC | 127 | C | O4'-C1'-N1 | 5.62 | 112.70 | 108.20 |
| 35 | AC | 12 | U | O4'-C1'-N1 | 5.62 | 112.70 | 108.20 |
| 34 | AA | 1779 | A | P-O3'-C3' | 5.62 | 126.44 | 119.70 |
| 34 | AA | 140 | A | O4'-C1'-N9 | 5.62 | 112.69 | 108.20 |
| 34 | AA | 3072 | A | O4'-C1'-N9 | 5.62 | 112.69 | 108.20 |
| 2 | 7 | 36 | A | P-O5'-C5' | 5.62 | 129.89 | 120.90 |
| 34 | AA | 1241 | G | O4'-C1'-N9 | 5.62 | 112.69 | 108.20 |
| 34 | AA | 3104 | C | O4'-C1'-N1 | 5.62 | 112.69 | 108.20 |
| 5 | G | 178 | ARG | NE-CZ-NH2 | 5.62 | 123.11 | 120.30 |
| 20 | B | 136 | ARG | NE-CZ-NH2 | 5.62 | 123.11 | 120.30 |
| 34 | AA | 2110 | C | O4'-C1'-N1 | 5.62 | 112.69 | 108.20 |
| 34 | AA | 1315 | C | O4'-C1'-N1 | 5.61 | 112.69 | 108.20 |
| 34 | AA | 3103 | C | O4'-C1'-N1 | 5.61 | 112.69 | 108.20 |
| 35 | AC | 66 | C | O4'-C1'-N1 | 5.61 | 112.69 | 108.20 |
| 1 | A | 1914 | U | O4'-C1'-N1 | 5.61 | 112.69 | 108.20 |
| 34 | AA | 1650 | U | O4'-C1'-N1 | 5.61 | 112.69 | 108.20 |
| 1 | A | 1720 | G | O4'-C1'-N9 | 5.61 | 112.69 | 108.20 |
| 1 | A | 1924 | U | O4'-C1'-N1 | 5.61 | 112.69 | 108.20 |
| 35 | AC | 54 | C | P-O3'-C3' | 5.61 | 126.43 | 119.70 |
| 1 | A | 121 | A | N1-C6-N6 | -5.61 | 115.24 | 118.60 |
| 1 | A | 2022 | A | O4'-C1'-N9 | 5.61 | 112.69 | 108.20 |
| 9 | W | 58 | MET | CG-SD-CE | -5.61 | 91.23 | 100.20 |
| 34 | AA | 134 | G | C5-C6-O6 | -5.61 | 125.24 | 128.60 |
| 34 | AA | 1048 | G | O4'-C1'-N9 | 5.61 | 112.69 | 108.20 |
| 36 | AB | 22 | G | O4'-C1'-N9 | 5.61 | 112.69 | 108.20 |
| 34 | AA | 2153 | A | O4'-C1'-N9 | 5.60 | 112.68 | 108.20 |
| 1 | A | 123 | U | O4'-C1'-N1 | 5.60 | 112.68 | 108.20 |
| 2 | 7 | 18 | G | O4'-C1'-N9 | 5.60 | 112.68 | 108.20 |
| 34 | AA | 834 | U | O4'-C1'-N1 | 5.60 | 112.68 | 108.20 |
| 34 | AA | 1903 | C | C2-N1-C1' | 5.60 | 124.96 | 118.80 |
| 24 | L | 51 | ARG | NE-CZ-NH2 | 5.60 | 123.10 | 120.30 |
| 34 | AA | 2146 | A | O4'-C1'-N9 | 5.60 | 112.68 | 108.20 |
| 34 | AA | 890 | G | O4'-C1'-N9 | 5.60 | 112.68 | 108.20 |
| 34 | AA | 1284 | C | O4'-C1'-N1 | 5.60 | 112.68 | 108.20 |
| 34 | AA | 2977 | U | O4'-C1'-N1 | 5.60 | 112.68 | 108.20 |
| 70 | AE | 305 | MET | CG-SD-CE | -5.60 | 91.24 | 100.20 |
| 35 | AC | 5 | A | O4'-C1'-N9 | 5.60 | 112.68 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 46 | Aa | 70 | ARG | NE-CZ-NH1 | 5.60 | 123.10 | 120.30 |
| 1 | A | 172 | U | O4'-C1'-N1 | 5.60 | 112.68 | 108.20 |
| 34 | AA | 1309 | U | P-O3'-C3' | 5.60 | 126.42 | 119.70 |
| 62 | AR | 23 | ARG | NE-CZ-NH1 | 5.60 | 123.10 | 120.30 |
| 1 | A | 1980 | A | C3'-C2'-C1' | -5.59 | 97.02 | 101.50 |
| 25 | N | 82 | ARG | NE-CZ-NH2 | 5.59 | 123.10 | 120.30 |
| 34 | AA | 1629 | G | P-O3'-C3' | -5.59 | 112.99 | 119.70 |
| 35 | AC | 139 | A | P-O3'-C3' | 5.59 | 126.41 | 119.70 |
| 34 | AA | 2499 | G | C5'-C4'-O4' | 5.59 | 115.81 | 109.10 |
| 1 | A | 16 | G | C5-C6-O6 | -5.59 | 125.25 | 128.60 |
| 1 | A | 1889 | G | O4'-C1'-N9 | 5.59 | 112.67 | 108.20 |
| 2 | 7 | 19 | G | C5-C6-O6 | -5.59 | 125.25 | 128.60 |
| 34 | AA | 646 | A | O4'-C1'-N9 | 5.59 | 112.67 | 108.20 |
| 34 | AA | 3048 | U | O4'-C1'-N1 | 5.59 | 112.67 | 108.20 |
| 34 | AA | 3074 | U | O4'-C1'-N1 | 5.59 | 112.67 | 108.20 |
| 34 | AA | 1201 | U | O4'-C1'-N1 | 5.59 | 112.67 | 108.20 |
| 34 | AA | 1575 | C | O4'-C1'-N1 | 5.59 | 112.67 | 108.20 |
| 34 | AA | 2455 | G | O4'-C1'-N9 | 5.59 | 112.67 | 108.20 |
| 34 | AA | 2670 | G | C5-C6-O6 | -5.59 | 125.25 | 128.60 |
| 34 | AA | 3149 | A | O4'-C1'-N9 | 5.59 | 112.67 | 108.20 |
| 34 | AA | 3376 | U | P-O3'-C3' | 5.59 | 126.41 | 119.70 |
| 34 | AA | 174 | U | P-O3'-C3' | 5.59 | 126.41 | 119.70 |
| 34 | AA | 3139 | C | C6-N1-C1' | -5.59 | 114.09 | 120.80 |
| 1 | A | 389 | G | O4'-C1'-N9 | 5.59 | 112.67 | 108.20 |
| 34 | AA | 366 | G | O4'-C1'-N9 | 5.59 | 112.67 | 108.20 |
| 34 | AA | 451 | C | C4'-C3'-C2' | 5.59 | 108.19 | 102.60 |
| 34 | AA | 1304 | C | O4'-C1'-N1 | 5.59 | 112.67 | 108.20 |
| 34 | AA | 1551 | C | O4'-C1'-N1 | 5.59 | 112.67 | 108.20 |
| 1 | A | 354 | C | O4'-C1'-N1 | 5.58 | 112.67 | 108.20 |
| 34 | AA | 2950 | U | O4'-C1'-N1 | 5.58 | 112.67 | 108.20 |
| 43 | AN | 133 | PHE | CB-CG-CD2 | -5.58 | 116.89 | 120.80 |
| 1 | A | 168 | U | O4'-C1'-N1 | 5.58 | 112.67 | 108.20 |
| 1 | A | 1975 | U | O4'-C1'-N1 | 5.58 | 112.66 | 108.20 |
| 32 | X | 123 | TYR | CB-CG-CD1 | -5.58 | 117.65 | 121.00 |
| 34 | AA | 2005 | A | O4'-C1'-N9 | 5.58 | 112.67 | 108.20 |
| 34 | AA | 3122 | A | N1-C6-N6 | 5.58 | 121.95 | 118.60 |
| 34 | AA | 3361 | U | O4'-C1'-N1 | 5.58 | 112.67 | 108.20 |
| 47 | Ab | 94 | ARG | NE-CZ-NH2 | 5.58 | 123.09 | 120.30 |
| 1 | A | 1257 | C | O4'-C1'-N1 | 5.58 | 112.66 | 108.20 |
| 73 | AU | 134 | ARG | NE-CZ-NH2 | 5.58 | 123.09 | 120.30 |
| 1 | A | 548 | A | O4'-C1'-N9 | 5.58 | 112.66 | 108.20 |
| 1 | A | 1605 | C | O4'-C1'-N1 | 5.58 | 112.66 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 1705 | C | O4'-C1'-N1 | 5.58 | 112.66 | 108.20 |
| 1 | A | 1861 | U | O4'-C1'-N1 | 5.58 | 112.66 | 108.20 |
| 34 | AA | 2482 | U | O4'-C1'-N1 | 5.58 | 112.66 | 108.20 |
| 1 | A | 24 | U | O4'-C1'-N1 | 5.58 | 112.66 | 108.20 |
| 1 | A | 399 | C | C6-N1-C2 | -5.58 | 118.07 | 120.30 |
| 1 | A | 923 | U | C5'-C4'-O4' | 5.58 | 115.79 | 109.10 |
| 1 | A | 1380 | C | O4'-C1'-N1 | 5.58 | 112.66 | 108.20 |
| 34 | AA | 1214 | C | O4'-C1'-N1 | 5.57 | 112.66 | 108.20 |
| 34 | AA | 3664 | G | O4'-C1'-N9 | 5.57 | 112.66 | 108.20 |
| 34 | AA | 2457 | C | O4'-C1'-N1 | 5.57 | 112.66 | 108.20 |
| 34 | AA | 859 | C | C6-N1-C2 | -5.57 | 118.07 | 120.30 |
| 34 | AA | 1154 | C | O4'-C1'-N1 | 5.57 | 112.66 | 108.20 |
| 35 | AC | 110 | G | N1-C6-O6 | 5.57 | 123.24 | 119.90 |
| 68 | A5 | 64 | TYR | CB-CG-CD2 | -5.57 | 117.66 | 121.00 |
| 1 | A | 1041 | G | O4'-C1'-N9 | 5.57 | 112.66 | 108.20 |
| 1 | A | 2023 | A | C5-C6-N6 | -5.57 | 119.25 | 123.70 |
| 34 | AA | 215 | C | O4'-C1'-N1 | 5.57 | 112.65 | 108.20 |
| 34 | AA | 2653 | C | O4'-C1'-N1 | 5.57 | 112.65 | 108.20 |
| 73 | AU | 124 | ARG | NE-CZ-NH2 | 5.57 | 123.08 | 120.30 |
| 1 | A | 957 | U | O4'-C1'-N1 | 5.57 | 112.65 | 108.20 |
| 1 | A | 1642 | U | O4'-C1'-N1 | 5.57 | 112.65 | 108.20 |
| 34 | AA | 2207 | G | O4'-C1'-N9 | 5.57 | 112.65 | 108.20 |
| 34 | AA | 2462 | C | O4'-C1'-N1 | 5.57 | 112.65 | 108.20 |
| 1 | A | 866 | A | O4'-C1'-N9 | 5.56 | 112.65 | 108.20 |
| 1 | A | 508 | U | O4'-C1'-N1 | 5.56 | 112.65 | 108.20 |
| 30 | U | 124 | ARG | NE-CZ-NH2 | 5.56 | 123.08 | 120.30 |
| 1 | A | 1940 | U | O4'-C1'-N1 | 5.56 | 112.65 | 108.20 |
| 1 | A | 272 | U | P-O5'-C5' | 5.56 | 129.80 | 120.90 |
| 34 | AA | 1277 | G | O4'-C1'-N9 | 5.56 | 112.65 | 108.20 |
| 34 | AA | 3238 | C | O4'-C1'-N1 | 5.56 | 112.65 | 108.20 |
| 1 | A | 1417 | U | O4'-C1'-N1 | 5.56 | 112.65 | 108.20 |
| 1 | A | 2030 | U | O4'-C1'-N1 | 5.56 | 112.65 | 108.20 |
| 34 | AA | 1643 | U | O4'-C1'-C2' | -5.56 | 100.24 | 105.80 |
| 34 | AA | 1053 | U | C2-N3-C4 | -5.56 | 123.67 | 127.00 |
| 34 | AA | 3099 | C | O4'-C1'-N1 | 5.56 | 112.64 | 108.20 |
| 34 | AA | 1254 | G | C5-C6-O6 | -5.55 | 125.27 | 128.60 |
| 2 | 7 | 37 | U | P-O5'-C5' | 5.55 | 129.78 | 120.90 |
| 1 | A | 1381 | C | O4'-C1'-N1 | 5.55 | 112.64 | 108.20 |
| 1 | A | 2051 | C | P-O3'-C3' | 5.55 | 126.36 | 119.70 |
| 6 | I | 86 | TYR | CB-CG-CD2 | 5.55 | 124.33 | 121.00 |
| 34 | AA | 1085 | U | O4'-C1'-N1 | 5.55 | 112.64 | 108.20 |
| 34 | AA | 2069 | C | O4'-C1'-N1 | 5.55 | 112.64 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 36 | AB | 14 | C | O4'-C1'-N1 | 5.55 | 112.64 | 108.20 |
| 34 | AA | 1218 | C | O4'-C1'-N1 | 5.55 | 112.64 | 108.20 |
| 34 | AA | 2004 | U | C6-N1-C1' | -5.55 | 113.43 | 121.20 |
| 34 | AA | 31 | C | O4'-C1'-N1 | 5.55 | 112.64 | 108.20 |
| 34 | AA | 184 | U | P-O3'-C3' | 5.55 | 126.36 | 119.70 |
| 1 | A | 2053 | U | C2'-C3'-O3' | 5.55 | 122.58 | 113.70 |
| 34 | AA | 338 | U | O4'-C1'-N1 | 5.55 | 112.64 | 108.20 |
| 34 | AA | 2111 | C | O4'-C1'-N1 | 5.55 | 112.64 | 108.20 |
| 2 | 7 | 63 | U | O4'-C1'-N1 | 5.54 | 112.64 | 108.20 |
| 57 | AK | 84 | ARG | NE-CZ-NH2 | 5.54 | 123.07 | 120.30 |
| 1 | A | 1878 | C | O4'-C1'-N1 | 5.54 | 112.64 | 108.20 |
| 34 | AA | 2215 | G | P-O3'-C3' | 5.54 | 126.35 | 119.70 |
| 1 | A | 82 | G | C5'-C4'-C3' | 5.54 | 124.86 | 116.00 |
| 1 | A | 2088 | C | P-O3'-C3' | 5.54 | 126.35 | 119.70 |
| 29 | T | 30 | ARG | NE-CZ-NH1 | 5.54 | 123.07 | 120.30 |
| 34 | AA | 170 | U | O4'-C1'-N1 | 5.54 | 112.63 | 108.20 |
| 34 | AA | 1872 | A | O4'-C1'-N9 | 5.54 | 112.63 | 108.20 |
| 35 | AC | 96 | U | O4'-C1'-N1 | 5.54 | 112.63 | 108.20 |
| 68 | A5 | 86 | ARG | NE-CZ-NH1 | 5.54 | 123.07 | 120.30 |
| 34 | AA | 2514 | G | C5-C6-O6 | -5.54 | 125.28 | 128.60 |
| 49 | Ae | 6 | ARG | NE-CZ-NH1 | 5.54 | 123.07 | 120.30 |
| 59 | AS | 151 | PHE | CB-CG-CD2 | -5.54 | 116.92 | 120.80 |
| 1 | A | 2008 | U | O4'-C1'-N1 | 5.54 | 112.63 | 108.20 |
| 34 | AA | 1034 | A | N1-C6-N6 | -5.54 | 115.28 | 118.60 |
| 34 | AA | 1666 | A | O4'-C1'-N9 | 5.54 | 112.63 | 108.20 |
| 34 | AA | 3546 | C | O4'-C1'-N1 | 5.54 | 112.63 | 108.20 |
| 60 | AO | 108 | PHE | CB-CG-CD2 | -5.54 | 116.92 | 120.80 |
| 1 | A | 428 | G | O4'-C1'-N9 | 5.53 | 112.63 | 108.20 |
| 24 | L | 188 | ARG | NE-CZ-NH1 | 5.53 | 123.07 | 120.30 |
| 34 | AA | 1019 | A | O4'-C1'-N9 | 5.53 | 112.63 | 108.20 |
| 34 | AA | 1276 | G | C5'-C4'-O4' | 5.53 | 115.74 | 109.10 |
| 1 | A | 530 | U | O4'-C1'-N1 | 5.53 | 112.62 | 108.20 |
| 2 | 7 | 29 | G | O4'-C1'-N9 | 5.53 | 112.62 | 108.20 |
| 9 | W | 67 | ARG | NE-CZ-NH2 | 5.53 | 123.06 | 120.30 |
| 34 | AA | 2030 | G | O4'-C1'-N9 | 5.53 | 112.62 | 108.20 |
| 1 | A | 1411 | G | O4'-C1'-N9 | 5.53 | 112.62 | 108.20 |
| 34 | AA | 187 | U | O4'-C1'-N1 | 5.53 | 112.62 | 108.20 |
| 34 | AA | 684 | G | C5-C6-O6 | -5.53 | 125.28 | 128.60 |
| 34 | AA | 1280 | G | P-O3'-C3' | 5.53 | 126.33 | 119.70 |
| 34 | AA | 2518 | U | O4'-C1'-N1 | 5.53 | 112.62 | 108.20 |
| 34 | AA | 3347 | C | O4'-C1'-N1 | 5.53 | 112.62 | 108.20 |
| 73 | AU | 116 | TYR | CB-CG-CD2 | -5.53 | 117.69 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 44 | A8 | 111 | ARG | NE-CZ-NH2 | 5.52 | 123.06 | 120.30 |
| 34 | AA | 1005 | C | O4'-C1'-N1 | 5.52 | 112.62 | 108.20 |
| 34 | AA | 1959 | G | O4'-C1'-N9 | 5.52 | 112.62 | 108.20 |
| 34 | AA | 2103 | C | P-O3'-C3' | -5.52 | 113.07 | 119.70 |
| 34 | AA | 3688 | G | P-O3'-C3' | 5.52 | 126.33 | 119.70 |
| 75 | AV | 131 | ARG | NE-CZ-NH2 | -5.52 | 117.54 | 120.30 |
| 1 | A | 1226 | A | O4'-C1'-N9 | 5.52 | 112.62 | 108.20 |
| 34 | AA | 285 | U | O4'-C1'-N1 | 5.52 | 112.62 | 108.20 |
| 34 | AA | 2976 | A | P-O3'-C3' | -5.52 | 113.07 | 119.70 |
| 1 | A | 973 | G | C5-C6-O6 | -5.52 | 125.29 | 128.60 |
| 1 | A | 1295 | A | O4'-C1'-N9 | 5.52 | 112.62 | 108.20 |
| 1 | A | 1638 | U | O4'-C1'-N1 | 5.52 | 112.61 | 108.20 |
| 34 | AA | 245 | U | C5'-C4'-O4' | 5.52 | 115.72 | 109.10 |
| 34 | AA | 1898 | U | O4'-C1'-N1 | 5.52 | 112.62 | 108.20 |
| 1 | A | 17 | C | C2-N1-C1' | 5.52 | 124.87 | 118.80 |
| 1 | A | 858 | U | O4'-C1'-N1 | 5.52 | 112.61 | 108.20 |
| 34 | AA | 618 | U | O4'-C1'-N1 | 5.52 | 112.61 | 108.20 |
| 34 | AA | 3450 | G | C5-C6-O6 | -5.52 | 125.29 | 128.60 |
| 57 | AK | 134 | TYR | CB-CG-CD1 | -5.52 | 117.69 | 121.00 |
| 78 | A0 | 57 | ARG | NE-CZ-NH1 | 5.52 | 123.06 | 120.30 |
| 1 | A | 1243 | A | O4'-C1'-N9 | 5.52 | 112.61 | 108.20 |
| 1 | A | 10 | G | O4'-C1'-N9 | 5.51 | 112.61 | 108.20 |
| 34 | AA | 230 | G | O4'-C1'-N9 | 5.51 | 112.61 | 108.20 |
| 34 | AA | 2182 | G | O4'-C1'-N9 | 5.51 | 112.61 | 108.20 |
| 1 | A | 591 | C | O4'-C1'-N1 | 5.51 | 112.61 | 108.20 |
| 1 | A | 809 | U | O4'-C1'-N1 | 5.51 | 112.61 | 108.20 |
| 1 | A | 1188 | A | O4'-C1'-N9 | 5.51 | 112.61 | 108.20 |
| 34 | AA | 969 | U | O4'-C1'-N1 | 5.51 | 112.61 | 108.20 |
| 34 | AA | 1119 | G | O4'-C1'-N9 | 5.51 | 112.61 | 108.20 |
| 34 | AA | 1424 | C | O4'-C1'-N1 | 5.51 | 112.61 | 108.20 |
| 34 | AA | 3748 | U | O4'-C1'-N1 | 5.51 | 112.61 | 108.20 |
| 1 | A | 103 | U | O4'-C1'-N1 | 5.51 | 112.61 | 108.20 |
| 34 | AA | 76 | G | C5-C6-O6 | -5.51 | 125.30 | 128.60 |
| 34 | AA | 964 | G | O4'-C1'-N9 | 5.51 | 112.61 | 108.20 |
| 34 | AA | 3110 | A | P-O3'-C3' | 5.51 | 126.31 | 119.70 |
| 12 | Y | 107 | ARG | NE-CZ-NH1 | 5.51 | 123.05 | 120.30 |
| 34 | AA | 41 | G | O4'-C1'-N9 | 5.51 | 112.61 | 108.20 |
| 34 | AA | 386 | U | O4'-C1'-N1 | 5.51 | 112.61 | 108.20 |
| 34 | AA | 1082 | G | O4'-C1'-N9 | 5.51 | 112.61 | 108.20 |
| 34 | AA | 1243 | G | N1-C6-O6 | 5.51 | 123.20 | 119.90 |
| 50 | Af | 46 | ARG | NE-CZ-NH1 | -5.51 | 117.55 | 120.30 |
| 1 | A | 896 | U | O4'-C1'-N1 | 5.50 | 112.60 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 1068 | U | O4'-C1'-N1 | 5.50 | 112.60 | 108.20 |
| 34 | AA | 2815 | G | C5-C6-O6 | -5.50 | 125.30 | 128.60 |
| 34 | AA | 1658 | G | O4'-C1'-N9 | 5.50 | 112.60 | 108.20 |
| 34 | AA | 3025 | U | O4'-C1'-N1 | 5.50 | 112.60 | 108.20 |
| 75 | AV | 37 | TYR | CB-CG-CD1 | 5.50 | 124.30 | 121.00 |
| 34 | AA | 337 | A | P-O3'-C3' | 5.50 | 126.30 | 119.70 |
| 34 | AA | 1705 | A | C2'-C3'-O3' | 5.50 | 122.50 | 113.70 |
| 34 | AA | 3508 | A | O4'-C1'-N9 | 5.50 | 112.60 | 108.20 |
| 2 | 7 | 40 | U | C5'-C4'-C3' | 5.50 | 124.80 | 116.00 |
| 34 | AA | 1530 | G | O4'-C1'-N9 | 5.50 | 112.60 | 108.20 |
| 1 | A | 161 | U | C6-N1-C1' | -5.50 | 113.50 | 121.20 |
| 34 | AA | 282 | U | O4'-C1'-N1 | 5.50 | 112.60 | 108.20 |
| 34 | AA | 586 | U | O4'-C1'-N1 | 5.50 | 112.60 | 108.20 |
| 34 | AA | 270 | U | O4'-C1'-N1 | 5.50 | 112.60 | 108.20 |
| 34 | AA | 575 | U | O4'-C1'-N1 | 5.50 | 112.60 | 108.20 |
| 34 | AA | 1600 | C | O4'-C1'-N1 | 5.50 | 112.60 | 108.20 |
| 1 | A | 304 | C | O4'-C1'-N1 | 5.50 | 112.60 | 108.20 |
| 34 | AA | 717 | G | O4'-C1'-N9 | 5.50 | 112.60 | 108.20 |
| 34 | AA | 1854 | U | O4'-C1'-N1 | 5.50 | 112.60 | 108.20 |
| 2 | 7 | 69 | U | O4'-C1'-N1 | 5.49 | 112.59 | 108.20 |
| 23 | J | 140 | ARG | NE-CZ-NH2 | 5.49 | 123.05 | 120.30 |
| 34 | AA | 3339 | U | O4'-C1'-N1 | 5.49 | 112.59 | 108.20 |
| 34 | AA | 3586 | U | O4'-C1'-N1 | 5.49 | 112.59 | 108.20 |
| 73 | AU | 93 | ARG | NE-CZ-NH1 | 5.49 | 123.05 | 120.30 |
| 34 | AA | 458 | A | O4'-C1'-N9 | 5.49 | 112.59 | 108.20 |
| 34 | AA | 3018 | A | O4'-C1'-N9 | 5.49 | 112.59 | 108.20 |
| 34 | AA | 2729 | U | O4'-C1'-N1 | 5.49 | 112.59 | 108.20 |
| 34 | AA | 3147 | A | P-O3'-C3' | 5.49 | 126.29 | 119.70 |
| 69 | AD | 65 | ARG | NE-CZ-NH1 | 5.49 | 123.05 | 120.30 |
| 34 | AA | 2942 | G | O4'-C1'-N9 | 5.49 | 112.59 | 108.20 |
| 37 | AL | 197 | ARG | NE-CZ-NH2 | 5.49 | 123.04 | 120.30 |
| 34 | AA | 1784 | G | N1-C2-N2 | -5.49 | 111.26 | 116.20 |
| 71 | AF | 291 | ARG | NE-CZ-NH1 | 5.49 | 123.04 | 120.30 |
| 34 | AA | 671 | U | O4'-C1'-N1 | 5.48 | 112.59 | 108.20 |
| 34 | AA | 1426 | C | O4'-C1'-N1 | 5.48 | 112.59 | 108.20 |
| 1 | A | 1654 | G | O4'-C1'-N9 | 5.48 | 112.58 | 108.20 |
| 34 | AA | 3582 | G | O4'-C1'-N9 | 5.48 | 112.58 | 108.20 |
| 1 | A | 1242 | G | O4'-C1'-N9 | 5.48 | 112.58 | 108.20 |
| 6 | I | 82 | ARG | NE-CZ-NH1 | 5.48 | 123.04 | 120.30 |
| 34 | AA | 3169 | C | O4'-C1'-N1 | 5.48 | 112.58 | 108.20 |
| 34 | AA | 3243 | C | O4'-C1'-N1 | 5.48 | 112.58 | 108.20 |
| 34 | AA | 1593 | G | C5-C6-O6 | -5.47 | 125.32 | 128.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 1718 | C | O4'-C1'-N1 | 5.47 | 112.58 | 108.20 |
| 34 | AA | 134 | G | N1-C6-O6 | 5.47 | 123.18 | 119.90 |
| 34 | AA | 650 | U | C5'-C4'-O4' | 5.47 | 115.67 | 109.10 |
| 6 | I | 62 | ARG | NE-CZ-NH1 | -5.47 | 117.56 | 120.30 |
| 34 | AA | 193 | C | O4'-C1'-N1 | 5.47 | 112.58 | 108.20 |
| 34 | AA | 659 | U | C5'-C4'-C3' | -5.47 | 107.25 | 116.00 |
| 34 | AA | 1026 | G | O4'-C1'-C2' | -5.47 | 100.33 | 105.80 |
| 34 | AA | 178 | U | O4'-C1'-N1 | 5.47 | 112.58 | 108.20 |
| 1 | A | 1409 | U | C2-N1-C1' | 5.47 | 124.26 | 117.70 |
| 1 | A | 1977 | G | O4'-C1'-N9 | 5.47 | 112.57 | 108.20 |
| 34 | AA | 545 | C | O4'-C1'-N1 | 5.47 | 112.57 | 108.20 |
| 34 | AA | 813 | G | C5-C6-O6 | -5.47 | 125.32 | 128.60 |
| 34 | AA | 826 | U | O4'-C1'-N1 | 5.47 | 112.57 | 108.20 |
| 34 | AA | 1008 | U | O4'-C1'-N1 | 5.47 | 112.57 | 108.20 |
| 34 | AA | 3568 | G | O4'-C1'-N9 | 5.47 | 112.57 | 108.20 |
| 34 | AA | 3785 | G | O4'-C1'-N9 | 5.47 | 112.57 | 108.20 |
| 50 | Af | 46 | ARG | NE-CZ-NH2 | 5.47 | 123.03 | 120.30 |
| 1 | A | 1384 | U | O4'-C1'-N1 | 5.46 | 112.57 | 108.20 |
| 34 | AA | 580 | A | O4'-C1'-N9 | 5.46 | 112.57 | 108.20 |
| 34 | AA | 703 | U | O4'-C1'-N1 | 5.46 | 112.57 | 108.20 |
| 51 | AP | 67 | ARG | NE-CZ-NH1 | -5.46 | 117.57 | 120.30 |
| 34 | AA | 1211 | U | O4'-C1'-N1 | 5.46 | 112.57 | 108.20 |
| 34 | AA | 3184 | C | O4'-C1'-N1 | 5.46 | 112.57 | 108.20 |
| 74 | AH | 80 | PHE | CB-CG-CD2 | -5.46 | 116.98 | 120.80 |
| 1 | A | 1173 | C | C6-N1-C2 | -5.46 | 118.11 | 120.30 |
| 34 | AA | 50 | U | O4'-C1'-N1 | 5.46 | 112.57 | 108.20 |
| 34 | AA | 117 | C | O4'-C1'-N1 | 5.46 | 112.57 | 108.20 |
| 34 | AA | 1021 | G | O4'-C1'-N9 | 5.46 | 112.57 | 108.20 |
| 34 | AA | 1332 | A | O4'-C1'-N9 | 5.46 | 112.57 | 108.20 |
| 41 | A6 | 89 | ARG | NE-CZ-NH1 | 5.46 | 123.03 | 120.30 |
| 34 | AA | 3033 | A | O4'-C1'-N9 | 5.46 | 112.57 | 108.20 |
| 34 | AA | 61 | A | C2'-C3'-O3' | 5.46 | 122.43 | 113.70 |
| 34 | AA | 991 | A | O4'-C1'-N9 | 5.46 | 112.56 | 108.20 |
| 34 | AA | 1197 | U | P-O3'-C3' | 5.46 | 126.25 | 119.70 |
| 34 | AA | 1238 | C | O4'-C1'-N1 | 5.46 | 112.57 | 108.20 |
| 34 | AA | 1790 | U | O4'-C1'-N1 | 5.46 | 112.56 | 108.20 |
| 34 | AA | 2455 | G | N1-C6-O6 | 5.46 | 123.17 | 119.90 |
| 1 | A | 624 | U | O4'-C1'-N1 | 5.45 | 112.56 | 108.20 |
| 34 | AA | 27 | U | O4'-C1'-N1 | 5.45 | 112.56 | 108.20 |
| 34 | AA | 244 | U | O4'-C1'-N1 | 5.45 | 112.56 | 108.20 |
| 63 | AW | 123 | ARG | NE-CZ-NH1 | 5.45 | 123.03 | 120.30 |
| 34 | AA | 1695 | A | O4'-C1'-N9 | 5.45 | 112.56 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 34 | AA | 2415 | G | O4'-C1'-N9 | 5.45 | 112.56 | 108.20 |
| 34 | AA | 220 | G | O4'-C1'-N9 | 5.45 | 112.56 | 108.20 |
| 1 | A | 1859 | A | O4'-C1'-N9 | 5.45 | 112.56 | 108.20 |
| 1 | A | 2085 | G | N1-C6-O6 | 5.45 | 123.17 | 119.90 |
| 34 | AA | 834 | U | P-O3'-C3' | 5.45 | 126.24 | 119.70 |
| 34 | AA | 1630 | A | C5'-C4'-C3' | -5.45 | 107.28 | 116.00 |
| 34 | AA | 2999 | C | O4'-C1'-N1 | 5.45 | 112.56 | 108.20 |
| 34 | AA | 3159 | G | N1-C6-O6 | 5.45 | 123.17 | 119.90 |
| 1 | A | 355 | U | O4'-C1'-N1 | 5.45 | 112.56 | 108.20 |
| 1 | A | 1950 | C | O4'-C1'-N1 | 5.45 | 112.56 | 108.20 |
| 34 | AA | 2472 | C | O4'-C1'-N1 | 5.45 | 112.56 | 108.20 |
| 35 | AC | 18 | U | O4'-C1'-N1 | 5.45 | 112.56 | 108.20 |
| 1 | A | 609 | U | O4'-C1'-N1 | 5.45 | 112.56 | 108.20 |
| 1 | A | 1051 | U | O4'-C1'-N1 | 5.45 | 112.56 | 108.20 |
| 34 | AA | 353 | G | C2'-C3'-O3' | 5.45 | 122.41 | 113.70 |
| 34 | AA | 1730 | A | N1-C6-N6 | -5.45 | 115.33 | 118.60 |
| 1 | A | 588 | U | P-O3'-C3' | 5.44 | 126.23 | 119.70 |
| 7 | K | 58 | SER | N-CA-CB | 5.44 | 118.67 | 110.50 |
| 1 | A | 90 | U | O4'-C1'-N1 | 5.44 | 112.55 | 108.20 |
| 1 | A | 575 | G | C5-C6-O6 | -5.44 | 125.33 | 128.60 |
| 34 | AA | 761 | U | O4'-C1'-N1 | 5.44 | 112.55 | 108.20 |
| 1 | A | 1046 | A | O4'-C1'-N9 | 5.44 | 112.55 | 108.20 |
| 34 | AA | 2095 | U | O4'-C1'-N1 | 5.44 | 112.55 | 108.20 |
| 66 | AZ | 83 | ARG | NE-CZ-NH2 | -5.44 | 117.58 | 120.30 |
| 1 | A | 1219 | U | O4'-C1'-N1 | 5.44 | 112.55 | 108.20 |
| 34 | AA | 974 | U | O4'-C1'-N1 | 5.44 | 112.55 | 108.20 |
| 1 | A | 212 | U | O4'-C1'-N1 | 5.44 | 112.55 | 108.20 |
| 1 | A | 472 | U | O4'-C1'-N1 | 5.44 | 112.55 | 108.20 |
| 1 | A | 1919 | G | O4'-C1'-N9 | 5.44 | 112.55 | 108.20 |
| 2 | 7 | 61 | C | O4'-C1'-N1 | 5.44 | 112.55 | 108.20 |
| 34 | AA | 1837 | U | O4'-C1'-N1 | 5.44 | 112.55 | 108.20 |
| 34 | AA | 3183 | G | O4'-C1'-N9 | 5.44 | 112.55 | 108.20 |
| 1 | A | 2004 | U | O4'-C1'-N1 | 5.44 | 112.55 | 108.20 |
| 34 | AA | 3260 | G | N1-C6-O6 | 5.44 | 123.16 | 119.90 |
| 34 | AA | 12 | U | O4'-C1'-N1 | 5.43 | 112.55 | 108.20 |
| 62 | AR | 85 | ARG | NE-CZ-NH1 | -5.43 | 117.58 | 120.30 |
| 1 | A | 1923 | U | O4'-C1'-N1 | 5.43 | 112.55 | 108.20 |
| 18 | 5 | 61 | ARG | NE-CZ-NH2 | 5.43 | 123.02 | 120.30 |
| 34 | AA | 97 | U | O4'-C1'-N1 | 5.43 | 112.55 | 108.20 |
| 34 | AA | 507 | G | O4'-C1'-N9 | 5.43 | 112.55 | 108.20 |
| 34 | AA | 879 | U | O4'-C1'-N1 | 5.43 | 112.55 | 108.20 |
| 34 | AA | 3188 | U | O4'-C1'-N1 | 5.43 | 112.55 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 34 | AA | 1685 | G | P-O5'-C5' | 5.43 | 129.59 | 120.90 |
| 1 | A | 180 | U | O4'-C1'-N1 | 5.43 | 112.54 | 108.20 |
| 34 | AA | 23 | C | O4'-C1'-N1 | 5.43 | 112.54 | 108.20 |
| 40 | A4 | 8 | THR | N-CA-CB | 5.43 | 120.61 | 110.30 |
| 66 | AZ | 45 | ARG | NE-CZ-NH2 | -5.43 | 117.58 | 120.30 |
| 12 | Y | 99 | ARG | NE-CZ-NH2 | 5.43 | 123.01 | 120.30 |
| 34 | AA | 1419 | A | P-O3'-C3' | 5.43 | 126.21 | 119.70 |
| 34 | AA | 3115 | C | P-O3'-C3' | 5.43 | 126.21 | 119.70 |
| 34 | AA | 1674 | G | O4'-C1'-N9 | 5.43 | 112.54 | 108.20 |
| 34 | AA | 2071 | U | P-O3'-C3' | -5.43 | 113.19 | 119.70 |
| 1 | A | 130 | U | C2-N1-C1' | 5.42 | 124.21 | 117.70 |
| 1 | A | 1635 | C | C6-N1-C1' | -5.42 | 114.29 | 120.80 |
| 34 | AA | 807 | U | C5'-C4'-C3' | 5.42 | 124.68 | 116.00 |
| 1 | A | 1236 | U | O4'-C1'-N1 | 5.42 | 112.54 | 108.20 |
| 2 | 7 | 12 | G | O4'-C1'-N9 | 5.42 | 112.54 | 108.20 |
| 34 | AA | 3119 | A | O4'-C1'-N9 | 5.42 | 112.54 | 108.20 |
| 34 | AA | 3318 | C | O4'-C1'-N1 | 5.42 | 112.54 | 108.20 |
| 1 | A | 1302 | G | O4'-C1'-N9 | 5.42 | 112.53 | 108.20 |
| 34 | AA | 831 | U | O4'-C1'-N1 | 5.42 | 112.53 | 108.20 |
| 1 | A | 1431 | A | C4'-C3'-C2' | -5.42 | 97.18 | 102.60 |
| 1 | A | 1843 | G | O4'-C1'-N9 | 5.42 | 112.53 | 108.20 |
| 6 | I | 118 | ARG | NE-CZ-NH1 | 5.42 | 123.01 | 120.30 |
| 34 | AA | 46 | U | O4'-C1'-N1 | 5.42 | 112.53 | 108.20 |
| 34 | AA | 1294 | G | O4'-C1'-N9 | 5.42 | 112.53 | 108.20 |
| 34 | AA | 1619 | U | O4'-C1'-N1 | 5.42 | 112.53 | 108.20 |
| 34 | AA | 2974 | A | C5-C6-N6 | -5.42 | 119.37 | 123.70 |
| 34 | AA | 499 | U | O4'-C1'-N1 | 5.42 | 112.53 | 108.20 |
| 34 | AA | 981 | U | O4'-C1'-N1 | 5.42 | 112.53 | 108.20 |
| 34 | AA | 1433 | U | O4'-C1'-N1 | 5.42 | 112.53 | 108.20 |
| 1 | A | 1387 | U | C4'-C3'-C2' | -5.41 | 97.19 | 102.60 |
| 72 | AG | 145 | ARG | NE-CZ-NH2 | 5.41 | 123.01 | 120.30 |
| 34 | AA | 3155 | G | O4'-C1'-N9 | 5.41 | 112.53 | 108.20 |
| 34 | AA | 3213 | U | O4'-C1'-N1 | 5.41 | 112.53 | 108.20 |
| 36 | AB | 53 | U | C6-N1-C1' | -5.41 | 113.63 | 121.20 |
| 36 | AB | 94 | C | O4'-C1'-N1 | 5.41 | 112.53 | 108.20 |
| 46 | Aa | 86 | ARG | NE-CZ-NH1 | 5.41 | 123.00 | 120.30 |
| 34 | AA | 1693 | U | O4'-C1'-N1 | 5.41 | 112.53 | 108.20 |
| 34 | AA | 2416 | G | O4'-C1'-N9 | 5.41 | 112.53 | 108.20 |
| 34 | AA | 3276 | G | O4'-C1'-N9 | 5.41 | 112.53 | 108.20 |
| 34 | AA | 3655 | U | O4'-C1'-N1 | 5.41 | 112.53 | 108.20 |
| 36 | AB | 8 | U | O4'-C1'-N1 | 5.41 | 112.53 | 108.20 |
| 1 | A | 7 | G | C5-C6-O6 | -5.41 | 125.36 | 128.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 34 | AA | 1309 | U | O4'-C1'-N1 | 5.41 | 112.53 | 108.20 |
| 34 | AA | 3362 | A | O4'-C1'-N9 | 5.41 | 112.53 | 108.20 |
| 74 | AH | 167 | ARG | NE-CZ-NH2 | 5.41 | 123.00 | 120.30 |
| 1 | A | 432 | G | P-O5'-C5' | -5.41 | 112.25 | 120.90 |
| 1 | A | 849 | U | O4'-C1'-N1 | 5.41 | 112.52 | 108.20 |
| 1 | A | 2070 | G | C5-C6-O6 | -5.41 | 125.36 | 128.60 |
| 14 | 1 | 61 | PHE | CB-CG-CD1 | 5.41 | 124.58 | 120.80 |
| 34 | AA | 823 | U | O4'-C1'-N1 | 5.41 | 112.52 | 108.20 |
| 34 | AA | 2814 | U | C2-N3-C4 | -5.41 | 123.76 | 127.00 |
| 27 | Q | 107 | PHE | CB-CG-CD1 | 5.40 | 124.58 | 120.80 |
| 1 | A | 13 | C | O4'-C1'-N1 | 5.40 | 112.52 | 108.20 |
| 1 | A | 1448 | U | C2-N1-C1' | 5.40 | 124.18 | 117.70 |
| 2 | 7 | 56 | U | O4'-C1'-N1 | 5.40 | 112.52 | 108.20 |
| 34 | AA | 247 | A | N1-C6-N6 | 5.40 | 121.84 | 118.60 |
| 34 | AA | 331 | A | O4'-C1'-N9 | 5.40 | 112.52 | 108.20 |
| 34 | AA | 453 | A | C5'-C4'-C3' | 5.40 | 124.64 | 116.00 |
| 34 | AA | 2216 | G | O4'-C1'-N9 | 5.40 | 112.52 | 108.20 |
| 34 | AA | 2954 | A | O4'-C1'-N9 | 5.40 | 112.52 | 108.20 |
| 70 | AE | 21 | ARG | NE-CZ-NH1 | 5.40 | 123.00 | 120.30 |
| 1 | A | 137 | A | C5'-C4'-O4' | 5.40 | 115.58 | 109.10 |
| 1 | A | 1935 | G | O4'-C1'-N9 | 5.40 | 112.52 | 108.20 |
| 34 | AA | 1583 | G | N1-C6-O6 | 5.40 | 123.14 | 119.90 |
| 51 | AP | 160 | ARG | NE-CZ-NH1 | 5.40 | 123.00 | 120.30 |
| 2 | 7 | 70 | A | C5'-C4'-O4' | 5.40 | 115.58 | 109.10 |
| 34 | AA | 3763 | G | O4'-C1'-N9 | 5.40 | 112.52 | 108.20 |
| 1 | A | 1426 | G | O4'-C1'-N9 | 5.39 | 112.52 | 108.20 |
| 1 | A | 1646 | U | O4'-C1'-N1 | 5.39 | 112.52 | 108.20 |
| 23 | J | 117 | ARG | NE-CZ-NH2 | -5.39 | 117.60 | 120.30 |
| 34 | AA | 903 | C | O4'-C1'-N1 | 5.39 | 112.52 | 108.20 |
| 35 | AC | 36 | C | C6-N1-C2 | -5.39 | 118.14 | 120.30 |
| 51 | AP | 71 | ARG | NE-CZ-NH2 | -5.39 | 117.60 | 120.30 |
| 1 | A | 816 | U | O4'-C1'-N1 | 5.39 | 112.51 | 108.20 |
| 1 | A | 868 | U | O4'-C1'-N1 | 5.39 | 112.51 | 108.20 |
| 34 | AA | 1245 | G | O4'-C1'-N9 | 5.39 | 112.51 | 108.20 |
| 34 | AA | 3293 | A | O4'-C1'-N9 | 5.39 | 112.51 | 108.20 |
| 60 | AO | 104 | ARG | NE-CZ-NH1 | 5.39 | 123.00 | 120.30 |
| 65 | AT | 80 | ARG | NE-CZ-NH2 | -5.39 | 117.60 | 120.30 |
| 68 | A5 | 154 | ARG | NE-CZ-NH1 | 5.39 | 123.00 | 120.30 |
| 1 | A | 1211 | G | O4'-C1'-N9 | 5.39 | 112.51 | 108.20 |
| 34 | AA | 3479 | U | O4'-C1'-N1 | 5.39 | 112.51 | 108.20 |
| 34 | AA | 3666 | U | O4'-C1'-N1 | 5.39 | 112.51 | 108.20 |
| 34 | AA | 2551 | U | O4'-C1'-N1 | 5.39 | 112.51 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 34 | AA | 310 | U | O4'-C1'-N1 | 5.39 | 112.51 | 108.20 |
| 1 | A | 2071 | U | O4'-C1'-N1 | 5.39 | 112.51 | 108.20 |
| 2 | 7 | 56 | U | C5'-C4'-O4' | 5.39 | 115.56 | 109.10 |
| 34 | AA | 685 | U | O4'-C1'-N1 | 5.39 | 112.51 | 108.20 |
| 34 | AA | 914 | G | O4'-C1'-N9 | 5.39 | 112.51 | 108.20 |
| 34 | AA | 1161 | C | O4'-C1'-N1 | 5.39 | 112.51 | 108.20 |
| 34 | AA | 2591 | U | C6-N1-C1' | -5.39 | 113.66 | 121.20 |
| 34 | AA | 3386 | A | O4'-C1'-N9 | 5.39 | 112.51 | 108.20 |
| 34 | AA | 266 | U | O4'-C1'-N1 | 5.38 | 112.51 | 108.20 |
| 34 | AA | 356 | A | O4'-C1'-N9 | 5.38 | 112.51 | 108.20 |
| 34 | AA | 2446 | U | O4'-C1'-N1 | 5.38 | 112.51 | 108.20 |
| 49 | Ae | 12 | ARG | NE-CZ-NH2 | -5.38 | 117.61 | 120.30 |
| 34 | AA | 3380 | U | O4'-C1'-N1 | 5.38 | 112.51 | 108.20 |
| 34 | AA | 664 | U | O4'-C1'-N1 | 5.38 | 112.50 | 108.20 |
| 34 | AA | 1273 | G | C5-C6-O6 | -5.38 | 125.37 | 128.60 |
| 34 | AA | 1773 | U | O4'-C1'-N1 | 5.38 | 112.50 | 108.20 |
| 34 | AA | 75 | U | O4'-C1'-N1 | 5.38 | 112.50 | 108.20 |
| 34 | AA | 2386 | A | O4'-C1'-N9 | 5.38 | 112.50 | 108.20 |
| 34 | AA | 3139 | C | O4'-C1'-N1 | 5.38 | 112.50 | 108.20 |
| 34 | AA | 3236 | G | O4'-C1'-N9 | 5.38 | 112.50 | 108.20 |
| 34 | AA | 3504 | C | O4'-C1'-N1 | 5.38 | 112.50 | 108.20 |
| 77 | AX | 102 | TYR | CB-CG-CD1 | 5.38 | 124.23 | 121.00 |
| 1 | A | 117 | G | C5-C6-O6 | -5.38 | 125.37 | 128.60 |
| 34 | AA | 667 | U | C6-N1-C1' | -5.38 | 113.67 | 121.20 |
| 34 | AA | 1427 | U | O4'-C1'-N1 | 5.38 | 112.50 | 108.20 |
| 34 | AA | 2408 | G | C5-C6-O6 | -5.38 | 125.37 | 128.60 |
| 70 | AE | 8 | ARG | NE-CZ-NH2 | 5.38 | 122.99 | 120.30 |
| 1 | A | 1932 | A | P-O3'-C3' | -5.38 | 113.25 | 119.70 |
| 1 | A | 2028 | U | O4'-C1'-N1 | 5.38 | 112.50 | 108.20 |
| 34 | AA | 221 | A | O4'-C1'-N9 | 5.38 | 112.50 | 108.20 |
| 34 | AA | 413 | C | O4'-C1'-N1 | 5.38 | 112.50 | 108.20 |
| 53 | Ai | 8 | ARG | NE-CZ-NH1 | 5.38 | 122.99 | 120.30 |
| 1 | A | 1807 | A | O4'-C1'-N9 | 5.38 | 112.50 | 108.20 |
| 1 | A | 618 | U | O4'-C1'-N1 | 5.37 | 112.50 | 108.20 |
| 34 | AA | 1990 | A | O4'-C1'-N9 | 5.37 | 112.50 | 108.20 |
| 34 | AA | 2689 | G | N3-C2-N2 | 5.37 | 123.66 | 119.90 |
| 34 | AA | 3474 | C | O4'-C1'-N1 | 5.37 | 112.50 | 108.20 |
| 59 | AS | 151 | PHE | CB-CG-CD1 | 5.37 | 124.56 | 120.80 |
| 62 | AR | 50 | ARG | NE-CZ-NH1 | 5.37 | 122.99 | 120.30 |
| 1 | A | 1407 | U | O4'-C1'-N1 | 5.37 | 112.50 | 108.20 |
| 34 | AA | 899 | A | O4'-C1'-N9 | 5.37 | 112.50 | 108.20 |
| 34 | AA | 2939 | C | O4'-C1'-N1 | 5.37 | 112.50 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 74 | AH | 92 | ARG | NE-CZ-NH1 | -5.37 | 117.61 | 120.30 |
| 60 | AO | 4 | ARG | NE-CZ-NH1 | 5.37 | 122.98 | 120.30 |
| 1 | A | 2020 | G | O4'-C1'-N9 | 5.37 | 112.50 | 108.20 |
| 2 | 7 | 12 | G | N1-C6-O6 | 5.37 | 123.12 | 119.90 |
| 34 | AA | 1807 | C | O4'-C1'-N1 | 5.37 | 112.50 | 108.20 |
| 34 | AA | 2148 | U | O4'-C1'-N1 | 5.37 | 112.49 | 108.20 |
| 34 | AA | 2555 | A | O4'-C1'-N9 | 5.37 | 112.50 | 108.20 |
| 34 | AA | 2697 | A | C1'-O4'-C4' | -5.37 | 105.61 | 109.90 |
| 34 | AA | 2720 | C | O4'-C1'-N1 | 5.37 | 112.50 | 108.20 |
| 34 | AA | 3330 | A | O4'-C1'-N9 | 5.37 | 112.50 | 108.20 |
| 1 | A | 1747 | U | O4'-C1'-N1 | 5.37 | 112.49 | 108.20 |
| 5 | G | 222 | PHE | CB-CG-CD1 | 5.37 | 124.56 | 120.80 |
| 34 | AA | 2012 | A | O4'-C1'-N9 | 5.37 | 112.49 | 108.20 |
| 1 | A | 207 | G | N1-C6-O6 | 5.36 | 123.12 | 119.90 |
| 1 | A | 1272 | A | O4'-C1'-N9 | 5.36 | 112.49 | 108.20 |
| 2 | 7 | 48 | U | O4'-C1'-N1 | 5.36 | 112.49 | 108.20 |
| 2 | 7 | 61 | C | C5'-C4'-O4' | 5.36 | 115.54 | 109.10 |
| 34 | AA | 1964 | G | C5-C6-O6 | -5.36 | 125.38 | 128.60 |
| 34 | AA | 2180 | U | O4'-C1'-N1 | 5.36 | 112.49 | 108.20 |
| 69 | AD | 193 | ARG | NE-CZ-NH1 | 5.36 | 122.98 | 120.30 |
| 1 | A | 638 | G | N1-C6-O6 | 5.36 | 123.12 | 119.90 |
| 1 | A | 1302 | G | C5'-C4'-O4' | 5.36 | 115.53 | 109.10 |
| 1 | A | 2007 | U | O4'-C1'-N1 | 5.36 | 112.49 | 108.20 |
| 34 | AA | 524 | U | O4'-C1'-N1 | 5.36 | 112.49 | 108.20 |
| 34 | AA | 1456 | C | O4'-C1'-N1 | 5.36 | 112.49 | 108.20 |
| 34 | AA | 1723 | C | C6-N1-C2 | -5.36 | 118.16 | 120.30 |
| 34 | AA | 1975 | A | N1-C6-N6 | -5.36 | 115.38 | 118.60 |
| 34 | AA | 1670 | G | N1-C6-O6 | 5.36 | 123.11 | 119.90 |
| 34 | AA | 3167 | A | C1'-O4'-C4' | -5.36 | 105.61 | 109.90 |
| 1 | A | 1383 | U | O4'-C1'-N1 | 5.36 | 112.48 | 108.20 |
| 34 | AA | 1445 | A | O4'-C1'-N9 | 5.35 | 112.48 | 108.20 |
| 34 | AA | 1504 | A | C1'-O4'-C4' | -5.35 | 105.62 | 109.90 |
| 34 | AA | 1744 | U | O4'-C1'-N1 | 5.35 | 112.48 | 108.20 |
| 34 | AA | 2009 | A | O4'-C1'-N9 | 5.35 | 112.48 | 108.20 |
| 34 | AA | 169 | U | O4'-C1'-N1 | 5.35 | 112.48 | 108.20 |
| 34 | AA | 915 | G | C5-C6-O6 | -5.35 | 125.39 | 128.60 |
| 34 | AA | 1640 | G | C5-C6-O6 | -5.35 | 125.39 | 128.60 |
| 1 | A | 63 | G | C5-C6-O6 | -5.35 | 125.39 | 128.60 |
| 34 | AA | 148 | G | P-O3'-C3' | 5.35 | 126.12 | 119.70 |
| 34 | AA | 3352 | G | N1-C6-O6 | 5.35 | 123.11 | 119.90 |
| 1 | A | 1000 | C | O4'-C1'-N1 | 5.35 | 112.48 | 108.20 |
| 1 | A | 3 | C | O4'-C1'-N1 | 5.34 | 112.48 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 34 | AA | 767 | U | O4'-C1'-N1 | 5.34 | 112.48 | 108.20 |
| 34 | AA | 1816 | G | O4'-C1'-N9 | 5.34 | 112.47 | 108.20 |
| 36 | AB | 37 | A | O4'-C1'-N9 | 5.34 | 112.48 | 108.20 |
| 34 | AA | 1202 | C | P-O5'-C5' | 5.34 | 129.45 | 120.90 |
| 1 | A | 2021 | U | O4'-C1'-N1 | 5.34 | 112.47 | 108.20 |
| 34 | AA | 2581 | G | C5-C6-O6 | -5.34 | 125.39 | 128.60 |
| 68 | A5 | 113 | ARG | NE-CZ-NH2 | 5.34 | 122.97 | 120.30 |
| 1 | A | 1676 | U | O4'-C1'-N1 | 5.34 | 112.47 | 108.20 |
| 8 | M | 123 | ARG | NE-CZ-NH2 | -5.34 | 117.63 | 120.30 |
| 34 | AA | 906 | G | O4'-C1'-N9 | 5.34 | 112.47 | 108.20 |
| 34 | AA | 2093 | U | C5'-C4'-C3' | -5.34 | 107.46 | 116.00 |
| 34 | AA | 2505 | C | O4'-C1'-N1 | 5.34 | 112.47 | 108.20 |
| 34 | AA | 3763 | G | N1-C6-O6 | 5.34 | 123.10 | 119.90 |
| 43 | AN | 120 | ARG | NE-CZ-NH1 | 5.34 | 122.97 | 120.30 |
| 70 | AE | 93 | ARG | NE-CZ-NH1 | 5.34 | 122.97 | 120.30 |
| 1 | A | 383 | G | O4'-C1'-N9 | 5.34 | 112.47 | 108.20 |
| 34 | AA | 2577 | C | C6-N1-C2 | -5.34 | 118.17 | 120.30 |
| 35 | AC | 36 | C | O4'-C1'-N1 | 5.33 | 112.47 | 108.20 |
| 62 | AR | 195 | ARG | NE-CZ-NH2 | 5.33 | 122.97 | 120.30 |
| 1 | A | 328 | G | N1-C6-O6 | 5.33 | 123.10 | 119.90 |
| 34 | AA | 22 | G | C5-C6-O6 | -5.33 | 125.40 | 128.60 |
| 34 | AA | 176 | A | O4'-C1'-N9 | 5.33 | 112.47 | 108.20 |
| 34 | AA | 1337 | G | O4'-C1'-N9 | 5.33 | 112.47 | 108.20 |
| 34 | AA | 3194 | C | O4'-C1'-N1 | 5.33 | 112.47 | 108.20 |
| 41 | A6 | 89 | ARG | NE-CZ-NH2 | -5.33 | 117.63 | 120.30 |
| 1 | A | 344 | C | C6-N1-C2 | -5.33 | 118.17 | 120.30 |
| 1 | A | 1188 | A | N1-C6-N6 | 5.33 | 121.80 | 118.60 |
| 1 | A | 1364 | G | C5-C6-O6 | -5.33 | 125.40 | 128.60 |
| 34 | AA | 1538 | U | C5'-C4'-O4' | 5.33 | 115.50 | 109.10 |
| 34 | AA | 3408 | G | O4'-C1'-N9 | 5.33 | 112.47 | 108.20 |
| 34 | AA | 935 | A | O4'-C1'-N9 | 5.33 | 112.46 | 108.20 |
| 34 | AA | 1028 | G | P-O3'-C3' | -5.33 | 113.30 | 119.70 |
| 34 | AA | 270 | U | C2'-C3'-O3' | 5.33 | 122.23 | 113.70 |
| 54 | AI | 44 | TYR | CB-CG-CD2 | 5.33 | 124.20 | 121.00 |
| 34 | AA | 812 | U | C5'-C4'-C3' | -5.33 | 107.48 | 116.00 |
| 34 | AA | 1188 | A | O4'-C1'-N9 | 5.33 | 112.46 | 108.20 |
| 34 | AA | 3520 | U | O4'-C1'-N1 | 5.33 | 112.46 | 108.20 |
| 1 | A | 981 | U | C5'-C4'-C3' | -5.33 | 107.48 | 116.00 |
| 2 | 7 | 64 | C | O4'-C1'-N1 | 5.33 | 112.46 | 108.20 |
| 34 | AA | 15 | U | O4'-C1'-N1 | 5.33 | 112.46 | 108.20 |
| 34 | AA | 1213 | U | O4'-C1'-N1 | 5.33 | 112.46 | 108.20 |
| 34 | AA | 3133 | U | O4'-C1'-N1 | 5.33 | 112.46 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 34 | AA | 13 | G | O4'-C1'-N9 | 5.32 | 112.46 | 108.20 |
| 34 | AA | 1480 | G | N1-C6-O6 | 5.32 | 123.09 | 119.90 |
| 34 | AA | 2826 | C | O4'-C1'-N1 | 5.32 | 112.46 | 108.20 |
| 70 | AE | 100 | ARG | NE-CZ-NH1 | 5.32 | 122.96 | 120.30 |
| 34 | AA | 824 | U | O4'-C1'-N1 | 5.32 | 112.46 | 108.20 |
| 34 | AA | 40 | A | O4'-C1'-N9 | 5.32 | 112.45 | 108.20 |
| 34 | AA | 1420 | C | C6-N1-C2 | -5.32 | 118.17 | 120.30 |
| 34 | AA | 2611 | U | O4'-C1'-N1 | 5.32 | 112.45 | 108.20 |
| 1 | A | 1453 | G | O4'-C1'-N9 | 5.32 | 112.45 | 108.20 |
| 34 | AA | 1189 | G | O4'-C1'-N9 | 5.32 | 112.45 | 108.20 |
| 34 | AA | 1331 | A | O4'-C1'-N9 | 5.32 | 112.45 | 108.20 |
| 34 | AA | 2137 | C | O4'-C1'-N1 | 5.32 | 112.45 | 108.20 |
| 34 | AA | 2735 | G | C5-C6-O6 | -5.32 | 125.41 | 128.60 |
| 34 | AA | 231 | G | C5'-C4'-O4' | 5.32 | 115.48 | 109.10 |
| 34 | AA | 1050 | C | O4'-C1'-N1 | 5.32 | 112.45 | 108.20 |
| 34 | AA | 1593 | G | N1-C6-O6 | 5.32 | 123.09 | 119.90 |
| 34 | AA | 1814 | U | O4'-C1'-N1 | 5.32 | 112.45 | 108.20 |
| 34 | AA | 2997 | G | C5-C6-O6 | -5.32 | 125.41 | 128.60 |
| 34 | AA | 3327 | G | O4'-C1'-N9 | 5.32 | 112.45 | 108.20 |
| 1 | A | 173 | G | C5-C6-O6 | -5.31 | 125.41 | 128.60 |
| 1 | A | 252 | U | O4'-C1'-N1 | 5.31 | 112.45 | 108.20 |
| 1 | A | 1095 | A | P-O3'-C3' | -5.31 | 113.32 | 119.70 |
| 34 | AA | 110 | G | O4'-C1'-N9 | 5.31 | 112.45 | 108.20 |
| 34 | AA | 259 | G | C5'-C4'-C3' | 5.31 | 124.50 | 116.00 |
| 34 | AA | 746 | A | O4'-C1'-N9 | 5.31 | 112.45 | 108.20 |
| 34 | AA | 1496 | U | C5'-C4'-C3' | 5.31 | 124.50 | 116.00 |
| 1 | A | 1445 | U | P-O3'-C3' | 5.31 | 126.07 | 119.70 |
| 1 | A | 1197 | C | P-O5'-C5' | 5.31 | 129.39 | 120.90 |
| 1 | A | 1971 | U | O4'-C1'-N1 | 5.31 | 112.45 | 108.20 |
| 11 | O | 88 | ARG | NE-CZ-NH1 | 5.31 | 122.95 | 120.30 |
| 24 | L | 49 | ARG | NE-CZ-NH1 | 5.31 | 122.95 | 120.30 |
| 34 | AA | 1694 | G | N1-C6-O6 | 5.31 | 123.09 | 119.90 |
| 59 | AS | 57 | ARG | NE-CZ-NH2 | 5.31 | 122.95 | 120.30 |
| 34 | AA | 246 | U | O4'-C1'-N1 | 5.31 | 112.45 | 108.20 |
| 34 | AA | 1537 | G | C5-C6-O6 | -5.31 | 125.42 | 128.60 |
| 1 | A | 2009 | C | O4'-C1'-N1 | 5.31 | 112.44 | 108.20 |
| 1 | A | 119 | C | O4'-C1'-N1 | 5.30 | 112.44 | 108.20 |
| 1 | A | 849 | U | P-O5'-C5' | 5.30 | 129.39 | 120.90 |
| 1 | A | 1816 | U | C5'-C4'-O4' | 5.30 | 115.47 | 109.10 |
| 34 | AA | 2592 | A | O4'-C1'-N9 | 5.30 | 112.44 | 108.20 |
| 59 | AS | 163 | ARG | NE-CZ-NH1 | 5.30 | 122.95 | 120.30 |
| 2 | 7 | 35 | C | O4'-C1'-N1 | 5.30 | 112.44 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 34 | AA | 2128 | G | O4'-C1'-N9 | 5.30 | 112.44 | 108.20 |
| 34 | AA | 2559 | U | O4'-C1'-N1 | 5.30 | 112.44 | 108.20 |
| 68 | A5 | 149 | THR | N-CA-CB | 5.30 | 120.38 | 110.30 |
| 2 | 7 | 68 | U | P-O3'-C3' | -5.30 | 113.34 | 119.70 |
| 31 | V | 106 | ARG | NE-CZ-NH1 | 5.30 | 122.95 | 120.30 |
| 2 | 7 | 49 | C | C5'-C4'-O4' | 5.30 | 115.46 | 109.10 |
| 34 | AA | 204 | G | C5-C6-O6 | -5.30 | 125.42 | 128.60 |
| 34 | AA | 1617 | A | O4'-C1'-N9 | 5.30 | 112.44 | 108.20 |
| 34 | AA | 530 | U | O4'-C1'-N1 | 5.30 | 112.44 | 108.20 |
| 34 | AA | 1299 | G | O4'-C1'-N9 | 5.30 | 112.44 | 108.20 |
| 1 | A | 461 | A | O4'-C1'-N9 | 5.30 | 112.44 | 108.20 |
| 34 | AA | 35 | A | O4'-C1'-N9 | 5.30 | 112.44 | 108.20 |
| 69 | AD | 69 | TYR | CB-CG-CD2 | -5.29 | 117.82 | 121.00 |
| 1 | A | 2061 | U | O4'-C1'-N1 | 5.29 | 112.44 | 108.20 |
| 34 | AA | 371 | G | O4'-C1'-N9 | 5.29 | 112.43 | 108.20 |
| 34 | AA | 1564 | G | C5-C6-O6 | -5.29 | 125.42 | 128.60 |
| 34 | AA | 581 | C | C2'-C3'-O3' | 5.29 | 122.17 | 113.70 |
| 34 | AA | 2436 | A | O4'-C1'-N9 | 5.29 | 112.43 | 108.20 |
| 34 | AA | 2805 | U | O4'-C1'-N1 | 5.29 | 112.43 | 108.20 |
| 34 | AA | 3312 | U | O4'-C1'-N1 | 5.29 | 112.43 | 108.20 |
| 54 | AI | 98 | ARG | NE-CZ-NH1 | 5.29 | 122.95 | 120.30 |
| 1 | A | 1735 | U | C2-N1-C1' | 5.29 | 124.05 | 117.70 |
| 34 | AA | 503 | A | P-O3'-C3' | 5.29 | 126.05 | 119.70 |
| 34 | AA | 1723 | C | O4'-C1'-N1 | 5.29 | 112.43 | 108.20 |
| 1 | A | 750 | U | O4'-C1'-N1 | 5.29 | 112.43 | 108.20 |
| 1 | A | 1454 | G | P-O5'-C5' | 5.29 | 129.36 | 120.90 |
| 1 | A | 1812 | A | N1-C6-N6 | 5.29 | 121.77 | 118.60 |
| 6 | I | 16 | TYR | CB-CG-CD1 | -5.29 | 117.83 | 121.00 |
| 16 | 3 | 87 | ARG | NE-CZ-NH1 | 5.29 | 122.94 | 120.30 |
| 34 | AA | 76 | G | N1-C6-O6 | 5.29 | 123.07 | 119.90 |
| 34 | AA | 1071 | A | P-O3'-C3' | 5.29 | 126.05 | 119.70 |
| 34 | AA | 1628 | U | O4'-C1'-N1 | 5.29 | 112.43 | 108.20 |
| 34 | AA | 3402 | A | O4'-C1'-N9 | 5.29 | 112.43 | 108.20 |
| 35 | AC | 157 | A | O4'-C1'-N9 | 5.29 | 112.43 | 108.20 |
| 1 | A | 933 | A | O4'-C1'-N9 | 5.29 | 112.43 | 108.20 |
| 1 | A | 2052 | G | C1'-O4'-C4' | 5.29 | 114.13 | 109.90 |
| 1 | A | 1858 | U | O4'-C1'-N1 | 5.29 | 112.43 | 108.20 |
| 2 | 7 | 2 | G | O4'-C1'-N9 | 5.29 | 112.43 | 108.20 |
| 7 | K | 57 | ARG | NE-CZ-NH2 | -5.29 | 117.66 | 120.30 |
| 34 | AA | 73 | U | O4'-C1'-N1 | 5.29 | 112.43 | 108.20 |
| 34 | AA | 1556 | G | N1-C6-O6 | 5.29 | 123.07 | 119.90 |
| 34 | AA | 1659 | A | P-O3'-C3' | -5.29 | 113.36 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 36 | AB | 86 | G | O4'-C1'-N9 | 5.29 | 112.43 | 108.20 |
| 33 | C | 116 | THR | N-CA-CB | 5.28 | 120.34 | 110.30 |
| 34 | AA | 263 | U | O4'-C1'-N1 | 5.28 | 112.43 | 108.20 |
| 34 | AA | 1507 | U | O4'-C1'-N1 | 5.28 | 112.43 | 108.20 |
| 34 | AA | 128 | U | O4'-C1'-N1 | 5.28 | 112.43 | 108.20 |
| 1 | A | 342 | G | C5-C6-O6 | -5.28 | 125.43 | 128.60 |
| 1 | A | 450 | C | O4'-C1'-N1 | 5.28 | 112.42 | 108.20 |
| 25 | N | 67 | SER | N-CA-CB | 5.28 | 118.42 | 110.50 |
| 34 | AA | 1338 | U | O4'-C1'-N1 | 5.28 | 112.42 | 108.20 |
| 34 | AA | 3249 | A | O4'-C1'-N9 | 5.28 | 112.42 | 108.20 |
| 34 | AA | 3338 | U | O4'-C1'-N1 | 5.28 | 112.42 | 108.20 |
| 34 | AA | 3422 | G | O4'-C1'-N9 | 5.28 | 112.42 | 108.20 |
| 1 | A | 1364 | G | O4'-C1'-N9 | 5.28 | 112.42 | 108.20 |
| 34 | AA | 497 | U | O4'-C1'-N1 | 5.28 | 112.42 | 108.20 |
| 34 | AA | 1283 | C | C6-N1-C2 | -5.28 | 118.19 | 120.30 |
| 34 | AA | 3740 | A | O4'-C1'-N9 | 5.28 | 112.42 | 108.20 |
| 35 | AC | 94 | C | C6-N1-C2 | -5.28 | 118.19 | 120.30 |
| 35 | AC | 125 | U | O4'-C1'-N1 | 5.28 | 112.42 | 108.20 |
| 1 | A | 758 | U | P-O5'-C5' | 5.28 | 129.34 | 120.90 |
| 34 | AA | 42 | C | O4'-C1'-N1 | 5.28 | 112.42 | 108.20 |
| 34 | AA | 2469 | U | O4'-C1'-N1 | 5.28 | 112.42 | 108.20 |
| 34 | AA | 2554 | G | N1-C6-O6 | 5.28 | 123.06 | 119.90 |
| 1 | A | 1944 | U | C5'-C4'-O4' | 5.27 | 115.43 | 109.10 |
| 34 | AA | 2746 | U | O4'-C1'-N1 | 5.27 | 112.42 | 108.20 |
| 53 | Ai | 57 | PHE | CB-CG-CD2 | 5.27 | 124.49 | 120.80 |
| 1 | A | 4 | C | O4'-C1'-N1 | 5.27 | 112.42 | 108.20 |
| 1 | A | 1723 | A | O4'-C1'-N9 | 5.27 | 112.42 | 108.20 |
| 34 | AA | 1648 | U | O4'-C1'-N1 | 5.27 | 112.42 | 108.20 |
| 1 | A | 560 | G | C5-C6-O6 | -5.27 | 125.44 | 128.60 |
| 1 | A | 634 | C | O4'-C1'-N1 | 5.27 | 112.42 | 108.20 |
| 16 | 3 | 39 | PHE | CB-CG-CD2 | -5.27 | 117.11 | 120.80 |
| 34 | AA | 56 | G | O4'-C1'-N9 | 5.27 | 112.42 | 108.20 |
| 34 | AA | 900 | G | O4'-C1'-N9 | 5.27 | 112.42 | 108.20 |
| 34 | AA | 2034 | G | C5'-C4'-O4' | -5.27 | 102.78 | 109.10 |
| 34 | AA | 2093 | U | C5'-C4'-O4' | 5.27 | 115.42 | 109.10 |
| 34 | AA | 2527 | G | O4'-C1'-N9 | 5.27 | 112.41 | 108.20 |
| 34 | AA | 2594 | U | O4'-C1'-N1 | 5.27 | 112.41 | 108.20 |
| 1 | A | 168 | U | P-O3'-C3' | -5.27 | 113.38 | 119.70 |
| 1 | A | 379 | G | C5'-C4'-C3' | -5.26 | 107.58 | 116.00 |
| 1 | A | 1375 | C | C2-N1-C1' | 5.26 | 124.59 | 118.80 |
| 34 | AA | 1573 | C | C6-N1-C1' | -5.26 | 114.48 | 120.80 |
| 34 | AA | 2489 | C | O4'-C1'-N1 | 5.26 | 112.41 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 34 | AA | 3124 | G | O4'-C1'-N9 | 5.26 | 112.41 | 108.20 |
| 1 | A | 99 | C | C6-N1-C2 | -5.26 | 118.19 | 120.30 |
| 1 | A | 490 | C | O4'-C1'-N1 | 5.26 | 112.41 | 108.20 |
| 1 | A | 1652 | A | O4'-C1'-N9 | 5.26 | 112.41 | 108.20 |
| 34 | AA | 975 | G | N1-C6-O6 | 5.26 | 123.06 | 119.90 |
| 34 | AA | 3086 | A | C5'-C4'-O4' | 5.26 | 115.41 | 109.10 |
| 59 | AS | 167 | ARG | NE-CZ-NH1 | 5.26 | 122.93 | 120.30 |
| 75 | AV | 98 | ARG | NE-CZ-NH1 | -5.26 | 117.67 | 120.30 |
| 1 | A | 795 | U | O4'-C1'-N1 | 5.26 | 112.41 | 108.20 |
| 1 | A | 1184 | G | C5-C6-O6 | -5.26 | 125.44 | 128.60 |
| 72 | AG | 35 | ARG | NE-CZ-NH2 | 5.26 | 122.93 | 120.30 |
| 1 | A | 1844 | A | P-O3'-C3' | -5.26 | 113.39 | 119.70 |
| 1 | A | 1964 | G | O4'-C1'-N9 | 5.26 | 112.41 | 108.20 |
| 4 | E | 126 | ARG | NE-CZ-NH2 | -5.26 | 117.67 | 120.30 |
| 34 | AA | 26 | A | O4'-C1'-N9 | 5.26 | 112.41 | 108.20 |
| 35 | AC | 4 | C | O4'-C1'-N1 | 5.26 | 112.41 | 108.20 |
| 36 | AB | 48 | G | O4'-C1'-N9 | 5.26 | 112.41 | 108.20 |
| 1 | A | 844 | G | C5'-C4'-C3' | 5.25 | 124.41 | 116.00 |
| 34 | AA | 1843 | U | O4'-C1'-N1 | 5.25 | 112.40 | 108.20 |
| 36 | AB | 108 | G | O4'-C1'-N9 | 5.25 | 112.40 | 108.20 |
| 1 | A | 379 | G | N1-C6-O6 | 5.25 | 123.05 | 119.90 |
| 1 | A | 1645 | C | C6-N1-C1' | -5.25 | 114.50 | 120.80 |
| 34 | AA | 1956 | U | O4'-C1'-N1 | 5.25 | 112.40 | 108.20 |
| 34 | AA | 2485 | C | C5'-C4'-C3' | -5.25 | 107.60 | 116.00 |
| 1 | A | 68 | U | C5'-C4'-O4' | 5.25 | 115.40 | 109.10 |
| 34 | AA | 636 | U | P-O3'-C3' | 5.25 | 126.00 | 119.70 |
| 1 | A | 931 | A | O4'-C1'-N9 | 5.25 | 112.40 | 108.20 |
| 34 | AA | 971 | U | O4'-C1'-N1 | 5.25 | 112.40 | 108.20 |
| 34 | AA | 2449 | U | O4'-C1'-N1 | 5.25 | 112.40 | 108.20 |
| 34 | AA | 3032 | U | O4'-C1'-N1 | 5.25 | 112.40 | 108.20 |
| 1 | A | 174 | C | O4'-C1'-N1 | 5.25 | 112.40 | 108.20 |
| 1 | A | 640 | U | O4'-C1'-N1 | 5.25 | 112.40 | 108.20 |
| 34 | AA | 229 | A | O4'-C1'-N9 | 5.25 | 112.40 | 108.20 |
| 34 | AA | 272 | U | O4'-C1'-N1 | 5.25 | 112.40 | 108.20 |
| 34 | AA | 721 | U | P-O3'-C3' | 5.25 | 126.00 | 119.70 |
| 34 | AA | 1240 | A | O4'-C1'-N9 | 5.25 | 112.40 | 108.20 |
| 34 | AA | 2582 | U | O4'-C1'-N1 | 5.25 | 112.40 | 108.20 |
| 63 | AW | 38 | ARG | NE-CZ-NH1 | 5.25 | 122.92 | 120.30 |
| 34 | AA | 2524 | C | C6-N1-C1' | -5.25 | 114.51 | 120.80 |
| 35 | AC | 37 | A | O4'-C1'-N9 | 5.25 | 112.40 | 108.20 |
| 1 | A | 1103 | C | O4'-C1'-N1 | 5.24 | 112.39 | 108.20 |
| 34 | AA | 280 | U | O4'-C1'-N1 | 5.24 | 112.39 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 34 | AA | 501 | U | C4'-C3'-C2' | -5.24 | 97.36 | 102.60 |
| 34 | AA | 985 | G | C5-C6-O6 | -5.24 | 125.45 | 128.60 |
| 34 | AA | 1059 | G | O4'-C1'-N9 | 5.24 | 112.39 | 108.20 |
| 1 | A | 1436 | U | O4'-C1'-N1 | 5.24 | 112.39 | 108.20 |
| 34 | AA | 714 | C | C4'-C3'-C2' | -5.24 | 97.36 | 102.60 |
| 34 | AA | 2663 | G | C5-C6-O6 | -5.24 | 125.45 | 128.60 |
| 1 | A | 554 | U | O4'-C1'-N1 | 5.24 | 112.39 | 108.20 |
| 1 | A | 1076 | C | P-O3'-C3' | -5.24 | 113.41 | 119.70 |
| 1 | A | 1403 | U | C5'-C4'-C3' | -5.24 | 107.62 | 116.00 |
| 34 | AA | 1252 | U | O4'-C1'-N1 | 5.24 | 112.39 | 108.20 |
| 34 | AA | 768 | C | C6-N1-C1' | -5.24 | 114.51 | 120.80 |
| 37 | AL | 198 | ARG | NE-CZ-NH2 | 5.24 | 122.92 | 120.30 |
| 1 | A | 1005 | G | O4'-C1'-N9 | 5.24 | 112.39 | 108.20 |
| 2 | 7 | 47 | G | O4'-C1'-N9 | 5.24 | 112.39 | 108.20 |
| 34 | AA | 415 | U | O4'-C1'-N1 | 5.24 | 112.39 | 108.20 |
| 57 | AK | 107 | MET | CG-SD-CE | -5.24 | 91.82 | 100.20 |
| 1 | A | 307 | G | C5-C6-O6 | -5.24 | 125.46 | 128.60 |
| 34 | AA | 584 | U | O4'-C1'-N1 | 5.24 | 112.39 | 108.20 |
| 34 | AA | 3334 | U | O4'-C1'-N1 | 5.24 | 112.39 | 108.20 |
| 26 | P | 37 | PHE | N-CA-CB | 5.23 | 120.02 | 110.60 |
| 34 | AA | 227 | A | O4'-C1'-N9 | 5.23 | 112.39 | 108.20 |
| 1 | A | 530 | U | P-O3'-C3' | -5.23 | 113.42 | 119.70 |
| 34 | AA | 517 | U | O4'-C1'-N1 | 5.23 | 112.39 | 108.20 |
| 34 | AA | 2715 | C | C6-N1-C2 | -5.23 | 118.21 | 120.30 |
| 1 | A | 1273 | G | O4'-C1'-N9 | 5.23 | 112.38 | 108.20 |
| 6 | I | 86 | TYR | CB-CG-CD1 | -5.23 | 117.86 | 121.00 |
| 1 | A | 560 | G | N1-C6-O6 | 5.23 | 123.04 | 119.90 |
| 1 | A | 1040 | A | O4'-C1'-N9 | 5.23 | 112.38 | 108.20 |
| 1 | A | 1321 | C | C5'-C4'-O4' | 5.23 | 115.37 | 109.10 |
| 34 | AA | 1140 | A | O4'-C1'-N9 | 5.23 | 112.38 | 108.20 |
| 34 | AA | 2509 | U | O4'-C1'-N1 | 5.23 | 112.38 | 108.20 |
| 34 | AA | 3275 | C | P-O3'-C3' | -5.23 | 113.43 | 119.70 |
| 1 | A | 33 | U | O4'-C1'-N1 | 5.23 | 112.38 | 108.20 |
| 27 | Q | 144 | ARG | NE-CZ-NH2 | -5.23 | 117.69 | 120.30 |
| 34 | AA | 1067 | U | O4'-C1'-N1 | 5.23 | 112.38 | 108.20 |
| 34 | AA | 1484 | A | O4'-C1'-N9 | 5.23 | 112.38 | 108.20 |
| 34 | AA | 3786 | U | O4'-C1'-N1 | 5.23 | 112.38 | 108.20 |
| 74 | AH | 172 | ARG | NH1-CZ-NH2 | -5.23 | 113.65 | 119.40 |
| 1 | A | 2085 | G | O4'-C1'-N9 | 5.22 | 112.38 | 108.20 |
| 34 | AA | 2807 | U | O4'-C1'-N1 | 5.22 | 112.38 | 108.20 |
| 1 | A | 846 | G | O4'-C1'-N9 | 5.22 | 112.38 | 108.20 |
| 12 | Y | 66 | ARG | NE-CZ-NH1 | -5.22 | 117.69 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 34 | AA | 3569 | C | O4'-C1'-N1 | 5.22 | 112.38 | 108.20 |
| 34 | AA | 130 | G | P-O3'-C3' | -5.22 | 113.43 | 119.70 |
| 1 | A | 861 | C | O4'-C1'-N1 | 5.22 | 112.38 | 108.20 |
| 7 | K | 120 | HIS | N-CA-CB | 5.22 | 120.00 | 110.60 |
| 20 | B | 165 | ARG | NE-CZ-NH1 | 5.22 | 122.91 | 120.30 |
| 34 | AA | 11 | A | N1-C6-N6 | 5.22 | 121.73 | 118.60 |
| 34 | AA | 1457 | G | P-O3'-C3' | 5.22 | 125.96 | 119.70 |
| 34 | AA | 1897 | G | O4'-C1'-N9 | 5.22 | 112.38 | 108.20 |
| 34 | AA | 3736 | A | O4'-C1'-N9 | 5.22 | 112.38 | 108.20 |
| 34 | AA | 199 | G | N1-C6-O6 | 5.22 | 123.03 | 119.90 |
| 34 | AA | 3239 | U | O4'-C1'-N1 | 5.22 | 112.37 | 108.20 |
| 1 | A | 1921 | C | O4'-C1'-N1 | 5.22 | 112.37 | 108.20 |
| 34 | AA | 3047 | U | O4'-C1'-N1 | 5.22 | 112.37 | 108.20 |
| 1 | A | 102 | A | O4'-C1'-N9 | 5.21 | 112.37 | 108.20 |
| 34 | AA | 340 | U | O4'-C1'-N1 | 5.21 | 112.37 | 108.20 |
| 34 | AA | 643 | G | C5-C6-O6 | -5.21 | 125.47 | 128.60 |
| 34 | AA | 2504 | U | O4'-C1'-N1 | 5.21 | 112.37 | 108.20 |
| 35 | AC | 69 | A | O4'-C1'-N9 | 5.21 | 112.37 | 108.20 |
| 46 | Aa | 8 | ARG | NE-CZ-NH1 | 5.21 | 122.91 | 120.30 |
| 78 | A0 | 63 | ARG | NE-CZ-NH1 | 5.21 | 122.91 | 120.30 |
| 1 | A | 1382 | G | P-O5'-C5' | 5.21 | 129.24 | 120.90 |
| 1 | A | 1957 | A | O4'-C1'-N9 | 5.21 | 112.37 | 108.20 |
| 34 | AA | 2090 | U | C5'-C4'-C3' | -5.21 | 107.66 | 116.00 |
| 1 | A | 557 | A | O4'-C1'-N9 | 5.21 | 112.37 | 108.20 |
| 1 | A | 2065 | C | O4'-C1'-N1 | 5.21 | 112.37 | 108.20 |
| 20 | B | 107 | ARG | NE-CZ-NH1 | 5.21 | 122.91 | 120.30 |
| 34 | AA | 384 | A | O4'-C1'-N9 | 5.21 | 112.37 | 108.20 |
| 34 | AA | 747 | A | N1-C6-N6 | 5.21 | 121.73 | 118.60 |
| 34 | AA | 833 | G | C5-C6-O6 | -5.21 | 125.47 | 128.60 |
| 1 | A | 799 | U | O4'-C1'-N1 | 5.21 | 112.37 | 108.20 |
| 34 | AA | 3008 | A | O4'-C1'-N9 | 5.21 | 112.37 | 108.20 |
| 1 | A | 1027 | C | O4'-C1'-N1 | 5.21 | 112.37 | 108.20 |
| 34 | AA | 490 | U | O4'-C1'-N1 | 5.21 | 112.37 | 108.20 |
| 34 | AA | 684 | G | O4'-C1'-N9 | 5.21 | 112.37 | 108.20 |
| 34 | AA | 1538 | U | C5'-C4'-C3' | -5.21 | 107.67 | 116.00 |
| 34 | AA | 1564 | G | N1-C6-O6 | 5.21 | 123.03 | 119.90 |
| 34 | AA | 2814 | U | O4'-C1'-N1 | 5.21 | 112.37 | 108.20 |
| 34 | AA | 3120 | U | C5'-C4'-O4' | 5.21 | 115.35 | 109.10 |
| 1 | A | 1173 | C | O4'-C1'-N1 | 5.21 | 112.37 | 108.20 |
| 1 | A | 1239 | A | N1-C6-N6 | -5.21 | 115.48 | 118.60 |
| 1 | A | 1821 | A | O4'-C1'-N9 | 5.21 | 112.36 | 108.20 |
| 34 | AA | 455 | U | O4'-C1'-N1 | 5.21 | 112.36 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 34 | AA | 2081 | U | O4'-C1'-N1 | 5.21 | 112.36 | 108.20 |
| 34 | AA | 2583 | C | O4'-C1'-N1 | 5.21 | 112.36 | 108.20 |
| 34 | AA | 3231 | A | O4'-C1'-N9 | 5.21 | 112.36 | 108.20 |
| 34 | AA | 3443 | A | N9-C1'-C2' | -5.21 | 106.27 | 112.00 |
| 1 | A | 91 | G | O4'-C1'-N9 | 5.20 | 112.36 | 108.20 |
| 1 | A | 542 | C | C6-N1-C2 | -5.20 | 118.22 | 120.30 |
| 1 | A | 986 | U | O4'-C1'-N1 | 5.20 | 112.36 | 108.20 |
| 1 | A | 1010 | A | O4'-C1'-N9 | 5.20 | 112.36 | 108.20 |
| 1 | A | 1108 | A | C4'-C3'-C2' | -5.20 | 97.40 | 102.60 |
| 34 | AA | 1598 | A | O4'-C1'-N9 | 5.20 | 112.36 | 108.20 |
| 34 | AA | 2534 | U | O4'-C1'-N1 | 5.20 | 112.36 | 108.20 |
| 34 | AA | 2728 | G | N1-C6-O6 | 5.20 | 123.02 | 119.90 |
| 1 | A | 884 | G | C5-C6-O6 | -5.20 | 125.48 | 128.60 |
| 34 | AA | 2994 | A | P-O5'-C5' | -5.20 | 112.58 | 120.90 |
| 34 | AA | 449 | A | P-O3'-C3' | 5.20 | 125.94 | 119.70 |
| 34 | AA | 582 | U | O4'-C1'-N1 | 5.20 | 112.36 | 108.20 |
| 34 | AA | 818 | C | O4'-C1'-N1 | 5.20 | 112.36 | 108.20 |
| 34 | AA | 3272 | U | O4'-C1'-N1 | 5.20 | 112.36 | 108.20 |
| 1 | A | 208 | U | O4'-C1'-N1 | 5.20 | 112.36 | 108.20 |
| 1 | A | 541 | C | O4'-C1'-N1 | 5.20 | 112.36 | 108.20 |
| 1 | A | 1097 | C | O4'-C1'-N1 | 5.20 | 112.36 | 108.20 |
| 1 | A | 1893 | C | C6-N1-C1' | -5.20 | 114.56 | 120.80 |
| 1 | A | 1943 | C | C5'-C4'-O4' | 5.20 | 115.34 | 109.10 |
| 34 | AA | 166 | U | O4'-C1'-N1 | 5.20 | 112.36 | 108.20 |
| 34 | AA | 856 | C | O4'-C1'-N1 | 5.20 | 112.36 | 108.20 |
| 34 | AA | 1751 | C | O4'-C1'-N1 | 5.20 | 112.36 | 108.20 |
| 35 | AC | 38 | G | C1'-O4'-C4' | -5.20 | 105.74 | 109.90 |
| 2 | 7 | 25 | G | O4'-C1'-N9 | 5.20 | 112.36 | 108.20 |
| 34 | AA | 287 | U | O4'-C1'-N1 | 5.20 | 112.36 | 108.20 |
| 34 | AA | 1968 | C | O4'-C1'-N1 | 5.20 | 112.36 | 108.20 |
| 34 | AA | 2075 | U | O4'-C1'-N1 | 5.20 | 112.36 | 108.20 |
| 1 | A | 578 | G | P-O3'-C3' | 5.19 | 125.93 | 119.70 |
| 1 | A | 911 | U | O4'-C1'-N1 | 5.19 | 112.35 | 108.20 |
| 1 | A | 928 | U | O4'-C1'-N1 | 5.19 | 112.35 | 108.20 |
| 34 | AA | 332 | A | P-O3'-C3' | 5.19 | 125.93 | 119.70 |
| 34 | AA | 1061 | U | O4'-C1'-N1 | 5.19 | 112.35 | 108.20 |
| 34 | AA | 2117 | A | O4'-C1'-N9 | 5.19 | 112.35 | 108.20 |
| 35 | AC | 11 | U | O4'-C1'-N1 | 5.19 | 112.35 | 108.20 |
| 35 | AC | 79 | G | C5-C6-O6 | -5.19 | 125.48 | 128.60 |
| 34 | AA | 2218 | C | O4'-C1'-N1 | 5.19 | 112.35 | 108.20 |
| 34 | AA | 3580 | G | C5'-C4'-O4' | 5.19 | 115.33 | 109.10 |
| 34 | AA | 511 | C | C6-N1-C2 | -5.19 | 118.22 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 34 | AA | 531 | U | O4'-C1'-N1 | 5.19 | 112.35 | 108.20 |
| 34 | AA | 2451 | A | O4'-C1'-N9 | 5.19 | 112.35 | 108.20 |
| 34 | AA | 2008 | G | O4'-C1'-N9 | 5.19 | 112.35 | 108.20 |
| 34 | AA | 2473 | A | O4'-C1'-N9 | 5.19 | 112.35 | 108.20 |
| 1 | A | 1118 | U | O4'-C1'-N1 | 5.19 | 112.35 | 108.20 |
| 34 | AA | 1066 | U | O4'-C1'-N1 | 5.19 | 112.35 | 108.20 |
| 34 | AA | 2189 | A | O4'-C1'-N9 | 5.19 | 112.35 | 108.20 |
| 34 | AA | 1222 | U | O4'-C1'-N1 | 5.18 | 112.35 | 108.20 |
| 34 | AA | 1254 | G | O4'-C1'-N9 | 5.18 | 112.35 | 108.20 |
| 1 | A | 105 | A | C2'-C3'-O3' | 5.18 | 121.99 | 113.70 |
| 1 | A | 1863 | U | C5'-C4'-C3' | -5.18 | 107.71 | 116.00 |
| 34 | AA | 1170 | A | O4'-C1'-N9 | 5.18 | 112.35 | 108.20 |
| 34 | AA | 1342 | U | O4'-C1'-N1 | 5.18 | 112.35 | 108.20 |
| 34 | AA | 3016 | G | C5'-C4'-O4' | 5.18 | 115.32 | 109.10 |
| 34 | AA | 3167 | A | C5'-C4'-O4' | 5.18 | 115.32 | 109.10 |
| 34 | AA | 3132 | C | O4'-C1'-N1 | 5.18 | 112.34 | 108.20 |
| 34 | AA | 544 | C | C2-N1-C1' | 5.18 | 124.50 | 118.80 |
| 34 | AA | 612 | G | O4'-C1'-N9 | 5.18 | 112.34 | 108.20 |
| 34 | AA | 2981 | A | O4'-C1'-N9 | 5.18 | 112.34 | 108.20 |
| 1 | A | 310 | U | O4'-C1'-N1 | 5.18 | 112.34 | 108.20 |
| 1 | A | 919 | U | P-O5'-C5' | 5.18 | 129.18 | 120.90 |
| 34 | AA | 1560 | U | O4'-C1'-N1 | 5.18 | 112.34 | 108.20 |
| 1 | A | 1848 | U | O4'-C1'-N1 | 5.18 | 112.34 | 108.20 |
| 34 | AA | 1277 | G | C5-C6-O6 | -5.18 | 125.50 | 128.60 |
| 35 | AC | 9 | U | O4'-C1'-N1 | 5.18 | 112.34 | 108.20 |
| 35 | AC | 56 | A | O4'-C1'-N9 | 5.18 | 112.34 | 108.20 |
| 70 | AE | 345 | ARG | NE-CZ-NH1 | 5.18 | 122.89 | 120.30 |
| 1 | A | 211 | U | O4'-C1'-N1 | 5.17 | 112.34 | 108.20 |
| 34 | AA | 673 | U | C6-N1-C1' | -5.17 | 113.95 | 121.20 |
| 34 | AA | 3613 | A | N1-C6-N6 | 5.17 | 121.70 | 118.60 |
| 34 | AA | 3395 | G | O4'-C1'-N9 | 5.17 | 112.34 | 108.20 |
| 1 | A | 44 | U | P-O3'-C3' | -5.17 | 113.50 | 119.70 |
| 34 | AA | 948 | G | O4'-C1'-N9 | 5.17 | 112.34 | 108.20 |
| 54 | AI | 68 | MET | CG-SD-CE | -5.17 | 91.93 | 100.20 |
| 70 | AE | 237 | ARG | NE-CZ-NH1 | 5.17 | 122.89 | 120.30 |
| 1 | A | 215 | U | O4'-C1'-N1 | 5.17 | 112.33 | 108.20 |
| 1 | A | 892 | U | O4'-C1'-N1 | 5.17 | 112.33 | 108.20 |
| 1 | A | 1798 | G | C5'-C4'-O4' | 5.17 | 115.30 | 109.10 |
| 1 | A | 1912 | C | O4'-C1'-N1 | 5.17 | 112.33 | 108.20 |
| 16 | 3 | 95 | ARG | NE-CZ-NH1 | 5.17 | 122.89 | 120.30 |
| 34 | AA | 389 | U | O4'-C1'-N1 | 5.17 | 112.33 | 108.20 |
| 34 | AA | 2514 | G | N1-C6-O6 | 5.17 | 123.00 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 34 | AA | 698 | G | C5-C6-O6 | -5.17 | 125.50 | 128.60 |
| 34 | AA | 1297 | A | O4'-C1'-N9 | 5.17 | 112.33 | 108.20 |
| 34 | AA | 2744 | G | O4'-C1'-N9 | 5.17 | 112.33 | 108.20 |
| 1 | A | 641 | G | O4'-C1'-N9 | 5.17 | 112.33 | 108.20 |
| 34 | AA | 155 | U | O4'-C1'-N1 | 5.17 | 112.33 | 108.20 |
| 34 | AA | 1250 | U | O4'-C1'-N1 | 5.17 | 112.33 | 108.20 |
| 34 | AA | 535 | U | O4'-C1'-N1 | 5.16 | 112.33 | 108.20 |
| 34 | AA | 3638 | A | N1-C6-N6 | -5.16 | 115.50 | 118.60 |
| 1 | A | 330 | U | O4'-C1'-N1 | 5.16 | 112.33 | 108.20 |
| 34 | AA | 610 | U | O4'-C1'-N1 | 5.16 | 112.33 | 108.20 |
| 1 | A | 376 | A | O4'-C1'-N9 | 5.16 | 112.33 | 108.20 |
| 1 | A | 1086 | U | O4'-C1'-N1 | 5.16 | 112.33 | 108.20 |
| 34 | AA | 1018 | C | O4'-C1'-N1 | 5.16 | 112.33 | 108.20 |
| 34 | AA | 2556 | C | O4'-C1'-N1 | 5.16 | 112.33 | 108.20 |
| 34 | AA | 951 | A | C5'-C4'-O4' | 5.16 | 115.29 | 109.10 |
| 34 | AA | 3190 | G | O4'-C1'-N9 | 5.16 | 112.33 | 108.20 |
| 1 | A | 1016 | U | O4'-C1'-N1 | 5.16 | 112.33 | 108.20 |
| 1 | A | 1075 | C | O4'-C1'-N1 | 5.16 | 112.32 | 108.20 |
| 34 | AA | 1747 | U | C6-N1-C1' | -5.16 | 113.98 | 121.20 |
| 34 | AA | 3050 | U | O4'-C1'-N1 | 5.16 | 112.33 | 108.20 |
| 1 | A | 955 | U | C5'-C4'-O4' | 5.15 | 115.28 | 109.10 |
| 34 | AA | 1699 | G | O4'-C1'-N9 | 5.15 | 112.32 | 108.20 |
| 75 | AV | 9 | ARG | NE-CZ-NH1 | 5.15 | 122.88 | 120.30 |
| 1 | A | 561 | C | O4'-C1'-N1 | 5.15 | 112.32 | 108.20 |
| 1 | A | 1464 | U | O4'-C1'-N1 | 5.15 | 112.32 | 108.20 |
| 14 | 1 | 106 | ARG | NE-CZ-NH1 | -5.15 | 117.72 | 120.30 |
| 34 | AA | 976 | G | O4'-C1'-N9 | 5.15 | 112.32 | 108.20 |
| 34 | AA | 3470 | G | C5-C6-O6 | -5.15 | 125.51 | 128.60 |
| 39 | A2 | 19 | PHE | CB-CG-CD2 | -5.15 | 117.19 | 120.80 |
| 1 | A | 1832 | U | C1'-O4'-C4' | -5.15 | 105.78 | 109.90 |
| 34 | AA | 1083 | G | O4'-C1'-N9 | 5.15 | 112.32 | 108.20 |
| 3 | D | 107 | ARG | NE-CZ-NH1 | 5.15 | 122.88 | 120.30 |
| 34 | AA | 1643 | U | C3'-C2'-C1' | -5.15 | 97.38 | 101.50 |
| 34 | AA | 2187 | G | N3-C2-N2 | 5.15 | 123.50 | 119.90 |
| 34 | AA | 1272 | U | C5'-C4'-O4' | 5.15 | 115.28 | 109.10 |
| 34 | AA | 3554 | U | C4'-C3'-C2' | 5.15 | 107.75 | 102.60 |
| 34 | AA | 3767 | U | P-O3'-C3' | 5.15 | 125.88 | 119.70 |
| 47 | Ab | 3 | ARG | NE-CZ-NH2 | 5.15 | 122.87 | 120.30 |
| 34 | AA | 3088 | G | C5-C6-O6 | -5.15 | 125.51 | 128.60 |
| 70 | AE | 272 | ARG | NE-CZ-NH2 | 5.15 | 122.87 | 120.30 |
| 1 | A | 636 | U | O4'-C1'-N1 | 5.14 | 112.32 | 108.20 |
| 34 | AA | 975 | G | P-O3'-C3' | 5.14 | 125.87 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 808 | U | O4'-C1'-N1 | 5.14 | 112.31 | 108.20 |
| 1 | A | 952 | U | P-O5'-C5' | 5.14 | 129.13 | 120.90 |
| 34 | AA | 226 | G | C5'-C4'-O4' | 5.14 | 115.27 | 109.10 |
| 34 | AA | 638 | G | C5-C6-O6 | -5.14 | 125.52 | 128.60 |
| 34 | AA | 2138 | U | O4'-C1'-N1 | 5.14 | 112.31 | 108.20 |
| 34 | AA | 2176 | A | O4'-C1'-N9 | 5.14 | 112.31 | 108.20 |
| 34 | AA | 3661 | A | O4'-C1'-N9 | 5.14 | 112.31 | 108.20 |
| 1 | A | 1722 | U | O4'-C1'-N1 | 5.14 | 112.31 | 108.20 |
| 21 | F | 253 | ARG | NE-CZ-NH1 | 5.14 | 122.87 | 120.30 |
| 34 | AA | 25 | A | O4'-C1'-N9 | 5.14 | 112.31 | 108.20 |
| 35 | AC | 92 | A | N1-C6-N6 | 5.14 | 121.68 | 118.60 |
| 1 | A | 43 | A | C5-C6-N6 | -5.14 | 119.59 | 123.70 |
| 1 | A | 201 | G | N1-C6-O6 | 5.14 | 122.98 | 119.90 |
| 1 | A | 1894 | A | O4'-C1'-N9 | 5.14 | 112.31 | 108.20 |
| 34 | AA | 892 | U | O4'-C1'-N1 | 5.14 | 112.31 | 108.20 |
| 34 | AA | 1517 | U | O4'-C1'-N1 | 5.14 | 112.31 | 108.20 |
| 34 | AA | 286 | U | O4'-C1'-N1 | 5.14 | 112.31 | 108.20 |
| 1 | A | 322 | G | O4'-C1'-N9 | 5.14 | 112.31 | 108.20 |
| 1 | A | 1220 | C | C6-N1-C2 | -5.14 | 118.25 | 120.30 |
| 2 | 7 | 36 | A | C5'-C4'-C3' | 5.14 | 124.22 | 116.00 |
| 6 | I | 46 | ARG | NE-CZ-NH2 | 5.14 | 122.87 | 120.30 |
| 34 | AA | 440 | A | N1-C6-N6 | 5.14 | 121.68 | 118.60 |
| 34 | AA | 579 | C | O4'-C1'-N1 | 5.14 | 112.31 | 108.20 |
| 34 | AA | 1550 | A | C5'-C4'-C3' | -5.14 | 107.78 | 116.00 |
| 34 | AA | 3583 | A | C5'-C4'-O4' | 5.14 | 115.26 | 109.10 |
| 34 | AA | 3726 | U | O4'-C1'-N1 | 5.14 | 112.31 | 108.20 |
| 67 | A3 | 50 | ARG | NE-CZ-NH1 | 5.14 | 122.87 | 120.30 |
| 34 | AA | 1550 | A | O4'-C1'-N9 | 5.13 | 112.31 | 108.20 |
| 34 | AA | 2562 | U | O4'-C1'-N1 | 5.13 | 112.31 | 108.20 |
| 53 | Ai | 86 | ARG | NE-CZ-NH1 | 5.13 | 122.87 | 120.30 |
| 44 | A8 | 24 | ARG | NH1-CZ-NH2 | -5.13 | 113.75 | 119.40 |
| 34 | AA | 81 | C | C6-N1-C2 | -5.13 | 118.25 | 120.30 |
| 34 | AA | 2410 | A | P-O3'-C3' | 5.13 | 125.86 | 119.70 |
| 34 | AA | 3109 | U | O4'-C1'-N1 | 5.13 | 112.31 | 108.20 |
| 58 | AM | 122 | ARG | NE-CZ-NH1 | 5.13 | 122.87 | 120.30 |
| 69 | AD | 23 | ARG | NE-CZ-NH1 | 5.13 | 122.86 | 120.30 |
| 34 | AA | 3679 | A | O3'-P-O5' | -5.13 | 94.25 | 104.00 |
| 1 | A | 367 | C | C6-N1-C2 | -5.13 | 118.25 | 120.30 |
| 1 | A | 853 | U | C5'-C4'-O4' | 5.13 | 115.25 | 109.10 |
| 68 | A5 | 97 | ARG | NE-CZ-NH1 | 5.13 | 122.86 | 120.30 |
| 1 | A | 1783 | U | O4'-C1'-N1 | 5.13 | 112.30 | 108.20 |
| 1 | A | 2070 | G | N1-C6-O6 | 5.13 | 122.98 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 34 | AA | 70 | A | O4'-C1'-N9 | 5.13 | 112.30 | 108.20 |
| 34 | AA | 1499 | U | O4'-C1'-N1 | 5.13 | 112.30 | 108.20 |
| 34 | AA | 2210 | U | O4'-C1'-N1 | 5.13 | 112.30 | 108.20 |
| 34 | AA | 3122 | A | C8-N9-C4 | 5.13 | 107.85 | 105.80 |
| 34 | AA | 3202 | U | O4'-C1'-N1 | 5.13 | 112.30 | 108.20 |
| 1 | A | 157 | G | C1'-O4'-C4' | -5.12 | 105.80 | 109.90 |
| 27 | Q | 95 | PHE | CB-CG-CD2 | 5.12 | 124.39 | 120.80 |
| 1 | A | 1008 | A | O4'-C1'-N9 | 5.12 | 112.30 | 108.20 |
| 1 | A | 1410 | G | O4'-C1'-N9 | 5.12 | 112.30 | 108.20 |
| 34 | AA | 1107 | U | O4'-C1'-N1 | 5.12 | 112.30 | 108.20 |
| 34 | AA | 2984 | G | O4'-C1'-N9 | 5.12 | 112.30 | 108.20 |
| 1 | A | 1864 | U | O4'-C1'-N1 | 5.12 | 112.30 | 108.20 |
| 34 | AA | 2125 | A | O4'-C1'-N9 | 5.12 | 112.30 | 108.20 |
| 34 | AA | 2466 | U | O4'-C1'-N1 | 5.12 | 112.30 | 108.20 |
| 34 | AA | 3106 | U | O4'-C1'-N1 | 5.12 | 112.30 | 108.20 |
| 1 | A | 1849 | U | O4'-C1'-N1 | 5.12 | 112.30 | 108.20 |
| 34 | AA | 382 | A | C5-C6-N6 | 5.12 | 127.80 | 123.70 |
| 34 | AA | 2554 | G | O4'-C1'-N9 | 5.12 | 112.30 | 108.20 |
| 34 | AA | 3243 | C | C6-N1-C2 | -5.12 | 118.25 | 120.30 |
| 1 | A | 1788 | U | C2-N1-C1' | 5.12 | 123.84 | 117.70 |
| 34 | AA | 2488 | C | O4'-C1'-N1 | 5.12 | 112.30 | 108.20 |
| 34 | AA | 3129 | U | C5'-C4'-O4' | 5.12 | 115.24 | 109.10 |
| 55 | AJ | 87 | ARG | NE-CZ-NH1 | 5.12 | 122.86 | 120.30 |
| 1 | A | 1653 | A | O4'-C1'-N9 | 5.12 | 112.29 | 108.20 |
| 1 | A | 2065 | C | C6-N1-C2 | -5.12 | 118.25 | 120.30 |
| 34 | AA | 365 | C | O4'-C1'-N1 | 5.12 | 112.29 | 108.20 |
| 34 | AA | 3693 | A | O4'-C1'-N9 | 5.12 | 112.29 | 108.20 |
| 36 | AB | 103 | A | N1-C6-N6 | 5.12 | 121.67 | 118.60 |
| 45 | A9 | 81 | ARG | NE-CZ-NH1 | 5.12 | 122.86 | 120.30 |
| 65 | AT | 8 | ARG | NE-CZ-NH1 | 5.12 | 122.86 | 120.30 |
| 34 | AA | 1762 | A | O4'-C1'-N9 | 5.11 | 112.29 | 108.20 |
| 34 | AA | 1800 | U | O4'-C1'-N1 | 5.11 | 112.29 | 108.20 |
| 34 | AA | 3068 | A | O4'-C1'-N9 | 5.11 | 112.29 | 108.20 |
| 34 | AA | 3111 | U | C5'-C4'-O4' | 5.11 | 115.24 | 109.10 |
| 2 | 7 | 44 | G | O4'-C1'-N9 | 5.11 | 112.29 | 108.20 |
| 34 | AA | 102 | A | C5'-C4'-O4' | 5.11 | 115.23 | 109.10 |
| 34 | AA | 3591 | U | O4'-C1'-N1 | 5.11 | 112.29 | 108.20 |
| 35 | AC | 79 | G | O4'-C1'-N9 | 5.11 | 112.29 | 108.20 |
| 62 | AR | 22 | ARG | NE-CZ-NH1 | 5.11 | 122.86 | 120.30 |
| 34 | AA | 3056 | U | O4'-C1'-N1 | 5.11 | 112.29 | 108.20 |
| 5 | G | 180 | ARG | NE-CZ-NH2 | 5.11 | 122.85 | 120.30 |
| 40 | A4 | 38 | ASN | N-CA-CB | 5.11 | 119.80 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 14 | 1 | 120 | ARG | NE-CZ-NH1 | 5.11 | 122.85 | 120.30 |
| 1 | A | 848 | U | O4'-C1'-N1 | 5.11 | 112.28 | 108.20 |
| 34 | AA | 1641 | G | O4'-C1'-N9 | 5.11 | 112.28 | 108.20 |
| 35 | AC | 89 | U | O4'-C1'-N1 | 5.11 | 112.28 | 108.20 |
| 1 | A | 1190 | U | O4'-C1'-N1 | 5.10 | 112.28 | 108.20 |
| 34 | AA | 1344 | C | O4'-C1'-N1 | 5.10 | 112.28 | 108.20 |
| 34 | AA | 1705 | A | C5'-C4'-C3' | 5.10 | 124.17 | 116.00 |
| 34 | AA | 2147 | A | O4'-C1'-N9 | 5.10 | 112.28 | 108.20 |
| 34 | AA | 3510 | C | O4'-C1'-N1 | 5.10 | 112.28 | 108.20 |
| 1 | A | 469 | U | O4'-C1'-N1 | 5.10 | 112.28 | 108.20 |
| 1 | A | 1186 | G | C5-C6-O6 | -5.10 | 125.54 | 128.60 |
| 1 | A | 1261 | A | O4'-C1'-N9 | 5.10 | 112.28 | 108.20 |
| 34 | AA | 34 | A | O4'-C1'-N9 | 5.10 | 112.28 | 108.20 |
| 34 | AA | 631 | U | O4'-C1'-N1 | 5.10 | 112.28 | 108.20 |
| 34 | AA | 938 | U | O4'-C1'-N1 | 5.10 | 112.28 | 108.20 |
| 34 | AA | 2501 | A | N1-C6-N6 | 5.10 | 121.66 | 118.60 |
| 34 | AA | 492 | U | O4'-C1'-N1 | 5.10 | 112.28 | 108.20 |
| 34 | AA | 3784 | U | O4'-C1'-N1 | 5.10 | 112.28 | 108.20 |
| 1 | A | 138 | U | P-O3'-C3' | 5.10 | 125.82 | 119.70 |
| 34 | AA | 379 | G | C5-C6-O6 | -5.10 | 125.54 | 128.60 |
| 34 | AA | 539 | G | P-O3'-C3' | 5.10 | 125.82 | 119.70 |
| 34 | AA | 873 | U | O4'-C1'-N1 | 5.10 | 112.28 | 108.20 |
| 34 | AA | 2118 | G | C5-C6-O6 | -5.10 | 125.54 | 128.60 |
| 34 | AA | 3332 | G | C5-C6-O6 | -5.10 | 125.54 | 128.60 |
| 37 | AL | 42 | ARG | NE-CZ-NH1 | 5.10 | 122.85 | 120.30 |
| 62 | AR | 207 | MET | CG-SD-CE | -5.10 | 92.04 | 100.20 |
| 1 | A | 1720 | G | N1-C6-O6 | 5.10 | 122.96 | 119.90 |
| 34 | AA | 1868 | U | O4'-C1'-N1 | 5.10 | 112.28 | 108.20 |
| 34 | AA | 2676 | C | O4'-C1'-N1 | 5.10 | 112.28 | 108.20 |
| 34 | AA | 3287 | C | C6-N1-C2 | -5.10 | 118.26 | 120.30 |
| 34 | AA | 417 | A | N1-C6-N6 | 5.10 | 121.66 | 118.60 |
| 36 | AB | 5 | U | O4'-C1'-N1 | 5.10 | 112.28 | 108.20 |
| 1 | A | 987 | U | O4'-C1'-N1 | 5.09 | 112.28 | 108.20 |
| 34 | AA | 206 | A | P-O3'-C3' | 5.09 | 125.81 | 119.70 |
| 34 | AA | 684 | G | N1-C6-O6 | 5.09 | 122.96 | 119.90 |
| 1 | A | 1624 | U | O4'-C1'-N1 | 5.09 | 112.27 | 108.20 |
| 1 | A | 1952 | A | C5-C6-N6 | -5.09 | 119.62 | 123.70 |
| 34 | AA | 1060 | G | O4'-C1'-N9 | 5.09 | 112.28 | 108.20 |
| 1 | A | 1696 | A | O4'-C1'-N9 | 5.09 | 112.27 | 108.20 |
| 24 | L | 210 | ARG | NE-CZ-NH2 | 5.09 | 122.84 | 120.30 |
| 34 | AA | 1641 | G | C5-C6-O6 | -5.09 | 125.55 | 128.60 |
| 34 | AA | 3388 | U | O4'-C1'-N1 | 5.09 | 112.27 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 1390 | U | O4'-C1'-N1 | 5.09 | 112.27 | 108.20 |
| 1 | A | 1688 | U | O4'-C1'-N1 | 5.09 | 112.27 | 108.20 |
| 34 | AA | 273 | C | O4'-C1'-N1 | 5.09 | 112.27 | 108.20 |
| 34 | AA | 1516 | G | N3-C2-N2 | 5.09 | 123.46 | 119.90 |
| 34 | AA | 2832 | A | P-O3'-C3' | 5.09 | 125.81 | 119.70 |
| 34 | AA | 3644 | G | O4'-C1'-N9 | 5.09 | 112.27 | 108.20 |
| 1 | A | 755 | A | O4'-C1'-N9 | 5.09 | 112.27 | 108.20 |
| 34 | AA | 1243 | G | C5-C6-O6 | -5.09 | 125.55 | 128.60 |
| 34 | AA | 1462 | C | O4'-C1'-N1 | 5.09 | 112.27 | 108.20 |
| 34 | AA | 1664 | A | N1-C6-N6 | -5.09 | 115.55 | 118.60 |
| 1 | A | 1370 | U | O4'-C1'-N1 | 5.09 | 112.27 | 108.20 |
| 1 | A | 1903 | U | O4'-C1'-N1 | 5.09 | 112.27 | 108.20 |
| 34 | AA | 1496 | U | O4'-C1'-N1 | 5.09 | 112.27 | 108.20 |
| 34 | AA | 2474 | C | O4'-C1'-N1 | 5.09 | 112.27 | 108.20 |
| 34 | AA | 2644 | U | O4'-C1'-N1 | 5.09 | 112.27 | 108.20 |
| 36 | AB | 88 | A | P-O3'-C3' | 5.09 | 125.81 | 119.70 |
| 1 | A | 164 | C | O4'-C1'-N1 | 5.08 | 112.27 | 108.20 |
| 1 | A | 296 | G | O4'-C1'-N9 | 5.08 | 112.27 | 108.20 |
| 1 | A | 385 | U | O4'-C1'-N1 | 5.08 | 112.27 | 108.20 |
| 1 | A | 1176 | U | O4'-C1'-N1 | 5.08 | 112.27 | 108.20 |
| 34 | AA | 537 | A | C5'-C4'-C3' | -5.08 | 107.87 | 116.00 |
| 34 | AA | 712 | C | O4'-C1'-N1 | 5.08 | 112.27 | 108.20 |
| 34 | AA | 1591 | U | O4'-C1'-N1 | 5.08 | 112.27 | 108.20 |
| 34 | AA | 3064 | U | O4'-C1'-N1 | 5.08 | 112.27 | 108.20 |
| 34 | AA | 3705 | C | C6-N1-C2 | -5.08 | 118.27 | 120.30 |
| 1 | A | 1809 | G | C5-C6-O6 | -5.08 | 125.55 | 128.60 |
| 34 | AA | 1690 | A | O4'-C1'-N9 | 5.08 | 112.27 | 108.20 |
| 34 | AA | 2408 | G | N1-C6-O6 | 5.08 | 122.95 | 119.90 |
| 34 | AA | 2736 | A | O4'-C1'-N9 | 5.08 | 112.27 | 108.20 |
| 56 | Ac | 68 | ARG | NE-CZ-NH1 | 5.08 | 122.84 | 120.30 |
| 1 | A | 970 | G | C5-C6-O6 | -5.08 | 125.55 | 128.60 |
| 1 | A | 1881 | G | N1-C6-O6 | 5.08 | 122.95 | 119.90 |
| 34 | AA | 254 | U | O4'-C1'-N1 | 5.08 | 112.26 | 108.20 |
| 34 | AA | 3384 | G | O4'-C1'-N9 | 5.08 | 112.26 | 108.20 |
| 1 | A | 794 | U | O4'-C1'-N1 | 5.08 | 112.26 | 108.20 |
| 1 | A | 1789 | U | P-O3'-C3' | 5.08 | 125.79 | 119.70 |
| 34 | AA | 1434 | G | C5-C6-O6 | -5.08 | 125.55 | 128.60 |
| 34 | AA | 1684 | A | N1-C6-N6 | 5.08 | 121.65 | 118.60 |
| 34 | AA | 522 | A | P-O5'-C5' | 5.08 | 129.02 | 120.90 |
| 34 | AA | 3282 | U | C5'-C4'-O4' | 5.08 | 115.19 | 109.10 |
| 1 | A | 390 | G | C5-C6-O6 | -5.08 | 125.55 | 128.60 |
| 1 | A | 453 | U | O4'-C1'-N1 | 5.08 | 112.26 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 1831 | G | C5-C6-O6 | -5.08 | 125.56 | 128.60 |
| 34 | AA | 957 | G | N1-C6-O6 | 5.08 | 122.94 | 119.90 |
| 34 | AA | 2711 | U | O4'-C1'-N1 | 5.08 | 112.26 | 108.20 |
| 34 | AA | 3137 | U | C2'-C3'-O3' | 5.08 | 121.82 | 113.70 |
| 1 | A | 832 | A | N1-C6-N6 | -5.07 | 115.56 | 118.60 |
| 1 | A | 1817 | U | O4'-C1'-N1 | 5.07 | 112.26 | 108.20 |
| 34 | AA | 1576 | U | O4'-C1'-N1 | 5.07 | 112.26 | 108.20 |
| 34 | AA | 1908 | U | O4'-C1'-N1 | 5.07 | 112.26 | 108.20 |
| 23 | J | 162 | ARG | NE-CZ-NH1 | 5.07 | 122.84 | 120.30 |
| 36 | AB | 116 | U | O4'-C1'-N1 | 5.07 | 112.26 | 108.20 |
| 1 | A | 922 | U | O4'-C1'-N1 | 5.07 | 112.26 | 108.20 |
| 1 | A | 1742 | A | C2'-C3'-O3' | 5.07 | 121.81 | 113.70 |
| 1 | A | 2053 | U | C5'-C4'-O4' | 5.07 | 115.19 | 109.10 |
| 34 | AA | 629 | A | O4'-C1'-N9 | 5.07 | 112.26 | 108.20 |
| 34 | AA | 832 | U | O4'-C1'-N1 | 5.07 | 112.26 | 108.20 |
| 34 | AA | 1099 | U | O4'-C1'-N1 | 5.07 | 112.26 | 108.20 |
| 34 | AA | 3443 | A | C4'-C3'-C2' | -5.07 | 97.53 | 102.60 |
| 34 | AA | 1080 | C | O4'-C1'-N1 | 5.07 | 112.25 | 108.20 |
| 34 | AA | 1136 | A | C5-C6-N6 | -5.07 | 119.64 | 123.70 |
| 34 | AA | 1839 | U | O4'-C1'-N1 | 5.07 | 112.26 | 108.20 |
| 34 | AA | 2170 | G | O4'-C1'-N9 | 5.07 | 112.25 | 108.20 |
| 35 | AC | 52 | A | O4'-C1'-N9 | 5.07 | 112.25 | 108.20 |
| 70 | AE | 115 | ARG | NE-CZ-NH1 | 5.07 | 122.83 | 120.30 |
| 1 | A | 69 | A | O4'-C1'-N9 | 5.07 | 112.25 | 108.20 |
| 1 | A | 1024 | A | O4'-C1'-N9 | 5.07 | 112.25 | 108.20 |
| 1 | A | 1665 | G | C5-C6-O6 | -5.07 | 125.56 | 128.60 |
| 34 | AA | 2405 | A | O4'-C1'-N9 | 5.07 | 112.25 | 108.20 |
| 72 | AG | 72 | ARG | NE-CZ-NH1 | 5.07 | 122.83 | 120.30 |
| 1 | A | 182 | U | O4'-C1'-N1 | 5.07 | 112.25 | 108.20 |
| 1 | A | 395 | G | C5-C6-O6 | -5.07 | 125.56 | 128.60 |
| 1 | A | 431 | A | P-O5'-C5' | 5.07 | 129.00 | 120.90 |
| 34 | AA | 1681 | C | P-O3'-C3' | 5.07 | 125.78 | 119.70 |
| 64 | AY | 95 | ARG | NE-CZ-NH1 | 5.07 | 122.83 | 120.30 |
| 74 | AH | 172 | ARG | NE-CZ-NH2 | 5.07 | 122.83 | 120.30 |
| 1 | A | 387 | C | C6-N1-C2 | -5.06 | 118.27 | 120.30 |
| 1 | A | 959 | C | O4'-C1'-N1 | 5.06 | 112.25 | 108.20 |
| 34 | AA | 506 | A | O4'-C1'-N9 | 5.06 | 112.25 | 108.20 |
| 34 | AA | 825 | G | N1-C6-O6 | 5.06 | 122.94 | 119.90 |
| 35 | AC | 62 | G | N3-C2-N2 | 5.06 | 123.44 | 119.90 |
| 16 | 3 | 15 | ARG | NE-CZ-NH1 | 5.06 | 122.83 | 120.30 |
| 34 | AA | 518 | G | C5-C6-O6 | -5.06 | 125.56 | 128.60 |
| 34 | AA | 1664 | A | O4'-C1'-N9 | 5.06 | 112.25 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 34 | AA | 3639 | G | C5'-C4'-C3' | -5.06 | 107.90 | 116.00 |
| 35 | AC | 145 | A | C5'-C4'-O4' | 5.06 | 115.17 | 109.10 |
| 1 | A | 1374 | G | N1-C6-O6 | 5.06 | 122.94 | 119.90 |
| 1 | A | 1711 | U | O4'-C1'-N1 | 5.06 | 112.25 | 108.20 |
| 34 | AA | 361 | G | N1-C6-O6 | 5.06 | 122.94 | 119.90 |
| 34 | AA | 1822 | A | O4'-C1'-N9 | 5.06 | 112.25 | 108.20 |
| 34 | AA | 2180 | U | C2'-C3'-O3' | 5.06 | 121.80 | 113.70 |
| 34 | AA | 3052 | U | C5'-C4'-O4' | 5.06 | 115.17 | 109.10 |
| 34 | AA | 3530 | A | C5'-C4'-O4' | 5.06 | 115.17 | 109.10 |
| 34 | AA | 3741 | A | O4'-C1'-N9 | 5.06 | 112.25 | 108.20 |
| 36 | AB | 21 | G | O4'-C1'-N9 | 5.06 | 112.25 | 108.20 |
| 1 | A | 204 | U | P-O3'-C3' | 5.06 | 125.77 | 119.70 |
| 1 | A | 1413 | U | C2'-C3'-O3' | 5.06 | 121.79 | 113.70 |
| 33 | C | 190 | ARG | NE-CZ-NH2 | 5.06 | 122.83 | 120.30 |
| 34 | AA | 889 | U | C2'-C3'-O3' | 5.06 | 121.79 | 113.70 |
| 34 | AA | 2092 | G | C5'-C4'-O4' | 5.06 | 115.17 | 109.10 |
| 35 | AC | 29 | G | O4'-C1'-N9 | 5.06 | 112.25 | 108.20 |
| 1 | A | 467 | G | O4'-C1'-N9 | 5.06 | 112.25 | 108.20 |
| 1 | A | 1374 | G | C5-C6-O6 | -5.05 | 125.57 | 128.60 |
| 29 | T | 17 | ARG | NE-CZ-NH1 | 5.05 | 122.83 | 120.30 |
| 34 | AA | 604 | G | P-O3'-C3' | 5.05 | 125.77 | 119.70 |
| 34 | AA | 639 | C | O4'-C1'-N1 | 5.05 | 112.24 | 108.20 |
| 34 | AA | 740 | U | O4'-C1'-N1 | 5.05 | 112.24 | 108.20 |
| 34 | AA | 1108 | U | O4'-C1'-N1 | 5.05 | 112.24 | 108.20 |
| 51 | AP | 63 | ARG | NE-CZ-NH2 | -5.05 | 117.77 | 120.30 |
| 1 | A | 1003 | C | C2-N1-C1' | 5.05 | 124.36 | 118.80 |
| 34 | AA | 3102 | U | O4'-C1'-N1 | 5.05 | 112.24 | 108.20 |
| 1 | A | 143 | A | O4'-C1'-N9 | 5.05 | 112.24 | 108.20 |
| 1 | A | 797 | C | O4'-C1'-N1 | 5.05 | 112.24 | 108.20 |
| 1 | A | 1088 | A | O4'-C1'-N9 | 5.05 | 112.24 | 108.20 |
| 34 | AA | 308 | U | O4'-C1'-N1 | 5.05 | 112.24 | 108.20 |
| 34 | AA | 2664 | G | C5-C6-O6 | -5.05 | 125.57 | 128.60 |
| 73 | AU | 126 | ARG | NE-CZ-NH2 | 5.05 | 122.83 | 120.30 |
| 34 | AA | 362 | U | O4'-C1'-N1 | 5.05 | 112.24 | 108.20 |
| 34 | AA | 2600 | G | C5-C6-O6 | -5.05 | 125.57 | 128.60 |
| 34 | AA | 3090 | G | C5-C6-O6 | -5.05 | 125.57 | 128.60 |
| 35 | AC | 48 | C | C6-N1-C2 | -5.05 | 118.28 | 120.30 |
| 36 | AB | 52 | U | O4'-C1'-N1 | 5.05 | 112.24 | 108.20 |
| 1 | A | 63 | G | N1-C6-O6 | 5.05 | 122.93 | 119.90 |
| 34 | AA | 277 | U | O4'-C1'-N1 | 5.05 | 112.24 | 108.20 |
| 34 | AA | 366 | G | C5-C6-O6 | -5.05 | 125.57 | 128.60 |
| 34 | AA | 533 | A | O4'-C1'-N9 | 5.05 | 112.24 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 34 | AA | 3271 | G | N1-C6-O6 | 5.05 | 122.93 | 119.90 |
| 1 | A | 603 | C | O4'-C1'-N1 | 5.04 | 112.24 | 108.20 |
| 6 | I | 42 | HIS | N-CA-CB | 5.04 | 119.68 | 110.60 |
| 38 | A1 | 65 | ARG | NE-CZ-NH1 | 5.04 | 122.82 | 120.30 |
| 1 | A | 1202 | G | C5-C6-O6 | -5.04 | 125.57 | 128.60 |
| 34 | AA | 1977 | U | O4'-C1'-N1 | 5.04 | 112.24 | 108.20 |
| 34 | AA | 3577 | A | P-O3'-C3' | 5.04 | 125.75 | 119.70 |
| 35 | AC | 78 | U | C6-N1-C1' | -5.04 | 114.14 | 121.20 |
| 1 | A | 1389 | G | O4'-C1'-N9 | 5.04 | 112.23 | 108.20 |
| 34 | AA | 724 | A | O4'-C1'-N9 | 5.04 | 112.23 | 108.20 |
| 34 | AA | 1113 | C | C6-N1-C2 | -5.04 | 118.28 | 120.30 |
| 34 | AA | 1508 | U | O4'-C1'-N1 | 5.04 | 112.23 | 108.20 |
| 1 | A | 1743 | A | N1-C6-N6 | 5.04 | 121.62 | 118.60 |
| 34 | AA | 928 | G | O4'-C1'-N9 | 5.04 | 112.23 | 108.20 |
| 34 | AA | 943 | G | C5-C6-O6 | -5.04 | 125.58 | 128.60 |
| 40 | A4 | 14 | ARG | NE-CZ-NH1 | 5.04 | 122.82 | 120.30 |
| 1 | A | 838 | U | O4'-C1'-N1 | 5.04 | 112.23 | 108.20 |
| 1 | A | 1101 | G | C5'-C4'-O4' | 5.04 | 115.14 | 109.10 |
| 34 | AA | 514 | C | O4'-C1'-N1 | 5.04 | 112.23 | 108.20 |
| 34 | AA | 681 | U | O4'-C1'-N1 | 5.04 | 112.23 | 108.20 |
| 1 | A | 51 | A | O4'-C1'-N9 | 5.04 | 112.23 | 108.20 |
| 1 | A | 790 | U | O4'-C1'-N1 | 5.04 | 112.23 | 108.20 |
| 34 | AA | 933 | U | O4'-C1'-N1 | 5.04 | 112.23 | 108.20 |
| 34 | AA | 1838 | U | O4'-C1'-N1 | 5.04 | 112.23 | 108.20 |
| 51 | AP | 30 | TYR | CB-CG-CD1 | 5.04 | 124.02 | 121.00 |
| 34 | AA | 79 | U | O4'-C1'-N1 | 5.03 | 112.23 | 108.20 |
| 34 | AA | 1060 | G | C5-C6-O6 | -5.03 | 125.58 | 128.60 |
| 34 | AA | 3322 | C | O4'-C1'-N1 | 5.03 | 112.23 | 108.20 |
| 34 | AA | 3377 | A | O4'-C1'-N9 | 5.03 | 112.23 | 108.20 |
| 34 | AA | 3715 | U | O4'-C1'-N1 | 5.03 | 112.23 | 108.20 |
| 34 | AA | 1900 | G | C5-C6-O6 | -5.03 | 125.58 | 128.60 |
| 34 | AA | 2091 | U | O4'-C1'-N1 | 5.03 | 112.22 | 108.20 |
| 1 | A | 456 | U | P-O3'-C3' | -5.03 | 113.66 | 119.70 |
| 4 | E | 6 | ARG | NE-CZ-NH1 | 5.03 | 122.81 | 120.30 |
| 26 | P | 141 | ARG | NH1-CZ-NH2 | -5.03 | 113.87 | 119.40 |
| 34 | AA | 1748 | A | C1'-O4'-C4' | -5.03 | 105.88 | 109.90 |
| 34 | AA | 3087 | A | O4'-C1'-N9 | 5.03 | 112.22 | 108.20 |
| 1 | A | 37 | U | O4'-C1'-N1 | 5.03 | 112.22 | 108.20 |
| 1 | A | 274 | A | O4'-C1'-N9 | 5.03 | 112.22 | 108.20 |
| 1 | A | 1863 | U | P-O3'-C3' | -5.03 | 113.67 | 119.70 |
| 1 | A | 1915 | C | O4'-C1'-N1 | 5.03 | 112.22 | 108.20 |
| 34 | AA | 757 | U | O4'-C1'-N1 | 5.03 | 112.22 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 34 | AA | 1469 | U | O4'-C1'-N1 | 5.03 | 112.22 | 108.20 |
| 57 | AK | 159 | ARG | NE-CZ-NH1 | 5.03 | 122.81 | 120.30 |
| 34 | AA | 3597 | C | C6-N1-C2 | -5.02 | 118.29 | 120.30 |
| 1 | A | 1072 | A | O4'-C1'-N9 | 5.02 | 112.22 | 108.20 |
| 1 | A | 1280 | G | O4'-C1'-N9 | 5.02 | 112.22 | 108.20 |
| 34 | AA | 632 | U | O4'-C1'-N1 | 5.02 | 112.22 | 108.20 |
| 34 | AA | 267 | U | O4'-C1'-N1 | 5.02 | 112.22 | 108.20 |
| 34 | AA | 3234 | U | O4'-C1'-N1 | 5.02 | 112.22 | 108.20 |
| 34 | AA | 3351 | U | O4'-C1'-N1 | 5.02 | 112.22 | 108.20 |
| 1 | A | 1292 | U | O4'-C1'-N1 | 5.02 | 112.22 | 108.20 |
| 1 | A | 1976 | G | C5'-C4'-C3' | -5.02 | 107.97 | 116.00 |
| 34 | AA | 113 | C | C6-N1-C2 | -5.02 | 118.29 | 120.30 |
| 34 | AA | 585 | C | O4'-C1'-N1 | 5.02 | 112.22 | 108.20 |
| 34 | AA | 1068 | C | C6-N1-C2 | -5.02 | 118.29 | 120.30 |
| 34 | AA | 1324 | U | P-O3'-C3' | -5.02 | 113.68 | 119.70 |
| 34 | AA | 3577 | A | O4'-C1'-N9 | 5.02 | 112.22 | 108.20 |
| 67 | A3 | 10 | ARG | NE-CZ-NH1 | 5.02 | 122.81 | 120.30 |
| 34 | AA | 163 | G | O4'-C1'-N9 | 5.02 | 112.21 | 108.20 |
| 34 | AA | 542 | A | C5'-C4'-O4' | 5.02 | 115.12 | 109.10 |
| 34 | AA | 1513 | U | O4'-C1'-N1 | 5.02 | 112.21 | 108.20 |
| 34 | AA | 3276 | G | C5-C6-O6 | -5.02 | 125.59 | 128.60 |
| 35 | AC | 144 | U | O4'-C1'-N1 | 5.02 | 112.21 | 108.20 |
| 63 | AW | 60 | PHE | CB-CG-CD2 | -5.02 | 117.29 | 120.80 |
| 73 | AU | 84 | TYR | CB-CG-CD1 | -5.02 | 117.99 | 121.00 |
| 1 | A | 251 | U | C2'-C3'-O3' | 5.02 | 121.72 | 113.70 |
| 1 | A | 1276 | U | O4'-C1'-N1 | 5.02 | 112.21 | 108.20 |
| 45 | A9 | 39 | ARG | NE-CZ-NH1 | 5.02 | 122.81 | 120.30 |
| 34 | AA | 33 | G | C5-C6-O6 | -5.01 | 125.59 | 128.60 |
| 1 | A | 850 | G | C5-C6-O6 | -5.01 | 125.59 | 128.60 |
| 1 | A | 1391 | U | O4'-C1'-N1 | 5.01 | 112.21 | 108.20 |
| 2 | 7 | 19 | G | N1-C6-O6 | 5.01 | 122.91 | 119.90 |
| 34 | AA | 803 | A | C1'-O4'-C4' | -5.01 | 105.89 | 109.90 |
| 34 | AA | 2401 | C | C6-N1-C2 | -5.01 | 118.30 | 120.30 |
| 34 | AA | 2567 | U | O4'-C1'-N1 | 5.01 | 112.21 | 108.20 |
| 34 | AA | 3646 | G | N1-C6-O6 | 5.01 | 122.91 | 119.90 |
| 34 | AA | 894 | U | O4'-C1'-N1 | 5.01 | 112.21 | 108.20 |
| 34 | AA | 2432 | A | O4'-C1'-N9 | 5.01 | 112.21 | 108.20 |
| 34 | AA | 760 | A | O4'-C1'-N9 | 5.01 | 112.21 | 108.20 |
| 1 | A | 984 | A | P-O5'-C5' | 5.01 | 128.91 | 120.90 |
| 34 | AA | 436 | G | C5-C6-O6 | -5.01 | 125.60 | 128.60 |
| 34 | AA | 1644 | U | O4'-C1'-N1 | 5.01 | 112.20 | 108.20 |
| 34 | AA | 3264 | U | O4'-C1'-N1 | 5.01 | 112.21 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 48 | Ad | 52 | MET | CG-SD-CE | -5.01 | 92.19 | 100.20 |
| 1 | A | 635 | G | P-O5'-C5' | 5.00 | 128.91 | 120.90 |
| 1 | A | 1011 | G | O4'-C1'-N9 | 5.00 | 112.20 | 108.20 |
| 2 | 7 | 72 | C | O4'-C1'-N1 | 5.00 | 112.20 | 108.20 |
| 9 | W | 97 | TYR | CB-CG-CD2 | -5.00 | 118.00 | 121.00 |
| 72 | AG | 72 | ARG | NE-CZ-NH2 | -5.00 | 117.80 | 120.30 |
| 1 | A | 1441 | C | P-O5'-C5' | 5.00 | 128.90 | 120.90 |
| 1 | A | 1704 | G | O4'-C1'-N9 | 5.00 | 112.20 | 108.20 |
| 34 | AA | 495 | U | O4'-C1'-N1 | 5.00 | 112.20 | 108.20 |
| 73 | AU | 145 | ARG | NE-CZ-NH1 | 5.00 | 122.80 | 120.30 |

All (1) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 34 | AA | 3018 | A | C3' |

All (1052) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 14 | 1 | 12 | TYR | Sidechain |
| 14 | 1 | 91 | ARG | Sidechain |
| 15 | 2 | 76 | ARG | Sidechain |
| 16 | 3 | 28 | ARG | Sidechain |
| 16 | 3 | 85 | ARG | Sidechain |
| 17 | 4 | 21 | ARG | Sidechain |
| 17 | 4 | 7 | ASN | Peptide |
| 17 | 4 | 77 | PHE | Sidechain |
| 19 | 6 | 10 | ARG | Sidechain |
| 19 | 6 | 43 | ARG | Sidechain |
| 2 | 7 | 1 | G | Sidechain |
| 2 | 7 | 12 | G | Sidechain |
| 2 | 7 | 14 | A | Sidechain |
| 2 | 7 | 15 | G | Sidechain |
| 2 | 7 | 27 | G | Sidechain |
| 2 | 7 | 29 | G | Sidechain |
| 2 | 7 | 3 | G | Sidechain |
| 2 | 7 | 31 | G | Sidechain |
| 2 | 7 | 36 | A | Sidechain |
| 2 | 7 | 37 | U | Sidechain |
| 2 | 7 | 46 | G | Sidechain |
| 2 | 7 | 52 | G | Sidechain |
| 2 | 7 | 55 | U | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 2 | 7 | 6 | A | Sidechain |
| 2 | 7 | 64 | C | Sidechain |
| 2 | 7 | 65 | A | Sidechain |
| 2 | 7 | 70 | A | Sidechain |
| 2 | 7 | 9 | G | Sidechain |
| 1 | A | 100 | U | Sidechain |
| 1 | A | 1000 | C | Sidechain |
| 1 | A | 1008 | A | Sidechain |
| 1 | A | 1014 | U | Sidechain |
| 1 | A | 1016 | U | Sidechain |
| 1 | A | 1020 | U | Sidechain |
| 1 | A | 1022 | A | Sidechain |
| 1 | A | 1025 | U | Sidechain |
| 1 | A | 104 | U | Sidechain |
| 1 | A | 1041 | G | Sidechain |
| 1 | A | 1056 | G | Sidechain |
| 1 | A | 1058 | G | Sidechain |
| 1 | A | 106 | A | Sidechain |
| 1 | A | 1061 | A | Sidechain |
| 1 | A | 1063 | G | Sidechain |
| 1 | A | 1071 | G | Sidechain |
| 1 | A | 1074 | A | Sidechain |
| 1 | A | 1080 | G | Sidechain |
| 1 | A | 1081 | U | Sidechain |
| 1 | A | 1083 | A | Sidechain |
| 1 | A | 1084 | U | Sidechain |
| 1 | A | 1086 | U | Sidechain |
| 1 | A | 1094 | A | Sidechain |
| 1 | A | 1100 | U | Sidechain |
| 1 | A | 1104 | G | Sidechain |
| 1 | A | 1107 | U | Sidechain |
| 1 | A | 114 | A | Sidechain |
| 1 | A | 118 | U | Sidechain |
| 1 | A | 1186 | G | Sidechain |
| 1 | A | 1187 | A | Sidechain |
| 1 | A | 1188 | A | Sidechain |
| 1 | A | 1189 | A | Sidechain |
| 1 | A | 120 | U | Sidechain |
| 1 | A | 1200 | U | Sidechain |
| 1 | A | 1208 | G | Sidechain |
| 1 | A | 1213 | G | Sidechain |
| 1 | A | 1214 | A | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | A | 1216 | U | Sidechain |
| 1 | A | 1221 | G | Sidechain |
| 1 | A | 1223 | G | Sidechain |
| 1 | A | 1224 | C | Sidechain |
| 1 | A | 1240 | A | Sidechain |
| 1 | A | 1241 | A | Sidechain |
| 1 | A | 1244 | A | Sidechain |
| 1 | A | 1250 | G | Sidechain |
| 1 | A | 1251 | G | Sidechain |
| 1 | A | 1264 | A | Sidechain |
| 1 | A | 1273 | G | Sidechain |
| 1 | A | 1275 | U | Sidechain |
| 1 | A | 1283 | U | Sidechain |
| 1 | A | 1287 | U | Sidechain |
| 1 | A | 1289 | G | Sidechain |
| 1 | A | 129 | U | Sidechain |
| 1 | A | 1290 | A | Sidechain |
| 1 | A | 1300 | G | Sidechain |
| 1 | A | 1307 | U | Sidechain |
| 1 | A | 1320 | A | Sidechain |
| 1 | A | 136 | U | Sidechain |
| 1 | A | 1363 | U | Sidechain |
| 1 | A | 1379 | G | Sidechain |
| 1 | A | 14 | U | Sidechain |
| 1 | A | 1401 | G | Sidechain |
| 1 | A | 1402 | A | Sidechain |
| 1 | A | 1409 | U | Sidechain |
| 1 | A | 141 | G | Sidechain |
| 1 | A | 1415 | A | Sidechain |
| 1 | A | 1423 | A | Sidechain |
| 1 | A | 1436 | U | Sidechain |
| 1 | A | 1442 | U | Sidechain |
| 1 | A | 1448 | U | Sidechain |
| 1 | A | 1454 | G | Sidechain |
| 1 | A | 15 | U | Sidechain |
| 1 | A | 153 | A | Sidechain |
| 1 | A | 159 | U | Sidechain |
| 1 | A | 1602 | G | Sidechain |
| 1 | A | 1607 | U | Sidechain |
| 1 | A | 161 | U | Sidechain |
| 1 | A | 1632 | G | Sidechain |
| 1 | A | 1646 | U | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | A | 1655 | G | Sidechain |
| 1 | A | 1656 | A | Sidechain |
| 1 | A | 1658 | G | Sidechain |
| 1 | A | 1660 | U | Sidechain |
| 1 | A | 1665 | G | Sidechain |
| 1 | A | 168 | U | Sidechain |
| 1 | A | 1683 | U | Sidechain |
| 1 | A | 1691 | G | Sidechain |
| 1 | A | 1692 | A | Sidechain |
| 1 | A | 1700 | G | Sidechain |
| 1 | A | 1718 | C | Sidechain |
| 1 | A | 1742 | A | Sidechain |
| 1 | A | 1743 | A | Sidechain |
| 1 | A | 1744 | A | Sidechain |
| 1 | A | 1745 | U | Sidechain |
| 1 | A | 1748 | G | Sidechain |
| 1 | A | 1792 | U | Sidechain |
| 1 | A | 1794 | C | Sidechain |
| 1 | A | 1807 | A | Sidechain |
| 1 | A | 1819 | U | Sidechain |
| 1 | A | 182 | U | Sidechain |
| 1 | A | 1823 | U | Sidechain |
| 1 | A | 1826 | A | Sidechain |
| 1 | A | 1832 | U | Sidechain |
| 1 | A | 1836 | G | Sidechain |
| 1 | A | 1839 | G | Sidechain |
| 1 | A | 1850 | G | Sidechain |
| 1 | A | 1858 | U | Sidechain |
| 1 | A | 1865 | G | Sidechain |
| 1 | A | 1872 | G | Sidechain |
| 1 | A | 1873 | A | Sidechain |
| 1 | A | 1879 | U | Sidechain |
| 1 | A | 1881 | G | Sidechain |
| 1 | A | 1882 | U | Sidechain |
| 1 | A | 1884 | A | Sidechain |
| 1 | A | 1891 | U | Sidechain |
| 1 | A | 1892 | U | Sidechain |
| 1 | A | 1904 | G | Sidechain |
| 1 | A | 1906 | U | Sidechain |
| 1 | A | 1914 | U | Sidechain |
| 1 | A | 1917 | C | Sidechain |
| 1 | A | 1940 | U | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | A | 1947 | U | Sidechain |
| 1 | A | 1955 | G | Sidechain |
| 1 | A | 1972 | G | Sidechain |
| 1 | A | 1977 | G | Sidechain |
| 1 | A | 1979 | C | Sidechain |
| 1 | A | 1980 | A | Sidechain |
| 1 | A | 1984 | A | Sidechain |
| 1 | A | 2014 | A | Sidechain |
| 1 | A | 2021 | U | Sidechain |
| 1 | A | 2028 | U | Sidechain |
| 1 | A | 2030 | U | Sidechain |
| 1 | A | 2031 | C | Sidechain |
| 1 | A | 2032 | U | Sidechain |
| 1 | A | 2033 | U | Sidechain |
| 1 | A | 2053 | U | Sidechain |
| 1 | A | 2055 | A | Sidechain |
| 1 | A | 2059 | G | Sidechain |
| 1 | A | 2060 | G | Sidechain |
| 1 | A | 2067 | U | Sidechain |
| 1 | A | 2072 | G | Sidechain |
| 1 | A | 2074 | A | Sidechain |
| 1 | A | 2075 | C | Sidechain |
| 1 | A | 2082 | A | Sidechain |
| 1 | A | 248 | G | Sidechain |
| 1 | A | 252 | U | Sidechain |
| 1 | A | 254 | U | Sidechain |
| 1 | A | 263 | A | Sidechain |
| 1 | A | 264 | G | Sidechain |
| 1 | A | 273 | A | Sidechain |
| 1 | A | 310 | U | Sidechain |
| 1 | A | 327 | U | Sidechain |
| 1 | A | 328 | G | Sidechain |
| 1 | A | 33 | U | Sidechain |
| 1 | A | 34 | G | Sidechain |
| 1 | A | 341 | U | Sidechain |
| 1 | A | 343 | G | Sidechain |
| 1 | A | 346 | U | Sidechain |
| 1 | A | 355 | U | Sidechain |
| 1 | A | 369 | G | Sidechain |
| 1 | A | 389 | G | Sidechain |
| 1 | A | 395 | G | Sidechain |
| 1 | A | 396 | G | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | A | 402 | G | Sidechain |
| 1 | A | 404 | G | Sidechain |
| 1 | A | 412 | U | Sidechain |
| 1 | A | 440 | G | Sidechain |
| 1 | A | 441 | U | Sidechain |
| 1 | A | 445 | U | Sidechain |
| 1 | A | 455 | C | Sidechain |
| 1 | A | 46 | A | Sidechain |
| 1 | A | 465 | G | Sidechain |
| 1 | A | 483 | A | Sidechain |
| 1 | A | 486 | A | Sidechain |
| 1 | A | 491 | A | Sidechain |
| 1 | A | 5 | U | Sidechain |
| 1 | A | 508 | U | Sidechain |
| 1 | A | 516 | G | Sidechain |
| 1 | A | 517 | G | Sidechain |
| 1 | A | 544 | G | Sidechain |
| 1 | A | 553 | U | Sidechain |
| 1 | A | 555 | G | Sidechain |
| 1 | A | 559 | G | Sidechain |
| 1 | A | 583 | G | Sidechain |
| 1 | A | 589 | U | Sidechain |
| 1 | A | 598 | A | Sidechain |
| 1 | A | 620 | G | Sidechain |
| 1 | A | 623 | G | Sidechain |
| 1 | A | 625 | U | Sidechain |
| 1 | A | 626 | A | Sidechain |
| 1 | A | 74 | U | Sidechain |
| 1 | A | 798 | U | Sidechain |
| 1 | A | 8 | U | Sidechain |
| 1 | A | 802 | A | Sidechain |
| 1 | A | 805 | A | Sidechain |
| 1 | A | 820 | A | Sidechain |
| 1 | A | 822 | G | Sidechain |
| 1 | A | 832 | A | Sidechain |
| 1 | A | 835 | G | Sidechain |
| 1 | A | 836 | C | Sidechain |
| 1 | A | 846 | G | Sidechain |
| 1 | A | 850 | G | Sidechain |
| 1 | A | 857 | A | Sidechain |
| 1 | A | 858 | U | Sidechain |
| 1 | A | 859 | A | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | A | 860 | G | Sidechain |
| 1 | A | 872 | A | Sidechain |
| 1 | A | 882 | A | Sidechain |
| 1 | A | 892 | U | Sidechain |
| 1 | A | 9 | U | Sidechain |
| 1 | A | 916 | G | Sidechain |
| 1 | A | 920 | A | Sidechain |
| 1 | A | 922 | U | Sidechain |
| 1 | A | 931 | A | Sidechain |
| 1 | A | 932 | U | Sidechain |
| 1 | A | 936 | A | Sidechain |
| 1 | A | 94 | A | Sidechain |
| 1 | A | 942 | U | Sidechain |
| 1 | A | 943 | U | Sidechain |
| 1 | A | 952 | U | Sidechain |
| 1 | A | 953 | C | Sidechain |
| 1 | A | 955 | U | Sidechain |
| 1 | A | 97 | G | Sidechain |
| 1 | A | 970 | G | Sidechain |
| 1 | A | 972 | U | Sidechain |
| 1 | A | 977 | U | Sidechain |
| 1 | A | 978 | U | Sidechain |
| 1 | A | 982 | A | Sidechain |
| 1 | A | 987 | U | Sidechain |
| 1 | A | 994 | G | Sidechain |
| 1 | A | 998 | A | Sidechain |
| 78 | A0 | 57 | ARG | Sidechain |
| 78 | A0 | 64 | ARG | Sidechain |
| 38 | A1 | 17 | ARG | Sidechain |
| 39 | A2 | 114 | ARG | Sidechain |
| 67 | A3 | 105 | ARG | Sidechain |
| 40 | A4 | 14 | ARG | Sidechain |
| 40 | A4 | 36 | ASP | Peptide |
| 68 | A5 | 119 | GLN | Peptide |
| 68 | A5 | 154 | ARG | Sidechain |
| 68 | A5 | 162 | TYR | Sidechain |
| 68 | A5 | 224 | ARG | Sidechain |
| 68 | A5 | 238 | ARG | Peptide,Sidechain |
| 68 | A5 | 56 | ARG | Sidechain |
| 41 | A6 | 30 | ARG | Sidechain |
| 41 | A6 | 56 | ARG | Sidechain |
| 41 | A6 | 62 | TYR | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 41 | A6 | 89 | ARG | Sidechain |
| 42 | A7 | 87 | ARG | Sidechain |
| 44 | A8 | 33 | ARG | Sidechain |
| 44 | A8 | 43 | ARG | Sidechain |
| 45 | A9 | 115 | ARG | Sidechain |
| 45 | A9 | 130 | ARG | Sidechain |
| 34 | AA | 1013 | U | Sidechain |
| 34 | AA | 1019 | A | Sidechain |
| 34 | AA | 102 | A | Sidechain |
| 34 | AA | 1023 | U | Sidechain |
| 34 | AA | 1033 | A | Sidechain |
| 34 | AA | 1047 | A | Sidechain |
| 34 | AA | 1050 | C | Sidechain |
| 34 | AA | 1053 | U | Sidechain |
| 34 | AA | 1055 | A | Sidechain |
| 34 | AA | 1056 | G | Sidechain |
| 34 | AA | 1058 | U | Sidechain |
| 34 | AA | 1064 | U | Sidechain |
| 34 | AA | 1065 | U | Sidechain |
| 34 | AA | 1067 | U | Sidechain |
| 34 | AA | 1073 | G | Sidechain |
| 34 | AA | 1075 | U | Sidechain |
| 34 | AA | 1079 | U | Sidechain |
| 34 | AA | 109 | A | Sidechain |
| 34 | AA | 1091 | G | Sidechain |
| 34 | AA | 1094 | U | Sidechain |
| 34 | AA | 1101 | A | Sidechain |
| 34 | AA | 1109 | U | Sidechain |
| 34 | AA | 1110 | U | Sidechain |
| 34 | AA | 1115 | G | Sidechain |
| 34 | AA | 1135 | G | Sidechain |
| 34 | AA | 114 | A | Sidechain |
| 34 | AA | 1142 | G | Sidechain |
| 34 | AA | 116 | A | Sidechain |
| 34 | AA | 1167 | U | Sidechain |
| 34 | AA | 1169 | A | Sidechain |
| 34 | AA | 1171 | A | Sidechain |
| 34 | AA | 1203 | A | Sidechain |
| 34 | AA | 1206 | U | Sidechain |
| 34 | AA | 1209 | U | Sidechain |
| 34 | AA | 1211 | U | Sidechain |
| 34 | AA | 1213 | U | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 34 | AA | 1217 | U | Sidechain |
| 34 | AA | 1220 | U | Sidechain |
| 34 | AA | 1222 | U | Sidechain |
| 34 | AA | 1223 | U | Sidechain |
| 34 | AA | 1224 | A | Sidechain |
| 34 | AA | 1231 | A | Sidechain |
| 34 | AA | 1232 | U | Sidechain |
| 34 | AA | 1239 | A | Sidechain |
| 34 | AA | 124 | U | Sidechain |
| 34 | AA | 1244 | G | Sidechain |
| 34 | AA | 1247 | C | Sidechain |
| 34 | AA | 1248 | A | Sidechain |
| 34 | AA | 1249 | U | Sidechain |
| 34 | AA | 1250 | U | Sidechain |
| 34 | AA | 1251 | U | Sidechain |
| 34 | AA | 1256 | U | Sidechain |
| 34 | AA | 1264 | A | Sidechain |
| 34 | AA | 1266 | U | Sidechain |
| 34 | AA | 127 | U | Sidechain |
| 34 | AA | 1273 | G | Sidechain |
| 34 | AA | 1276 | G | Sidechain |
| 34 | AA | 1280 | G | Sidechain |
| 34 | AA | 1297 | A | Sidechain |
| 34 | AA | 1318 | A | Sidechain |
| 34 | AA | 1321 | A | Sidechain |
| 34 | AA | 1327 | C | Sidechain |
| 34 | AA | 1329 | U | Sidechain |
| 34 | AA | 1330 | A | Sidechain |
| 34 | AA | 1331 | A | Sidechain |
| 34 | AA | 136 | U | Sidechain |
| 34 | AA | 14 | U | Sidechain |
| 34 | AA | 1416 | U | Sidechain |
| 34 | AA | 1417 | G | Sidechain |
| 34 | AA | 1423 | G | Sidechain |
| 34 | AA | 1429 | A | Sidechain |
| 34 | AA | 1434 | G | Sidechain |
| 34 | AA | 1445 | A | Sidechain |
| 34 | AA | 1447 | G | Sidechain |
| 34 | AA | 1453 | U | Sidechain |
| 34 | AA | 1457 | G | Sidechain |
| 34 | AA | 1459 | U | Sidechain |
| 34 | AA | 146 | U | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 34 | AA | 147 | C | Sidechain |
| 34 | AA | 1473 | A | Sidechain |
| 34 | AA | 1476 | A | Sidechain |
| 34 | AA | 148 | G | Sidechain |
| 34 | AA | 149 | A | Sidechain |
| 34 | AA | 1493 | U | Sidechain |
| 34 | AA | 1497 | U | Sidechain |
| 34 | AA | 1499 | U | Sidechain |
| 34 | AA | 1503 | A | Sidechain |
| 34 | AA | 1507 | U | Sidechain |
| 34 | AA | 1510 | U | Sidechain |
| 34 | AA | 1511 | U | Sidechain |
| 34 | AA | 1513 | U | Sidechain |
| 34 | AA | 1516 | G | Sidechain |
| 34 | AA | 1518 | A | Sidechain |
| 34 | AA | 1524 | U | Sidechain |
| 34 | AA | 1534 | U | Sidechain |
| 34 | AA | 1549 | U | Sidechain |
| 34 | AA | 1552 | G | Sidechain |
| 34 | AA | 1553 | U | Sidechain |
| 34 | AA | 1554 | G | Sidechain |
| 34 | AA | 156 | U | Sidechain |
| 34 | AA | 1572 | U | Sidechain |
| 34 | AA | 1574 | C | Sidechain |
| 34 | AA | 1583 | G | Sidechain |
| 34 | AA | 1585 | U | Sidechain |
| 34 | AA | 1588 | U | Sidechain |
| 34 | AA | 1595 | A | Sidechain |
| 34 | AA | 1597 | U | Sidechain |
| 34 | AA | 1598 | A | Sidechain |
| 34 | AA | 160 | G | Sidechain |
| 34 | AA | 1602 | A | Sidechain |
| 34 | AA | 1606 | U | Sidechain |
| 34 | AA | 1613 | G | Sidechain |
| 34 | AA | 1617 | A | Sidechain |
| 34 | AA | 1619 | U | Sidechain |
| 34 | AA | 1625 | G | Sidechain |
| 34 | AA | 1628 | U | Sidechain |
| 34 | AA | 1629 | G | Sidechain |
| 34 | AA | 1635 | G | Sidechain |
| 34 | AA | 1643 | U | Sidechain |
| 34 | AA | 1644 | U | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 34 | AA | 1645 | U | Sidechain |
| 34 | AA | 1647 | U | Sidechain |
| 34 | AA | 1650 | U | Sidechain |
| 34 | AA | 1655 | U | Sidechain |
| 34 | AA | 1658 | G | Sidechain |
| 34 | AA | 1671 | U | Sidechain |
| 34 | AA | 1695 | A | Sidechain |
| 34 | AA | 170 | U | Sidechain |
| 34 | AA | 1700 | U | Sidechain |
| 34 | AA | 1701 | G | Sidechain |
| 34 | AA | 1726 | C | Sidechain |
| 34 | AA | 1731 | A | Sidechain |
| 34 | AA | 1735 | G | Sidechain |
| 34 | AA | 1737 | A | Sidechain |
| 34 | AA | 174 | U | Sidechain |
| 34 | AA | 1740 | A | Sidechain |
| 34 | AA | 1745 | G | Sidechain |
| 34 | AA | 1747 | U | Sidechain |
| 34 | AA | 1755 | U | Sidechain |
| 34 | AA | 1763 | G | Sidechain |
| 34 | AA | 1784 | G | Sidechain |
| 34 | AA | 1785 | U | Sidechain |
| 34 | AA | 1786 | A | Sidechain |
| 34 | AA | 1787 | A | Sidechain |
| 34 | AA | 1797 | A | Sidechain |
| 34 | AA | 1798 | A | Sidechain |
| 34 | AA | 1805 | U | Sidechain |
| 34 | AA | 1815 | A | Sidechain |
| 34 | AA | 1820 | U | Sidechain |
| 34 | AA | 1821 | U | Sidechain |
| 34 | AA | 1829 | G | Sidechain |
| 34 | AA | 1830 | G | Sidechain |
| 34 | AA | 1832 | U | Sidechain |
| 34 | AA | 1835 | G | Sidechain |
| 34 | AA | 1836 | U | Sidechain |
| 34 | AA | 1841 | U | Sidechain |
| 34 | AA | 1842 | U | Sidechain |
| 34 | AA | 1844 | G | Sidechain |
| 34 | AA | 1846 | A | Sidechain |
| 34 | AA | 1848 | U | Sidechain |
| 34 | AA | 1851 | A | Sidechain |
| 34 | AA | 1872 | A | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 34 | AA | 1878 | U | Sidechain |
| 34 | AA | 1882 | U | Sidechain |
| 34 | AA | 1886 | A | Sidechain |
| 34 | AA | 1889 | A | Sidechain |
| 34 | AA | 1894 | U | Sidechain |
| 34 | AA | 1899 | U | Sidechain |
| 34 | AA | 1902 | A | Sidechain |
| 34 | AA | 1906 | A | Sidechain |
| 34 | AA | 1958 | U | Sidechain |
| 34 | AA | 1960 | U | Sidechain |
| 34 | AA | 1969 | A | Sidechain |
| 34 | AA | 1981 | U | Sidechain |
| 34 | AA | 1997 | G | Sidechain |
| 34 | AA | 200 | A | Sidechain |
| 34 | AA | 2000 | G | Sidechain |
| 34 | AA | 2001 | U | Sidechain |
| 34 | AA | 2004 | U | Sidechain |
| 34 | AA | 2018 | G | Sidechain |
| 34 | AA | 2019 | A | Sidechain |
| 34 | AA | 2030 | G | Sidechain |
| 34 | AA | 205 | G | Sidechain |
| 34 | AA | 207 | A | Sidechain |
| 34 | AA | 2072 | U | Sidechain |
| 34 | AA | 208 | U | Sidechain |
| 34 | AA | 2080 | C | Sidechain |
| 34 | AA | 2081 | U | Sidechain |
| 34 | AA | 2102 | A | Sidechain |
| 34 | AA | 2103 | C | Sidechain |
| 34 | AA | 2104 | C | Sidechain |
| 34 | AA | 2108 | A | Sidechain |
| 34 | AA | 2109 | A | Sidechain |
| 34 | AA | 211 | U | Sidechain |
| 34 | AA | 2112 | G | Sidechain |
| 34 | AA | 2117 | A | Sidechain |
| 34 | AA | 2127 | G | Sidechain |
| 34 | AA | 2137 | C | Sidechain |
| 34 | AA | 2138 | U | Sidechain |
| 34 | AA | 2141 | G | Sidechain |
| 34 | AA | 2148 | U | Sidechain |
| 34 | AA | 216 | C | Sidechain |
| 34 | AA | 2161 | G | Sidechain |
| 34 | AA | 2165 | G | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 34 | AA | 2173 | G | Sidechain |
| 34 | AA | 2176 | A | Sidechain |
| 34 | AA | 2178 | A | Sidechain |
| 34 | AA | 2180 | U | Sidechain |
| 34 | AA | 2184 | U | Sidechain |
| 34 | AA | 2194 | C | Sidechain |
| 34 | AA | 2198 | A | Sidechain |
| 34 | AA | 2214 | A | Sidechain |
| 34 | AA | 2393 | A | Sidechain |
| 34 | AA | 2396 | C | Sidechain |
| 34 | AA | 2409 | G | Sidechain |
| 34 | AA | 2411 | C | Sidechain |
| 34 | AA | 2412 | A | Sidechain |
| 34 | AA | 2423 | G | Sidechain |
| 34 | AA | 2424 | A | Sidechain |
| 34 | AA | 2429 | U | Sidechain |
| 34 | AA | 2432 | A | Sidechain |
| 34 | AA | 2433 | U | Sidechain |
| 34 | AA | 2434 | U | Sidechain |
| 34 | AA | 244 | U | Sidechain |
| 34 | AA | 2441 | U | Sidechain |
| 34 | AA | 2443 | G | Sidechain |
| 34 | AA | 2457 | C | Sidechain |
| 34 | AA | 2460 | A | Sidechain |
| 34 | AA | 2463 | U | Sidechain |
| 34 | AA | 2473 | A | Sidechain |
| 34 | AA | 2481 | A | Sidechain |
| 34 | AA | 2482 | U | Sidechain |
| 34 | AA | 2484 | U | Sidechain |
| 34 | AA | 2486 | U | Sidechain |
| 34 | AA | 2497 | U | Sidechain |
| 34 | AA | 2499 | G | Sidechain |
| 34 | AA | 2503 | G | Sidechain |
| 34 | AA | 2506 | A | Sidechain |
| 34 | AA | 2510 | U | Sidechain |
| 34 | AA | 2514 | G | Sidechain |
| 34 | AA | 2518 | U | Sidechain |
| 34 | AA | 2534 | U | Sidechain |
| 34 | AA | 2552 | A | Sidechain |
| 34 | AA | 2554 | G | Sidechain |
| 34 | AA | 2563 | A | Sidechain |
| 34 | AA | 2565 | G | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 34 | AA | 2566 | G | Sidechain |
| 34 | AA | 2567 | U | Sidechain |
| 34 | AA | 2573 | A | Sidechain |
| 34 | AA | 2575 | U | Sidechain |
| 34 | AA | 2577 | C | Sidechain |
| 34 | AA | 2579 | U | Sidechain |
| 34 | AA | 258 | U | Sidechain |
| 34 | AA | 2587 | U | Sidechain |
| 34 | AA | 2589 | A | Sidechain |
| 34 | AA | 2590 | U | Sidechain |
| 34 | AA | 2600 | G | Sidechain |
| 34 | AA | 2603 | U | Sidechain |
| 34 | AA | 262 | A | Sidechain |
| 34 | AA | 2629 | U | Sidechain |
| 34 | AA | 2636 | U | Sidechain |
| 34 | AA | 2644 | U | Sidechain |
| 34 | AA | 2649 | A | Sidechain |
| 34 | AA | 265 | U | Sidechain |
| 34 | AA | 2654 | A | Sidechain |
| 34 | AA | 2660 | A | Sidechain |
| 34 | AA | 2662 | G | Sidechain |
| 34 | AA | 2669 | G | Sidechain |
| 34 | AA | 2670 | G | Sidechain |
| 34 | AA | 2672 | U | Sidechain |
| 34 | AA | 2681 | U | Sidechain |
| 34 | AA | 2690 | A | Sidechain |
| 34 | AA | 2693 | G | Sidechain |
| 34 | AA | 27 | U | Sidechain |
| 34 | AA | 270 | U | Sidechain |
| 34 | AA | 2707 | G | Sidechain |
| 34 | AA | 2709 | U | Sidechain |
| 34 | AA | 271 | G | Sidechain |
| 34 | AA | 2711 | U | Sidechain |
| 34 | AA | 2716 | U | Sidechain |
| 34 | AA | 2727 | U | Sidechain |
| 34 | AA | 2809 | A | Sidechain |
| 34 | AA | 2811 | A | Sidechain |
| 34 | AA | 2814 | U | Sidechain |
| 34 | AA | 2822 | U | Sidechain |
| 34 | AA | 288 | G | Sidechain |
| 34 | AA | 2915 | U | Sidechain |
| 34 | AA | 2920 | A | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 34 | AA | 2925 | U | Sidechain |
| 34 | AA | 2951 | U | Sidechain |
| 34 | AA | 2957 | G | Sidechain |
| 34 | AA | 2968 | U | Sidechain |
| 34 | AA | 2971 | G | Sidechain |
| 34 | AA | 2975 | A | Sidechain |
| 34 | AA | 2977 | U | Sidechain |
| 34 | AA | 2979 | U | Sidechain |
| 34 | AA | 2981 | A | Sidechain |
| 34 | AA | 2987 | G | Sidechain |
| 34 | AA | 2994 | A | Sidechain |
| 34 | AA | 3016 | G | Sidechain |
| 34 | AA | 3020 | U | Sidechain |
| 34 | AA | 3033 | A | Sidechain |
| 34 | AA | 3035 | A | Sidechain |
| 34 | AA | 3038 | G | Sidechain |
| 34 | AA | 304 | U | Sidechain |
| 34 | AA | 3044 | A | Sidechain |
| 34 | AA | 3049 | G | Sidechain |
| 34 | AA | 3052 | U | Sidechain |
| 34 | AA | 3062 | U | Sidechain |
| 34 | AA | 3063 | U | Sidechain |
| 34 | AA | 3064 | U | Sidechain |
| 34 | AA | 3065 | C | Sidechain |
| 34 | AA | 3068 | A | Sidechain |
| 34 | AA | 308 | U | Sidechain |
| 34 | AA | 3080 | A | Sidechain |
| 34 | AA | 3084 | G | Sidechain |
| 34 | AA | 3088 | G | Sidechain |
| 34 | AA | 3092 | G | Sidechain |
| 34 | AA | 3097 | A | Sidechain |
| 34 | AA | 3109 | U | Sidechain |
| 34 | AA | 3111 | U | Sidechain |
| 34 | AA | 3114 | G | Sidechain |
| 34 | AA | 3122 | A | Sidechain |
| 34 | AA | 3137 | U | Sidechain |
| 34 | AA | 3141 | G | Sidechain |
| 34 | AA | 3142 | U | Sidechain |
| 34 | AA | 3182 | G | Sidechain |
| 34 | AA | 3183 | G | Sidechain |
| 34 | AA | 3186 | U | Sidechain |
| 34 | AA | 3192 | U | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 34 | AA | 3203 | C | Sidechain |
| 34 | AA | 3205 | U | Sidechain |
| 34 | AA | 3212 | G | Sidechain |
| 34 | AA | 3219 | U | Sidechain |
| 34 | AA | 3220 | U | Sidechain |
| 34 | AA | 3241 | U | Sidechain |
| 34 | AA | 3247 | U | Sidechain |
| 34 | AA | 3255 | A | Sidechain |
| 34 | AA | 3257 | G | Sidechain |
| 34 | AA | 3264 | U | Sidechain |
| 34 | AA | 3277 | G | Sidechain |
| 34 | AA | 3278 | A | Sidechain |
| 34 | AA | 3279 | U | Sidechain |
| 34 | AA | 3280 | U | Sidechain |
| 34 | AA | 3281 | G | Sidechain |
| 34 | AA | 3300 | A | Sidechain |
| 34 | AA | 3309 | G | Sidechain |
| 34 | AA | 331 | A | Sidechain |
| 34 | AA | 332 | A | Sidechain |
| 34 | AA | 3323 | G | Sidechain |
| 34 | AA | 3325 | G | Sidechain |
| 34 | AA | 3328 | A | Sidechain |
| 34 | AA | 3335 | A | Sidechain |
| 34 | AA | 3359 | A | Sidechain |
| 34 | AA | 3362 | A | Sidechain |
| 34 | AA | 3365 | U | Sidechain |
| 34 | AA | 3374 | U | Sidechain |
| 34 | AA | 3387 | U | Sidechain |
| 34 | AA | 339 | G | Sidechain |
| 34 | AA | 3391 | G | Sidechain |
| 34 | AA | 3402 | A | Sidechain |
| 34 | AA | 3413 | A | Sidechain |
| 34 | AA | 3418 | A | Sidechain |
| 34 | AA | 3427 | U | Sidechain |
| 34 | AA | 3441 | A | Sidechain |
| 34 | AA | 3444 | G | Sidechain |
| 34 | AA | 3449 | U | Sidechain |
| 34 | AA | 3452 | U | Sidechain |
| 34 | AA | 3470 | G | Sidechain |
| 34 | AA | 3472 | A | Sidechain |
| 34 | AA | 3480 | C | Sidechain |
| 34 | AA | 3483 | U | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 34 | AA | 3484 | U | Sidechain |
| 34 | AA | 3488 | U | Sidechain |
| 34 | AA | 349 | G | Sidechain |
| 34 | AA | 3495 | U | Sidechain |
| 34 | AA | 3499 | C | Sidechain |
| 34 | AA | 3503 | U | Sidechain |
| 34 | AA | 3505 | U | Sidechain |
| 34 | AA | 3508 | A | Sidechain |
| 34 | AA | 351 | U | Sidechain |
| 34 | AA | 3515 | A | Sidechain |
| 34 | AA | 3516 | A | Sidechain |
| 34 | AA | 352 | A | Sidechain |
| 34 | AA | 3526 | U | Sidechain |
| 34 | AA | 3532 | A | Sidechain |
| 34 | AA | 3535 | A | Sidechain |
| 34 | AA | 3545 | U | Sidechain |
| 34 | AA | 3546 | C | Sidechain |
| 34 | AA | 3549 | U | Sidechain |
| 34 | AA | 356 | A | Sidechain |
| 34 | AA | 357 | A | Sidechain |
| 34 | AA | 3571 | A | Sidechain |
| 34 | AA | 3574 | G | Sidechain |
| 34 | AA | 3581 | A | Sidechain |
| 34 | AA | 3585 | A | Sidechain |
| 34 | AA | 3591 | U | Sidechain |
| 34 | AA | 3594 | G | Sidechain |
| 34 | AA | 361 | G | Sidechain |
| 34 | AA | 362 | U | Sidechain |
| 34 | AA | 3624 | U | Sidechain |
| 34 | AA | 3629 | U | Sidechain |
| 34 | AA | 3632 | U | Sidechain |
| 34 | AA | 3639 | G | Sidechain |
| 34 | AA | 3646 | G | Sidechain |
| 34 | AA | 3648 | U | Sidechain |
| 34 | AA | 3658 | G | Sidechain |
| 34 | AA | 366 | G | Sidechain |
| 34 | AA | 3660 | A | Sidechain |
| 34 | AA | 3666 | U | Sidechain |
| 34 | AA | 367 | U | Sidechain |
| 34 | AA | 3672 | A | Sidechain |
| 34 | AA | 368 | G | Sidechain |
| 34 | AA | 3688 | G | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 34 | AA | 3692 | A | Sidechain |
| 34 | AA | 3698 | U | Sidechain |
| 34 | AA | 37 | U | Sidechain |
| 34 | AA | 3706 | U | Sidechain |
| 34 | AA | 3707 | U | Sidechain |
| 34 | AA | 3708 | U | Sidechain |
| 34 | AA | 3709 | U | Sidechain |
| 34 | AA | 3726 | U | Sidechain |
| 34 | AA | 3736 | A | Sidechain |
| 34 | AA | 3738 | U | Sidechain |
| 34 | AA | 3739 | A | Sidechain |
| 34 | AA | 374 | A | Sidechain |
| 34 | AA | 3740 | A | Sidechain |
| 34 | AA | 3749 | U | Sidechain |
| 34 | AA | 3754 | A | Sidechain |
| 34 | AA | 3767 | U | Sidechain |
| 34 | AA | 3775 | G | Sidechain |
| 34 | AA | 3776 | U | Sidechain |
| 34 | AA | 3782 | A | Sidechain |
| 34 | AA | 3783 | G | Sidechain |
| 34 | AA | 379 | G | Sidechain |
| 34 | AA | 38 | U | Sidechain |
| 34 | AA | 380 | A | Sidechain |
| 34 | AA | 389 | U | Sidechain |
| 34 | AA | 392 | G | Sidechain |
| 34 | AA | 393 | G | Sidechain |
| 34 | AA | 406 | A | Sidechain |
| 34 | AA | 416 | G | Sidechain |
| 34 | AA | 418 | A | Sidechain |
| 34 | AA | 422 | G | Sidechain |
| 34 | AA | 424 | U | Sidechain |
| 34 | AA | 439 | U | Sidechain |
| 34 | AA | 440 | A | Sidechain |
| 34 | AA | 441 | A | Sidechain |
| 34 | AA | 446 | G | Sidechain |
| 34 | AA | 449 | A | Sidechain |
| 34 | AA | 458 | A | Sidechain |
| 34 | AA | 490 | U | Sidechain |
| 34 | AA | 495 | U | Sidechain |
| 34 | AA | 498 | U | Sidechain |
| 34 | AA | 500 | A | Sidechain |
| 34 | AA | 507 | G | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 34 | AA | 520 | U | Sidechain |
| 34 | AA | 525 | U | Sidechain |
| 34 | AA | 527 | A | Sidechain |
| 34 | AA | 544 | C | Sidechain |
| 34 | AA | 55 | G | Sidechain |
| 34 | AA | 578 | U | Sidechain |
| 34 | AA | 579 | C | Sidechain |
| 34 | AA | 582 | U | Sidechain |
| 34 | AA | 583 | U | Sidechain |
| 34 | AA | 596 | A | Sidechain |
| 34 | AA | 60 | A | Sidechain |
| 34 | AA | 606 | A | Sidechain |
| 34 | AA | 607 | A | Sidechain |
| 34 | AA | 609 | C | Sidechain |
| 34 | AA | 614 | U | Sidechain |
| 34 | AA | 623 | U | Sidechain |
| 34 | AA | 629 | A | Sidechain |
| 34 | AA | 630 | U | Sidechain |
| 34 | AA | 633 | U | Sidechain |
| 34 | AA | 634 | U | Sidechain |
| 34 | AA | 637 | U | Sidechain |
| 34 | AA | 640 | U | Sidechain |
| 34 | AA | 641 | G | Sidechain |
| 34 | AA | 644 | G | Sidechain |
| 34 | AA | 649 | U | Sidechain |
| 34 | AA | 65 | A | Sidechain |
| 34 | AA | 656 | U | Sidechain |
| 34 | AA | 670 | U | Sidechain |
| 34 | AA | 671 | U | Sidechain |
| 34 | AA | 673 | U | Sidechain |
| 34 | AA | 679 | U | Sidechain |
| 34 | AA | 68 | A | Sidechain |
| 34 | AA | 683 | A | Sidechain |
| 34 | AA | 684 | G | Sidechain |
| 34 | AA | 688 | U | Sidechain |
| 34 | AA | 69 | U | Sidechain |
| 34 | AA | 696 | C | Sidechain |
| 34 | AA | 70 | A | Sidechain |
| 34 | AA | 702 | U | Sidechain |
| 34 | AA | 703 | U | Sidechain |
| 34 | AA | 704 | U | Sidechain |
| 34 | AA | 706 | U | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 34 | AA | 708 | A | Sidechain |
| 34 | AA | 71 | A | Sidechain |
| 34 | AA | 714 | C | Sidechain |
| 34 | AA | 716 | C | Sidechain |
| 34 | AA | 722 | G | Sidechain |
| 34 | AA | 729 | G | Sidechain |
| 34 | AA | 734 | A | Sidechain |
| 34 | AA | 739 | G | Sidechain |
| 34 | AA | 744 | G | Sidechain |
| 34 | AA | 746 | A | Sidechain |
| 34 | AA | 75 | U | Sidechain |
| 34 | AA | 754 | A | Sidechain |
| 34 | AA | 760 | A | Sidechain |
| 34 | AA | 764 | G | Sidechain |
| 34 | AA | 77 | A | Sidechain |
| 34 | AA | 770 | U | Sidechain |
| 34 | AA | 771 | U | Sidechain |
| 34 | AA | 773 | A | Sidechain |
| 34 | AA | 774 | A | Sidechain |
| 34 | AA | 825 | G | Sidechain |
| 34 | AA | 826 | U | Sidechain |
| 34 | AA | 828 | G | Sidechain |
| 34 | AA | 831 | U | Sidechain |
| 34 | AA | 835 | G | Sidechain |
| 34 | AA | 86 | G | Sidechain |
| 34 | AA | 869 | A | Sidechain |
| 34 | AA | 888 | A | Sidechain |
| 34 | AA | 911 | U | Sidechain |
| 34 | AA | 912 | U | Sidechain |
| 34 | AA | 913 | U | Sidechain |
| 34 | AA | 92 | G | Sidechain |
| 34 | AA | 920 | A | Sidechain |
| 34 | AA | 925 | A | Sidechain |
| 34 | AA | 926 | G | Sidechain |
| 34 | AA | 93 | C | Sidechain |
| 34 | AA | 931 | U | Sidechain |
| 34 | AA | 933 | U | Sidechain |
| 34 | AA | 937 | C | Sidechain |
| 34 | AA | 938 | U | Sidechain |
| 34 | AA | 94 | G | Sidechain |
| 34 | AA | 943 | G | Sidechain |
| 34 | AA | 95 | A | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 34 | AA | 950 | G | Sidechain |
| 34 | AA | 954 | G | Sidechain |
| 34 | AA | 965 | A | Sidechain |
| 34 | AA | 966 | A | Sidechain |
| 34 | AA | 977 | A | Sidechain |
| 34 | AA | 981 | U | Sidechain |
| 36 | AB | 109 | U | Sidechain |
| 36 | AB | 11 | A | Sidechain |
| 36 | AB | 22 | G | Sidechain |
| 36 | AB | 24 | U | Sidechain |
| 36 | AB | 26 | C | Sidechain |
| 36 | AB | 48 | G | Sidechain |
| 36 | AB | 53 | U | Sidechain |
| 36 | AB | 55 | A | Sidechain |
| 36 | AB | 61 | G | Sidechain |
| 36 | AB | 69 | U | Sidechain |
| 36 | AB | 73 | U | Sidechain |
| 36 | AB | 75 | G | Sidechain |
| 36 | AB | 97 | G | Sidechain |
| 36 | AB | 98 | G | Sidechain |
| 35 | AC | 106 | G | Sidechain |
| 35 | AC | 12 | U | Sidechain |
| 35 | AC | 125 | U | Sidechain |
| 35 | AC | 127 | C | Sidechain |
| 35 | AC | 129 | U | Sidechain |
| 35 | AC | 156 | A | Sidechain |
| 35 | AC | 20 | G | Sidechain |
| 35 | AC | 25 | C | Sidechain |
| 35 | AC | 27 | U | Sidechain |
| 35 | AC | 3 | G | Sidechain |
| 35 | AC | 30 | U | Sidechain |
| 35 | AC | 31 | U | Sidechain |
| 35 | AC | 4 | C | Sidechain |
| 35 | AC | 40 | G | Sidechain |
| 35 | AC | 42 | U | Sidechain |
| 35 | AC | 53 | G | Sidechain |
| 35 | AC | 64 | U | Sidechain |
| 35 | AC | 78 | U | Sidechain |
| 35 | AC | 85 | A | Sidechain |
| 69 | AD | 11 | GLY | Peptide |
| 69 | AD | 163 | ARG | Sidechain |
| 69 | AD | 20 | ASN | Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 69 | AD | 23 | ARG | Sidechain |
| 69 | AD | 242 | ARG | Sidechain |
| 69 | AD | 54 | ARG | Sidechain |
| 70 | AE | 119 | TYR | Sidechain |
| 70 | AE | 241 | ARG | Sidechain |
| 70 | AE | 272 | ARG | Sidechain |
| 70 | AE | 331 | ARG | Sidechain |
| 71 | AF | 140 | ARG | Sidechain |
| 71 | AF | 199 | ARG | Sidechain |
| 71 | AF | 264 | TYR | Peptide |
| 71 | AF | 48 | ARG | Sidechain |
| 71 | AF | 49 | ARG | Sidechain |
| 71 | AF | 60 | TYR | Sidechain |
| 72 | AG | 141 | ARG | Peptide |
| 72 | AG | 32 | ARG | Sidechain |
| 72 | AG | 41 | THR | Peptide |
| 74 | AH | 144 | TYR | Sidechain |
| 74 | AH | 179 | TYR | Sidechain |
| 74 | AH | 39 | ARG | Sidechain |
| 54 | AI | 11 | TYR | Sidechain |
| 54 | AI | 48 | ARG | Sidechain |
| 55 | AJ | 116 | TYR | Sidechain |
| 55 | AJ | 172 | ASN | Peptide |
| 57 | AK | 17 | ARG | Sidechain |
| 57 | AK | 31 | ARG | Sidechain |
| 57 | AK | 58 | ARG | Sidechain |
| 57 | AK | 81 | ARG | Sidechain |
| 57 | AK | 84 | ARG | Sidechain |
| 37 | AL | 197 | ARG | Sidechain |
| 37 | AL | 34 | ARG | Sidechain |
| 37 | AL | 63 | ARG | Sidechain |
| 37 | AL | 69 | ARG | Sidechain |
| 37 | AL | 96 | TYR | Peptide |
| 58 | AM | 122 | ARG | Sidechain |
| 58 | AM | 37 | TYR | Sidechain |
| 58 | AM | 50 | ARG | Sidechain |
| 58 | AM | 72 | ARG | Sidechain |
| 58 | AM | 82 | ARG | Sidechain |
| 43 | AN | 35 | TYR | Sidechain |
| 43 | AN | 66 | ARG | Sidechain |
| 43 | AN | 93 | ARG | Sidechain |
| 60 | AO | 127 | ARG | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 60 | AO | 28 | HIS | Peptide |
| 60 | AO | 48 | TYR | Sidechain |
| 51 | AP | 160 | ARG | Sidechain |
| 51 | AP | 176 | ARG | Sidechain |
| 51 | AP | 186 | ARG | Sidechain |
| 51 | AP | 44 | ARG | Sidechain |
| 51 | AP | 49 | ARG | Sidechain |
| 51 | AP | 68 | ARG | Sidechain |
| 61 | AQ | 154 | ARG | Sidechain |
| 61 | AQ | 189 | ARG | Sidechain |
| 61 | AQ | 3 | ARG | Sidechain |
| 61 | AQ | 34 | TYR | Sidechain |
| 62 | AR | 181 | ARG | Sidechain |
| 62 | AR | 24 | ARG | Sidechain |
| 62 | AR | 278 | ARG | Sidechain |
| 62 | AR | 50 | ARG | Sidechain |
| 59 | AS | 111 | ARG | Sidechain |
| 59 | AS | 139 | ARG | Sidechain |
| 59 | AS | 157 | LYS | Peptide |
| 59 | AS | 165 | TYR | Sidechain |
| 59 | AS | 177 | ARG | Sidechain |
| 59 | AS | 183 | ARG | Sidechain |
| 59 | AS | 39 | ARG | Sidechain |
| 59 | AS | 57 | ARG | Sidechain |
| 65 | AT | 109 | ARG | Sidechain |
| 65 | AT | 116 | ARG | Sidechain |
| 65 | AT | 162 | ARG | Sidechain |
| 65 | AT | 37 | ARG | Sidechain |
| 65 | AT | 87 | ARG | Sidechain |
| 65 | AT | 99 | ARG | Sidechain |
| 73 | AU | 122 | ARG | Sidechain |
| 73 | AU | 134 | ARG | Sidechain |
| 73 | AU | 157 | ARG | Sidechain |
| 73 | AU | 170 | TYR | Sidechain |
| 73 | AU | 21 | ARG | Sidechain |
| 73 | AU | 35 | ARG | Sidechain |
| 73 | AU | 76 | ARG | Sidechain |
| 75 | AV | 109 | ARG | Sidechain |
| 75 | AV | 13 | ARG | Sidechain |
| 75 | AV | 21 | ARG | Sidechain |
| 75 | AV | 71 | ARG | Sidechain |
| 75 | AV | 80 | ARG | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 63 | AW | 131 | LYS | Peptide |
| 63 | AW | 30 | TYR | Sidechain |
| 63 | AW | 37 | ARG | Sidechain |
| 63 | AW | 47 | TYR | Sidechain |
| 63 | AW | 56 | ARG | Sidechain |
| 63 | AW | 63 | TYR | Peptide |
| 77 | AX | 101 | ARG | Sidechain |
| 64 | AY | 173 | ARG | Sidechain |
| 66 | AZ | 114 | ARG | Sidechain |
| 66 | AZ | 15 | ARG | Sidechain |
| 66 | AZ | 83 | ARG | Sidechain |
| 66 | AZ | 86 | ARG | Sidechain |
| 46 | Aa | 4 | ARG | Sidechain |
| 46 | Aa | 74 | ARG | Sidechain |
| 46 | Aa | 76 | TYR | Sidechain |
| 46 | Aa | 88 | ARG | Sidechain |
| 47 | Ab | 106 | ARG | Sidechain |
| 56 | Ac | 14 | ARG | Sidechain |
| 56 | Ac | 48 | ARG | Sidechain |
| 56 | Ac | 69 | TYR | Sidechain |
| 49 | Ae | 18 | ARG | Sidechain |
| 49 | Ae | 28 | ARG | Sidechain |
| 49 | Ae | 42 | ARG | Sidechain |
| 49 | Ae | 45 | ARG | Sidechain |
| 49 | Ae | 6 | ARG | Sidechain |
| 50 | Af | 41 | ARG | Sidechain |
| 50 | Af | 46 | ARG | Sidechain |
| 76 | Ag | 16 | ARG | Sidechain |
| 76 | Ag | 37 | ARG | Sidechain |
| 52 | Ah | 17 | ARG | Sidechain |
| 52 | Ah | 7 | LYS | Peptide |
| 53 | Ai | 40 | ARG | Sidechain |
| 53 | Ai | 42 | TYR | Sidechain |
| 53 | Ai | 54 | LYS | Peptide |
| 20 | B | 146 | ARG | Peptide |
| 20 | B | 190 | PRO | Peptide |
| 20 | B | 213 | ARG | Sidechain |
| 20 | B | 64 | ARG | Sidechain |
| 33 | C | 103 | THR | Peptide |
| 33 | C | 119 | ARG | Sidechain |
| 33 | C | 151 | SER | Peptide |
| 33 | C | 62 | ARG | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 33 | C | 79 | ARG | Sidechain |
| 33 | C | 84 | ARG | Sidechain |
| 3 | D | 117 | ARG | Sidechain |
| 4 | E | 108 | ARG | Sidechain |
| 4 | E | 14 | ASN | Peptide |
| 4 | E | 168 | ARG | Peptide |
| 4 | E | 171 | ARG | Sidechain |
| 4 | E | 69 | ARG | Sidechain |
| 4 | E | 78 | ARG | Sidechain |
| 21 | F | 100 | ARG | Sidechain |
| 21 | F | 103 | TYR | Sidechain |
| 21 | F | 108 | ARG | Sidechain |
| 21 | F | 11 | ARG | Sidechain |
| 21 | F | 191 | ARG | Sidechain |
| 5 | G | 107 | ARG | Sidechain |
| 5 | G | 236 | TYR | Sidechain |
| 5 | G | 63 | TYR | Sidechain |
| 5 | G | 80 | GLN | Peptide |
| 22 | H | 137 | ARG | Sidechain |
| 22 | H | 154 | ARG | Sidechain |
| 22 | H | 82 | LYS | Peptide |
| 6 | I | 136 | ARG | Sidechain |
| 6 | I | 150 | ARG | Sidechain |
| 6 | I | 195 | ARG | Sidechain |
| 6 | I | 62 | ARG | Sidechain |
| 23 | J | 115 | ARG | Sidechain |
| 23 | J | 12 | ASN | Peptide |
| 23 | J | 123 | TYR | Sidechain |
| 23 | J | 69 | TYR | Sidechain |
| 23 | J | 98 | ARG | Sidechain |
| 7 | K | 118 | ARG | Sidechain |
| 7 | K | 46 | TYR | Sidechain |
| 24 | L | 217 | ARG | Sidechain |
| 24 | L | 25 | ARG | Sidechain |
| 24 | L | 53 | TYR | Sidechain |
| 8 | M | 115 | ARG | Sidechain |
| 25 | N | 82 | ARG | Sidechain |
| 11 | O | 63 | ARG | Sidechain |
| 26 | P | 149 | ARG | Sidechain |
| 26 | P | 37 | PHE | Peptide |
| 26 | P | 50 | ARG | Sidechain |
| 27 | Q | 109 | ARG | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 27 | Q | 137 | LYS | Peptide |
| 29 | T | 54 | ARG | Sidechain |
| 30 | U | 114 | ARG | Sidechain |
| 30 | U | 141 | TYR | Sidechain |
| 31 | V | 102 | ARG | Sidechain |
| 31 | V | 106 | ARG | Sidechain |
| 31 | V | 11 | ARG | Sidechain |
| 31 | V | 36 | ARG | Sidechain |
| 31 | V | 70 | ARG | Sidechain |
| 31 | V | 90 | ARG | Sidechain |
| 9 | W | 11 | ARG | Sidechain |
| 9 | W | 21 | TYR | Sidechain |
| 9 | W | 3 | ARG | Sidechain |
| 32 | X | 40 | ARG | Sidechain |
| 12 | Y | 108 | ARG | Sidechain |
| 12 | Y | 141 | LYS | Peptide |
| 12 | Y | 148 | THR | Peptide |
| 12 | Y | 161 | TYR | Sidechain |
| 12 | Y | 39 | ARG | Sidechain |
| 12 | Y | 53 | TYR | Peptide |

## 5.2 Too-close contacts (i)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | A | 34207 | 0 | 17266 | 123 | 0 |
| 2 | 7 | 1571 | 0 | 797 | 12 | 0 |
| 3 | D | 1229 | 0 | 1311 | 0 | 0 |
| 4 | E | 1515 | 0 | 1605 | 2 | 0 |
| 5 | G | 1758 | 0 | 1811 | 1 | 0 |
| 6 | I | 1424 | 0 | 1471 | 0 | 0 |
| 7 | K | 1037 | 0 | 1099 | 2 | 0 |
| 8 | M | 1099 | 0 | 1183 | 1 | 0 |
| 9 | W | 786 | 0 | 858 | 1 | 0 |
| 10 | R | 747 | 0 | 754 | 0 | 0 |
| 11 | O | 687 | 0 | 695 | 0 | 0 |
| 12 | Y | 1267 | 0 | 1316 | 1 | 0 |
| 13 | Z | 557 | 0 | 558 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 14 | 1 | 986 | 0 | 1076 | 0 | 0 |
| 15 | 2 | 321 | 0 | 338 | 0 | 0 |
| 16 | 3 | 782 | 0 | 820 | 0 | 0 |
| 17 | 4 | 586 | 0 | 604 | 1 | 0 |
| 18 | 5 | 458 | 0 | 496 | 0 | 0 |
| 19 | 6 | 346 | 0 | 381 | 0 | 0 |
| 20 | B | 1714 | 0 | 1838 | 0 | 0 |
| 21 | F | 2062 | 0 | 2200 | 3 | 0 |
| 22 | H | 1648 | 0 | 1803 | 0 | 0 |
| 23 | J | 1529 | 0 | 1680 | 0 | 0 |
| 24 | L | 1383 | 0 | 1434 | 3 | 0 |
| 25 | N | 772 | 0 | 813 | 1 | 0 |
| 26 | P | 954 | 0 | 997 | 0 | 0 |
| 27 | Q | 1129 | 0 | 1196 | 0 | 0 |
| 28 | S | 1047 | 0 | 1101 | 2 | 0 |
| 29 | T | 405 | 0 | 419 | 0 | 0 |
| 30 | U | 1202 | 0 | 1299 | 1 | 0 |
| 31 | V | 1206 | 0 | 1239 | 1 | 0 |
| 32 | X | 777 | 0 | 832 | 1 | 0 |
| 33 | C | 1539 | 0 | 1600 | 1 | 0 |
| 34 | AA | 67884 | 0 | 34244 | 322 | 0 |
| 35 | AC | 3215 | 0 | 1633 | 8 | 0 |
| 36 | AB | 2522 | 0 | 1275 | 9 | 0 |
| 37 | AL | 1757 | 0 | 1888 | 0 | 0 |
| 38 | A1 | 1134 | 0 | 1245 | 2 | 0 |
| 39 | A2 | 831 | 0 | 887 | 1 | 0 |
| 40 | A4 | 555 | 0 | 599 | 4 | 0 |
| 41 | A6 | 741 | 0 | 763 | 1 | 0 |
| 42 | A7 | 794 | 0 | 869 | 2 | 0 |
| 43 | AN | 1202 | 0 | 1316 | 2 | 0 |
| 44 | A8 | 1037 | 0 | 1139 | 2 | 0 |
| 45 | A9 | 845 | 0 | 886 | 3 | 0 |
| 46 | Aa | 859 | 0 | 912 | 0 | 0 |
| 47 | Ab | 757 | 0 | 842 | 0 | 0 |
| 48 | Ad | 604 | 0 | 686 | 0 | 0 |
| 49 | Ae | 388 | 0 | 421 | 0 | 0 |
| 50 | Af | 414 | 0 | 452 | 0 | 0 |
| 51 | AP | 1697 | 0 | 1802 | 2 | 0 |
| 52 | Ah | 659 | 0 | 727 | 0 | 0 |
| 53 | Ai | 779 | 0 | 861 | 0 | 0 |
| 54 | AI | 1685 | 0 | 1849 | 0 | 0 |
| 55 | AJ | 1813 | 0 | 1985 | 1 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 56 | Ac | 710 | 0 | 761 | 0 | 0 |
| 57 | AK | 1660 | 0 | 1785 | 2 | 0 |
| 58 | AM | 996 | 0 | 1044 | 0 | 0 |
| 59 | AS | 1503 | 0 | 1636 | 1 | 0 |
| 60 | AO | 1172 | 0 | 1230 | 3 | 0 |
| 61 | AQ | 1545 | 0 | 1582 | 0 | 0 |
| 62 | AR | 2050 | 0 | 2140 | 1 | 0 |
| 63 | AW | 1319 | 0 | 1304 | 1 | 0 |
| 64 | AY | 797 | 0 | 850 | 0 | 0 |
| 65 | AT | 1509 | 0 | 1682 | 0 | 0 |
| 66 | AZ | 1001 | 0 | 1099 | 0 | 0 |
| 67 | A3 | 995 | 0 | 1121 | 0 | 0 |
| 68 | A5 | 1879 | 0 | 2005 | 3 | 0 |
| 69 | AD | 1867 | 0 | 1964 | 4 | 0 |
| 70 | AE | 3062 | 0 | 3205 | 5 | 0 |
| 71 | AF | 3095 | 0 | 3333 | 1 | 0 |
| 72 | AG | 1011 | 0 | 1073 | 1 | 0 |
| 73 | AU | 1497 | 0 | 1556 | 2 | 0 |
| 74 | AH | 1476 | 0 | 1574 | 2 | 0 |
| 75 | AV | 1276 | 0 | 1355 | 0 | 0 |
| 76 | Ag | 343 | 0 | 388 | 0 | 0 |
| 77 | AX | 825 | 0 | 882 | 0 | 0 |
| 78 | A0 | 522 | 0 | 539 | 0 | 0 |
| All | All | 193012 | 0 | 144279 | 522 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (522) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 70:AE:353:LEU:H | 70:AE:353:LEU:HD23 | 1.55 | 0.71 |
| 34:AA:3632:U:H3 | 34:AA:3653:G:H1 | 1.42 | 0.65 |
| 34:AA:123:A:H3' | 34:AA:124:U:H5" | 1.81 | 0.62 |
| 34:AA:744:G:H1 | 34:AA:915:G:H1 | 1.47 | 0.62 |
| 34:AA:642:A:C6 | 34:AA:684:G:C8 | 2.89 | 0.61 |
| 28:S:29:ILE:HD13 | 28:S:29:ILE:H | 1.65 | 0.61 |
| 34:AA:440:A:H2' | 34:AA:441:A:C8 | 2.36 | 0.61 |
| 1:A:1982:G:H1 | 1:A:2008:U:H3 | 1.48 | 0.60 |
| 34:AA:2735:G:H1 | 34:AA:2814:U:H3 | 1.50 | 0.59 |
| 34:AA:3626:A:H3' | 34:AA:3627:C:H5" | 1.86 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 34:AA:746:A:H2' | 34:AA:747:A:C8 | 2.39 | 0.58 |
| 1:A:955:U:H2' | 1:A:956:A:C8 | 2.39 | 0.57 |
| 1:A:1022:A:H2' | 1:A:1023:A:C8 | 2.39 | 0.57 |
| 2:7:6:A:H61 | 2:7:65:A:H61 | 1.51 | 0.57 |
| 34:AA:1072:A:H4' | 34:AA:1073:G:H21 | 1.70 | 0.57 |
| 40:A4:7:HIS:CG | 40:A4:8:THR:N | 2.72 | 0.57 |
| 34:AA:1259:G:C4 | 34:AA:2666:A:C2 | 2.93 | 0.57 |
| 34:AA:1822:A:N1 | 34:AA:2004:U:C4 | 2.73 | 0.56 |
| 34:AA:681:U:C6 | 34:AA:681:U:H5" | 2.40 | 0.56 |
| 1:A:1187:A:H2' | 1:A:1188:A:C8 | 2.40 | 0.56 |
| 74:AH:46:ARG:HH11 | 74:AH:46:ARG:HB3 | 1.70 | 0.56 |
| 34:AA:1644:U:C4 | 34:AA:2102:A:N1 | 2.74 | 0.55 |
| 21:F:36:HIS:CD2 | 21:F:86:LEU:H | 2.24 | 0.55 |
| 34:AA:445:A:C2 | 34:AA:446:G:C4 | 2.95 | 0.55 |
| 12:Y:44:HIS:CE1 | 12:Y:48:HIS:CE1 | 2.94 | 0.54 |
| 70:AE:85:VAL:HB | 70:AE:160:HIS:CE1 | 2.41 | 0.54 |
| 1:A:149:A:C2 | 1:A:161:U:C4 | 2.95 | 0.54 |
| 62:AR:49:LEU:H | 62:AR:49:LEU:HD12 | 1.71 | 0.54 |
| 34:AA:136:U:C4 | 34:AA:141:A:C2 | 2.96 | 0.54 |
| 35:AC:30:U:H2' | 35:AC:31:U:C6 | 2.43 | 0.54 |
| 34:AA:124:U:H5' | 34:AA:124:U:C6 | 2.43 | 0.53 |
| 34:AA:343:G:H2' | 34:AA:344:A:H5" | 1.90 | 0.53 |
| 63:AW:20:VAL:O | 63:AW:145:HIS:CD2 | 2.62 | 0.53 |
| 34:AA:320:C:H2' | 34:AA:321:A:C8 | 2.44 | 0.53 |
| 73:AU:107:THR:HG23 | 73:AU:110:GLY:H | 1.73 | 0.53 |
| 34:AA:2506:A:H2' | 34:AA:2507:A:C8 | 2.43 | 0.53 |
| 34:AA:965:A:C6 | 34:AA:966:A:C2 | 2.97 | 0.53 |
| 34:AA:506:A:H2' | 34:AA:507:G:C8 | 2.43 | 0.53 |
| 34:AA:173:A:H3' | 34:AA:174:U:H5" | 1.91 | 0.53 |
| 41:A6:54:ILE:HD12 | 41:A6:54:ILE:H | 1.74 | 0.52 |
| 1:A:520:U:H2' | 1:A:521:G:C8 | 2.44 | 0.52 |
| 1:A:1734:G:H3' | 1:A:1811:A:H61 | 1.74 | 0.52 |
| 30:U:101:HIS:CE1 | 30:U:105:ASN:HD22 | 2.28 | 0.52 |
| 34:AA:1531:G:H1 | 34:AA:1573:C:H5 | 1.55 | 0.52 |
| 34:AA:445:A:N1 | 34:AA:702:U:C4 | 2.77 | 0.52 |
| 34:AA:912:U:H2' | 34:AA:913:U:C6 | 2.45 | 0.52 |
| 9:W:99:GLU:H | 9:W:99:GLU:CD | 2.12 | 0.52 |
| 34:AA:3164:G:C5 | 34:AA:3165:U:C5 | 2.97 | 0.52 |
| 34:AA:3768:A:C5 | 42:A7:29:HIS:CE1 | 2.98 | 0.52 |
| 24:L:168:ILE:HG12 | 24:L:169:ASP:H | 1.75 | 0.51 |
| 34:AA:1675:C:H4' | 34:AA:1737:A:C5 | 2.45 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 34:AA:2525:A:H2' | 34:AA:2526:A:C8 | 2.45 | 0.51 |
| 1:A:1040:A:H61 | 34:AA:965:A:H61 | 1.58 | 0.51 |
| 39:A2:119:TYR:C | 44:A8:111:ARG:HH22 | 2.13 | 0.51 |
| 1:A:2072:G:H2' | 1:A:2073:A:C8 | 2.45 | 0.51 |
| 34:AA:445:A:C2 | 34:AA:702:U:C4 | 2.98 | 0.51 |
| 34:AA:914:G:H2' | 34:AA:915:G:C8 | 2.45 | 0.51 |
| 34:AA:1588:U:H2' | 34:AA:1589:G:C8 | 2.46 | 0.51 |
| 34:AA:2709:U:H2' | 34:AA:2710:U:C6 | 2.45 | 0.51 |
| 34:AA:3054:A:C2 | 34:AA:3092:G:C6 | 2.99 | 0.51 |
| 34:AA:3555:U:C4 | 45:A9:91:HIS:CE1 | 2.99 | 0.51 |
| 1:A:1976:G:H3' | 1:A:1977:G:C8 | 2.46 | 0.51 |
| 34:AA:1786:A:C5 | 34:AA:1787:A:C6 | 2.99 | 0.50 |
| 40:A4:7:HIS:CG | 40:A4:8:THR:H | 2.29 | 0.50 |
| 1:A:1859:A:H2' | 1:A:1860:A:C8 | 2.46 | 0.50 |
| 34:AA:1770:G:H1' | 34:AA:1797:A:H61 | 1.76 | 0.50 |
| 1:A:808:U:C5 | 1:A:809:U:C5 | 2.99 | 0.50 |
| 2:7:6:A:N1 | 2:7:65:A:N1 | 2.59 | 0.50 |
| 34:AA:1219:A:C5 | 34:AA:1220:U:C5 | 2.99 | 0.50 |
| 1:A:1041:G:H1' | 34:AA:966:A:H61 | 1.76 | 0.50 |
| 34:AA:136:U:O4 | 34:AA:141:A:C2 | 2.65 | 0.50 |
| 34:AA:2657:G:H22 | 34:AA:2689:G:H1' | 1.75 | 0.50 |
| 1:A:107:A:C5 | 1:A:108:A:C5 | 3.00 | 0.50 |
| 1:A:1261:A:H2' | 1:A:1262:C:C6 | 2.47 | 0.50 |
| 1:A:597:C:H2' | 1:A:598:A:C8 | 2.46 | 0.50 |
| 34:AA:1064:U:H2' | 34:AA:1065:U:C6 | 2.46 | 0.50 |
| 34:AA:66:A:C2 | 34:AA:68:A:H1' | 2.46 | 0.50 |
| 35:AC:13:A:H2' | 35:AC:14:A:C8 | 2.47 | 0.50 |
| 34:AA:1511:U:H2' | 34:AA:1512:A:C8 | 2.47 | 0.50 |
| 34:AA:75:U:C4 | 34:AA:76:G:C6 | 3.00 | 0.49 |
| 34:AA:1433:U:C2 | 70:AE:254:PRO:HB3 | 2.47 | 0.49 |
| 34:AA:606:A:H2' | 34:AA:607:A:C8 | 2.47 | 0.49 |
| 36:AB:24:U:C5 | 36:AB:25:A:C8 | 3.01 | 0.49 |
| 2:7:15:G:H21 | 2:7:19:G:H1 | 1.61 | 0.49 |
| 34:AA:1738:A:C4 | 34:AA:1739:C:C5 | 3.01 | 0.49 |
| 34:AA:2158:U:H2' | 34:AA:2159:A:C8 | 2.48 | 0.49 |
| 69:AD:50:HIS:CG | 69:AD:51:ASP:H | 2.30 | 0.49 |
| 34:AA:642:A:C5 | 34:AA:684:G:C8 | 3.01 | 0.49 |
| 34:AA:715:U:H2' | 34:AA:716:C:C5 | 2.48 | 0.49 |
| 4:E:141:VAL:HG22 | 4:E:143:ILE:H | 1.77 | 0.49 |
| 34:AA:2401:C:H1' | 34:AA:3736:A:C8 | 2.48 | 0.49 |
| 34:AA:2950:U:H2' | 34:AA:2951:U:C6 | 2.48 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:952:U:H2' | 1:A:953:C:C6 | 2.48 | 0.49 |
| 34:AA:3241:U:H2' | 34:AA:3242:U:C6 | 2.48 | 0.49 |
| 34:AA:3402:A:H2' | 34:AA:3403:A:C8 | 2.48 | 0.49 |
| 1:A:755:A:C2 | 1:A:756:A:C4 | 3.01 | 0.49 |
| 34:AA:983:G:C5 | 34:AA:1012:U:C4 | 3.01 | 0.49 |
| 34:AA:1416:U:H2' | 34:AA:1417:G:C8 | 2.47 | 0.49 |
| 1:A:886:U:H2' | 1:A:887:A:C8 | 2.48 | 0.48 |
| 34:AA:220:G:C6 | 34:AA:230:G:C5 | 3.01 | 0.48 |
| 21:F:249:ILE:HD12 | 21:F:249:ILE:H | 1.78 | 0.48 |
| 34:AA:1093:G:H2' | 34:AA:1094:U:C6 | 2.48 | 0.48 |
| 34:AA:1541:A:C2 | 34:AA:1542:A:C4 | 3.02 | 0.48 |
| 34:AA:2430:U:C6 | 34:AA:2434:U:C4 | 3.01 | 0.48 |
| 7:K:115:GLU:CD | 7:K:118:ARG:HH22 | 2.16 | 0.48 |
| 34:AA:3320:G:H2' | 34:AA:3321:U:C6 | 2.48 | 0.48 |
| 1:A:1061:A:C2 | 1:A:1082:A:C4 | 3.02 | 0.48 |
| 34:AA:2132:A:C5 | 34:AA:2134:A:C5 | 3.01 | 0.48 |
| 57:AK:84:ARG:HE | 57:AK:89:HIS:CD2 | 2.32 | 0.48 |
| 34:AA:909:U:H2' | 34:AA:910:A:C8 | 2.49 | 0.48 |
| 51:AP:189:ILE:HD12 | 51:AP:189:ILE:H | 1.79 | 0.48 |
| 1:A:246:A:H2' | 1:A:247:G:C8 | 2.49 | 0.48 |
| 34:AA:687:G:H2' | 34:AA:688:U:C6 | 2.49 | 0.48 |
| 51:AP:140:HIS:CD2 | 51:AP:142:ALA:H | 2.32 | 0.48 |
| 1:A:993:A:H2' | 1:A:994:G:C8 | 2.48 | 0.48 |
| 34:AA:352:A:C5 | 34:AA:353:G:C5 | 3.01 | 0.48 |
| 34:AA:1031:G:H1 | 69:AD:208:GLU:CD | 2.17 | 0.48 |
| 34:AA:1536:U:H3' | 34:AA:1537:G:H5" | 1.95 | 0.48 |
| 72:AG:43:GLN:CD | 72:AG:43:GLN:H | 2.17 | 0.48 |
| 34:AA:3726:U:H4' | 34:AA:3727:A:H5" | 1.94 | 0.48 |
| 34:AA:2679:A:C4 | 34:AA:3353:A:C2 | 3.01 | 0.47 |
| 34:AA:2926:A:H2' | 34:AA:2927:U:C6 | 2.48 | 0.47 |
| 2:7:45:A:H3' | 2:7:46:G:H5' | 1.96 | 0.47 |
| 34:AA:1106:A:C5 | 40:A4:17:HIS:CG | 3.02 | 0.47 |
| 34:AA:2183:A:H2' | 34:AA:2184:U:C6 | 2.49 | 0.47 |
| 34:AA:525:U:H2' | 34:AA:526:U:C6 | 2.49 | 0.47 |
| 34:AA:1506:C:H2' | 34:AA:1507:U:C6 | 2.49 | 0.47 |
| 34:AA:2569:G:C5 | 34:AA:2570:C:C5 | 3.02 | 0.47 |
| 1:A:262:A:C5 | 1:A:263:A:H1' | 2.50 | 0.47 |
| 34:AA:1302:G:C6 | 34:AA:1446:A:C2 | 3.03 | 0.47 |
| 34:AA:2134:A:C6 | 34:AA:2135:G:C5 | 3.02 | 0.47 |
| 34:AA:3451:G:C6 | 34:AA:3452:U:C4 | 3.02 | 0.47 |
| 34:AA:1109:U:H2' | 34:AA:1110:U:C6 | 2.50 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:149:A:N1 | 1:A:161:U:C4 | 2.83 | 0.47 |
| 1:A:930:A:C2 | 1:A:1032:A:C4 | 3.02 | 0.47 |
| 34:AA:593:A:H4' | 34:AA:594:C:H5' | 1.96 | 0.47 |
| 34:AA:2473:A:H2' | 34:AA:2474:C:C6 | 2.50 | 0.47 |
| 44:A8:98:HIS:CD2 | 44:A8:99:ASN:H | 2.33 | 0.47 |
| 60:AO:61:LEU:HD22 | 60:AO:61:LEU:H | 1.79 | 0.47 |
| 34:AA:1034:A:C5 | 34:AA:1036:A:H1' | 2.49 | 0.47 |
| 34:AA:1100:A:C5 | 68:A5:185:HIS:CE1 | 3.03 | 0.47 |
| 34:AA:1905:C:H2' | 34:AA:1906:A:C8 | 2.50 | 0.47 |
| 34:AA:2441:U:H2' | 34:AA:2442:A:C5 | 2.50 | 0.47 |
| 34:AA:2663:G:C6 | 34:AA:2664:G:C6 | 3.03 | 0.47 |
| 1:A:1424:A:H2' | 1:A:1425:C:C6 | 2.50 | 0.47 |
| 8:M:44:ILE:HD12 | 8:M:44:ILE:H | 1.80 | 0.47 |
| 34:AA:1210:A:H2' | 34:AA:1211:U:C6 | 2.50 | 0.47 |
| 1:A:491:A:H2' | 1:A:492:A:C8 | 2.50 | 0.46 |
| 2:7:23:G:C5 | 2:7:24:C:C5 | 3.04 | 0.46 |
| 34:AA:1103:A:C5 | 34:AA:1231:A:C2 | 3.03 | 0.46 |
| 34:AA:1203:A:C6 | 34:AA:1204:A:C6 | 3.03 | 0.46 |
| 34:AA:1628:U:C5 | 34:AA:1629:G:C5 | 3.03 | 0.46 |
| 34:AA:1683:A:H2' | 34:AA:1684:A:C8 | 2.50 | 0.46 |
| 34:AA:3263:G:H2' | 34:AA:3264:U:C6 | 2.50 | 0.46 |
| 34:AA:1083:G:H2' | 34:AA:1084:A:C8 | 2.50 | 0.46 |
| 34:AA:2020:A:H2' | 34:AA:2021:A:C8 | 2.51 | 0.46 |
| 34:AA:2433:U:C2 | 34:AA:3337:U:C5 | 3.03 | 0.46 |
| 1:A:149:A:C2 | 1:A:150:C:C2 | 3.04 | 0.46 |
| 34:AA:3325:G:C5 | 34:AA:3326:A:C6 | 3.04 | 0.46 |
| 34:AA:40:A:C5 | 34:AA:1056:G:C6 | 3.03 | 0.46 |
| 36:AB:75:G:C4 | 36:AB:99:G:C6 | 3.04 | 0.46 |
| 69:AD:235:VAL:HG13 | 69:AD:236:GLY:H | 1.81 | 0.46 |
| 1:A:995:A:H2' | 1:A:996:C:C6 | 2.51 | 0.46 |
| 1:A:1444:C:H3' | 1:A:1445:U:H5' | 1.98 | 0.46 |
| 34:AA:1644:U:C5 | 34:AA:2102:A:C2 | 3.04 | 0.46 |
| 1:A:458:A:H3' | 1:A:459:A:C5' | 2.45 | 0.46 |
| 1:A:1743:A:H2' | 1:A:1744:A:C8 | 2.51 | 0.46 |
| 34:AA:967:A:C5 | 34:AA:968:G:H1' | 2.51 | 0.46 |
| 34:AA:1106:A:C4 | 40:A4:17:HIS:CD2 | 3.03 | 0.46 |
| 34:AA:3242:U:H2' | 34:AA:3243:C:C6 | 2.51 | 0.46 |
| 1:A:122:C:C5 | 1:A:123:U:C5 | 3.04 | 0.46 |
| 24:L:13:LEU:HD22 | 24:L:13:LEU:H | 1.81 | 0.46 |
| 34:AA:1043:G:C4 | 34:AA:3168:C:C2 | 3.03 | 0.46 |
| 34:AA:1786:A:H4' | 38:A1:79:HIS:CE1 | 2.51 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 34:AA:1118:A:C2 | 34:AA:1177:A:C4 | 3.03 | 0.46 |
| 34:AA:2176:A:C5 | 34:AA:2177:A:C5 | 3.04 | 0.46 |
| 1:A:441:U:C4 | 1:A:442:A:C6 | 3.04 | 0.45 |
| 34:AA:918:G:C6 | 34:AA:920:A:C4 | 3.04 | 0.45 |
| 34:AA:1980:G:C8 | 34:AA:1981:U:C4 | 3.04 | 0.45 |
| 36:AB:95:U:H2' | 36:AB:96:C:C6 | 2.51 | 0.45 |
| 1:A:1251:G:C6 | 1:A:2060:G:C5 | 3.04 | 0.45 |
| 34:AA:3386:A:H2' | 34:AA:3387:U:C6 | 2.51 | 0.45 |
| 45:A9:66:LYS:HA | 57:AK:2:TYR:CZ | 2.51 | 0.45 |
| 1:A:118:U:H2' | 1:A:119:C:C6 | 2.51 | 0.45 |
| 1:A:1208:G:C5 | 1:A:1209:G:C6 | 3.05 | 0.45 |
| 1:A:1873:A:C5 | 1:A:1874:A:H1' | 2.52 | 0.45 |
| 2:7:14:A:C6 | 2:7:15:G:C2 | 3.04 | 0.45 |
| 24:L:213:ASP:C | 24:L:217:ARG:HE | 2.19 | 0.45 |
| 34:AA:1216:C:H2' | 34:AA:1217:U:H5' | 1.98 | 0.45 |
| 1:A:1272:A:H2' | 1:A:1273:G:C8 | 2.51 | 0.45 |
| 34:AA:1259:G:C2 | 34:AA:2666:A:C4 | 3.05 | 0.45 |
| 34:AA:1831:G:C5 | 34:AA:1832:U:C5 | 3.04 | 0.45 |
| 34:AA:2106:A:C4 | 34:AA:2110:C:C5 | 3.05 | 0.45 |
| 34:AA:3140:U:H4' | 34:AA:3141:G:OP1 | 2.16 | 0.45 |
| 1:A:1957:A:C2 | 1:A:2033:U:C2 | 3.05 | 0.45 |
| 34:AA:307:G:C5 | 34:AA:308:U:C4 | 3.05 | 0.45 |
| 34:AA:1036:A:C5 | 34:AA:1037:C:C5 | 3.04 | 0.45 |
| 34:AA:1214:C:H3' | 34:AA:1215:A:H5" | 1.99 | 0.45 |
| 34:AA:1662:G:C6 | 34:AA:1664:A:C5 | 3.05 | 0.45 |
| 34:AA:1793:A:C6 | 34:AA:1797:A:C8 | 3.05 | 0.45 |
| 1:A:392:G:H2' | 1:A:393:A:C8 | 2.52 | 0.45 |
| 34:AA:262:A:H2' | 34:AA:263:U:C6 | 2.52 | 0.45 |
| 34:AA:2590:U:H2' | 34:AA:2590:U:O2 | 2.15 | 0.45 |
| 1:A:1008:A:C6 | 1:A:1009:A:C6 | 3.05 | 0.45 |
| 34:AA:70:A:C6 | 34:AA:71:A:C6 | 3.05 | 0.45 |
| 34:AA:510:A:H2' | 34:AA:511:C:C6 | 2.52 | 0.45 |
| 34:AA:3164:G:C6 | 34:AA:3165:U:C4 | 3.05 | 0.45 |
| 43:AN:79:GLU:CD | 43:AN:79:GLU:H | 2.20 | 0.45 |
| 45:A9:134:LEU:H | 45:A9:134:LEU:HD22 | 1.82 | 0.45 |
| 1:A:1239:A:C4 | 1:A:1240:A:N7 | 2.85 | 0.45 |
| 34:AA:63:A:H2' | 34:AA:64:G:C8 | 2.52 | 0.45 |
| 34:AA:378:U:C4 | 34:AA:379:G:C5 | 3.05 | 0.45 |
| 34:AA:1244:G:C4 | 34:AA:3176:A:C2 | 3.05 | 0.45 |
| 1:A:413:A:H2' | 1:A:414:C:C6 | 2.52 | 0.44 |
| 1:A:805:A:C2 | 1:A:806:A:C4 | 3.04 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1225:A:H2' | 1:A:1226:A:C8 | 2.52 | 0.44 |
| 34:AA:734:A:H2' | 34:AA:735:A:C8 | 2.52 | 0.44 |
| 34:AA:965:A:N6 | 34:AA:966:A:C2 | 2.85 | 0.44 |
| 34:AA:1646:C:H2' | 34:AA:1647:U:C6 | 2.52 | 0.44 |
| 70:AE:68:HIS:CG | 70:AE:69:LYS:N | 2.86 | 0.44 |
| 1:A:1378:G:C4 | 1:A:1682:A:C2 | 3.05 | 0.44 |
| 25:N:21:ILE:HD13 | 25:N:23:LEU:HD21 | 1.99 | 0.44 |
| 34:AA:609:C:H3' | 34:AA:610:U:H5' | 2.00 | 0.44 |
| 34:AA:2723:G:H2' | 34:AA:2724:C:C6 | 2.52 | 0.44 |
| 34:AA:3022:U:H2' | 34:AA:3023:C:C6 | 2.52 | 0.44 |
| 1:A:91:G:C6 | 1:A:92:C:C4 | 3.06 | 0.44 |
| 1:A:850:G:H2' | 1:A:851:A:C8 | 2.52 | 0.44 |
| 1:A:1400:U:H5 | 1:A:1401:G:C5 | 2.36 | 0.44 |
| 1:A:1692:A:C4 | 1:A:1694:G:C8 | 3.05 | 0.44 |
| 34:AA:88:A:C2 | 34:AA:99:A:C4 | 3.05 | 0.44 |
| 34:AA:1186:A:C5 | 34:AA:1224:A:C6 | 3.05 | 0.44 |
| 34:AA:2181:A:C5 | 34:AA:2413:A:C2 | 3.05 | 0.44 |
| 34:AA:2189:A:C6 | 34:AA:2200:A:C2 | 3.05 | 0.44 |
| 1:A:872:A:C6 | 1:A:873:A:C2 | 3.06 | 0.44 |
| 1:A:1188:A:H2' | 1:A:1189:A:C8 | 2.52 | 0.44 |
| 34:AA:350:A:C5 | 34:AA:376:G:C5 | 3.06 | 0.44 |
| 34:AA:1681:C:H2' | 34:AA:1682:U:C6 | 2.53 | 0.44 |
| 34:AA:2737:C:H2' | 34:AA:2738:U:C6 | 2.51 | 0.44 |
| 34:AA:2946:G:C6 | 34:AA:2947:G:C5 | 3.05 | 0.44 |
| 34:AA:3768:A:C6 | 42:A7:29:HIS:CE1 | 3.06 | 0.44 |
| 1:A:598:A:H2' | 1:A:599:A:C8 | 2.53 | 0.44 |
| 1:A:1109:G:H4' | 33:C:31:ASN:HD22 | 1.83 | 0.44 |
| 34:AA:916:U:H2' | 34:AA:917:A:C8 | 2.52 | 0.44 |
| 34:AA:1572:U:C5 | 34:AA:1573:C:C5 | 3.06 | 0.44 |
| 34:AA:685:U:C5 | 34:AA:686:U:C4 | 3.06 | 0.44 |
| 34:AA:1121:G:C2 | 34:AA:1122:A:C2 | 3.06 | 0.44 |
| 34:AA:2439:C:H2' | 34:AA:2440:A:C8 | 2.53 | 0.44 |
| 34:AA:3347:C:H2' | 34:AA:3348:U:C6 | 2.53 | 0.44 |
| 21:F:36:HIS:CG | 21:F:85:GLY:HA2 | 2.52 | 0.44 |
| 34:AA:3615:A:H3' | 34:AA:3615:A:C8 | 2.51 | 0.44 |
| 34:AA:3727:A:C2 | 34:AA:3728:A:C4 | 3.05 | 0.44 |
| 1:A:43:A:C2 | 1:A:384:A:C5 | 3.05 | 0.44 |
| 1:A:95:A:C6 | 1:A:404:G:C6 | 3.06 | 0.44 |
| 1:A:161:U:O4 | 1:A:162:A:C6 | 2.70 | 0.44 |
| 1:A:970:G:C6 | 1:A:971:G:C5 | 3.06 | 0.44 |
| 34:AA:3086:A:H2' | 34:AA:3087:A:C8 | 2.53 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 34:AA:3171:C:H2' | 34:AA:3172:A:C8 | 2.52 | 0.44 |
| 34:AA:202:C:H2' | 34:AA:203:A:C8 | 2.53 | 0.44 |
| 34:AA:228:A:C5 | 34:AA:1537:G:C6 | 3.06 | 0.44 |
| 34:AA:1793:A:C6 | 34:AA:1795:A:C4 | 3.06 | 0.44 |
| 35:AC:29:G:C5 | 35:AC:30:U:C5 | 3.05 | 0.44 |
| 55:AJ:44:LEU:HD23 | 55:AJ:44:LEU:H | 1.82 | 0.44 |
| 68:A5:141:PRO:HA | 68:A5:242:TRP:CD2 | 2.52 | 0.44 |
| 1:A:943:U:H2' | 1:A:944:G:C8 | 2.52 | 0.43 |
| 34:AA:1184:A:H2' | 34:AA:1185:A:C8 | 2.53 | 0.43 |
| 34:AA:2577:C:C5 | 34:AA:2578:C:C2 | 3.06 | 0.43 |
| 34:AA:1113:C:H2' | 34:AA:1114:A:C8 | 2.53 | 0.43 |
| 34:AA:1875:A:H2' | 34:AA:1876:A:C8 | 2.53 | 0.43 |
| 34:AA:3035:A:H3' | 34:AA:3036:A:C8 | 2.54 | 0.43 |
| 1:A:26:A:C4 | 1:A:27:U:C5 | 3.05 | 0.43 |
| 1:A:162:A:C6 | 1:A:163:G:C5 | 3.07 | 0.43 |
| 1:A:1061:A:C2 | 1:A:1081:U:O4 | 2.70 | 0.43 |
| 2:7:12:G:N2 | 2:7:22:A:C2 | 2.86 | 0.43 |
| 34:AA:1844:G:C5 | 34:AA:1845:C:C5 | 3.06 | 0.43 |
| 34:AA:3387:U:H2' | 34:AA:3388:U:C6 | 2.54 | 0.43 |
| 1:A:1904:G:H2' | 1:A:1905:C:C6 | 2.53 | 0.43 |
| 2:7:54:G:C6 | 2:7:55:U:C2 | 3.07 | 0.43 |
| 34:AA:1973:G:C6 | 34:AA:1974:U:C4 | 3.05 | 0.43 |
| 34:AA:1974:U:H2' | 34:AA:1975:A:C8 | 2.53 | 0.43 |
| 34:AA:3066:A:C6 | 34:AA:3068:A:C5 | 3.06 | 0.43 |
| 1:A:1040:A:H61 | 34:AA:965:A:N6 | 2.15 | 0.43 |
| 1:A:2033:U:H2' | 1:A:2034:U:C6 | 2.52 | 0.43 |
| 34:AA:1237:C:H2' | 34:AA:1238:C:C6 | 2.54 | 0.43 |
| 69:AD:50:HIS:CG | 69:AD:51:ASP:N | 2.86 | 0.43 |
| 1:A:1061:A:C2 | 1:A:1082:A:C5 | 3.06 | 0.43 |
| 34:AA:141:A:C2 | 34:AA:142:C:C4 | 3.06 | 0.43 |
| 34:AA:205:G:C6 | 34:AA:405:A:C5 | 3.07 | 0.43 |
| 34:AA:723:A:C8 | 34:AA:727:A:C6 | 3.07 | 0.43 |
| 36:AB:13:A:C5 | 36:AB:110:G:C6 | 3.06 | 0.43 |
| 36:AB:77:A:C2 | 36:AB:100:A:C4 | 3.07 | 0.43 |
| 34:AA:2079:A:H2' | 34:AA:2080:C:C6 | 2.54 | 0.43 |
| 34:AA:2516:A:H2' | 34:AA:2517:A:C8 | 2.54 | 0.43 |
| 34:AA:3268:A:H3' | 34:AA:3269:A:H5" | 2.00 | 0.43 |
| 36:AB:66:G:C6 | 36:AB:67:C:C4 | 3.06 | 0.43 |
| 1:A:403:A:H2' | 1:A:404:G:C8 | 2.53 | 0.43 |
| 1:A:1968:A:C4 | 1:A:1969:A:C8 | 3.07 | 0.43 |
| 34:AA:30:G:C6 | 34:AA:55:G:C6 | 3.07 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 34:AA:344:A:C2 | 34:AA:345:G:C5 | 3.07 | 0.43 |
| 34:AA:2700:C:H5' | 34:AA:2958:G:H21 | 1.83 | 0.43 |
| 34:AA:3055:U:H2' | 34:AA:3056:U:C6 | 2.53 | 0.43 |
| 34:AA:888:A:C8 | 34:AA:890:G:H1' | 2.53 | 0.43 |
| 34:AA:999:G:C4 | 34:AA:1001:A:C6 | 3.07 | 0.43 |
| 34:AA:1696:A:H2' | 34:AA:1697:A:C8 | 2.54 | 0.43 |
| 34:AA:1699:G:C5 | 34:AA:1700:U:C5 | 3.07 | 0.43 |
| 35:AC:44:A:H2' | 35:AC:45:A:C8 | 2.54 | 0.43 |
| 1:A:107:A:C4 | 1:A:108:A:C8 | 3.07 | 0.43 |
| 34:AA:423:U:H2' | 34:AA:424:U:C6 | 2.54 | 0.43 |
| 34:AA:583:U:H5" | 34:AA:583:U:H6 | 1.84 | 0.43 |
| 34:AA:983:G:C6 | 34:AA:1012:U:C5 | 3.07 | 0.43 |
| 1:A:1386:U:C4 | 1:A:1667:A:C5 | 3.07 | 0.42 |
| 34:AA:48:A:C4 | 34:AA:50:U:C4 | 3.07 | 0.42 |
| 34:AA:977:A:C6 | 34:AA:978:G:C6 | 3.06 | 0.42 |
| 34:AA:1212:U:H2' | 34:AA:1213:U:C6 | 2.54 | 0.42 |
| 34:AA:3165:U:H2' | 34:AA:3166:U:C6 | 2.53 | 0.42 |
| 34:AA:3443:A:H2' | 34:AA:3444:G:H5' | 2.01 | 0.42 |
| 34:AA:714:C:C2 | 34:AA:724:A:H1' | 2.53 | 0.42 |
| 34:AA:1331:A:H2' | 34:AA:1332:A:C8 | 2.54 | 0.42 |
| 34:AA:2021:A:C2 | 34:AA:2022:A:C4 | 3.07 | 0.42 |
| 34:AA:2400:A:C5 | 34:AA:2401:C:C5 | 3.08 | 0.42 |
| 1:A:887:A:C2 | 1:A:916:G:C2 | 3.06 | 0.42 |
| 1:A:1304:A:C6 | 1:A:1852:A:C6 | 3.07 | 0.42 |
| 34:AA:332:A:H2' | 34:AA:333:A:C8 | 2.54 | 0.42 |
| 34:AA:1431:A:C4 | 34:AA:1432:A:C2 | 3.08 | 0.42 |
| 34:AA:3262:A:C2 | 34:AA:3263:G:H1' | 2.55 | 0.42 |
| 43:AN:76:LEU:H | 43:AN:76:LEU:HD12 | 1.85 | 0.42 |
| 70:AE:11:HIS:CD2 | 70:AE:232:VAL:HA | 2.54 | 0.42 |
| 74:AH:40:HIS:CE1 | 74:AH:41:LEU:HB2 | 2.54 | 0.42 |
| 1:A:632:C:H2' | 1:A:633:U:C6 | 2.54 | 0.42 |
| 1:A:1271:G:C2 | 1:A:1272:A:C8 | 3.07 | 0.42 |
| 1:A:1401:G:H2' | 1:A:1402:A:C8 | 2.54 | 0.42 |
| 34:AA:302:A:H2' | 34:AA:303:A:C8 | 2.54 | 0.42 |
| 34:AA:1103:A:C6 | 34:AA:1231:A:C2 | 3.07 | 0.42 |
| 34:AA:1120:A:C2 | 34:AA:1121:G:C4 | 3.07 | 0.42 |
| 34:AA:1598:A:C2 | 34:AA:2649:A:C4 | 3.07 | 0.42 |
| 34:AA:2932:A:H4' | 34:AA:2933:C:O5' | 2.19 | 0.42 |
| 34:AA:3578:A:C2 | 34:AA:3579:A:C4 | 3.08 | 0.42 |
| 1:A:318:A:C4 | 1:A:320:C:C5 | 3.08 | 0.42 |
| 34:AA:382:A:C2 | 34:AA:384:A:C4 | 3.08 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 34:AA:1683:A:C2 | 34:AA:1684:A:C4 | 3.08 | 0.42 |
| 34:AA:2573:A:C6 | 34:AA:2575:U:C4 | 3.08 | 0.42 |
| 34:AA:2801:C:H2' | 34:AA:2802:U:C6 | 2.55 | 0.42 |
| 34:AA:3717:A:H2' | 34:AA:3718:G:C8 | 2.54 | 0.42 |
| 2:7:6:A:N6 | 2:7:65:A:H61 | 2.17 | 0.42 |
| 34:AA:229:A:C5 | 34:AA:232:C:C4 | 3.07 | 0.42 |
| 34:AA:695:A:C5 | 34:AA:696:C:C4 | 3.08 | 0.42 |
| 34:AA:2021:A:H2' | 34:AA:2022:A:C8 | 2.55 | 0.42 |
| 34:AA:3333:U:H2' | 34:AA:3334:U:C6 | 2.54 | 0.42 |
| 34:AA:3776:U:H2' | 34:AA:3777:G:C8 | 2.54 | 0.42 |
| 1:A:643:A:C2 | 1:A:929:U:C2 | 3.08 | 0.42 |
| 1:A:1379:G:C5 | 1:A:1380:C:C4 | 3.08 | 0.42 |
| 34:AA:26:A:H2' | 34:AA:27:U:C6 | 2.55 | 0.42 |
| 34:AA:685:U:HO2' | 34:AA:686:U:H6 | 1.63 | 0.42 |
| 34:AA:706:U:H2' | 34:AA:707:U:C6 | 2.55 | 0.42 |
| 34:AA:718:U:H2' | 34:AA:719:C:C6 | 2.54 | 0.42 |
| 34:AA:742:U:H2' | 34:AA:743:A:C8 | 2.55 | 0.42 |
| 34:AA:2004:U:O4 | 34:AA:2005:A:C6 | 2.72 | 0.42 |
| 34:AA:2571:C:C5 | 34:AA:2598:G:C6 | 3.08 | 0.42 |
| 1:A:116:A:C6 | 1:A:249:A:C6 | 3.08 | 0.42 |
| 1:A:970:G:C6 | 1:A:971:G:C6 | 3.08 | 0.42 |
| 1:A:1046:A:C2 | 1:A:1047:A:H1' | 2.55 | 0.42 |
| 4:E:90:GLU:CD | 4:E:90:GLU:H | 2.23 | 0.42 |
| 34:AA:302:A:C2 | 34:AA:303:A:C4 | 3.08 | 0.42 |
| 34:AA:607:A:H2' | 34:AA:608:A:C8 | 2.55 | 0.42 |
| 34:AA:1423:G:H5' | 73:AU:93:ARG:NH2 | 2.34 | 0.42 |
| 34:AA:1781:A:C6 | 34:AA:1782:U:C5 | 3.08 | 0.42 |
| 34:AA:3635:G:H1 | 34:AA:3650:U:H3 | 1.68 | 0.42 |
| 1:A:379:G:C6 | 1:A:380:U:C4 | 3.07 | 0.42 |
| 1:A:806:A:C6 | 1:A:807:A:C5 | 3.08 | 0.42 |
| 1:A:1189:A:C5 | 1:A:1190:U:H1' | 2.54 | 0.42 |
| 34:AA:84:U:C4 | 34:AA:85:A:C5 | 3.08 | 0.42 |
| 34:AA:658:U:C4 | 34:AA:659:U:C4 | 3.08 | 0.42 |
| 34:AA:949:A:C2 | 34:AA:984:A:C5 | 3.07 | 0.42 |
| 1:A:1846:U:C5 | 32:X:39:ALA:HB3 | 2.54 | 0.42 |
| 1:A:2058:A:C4 | 1:A:2086:A:C2 | 3.08 | 0.42 |
| 34:AA:69:U:H2' | 34:AA:70:A:O4' | 2.20 | 0.42 |
| 34:AA:207:A:C2 | 34:AA:209:G:C5 | 3.07 | 0.42 |
| 34:AA:280:U:H2' | 34:AA:281:G:C8 | 2.54 | 0.42 |
| 34:AA:659:U:H2' | 34:AA:660:U:C6 | 2.54 | 0.42 |
| 34:AA:995:A:C5 | 34:AA:996:C:C5 | 3.08 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 34:AA:1053:U:O2 | 34:AA:1053:U:H2' | 2.20 | 0.42 |
| 34:AA:1219:A:C6 | 34:AA:1220:U:C4 | 3.08 | 0.42 |
| 34:AA:1301:U:H2' | 34:AA:1308:A:C8 | 2.55 | 0.42 |
| 34:AA:3200:G:C5 | 34:AA:3203:C:C4 | 3.07 | 0.42 |
| 1:A:34:G:H3' | 1:A:35:U:H5" | 2.01 | 0.41 |
| 1:A:1703:U:H1' | 28:S:137:HIS:CE1 | 2.55 | 0.41 |
| 1:A:2072:G:C6 | 1:A:2073:A:C6 | 3.07 | 0.41 |
| 1:A:2082:A:H2' | 1:A:2083:A:C8 | 2.55 | 0.41 |
| 17:4:44:LEU:HD12 | 17:4:45:PHE:H | 1.85 | 0.41 |
| 34:AA:219:A:C5 | 34:AA:237:A:C2 | 3.08 | 0.41 |
| 34:AA:733:C:H2' | 34:AA:734:A:C8 | 2.55 | 0.41 |
| 34:AA:1813:A:C4 | 34:AA:2018:G:C5 | 3.08 | 0.41 |
| 34:AA:2613:A:C6 | 34:AA:2614:A:C4 | 3.08 | 0.41 |
| 34:AA:2621:U:H2' | 34:AA:2622:C:C6 | 2.55 | 0.41 |
| 1:A:638:G:C5 | 1:A:639:U:C5 | 3.08 | 0.41 |
| 1:A:2034:U:C4 | 1:A:2035:U:C4 | 3.08 | 0.41 |
| 34:AA:374:A:C5 | 34:AA:375:A:C5 | 3.08 | 0.41 |
| 34:AA:418:A:C2 | 34:AA:419:A:C4 | 3.08 | 0.41 |
| 34:AA:703:U:H2' | 34:AA:704:U:C6 | 2.54 | 0.41 |
| 34:AA:1203:A:C5 | 34:AA:1204:A:C5 | 3.07 | 0.41 |
| 34:AA:1285:U:C4 | 34:AA:1286:A:C5 | 3.08 | 0.41 |
| 34:AA:2712:A:H2' | 34:AA:2713:C:C6 | 2.55 | 0.41 |
| 34:AA:3638:A:H61 | 34:AA:3647:C:H42 | 1.66 | 0.41 |
| 1:A:1193:A:C5 | 1:A:1195:G:C8 | 3.08 | 0.41 |
| 2:7:70:A:C2 | 2:7:71:C:C6 | 3.08 | 0.41 |
| 34:AA:934:G:C5 | 34:AA:1025:A:C6 | 3.09 | 0.41 |
| 34:AA:1170:A:N7 | 34:AA:1171:A:C5 | 2.88 | 0.41 |
| 34:AA:1683:A:C2 | 34:AA:1684:A:C5 | 3.08 | 0.41 |
| 34:AA:2601:C:C4 | 34:AA:2602:A:C5 | 3.08 | 0.41 |
| 34:AA:3248:C:C5 | 34:AA:3295:A:C4 | 3.07 | 0.41 |
| 1:A:1054:G:C6 | 1:A:1055:G:C4 | 3.07 | 0.41 |
| 1:A:1083:A:C5 | 1:A:1084:U:C5 | 3.09 | 0.41 |
| 34:AA:60:A:C8 | 34:AA:335:A:C6 | 3.08 | 0.41 |
| 34:AA:795:G:C5 | 34:AA:796:C:C4 | 3.08 | 0.41 |
| 34:AA:1302:G:C6 | 34:AA:1303:C:C4 | 3.08 | 0.41 |
| 34:AA:1540:G:C8 | 34:AA:1565:G:C2 | 3.09 | 0.41 |
| 34:AA:2593:G:C5 | 34:AA:2594:U:C5 | 3.08 | 0.41 |
| 34:AA:3316:G:C5 | 34:AA:3317:A:C8 | 3.08 | 0.41 |
| 1:A:1188:A:C2 | 1:A:1189:A:C4 | 3.09 | 0.41 |
| 34:AA:700:A:C5 | 34:AA:701:C:C5 | 3.08 | 0.41 |
| 34:AA:702:U:O4 | 34:AA:703:U:C2 | 2.74 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 34:AA:2014:C:C2 | 34:AA:2017:U:C5 | 3.08 | 0.41 |
| 34:AA:2083:U:H2' | 34:AA:2084:U:C6 | 2.56 | 0.41 |
| 34:AA:2491:A:C8 | 34:AA:2563:A:H1' | 2.56 | 0.41 |
| 35:AC:44:A:C2 | 35:AC:45:A:C4 | 3.08 | 0.41 |
| 38:A1:13:ILE:HG22 | 38:A1:15:ASN:H | 1.85 | 0.41 |
| 1:A:10:G:C2 | 1:A:11:A:C4 | 3.08 | 0.41 |
| 1:A:608:A:C5 | 1:A:609:U:C5 | 3.09 | 0.41 |
| 34:AA:63:A:C6 | 34:AA:64:G:C6 | 3.08 | 0.41 |
| 34:AA:110:G:C2 | 34:AA:111:C:H1' | 2.56 | 0.41 |
| 34:AA:113:C:C2 | 34:AA:114:A:C8 | 3.08 | 0.41 |
| 34:AA:221:A:C6 | 34:AA:222:G:C4 | 3.09 | 0.41 |
| 34:AA:350:A:C6 | 34:AA:376:G:C4 | 3.09 | 0.41 |
| 34:AA:643:G:N7 | 34:AA:644:G:C6 | 2.89 | 0.41 |
| 34:AA:2131:A:N7 | 34:AA:2132:A:C5 | 2.89 | 0.41 |
| 34:AA:3399:U:H2' | 34:AA:3400:C:C6 | 2.56 | 0.41 |
| 34:AA:3471:A:C4 | 34:AA:3472:A:C8 | 3.09 | 0.41 |
| 36:AB:82:G:H2' | 36:AB:83:G:C8 | 2.55 | 0.41 |
| 1:A:97:G:C6 | 1:A:98:G:C4 | 3.08 | 0.41 |
| 1:A:857:A:H2' | 1:A:858:U:C6 | 2.56 | 0.41 |
| 1:A:1082:A:C4 | 1:A:1083:A:C8 | 3.09 | 0.41 |
| 1:A:1101:G:C6 | 1:A:1102:C:C4 | 3.08 | 0.41 |
| 1:A:1225:A:C6 | 1:A:1226:A:C6 | 3.08 | 0.41 |
| 1:A:1376:A:C2 | 1:A:1684:G:H1' | 2.54 | 0.41 |
| 34:AA:141:A:C2 | 34:AA:142:C:N3 | 2.89 | 0.41 |
| 34:AA:1015:A:C2 | 34:AA:1032:A:C2 | 3.09 | 0.41 |
| 34:AA:1060:G:C5 | 34:AA:1061:U:C5 | 3.09 | 0.41 |
| 34:AA:3001:A:H2' | 34:AA:3002:G:C8 | 2.56 | 0.41 |
| 34:AA:3763:G:C6 | 34:AA:3764:G:C5 | 3.09 | 0.41 |
| 34:AA:1730:A:C5 | 34:AA:1733:G:C5 | 3.09 | 0.41 |
| 34:AA:2492:G:C6 | 34:AA:2493:U:C4 | 3.08 | 0.41 |
| 34:AA:2695:A:C2 | 34:AA:3230:G:C5 | 3.09 | 0.41 |
| 34:AA:3198:G:C6 | 34:AA:3199:C:C5 | 3.09 | 0.41 |
| 71:AF:211:TYR:O | 71:AF:232:VAL:HG23 | 2.20 | 0.41 |
| 1:A:1305:A:N6 | 1:A:1894:A:H62 | 2.18 | 0.41 |
| 1:A:1832:U:H1' | 1:A:1833:G:C2 | 2.56 | 0.41 |
| 1:A:1837:G:C6 | 1:A:1838:G:C4 | 3.09 | 0.41 |
| 1:A:1957:A:H2' | 1:A:1958:A:C8 | 2.56 | 0.41 |
| 2:7:25:G:C6 | 2:7:26:C:C4 | 3.09 | 0.41 |
| 34:AA:26:A:C5 | 34:AA:338:U:C2 | 3.09 | 0.41 |
| 34:AA:331:A:C6 | 34:AA:332:A:C6 | 3.09 | 0.41 |
| 34:AA:997:G:H1' | 34:AA:999:G:H21 | 1.86 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 34:AA:1067:U:H2' | 34:AA:1068:C:C6 | 2.56 | 0.41 |
| 34:AA:1070:A:C4 | 34:AA:1518:A:C2 | 3.09 | 0.41 |
| 34:AA:1435:G:C5 | 34:AA:1436:A:C6 | 3.09 | 0.41 |
| 34:AA:1740:A:H2' | 34:AA:1741:G:C8 | 2.56 | 0.41 |
| 34:AA:1781:A:C5 | 34:AA:1782:U:C5 | 3.09 | 0.41 |
| 34:AA:2460:A:H2' | 34:AA:2461:A:C8 | 2.56 | 0.41 |
| 34:AA:2516:A:C2 | 34:AA:2517:A:C4 | 3.09 | 0.41 |
| 34:AA:3443:A:C5 | 34:AA:3471:A:C5 | 3.09 | 0.41 |
| 35:AC:148:C:H2' | 35:AC:149:C:C6 | 2.56 | 0.41 |
| 59:AS:156:GLY:HA3 | 60:AO:50:PRO:HG3 | 2.03 | 0.41 |
| 68:A5:232:HIS:CE1 | 68:A5:238:ARG:NH2 | 2.88 | 0.41 |
| 1:A:2072:G:C5 | 1:A:2073:A:C6 | 3.09 | 0.41 |
| 34:AA:163:G:C5 | 34:AA:269:A:C2 | 3.09 | 0.41 |
| 34:AA:200:A:C6 | 34:AA:201:G:C5 | 3.09 | 0.41 |
| 34:AA:345:G:C6 | 34:AA:347:C:C4 | 3.08 | 0.41 |
| 34:AA:352:A:C6 | 34:AA:353:G:C5 | 3.09 | 0.41 |
| 34:AA:1736:A:N7 | 34:AA:1737:A:C5 | 2.88 | 0.41 |
| 34:AA:2004:U:O4 | 34:AA:2005:A:C5 | 2.73 | 0.41 |
| 34:AA:2613:A:C6 | 34:AA:2614:A:C5 | 3.09 | 0.41 |
| 34:AA:2710:U:C4 | 34:AA:2945:G:C6 | 3.09 | 0.41 |
| 34:AA:3153:G:C5 | 34:AA:3154:U:C4 | 3.09 | 0.41 |
| 35:AC:8:G:C6 | 35:AC:9:U:C4 | 3.09 | 0.41 |
| 36:AB:88:A:C6 | 36:AB:89:G:C4 | 3.08 | 0.41 |
| 34:AA:307:G:C6 | 34:AA:308:U:C4 | 3.09 | 0.40 |
| 34:AA:380:A:C6 | 34:AA:381:A:C5 | 3.10 | 0.40 |
| 34:AA:1535:G:C6 | 34:AA:1569:A:C6 | 3.09 | 0.40 |
| 34:AA:2401:C:H1' | 34:AA:3736:A:H8 | 1.86 | 0.40 |
| 34:AA:2563:A:C6 | 34:AA:2564:A:C6 | 3.09 | 0.40 |
| 35:AC:143:G:C5 | 35:AC:144:U:C5 | 3.09 | 0.40 |
| 1:A:1009:A:C6 | 1:A:1010:A:C5 | 3.10 | 0.40 |
| 1:A:1444:C:C5 | 1:A:1445:U:C5 | 3.10 | 0.40 |
| 2:7:36:A:H2' | 2:7:37:U:H5' | 2.02 | 0.40 |
| 31:V:10:GLU:H | 31:V:10:GLU:CD | 2.23 | 0.40 |
| 34:AA:3444:G:C5 | 34:AA:3445:C:C5 | 3.09 | 0.40 |
| 1:A:161:U:O4 | 1:A:162:A:C5 | 2.75 | 0.40 |
| 1:A:593:G:C6 | 1:A:594:C:C4 | 3.10 | 0.40 |
| 1:A:865:G:H21 | 7:K:107:PRO:HG3 | 1.86 | 0.40 |
| 1:A:1043:A:C5 | 1:A:1044:C:C5 | 3.09 | 0.40 |
| 1:A:1729:A:C2 | 1:A:1730:A:C4 | 3.09 | 0.40 |
| 34:AA:261:A:H2' | 34:AA:262:A:C8 | 2.57 | 0.40 |
| 34:AA:363:A:C2 | 34:AA:373:A:C4 | 3.09 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 34:AA:3316:G:C5 | 34:AA:3335:A:C2 | 3.09 | 0.40 |
| 34:AA:3701:A:C5 | 34:AA:3702:C:C5 | 3.10 | 0.40 |
| 1:A:1008:A:H2' | 1:A:1009:A:C8 | 2.55 | 0.40 |
| 1:A:1239:A:C6 | 1:A:1240:A:C5 | 3.10 | 0.40 |
| 1:A:2073:A:C2 | 1:A:2074:A:C4 | 3.09 | 0.40 |
| 34:AA:3697:G:C4 | 34:AA:3699:A:C5 | 3.10 | 0.40 |
| 34:AA:3778:G:C5 | 34:AA:3779:U:C4 | 3.10 | 0.40 |
| 60:AO:13:GLY:O | 60:AO:14:HIS:CD2 | 2.74 | 0.40 |
| 1:A:98:G:C6 | 1:A:99:C:C4 | 3.09 | 0.40 |
| 1:A:1045:G:C6 | 1:A:1092:A:C4 | 3.09 | 0.40 |
| 1:A:2068:A:H2' | 1:A:2069:G:C8 | 2.57 | 0.40 |
| 5:G:75:ILE:H | 5:G:75:ILE:HD12 | 1.86 | 0.40 |
| 34:AA:519:A:C2 | 34:AA:520:U:H1' | 2.56 | 0.40 |
| 34:AA:906:G:H2' | 34:AA:907:C:C6 | 2.57 | 0.40 |
| 34:AA:2981:A:H2' | 34:AA:2982:A:C8 | 2.56 | 0.40 |
| 34:AA:3455:A:C5 | 34:AA:3456:C:C5 | 3.09 | 0.40 |
| 34:AA:3479:U:H2' | 34:AA:3480:C:C6 | 2.57 | 0.40 |
| 34:AA:3641:U:H3 | 34:AA:3644:G:H1 | 1.70 | 0.40 |
| 34:AA:3762:A:C2 | 34:AA:3763:G:C4 | 3.10 | 0.40 |
| 36:AB:13:A:C8 | 36:AB:110:G:C5 | 3.10 | 0.40 |

There are no symmetry-related clashes.

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 3 | D | 149/209 (71%) | 142 (95%) | 7 (5%) | 0 | 100 | 100 |
| 4 | E | 183/185 (99%) | 171 (93%) | 11 (6%) | 1 (0%) | 29 | 69 |
| 5 | G | 222/224 (99%) | 204 (92%) | 16 (7%) | 2 (1%) | 17 | 57 |
| 6 | I | 176/189 (93%) | 165 (94%) | 9 (5%) | 2 (1%) | 14 | 52 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 7 | K | 127/129 (98%) | 113 (89%) | 9 (7%) | 5 (4%) | 3 | 23 |
| 8 | M | 136/138 (99%) | 125 (92%) | 9 (7%) | 2 (2%) | 10 | 46 |
| 9 | W | 91/108 (84%) | 82 (90%) | 6 (7%) | 3 (3%) | 4 | 26 |
| 10 | R | 92/114 (81%) | 80 (87%) | 7 (8%) | 5 (5%) | 2 | 19 |
| 11 | O | 77/79 (98%) | 69 (90%) | 5 (6%) | 3 (4%) | 3 | 23 |
| 12 | Y | 152/154 (99%) | 145 (95%) | 4 (3%) | 3 (2%) | 7 | 38 |
| 13 | Z | 70/72 (97%) | 64 (91%) | 5 (7%) | 1 (1%) | 11 | 46 |
| 14 | 1 | 118/120 (98%) | 112 (95%) | 5 (4%) | 1 (1%) | 19 | 60 |
| 15 | 2 | 35/68 (52%) | 33 (94%) | 2 (6%) | 0 | 100 | 100 |
| 16 | 3 | 93/95 (98%) | 82 (88%) | 10 (11%) | 1 (1%) | 14 | 52 |
| 17 | 4 | 74/76 (97%) | 62 (84%) | 8 (11%) | 4 (5%) | 2 | 19 |
| 18 | 5 | 54/65 (83%) | 53 (98%) | 1 (2%) | 0 | 100 | 100 |
| 19 | 6 | 41/43 (95%) | 33 (80%) | 7 (17%) | 1 (2%) | 6 | 33 |
| 20 | B | 208/210 (99%) | 189 (91%) | 11 (5%) | 8 (4%) | 3 | 24 |
| 21 | F | 255/257 (99%) | 232 (91%) | 18 (7%) | 5 (2%) | 7 | 38 |
| 22 | H | 200/214 (94%) | 187 (94%) | 10 (5%) | 3 (2%) | 10 | 46 |
| 23 | J | 186/188 (99%) | 169 (91%) | 9 (5%) | 8 (4%) | 2 | 22 |
| 24 | L | 165/214 (77%) | 146 (88%) | 14 (8%) | 5 (3%) | 4 | 28 |
| 25 | N | 96/98 (98%) | 90 (94%) | 4 (4%) | 2 (2%) | 7 | 36 |
| 26 | P | 125/127 (98%) | 109 (87%) | 13 (10%) | 3 (2%) | 6 | 33 |
| 27 | Q | 142/144 (99%) | 127 (89%) | 13 (9%) | 2 (1%) | 11 | 46 |
| 28 | S | 126/128 (98%) | 107 (85%) | 12 (10%) | 7 (6%) | 2 | 18 |
| 29 | T | 46/48 (96%) | 45 (98%) | 1 (2%) | 0 | 100 | 100 |
| 30 | U | 147/149 (99%) | 141 (96%) | 4 (3%) | 2 (1%) | 11 | 46 |
| 31 | V | 142/156 (91%) | 128 (90%) | 11 (8%) | 3 (2%) | 7 | 36 |
| 32 | X | 92/103 (89%) | 78 (85%) | 11 (12%) | 3 (3%) | 4 | 26 |
| 33 | C | 193/195 (99%) | 171 (89%) | 17 (9%) | 5 (3%) | 5 | 31 |
| 37 | AL | 209/211 (99%) | 191 (91%) | 14 (7%) | 4 (2%) | 8 | 38 |
| 38 | A1 | 136/145 (94%) | 125 (92%) | 8 (6%) | 3 (2%) | 6 | 35 |
| 39 | A2 | 96/118 (81%) | 90 (94%) | 4 (4%) | 2 (2%) | 7 | 36 |
| 40 | A4 | 64/66 (97%) | 60 (94%) | 1 (2%) | 3 (5%) | 2 | 21 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 41 | A6 | 96/98 (98%) | 93 (97%) | 3 (3%) | 0 | 100 | 100 |
| 42 | A7 | 92/102 (90%) | 87 (95%) | 5 (5%) | 0 | 100 | 100 |
| 43 | AN | 144/146 (99%) | 137 (95%) | 5 (4%) | 2 (1%) | 11 | 46 |
| 44 | A8 | 123/125 (98%) | 102 (83%) | 21 (17%) | 0 | 100 | 100 |
| 45 | A9 | 101/103 (98%) | 92 (91%) | 7 (7%) | 2 (2%) | 7 | 38 |
| 46 | Aa | 104/106 (98%) | 96 (92%) | 6 (6%) | 2 (2%) | 8 | 38 |
| 47 | Ab | 91/105 (87%) | 85 (93%) | 5 (6%) | 1 (1%) | 14 | 52 |
| 48 | Ad | 68/76 (90%) | 65 (96%) | 3 (4%) | 0 | 100 | 100 |
| 49 | Ae | 39/50 (78%) | 36 (92%) | 3 (8%) | 0 | 100 | 100 |
| 50 | Af | 49/51 (96%) | 43 (88%) | 6 (12%) | 0 | 100 | 100 |
| 51 | AP | 202/204 (99%) | 187 (93%) | 7 (4%) | 8 (4%) | 3 | 23 |
| 52 | Ah | 83/85 (98%) | 78 (94%) | 4 (5%) | 1 (1%) | 13 | 50 |
| 53 | Ai | 93/95 (98%) | 87 (94%) | 4 (4%) | 2 (2%) | 6 | 35 |
| 54 | AI | 203/213 (95%) | 183 (90%) | 17 (8%) | 3 (2%) | 10 | 46 |
| 55 | AJ | 216/244 (88%) | 202 (94%) | 12 (6%) | 2 (1%) | 17 | 57 |
| 56 | Ac | 87/89 (98%) | 76 (87%) | 7 (8%) | 4 (5%) | 2 | 21 |
| 57 | AK | 199/201 (99%) | 192 (96%) | 5 (2%) | 2 (1%) | 15 | 54 |
| 58 | AM | 130/132 (98%) | 123 (95%) | 7 (5%) | 0 | 100 | 100 |
| 59 | AS | 184/186 (99%) | 168 (91%) | 14 (8%) | 2 (1%) | 14 | 52 |
| 60 | AO | 145/147 (99%) | 132 (91%) | 12 (8%) | 1 (1%) | 22 | 63 |
| 61 | AQ | 185/205 (90%) | 161 (87%) | 19 (10%) | 5 (3%) | 5 | 31 |
| 62 | AR | 244/289 (84%) | 224 (92%) | 13 (5%) | 7 (3%) | 4 | 29 |
| 63 | AW | 149/170 (88%) | 133 (89%) | 10 (7%) | 6 (4%) | 3 | 23 |
| 64 | AY | 99/101 (98%) | 95 (96%) | 3 (3%) | 1 (1%) | 15 | 54 |
| 65 | AT | 179/181 (99%) | 171 (96%) | 5 (3%) | 3 (2%) | 9 | 42 |
| 66 | AZ | 119/121 (98%) | 110 (92%) | 7 (6%) | 2 (2%) | 9 | 42 |
| 67 | A3 | 117/119 (98%) | 107 (92%) | 9 (8%) | 1 (1%) | 17 | 57 |
| 68 | A5 | 221/223 (99%) | 195 (88%) | 21 (10%) | 5 (2%) | 6 | 34 |
| 69 | AD | 245/247 (99%) | 223 (91%) | 20 (8%) | 2 (1%) | 19 | 60 |
| 70 | AE | 378/380 (100%) | 353 (93%) | 21 (6%) | 4 (1%) | 14 | 52 |
| 71 | AF | 388/390 (100%) | 356 (92%) | 26 (7%) | 6 (2%) | 10 | 46 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 72 | AG | 116/159 (73%) | 104 (90%) | 11 (10%) | 1 (1%) | 17 57 |
| 73 | AU | 178/180 (99%) | 169 (95%) | 6 (3%) | 3 (2%) | 9 42 |
| 74 | AH | 183/185 (99%) | 166 (91%) | 14 (8%) | 3 (2%) | 9 44 |
| 75 | AV | 153/155 (99%) | 141 (92%) | 9 (6%) | 3 (2%) | 7 38 |
| 76 | Ag | 35/37 (95%) | 30 (86%) | 3 (9%) | 2 (6%) | 1 18 |
| 77 | AX | 95/97 (98%) | 88 (93%) | 5 (5%) | 2 (2%) | 7 36 |
| 78 | A0 | 60/62 (97%) | 59 (98%) | 1 (2%) | 0 | 100 100 |
| All | All | 10111/10698 (94%) | 9269 (92%) | 652 (6%) | 190 (2%) | 11 38 |

All (190) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 6 | I | 42 | HIS |
| 6 | I | 70 | HIS |
| 8 | M | 41 | GLU |
| 9 | W | 4 | VAL |
| 10 | R | 42 | ILE |
| 17 | 4 | 10 | PRO |
| 17 | 4 | 20 | LYS |
| 20 | B | 93 | ASN |
| 20 | B | 146 | ARG |
| 22 | H | 25 | LEU |
| 23 | J | 13 | PRO |
| 23 | J | 112 | ILE |
| 23 | J | 156 | ASP |
| 26 | P | 100 | SER |
| 27 | Q | 137 | LYS |
| 32 | X | 52 | LYS |
| 37 | AL | 169 | PRO |
| 45 | A9 | 66 | LYS |
| 51 | AP | 51 | LEU |
| 51 | AP | 149 | ILE |
| 55 | AJ | 57 | VAL |
| 55 | AJ | 65 | LEU |
| 56 | Ac | 42 | TYR |
| 61 | AQ | 57 | TYR |
| 65 | AT | 129 | ASN |
| 68 | A5 | 116 | ARG |
| 70 | AE | 196 | LEU |
| 73 | AU | 183 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 76 | Ag | 7 | ARG |
| 4 | E | 167 | ALA |
| 5 | G | 41 | TRP |
| 7 | K | 57 | ARG |
| 7 | K | 120 | HIS |
| 7 | K | 121 | THR |
| 8 | M | 99 | ASP |
| 10 | R | 41 | GLY |
| 17 | 4 | 18 | LYS |
| 19 | 6 | 28 | LYS |
| 20 | B | 50 | LYS |
| 22 | H | 178 | LEU |
| 23 | J | 157 | SER |
| 23 | J | 165 | ILE |
| 24 | L | 119 | THR |
| 24 | L | 168 | ILE |
| 28 | S | 17 | ILE |
| 28 | S | 101 | ILE |
| 30 | U | 10 | GLY |
| 31 | V | 41 | VAL |
| 32 | X | 51 | LYS |
| 33 | C | 116 | THR |
| 37 | AL | 144 | ASP |
| 39 | A2 | 95 | GLN |
| 40 | A4 | 38 | ASN |
| 46 | Aa | 77 | GLY |
| 51 | AP | 72 | LYS |
| 51 | AP | 138 | PRO |
| 51 | AP | 150 | ASN |
| 51 | AP | 188 | SER |
| 53 | Ai | 85 | LYS |
| 54 | AI | 88 | PRO |
| 56 | Ac | 5 | GLY |
| 62 | AR | 114 | ASN |
| 62 | AR | 152 | ILE |
| 62 | AR | 229 | ASN |
| 63 | AW | 106 | ASN |
| 65 | AT | 15 | LYS |
| 71 | AF | 19 | VAL |
| 71 | AF | 95 | MET |
| 71 | AF | 313 | LEU |
| 72 | AG | 26 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 74 | AH | 43 | ILE |
| 74 | AH | 110 | ARG |
| 74 | AH | 166 | CYS |
| 75 | AV | 134 | GLU |
| 7 | K | 29 | PRO |
| 9 | W | 62 | GLN |
| 11 | O | 70 | TYR |
| 13 | Z | 76 | LYS |
| 17 | 4 | 47 | HIS |
| 20 | B | 49 | THR |
| 21 | F | 104 | ASP |
| 21 | F | 177 | VAL |
| 23 | J | 132 | SER |
| 26 | P | 39 | ASP |
| 28 | S | 13 | HIS |
| 28 | S | 24 | GLY |
| 28 | S | 34 | ALA |
| 28 | S | 120 | ARG |
| 30 | U | 141 | TYR |
| 32 | X | 121 | ILE |
| 33 | C | 27 | LYS |
| 37 | AL | 61 | THR |
| 38 | A1 | 42 | LEU |
| 40 | A4 | 8 | THR |
| 43 | AN | 87 | CYS |
| 47 | Ab | 10 | ALA |
| 51 | AP | 108 | LYS |
| 54 | AI | 19 | VAL |
| 56 | Ac | 48 | ARG |
| 60 | AO | 24 | LYS |
| 61 | AQ | 24 | ARG |
| 62 | AR | 59 | GLN |
| 62 | AR | 172 | GLY |
| 62 | AR | 233 | ASP |
| 63 | AW | 132 | ALA |
| 65 | AT | 4 | THR |
| 67 | A3 | 37 | LEU |
| 68 | A5 | 83 | CYS |
| 68 | A5 | 172 | ALA |
| 71 | AF | 68 | GLY |
| 71 | AF | 346 | SER |
| 5 | G | 121 | GLY |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 9 | W | 69 | ILE |
| 12 | Y | 142 | LYS |
| 14 | 1 | 11 | LYS |
| 21 | F | 176 | GLN |
| 23 | J | 106 | LYS |
| 24 | L | 29 | LEU |
| 24 | L | 86 | SER |
| 25 | N | 52 | PRO |
| 26 | P | 57 | THR |
| 28 | S | 40 | LYS |
| 31 | V | 56 | TYR |
| 33 | C | 29 | LEU |
| 33 | C | 30 | GLU |
| 37 | AL | 129 | LYS |
| 38 | A1 | 30 | GLU |
| 39 | A2 | 17 | ASN |
| 40 | A4 | 36 | ASP |
| 46 | Aa | 52 | GLN |
| 51 | AP | 183 | ALA |
| 53 | Ai | 95 | ASP |
| 61 | AQ | 13 | LYS |
| 61 | AQ | 47 | SER |
| 62 | AR | 183 | PRO |
| 63 | AW | 37 | ARG |
| 63 | AW | 61 | ARG |
| 66 | AZ | 84 | VAL |
| 70 | AE | 12 | GLY |
| 70 | AE | 239 | THR |
| 71 | AF | 268 | HIS |
| 73 | AU | 167 | GLN |
| 75 | AV | 13 | ARG |
| 77 | AX | 78 | LYS |
| 7 | K | 58 | SER |
| 10 | R | 36 | ASP |
| 10 | R | 37 | GLY |
| 11 | O | 35 | GLU |
| 20 | B | 98 | THR |
| 20 | B | 150 | THR |
| 21 | F | 195 | ILE |
| 22 | H | 105 | ASP |
| 23 | J | 58 | LYS |
| 25 | N | 67 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 27 | Q | 143 | PRO |
| 33 | C | 143 | VAL |
| 45 | A9 | 47 | LEU |
| 54 | AI | 49 | LYS |
| 57 | AK | 72 | LEU |
| 61 | AQ | 60 | ILE |
| 63 | AW | 9 | ARG |
| 63 | AW | 20 | VAL |
| 68 | A5 | 168 | VAL |
| 69 | AD | 199 | VAL |
| 75 | AV | 56 | ASN |
| 10 | R | 127 | ALA |
| 12 | Y | 21 | PRO |
| 12 | Y | 49 | ASN |
| 16 | 3 | 46 | ASP |
| 20 | B | 209 | ASN |
| 31 | V | 9 | HIS |
| 38 | A1 | 37 | PRO |
| 56 | Ac | 40 | CYS |
| 57 | AK | 88 | PRO |
| 59 | AS | 130 | PRO |
| 64 | AY | 89 | ARG |
| 66 | AZ | 70 | VAL |
| 70 | AE | 107 | ALA |
| 73 | AU | 134 | ARG |
| 76 | Ag | 9 | LYS |
| 59 | AS | 82 | VAL |
| 69 | AD | 127 | VAL |
| 77 | AX | 68 | ILE |
| 11 | O | 41 | PRO |
| 20 | B | 190 | PRO |
| 21 | F | 189 | VAL |
| 43 | AN | 46 | VAL |
| 24 | L | 202 | GLY |
| 52 | Ah | 52 | VAL |
| 68 | A5 | 100 | 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 | |
|---|---|---|---|---|---|---|
| 3 | D | 132/177 (75%) | 128 (97%) | 4 (3%) | 41 | 63 |
| 4 | E | 161/164 (98%) | 156 (97%) | 5 (3%) | 40 | 62 |
| 5 | G | 191/191 (100%) | 185 (97%) | 6 (3%) | 40 | 62 |
| 6 | I | 154/160 (96%) | 151 (98%) | 3 (2%) | 57 | 75 |
| 7 | K | 115/115 (100%) | 113 (98%) | 2 (2%) | 60 | 78 |
| 8 | M | 116/116 (100%) | 115 (99%) | 1 (1%) | 78 | 87 |
| 9 | W | 86/99 (87%) | 83 (96%) | 3 (4%) | 36 | 59 |
| 10 | R | 83/97 (86%) | 81 (98%) | 2 (2%) | 49 | 69 |
| 11 | O | 76/76 (100%) | 71 (93%) | 5 (7%) | 16 | 41 |
| 12 | Y | 137/137 (100%) | 132 (96%) | 5 (4%) | 35 | 59 |
| 13 | Z | 60/60 (100%) | 59 (98%) | 1 (2%) | 60 | 78 |
| 14 | 1 | 104/104 (100%) | 100 (96%) | 4 (4%) | 33 | 57 |
| 15 | 2 | 35/61 (57%) | 34 (97%) | 1 (3%) | 42 | 64 |
| 16 | 3 | 87/87 (100%) | 83 (95%) | 4 (5%) | 27 | 52 |
| 17 | 4 | 70/70 (100%) | 69 (99%) | 1 (1%) | 67 | 80 |
| 18 | 5 | 47/52 (90%) | 46 (98%) | 1 (2%) | 53 | 72 |
| 19 | 6 | 36/36 (100%) | 35 (97%) | 1 (3%) | 43 | 65 |
| 20 | B | 195/195 (100%) | 191 (98%) | 4 (2%) | 53 | 72 |
| 21 | F | 233/233 (100%) | 223 (96%) | 10 (4%) | 29 | 54 |
| 22 | H | 182/190 (96%) | 173 (95%) | 9 (5%) | 25 | 50 |
| 23 | J | 177/177 (100%) | 171 (97%) | 6 (3%) | 37 | 60 |
| 24 | L | 151/190 (80%) | 144 (95%) | 7 (5%) | 27 | 52 |
| 25 | N | 91/91 (100%) | 89 (98%) | 2 (2%) | 52 | 71 |
| 26 | P | 99/99 (100%) | 97 (98%) | 2 (2%) | 55 | 74 |
| 27 | Q | 120/120 (100%) | 119 (99%) | 1 (1%) | 81 | 89 |
| 28 | S | 114/114 (100%) | 109 (96%) | 5 (4%) | 28 | 53 |
| 29 | T | 43/43 (100%) | 40 (93%) | 3 (7%) | 15 | 40 |
| 30 | U | 132/132 (100%) | 129 (98%) | 3 (2%) | 50 | 70 |
| 31 | V | 131/140 (94%) | 128 (98%) | 3 (2%) | 50 | 70 |
| 32 | X | 88/94 (94%) | 88 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 33 | C | 167/167 (100%) | 161 (96%) | 6 (4%) | 35 59 |
| 37 | AL | 190/190 (100%) | 188 (99%) | 2 (1%) | 73 84 |
| 38 | A1 | 127/131 (97%) | 124 (98%) | 3 (2%) | 49 69 |
| 39 | A2 | 97/109 (89%) | 96 (99%) | 1 (1%) | 76 86 |
| 40 | A4 | 60/60 (100%) | 57 (95%) | 3 (5%) | 24 49 |
| 41 | A6 | 83/83 (100%) | 76 (92%) | 7 (8%) | 11 33 |
| 42 | A7 | 90/96 (94%) | 87 (97%) | 3 (3%) | 38 61 |
| 43 | AN | 135/135 (100%) | 130 (96%) | 5 (4%) | 34 58 |
| 44 | A8 | 114/114 (100%) | 108 (95%) | 6 (5%) | 22 47 |
| 45 | A9 | 90/90 (100%) | 86 (96%) | 4 (4%) | 28 53 |
| 46 | Aa | 89/89 (100%) | 85 (96%) | 4 (4%) | 27 52 |
| 47 | Ab | 82/92 (89%) | 81 (99%) | 1 (1%) | 71 83 |
| 48 | Ad | 69/73 (94%) | 68 (99%) | 1 (1%) | 67 80 |
| 49 | Ae | 40/47 (85%) | 38 (95%) | 2 (5%) | 24 49 |
| 50 | Af | 45/45 (100%) | 45 (100%) | 0 | 100 100 |
| 51 | AP | 179/179 (100%) | 175 (98%) | 4 (2%) | 52 71 |
| 52 | Ah | 70/70 (100%) | 70 (100%) | 0 | 100 100 |
| 53 | Ai | 87/87 (100%) | 87 (100%) | 0 | 100 100 |
| 54 | AI | 189/195 (97%) | 183 (97%) | 6 (3%) | 39 61 |
| 55 | AJ | 204/224 (91%) | 200 (98%) | 4 (2%) | 55 74 |
| 56 | Ac | 74/74 (100%) | 68 (92%) | 6 (8%) | 11 35 |
| 57 | AK | 181/181 (100%) | 178 (98%) | 3 (2%) | 60 78 |
| 58 | AM | 106/106 (100%) | 104 (98%) | 2 (2%) | 57 75 |
| 59 | AS | 158/158 (100%) | 151 (96%) | 7 (4%) | 28 53 |
| 60 | AO | 121/121 (100%) | 119 (98%) | 2 (2%) | 60 78 |
| 61 | AQ | 165/176 (94%) | 160 (97%) | 5 (3%) | 41 63 |
| 62 | AR | 215/250 (86%) | 208 (97%) | 7 (3%) | 38 61 |
| 63 | AW | 128/128 (100%) | 126 (98%) | 2 (2%) | 62 79 |
| 64 | AY | 90/90 (100%) | 88 (98%) | 2 (2%) | 52 71 |
| 65 | AT | 162/162 (100%) | 161 (99%) | 1 (1%) | 86 92 |
| 66 | AZ | 111/111 (100%) | 111 (100%) | 0 | 100 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 67 | A3 | 110/110 (100%) | 108 (98%) | 2 (2%) | 59 77 |
| 68 | A5 | 201/201 (100%) | 196 (98%) | 5 (2%) | 47 68 |
| 69 | AD | 191/191 (100%) | 185 (97%) | 6 (3%) | 40 62 |
| 70 | AE | 335/335 (100%) | 329 (98%) | 6 (2%) | 59 77 |
| 71 | AF | 336/336 (100%) | 327 (97%) | 9 (3%) | 44 65 |
| 72 | AG | 110/142 (78%) | 106 (96%) | 4 (4%) | 35 59 |
| 73 | AU | 162/162 (100%) | 158 (98%) | 4 (2%) | 47 68 |
| 74 | AH | 168/168 (100%) | 164 (98%) | 4 (2%) | 49 69 |
| 75 | AV | 140/140 (100%) | 137 (98%) | 3 (2%) | 53 72 |
| 76 | Ag | 34/34 (100%) | 33 (97%) | 1 (3%) | 42 64 |
| 77 | AX | 92/92 (100%) | 91 (99%) | 1 (1%) | 73 84 |
| 78 | A0 | 53/53 (100%) | 52 (98%) | 1 (2%) | 57 75 |
| All | All | 9096/9417 (97%) | 8847 (97%) | 249 (3%) | 48 65 |

All (249) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | D | 76 | ARG |
| 3 | D | 107 | ARG |
| 3 | D | 158 | LEU |
| 3 | D | 190 | MET |
| 4 | E | 36 | LEU |
| 4 | E | 53 | ARG |
| 4 | E | 69 | ARG |
| 4 | E | 121 | SER |
| 4 | E | 181 | LYS |
| 5 | G | 41 | TRP |
| 5 | G | 168 | MET |
| 5 | G | 179 | ILE |
| 5 | G | 182 | VAL |
| 5 | G | 234 | TYR |
| 5 | G | 242 | TRP |
| 6 | I | 16 | TYR |
| 6 | I | 89 | GLU |
| 6 | I | 118 | ARG |
| 7 | K | 46 | TYR |
| 7 | K | 112 | ASP |
| 8 | M | 116 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 9 | W | 18 | GLU |
| 9 | W | 45 | ARG |
| 9 | W | 101 | ASP |
| 10 | R | 43 | ARG |
| 10 | R | 61 | ASP |
| 11 | O | 17 | GLN |
| 11 | O | 18 | ASN |
| 11 | O | 26 | LEU |
| 11 | O | 42 | ARG |
| 11 | O | 68 | GLU |
| 12 | Y | 27 | ASN |
| 12 | Y | 64 | LYS |
| 12 | Y | 72 | ASN |
| 12 | Y | 105 | LYS |
| 12 | Y | 160 | ARG |
| 13 | Z | 81 | GLN |
| 14 | 1 | 20 | ARG |
| 14 | 1 | 94 | ARG |
| 14 | 1 | 113 | LYS |
| 14 | 1 | 118 | LYS |
| 15 | 2 | 99 | LYS |
| 16 | 3 | 2 | PRO |
| 16 | 3 | 38 | ARG |
| 16 | 3 | 39 | PHE |
| 16 | 3 | 85 | ARG |
| 17 | 4 | 77 | PHE |
| 18 | 5 | 29 | PHE |
| 19 | 6 | 17 | GLN |
| 20 | B | 31 | ASP |
| 20 | B | 49 | THR |
| 20 | B | 124 | HIS |
| 20 | B | 209 | ASN |
| 21 | F | 5 | ILE |
| 21 | F | 18 | TRP |
| 21 | F | 42 | ILE |
| 21 | F | 88 | ASP |
| 21 | F | 93 | THR |
| 21 | F | 108 | ARG |
| 21 | F | 132 | ARG |
| 21 | F | 142 | HIS |
| 21 | F | 174 | LYS |
| 21 | F | 224 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 22 | H | 14 | LYS |
| 22 | H | 25 | LEU |
| 22 | H | 51 | ARG |
| 22 | H | 68 | LEU |
| 22 | H | 136 | LYS |
| 22 | H | 140 | LYS |
| 22 | H | 147 | LEU |
| 22 | H | 158 | ILE |
| 22 | H | 159 | ILE |
| 23 | J | 44 | LEU |
| 23 | J | 51 | GLU |
| 23 | J | 111 | LYS |
| 23 | J | 142 | SER |
| 23 | J | 166 | GLU |
| 23 | J | 183 | ASP |
| 24 | L | 26 | LYS |
| 24 | L | 37 | LYS |
| 24 | L | 41 | ARG |
| 24 | L | 92 | ARG |
| 24 | L | 119 | THR |
| 24 | L | 176 | PHE |
| 24 | L | 201 | GLU |
| 25 | N | 31 | ILE |
| 25 | N | 43 | LYS |
| 26 | P | 34 | PHE |
| 26 | P | 41 | PHE |
| 27 | Q | 103 | LEU |
| 28 | S | 29 | ILE |
| 28 | S | 36 | LYS |
| 28 | S | 86 | LEU |
| 28 | S | 94 | GLU |
| 28 | S | 110 | ARG |
| 29 | T | 35 | ASN |
| 29 | T | 39 | GLN |
| 29 | T | 54 | ARG |
| 30 | U | 3 | ARG |
| 30 | U | 47 | PRO |
| 30 | U | 78 | GLN |
| 31 | V | 6 | ASP |
| 31 | V | 70 | ARG |
| 31 | V | 130 | GLN |
| 33 | C | 22 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 33 | C | 58 | GLN |
| 33 | C | 121 | LEU |
| 33 | C | 135 | GLU |
| 33 | C | 172 | LEU |
| 33 | C | 204 | ARG |
| 37 | AL | 160 | ILE |
| 37 | AL | 193 | LYS |
| 38 | A1 | 86 | GLN |
| 38 | A1 | 105 | LYS |
| 38 | A1 | 121 | LYS |
| 39 | A2 | 94 | GLN |
| 40 | A4 | 5 | LYS |
| 40 | A4 | 25 | LYS |
| 40 | A4 | 30 | MET |
| 41 | A6 | 14 | ASN |
| 41 | A6 | 19 | LEU |
| 41 | A6 | 28 | PHE |
| 41 | A6 | 44 | LEU |
| 41 | A6 | 62 | TYR |
| 41 | A6 | 65 | LEU |
| 41 | A6 | 89 | ARG |
| 42 | A7 | 52 | MET |
| 42 | A7 | 74 | ASN |
| 42 | A7 | 95 | GLU |
| 43 | AN | 56 | VAL |
| 43 | AN | 79 | GLU |
| 43 | AN | 80 | ARG |
| 43 | AN | 82 | LYS |
| 43 | AN | 133 | PHE |
| 44 | A8 | 4 | LYS |
| 44 | A8 | 21 | GLN |
| 44 | A8 | 33 | ARG |
| 44 | A8 | 34 | LYS |
| 44 | A8 | 61 | LYS |
| 44 | A8 | 77 | LYS |
| 45 | A9 | 54 | ARG |
| 45 | A9 | 130 | ARG |
| 45 | A9 | 134 | LEU |
| 45 | A9 | 136 | TYR |
| 46 | Aa | 6 | HIS |
| 46 | Aa | 11 | ASN |
| 46 | Aa | 32 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 46 | Aa | 66 | ARG |
| 47 | Ab | 106 | ARG |
| 48 | Ad | 47 | LYS |
| 49 | Ae | 17 | ARG |
| 49 | Ae | 30 | LYS |
| 51 | AP | 56 | ILE |
| 51 | AP | 85 | LYS |
| 51 | AP | 161 | GLU |
| 51 | AP | 162 | LEU |
| 54 | AI | 10 | HIS |
| 54 | AI | 42 | LYS |
| 54 | AI | 63 | LEU |
| 54 | AI | 88 | PRO |
| 54 | AI | 115 | GLU |
| 54 | AI | 149 | LEU |
| 55 | AJ | 55 | ILE |
| 55 | AJ | 60 | ARG |
| 55 | AJ | 120 | SER |
| 55 | AJ | 172 | ASN |
| 56 | Ac | 20 | PHE |
| 56 | Ac | 48 | ARG |
| 56 | Ac | 49 | ARG |
| 56 | Ac | 55 | LYS |
| 56 | Ac | 76 | LYS |
| 56 | Ac | 90 | LYS |
| 57 | AK | 38 | GLU |
| 57 | AK | 116 | LYS |
| 57 | AK | 134 | TYR |
| 58 | AM | 29 | ASP |
| 58 | AM | 49 | ASN |
| 59 | AS | 26 | LEU |
| 59 | AS | 58 | TYR |
| 59 | AS | 74 | HIS |
| 59 | AS | 96 | GLN |
| 59 | AS | 133 | LYS |
| 59 | AS | 177 | ARG |
| 59 | AS | 187 | LYS |
| 60 | AO | 32 | ARG |
| 60 | AO | 63 | LEU |
| 61 | AQ | 35 | ASP |
| 61 | AQ | 59 | GLN |
| 61 | AQ | 125 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 61 | AQ | 126 | VAL |
| 61 | AQ | 193 | ASP |
| 62 | AR | 21 | ARG |
| 62 | AR | 23 | ARG |
| 62 | AR | 39 | GLN |
| 62 | AR | 56 | THR |
| 62 | AR | 70 | GLU |
| 62 | AR | 77 | GLU |
| 62 | AR | 249 | ASN |
| 63 | AW | 94 | ILE |
| 63 | AW | 97 | ASN |
| 64 | AY | 96 | ILE |
| 64 | AY | 133 | MET |
| 65 | AT | 162 | ARG |
| 67 | A3 | 78 | LYS |
| 67 | A3 | 111 | GLN |
| 68 | A5 | 59 | ARG |
| 68 | A5 | 149 | THR |
| 68 | A5 | 169 | ARG |
| 68 | A5 | 170 | ARG |
| 68 | A5 | 195 | GLU |
| 69 | AD | 12 | ARG |
| 69 | AD | 118 | HIS |
| 69 | AD | 163 | ARG |
| 69 | AD | 207 | VAL |
| 69 | AD | 221 | HIS |
| 69 | AD | 242 | ARG |
| 70 | AE | 71 | GLU |
| 70 | AE | 140 | THR |
| 70 | AE | 214 | VAL |
| 70 | AE | 269 | TYR |
| 70 | AE | 353 | LEU |
| 70 | AE | 361 | LYS |
| 71 | AF | 77 | PRO |
| 71 | AF | 86 | ARG |
| 71 | AF | 101 | MET |
| 71 | AF | 122 | TYR |
| 71 | AF | 140 | ARG |
| 71 | AF | 190 | ARG |
| 71 | AF | 313 | LEU |
| 71 | AF | 344 | ARG |
| 71 | AF | 366 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 72 | AG | 35 | ARG |
| 72 | AG | 134 | SER |
| 72 | AG | 141 | ARG |
| 72 | AG | 166 | LYS |
| 73 | AU | 90 | TYR |
| 73 | AU | 107 | THR |
| 73 | AU | 157 | ARG |
| 73 | AU | 166 | LEU |
| 74 | AH | 46 | ARG |
| 74 | AH | 57 | VAL |
| 74 | AH | 140 | LYS |
| 74 | AH | 159 | LEU |
| 75 | AV | 83 | HIS |
| 75 | AV | 97 | VAL |
| 75 | AV | 104 | GLU |
| 76 | Ag | 19 | TRP |
| 77 | AX | 44 | LEU |
| 78 | A0 | 37 | PHE |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | D | 102 | GLN |
| 4 | E | 133 | HIS |
| 4 | E | 155 | HIS |
| 7 | K | 56 | HIS |
| 7 | K | 113 | HIS |
| 10 | R | 52 | GLN |
| 12 | Y | 44 | HIS |
| 17 | 4 | 58 | ASN |
| 20 | B | 124 | HIS |
| 21 | F | 112 | HIS |
| 26 | P | 32 | HIS |
| 30 | U | 105 | ASN |
| 33 | C | 23 | HIS |
| 37 | AL | 4 | HIS |
| 38 | A1 | 79 | HIS |
| 39 | A2 | 53 | ASN |
| 40 | A4 | 27 | HIS |
| 42 | A7 | 29 | HIS |
| 43 | AN | 130 | GLN |
| 44 | A8 | 98 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 45 | A9 | 53 | GLN |
| 52 | Ah | 34 | HIS |
| 53 | Ai | 26 | GLN |
| 60 | AO | 19 | HIS |
| 60 | AO | 40 | HIS |
| 60 | AO | 60 | HIS |
| 60 | AO | 62 | ASN |
| 60 | AO | 118 | HIS |
| 60 | AO | 119 | ASN |
| 63 | AW | 25 | HIS |
| 63 | AW | 145 | HIS |
| 68 | A5 | 51 | ASN |
| 68 | A5 | 232 | HIS |
| 69 | AD | 118 | HIS |
| 69 | AD | 216 | HIS |
| 71 | AF | 286 | ASN |
| 73 | AU | 97 | HIS |
| 73 | AU | 162 | HIS |
| 77 | AX | 114 | HIS |

### 5.3.3 RNA

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 1 | A | 1588/1608 (98%) | 476 (29%) | 86 (5%) |
| 2 | 7 | 73/74 (98%) | 23 (31%) | 3 (4%) |
| 34 | AA | 3167/3193 (99%) | 966 (30%) | 190 (5%) |
| 35 | AC | 148/151 (98%) | 51 (34%) | 6 (4%) |
| 36 | AB | 117/118 (99%) | 28 (23%) | 4 (3%) |
| All | All | 5093/5144 (99%) | 1544 (30%) | 289 (5%) |

All (1544) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 17 | C |
| 1 | A | 25 | C |
| 1 | A | 26 | A |
| 1 | A | 27 | U |
| 1 | A | 34 | G |
| 1 | A | 35 | U |
| 1 | A | 40 | A |
| 1 | A | 42 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 43 | A |
| 1 | A | 47 | A |
| 1 | A | 50 | C |
| 1 | A | 52 | U |
| 1 | A | 57 | G |
| 1 | A | 59 | G |
| 1 | A | 60 | A |
| 1 | A | 67 | A |
| 1 | A | 68 | U |
| 1 | A | 71 | A |
| 1 | A | 79 | U |
| 1 | A | 81 | U |
| 1 | A | 82 | G |
| 1 | A | 84 | A |
| 1 | A | 106 | A |
| 1 | A | 113 | U |
| 1 | A | 116 | A |
| 1 | A | 125 | G |
| 1 | A | 128 | A |
| 1 | A | 129 | U |
| 1 | A | 130 | U |
| 1 | A | 138 | U |
| 1 | A | 139 | A |
| 1 | A | 140 | A |
| 1 | A | 142 | G |
| 1 | A | 143 | A |
| 1 | A | 144 | U |
| 1 | A | 151 | G |
| 1 | A | 157 | G |
| 1 | A | 158 | C |
| 1 | A | 159 | U |
| 1 | A | 161 | U |
| 1 | A | 164 | C |
| 1 | A | 165 | U |
| 1 | A | 168 | U |
| 1 | A | 182 | U |
| 1 | A | 183 | C |
| 1 | A | 206 | A |
| 1 | A | 207 | G |
| 1 | A | 208 | U |
| 1 | A | 209 | A |
| 1 | A | 217 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 247 | G |
| 1 | A | 249 | A |
| 1 | A | 251 | U |
| 1 | A | 252 | U |
| 1 | A | 254 | U |
| 1 | A | 255 | A |
| 1 | A | 258 | A |
| 1 | A | 260 | A |
| 1 | A | 262 | A |
| 1 | A | 264 | G |
| 1 | A | 266 | A |
| 1 | A | 267 | A |
| 1 | A | 268 | C |
| 1 | A | 272 | U |
| 1 | A | 273 | A |
| 1 | A | 274 | A |
| 1 | A | 292 | G |
| 1 | A | 305 | G |
| 1 | A | 308 | U |
| 1 | A | 320 | C |
| 1 | A | 322 | G |
| 1 | A | 323 | C |
| 1 | A | 326 | U |
| 1 | A | 330 | U |
| 1 | A | 335 | G |
| 1 | A | 339 | A |
| 1 | A | 342 | G |
| 1 | A | 343 | G |
| 1 | A | 344 | C |
| 1 | A | 345 | C |
| 1 | A | 349 | C |
| 1 | A | 358 | G |
| 1 | A | 361 | G |
| 1 | A | 365 | A |
| 1 | A | 367 | C |
| 1 | A | 375 | U |
| 1 | A | 378 | A |
| 1 | A | 379 | G |
| 1 | A | 384 | A |
| 1 | A | 385 | U |
| 1 | A | 396 | G |
| 1 | A | 399 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 405 | A |
| 1 | A | 406 | A |
| 1 | A | 407 | A |
| 1 | A | 408 | U |
| 1 | A | 409 | A |
| 1 | A | 410 | G |
| 1 | A | 422 | A |
| 1 | A | 423 | A |
| 1 | A | 424 | G |
| 1 | A | 430 | C |
| 1 | A | 431 | A |
| 1 | A | 432 | G |
| 1 | A | 434 | A |
| 1 | A | 440 | G |
| 1 | A | 441 | U |
| 1 | A | 445 | U |
| 1 | A | 446 | U |
| 1 | A | 450 | C |
| 1 | A | 451 | A |
| 1 | A | 454 | U |
| 1 | A | 458 | A |
| 1 | A | 459 | A |
| 1 | A | 466 | A |
| 1 | A | 467 | G |
| 1 | A | 470 | A |
| 1 | A | 475 | C |
| 1 | A | 483 | A |
| 1 | A | 488 | U |
| 1 | A | 508 | U |
| 1 | A | 509 | U |
| 1 | A | 515 | U |
| 1 | A | 516 | G |
| 1 | A | 521 | G |
| 1 | A | 526 | G |
| 1 | A | 527 | A |
| 1 | A | 543 | A |
| 1 | A | 545 | A |
| 1 | A | 546 | G |
| 1 | A | 547 | U |
| 1 | A | 548 | A |
| 1 | A | 549 | A |
| 1 | A | 562 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 564 | G |
| 1 | A | 565 | U |
| 1 | A | 566 | C |
| 1 | A | 568 | G |
| 1 | A | 575 | G |
| 1 | A | 584 | G |
| 1 | A | 587 | A |
| 1 | A | 590 | C |
| 1 | A | 601 | A |
| 1 | A | 602 | G |
| 1 | A | 613 | A |
| 1 | A | 614 | A |
| 1 | A | 616 | U |
| 1 | A | 617 | G |
| 1 | A | 618 | U |
| 1 | A | 620 | G |
| 1 | A | 626 | A |
| 1 | A | 627 | A |
| 1 | A | 629 | A |
| 1 | A | 630 | C |
| 1 | A | 631 | G |
| 1 | A | 641 | G |
| 1 | A | 642 | A |
| 1 | A | 646 | U |
| 1 | A | 648 | A |
| 1 | A | 752 | U |
| 1 | A | 753 | U |
| 1 | A | 756 | A |
| 1 | A | 760 | C |
| 1 | A | 790 | U |
| 1 | A | 791 | U |
| 1 | A | 792 | U |
| 1 | A | 793 | G |
| 1 | A | 794 | U |
| 1 | A | 800 | U |
| 1 | A | 801 | G |
| 1 | A | 804 | U |
| 1 | A | 805 | A |
| 1 | A | 806 | A |
| 1 | A | 815 | G |
| 1 | A | 816 | U |
| 1 | A | 824 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 828 | A |
| 1 | A | 832 | A |
| 1 | A | 833 | A |
| 1 | A | 837 | A |
| 1 | A | 844 | G |
| 1 | A | 845 | U |
| 1 | A | 846 | G |
| 1 | A | 849 | U |
| 1 | A | 851 | A |
| 1 | A | 852 | A |
| 1 | A | 853 | U |
| 1 | A | 857 | A |
| 1 | A | 858 | U |
| 1 | A | 866 | A |
| 1 | A | 867 | A |
| 1 | A | 869 | A |
| 1 | A | 870 | A |
| 1 | A | 875 | A |
| 1 | A | 876 | U |
| 1 | A | 877 | U |
| 1 | A | 879 | A |
| 1 | A | 881 | C |
| 1 | A | 882 | A |
| 1 | A | 887 | A |
| 1 | A | 888 | A |
| 1 | A | 896 | U |
| 1 | A | 908 | U |
| 1 | A | 915 | G |
| 1 | A | 917 | C |
| 1 | A | 920 | A |
| 1 | A | 921 | G |
| 1 | A | 922 | U |
| 1 | A | 924 | A |
| 1 | A | 925 | C |
| 1 | A | 927 | A |
| 1 | A | 928 | U |
| 1 | A | 929 | U |
| 1 | A | 930 | A |
| 1 | A | 931 | A |
| 1 | A | 941 | C |
| 1 | A | 942 | U |
| 1 | A | 945 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 962 | A |
| 1 | A | 965 | U |
| 1 | A | 966 | C |
| 1 | A | 967 | A |
| 1 | A | 973 | G |
| 1 | A | 974 | A |
| 1 | A | 982 | A |
| 1 | A | 983 | G |
| 1 | A | 984 | A |
| 1 | A | 990 | U |
| 1 | A | 999 | A |
| 1 | A | 1002 | A |
| 1 | A | 1003 | C |
| 1 | A | 1004 | U |
| 1 | A | 1011 | G |
| 1 | A | 1013 | A |
| 1 | A | 1021 | A |
| 1 | A | 1029 | U |
| 1 | A | 1035 | A |
| 1 | A | 1038 | C |
| 1 | A | 1051 | U |
| 1 | A | 1054 | G |
| 1 | A | 1057 | A |
| 1 | A | 1061 | A |
| 1 | A | 1062 | A |
| 1 | A | 1065 | C |
| 1 | A | 1072 | A |
| 1 | A | 1073 | U |
| 1 | A | 1074 | A |
| 1 | A | 1082 | A |
| 1 | A | 1089 | A |
| 1 | A | 1090 | C |
| 1 | A | 1092 | A |
| 1 | A | 1093 | U |
| 1 | A | 1094 | A |
| 1 | A | 1095 | A |
| 1 | A | 1097 | C |
| 1 | A | 1098 | U |
| 1 | A | 1099 | A |
| 1 | A | 1100 | U |
| 1 | A | 1101 | G |
| 1 | A | 1107 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 1108 | A |
| 1 | A | 1109 | G |
| 1 | A | 1112 | G |
| 1 | A | 1116 | G |
| 1 | A | 1119 | G |
| 1 | A | 1175 | G |
| 1 | A | 1177 | A |
| 1 | A | 1183 | U |
| 1 | A | 1193 | A |
| 1 | A | 1195 | G |
| 1 | A | 1197 | C |
| 1 | A | 1198 | U |
| 1 | A | 1199 | U |
| 1 | A | 1209 | G |
| 1 | A | 1210 | G |
| 1 | A | 1212 | C |
| 1 | A | 1227 | G |
| 1 | A | 1230 | A |
| 1 | A | 1239 | A |
| 1 | A | 1247 | G |
| 1 | A | 1251 | G |
| 1 | A | 1252 | A |
| 1 | A | 1255 | G |
| 1 | A | 1259 | C |
| 1 | A | 1260 | C |
| 1 | A | 1261 | A |
| 1 | A | 1265 | G |
| 1 | A | 1268 | G |
| 1 | A | 1271 | G |
| 1 | A | 1274 | C |
| 1 | A | 1279 | G |
| 1 | A | 1284 | A |
| 1 | A | 1285 | A |
| 1 | A | 1286 | U |
| 1 | A | 1287 | U |
| 1 | A | 1292 | U |
| 1 | A | 1295 | A |
| 1 | A | 1296 | C |
| 1 | A | 1297 | A |
| 1 | A | 1301 | G |
| 1 | A | 1302 | G |
| 1 | A | 1303 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 1304 | A |
| 1 | A | 1307 | U |
| 1 | A | 1308 | C |
| 1 | A | 1315 | U |
| 1 | A | 1318 | A |
| 1 | A | 1319 | G |
| 1 | A | 1321 | C |
| 1 | A | 1363 | U |
| 1 | A | 1366 | A |
| 1 | A | 1367 | U |
| 1 | A | 1374 | G |
| 1 | A | 1375 | C |
| 1 | A | 1382 | G |
| 1 | A | 1383 | U |
| 1 | A | 1384 | U |
| 1 | A | 1385 | U |
| 1 | A | 1386 | U |
| 1 | A | 1387 | U |
| 1 | A | 1388 | A |
| 1 | A | 1401 | G |
| 1 | A | 1409 | U |
| 1 | A | 1414 | A |
| 1 | A | 1415 | A |
| 1 | A | 1416 | U |
| 1 | A | 1417 | U |
| 1 | A | 1422 | U |
| 1 | A | 1423 | A |
| 1 | A | 1427 | A |
| 1 | A | 1431 | A |
| 1 | A | 1432 | G |
| 1 | A | 1433 | A |
| 1 | A | 1437 | U |
| 1 | A | 1443 | G |
| 1 | A | 1444 | C |
| 1 | A | 1445 | U |
| 1 | A | 1449 | U |
| 1 | A | 1450 | A |
| 1 | A | 1451 | G |
| 1 | A | 1453 | G |
| 1 | A | 1454 | G |
| 1 | A | 1456 | G |
| 1 | A | 1459 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 1462 | A |
| 1 | A | 1463 | C |
| 1 | A | 1464 | U |
| 1 | A | 1607 | U |
| 1 | A | 1623 | U |
| 1 | A | 1624 | U |
| 1 | A | 1625 | C |
| 1 | A | 1626 | U |
| 1 | A | 1635 | C |
| 1 | A | 1636 | A |
| 1 | A | 1644 | U |
| 1 | A | 1645 | C |
| 1 | A | 1646 | U |
| 1 | A | 1648 | A |
| 1 | A | 1649 | C |
| 1 | A | 1656 | A |
| 1 | A | 1659 | U |
| 1 | A | 1660 | U |
| 1 | A | 1661 | U |
| 1 | A | 1664 | G |
| 1 | A | 1668 | A |
| 1 | A | 1673 | A |
| 1 | A | 1674 | G |
| 1 | A | 1677 | C |
| 1 | A | 1678 | U |
| 1 | A | 1679 | G |
| 1 | A | 1691 | G |
| 1 | A | 1692 | A |
| 1 | A | 1693 | U |
| 1 | A | 1703 | U |
| 1 | A | 1705 | C |
| 1 | A | 1706 | A |
| 1 | A | 1715 | A |
| 1 | A | 1716 | C |
| 1 | A | 1717 | A |
| 1 | A | 1718 | C |
| 1 | A | 1719 | U |
| 1 | A | 1720 | G |
| 1 | A | 1721 | A |
| 1 | A | 1723 | A |
| 1 | A | 1727 | A |
| 1 | A | 1728 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 1732 | G |
| 1 | A | 1735 | U |
| 1 | A | 1742 | A |
| 1 | A | 1749 | C |
| 1 | A | 1750 | U |
| 1 | A | 1787 | U |
| 1 | A | 1790 | C |
| 1 | A | 1792 | U |
| 1 | A | 1795 | G |
| 1 | A | 1796 | C |
| 1 | A | 1801 | A |
| 1 | A | 1802 | G |
| 1 | A | 1806 | U |
| 1 | A | 1810 | U |
| 1 | A | 1812 | A |
| 1 | A | 1813 | U |
| 1 | A | 1817 | U |
| 1 | A | 1818 | A |
| 1 | A | 1819 | U |
| 1 | A | 1820 | C |
| 1 | A | 1824 | A |
| 1 | A | 1825 | U |
| 1 | A | 1830 | C |
| 1 | A | 1833 | G |
| 1 | A | 1834 | A |
| 1 | A | 1835 | U |
| 1 | A | 1837 | G |
| 1 | A | 1846 | U |
| 1 | A | 1850 | G |
| 1 | A | 1854 | U |
| 1 | A | 1856 | A |
| 1 | A | 1861 | U |
| 1 | A | 1866 | A |
| 1 | A | 1868 | C |
| 1 | A | 1870 | A |
| 1 | A | 1871 | G |
| 1 | A | 1881 | G |
| 1 | A | 1882 | U |
| 1 | A | 1887 | A |
| 1 | A | 1892 | U |
| 1 | A | 1897 | A |
| 1 | A | 1898 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 1902 | G |
| 1 | A | 1904 | G |
| 1 | A | 1907 | A |
| 1 | A | 1908 | A |
| 1 | A | 1911 | A |
| 1 | A | 1912 | C |
| 1 | A | 1913 | G |
| 1 | A | 1915 | C |
| 1 | A | 1916 | C |
| 1 | A | 1927 | U |
| 1 | A | 1928 | A |
| 1 | A | 1929 | C |
| 1 | A | 1930 | A |
| 1 | A | 1932 | A |
| 1 | A | 1938 | C |
| 1 | A | 1944 | U |
| 1 | A | 1954 | U |
| 1 | A | 1955 | G |
| 1 | A | 1961 | U |
| 1 | A | 1977 | G |
| 1 | A | 1978 | A |
| 1 | A | 1979 | C |
| 1 | A | 1980 | A |
| 1 | A | 1981 | A |
| 1 | A | 1982 | G |
| 1 | A | 1983 | A |
| 1 | A | 2012 | G |
| 1 | A | 2016 | A |
| 1 | A | 2019 | C |
| 1 | A | 2020 | G |
| 1 | A | 2021 | U |
| 1 | A | 2028 | U |
| 1 | A | 2034 | U |
| 1 | A | 2042 | A |
| 1 | A | 2048 | A |
| 1 | A | 2049 | G |
| 1 | A | 2054 | A |
| 1 | A | 2058 | A |
| 1 | A | 2061 | U |
| 1 | A | 2072 | G |
| 1 | A | 2075 | C |
| 1 | A | 2084 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 2085 | G |
| 1 | A | 2086 | A |
| 1 | A | 2087 | U |
| 1 | A | 2088 | C |
| 1 | A | 2089 | A |
| 1 | A | 2090 | U |
| 2 | 7 | 8 | U |
| 2 | 7 | 13 | C |
| 2 | 7 | 16 | U |
| 2 | 7 | 17 | U |
| 2 | 7 | 18 | G |
| 2 | 7 | 19 | G |
| 2 | 7 | 20 | U |
| 2 | 7 | 21 | U |
| 2 | 7 | 32 | U |
| 2 | 7 | 33 | C |
| 2 | 7 | 34 | U |
| 2 | 7 | 41 | C |
| 2 | 7 | 43 | C |
| 2 | 7 | 46 | G |
| 2 | 7 | 50 | G |
| 2 | 7 | 53 | A |
| 2 | 7 | 55 | U |
| 2 | 7 | 56 | U |
| 2 | 7 | 69 | U |
| 2 | 7 | 70 | A |
| 2 | 7 | 72 | C |
| 2 | 7 | 73 | C |
| 2 | 7 | 74 | A |
| 34 | AA | 11 | A |
| 34 | AA | 12 | U |
| 34 | AA | 13 | G |
| 34 | AA | 14 | U |
| 34 | AA | 16 | A |
| 34 | AA | 18 | G |
| 34 | AA | 25 | A |
| 34 | AA | 26 | A |
| 34 | AA | 30 | G |
| 34 | AA | 32 | C |
| 34 | AA | 40 | A |
| 34 | AA | 43 | A |
| 34 | AA | 44 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 34 | AA | 45 | A |
| 34 | AA | 49 | U |
| 34 | AA | 55 | G |
| 34 | AA | 57 | A |
| 34 | AA | 59 | G |
| 34 | AA | 60 | A |
| 34 | AA | 62 | A |
| 34 | AA | 63 | A |
| 34 | AA | 66 | A |
| 34 | AA | 73 | U |
| 34 | AA | 75 | U |
| 34 | AA | 83 | U |
| 34 | AA | 85 | A |
| 34 | AA | 87 | U |
| 34 | AA | 92 | G |
| 34 | AA | 105 | G |
| 34 | AA | 109 | A |
| 34 | AA | 110 | G |
| 34 | AA | 111 | C |
| 34 | AA | 113 | C |
| 34 | AA | 121 | U |
| 34 | AA | 122 | A |
| 34 | AA | 124 | U |
| 34 | AA | 125 | C |
| 34 | AA | 130 | G |
| 34 | AA | 133 | U |
| 34 | AA | 134 | G |
| 34 | AA | 135 | G |
| 34 | AA | 136 | U |
| 34 | AA | 137 | G |
| 34 | AA | 144 | U |
| 34 | AA | 145 | U |
| 34 | AA | 147 | C |
| 34 | AA | 148 | G |
| 34 | AA | 149 | A |
| 34 | AA | 152 | G |
| 34 | AA | 157 | G |
| 34 | AA | 163 | G |
| 34 | AA | 165 | A |
| 34 | AA | 167 | U |
| 34 | AA | 168 | A |
| 34 | AA | 172 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 34 | AA | 173 | A |
| 34 | AA | 174 | U |
| 34 | AA | 175 | G |
| 34 | AA | 180 | C |
| 34 | AA | 182 | U |
| 34 | AA | 183 | U |
| 34 | AA | 185 | A |
| 34 | AA | 186 | A |
| 34 | AA | 189 | U |
| 34 | AA | 190 | G |
| 34 | AA | 191 | A |
| 34 | AA | 192 | G |
| 34 | AA | 195 | A |
| 34 | AA | 197 | G |
| 34 | AA | 198 | U |
| 34 | AA | 199 | G |
| 34 | AA | 200 | A |
| 34 | AA | 201 | G |
| 34 | AA | 207 | A |
| 34 | AA | 208 | U |
| 34 | AA | 211 | U |
| 34 | AA | 215 | C |
| 34 | AA | 216 | C |
| 34 | AA | 219 | A |
| 34 | AA | 220 | G |
| 34 | AA | 221 | A |
| 34 | AA | 226 | G |
| 34 | AA | 227 | A |
| 34 | AA | 228 | A |
| 34 | AA | 229 | A |
| 34 | AA | 231 | G |
| 34 | AA | 235 | A |
| 34 | AA | 239 | U |
| 34 | AA | 242 | U |
| 34 | AA | 246 | U |
| 34 | AA | 247 | A |
| 34 | AA | 250 | U |
| 34 | AA | 258 | U |
| 34 | AA | 263 | U |
| 34 | AA | 265 | U |
| 34 | AA | 268 | C |
| 34 | AA | 269 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 34 | AA | 271 | G |
| 34 | AA | 276 | G |
| 34 | AA | 290 | G |
| 34 | AA | 292 | U |
| 34 | AA | 293 | U |
| 34 | AA | 302 | A |
| 34 | AA | 303 | A |
| 34 | AA | 304 | U |
| 34 | AA | 305 | A |
| 34 | AA | 307 | G |
| 34 | AA | 308 | U |
| 34 | AA | 309 | G |
| 34 | AA | 310 | U |
| 34 | AA | 313 | U |
| 34 | AA | 315 | C |
| 34 | AA | 317 | U |
| 34 | AA | 319 | U |
| 34 | AA | 324 | U |
| 34 | AA | 325 | A |
| 34 | AA | 333 | A |
| 34 | AA | 336 | U |
| 34 | AA | 337 | A |
| 34 | AA | 338 | U |
| 34 | AA | 342 | G |
| 34 | AA | 344 | A |
| 34 | AA | 345 | G |
| 34 | AA | 347 | C |
| 34 | AA | 351 | U |
| 34 | AA | 354 | C |
| 34 | AA | 359 | A |
| 34 | AA | 360 | A |
| 34 | AA | 362 | U |
| 34 | AA | 378 | U |
| 34 | AA | 382 | A |
| 34 | AA | 384 | A |
| 34 | AA | 385 | G |
| 34 | AA | 386 | U |
| 34 | AA | 392 | G |
| 34 | AA | 396 | U |
| 34 | AA | 400 | C |
| 34 | AA | 401 | A |
| 34 | AA | 402 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 34 | AA | 405 | A |
| 34 | AA | 408 | U |
| 34 | AA | 409 | A |
| 34 | AA | 411 | U |
| 34 | AA | 412 | A |
| 34 | AA | 413 | C |
| 34 | AA | 431 | G |
| 34 | AA | 432 | A |
| 34 | AA | 433 | A |
| 34 | AA | 439 | U |
| 34 | AA | 442 | G |
| 34 | AA | 444 | G |
| 34 | AA | 447 | A |
| 34 | AA | 448 | A |
| 34 | AA | 449 | A |
| 34 | AA | 450 | A |
| 34 | AA | 451 | C |
| 34 | AA | 458 | A |
| 34 | AA | 459 | G |
| 34 | AA | 462 | G |
| 34 | AA | 463 | G |
| 34 | AA | 467 | U |
| 34 | AA | 489 | U |
| 34 | AA | 494 | U |
| 34 | AA | 495 | U |
| 34 | AA | 497 | U |
| 34 | AA | 498 | U |
| 34 | AA | 499 | U |
| 34 | AA | 500 | A |
| 34 | AA | 501 | U |
| 34 | AA | 502 | U |
| 34 | AA | 503 | A |
| 34 | AA | 504 | A |
| 34 | AA | 505 | A |
| 34 | AA | 506 | A |
| 34 | AA | 509 | A |
| 34 | AA | 510 | A |
| 34 | AA | 514 | C |
| 34 | AA | 521 | U |
| 34 | AA | 522 | A |
| 34 | AA | 523 | A |
| 34 | AA | 527 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 34 | AA | 530 | U |
| 34 | AA | 532 | C |
| 34 | AA | 534 | A |
| 34 | AA | 536 | A |
| 34 | AA | 538 | A |
| 34 | AA | 539 | G |
| 34 | AA | 542 | A |
| 34 | AA | 543 | U |
| 34 | AA | 545 | C |
| 34 | AA | 547 | C |
| 34 | AA | 549 | G |
| 34 | AA | 573 | U |
| 34 | AA | 579 | C |
| 34 | AA | 580 | A |
| 34 | AA | 581 | C |
| 34 | AA | 582 | U |
| 34 | AA | 583 | U |
| 34 | AA | 585 | C |
| 34 | AA | 586 | U |
| 34 | AA | 592 | C |
| 34 | AA | 594 | C |
| 34 | AA | 595 | U |
| 34 | AA | 598 | U |
| 34 | AA | 599 | G |
| 34 | AA | 601 | G |
| 34 | AA | 604 | G |
| 34 | AA | 605 | A |
| 34 | AA | 608 | A |
| 34 | AA | 610 | U |
| 34 | AA | 615 | U |
| 34 | AA | 617 | A |
| 34 | AA | 618 | U |
| 34 | AA | 620 | U |
| 34 | AA | 621 | C |
| 34 | AA | 622 | U |
| 34 | AA | 623 | U |
| 34 | AA | 628 | U |
| 34 | AA | 631 | U |
| 34 | AA | 636 | U |
| 34 | AA | 637 | U |
| 34 | AA | 641 | G |
| 34 | AA | 642 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 34 | AA | 645 | A |
| 34 | AA | 646 | A |
| 34 | AA | 648 | U |
| 34 | AA | 649 | U |
| 34 | AA | 650 | U |
| 34 | AA | 651 | A |
| 34 | AA | 653 | A |
| 34 | AA | 659 | U |
| 34 | AA | 662 | A |
| 34 | AA | 666 | U |
| 34 | AA | 671 | U |
| 34 | AA | 672 | C |
| 34 | AA | 674 | U |
| 34 | AA | 675 | A |
| 34 | AA | 677 | A |
| 34 | AA | 678 | A |
| 34 | AA | 679 | U |
| 34 | AA | 681 | U |
| 34 | AA | 682 | A |
| 34 | AA | 683 | A |
| 34 | AA | 684 | G |
| 34 | AA | 685 | U |
| 34 | AA | 694 | U |
| 34 | AA | 697 | A |
| 34 | AA | 698 | G |
| 34 | AA | 699 | U |
| 34 | AA | 704 | U |
| 34 | AA | 707 | U |
| 34 | AA | 708 | A |
| 34 | AA | 714 | C |
| 34 | AA | 715 | U |
| 34 | AA | 716 | C |
| 34 | AA | 722 | G |
| 34 | AA | 727 | A |
| 34 | AA | 729 | G |
| 34 | AA | 738 | A |
| 34 | AA | 755 | A |
| 34 | AA | 760 | A |
| 34 | AA | 761 | U |
| 34 | AA | 763 | U |
| 34 | AA | 765 | A |
| 34 | AA | 767 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 34 | AA | 769 | U |
| 34 | AA | 771 | U |
| 34 | AA | 773 | A |
| 34 | AA | 774 | A |
| 34 | AA | 778 | U |
| 34 | AA | 779 | U |
| 34 | AA | 793 | A |
| 34 | AA | 794 | C |
| 34 | AA | 806 | G |
| 34 | AA | 809 | A |
| 34 | AA | 810 | U |
| 34 | AA | 811 | A |
| 34 | AA | 812 | U |
| 34 | AA | 813 | G |
| 34 | AA | 822 | A |
| 34 | AA | 825 | G |
| 34 | AA | 833 | G |
| 34 | AA | 834 | U |
| 34 | AA | 835 | G |
| 34 | AA | 859 | C |
| 34 | AA | 860 | A |
| 34 | AA | 862 | U |
| 34 | AA | 873 | U |
| 34 | AA | 874 | A |
| 34 | AA | 880 | A |
| 34 | AA | 885 | A |
| 34 | AA | 889 | U |
| 34 | AA | 890 | G |
| 34 | AA | 893 | U |
| 34 | AA | 896 | U |
| 34 | AA | 899 | A |
| 34 | AA | 900 | G |
| 34 | AA | 903 | C |
| 34 | AA | 905 | A |
| 34 | AA | 918 | G |
| 34 | AA | 920 | A |
| 34 | AA | 925 | A |
| 34 | AA | 927 | A |
| 34 | AA | 934 | G |
| 34 | AA | 936 | A |
| 34 | AA | 937 | C |
| 34 | AA | 945 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 34 | AA | 946 | A |
| 34 | AA | 951 | A |
| 34 | AA | 955 | A |
| 34 | AA | 956 | A |
| 34 | AA | 965 | A |
| 34 | AA | 966 | A |
| 34 | AA | 968 | G |
| 34 | AA | 970 | C |
| 34 | AA | 976 | G |
| 34 | AA | 980 | A |
| 34 | AA | 984 | A |
| 34 | AA | 988 | G |
| 34 | AA | 989 | A |
| 34 | AA | 993 | U |
| 34 | AA | 998 | U |
| 34 | AA | 999 | G |
| 34 | AA | 1013 | U |
| 34 | AA | 1014 | C |
| 34 | AA | 1015 | A |
| 34 | AA | 1016 | A |
| 34 | AA | 1024 | U |
| 34 | AA | 1026 | G |
| 34 | AA | 1027 | G |
| 34 | AA | 1033 | A |
| 34 | AA | 1034 | A |
| 34 | AA | 1035 | G |
| 34 | AA | 1036 | A |
| 34 | AA | 1040 | A |
| 34 | AA | 1042 | C |
| 34 | AA | 1043 | G |
| 34 | AA | 1053 | U |
| 34 | AA | 1056 | G |
| 34 | AA | 1062 | U |
| 34 | AA | 1063 | A |
| 34 | AA | 1070 | A |
| 34 | AA | 1072 | A |
| 34 | AA | 1073 | G |
| 34 | AA | 1078 | C |
| 34 | AA | 1079 | U |
| 34 | AA | 1081 | A |
| 34 | AA | 1086 | C |
| 34 | AA | 1087 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 34 | AA | 1092 | A |
| 34 | AA | 1099 | U |
| 34 | AA | 1100 | A |
| 34 | AA | 1101 | A |
| 34 | AA | 1102 | U |
| 34 | AA | 1106 | A |
| 34 | AA | 1109 | U |
| 34 | AA | 1111 | A |
| 34 | AA | 1113 | C |
| 34 | AA | 1114 | A |
| 34 | AA | 1115 | G |
| 34 | AA | 1116 | G |
| 34 | AA | 1121 | G |
| 34 | AA | 1122 | A |
| 34 | AA | 1123 | U |
| 34 | AA | 1124 | A |
| 34 | AA | 1132 | G |
| 34 | AA | 1136 | A |
| 34 | AA | 1158 | G |
| 34 | AA | 1164 | U |
| 34 | AA | 1168 | C |
| 34 | AA | 1169 | A |
| 34 | AA | 1170 | A |
| 34 | AA | 1172 | C |
| 34 | AA | 1174 | C |
| 34 | AA | 1186 | A |
| 34 | AA | 1187 | A |
| 34 | AA | 1188 | A |
| 34 | AA | 1193 | G |
| 34 | AA | 1194 | A |
| 34 | AA | 1196 | A |
| 34 | AA | 1197 | U |
| 34 | AA | 1198 | A |
| 34 | AA | 1199 | A |
| 34 | AA | 1200 | C |
| 34 | AA | 1202 | C |
| 34 | AA | 1205 | U |
| 34 | AA | 1206 | U |
| 34 | AA | 1207 | U |
| 34 | AA | 1210 | A |
| 34 | AA | 1215 | A |
| 34 | AA | 1217 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 34 | AA | 1218 | C |
| 34 | AA | 1219 | A |
| 34 | AA | 1221 | A |
| 34 | AA | 1222 | U |
| 34 | AA | 1223 | U |
| 34 | AA | 1224 | A |
| 34 | AA | 1225 | A |
| 34 | AA | 1226 | A |
| 34 | AA | 1229 | A |
| 34 | AA | 1230 | A |
| 34 | AA | 1231 | A |
| 34 | AA | 1232 | U |
| 34 | AA | 1233 | A |
| 34 | AA | 1234 | A |
| 34 | AA | 1239 | A |
| 34 | AA | 1240 | A |
| 34 | AA | 1245 | G |
| 34 | AA | 1257 | A |
| 34 | AA | 1259 | G |
| 34 | AA | 1263 | A |
| 34 | AA | 1272 | U |
| 34 | AA | 1273 | G |
| 34 | AA | 1279 | U |
| 34 | AA | 1281 | C |
| 34 | AA | 1283 | C |
| 34 | AA | 1287 | A |
| 34 | AA | 1288 | C |
| 34 | AA | 1291 | U |
| 34 | AA | 1295 | A |
| 34 | AA | 1299 | G |
| 34 | AA | 1300 | G |
| 34 | AA | 1306 | A |
| 34 | AA | 1309 | U |
| 34 | AA | 1310 | A |
| 34 | AA | 1313 | C |
| 34 | AA | 1314 | G |
| 34 | AA | 1320 | G |
| 34 | AA | 1321 | A |
| 34 | AA | 1324 | U |
| 34 | AA | 1325 | C |
| 34 | AA | 1329 | U |
| 34 | AA | 1334 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 34 | AA | 1337 | G |
| 34 | AA | 1340 | G |
| 34 | AA | 1341 | G |
| 34 | AA | 1344 | C |
| 34 | AA | 1345 | A |
| 34 | AA | 1346 | U |
| 34 | AA | 1416 | U |
| 34 | AA | 1418 | A |
| 34 | AA | 1420 | C |
| 34 | AA | 1423 | G |
| 34 | AA | 1431 | A |
| 34 | AA | 1432 | A |
| 34 | AA | 1433 | U |
| 34 | AA | 1435 | G |
| 34 | AA | 1436 | A |
| 34 | AA | 1437 | U |
| 34 | AA | 1441 | G |
| 34 | AA | 1444 | A |
| 34 | AA | 1445 | A |
| 34 | AA | 1450 | G |
| 34 | AA | 1451 | A |
| 34 | AA | 1453 | U |
| 34 | AA | 1458 | A |
| 34 | AA | 1460 | A |
| 34 | AA | 1473 | A |
| 34 | AA | 1476 | A |
| 34 | AA | 1480 | G |
| 34 | AA | 1481 | A |
| 34 | AA | 1486 | A |
| 34 | AA | 1498 | U |
| 34 | AA | 1499 | U |
| 34 | AA | 1503 | A |
| 34 | AA | 1504 | A |
| 34 | AA | 1506 | C |
| 34 | AA | 1524 | U |
| 34 | AA | 1535 | G |
| 34 | AA | 1537 | G |
| 34 | AA | 1539 | U |
| 34 | AA | 1540 | G |
| 34 | AA | 1549 | U |
| 34 | AA | 1550 | A |
| 34 | AA | 1556 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 34 | AA | 1565 | G |
| 34 | AA | 1567 | A |
| 34 | AA | 1572 | U |
| 34 | AA | 1575 | C |
| 34 | AA | 1578 | G |
| 34 | AA | 1583 | G |
| 34 | AA | 1586 | C |
| 34 | AA | 1592 | G |
| 34 | AA | 1595 | A |
| 34 | AA | 1599 | G |
| 34 | AA | 1601 | A |
| 34 | AA | 1602 | A |
| 34 | AA | 1605 | A |
| 34 | AA | 1619 | U |
| 34 | AA | 1626 | A |
| 34 | AA | 1630 | A |
| 34 | AA | 1631 | A |
| 34 | AA | 1635 | G |
| 34 | AA | 1636 | A |
| 34 | AA | 1637 | G |
| 34 | AA | 1642 | G |
| 34 | AA | 1643 | U |
| 34 | AA | 1649 | G |
| 34 | AA | 1651 | C |
| 34 | AA | 1657 | U |
| 34 | AA | 1659 | A |
| 34 | AA | 1661 | U |
| 34 | AA | 1668 | G |
| 34 | AA | 1676 | C |
| 34 | AA | 1677 | G |
| 34 | AA | 1685 | G |
| 34 | AA | 1688 | A |
| 34 | AA | 1691 | G |
| 34 | AA | 1693 | U |
| 34 | AA | 1703 | U |
| 34 | AA | 1704 | U |
| 34 | AA | 1705 | A |
| 34 | AA | 1706 | A |
| 34 | AA | 1707 | A |
| 34 | AA | 1721 | C |
| 34 | AA | 1725 | U |
| 34 | AA | 1730 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 34 | AA | 1732 | A |
| 34 | AA | 1733 | G |
| 34 | AA | 1736 | A |
| 34 | AA | 1737 | A |
| 34 | AA | 1739 | C |
| 34 | AA | 1748 | A |
| 34 | AA | 1750 | U |
| 34 | AA | 1751 | C |
| 34 | AA | 1756 | G |
| 34 | AA | 1762 | A |
| 34 | AA | 1763 | G |
| 34 | AA | 1766 | U |
| 34 | AA | 1767 | U |
| 34 | AA | 1768 | A |
| 34 | AA | 1769 | U |
| 34 | AA | 1770 | G |
| 34 | AA | 1771 | A |
| 34 | AA | 1774 | U |
| 34 | AA | 1780 | G |
| 34 | AA | 1781 | A |
| 34 | AA | 1782 | U |
| 34 | AA | 1783 | G |
| 34 | AA | 1788 | C |
| 34 | AA | 1794 | U |
| 34 | AA | 1797 | A |
| 34 | AA | 1798 | A |
| 34 | AA | 1799 | A |
| 34 | AA | 1800 | U |
| 34 | AA | 1801 | G |
| 34 | AA | 1805 | U |
| 34 | AA | 1806 | C |
| 34 | AA | 1812 | C |
| 34 | AA | 1817 | G |
| 34 | AA | 1832 | U |
| 34 | AA | 1842 | U |
| 34 | AA | 1850 | U |
| 34 | AA | 1852 | C |
| 34 | AA | 1855 | U |
| 34 | AA | 1856 | U |
| 34 | AA | 1857 | A |
| 34 | AA | 1871 | A |
| 34 | AA | 1872 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 34 | AA | 1874 | C |
| 34 | AA | 1881 | C |
| 34 | AA | 1882 | U |
| 34 | AA | 1886 | A |
| 34 | AA | 1887 | G |
| 34 | AA | 1888 | A |
| 34 | AA | 1898 | U |
| 34 | AA | 1899 | U |
| 34 | AA | 1900 | G |
| 34 | AA | 1902 | A |
| 34 | AA | 1903 | C |
| 34 | AA | 1904 | U |
| 34 | AA | 1905 | C |
| 34 | AA | 1914 | A |
| 34 | AA | 1915 | A |
| 34 | AA | 1963 | U |
| 34 | AA | 1964 | G |
| 34 | AA | 1965 | U |
| 34 | AA | 1966 | A |
| 34 | AA | 1969 | A |
| 34 | AA | 1970 | A |
| 34 | AA | 1971 | U |
| 34 | AA | 1976 | A |
| 34 | AA | 1978 | U |
| 34 | AA | 1981 | U |
| 34 | AA | 1990 | A |
| 34 | AA | 1991 | U |
| 34 | AA | 1996 | C |
| 34 | AA | 1997 | G |
| 34 | AA | 1998 | A |
| 34 | AA | 1999 | A |
| 34 | AA | 2000 | G |
| 34 | AA | 2003 | G |
| 34 | AA | 2010 | C |
| 34 | AA | 2018 | G |
| 34 | AA | 2019 | A |
| 34 | AA | 2030 | G |
| 34 | AA | 2034 | G |
| 34 | AA | 2072 | U |
| 34 | AA | 2082 | C |
| 34 | AA | 2084 | U |
| 34 | AA | 2090 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 34 | AA | 2092 | G |
| 34 | AA | 2093 | U |
| 34 | AA | 2096 | G |
| 34 | AA | 2097 | A |
| 34 | AA | 2102 | A |
| 34 | AA | 2106 | A |
| 34 | AA | 2107 | C |
| 34 | AA | 2108 | A |
| 34 | AA | 2109 | A |
| 34 | AA | 2113 | C |
| 34 | AA | 2114 | A |
| 34 | AA | 2115 | U |
| 34 | AA | 2125 | A |
| 34 | AA | 2136 | C |
| 34 | AA | 2145 | A |
| 34 | AA | 2146 | A |
| 34 | AA | 2147 | A |
| 34 | AA | 2148 | U |
| 34 | AA | 2149 | A |
| 34 | AA | 2154 | A |
| 34 | AA | 2160 | G |
| 34 | AA | 2161 | G |
| 34 | AA | 2174 | G |
| 34 | AA | 2181 | A |
| 34 | AA | 2186 | C |
| 34 | AA | 2203 | G |
| 34 | AA | 2218 | C |
| 34 | AA | 2219 | A |
| 34 | AA | 2220 | U |
| 34 | AA | 2389 | G |
| 34 | AA | 2394 | C |
| 34 | AA | 2395 | U |
| 34 | AA | 2400 | A |
| 34 | AA | 2403 | G |
| 34 | AA | 2404 | A |
| 34 | AA | 2405 | A |
| 34 | AA | 2410 | A |
| 34 | AA | 2415 | G |
| 34 | AA | 2419 | A |
| 34 | AA | 2424 | A |
| 34 | AA | 2427 | G |
| 34 | AA | 2433 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 34 | AA | 2437 | A |
| 34 | AA | 2438 | A |
| 34 | AA | 2451 | A |
| 34 | AA | 2453 | A |
| 34 | AA | 2463 | U |
| 34 | AA | 2464 | G |
| 34 | AA | 2465 | G |
| 34 | AA | 2477 | U |
| 34 | AA | 2486 | U |
| 34 | AA | 2489 | C |
| 34 | AA | 2500 | A |
| 34 | AA | 2501 | A |
| 34 | AA | 2510 | U |
| 34 | AA | 2516 | A |
| 34 | AA | 2518 | U |
| 34 | AA | 2521 | A |
| 34 | AA | 2524 | C |
| 34 | AA | 2536 | A |
| 34 | AA | 2537 | A |
| 34 | AA | 2539 | G |
| 34 | AA | 2542 | G |
| 34 | AA | 2544 | G |
| 34 | AA | 2545 | A |
| 34 | AA | 2548 | A |
| 34 | AA | 2549 | A |
| 34 | AA | 2550 | C |
| 34 | AA | 2552 | A |
| 34 | AA | 2555 | A |
| 34 | AA | 2556 | C |
| 34 | AA | 2565 | G |
| 34 | AA | 2566 | G |
| 34 | AA | 2573 | A |
| 34 | AA | 2574 | A |
| 34 | AA | 2575 | U |
| 34 | AA | 2581 | G |
| 34 | AA | 2584 | A |
| 34 | AA | 2589 | A |
| 34 | AA | 2591 | U |
| 34 | AA | 2596 | A |
| 34 | AA | 2600 | G |
| 34 | AA | 2602 | A |
| 34 | AA | 2603 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 34 | AA | 2606 | A |
| 34 | AA | 2608 | G |
| 34 | AA | 2618 | G |
| 34 | AA | 2627 | U |
| 34 | AA | 2628 | G |
| 34 | AA | 2629 | U |
| 34 | AA | 2640 | U |
| 34 | AA | 2666 | A |
| 34 | AA | 2667 | C |
| 34 | AA | 2668 | G |
| 34 | AA | 2671 | C |
| 34 | AA | 2676 | C |
| 34 | AA | 2681 | U |
| 34 | AA | 2684 | G |
| 34 | AA | 2686 | G |
| 34 | AA | 2690 | A |
| 34 | AA | 2695 | A |
| 34 | AA | 2696 | G |
| 34 | AA | 2697 | A |
| 34 | AA | 2698 | C |
| 34 | AA | 2703 | U |
| 34 | AA | 2704 | U |
| 34 | AA | 2705 | G |
| 34 | AA | 2710 | U |
| 34 | AA | 2711 | U |
| 34 | AA | 2712 | A |
| 34 | AA | 2727 | U |
| 34 | AA | 2728 | G |
| 34 | AA | 2730 | G |
| 34 | AA | 2745 | G |
| 34 | AA | 2803 | A |
| 34 | AA | 2809 | A |
| 34 | AA | 2810 | A |
| 34 | AA | 2811 | A |
| 34 | AA | 2817 | U |
| 34 | AA | 2822 | U |
| 34 | AA | 2823 | U |
| 34 | AA | 2824 | A |
| 34 | AA | 2833 | U |
| 34 | AA | 2835 | G |
| 34 | AA | 2837 | G |
| 34 | AA | 2884 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 34 | AA | 2886 | A |
| 34 | AA | 2887 | U |
| 34 | AA | 2888 | U |
| 34 | AA | 2920 | A |
| 34 | AA | 2928 | G |
| 34 | AA | 2932 | A |
| 34 | AA | 2933 | C |
| 34 | AA | 2945 | G |
| 34 | AA | 2946 | G |
| 34 | AA | 2953 | G |
| 34 | AA | 2959 | G |
| 34 | AA | 2960 | G |
| 34 | AA | 2967 | A |
| 34 | AA | 2968 | U |
| 34 | AA | 2975 | A |
| 34 | AA | 2980 | U |
| 34 | AA | 2981 | A |
| 34 | AA | 2987 | G |
| 34 | AA | 2990 | G |
| 34 | AA | 2991 | U |
| 34 | AA | 2995 | A |
| 34 | AA | 2996 | A |
| 34 | AA | 3005 | C |
| 34 | AA | 3013 | A |
| 34 | AA | 3015 | A |
| 34 | AA | 3016 | G |
| 34 | AA | 3017 | A |
| 34 | AA | 3018 | A |
| 34 | AA | 3019 | A |
| 34 | AA | 3020 | U |
| 34 | AA | 3028 | A |
| 34 | AA | 3029 | G |
| 34 | AA | 3030 | A |
| 34 | AA | 3033 | A |
| 34 | AA | 3034 | A |
| 34 | AA | 3035 | A |
| 34 | AA | 3044 | A |
| 34 | AA | 3053 | G |
| 34 | AA | 3059 | U |
| 34 | AA | 3068 | A |
| 34 | AA | 3076 | G |
| 34 | AA | 3079 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 34 | AA | 3081 | C |
| 34 | AA | 3086 | A |
| 34 | AA | 3088 | G |
| 34 | AA | 3091 | U |
| 34 | AA | 3092 | G |
| 34 | AA | 3094 | C |
| 34 | AA | 3100 | G |
| 34 | AA | 3108 | A |
| 34 | AA | 3111 | U |
| 34 | AA | 3112 | U |
| 34 | AA | 3113 | U |
| 34 | AA | 3116 | A |
| 34 | AA | 3118 | A |
| 34 | AA | 3123 | C |
| 34 | AA | 3124 | G |
| 34 | AA | 3126 | A |
| 34 | AA | 3127 | A |
| 34 | AA | 3130 | U |
| 34 | AA | 3131 | A |
| 34 | AA | 3135 | A |
| 34 | AA | 3138 | A |
| 34 | AA | 3139 | C |
| 34 | AA | 3140 | U |
| 34 | AA | 3141 | G |
| 34 | AA | 3146 | U |
| 34 | AA | 3155 | G |
| 34 | AA | 3158 | U |
| 34 | AA | 3159 | G |
| 34 | AA | 3160 | A |
| 34 | AA | 3161 | A |
| 34 | AA | 3167 | A |
| 34 | AA | 3168 | C |
| 34 | AA | 3169 | C |
| 34 | AA | 3173 | G |
| 34 | AA | 3175 | G |
| 34 | AA | 3176 | A |
| 34 | AA | 3180 | C |
| 34 | AA | 3187 | G |
| 34 | AA | 3193 | G |
| 34 | AA | 3201 | C |
| 34 | AA | 3204 | C |
| 34 | AA | 3208 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 34 | AA | 3209 | G |
| 34 | AA | 3212 | G |
| 34 | AA | 3220 | U |
| 34 | AA | 3222 | G |
| 34 | AA | 3225 | C |
| 34 | AA | 3230 | G |
| 34 | AA | 3231 | A |
| 34 | AA | 3232 | U |
| 34 | AA | 3235 | C |
| 34 | AA | 3245 | U |
| 34 | AA | 3246 | A |
| 34 | AA | 3248 | C |
| 34 | AA | 3253 | G |
| 34 | AA | 3257 | G |
| 34 | AA | 3258 | C |
| 34 | AA | 3269 | A |
| 34 | AA | 3277 | G |
| 34 | AA | 3282 | U |
| 34 | AA | 3287 | C |
| 34 | AA | 3292 | A |
| 34 | AA | 3294 | U |
| 34 | AA | 3295 | A |
| 34 | AA | 3297 | G |
| 34 | AA | 3301 | C |
| 34 | AA | 3302 | G |
| 34 | AA | 3304 | G |
| 34 | AA | 3305 | A |
| 34 | AA | 3306 | G |
| 34 | AA | 3330 | A |
| 34 | AA | 3336 | G |
| 34 | AA | 3337 | U |
| 34 | AA | 3342 | C |
| 34 | AA | 3343 | C |
| 34 | AA | 3349 | G |
| 34 | AA | 3351 | U |
| 34 | AA | 3353 | A |
| 34 | AA | 3356 | U |
| 34 | AA | 3357 | U |
| 34 | AA | 3358 | U |
| 34 | AA | 3359 | A |
| 34 | AA | 3361 | U |
| 34 | AA | 3362 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 34 | AA | 3374 | U |
| 34 | AA | 3375 | A |
| 34 | AA | 3378 | C |
| 34 | AA | 3379 | A |
| 34 | AA | 3380 | U |
| 34 | AA | 3381 | A |
| 34 | AA | 3382 | U |
| 34 | AA | 3383 | A |
| 34 | AA | 3389 | G |
| 34 | AA | 3391 | G |
| 34 | AA | 3398 | A |
| 34 | AA | 3414 | G |
| 34 | AA | 3415 | A |
| 34 | AA | 3416 | G |
| 34 | AA | 3418 | A |
| 34 | AA | 3421 | A |
| 34 | AA | 3432 | A |
| 34 | AA | 3434 | A |
| 34 | AA | 3435 | A |
| 34 | AA | 3442 | C |
| 34 | AA | 3443 | A |
| 34 | AA | 3444 | G |
| 34 | AA | 3445 | C |
| 34 | AA | 3459 | A |
| 34 | AA | 3463 | G |
| 34 | AA | 3464 | U |
| 34 | AA | 3468 | G |
| 34 | AA | 3471 | A |
| 34 | AA | 3472 | A |
| 34 | AA | 3476 | A |
| 34 | AA | 3477 | A |
| 34 | AA | 3483 | U |
| 34 | AA | 3488 | U |
| 34 | AA | 3493 | G |
| 34 | AA | 3500 | G |
| 34 | AA | 3507 | A |
| 34 | AA | 3510 | C |
| 34 | AA | 3513 | G |
| 34 | AA | 3515 | A |
| 34 | AA | 3516 | A |
| 34 | AA | 3526 | U |
| 34 | AA | 3527 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 34 | AA | 3528 | A |
| 34 | AA | 3530 | A |
| 34 | AA | 3568 | G |
| 34 | AA | 3571 | A |
| 34 | AA | 3573 | U |
| 34 | AA | 3575 | U |
| 34 | AA | 3576 | A |
| 34 | AA | 3578 | A |
| 34 | AA | 3580 | G |
| 34 | AA | 3581 | A |
| 34 | AA | 3582 | G |
| 34 | AA | 3585 | A |
| 34 | AA | 3586 | U |
| 34 | AA | 3588 | A |
| 34 | AA | 3589 | U |
| 34 | AA | 3590 | A |
| 34 | AA | 3591 | U |
| 34 | AA | 3594 | G |
| 34 | AA | 3597 | C |
| 34 | AA | 3612 | U |
| 34 | AA | 3615 | A |
| 34 | AA | 3616 | U |
| 34 | AA | 3617 | A |
| 34 | AA | 3618 | A |
| 34 | AA | 3623 | A |
| 34 | AA | 3624 | U |
| 34 | AA | 3626 | A |
| 34 | AA | 3627 | C |
| 34 | AA | 3632 | U |
| 34 | AA | 3635 | G |
| 34 | AA | 3658 | G |
| 34 | AA | 3659 | C |
| 34 | AA | 3663 | A |
| 34 | AA | 3664 | G |
| 34 | AA | 3665 | U |
| 34 | AA | 3667 | C |
| 34 | AA | 3668 | U |
| 34 | AA | 3670 | U |
| 34 | AA | 3671 | A |
| 34 | AA | 3676 | C |
| 34 | AA | 3677 | A |
| 34 | AA | 3680 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 34 | AA | 3683 | G |
| 34 | AA | 3684 | A |
| 34 | AA | 3689 | C |
| 34 | AA | 3697 | G |
| 34 | AA | 3698 | U |
| 34 | AA | 3707 | U |
| 34 | AA | 3711 | U |
| 34 | AA | 3712 | G |
| 34 | AA | 3716 | C |
| 34 | AA | 3727 | A |
| 34 | AA | 3728 | A |
| 34 | AA | 3732 | U |
| 34 | AA | 3733 | G |
| 34 | AA | 3736 | A |
| 34 | AA | 3737 | G |
| 34 | AA | 3739 | A |
| 34 | AA | 3740 | A |
| 34 | AA | 3741 | A |
| 34 | AA | 3752 | C |
| 34 | AA | 3761 | G |
| 34 | AA | 3767 | U |
| 34 | AA | 3768 | A |
| 34 | AA | 3770 | C |
| 34 | AA | 3774 | A |
| 34 | AA | 3775 | G |
| 34 | AA | 3778 | G |
| 34 | AA | 3779 | U |
| 34 | AA | 3782 | A |
| 34 | AA | 3783 | G |
| 35 | AC | 5 | A |
| 35 | AC | 25 | C |
| 35 | AC | 36 | C |
| 35 | AC | 37 | A |
| 35 | AC | 38 | G |
| 35 | AC | 39 | C |
| 35 | AC | 43 | G |
| 35 | AC | 44 | A |
| 35 | AC | 50 | G |
| 35 | AC | 53 | G |
| 35 | AC | 55 | A |
| 35 | AC | 56 | A |
| 35 | AC | 63 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 35 | AC | 64 | U |
| 35 | AC | 66 | C |
| 35 | AC | 67 | G |
| 35 | AC | 73 | A |
| 35 | AC | 75 | A |
| 35 | AC | 78 | U |
| 35 | AC | 79 | G |
| 35 | AC | 80 | C |
| 35 | AC | 82 | G |
| 35 | AC | 85 | A |
| 35 | AC | 90 | G |
| 35 | AC | 91 | A |
| 35 | AC | 92 | A |
| 35 | AC | 94 | C |
| 35 | AC | 98 | A |
| 35 | AC | 99 | G |
| 35 | AC | 107 | A |
| 35 | AC | 108 | A |
| 35 | AC | 109 | U |
| 35 | AC | 111 | U |
| 35 | AC | 112 | A |
| 35 | AC | 114 | A |
| 35 | AC | 115 | C |
| 35 | AC | 116 | U |
| 35 | AC | 117 | A |
| 35 | AC | 119 | A |
| 35 | AC | 122 | A |
| 35 | AC | 123 | A |
| 35 | AC | 135 | G |
| 35 | AC | 136 | A |
| 35 | AC | 137 | A |
| 35 | AC | 138 | U |
| 35 | AC | 139 | A |
| 35 | AC | 140 | G |
| 35 | AC | 142 | G |
| 35 | AC | 145 | A |
| 35 | AC | 146 | C |
| 35 | AC | 156 | A |
| 36 | AB | 3 | A |
| 36 | AB | 7 | G |
| 36 | AB | 13 | A |
| 36 | AB | 16 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 36 | AB | 18 | A |
| 36 | AB | 22 | G |
| 36 | AB | 25 | A |
| 36 | AB | 26 | C |
| 36 | AB | 27 | A |
| 36 | AB | 33 | U |
| 36 | AB | 38 | U |
| 36 | AB | 39 | C |
| 36 | AB | 40 | A |
| 36 | AB | 48 | G |
| 36 | AB | 51 | G |
| 36 | AB | 53 | U |
| 36 | AB | 54 | A |
| 36 | AB | 63 | A |
| 36 | AB | 64 | A |
| 36 | AB | 69 | U |
| 36 | AB | 71 | G |
| 36 | AB | 74 | A |
| 36 | AB | 76 | U |
| 36 | AB | 89 | G |
| 36 | AB | 93 | G |
| 36 | AB | 97 | G |
| 36 | AB | 100 | A |
| 36 | AB | 110 | G |

All (289) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 25 | C |
| 1 | A | 39 | A |
| 1 | A | 45 | U |
| 1 | A | 105 | A |
| 1 | A | 116 | A |
| 1 | A | 138 | U |
| 1 | A | 139 | A |
| 1 | A | 156 | A |
| 1 | A | 157 | G |
| 1 | A | 161 | U |
| 1 | A | 206 | A |
| 1 | A | 246 | A |
| 1 | A | 248 | G |
| 1 | A | 250 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 251 | U |
| 1 | A | 273 | A |
| 1 | A | 291 | A |
| 1 | A | 383 | G |
| 1 | A | 386 | U |
| 1 | A | 423 | A |
| 1 | A | 474 | A |
| 1 | A | 525 | G |
| 1 | A | 544 | G |
| 1 | A | 586 | A |
| 1 | A | 589 | U |
| 1 | A | 614 | A |
| 1 | A | 752 | U |
| 1 | A | 753 | U |
| 1 | A | 789 | U |
| 1 | A | 790 | U |
| 1 | A | 793 | G |
| 1 | A | 805 | A |
| 1 | A | 815 | G |
| 1 | A | 844 | G |
| 1 | A | 876 | U |
| 1 | A | 919 | U |
| 1 | A | 930 | A |
| 1 | A | 973 | G |
| 1 | A | 975 | A |
| 1 | A | 981 | U |
| 1 | A | 983 | G |
| 1 | A | 1028 | U |
| 1 | A | 1071 | G |
| 1 | A | 1073 | U |
| 1 | A | 1099 | A |
| 1 | A | 1100 | U |
| 1 | A | 1182 | A |
| 1 | A | 1209 | G |
| 1 | A | 1259 | C |
| 1 | A | 1283 | U |
| 1 | A | 1284 | A |
| 1 | A | 1295 | A |
| 1 | A | 1381 | C |
| 1 | A | 1386 | U |
| 1 | A | 1400 | U |
| 1 | A | 1413 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 1414 | A |
| 1 | A | 1421 | A |
| 1 | A | 1423 | A |
| 1 | A | 1430 | G |
| 1 | A | 1431 | A |
| 1 | A | 1448 | U |
| 1 | A | 1455 | C |
| 1 | A | 1623 | U |
| 1 | A | 1624 | U |
| 1 | A | 1645 | C |
| 1 | A | 1660 | U |
| 1 | A | 1673 | A |
| 1 | A | 1692 | A |
| 1 | A | 1703 | U |
| 1 | A | 1705 | C |
| 1 | A | 1786 | U |
| 1 | A | 1817 | U |
| 1 | A | 1818 | A |
| 1 | A | 1819 | U |
| 1 | A | 1834 | A |
| 1 | A | 1865 | G |
| 1 | A | 1870 | A |
| 1 | A | 1897 | A |
| 1 | A | 1898 | G |
| 1 | A | 1912 | C |
| 1 | A | 1976 | G |
| 1 | A | 1977 | G |
| 1 | A | 2048 | A |
| 1 | A | 2053 | U |
| 1 | A | 2071 | U |
| 2 | 7 | 32 | U |
| 2 | 7 | 33 | C |
| 2 | 7 | 56 | U |
| 34 | AA | 10 | G |
| 34 | AA | 11 | A |
| 34 | AA | 13 | G |
| 34 | AA | 21 | G |
| 34 | AA | 25 | A |
| 34 | AA | 40 | A |
| 34 | AA | 43 | A |
| 34 | AA | 61 | A |
| 34 | AA | 62 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 34 | AA | 65 | A |
| 34 | AA | 124 | U |
| 34 | AA | 149 | A |
| 34 | AA | 162 | U |
| 34 | AA | 179 | G |
| 34 | AA | 181 | C |
| 34 | AA | 206 | A |
| 34 | AA | 215 | C |
| 34 | AA | 257 | U |
| 34 | AA | 270 | U |
| 34 | AA | 289 | A |
| 34 | AA | 337 | A |
| 34 | AA | 344 | A |
| 34 | AA | 353 | G |
| 34 | AA | 358 | C |
| 34 | AA | 385 | G |
| 34 | AA | 411 | U |
| 34 | AA | 416 | G |
| 34 | AA | 432 | A |
| 34 | AA | 500 | A |
| 34 | AA | 501 | U |
| 34 | AA | 504 | A |
| 34 | AA | 505 | A |
| 34 | AA | 579 | C |
| 34 | AA | 580 | A |
| 34 | AA | 581 | C |
| 34 | AA | 583 | U |
| 34 | AA | 593 | A |
| 34 | AA | 594 | C |
| 34 | AA | 597 | A |
| 34 | AA | 607 | A |
| 34 | AA | 608 | A |
| 34 | AA | 620 | U |
| 34 | AA | 621 | C |
| 34 | AA | 641 | G |
| 34 | AA | 645 | A |
| 34 | AA | 652 | A |
| 34 | AA | 666 | U |
| 34 | AA | 667 | U |
| 34 | AA | 673 | U |
| 34 | AA | 674 | U |
| 34 | AA | 681 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 34 | AA | 683 | A |
| 34 | AA | 697 | A |
| 34 | AA | 698 | G |
| 34 | AA | 702 | U |
| 34 | AA | 703 | U |
| 34 | AA | 715 | U |
| 34 | AA | 721 | U |
| 34 | AA | 754 | A |
| 34 | AA | 764 | G |
| 34 | AA | 809 | A |
| 34 | AA | 821 | C |
| 34 | AA | 859 | C |
| 34 | AA | 888 | A |
| 34 | AA | 889 | U |
| 34 | AA | 935 | A |
| 34 | AA | 965 | A |
| 34 | AA | 998 | U |
| 34 | AA | 1013 | U |
| 34 | AA | 1032 | A |
| 34 | AA | 1035 | G |
| 34 | AA | 1042 | C |
| 34 | AA | 1078 | C |
| 34 | AA | 1080 | C |
| 34 | AA | 1101 | A |
| 34 | AA | 1115 | G |
| 34 | AA | 1197 | U |
| 34 | AA | 1204 | A |
| 34 | AA | 1205 | U |
| 34 | AA | 1206 | U |
| 34 | AA | 1217 | U |
| 34 | AA | 1222 | U |
| 34 | AA | 1224 | A |
| 34 | AA | 1230 | A |
| 34 | AA | 1234 | A |
| 34 | AA | 1272 | U |
| 34 | AA | 1336 | U |
| 34 | AA | 1422 | A |
| 34 | AA | 1431 | A |
| 34 | AA | 1435 | G |
| 34 | AA | 1457 | G |
| 34 | AA | 1459 | U |
| 34 | AA | 1503 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 34 | AA | 1504 | A |
| 34 | AA | 1538 | U |
| 34 | AA | 1566 | A |
| 34 | AA | 1574 | C |
| 34 | AA | 1632 | G |
| 34 | AA | 1642 | G |
| 34 | AA | 1643 | U |
| 34 | AA | 1658 | G |
| 34 | AA | 1705 | A |
| 34 | AA | 1736 | A |
| 34 | AA | 1748 | A |
| 34 | AA | 1750 | U |
| 34 | AA | 1779 | A |
| 34 | AA | 1794 | U |
| 34 | AA | 1805 | U |
| 34 | AA | 1841 | U |
| 34 | AA | 1873 | U |
| 34 | AA | 1881 | C |
| 34 | AA | 1898 | U |
| 34 | AA | 1913 | A |
| 34 | AA | 1964 | G |
| 34 | AA | 1980 | G |
| 34 | AA | 1989 | A |
| 34 | AA | 1990 | A |
| 34 | AA | 1996 | C |
| 34 | AA | 1999 | A |
| 34 | AA | 2015 | C |
| 34 | AA | 2033 | C |
| 34 | AA | 2096 | G |
| 34 | AA | 2109 | A |
| 34 | AA | 2146 | A |
| 34 | AA | 2153 | A |
| 34 | AA | 2180 | U |
| 34 | AA | 2193 | U |
| 34 | AA | 2219 | A |
| 34 | AA | 2394 | C |
| 34 | AA | 2437 | A |
| 34 | AA | 2523 | U |
| 34 | AA | 2590 | U |
| 34 | AA | 2618 | G |
| 34 | AA | 2665 | A |
| 34 | AA | 2696 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 34 | AA | 2697 | A |
| 34 | AA | 2727 | U |
| 34 | AA | 2816 | U |
| 34 | AA | 2822 | U |
| 34 | AA | 2832 | A |
| 34 | AA | 2883 | U |
| 34 | AA | 2885 | A |
| 34 | AA | 2886 | A |
| 34 | AA | 2919 | A |
| 34 | AA | 2932 | A |
| 34 | AA | 2958 | G |
| 34 | AA | 2959 | G |
| 34 | AA | 3016 | G |
| 34 | AA | 3018 | A |
| 34 | AA | 3034 | A |
| 34 | AA | 3067 | G |
| 34 | AA | 3111 | U |
| 34 | AA | 3130 | U |
| 34 | AA | 3137 | U |
| 34 | AA | 3139 | C |
| 34 | AA | 3140 | U |
| 34 | AA | 3160 | A |
| 34 | AA | 3167 | A |
| 34 | AA | 3229 | C |
| 34 | AA | 3230 | G |
| 34 | AA | 3232 | U |
| 34 | AA | 3245 | U |
| 34 | AA | 3309 | G |
| 34 | AA | 3361 | U |
| 34 | AA | 3379 | A |
| 34 | AA | 3381 | A |
| 34 | AA | 3382 | U |
| 34 | AA | 3391 | G |
| 34 | AA | 3414 | G |
| 34 | AA | 3434 | A |
| 34 | AA | 3476 | A |
| 34 | AA | 3505 | U |
| 34 | AA | 3526 | U |
| 34 | AA | 3575 | U |
| 34 | AA | 3577 | A |
| 34 | AA | 3585 | A |
| 34 | AA | 3588 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 34 | AA | 3590 | A |
| 34 | AA | 3627 | C |
| 34 | AA | 3658 | G |
| 34 | AA | 3662 | U |
| 34 | AA | 3664 | G |
| 34 | AA | 3667 | C |
| 34 | AA | 3698 | U |
| 34 | AA | 3711 | U |
| 34 | AA | 3727 | A |
| 34 | AA | 3736 | A |
| 34 | AA | 3767 | U |
| 34 | AA | 3769 | U |
| 34 | AA | 3782 | A |
| 35 | AC | 35 | A |
| 35 | AC | 37 | A |
| 35 | AC | 75 | A |
| 35 | AC | 134 | G |
| 35 | AC | 139 | A |
| 35 | AC | 145 | A |
| 36 | AB | 13 | A |
| 36 | AB | 39 | C |
| 36 | AB | 84 | U |
| 36 | AB | 88 | A |

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

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

## 5.5 Carbohydrates

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

There are no ligands in this entry.

## 5.7 Other polymers

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 |
|---|---|---|
| 63 | AW | 1 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|---|---|---|---|---|---|---|
| 1 | AW | 154:ASN | C | 197:UNK | N | 30.56 |

# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-6454. 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

This section was not generated.

## 6.2 Central slices

This section was not generated.

## 6.3 Largest variance slices

This section was not generated.

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

This section was not generated.

## 6.5 Orthogonal surface views

This section was not generated.

## 6.6 Mask visualisation

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

# 7 Map analysis

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

## 7.1 Map-value distribution

This section was not generated.

## 7.2 Volume estimate versus contour level

This section was not generated.

## 7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

# 8 Fourier-Shell correlation

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

# 9 Map-model fit

This section was not generated.