# Full wwPDB EM Validation Report (i)

Jul 3, 2024 – 06:47 am BST

| | | |
|---|---|---|
| PDB ID | : | 7NPN |
| EMDB ID | : | EMD-12516 |
| Title | : | B-brick bare in 5 mM Mg2+ |
| Authors | : | Bertosin, E.; Stoemmer, P.; Feigl, E.; Wenig, M.; Honemann, M.; Dietz, H. |
| Deposited on | : | 2021-02-27 |
| Resolution | : | 10.38 Å(reported) |

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

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

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

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

| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev92 |
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | 1.9.13 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.37.1 |

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 10.38 Å.

There are no overall percentile quality scores available for this entry.

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

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | AA | 2873 | 59% 34% 7% |
| 2 | AB | 34 | 68% 29% • |
| 3 | AC | 48 | 65% 29% 6% |
| 4 | AD | 34 | 62% 35% • |
| 5 | AE | 41 | 63% 32% 5% |
| 6 | AF | 41 | 68% 29% • |
| 7 | AG | 34 | 56% 35% 9% |
| 8 | AH | 42 | 50% 43% 7% |
| 9 | AI | 28 | 54% 46% |
| 10 | AJ | 34 | 12% 47% 41% 12% |
| 11 | AK | 42 | 57% 36% 7% |
| 12 | AL | 42 | 57% 33% 10% |
| 13 | AM | 42 | 57% 40% • |
| 14 | AN | 42 | 64% 33% • |
| 15 | AO | 49 | 61% 37% • |
| 16 | AP | 49 | 73% 22% • |
| 17 | AQ | 28 | • 50% 50% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 18 | AR | 28 | 54% 43% • |
| 19 | AS | 42 | • 57% 38% 5% |
| 20 | AT | 52 | 65% 33% • |
| 21 | AU | 49 | 65% 22% 12% |
| 22 | AV | 52 | 56% 42% • |
| 23 | AW | 42 | 64% 33% • |
| 24 | AX | 38 | 55% 45% |
| 25 | AY | 31 | 71% 19% 10% |
| 26 | AZ | 49 | 63% 29% 8% |
| 27 | Aa | 41 | 71% 27% • |
| 28 | Ab | 42 | 52% 43% 5% |
| 29 | Ac | 42 | 64% 29% 7% |
| 30 | Ad | 34 | • 68% 29% • |
| 31 | Ae | 41 | • 66% 29% 5% |
| 32 | Af | 42 | 64% 31% 5% |
| 33 | Ag | 28 | 61% 36% • |
| 34 | Ah | 34 | 50% 41% 9% |
| 35 | Ai | 49 | 63% 35% • |
| 36 | Aj | 42 | 81% 14% 5% |
| 37 | Ak | 59 | • 69% 25% 5% |
| 38 | Al | 42 | 64% 29% 7% |
| 39 | Am | 42 | 64% 24% 12% |
| 40 | An | 42 | 62% 33% 5% |
| 41 | Ao | 28 | 43% 50% 7% |
| 42 | Ap | 28 | 46% 54% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 43 | Aq | 41 | 5% 66% 29% 5% |
| 44 | Ar | 52 | 69% 25% 6% |
| 45 | As | 49 | 59% 39% • |
| 46 | At | 52 | 67% 31% • |
| 47 | Au | 52 | • 73% 23% • |
| 48 | Av | 42 | 64% 31% 5% |
| 49 | Aw | 42 | 69% 24% 7% |
| 50 | Ax | 42 | 45% 45% 10% |
| 51 | Ay | 41 | 56% 37% 7% |
| 52 | Az | 35 | 57% 37% 6% |
| 53 | A0 | 41 | 76% 22% • |
| 54 | A1 | 45 | 7% 62% 31% 7% |
| 55 | A2 | 34 | • 53% 44% • |
| 56 | A3 | 41 | 56% 32% 12% |
| 57 | A4 | 42 | 74% 24% • |
| 58 | A5 | 31 | 61% 35% • |
| 59 | A6 | 28 | 68% 25% 7% |
| 60 | A7 | 34 | • 62% 38% |
| 61 | A8 | 34 | 68% 32% |
| 62 | A9 | 42 | 64% 33% • |
| 63 | BA | 35 | 63% 26% 11% |
| 64 | BB | 45 | 58% 38% • |
| 65 | BC | 35 | 57% 34% 9% |
| 66 | BD | 28 | • 71% 25% • |
| 67 | BE | 28 | 64% 36% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 68 | BF | 41 | 5% 51% 44% 5% |
| 69 | BG | 35 | 54% 40% 6% |
| 70 | BH | 42 | 76% 21% • |
| 71 | BI | 42 | 69% 26% 5% |
| 72 | BJ | 45 | 62% 36% • |
| 73 | BK | 31 | 77% 23% |
| 74 | BL | 42 | 67% 31% • |
| 75 | BM | 49 | 59% 29% 12% |
| 76 | BN | 41 | 59% 29% 12% |
| 77 | BO | 42 | 71% 24% 5% |
| 78 | BP | 34 | • 59% 38% • |
| 79 | BQ | 37 | 62% 35% • |

# 2 Entry composition (i)

There are 79 unique types of molecules in this entry. The entry contains 122511 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 DNA chain called SCAFFOLD STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 1 | AA | 2873 | 58849 | 28004 | 10702 | 17271 | 2872 | 0 | 0 |

- Molecule 2 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 2 | AB | 34 | 691 | 331 | 125 | 202 | 33 | 0 | 0 |

- Molecule 3 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 3 | AC | 48 | 967 | 464 | 160 | 296 | 47 | 0 | 0 |

- Molecule 4 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 4 | AD | 34 | 702 | 337 | 134 | 198 | 33 | 0 | 0 |

- Molecule 5 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 5 | AE | 41 | 838 | 400 | 155 | 243 | 40 | 0 | 0 |

- Molecule 6 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 6 | AF | 41 | 831 | 398 | 145 | 248 | 40 | 0 | 0 |

- Molecule 7 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 7 | AG | 34 | 688 | 331 | 119 | 205 | 33 | 0 | 0 |

- Molecule 8 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 8 | AH | 42 | 857 | 409 | 149 | 258 | 41 | 0 | 0 |

- Molecule 9 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 9 | AI | 28 | 575 | 275 | 109 | 164 | 27 | 0 | 0 |

- Molecule 10 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 10 | AJ | 34 | 674 | 329 | 94 | 218 | 33 | 0 | 0 |

- Molecule 11 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 11 | AK | 42 | 859 | 413 | 151 | 254 | 41 | 0 | 0 |

- Molecule 12 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 12 | AL | 42 | 865 | 411 | 162 | 251 | 41 | 0 | 0 |

- Molecule 13 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 13 | AM | 42 | 864 | 412 | 161 | 250 | 41 | 0 | 0 |

- Molecule 14 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 14 | AN | 42 | 877 | 410 | 184 | 242 | 41 | 0 | 0 |

- Molecule 15 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 15 | AO | 49 | 1007 | 478 | 194 | 287 | 48 | 0 | 0 |

- Molecule 16 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 16 | AP | 49 | 999 | 479 | 178 | 294 | 48 | 0 | 0 |

- Molecule 17 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 17 | AQ | 28 | 561 | 271 | 86 | 177 | 27 | 0 | 0 |

- Molecule 18 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 18 | AR | 28 | 564 | 273 | 90 | 174 | 27 | 0 | 0 |

- Molecule 19 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 19 | AS | 42 | 857 | 412 | 143 | 261 | 41 | 0 | 0 |

- Molecule 20 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 20 | AT | 52 | 1049 | 503 | 181 | 314 | 51 | 0 | 0 |

- Molecule 21 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 21 | AU | 49 | 1011 | 479 | 187 | 297 | 48 | 0 | 0 |

- Molecule 22 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 22 | AV | 52 | 1064 | 507 | 195 | 311 | 51 | 0 | 0 |

- Molecule 23 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 23 | AW | 42 | 860 | 408 | 165 | 246 | 41 | 0 | 0 |

- Molecule 24 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 24 | AX | 38 | 762 | 369 | 117 | 239 | 37 | 0 | 0 |

- Molecule 25 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 25 | AY | 31 | 628 | 304 | 107 | 187 | 30 | 0 | 0 |

- Molecule 26 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 26 | AZ | 49 | 1000 | 478 | 185 | 289 | 48 | 0 | 0 |

- Molecule 27 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 27 | Aa | 41 | 832 | 398 | 163 | 231 | 40 | 0 | 0 |

- Molecule 28 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 28 | Ab | 42 | 856 | 407 | 163 | 245 | 41 | 0 | 0 |

- Molecule 29 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 29 | Ac | 42 | 860 | 410 | 154 | 255 | 41 | 0 | 0 |

- Molecule 30 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 30 | Ad | 34 | 697 | 337 | 116 | 211 | 33 | 0 | 0 |

- Molecule 31 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 31 | Ae | 41 | 826 | 401 | 130 | 255 | 40 | 0 | 0 |

- Molecule 32 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 32 | Af | 42 | 865 | 415 | 155 | 254 | 41 | 0 | 0 |

- Molecule 33 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 33 | Ag | 28 | 569 | 275 | 94 | 173 | 27 | 0 | 0 |

- Molecule 34 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 34 | Ah | 34 | 688 | 336 | 105 | 214 | 33 | 0 | 0 |

- Molecule 35 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 35 | Ai | 49 | 1007 | 481 | 194 | 284 | 48 | 0 | 0 |

- Molecule 36 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 36 | Aj | 42 | 851 | 407 | 154 | 249 | 41 | 0 | 0 |

- Molecule 37 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 37 | Ak | 59 | 1199 | 574 | 203 | 364 | 58 | 0 | 0 |

- Molecule 38 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 38 | Al | 42 | 861 | 409 | 170 | 241 | 41 | 0 | 0 |

- Molecule 39 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 39 | Am | 42 | 862 | 410 | 163 | 248 | 41 | 0 | 0 |

- Molecule 40 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 40 | An | 42 | 862 | 411 | 159 | 251 | 41 | 0 | 0 |

- Molecule 41 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 41 | Ao | 28 | 573 | 274 | 104 | 168 | 27 | 0 | 0 |

- Molecule 42 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 42 | Ap | 28 | 569 | 276 | 90 | 176 | 27 | 0 | 0 |

- Molecule 43 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 43 | Aq | 41 | 832 | 400 | 140 | 252 | 40 | 0 | 0 |

- Molecule 44 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 44 | Ar | 52 | 1052 | 510 | 165 | 326 | 51 | 0 | 0 |

- Molecule 45 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 45 | As | 49 | 985 | 470 | 169 | 298 | 48 | 0 | 0 |

- Molecule 46 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 46 | At | 52 | 1067 | 507 | 192 | 317 | 51 | 0 | 0 |

- Molecule 47 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 47 | Au | 52 | 1063 | 507 | 198 | 307 | 51 | 0 | 0 |

- Molecule 48 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 48 | Av | 42 | 849 | 404 | 160 | 244 | 41 | 0 | 0 |

- Molecule 49 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 49 | Aw | 42 | 872 | 409 | 179 | 243 | 41 | 0 | 0 |

- Molecule 50 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 50 | Ax | 42 | 859 | 407 | 163 | 248 | 41 | 0 | 0 |

- Molecule 51 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 51 | Ay | 41 | 841 | 402 | 150 | 249 | 40 | 0 | 0 |

- Molecule 52 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 52 | Az | 35 | 717 | 339 | 141 | 203 | 34 | 0 | 0 |

- Molecule 53 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 53 | A0 | 41 | 840 | 401 | 151 | 248 | 40 | 0 | 0 |

- Molecule 54 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 54 | A1 | 45 | 923 | 439 | 167 | 273 | 44 | 0 | 0 |

- Molecule 55 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 55 | A2 | 34 | 697 | 338 | 115 | 211 | 33 | 0 | 0 |

- Molecule 56 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 56 | A3 | 41 | 835 | 404 | 136 | 255 | 40 | 0 | 0 |

- Molecule 57 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 57 | A4 | 42 | 852 | 409 | 158 | 244 | 41 | 0 | 0 |

- Molecule 58 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 58 | A5 | 31 | 627 | 302 | 115 | 180 | 30 | 0 | 0 |

- Molecule 59 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 59 | A6 | 28 | 573 | 277 | 95 | 174 | 27 | 0 | 0 |

- Molecule 60 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 60 | A7 | 34 | 682 | 331 | 104 | 214 | 33 | 0 | 0 |

- Molecule 61 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 61 | A8 | 34 | 697 | 335 | 127 | 202 | 33 | 0 | 0 |

- Molecule 62 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 62 | A9 | 42 | 867 | 413 | 166 | 247 | 41 | 0 | 0 |

- Molecule 63 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 63 | BA | 35 | 708 | 337 | 137 | 200 | 34 | 0 | 0 |

- Molecule 64 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 64 | BB | 45 | 909 | 441 | 153 | 271 | 44 | 0 | 0 |

- Molecule 65 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 65 | BC | 35 | 725 | 346 | 137 | 208 | 34 | 0 | 0 |

- Molecule 66 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 66 | BD | 28 | 570 | 277 | 92 | 174 | 27 | 0 | 0 |

- Molecule 67 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 67 | BE | 28 | 573 | 280 | 86 | 180 | 27 | 0 | 0 |

- Molecule 68 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 68 | BF | 41 | 827 | 401 | 124 | 262 | 40 | 0 | 0 |

- Molecule 69 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 69 | BG | 35 | 712 | 344 | 124 | 210 | 34 | 0 | 0 |

- Molecule 70 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 70 | BH | 42 | 863 | 413 | 160 | 249 | 41 | 0 | 0 |

- Molecule 71 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 71 | BI | 42 | 873 | 415 | 182 | 235 | 41 | 0 | 0 |

- Molecule 72 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 72 | BJ | 45 | 924 | 445 | 161 | 274 | 44 | 0 | 0 |

- Molecule 73 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 73 | BK | 31 | 633 | 305 | 112 | 186 | 30 | 0 | 0 |

- Molecule 74 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 74 | BL | 42 | 852 | 405 | 153 | 253 | 41 | 0 | 0 |

- Molecule 75 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 75 | BM | 49 | 1002 | 477 | 195 | 282 | 48 | 0 | 0 |

- Molecule 76 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 76 | BN | 41 | 840 | 401 | 151 | 248 | 40 | 0 | 0 |

- Molecule 77 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 77 | BO | 42 | 852 | 412 | 143 | 256 | 41 | 0 | 0 |

- Molecule 78 is a DNA chain called STAPLE STRAND.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 78 | BP | 34 | 687 | 335 | 103 | 216 | 33 | 0 | 0 |

- Molecule 79 is a DNA chain called STAPLE STRAND.

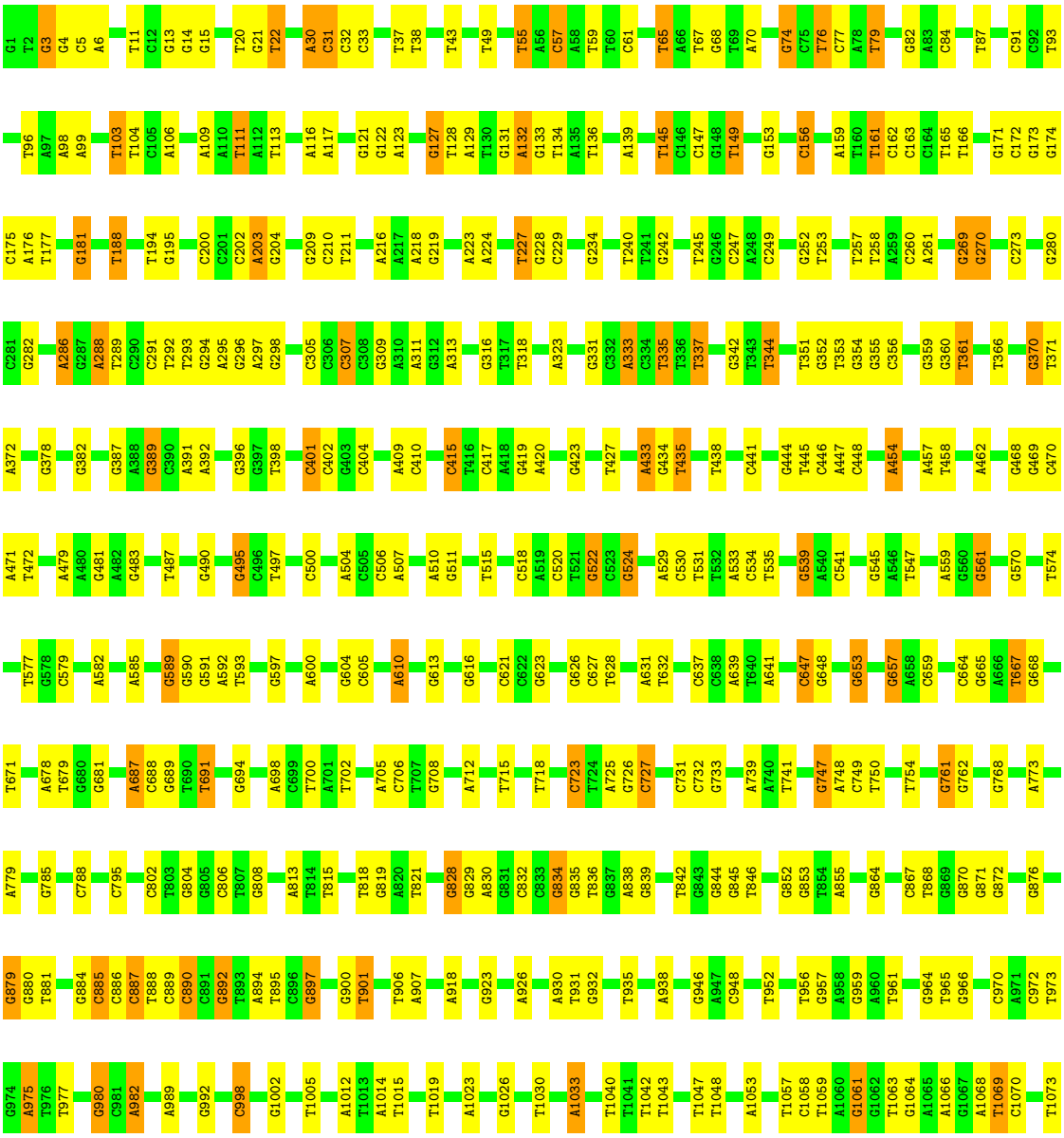
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 79 | BQ | 37 | 755 | 362 | 133 | 224 | 36 | 0 | 0 |

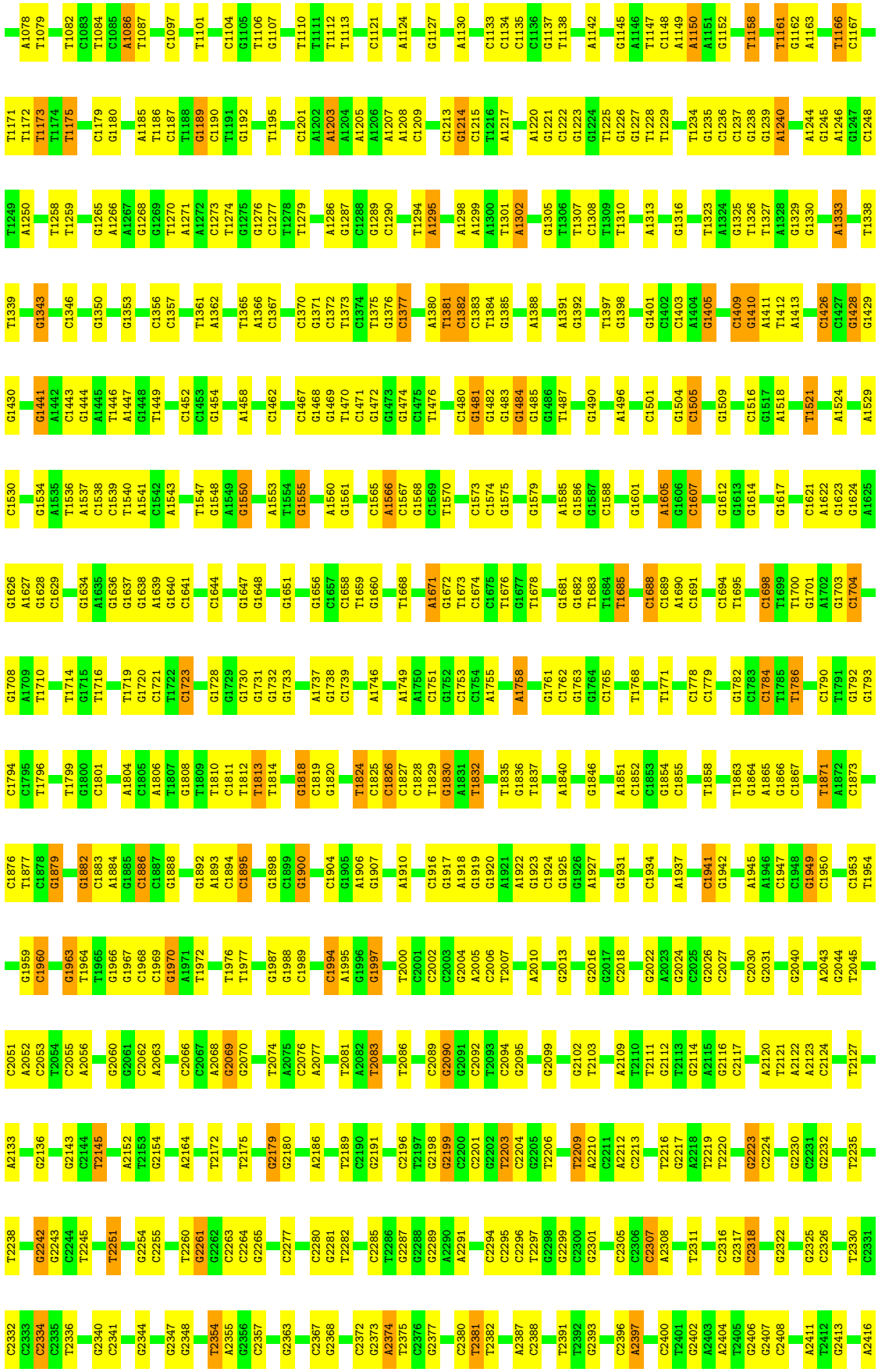
# 3 Residue-property plots (i)

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

- Molecule 1: SCAFFOLD STRAND

Chain AA: 59% 34% 7%




A1078 T1079
T1082 C1083 T1084 C1085 A1086 T1087
C1097
T1101
C1104 G1105 T1106 G1107
T1110 T1111 T1112 T1113
C1121
A1124
G1127
A1130
C1133 C1134 C1135 C1136 G1137 T1138
A1142
G1145 A1146 T1147 C1148 A1149 A1150 A1151 G1152
T1158
T1161 G1162 A1163
T1166 C1167
T1171 T1172 T1173 T1174 T1175
C1179 G1180
A1185 T1186 C1187 T1188 G1189 C1190
T1191 G1192
T1195
C1201 A1202 A1203 A1204 A1205 A1206 A1207 A1208 C1209
C1213 G1214 C1215
T1216 A1217
A1220 G1221 C1222 G1223 G1224 T1225 G1226 G1227 T1228 T1229
T1234 G1235 C1236 C1237 G1238 G1239 A1240
A1244 G1245 A1246 G1247 C1248
T1249 A1250
T1258 T1259
G1265 A1266 A1267 G1268 G1269 T1270 A1271 A1272 C1273 T1274 G1275 G1276 C1277 T1278 T1279
A1286 A1287 C1288 G1289 C1290
T1294 A1295
A1298 A1299 A1300 T1301 A1302
G1305 T1306 T1307 C1308 T1309 T1310
A1313
G1316
T1323 A1324 G1325 T1326 T1327 A1328 G1329 G1330
A1333
T1338
T1339 G1343
C1346
G1350
G1353
C1356 C1357
T1361 A1362
T1365 A1366 C1367
C1370 G1371 C1372 T1373 C1374 T1375 G1376 C1377
A1380 T1381 C1382 C1383 T1384 G1385
A1388
A1391 G1392
T1397 G1398
G1401 C1402 C1403 A1404 G1405
C1409 G1410 A1411 T1412 A1413
C1426 C1427 G1428 G1429
G1430 G1441 A1442 C1443 G1444 A1445 T1446 A1447 G1448 T1449
C1452 C1453 G1454
A1458
C1462
C1467 G1468 G1469 T1470 C1471 G1472 G1473 G1474 C1475 T1476
C1480 G1481 G1482 G1483 G1484 G1485 G1486 T1487
G1490
A1496
C1501
G1504 C1505
G1509
C1516 G1517 A1518
T1521
A1524
A1529
C1530 G1534 A1535 T1536 A1537 C1538 C1539 T1540 A1541 C1542 A1543
T1547 G1548 A1549 G1550
A1553 T1554 G1555
A1560 G1561
C1565 A1566 C1567 G1568 C1569 T1570
C1573 C1574 G1575
G1579
A1585 G1586 G1587 C1588
G1601
A1605 G1606 C1607
G1612 G1613 G1614
G1617
C1621 A1622 G1623 G1624 A1625
G1626 A1627 G1628 C1629
G1634 A1635 G1636 G1637 G1638 A1639 G1640 C1641
C1644
G1647 G1648
G1651
G1656 C1657 C1658 T1659 G1660
T1668
A1671 G1672 T1673 C1674 C1675 T1676 G1677 T1678
G1681 G1682 T1683 T1684 T1685
C1688 C1689 A1690 C1691
C1694 T1695
C1698 T1699 T1700 G1701 A1702 G1703 C1704
G1708 A1709 T1710
T1714 G1715 T1716
T1719 G1720 C1721 T1722 C1723
G1728 G1729 G1730 G1731 G1732 G1733
A1737 G1738 C1739
A1746
A1749 A1750 C1751 G1752 C1753 C1754 A1755
A1758
G1761 C1762 G1763 G1764 C1765
T1768
T1771
C1778 C1779
G1782 C1783 C1784 T1785 T1786
C1790 T1791 G1792 G1793
C1794 C1795 T1796
T1799 G1800 C1801
A1804 C1805 A1806 T1807 G1808 T1809 T1810 C1811 T1812 T1813 T1814
G1818 C1819 G1820
T1824 C1825 C1826
C1827 C1828 T1829 G1830 A1831 T1832
T1835 G1836 T1837
A1840
G1846
A1851 C1852 C1853 G1854 C1855
T1858
T1863 G1864 A1865 G1866 C1867
T1871 A1872 C1873
C1876 T1877 C1878 G1879
G1882 C1883 A1884 C1885 C1886 C1887 G1888
G1892 A1893 C1894 C1895
G1898 C1899 G1900
C1904 C1905 A1906 G1907
A1910
C1916 G1917 A1918 G1919 G1920 A1921 A1922 G1923 C1924 G1925 G1926 A1927
G1931
C1934
A1937
C1941 G1942
A1945 A1946 C1947 C1948 G1949 C1950
C1953 T1954
G1959 C1960
G1963 T1964 T1965 G1966 G1967 G1968 C1969 G1970 A1971 T1972
T1976 T1977
G1987 G1988 C1989
C1994 A1995 G1996 G1997
T2000 C2001 C2002 C2003 G2004 A2005 C2006 T2007
A2010
G2013
G2016 G2017 C2018
G2022 A2023 G2024 C2025 G2026 C2027
C2030 G2031
G2040
A2043 G2044 T2045
C2051 A2052 C2053 T2054 C2055 A2056
G2060 G2061 C2062 A2063
C2066 C2067 A2068 G2069 G2070
T2074 A2075 C2076 A2077
T2081 A2082 T2083
T2086
C2089 G2090 G2091 C2092 T2093 C2094 G2095
G2099
G2102 T2103
A2109 T2110 T2111 G2112 T2113 G2114 A2115 G2116 C2117
A2120 T2121 A2122 A2123 C2124
T2127
A2133 G2136
G2143 C2144 T2145
A2152 T2153 G2154
A2164
T2172
T2175
G2179 G2180
A2186
T2189 C2190 G2191
C2196 T2197 G2198 G2199 C2200 C2201 G2202 T2203 C2204 G2205 T2206
T2209 A2210 C2211 A2212 C2213
T2216 G2217 A2218 T2219 T2220
G2223 C2224
G2230 C2231 G2232
T2235
T2238 G2242 G2243 C2244 T2245
T2251
G2254 C2255
T2260 G2261 G2262 C2263 C2264 G2265
C2277
C2280 G2281 T2282
C2285 T2286 G2287 G2288 G2289 A2290 A2291
C2294 C2295 C2296 T2297 G2298 G2299 C2300 G2301
C2305 C2306 C2307 A2308
T2311
C2316 G2317 C2318
G2322
G2325 C2326
T2330 G2331
C2332 C2333 C2334 C2335 T2336
G2340 C2341
G2344
G2347 G2348
T2354 A2355 G2356 C2357
G2363
C2367 G2368
C2372 G2373 A2374 T2375 C2376 G2377
C2380 T2381 T2382
A2387 C2388
T2391 T2392 G2393
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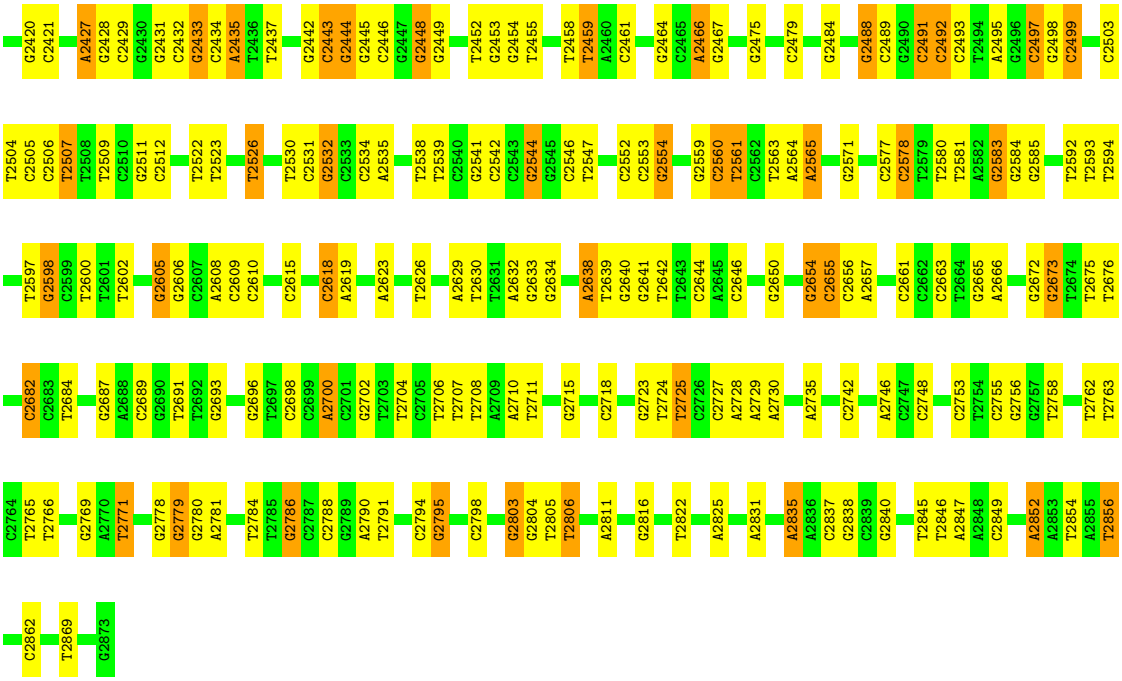
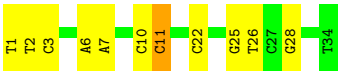
C2400 T2401 G2402 A2403 A2404 T2405 G2406 G2407 C2408
A2411 T2412 G2413
A2416



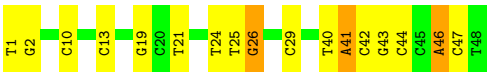

- Molecule 2: STAPLE STRAND

Chain AB:




- Molecule 3: STAPLE STRAND

Chain AC:

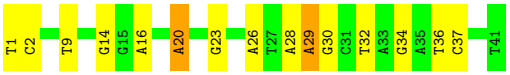



- Molecule 4: STAPLE STRAND

Chain AD:

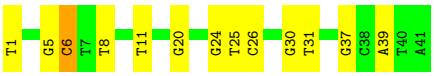
- Molecule 5: STAPLE STRAND

Chain AE:



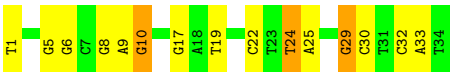

- Molecule 6: STAPLE STRAND

Chain AF: 68% 29% •



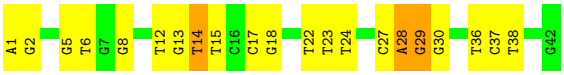

• Molecule 7: STAPLE STRAND

Chain AG: 56% 35% 9%




• Molecule 8: STAPLE STRAND

Chain AH: 50% 43% 7%

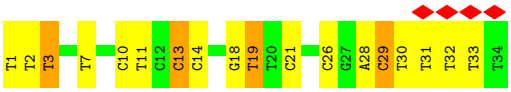



• Molecule 9: STAPLE STRAND

Chain AI: 54% 46%

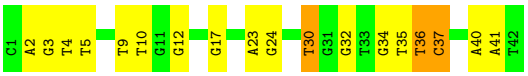
• Molecule 10: STAPLE STRAND

Chain AJ: 12% 47% 41% 12%



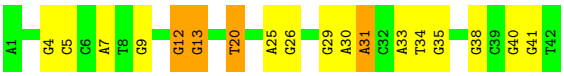

• Molecule 11: STAPLE STRAND

Chain AK: 57% 36% 7%



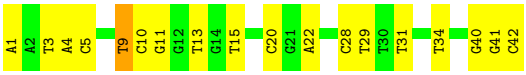

• Molecule 12: STAPLE STRAND

Chain AL: 57% 33% 10%



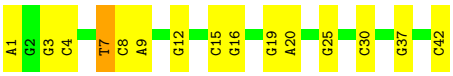

• Molecule 13: STAPLE STRAND

Chain AM: 57% 40% •




• Molecule 14: STAPLE STRAND

Chain AN: 64% 33% •

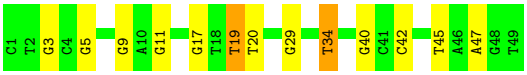



• Molecule 15: STAPLE STRAND

Chain AO: 61% 37% •

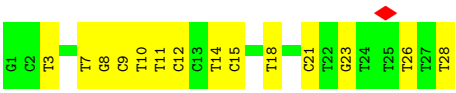
• Molecule 16: STAPLE STRAND

Chain AP: 73% 22% •



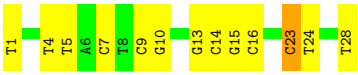

• Molecule 17: STAPLE STRAND

Chain AQ: 50% 50%




• Molecule 18: STAPLE STRAND

Chain AR: 54% 43% •

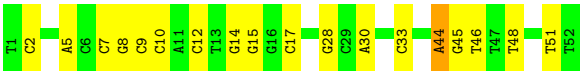



• Molecule 19: STAPLE STRAND

Chain AS: 57% 38% 5%

• Molecule 20: STAPLE STRAND

Chain AT: 65% 33% •




• Molecule 21: STAPLE STRAND

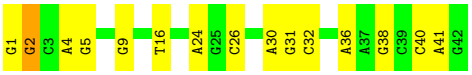
Chain AU: 65% 22% 12%

• Molecule 22: STAPLE STRAND

Chain AV: 56% 42% •

• Molecule 23: STAPLE STRAND

Chain AW: 64% 33% •




• Molecule 24: STAPLE STRAND

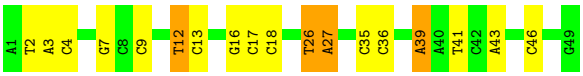
Chain AX: 55% 45%

• Molecule 25: STAPLE STRAND

Chain AY: 71% 19% 10%

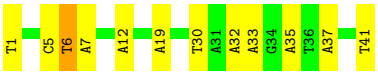
• Molecule 26: STAPLE STRAND

Chain AZ: 63% 29% 8%




• Molecule 27: STAPLE STRAND

Chain Aa: 71% 27% •




• Molecule 28: STAPLE STRAND

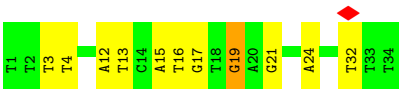
Chain Ab:

• Molecule 29: STAPLE STRAND

Chain Ac:

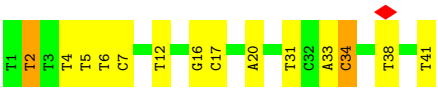
• Molecule 30: STAPLE STRAND

Chain Ad:



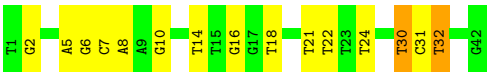

• Molecule 31: STAPLE STRAND

Chain Ae:



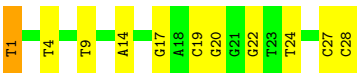

• Molecule 32: STAPLE STRAND

Chain Af:



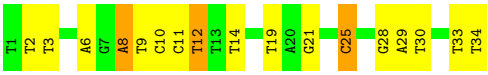

• Molecule 33: STAPLE STRAND

Chain Ag:



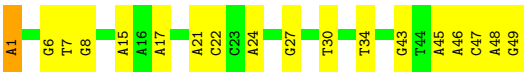

• Molecule 34: STAPLE STRAND

Chain Ah:



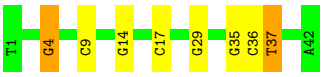

• Molecule 35: STAPLE STRAND

Chain Ai:



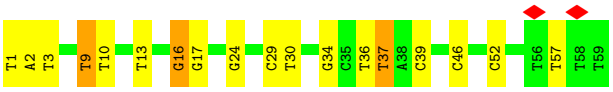

• Molecule 36: STAPLE STRAND

Chain Aj:



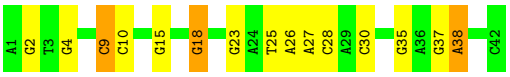

• Molecule 37: STAPLE STRAND

Chain Ak:



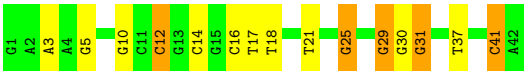

• Molecule 38: STAPLE STRAND

Chain Al:



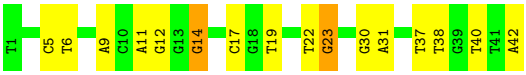

• Molecule 39: STAPLE STRAND

Chain Am:



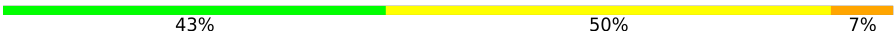

• Molecule 40: STAPLE STRAND

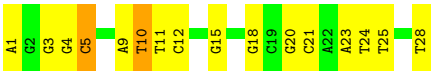
Chain An:




• Molecule 41: STAPLE STRAND

Chain Ao:



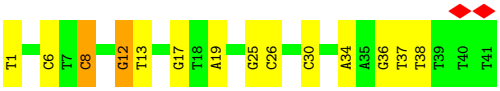



• Molecule 42: STAPLE STRAND

Chain Ap:

• Molecule 43: STAPLE STRAND

Chain Aq:

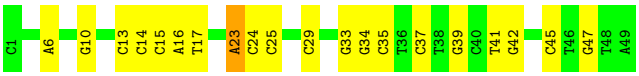



• Molecule 44: STAPLE STRAND

Chain Ar:

• Molecule 45: STAPLE STRAND

Chain As:

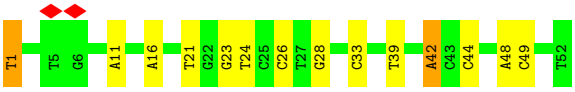



• Molecule 46: STAPLE STRAND

Chain At:

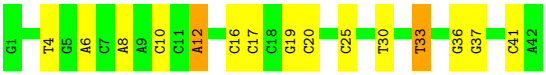
• Molecule 47: STAPLE STRAND

Chain Au:



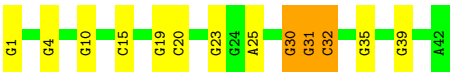

• Molecule 48: STAPLE STRAND

Chain Av:



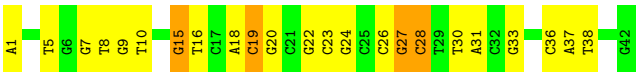

• Molecule 49: STAPLE STRAND

Chain Aw:

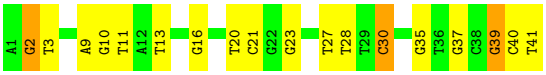

• Molecule 50: STAPLE STRAND

Chain Ax:

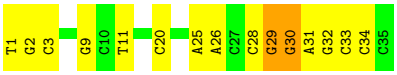

• Molecule 51: STAPLE STRAND

Chain Ay:


• Molecule 52: STAPLE STRAND

Chain Az:

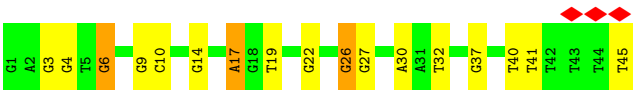




• Molecule 53: STAPLE STRAND

Chain A0:

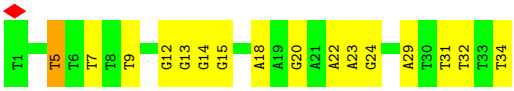

• Molecule 54: STAPLE STRAND

Chain A1:

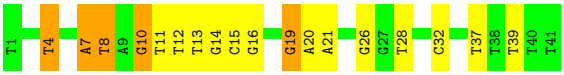

• Molecule 55: STAPLE STRAND

Chain A2:



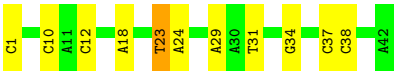

• Molecule 56: STAPLE STRAND

Chain A3:

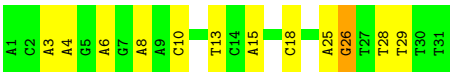

• Molecule 57: STAPLE STRAND

Chain A4:

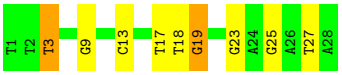

• Molecule 58: STAPLE STRAND

Chain A5:

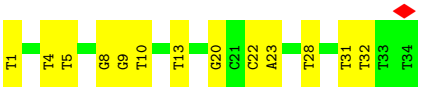

• Molecule 59: STAPLE STRAND

Chain A6:

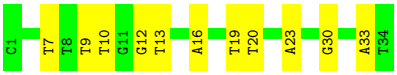

• Molecule 60: STAPLE STRAND

Chain A7:

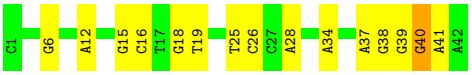

• Molecule 61: STAPLE STRAND

Chain A8:


• Molecule 62: STAPLE STRAND

Chain A9:

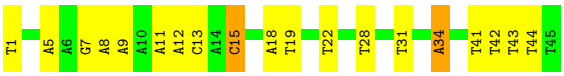



• Molecule 63: STAPLE STRAND

Chain BA: 63% 26% 11%

• Molecule 64: STAPLE STRAND

Chain BB: 58% 38%

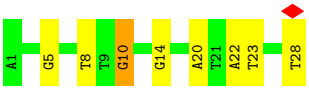



• Molecule 65: STAPLE STRAND

Chain BC: 57% 34% 9%

• Molecule 66: STAPLE STRAND

Chain BD: 71% 25%

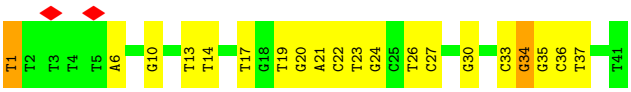



• Molecule 67: STAPLE STRAND

Chain BE: 64% 36%

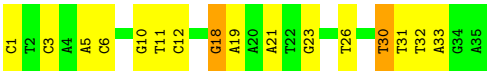
• Molecule 68: STAPLE STRAND

Chain BF: 5% 51% 44% 5%



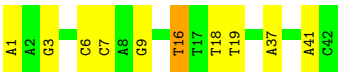

• Molecule 69: STAPLE STRAND

Chain BG: 54% 40% 6%



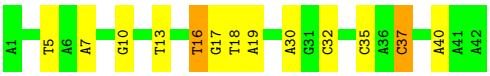

• Molecule 70: STAPLE STRAND

Chain BH: 76% 21% •



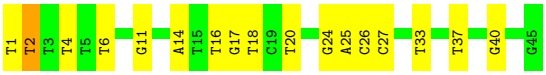

• Molecule 71: STAPLE STRAND

Chain BI: 69% 26% 5%



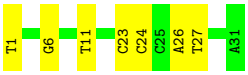

• Molecule 72: STAPLE STRAND

Chain BJ: 62% 36% •



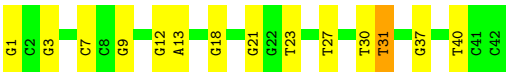

• Molecule 73: STAPLE STRAND

Chain BK: 77% 23%




• Molecule 74: STAPLE STRAND

Chain BL: 67% 31% •

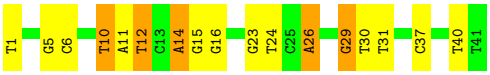



• Molecule 75: STAPLE STRAND

Chain BM: 59% 29% 12%

• Molecule 76: STAPLE STRAND

Chain BN: 59% 29% 12%

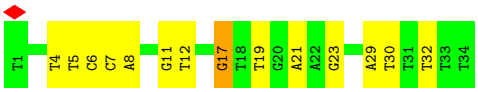



- Molecule 77: STAPLE STRAND

Chain BO:

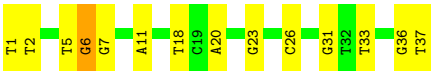
- Molecule 78: STAPLE STRAND

Chain BP:




- Molecule 79: STAPLE STRAND

Chain BQ:



# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 42209 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | NONE | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 50 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | Not provided | |
| Image detector | FEI FALCON III (4k x 4k) | Depositor |
| Maximum map value | 0.372 | Depositor |
| Minimum map value | -0.063 | Depositor |
| Average map value | 0.002 | Depositor |
| Map value standard deviation | 0.015 | Depositor |
| Recommended contour level | 0.0628 | Depositor |
| Map size (Å) | 695.7, 695.7, 695.7 | wwPDB |
| Map dimensions | 300, 300, 300 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 2.319, 2.319, 2.319 | Depositor |

# 5 Model quality (i)

## 5.1 Standard geometry (i)

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

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | $\#\|Z\|>5$ | RMSZ | $\#\|Z\|>5$ |
| 1 | AA | 1.23 | 5/66004 (0.0%) | 1.43 | 971/101868 (1.0%) |
| 2 | AB | 1.27 | 0/774 | 1.37 | 5/1192 (0.4%) |
| 3 | AC | 1.22 | 0/1078 | 1.46 | 19/1660 (1.1%) |
| 4 | AD | 1.19 | 0/790 | 1.49 | 11/1219 (0.9%) |
| 5 | AE | 1.25 | 0/940 | 1.42 | 8/1449 (0.6%) |
| 6 | AF | 1.22 | 0/929 | 1.41 | 11/1431 (0.8%) |
| 7 | AG | 1.20 | 0/769 | 1.48 | 12/1184 (1.0%) |
| 8 | AH | 1.27 | 0/958 | 1.47 | 18/1478 (1.2%) |
| 9 | AI | 1.22 | 0/646 | 1.31 | 6/996 (0.6%) |
| 10 | AJ | 1.22 | 0/746 | 1.68 | 24/1147 (2.1%) |
| 11 | AK | 1.22 | 0/962 | 1.35 | 9/1484 (0.6%) |
| 12 | AL | 1.22 | 0/971 | 1.36 | 11/1499 (0.7%) |
| 13 | AM | 1.24 | 0/970 | 1.45 | 17/1497 (1.1%) |
| 14 | AN | 1.31 | 0/990 | 1.38 | 11/1530 (0.7%) |
| 15 | AO | 1.26 | 0/1132 | 1.43 | 17/1746 (1.0%) |
| 16 | AP | 1.23 | 0/1119 | 1.33 | 10/1725 (0.6%) |
| 17 | AQ | 1.23 | 0/623 | 1.42 | 5/959 (0.5%) |
| 18 | AR | 1.23 | 0/628 | 1.56 | 16/967 (1.7%) |
| 19 | AS | 1.22 | 0/957 | 1.38 | 13/1477 (0.9%) |
| 20 | AT | 1.21 | 0/1172 | 1.28 | 3/1804 (0.2%) |
| 21 | AU | 1.31 | 0/1134 | 1.44 | 12/1752 (0.7%) |
| 22 | AV | 1.26 | 0/1193 | 1.52 | 27/1840 (1.5%) |
| 23 | AW | 1.22 | 0/966 | 1.37 | 10/1489 (0.7%) |
| 24 | AX | 1.21 | 0/847 | 1.35 | 7/1304 (0.5%) |
| 25 | AY | 1.21 | 0/702 | 1.32 | 8/1081 (0.7%) |
| 26 | AZ | 1.22 | 0/1122 | 1.38 | 11/1729 (0.6%) |
| 27 | Aa | 1.16 | 0/936 | 1.37 | 10/1439 (0.7%) |
| 28 | Ab | 1.31 | 1/961 (0.1%) | 1.64 | 25/1480 (1.7%) |
| 29 | Ac | 1.26 | 0/963 | 1.43 | 11/1486 (0.7%) |
| 30 | Ad | 1.20 | 1/779 (0.1%) | 1.21 | 3/1203 (0.2%) |
| 31 | Ae | 1.22 | 1/920 (0.1%) | 1.42 | 9/1417 (0.6%) |
| 32 | Af | 1.24 | 0/970 | 1.42 | 16/1498 (1.1%) |
| 33 | Ag | 1.19 | 0/635 | 1.29 | 7/979 (0.7%) |
| 34 | Ah | 1.24 | 0/766 | 1.62 | 17/1181 (1.4%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 35 | Ai | 1.22 | 0/1133 | 1.37 | 15/1747 (0.9%) |
| 36 | Aj | 1.25 | 0/953 | 1.33 | 5/1467 (0.3%) |
| 37 | Ak | 1.23 | 0/1339 | 1.34 | 13/2065 (0.6%) |
| 38 | Al | 1.26 | 0/969 | 1.40 | 11/1493 (0.7%) |
| 39 | Am | 1.28 | 0/968 | 1.46 | 14/1493 (0.9%) |
| 40 | An | 1.28 | 1/967 (0.1%) | 1.34 | 10/1492 (0.7%) |
| 41 | Ao | 1.19 | 0/642 | 1.47 | 13/990 (1.3%) |
| 42 | Ap | 1.21 | 0/634 | 1.60 | 19/978 (1.9%) |
| 43 | Aq | 1.21 | 0/929 | 1.34 | 9/1432 (0.6%) |
| 44 | Ar | 1.18 | 0/1172 | 1.30 | 12/1807 (0.7%) |
| 45 | As | 1.26 | 0/1099 | 1.47 | 16/1691 (0.9%) |
| 46 | At | 1.26 | 0/1195 | 1.45 | 15/1845 (0.8%) |
| 47 | Au | 1.22 | 0/1193 | 1.25 | 8/1839 (0.4%) |
| 48 | Av | 1.21 | 0/952 | 1.34 | 9/1464 (0.6%) |
| 49 | Aw | 1.28 | 0/983 | 1.41 | 14/1518 (0.9%) |
| 50 | Ax | 1.31 | 1/964 (0.1%) | 1.38 | 13/1486 (0.9%) |
| 51 | Ay | 1.26 | 0/942 | 1.40 | 12/1454 (0.8%) |
| 52 | Az | 1.29 | 1/806 (0.1%) | 1.46 | 16/1242 (1.3%) |
| 53 | A0 | 1.20 | 0/941 | 1.33 | 6/1452 (0.4%) |
| 54 | A1 | 1.27 | 0/1034 | 1.44 | 13/1596 (0.8%) |
| 55 | A2 | 1.21 | 0/779 | 1.40 | 8/1203 (0.7%) |
| 56 | A3 | 1.23 | 0/932 | 1.42 | 17/1438 (1.2%) |
| 57 | A4 | 1.21 | 0/956 | 1.32 | 2/1471 (0.1%) |
| 58 | A5 | 1.17 | 0/703 | 1.35 | 8/1081 (0.7%) |
| 59 | A6 | 1.23 | 0/640 | 1.47 | 9/988 (0.9%) |
| 60 | A7 | 1.22 | 1/758 (0.1%) | 1.40 | 7/1167 (0.6%) |
| 61 | A8 | 1.20 | 0/782 | 1.40 | 11/1206 (0.9%) |
| 62 | A9 | 1.26 | 0/975 | 1.37 | 7/1505 (0.5%) |
| 63 | BA | 1.27 | 0/795 | 1.48 | 16/1222 (1.3%) |
| 64 | BB | 1.17 | 0/1016 | 1.30 | 10/1564 (0.6%) |
| 65 | BC | 1.26 | 0/815 | 1.49 | 19/1259 (1.5%) |
| 66 | BD | 1.18 | 0/636 | 1.20 | 3/981 (0.3%) |
| 67 | BE | 1.18 | 0/638 | 1.23 | 7/986 (0.7%) |
| 68 | BF | 1.24 | 0/919 | 1.40 | 16/1417 (1.1%) |
| 69 | BG | 1.18 | 0/797 | 1.41 | 11/1228 (0.9%) |
| 70 | BH | 1.24 | 0/969 | 1.38 | 8/1495 (0.5%) |
| 71 | BI | 1.19 | 0/987 | 1.35 | 12/1523 (0.8%) |
| 72 | BJ | 1.25 | 0/1035 | 1.41 | 16/1598 (1.0%) |
| 73 | BK | 1.22 | 0/709 | 1.30 | 6/1093 (0.5%) |
| 74 | BL | 1.24 | 0/953 | 1.41 | 15/1468 (1.0%) |
| 75 | BM | 1.30 | 0/1127 | 1.47 | 16/1736 (0.9%) |
| 76 | BN | 1.28 | 0/941 | 1.39 | 15/1452 (1.0%) |
| 77 | BO | 1.20 | 1/952 (0.1%) | 1.34 | 7/1467 (0.5%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 78 | BP | 1.21 | 0/764 | 1.66 | 21/1178 (1.8%) |
| 79 | BQ | 1.18 | 0/845 | 1.45 | 12/1303 (0.9%) |
| All | All | 1.23 | 13/137290 (0.0%) | 1.42 | 1892/211770 (0.9%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 1 | AA | 10 | 739 |
| 2 | AB | 0 | 8 |
| 3 | AC | 0 | 9 |
| 4 | AD | 0 | 8 |
| 5 | AE | 0 | 10 |
| 6 | AF | 0 | 8 |
| 7 | AG | 0 | 10 |
| 8 | AH | 0 | 12 |
| 9 | AI | 0 | 9 |
| 10 | AJ | 0 | 10 |
| 11 | AK | 0 | 13 |
| 12 | AL | 0 | 13 |
| 13 | AM | 0 | 10 |
| 14 | AN | 0 | 11 |
| 15 | AO | 0 | 9 |
| 16 | AP | 0 | 8 |
| 17 | AQ | 0 | 10 |
| 18 | AR | 0 | 7 |
| 19 | AS | 1 | 11 |
| 20 | AT | 0 | 16 |
| 21 | AU | 0 | 13 |
| 22 | AV | 0 | 8 |
| 23 | AW | 0 | 9 |
| 24 | AX | 0 | 10 |
| 25 | AY | 1 | 5 |
| 26 | AZ | 0 | 13 |
| 27 | Aa | 0 | 7 |
| 28 | Ab | 0 | 8 |
| 29 | Ac | 0 | 10 |
| 30 | Ad | 0 | 9 |
| 31 | Ae | 0 | 10 |
| 32 | Af | 0 | 8 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 33 | Ag | 0 | 6 |
| 34 | Ah | 0 | 11 |
| 35 | Ai | 0 | 9 |
| 36 | Aj | 0 | 6 |
| 37 | Ak | 0 | 11 |
| 38 | Al | 0 | 11 |
| 39 | Am | 0 | 12 |
| 40 | An | 0 | 12 |
| 41 | Ao | 0 | 10 |
| 42 | Ap | 0 | 6 |
| 43 | Aq | 0 | 8 |
| 44 | Ar | 0 | 12 |
| 45 | As | 0 | 11 |
| 46 | At | 0 | 9 |
| 47 | Au | 0 | 9 |
| 48 | Av | 0 | 9 |
| 49 | Aw | 0 | 9 |
| 50 | Ax | 0 | 19 |
| 51 | Ay | 0 | 13 |
| 52 | Az | 0 | 5 |
| 53 | A0 | 0 | 6 |
| 54 | A1 | 0 | 10 |
| 55 | A2 | 0 | 13 |
| 56 | A3 | 0 | 11 |
| 57 | A4 | 0 | 10 |
| 58 | A5 | 0 | 7 |
| 59 | A6 | 0 | 5 |
| 60 | A7 | 0 | 6 |
| 61 | A8 | 0 | 4 |
| 62 | A9 | 0 | 10 |
| 63 | BA | 0 | 8 |
| 64 | BB | 0 | 13 |
| 65 | BC | 0 | 8 |
| 66 | BD | 0 | 6 |
| 67 | BE | 0 | 6 |
| 68 | BF | 0 | 10 |
| 69 | BG | 0 | 11 |
| 70 | BH | 0 | 6 |
| 71 | BI | 0 | 7 |
| 72 | BJ | 0 | 10 |
| 73 | BK | 0 | 4 |
| 74 | BL | 0 | 7 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 75 | BM | 0 | 14 |
| 76 | BN | 0 | 10 |
| 77 | BO | 0 | 9 |
| 78 | BP | 0 | 3 |
| 79 | BQ | 0 | 6 |
| All | All | 12 | 1459 |

All (13) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | AA | 1302 | DA | C5'-C4' | 5.50 | 1.57 | 1.51 |
| 30 | Ad | 32 | DT | C5'-C4' | 5.45 | 1.57 | 1.51 |
| 50 | Ax | 15 | DG | C2-N2 | -5.25 | 1.29 | 1.34 |
| 1 | AA | 2655 | DC | C5'-C4' | 5.23 | 1.57 | 1.51 |
| 1 | AA | 1452 | DC | C5'-C4' | 5.23 | 1.57 | 1.51 |
| 28 | Ab | 37 | DT | O3'-P | -5.17 | 1.54 | 1.61 |
| 1 | AA | 828 | DG | C4'-C3' | 5.16 | 1.58 | 1.53 |
| 60 | A7 | 4 | DT | C5'-C4' | 5.10 | 1.56 | 1.51 |
| 40 | An | 30 | DG | C4'-C3' | 5.09 | 1.58 | 1.53 |
| 1 | AA | 923 | DG | C2-N2 | -5.07 | 1.29 | 1.34 |
| 31 | Ae | 38 | DT | C5'-C4' | 5.05 | 1.56 | 1.51 |
| 52 | Az | 32 | DG | C2-N2 | -5.02 | 1.29 | 1.34 |
| 77 | BO | 38 | DA | N9-C4 | -5.01 | 1.34 | 1.37 |

All (1892) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 34 | Ah | 12 | DT | P-O3'-C3' | 15.81 | 138.68 | 119.70 |
| 1 | AA | 1873 | DC | P-O3'-C3' | 15.25 | 138.00 | 119.70 |
| 1 | AA | 175 | DC | P-O3'-C3' | 15.17 | 137.90 | 119.70 |
| 54 | A1 | 9 | DG | P-O3'-C3' | 15.13 | 137.85 | 119.70 |
| 1 | AA | 409 | DA | P-O3'-C3' | 14.92 | 137.60 | 119.70 |
| 1 | AA | 2803 | DG | P-O3'-C3' | 14.80 | 137.46 | 119.70 |
| 26 | AZ | 9 | DC | P-O3'-C3' | 14.64 | 137.27 | 119.70 |
| 1 | AA | 2682 | DC | P-O3'-C3' | 14.47 | 137.07 | 119.70 |
| 1 | AA | 1410 | DG | P-O3'-C3' | 14.45 | 137.04 | 119.70 |
| 39 | Am | 14 | DC | P-O3'-C3' | 14.21 | 136.75 | 119.70 |
| 1 | AA | 57 | DC | P-O3'-C3' | 14.16 | 136.69 | 119.70 |
| 71 | BI | 37 | DC | P-O3'-C3' | 14.07 | 136.59 | 119.70 |
| 77 | BO | 30 | DA | P-O3'-C3' | 13.99 | 136.49 | 119.70 |
| 38 | Al | 30 | DC | P-O3'-C3' | 13.96 | 136.46 | 119.70 |
| 78 | BP | 29 | DA | P-O3'-C3' | 13.92 | 136.40 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 34 | Ah | 9 | DT | P-O3'-C3' | 13.83 | 136.29 | 119.70 |
| 28 | Ab | 37 | DT | P-O3'-C3' | 13.75 | 136.20 | 119.70 |
| 6 | AF | 11 | DT | P-O3'-C3' | 13.68 | 136.12 | 119.70 |
| 1 | AA | 1383 | DC | P-O3'-C3' | 13.67 | 136.11 | 119.70 |
| 1 | AA | 288 | DA | P-O3'-C3' | 13.61 | 136.03 | 119.70 |
| 46 | At | 47 | DT | P-O3'-C3' | 13.47 | 135.87 | 119.70 |
| 1 | AA | 610 | DA | P-O3'-C3' | 13.45 | 135.84 | 119.70 |
| 1 | AA | 2124 | DC | P-O3'-C3' | 13.43 | 135.82 | 119.70 |
| 1 | AA | 1778 | DC | P-O3'-C3' | 13.40 | 135.78 | 119.70 |
| 1 | AA | 1651 | DG | P-O3'-C3' | 13.38 | 135.75 | 119.70 |
| 17 | AQ | 28 | DT | O4'-C4'-C3' | -13.38 | 97.97 | 106.00 |
| 1 | AA | 1540 | DT | P-O3'-C3' | 13.35 | 135.72 | 119.70 |
| 45 | As | 35 | DC | P-O3'-C3' | 13.35 | 135.72 | 119.70 |
| 42 | Ap | 5 | DT | O4'-C4'-C3' | -13.32 | 98.00 | 106.00 |
| 1 | AA | 337 | DT | P-O3'-C3' | 13.32 | 135.68 | 119.70 |
| 78 | BP | 32 | DT | P-O3'-C3' | 13.08 | 135.40 | 119.70 |
| 1 | AA | 1205 | DA | P-O3'-C3' | 13.07 | 135.39 | 119.70 |
| 1 | AA | 2728 | DA | P-O3'-C3' | 13.07 | 135.38 | 119.70 |
| 4 | AD | 29 | DA | P-O3'-C3' | 12.98 | 135.28 | 119.70 |
| 52 | Az | 1 | DT | P-O3'-C3' | 12.98 | 135.27 | 119.70 |
| 1 | AA | 2053 | DC | P-O3'-C3' | 12.97 | 135.26 | 119.70 |
| 1 | AA | 2062 | DC | P-O3'-C3' | 12.94 | 135.23 | 119.70 |
| 1 | AA | 240 | DT | P-O3'-C3' | 12.89 | 135.17 | 119.70 |
| 1 | AA | 2382 | DT | O4'-C4'-C3' | -12.86 | 98.28 | 106.00 |
| 39 | Am | 29 | DG | P-O3'-C3' | 12.81 | 135.07 | 119.70 |
| 22 | AV | 9 | DC | P-O3'-C3' | 12.78 | 135.04 | 119.70 |
| 64 | BB | 9 | DA | P-O3'-C3' | 12.71 | 134.96 | 119.70 |
| 45 | As | 37 | DC | P-O3'-C3' | 12.67 | 134.90 | 119.70 |
| 28 | Ab | 34 | DT | O4'-C4'-C3' | -12.63 | 98.42 | 106.00 |
| 1 | AA | 1836 | DG | O4'-C4'-C3' | -12.62 | 98.42 | 106.00 |
| 29 | Ac | 30 | DG | P-O3'-C3' | 12.54 | 134.75 | 119.70 |
| 72 | BJ | 26 | DC | P-O3'-C3' | 12.46 | 134.65 | 119.70 |
| 4 | AD | 22 | DA | P-O3'-C3' | 12.44 | 134.63 | 119.70 |
| 1 | AA | 1641 | DC | P-O3'-C3' | 12.44 | 134.62 | 119.70 |
| 1 | AA | 2639 | DT | O4'-C4'-C3' | -12.39 | 98.56 | 106.00 |
| 1 | AA | 1441 | DG | P-O3'-C3' | 12.33 | 134.50 | 119.70 |
| 1 | AA | 2507 | DT | O4'-C4'-C3' | -12.32 | 98.61 | 106.00 |
| 1 | AA | 2092 | DC | P-O3'-C3' | 12.26 | 134.41 | 119.70 |
| 5 | AE | 1 | DT | O4'-C4'-C3' | -12.18 | 98.69 | 106.00 |
| 32 | Af | 8 | DA | P-O3'-C3' | 12.17 | 134.30 | 119.70 |
| 51 | Ay | 9 | DA | P-O3'-C3' | 12.16 | 134.29 | 119.70 |
| 1 | AA | 1628 | DG | P-O3'-C3' | 12.16 | 134.29 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | AA | 1222 | DC | P-O3'-C3' | 12.15 | 134.28 | 119.70 |
| 1 | AA | 2355 | DA | P-O3'-C3' | 12.15 | 134.28 | 119.70 |
| 1 | AA | 269 | DG | P-O3'-C3' | 12.13 | 134.26 | 119.70 |
| 62 | A9 | 34 | DA | P-O3'-C3' | 12.13 | 134.26 | 119.70 |
| 60 | A7 | 4 | DT | P-O3'-C3' | 12.11 | 134.23 | 119.70 |
| 1 | AA | 2491 | DC | P-O3'-C3' | 12.11 | 134.23 | 119.70 |
| 14 | AN | 30 | DC | P-O3'-C3' | 12.10 | 134.22 | 119.70 |
| 62 | A9 | 12 | DA | P-O3'-C3' | 12.07 | 134.18 | 119.70 |
| 1 | AA | 2673 | DG | P-O3'-C3' | 12.06 | 134.17 | 119.70 |
| 1 | AA | 1941 | DC | P-O3'-C3' | 12.01 | 134.11 | 119.70 |
| 1 | AA | 931 | DT | O4'-C4'-C3' | -11.99 | 98.81 | 106.00 |
| 7 | AG | 22 | DC | P-O3'-C3' | 11.97 | 134.07 | 119.70 |
| 1 | AA | 1607 | DC | P-O3'-C3' | 11.97 | 134.06 | 119.70 |
| 1 | AA | 1540 | DT | O4'-C4'-C3' | -11.94 | 98.83 | 106.00 |
| 1 | AA | 149 | DT | P-O3'-C3' | 11.93 | 134.02 | 119.70 |
| 41 | Ao | 21 | DC | O4'-C4'-C3' | -11.92 | 98.85 | 106.00 |
| 36 | Aj | 37 | DT | P-O3'-C3' | 11.91 | 134.00 | 119.70 |
| 3 | AC | 21 | DT | P-O3'-C3' | 11.88 | 133.96 | 119.70 |
| 1 | AA | 845 | DG | O4'-C4'-C3' | -11.86 | 98.89 | 106.00 |
| 1 | AA | 1033 | DA | O4'-C4'-C3' | -11.84 | 98.90 | 106.00 |
| 75 | BM | 48 | DA | P-O3'-C3' | 11.81 | 133.87 | 119.70 |
| 1 | AA | 1575 | DG | O4'-C4'-C3' | -11.81 | 98.92 | 106.00 |
| 34 | Ah | 25 | DC | P-O3'-C3' | 11.79 | 133.85 | 119.70 |
| 13 | AM | 1 | DA | O4'-C4'-C3' | -11.76 | 98.94 | 106.00 |
| 1 | AA | 574 | DT | P-O3'-C3' | 11.73 | 133.78 | 119.70 |
| 1 | AA | 2781 | DA | P-O3'-C3' | 11.70 | 133.74 | 119.70 |
| 1 | AA | 1970 | DG | P-O3'-C3' | 11.68 | 133.72 | 119.70 |
| 21 | AU | 44 | DG | P-O3'-C3' | 11.66 | 133.70 | 119.70 |
| 1 | AA | 1064 | DG | O4'-C4'-C3' | -11.66 | 99.00 | 106.00 |
| 32 | Af | 10 | DG | O4'-C4'-C3' | -11.64 | 99.01 | 106.00 |
| 1 | AA | 2069 | DG | P-O3'-C3' | 11.63 | 133.66 | 119.70 |
| 12 | AL | 9 | DG | O4'-C4'-C3' | -11.57 | 99.06 | 106.00 |
| 39 | Am | 31 | DG | O4'-C4'-C3' | -11.52 | 99.09 | 106.00 |
| 1 | AA | 417 | DC | P-O3'-C3' | 11.52 | 133.52 | 119.70 |
| 1 | AA | 2638 | DA | P-O3'-C3' | 11.52 | 133.52 | 119.70 |
| 15 | AO | 43 | DA | P-O3'-C3' | 11.49 | 133.49 | 119.70 |
| 28 | Ab | 34 | DT | P-O3'-C3' | 11.47 | 133.46 | 119.70 |
| 1 | AA | 1565 | DC | P-O3'-C3' | 11.46 | 133.45 | 119.70 |
| 73 | BK | 1 | DT | O4'-C4'-C3' | -11.40 | 99.16 | 106.00 |
| 53 | A0 | 40 | DT | P-O3'-C3' | 11.37 | 133.34 | 119.70 |
| 67 | BE | 17 | DG | O4'-C4'-C3' | -11.35 | 99.19 | 106.00 |
| 1 | AA | 541 | DC | P-O3'-C3' | 11.34 | 133.31 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | AA | 1892 | DG | O4'-C4'-C3' | -11.31 | 99.21 | 106.00 |
| 22 | AV | 29 | DG | P-O3'-C3' | 11.27 | 133.22 | 119.70 |
| 10 | AJ | 3 | DT | O4'-C4'-C3' | -11.26 | 99.25 | 106.00 |
| 47 | Au | 1 | DT | P-O3'-C3' | 11.24 | 133.19 | 119.70 |
| 75 | BM | 23 | DC | P-O3'-C3' | 11.23 | 133.18 | 119.70 |
| 7 | AG | 1 | DT | O4'-C4'-C3' | -11.18 | 99.30 | 106.00 |
| 59 | A6 | 19 | DG | P-O3'-C3' | 11.17 | 133.10 | 119.70 |
| 1 | AA | 2040 | DG | O4'-C4'-C3' | -11.16 | 99.30 | 106.00 |
| 1 | AA | 659 | DC | P-O3'-C3' | 11.16 | 133.09 | 119.70 |
| 1 | AA | 2702 | DG | O4'-C4'-C3' | -11.16 | 99.31 | 106.00 |
| 46 | At | 21 | DG | O4'-C4'-C3' | -11.13 | 99.32 | 106.00 |
| 31 | Ae | 17 | DC | O4'-C4'-C3' | -11.10 | 99.34 | 106.00 |
| 1 | AA | 821 | DT | P-O3'-C3' | 11.09 | 133.00 | 119.70 |
| 22 | AV | 27 | DC | P-O3'-C3' | 11.08 | 133.00 | 119.70 |
| 65 | BC | 1 | DA | P-O3'-C3' | 11.06 | 132.98 | 119.70 |
| 1 | AA | 597 | DG | O4'-C4'-C3' | -11.06 | 99.36 | 106.00 |
| 65 | BC | 29 | DT | O4'-C4'-C3' | -11.04 | 99.37 | 106.00 |
| 1 | AA | 1732 | DG | O4'-C4'-C3' | -11.04 | 99.38 | 106.00 |
| 11 | AK | 41 | DA | P-O3'-C3' | 11.02 | 132.93 | 119.70 |
| 1 | AA | 2791 | DT | O4'-C4'-C3' | -11.00 | 99.40 | 106.00 |
| 1 | AA | 2296 | DC | P-O3'-C3' | 10.96 | 132.85 | 119.70 |
| 1 | AA | 2693 | DG | O4'-C4'-C3' | -10.94 | 99.43 | 106.00 |
| 13 | AM | 40 | DG | P-O3'-C3' | 10.94 | 132.83 | 119.70 |
| 1 | AA | 1710 | DT | O4'-C4'-C3' | -10.91 | 99.46 | 106.00 |
| 79 | BQ | 36 | DG | P-O3'-C3' | 10.90 | 132.78 | 119.70 |
| 1 | AA | 68 | DG | O4'-C4'-C3' | -10.88 | 99.47 | 106.00 |
| 1 | AA | 2499 | DC | P-O3'-C3' | 10.88 | 132.75 | 119.70 |
| 1 | AA | 733 | DG | P-O3'-C3' | 10.86 | 132.73 | 119.70 |
| 1 | AA | 22 | DT | P-O3'-C3' | 10.83 | 132.70 | 119.70 |
| 1 | AA | 1804 | DA | P-O3'-C3' | 10.83 | 132.70 | 119.70 |
| 1 | AA | 665 | DG | O4'-C4'-C3' | -10.82 | 99.51 | 106.00 |
| 1 | AA | 1879 | DG | O4'-C4'-C3' | -10.77 | 99.54 | 106.00 |
| 49 | Aw | 25 | DA | O4'-C4'-C3' | -10.71 | 99.57 | 106.00 |
| 1 | AA | 1836 | DG | P-O3'-C3' | 10.70 | 132.54 | 119.70 |
| 1 | AA | 1033 | DA | P-O3'-C3' | 10.69 | 132.53 | 119.70 |
| 35 | Ai | 1 | DA | O4'-C4'-C3' | -10.69 | 99.59 | 106.00 |
| 3 | AC | 47 | DC | P-O3'-C3' | 10.67 | 132.50 | 119.70 |
| 49 | Aw | 32 | DC | P-O3'-C3' | 10.66 | 132.50 | 119.70 |
| 59 | A6 | 27 | DT | P-O3'-C3' | 10.63 | 132.46 | 119.70 |
| 5 | AE | 37 | DC | P-O3'-C3' | 10.63 | 132.45 | 119.70 |
| 1 | AA | 881 | DT | O4'-C4'-C3' | -10.57 | 99.66 | 106.00 |
| 1 | AA | 2223 | DG | P-O3'-C3' | 10.57 | 132.38 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | AA | 2434 | DC | P-O3'-C3' | 10.51 | 132.31 | 119.70 |
| 1 | AA | 1723 | DC | P-O3'-C3' | 10.50 | 132.30 | 119.70 |
| 37 | Ak | 9 | DT | O4'-C4'-C3' | -10.40 | 99.76 | 106.00 |
| 13 | AM | 40 | DG | O4'-C4'-C3' | -10.40 | 99.76 | 106.00 |
| 1 | AA | 520 | DC | P-O3'-C3' | 10.38 | 132.16 | 119.70 |
| 56 | A3 | 8 | DT | O4'-C4'-C3' | -10.38 | 99.78 | 106.00 |
| 18 | AR | 1 | DT | O4'-C4'-C3' | -10.34 | 99.80 | 106.00 |
| 1 | AA | 1365 | DT | O4'-C4'-C3' | -10.33 | 99.80 | 106.00 |
| 22 | AV | 44 | DT | O4'-C4'-C3' | -10.33 | 99.80 | 106.00 |
| 41 | Ao | 10 | DT | O4'-C4'-C3' | -10.31 | 99.81 | 106.00 |
| 74 | BL | 18 | DG | O4'-C4'-C3' | -10.31 | 99.81 | 106.00 |
| 78 | BP | 8 | DA | O4'-C4'-C3' | -10.28 | 99.83 | 106.00 |
| 3 | AC | 26 | DG | P-O3'-C3' | 10.28 | 132.04 | 119.70 |
| 21 | AU | 23 | DC | P-O3'-C3' | 10.27 | 132.02 | 119.70 |
| 74 | BL | 37 | DG | P-O3'-C3' | 10.27 | 132.02 | 119.70 |
| 1 | AA | 520 | DC | O4'-C4'-C3' | -10.21 | 99.87 | 106.00 |
| 38 | Al | 38 | DA | P-O3'-C3' | 10.20 | 131.94 | 119.70 |
| 1 | AA | 1444 | DG | P-O3'-C3' | 10.14 | 131.87 | 119.70 |
| 28 | Ab | 31 | DG | O4'-C4'-C3' | -10.12 | 99.93 | 106.00 |
| 4 | AD | 16 | DG | O4'-C4'-C3' | -10.10 | 99.94 | 106.00 |
| 70 | BH | 37 | DA | P-O3'-C3' | 10.08 | 131.79 | 119.70 |
| 1 | AA | 828 | DG | P-O3'-C3' | 10.07 | 131.78 | 119.70 |
| 1 | AA | 1521 | DT | O4'-C4'-C3' | -10.04 | 99.98 | 106.00 |
| 1 | AA | 2526 | DT | O4'-C4'-C3' | -10.02 | 99.99 | 106.00 |
| 31 | Ae | 2 | DT | O4'-C4'-C3' | -10.00 | 100.00 | 106.00 |
| 1 | AA | 359 | DG | O4'-C4'-C3' | -9.98 | 100.01 | 106.00 |
| 42 | Ap | 13 | DG | O4'-C4'-C3' | -9.98 | 100.01 | 106.00 |
| 62 | A9 | 18 | DG | O4'-C4'-C3' | -9.96 | 100.02 | 106.00 |
| 1 | AA | 2341 | DC | P-O3'-C3' | 9.96 | 131.65 | 119.70 |
| 10 | AJ | 7 | DT | O4'-C4'-C3' | -9.95 | 100.03 | 106.00 |
| 1 | AA | 1391 | DA | P-O3'-C3' | 9.93 | 131.62 | 119.70 |
| 61 | A8 | 33 | DA | P-O3'-C3' | 9.89 | 131.57 | 119.70 |
| 4 | AD | 10 | DT | O4'-C4'-C3' | -9.88 | 100.07 | 106.00 |
| 33 | Ag | 1 | DT | O4'-C4'-C3' | -9.86 | 100.08 | 106.00 |
| 18 | AR | 23 | DC | C2-N1-C1' | 9.83 | 129.61 | 118.80 |
| 1 | AA | 1302 | DA | O4'-C4'-C3' | -9.80 | 100.12 | 106.00 |
| 29 | Ac | 4 | DT | O4'-C4'-C3' | -9.79 | 100.12 | 106.00 |
| 1 | AA | 1883 | DC | P-O3'-C3' | 9.78 | 131.44 | 119.70 |
| 27 | Aa | 1 | DT | P-O3'-C3' | 9.78 | 131.44 | 119.70 |
| 69 | BG | 19 | DA | P-O3'-C3' | 9.75 | 131.40 | 119.70 |
| 38 | Al | 25 | DT | O4'-C4'-C3' | -9.74 | 100.16 | 106.00 |
| 61 | A8 | 10 | DT | P-O3'-C3' | 9.71 | 131.35 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | AA | 901 | DT | P-O3'-C3' | 9.69 | 131.32 | 119.70 |
| 1 | AA | 1627 | DA | P-O3'-C3' | 9.66 | 131.29 | 119.70 |
| 54 | A1 | 19 | DT | O4'-C4'-C3' | -9.64 | 100.22 | 106.00 |
| 1 | AA | 389 | DG | P-O3'-C3' | 9.62 | 131.25 | 119.70 |
| 1 | AA | 2435 | DA | P-O3'-C3' | 9.61 | 131.24 | 119.70 |
| 17 | AQ | 3 | DT | O4'-C4'-C3' | -9.61 | 100.23 | 106.00 |
| 1 | AA | 1626 | DG | P-O3'-C3' | 9.57 | 131.19 | 119.70 |
| 79 | BQ | 31 | DG | O4'-C4'-C3' | -9.57 | 100.26 | 106.00 |
| 1 | AA | 200 | DC | P-O3'-C3' | 9.52 | 131.13 | 119.70 |
| 1 | AA | 1134 | DC | O4'-C4'-C3' | -9.51 | 100.29 | 106.00 |
| 48 | Av | 4 | DT | O4'-C4'-C3' | -9.51 | 100.30 | 106.00 |
| 48 | Av | 33 | DT | P-O3'-C3' | 9.49 | 131.08 | 119.70 |
| 69 | BG | 19 | DA | O4'-C1'-C2' | -9.47 | 98.32 | 105.90 |
| 1 | AA | 616 | DG | O4'-C4'-C3' | -9.41 | 100.35 | 106.00 |
| 1 | AA | 1723 | DC | O4'-C1'-C2' | -9.38 | 98.39 | 105.90 |
| 1 | AA | 1941 | DC | O4'-C1'-C2' | -9.38 | 98.40 | 105.90 |
| 1 | AA | 2260 | DT | P-O3'-C3' | 9.38 | 130.95 | 119.70 |
| 15 | AO | 41 | DG | P-O3'-C3' | 9.36 | 130.93 | 119.70 |
| 41 | Ao | 23 | DA | P-O3'-C3' | 9.36 | 130.93 | 119.70 |
| 56 | A3 | 32 | DC | P-O3'-C3' | 9.35 | 130.91 | 119.70 |
| 1 | AA | 890 | DC | P-O3'-C3' | 9.33 | 130.90 | 119.70 |
| 15 | AO | 12 | DA | P-O3'-C3' | 9.30 | 130.86 | 119.70 |
| 78 | BP | 30 | DT | O4'-C4'-C3' | -9.30 | 100.42 | 106.00 |
| 1 | AA | 836 | DT | O4'-C4'-C3' | -9.29 | 100.43 | 106.00 |
| 28 | Ab | 13 | DA | P-O3'-C3' | 9.28 | 130.84 | 119.70 |
| 1 | AA | 2577 | DC | P-O3'-C3' | 9.28 | 130.83 | 119.70 |
| 1 | AA | 2069 | DG | O4'-C1'-C2' | -9.27 | 98.48 | 105.90 |
| 1 | AA | 2532 | DG | P-O3'-C3' | 9.27 | 130.82 | 119.70 |
| 14 | AN | 9 | DA | P-O3'-C3' | 9.26 | 130.81 | 119.70 |
| 1 | AA | 2715 | DG | O4'-C4'-C3' | -9.26 | 100.45 | 106.00 |
| 1 | AA | 240 | DT | O4'-C1'-C2' | -9.25 | 98.50 | 105.90 |
| 50 | Ax | 19 | DC | P-O3'-C3' | 9.24 | 130.79 | 119.70 |
| 1 | AA | 821 | DT | O4'-C1'-C2' | -9.23 | 98.51 | 105.90 |
| 42 | Ap | 11 | DG | C5-C6-O6 | -9.21 | 123.07 | 128.60 |
| 23 | AW | 5 | DG | P-O3'-C3' | 9.21 | 130.75 | 119.70 |
| 79 | BQ | 26 | DC | P-O3'-C3' | 9.18 | 130.72 | 119.70 |
| 1 | AA | 2092 | DC | O4'-C1'-C2' | -9.15 | 98.58 | 105.90 |
| 1 | AA | 1333 | DA | P-O3'-C3' | 9.14 | 130.67 | 119.70 |
| 6 | AF | 11 | DT | O4'-C1'-C2' | -9.14 | 98.59 | 105.90 |
| 18 | AR | 23 | DC | O4'-C1'-N1 | 9.10 | 114.37 | 108.00 |
| 41 | Ao | 5 | DC | P-O3'-C3' | 9.05 | 130.56 | 119.70 |
| 14 | AN | 4 | DC | P-O3'-C3' | 9.03 | 130.53 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | AY | 24 | DC | P-O3'-C3' | 9.02 | 130.53 | 119.70 |
| 1 | AA | 885 | DC | C6-N1-C2 | -9.00 | 116.70 | 120.30 |
| 1 | AA | 1087 | DT | P-O3'-C3' | 9.00 | 130.50 | 119.70 |
| 10 | AJ | 19 | DT | P-O3'-C3' | 8.99 | 130.49 | 119.70 |
| 1 | AA | 2838 | DG | P-O3'-C3' | 8.98 | 130.48 | 119.70 |
| 1 | AA | 723 | DC | P-O3'-C3' | 8.97 | 130.47 | 119.70 |
| 51 | Ay | 27 | DT | C6-C5-C7 | -8.96 | 117.52 | 122.90 |
| 1 | AA | 2491 | DC | O4'-C1'-C2' | -8.96 | 98.73 | 105.90 |
| 47 | Au | 11 | DA | P-O3'-C3' | 8.94 | 130.43 | 119.70 |
| 65 | BC | 1 | DA | O4'-C1'-C2' | -8.93 | 98.75 | 105.90 |
| 1 | AA | 2242 | DG | O4'-C1'-C2' | -8.93 | 98.76 | 105.90 |
| 1 | AA | 210 | DC | O4'-C1'-C2' | -8.91 | 98.77 | 105.90 |
| 22 | AV | 37 | DG | P-O3'-C3' | 8.91 | 130.39 | 119.70 |
| 43 | Aq | 1 | DT | O4'-C1'-C2' | -8.91 | 98.78 | 105.90 |
| 1 | AA | 1651 | DG | O4'-C1'-C2' | -8.90 | 98.78 | 105.90 |
| 1 | AA | 1700 | DT | O4'-C4'-C3' | -8.90 | 100.66 | 106.00 |
| 1 | AA | 2626 | DT | P-O3'-C3' | 8.88 | 130.36 | 119.70 |
| 22 | AV | 33 | DA | O4'-C4'-C3' | -8.87 | 100.68 | 106.00 |
| 1 | AA | 2242 | DG | P-O3'-C3' | 8.87 | 130.34 | 119.70 |
| 1 | AA | 795 | DC | P-O3'-C3' | 8.86 | 130.34 | 119.70 |
| 1 | AA | 1960 | DC | P-O3'-C3' | 8.86 | 130.34 | 119.70 |
| 1 | AA | 2673 | DG | O4'-C1'-C2' | -8.86 | 98.81 | 105.90 |
| 72 | BJ | 1 | DT | O4'-C1'-C2' | -8.86 | 98.81 | 105.90 |
| 1 | AA | 980 | DG | O4'-C4'-C3' | -8.85 | 100.69 | 106.00 |
| 1 | AA | 149 | DT | O4'-C1'-C2' | -8.85 | 98.82 | 105.90 |
| 1 | AA | 2437 | DT | P-O3'-C3' | 8.80 | 130.26 | 119.70 |
| 63 | BA | 10 | DC | P-O3'-C3' | 8.79 | 130.24 | 119.70 |
| 1 | AA | 577 | DT | O4'-C4'-C3' | -8.78 | 100.73 | 106.00 |
| 1 | AA | 1235 | DG | O4'-C4'-C3' | -8.78 | 100.73 | 106.00 |
| 1 | AA | 446 | DC | P-O3'-C3' | 8.77 | 130.23 | 119.70 |
| 31 | Ae | 34 | DC | O4'-C1'-N1 | 8.76 | 114.13 | 108.00 |
| 1 | AA | 1410 | DG | O4'-C1'-C2' | -8.70 | 98.94 | 105.90 |
| 31 | Ae | 34 | DC | O4'-C1'-C2' | -8.65 | 98.98 | 105.90 |
| 53 | A0 | 8 | DG | O4'-C4'-C3' | -8.65 | 100.81 | 106.00 |
| 40 | An | 30 | DG | P-O3'-C3' | 8.64 | 130.07 | 119.70 |
| 78 | BP | 30 | DT | O4'-C1'-C2' | -8.64 | 98.99 | 105.90 |
| 65 | BC | 6 | DC | P-O3'-C3' | 8.63 | 130.06 | 119.70 |
| 1 | AA | 1970 | DG | O4'-C1'-C2' | -8.62 | 99.00 | 105.90 |
| 68 | BF | 19 | DT | P-O3'-C3' | 8.62 | 130.05 | 119.70 |
| 70 | BH | 16 | DT | P-O3'-C3' | 8.59 | 130.01 | 119.70 |
| 3 | AC | 46 | DA | N1-C6-N6 | -8.59 | 113.45 | 118.60 |
| 1 | AA | 733 | DG | O4'-C1'-C2' | -8.59 | 99.03 | 105.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | AV | 31 | DG | O4'-C1'-C2' | -8.59 | 99.03 | 105.90 |
| 1 | AA | 2779 | DG | P-O3'-C3' | 8.57 | 129.98 | 119.70 |
| 1 | AA | 181 | DG | O4'-C4'-C3' | -8.55 | 100.87 | 106.00 |
| 69 | BG | 1 | DC | O4'-C1'-C2' | -8.55 | 99.06 | 105.90 |
| 1 | AA | 647 | DC | P-O3'-C3' | 8.54 | 129.95 | 119.70 |
| 1 | AA | 354 | DG | P-O3'-C3' | 8.53 | 129.94 | 119.70 |
| 55 | A2 | 34 | DT | O4'-C4'-C3' | -8.53 | 100.88 | 106.00 |
| 65 | BC | 14 | DG | O4'-C1'-C2' | -8.52 | 99.08 | 105.90 |
| 1 | AA | 1377 | DC | P-O3'-C3' | 8.52 | 129.92 | 119.70 |
| 10 | AJ | 11 | DT | O4'-C1'-C2' | -8.51 | 99.09 | 105.90 |
| 1 | AA | 161 | DT | P-O3'-C3' | 8.49 | 129.89 | 119.70 |
| 1 | AA | 1682 | DG | O4'-C4'-C3' | -8.49 | 100.90 | 106.00 |
| 78 | BP | 4 | DT | O4'-C4'-C3' | -8.49 | 100.91 | 106.00 |
| 1 | AA | 1391 | DA | O4'-C4'-C3' | -8.49 | 100.91 | 106.00 |
| 6 | AF | 37 | DG | O4'-C4'-C3' | -8.48 | 100.91 | 106.00 |
| 9 | AI | 19 | DC | O4'-C1'-C2' | -8.48 | 99.12 | 105.90 |
| 28 | Ab | 14 | DA | P-O3'-C3' | 8.48 | 129.87 | 119.70 |
| 1 | AA | 733 | DG | O4'-C4'-C3' | -8.46 | 100.92 | 106.00 |
| 10 | AJ | 26 | DC | O4'-C1'-C2' | -8.46 | 99.13 | 105.90 |
| 43 | Aq | 38 | DT | P-O3'-C3' | 8.45 | 129.84 | 119.70 |
| 10 | AJ | 11 | DT | P-O3'-C3' | 8.45 | 129.84 | 119.70 |
| 52 | Az | 30 | DG | P-O3'-C3' | 8.44 | 129.83 | 119.70 |
| 1 | AA | 1441 | DG | O4'-C1'-N9 | 8.44 | 113.91 | 108.00 |
| 1 | AA | 1970 | DG | O4'-C4'-C3' | -8.44 | 100.94 | 106.00 |
| 3 | AC | 41 | DA | P-O3'-C3' | 8.44 | 129.82 | 119.70 |
| 13 | AM | 1 | DA | P-O3'-C3' | 8.40 | 129.78 | 119.70 |
| 63 | BA | 28 | DG | O4'-C4'-C3' | -8.39 | 100.97 | 106.00 |
| 42 | Ap | 13 | DG | P-O3'-C3' | 8.37 | 129.75 | 119.70 |
| 71 | BI | 7 | DA | O4'-C1'-C2' | -8.37 | 99.21 | 105.90 |
| 1 | AA | 1730 | DG | O4'-C1'-C2' | -8.36 | 99.22 | 105.90 |
| 1 | AA | 417 | DC | O4'-C1'-C2' | -8.34 | 99.23 | 105.90 |
| 1 | AA | 2654 | DG | O4'-C1'-C2' | -8.34 | 99.23 | 105.90 |
| 18 | AR | 23 | DC | C6-N1-C1' | -8.32 | 110.81 | 120.80 |
| 56 | A3 | 19 | DG | P-O3'-C3' | 8.32 | 129.69 | 119.70 |
| 1 | AA | 2355 | DA | O4'-C1'-C2' | -8.31 | 99.25 | 105.90 |
| 10 | AJ | 30 | DT | O4'-C1'-C2' | -8.29 | 99.27 | 105.90 |
| 23 | AW | 9 | DG | O4'-C1'-C2' | -8.29 | 99.27 | 105.90 |
| 1 | AA | 1804 | DA | O4'-C1'-C2' | -8.29 | 99.27 | 105.90 |
| 78 | BP | 5 | DT | O4'-C4'-C3' | -8.28 | 101.03 | 106.00 |
| 8 | AH | 14 | DT | P-O3'-C3' | 8.22 | 129.56 | 119.70 |
| 51 | Ay | 27 | DT | C4-C5-C7 | 8.21 | 123.93 | 119.00 |
| 14 | AN | 30 | DC | O4'-C1'-C2' | -8.20 | 99.34 | 105.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | AA | 1751 | DC | O4'-C4'-C3' | -8.20 | 101.08 | 106.00 |
| 67 | BE | 22 | DG | O4'-C1'-C2' | -8.20 | 99.34 | 105.90 |
| 61 | A8 | 9 | DT | O4'-C4'-C3' | -8.19 | 101.08 | 106.00 |
| 73 | BK | 6 | DG | O4'-C1'-C2' | -8.19 | 99.35 | 105.90 |
| 1 | AA | 98 | DA | O4'-C1'-C2' | -8.18 | 99.36 | 105.90 |
| 41 | Ao | 10 | DT | C1'-O4'-C4' | -8.18 | 101.92 | 110.10 |
| 1 | AA | 1444 | DG | O4'-C4'-C3' | -8.17 | 101.10 | 106.00 |
| 31 | Ae | 34 | DC | C1'-O4'-C4' | -8.17 | 101.93 | 110.10 |
| 1 | AA | 2554 | DG | O4'-C1'-C2' | -8.15 | 99.38 | 105.90 |
| 1 | AA | 900 | DG | O4'-C1'-C2' | -8.14 | 99.39 | 105.90 |
| 13 | AM | 1 | DA | C1'-O4'-C4' | -8.13 | 101.97 | 110.10 |
| 13 | AM | 40 | DG | O4'-C1'-C2' | -8.11 | 99.41 | 105.90 |
| 1 | AA | 252 | DG | O4'-C1'-C2' | -8.11 | 99.41 | 105.90 |
| 1 | AA | 2069 | DG | C1'-O4'-C4' | -8.11 | 102.00 | 110.10 |
| 34 | Ah | 12 | DT | O4'-C1'-C2' | -8.11 | 99.42 | 105.90 |
| 1 | AA | 2051 | DC | O4'-C1'-C2' | -8.10 | 99.42 | 105.90 |
| 1 | AA | 1401 | DG | O4'-C1'-C2' | -8.09 | 99.42 | 105.90 |
| 1 | AA | 2092 | DC | O4'-C4'-C3' | -8.09 | 101.14 | 106.00 |
| 78 | BP | 5 | DT | O4'-C1'-C2' | -8.09 | 99.43 | 105.90 |
| 1 | AA | 2434 | DC | O4'-C1'-C2' | -8.09 | 99.43 | 105.90 |
| 1 | AA | 1614 | DG | O4'-C4'-C3' | -8.08 | 101.15 | 106.00 |
| 34 | Ah | 14 | DT | O4'-C4'-C3' | -8.08 | 101.15 | 106.00 |
| 1 | AA | 1605 | DA | O4'-C1'-C2' | -8.07 | 99.44 | 105.90 |
| 1 | AA | 2090 | DG | O4'-C1'-C2' | -8.06 | 99.45 | 105.90 |
| 1 | AA | 2382 | DT | C1'-O4'-C4' | -8.06 | 102.04 | 110.10 |
| 1 | AA | 1441 | DG | O4'-C1'-C2' | -8.05 | 99.46 | 105.90 |
| 1 | AA | 828 | DG | O4'-C1'-C2' | -8.05 | 99.46 | 105.90 |
| 1 | AA | 2296 | DC | O4'-C4'-C3' | -8.04 | 101.18 | 106.00 |
| 8 | AH | 12 | DT | C4'-C3'-C2' | -8.04 | 95.86 | 103.10 |
| 9 | AI | 19 | DC | P-O3'-C3' | 8.02 | 129.32 | 119.70 |
| 22 | AV | 39 | DG | O4'-C1'-C2' | -8.02 | 99.49 | 105.90 |
| 1 | AA | 946 | DG | O4'-C1'-C2' | -8.01 | 99.49 | 105.90 |
| 1 | AA | 659 | DC | O4'-C1'-C2' | -8.00 | 99.50 | 105.90 |
| 32 | Af | 10 | DG | C1'-O4'-C4' | -8.00 | 102.10 | 110.10 |
| 1 | AA | 269 | DG | O4'-C1'-C2' | -7.99 | 99.51 | 105.90 |
| 1 | AA | 1372 | DC | O4'-C1'-C2' | -7.98 | 99.51 | 105.90 |
| 1 | AA | 1033 | DA | C1'-O4'-C4' | -7.98 | 102.12 | 110.10 |
| 34 | Ah | 8 | DA | P-O3'-C3' | 7.98 | 129.27 | 119.70 |
| 24 | AX | 33 | DG | P-O3'-C3' | 7.97 | 129.27 | 119.70 |
| 3 | AC | 47 | DC | O4'-C1'-C2' | -7.97 | 99.53 | 105.90 |
| 28 | Ab | 40 | DG | P-O3'-C3' | 7.95 | 129.24 | 119.70 |
| 19 | AS | 1 | DT | O4'-C4'-C3' | -7.94 | 101.24 | 106.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 72 | BJ | 24 | DG | O4'-C1'-C2' | -7.93 | 99.55 | 105.90 |
| 74 | BL | 1 | DG | O4'-C1'-C2' | -7.92 | 99.56 | 105.90 |
| 76 | BN | 1 | DT | O4'-C1'-C2' | -7.92 | 99.56 | 105.90 |
| 22 | AV | 9 | DC | O4'-C1'-C2' | -7.92 | 99.56 | 105.90 |
| 68 | BF | 26 | DT | P-O3'-C3' | 7.92 | 129.20 | 119.70 |
| 52 | Az | 34 | DC | P-O3'-C3' | 7.90 | 129.19 | 119.70 |
| 1 | AA | 337 | DT | O4'-C1'-C2' | -7.90 | 99.58 | 105.90 |
| 19 | AS | 36 | DT | O4'-C1'-C2' | -7.90 | 99.58 | 105.90 |
| 1 | AA | 454 | DA | O4'-C1'-C2' | -7.89 | 99.58 | 105.90 |
| 1 | AA | 1605 | DA | P-O3'-C3' | 7.89 | 129.17 | 119.70 |
| 1 | AA | 1238 | DG | O4'-C1'-C2' | -7.88 | 99.59 | 105.90 |
| 1 | AA | 2006 | DC | O4'-C4'-C3' | -7.88 | 101.27 | 106.00 |
| 1 | AA | 1779 | DC | O4'-C1'-C2' | -7.87 | 99.61 | 105.90 |
| 1 | AA | 2511 | DG | O4'-C1'-C2' | -7.87 | 99.61 | 105.90 |
| 18 | AR | 28 | DT | O4'-C1'-C2' | -7.85 | 99.62 | 105.90 |
| 1 | AA | 1391 | DA | O4'-C1'-C2' | -7.84 | 99.63 | 105.90 |
| 1 | AA | 1629 | DC | O4'-C1'-C2' | -7.83 | 99.63 | 105.90 |
| 1 | AA | 1487 | DT | O4'-C4'-C3' | -7.83 | 101.30 | 106.00 |
| 1 | AA | 1626 | DG | O4'-C1'-C2' | -7.83 | 99.64 | 105.90 |
| 1 | AA | 1441 | DG | C1'-O4'-C4' | -7.83 | 102.27 | 110.10 |
| 41 | Ao | 21 | DC | C1'-O4'-C4' | -7.83 | 102.27 | 110.10 |
| 58 | A5 | 10 | DC | O4'-C1'-C2' | -7.82 | 99.65 | 105.90 |
| 1 | AA | 589 | DG | P-O3'-C3' | 7.81 | 129.07 | 119.70 |
| 1 | AA | 1158 | DT | P-O3'-C3' | 7.80 | 129.06 | 119.70 |
| 1 | AA | 1370 | DC | O4'-C1'-C2' | -7.80 | 99.66 | 105.90 |
| 1 | AA | 2285 | DC | O4'-C4'-C3' | -7.79 | 101.33 | 106.00 |
| 1 | AA | 2444 | DG | O4'-C1'-C2' | -7.79 | 99.67 | 105.90 |
| 1 | AA | 2341 | DC | O4'-C1'-C2' | -7.78 | 99.67 | 105.90 |
| 31 | Ae | 34 | DC | P-O3'-C3' | 7.78 | 129.04 | 119.70 |
| 1 | AA | 1659 | DT | C1'-O4'-C4' | -7.77 | 102.33 | 110.10 |
| 29 | Ac | 29 | DA | O4'-C1'-C2' | -7.77 | 99.68 | 105.90 |
| 42 | Ap | 8 | DG | O4'-C4'-C3' | -7.77 | 101.34 | 106.00 |
| 66 | BD | 20 | DA | O4'-C1'-C2' | -7.77 | 99.68 | 105.90 |
| 1 | AA | 1614 | DG | O4'-C1'-C2' | -7.76 | 99.69 | 105.90 |
| 35 | Ai | 43 | DG | P-O3'-C3' | 7.76 | 129.01 | 119.70 |
| 1 | AA | 2497 | DC | C6-N1-C2 | -7.75 | 117.20 | 120.30 |
| 1 | AA | 2522 | DT | O4'-C4'-C3' | -7.75 | 101.35 | 106.00 |
| 1 | AA | 1428 | DG | O4'-C1'-C2' | -7.75 | 99.70 | 105.90 |
| 55 | A2 | 23 | DA | O4'-C1'-C2' | -7.75 | 99.70 | 105.90 |
| 4 | AD | 22 | DA | O4'-C1'-C2' | -7.74 | 99.71 | 105.90 |
| 1 | AA | 2781 | DA | O4'-C1'-C2' | -7.73 | 99.71 | 105.90 |
| 46 | At | 40 | DG | O4'-C1'-C2' | -7.73 | 99.72 | 105.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 65 | BC | 1 | DA | O4'-C4'-C3' | -7.72 | 101.37 | 106.00 |
| 1 | AA | 2598 | DG | O4'-C4'-C3' | -7.71 | 101.37 | 106.00 |
| 8 | AH | 12 | DT | O4'-C4'-C3' | -7.71 | 101.37 | 106.00 |
| 29 | Ac | 16 | DC | P-O3'-C3' | 7.70 | 128.94 | 119.70 |
| 42 | Ap | 11 | DG | N1-C6-O6 | 7.70 | 124.52 | 119.90 |
| 1 | AA | 1480 | DC | O4'-C1'-C2' | -7.69 | 99.75 | 105.90 |
| 1 | AA | 705 | DA | P-O3'-C3' | 7.68 | 128.91 | 119.70 |
| 46 | At | 13 | DG | O4'-C1'-C2' | -7.67 | 99.76 | 105.90 |
| 1 | AA | 1397 | DT | O4'-C1'-C2' | -7.67 | 99.77 | 105.90 |
| 8 | AH | 28 | DA | P-O3'-C3' | 7.66 | 128.89 | 119.70 |
| 1 | AA | 610 | DA | O4'-C1'-C2' | -7.66 | 99.77 | 105.90 |
| 29 | Ac | 30 | DG | O4'-C1'-C2' | -7.65 | 99.78 | 105.90 |
| 1 | AA | 1047 | DT | O4'-C1'-C2' | -7.64 | 99.79 | 105.90 |
| 65 | BC | 4 | DG | P-O3'-C3' | 7.64 | 128.87 | 119.70 |
| 7 | AG | 5 | DG | O4'-C1'-C2' | -7.64 | 99.79 | 105.90 |
| 28 | Ab | 9 | DA | O4'-C1'-C2' | -7.64 | 99.79 | 105.90 |
| 1 | AA | 2242 | DG | C1'-O4'-C4' | -7.63 | 102.47 | 110.10 |
| 1 | AA | 76 | DT | C4'-C3'-C2' | -7.63 | 96.23 | 103.10 |
| 63 | BA | 8 | DC | P-O3'-C3' | 7.63 | 128.85 | 119.70 |
| 1 | AA | 1659 | DT | O4'-C4'-C3' | -7.62 | 101.42 | 106.00 |
| 1 | AA | 2495 | DA | O4'-C1'-C2' | -7.62 | 99.80 | 105.90 |
| 59 | A6 | 13 | DC | O4'-C1'-C2' | -7.62 | 99.80 | 105.90 |
| 1 | AA | 2673 | DG | C1'-O4'-C4' | -7.62 | 102.48 | 110.10 |
| 42 | Ap | 8 | DG | C5-C6-O6 | -7.62 | 124.03 | 128.60 |
| 1 | AA | 2216 | DT | O4'-C1'-C2' | -7.61 | 99.81 | 105.90 |
| 1 | AA | 2230 | DG | O4'-C1'-C2' | -7.60 | 99.82 | 105.90 |
| 1 | AA | 1636 | DG | O4'-C1'-C2' | -7.60 | 99.82 | 105.90 |
| 1 | AA | 472 | DT | O4'-C1'-C2' | -7.60 | 99.82 | 105.90 |
| 60 | A7 | 22 | DC | P-O3'-C3' | 7.59 | 128.81 | 119.70 |
| 49 | Aw | 35 | DG | O4'-C1'-C2' | -7.59 | 99.83 | 105.90 |
| 1 | AA | 1372 | DC | O4'-C4'-C3' | -7.59 | 101.45 | 106.00 |
| 1 | AA | 76 | DT | O4'-C4'-C3' | -7.58 | 101.45 | 106.00 |
| 1 | AA | 1087 | DT | O4'-C1'-C2' | -7.58 | 99.83 | 105.90 |
| 52 | Az | 31 | DA | P-O3'-C3' | 7.58 | 128.79 | 119.70 |
| 10 | AJ | 3 | DT | C1'-O4'-C4' | -7.57 | 102.53 | 110.10 |
| 8 | AH | 22 | DT | P-O3'-C3' | 7.57 | 128.78 | 119.70 |
| 19 | AS | 36 | DT | O4'-C4'-C3' | -7.57 | 101.46 | 106.00 |
| 1 | AA | 1371 | DG | O4'-C1'-C2' | -7.56 | 99.85 | 105.90 |
| 1 | AA | 691 | DT | C4'-C3'-C2' | -7.56 | 96.30 | 103.10 |
| 3 | AC | 29 | DC | P-O3'-C3' | 7.56 | 128.77 | 119.70 |
| 25 | AY | 4 | DT | P-O3'-C3' | 7.55 | 128.77 | 119.70 |
| 53 | A0 | 1 | DC | O4'-C4'-C3' | -7.55 | 101.47 | 106.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | AA | 1659 | DT | O4'-C1'-C2' | -7.55 | 99.86 | 105.90 |
| 18 | AR | 14 | DC | O4'-C1'-C2' | -7.55 | 99.86 | 105.90 |
| 64 | BB | 43 | DT | C4'-C3'-C2' | -7.54 | 96.31 | 103.10 |
| 27 | Aa | 1 | DT | O4'-C4'-C3' | -7.54 | 101.47 | 106.00 |
| 1 | AA | 1454 | DG | O4'-C1'-C2' | -7.54 | 99.87 | 105.90 |
| 1 | AA | 1487 | DT | C4'-C3'-C2' | -7.54 | 96.32 | 103.10 |
| 1 | AA | 1064 | DG | C1'-O4'-C4' | -7.53 | 102.57 | 110.10 |
| 1 | AA | 2374 | DA | P-O3'-C3' | 7.53 | 128.73 | 119.70 |
| 1 | AA | 1238 | DG | P-O3'-C3' | 7.52 | 128.73 | 119.70 |
| 1 | AA | 2673 | DG | O4'-C1'-N9 | 7.52 | 113.27 | 108.00 |
| 75 | BM | 30 | DG | O4'-C4'-C3' | -7.52 | 101.49 | 106.00 |
| 17 | AQ | 28 | DT | C1'-O4'-C4' | -7.52 | 102.58 | 110.10 |
| 10 | AJ | 1 | DT | O4'-C1'-C2' | -7.52 | 99.89 | 105.90 |
| 1 | AA | 2223 | DG | O4'-C4'-C3' | -7.51 | 101.49 | 106.00 |
| 1 | AA | 409 | DA | O4'-C1'-N9 | 7.51 | 113.26 | 108.00 |
| 1 | AA | 879 | DG | O4'-C1'-C2' | -7.51 | 99.89 | 105.90 |
| 1 | AA | 2006 | DC | P-O3'-C3' | 7.51 | 128.71 | 119.70 |
| 1 | AA | 1222 | DC | O4'-C1'-C2' | -7.50 | 99.90 | 105.90 |
| 7 | AG | 29 | DG | O4'-C1'-N9 | 7.50 | 113.25 | 108.00 |
| 42 | Ap | 21 | DC | O4'-C1'-C2' | -7.49 | 99.91 | 105.90 |
| 75 | BM | 30 | DG | O4'-C1'-C2' | -7.48 | 99.92 | 105.90 |
| 55 | A2 | 34 | DT | O4'-C1'-C2' | -7.48 | 99.92 | 105.90 |
| 1 | AA | 1058 | DC | O4'-C4'-C3' | -7.47 | 101.51 | 104.50 |
| 1 | AA | 2583 | DG | P-O3'-C3' | 7.47 | 128.67 | 119.70 |
| 1 | AA | 1723 | DC | O4'-C4'-C3' | -7.47 | 101.51 | 104.50 |
| 1 | AA | 2220 | DT | C4'-C3'-C2' | -7.47 | 96.38 | 103.10 |
| 76 | BN | 16 | DG | P-O3'-C3' | 7.46 | 128.66 | 119.70 |
| 76 | BN | 29 | DG | O4'-C1'-C2' | -7.46 | 99.93 | 105.90 |
| 1 | AA | 2602 | DT | O4'-C4'-C3' | -7.46 | 101.52 | 104.50 |
| 1 | AA | 3 | DG | O4'-C1'-C2' | -7.45 | 99.94 | 105.90 |
| 1 | AA | 378 | DG | O4'-C4'-C3' | -7.44 | 101.53 | 104.50 |
| 1 | AA | 2180 | DG | O4'-C1'-C2' | -7.43 | 99.95 | 105.90 |
| 75 | BM | 13 | DG | O4'-C1'-C2' | -7.42 | 99.96 | 105.90 |
| 19 | AS | 1 | DT | P-O3'-C3' | -7.42 | 110.80 | 119.70 |
| 69 | BG | 19 | DA | C1'-O4'-C4' | -7.41 | 102.69 | 110.10 |
| 46 | At | 46 | DG | P-O3'-C3' | 7.41 | 128.59 | 119.70 |
| 16 | AP | 9 | DG | O4'-C1'-C2' | -7.41 | 99.97 | 105.90 |
| 37 | Ak | 52 | DC | O4'-C1'-C2' | -7.41 | 99.98 | 105.90 |
| 70 | BH | 16 | DT | O4'-C1'-C2' | -7.41 | 99.97 | 105.90 |
| 1 | AA | 1836 | DG | C1'-O4'-C4' | -7.40 | 102.70 | 110.10 |
| 28 | Ab | 40 | DG | O4'-C1'-C2' | -7.39 | 99.98 | 105.90 |
| 78 | BP | 6 | DC | O4'-C1'-C2' | -7.39 | 99.99 | 105.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 49 | Aw | 4 | DG | O4'-C1'-C2' | -7.38 | 99.99 | 105.90 |
| 35 | Ai | 43 | DG | O4'-C1'-C2' | -7.38 | 100.00 | 105.90 |
| 72 | BJ | 2 | DT | P-O3'-C3' | 7.38 | 128.55 | 119.70 |
| 7 | AG | 24 | DT | O4'-C4'-C3' | -7.38 | 101.55 | 104.50 |
| 77 | BO | 30 | DA | O4'-C1'-C2' | -7.38 | 100.00 | 105.90 |
| 1 | AA | 1518 | DA | P-O3'-C3' | 7.37 | 128.55 | 119.70 |
| 68 | BF | 20 | DG | O4'-C1'-C2' | -7.37 | 100.00 | 105.90 |
| 1 | AA | 1186 | DT | P-O3'-C3' | 7.37 | 128.54 | 119.70 |
| 68 | BF | 10 | DG | O4'-C1'-C2' | -7.37 | 100.01 | 105.90 |
| 1 | AA | 561 | DG | O4'-C1'-C2' | -7.37 | 100.01 | 105.90 |
| 58 | A5 | 28 | DT | O4'-C1'-C2' | -7.37 | 100.01 | 105.90 |
| 1 | AA | 2341 | DC | O4'-C4'-C3' | -7.36 | 101.56 | 104.50 |
| 1 | AA | 1238 | DG | C1'-O4'-C4' | -7.35 | 102.75 | 110.10 |
| 1 | AA | 55 | DT | O4'-C4'-C3' | -7.35 | 101.56 | 104.50 |
| 1 | AA | 2263 | DC | P-O3'-C3' | 7.34 | 128.51 | 119.70 |
| 15 | AO | 1 | DC | O4'-C1'-C2' | -7.34 | 100.02 | 105.90 |
| 1 | AA | 2199 | DG | O4'-C1'-C2' | -7.34 | 100.03 | 105.90 |
| 34 | Ah | 30 | DT | O4'-C4'-C3' | -7.34 | 101.56 | 104.50 |
| 14 | AN | 30 | DC | O4'-C4'-C3' | -7.34 | 101.56 | 104.50 |
| 62 | A9 | 16 | DC | P-O3'-C3' | 7.33 | 128.50 | 119.70 |
| 7 | AG | 17 | DG | O4'-C1'-C2' | -7.33 | 100.04 | 105.90 |
| 1 | AA | 3 | DG | P-O3'-C3' | 7.31 | 128.47 | 119.70 |
| 1 | AA | 55 | DT | C4'-C3'-C2' | -7.29 | 96.54 | 103.10 |
| 1 | AA | 2795 | DG | P-O3'-C3' | 7.29 | 128.45 | 119.70 |
| 55 | A2 | 34 | DT | C1'-O4'-C4' | -7.29 | 102.81 | 110.10 |
| 9 | AI | 19 | DC | C1'-O4'-C4' | -7.29 | 102.81 | 110.10 |
| 1 | AA | 2301 | DG | C4'-C3'-C2' | -7.28 | 96.55 | 103.10 |
| 15 | AO | 44 | DG | P-O3'-C3' | 7.27 | 128.43 | 119.70 |
| 1 | AA | 1963 | DG | O4'-C1'-C2' | -7.27 | 100.09 | 105.90 |
| 1 | AA | 2592 | DT | C4'-C3'-C2' | -7.26 | 96.56 | 103.10 |
| 1 | AA | 2069 | DG | O4'-C4'-C3' | -7.24 | 101.61 | 104.50 |
| 56 | A3 | 8 | DT | C1'-O4'-C4' | -7.24 | 102.86 | 110.10 |
| 61 | A8 | 9 | DT | C4'-C3'-C2' | -7.23 | 96.59 | 103.10 |
| 1 | AA | 1481 | DG | C1'-O4'-C4' | -7.22 | 102.88 | 110.10 |
| 1 | AA | 2488 | DG | O4'-C1'-C2' | -7.22 | 100.12 | 105.90 |
| 72 | BJ | 26 | DC | O4'-C1'-C2' | -7.22 | 100.12 | 105.90 |
| 1 | AA | 132 | DA | P-O3'-C3' | 7.22 | 128.36 | 119.70 |
| 1 | AA | 2835 | DA | P-O3'-C3' | 7.22 | 128.36 | 119.70 |
| 3 | AC | 40 | DT | C4'-C3'-C2' | -7.21 | 96.61 | 103.10 |
| 1 | AA | 2069 | DG | O4'-C1'-N9 | 7.21 | 113.04 | 108.00 |
| 43 | Aq | 26 | DC | O4'-C1'-C2' | -7.20 | 100.14 | 105.90 |
| 1 | AA | 980 | DG | C4'-C3'-C2' | -7.20 | 96.62 | 103.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | AA | 1621 | DC | O4'-C4'-C3' | -7.20 | 101.62 | 104.50 |
| 8 | AH | 8 | DG | C4'-C3'-C2' | -7.20 | 96.62 | 103.10 |
| 1 | AA | 462 | DA | P-O3'-C3' | 7.19 | 128.33 | 119.70 |
| 1 | AA | 1166 | DT | C4'-C3'-C2' | -7.19 | 96.63 | 103.10 |
| 1 | AA | 2491 | DC | O4'-C4'-C3' | -7.18 | 101.63 | 104.50 |
| 1 | AA | 2301 | DG | O4'-C4'-C3' | -7.18 | 101.63 | 104.50 |
| 38 | Al | 9 | DC | O4'-C1'-N1 | 7.18 | 113.03 | 108.00 |
| 1 | AA | 2179 | DG | O4'-C1'-C2' | -7.18 | 100.16 | 105.90 |
| 1 | AA | 247 | DC | O4'-C4'-C3' | -7.17 | 101.63 | 104.50 |
| 1 | AA | 715 | DT | C4'-C3'-C2' | -7.17 | 96.65 | 103.10 |
| 43 | Aq | 17 | DG | O4'-C1'-C2' | -7.16 | 100.17 | 105.90 |
| 1 | AA | 1444 | DG | O4'-C1'-C2' | -7.16 | 100.17 | 105.90 |
| 3 | AC | 21 | DT | O4'-C1'-C2' | -7.15 | 100.18 | 105.90 |
| 6 | AF | 11 | DT | O4'-C4'-C3' | -7.15 | 101.64 | 104.50 |
| 1 | AA | 1521 | DT | P-O3'-C3' | 7.15 | 128.28 | 119.70 |
| 69 | BG | 19 | DA | O4'-C4'-C3' | -7.15 | 101.64 | 104.50 |
| 1 | AA | 1484 | DG | O4'-C1'-C2' | -7.15 | 100.18 | 105.90 |
| 59 | A6 | 19 | DG | O4'-C1'-C2' | -7.13 | 100.19 | 105.90 |
| 78 | BP | 30 | DT | P-O3'-C3' | 7.13 | 128.26 | 119.70 |
| 27 | Aa | 37 | DA | C4'-C3'-C2' | -7.12 | 96.69 | 103.10 |
| 74 | BL | 1 | DG | C1'-O4'-C4' | -7.12 | 102.98 | 110.10 |
| 1 | AA | 1922 | DA | O4'-C1'-C2' | -7.10 | 100.22 | 105.90 |
| 1 | AA | 541 | DC | O4'-C1'-C2' | -7.10 | 100.22 | 105.90 |
| 1 | AA | 1945 | DA | P-O3'-C3' | 7.08 | 128.20 | 119.70 |
| 28 | Ab | 16 | DC | O4'-C4'-C3' | -7.08 | 101.67 | 104.50 |
| 39 | Am | 12 | DC | C2-N1-C1' | 7.08 | 126.59 | 118.80 |
| 1 | AA | 2526 | DT | C4'-C3'-C2' | -7.08 | 96.73 | 103.10 |
| 1 | AA | 1430 | DG | O4'-C1'-C2' | -7.06 | 100.25 | 105.90 |
| 1 | AA | 2318 | DC | O4'-C1'-C2' | -7.06 | 100.25 | 105.90 |
| 7 | AG | 24 | DT | C4'-C3'-C2' | -7.06 | 96.75 | 103.10 |
| 59 | A6 | 23 | DG | O4'-C1'-C2' | -7.06 | 100.25 | 105.90 |
| 1 | AA | 2164 | DA | P-O3'-C3' | 7.06 | 128.17 | 119.70 |
| 1 | AA | 1804 | DA | O4'-C4'-C3' | -7.05 | 101.68 | 104.50 |
| 1 | AA | 2728 | DA | O4'-C1'-C2' | -7.05 | 100.26 | 105.90 |
| 44 | Ar | 37 | DA | P-O3'-C3' | 7.05 | 128.16 | 119.70 |
| 1 | AA | 653 | DG | C4'-C3'-C2' | -7.05 | 96.76 | 103.10 |
| 28 | Ab | 42 | DG | O4'-C1'-C2' | -7.05 | 100.26 | 105.90 |
| 1 | AA | 1898 | DG | O4'-C4'-C3' | -7.05 | 101.68 | 104.50 |
| 1 | AA | 2136 | DG | O4'-C1'-C2' | -7.05 | 100.26 | 105.90 |
| 1 | AA | 2786 | DG | C4'-C3'-C2' | -7.05 | 96.76 | 103.10 |
| 1 | AA | 1481 | DG | O4'-C1'-C2' | -7.04 | 100.27 | 105.90 |
| 1 | AA | 547 | DT | O4'-C1'-C2' | -7.04 | 100.27 | 105.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | AA | 2189 | DT | O4'-C4'-C3' | -7.04 | 101.68 | 104.50 |
| 54 | A1 | 3 | DG | O4'-C1'-C2' | -7.04 | 100.27 | 105.90 |
| 32 | Af | 5 | DA | O4'-C1'-C2' | -7.03 | 100.28 | 105.90 |
| 1 | AA | 2672 | DG | O4'-C1'-C2' | -7.02 | 100.28 | 105.90 |
| 51 | Ay | 39 | DG | O4'-C1'-C2' | -7.01 | 100.29 | 105.90 |
| 1 | AA | 1793 | DG | C4'-C3'-C2' | -7.00 | 96.80 | 103.10 |
| 45 | As | 24 | DC | P-O3'-C3' | 6.99 | 128.09 | 119.70 |
| 72 | BJ | 20 | DT | O4'-C1'-C2' | -6.99 | 100.31 | 105.90 |
| 1 | AA | 145 | DT | C4'-C3'-C2' | -6.99 | 96.81 | 103.10 |
| 6 | AF | 37 | DG | C4'-C3'-C2' | -6.99 | 96.81 | 103.10 |
| 75 | BM | 23 | DC | O4'-C1'-C2' | -6.99 | 100.31 | 105.90 |
| 10 | AJ | 26 | DC | O4'-C1'-N1 | 6.99 | 112.89 | 108.00 |
| 1 | AA | 1629 | DC | O4'-C1'-N1 | 6.98 | 112.89 | 108.00 |
| 1 | AA | 1148 | DC | P-O3'-C3' | 6.98 | 128.08 | 119.70 |
| 1 | AA | 121 | DG | O4'-C1'-C2' | -6.98 | 100.32 | 105.90 |
| 1 | AA | 409 | DA | O4'-C1'-C2' | -6.98 | 100.32 | 105.90 |
| 54 | A1 | 26 | DG | O4'-C1'-C2' | -6.97 | 100.32 | 105.90 |
| 1 | AA | 589 | DG | O4'-C1'-C2' | -6.97 | 100.32 | 105.90 |
| 1 | AA | 181 | DG | C4'-C3'-C2' | -6.96 | 96.83 | 103.10 |
| 1 | AA | 1073 | DT | C4'-C3'-C2' | -6.96 | 96.84 | 103.10 |
| 79 | BQ | 36 | DG | O4'-C1'-C2' | -6.96 | 100.33 | 105.90 |
| 28 | Ab | 37 | DT | O4'-C1'-C2' | -6.96 | 100.33 | 105.90 |
| 1 | AA | 1904 | DC | O4'-C1'-C2' | -6.96 | 100.33 | 105.90 |
| 1 | AA | 2585 | DG | P-O3'-C3' | 6.96 | 128.05 | 119.70 |
| 45 | As | 34 | DG | O4'-C1'-C2' | -6.96 | 100.33 | 105.90 |
| 1 | AA | 361 | DT | C4'-C3'-C2' | -6.96 | 96.84 | 103.10 |
| 1 | AA | 1851 | DA | P-O3'-C3' | 6.95 | 128.04 | 119.70 |
| 1 | AA | 852 | DG | P-O3'-C3' | 6.95 | 128.03 | 119.70 |
| 1 | AA | 487 | DT | O4'-C4'-C3' | -6.94 | 101.72 | 104.50 |
| 59 | A6 | 25 | DG | O4'-C1'-C2' | -6.94 | 100.35 | 105.90 |
| 75 | BM | 36 | DT | O4'-C1'-C2' | -6.94 | 100.35 | 105.90 |
| 1 | AA | 161 | DT | C4'-C3'-C2' | -6.94 | 96.86 | 103.10 |
| 1 | AA | 998 | DC | C4'-C3'-C2' | -6.94 | 96.86 | 103.10 |
| 1 | AA | 70 | DA | O4'-C1'-C2' | -6.93 | 100.35 | 105.90 |
| 39 | Am | 25 | DG | P-O3'-C3' | 6.93 | 128.02 | 119.70 |
| 2 | AB | 7 | DA | O4'-C1'-C2' | -6.92 | 100.36 | 105.90 |
| 27 | Aa | 1 | DT | O4'-C1'-C2' | -6.92 | 100.36 | 105.90 |
| 1 | AA | 2561 | DT | C4-C5-C7 | -6.92 | 114.85 | 119.00 |
| 64 | BB | 9 | DA | O4'-C1'-C2' | -6.92 | 100.36 | 105.90 |
| 29 | Ac | 41 | DC | P-O3'-C3' | 6.92 | 128.00 | 119.70 |
| 46 | At | 40 | DG | P-O3'-C3' | 6.92 | 128.00 | 119.70 |
| 13 | AM | 11 | DG | P-O3'-C3' | 6.91 | 127.99 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | AA | 1614 | DG | C1'-O4'-C4' | -6.91 | 103.19 | 110.10 |
| 1 | AA | 2114 | DG | O4'-C1'-C2' | -6.91 | 100.37 | 105.90 |
| 1 | AA | 1339 | DT | C4'-C3'-C2' | -6.91 | 96.88 | 103.10 |
| 1 | AA | 1555 | DG | O4'-C1'-C2' | -6.90 | 100.38 | 105.90 |
| 43 | Aq | 34 | DA | O4'-C1'-C2' | -6.90 | 100.38 | 105.90 |
| 1 | AA | 2665 | DG | O4'-C1'-C2' | -6.89 | 100.39 | 105.90 |
| 1 | AA | 2673 | DG | O4'-C4'-C3' | -6.89 | 101.75 | 104.50 |
| 1 | AA | 1628 | DG | O4'-C1'-C2' | -6.89 | 100.39 | 105.90 |
| 45 | As | 13 | DC | P-O3'-C3' | 6.89 | 127.96 | 119.70 |
| 39 | Am | 31 | DG | C1'-O4'-C4' | -6.88 | 103.22 | 110.10 |
| 39 | Am | 12 | DC | O4'-C1'-N1 | 6.88 | 112.82 | 108.00 |
| 56 | A3 | 19 | DG | O4'-C1'-N9 | 6.88 | 112.81 | 108.00 |
| 26 | AZ | 12 | DT | C4'-C3'-C2' | -6.87 | 96.92 | 103.10 |
| 68 | BF | 33 | DC | O4'-C1'-C2' | -6.87 | 100.40 | 105.90 |
| 28 | Ab | 31 | DG | C4'-C3'-C2' | -6.87 | 96.92 | 103.10 |
| 35 | Ai | 1 | DA | C4'-C3'-C2' | -6.87 | 96.92 | 103.10 |
| 1 | AA | 2532 | DG | O4'-C1'-N9 | 6.87 | 112.81 | 108.00 |
| 4 | AD | 22 | DA | O4'-C4'-C3' | -6.86 | 101.75 | 104.50 |
| 47 | Au | 33 | DC | O4'-C1'-C2' | -6.86 | 100.41 | 105.90 |
| 61 | A8 | 16 | DA | C4'-C3'-C2' | -6.86 | 96.93 | 103.10 |
| 1 | AA | 1888 | DG | O4'-C1'-C2' | -6.86 | 100.42 | 105.90 |
| 19 | AS | 24 | DA | O4'-C1'-C2' | -6.86 | 100.42 | 105.90 |
| 50 | Ax | 9 | DG | O4'-C1'-C2' | -6.86 | 100.42 | 105.90 |
| 1 | AA | 1678 | DT | O4'-C1'-C2' | -6.85 | 100.42 | 105.90 |
| 1 | AA | 639 | DA | C4'-C3'-C2' | -6.84 | 96.94 | 103.10 |
| 1 | AA | 1941 | DC | O4'-C4'-C3' | -6.84 | 101.76 | 104.50 |
| 1 | AA | 2728 | DA | O4'-C1'-N9 | 6.84 | 112.79 | 108.00 |
| 1 | AA | 657 | DG | P-O3'-C3' | 6.84 | 127.90 | 119.70 |
| 69 | BG | 23 | DG | O4'-C1'-C2' | -6.83 | 100.44 | 105.90 |
| 1 | AA | 1779 | DC | C1'-O4'-C4' | -6.82 | 103.28 | 110.10 |
| 1 | AA | 2199 | DG | O4'-C1'-N9 | 6.82 | 112.78 | 108.00 |
| 1 | AA | 966 | DG | C4'-C3'-C2' | -6.82 | 96.96 | 103.10 |
| 1 | AA | 1086 | DA | N1-C6-N6 | -6.81 | 114.51 | 118.60 |
| 28 | Ab | 34 | DT | C1'-O4'-C4' | -6.81 | 103.29 | 110.10 |
| 61 | A8 | 16 | DA | O4'-C4'-C3' | -6.81 | 101.78 | 104.50 |
| 1 | AA | 487 | DT | C4'-C3'-C2' | -6.80 | 96.98 | 103.10 |
| 56 | A3 | 19 | DG | C1'-O4'-C4' | -6.80 | 103.30 | 110.10 |
| 16 | AP | 20 | DT | C4'-C3'-C2' | -6.80 | 96.98 | 103.10 |
| 1 | AA | 965 | DT | C4'-C3'-C2' | -6.80 | 96.98 | 103.10 |
| 1 | AA | 1201 | DC | P-O3'-C3' | 6.79 | 127.85 | 119.70 |
| 28 | Ab | 16 | DC | C4'-C3'-C2' | -6.79 | 96.99 | 103.10 |
| 1 | AA | 288 | DA | O4'-C1'-C2' | -6.79 | 100.47 | 105.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | AA | 2427 | DA | O4'-C1'-N9 | 6.79 | 112.75 | 108.00 |
| 1 | AA | 378 | DG | O4'-C1'-C2' | -6.78 | 100.47 | 105.90 |
| 1 | AA | 2646 | DC | O4'-C1'-C2' | -6.78 | 100.48 | 105.90 |
| 1 | AA | 1061 | DG | O4'-C1'-C2' | -6.78 | 100.48 | 105.90 |
| 78 | BP | 29 | DA | O4'-C1'-C2' | -6.78 | 100.48 | 105.90 |
| 1 | AA | 2294 | DC | C4'-C3'-C2' | -6.77 | 97.00 | 103.10 |
| 31 | Ae | 33 | DA | O4'-C1'-C2' | -6.77 | 100.49 | 105.90 |
| 53 | A0 | 30 | DT | C4'-C3'-C2' | -6.76 | 97.01 | 103.10 |
| 1 | AA | 1220 | DA | O4'-C1'-C2' | -6.76 | 100.49 | 105.90 |
| 34 | Ah | 14 | DT | C4'-C3'-C2' | -6.76 | 97.02 | 103.10 |
| 42 | Ap | 5 | DT | C1'-O4'-C4' | -6.75 | 103.35 | 110.10 |
| 58 | A5 | 10 | DC | C1'-O4'-C4' | -6.75 | 103.35 | 110.10 |
| 37 | Ak | 16 | DG | O4'-C1'-C2' | -6.75 | 100.50 | 105.90 |
| 1 | AA | 1516 | DC | O4'-C1'-C2' | -6.75 | 100.50 | 105.90 |
| 1 | AA | 1444 | DG | C1'-O4'-C4' | -6.75 | 103.35 | 110.10 |
| 1 | AA | 218 | DA | O4'-C1'-C2' | -6.74 | 100.51 | 105.90 |
| 1 | AA | 163 | DC | O4'-C1'-C2' | -6.74 | 100.51 | 105.90 |
| 1 | AA | 1560 | DA | O4'-C1'-C2' | -6.73 | 100.51 | 105.90 |
| 1 | AA | 1073 | DT | O4'-C4'-C3' | -6.73 | 101.81 | 104.50 |
| 1 | AA | 1097 | DC | O4'-C1'-C2' | -6.72 | 100.52 | 105.90 |
| 1 | AA | 1688 | DC | O4'-C1'-C2' | -6.72 | 100.53 | 105.90 |
| 1 | AA | 1799 | DT | C4'-C3'-C2' | -6.72 | 97.06 | 103.10 |
| 56 | A3 | 19 | DG | O4'-C1'-C2' | -6.71 | 100.53 | 105.90 |
| 1 | AA | 2189 | DT | C4'-C3'-C2' | -6.71 | 97.06 | 103.10 |
| 38 | Al | 18 | DG | C5-C6-O6 | -6.71 | 124.57 | 128.60 |
| 1 | AA | 522 | DG | O4'-C4'-C3' | -6.71 | 101.82 | 104.50 |
| 1 | AA | 372 | DA | O4'-C1'-C2' | -6.71 | 100.53 | 105.90 |
| 8 | AH | 14 | DT | O4'-C1'-C2' | -6.71 | 100.54 | 105.90 |
| 1 | AA | 1813 | DT | O4'-C1'-C2' | -6.70 | 100.54 | 105.90 |
| 52 | Az | 29 | DG | O4'-C1'-C2' | -6.69 | 100.54 | 105.90 |
| 28 | Ab | 18 | DG | O4'-C1'-C2' | -6.69 | 100.55 | 105.90 |
| 12 | AL | 31 | DA | C4'-C3'-C2' | -6.69 | 97.08 | 103.10 |
| 1 | AA | 1079 | DT | O4'-C1'-C2' | -6.69 | 100.55 | 105.90 |
| 18 | AR | 23 | DC | O4'-C1'-C2' | -6.69 | 100.55 | 105.90 |
| 1 | AA | 1053 | DA | O4'-C1'-C2' | -6.68 | 100.55 | 105.90 |
| 5 | AE | 16 | DA | P-O3'-C3' | 6.68 | 127.72 | 119.70 |
| 34 | Ah | 19 | DT | O4'-C1'-C2' | -6.68 | 100.55 | 105.90 |
| 54 | A1 | 6 | DG | O4'-C1'-C2' | -6.68 | 100.55 | 105.90 |
| 1 | AA | 623 | DG | O4'-C1'-C2' | -6.68 | 100.56 | 105.90 |
| 1 | AA | 1644 | DC | P-O5'-C5' | 6.67 | 131.58 | 120.90 |
| 53 | A0 | 30 | DT | O4'-C4'-C3' | -6.67 | 101.83 | 104.50 |
| 1 | AA | 828 | DG | C1'-O4'-C4' | -6.67 | 103.43 | 110.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | AA | 1906 | DA | O4'-C1'-C2' | -6.67 | 100.57 | 105.90 |
| 1 | AA | 2598 | DG | C4'-C3'-C2' | -6.66 | 97.10 | 103.10 |
| 1 | AA | 1175 | DT | C4'-C3'-C2' | -6.66 | 97.11 | 103.10 |
| 1 | AA | 1621 | DC | C4'-C3'-C2' | -6.66 | 97.11 | 103.10 |
| 26 | AZ | 13 | DC | P-O3'-C3' | 6.66 | 127.69 | 119.70 |
| 1 | AA | 1248 | DC | P-O3'-C3' | 6.66 | 127.69 | 119.70 |
| 65 | BC | 6 | DC | C4'-C3'-C2' | -6.66 | 97.11 | 103.10 |
| 1 | AA | 415 | DC | P-O3'-C3' | 6.65 | 127.68 | 119.70 |
| 1 | AA | 1235 | DG | C4'-C3'-C2' | -6.65 | 97.12 | 103.10 |
| 79 | BQ | 26 | DC | O4'-C1'-C2' | -6.65 | 100.58 | 105.90 |
| 13 | AM | 5 | DC | P-O3'-C3' | 6.65 | 127.67 | 119.70 |
| 15 | AO | 1 | DC | O4'-C4'-C3' | -6.65 | 101.84 | 104.50 |
| 3 | AC | 1 | DT | O4'-C4'-C3' | -6.64 | 101.84 | 104.50 |
| 9 | AI | 14 | DG | O4'-C1'-C2' | -6.64 | 100.59 | 105.90 |
| 26 | AZ | 27 | DA | P-O3'-C3' | 6.64 | 127.66 | 119.70 |
| 8 | AH | 37 | DC | O4'-C1'-C2' | -6.63 | 100.59 | 105.90 |
| 1 | AA | 2602 | DT | C4'-C3'-C2' | -6.63 | 97.13 | 103.10 |
| 74 | BL | 23 | DT | P-O3'-C3' | 6.63 | 127.66 | 119.70 |
| 1 | AA | 1682 | DG | C4'-C3'-C2' | -6.63 | 97.13 | 103.10 |
| 1 | AA | 1925 | DG | O4'-C1'-C2' | -6.62 | 100.60 | 105.90 |
| 48 | Av | 16 | DC | O4'-C1'-C2' | -6.62 | 100.60 | 105.90 |
| 69 | BG | 18 | DG | O4'-C1'-C2' | -6.62 | 100.60 | 105.90 |
| 33 | Ag | 1 | DT | C4'-C3'-C2' | -6.62 | 97.14 | 103.10 |
| 1 | AA | 1295 | DA | P-O3'-C3' | 6.62 | 127.64 | 119.70 |
| 1 | AA | 2654 | DG | O4'-C1'-N9 | 6.62 | 112.63 | 108.00 |
| 8 | AH | 1 | DA | O4'-C1'-C2' | -6.62 | 100.61 | 105.90 |
| 32 | Af | 30 | DT | O4'-C1'-C2' | -6.61 | 100.61 | 105.90 |
| 1 | AA | 2406 | DG | O4'-C1'-C2' | -6.61 | 100.61 | 105.90 |
| 12 | AL | 26 | DG | O4'-C1'-C2' | -6.61 | 100.61 | 105.90 |
| 1 | AA | 885 | DC | O4'-C1'-C2' | -6.61 | 100.61 | 105.90 |
| 72 | BJ | 1 | DT | O4'-C4'-C3' | -6.61 | 101.86 | 104.50 |
| 1 | AA | 22 | DT | O4'-C4'-C3' | -6.61 | 101.86 | 104.50 |
| 1 | AA | 653 | DG | O4'-C4'-C3' | -6.61 | 101.86 | 104.50 |
| 25 | AY | 5 | DT | O4'-C4'-C3' | -6.61 | 101.86 | 104.50 |
| 50 | Ax | 18 | DA | N1-C6-N6 | -6.61 | 114.64 | 118.60 |
| 76 | BN | 37 | DC | O4'-C1'-C2' | -6.61 | 100.61 | 105.90 |
| 18 | AR | 9 | DC | O4'-C1'-C2' | -6.60 | 100.62 | 105.90 |
| 42 | Ap | 8 | DG | C4'-C3'-C2' | -6.60 | 97.16 | 103.10 |
| 1 | AA | 591 | DG | O4'-C1'-C2' | -6.59 | 100.62 | 105.90 |
| 42 | Ap | 13 | DG | C1'-O4'-C4' | -6.59 | 103.51 | 110.10 |
| 52 | Az | 26 | DA | C4'-C3'-C2' | -6.59 | 97.17 | 103.10 |
| 1 | AA | 2492 | DC | P-O5'-C5' | 6.59 | 131.44 | 120.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 61 | A8 | 33 | DA | O4'-C1'-C2' | -6.59 | 100.63 | 105.90 |
| 1 | AA | 754 | DT | O4'-C4'-C3' | -6.58 | 101.87 | 104.50 |
| 1 | AA | 2634 | DG | P-O3'-C3' | 6.58 | 127.60 | 119.70 |
| 1 | AA | 479 | DA | O4'-C1'-C2' | -6.58 | 100.63 | 105.90 |
| 22 | AV | 9 | DC | O4'-C4'-C3' | -6.58 | 101.87 | 104.50 |
| 71 | BI | 35 | DC | P-O3'-C3' | 6.58 | 127.60 | 119.70 |
| 68 | BF | 17 | DT | C4'-C3'-C2' | -6.57 | 97.19 | 103.10 |
| 1 | AA | 715 | DT | O4'-C4'-C3' | -6.56 | 101.88 | 104.50 |
| 1 | AA | 1152 | DG | O4'-C1'-C2' | -6.56 | 100.65 | 105.90 |
| 4 | AD | 22 | DA | C1'-O4'-C4' | -6.56 | 103.54 | 110.10 |
| 49 | Aw | 4 | DG | P-O3'-C3' | 6.56 | 127.57 | 119.70 |
| 1 | AA | 22 | DT | O4'-C1'-C2' | -6.56 | 100.65 | 105.90 |
| 1 | AA | 2684 | DT | C4'-C3'-C2' | -6.56 | 97.20 | 103.10 |
| 1 | AA | 2771 | DT | O4'-C1'-C2' | -6.55 | 100.66 | 105.90 |
| 1 | AA | 1295 | DA | O4'-C1'-C2' | -6.55 | 100.66 | 105.90 |
| 68 | BF | 24 | DG | O4'-C1'-C2' | -6.55 | 100.66 | 105.90 |
| 1 | AA | 316 | DG | O4'-C1'-C2' | -6.55 | 100.66 | 105.90 |
| 1 | AA | 2199 | DG | C1'-O4'-C4' | -6.53 | 103.57 | 110.10 |
| 34 | Ah | 34 | DT | O4'-C1'-C2' | -6.53 | 100.67 | 105.90 |
| 15 | AO | 2 | DA | P-O3'-C3' | 6.53 | 127.54 | 119.70 |
| 1 | AA | 900 | DG | O4'-C4'-C3' | -6.53 | 101.89 | 104.50 |
| 74 | BL | 18 | DG | C1'-O4'-C4' | -6.53 | 103.57 | 110.10 |
| 79 | BQ | 18 | DT | O4'-C4'-C3' | -6.53 | 101.89 | 104.50 |
| 49 | Aw | 35 | DG | O4'-C4'-C3' | -6.53 | 101.89 | 104.50 |
| 1 | AA | 2619 | DA | P-O3'-C3' | 6.52 | 127.53 | 119.70 |
| 1 | AA | 68 | DG | C1'-O4'-C4' | -6.52 | 103.58 | 110.10 |
| 63 | BA | 31 | DC | P-O3'-C3' | 6.52 | 127.52 | 119.70 |
| 24 | AX | 20 | DG | O4'-C1'-C2' | -6.51 | 100.69 | 105.90 |
| 1 | AA | 975 | DA | P-O3'-C3' | 6.51 | 127.51 | 119.70 |
| 1 | AA | 2769 | DG | P-O3'-C3' | 6.51 | 127.52 | 119.70 |
| 1 | AA | 2280 | DC | O4'-C1'-C2' | -6.50 | 100.70 | 105.90 |
| 1 | AA | 2532 | DG | O4'-C1'-C2' | -6.50 | 100.70 | 105.90 |
| 8 | AH | 23 | DT | P-O3'-C3' | 6.50 | 127.50 | 119.70 |
| 19 | AS | 31 | DA | O4'-C1'-C2' | -6.50 | 100.70 | 105.90 |
| 1 | AA | 2420 | DG | O4'-C4'-C3' | -6.49 | 101.90 | 104.50 |
| 68 | BF | 20 | DG | P-O3'-C3' | 6.48 | 127.48 | 119.70 |
| 1 | AA | 210 | DC | C1'-O4'-C4' | -6.48 | 103.62 | 110.10 |
| 1 | AA | 754 | DT | C4'-C3'-C2' | -6.48 | 97.27 | 103.10 |
| 1 | AA | 359 | DG | C1'-O4'-C4' | -6.48 | 103.62 | 110.10 |
| 1 | AA | 2355 | DA | O4'-C4'-C3' | -6.48 | 101.91 | 104.50 |
| 26 | AZ | 41 | DT | O4'-C4'-C3' | -6.47 | 101.91 | 104.50 |
| 1 | AA | 1714 | DT | C4'-C3'-C2' | -6.46 | 97.28 | 103.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 71 | BI | 7 | DA | C1'-O4'-C4' | -6.46 | 103.64 | 110.10 |
| 75 | BM | 30 | DG | P-O3'-C3' | 6.46 | 127.45 | 119.70 |
| 1 | AA | 1401 | DG | P-O3'-C3' | 6.46 | 127.45 | 119.70 |
| 4 | AD | 1 | DT | O4'-C1'-C2' | -6.46 | 100.73 | 105.90 |
| 1 | AA | 65 | DT | O4'-C1'-C2' | -6.45 | 100.74 | 105.90 |
| 1 | AA | 845 | DG | C1'-O4'-C4' | -6.45 | 103.65 | 110.10 |
| 37 | Ak | 16 | DG | C1'-O4'-C4' | -6.45 | 103.65 | 110.10 |
| 1 | AA | 894 | DA | O4'-C1'-C2' | -6.45 | 100.74 | 105.90 |
| 1 | AA | 1970 | DG | C1'-O4'-C4' | -6.45 | 103.65 | 110.10 |
| 14 | AN | 9 | DA | O4'-C1'-C2' | -6.45 | 100.74 | 105.90 |
| 1 | AA | 2285 | DC | O4'-C1'-C2' | -6.45 | 100.74 | 105.90 |
| 1 | AA | 2223 | DG | C4'-C3'-C2' | -6.44 | 97.30 | 103.10 |
| 5 | AE | 1 | DT | C1'-O4'-C4' | -6.44 | 103.66 | 110.10 |
| 1 | AA | 923 | DG | O4'-C1'-C2' | -6.44 | 100.75 | 105.90 |
| 19 | AS | 16 | DT | C4'-C3'-C2' | -6.44 | 97.30 | 103.10 |
| 22 | AV | 19 | DC | P-O3'-C3' | 6.44 | 127.43 | 119.70 |
| 44 | Ar | 47 | DG | C5-C6-O6 | -6.43 | 124.74 | 128.60 |
| 22 | AV | 33 | DA | C1'-O4'-C4' | -6.43 | 103.67 | 110.10 |
| 46 | At | 26 | DA | O4'-C1'-C2' | -6.43 | 100.76 | 105.90 |
| 69 | BG | 30 | DT | C4'-C3'-C2' | -6.43 | 97.31 | 103.10 |
| 4 | AD | 29 | DA | O4'-C1'-C2' | -6.43 | 100.76 | 105.90 |
| 73 | BK | 6 | DG | O4'-C4'-C3' | -6.42 | 101.93 | 104.50 |
| 1 | AA | 946 | DG | C1'-O4'-C4' | -6.42 | 103.68 | 110.10 |
| 7 | AG | 10 | DG | O4'-C1'-C2' | -6.42 | 100.77 | 105.90 |
| 1 | AA | 1851 | DA | O4'-C1'-C2' | -6.42 | 100.77 | 105.90 |
| 1 | AA | 2212 | DA | P-O3'-C3' | 6.42 | 127.40 | 119.70 |
| 1 | AA | 1265 | DG | P-O3'-C3' | 6.41 | 127.40 | 119.70 |
| 1 | AA | 247 | DC | C4'-C3'-C2' | -6.41 | 97.33 | 103.10 |
| 44 | Ar | 23 | DA | C1'-O4'-C4' | -6.41 | 103.69 | 110.10 |
| 1 | AA | 1133 | DC | O4'-C1'-C2' | -6.41 | 100.78 | 105.90 |
| 1 | AA | 2541 | DG | P-O3'-C3' | 6.41 | 127.39 | 119.70 |
| 51 | Ay | 9 | DA | O4'-C1'-C2' | -6.41 | 100.78 | 105.90 |
| 1 | AA | 139 | DA | N1-C6-N6 | -6.40 | 114.76 | 118.60 |
| 5 | AE | 20 | DA | O4'-C1'-N9 | -6.40 | 103.52 | 108.00 |
| 32 | Af | 32 | DT | C4'-C3'-C2' | -6.40 | 97.34 | 103.10 |
| 1 | AA | 298 | DG | O4'-C1'-C2' | -6.40 | 100.78 | 105.90 |
| 1 | AA | 404 | DC | O4'-C1'-C2' | -6.40 | 100.78 | 105.90 |
| 26 | AZ | 9 | DC | O4'-C1'-C2' | -6.40 | 100.78 | 105.90 |
| 1 | AA | 396 | DG | O4'-C1'-C2' | -6.39 | 100.78 | 105.90 |
| 44 | Ar | 7 | DC | O4'-C1'-C2' | -6.39 | 100.78 | 105.90 |
| 23 | AW | 16 | DT | O4'-C4'-C3' | -6.39 | 101.94 | 104.50 |
| 1 | AA | 468 | DG | O4'-C1'-C2' | -6.39 | 100.79 | 105.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | AA | 1409 | DC | P-O3'-C3' | 6.39 | 127.37 | 119.70 |
| 12 | AL | 20 | DT | C4'-C3'-C2' | -6.39 | 97.35 | 103.10 |
| 62 | A9 | 40 | DG | N1-C6-O6 | 6.38 | 123.73 | 119.90 |
| 1 | AA | 2443 | DC | P-O3'-C3' | 6.38 | 127.36 | 119.70 |
| 1 | AA | 2657 | DA | C4'-C3'-C2' | -6.38 | 97.36 | 103.10 |
| 42 | Ap | 14 | DA | O4'-C1'-C2' | -6.38 | 100.80 | 105.90 |
| 72 | BJ | 17 | DG | O4'-C1'-C2' | -6.38 | 100.80 | 105.90 |
| 1 | AA | 454 | DA | C1'-O4'-C4' | -6.37 | 103.73 | 110.10 |
| 13 | AM | 40 | DG | C1'-O4'-C4' | -6.37 | 103.73 | 110.10 |
| 1 | AA | 531 | DT | P-O3'-C3' | 6.37 | 127.34 | 119.70 |
| 1 | AA | 1910 | DA | O4'-C1'-C2' | -6.37 | 100.80 | 105.90 |
| 49 | Aw | 35 | DG | C1'-O4'-C4' | -6.37 | 103.73 | 110.10 |
| 1 | AA | 2504 | DT | P-O3'-C3' | 6.37 | 127.34 | 119.70 |
| 1 | AA | 1195 | DT | C4'-C3'-C2' | -6.36 | 97.38 | 103.10 |
| 32 | Af | 30 | DT | C1'-O4'-C4' | -6.36 | 103.74 | 110.10 |
| 1 | AA | 1538 | DC | O4'-C4'-C3' | -6.36 | 101.96 | 104.50 |
| 1 | AA | 1826 | DC | C6-N1-C2 | -6.36 | 117.76 | 120.30 |
| 1 | AA | 705 | DA | O4'-C1'-C2' | -6.35 | 100.82 | 105.90 |
| 1 | AA | 989 | DA | O4'-C1'-C2' | -6.35 | 100.82 | 105.90 |
| 1 | AA | 1784 | DC | C6-N1-C2 | -6.34 | 117.76 | 120.30 |
| 1 | AA | 2199 | DG | P-O3'-C3' | 6.34 | 127.31 | 119.70 |
| 58 | A5 | 28 | DT | P-O3'-C3' | 6.33 | 127.30 | 119.70 |
| 61 | A8 | 20 | DT | C4'-C3'-C2' | -6.33 | 97.40 | 103.10 |
| 1 | AA | 1286 | DA | P-O3'-C3' | 6.33 | 127.30 | 119.70 |
| 15 | AO | 41 | DG | N1-C6-O6 | 6.33 | 123.70 | 119.90 |
| 65 | BC | 6 | DC | O4'-C4'-C3' | -6.33 | 101.97 | 104.50 |
| 1 | AA | 1898 | DG | C4'-C3'-C2' | -6.33 | 97.41 | 103.10 |
| 1 | AA | 2090 | DG | C5-C6-O6 | -6.32 | 124.81 | 128.60 |
| 71 | BI | 10 | DG | O4'-C1'-C2' | -6.32 | 100.84 | 105.90 |
| 1 | AA | 1818 | DG | O4'-C1'-C2' | -6.32 | 100.84 | 105.90 |
| 41 | Ao | 10 | DT | P-O3'-C3' | 6.32 | 127.28 | 119.70 |
| 54 | A1 | 17 | DA | O4'-C1'-C2' | -6.32 | 100.85 | 105.90 |
| 1 | AA | 881 | DT | C1'-O4'-C4' | -6.31 | 103.79 | 110.10 |
| 3 | AC | 10 | DC | P-O3'-C3' | 6.31 | 127.28 | 119.70 |
| 1 | AA | 2296 | DC | O4'-C1'-C2' | -6.31 | 100.85 | 105.90 |
| 1 | AA | 2340 | DG | O4'-C1'-C2' | -6.31 | 100.85 | 105.90 |
| 1 | AA | 779 | DA | O4'-C1'-C2' | -6.31 | 100.85 | 105.90 |
| 60 | A7 | 8 | DG | O4'-C1'-C2' | -6.31 | 100.85 | 105.90 |
| 1 | AA | 123 | DA | P-O3'-C3' | 6.30 | 127.27 | 119.70 |
| 1 | AA | 918 | DA | O4'-C1'-C2' | -6.30 | 100.86 | 105.90 |
| 1 | AA | 2791 | DT | C4'-C3'-C2' | -6.30 | 97.43 | 103.10 |
| 68 | BF | 22 | DC | P-O3'-C3' | 6.30 | 127.26 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | AA | 2479 | DC | P-O3'-C3' | 6.30 | 127.26 | 119.70 |
| 1 | AA | 1624 | DG | P-O3'-C3' | 6.30 | 127.26 | 119.70 |
| 1 | AA | 15 | DG | O4'-C1'-C2' | -6.29 | 100.86 | 105.90 |
| 10 | AJ | 3 | DT | O4'-C1'-C2' | -6.29 | 100.87 | 105.90 |
| 41 | Ao | 21 | DC | O4'-C1'-N1 | 6.29 | 112.41 | 108.00 |
| 1 | AA | 1947 | DC | P-O3'-C3' | 6.28 | 127.23 | 119.70 |
| 5 | AE | 29 | DA | P-O3'-C3' | 6.28 | 127.24 | 119.70 |
| 1 | AA | 1305 | DG | O4'-C1'-C2' | -6.28 | 100.88 | 105.90 |
| 16 | AP | 9 | DG | C1'-O4'-C4' | -6.28 | 103.82 | 110.10 |
| 1 | AA | 511 | DG | O4'-C1'-C2' | -6.28 | 100.88 | 105.90 |
| 27 | Aa | 30 | DT | O4'-C1'-C2' | -6.28 | 100.88 | 105.90 |
| 43 | Aq | 1 | DT | C1'-O4'-C4' | -6.28 | 103.83 | 110.10 |
| 27 | Aa | 41 | DT | O4'-C4'-C3' | -6.27 | 101.99 | 104.50 |
| 1 | AA | 2280 | DC | O4'-C1'-N1 | 6.27 | 112.39 | 108.00 |
| 19 | AS | 12 | DG | C4'-C3'-C2' | -6.27 | 97.46 | 103.10 |
| 10 | AJ | 19 | DT | O4'-C1'-C2' | -6.26 | 100.89 | 105.90 |
| 1 | AA | 1430 | DG | P-O3'-C3' | 6.26 | 127.22 | 119.70 |
| 1 | AA | 435 | DT | P-O3'-C3' | 6.26 | 127.22 | 119.70 |
| 1 | AA | 1203 | DA | N1-C6-N6 | -6.26 | 114.84 | 118.60 |
| 1 | AA | 2285 | DC | C1'-O4'-C4' | -6.25 | 103.84 | 110.10 |
| 79 | BQ | 18 | DT | C4'-C3'-C2' | -6.25 | 97.47 | 103.10 |
| 1 | AA | 1994 | DC | O4'-C1'-C2' | -6.25 | 100.90 | 105.90 |
| 1 | AA | 433 | DA | P-O3'-C3' | 6.24 | 127.18 | 119.70 |
| 63 | BA | 22 | DA | O4'-C1'-C2' | -6.24 | 100.91 | 105.90 |
| 40 | An | 14 | DG | O4'-C4'-C3' | -6.24 | 102.01 | 104.50 |
| 1 | AA | 2822 | DT | C4'-C3'-C2' | -6.23 | 97.49 | 103.10 |
| 38 | Al | 18 | DG | N1-C6-O6 | 6.23 | 123.64 | 119.90 |
| 1 | AA | 1671 | DA | O4'-C1'-C2' | -6.23 | 100.92 | 105.90 |
| 45 | As | 16 | DA | P-O3'-C3' | 6.23 | 127.18 | 119.70 |
| 76 | BN | 12 | DT | C4'-C3'-C2' | -6.23 | 97.49 | 103.10 |
| 1 | AA | 1150 | DA | P-O3'-C3' | 6.23 | 127.17 | 119.70 |
| 1 | AA | 2026 | DG | O4'-C1'-C2' | -6.23 | 100.92 | 105.90 |
| 1 | AA | 2461 | DC | O4'-C1'-C2' | -6.23 | 100.92 | 105.90 |
| 42 | Ap | 25 | DT | P-O3'-C3' | 6.22 | 127.17 | 119.70 |
| 1 | AA | 2491 | DC | C1'-O4'-C4' | -6.22 | 103.88 | 110.10 |
| 70 | BH | 16 | DT | C1'-O4'-C4' | -6.22 | 103.88 | 110.10 |
| 1 | AA | 1540 | DT | C1'-O4'-C4' | -6.22 | 103.88 | 110.10 |
| 42 | Ap | 8 | DG | N1-C6-O6 | 6.22 | 123.63 | 119.90 |
| 71 | BI | 30 | DA | C4'-C3'-C2' | -6.22 | 97.50 | 103.10 |
| 44 | Ar | 47 | DG | N1-C6-O6 | 6.22 | 123.63 | 119.90 |
| 9 | AI | 23 | DC | O4'-C1'-C2' | -6.21 | 100.93 | 105.90 |
| 1 | AA | 2393 | DG | C4'-C3'-C2' | -6.21 | 97.51 | 103.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | AA | 2242 | DG | O4'-C4'-C3' | -6.21 | 102.02 | 104.50 |
| 1 | AA | 980 | DG | N1-C6-O6 | 6.21 | 123.62 | 119.90 |
| 1 | AA | 2318 | DC | C1'-O4'-C4' | -6.20 | 103.90 | 110.10 |
| 1 | AA | 1365 | DT | C1'-O4'-C4' | -6.20 | 103.90 | 110.10 |
| 28 | Ab | 9 | DA | P-O3'-C3' | 6.20 | 127.14 | 119.70 |
| 27 | Aa | 37 | DA | O4'-C4'-C3' | -6.19 | 102.02 | 104.50 |
| 69 | BG | 6 | DC | P-O5'-C5' | 6.19 | 130.81 | 120.90 |
| 1 | AA | 2388 | DC | O4'-C1'-C2' | -6.19 | 100.95 | 105.90 |
| 37 | Ak | 37 | DT | C4'-C3'-C2' | -6.19 | 97.53 | 103.10 |
| 11 | AK | 30 | DT | C4'-C3'-C2' | -6.18 | 97.54 | 103.10 |
| 16 | AP | 5 | DG | O4'-C1'-C2' | -6.18 | 100.96 | 105.90 |
| 60 | A7 | 10 | DT | C4'-C3'-C2' | -6.18 | 97.54 | 103.10 |
| 12 | AL | 5 | DC | O4'-C4'-C3' | -6.17 | 102.03 | 104.50 |
| 27 | Aa | 1 | DT | C1'-O4'-C4' | -6.17 | 103.93 | 110.10 |
| 1 | AA | 2074 | DT | C4'-C3'-C2' | -6.17 | 97.55 | 103.10 |
| 1 | AA | 387 | DG | O4'-C1'-C2' | -6.17 | 100.97 | 105.90 |
| 61 | A8 | 30 | DG | O4'-C1'-C2' | -6.16 | 100.97 | 105.90 |
| 74 | BL | 31 | DT | O4'-C4'-C3' | -6.16 | 102.03 | 104.50 |
| 46 | At | 34 | DG | O4'-C1'-C2' | -6.16 | 100.97 | 105.90 |
| 1 | AA | 1900 | DG | O4'-C4'-C3' | -6.16 | 102.04 | 104.50 |
| 50 | Ax | 9 | DG | C1'-O4'-C4' | -6.16 | 103.94 | 110.10 |
| 1 | AA | 761 | DG | O4'-C1'-C2' | -6.16 | 100.97 | 105.90 |
| 43 | Aq | 19 | DA | O4'-C1'-C2' | -6.16 | 100.97 | 105.90 |
| 1 | AA | 1504 | DG | C4'-C3'-C2' | -6.15 | 97.56 | 103.10 |
| 57 | A4 | 10 | DC | P-O3'-C3' | 6.15 | 127.08 | 119.70 |
| 10 | AJ | 30 | DT | O4'-C1'-N1 | 6.14 | 112.30 | 108.00 |
| 35 | Ai | 27 | DG | O4'-C1'-C2' | -6.14 | 100.99 | 105.90 |
| 1 | AA | 1518 | DA | O4'-C1'-N9 | 6.13 | 112.30 | 108.00 |
| 1 | AA | 1057 | DT | C6-C5-C7 | -6.13 | 119.22 | 122.90 |
| 1 | AA | 2539 | DT | O4'-C4'-C3' | -6.13 | 102.05 | 104.50 |
| 21 | AU | 10 | DG | O4'-C1'-C2' | -6.13 | 101.00 | 105.90 |
| 40 | An | 12 | DG | O4'-C1'-C2' | -6.13 | 101.00 | 105.90 |
| 1 | AA | 2488 | DG | P-O3'-C3' | 6.13 | 127.06 | 119.70 |
| 54 | A1 | 45 | DT | O4'-C1'-N1 | 6.13 | 112.29 | 108.00 |
| 74 | BL | 31 | DT | C4'-C3'-C2' | -6.13 | 97.58 | 103.10 |
| 22 | AV | 37 | DG | O4'-C1'-C2' | -6.13 | 101.00 | 105.90 |
| 1 | AA | 20 | DT | C4'-C3'-C2' | -6.13 | 97.59 | 103.10 |
| 1 | AA | 2798 | DC | O4'-C1'-C2' | -6.13 | 101.00 | 105.90 |
| 49 | Aw | 30 | DG | O4'-C1'-N9 | 6.12 | 112.29 | 108.00 |
| 1 | AA | 832 | DC | P-O5'-C5' | 6.12 | 130.69 | 120.90 |
| 18 | AR | 28 | DT | C1'-O4'-C4' | -6.12 | 103.98 | 110.10 |
| 1 | AA | 547 | DT | P-O3'-C3' | 6.12 | 127.04 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 15 | AO | 41 | DG | C5-C6-O6 | -6.11 | 124.93 | 128.60 |
| 74 | BL | 9 | DG | O4'-C1'-C2' | -6.11 | 101.01 | 105.90 |
| 1 | AA | 2434 | DC | O4'-C4'-C3' | -6.11 | 102.06 | 104.50 |
| 58 | A5 | 13 | DT | C4'-C3'-C2' | -6.10 | 97.61 | 103.10 |
| 1 | AA | 879 | DG | O4'-C1'-N9 | 6.10 | 112.27 | 108.00 |
| 49 | Aw | 4 | DG | C1'-O4'-C4' | -6.10 | 104.00 | 110.10 |
| 60 | A7 | 20 | DG | O4'-C1'-C2' | -6.10 | 101.02 | 105.90 |
| 72 | BJ | 24 | DG | O4'-C4'-C3' | -6.10 | 102.06 | 104.50 |
| 24 | AX | 23 | DG | O4'-C1'-C2' | -6.10 | 101.02 | 105.90 |
| 1 | AA | 1019 | DT | C4'-C3'-C2' | -6.10 | 97.61 | 103.10 |
| 1 | AA | 1470 | DT | P-O3'-C3' | 6.09 | 127.01 | 119.70 |
| 13 | AM | 34 | DT | O4'-C4'-C3' | -6.09 | 102.06 | 104.50 |
| 42 | Ap | 16 | DA | O4'-C1'-C2' | -6.09 | 101.03 | 105.90 |
| 2 | AB | 2 | DT | O4'-C1'-C2' | -6.09 | 101.03 | 105.90 |
| 1 | AA | 2778 | DG | O4'-C1'-C2' | -6.09 | 101.03 | 105.90 |
| 65 | BC | 29 | DT | C1'-O4'-C4' | -6.09 | 104.01 | 110.10 |
| 70 | BH | 37 | DA | O4'-C1'-C2' | -6.08 | 101.04 | 105.90 |
| 1 | AA | 1994 | DC | P-O3'-C3' | 6.08 | 127.00 | 119.70 |
| 68 | BF | 1 | DT | O4'-C1'-C2' | -6.08 | 101.04 | 105.90 |
| 1 | AA | 1410 | DG | O4'-C1'-N9 | 6.07 | 112.25 | 108.00 |
| 60 | A7 | 1 | DT | O4'-C1'-N1 | 6.07 | 112.25 | 108.00 |
| 1 | AA | 1265 | DG | O4'-C1'-C2' | -6.07 | 101.05 | 105.90 |
| 1 | AA | 166 | DT | C4'-C3'-C2' | -6.06 | 97.64 | 103.10 |
| 19 | AS | 16 | DT | O4'-C4'-C3' | -6.06 | 102.07 | 104.50 |
| 1 | AA | 836 | DT | P-O3'-C3' | 6.06 | 126.97 | 119.70 |
| 1 | AA | 2532 | DG | C5-C6-O6 | -6.06 | 124.96 | 128.60 |
| 47 | Au | 24 | DT | C4'-C3'-C2' | -6.06 | 97.64 | 103.10 |
| 1 | AA | 1189 | DG | O4'-C1'-N9 | 6.06 | 112.24 | 108.00 |
| 1 | AA | 1886 | DC | C6-N1-C2 | -6.05 | 117.88 | 120.30 |
| 1 | AA | 1895 | DC | C6-N1-C2 | -6.05 | 117.88 | 120.30 |
| 62 | A9 | 40 | DG | C5-C6-O6 | -6.05 | 124.97 | 128.60 |
| 6 | AF | 1 | DT | O4'-C1'-C2' | -6.05 | 101.06 | 105.90 |
| 2 | AB | 22 | DC | O4'-C1'-C2' | -6.04 | 101.07 | 105.90 |
| 1 | AA | 156 | DC | P-O3'-C3' | 6.04 | 126.95 | 119.70 |
| 1 | AA | 631 | DA | C4'-C3'-C2' | -6.04 | 97.66 | 103.10 |
| 1 | AA | 956 | DT | C4'-C3'-C2' | -6.04 | 97.67 | 103.10 |
| 1 | AA | 1474 | DG | C4'-C3'-C2' | -6.04 | 97.67 | 103.10 |
| 1 | AA | 1524 | DA | C4'-C3'-C2' | -6.04 | 97.67 | 103.10 |
| 28 | Ab | 40 | DG | C1'-O4'-C4' | -6.04 | 104.06 | 110.10 |
| 63 | BA | 10 | DC | O4'-C4'-C3' | -6.03 | 102.09 | 104.50 |
| 56 | A3 | 14 | DG | O4'-C1'-C2' | -6.03 | 101.08 | 105.90 |
| 75 | BM | 39 | DC | P-O3'-C3' | 6.02 | 126.93 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | BP | 19 | DT | P-O3'-C3' | 6.02 | 126.93 | 119.70 |
| 1 | AA | 84 | DC | O4'-C1'-C2' | -6.02 | 101.09 | 105.90 |
| 1 | AA | 2099 | DG | O4'-C1'-C2' | -6.02 | 101.09 | 105.90 |
| 10 | AJ | 30 | DT | C1'-O4'-C4' | -6.02 | 104.08 | 110.10 |
| 1 | AA | 2605 | DG | O4'-C1'-C2' | -6.01 | 101.09 | 105.90 |
| 23 | AW | 16 | DT | C4'-C3'-C2' | -6.01 | 97.69 | 103.10 |
| 46 | At | 40 | DG | C1'-O4'-C4' | -6.01 | 104.09 | 110.10 |
| 1 | AA | 1005 | DT | C4'-C3'-C2' | -6.00 | 97.69 | 103.10 |
| 1 | AA | 2090 | DG | N1-C6-O6 | 6.00 | 123.50 | 119.90 |
| 77 | BO | 16 | DC | O4'-C1'-C2' | -6.00 | 101.10 | 105.90 |
| 1 | AA | 2639 | DT | C1'-O4'-C4' | -6.00 | 104.10 | 110.10 |
| 1 | AA | 33 | DC | C4'-C3'-C2' | -5.99 | 97.71 | 103.10 |
| 1 | AA | 952 | DT | C4'-C3'-C2' | -5.99 | 97.71 | 103.10 |
| 15 | AO | 43 | DA | O4'-C1'-C2' | -5.99 | 101.11 | 105.90 |
| 1 | AA | 417 | DC | O4'-C4'-C3' | -5.99 | 102.11 | 104.50 |
| 1 | AA | 1871 | DT | O4'-C1'-C2' | -5.99 | 101.11 | 105.90 |
| 1 | AA | 1279 | DT | C4'-C3'-C2' | -5.98 | 97.72 | 103.10 |
| 67 | BE | 23 | DT | O4'-C1'-C2' | -5.98 | 101.11 | 105.90 |
| 1 | AA | 2654 | DG | C1'-O4'-C4' | -5.98 | 104.12 | 110.10 |
| 12 | AL | 20 | DT | O4'-C4'-C3' | -5.98 | 102.11 | 104.50 |
| 25 | AY | 19 | DT | O4'-C4'-C3' | -5.98 | 102.11 | 104.50 |
| 1 | AA | 935 | DT | C4'-C3'-C2' | -5.97 | 97.72 | 103.10 |
| 1 | AA | 1207 | DA | O4'-C4'-C3' | -5.97 | 102.11 | 104.50 |
| 1 | AA | 889 | DC | O4'-C1'-C2' | -5.97 | 101.12 | 105.90 |
| 1 | AA | 1685 | DT | P-O3'-C3' | 5.97 | 126.87 | 119.70 |
| 63 | BA | 9 | DG | O4'-C1'-C2' | -5.97 | 101.12 | 105.90 |
| 34 | Ah | 9 | DT | O4'-C1'-N1 | 5.97 | 112.18 | 108.00 |
| 1 | AA | 2626 | DT | O4'-C1'-C2' | -5.97 | 101.13 | 105.90 |
| 35 | Ai | 15 | DA | P-O3'-C3' | 5.97 | 126.86 | 119.70 |
| 64 | BB | 34 | DA | O4'-C1'-C2' | -5.96 | 101.13 | 105.90 |
| 65 | BC | 23 | DT | C4'-C3'-C2' | -5.96 | 97.73 | 103.10 |
| 33 | Ag | 14 | DA | O4'-C1'-C2' | -5.96 | 101.13 | 105.90 |
| 65 | BC | 14 | DG | C1'-O4'-C4' | -5.96 | 104.14 | 110.10 |
| 1 | AA | 1410 | DG | C1'-O4'-C4' | -5.96 | 104.14 | 110.10 |
| 1 | AA | 2263 | DC | C4'-C3'-C2' | -5.96 | 97.74 | 103.10 |
| 68 | BF | 19 | DT | O4'-C1'-C2' | -5.95 | 101.14 | 105.90 |
| 1 | AA | 261 | DA | N1-C6-N6 | -5.95 | 115.03 | 118.60 |
| 1 | AA | 1950 | DC | O4'-C1'-C2' | -5.95 | 101.14 | 105.90 |
| 77 | BO | 30 | DA | O4'-C4'-C3' | -5.95 | 102.12 | 104.50 |
| 1 | AA | 2154 | DG | C5-C6-O6 | -5.95 | 125.03 | 128.60 |
| 13 | AM | 22 | DA | P-O3'-C3' | 5.95 | 126.84 | 119.70 |
| 1 | AA | 1864 | DG | P-O3'-C3' | 5.95 | 126.84 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | AV | 11 | DA | O4'-C1'-C2' | -5.95 | 101.14 | 105.90 |
| 1 | AA | 1301 | DT | C4'-C3'-C2' | -5.94 | 97.75 | 103.10 |
| 1 | AA | 1575 | DG | C1'-O4'-C4' | -5.94 | 104.16 | 110.10 |
| 52 | Az | 31 | DA | O4'-C1'-C2' | -5.94 | 101.15 | 105.90 |
| 1 | AA | 1385 | DG | O4'-C1'-C2' | -5.94 | 101.15 | 105.90 |
| 36 | Aj | 4 | DG | O4'-C1'-C2' | -5.94 | 101.15 | 105.90 |
| 1 | AA | 1538 | DC | C4'-C3'-C2' | -5.93 | 97.76 | 103.10 |
| 35 | Ai | 8 | DG | N1-C6-O6 | 5.93 | 123.46 | 119.90 |
| 1 | AA | 821 | DT | O4'-C4'-C3' | -5.93 | 102.13 | 104.50 |
| 1 | AA | 1524 | DA | N1-C6-N6 | -5.93 | 115.04 | 118.60 |
| 1 | AA | 2845 | DT | O4'-C4'-C3' | -5.93 | 102.13 | 104.50 |
| 4 | AD | 10 | DT | C4'-C3'-C2' | -5.93 | 97.77 | 103.10 |
| 1 | AA | 200 | DC | O4'-C1'-C2' | -5.92 | 101.16 | 105.90 |
| 1 | AA | 1313 | DA | O4'-C1'-C2' | -5.92 | 101.16 | 105.90 |
| 35 | Ai | 22 | DC | P-O5'-C5' | 5.92 | 130.38 | 120.90 |
| 1 | AA | 1804 | DA | C1'-O4'-C4' | -5.92 | 104.18 | 110.10 |
| 1 | AA | 518 | DC | O4'-C1'-C2' | -5.92 | 101.17 | 105.90 |
| 1 | AA | 539 | DG | O4'-C1'-C2' | -5.92 | 101.17 | 105.90 |
| 1 | AA | 1585 | DA | P-O3'-C3' | 5.92 | 126.80 | 119.70 |
| 1 | AA | 2585 | DG | O4'-C1'-C2' | -5.92 | 101.17 | 105.90 |
| 15 | AO | 1 | DC | C1'-O4'-C4' | -5.92 | 104.18 | 110.10 |
| 45 | As | 39 | DG | C4'-C3'-C2' | -5.92 | 97.78 | 103.10 |
| 78 | BP | 19 | DT | O4'-C1'-C2' | -5.92 | 101.17 | 105.90 |
| 1 | AA | 2641 | DG | O4'-C1'-C2' | -5.92 | 101.17 | 105.90 |
| 34 | Ah | 12 | DT | C1'-O4'-C4' | -5.92 | 104.19 | 110.10 |
| 1 | AA | 1719 | DT | O4'-C4'-C3' | -5.91 | 102.14 | 104.50 |
| 1 | AA | 1934 | DC | O4'-C4'-C3' | -5.91 | 102.14 | 104.50 |
| 1 | AA | 2459 | DT | C4'-C3'-C2' | -5.91 | 97.78 | 103.10 |
| 30 | Ad | 19 | DG | O4'-C1'-C2' | -5.91 | 101.17 | 105.90 |
| 1 | AA | 361 | DT | O4'-C4'-C3' | -5.91 | 102.14 | 104.50 |
| 27 | Aa | 6 | DT | P-O3'-C3' | 5.91 | 126.79 | 119.70 |
| 40 | An | 9 | DA | P-O3'-C3' | 5.91 | 126.79 | 119.70 |
| 6 | AF | 11 | DT | C1'-O4'-C4' | -5.91 | 104.19 | 110.10 |
| 56 | A3 | 39 | DT | C4'-C3'-C2' | -5.91 | 97.79 | 103.10 |
| 62 | A9 | 39 | DG | P-O3'-C3' | 5.90 | 126.78 | 119.70 |
| 1 | AA | 1134 | DC | O4'-C1'-C2' | -5.90 | 101.18 | 105.90 |
| 15 | AO | 17 | DT | C4'-C3'-C2' | -5.90 | 97.79 | 103.10 |
| 56 | A3 | 4 | DT | O4'-C1'-C2' | -5.90 | 101.18 | 105.90 |
| 1 | AA | 188 | DT | C4'-C3'-C2' | -5.90 | 97.79 | 103.10 |
| 23 | AW | 9 | DG | C1'-O4'-C4' | -5.90 | 104.20 | 110.10 |
| 52 | Az | 30 | DG | O4'-C1'-N9 | 5.89 | 112.12 | 108.00 |
| 1 | AA | 445 | DT | C4'-C3'-C2' | -5.89 | 97.80 | 103.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | AA | 1258 | DT | O4'-C1'-C2' | -5.89 | 101.19 | 105.90 |
| 28 | Ab | 9 | DA | C1'-O4'-C4' | -5.89 | 104.21 | 110.10 |
| 9 | AI | 18 | DG | O4'-C1'-C2' | -5.89 | 101.19 | 105.90 |
| 1 | AA | 2619 | DA | O4'-C1'-C2' | -5.89 | 101.19 | 105.90 |
| 1 | AA | 2856 | DT | C4'-C3'-C2' | -5.89 | 97.80 | 103.10 |
| 35 | Ai | 49 | DG | C5-C6-O6 | -5.89 | 125.07 | 128.60 |
| 1 | AA | 1626 | DG | C1'-O4'-C4' | -5.89 | 104.21 | 110.10 |
| 6 | AF | 6 | DC | P-O5'-C5' | 5.88 | 130.32 | 120.90 |
| 16 | AP | 9 | DG | P-O3'-C3' | 5.88 | 126.76 | 119.70 |
| 1 | AA | 879 | DG | C1'-O4'-C4' | -5.88 | 104.22 | 110.10 |
| 1 | AA | 1302 | DA | C4'-C3'-C2' | -5.88 | 97.81 | 103.10 |
| 1 | AA | 2263 | DC | O4'-C4'-C3' | -5.88 | 102.15 | 104.50 |
| 76 | BN | 29 | DG | O4'-C4'-C3' | -5.88 | 102.15 | 104.50 |
| 26 | AZ | 41 | DT | P-O3'-C3' | 5.87 | 126.75 | 119.70 |
| 58 | A5 | 15 | DA | C4'-C3'-C2' | -5.87 | 97.81 | 103.10 |
| 1 | AA | 1057 | DT | C4-C5-C7 | 5.87 | 122.52 | 119.00 |
| 29 | Ac | 33 | DG | O4'-C1'-C2' | -5.87 | 101.20 | 105.90 |
| 63 | BA | 5 | DG | C5-C6-O6 | -5.87 | 125.08 | 128.60 |
| 1 | AA | 109 | DA | N1-C6-N6 | -5.87 | 115.08 | 118.60 |
| 1 | AA | 1104 | DC | C4'-C3'-C2' | -5.87 | 97.82 | 103.10 |
| 1 | AA | 1804 | DA | O4'-C1'-N9 | 5.87 | 112.11 | 108.00 |
| 67 | BE | 22 | DG | O4'-C4'-C3' | -5.87 | 102.15 | 104.50 |
| 1 | AA | 1330 | DG | N1-C6-O6 | 5.87 | 123.42 | 119.90 |
| 68 | BF | 34 | DG | O4'-C1'-C2' | -5.87 | 101.21 | 105.90 |
| 1 | AA | 1376 | DG | O4'-C1'-C2' | -5.86 | 101.21 | 105.90 |
| 1 | AA | 311 | DA | O4'-C1'-C2' | -5.86 | 101.21 | 105.90 |
| 37 | Ak | 10 | DT | C4'-C3'-C2' | -5.86 | 97.83 | 103.10 |
| 1 | AA | 539 | DG | O4'-C1'-N9 | 5.86 | 112.10 | 108.00 |
| 1 | AA | 2322 | DG | O4'-C1'-C2' | -5.86 | 101.21 | 105.90 |
| 33 | Ag | 17 | DG | O4'-C1'-C2' | -5.86 | 101.21 | 105.90 |
| 34 | Ah | 9 | DT | O4'-C1'-C2' | -5.86 | 101.22 | 105.90 |
| 1 | AA | 1825 | DC | C6-N1-C2 | -5.85 | 117.96 | 120.30 |
| 1 | AA | 2387 | DA | C5-C6-N6 | -5.85 | 119.02 | 123.70 |
| 16 | AP | 19 | DT | C4'-C3'-C2' | -5.85 | 97.83 | 103.10 |
| 1 | AA | 2261 | DG | P-O3'-C3' | 5.85 | 126.72 | 119.70 |
| 50 | Ax | 27 | DG | N1-C6-O6 | 5.85 | 123.41 | 119.90 |
| 1 | AA | 1947 | DC | O4'-C1'-C2' | -5.85 | 101.22 | 105.90 |
| 1 | AA | 1900 | DG | C4'-C3'-C2' | -5.84 | 97.84 | 103.10 |
| 1 | AA | 2696 | DG | C4'-C3'-C2' | -5.84 | 97.84 | 103.10 |
| 34 | Ah | 12 | DT | O4'-C1'-N1 | 5.84 | 112.09 | 108.00 |
| 1 | AA | 1501 | DC | C4'-C3'-C2' | -5.84 | 97.84 | 103.10 |
| 37 | Ak | 16 | DG | O4'-C1'-N9 | 5.84 | 112.09 | 108.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | AA | 1047 | DT | O4'-C4'-C3' | -5.84 | 102.17 | 104.50 |
| 1 | AA | 398 | DT | O4'-C4'-C3' | -5.83 | 102.17 | 104.50 |
| 72 | BJ | 1 | DT | C1'-O4'-C4' | -5.83 | 104.27 | 110.10 |
| 70 | BH | 6 | DC | C4'-C3'-C2' | -5.83 | 97.85 | 103.10 |
| 1 | AA | 539 | DG | C1'-O4'-C4' | -5.83 | 104.27 | 110.10 |
| 1 | AA | 2534 | DC | O4'-C1'-C2' | -5.83 | 101.24 | 105.90 |
| 2 | AB | 7 | DA | N1-C6-N6 | 5.83 | 122.10 | 118.60 |
| 8 | AH | 18 | DG | P-O3'-C3' | 5.83 | 126.69 | 119.70 |
| 63 | BA | 9 | DG | C1'-O4'-C4' | -5.83 | 104.27 | 110.10 |
| 45 | As | 23 | DA | P-O3'-C3' | 5.83 | 126.69 | 119.70 |
| 1 | AA | 1888 | DG | C1'-O4'-C4' | -5.82 | 104.28 | 110.10 |
| 14 | AN | 9 | DA | C1'-O4'-C4' | -5.82 | 104.28 | 110.10 |
| 28 | Ab | 28 | DC | P-O3'-C3' | 5.82 | 126.69 | 119.70 |
| 1 | AA | 522 | DG | C4'-C3'-C2' | -5.82 | 97.86 | 103.10 |
| 3 | AC | 47 | DC | O4'-C4'-C3' | -5.82 | 102.17 | 104.50 |
| 55 | A2 | 23 | DA | C1'-O4'-C4' | -5.82 | 104.28 | 110.10 |
| 53 | A0 | 15 | DA | P-O3'-C3' | 5.82 | 126.68 | 119.70 |
| 50 | Ax | 37 | DA | O4'-C1'-C2' | -5.82 | 101.25 | 105.90 |
| 1 | AA | 589 | DG | C1'-O4'-C4' | -5.81 | 104.29 | 110.10 |
| 1 | AA | 1782 | DG | O4'-C1'-C2' | -5.81 | 101.25 | 105.90 |
| 44 | Ar | 16 | DT | P-O3'-C3' | 5.81 | 126.67 | 119.70 |
| 65 | BC | 16 | DT | C4'-C3'-C2' | -5.81 | 97.88 | 103.10 |
| 33 | Ag | 22 | DG | O4'-C1'-C2' | -5.80 | 101.26 | 105.90 |
| 75 | BM | 31 | DG | O4'-C1'-C2' | -5.80 | 101.26 | 105.90 |
| 17 | AQ | 9 | DC | O4'-C1'-C2' | -5.80 | 101.26 | 105.90 |
| 56 | A3 | 12 | DT | O4'-C1'-C2' | -5.80 | 101.26 | 105.90 |
| 1 | AA | 344 | DT | C4'-C3'-C2' | -5.80 | 97.88 | 103.10 |
| 1 | AA | 972 | DC | P-O3'-C3' | 5.80 | 126.66 | 119.70 |
| 1 | AA | 2448 | DG | O4'-C1'-C2' | -5.80 | 101.26 | 105.90 |
| 25 | AY | 19 | DT | C4'-C3'-C2' | -5.80 | 97.88 | 103.10 |
| 69 | BG | 3 | DC | C4'-C3'-C2' | -5.80 | 97.88 | 103.10 |
| 1 | AA | 1147 | DT | C4'-C3'-C2' | -5.79 | 97.89 | 103.10 |
| 1 | AA | 2427 | DA | P-O3'-C3' | 5.79 | 126.65 | 119.70 |
| 1 | AA | 1446 | DT | C4'-C3'-C2' | -5.79 | 97.89 | 103.10 |
| 64 | BB | 15 | DC | C4'-C3'-C2' | -5.79 | 97.89 | 103.10 |
| 1 | AA | 117 | DA | P-O3'-C3' | 5.79 | 126.64 | 119.70 |
| 1 | AA | 887 | DC | P-O3'-C3' | 5.79 | 126.64 | 119.70 |
| 1 | AA | 323 | DA | O4'-C1'-C2' | -5.78 | 101.27 | 105.90 |
| 52 | Az | 9 | DG | C4'-C3'-C2' | -5.78 | 97.90 | 103.10 |
| 1 | AA | 370 | DG | C5-C6-O6 | -5.78 | 125.14 | 128.60 |
| 1 | AA | 1366 | DA | N1-C6-N6 | -5.77 | 115.14 | 118.60 |
| 1 | AA | 1710 | DT | C1'-O4'-C4' | -5.77 | 104.33 | 110.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 8 | AH | 23 | DT | O4'-C1'-C2' | -5.77 | 101.28 | 105.90 |
| 1 | AA | 1950 | DC | O4'-C1'-N1 | 5.77 | 112.04 | 108.00 |
| 13 | AM | 11 | DG | O4'-C1'-C2' | -5.77 | 101.29 | 105.90 |
| 1 | AA | 980 | DG | C5-C6-O6 | -5.77 | 125.14 | 128.60 |
| 1 | AA | 2242 | DG | O4'-C1'-N9 | 5.76 | 112.03 | 108.00 |
| 72 | BJ | 40 | DG | C5-C6-O6 | -5.76 | 125.14 | 128.60 |
| 1 | AA | 291 | DC | O4'-C1'-C2' | -5.76 | 101.29 | 105.90 |
| 48 | Av | 25 | DC | C4'-C3'-C2' | -5.76 | 97.92 | 103.10 |
| 63 | BA | 10 | DC | C4'-C3'-C2' | -5.76 | 97.92 | 103.10 |
| 72 | BJ | 2 | DT | O4'-C1'-C2' | -5.76 | 101.29 | 105.90 |
| 1 | AA | 1391 | DA | C1'-O4'-C4' | -5.76 | 104.34 | 110.10 |
| 78 | BP | 7 | DC | O4'-C1'-C2' | -5.76 | 101.29 | 105.90 |
| 32 | Af | 5 | DA | N1-C6-N6 | -5.76 | 115.15 | 118.60 |
| 1 | AA | 2577 | DC | O4'-C1'-C2' | -5.75 | 101.30 | 105.90 |
| 74 | BL | 3 | DG | P-O3'-C3' | 5.75 | 126.60 | 119.70 |
| 1 | AA | 2381 | DT | O4'-C1'-C2' | -5.75 | 101.30 | 105.90 |
| 16 | AP | 3 | DG | N1-C6-O6 | 5.75 | 123.35 | 119.90 |
| 1 | AA | 1920 | DG | P-O3'-C3' | 5.75 | 126.60 | 119.70 |
| 39 | Am | 12 | DC | C6-N1-C1' | -5.75 | 113.90 | 120.80 |
| 1 | AA | 1208 | DA | O4'-C1'-C2' | -5.75 | 101.30 | 105.90 |
| 1 | AA | 1786 | DT | C4'-C3'-C2' | -5.75 | 97.93 | 103.10 |
| 26 | AZ | 39 | DA | O4'-C1'-C2' | -5.75 | 101.30 | 105.90 |
| 50 | Ax | 16 | DT | C4'-C3'-C2' | -5.75 | 97.93 | 103.10 |
| 1 | AA | 2334 | DC | O4'-C1'-N1 | -5.75 | 103.98 | 108.00 |
| 10 | AJ | 26 | DC | C1'-O4'-C4' | -5.74 | 104.36 | 110.10 |
| 41 | Ao | 4 | DG | C4'-C3'-C2' | -5.74 | 97.93 | 103.10 |
| 15 | AO | 10 | DT | C4'-C3'-C2' | -5.74 | 97.93 | 103.10 |
| 23 | AW | 9 | DG | O4'-C4'-C3' | -5.74 | 102.20 | 104.50 |
| 1 | AA | 335 | DT | P-O3'-C3' | 5.74 | 126.58 | 119.70 |
| 18 | AR | 13 | DG | N1-C6-O6 | 5.74 | 123.34 | 119.90 |
| 65 | BC | 14 | DG | P-O3'-C3' | 5.74 | 126.58 | 119.70 |
| 1 | AA | 240 | DT | O4'-C4'-C3' | -5.73 | 102.21 | 104.50 |
| 1 | AA | 2561 | DT | C6-C5-C7 | 5.73 | 126.34 | 122.90 |
| 51 | Ay | 30 | DC | O4'-C1'-C2' | -5.73 | 101.31 | 105.90 |
| 1 | AA | 333 | DA | O4'-C1'-C2' | -5.73 | 101.31 | 105.90 |
| 1 | AA | 1704 | DC | C4'-C3'-C2' | -5.73 | 97.94 | 103.10 |
| 78 | BP | 17 | DG | O4'-C1'-C2' | -5.73 | 101.31 | 105.90 |
| 1 | AA | 631 | DA | O4'-C4'-C3' | -5.73 | 102.21 | 104.50 |
| 1 | AA | 2798 | DC | C1'-O4'-C4' | -5.73 | 104.37 | 110.10 |
| 1 | AA | 1801 | DC | P-O5'-C5' | 5.73 | 130.06 | 120.90 |
| 54 | A1 | 14 | DG | P-O3'-C3' | 5.73 | 126.57 | 119.70 |
| 67 | BE | 17 | DG | C1'-O4'-C4' | -5.73 | 104.37 | 110.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | AA | 2845 | DT | C4'-C3'-C2' | -5.73 | 97.95 | 103.10 |
| 1 | AA | 2837 | DC | O4'-C1'-C2' | -5.72 | 101.32 | 105.90 |
| 63 | BA | 28 | DG | C4'-C3'-C2' | -5.72 | 97.95 | 103.10 |
| 21 | AU | 15 | DG | O4'-C1'-N9 | 5.72 | 112.01 | 108.00 |
| 65 | BC | 34 | DA | P-O3'-C3' | 5.72 | 126.57 | 119.70 |
| 76 | BN | 6 | DC | P-O5'-C5' | 5.72 | 130.06 | 120.90 |
| 76 | BN | 29 | DG | C1'-O4'-C4' | -5.72 | 104.38 | 110.10 |
| 1 | AA | 828 | DG | O4'-C1'-N9 | 5.72 | 112.00 | 108.00 |
| 1 | AA | 2605 | DG | O4'-C1'-N9 | 5.72 | 112.00 | 108.00 |
| 1 | AA | 665 | DG | P-O3'-C3' | 5.72 | 126.56 | 119.70 |
| 1 | AA | 2532 | DG | C1'-O4'-C4' | -5.72 | 104.38 | 110.10 |
| 1 | AA | 2006 | DC | C4'-C3'-C2' | -5.71 | 97.96 | 103.10 |
| 28 | Ab | 42 | DG | O4'-C4'-C3' | -5.71 | 102.22 | 104.50 |
| 29 | Ac | 30 | DG | O4'-C4'-C3' | -5.71 | 102.22 | 104.50 |
| 1 | AA | 2074 | DT | O4'-C4'-C3' | -5.71 | 102.22 | 104.50 |
| 1 | AA | 1388 | DA | O4'-C1'-C2' | -5.70 | 101.34 | 105.90 |
| 1 | AA | 2693 | DG | C1'-O4'-C4' | -5.70 | 104.40 | 110.10 |
| 19 | AS | 5 | DT | O4'-C1'-N1 | 5.70 | 111.99 | 108.00 |
| 1 | AA | 127 | DG | O4'-C1'-C2' | -5.70 | 101.34 | 105.90 |
| 1 | AA | 245 | DT | C4'-C3'-C2' | -5.70 | 97.97 | 103.10 |
| 1 | AA | 1954 | DT | C4'-C3'-C2' | -5.70 | 97.97 | 103.10 |
| 1 | AA | 2806 | DT | C4'-C3'-C2' | -5.70 | 97.97 | 103.10 |
| 1 | AA | 2347 | DG | O4'-C1'-C2' | -5.70 | 101.34 | 105.90 |
| 48 | Av | 16 | DC | C1'-O4'-C4' | -5.69 | 104.41 | 110.10 |
| 1 | AA | 261 | DA | O4'-C1'-C2' | -5.69 | 101.35 | 105.90 |
| 45 | As | 16 | DA | O4'-C1'-C2' | -5.69 | 101.35 | 105.90 |
| 68 | BF | 1 | DT | O4'-C4'-C3' | -5.69 | 102.22 | 104.50 |
| 55 | A2 | 23 | DA | P-O3'-C3' | 5.69 | 126.53 | 119.70 |
| 1 | AA | 2672 | DG | C5-C6-O6 | -5.69 | 125.19 | 128.60 |
| 1 | AA | 227 | DT | O4'-C1'-C2' | -5.69 | 101.35 | 105.90 |
| 1 | AA | 839 | DG | O4'-C4'-C3' | -5.68 | 102.23 | 104.50 |
| 1 | AA | 2831 | DA | O4'-C4'-C3' | -5.68 | 102.23 | 104.50 |
| 20 | AT | 9 | DC | P-O3'-C3' | 5.68 | 126.52 | 119.70 |
| 1 | AA | 145 | DT | O4'-C4'-C3' | -5.68 | 102.23 | 104.50 |
| 1 | AA | 785 | DG | O4'-C1'-C2' | -5.68 | 101.35 | 105.90 |
| 1 | AA | 2363 | DG | C4'-C3'-C2' | -5.68 | 97.98 | 103.10 |
| 64 | BB | 11 | DA | N1-C6-N6 | -5.68 | 115.19 | 118.60 |
| 1 | AA | 1629 | DC | C1'-O4'-C4' | -5.67 | 104.42 | 110.10 |
| 73 | BK | 24 | DC | C2-N1-C1' | 5.67 | 125.04 | 118.80 |
| 1 | AA | 441 | DC | O4'-C4'-C3' | -5.67 | 102.23 | 104.50 |
| 1 | AA | 1688 | DC | P-O3'-C3' | 5.67 | 126.51 | 119.70 |
| 1 | AA | 2532 | DG | N1-C6-O6 | 5.67 | 123.30 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 71 | BI | 35 | DC | O4'-C1'-C2' | -5.67 | 101.36 | 105.90 |
| 1 | AA | 37 | DT | C4'-C3'-C2' | -5.67 | 98.00 | 103.10 |
| 10 | AJ | 2 | DT | O4'-C1'-C2' | -5.67 | 101.37 | 105.90 |
| 1 | AA | 2354 | DT | O4'-C1'-C2' | -5.67 | 101.37 | 105.90 |
| 22 | AV | 33 | DA | O4'-C1'-C2' | -5.67 | 101.37 | 105.90 |
| 1 | AA | 768 | DG | C4'-C3'-C2' | -5.66 | 98.00 | 103.10 |
| 1 | AA | 885 | DC | C2-N1-C1' | 5.66 | 125.03 | 118.80 |
| 1 | AA | 1966 | DG | O4'-C1'-C2' | -5.66 | 101.37 | 105.90 |
| 61 | A8 | 20 | DT | O4'-C4'-C3' | -5.66 | 102.23 | 104.50 |
| 26 | AZ | 16 | DG | O4'-C1'-C2' | -5.66 | 101.37 | 105.90 |
| 28 | Ab | 37 | DT | C1'-O4'-C4' | -5.66 | 104.44 | 110.10 |
| 20 | AT | 44 | DA | O4'-C1'-C2' | -5.66 | 101.37 | 105.90 |
| 46 | At | 21 | DG | C1'-O4'-C4' | -5.66 | 104.44 | 110.10 |
| 1 | AA | 1069 | DT | C4'-C3'-C2' | -5.66 | 98.01 | 103.10 |
| 77 | BO | 30 | DA | C1'-O4'-C4' | -5.66 | 104.44 | 110.10 |
| 1 | AA | 749 | DC | O4'-C1'-C2' | -5.65 | 101.38 | 105.90 |
| 45 | As | 14 | DC | C2-N1-C1' | 5.65 | 125.02 | 118.80 |
| 12 | AL | 34 | DT | C4'-C3'-C2' | -5.65 | 98.01 | 103.10 |
| 31 | Ae | 12 | DT | C4'-C3'-C2' | -5.65 | 98.01 | 103.10 |
| 23 | AW | 24 | DA | P-O3'-C3' | 5.65 | 126.48 | 119.70 |
| 39 | Am | 30 | DG | P-O3'-C3' | 5.65 | 126.48 | 119.70 |
| 61 | A8 | 23 | DA | C4'-C3'-C2' | -5.65 | 98.02 | 103.10 |
| 1 | AA | 1719 | DT | C4'-C3'-C2' | -5.64 | 98.02 | 103.10 |
| 1 | AA | 2413 | DG | O4'-C1'-C2' | -5.64 | 101.38 | 105.90 |
| 69 | BG | 3 | DC | O4'-C4'-C3' | -5.64 | 102.24 | 104.50 |
| 1 | AA | 1012 | DA | C4'-C3'-C2' | -5.63 | 98.03 | 103.10 |
| 1 | AA | 2507 | DT | C1'-O4'-C4' | -5.63 | 104.47 | 110.10 |
| 1 | AA | 106 | DA | O4'-C1'-C2' | -5.63 | 101.39 | 105.90 |
| 21 | AU | 7 | DA | O4'-C1'-C2' | -5.63 | 101.40 | 105.90 |
| 44 | Ar | 23 | DA | O4'-C1'-C2' | -5.63 | 101.39 | 105.90 |
| 1 | AA | 733 | DG | C1'-O4'-C4' | -5.63 | 104.47 | 110.10 |
| 1 | AA | 370 | DG | N1-C6-O6 | 5.63 | 123.28 | 119.90 |
| 1 | AA | 1070 | DC | P-O3'-C3' | 5.62 | 126.45 | 119.70 |
| 1 | AA | 2326 | DC | P-O3'-C3' | 5.62 | 126.45 | 119.70 |
| 1 | AA | 1799 | DT | O4'-C4'-C3' | -5.62 | 102.25 | 104.50 |
| 39 | Am | 5 | DG | C4'-C3'-C2' | -5.62 | 98.04 | 103.10 |
| 1 | AA | 219 | DG | O4'-C1'-C2' | -5.62 | 101.40 | 105.90 |
| 1 | AA | 441 | DC | C4'-C3'-C2' | -5.62 | 98.04 | 103.10 |
| 1 | AA | 203 | DA | P-O3'-C3' | 5.62 | 126.44 | 119.70 |
| 1 | AA | 819 | DG | P-O3'-C3' | 5.62 | 126.44 | 119.70 |
| 13 | AM | 9 | DT | C4'-C3'-C2' | -5.62 | 98.04 | 103.10 |
| 1 | AA | 372 | DA | C1'-O4'-C4' | -5.62 | 104.48 | 110.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | AA | 2623 | DA | P-O3'-C3' | 5.62 | 126.44 | 119.70 |
| 56 | A3 | 7 | DA | O4'-C1'-C2' | -5.62 | 101.41 | 105.90 |
| 1 | AA | 79 | DT | O4'-C1'-C2' | -5.62 | 101.41 | 105.90 |
| 1 | AA | 2016 | DG | P-O3'-C3' | 5.61 | 126.44 | 119.70 |
| 12 | AL | 7 | DA | O4'-C1'-N9 | -5.61 | 104.07 | 108.00 |
| 24 | AX | 26 | DT | P-O3'-C3' | 5.61 | 126.43 | 119.70 |
| 28 | Ab | 21 | DC | P-O3'-C3' | 5.61 | 126.43 | 119.70 |
| 1 | AA | 1166 | DT | O4'-C4'-C3' | -5.61 | 102.26 | 104.50 |
| 1 | AA | 2605 | DG | C1'-O4'-C4' | -5.61 | 104.49 | 110.10 |
| 71 | BI | 7 | DA | P-O3'-C3' | 5.61 | 126.43 | 119.70 |
| 1 | AA | 613 | DG | O4'-C1'-C2' | -5.61 | 101.42 | 105.90 |
| 16 | AP | 3 | DG | C5-C6-O6 | -5.61 | 125.24 | 128.60 |
| 1 | AA | 533 | DA | O4'-C1'-C2' | -5.60 | 101.42 | 105.90 |
| 10 | AJ | 11 | DT | C1'-O4'-C4' | -5.60 | 104.50 | 110.10 |
| 1 | AA | 149 | DT | O4'-C4'-C3' | -5.60 | 102.26 | 104.50 |
| 15 | AO | 13 | DC | P-O3'-C3' | 5.60 | 126.42 | 119.70 |
| 1 | AA | 1884 | DA | N1-C6-N6 | -5.60 | 115.24 | 118.60 |
| 1 | AA | 2175 | DT | O4'-C1'-C2' | -5.60 | 101.42 | 105.90 |
| 36 | Aj | 9 | DC | P-O3'-C3' | 5.60 | 126.42 | 119.70 |
| 64 | BB | 11 | DA | P-O3'-C3' | 5.60 | 126.42 | 119.70 |
| 21 | AU | 15 | DG | P-O3'-C3' | 5.59 | 126.41 | 119.70 |
| 21 | AU | 16 | DC | O4'-C1'-C2' | -5.59 | 101.43 | 105.90 |
| 1 | AA | 2387 | DA | N1-C6-N6 | 5.59 | 121.95 | 118.60 |
| 1 | AA | 2534 | DC | P-O3'-C3' | 5.59 | 126.41 | 119.70 |
| 32 | Af | 2 | DG | O4'-C1'-C2' | -5.59 | 101.43 | 105.90 |
| 79 | BQ | 7 | DG | O4'-C1'-C2' | -5.59 | 101.43 | 105.90 |
| 18 | AR | 28 | DT | O4'-C4'-C3' | -5.59 | 102.27 | 104.50 |
| 26 | AZ | 7 | DG | O4'-C1'-C2' | -5.59 | 101.43 | 105.90 |
| 1 | AA | 616 | DG | C1'-O4'-C4' | -5.58 | 104.52 | 110.10 |
| 1 | AA | 1381 | DT | C4'-C3'-C2' | -5.58 | 98.08 | 103.10 |
| 1 | AA | 1397 | DT | C1'-O4'-C4' | -5.58 | 104.52 | 110.10 |
| 72 | BJ | 33 | DT | O4'-C1'-C2' | -5.58 | 101.43 | 105.90 |
| 1 | AA | 975 | DA | O4'-C1'-C2' | -5.58 | 101.44 | 105.90 |
| 1 | AA | 1248 | DC | O4'-C1'-C2' | -5.58 | 101.44 | 105.90 |
| 8 | AH | 24 | DT | C4'-C3'-C2' | -5.58 | 98.08 | 103.10 |
| 1 | AA | 972 | DC | O4'-C1'-C2' | -5.57 | 101.44 | 105.90 |
| 51 | Ay | 37 | DG | O4'-C1'-C2' | -5.57 | 101.44 | 105.90 |
| 6 | AF | 24 | DG | O4'-C1'-C2' | -5.57 | 101.44 | 105.90 |
| 25 | AY | 30 | DA | P-O3'-C3' | 5.57 | 126.38 | 119.70 |
| 5 | AE | 23 | DG | O4'-C1'-C2' | -5.56 | 101.45 | 105.90 |
| 64 | BB | 28 | DT | C4'-C3'-C2' | -5.56 | 98.09 | 103.10 |
| 1 | AA | 210 | DC | O4'-C4'-C3' | -5.56 | 102.28 | 104.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 47 | Au | 16 | DA | O4'-C1'-C2' | -5.56 | 101.45 | 105.90 |
| 75 | BM | 10 | DA | C4'-C3'-C2' | -5.56 | 98.10 | 103.10 |
| 1 | AA | 495 | DG | O4'-C1'-N9 | 5.56 | 111.89 | 108.00 |
| 1 | AA | 2373 | DG | N1-C6-O6 | 5.56 | 123.23 | 119.90 |
| 35 | Ai | 47 | DC | O4'-C1'-C2' | -5.56 | 101.45 | 105.90 |
| 23 | AW | 2 | DG | C5-C6-O6 | -5.56 | 125.27 | 128.60 |
| 47 | Au | 23 | DG | O4'-C1'-C2' | -5.56 | 101.45 | 105.90 |
| 42 | Ap | 5 | DT | O4'-C1'-N1 | 5.55 | 111.89 | 108.00 |
| 71 | BI | 40 | DA | P-O3'-C3' | 5.55 | 126.37 | 119.70 |
| 1 | AA | 1879 | DG | C1'-O4'-C4' | -5.55 | 104.55 | 110.10 |
| 1 | AA | 161 | DT | O4'-C4'-C3' | -5.55 | 102.28 | 104.50 |
| 1 | AA | 1405 | DG | O4'-C4'-C3' | -5.55 | 102.28 | 104.50 |
| 1 | AA | 946 | DG | O4'-C4'-C3' | -5.54 | 102.28 | 104.50 |
| 1 | AA | 1674 | DC | P-O5'-C5' | 5.54 | 129.77 | 120.90 |
| 38 | Al | 38 | DA | O4'-C4'-C3' | -5.54 | 102.28 | 104.50 |
| 1 | AA | 708 | DG | O4'-C1'-C2' | -5.54 | 101.47 | 105.90 |
| 1 | AA | 1949 | DG | N1-C6-O6 | 5.54 | 123.22 | 119.90 |
| 1 | AA | 2031 | DG | N1-C6-O6 | 5.54 | 123.22 | 119.90 |
| 12 | AL | 12 | DG | O4'-C1'-C2' | -5.54 | 101.47 | 105.90 |
| 1 | AA | 1207 | DA | C4'-C3'-C2' | -5.53 | 98.12 | 103.10 |
| 7 | AG | 6 | DG | C5-C6-O6 | -5.53 | 125.28 | 128.60 |
| 1 | AA | 2305 | DC | C4'-C3'-C2' | -5.53 | 98.12 | 103.10 |
| 37 | Ak | 29 | DC | P-O3'-C3' | 5.53 | 126.34 | 119.70 |
| 45 | As | 34 | DG | C1'-O4'-C4' | -5.53 | 104.57 | 110.10 |
| 1 | AA | 247 | DC | P-O3'-C3' | 5.53 | 126.33 | 119.70 |
| 1 | AA | 1765 | DC | O4'-C1'-C2' | -5.53 | 101.48 | 105.90 |
| 8 | AH | 1 | DA | C1'-O4'-C4' | -5.53 | 104.57 | 110.10 |
| 18 | AR | 14 | DC | O4'-C1'-N1 | 5.53 | 111.87 | 108.00 |
| 3 | AC | 44 | DC | P-O3'-C3' | 5.52 | 126.33 | 119.70 |
| 40 | An | 38 | DT | C4'-C3'-C2' | -5.52 | 98.13 | 103.10 |
| 1 | AA | 1694 | DC | P-O5'-C5' | 5.52 | 129.73 | 120.90 |
| 1 | AA | 2308 | DA | O4'-C1'-C2' | -5.52 | 101.48 | 105.90 |
| 1 | AA | 2522 | DT | C4'-C3'-C2' | -5.52 | 98.13 | 103.10 |
| 17 | AQ | 10 | DT | C4'-C3'-C2' | -5.52 | 98.13 | 103.10 |
| 18 | AR | 13 | DG | C5-C6-O6 | -5.52 | 125.29 | 128.60 |
| 3 | AC | 40 | DT | O4'-C4'-C3' | -5.52 | 102.29 | 104.50 |
| 19 | AS | 21 | DG | O4'-C1'-C2' | -5.52 | 101.49 | 105.90 |
| 1 | AA | 2585 | DG | O4'-C1'-N9 | 5.52 | 111.86 | 108.00 |
| 45 | As | 23 | DA | O4'-C1'-N9 | 5.52 | 111.86 | 108.00 |
| 1 | AA | 815 | DT | C4'-C3'-C2' | -5.51 | 98.14 | 103.10 |
| 70 | BH | 7 | DC | C2-N1-C1' | 5.51 | 124.86 | 118.80 |
| 77 | BO | 39 | DT | C4'-C3'-C2' | -5.51 | 98.14 | 103.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | AA | 1543 | DA | O4'-C1'-C2' | -5.51 | 101.49 | 105.90 |
| 3 | AC | 44 | DC | O4'-C1'-C2' | -5.51 | 101.49 | 105.90 |
| 44 | Ar | 37 | DA | O4'-C1'-C2' | -5.51 | 101.49 | 105.90 |
| 75 | BM | 44 | DA | N1-C6-N6 | -5.51 | 115.30 | 118.60 |
| 1 | AA | 1866 | DG | O4'-C1'-C2' | -5.51 | 101.50 | 105.90 |
| 38 | Al | 28 | DC | C4'-C3'-C2' | -5.51 | 98.14 | 103.10 |
| 1 | AA | 313 | DA | P-O3'-C3' | 5.50 | 126.31 | 119.70 |
| 1 | AA | 2639 | DT | O4'-C1'-C2' | -5.50 | 101.50 | 105.90 |
| 44 | Ar | 33 | DT | C4'-C3'-C2' | -5.50 | 98.15 | 103.10 |
| 1 | AA | 2294 | DC | O4'-C4'-C3' | -5.50 | 102.30 | 104.50 |
| 1 | AA | 55 | DT | P-O3'-C3' | -5.50 | 113.10 | 119.70 |
| 1 | AA | 252 | DG | O4'-C4'-C3' | -5.50 | 102.30 | 104.50 |
| 1 | AA | 1588 | DC | O4'-C1'-C2' | -5.50 | 101.50 | 105.90 |
| 1 | AA | 2081 | DT | C4'-C3'-C2' | -5.50 | 98.15 | 103.10 |
| 1 | AA | 1362 | DA | O4'-C1'-C2' | -5.49 | 101.50 | 105.90 |
| 37 | Ak | 57 | DT | P-O3'-C3' | 5.49 | 126.29 | 119.70 |
| 1 | AA | 2251 | DT | O4'-C1'-C2' | -5.49 | 101.51 | 105.90 |
| 1 | AA | 1343 | DG | C5-C6-O6 | -5.49 | 125.31 | 128.60 |
| 1 | AA | 1810 | DT | O4'-C4'-C3' | -5.49 | 102.30 | 104.50 |
| 1 | AA | 2377 | DG | C4'-C3'-C2' | -5.49 | 98.16 | 103.10 |
| 31 | Ae | 33 | DA | C1'-O4'-C4' | -5.49 | 104.61 | 110.10 |
| 1 | AA | 1832 | DT | C4'-C3'-C2' | -5.49 | 98.16 | 103.10 |
| 1 | AA | 1825 | DC | C4'-C3'-C2' | -5.49 | 98.16 | 103.10 |
| 1 | AA | 2753 | DC | P-O5'-C5' | 5.49 | 129.68 | 120.90 |
| 66 | BD | 10 | DG | O4'-C1'-C2' | -5.49 | 101.51 | 105.90 |
| 1 | AA | 2849 | DC | C4'-C3'-C2' | -5.48 | 98.17 | 103.10 |
| 1 | AA | 30 | DA | O4'-C1'-C2' | -5.48 | 101.51 | 105.90 |
| 1 | AA | 1779 | DC | O4'-C1'-N1 | 5.48 | 111.84 | 108.00 |
| 1 | AA | 2387 | DA | O4'-C1'-C2' | -5.48 | 101.51 | 105.90 |
| 32 | Af | 31 | DC | C2-N1-C1' | 5.48 | 124.83 | 118.80 |
| 5 | AE | 26 | DA | C4'-C3'-C2' | -5.48 | 98.17 | 103.10 |
| 71 | BI | 13 | DT | O4'-C4'-C3' | -5.48 | 102.31 | 104.50 |
| 51 | Ay | 30 | DC | P-O3'-C3' | 5.48 | 126.27 | 119.70 |
| 1 | AA | 435 | DT | O4'-C1'-C2' | -5.48 | 101.52 | 105.90 |
| 8 | AH | 23 | DT | C1'-O4'-C4' | -5.47 | 104.62 | 110.10 |
| 35 | Ai | 49 | DG | N1-C6-O6 | 5.47 | 123.19 | 119.90 |
| 1 | AA | 1286 | DA | O4'-C1'-C2' | -5.47 | 101.52 | 105.90 |
| 1 | AA | 982 | DA | O4'-C1'-C2' | -5.47 | 101.52 | 105.90 |
| 1 | AA | 667 | DT | P-O3'-C3' | 5.47 | 126.26 | 119.70 |
| 1 | AA | 68 | DG | O4'-C1'-C2' | -5.47 | 101.53 | 105.90 |
| 1 | AA | 839 | DG | C4'-C3'-C2' | -5.46 | 98.18 | 103.10 |
| 1 | AA | 1824 | DT | P-O3'-C3' | 5.46 | 126.26 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | AA | 2560 | DC | O4'-C1'-N1 | 5.46 | 111.82 | 108.00 |
| 1 | AA | 1751 | DC | P-O3'-C3' | 5.46 | 126.25 | 119.70 |
| 1 | AA | 892 | DG | O4'-C1'-C2' | -5.46 | 101.53 | 105.90 |
| 1 | AA | 1058 | DC | C4'-C3'-C2' | -5.46 | 98.19 | 103.10 |
| 1 | AA | 1484 | DG | C1'-O4'-C4' | -5.45 | 104.65 | 110.10 |
| 48 | Av | 10 | DC | C4'-C3'-C2' | -5.45 | 98.19 | 103.10 |
| 1 | AA | 2781 | DA | O4'-C4'-C3' | -5.45 | 102.32 | 104.50 |
| 58 | A5 | 26 | DG | C4'-C3'-C2' | -5.45 | 98.20 | 103.10 |
| 1 | AA | 1689 | DC | P-O3'-C3' | 5.45 | 126.23 | 119.70 |
| 76 | BN | 14 | DA | O4'-C1'-N9 | -5.45 | 104.19 | 108.00 |
| 14 | AN | 7 | DT | O4'-C4'-C3' | -5.44 | 102.32 | 104.50 |
| 10 | AJ | 7 | DT | C1'-O4'-C4' | -5.44 | 104.66 | 110.10 |
| 58 | A5 | 4 | DA | O4'-C1'-C2' | -5.44 | 101.55 | 105.90 |
| 3 | AC | 42 | DC | C4'-C3'-C2' | -5.44 | 98.20 | 103.10 |
| 52 | Az | 28 | DC | O4'-C1'-C2' | -5.44 | 101.55 | 105.90 |
| 1 | AA | 2539 | DT | C4'-C3'-C2' | -5.44 | 98.20 | 103.10 |
| 1 | AA | 2633 | DG | O4'-C1'-C2' | -5.44 | 101.55 | 105.90 |
| 1 | AA | 808 | DG | O4'-C1'-C2' | -5.44 | 101.55 | 105.90 |
| 32 | Af | 14 | DT | C4'-C3'-C2' | -5.44 | 98.21 | 103.10 |
| 46 | At | 17 | DT | C4'-C3'-C2' | -5.44 | 98.21 | 103.10 |
| 46 | At | 40 | DG | O4'-C1'-N9 | 5.44 | 111.81 | 108.00 |
| 78 | BP | 11 | DG | O4'-C1'-C2' | -5.44 | 101.55 | 105.90 |
| 1 | AA | 307 | DC | O4'-C1'-N1 | -5.43 | 104.20 | 108.00 |
| 1 | AA | 834 | DG | O4'-C1'-C2' | -5.43 | 101.55 | 105.90 |
| 6 | AF | 8 | DT | C4'-C3'-C2' | -5.43 | 98.21 | 103.10 |
| 38 | Al | 25 | DT | C1'-O4'-C4' | -5.43 | 104.67 | 110.10 |
| 1 | AA | 11 | DT | C4'-C3'-C2' | -5.43 | 98.21 | 103.10 |
| 7 | AG | 29 | DG | P-O3'-C3' | 5.43 | 126.22 | 119.70 |
| 21 | AU | 10 | DG | P-O3'-C3' | 5.43 | 126.22 | 119.70 |
| 76 | BN | 10 | DT | C4'-C3'-C2' | -5.43 | 98.21 | 103.10 |
| 56 | A3 | 10 | DG | C4'-C3'-C2' | -5.43 | 98.21 | 103.10 |
| 1 | AA | 1426 | DC | P-O5'-C5' | 5.43 | 129.59 | 120.90 |
| 12 | AL | 5 | DC | C4'-C3'-C2' | -5.43 | 98.21 | 103.10 |
| 28 | Ab | 10 | DG | O4'-C1'-C2' | -5.43 | 101.56 | 105.90 |
| 40 | An | 9 | DA | O4'-C1'-C2' | -5.43 | 101.56 | 105.90 |
| 1 | AA | 1012 | DA | O4'-C4'-C3' | -5.43 | 102.33 | 104.50 |
| 22 | AV | 23 | DC | O4'-C1'-C2' | -5.43 | 101.56 | 105.90 |
| 1 | AA | 409 | DA | C1'-O4'-C4' | -5.43 | 104.67 | 110.10 |
| 1 | AA | 2445 | DG | N1-C6-O6 | 5.43 | 123.16 | 119.90 |
| 46 | At | 26 | DA | P-O3'-C3' | 5.43 | 126.21 | 119.70 |
| 1 | AA | 2355 | DA | C1'-O4'-C4' | -5.42 | 104.67 | 110.10 |
| 13 | AM | 34 | DT | C4'-C3'-C2' | -5.42 | 98.22 | 103.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | AV | 39 | DG | C1'-O4'-C4' | -5.42 | 104.67 | 110.10 |
| 1 | AA | 1175 | DT | O4'-C4'-C3' | -5.42 | 102.33 | 104.50 |
| 10 | AJ | 29 | DC | O4'-C4'-C3' | -5.42 | 102.33 | 104.50 |
| 39 | Am | 25 | DG | O4'-C1'-C2' | -5.42 | 101.56 | 105.90 |
| 1 | AA | 500 | DC | O4'-C1'-C2' | -5.42 | 101.56 | 105.90 |
| 1 | AA | 700 | DT | O4'-C1'-C2' | -5.42 | 101.56 | 105.90 |
| 1 | AA | 2779 | DG | C5-C6-O6 | -5.42 | 125.35 | 128.60 |
| 24 | AX | 18 | DG | O4'-C1'-C2' | -5.42 | 101.56 | 105.90 |
| 1 | AA | 1518 | DA | O4'-C1'-C2' | -5.42 | 101.56 | 105.90 |
| 22 | AV | 47 | DC | O4'-C1'-C2' | -5.42 | 101.57 | 105.90 |
| 1 | AA | 907 | DA | C4'-C3'-C2' | -5.42 | 98.22 | 103.10 |
| 1 | AA | 2578 | DC | C6-N1-C2 | -5.42 | 118.13 | 120.30 |
| 14 | AN | 4 | DC | P-O5'-C5' | 5.42 | 129.57 | 120.90 |
| 1 | AA | 2546 | DC | O4'-C1'-C2' | -5.41 | 101.57 | 105.90 |
| 1 | AA | 3 | DG | C1'-O4'-C4' | -5.41 | 104.69 | 110.10 |
| 1 | AA | 2707 | DT | C4'-C3'-C2' | -5.41 | 98.23 | 103.10 |
| 22 | AV | 25 | DC | P-O5'-C5' | 5.41 | 129.55 | 120.90 |
| 22 | AV | 39 | DG | O4'-C4'-C3' | -5.41 | 102.34 | 104.50 |
| 1 | AA | 2448 | DG | C1'-O4'-C4' | -5.40 | 104.70 | 110.10 |
| 29 | Ac | 27 | DG | O4'-C1'-C2' | -5.40 | 101.58 | 105.90 |
| 64 | BB | 22 | DT | C4'-C3'-C2' | -5.40 | 98.24 | 103.10 |
| 1 | AA | 2608 | DA | P-O3'-C3' | 5.40 | 126.18 | 119.70 |
| 19 | AS | 13 | DC | P-O3'-C3' | 5.40 | 126.18 | 119.70 |
| 37 | Ak | 2 | DA | N1-C6-N6 | -5.40 | 115.36 | 118.60 |
| 1 | AA | 457 | DA | O4'-C1'-C2' | -5.40 | 101.58 | 105.90 |
| 42 | Ap | 4 | DT | O4'-C1'-C2' | -5.40 | 101.58 | 105.90 |
| 51 | Ay | 20 | DT | C4'-C3'-C2' | -5.40 | 98.24 | 103.10 |
| 1 | AA | 1286 | DA | C1'-O4'-C4' | -5.40 | 104.70 | 110.10 |
| 52 | Az | 25 | DA | C4'-C3'-C2' | -5.40 | 98.24 | 103.10 |
| 50 | Ax | 37 | DA | P-O3'-C3' | 5.40 | 126.17 | 119.70 |
| 68 | BF | 22 | DC | O4'-C1'-C2' | -5.40 | 101.58 | 105.90 |
| 13 | AM | 42 | DC | C2-N1-C1' | 5.39 | 124.73 | 118.80 |
| 37 | Ak | 24 | DG | O4'-C1'-C2' | -5.39 | 101.59 | 105.90 |
| 1 | AA | 1430 | DG | C1'-O4'-C4' | -5.39 | 104.71 | 110.10 |
| 1 | AA | 559 | DA | C4'-C3'-C2' | -5.39 | 98.25 | 103.10 |
| 41 | Ao | 20 | DG | O4'-C1'-C2' | -5.39 | 101.59 | 105.90 |
| 63 | BA | 22 | DA | P-O3'-C3' | 5.38 | 126.16 | 119.70 |
| 54 | A1 | 40 | DT | C6-C5-C7 | -5.38 | 119.67 | 122.90 |
| 1 | AA | 1268 | DG | O4'-C1'-C2' | -5.38 | 101.59 | 105.90 |
| 52 | Az | 11 | DT | P-O3'-C3' | 5.38 | 126.16 | 119.70 |
| 1 | AA | 931 | DT | C1'-O4'-C4' | -5.38 | 104.72 | 110.10 |
| 1 | AA | 1179 | DC | C4'-C3'-C2' | -5.38 | 98.26 | 103.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 21 | AU | 37 | DG | O4'-C1'-C2' | -5.38 | 101.60 | 105.90 |
| 1 | AA | 2004 | DG | N1-C6-O6 | 5.38 | 123.13 | 119.90 |
| 1 | AA | 252 | DG | C1'-O4'-C4' | -5.37 | 104.73 | 110.10 |
| 1 | AA | 1771 | DT | C4'-C3'-C2' | -5.37 | 98.26 | 103.10 |
| 46 | At | 15 | DG | O4'-C1'-C2' | -5.37 | 101.60 | 105.90 |
| 68 | BF | 36 | DC | O4'-C1'-C2' | -5.37 | 101.60 | 105.90 |
| 1 | AA | 1161 | DT | O4'-C1'-C2' | -5.37 | 101.61 | 105.90 |
| 1 | AA | 2083 | DT | P-O3'-C3' | 5.37 | 126.14 | 119.70 |
| 1 | AA | 472 | DT | C1'-O4'-C4' | -5.37 | 104.73 | 110.10 |
| 45 | As | 47 | DG | O4'-C1'-C2' | -5.37 | 101.61 | 105.90 |
| 1 | AA | 1019 | DT | O4'-C4'-C3' | -5.36 | 102.35 | 104.50 |
| 40 | An | 30 | DG | O4'-C1'-C2' | -5.36 | 101.61 | 105.90 |
| 74 | BL | 37 | DG | O4'-C1'-C2' | -5.36 | 101.61 | 105.90 |
| 65 | BC | 14 | DG | O4'-C1'-N9 | 5.36 | 111.75 | 108.00 |
| 1 | AA | 2004 | DG | C5-C6-O6 | -5.36 | 125.39 | 128.60 |
| 24 | AX | 13 | DT | C4'-C3'-C2' | -5.36 | 98.28 | 103.10 |
| 1 | AA | 293 | DT | C4'-C3'-C2' | -5.36 | 98.28 | 103.10 |
| 1 | AA | 2254 | DG | P-O3'-C3' | 5.36 | 126.13 | 119.70 |
| 1 | AA | 2856 | DT | O4'-C4'-C3' | -5.35 | 102.36 | 104.50 |
| 1 | AA | 2618 | DC | C6-N1-C2 | -5.35 | 118.16 | 120.30 |
| 1 | AA | 2779 | DG | N1-C6-O6 | 5.35 | 123.11 | 119.90 |
| 10 | AJ | 14 | DC | C4'-C3'-C2' | -5.35 | 98.28 | 103.10 |
| 78 | BP | 30 | DT | C1'-O4'-C4' | -5.35 | 104.75 | 110.10 |
| 1 | AA | 104 | DT | P-O3'-C3' | 5.35 | 126.12 | 119.70 |
| 74 | BL | 18 | DG | O4'-C1'-C2' | -5.35 | 101.62 | 105.90 |
| 1 | AA | 959 | DG | O4'-C1'-N9 | 5.34 | 111.74 | 108.00 |
| 1 | AA | 1950 | DC | P-O3'-C3' | 5.34 | 126.11 | 119.70 |
| 59 | A6 | 23 | DG | C1'-O4'-C4' | -5.34 | 104.76 | 110.10 |
| 1 | AA | 1382 | DC | C6-N1-C2 | -5.34 | 118.16 | 120.30 |
| 1 | AA | 1830 | DG | P-O3'-C3' | 5.34 | 126.11 | 119.70 |
| 1 | AA | 2771 | DT | P-O3'-C3' | 5.34 | 126.11 | 119.70 |
| 1 | AA | 1651 | DG | O4'-C4'-C3' | -5.34 | 102.36 | 104.50 |
| 21 | AU | 31 | DG | C4'-C3'-C2' | -5.34 | 98.30 | 103.10 |
| 22 | AV | 44 | DT | C1'-O4'-C4' | -5.33 | 104.77 | 110.10 |
| 1 | AA | 366 | DT | C4'-C3'-C2' | -5.33 | 98.30 | 103.10 |
| 1 | AA | 1214 | DG | C5-C6-O6 | -5.33 | 125.40 | 128.60 |
| 1 | AA | 2102 | DG | O4'-C1'-C2' | -5.33 | 101.63 | 105.90 |
| 1 | AA | 270 | DG | C5-C6-O6 | -5.33 | 125.40 | 128.60 |
| 19 | AS | 36 | DT | C1'-O4'-C4' | -5.33 | 104.77 | 110.10 |
| 40 | An | 30 | DG | C1'-O4'-C4' | -5.33 | 104.77 | 110.10 |
| 56 | A3 | 37 | DT | C4'-C3'-C2' | -5.33 | 98.30 | 103.10 |
| 63 | BA | 9 | DG | O4'-C1'-N9 | 5.33 | 111.73 | 108.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | AA | 739 | DA | O4'-C1'-N9 | 5.32 | 111.73 | 108.00 |
| 1 | AA | 1472 | DG | O4'-C1'-C2' | -5.32 | 101.64 | 105.90 |
| 10 | AJ | 1 | DT | C1'-O4'-C4' | -5.32 | 104.78 | 110.10 |
| 1 | AA | 448 | DC | P-O3'-C3' | 5.32 | 126.09 | 119.70 |
| 1 | AA | 1882 | DG | N3-C2-N2 | 5.32 | 123.62 | 119.90 |
| 1 | AA | 2133 | DA | C4'-C3'-C2' | -5.32 | 98.31 | 103.10 |
| 1 | AA | 2689 | DC | O4'-C1'-C2' | -5.32 | 101.64 | 105.90 |
| 11 | AK | 37 | DC | O4'-C1'-C2' | -5.32 | 101.64 | 105.90 |
| 1 | AA | 520 | DC | O4'-C1'-C2' | -5.32 | 101.64 | 105.90 |
| 21 | AU | 35 | DC | C2-N1-C1' | 5.32 | 124.65 | 118.80 |
| 39 | Am | 41 | DC | P-O3'-C3' | 5.32 | 126.08 | 119.70 |
| 49 | Aw | 30 | DG | O4'-C1'-C2' | -5.32 | 101.65 | 105.90 |
| 1 | AA | 31 | DC | O4'-C1'-C2' | -5.32 | 101.65 | 105.90 |
| 1 | AA | 1265 | DG | C1'-O4'-C4' | -5.32 | 104.78 | 110.10 |
| 30 | Ad | 19 | DG | O4'-C1'-N9 | 5.31 | 111.72 | 108.00 |
| 52 | Az | 20 | DC | C4'-C3'-C2' | -5.31 | 98.32 | 103.10 |
| 38 | Al | 2 | DG | C4'-C3'-C2' | -5.31 | 98.32 | 103.10 |
| 39 | Am | 14 | DC | O4'-C1'-C2' | -5.31 | 101.65 | 105.90 |
| 71 | BI | 16 | DT | C4'-C3'-C2' | -5.31 | 98.32 | 103.10 |
| 1 | AA | 2488 | DG | O4'-C1'-N9 | 5.31 | 111.72 | 108.00 |
| 65 | BC | 9 | DT | C4'-C3'-C2' | -5.31 | 98.32 | 103.10 |
| 72 | BJ | 26 | DC | O4'-C4'-C3' | -5.31 | 102.38 | 104.50 |
| 55 | A2 | 5 | DT | C4'-C3'-C2' | -5.31 | 98.32 | 103.10 |
| 60 | A7 | 13 | DT | C4'-C3'-C2' | -5.31 | 98.32 | 103.10 |
| 1 | AA | 961 | DT | C4'-C3'-C2' | -5.31 | 98.32 | 103.10 |
| 6 | AF | 11 | DT | O4'-C1'-N1 | 5.31 | 111.72 | 108.00 |
| 1 | AA | 1410 | DG | C5-C6-O6 | -5.30 | 125.42 | 128.60 |
| 1 | AA | 2154 | DG | N1-C6-O6 | 5.30 | 123.08 | 119.90 |
| 67 | BE | 22 | DG | C1'-O4'-C4' | -5.30 | 104.80 | 110.10 |
| 1 | AA | 1873 | DC | O4'-C1'-C2' | -5.30 | 101.66 | 105.90 |
| 1 | AA | 689 | DG | C4'-C3'-C2' | -5.30 | 98.33 | 103.10 |
| 50 | Ax | 19 | DC | C4'-C3'-C2' | -5.30 | 98.33 | 103.10 |
| 1 | AA | 2077 | DA | O4'-C1'-C2' | -5.30 | 101.66 | 105.90 |
| 10 | AJ | 10 | DC | P-O5'-C5' | 5.30 | 129.38 | 120.90 |
| 39 | Am | 12 | DC | O4'-C1'-C2' | -5.30 | 101.66 | 105.90 |
| 1 | AA | 1330 | DG | C5-C6-O6 | -5.29 | 125.42 | 128.60 |
| 3 | AC | 1 | DT | C4'-C3'-C2' | -5.29 | 98.33 | 103.10 |
| 55 | A2 | 12 | DG | O4'-C1'-C2' | -5.29 | 101.67 | 105.90 |
| 1 | AA | 2615 | DC | C4'-C3'-C2' | -5.29 | 98.34 | 103.10 |
| 29 | Ac | 16 | DC | O4'-C1'-C2' | -5.29 | 101.67 | 105.90 |
| 1 | AA | 2854 | DT | C4'-C3'-C2' | -5.29 | 98.34 | 103.10 |
| 25 | AY | 22 | DT | C4'-C3'-C2' | -5.28 | 98.34 | 103.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 76 | BN | 31 | DT | O4'-C1'-C2' | -5.28 | 101.67 | 105.90 |
| 1 | AA | 288 | DA | O4'-C1'-N9 | 5.28 | 111.70 | 108.00 |
| 1 | AA | 2136 | DG | C1'-O4'-C4' | -5.28 | 104.82 | 110.10 |
| 1 | AA | 410 | DC | P-O5'-C5' | 5.28 | 129.35 | 120.90 |
| 1 | AA | 389 | DG | C5-C6-O6 | -5.28 | 125.43 | 128.60 |
| 41 | Ao | 1 | DA | O4'-C4'-C3' | -5.28 | 102.39 | 104.50 |
| 56 | A3 | 26 | DG | O4'-C1'-C2' | -5.28 | 101.68 | 105.90 |
| 14 | AN | 3 | DG | C4'-C3'-C2' | -5.27 | 98.35 | 103.10 |
| 1 | AA | 779 | DA | N1-C6-N6 | -5.27 | 115.44 | 118.60 |
| 1 | AA | 2373 | DG | C5-C6-O6 | -5.27 | 125.44 | 128.60 |
| 54 | A1 | 26 | DG | C1'-O4'-C4' | -5.27 | 104.83 | 110.10 |
| 1 | AA | 2164 | DA | O4'-C1'-C2' | -5.27 | 101.68 | 105.90 |
| 40 | An | 14 | DG | C4'-C3'-C2' | -5.27 | 98.36 | 103.10 |
| 1 | AA | 1325 | DG | O4'-C1'-C2' | -5.27 | 101.68 | 105.90 |
| 1 | AA | 1371 | DG | C1'-O4'-C4' | -5.27 | 104.83 | 110.10 |
| 1 | AA | 547 | DT | C1'-O4'-C4' | -5.27 | 104.83 | 110.10 |
| 1 | AA | 1271 | DA | O4'-C1'-C2' | -5.27 | 101.69 | 105.90 |
| 1 | AA | 1428 | DG | C3'-C2'-C1' | -5.27 | 96.18 | 102.50 |
| 1 | AA | 2498 | DG | C5-C6-O6 | -5.27 | 125.44 | 128.60 |
| 13 | AM | 13 | DT | C4'-C3'-C2' | -5.27 | 98.36 | 103.10 |
| 22 | AV | 16 | DG | O4'-C1'-C2' | -5.27 | 101.69 | 105.90 |
| 79 | BQ | 6 | DG | N3-C2-N2 | 5.27 | 123.59 | 119.90 |
| 1 | AA | 1739 | DC | O4'-C1'-C2' | -5.27 | 101.69 | 105.90 |
| 1 | AA | 391 | DA | N1-C6-N6 | -5.26 | 115.44 | 118.60 |
| 49 | Aw | 10 | DG | O4'-C1'-C2' | -5.26 | 101.69 | 105.90 |
| 1 | AA | 2466 | DA | O4'-C1'-C2' | -5.26 | 101.69 | 105.90 |
| 59 | A6 | 3 | DT | P-O3'-C3' | 5.26 | 126.01 | 119.70 |
| 32 | Af | 22 | DT | C6-C5-C7 | -5.26 | 119.75 | 122.90 |
| 57 | A4 | 23 | DT | C1'-O4'-C4' | -5.26 | 104.84 | 110.10 |
| 1 | AA | 2408 | DC | O4'-C1'-C2' | -5.25 | 101.70 | 105.90 |
| 1 | AA | 1298 | DA | N1-C6-N6 | -5.25 | 115.45 | 118.60 |
| 3 | AC | 47 | DC | C1'-O4'-C4' | -5.25 | 104.85 | 110.10 |
| 76 | BN | 15 | DG | O4'-C1'-C2' | -5.25 | 101.70 | 105.90 |
| 76 | BN | 26 | DA | N1-C6-N6 | -5.25 | 115.45 | 118.60 |
| 1 | AA | 1298 | DA | O4'-C1'-C2' | -5.25 | 101.70 | 105.90 |
| 1 | AA | 1612 | DG | O4'-C1'-C2' | -5.25 | 101.70 | 105.90 |
| 15 | AO | 2 | DA | O4'-C1'-C2' | -5.25 | 101.70 | 105.90 |
| 1 | AA | 309 | DG | O4'-C1'-C2' | -5.25 | 101.70 | 105.90 |
| 1 | AA | 1963 | DG | C1'-O4'-C4' | -5.25 | 104.85 | 110.10 |
| 25 | AY | 3 | DT | P-O3'-C3' | 5.25 | 126.00 | 119.70 |
| 32 | Af | 14 | DT | O4'-C4'-C3' | -5.25 | 102.40 | 104.50 |
| 36 | Aj | 9 | DC | O4'-C1'-C2' | -5.25 | 101.70 | 105.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | AA | 2052 | DA | N1-C6-N6 | -5.25 | 115.45 | 118.60 |
| 1 | AA | 1628 | DG | C1'-O4'-C4' | -5.24 | 104.86 | 110.10 |
| 1 | AA | 1454 | DG | C1'-O4'-C4' | -5.24 | 104.86 | 110.10 |
| 1 | AA | 2702 | DG | N1-C6-O6 | 5.24 | 123.05 | 119.90 |
| 4 | AD | 14 | DT | P-O3'-C3' | 5.24 | 125.99 | 119.70 |
| 47 | Au | 33 | DC | C1'-O4'-C4' | -5.24 | 104.86 | 110.10 |
| 1 | AA | 2433 | DG | O4'-C1'-C2' | -5.24 | 101.71 | 105.90 |
| 63 | BA | 17 | DA | O4'-C1'-C2' | -5.24 | 101.71 | 105.90 |
| 72 | BJ | 33 | DT | C1'-O4'-C4' | -5.24 | 104.86 | 110.10 |
| 1 | AA | 887 | DC | O4'-C1'-N1 | 5.23 | 111.66 | 108.00 |
| 1 | AA | 2565 | DA | N1-C6-N6 | -5.23 | 115.46 | 118.60 |
| 49 | Aw | 32 | DC | C4'-C3'-C2' | -5.23 | 98.39 | 103.10 |
| 1 | AA | 4 | DG | C5-C6-O6 | -5.23 | 125.46 | 128.60 |
| 1 | AA | 1316 | DG | O4'-C1'-C2' | -5.23 | 101.72 | 105.90 |
| 78 | BP | 8 | DA | C1'-O4'-C4' | -5.23 | 104.87 | 110.10 |
| 1 | AA | 479 | DA | C1'-O4'-C4' | -5.23 | 104.87 | 110.10 |
| 63 | BA | 5 | DG | C4'-C3'-C2' | -5.22 | 98.40 | 103.10 |
| 1 | AA | 2448 | DG | P-O3'-C3' | 5.22 | 125.97 | 119.70 |
| 1 | AA | 2203 | DT | C6-C5-C7 | 5.22 | 126.03 | 122.90 |
| 11 | AK | 9 | DT | O4'-C1'-C2' | -5.22 | 101.72 | 105.90 |
| 48 | Av | 37 | DG | P-O3'-C3' | 5.22 | 125.96 | 119.70 |
| 1 | AA | 2544 | DG | P-O3'-C3' | 5.22 | 125.96 | 119.70 |
| 65 | BC | 1 | DA | N1-C6-N6 | -5.22 | 115.47 | 118.60 |
| 74 | BL | 37 | DG | C1'-O4'-C4' | -5.22 | 104.88 | 110.10 |
| 1 | AA | 2650 | DG | O4'-C1'-C2' | -5.21 | 101.73 | 105.90 |
| 16 | AP | 34 | DT | O4'-C1'-C2' | -5.21 | 101.73 | 105.90 |
| 51 | Ay | 2 | DG | C4'-C3'-C2' | -5.21 | 98.41 | 103.10 |
| 48 | Av | 20 | DC | C4'-C3'-C2' | -5.21 | 98.41 | 103.10 |
| 54 | A1 | 45 | DT | C2-N1-C1' | 5.21 | 126.54 | 118.20 |
| 1 | AA | 1660 | DG | O4'-C1'-C2' | -5.21 | 101.73 | 105.90 |
| 1 | AA | 1884 | DA | P-O3'-C3' | 5.21 | 125.95 | 119.70 |
| 1 | AA | 2420 | DG | C4'-C3'-C2' | -5.21 | 98.41 | 103.10 |
| 42 | Ap | 11 | DG | O4'-C1'-C2' | -5.21 | 101.73 | 105.90 |
| 1 | AA | 582 | DA | O4'-C1'-C2' | -5.21 | 101.74 | 105.90 |
| 1 | AA | 639 | DA | O4'-C4'-C3' | -5.21 | 102.42 | 104.50 |
| 1 | AA | 2330 | DT | C4'-C3'-C2' | -5.21 | 98.41 | 103.10 |
| 52 | Az | 32 | DG | O4'-C1'-C2' | -5.21 | 101.73 | 105.90 |
| 1 | AA | 149 | DT | C1'-O4'-C4' | -5.21 | 104.89 | 110.10 |
| 35 | Ai | 8 | DG | C5-C6-O6 | -5.20 | 125.48 | 128.60 |
| 1 | AA | 507 | DA | O4'-C1'-C2' | -5.20 | 101.74 | 105.90 |
| 1 | AA | 1333 | DA | O4'-C1'-C2' | -5.20 | 101.74 | 105.90 |
| 1 | AA | 2644 | DC | P-O5'-C5' | 5.20 | 129.22 | 120.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | AA | 2397 | DA | P-O3'-C3' | 5.20 | 125.94 | 119.70 |
| 1 | AA | 2431 | DG | C4'-C3'-C2' | -5.20 | 98.42 | 103.10 |
| 2 | AB | 11 | DC | C6-N1-C2 | -5.20 | 118.22 | 120.30 |
| 34 | Ah | 8 | DA | O4'-C1'-C2' | -5.20 | 101.74 | 105.90 |
| 1 | AA | 1550 | DG | O4'-C1'-N9 | 5.20 | 111.64 | 108.00 |
| 75 | BM | 26 | DG | O4'-C1'-C2' | -5.20 | 101.74 | 105.90 |
| 8 | AH | 29 | DG | O4'-C1'-N9 | 5.20 | 111.64 | 108.00 |
| 52 | Az | 32 | DG | O4'-C1'-N9 | 5.20 | 111.64 | 108.00 |
| 1 | AA | 687 | DA | N1-C6-N6 | 5.19 | 121.72 | 118.60 |
| 1 | AA | 747 | DG | O4'-C1'-N9 | 5.19 | 111.64 | 108.00 |
| 1 | AA | 1214 | DG | N1-C6-O6 | 5.19 | 123.02 | 119.90 |
| 1 | AA | 1286 | DA | O4'-C1'-N9 | 5.19 | 111.64 | 108.00 |
| 15 | AO | 8 | DG | O4'-C1'-C2' | -5.19 | 101.75 | 105.90 |
| 63 | BA | 30 | DA | O4'-C1'-N9 | 5.19 | 111.64 | 108.00 |
| 1 | AA | 1142 | DA | P-O3'-C3' | 5.19 | 125.93 | 119.70 |
| 1 | AA | 1356 | DC | P-O3'-C3' | 5.19 | 125.93 | 119.70 |
| 1 | AA | 2725 | DT | C4'-C3'-C2' | -5.19 | 98.43 | 103.10 |
| 1 | AA | 318 | DT | C4'-C3'-C2' | -5.18 | 98.43 | 103.10 |
| 15 | AO | 16 | DA | C4'-C3'-C2' | -5.18 | 98.43 | 103.10 |
| 29 | Ac | 19 | DG | O4'-C1'-N9 | 5.18 | 111.63 | 108.00 |
| 75 | BM | 4 | DT | C4'-C3'-C2' | -5.18 | 98.44 | 103.10 |
| 1 | AA | 600 | DA | C4'-C3'-C2' | -5.18 | 98.44 | 103.10 |
| 18 | AR | 4 | DT | C6-C5-C7 | -5.18 | 119.79 | 122.90 |
| 22 | AV | 28 | DC | O4'-C1'-C2' | -5.18 | 101.75 | 105.90 |
| 34 | Ah | 12 | DT | O4'-C4'-C3' | -5.18 | 102.43 | 104.50 |
| 1 | AA | 103 | DT | C4'-C3'-C2' | -5.18 | 98.44 | 103.10 |
| 1 | AA | 2374 | DA | O4'-C1'-C2' | -5.18 | 101.76 | 105.90 |
| 37 | Ak | 9 | DT | C1'-O4'-C4' | -5.18 | 104.92 | 110.10 |
| 64 | BB | 41 | DT | P-O3'-C3' | 5.18 | 125.91 | 119.70 |
| 1 | AA | 156 | DC | O4'-C1'-C2' | -5.18 | 101.76 | 105.90 |
| 1 | AA | 597 | DG | C1'-O4'-C4' | -5.17 | 104.93 | 110.10 |
| 1 | AA | 1244 | DA | N1-C6-N6 | 5.17 | 121.70 | 118.60 |
| 1 | AA | 117 | DA | O4'-C1'-C2' | -5.17 | 101.76 | 105.90 |
| 1 | AA | 2852 | DA | O4'-C4'-C3' | -5.17 | 102.43 | 104.50 |
| 10 | AJ | 13 | DC | C2-N1-C1' | 5.17 | 124.49 | 118.80 |
| 1 | AA | 2435 | DA | N1-C6-N6 | -5.17 | 115.50 | 118.60 |
| 35 | Ai | 6 | DG | N1-C6-O6 | 5.17 | 123.00 | 119.90 |
| 1 | AA | 2672 | DG | N1-C6-O6 | 5.17 | 123.00 | 119.90 |
| 1 | AA | 1851 | DA | C1'-O4'-C4' | -5.16 | 104.94 | 110.10 |
| 7 | AG | 29 | DG | C1'-O4'-C4' | -5.16 | 104.94 | 110.10 |
| 28 | Ab | 29 | DG | N1-C6-O6 | 5.16 | 123.00 | 119.90 |
| 74 | BL | 3 | DG | O4'-C1'-C2' | -5.16 | 101.77 | 105.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | AA | 897 | DG | O4'-C1'-C2' | -5.16 | 101.77 | 105.90 |
| 10 | AJ | 13 | DC | C6-N1-C2 | -5.16 | 118.24 | 120.30 |
| 1 | AA | 371 | DT | P-O3'-C3' | 5.16 | 125.89 | 119.70 |
| 1 | AA | 1547 | DT | O4'-C4'-C3' | -5.16 | 102.44 | 104.50 |
| 1 | AA | 1968 | DC | O4'-C1'-C2' | -5.16 | 101.77 | 105.90 |
| 1 | AA | 804 | DG | O4'-C1'-C2' | -5.16 | 101.77 | 105.90 |
| 26 | AZ | 26 | DT | O4'-C1'-C2' | -5.16 | 101.77 | 105.90 |
| 1 | AA | 1829 | DT | C4'-C3'-C2' | -5.16 | 98.46 | 103.10 |
| 40 | An | 23 | DG | O4'-C1'-C2' | -5.15 | 101.78 | 105.90 |
| 76 | BN | 30 | DT | P-O3'-C3' | 5.15 | 125.89 | 119.70 |
| 1 | AA | 1458 | DA | O4'-C1'-C2' | -5.15 | 101.78 | 105.90 |
| 1 | AA | 2122 | DA | O4'-C1'-C2' | -5.15 | 101.78 | 105.90 |
| 1 | AA | 1997 | DG | O4'-C1'-C2' | -5.15 | 101.78 | 105.90 |
| 22 | AV | 31 | DG | O4'-C4'-C3' | -5.15 | 102.44 | 104.50 |
| 1 | AA | 604 | DG | P-O3'-C3' | 5.15 | 125.88 | 119.70 |
| 1 | AA | 282 | DG | O4'-C1'-C2' | -5.15 | 101.78 | 105.90 |
| 1 | AA | 1375 | DT | O4'-C1'-C2' | -5.15 | 101.78 | 105.90 |
| 21 | AU | 17 | DT | C4'-C3'-C2' | -5.15 | 98.47 | 103.10 |
| 78 | BP | 12 | DT | C4'-C3'-C2' | -5.15 | 98.47 | 103.10 |
| 1 | AA | 1601 | DG | O4'-C1'-C2' | -5.15 | 101.78 | 105.90 |
| 11 | AK | 10 | DT | C4'-C3'-C2' | -5.15 | 98.47 | 103.10 |
| 1 | AA | 506 | DC | C2-N1-C1' | 5.14 | 124.46 | 118.80 |
| 78 | BP | 6 | DC | C1'-O4'-C4' | -5.14 | 104.96 | 110.10 |
| 79 | BQ | 20 | DA | P-O3'-C3' | 5.14 | 125.87 | 119.70 |
| 1 | AA | 679 | DT | O4'-C1'-C2' | -5.14 | 101.79 | 105.90 |
| 1 | AA | 1385 | DG | O4'-C1'-N9 | 5.14 | 111.60 | 108.00 |
| 1 | AA | 2665 | DG | C1'-O4'-C4' | -5.14 | 104.96 | 110.10 |
| 18 | AR | 23 | DC | C1'-O4'-C4' | -5.13 | 104.97 | 110.10 |
| 41 | Ao | 9 | DA | O4'-C1'-C2' | -5.13 | 101.79 | 105.90 |
| 1 | AA | 1673 | DT | C4'-C3'-C2' | -5.13 | 98.48 | 103.10 |
| 36 | Aj | 29 | DG | O4'-C1'-C2' | -5.13 | 101.79 | 105.90 |
| 1 | AA | 1749 | DA | N1-C6-N6 | -5.13 | 115.52 | 118.60 |
| 30 | Ad | 24 | DA | C4'-C3'-C2' | -5.13 | 98.48 | 103.10 |
| 1 | AA | 511 | DG | C1'-O4'-C4' | -5.13 | 104.97 | 110.10 |
| 14 | AN | 7 | DT | C4'-C3'-C2' | -5.13 | 98.48 | 103.10 |
| 1 | AA | 1698 | DC | C4'-C3'-C2' | -5.13 | 98.48 | 103.10 |
| 1 | AA | 1786 | DT | O4'-C4'-C3' | -5.13 | 102.45 | 104.50 |
| 1 | AA | 2204 | DC | P-O3'-C3' | 5.13 | 125.85 | 119.70 |
| 56 | A3 | 16 | DG | C1'-O4'-C4' | -5.13 | 104.97 | 110.10 |
| 73 | BK | 6 | DG | C1'-O4'-C4' | -5.13 | 104.97 | 110.10 |
| 1 | AA | 2040 | DG | C1'-O4'-C4' | -5.13 | 104.97 | 110.10 |
| 1 | AA | 2145 | DT | C4'-C3'-C2' | -5.13 | 98.49 | 103.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | AA | 128 | DT | C4'-C3'-C2' | -5.12 | 98.49 | 103.10 |
| 1 | AA | 1790 | DC | C4'-C3'-C2' | -5.12 | 98.49 | 103.10 |
| 11 | AK | 40 | DA | P-O3'-C3' | 5.12 | 125.85 | 119.70 |
| 12 | AL | 13 | DG | C5-C6-O6 | -5.12 | 125.53 | 128.60 |
| 34 | Ah | 21 | DG | O4'-C1'-C2' | -5.12 | 101.80 | 105.90 |
| 43 | Aq | 12 | DG | C5-C6-O6 | -5.12 | 125.53 | 128.60 |
| 1 | AA | 260 | DC | O4'-C1'-C2' | -5.12 | 101.80 | 105.90 |
| 78 | BP | 30 | DT | C4-C5-C7 | -5.12 | 115.93 | 119.00 |
| 1 | AA | 520 | DC | C1'-O4'-C4' | -5.12 | 104.98 | 110.10 |
| 13 | AM | 42 | DC | O4'-C1'-N1 | -5.12 | 104.42 | 108.00 |
| 38 | Al | 9 | DC | O4'-C1'-C2' | -5.12 | 101.81 | 105.90 |
| 1 | AA | 1586 | DG | O4'-C1'-C2' | -5.12 | 101.81 | 105.90 |
| 8 | AH | 15 | DT | C4'-C3'-C2' | -5.11 | 98.50 | 103.10 |
| 11 | AK | 35 | DT | O4'-C1'-C2' | -5.11 | 101.81 | 105.90 |
| 1 | AA | 855 | DA | O4'-C1'-C2' | -5.11 | 101.81 | 105.90 |
| 1 | AA | 886 | DC | O4'-C1'-N1 | 5.11 | 111.58 | 108.00 |
| 1 | AA | 900 | DG | C1'-O4'-C4' | -5.11 | 104.99 | 110.10 |
| 1 | AA | 1240 | DA | O4'-C1'-C2' | -5.11 | 101.81 | 105.90 |
| 1 | AA | 1566 | DA | P-O3'-C3' | 5.11 | 125.83 | 119.70 |
| 16 | AP | 47 | DA | C4'-C3'-C2' | -5.11 | 98.50 | 103.10 |
| 22 | AV | 21 | DA | P-O3'-C3' | 5.11 | 125.83 | 119.70 |
| 59 | A6 | 23 | DG | C5-C6-O6 | -5.11 | 125.53 | 128.60 |
| 77 | BO | 25 | DA | O4'-C4'-C3' | -5.11 | 102.46 | 104.50 |
| 1 | AA | 74 | DG | C4'-C3'-C2' | -5.11 | 98.50 | 103.10 |
| 1 | AA | 359 | DG | O4'-C1'-C2' | -5.11 | 101.81 | 105.90 |
| 1 | AA | 1343 | DG | N1-C6-O6 | 5.11 | 122.96 | 119.90 |
| 11 | AK | 36 | DT | C6-C5-C7 | -5.11 | 119.84 | 122.90 |
| 45 | As | 34 | DG | O4'-C4'-C3' | -5.11 | 102.46 | 104.50 |
| 27 | Aa | 12 | DA | O4'-C1'-C2' | -5.10 | 101.82 | 105.90 |
| 1 | AA | 1605 | DA | C1'-O4'-C4' | -5.10 | 105.00 | 110.10 |
| 1 | AA | 2444 | DG | C1'-O4'-C4' | -5.10 | 105.00 | 110.10 |
| 41 | Ao | 10 | DT | O4'-C1'-C2' | -5.10 | 101.82 | 105.90 |
| 1 | AA | 1882 | DG | C5-C6-O6 | -5.10 | 125.54 | 128.60 |
| 1 | AA | 1325 | DG | P-O3'-C3' | 5.10 | 125.82 | 119.70 |
| 44 | Ar | 47 | DG | O4'-C1'-C2' | -5.10 | 101.82 | 105.90 |
| 1 | AA | 2307 | DC | C6-N1-C2 | -5.10 | 118.26 | 120.30 |
| 1 | AA | 2693 | DG | O4'-C1'-C2' | -5.10 | 101.82 | 105.90 |
| 1 | AA | 1307 | DT | C4'-C3'-C2' | -5.09 | 98.52 | 103.10 |
| 1 | AA | 1910 | DA | P-O3'-C3' | 5.09 | 125.81 | 119.70 |
| 7 | AG | 10 | DG | C1'-O4'-C4' | -5.09 | 105.01 | 110.10 |
| 11 | AK | 41 | DA | O4'-C1'-C2' | -5.09 | 101.83 | 105.90 |
| 35 | Ai | 27 | DG | C5-C6-O6 | -5.09 | 125.55 | 128.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | AA | 524 | DG | O4'-C1'-N9 | 5.09 | 111.56 | 108.00 |
| 1 | AA | 2498 | DG | N1-C6-O6 | 5.09 | 122.95 | 119.90 |
| 75 | BM | 30 | DG | C1'-O4'-C4' | -5.09 | 105.01 | 110.10 |
| 3 | AC | 21 | DT | O4'-C4'-C3' | -5.09 | 102.47 | 104.50 |
| 75 | BM | 37 | DG | O4'-C1'-C2' | -5.09 | 101.83 | 105.90 |
| 1 | AA | 1043 | DT | P-O3'-C3' | 5.09 | 125.80 | 119.70 |
| 1 | AA | 1622 | DA | P-O5'-C5' | 5.08 | 129.03 | 120.90 |
| 22 | AV | 9 | DC | C1'-O4'-C4' | -5.08 | 105.02 | 110.10 |
| 51 | Ay | 23 | DG | O4'-C1'-C2' | -5.08 | 101.83 | 105.90 |
| 1 | AA | 1529 | DA | O4'-C1'-C2' | -5.08 | 101.83 | 105.90 |
| 32 | Af | 30 | DT | P-O3'-C3' | 5.08 | 125.80 | 119.70 |
| 52 | Az | 31 | DA | C1'-O4'-C4' | -5.08 | 105.02 | 110.10 |
| 1 | AA | 121 | DG | C1'-O4'-C4' | -5.08 | 105.02 | 110.10 |
| 47 | Au | 42 | DA | O4'-C1'-C2' | -5.08 | 101.84 | 105.90 |
| 1 | AA | 2700 | DA | O4'-C1'-C2' | -5.08 | 101.84 | 105.90 |
| 1 | AA | 561 | DG | C1'-O4'-C4' | -5.08 | 105.02 | 110.10 |
| 1 | AA | 1678 | DT | C1'-O4'-C4' | -5.08 | 105.02 | 110.10 |
| 1 | AA | 2213 | DC | O4'-C1'-N1 | 5.08 | 111.55 | 108.00 |
| 50 | Ax | 18 | DA | C5-C6-N6 | 5.08 | 127.76 | 123.70 |
| 50 | Ax | 28 | DC | C6-N1-C2 | -5.08 | 118.27 | 120.30 |
| 33 | Ag | 24 | DT | C4'-C3'-C2' | -5.07 | 98.53 | 103.10 |
| 1 | AA | 1937 | DA | N1-C6-N6 | 5.07 | 121.64 | 118.60 |
| 49 | Aw | 31 | DG | C5-C6-O6 | -5.07 | 125.56 | 128.60 |
| 1 | AA | 959 | DG | O4'-C1'-C2' | -5.07 | 101.85 | 105.90 |
| 1 | AA | 2427 | DA | C1'-O4'-C4' | -5.07 | 105.03 | 110.10 |
| 32 | Af | 8 | DA | O4'-C1'-C2' | -5.07 | 101.85 | 105.90 |
| 1 | AA | 727 | DC | P-O5'-C5' | 5.07 | 129.00 | 120.90 |
| 1 | AA | 1145 | DG | O4'-C1'-C2' | -5.07 | 101.85 | 105.90 |
| 1 | AA | 1313 | DA | C1'-O4'-C4' | -5.06 | 105.04 | 110.10 |
| 54 | A1 | 27 | DG | P-O3'-C3' | 5.06 | 125.78 | 119.70 |
| 1 | AA | 1553 | DA | C4'-C3'-C2' | -5.06 | 98.54 | 103.10 |
| 1 | AA | 2507 | DT | O4'-C1'-C2' | -5.06 | 101.85 | 105.90 |
| 42 | Ap | 5 | DT | O4'-C1'-C2' | -5.06 | 101.85 | 105.90 |
| 74 | BL | 12 | DG | O4'-C1'-C2' | -5.06 | 101.85 | 105.90 |
| 1 | AA | 1454 | DG | O4'-C1'-N9 | 5.06 | 111.54 | 108.00 |
| 1 | AA | 1505 | DC | O4'-C1'-N1 | 5.06 | 111.54 | 108.00 |
| 1 | AA | 1647 | DG | O4'-C1'-C2' | -5.06 | 101.85 | 105.90 |
| 1 | AA | 2421 | DC | P-O5'-C5' | 5.06 | 129.00 | 120.90 |
| 8 | AH | 1 | DA | O4'-C4'-C3' | -5.06 | 102.48 | 104.50 |
| 44 | Ar | 23 | DA | C3'-C2'-C1' | -5.06 | 96.43 | 102.50 |
| 1 | AA | 2209 | DT | C4'-C3'-C2' | -5.06 | 98.55 | 103.10 |
| 1 | AA | 2511 | DG | C5-C6-O6 | -5.06 | 125.56 | 128.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 51 | Ay | 27 | DT | O4'-C1'-N1 | -5.06 | 104.46 | 108.00 |
| 1 | AA | 22 | DT | C1'-O4'-C4' | -5.05 | 105.05 | 110.10 |
| 1 | AA | 2488 | DG | C1'-O4'-C4' | -5.05 | 105.05 | 110.10 |
| 1 | AA | 2838 | DG | C4'-C3'-C2' | -5.05 | 98.55 | 103.10 |
| 72 | BJ | 40 | DG | N1-C6-O6 | 5.05 | 122.93 | 119.90 |
| 79 | BQ | 33 | DT | C4'-C3'-C2' | -5.05 | 98.55 | 103.10 |
| 1 | AA | 1483 | DG | N3-C2-N2 | 5.05 | 123.44 | 119.90 |
| 18 | AR | 4 | DT | C4-C5-C7 | 5.05 | 122.03 | 119.00 |
| 1 | AA | 1107 | DG | O4'-C1'-C2' | -5.05 | 101.86 | 105.90 |
| 1 | AA | 1405 | DG | C4'-C3'-C2' | -5.05 | 98.56 | 103.10 |
| 1 | AA | 539 | DG | P-O3'-C3' | 5.05 | 125.75 | 119.70 |
| 1 | AA | 1250 | DA | P-O3'-C3' | 5.05 | 125.76 | 119.70 |
| 37 | Ak | 13 | DT | O4'-C4'-C3' | -5.04 | 102.48 | 104.50 |
| 65 | BC | 10 | DA | P-O3'-C3' | 5.04 | 125.75 | 119.70 |
| 46 | At | 46 | DG | O4'-C1'-C2' | -5.04 | 101.86 | 105.90 |
| 1 | AA | 111 | DT | O4'-C1'-C2' | -5.04 | 101.87 | 105.90 |
| 1 | AA | 1708 | DG | O4'-C1'-C2' | -5.04 | 101.87 | 105.90 |
| 1 | AA | 2475 | DG | N1-C6-O6 | 5.04 | 122.92 | 119.90 |
| 54 | A1 | 45 | DT | C6-N1-C1' | -5.04 | 112.84 | 120.40 |
| 79 | BQ | 1 | DT | O4'-C4'-C3' | -5.04 | 102.48 | 104.50 |
| 1 | AA | 1538 | DC | P-O3'-C3' | -5.04 | 113.65 | 119.70 |
| 33 | Ag | 20 | DG | O4'-C1'-C2' | -5.04 | 101.87 | 105.90 |
| 1 | AA | 286 | DA | N1-C6-N6 | -5.04 | 115.58 | 118.60 |
| 1 | AA | 2031 | DG | C5-C6-O6 | -5.04 | 125.58 | 128.60 |
| 1 | AA | 2698 | DC | P-O3'-C3' | 5.04 | 125.75 | 119.70 |
| 1 | AA | 2822 | DT | O4'-C4'-C3' | -5.04 | 102.48 | 104.50 |
| 76 | BN | 1 | DT | C1'-O4'-C4' | -5.04 | 105.06 | 110.10 |
| 1 | AA | 1547 | DT | C4'-C3'-C2' | -5.04 | 98.57 | 103.10 |
| 50 | Ax | 37 | DA | C3'-C2'-C1' | -5.04 | 96.46 | 102.50 |
| 23 | AW | 41 | DA | P-O3'-C3' | 5.04 | 125.74 | 119.70 |
| 73 | BK | 1 | DT | C4'-C3'-C2' | -5.03 | 98.57 | 103.10 |
| 35 | Ai | 21 | DA | C4'-C3'-C2' | -5.03 | 98.57 | 103.10 |
| 1 | AA | 372 | DA | P-O3'-C3' | 5.03 | 125.74 | 119.70 |
| 1 | AA | 401 | DC | O4'-C1'-N1 | 5.03 | 111.52 | 108.00 |
| 1 | AA | 605 | DC | C6-N1-C2 | -5.03 | 118.29 | 120.30 |
| 1 | AA | 1755 | DA | O4'-C1'-C2' | -5.03 | 101.88 | 105.90 |
| 1 | AA | 1997 | DG | O4'-C1'-N9 | 5.03 | 111.52 | 108.00 |
| 1 | AA | 2657 | DA | O4'-C4'-C3' | -5.03 | 102.49 | 104.50 |
| 1 | AA | 1225 | DT | C4'-C3'-C2' | -5.03 | 98.57 | 103.10 |
| 1 | AA | 876 | DG | O4'-C1'-C2' | -5.03 | 101.88 | 105.90 |
| 1 | AA | 2794 | DC | C4'-C3'-C2' | -5.03 | 98.58 | 103.10 |
| 20 | AT | 30 | DA | C1'-O4'-C4' | -5.03 | 105.07 | 110.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 44 | Ar | 20 | DT | C4'-C3'-C2' | -5.03 | 98.58 | 103.10 |
| 70 | BH | 9 | DG | O4'-C1'-C2' | -5.03 | 101.88 | 105.90 |
| 1 | AA | 1026 | DG | O4'-C1'-C2' | -5.02 | 101.88 | 105.90 |
| 1 | AA | 1937 | DA | C5-C6-N6 | -5.02 | 119.68 | 123.70 |
| 1 | AA | 1758 | DA | N1-C6-N6 | -5.02 | 115.59 | 118.60 |
| 22 | AV | 16 | DG | P-O3'-C3' | 5.02 | 125.72 | 119.70 |
| 67 | BE | 9 | DG | P-O3'-C3' | 5.02 | 125.72 | 119.70 |
| 71 | BI | 40 | DA | O4'-C1'-C2' | -5.02 | 101.89 | 105.90 |
| 1 | AA | 6 | DA | P-O5'-C5' | 5.02 | 128.93 | 120.90 |
| 1 | AA | 1941 | DC | C1'-O4'-C4' | -5.02 | 105.08 | 110.10 |
| 1 | AA | 2763 | DT | C4'-C3'-C2' | -5.02 | 98.58 | 103.10 |
| 68 | BF | 30 | DG | C4'-C3'-C2' | -5.02 | 98.58 | 103.10 |
| 56 | A3 | 16 | DG | O4'-C1'-C2' | -5.02 | 101.89 | 105.90 |
| 1 | AA | 1173 | DT | C4'-C3'-C2' | -5.01 | 98.59 | 103.10 |
| 50 | Ax | 27 | DG | C5-C6-O6 | -5.01 | 125.59 | 128.60 |
| 1 | AA | 570 | DG | O4'-C1'-C2' | -5.01 | 101.89 | 105.90 |
| 23 | AW | 40 | DC | C2-N1-C1' | 5.01 | 124.31 | 118.80 |
| 1 | AA | 2219 | DT | C6-C5-C7 | -5.01 | 119.89 | 122.90 |
| 32 | Af | 5 | DA | C1'-O4'-C4' | -5.01 | 105.09 | 110.10 |
| 49 | Aw | 30 | DG | C1'-O4'-C4' | -5.01 | 105.09 | 110.10 |
| 1 | AA | 881 | DT | O4'-C1'-C2' | -5.01 | 101.89 | 105.90 |
| 24 | AX | 24 | DC | C2-N1-C1' | 5.01 | 124.31 | 118.80 |
| 1 | AA | 1187 | DC | C2-N1-C1' | 5.00 | 124.31 | 118.80 |
| 48 | Av | 12 | DA | P-O3'-C3' | 5.00 | 125.70 | 119.70 |
| 1 | AA | 1818 | DG | O4'-C1'-N9 | 5.00 | 111.50 | 108.00 |
| 43 | Aq | 8 | DC | C4'-C3'-C2' | -5.00 | 98.60 | 103.10 |
| 45 | As | 23 | DA | C1'-O4'-C4' | -5.00 | 105.10 | 110.10 |
| 45 | As | 37 | DC | O4'-C1'-C2' | -5.00 | 101.90 | 105.90 |
| 66 | BD | 5 | DG | O4'-C1'-C2' | -5.00 | 101.90 | 105.90 |

All (12) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 1 | AA | 342 | DG | C3' |
| 1 | AA | 738 | DC | C3' |
| 1 | AA | 1302 | DA | C3' |
| 1 | AA | 1360 | DC | C3' |
| 1 | AA | 1774 | DG | C3' |
| 1 | AA | 1908 | DT | C3' |
| 1 | AA | 2278 | DG | C3' |
| 1 | AA | 2390 | DG | C3' |
| 1 | AA | 2740 | DC | C3' |

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| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 1 | AA | 2852 | DA | C3' |
| 19 | AS | 37 | DG | C3' |
| 25 | AY | 5 | DT | C3' |

All (1459) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 53 | A0 | 18 | DA | Sidechain |
| 53 | A0 | 2 | DC | Sidechain |
| 53 | A0 | 22 | DC | Sidechain |
| 53 | A0 | 6 | DG | Sidechain |
| 53 | A0 | 8 | DG | Sidechain |
| 53 | A0 | 9 | DT | Sidechain |
| 54 | A1 | 10 | DC | Sidechain |
| 54 | A1 | 17 | DA | Sidechain |
| 54 | A1 | 22 | DG | Sidechain |
| 54 | A1 | 26 | DG | Sidechain |
| 54 | A1 | 30 | DA | Sidechain |
| 54 | A1 | 32 | DT | Sidechain |
| 54 | A1 | 37 | DG | Sidechain |
| 54 | A1 | 4 | DG | Sidechain |
| 54 | A1 | 41 | DT | Sidechain |
| 54 | A1 | 6 | DG | Sidechain |
| 55 | A2 | 13 | DG | Sidechain |
| 55 | A2 | 14 | DG | Sidechain |
| 55 | A2 | 15 | DG | Sidechain |
| 55 | A2 | 18 | DA | Sidechain |
| 55 | A2 | 20 | DG | Sidechain |
| 55 | A2 | 22 | DA | Sidechain |
| 55 | A2 | 24 | DG | Sidechain |
| 55 | A2 | 29 | DA | Sidechain |
| 55 | A2 | 31 | DT | Sidechain |
| 55 | A2 | 32 | DT | Sidechain |
| 55 | A2 | 5 | DT | Sidechain |
| 55 | A2 | 7 | DT | Sidechain |
| 55 | A2 | 9 | DT | Sidechain |
| 56 | A3 | 10 | DG | Sidechain |
| 56 | A3 | 11 | DT | Sidechain |
| 56 | A3 | 13 | DT | Sidechain |
| 56 | A3 | 15 | DC | Sidechain |
| 56 | A3 | 19 | DG | Sidechain |
| 56 | A3 | 20 | DA | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 56 | A3 | 21 | DA | Sidechain |
| 56 | A3 | 28 | DT | Sidechain |
| 56 | A3 | 4 | DT | Sidechain |
| 56 | A3 | 7 | DA | Sidechain |
| 56 | A3 | 8 | DT | Sidechain |
| 57 | A4 | 1 | DC | Sidechain |
| 57 | A4 | 12 | DC | Sidechain |
| 57 | A4 | 18 | DA | Sidechain |
| 57 | A4 | 23 | DT | Sidechain |
| 57 | A4 | 24 | DA | Sidechain |
| 57 | A4 | 29 | DA | Sidechain |
| 57 | A4 | 31 | DT | Sidechain |
| 57 | A4 | 34 | DG | Sidechain |
| 57 | A4 | 37 | DC | Sidechain |
| 57 | A4 | 38 | DC | Sidechain |
| 58 | A5 | 18 | DC | Sidechain |
| 58 | A5 | 25 | DA | Sidechain |
| 58 | A5 | 26 | DG | Sidechain |
| 58 | A5 | 29 | DT | Sidechain |
| 58 | A5 | 3 | DA | Sidechain |
| 58 | A5 | 6 | DA | Sidechain |
| 58 | A5 | 8 | DA | Sidechain |
| 59 | A6 | 17 | DT | Sidechain |
| 59 | A6 | 18 | DT | Sidechain |
| 59 | A6 | 19 | DG | Sidechain |
| 59 | A6 | 3 | DT | Sidechain |
| 59 | A6 | 9 | DG | Sidechain |
| 60 | A7 | 23 | DA | Sidechain |
| 60 | A7 | 28 | DT | Sidechain |
| 60 | A7 | 31 | DT | Sidechain |
| 60 | A7 | 32 | DT | Sidechain |
| 60 | A7 | 5 | DT | Sidechain |
| 60 | A7 | 9 | DG | Sidechain |
| 61 | A8 | 12 | DG | Sidechain |
| 61 | A8 | 13 | DT | Sidechain |
| 61 | A8 | 19 | DT | Sidechain |
| 61 | A8 | 7 | DT | Sidechain |
| 62 | A9 | 15 | DG | Sidechain |
| 62 | A9 | 19 | DT | Sidechain |
| 62 | A9 | 25 | DT | Sidechain |
| 62 | A9 | 26 | DC | Sidechain |
| 62 | A9 | 28 | DA | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 62 | A9 | 37 | DA | Sidechain |
| 62 | A9 | 38 | DG | Sidechain |
| 62 | A9 | 40 | DG | Sidechain |
| 62 | A9 | 41 | DA | Sidechain |
| 62 | A9 | 6 | DG | Sidechain |
| 1 | AA | 1002 | DG | Sidechain |
| 1 | AA | 1014 | DA | Sidechain |
| 1 | AA | 1015 | DT | Sidechain |
| 1 | AA | 1023 | DA | Sidechain |
| 1 | AA | 103 | DT | Sidechain |
| 1 | AA | 1030 | DT | Sidechain |
| 1 | AA | 1033 | DA | Sidechain |
| 1 | AA | 1040 | DT | Sidechain |
| 1 | AA | 1042 | DT | Sidechain |
| 1 | AA | 1048 | DT | Sidechain |
| 1 | AA | 1059 | DT | Sidechain |
| 1 | AA | 1061 | DG | Sidechain |
| 1 | AA | 1063 | DT | Sidechain |
| 1 | AA | 1066 | DA | Sidechain |
| 1 | AA | 1068 | DA | Sidechain |
| 1 | AA | 1069 | DT | Sidechain |
| 1 | AA | 1078 | DA | Sidechain |
| 1 | AA | 1082 | DT | Sidechain |
| 1 | AA | 1084 | DT | Sidechain |
| 1 | AA | 1086 | DA | Sidechain |
| 1 | AA | 1101 | DT | Sidechain |
| 1 | AA | 1106 | DT | Sidechain |
| 1 | AA | 111 | DT | Sidechain |
| 1 | AA | 1110 | DT | Sidechain |
| 1 | AA | 1112 | DT | Sidechain |
| 1 | AA | 1113 | DT | Sidechain |
| 1 | AA | 1121 | DC | Sidechain |
| 1 | AA | 1124 | DA | Sidechain |
| 1 | AA | 1127 | DG | Sidechain |
| 1 | AA | 113 | DT | Sidechain |
| 1 | AA | 1130 | DA | Sidechain |
| 1 | AA | 1135 | DC | Sidechain |
| 1 | AA | 1137 | DG | Sidechain |
| 1 | AA | 1138 | DT | Sidechain |
| 1 | AA | 1149 | DA | Sidechain |
| 1 | AA | 1150 | DA | Sidechain |
| 1 | AA | 1158 | DT | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | AA | 116 | DA | Sidechain |
| 1 | AA | 1161 | DT | Sidechain |
| 1 | AA | 1162 | DG | Sidechain |
| 1 | AA | 1163 | DA | Sidechain |
| 1 | AA | 1166 | DT | Sidechain |
| 1 | AA | 1167 | DC | Sidechain |
| 1 | AA | 1171 | DT | Sidechain |
| 1 | AA | 1172 | DT | Sidechain |
| 1 | AA | 1173 | DT | Sidechain |
| 1 | AA | 1175 | DT | Sidechain |
| 1 | AA | 1180 | DG | Sidechain |
| 1 | AA | 1185 | DA | Sidechain |
| 1 | AA | 1189 | DG | Sidechain |
| 1 | AA | 1190 | DC | Sidechain |
| 1 | AA | 1192 | DG | Sidechain |
| 1 | AA | 1203 | DA | Sidechain |
| 1 | AA | 1209 | DC | Sidechain |
| 1 | AA | 1213 | DC | Sidechain |
| 1 | AA | 1214 | DG | Sidechain |
| 1 | AA | 1215 | DC | Sidechain |
| 1 | AA | 1217 | DA | Sidechain |
| 1 | AA | 122 | DG | Sidechain |
| 1 | AA | 1221 | DG | Sidechain |
| 1 | AA | 1223 | DG | Sidechain |
| 1 | AA | 1226 | DG | Sidechain |
| 1 | AA | 1227 | DG | Sidechain |
| 1 | AA | 1228 | DT | Sidechain |
| 1 | AA | 1229 | DT | Sidechain |
| 1 | AA | 1234 | DT | Sidechain |
| 1 | AA | 1236 | DC | Sidechain |
| 1 | AA | 1237 | DC | Sidechain |
| 1 | AA | 1239 | DG | Sidechain |
| 1 | AA | 1240 | DA | Sidechain |
| 1 | AA | 1245 | DG | Sidechain |
| 1 | AA | 1246 | DA | Sidechain |
| 1 | AA | 1259 | DT | Sidechain |
| 1 | AA | 1266 | DA | Sidechain |
| 1 | AA | 127 | DG | Sidechain |
| 1 | AA | 1270 | DT | Sidechain |
| 1 | AA | 1273 | DC | Sidechain |
| 1 | AA | 1274 | DT | Sidechain |
| 1 | AA | 1276 | DG | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | AA | 1277 | DC | Sidechain |
| 1 | AA | 1287 | DG | Sidechain |
| 1 | AA | 1289 | DG | Sidechain |
| 1 | AA | 129 | DA | Sidechain |
| 1 | AA | 1290 | DC | Sidechain |
| 1 | AA | 1294 | DT | Sidechain |
| 1 | AA | 1295 | DA | Sidechain |
| 1 | AA | 1299 | DA | Sidechain |
| 1 | AA | 13 | DG | Sidechain |
| 1 | AA | 1302 | DA | Sidechain |
| 1 | AA | 1308 | DC | Sidechain |
| 1 | AA | 131 | DG | Sidechain |
| 1 | AA | 1310 | DT | Sidechain |
| 1 | AA | 132 | DA | Sidechain |
| 1 | AA | 1323 | DT | Sidechain |
| 1 | AA | 1326 | DT | Sidechain |
| 1 | AA | 1327 | DT | Sidechain |
| 1 | AA | 1329 | DG | Sidechain |
| 1 | AA | 133 | DG | Sidechain |
| 1 | AA | 1333 | DA | Sidechain |
| 1 | AA | 1338 | DT | Sidechain |
| 1 | AA | 134 | DT | Sidechain |
| 1 | AA | 1343 | DG | Sidechain |
| 1 | AA | 1346 | DC | Sidechain |
| 1 | AA | 1350 | DG | Sidechain |
| 1 | AA | 1353 | DG | Sidechain |
| 1 | AA | 1357 | DC | Sidechain |
| 1 | AA | 136 | DT | Sidechain |
| 1 | AA | 1361 | DT | Sidechain |
| 1 | AA | 1367 | DC | Sidechain |
| 1 | AA | 1373 | DT | Sidechain |
| 1 | AA | 1377 | DC | Sidechain |
| 1 | AA | 1380 | DA | Sidechain |
| 1 | AA | 1381 | DT | Sidechain |
| 1 | AA | 1382 | DC | Sidechain |
| 1 | AA | 1384 | DT | Sidechain |
| 1 | AA | 1392 | DG | Sidechain |
| 1 | AA | 1398 | DG | Sidechain |
| 1 | AA | 14 | DG | Sidechain |
| 1 | AA | 1403 | DC | Sidechain |
| 1 | AA | 1405 | DG | Sidechain |
| 1 | AA | 1409 | DC | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | AA | 1410 | DG | Sidechain |
| 1 | AA | 1411 | DA | Sidechain |
| 1 | AA | 1412 | DT | Sidechain |
| 1 | AA | 1413 | DA | Sidechain |
| 1 | AA | 1426 | DC | Sidechain |
| 1 | AA | 1428 | DG | Sidechain |
| 1 | AA | 1429 | DG | Sidechain |
| 1 | AA | 1441 | DG | Sidechain |
| 1 | AA | 1443 | DC | Sidechain |
| 1 | AA | 1447 | DA | Sidechain |
| 1 | AA | 1449 | DT | Sidechain |
| 1 | AA | 145 | DT | Sidechain |
| 1 | AA | 1462 | DC | Sidechain |
| 1 | AA | 1467 | DC | Sidechain |
| 1 | AA | 1468 | DG | Sidechain |
| 1 | AA | 1469 | DG | Sidechain |
| 1 | AA | 147 | DC | Sidechain |
| 1 | AA | 1471 | DC | Sidechain |
| 1 | AA | 1476 | DT | Sidechain |
| 1 | AA | 1481 | DG | Sidechain |
| 1 | AA | 1482 | DG | Sidechain |
| 1 | AA | 1484 | DG | Sidechain |
| 1 | AA | 1485 | DG | Sidechain |
| 1 | AA | 149 | DT | Sidechain |
| 1 | AA | 1490 | DG | Sidechain |
| 1 | AA | 1496 | DA | Sidechain |
| 1 | AA | 1505 | DC | Sidechain |
| 1 | AA | 1509 | DG | Sidechain |
| 1 | AA | 1521 | DT | Sidechain |
| 1 | AA | 153 | DG | Sidechain |
| 1 | AA | 1530 | DC | Sidechain |
| 1 | AA | 1534 | DG | Sidechain |
| 1 | AA | 1536 | DT | Sidechain |
| 1 | AA | 1537 | DA | Sidechain |
| 1 | AA | 1539 | DC | Sidechain |
| 1 | AA | 1541 | DA | Sidechain |
| 1 | AA | 1548 | DG | Sidechain |
| 1 | AA | 1550 | DG | Sidechain |
| 1 | AA | 1555 | DG | Sidechain |
| 1 | AA | 156 | DC | Sidechain |
| 1 | AA | 1561 | DG | Sidechain |
| 1 | AA | 1566 | DA | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | AA | 1567 | DC | Sidechain |
| 1 | AA | 1568 | DG | Sidechain |
| 1 | AA | 1570 | DT | Sidechain |
| 1 | AA | 1573 | DC | Sidechain |
| 1 | AA | 1574 | DC | Sidechain |
| 1 | AA | 1579 | DG | Sidechain |
| 1 | AA | 159 | DA | Sidechain |
| 1 | AA | 1605 | DA | Sidechain |
| 1 | AA | 1607 | DC | Sidechain |
| 1 | AA | 161 | DT | Sidechain |
| 1 | AA | 1617 | DG | Sidechain |
| 1 | AA | 162 | DC | Sidechain |
| 1 | AA | 1623 | DG | Sidechain |
| 1 | AA | 1634 | DG | Sidechain |
| 1 | AA | 1637 | DG | Sidechain |
| 1 | AA | 1638 | DG | Sidechain |
| 1 | AA | 1639 | DA | Sidechain |
| 1 | AA | 1640 | DG | Sidechain |
| 1 | AA | 1648 | DG | Sidechain |
| 1 | AA | 165 | DT | Sidechain |
| 1 | AA | 1656 | DG | Sidechain |
| 1 | AA | 1658 | DC | Sidechain |
| 1 | AA | 1668 | DT | Sidechain |
| 1 | AA | 1671 | DA | Sidechain |
| 1 | AA | 1672 | DG | Sidechain |
| 1 | AA | 1676 | DT | Sidechain |
| 1 | AA | 1681 | DG | Sidechain |
| 1 | AA | 1683 | DT | Sidechain |
| 1 | AA | 1685 | DT | Sidechain |
| 1 | AA | 1688 | DC | Sidechain |
| 1 | AA | 1690 | DA | Sidechain |
| 1 | AA | 1691 | DC | Sidechain |
| 1 | AA | 1695 | DT | Sidechain |
| 1 | AA | 1698 | DC | Sidechain |
| 1 | AA | 1701 | DG | Sidechain |
| 1 | AA | 1703 | DG | Sidechain |
| 1 | AA | 1704 | DC | Sidechain |
| 1 | AA | 171 | DG | Sidechain |
| 1 | AA | 1716 | DT | Sidechain |
| 1 | AA | 172 | DC | Sidechain |
| 1 | AA | 1720 | DG | Sidechain |
| 1 | AA | 1721 | DC | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | AA | 1723 | DC | Sidechain |
| 1 | AA | 1728 | DG | Sidechain |
| 1 | AA | 173 | DG | Sidechain |
| 1 | AA | 1731 | DG | Sidechain |
| 1 | AA | 1733 | DG | Sidechain |
| 1 | AA | 1737 | DA | Sidechain |
| 1 | AA | 1738 | DG | Sidechain |
| 1 | AA | 174 | DG | Sidechain |
| 1 | AA | 1746 | DA | Sidechain |
| 1 | AA | 1753 | DC | Sidechain |
| 1 | AA | 1758 | DA | Sidechain |
| 1 | AA | 176 | DA | Sidechain |
| 1 | AA | 1761 | DG | Sidechain |
| 1 | AA | 1762 | DC | Sidechain |
| 1 | AA | 1763 | DG | Sidechain |
| 1 | AA | 1768 | DT | Sidechain |
| 1 | AA | 177 | DT | Sidechain |
| 1 | AA | 1784 | DC | Sidechain |
| 1 | AA | 1786 | DT | Sidechain |
| 1 | AA | 1792 | DG | Sidechain |
| 1 | AA | 1794 | DC | Sidechain |
| 1 | AA | 1796 | DT | Sidechain |
| 1 | AA | 1806 | DA | Sidechain |
| 1 | AA | 1808 | DG | Sidechain |
| 1 | AA | 181 | DG | Sidechain |
| 1 | AA | 1811 | DC | Sidechain |
| 1 | AA | 1812 | DT | Sidechain |
| 1 | AA | 1813 | DT | Sidechain |
| 1 | AA | 1814 | DT | Sidechain |
| 1 | AA | 1818 | DG | Sidechain |
| 1 | AA | 1819 | DC | Sidechain |
| 1 | AA | 1820 | DG | Sidechain |
| 1 | AA | 1824 | DT | Sidechain |
| 1 | AA | 1826 | DC | Sidechain |
| 1 | AA | 1827 | DC | Sidechain |
| 1 | AA | 1828 | DC | Sidechain |
| 1 | AA | 1830 | DG | Sidechain |
| 1 | AA | 1832 | DT | Sidechain |
| 1 | AA | 1835 | DT | Sidechain |
| 1 | AA | 1837 | DT | Sidechain |
| 1 | AA | 1840 | DA | Sidechain |
| 1 | AA | 1846 | DG | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | AA | 1852 | DC | Sidechain |
| 1 | AA | 1854 | DG | Sidechain |
| 1 | AA | 1855 | DC | Sidechain |
| 1 | AA | 1858 | DT | Sidechain |
| 1 | AA | 1863 | DT | Sidechain |
| 1 | AA | 1865 | DA | Sidechain |
| 1 | AA | 1867 | DC | Sidechain |
| 1 | AA | 1871 | DT | Sidechain |
| 1 | AA | 1876 | DC | Sidechain |
| 1 | AA | 1877 | DT | Sidechain |
| 1 | AA | 1879 | DG | Sidechain |
| 1 | AA | 188 | DT | Sidechain |
| 1 | AA | 1882 | DG | Sidechain |
| 1 | AA | 1886 | DC | Sidechain |
| 1 | AA | 1893 | DA | Sidechain |
| 1 | AA | 1894 | DC | Sidechain |
| 1 | AA | 1895 | DC | Sidechain |
| 1 | AA | 1900 | DG | Sidechain |
| 1 | AA | 1907 | DG | Sidechain |
| 1 | AA | 1916 | DC | Sidechain |
| 1 | AA | 1917 | DG | Sidechain |
| 1 | AA | 1918 | DA | Sidechain |
| 1 | AA | 1919 | DG | Sidechain |
| 1 | AA | 1923 | DG | Sidechain |
| 1 | AA | 1924 | DC | Sidechain |
| 1 | AA | 1927 | DA | Sidechain |
| 1 | AA | 1931 | DG | Sidechain |
| 1 | AA | 194 | DT | Sidechain |
| 1 | AA | 1941 | DC | Sidechain |
| 1 | AA | 1942 | DG | Sidechain |
| 1 | AA | 1949 | DG | Sidechain |
| 1 | AA | 195 | DG | Sidechain |
| 1 | AA | 1953 | DC | Sidechain |
| 1 | AA | 1959 | DG | Sidechain |
| 1 | AA | 1960 | DC | Sidechain |
| 1 | AA | 1963 | DG | Sidechain |
| 1 | AA | 1964 | DT | Sidechain |
| 1 | AA | 1967 | DG | Sidechain |
| 1 | AA | 1969 | DC | Sidechain |
| 1 | AA | 1970 | DG | Sidechain |
| 1 | AA | 1972 | DT | Sidechain |
| 1 | AA | 1976 | DT | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | AA | 1977 | DT | Sidechain |
| 1 | AA | 1987 | DG | Sidechain |
| 1 | AA | 1988 | DG | Sidechain |
| 1 | AA | 1989 | DC | Sidechain |
| 1 | AA | 1994 | DC | Sidechain |
| 1 | AA | 1995 | DA | Sidechain |
| 1 | AA | 1997 | DG | Sidechain |
| 1 | AA | 2000 | DT | Sidechain |
| 1 | AA | 2002 | DC | Sidechain |
| 1 | AA | 2005 | DA | Sidechain |
| 1 | AA | 2007 | DT | Sidechain |
| 1 | AA | 2010 | DA | Sidechain |
| 1 | AA | 2013 | DG | Sidechain |
| 1 | AA | 2018 | DC | Sidechain |
| 1 | AA | 202 | DC | Sidechain |
| 1 | AA | 2022 | DG | Sidechain |
| 1 | AA | 2024 | DG | Sidechain |
| 1 | AA | 2027 | DC | Sidechain |
| 1 | AA | 203 | DA | Sidechain |
| 1 | AA | 2030 | DC | Sidechain |
| 1 | AA | 204 | DG | Sidechain |
| 1 | AA | 2043 | DA | Sidechain |
| 1 | AA | 2044 | DG | Sidechain |
| 1 | AA | 2045 | DT | Sidechain |
| 1 | AA | 2055 | DC | Sidechain |
| 1 | AA | 2056 | DA | Sidechain |
| 1 | AA | 2060 | DG | Sidechain |
| 1 | AA | 2063 | DA | Sidechain |
| 1 | AA | 2066 | DC | Sidechain |
| 1 | AA | 2068 | DA | Sidechain |
| 1 | AA | 2069 | DG | Sidechain |
| 1 | AA | 2070 | DG | Sidechain |
| 1 | AA | 2076 | DC | Sidechain |
| 1 | AA | 2083 | DT | Sidechain |
| 1 | AA | 2086 | DT | Sidechain |
| 1 | AA | 2089 | DC | Sidechain |
| 1 | AA | 209 | DG | Sidechain |
| 1 | AA | 2090 | DG | Sidechain |
| 1 | AA | 2094 | DC | Sidechain |
| 1 | AA | 2095 | DG | Sidechain |
| 1 | AA | 21 | DG | Sidechain |
| 1 | AA | 2103 | DT | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | AA | 2109 | DA | Sidechain |
| 1 | AA | 211 | DT | Sidechain |
| 1 | AA | 2111 | DT | Sidechain |
| 1 | AA | 2112 | DG | Sidechain |
| 1 | AA | 2116 | DG | Sidechain |
| 1 | AA | 2117 | DC | Sidechain |
| 1 | AA | 2120 | DA | Sidechain |
| 1 | AA | 2121 | DT | Sidechain |
| 1 | AA | 2123 | DA | Sidechain |
| 1 | AA | 2127 | DT | Sidechain |
| 1 | AA | 2143 | DG | Sidechain |
| 1 | AA | 2145 | DT | Sidechain |
| 1 | AA | 2152 | DA | Sidechain |
| 1 | AA | 216 | DA | Sidechain |
| 1 | AA | 2172 | DT | Sidechain |
| 1 | AA | 2179 | DG | Sidechain |
| 1 | AA | 2186 | DA | Sidechain |
| 1 | AA | 2191 | DG | Sidechain |
| 1 | AA | 2196 | DC | Sidechain |
| 1 | AA | 2198 | DG | Sidechain |
| 1 | AA | 2199 | DG | Sidechain |
| 1 | AA | 22 | DT | Sidechain |
| 1 | AA | 2201 | DC | Sidechain |
| 1 | AA | 2203 | DT | Sidechain |
| 1 | AA | 2206 | DT | Sidechain |
| 1 | AA | 2209 | DT | Sidechain |
| 1 | AA | 2210 | DA | Sidechain |
| 1 | AA | 2217 | DG | Sidechain |
| 1 | AA | 2223 | DG | Sidechain |
| 1 | AA | 2224 | DC | Sidechain |
| 1 | AA | 223 | DA | Sidechain |
| 1 | AA | 2232 | DG | Sidechain |
| 1 | AA | 2235 | DT | Sidechain |
| 1 | AA | 2238 | DT | Sidechain |
| 1 | AA | 224 | DA | Sidechain |
| 1 | AA | 2242 | DG | Sidechain |
| 1 | AA | 2243 | DG | Sidechain |
| 1 | AA | 2245 | DT | Sidechain |
| 1 | AA | 2251 | DT | Sidechain |
| 1 | AA | 2255 | DC | Sidechain |
| 1 | AA | 2261 | DG | Sidechain |
| 1 | AA | 2264 | DC | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | AA | 2265 | DG | Sidechain |
| 1 | AA | 227 | DT | Sidechain |
| 1 | AA | 2277 | DC | Sidechain |
| 1 | AA | 228 | DG | Sidechain |
| 1 | AA | 2281 | DG | Sidechain |
| 1 | AA | 2282 | DT | Sidechain |
| 1 | AA | 2287 | DG | Sidechain |
| 1 | AA | 2289 | DG | Sidechain |
| 1 | AA | 229 | DC | Sidechain |
| 1 | AA | 2291 | DA | Sidechain |
| 1 | AA | 2295 | DC | Sidechain |
| 1 | AA | 2297 | DT | Sidechain |
| 1 | AA | 2299 | DG | Sidechain |
| 1 | AA | 2307 | DC | Sidechain |
| 1 | AA | 2311 | DT | Sidechain |
| 1 | AA | 2316 | DC | Sidechain |
| 1 | AA | 2317 | DG | Sidechain |
| 1 | AA | 2318 | DC | Sidechain |
| 1 | AA | 2325 | DG | Sidechain |
| 1 | AA | 2332 | DC | Sidechain |
| 1 | AA | 2334 | DC | Sidechain |
| 1 | AA | 2336 | DT | Sidechain |
| 1 | AA | 234 | DG | Sidechain |
| 1 | AA | 2344 | DG | Sidechain |
| 1 | AA | 2348 | DG | Sidechain |
| 1 | AA | 2354 | DT | Sidechain |
| 1 | AA | 2357 | DC | Sidechain |
| 1 | AA | 2367 | DC | Sidechain |
| 1 | AA | 2368 | DG | Sidechain |
| 1 | AA | 2372 | DC | Sidechain |
| 1 | AA | 2374 | DA | Sidechain |
| 1 | AA | 2375 | DT | Sidechain |
| 1 | AA | 2380 | DC | Sidechain |
| 1 | AA | 2381 | DT | Sidechain |
| 1 | AA | 2391 | DT | Sidechain |
| 1 | AA | 2396 | DC | Sidechain |
| 1 | AA | 2397 | DA | Sidechain |
| 1 | AA | 2400 | DC | Sidechain |
| 1 | AA | 2402 | DG | Sidechain |
| 1 | AA | 2404 | DA | Sidechain |
| 1 | AA | 2407 | DG | Sidechain |
| 1 | AA | 2411 | DA | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | AA | 2416 | DA | Sidechain |
| 1 | AA | 242 | DG | Sidechain |
| 1 | AA | 2427 | DA | Sidechain |
| 1 | AA | 2428 | DG | Sidechain |
| 1 | AA | 2429 | DC | Sidechain |
| 1 | AA | 2432 | DC | Sidechain |
| 1 | AA | 2433 | DG | Sidechain |
| 1 | AA | 2435 | DA | Sidechain |
| 1 | AA | 2442 | DG | Sidechain |
| 1 | AA | 2443 | DC | Sidechain |
| 1 | AA | 2444 | DG | Sidechain |
| 1 | AA | 2446 | DC | Sidechain |
| 1 | AA | 2448 | DG | Sidechain |
| 1 | AA | 2449 | DG | Sidechain |
| 1 | AA | 2452 | DT | Sidechain |
| 1 | AA | 2453 | DG | Sidechain |
| 1 | AA | 2454 | DG | Sidechain |
| 1 | AA | 2455 | DT | Sidechain |
| 1 | AA | 2458 | DT | Sidechain |
| 1 | AA | 2459 | DT | Sidechain |
| 1 | AA | 2464 | DG | Sidechain |
| 1 | AA | 2466 | DA | Sidechain |
| 1 | AA | 2467 | DG | Sidechain |
| 1 | AA | 2484 | DG | Sidechain |
| 1 | AA | 2488 | DG | Sidechain |
| 1 | AA | 2489 | DC | Sidechain |
| 1 | AA | 249 | DC | Sidechain |
| 1 | AA | 2491 | DC | Sidechain |
| 1 | AA | 2492 | DC | Sidechain |
| 1 | AA | 2493 | DC | Sidechain |
| 1 | AA | 2497 | DC | Sidechain |
| 1 | AA | 2499 | DC | Sidechain |
| 1 | AA | 2503 | DC | Sidechain |
| 1 | AA | 2505 | DC | Sidechain |
| 1 | AA | 2506 | DC | Sidechain |
| 1 | AA | 2507 | DT | Sidechain |
| 1 | AA | 2509 | DT | Sidechain |
| 1 | AA | 2512 | DC | Sidechain |
| 1 | AA | 2523 | DT | Sidechain |
| 1 | AA | 2526 | DT | Sidechain |
| 1 | AA | 253 | DT | Sidechain |
| 1 | AA | 2530 | DT | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | AA | 2531 | DC | Sidechain |
| 1 | AA | 2532 | DG | Sidechain |
| 1 | AA | 2535 | DA | Sidechain |
| 1 | AA | 2538 | DT | Sidechain |
| 1 | AA | 2542 | DC | Sidechain |
| 1 | AA | 2544 | DG | Sidechain |
| 1 | AA | 2547 | DT | Sidechain |
| 1 | AA | 2552 | DC | Sidechain |
| 1 | AA | 2553 | DC | Sidechain |
| 1 | AA | 2554 | DG | Sidechain |
| 1 | AA | 2559 | DG | Sidechain |
| 1 | AA | 2560 | DC | Sidechain |
| 1 | AA | 2561 | DT | Sidechain |
| 1 | AA | 2563 | DT | Sidechain |
| 1 | AA | 2564 | DA | Sidechain |
| 1 | AA | 2565 | DA | Sidechain |
| 1 | AA | 257 | DT | Sidechain |
| 1 | AA | 2571 | DG | Sidechain |
| 1 | AA | 2578 | DC | Sidechain |
| 1 | AA | 258 | DT | Sidechain |
| 1 | AA | 2580 | DT | Sidechain |
| 1 | AA | 2581 | DT | Sidechain |
| 1 | AA | 2583 | DG | Sidechain |
| 1 | AA | 2584 | DG | Sidechain |
| 1 | AA | 2593 | DT | Sidechain |
| 1 | AA | 2594 | DT | Sidechain |
| 1 | AA | 2597 | DT | Sidechain |
| 1 | AA | 2598 | DG | Sidechain |
| 1 | AA | 2600 | DT | Sidechain |
| 1 | AA | 2605 | DG | Sidechain |
| 1 | AA | 2606 | DG | Sidechain |
| 1 | AA | 2609 | DC | Sidechain |
| 1 | AA | 2610 | DC | Sidechain |
| 1 | AA | 2618 | DC | Sidechain |
| 1 | AA | 2629 | DA | Sidechain |
| 1 | AA | 2630 | DT | Sidechain |
| 1 | AA | 2632 | DA | Sidechain |
| 1 | AA | 2638 | DA | Sidechain |
| 1 | AA | 2640 | DG | Sidechain |
| 1 | AA | 2642 | DT | Sidechain |
| 1 | AA | 2654 | DG | Sidechain |
| 1 | AA | 2655 | DC | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | AA | 2656 | DC | Sidechain |
| 1 | AA | 2661 | DC | Sidechain |
| 1 | AA | 2663 | DC | Sidechain |
| 1 | AA | 2666 | DA | Sidechain |
| 1 | AA | 2673 | DG | Sidechain |
| 1 | AA | 2675 | DT | Sidechain |
| 1 | AA | 2676 | DT | Sidechain |
| 1 | AA | 2682 | DC | Sidechain |
| 1 | AA | 2687 | DG | Sidechain |
| 1 | AA | 269 | DG | Sidechain |
| 1 | AA | 2691 | DT | Sidechain |
| 1 | AA | 270 | DG | Sidechain |
| 1 | AA | 2700 | DA | Sidechain |
| 1 | AA | 2704 | DT | Sidechain |
| 1 | AA | 2706 | DT | Sidechain |
| 1 | AA | 2708 | DT | Sidechain |
| 1 | AA | 2710 | DA | Sidechain |
| 1 | AA | 2711 | DT | Sidechain |
| 1 | AA | 2718 | DC | Sidechain |
| 1 | AA | 2723 | DG | Sidechain |
| 1 | AA | 2724 | DT | Sidechain |
| 1 | AA | 2725 | DT | Sidechain |
| 1 | AA | 2727 | DC | Sidechain |
| 1 | AA | 2729 | DA | Sidechain |
| 1 | AA | 273 | DC | Sidechain |
| 1 | AA | 2730 | DA | Sidechain |
| 1 | AA | 2735 | DA | Sidechain |
| 1 | AA | 2742 | DC | Sidechain |
| 1 | AA | 2746 | DA | Sidechain |
| 1 | AA | 2748 | DC | Sidechain |
| 1 | AA | 2755 | DC | Sidechain |
| 1 | AA | 2756 | DG | Sidechain |
| 1 | AA | 2758 | DT | Sidechain |
| 1 | AA | 2762 | DT | Sidechain |
| 1 | AA | 2765 | DT | Sidechain |
| 1 | AA | 2766 | DT | Sidechain |
| 1 | AA | 2771 | DT | Sidechain |
| 1 | AA | 2779 | DG | Sidechain |
| 1 | AA | 2780 | DG | Sidechain |
| 1 | AA | 2784 | DT | Sidechain |
| 1 | AA | 2786 | DG | Sidechain |
| 1 | AA | 2788 | DC | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | AA | 2790 | DA | Sidechain |
| 1 | AA | 2795 | DG | Sidechain |
| 1 | AA | 280 | DG | Sidechain |
| 1 | AA | 2803 | DG | Sidechain |
| 1 | AA | 2804 | DG | Sidechain |
| 1 | AA | 2805 | DT | Sidechain |
| 1 | AA | 2806 | DT | Sidechain |
| 1 | AA | 2811 | DA | Sidechain |
| 1 | AA | 2816 | DG | Sidechain |
| 1 | AA | 2825 | DA | Sidechain |
| 1 | AA | 2835 | DA | Sidechain |
| 1 | AA | 2840 | DG | Sidechain |
| 1 | AA | 2846 | DT | Sidechain |
| 1 | AA | 2847 | DA | Sidechain |
| 1 | AA | 2852 | DA | Sidechain |
| 1 | AA | 2856 | DT | Sidechain |
| 1 | AA | 286 | DA | Sidechain |
| 1 | AA | 2862 | DC | Sidechain |
| 1 | AA | 2869 | DT | Sidechain |
| 1 | AA | 288 | DA | Sidechain |
| 1 | AA | 289 | DT | Sidechain |
| 1 | AA | 292 | DT | Sidechain |
| 1 | AA | 294 | DG | Sidechain |
| 1 | AA | 295 | DA | Sidechain |
| 1 | AA | 296 | DG | Sidechain |
| 1 | AA | 297 | DA | Sidechain |
| 1 | AA | 3 | DG | Sidechain |
| 1 | AA | 30 | DA | Sidechain |
| 1 | AA | 305 | DC | Sidechain |
| 1 | AA | 307 | DC | Sidechain |
| 1 | AA | 31 | DC | Sidechain |
| 1 | AA | 32 | DC | Sidechain |
| 1 | AA | 331 | DG | Sidechain |
| 1 | AA | 333 | DA | Sidechain |
| 1 | AA | 335 | DT | Sidechain |
| 1 | AA | 337 | DT | Sidechain |
| 1 | AA | 342 | DG | Sidechain |
| 1 | AA | 344 | DT | Sidechain |
| 1 | AA | 351 | DT | Sidechain |
| 1 | AA | 352 | DG | Sidechain |
| 1 | AA | 353 | DT | Sidechain |
| 1 | AA | 355 | DG | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | AA | 356 | DC | Sidechain |
| 1 | AA | 360 | DG | Sidechain |
| 1 | AA | 361 | DT | Sidechain |
| 1 | AA | 370 | DG | Sidechain |
| 1 | AA | 38 | DT | Sidechain |
| 1 | AA | 382 | DG | Sidechain |
| 1 | AA | 389 | DG | Sidechain |
| 1 | AA | 392 | DA | Sidechain |
| 1 | AA | 401 | DC | Sidechain |
| 1 | AA | 402 | DC | Sidechain |
| 1 | AA | 415 | DC | Sidechain |
| 1 | AA | 419 | DG | Sidechain |
| 1 | AA | 420 | DA | Sidechain |
| 1 | AA | 423 | DG | Sidechain |
| 1 | AA | 427 | DT | Sidechain |
| 1 | AA | 43 | DT | Sidechain |
| 1 | AA | 433 | DA | Sidechain |
| 1 | AA | 434 | DG | Sidechain |
| 1 | AA | 435 | DT | Sidechain |
| 1 | AA | 438 | DT | Sidechain |
| 1 | AA | 444 | DG | Sidechain |
| 1 | AA | 447 | DA | Sidechain |
| 1 | AA | 454 | DA | Sidechain |
| 1 | AA | 458 | DT | Sidechain |
| 1 | AA | 469 | DG | Sidechain |
| 1 | AA | 470 | DC | Sidechain |
| 1 | AA | 471 | DA | Sidechain |
| 1 | AA | 481 | DG | Sidechain |
| 1 | AA | 483 | DG | Sidechain |
| 1 | AA | 49 | DT | Sidechain |
| 1 | AA | 490 | DG | Sidechain |
| 1 | AA | 495 | DG | Sidechain |
| 1 | AA | 497 | DT | Sidechain |
| 1 | AA | 5 | DC | Sidechain |
| 1 | AA | 504 | DA | Sidechain |
| 1 | AA | 510 | DA | Sidechain |
| 1 | AA | 515 | DT | Sidechain |
| 1 | AA | 522 | DG | Sidechain |
| 1 | AA | 524 | DG | Sidechain |
| 1 | AA | 529 | DA | Sidechain |
| 1 | AA | 530 | DC | Sidechain |
| 1 | AA | 534 | DC | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | AA | 535 | DT | Sidechain |
| 1 | AA | 539 | DG | Sidechain |
| 1 | AA | 545 | DG | Sidechain |
| 1 | AA | 55 | DT | Sidechain |
| 1 | AA | 561 | DG | Sidechain |
| 1 | AA | 57 | DC | Sidechain |
| 1 | AA | 579 | DC | Sidechain |
| 1 | AA | 585 | DA | Sidechain |
| 1 | AA | 589 | DG | Sidechain |
| 1 | AA | 59 | DT | Sidechain |
| 1 | AA | 590 | DG | Sidechain |
| 1 | AA | 592 | DA | Sidechain |
| 1 | AA | 593 | DT | Sidechain |
| 1 | AA | 61 | DC | Sidechain |
| 1 | AA | 610 | DA | Sidechain |
| 1 | AA | 621 | DC | Sidechain |
| 1 | AA | 626 | DG | Sidechain |
| 1 | AA | 627 | DC | Sidechain |
| 1 | AA | 628 | DT | Sidechain |
| 1 | AA | 632 | DT | Sidechain |
| 1 | AA | 637 | DC | Sidechain |
| 1 | AA | 641 | DA | Sidechain |
| 1 | AA | 647 | DC | Sidechain |
| 1 | AA | 648 | DG | Sidechain |
| 1 | AA | 65 | DT | Sidechain |
| 1 | AA | 653 | DG | Sidechain |
| 1 | AA | 657 | DG | Sidechain |
| 1 | AA | 664 | DC | Sidechain |
| 1 | AA | 667 | DT | Sidechain |
| 1 | AA | 668 | DG | Sidechain |
| 1 | AA | 67 | DT | Sidechain |
| 1 | AA | 671 | DT | Sidechain |
| 1 | AA | 678 | DA | Sidechain |
| 1 | AA | 681 | DG | Sidechain |
| 1 | AA | 687 | DA | Sidechain |
| 1 | AA | 688 | DC | Sidechain |
| 1 | AA | 691 | DT | Sidechain |
| 1 | AA | 694 | DG | Sidechain |
| 1 | AA | 698 | DA | Sidechain |
| 1 | AA | 702 | DT | Sidechain |
| 1 | AA | 706 | DC | Sidechain |
| 1 | AA | 712 | DA | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | AA | 718 | DT | Sidechain |
| 1 | AA | 723 | DC | Sidechain |
| 1 | AA | 725 | DA | Sidechain |
| 1 | AA | 726 | DG | Sidechain |
| 1 | AA | 727 | DC | Sidechain |
| 1 | AA | 731 | DC | Sidechain |
| 1 | AA | 732 | DC | Sidechain |
| 1 | AA | 74 | DG | Sidechain |
| 1 | AA | 741 | DT | Sidechain |
| 1 | AA | 747 | DG | Sidechain |
| 1 | AA | 748 | DA | Sidechain |
| 1 | AA | 750 | DT | Sidechain |
| 1 | AA | 76 | DT | Sidechain |
| 1 | AA | 761 | DG | Sidechain |
| 1 | AA | 762 | DG | Sidechain |
| 1 | AA | 77 | DC | Sidechain |
| 1 | AA | 773 | DA | Sidechain |
| 1 | AA | 788 | DC | Sidechain |
| 1 | AA | 79 | DT | Sidechain |
| 1 | AA | 802 | DC | Sidechain |
| 1 | AA | 806 | DC | Sidechain |
| 1 | AA | 813 | DA | Sidechain |
| 1 | AA | 818 | DT | Sidechain |
| 1 | AA | 82 | DG | Sidechain |
| 1 | AA | 828 | DG | Sidechain |
| 1 | AA | 829 | DG | Sidechain |
| 1 | AA | 830 | DA | Sidechain |
| 1 | AA | 834 | DG | Sidechain |
| 1 | AA | 835 | DG | Sidechain |
| 1 | AA | 838 | DA | Sidechain |
| 1 | AA | 842 | DT | Sidechain |
| 1 | AA | 844 | DG | Sidechain |
| 1 | AA | 846 | DT | Sidechain |
| 1 | AA | 853 | DG | Sidechain |
| 1 | AA | 864 | DG | Sidechain |
| 1 | AA | 867 | DC | Sidechain |
| 1 | AA | 868 | DT | Sidechain |
| 1 | AA | 87 | DT | Sidechain |
| 1 | AA | 870 | DG | Sidechain |
| 1 | AA | 871 | DG | Sidechain |
| 1 | AA | 872 | DG | Sidechain |
| 1 | AA | 879 | DG | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | AA | 880 | DG | Sidechain |
| 1 | AA | 884 | DG | Sidechain |
| 1 | AA | 885 | DC | Sidechain |
| 1 | AA | 887 | DC | Sidechain |
| 1 | AA | 888 | DT | Sidechain |
| 1 | AA | 890 | DC | Sidechain |
| 1 | AA | 892 | DG | Sidechain |
| 1 | AA | 895 | DT | Sidechain |
| 1 | AA | 897 | DG | Sidechain |
| 1 | AA | 901 | DT | Sidechain |
| 1 | AA | 906 | DT | Sidechain |
| 1 | AA | 91 | DC | Sidechain |
| 1 | AA | 926 | DA | Sidechain |
| 1 | AA | 93 | DT | Sidechain |
| 1 | AA | 930 | DA | Sidechain |
| 1 | AA | 932 | DG | Sidechain |
| 1 | AA | 938 | DA | Sidechain |
| 1 | AA | 948 | DC | Sidechain |
| 1 | AA | 957 | DG | Sidechain |
| 1 | AA | 96 | DT | Sidechain |
| 1 | AA | 964 | DG | Sidechain |
| 1 | AA | 970 | DC | Sidechain |
| 1 | AA | 973 | DT | Sidechain |
| 1 | AA | 975 | DA | Sidechain |
| 1 | AA | 977 | DT | Sidechain |
| 1 | AA | 980 | DG | Sidechain |
| 1 | AA | 982 | DA | Sidechain |
| 1 | AA | 99 | DA | Sidechain |
| 1 | AA | 992 | DG | Sidechain |
| 1 | AA | 998 | DC | Sidechain |
| 2 | AB | 1 | DT | Sidechain |
| 2 | AB | 10 | DC | Sidechain |
| 2 | AB | 11 | DC | Sidechain |
| 2 | AB | 25 | DG | Sidechain |
| 2 | AB | 26 | DT | Sidechain |
| 2 | AB | 28 | DG | Sidechain |
| 2 | AB | 3 | DC | Sidechain |
| 2 | AB | 6 | DA | Sidechain |
| 3 | AC | 13 | DC | Sidechain |
| 3 | AC | 19 | DG | Sidechain |
| 3 | AC | 2 | DG | Sidechain |
| 3 | AC | 24 | DT | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 3 | AC | 25 | DT | Sidechain |
| 3 | AC | 26 | DG | Sidechain |
| 3 | AC | 41 | DA | Sidechain |
| 3 | AC | 43 | DG | Sidechain |
| 3 | AC | 46 | DA | Sidechain |
| 4 | AD | 11 | DC | Sidechain |
| 4 | AD | 12 | DC | Sidechain |
| 4 | AD | 19 | DC | Sidechain |
| 4 | AD | 2 | DA | Sidechain |
| 4 | AD | 21 | DA | Sidechain |
| 4 | AD | 22 | DA | Sidechain |
| 4 | AD | 4 | DG | Sidechain |
| 4 | AD | 6 | DA | Sidechain |
| 5 | AE | 14 | DG | Sidechain |
| 5 | AE | 2 | DC | Sidechain |
| 5 | AE | 20 | DA | Sidechain |
| 5 | AE | 28 | DA | Sidechain |
| 5 | AE | 29 | DA | Sidechain |
| 5 | AE | 30 | DG | Sidechain |
| 5 | AE | 32 | DT | Sidechain |
| 5 | AE | 34 | DG | Sidechain |
| 5 | AE | 36 | DT | Sidechain |
| 5 | AE | 9 | DT | Sidechain |
| 6 | AF | 20 | DG | Sidechain |
| 6 | AF | 25 | DT | Sidechain |
| 6 | AF | 26 | DC | Sidechain |
| 6 | AF | 30 | DG | Sidechain |
| 6 | AF | 31 | DT | Sidechain |
| 6 | AF | 39 | DA | Sidechain |
| 6 | AF | 5 | DG | Sidechain |
| 6 | AF | 6 | DC | Sidechain |
| 7 | AG | 10 | DG | Sidechain |
| 7 | AG | 19 | DT | Sidechain |
| 7 | AG | 24 | DT | Sidechain |
| 7 | AG | 25 | DA | Sidechain |
| 7 | AG | 29 | DG | Sidechain |
| 7 | AG | 30 | DC | Sidechain |
| 7 | AG | 32 | DC | Sidechain |
| 7 | AG | 33 | DA | Sidechain |
| 7 | AG | 8 | DG | Sidechain |
| 7 | AG | 9 | DA | Sidechain |
| 8 | AH | 13 | DG | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 8 | AH | 14 | DT | Sidechain |
| 8 | AH | 17 | DC | Sidechain |
| 8 | AH | 2 | DG | Sidechain |
| 8 | AH | 27 | DC | Sidechain |
| 8 | AH | 28 | DA | Sidechain |
| 8 | AH | 29 | DG | Sidechain |
| 8 | AH | 30 | DG | Sidechain |
| 8 | AH | 36 | DT | Sidechain |
| 8 | AH | 38 | DT | Sidechain |
| 8 | AH | 5 | DG | Sidechain |
| 8 | AH | 6 | DT | Sidechain |
| 9 | AI | 11 | DA | Sidechain |
| 9 | AI | 12 | DA | Sidechain |
| 9 | AI | 15 | DG | Sidechain |
| 9 | AI | 20 | DG | Sidechain |
| 9 | AI | 21 | DT | Sidechain |
| 9 | AI | 22 | DG | Sidechain |
| 9 | AI | 28 | DG | Sidechain |
| 9 | AI | 3 | DT | Sidechain |
| 9 | AI | 5 | DT | Sidechain |
| 10 | AJ | 13 | DC | Sidechain |
| 10 | AJ | 18 | DG | Sidechain |
| 10 | AJ | 19 | DT | Sidechain |
| 10 | AJ | 21 | DC | Sidechain |
| 10 | AJ | 28 | DA | Sidechain |
| 10 | AJ | 29 | DC | Sidechain |
| 10 | AJ | 3 | DT | Sidechain |
| 10 | AJ | 31 | DT | Sidechain |
| 10 | AJ | 32 | DT | Sidechain |
| 10 | AJ | 33 | DT | Sidechain |
| 11 | AK | 12 | DG | Sidechain |
| 11 | AK | 17 | DG | Sidechain |
| 11 | AK | 2 | DA | Sidechain |
| 11 | AK | 23 | DA | Sidechain |
| 11 | AK | 24 | DG | Sidechain |
| 11 | AK | 3 | DG | Sidechain |
| 11 | AK | 30 | DT | Sidechain |
| 11 | AK | 32 | DG | Sidechain |
| 11 | AK | 34 | DG | Sidechain |
| 11 | AK | 36 | DT | Sidechain |
| 11 | AK | 37 | DC | Sidechain |
| 11 | AK | 4 | DT | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 11 | AK | 5 | DT | Sidechain |
| 12 | AL | 12 | DG | Sidechain |
| 12 | AL | 13 | DG | Sidechain |
| 12 | AL | 20 | DT | Sidechain |
| 12 | AL | 25 | DA | Sidechain |
| 12 | AL | 29 | DG | Sidechain |
| 12 | AL | 30 | DA | Sidechain |
| 12 | AL | 31 | DA | Sidechain |
| 12 | AL | 33 | DA | Sidechain |
| 12 | AL | 35 | DG | Sidechain |
| 12 | AL | 38 | DG | Sidechain |
| 12 | AL | 4 | DG | Sidechain |
| 12 | AL | 40 | DG | Sidechain |
| 12 | AL | 41 | DG | Sidechain |
| 13 | AM | 10 | DC | Sidechain |
| 13 | AM | 15 | DT | Sidechain |
| 13 | AM | 20 | DC | Sidechain |
| 13 | AM | 28 | DC | Sidechain |
| 13 | AM | 29 | DT | Sidechain |
| 13 | AM | 3 | DT | Sidechain |
| 13 | AM | 31 | DT | Sidechain |
| 13 | AM | 4 | DA | Sidechain |
| 13 | AM | 41 | DG | Sidechain |
| 13 | AM | 9 | DT | Sidechain |
| 14 | AN | 1 | DA | Sidechain |
| 14 | AN | 12 | DG | Sidechain |
| 14 | AN | 15 | DC | Sidechain |
| 14 | AN | 16 | DG | Sidechain |
| 14 | AN | 19 | DG | Sidechain |
| 14 | AN | 20 | DA | Sidechain |
| 14 | AN | 25 | DG | Sidechain |
| 14 | AN | 37 | DG | Sidechain |
| 14 | AN | 42 | DC | Sidechain |
| 14 | AN | 7 | DT | Sidechain |
| 14 | AN | 8 | DC | Sidechain |
| 15 | AO | 11 | DA | Sidechain |
| 15 | AO | 12 | DA | Sidechain |
| 15 | AO | 14 | DG | Sidechain |
| 15 | AO | 15 | DT | Sidechain |
| 15 | AO | 27 | DG | Sidechain |
| 15 | AO | 34 | DG | Sidechain |
| 15 | AO | 35 | DC | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 15 | AO | 39 | DG | Sidechain |
| 15 | AO | 45 | DG | Sidechain |
| 16 | AP | 11 | DG | Sidechain |
| 16 | AP | 17 | DG | Sidechain |
| 16 | AP | 19 | DT | Sidechain |
| 16 | AP | 29 | DG | Sidechain |
| 16 | AP | 34 | DT | Sidechain |
| 16 | AP | 40 | DG | Sidechain |
| 16 | AP | 42 | DC | Sidechain |
| 16 | AP | 45 | DT | Sidechain |
| 17 | AQ | 11 | DT | Sidechain |
| 17 | AQ | 12 | DC | Sidechain |
| 17 | AQ | 14 | DT | Sidechain |
| 17 | AQ | 15 | DC | Sidechain |
| 17 | AQ | 18 | DT | Sidechain |
| 17 | AQ | 21 | DC | Sidechain |
| 17 | AQ | 23 | DG | Sidechain |
| 17 | AQ | 26 | DT | Sidechain |
| 17 | AQ | 7 | DT | Sidechain |
| 17 | AQ | 8 | DG | Sidechain |
| 18 | AR | 10 | DG | Sidechain |
| 18 | AR | 15 | DG | Sidechain |
| 18 | AR | 16 | DC | Sidechain |
| 18 | AR | 23 | DC | Sidechain |
| 18 | AR | 24 | DT | Sidechain |
| 18 | AR | 5 | DT | Sidechain |
| 18 | AR | 7 | DC | Sidechain |
| 19 | AS | 1 | DT | Sidechain |
| 19 | AS | 2 | DT | Sidechain |
| 19 | AS | 22 | DG | Sidechain |
| 19 | AS | 25 | DA | Sidechain |
| 19 | AS | 26 | DG | Sidechain |
| 19 | AS | 27 | DA | Sidechain |
| 19 | AS | 33 | DG | Sidechain |
| 19 | AS | 37 | DG | Sidechain |
| 19 | AS | 38 | DT | Sidechain |
| 19 | AS | 39 | DT | Sidechain |
| 19 | AS | 5 | DT | Sidechain |
| 20 | AT | 10 | DC | Sidechain |
| 20 | AT | 12 | DC | Sidechain |
| 20 | AT | 14 | DG | Sidechain |
| 20 | AT | 15 | DG | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 20 | AT | 17 | DC | Sidechain |
| 20 | AT | 2 | DC | Sidechain |
| 20 | AT | 28 | DG | Sidechain |
| 20 | AT | 33 | DC | Sidechain |
| 20 | AT | 44 | DA | Sidechain |
| 20 | AT | 45 | DG | Sidechain |
| 20 | AT | 46 | DT | Sidechain |
| 20 | AT | 48 | DT | Sidechain |
| 20 | AT | 5 | DA | Sidechain |
| 20 | AT | 51 | DT | Sidechain |
| 20 | AT | 7 | DC | Sidechain |
| 20 | AT | 8 | DG | Sidechain |
| 21 | AU | 16 | DC | Sidechain |
| 21 | AU | 23 | DC | Sidechain |
| 21 | AU | 25 | DG | Sidechain |
| 21 | AU | 28 | DG | Sidechain |
| 21 | AU | 29 | DG | Sidechain |
| 21 | AU | 31 | DG | Sidechain |
| 21 | AU | 34 | DT | Sidechain |
| 21 | AU | 35 | DC | Sidechain |
| 21 | AU | 43 | DC | Sidechain |
| 21 | AU | 44 | DG | Sidechain |
| 21 | AU | 6 | DT | Sidechain |
| 21 | AU | 7 | DA | Sidechain |
| 21 | AU | 9 | DT | Sidechain |
| 22 | AV | 1 | DG | Sidechain |
| 22 | AV | 14 | DG | Sidechain |
| 22 | AV | 2 | DA | Sidechain |
| 22 | AV | 30 | DG | Sidechain |
| 22 | AV | 37 | DG | Sidechain |
| 22 | AV | 4 | DT | Sidechain |
| 22 | AV | 6 | DG | Sidechain |
| 22 | AV | 7 | DC | Sidechain |
| 23 | AW | 1 | DG | Sidechain |
| 23 | AW | 2 | DG | Sidechain |
| 23 | AW | 26 | DC | Sidechain |
| 23 | AW | 30 | DA | Sidechain |
| 23 | AW | 31 | DG | Sidechain |
| 23 | AW | 32 | DC | Sidechain |
| 23 | AW | 36 | DA | Sidechain |
| 23 | AW | 38 | DG | Sidechain |
| 23 | AW | 4 | DA | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 24 | AX | 16 | DT | Sidechain |
| 24 | AX | 21 | DT | Sidechain |
| 24 | AX | 25 | DC | Sidechain |
| 24 | AX | 27 | DC | Sidechain |
| 24 | AX | 32 | DC | Sidechain |
| 24 | AX | 35 | DT | Sidechain |
| 24 | AX | 37 | DG | Sidechain |
| 24 | AX | 38 | DG | Sidechain |
| 24 | AX | 6 | DC | Sidechain |
| 24 | AX | 9 | DA | Sidechain |
| 25 | AY | 14 | DC | Sidechain |
| 25 | AY | 18 | DT | Sidechain |
| 25 | AY | 19 | DT | Sidechain |
| 25 | AY | 4 | DT | Sidechain |
| 25 | AY | 5 | DT | Sidechain |
| 26 | AZ | 12 | DT | Sidechain |
| 26 | AZ | 17 | DC | Sidechain |
| 26 | AZ | 18 | DC | Sidechain |
| 26 | AZ | 2 | DT | Sidechain |
| 26 | AZ | 26 | DT | Sidechain |
| 26 | AZ | 27 | DA | Sidechain |
| 26 | AZ | 3 | DA | Sidechain |
| 26 | AZ | 35 | DC | Sidechain |
| 26 | AZ | 36 | DC | Sidechain |
| 26 | AZ | 39 | DA | Sidechain |
| 26 | AZ | 4 | DC | Sidechain |
| 26 | AZ | 43 | DA | Sidechain |
| 26 | AZ | 46 | DC | Sidechain |
| 27 | Aa | 19 | DA | Sidechain |
| 27 | Aa | 32 | DA | Sidechain |
| 27 | Aa | 33 | DA | Sidechain |
| 27 | Aa | 35 | DA | Sidechain |
| 27 | Aa | 5 | DC | Sidechain |
| 27 | Aa | 6 | DT | Sidechain |
| 27 | Aa | 7 | DA | Sidechain |
| 28 | Ab | 13 | DA | Sidechain |
| 28 | Ab | 19 | DC | Sidechain |
| 28 | Ab | 20 | DC | Sidechain |
| 28 | Ab | 21 | DC | Sidechain |
| 28 | Ab | 23 | DC | Sidechain |
| 28 | Ab | 33 | DA | Sidechain |
| 28 | Ab | 39 | DA | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 28 | Ab | 41 | DG | Sidechain |
| 29 | Ac | 1 | DC | Sidechain |
| 29 | Ac | 15 | DG | Sidechain |
| 29 | Ac | 16 | DC | Sidechain |
| 29 | Ac | 19 | DG | Sidechain |
| 29 | Ac | 2 | DT | Sidechain |
| 29 | Ac | 28 | DT | Sidechain |
| 29 | Ac | 3 | DG | Sidechain |
| 29 | Ac | 35 | DT | Sidechain |
| 29 | Ac | 41 | DC | Sidechain |
| 29 | Ac | 9 | DG | Sidechain |
| 30 | Ad | 12 | DA | Sidechain |
| 30 | Ad | 13 | DT | Sidechain |
| 30 | Ad | 15 | DA | Sidechain |
| 30 | Ad | 16 | DT | Sidechain |
| 30 | Ad | 17 | DG | Sidechain |
| 30 | Ad | 19 | DG | Sidechain |
| 30 | Ad | 21 | DG | Sidechain |
| 30 | Ad | 3 | DT | Sidechain |
| 30 | Ad | 4 | DT | Sidechain |
| 31 | Ae | 16 | DG | Sidechain |
| 31 | Ae | 2 | DT | Sidechain |
| 31 | Ae | 20 | DA | Sidechain |
| 31 | Ae | 31 | DT | Sidechain |
| 31 | Ae | 34 | DC | Sidechain |
| 31 | Ae | 4 | DT | Sidechain |
| 31 | Ae | 41 | DT | Sidechain |
| 31 | Ae | 5 | DT | Sidechain |
| 31 | Ae | 6 | DT | Sidechain |
| 31 | Ae | 7 | DC | Sidechain |
| 32 | Af | 16 | DG | Sidechain |
| 32 | Af | 18 | DT | Sidechain |
| 32 | Af | 21 | DT | Sidechain |
| 32 | Af | 24 | DT | Sidechain |
| 32 | Af | 30 | DT | Sidechain |
| 32 | Af | 32 | DT | Sidechain |
| 32 | Af | 6 | DG | Sidechain |
| 32 | Af | 7 | DC | Sidechain |
| 33 | Ag | 1 | DT | Sidechain |
| 33 | Ag | 19 | DC | Sidechain |
| 33 | Ag | 27 | DC | Sidechain |
| 33 | Ag | 28 | DC | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 33 | Ag | 4 | DT | Sidechain |
| 33 | Ag | 9 | DT | Sidechain |
| 34 | Ah | 10 | DC | Sidechain |
| 34 | Ah | 11 | DC | Sidechain |
| 34 | Ah | 12 | DT | Sidechain |
| 34 | Ah | 2 | DT | Sidechain |
| 34 | Ah | 25 | DC | Sidechain |
| 34 | Ah | 28 | DG | Sidechain |
| 34 | Ah | 29 | DA | Sidechain |
| 34 | Ah | 3 | DT | Sidechain |
| 34 | Ah | 33 | DT | Sidechain |
| 34 | Ah | 6 | DA | Sidechain |
| 34 | Ah | 8 | DA | Sidechain |
| 35 | Ai | 1 | DA | Sidechain |
| 35 | Ai | 17 | DA | Sidechain |
| 35 | Ai | 24 | DA | Sidechain |
| 35 | Ai | 30 | DT | Sidechain |
| 35 | Ai | 34 | DT | Sidechain |
| 35 | Ai | 45 | DA | Sidechain |
| 35 | Ai | 46 | DA | Sidechain |
| 35 | Ai | 48 | DA | Sidechain |
| 35 | Ai | 7 | DT | Sidechain |
| 36 | Aj | 14 | DG | Sidechain |
| 36 | Aj | 17 | DC | Sidechain |
| 36 | Aj | 35 | DG | Sidechain |
| 36 | Aj | 36 | DC | Sidechain |
| 36 | Aj | 37 | DT | Sidechain |
| 36 | Aj | 4 | DG | Sidechain |
| 37 | Ak | 1 | DT | Sidechain |
| 37 | Ak | 16 | DG | Sidechain |
| 37 | Ak | 17 | DG | Sidechain |
| 37 | Ak | 3 | DT | Sidechain |
| 37 | Ak | 30 | DT | Sidechain |
| 37 | Ak | 34 | DG | Sidechain |
| 37 | Ak | 36 | DT | Sidechain |
| 37 | Ak | 37 | DT | Sidechain |
| 37 | Ak | 39 | DC | Sidechain |
| 37 | Ak | 46 | DC | Sidechain |
| 37 | Ak | 9 | DT | Sidechain |
| 38 | Al | 10 | DC | Sidechain |
| 38 | Al | 15 | DG | Sidechain |
| 38 | Al | 18 | DG | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 38 | Al | 23 | DG | Sidechain |
| 38 | Al | 26 | DA | Sidechain |
| 38 | Al | 27 | DA | Sidechain |
| 38 | Al | 35 | DG | Sidechain |
| 38 | Al | 37 | DG | Sidechain |
| 38 | Al | 38 | DA | Sidechain |
| 38 | Al | 4 | DG | Sidechain |
| 38 | Al | 9 | DC | Sidechain |
| 39 | Am | 10 | DG | Sidechain |
| 39 | Am | 12 | DC | Sidechain |
| 39 | Am | 16 | DC | Sidechain |
| 39 | Am | 17 | DT | Sidechain |
| 39 | Am | 18 | DT | Sidechain |
| 39 | Am | 21 | DT | Sidechain |
| 39 | Am | 25 | DG | Sidechain |
| 39 | Am | 29 | DG | Sidechain |
| 39 | Am | 3 | DA | Sidechain |
| 39 | Am | 31 | DG | Sidechain |
| 39 | Am | 37 | DT | Sidechain |
| 39 | Am | 41 | DC | Sidechain |
| 40 | An | 11 | DA | Sidechain |
| 40 | An | 14 | DG | Sidechain |
| 40 | An | 17 | DC | Sidechain |
| 40 | An | 19 | DT | Sidechain |
| 40 | An | 22 | DT | Sidechain |
| 40 | An | 23 | DG | Sidechain |
| 40 | An | 31 | DA | Sidechain |
| 40 | An | 37 | DT | Sidechain |
| 40 | An | 40 | DT | Sidechain |
| 40 | An | 42 | DA | Sidechain |
| 40 | An | 5 | DC | Sidechain |
| 40 | An | 6 | DT | Sidechain |
| 41 | Ao | 10 | DT | Sidechain |
| 41 | Ao | 11 | DT | Sidechain |
| 41 | Ao | 12 | DC | Sidechain |
| 41 | Ao | 15 | DG | Sidechain |
| 41 | Ao | 18 | DG | Sidechain |
| 41 | Ao | 24 | DT | Sidechain |
| 41 | Ao | 25 | DT | Sidechain |
| 41 | Ao | 28 | DT | Sidechain |
| 41 | Ao | 3 | DG | Sidechain |
| 41 | Ao | 5 | DC | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 42 | Ap | 17 | DG | Sidechain |
| 42 | Ap | 2 | DT | Sidechain |
| 42 | Ap | 22 | DG | Sidechain |
| 42 | Ap | 23 | DA | Sidechain |
| 42 | Ap | 26 | DT | Sidechain |
| 42 | Ap | 9 | DT | Sidechain |
| 43 | Aq | 12 | DG | Sidechain |
| 43 | Aq | 13 | DT | Sidechain |
| 43 | Aq | 25 | DG | Sidechain |
| 43 | Aq | 30 | DC | Sidechain |
| 43 | Aq | 36 | DG | Sidechain |
| 43 | Aq | 37 | DT | Sidechain |
| 43 | Aq | 6 | DC | Sidechain |
| 43 | Aq | 8 | DC | Sidechain |
| 44 | Ar | 10 | DA | Sidechain |
| 44 | Ar | 17 | DT | Sidechain |
| 44 | Ar | 20 | DT | Sidechain |
| 44 | Ar | 27 | DT | Sidechain |
| 44 | Ar | 3 | DC | Sidechain |
| 44 | Ar | 33 | DT | Sidechain |
| 44 | Ar | 38 | DA | Sidechain |
| 44 | Ar | 46 | DC | Sidechain |
| 44 | Ar | 47 | DG | Sidechain |
| 44 | Ar | 48 | DT | Sidechain |
| 44 | Ar | 49 | DT | Sidechain |
| 44 | Ar | 8 | DA | Sidechain |
| 45 | As | 10 | DG | Sidechain |
| 45 | As | 15 | DC | Sidechain |
| 45 | As | 17 | DT | Sidechain |
| 45 | As | 23 | DA | Sidechain |
| 45 | As | 25 | DC | Sidechain |
| 45 | As | 29 | DC | Sidechain |
| 45 | As | 33 | DG | Sidechain |
| 45 | As | 41 | DT | Sidechain |
| 45 | As | 42 | DG | Sidechain |
| 45 | As | 45 | DC | Sidechain |
| 45 | As | 6 | DA | Sidechain |
| 46 | At | 10 | DC | Sidechain |
| 46 | At | 11 | DG | Sidechain |
| 46 | At | 16 | DC | Sidechain |
| 46 | At | 20 | DG | Sidechain |
| 46 | At | 26 | DA | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 46 | At | 37 | DG | Sidechain |
| 46 | At | 38 | DC | Sidechain |
| 46 | At | 39 | DT | Sidechain |
| 46 | At | 9 | DG | Sidechain |
| 47 | Au | 1 | DT | Sidechain |
| 47 | Au | 21 | DT | Sidechain |
| 47 | Au | 26 | DC | Sidechain |
| 47 | Au | 28 | DG | Sidechain |
| 47 | Au | 39 | DT | Sidechain |
| 47 | Au | 42 | DA | Sidechain |
| 47 | Au | 44 | DC | Sidechain |
| 47 | Au | 48 | DA | Sidechain |
| 47 | Au | 49 | DC | Sidechain |
| 48 | Av | 12 | DA | Sidechain |
| 48 | Av | 17 | DC | Sidechain |
| 48 | Av | 19 | DG | Sidechain |
| 48 | Av | 30 | DT | Sidechain |
| 48 | Av | 33 | DT | Sidechain |
| 48 | Av | 36 | DG | Sidechain |
| 48 | Av | 41 | DC | Sidechain |
| 48 | Av | 6 | DA | Sidechain |
| 48 | Av | 8 | DA | Sidechain |
| 49 | Aw | 1 | DG | Sidechain |
| 49 | Aw | 15 | DC | Sidechain |
| 49 | Aw | 19 | DG | Sidechain |
| 49 | Aw | 20 | DC | Sidechain |
| 49 | Aw | 23 | DG | Sidechain |
| 49 | Aw | 30 | DG | Sidechain |
| 49 | Aw | 31 | DG | Sidechain |
| 49 | Aw | 32 | DC | Sidechain |
| 49 | Aw | 39 | DG | Sidechain |
| 50 | Ax | 1 | DA | Sidechain |
| 50 | Ax | 10 | DT | Sidechain |
| 50 | Ax | 15 | DG | Sidechain |
| 50 | Ax | 19 | DC | Sidechain |
| 50 | Ax | 20 | DG | Sidechain |
| 50 | Ax | 22 | DG | Sidechain |
| 50 | Ax | 23 | DC | Sidechain |
| 50 | Ax | 24 | DG | Sidechain |
| 50 | Ax | 26 | DC | Sidechain |
| 50 | Ax | 27 | DG | Sidechain |
| 50 | Ax | 28 | DC | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 50 | Ax | 30 | DT | Sidechain |
| 50 | Ax | 31 | DA | Sidechain |
| 50 | Ax | 33 | DG | Sidechain |
| 50 | Ax | 36 | DC | Sidechain |
| 50 | Ax | 38 | DT | Sidechain |
| 50 | Ax | 5 | DT | Sidechain |
| 50 | Ax | 7 | DG | Sidechain |
| 50 | Ax | 8 | DT | Sidechain |
| 51 | Ay | 10 | DG | Sidechain |
| 51 | Ay | 11 | DT | Sidechain |
| 51 | Ay | 13 | DT | Sidechain |
| 51 | Ay | 16 | DG | Sidechain |
| 51 | Ay | 2 | DG | Sidechain |
| 51 | Ay | 21 | DC | Sidechain |
| 51 | Ay | 28 | DT | Sidechain |
| 51 | Ay | 3 | DT | Sidechain |
| 51 | Ay | 30 | DC | Sidechain |
| 51 | Ay | 35 | DG | Sidechain |
| 51 | Ay | 39 | DG | Sidechain |
| 51 | Ay | 40 | DC | Sidechain |
| 51 | Ay | 41 | DT | Sidechain |
| 52 | Az | 2 | DG | Sidechain |
| 52 | Az | 29 | DG | Sidechain |
| 52 | Az | 3 | DC | Sidechain |
| 52 | Az | 30 | DG | Sidechain |
| 52 | Az | 33 | DC | Sidechain |
| 63 | BA | 15 | DG | Sidechain |
| 63 | BA | 17 | DA | Sidechain |
| 63 | BA | 27 | DT | Sidechain |
| 63 | BA | 28 | DG | Sidechain |
| 63 | BA | 3 | DC | Sidechain |
| 63 | BA | 30 | DA | Sidechain |
| 63 | BA | 4 | DG | Sidechain |
| 63 | BA | 5 | DG | Sidechain |
| 64 | BB | 1 | DT | Sidechain |
| 64 | BB | 12 | DA | Sidechain |
| 64 | BB | 13 | DC | Sidechain |
| 64 | BB | 15 | DC | Sidechain |
| 64 | BB | 18 | DA | Sidechain |
| 64 | BB | 19 | DT | Sidechain |
| 64 | BB | 31 | DT | Sidechain |
| 64 | BB | 34 | DA | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 64 | BB | 42 | DT | Sidechain |
| 64 | BB | 44 | DT | Sidechain |
| 64 | BB | 5 | DA | Sidechain |
| 64 | BB | 7 | DG | Sidechain |
| 64 | BB | 8 | DA | Sidechain |
| 65 | BC | 10 | DA | Sidechain |
| 65 | BC | 13 | DG | Sidechain |
| 65 | BC | 16 | DT | Sidechain |
| 65 | BC | 2 | DT | Sidechain |
| 65 | BC | 20 | DC | Sidechain |
| 65 | BC | 23 | DT | Sidechain |
| 65 | BC | 24 | DT | Sidechain |
| 65 | BC | 35 | DA | Sidechain |
| 66 | BD | 10 | DG | Sidechain |
| 66 | BD | 14 | DG | Sidechain |
| 66 | BD | 22 | DA | Sidechain |
| 66 | BD | 23 | DT | Sidechain |
| 66 | BD | 28 | DT | Sidechain |
| 66 | BD | 8 | DT | Sidechain |
| 67 | BE | 14 | DA | Sidechain |
| 67 | BE | 18 | DT | Sidechain |
| 67 | BE | 20 | DG | Sidechain |
| 67 | BE | 3 | DT | Sidechain |
| 67 | BE | 4 | DT | Sidechain |
| 67 | BE | 6 | DT | Sidechain |
| 68 | BF | 1 | DT | Sidechain |
| 68 | BF | 13 | DT | Sidechain |
| 68 | BF | 14 | DT | Sidechain |
| 68 | BF | 21 | DA | Sidechain |
| 68 | BF | 23 | DT | Sidechain |
| 68 | BF | 27 | DC | Sidechain |
| 68 | BF | 34 | DG | Sidechain |
| 68 | BF | 35 | DG | Sidechain |
| 68 | BF | 37 | DT | Sidechain |
| 68 | BF | 6 | DA | Sidechain |
| 69 | BG | 10 | DG | Sidechain |
| 69 | BG | 11 | DT | Sidechain |
| 69 | BG | 12 | DC | Sidechain |
| 69 | BG | 18 | DG | Sidechain |
| 69 | BG | 21 | DA | Sidechain |
| 69 | BG | 26 | DT | Sidechain |
| 69 | BG | 30 | DT | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 69 | BG | 31 | DT | Sidechain |
| 69 | BG | 32 | DT | Sidechain |
| 69 | BG | 33 | DA | Sidechain |
| 69 | BG | 5 | DA | Sidechain |
| 70 | BH | 1 | DA | Sidechain |
| 70 | BH | 16 | DT | Sidechain |
| 70 | BH | 18 | DT | Sidechain |
| 70 | BH | 19 | DT | Sidechain |
| 70 | BH | 3 | DG | Sidechain |
| 70 | BH | 41 | DA | Sidechain |
| 71 | BI | 16 | DT | Sidechain |
| 71 | BI | 17 | DG | Sidechain |
| 71 | BI | 18 | DT | Sidechain |
| 71 | BI | 19 | DA | Sidechain |
| 71 | BI | 32 | DC | Sidechain |
| 71 | BI | 37 | DC | Sidechain |
| 71 | BI | 5 | DT | Sidechain |
| 72 | BJ | 11 | DG | Sidechain |
| 72 | BJ | 14 | DA | Sidechain |
| 72 | BJ | 16 | DT | Sidechain |
| 72 | BJ | 18 | DT | Sidechain |
| 72 | BJ | 2 | DT | Sidechain |
| 72 | BJ | 25 | DA | Sidechain |
| 72 | BJ | 27 | DC | Sidechain |
| 72 | BJ | 37 | DT | Sidechain |
| 72 | BJ | 4 | DT | Sidechain |
| 72 | BJ | 6 | DT | Sidechain |
| 73 | BK | 11 | DT | Sidechain |
| 73 | BK | 23 | DC | Sidechain |
| 73 | BK | 26 | DA | Sidechain |
| 73 | BK | 27 | DT | Sidechain |
| 74 | BL | 13 | DA | Sidechain |
| 74 | BL | 21 | DG | Sidechain |
| 74 | BL | 27 | DT | Sidechain |
| 74 | BL | 30 | DT | Sidechain |
| 74 | BL | 31 | DT | Sidechain |
| 74 | BL | 40 | DT | Sidechain |
| 74 | BL | 7 | DC | Sidechain |
| 75 | BM | 10 | DA | Sidechain |
| 75 | BM | 15 | DA | Sidechain |
| 75 | BM | 20 | DC | Sidechain |
| 75 | BM | 22 | DA | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 75 | BM | 3 | DC | Sidechain |
| 75 | BM | 30 | DG | Sidechain |
| 75 | BM | 37 | DG | Sidechain |
| 75 | BM | 38 | DG | Sidechain |
| 75 | BM | 39 | DC | Sidechain |
| 75 | BM | 4 | DT | Sidechain |
| 75 | BM | 43 | DC | Sidechain |
| 75 | BM | 46 | DT | Sidechain |
| 75 | BM | 48 | DA | Sidechain |
| 75 | BM | 49 | DA | Sidechain |
| 76 | BN | 10 | DT | Sidechain |
| 76 | BN | 11 | DA | Sidechain |
| 76 | BN | 12 | DT | Sidechain |
| 76 | BN | 14 | DA | Sidechain |
| 76 | BN | 23 | DG | Sidechain |
| 76 | BN | 24 | DT | Sidechain |
| 76 | BN | 26 | DA | Sidechain |
| 76 | BN | 29 | DG | Sidechain |
| 76 | BN | 40 | DT | Sidechain |
| 76 | BN | 5 | DG | Sidechain |
| 77 | BO | 10 | DT | Sidechain |
| 77 | BO | 17 | DA | Sidechain |
| 77 | BO | 18 | DT | Sidechain |
| 77 | BO | 24 | DA | Sidechain |
| 77 | BO | 25 | DA | Sidechain |
| 77 | BO | 29 | DC | Sidechain |
| 77 | BO | 34 | DT | Sidechain |
| 77 | BO | 37 | DC | Sidechain |
| 77 | BO | 39 | DT | Sidechain |
| 78 | BP | 17 | DG | Sidechain |
| 78 | BP | 21 | DA | Sidechain |
| 78 | BP | 23 | DG | Sidechain |
| 79 | BQ | 11 | DA | Sidechain |
| 79 | BQ | 2 | DT | Sidechain |
| 79 | BQ | 23 | DG | Sidechain |
| 79 | BQ | 37 | DT | Sidechain |
| 79 | BQ | 5 | DT | Sidechain |
| 79 | BQ | 6 | DG | Sidechain |

## 5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

There are no protein molecules in this entry.

### 5.3.2 Protein sidechains (i)

There are no protein molecules in this entry.

### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

There are no ligands in this entry.

## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

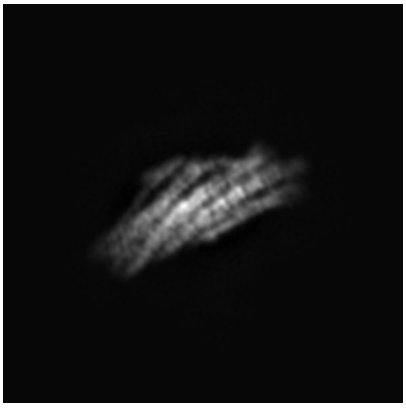
# 6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-12516. These allow visual inspection of the internal detail of the map and identification of artifacts.

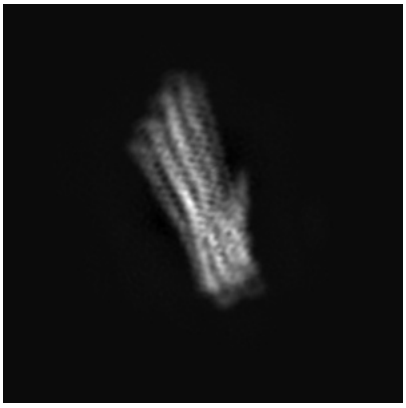
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

## 6.1 Orthogonal projections (i)

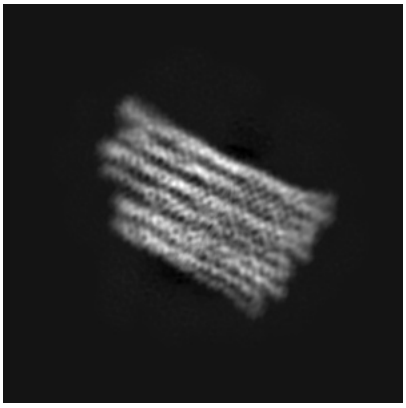
### 6.1.1 Primary map



X



Y



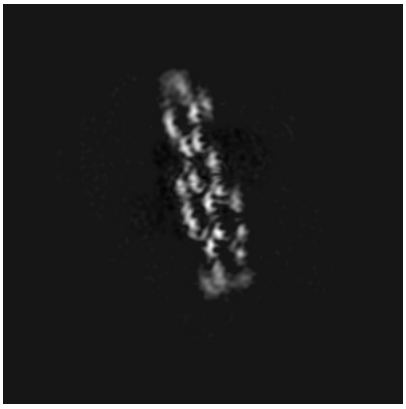
Z

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

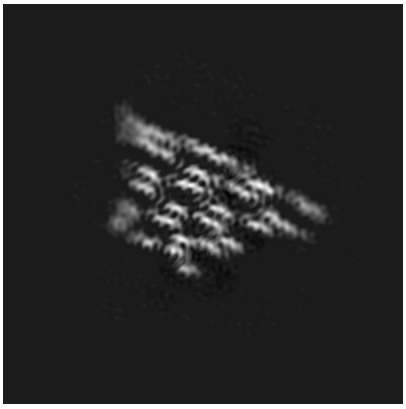
## 6.2 Central slices (i)

### 6.2.1 Primary map

X Index: 150



Y Index: 150

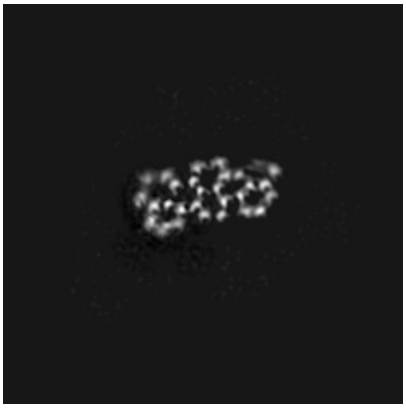


Z Index: 150

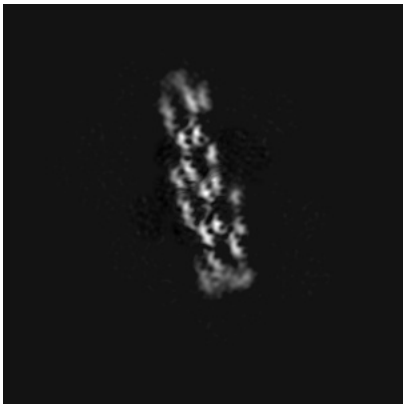
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

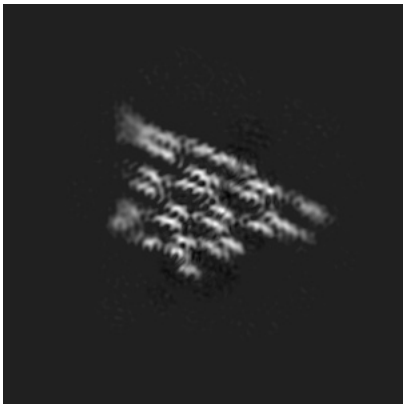
### 6.3.1 Primary map



X Index: 133



Y Index: 147

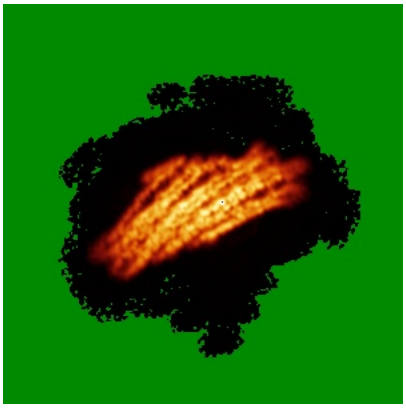


Z Index: 149

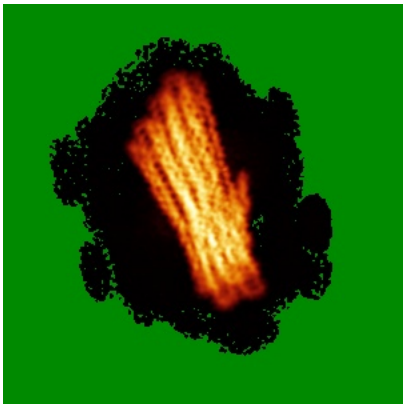
The images above show the largest variance slices of the map in three orthogonal directions.

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

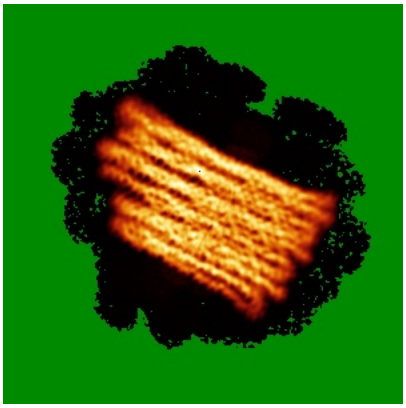
### 6.4.1 Primary map



X



Y



Z

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

## 6.5 Orthogonal surface views (i)

### 6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0628. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

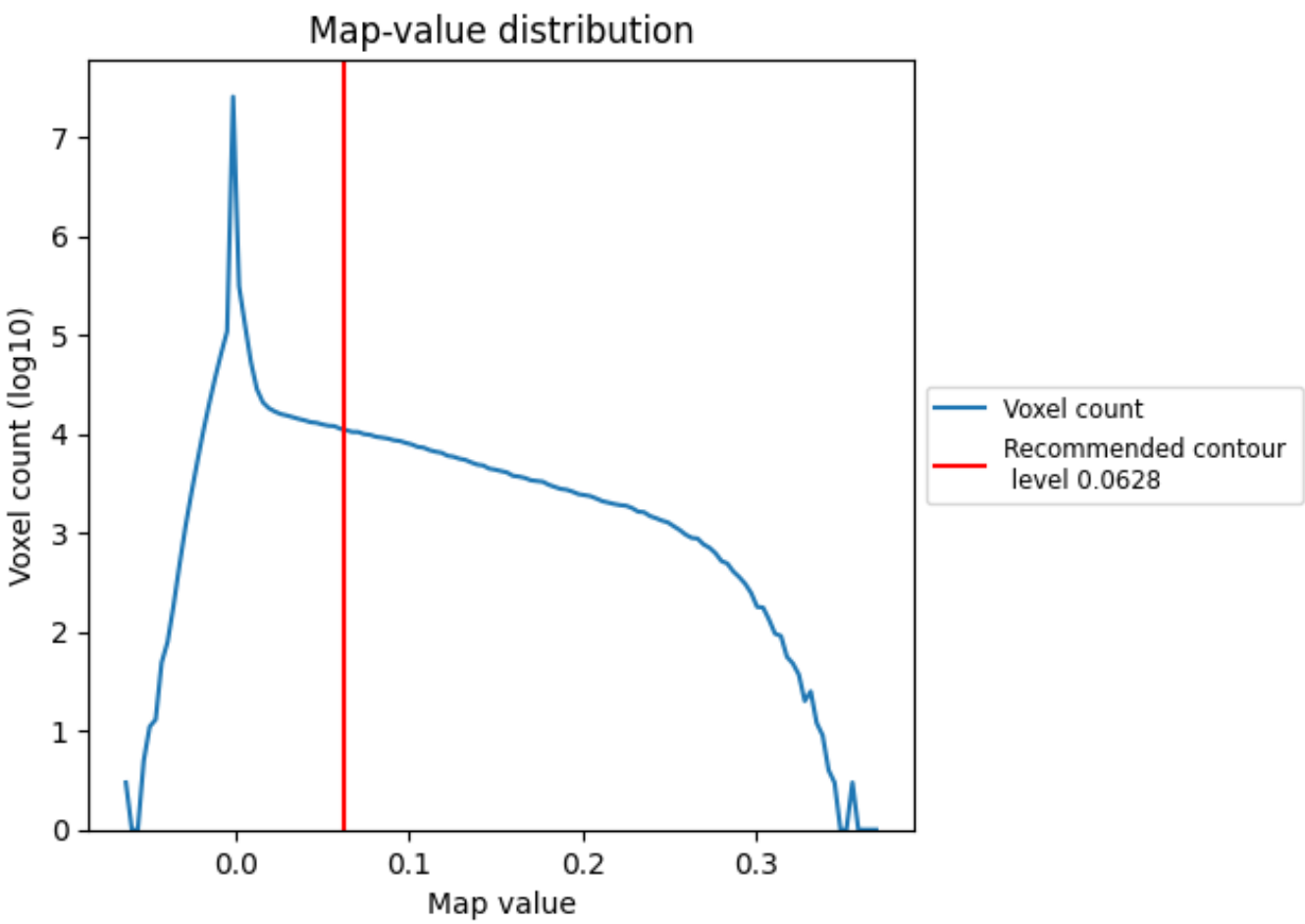
## 6.6 Mask visualisation (i)

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

# 7 Map analysis (i)

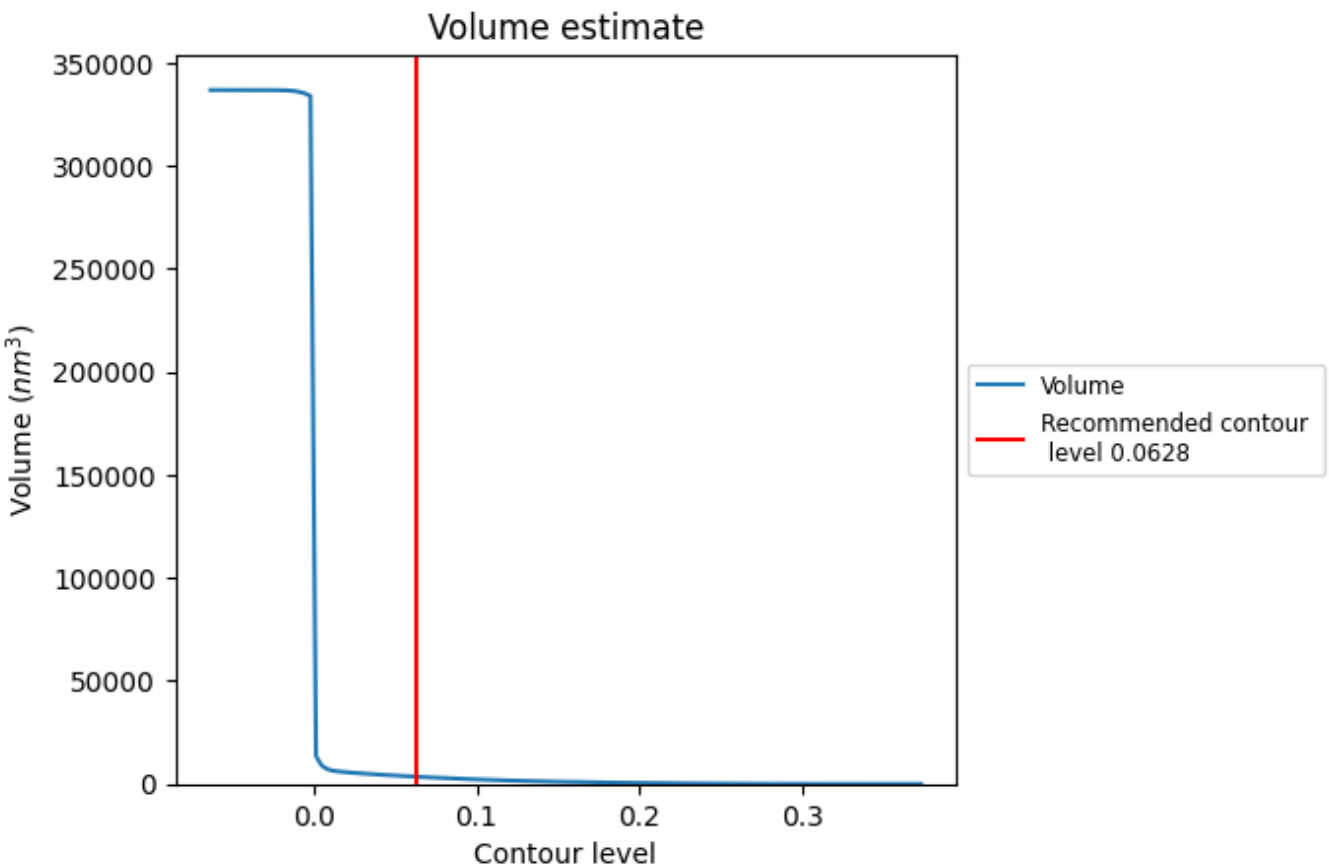
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution (i)




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

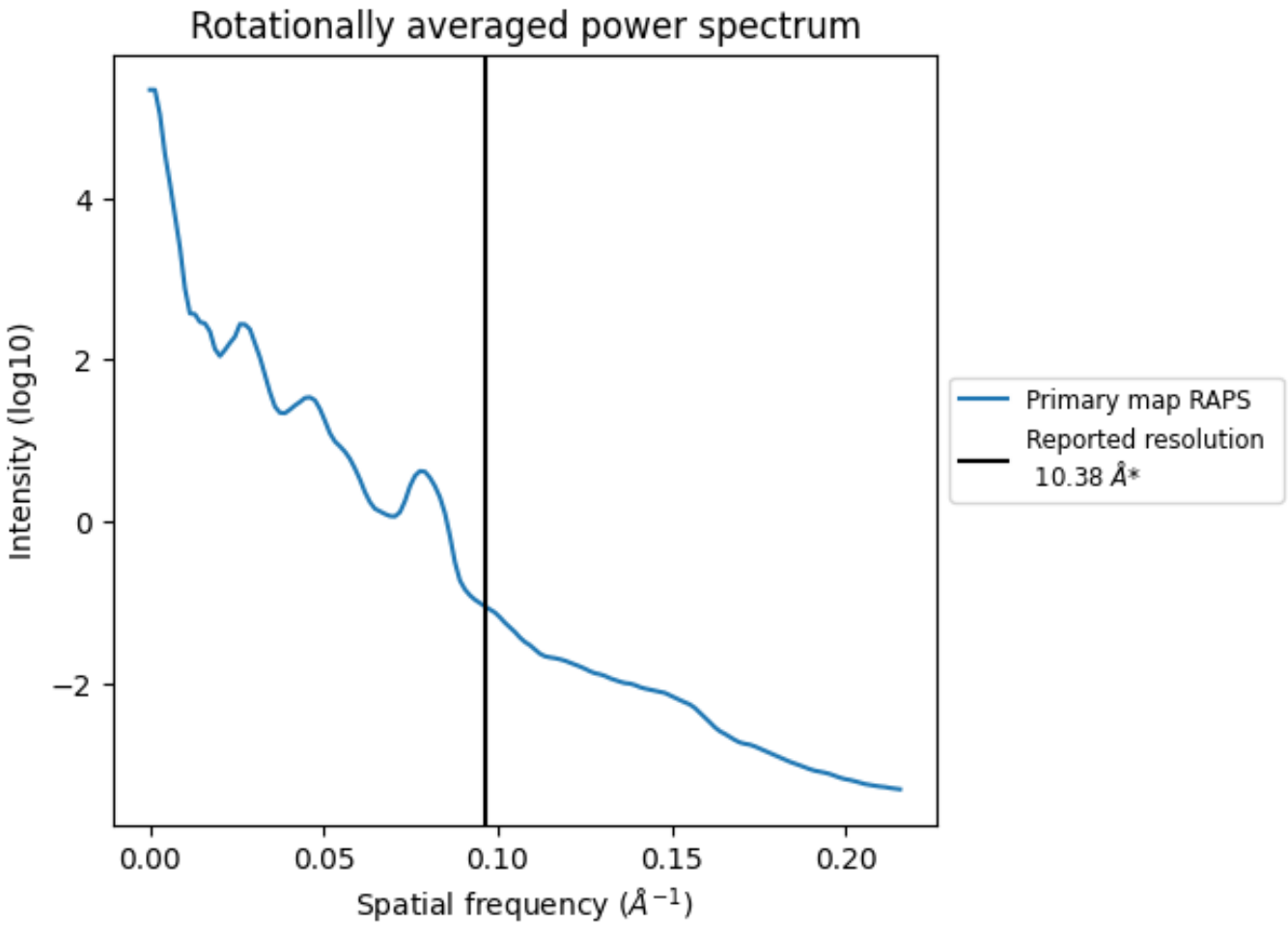
## 7.2 Volume estimate (i)




The volume at the recommended contour level is 3511 $nm^3$; this corresponds to an approximate mass of 3171 kDa.

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

## 7.3 Rotationally averaged power spectrum (i)

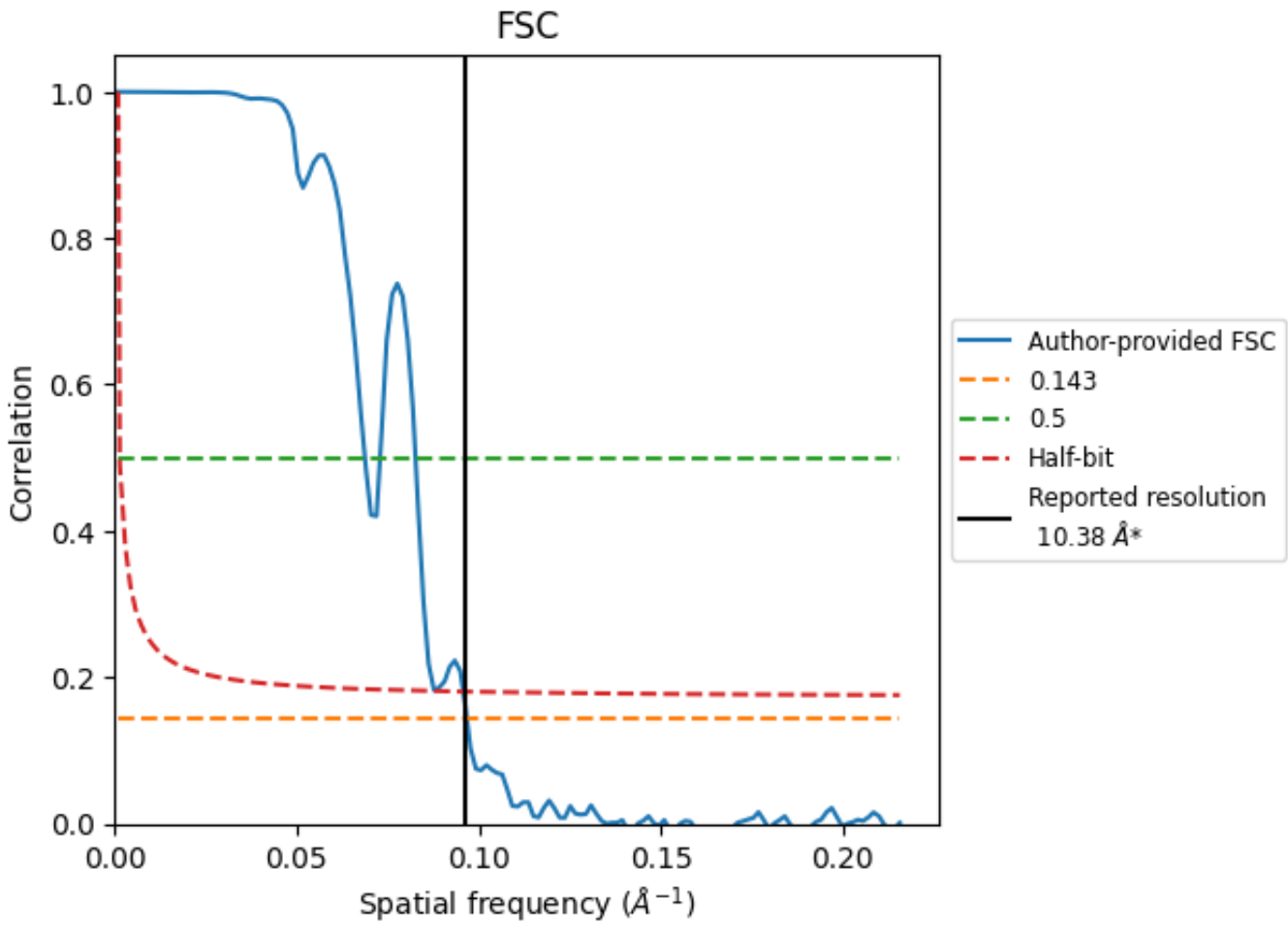



*Reported resolution corresponds to spatial frequency of 0.096 Å$^{-1}$

# 8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

## 8.1 FSC (i)




*Reported resolution corresponds to spatial frequency of 0.096 Å$^{-1}$

## 8.2 Resolution estimates (i)

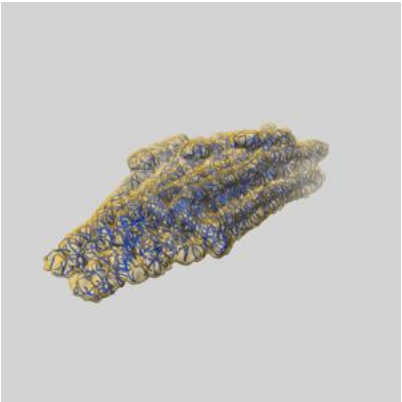
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 10.38 | - | - |
| Author-provided FSC curve | 10.34 | 14.56 | 10.45 |
| Unmasked-calculated* | - | - | - |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

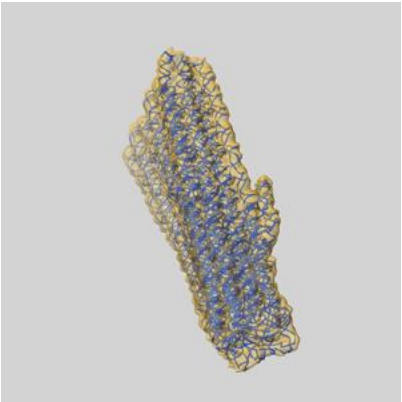
# 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-12516 and PDB model 7NPN. Per-residue inclusion information can be found in section 3 on page 18.

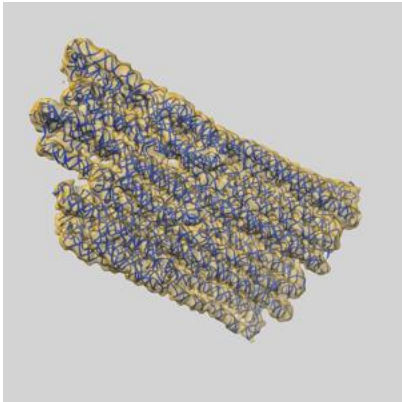
## 9.1 Map-model overlay (i)



X



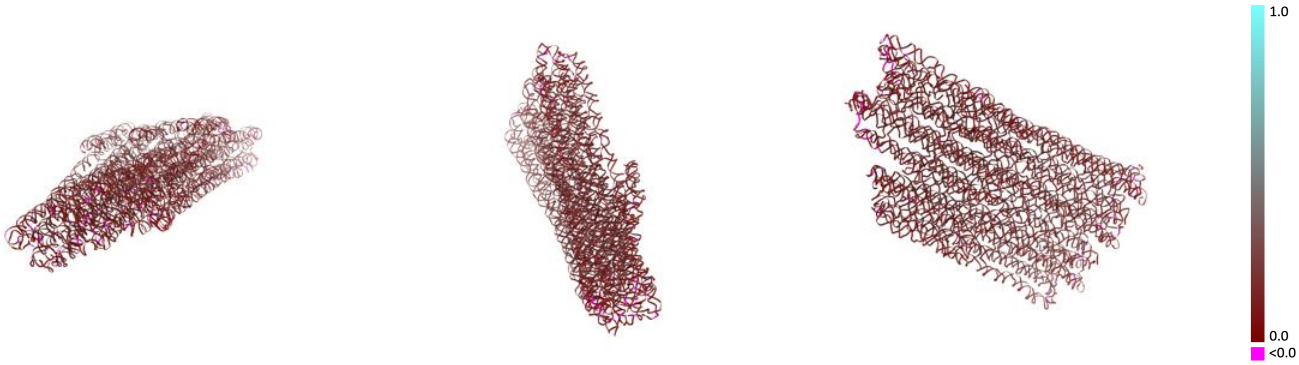
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0628 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

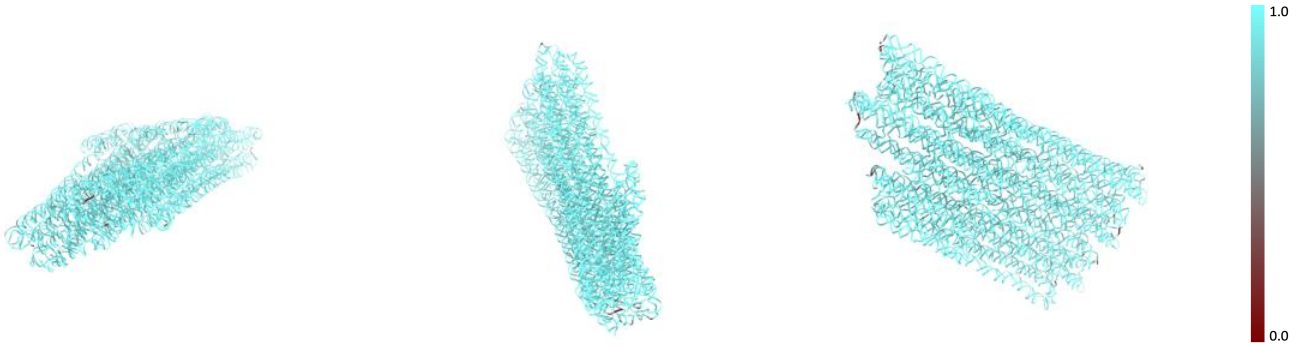
## 9.2 Q-score mapped to coordinate model (i)




X Y Z

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

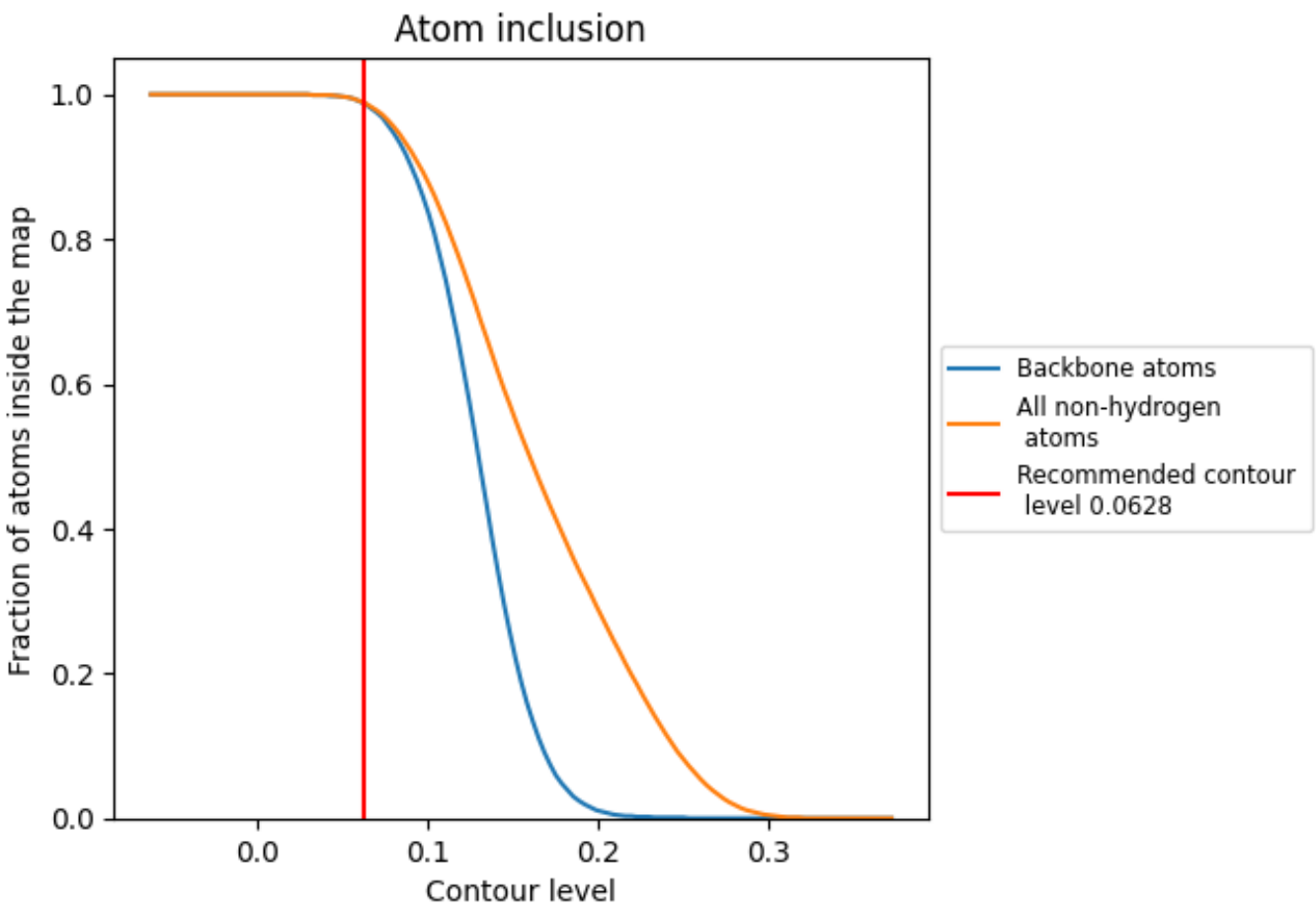
## 9.3 Atom inclusion mapped to coordinate model (i)




X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0628).

## 9.4 Atom inclusion (i)




At the recommended contour level, 99% of all backbone atoms, 99% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0628) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.9880 | 0.1650 |
| A0 | 0.9980 | 0.1910 |
| A1 | 0.9310 | 0.1530 |
| A2 | 0.9600 | 0.1210 |
| A3 | 0.9880 | 0.1620 |
| A4 | 0.9980 | 0.1810 |
| A5 | 0.9860 | 0.1520 |
| A6 | 0.9840 | 0.1280 |
| A7 | 0.9310 | 0.1230 |
| A8 | 0.9990 | 0.1930 |
| A9 | 1.0000 | 0.1800 |
| AA | 0.9950 | 0.1700 |
| AB | 0.9970 | 0.1520 |
| AC | 0.9870 | 0.1460 |
| AD | 0.9960 | 0.1910 |
| AE | 0.9910 | 0.1720 |
| AF | 0.9940 | 0.1810 |
| AG | 0.9900 | 0.1510 |
| AH | 1.0000 | 0.1630 |
| AI | 0.9790 | 0.1480 |
| AJ | 0.8720 | 0.1060 |
| AK | 1.0000 | 0.1910 |
| AL | 0.9990 | 0.1710 |
| AM | 1.0000 | 0.1920 |
| AN | 1.0000 | 0.1700 |
| AO | 1.0000 | 0.1700 |
| AP | 1.0000 | 0.1770 |
| AQ | 0.9220 | 0.1280 |
| AR | 0.9660 | 0.1080 |
| AS | 0.9480 | 0.0840 |
| AT | 0.9980 | 0.1780 |
| AU | 1.0000 | 0.1720 |
| AV | 0.9900 | 0.1510 |
| AW | 0.9980 | 0.1850 |
| AX | 0.9960 | 0.1330 |

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| Chain | Atom inclusion | Q-score |
|---|---|---|
| AY | 0.9520 | 0.1430 |
| AZ | 1.0000 | 0.1870 |
| Aa | 0.9980 | 0.1670 |
| Ab | 0.9980 | 0.1780 |
| Ac | 0.9990 | 0.1680 |
| Ad | 0.9600 | 0.1260 |
| Ae | 0.9530 | 0.1370 |
| Af | 1.0000 | 0.1850 |
| Ag | 0.9740 | 0.1330 |
| Ah | 0.9350 | 0.1090 |
| Ai | 1.0000 | 0.1750 |
| Aj | 1.0000 | 0.1670 |
| Ak | 0.9540 | 0.1480 |
| Al | 0.9970 | 0.1940 |
| Am | 0.9980 | 0.1710 |
| An | 0.9990 | 0.1740 |
| Ao | 0.9810 | 0.1430 |
| Ap | 0.9260 | 0.0890 |
| Aq | 0.9280 | 0.1090 |
| Ar | 0.9980 | 0.1790 |
| As | 1.0000 | 0.1880 |
| At | 0.9840 | 0.1500 |
| Au | 0.9210 | 0.1380 |
| Av | 0.9980 | 0.1940 |
| Aw | 0.9950 | 0.1890 |
| Ax | 0.9980 | 0.1800 |
| Ay | 0.9980 | 0.1610 |
| Az | 1.0000 | 0.1760 |
| BA | 0.9990 | 0.1670 |
| BB | 0.9600 | 0.1370 |
| BC | 1.0000 | 0.1650 |
| BD | 0.9510 | 0.1430 |
| BE | 0.9600 | 0.1340 |
| BF | 0.9300 | 0.1210 |
| BG | 0.9890 | 0.1660 |
| BH | 0.9990 | 0.1760 |
| BI | 1.0000 | 0.1960 |
| BJ | 0.9910 | 0.1620 |
| BK | 0.9560 | 0.1450 |
| BL | 1.0000 | 0.1710 |
| BM | 0.9980 | 0.1830 |
| BN | 0.9990 | 0.1710 |

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| Chain | Atom inclusion | Q-score |
|---|---|---|
| BO | 0.9990 | 0.1780 |
| BP | 0.9560 | 0.1420 |
| BQ | 0.9920 | 0.1530 |