# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2023 – 04:45 AM EDT

| | | |
|---|---|---|
| PDB ID | : | 1K82 |
| Title | : | Crystal structure of E.coli formamidopyrimidine-DNA glycosylase (Fpg) covalently trapped with DNA |
| Authors | : | Gilboa, R.; Zharkov, D.O.; Golan, G.; Fernandes, A.S.; Gerchman, S.E.; Matz, E.; Kycia, J.H.; Grollman, A.P.; Shoham, G. |
| Deposited on | : | 2001-10-22 |
| Resolution | : | 2.10 Å(reported) |

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

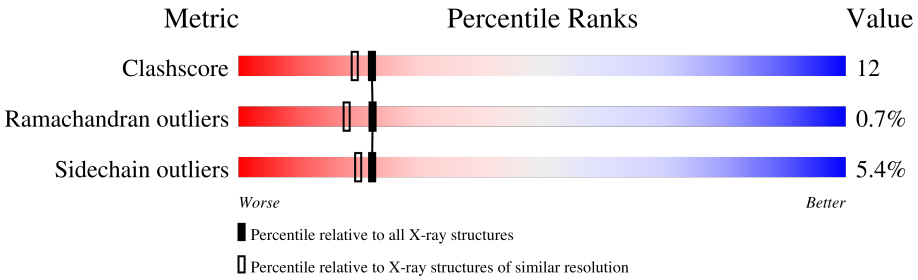
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| Xtriage (Phenix) | : | NOT EXECUTED |
| EDS | : | NOT EXECUTED |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.35 |

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 Å.

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




| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|---|---|---|
| Clashscore | 141614 | 5710 (2.10-2.10) |
| Ramachandran outliers | 138981 | 5647 (2.10-2.10) |
| Sidechain outliers | 138945 | 5648 (2.10-2.10) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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%

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | E | 13 | 62% 38% |
| 1 | F | 13 | 69% 31% |
| 1 | G | 13 | 69% 31% |
| 1 | H | 13 | 69% 31% |
| 2 | I | 13 | 8% 62% 31% |
| 2 | J | 13 | 8% 54% 38% |
| 2 | K | 13 | 8% 69% 23% |
| 2 | L | 13 | 8% 54% 38% |

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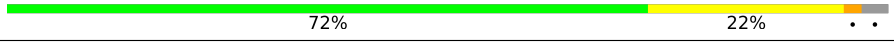
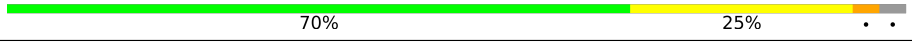
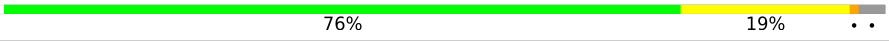
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 3 | A | 268 |   |
| 3 | B | 268 |   |
| 3 | C | 268 |   |
| 3 | D | 268 |   |

## 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 10716 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 5'-D(*GP*GP*CP*TP*TP*CP*CP*TP*CP*CP*TP*GP *G)-3'.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | E | 13 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 260 | 125 | 43 | 80 | 12 | | | |
| 1 | F | 13 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 260 | 125 | 43 | 80 | 12 | | | |
| 1 | G | 13 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 260 | 125 | 43 | 80 | 12 | | | |
| 1 | H | 13 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 260 | 125 | 43 | 80 | 12 | | | |

- Molecule 2 is a DNA chain called 5'-D(*CP*CP*AP*GP*GP*AP*(PED)P*GP*AP*AP*G P*CP*C)-3'.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 2 | I | 13 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 256 | 121 | 52 | 71 | 12 | | | |
| 2 | J | 13 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 256 | 121 | 52 | 71 | 12 | | | |
| 2 | K | 13 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 256 | 121 | 52 | 71 | 12 | | | |
| 2 | L | 13 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 256 | 121 | 52 | 71 | 12 | | | |

- Molecule 3 is a protein called formamidopyrimidine-DNA glycosylase.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 3 | A | 260 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2038 | 1297 | 370 | 362 | 9 | | | |
| 3 | B | 260 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2030 | 1293 | 367 | 361 | 9 | | | |
| 3 | C | 260 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2042 | 1299 | 368 | 366 | 9 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 3 | D | 260 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2039 | 1298 | 370 | 362 | 9 | | | |

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| 4 | A | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 4 | B | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 4 | C | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 4 | D | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 5 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| 5 | E | 15 | Total | O | 0 | 0 |
| | | | 15 | 15 | | |
| 5 | I | 23 | Total | O | 0 | 0 |
| | | | 23 | 23 | | |
| 5 | F | 16 | Total | O | 0 | 0 |
| | | | 16 | 16 | | |
| 5 | J | 24 | Total | O | 0 | 0 |
| | | | 24 | 24 | | |
| 5 | G | 18 | Total | O | 0 | 0 |
| | | | 18 | 18 | | |
| 5 | K | 20 | Total | O | 0 | 0 |
| | | | 20 | 20 | | |
| 5 | H | 18 | Total | O | 0 | 0 |
| | | | 18 | 18 | | |
| 5 | L | 21 | Total | O | 0 | 0 |
| | | | 21 | 21 | | |
| 5 | A | 93 | Total | O | 0 | 0 |
| | | | 93 | 93 | | |
| 5 | B | 82 | Total | O | 0 | 0 |
| | | | 82 | 82 | | |
| 5 | C | 77 | Total | O | 0 | 0 |
| | | | 77 | 77 | | |
| 5 | D | 92 | Total | O | 0 | 0 |
| | | | 92 | 92 | | |

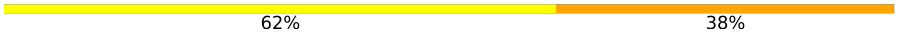
# 3 Residue-property plots (i)

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

Note EDS was not executed.

• Molecule 1: 5'-D(*GP*GP*CP*TP*TP*CP*CP*TP*CP*CP*TP*GP*G)-3'

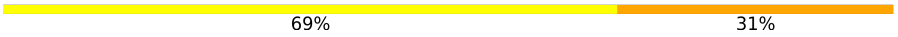
Chain E:





• Molecule 1: 5'-D(*GP*GP*CP*TP*TP*CP*CP*TP*CP*CP*TP*GP*G)-3'

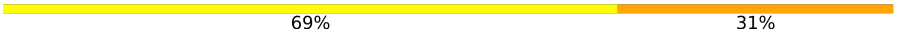
Chain F:





• Molecule 1: 5'-D(*GP*GP*CP*TP*TP*CP*CP*TP*CP*CP*TP*GP*G)-3'

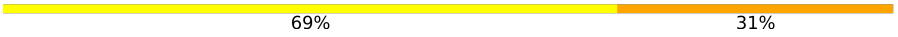
Chain G:





• Molecule 1: 5'-D(*GP*GP*CP*TP*TP*CP*CP*TP*CP*CP*TP*GP*G)-3'

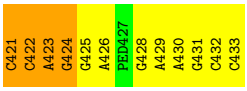
Chain H:





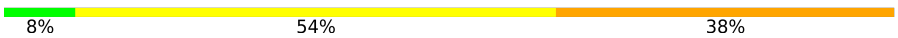
• Molecule 2: 5'-D(*CP*CP*AP*GP*GP*AP*(PED)P*GP*AP*AP*GP*CP*C)-3'

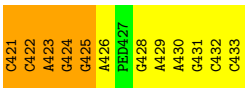
Chain I:


• Molecule 2: 5'-D(*CP*CP*AP*GP*GP*AP*(PED)P*GP*AP*AP*GP*CP*C)-3'

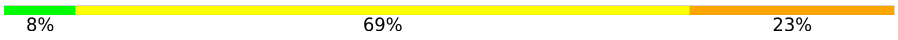
Chain J:

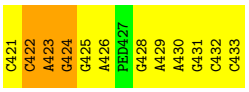





• Molecule 2: 5'-D(*CP*CP*AP*GP*GP*AP*(PED)P*GP*AP*AP*GP*CP*C)-3'

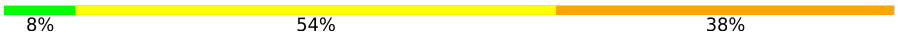
Chain K:

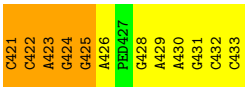



• Molecule 2: 5'-D(*CP*CP*AP*GP*GP*AP*(PED)P*GP*AP*AP*GP*CP*C)-3'

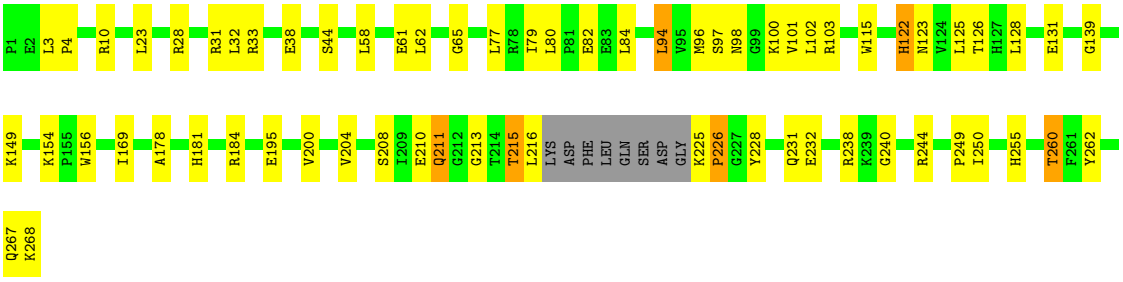
Chain L:



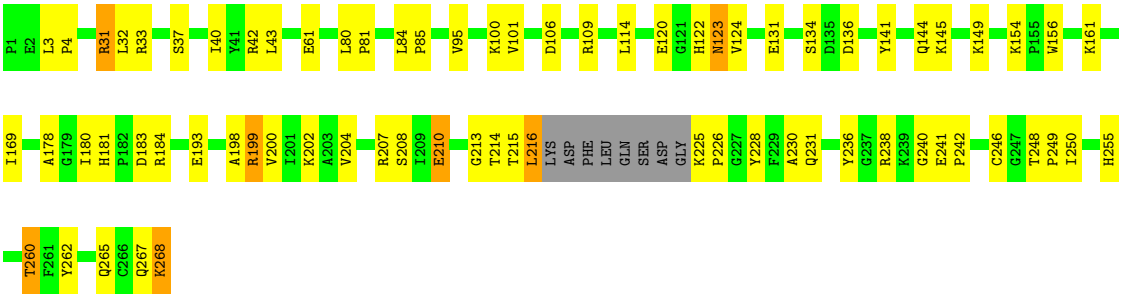

• Molecule 3: formamidopyrimidine-DNA glycosylase

Chain A:

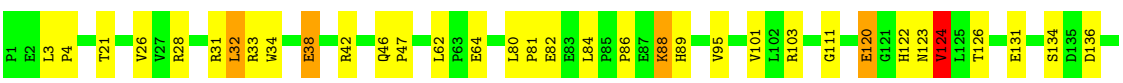

• Molecule 3: formamidopyrimidine-DNA glycosylase

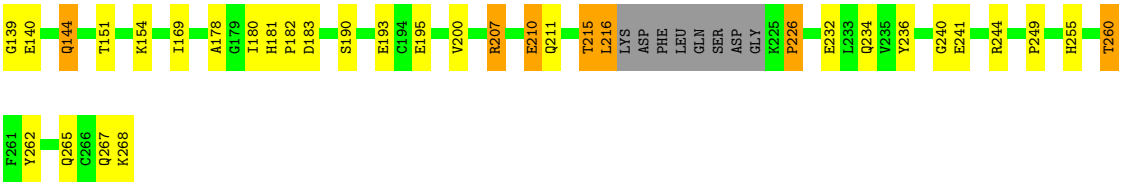
Chain B:

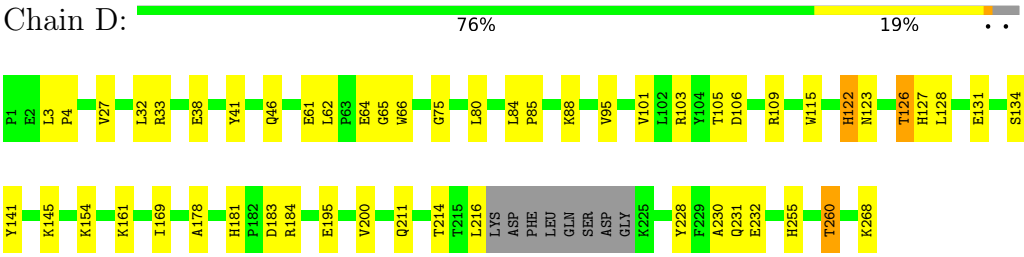

• Molecule 3: formamidopyrimidine-DNA glycosylase

Chain C:




• Molecule 3: formamidopyrimidine-DNA glycosylase



# 4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

| Property | Value | Source |
|---|---|---|
| Space group | P 1 21 1 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 80.70Å 96.03Å 96.23Å<br>90.00° 96.80° 90.00° | Depositor |
| Resolution (Å) | 34.00 – 2.10 | Depositor |
| % Data completeness<br>(in resolution range) | (Not available) (34.00-2.10) | Depositor |
| $R_{merge}$ | (Not available) | Depositor |
| $R_{sym}$ | 0.07 | Depositor |
| Refinement program | CNS 1.0 | Depositor |
| R, $R_{free}$ | 0.214 , 0.265 | Depositor |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| Total number of atoms | 10716 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 37.0 | wwPDB-VP |

# 5 Model quality (i)

## 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PED, ZN

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 | E | 3.03 | 18/289 (6.2%) | 5.96 | 96/444 (21.6%) |
| 1 | F | 2.97 | 19/289 (6.6%) | 5.76 | 97/444 (21.8%) |
| 1 | G | 2.99 | 17/289 (5.9%) | 5.90 | 95/444 (21.4%) |
| 1 | H | 2.98 | 18/289 (6.2%) | 6.06 | 99/444 (22.3%) |
| 2 | I | 1.76 | 10/275 (3.6%) | 5.55 | 86/420 (20.5%) |
| 2 | J | 1.74 | 9/275 (3.3%) | 5.82 | 91/420 (21.7%) |
| 2 | K | 1.73 | 9/275 (3.3%) | 5.59 | 81/420 (19.3%) |
| 2 | L | 1.74 | 10/275 (3.6%) | 5.70 | 83/420 (19.8%) |
| 3 | A | 0.33 | 0/2085 | 0.79 | 1/2826 (0.0%) |
| 3 | B | 0.31 | 0/2076 | 0.80 | 3/2815 (0.1%) |
| 3 | C | 0.33 | 0/2088 | 0.78 | 0/2830 |
| 3 | D | 0.32 | 0/2086 | 0.77 | 0/2828 |
| All | All | 1.17 | 110/10591 (1.0%) | 2.89 | 732/14755 (5.0%) |

All (110) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | E | 404 | DT | C5-C7 | 18.17 | 1.60 | 1.50 |
| 1 | F | 411 | DT | C5-C7 | 17.36 | 1.60 | 1.50 |
| 1 | G | 411 | DT | C5-C7 | 17.27 | 1.60 | 1.50 |
| 1 | G | 404 | DT | C5-C7 | 17.03 | 1.60 | 1.50 |
| 1 | E | 405 | DT | C5-C7 | 16.97 | 1.60 | 1.50 |
| 1 | G | 408 | DT | C5-C7 | 16.90 | 1.60 | 1.50 |
| 1 | E | 411 | DT | C5-C7 | 16.89 | 1.60 | 1.50 |
| 1 | H | 411 | DT | C5-C7 | 16.87 | 1.60 | 1.50 |
| 1 | F | 404 | DT | C5-C7 | 16.79 | 1.60 | 1.50 |
| 1 | E | 408 | DT | C5-C7 | 16.78 | 1.60 | 1.50 |
| 1 | H | 408 | DT | C5-C7 | 16.49 | 1.59 | 1.50 |
| 1 | F | 405 | DT | C5-C7 | 16.46 | 1.59 | 1.50 |
| 1 | F | 408 | DT | C5-C7 | 16.37 | 1.59 | 1.50 |
| 1 | H | 405 | DT | C5-C7 | 16.21 | 1.59 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | H | 404 | DT | C5-C7 | 16.15 | 1.59 | 1.50 |
| 1 | G | 405 | DT | C5-C7 | 16.06 | 1.59 | 1.50 |
| 1 | G | 404 | DT | C2-N3 | 11.19 | 1.46 | 1.37 |
| 1 | E | 404 | DT | C2-N3 | 11.12 | 1.46 | 1.37 |
| 1 | E | 408 | DT | C2-N3 | 11.12 | 1.46 | 1.37 |
| 1 | H | 411 | DT | C2-N3 | 11.12 | 1.46 | 1.37 |
| 1 | F | 411 | DT | C2-N3 | 11.08 | 1.46 | 1.37 |
| 1 | H | 405 | DT | C2-N3 | 10.97 | 1.46 | 1.37 |
| 1 | G | 411 | DT | C2-N3 | 10.96 | 1.46 | 1.37 |
| 1 | F | 404 | DT | C2-N3 | 10.82 | 1.46 | 1.37 |
| 1 | F | 408 | DT | C2-N3 | 10.62 | 1.46 | 1.37 |
| 1 | F | 405 | DT | C2-N3 | 10.46 | 1.46 | 1.37 |
| 1 | G | 408 | DT | C2-N3 | 10.45 | 1.46 | 1.37 |
| 1 | E | 411 | DT | C2-N3 | 10.41 | 1.46 | 1.37 |
| 1 | H | 408 | DT | C2-N3 | 10.39 | 1.46 | 1.37 |
| 1 | E | 405 | DT | C2-N3 | 10.19 | 1.46 | 1.37 |
| 1 | H | 404 | DT | C2-N3 | 10.08 | 1.45 | 1.37 |
| 1 | G | 405 | DT | C2-N3 | 10.00 | 1.45 | 1.37 |
| 1 | F | 402 | DG | C5-C4 | 6.34 | 1.42 | 1.38 |
| 1 | H | 413 | DG | C5-C4 | 6.25 | 1.42 | 1.38 |
| 1 | H | 412 | DG | C5-C4 | 6.15 | 1.42 | 1.38 |
| 1 | E | 402 | DG | C5-C4 | 6.10 | 1.42 | 1.38 |
| 1 | E | 412 | DG | C5-C4 | 6.05 | 1.42 | 1.38 |
| 1 | E | 413 | DG | C5-C4 | 6.02 | 1.42 | 1.38 |
| 2 | I | 424 | DG | C5-C4 | 5.94 | 1.42 | 1.38 |
| 2 | L | 428 | DG | N3-C4 | 5.93 | 1.39 | 1.35 |
| 2 | I | 431 | DG | C5-C4 | 5.87 | 1.42 | 1.38 |
| 2 | K | 431 | DG | C5-C4 | 5.83 | 1.42 | 1.38 |
| 1 | H | 402 | DG | C5-C4 | 5.80 | 1.42 | 1.38 |
| 2 | L | 428 | DG | C5-C4 | 5.79 | 1.42 | 1.38 |
| 1 | G | 401 | DG | C5-C4 | 5.77 | 1.42 | 1.38 |
| 1 | G | 401 | DG | N3-C4 | 5.75 | 1.39 | 1.35 |
| 1 | F | 413 | DG | C5-C4 | 5.72 | 1.42 | 1.38 |
| 1 | H | 401 | DG | C5-C6 | 5.71 | 1.48 | 1.42 |
| 2 | I | 428 | DG | C5-C4 | 5.68 | 1.42 | 1.38 |
| 2 | J | 431 | DG | C5-C4 | 5.68 | 1.42 | 1.38 |
| 2 | J | 428 | DG | C5-C4 | 5.68 | 1.42 | 1.38 |
| 1 | G | 401 | DG | C5-C6 | 5.66 | 1.48 | 1.42 |
| 1 | E | 413 | DG | C5-C6 | 5.64 | 1.48 | 1.42 |
| 2 | L | 424 | DG | C5-C4 | 5.64 | 1.42 | 1.38 |
| 2 | J | 431 | DG | C5-C6 | 5.63 | 1.48 | 1.42 |
| 2 | K | 424 | DG | N3-C4 | 5.62 | 1.39 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | J | 424 | DG | C5-C4 | 5.61 | 1.42 | 1.38 |
| 1 | F | 412 | DG | C5-C4 | 5.60 | 1.42 | 1.38 |
| 1 | G | 413 | DG | C5-C4 | 5.57 | 1.42 | 1.38 |
| 2 | L | 424 | DG | C5-C6 | 5.54 | 1.47 | 1.42 |
| 1 | G | 402 | DG | C5-C6 | 5.50 | 1.47 | 1.42 |
| 1 | E | 401 | DG | N3-C4 | 5.49 | 1.39 | 1.35 |
| 1 | E | 412 | DG | C5-C6 | 5.49 | 1.47 | 1.42 |
| 1 | H | 413 | DG | C5-C6 | 5.48 | 1.47 | 1.42 |
| 1 | F | 413 | DG | C5-C6 | 5.48 | 1.47 | 1.42 |
| 1 | E | 401 | DG | C5-C4 | 5.47 | 1.42 | 1.38 |
| 2 | J | 425 | DG | C5-C4 | 5.47 | 1.42 | 1.38 |
| 2 | K | 425 | DG | C5-C4 | 5.46 | 1.42 | 1.38 |
| 2 | K | 431 | DG | N3-C4 | 5.45 | 1.39 | 1.35 |
| 2 | K | 424 | DG | C5-C6 | 5.42 | 1.47 | 1.42 |
| 2 | K | 425 | DG | C5-C6 | 5.41 | 1.47 | 1.42 |
| 1 | F | 401 | DG | N3-C4 | 5.41 | 1.39 | 1.35 |
| 2 | J | 428 | DG | N3-C4 | 5.39 | 1.39 | 1.35 |
| 2 | I | 424 | DG | C5-C6 | 5.38 | 1.47 | 1.42 |
| 2 | K | 428 | DG | C5-C6 | 5.37 | 1.47 | 1.42 |
| 2 | I | 425 | DG | C5-C6 | 5.36 | 1.47 | 1.42 |
| 2 | K | 424 | DG | C5-C4 | 5.36 | 1.42 | 1.38 |
| 1 | E | 401 | DG | C5-C6 | 5.33 | 1.47 | 1.42 |
| 2 | I | 431 | DG | C5-C6 | 5.33 | 1.47 | 1.42 |
| 1 | H | 401 | DG | N3-C4 | 5.33 | 1.39 | 1.35 |
| 1 | G | 413 | DG | C5-C6 | 5.29 | 1.47 | 1.42 |
| 2 | L | 424 | DG | N3-C4 | 5.27 | 1.39 | 1.35 |
| 2 | I | 428 | DG | N3-C4 | 5.26 | 1.39 | 1.35 |
| 1 | H | 412 | DG | C5-C6 | 5.26 | 1.47 | 1.42 |
| 1 | F | 412 | DG | C5-C6 | 5.25 | 1.47 | 1.42 |
| 2 | L | 425 | DG | C5-C6 | 5.25 | 1.47 | 1.42 |
| 1 | F | 401 | DG | C5-C6 | 5.24 | 1.47 | 1.42 |
| 2 | L | 431 | DG | C5-C6 | 5.24 | 1.47 | 1.42 |
| 2 | I | 431 | DG | N3-C4 | 5.24 | 1.39 | 1.35 |
| 1 | F | 412 | DG | N3-C4 | 5.24 | 1.39 | 1.35 |
| 1 | F | 401 | DG | C5-C4 | 5.22 | 1.42 | 1.38 |
| 1 | G | 402 | DG | C5-C4 | 5.21 | 1.42 | 1.38 |
| 1 | F | 402 | DG | C5-C6 | 5.20 | 1.47 | 1.42 |
| 2 | L | 425 | DG | C5-C4 | 5.20 | 1.42 | 1.38 |
| 1 | H | 413 | DG | N3-C4 | 5.19 | 1.39 | 1.35 |
| 2 | J | 424 | DG | C5-C6 | 5.18 | 1.47 | 1.42 |
| 1 | E | 402 | DG | C5-C6 | 5.18 | 1.47 | 1.42 |
| 2 | J | 424 | DG | N3-C4 | 5.14 | 1.39 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | G | 413 | DG | N3-C4 | 5.14 | 1.39 | 1.35 |
| 2 | L | 428 | DG | C5-C6 | 5.14 | 1.47 | 1.42 |
| 2 | I | 428 | DG | C5-C6 | 5.13 | 1.47 | 1.42 |
| 1 | H | 402 | DG | C5-C6 | 5.12 | 1.47 | 1.42 |
| 1 | F | 413 | DG | N3-C4 | 5.12 | 1.39 | 1.35 |
| 2 | J | 425 | DG | C5-C6 | 5.12 | 1.47 | 1.42 |
| 2 | I | 425 | DG | C5-C4 | 5.08 | 1.42 | 1.38 |
| 2 | L | 425 | DG | N3-C4 | 5.07 | 1.39 | 1.35 |
| 2 | K | 428 | DG | C5-C4 | 5.05 | 1.41 | 1.38 |
| 1 | H | 401 | DG | C5-C4 | 5.03 | 1.41 | 1.38 |
| 1 | G | 412 | DG | C5-C4 | 5.02 | 1.41 | 1.38 |
| 1 | E | 412 | DG | N3-C4 | 5.00 | 1.39 | 1.35 |

All (732) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | E | 413 | DG | N7-C8-N9 | 22.34 | 124.27 | 113.10 |
| 1 | H | 413 | DG | N7-C8-N9 | 21.92 | 124.06 | 113.10 |
| 1 | F | 412 | DG | N7-C8-N9 | 21.85 | 124.02 | 113.10 |
| 2 | L | 424 | DG | N7-C8-N9 | 21.82 | 124.01 | 113.10 |
| 2 | J | 431 | DG | N7-C8-N9 | 21.74 | 123.97 | 113.10 |
| 2 | L | 431 | DG | N7-C8-N9 | 21.72 | 123.96 | 113.10 |
| 1 | E | 412 | DG | N7-C8-N9 | 21.66 | 123.93 | 113.10 |
| 1 | H | 412 | DG | N3-C4-C5 | -21.61 | 117.79 | 128.60 |
| 2 | J | 422 | DC | C2-N3-C4 | 21.54 | 130.67 | 119.90 |
| 2 | I | 424 | DG | N7-C8-N9 | 21.50 | 123.85 | 113.10 |
| 1 | G | 413 | DG | N7-C8-N9 | 21.39 | 123.80 | 113.10 |
| 1 | H | 402 | DG | N7-C8-N9 | 21.37 | 123.78 | 113.10 |
| 2 | L | 425 | DG | N7-C8-N9 | 21.33 | 123.77 | 113.10 |
| 2 | J | 424 | DG | N7-C8-N9 | 21.26 | 123.73 | 113.10 |
| 1 | H | 412 | DG | N7-C8-N9 | 21.19 | 123.69 | 113.10 |
| 1 | F | 402 | DG | N7-C8-N9 | 21.18 | 123.69 | 113.10 |
| 1 | G | 402 | DG | N7-C8-N9 | 21.14 | 123.67 | 113.10 |
| 1 | G | 412 | DG | N7-C8-N9 | 21.11 | 123.66 | 113.10 |
| 2 | K | 424 | DG | N7-C8-N9 | 20.94 | 123.57 | 113.10 |
| 1 | E | 402 | DG | N7-C8-N9 | 20.75 | 123.48 | 113.10 |
| 2 | K | 431 | DG | N7-C8-N9 | 20.75 | 123.47 | 113.10 |
| 1 | F | 413 | DG | N7-C8-N9 | 20.70 | 123.45 | 113.10 |
| 1 | E | 413 | DG | C8-N9-C4 | -20.66 | 98.13 | 106.40 |
| 2 | J | 428 | DG | N7-C8-N9 | 20.64 | 123.42 | 113.10 |
| 2 | J | 431 | DG | C8-N9-C4 | -20.60 | 98.16 | 106.40 |
| 2 | K | 425 | DG | N3-C4-C5 | -20.59 | 118.31 | 128.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | I | 428 | DG | N7-C8-N9 | 20.55 | 123.38 | 113.10 |
| 2 | I | 425 | DG | N7-C8-N9 | 20.21 | 123.21 | 113.10 |
| 2 | L | 428 | DG | N7-C8-N9 | 20.17 | 123.19 | 113.10 |
| 1 | H | 413 | DG | N3-C4-C5 | -20.12 | 118.54 | 128.60 |
| 2 | I | 424 | DG | C8-N9-C4 | -20.08 | 98.37 | 106.40 |
| 1 | E | 412 | DG | C8-N9-C4 | -20.06 | 98.38 | 106.40 |
| 1 | H | 413 | DG | C8-N9-C4 | -20.06 | 98.38 | 106.40 |
| 2 | L | 433 | DC | C2-N3-C4 | 19.98 | 129.89 | 119.90 |
| 2 | K | 425 | DG | N7-C8-N9 | 19.96 | 123.08 | 113.10 |
| 1 | G | 401 | DG | N7-C8-N9 | 19.88 | 123.04 | 113.10 |
| 1 | E | 412 | DG | N3-C4-C5 | -19.86 | 118.67 | 128.60 |
| 2 | K | 428 | DG | N7-C8-N9 | 19.77 | 122.98 | 113.10 |
| 1 | H | 401 | DG | N7-C8-N9 | 19.72 | 122.96 | 113.10 |
| 1 | F | 413 | DG | C8-N9-C4 | -19.71 | 98.52 | 106.40 |
| 1 | G | 412 | DG | N3-C4-C5 | -19.70 | 118.75 | 128.60 |
| 1 | G | 413 | DG | N3-C4-C5 | -19.67 | 118.76 | 128.60 |
| 2 | L | 424 | DG | C8-N9-C4 | -19.66 | 98.53 | 106.40 |
| 1 | F | 412 | DG | C8-N9-C4 | -19.60 | 98.56 | 106.40 |
| 2 | J | 421 | DC | C2-N3-C4 | 19.54 | 129.67 | 119.90 |
| 1 | E | 402 | DG | N3-C4-C5 | -19.37 | 118.91 | 128.60 |
| 2 | J | 431 | DG | N3-C4-C5 | -19.28 | 118.96 | 128.60 |
| 1 | G | 402 | DG | C8-N9-C4 | -19.26 | 98.69 | 106.40 |
| 1 | H | 401 | DG | N3-C4-C5 | -19.26 | 118.97 | 128.60 |
| 2 | K | 424 | DG | C8-N9-C4 | -19.25 | 98.70 | 106.40 |
| 2 | J | 428 | DG | N3-C4-C5 | -19.25 | 118.98 | 128.60 |
| 1 | H | 410 | DC | C2-N3-C4 | 19.24 | 129.52 | 119.90 |
| 1 | H | 402 | DG | C8-N9-C4 | -19.22 | 98.71 | 106.40 |
| 2 | I | 425 | DG | N3-C4-C5 | -19.21 | 118.99 | 128.60 |
| 1 | G | 413 | DG | C8-N9-C4 | -19.19 | 98.72 | 106.40 |
| 1 | G | 402 | DG | N3-C4-C5 | -19.17 | 119.01 | 128.60 |
| 2 | K | 431 | DG | N3-C4-C5 | -19.16 | 119.02 | 128.60 |
| 2 | J | 425 | DG | N7-C8-N9 | 19.07 | 122.63 | 113.10 |
| 2 | J | 424 | DG | N3-C4-C5 | -18.99 | 119.10 | 128.60 |
| 1 | G | 412 | DG | C8-N9-C4 | -18.98 | 98.81 | 106.40 |
| 1 | F | 401 | DG | N7-C8-N9 | 18.93 | 122.57 | 113.10 |
| 1 | H | 402 | DG | N3-C4-C5 | -18.86 | 119.17 | 128.60 |
| 1 | E | 401 | DG | N7-C8-N9 | 18.86 | 122.53 | 113.10 |
| 1 | H | 412 | DG | C8-N9-C4 | -18.85 | 98.86 | 106.40 |
| 1 | F | 402 | DG | C8-N9-C4 | -18.85 | 98.86 | 106.40 |
| 1 | E | 401 | DG | N3-C4-C5 | -18.72 | 119.24 | 128.60 |
| 2 | J | 424 | DG | C8-N9-C4 | -18.67 | 98.93 | 106.40 |
| 2 | I | 424 | DG | N3-C4-C5 | -18.60 | 119.30 | 128.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | L | 428 | DG | C8-N9-C4 | -18.60 | 98.96 | 106.40 |
| 2 | I | 425 | DG | C8-N9-C4 | -18.57 | 98.97 | 106.40 |
| 2 | L | 431 | DG | C8-N9-C4 | -18.55 | 98.98 | 106.40 |
| 2 | L | 431 | DG | N3-C4-C5 | -18.52 | 119.34 | 128.60 |
| 1 | F | 406 | DC | C2-N3-C4 | 18.48 | 129.14 | 119.90 |
| 2 | L | 425 | DG | C8-N9-C4 | -18.43 | 99.03 | 106.40 |
| 2 | K | 431 | DG | C8-N9-C4 | -18.36 | 99.06 | 106.40 |
| 1 | E | 413 | DG | N3-C4-C5 | -18.36 | 119.42 | 128.60 |
| 1 | G | 413 | DG | C2-N3-C4 | 18.36 | 121.08 | 111.90 |
| 1 | F | 402 | DG | N3-C4-C5 | -18.30 | 119.45 | 128.60 |
| 2 | I | 422 | DC | C2-N3-C4 | 18.27 | 129.04 | 119.90 |
| 2 | K | 425 | DG | C8-N9-C4 | -18.23 | 99.11 | 106.40 |
| 2 | J | 422 | DC | N3-C4-C5 | -18.21 | 114.62 | 121.90 |
| 2 | J | 428 | DG | C8-N9-C4 | -18.16 | 99.14 | 106.40 |
| 1 | H | 403 | DC | N3-C4-C5 | -18.05 | 114.68 | 121.90 |
| 1 | G | 401 | DG | N3-C4-C5 | -18.05 | 119.58 | 128.60 |
| 1 | E | 402 | DG | C8-N9-C4 | -17.95 | 99.22 | 106.40 |
| 2 | I | 428 | DG | N3-C4-C5 | -17.95 | 119.63 | 128.60 |
| 1 | G | 401 | DG | C8-N9-C4 | -17.89 | 99.24 | 106.40 |
| 1 | H | 401 | DG | C2-N3-C4 | 17.88 | 120.84 | 111.90 |
| 2 | K | 425 | DG | C2-N3-C4 | 17.87 | 120.84 | 111.90 |
| 1 | H | 401 | DG | C8-N9-C4 | -17.84 | 99.26 | 106.40 |
| 2 | L | 432 | DC | C2-N3-C4 | 17.81 | 128.81 | 119.90 |
| 2 | I | 425 | DG | C2-N3-C4 | 17.80 | 120.80 | 111.90 |
| 2 | K | 428 | DG | N3-C4-C5 | -17.78 | 119.71 | 128.60 |
| 2 | L | 433 | DC | N3-C4-C5 | -17.74 | 114.81 | 121.90 |
| 1 | F | 413 | DG | N3-C4-C5 | -17.73 | 119.74 | 128.60 |
| 2 | K | 424 | DG | N3-C4-C5 | -17.71 | 119.75 | 128.60 |
| 2 | I | 428 | DG | C8-N9-C4 | -17.67 | 99.33 | 106.40 |
| 2 | L | 428 | DG | N3-C4-C5 | -17.67 | 119.77 | 128.60 |
| 1 | F | 401 | DG | N3-C4-C5 | -17.65 | 119.78 | 128.60 |
| 2 | L | 424 | DG | N3-C4-C5 | -17.52 | 119.84 | 128.60 |
| 1 | H | 412 | DG | C2-N3-C4 | 17.44 | 120.62 | 111.90 |
| 1 | H | 409 | DC | N3-C4-C5 | -17.42 | 114.93 | 121.90 |
| 2 | I | 431 | DG | N7-C8-N9 | 17.36 | 121.78 | 113.10 |
| 2 | I | 422 | DC | N3-C4-C5 | -17.30 | 114.98 | 121.90 |
| 2 | J | 425 | DG | C8-N9-C4 | -17.26 | 99.50 | 106.40 |
| 1 | H | 410 | DC | N3-C4-C5 | -17.14 | 115.05 | 121.90 |
| 1 | H | 409 | DC | C2-N3-C4 | 17.07 | 128.43 | 119.90 |
| 2 | I | 421 | DC | C2-N3-C4 | 16.99 | 128.40 | 119.90 |
| 1 | E | 402 | DG | C2-N3-C4 | 16.96 | 120.38 | 111.90 |
| 1 | G | 412 | DG | C2-N3-C4 | 16.95 | 120.38 | 111.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | E | 401 | DG | C2-N3-C4 | 16.92 | 120.36 | 111.90 |
| 2 | J | 425 | DG | N3-C4-C5 | -16.86 | 120.17 | 128.60 |
| 2 | J | 421 | DC | N3-C4-C5 | -16.82 | 115.17 | 121.90 |
| 1 | F | 401 | DG | C8-N9-C4 | -16.81 | 99.68 | 106.40 |
| 1 | E | 406 | DC | C2-N3-C4 | 16.76 | 128.28 | 119.90 |
| 2 | K | 428 | DG | C8-N9-C4 | -16.72 | 99.71 | 106.40 |
| 2 | L | 431 | DG | C2-N3-C4 | 16.71 | 120.26 | 111.90 |
| 2 | I | 431 | DG | N3-C4-C5 | -16.71 | 120.25 | 128.60 |
| 2 | J | 431 | DG | C2-N3-C4 | 16.66 | 120.23 | 111.90 |
| 2 | K | 428 | DG | C2-N3-C4 | 16.63 | 120.21 | 111.90 |
| 1 | E | 412 | DG | C2-N3-C4 | 16.58 | 120.19 | 111.90 |
| 2 | I | 432 | DC | C2-N3-C4 | 16.40 | 128.10 | 119.90 |
| 2 | J | 428 | DG | C2-N3-C4 | 16.39 | 120.10 | 111.90 |
| 1 | G | 402 | DG | C2-N3-C4 | 16.38 | 120.09 | 111.90 |
| 1 | F | 406 | DC | N3-C4-C5 | -16.33 | 115.37 | 121.90 |
| 2 | I | 431 | DG | C8-N9-C4 | -16.29 | 99.88 | 106.40 |
| 1 | E | 403 | DC | N3-C4-C5 | -16.28 | 115.39 | 121.90 |
| 2 | L | 421 | DC | C2-N3-C4 | 16.18 | 127.99 | 119.90 |
| 2 | L | 425 | DG | N3-C4-C5 | -16.11 | 120.54 | 128.60 |
| 1 | H | 413 | DG | C2-N3-C4 | 16.09 | 119.95 | 111.90 |
| 1 | F | 409 | DC | C2-N3-C4 | 16.03 | 127.91 | 119.90 |
| 1 | E | 407 | DC | C2-N3-C4 | 16.00 | 127.90 | 119.90 |
| 2 | J | 432 | DC | C2-N3-C4 | 15.99 | 127.90 | 119.90 |
| 2 | L | 424 | DG | C2-N3-C4 | 15.98 | 119.89 | 111.90 |
| 1 | G | 407 | DC | C2-N3-C4 | 15.91 | 127.85 | 119.90 |
| 2 | J | 425 | DG | C2-N3-C4 | 15.89 | 119.85 | 111.90 |
| 2 | J | 424 | DG | C2-N3-C4 | 15.85 | 119.82 | 111.90 |
| 1 | G | 410 | DC | C2-N3-C4 | 15.84 | 127.82 | 119.90 |
| 1 | H | 402 | DG | C2-N3-C4 | 15.81 | 119.80 | 111.90 |
| 2 | I | 421 | DC | N3-C4-C5 | -15.75 | 115.60 | 121.90 |
| 1 | H | 403 | DC | C2-N3-C4 | 15.66 | 127.73 | 119.90 |
| 2 | K | 422 | DC | C2-N3-C4 | 15.64 | 127.72 | 119.90 |
| 1 | F | 410 | DC | N3-C4-C5 | -15.61 | 115.66 | 121.90 |
| 2 | I | 433 | DC | C2-N3-C4 | 15.56 | 127.68 | 119.90 |
| 2 | L | 421 | DC | N3-C4-C5 | -15.56 | 115.68 | 121.90 |
| 1 | F | 413 | DG | C2-N3-C4 | 15.55 | 119.67 | 111.90 |
| 1 | E | 410 | DC | C2-N3-C4 | 15.52 | 127.66 | 119.90 |
| 1 | E | 406 | DC | N3-C4-C5 | -15.51 | 115.70 | 121.90 |
| 2 | I | 428 | DG | C2-N3-C4 | 15.50 | 119.65 | 111.90 |
| 2 | I | 424 | DG | C2-N3-C4 | 15.49 | 119.64 | 111.90 |
| 2 | J | 432 | DC | N3-C4-C5 | -15.38 | 115.75 | 121.90 |
| 1 | E | 403 | DC | C2-N3-C4 | 15.37 | 127.59 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | L | 422 | DC | N3-C4-C5 | -15.37 | 115.75 | 121.90 |
| 1 | F | 407 | DC | C2-N3-C4 | 15.31 | 127.55 | 119.90 |
| 2 | L | 432 | DC | N3-C4-C5 | -15.30 | 115.78 | 121.90 |
| 1 | F | 402 | DG | C2-N3-C4 | 15.23 | 119.52 | 111.90 |
| 1 | E | 413 | DG | C2-N3-C4 | 15.22 | 119.51 | 111.90 |
| 1 | G | 403 | DC | C2-N3-C4 | 15.10 | 127.45 | 119.90 |
| 1 | F | 407 | DC | N3-C4-C5 | -15.09 | 115.86 | 121.90 |
| 1 | F | 410 | DC | C2-N3-C4 | 15.08 | 127.44 | 119.90 |
| 1 | E | 401 | DG | C8-N9-C4 | -15.04 | 100.38 | 106.40 |
| 1 | G | 409 | DC | C2-N3-C4 | 15.00 | 127.40 | 119.90 |
| 1 | E | 410 | DC | N3-C4-C5 | -14.98 | 115.91 | 121.90 |
| 2 | I | 432 | DC | N3-C4-C5 | -14.93 | 115.93 | 121.90 |
| 2 | L | 431 | DG | C5-N7-C8 | -14.93 | 96.84 | 104.30 |
| 1 | H | 406 | DC | C2-N3-C4 | 14.90 | 127.35 | 119.90 |
| 2 | K | 431 | DG | C2-N3-C4 | 14.88 | 119.34 | 111.90 |
| 1 | H | 407 | DC | C2-N3-C4 | 14.88 | 127.34 | 119.90 |
| 1 | F | 412 | DG | N3-C4-C5 | -14.84 | 121.18 | 128.60 |
| 1 | G | 410 | DC | N3-C4-C5 | -14.82 | 115.97 | 121.90 |
| 2 | L | 425 | DG | C2-N3-C4 | 14.78 | 119.29 | 111.90 |
| 2 | K | 421 | DC | C2-N3-C4 | 14.75 | 127.27 | 119.90 |
| 2 | I | 431 | DG | C2-N3-C4 | 14.70 | 119.25 | 111.90 |
| 2 | K | 432 | DC | C2-N3-C4 | 14.68 | 127.24 | 119.90 |
| 1 | G | 409 | DC | N3-C4-C5 | -14.64 | 116.04 | 121.90 |
| 1 | H | 406 | DC | N3-C4-C5 | -14.64 | 116.04 | 121.90 |
| 1 | E | 409 | DC | C2-N3-C4 | 14.64 | 127.22 | 119.90 |
| 2 | K | 426 | DA | O4'-C1'-N9 | 14.63 | 118.24 | 108.00 |
| 1 | G | 403 | DC | N3-C4-C5 | -14.63 | 116.05 | 121.90 |
| 1 | F | 401 | DG | C2-N3-C4 | 14.61 | 119.21 | 111.90 |
| 1 | E | 404 | DT | N3-C2-O2 | -14.57 | 113.56 | 122.30 |
| 2 | K | 424 | DG | C2-N3-C4 | 14.56 | 119.18 | 111.90 |
| 2 | L | 425 | DG | C5-N7-C8 | -14.56 | 97.02 | 104.30 |
| 2 | L | 428 | DG | C2-N3-C4 | 14.56 | 119.18 | 111.90 |
| 1 | F | 403 | DC | C2-N3-C4 | 14.51 | 127.15 | 119.90 |
| 2 | K | 422 | DC | N3-C4-C5 | -14.47 | 116.11 | 121.90 |
| 2 | L | 422 | DC | C2-N3-C4 | 14.43 | 127.11 | 119.90 |
| 2 | K | 433 | DC | C2-N3-C4 | 14.42 | 127.11 | 119.90 |
| 2 | K | 421 | DC | N3-C4-C5 | -14.37 | 116.15 | 121.90 |
| 1 | H | 402 | DG | C5-N7-C8 | -14.34 | 97.13 | 104.30 |
| 1 | E | 407 | DC | N3-C4-C5 | -14.14 | 116.24 | 121.90 |
| 2 | J | 424 | DG | C5-N7-C8 | -14.09 | 97.26 | 104.30 |
| 2 | L | 424 | DG | C5-N7-C8 | -14.07 | 97.27 | 104.30 |
| 1 | H | 412 | DG | C5-N7-C8 | -13.99 | 97.30 | 104.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | F | 403 | DC | N3-C4-C5 | -13.99 | 116.30 | 121.90 |
| 1 | F | 409 | DC | N3-C4-C5 | -13.99 | 116.31 | 121.90 |
| 2 | K | 431 | DG | C5-N7-C8 | -13.98 | 97.31 | 104.30 |
| 2 | J | 433 | DC | C2-N3-C4 | 13.98 | 126.89 | 119.90 |
| 2 | K | 432 | DC | N3-C4-C5 | -13.95 | 116.32 | 121.90 |
| 1 | H | 412 | DG | N3-C4-N9 | 13.94 | 134.36 | 126.00 |
| 1 | G | 401 | DG | C2-N3-C4 | 13.92 | 118.86 | 111.90 |
| 2 | I | 428 | DG | C5-N7-C8 | -13.88 | 97.36 | 104.30 |
| 1 | H | 413 | DG | C5-N7-C8 | -13.86 | 97.37 | 104.30 |
| 2 | L | 431 | DG | C5-C6-O6 | -13.85 | 120.29 | 128.60 |
| 1 | E | 411 | DT | O4'-C1'-N1 | 13.85 | 117.69 | 108.00 |
| 1 | F | 411 | DT | C2-N3-C4 | -13.82 | 118.91 | 127.20 |
| 1 | G | 412 | DG | C5-N7-C8 | -13.81 | 97.39 | 104.30 |
| 2 | I | 433 | DC | N3-C4-C5 | -13.80 | 116.38 | 121.90 |
| 1 | F | 412 | DG | C5-N7-C8 | -13.79 | 97.41 | 104.30 |
| 1 | G | 411 | DT | C2-N3-C4 | -13.72 | 118.97 | 127.20 |
| 1 | G | 402 | DG | C5-N7-C8 | -13.70 | 97.45 | 104.30 |
| 1 | G | 413 | DG | C5-N7-C8 | -13.68 | 97.46 | 104.30 |
| 1 | E | 401 | DG | N3-C4-N9 | 13.57 | 134.14 | 126.00 |
| 1 | E | 413 | DG | C5-N7-C8 | -13.57 | 97.51 | 104.30 |
| 1 | E | 401 | DG | C5-N7-C8 | -13.56 | 97.52 | 104.30 |
| 1 | F | 402 | DG | C5-N7-C8 | -13.51 | 97.55 | 104.30 |
| 1 | E | 409 | DC | N3-C4-C5 | -13.49 | 116.50 | 121.90 |
| 1 | E | 402 | DG | C5-N7-C8 | -13.49 | 97.56 | 104.30 |
| 1 | E | 408 | DT | N3-C2-O2 | -13.46 | 114.22 | 122.30 |
| 1 | E | 412 | DG | C5-N7-C8 | -13.45 | 97.58 | 104.30 |
| 2 | K | 428 | DG | C5-N7-C8 | -13.41 | 97.59 | 104.30 |
| 2 | J | 429 | DA | O4'-C1'-N9 | 13.39 | 117.38 | 108.00 |
| 1 | F | 412 | DG | C2-N3-C4 | 13.37 | 118.58 | 111.90 |
| 2 | J | 428 | DG | C5-N7-C8 | -13.34 | 97.63 | 104.30 |
| 2 | K | 424 | DG | C5-N7-C8 | -13.33 | 97.63 | 104.30 |
| 1 | G | 413 | DG | C5-C6-N1 | 13.30 | 118.15 | 111.50 |
| 2 | L | 428 | DG | C5-N7-C8 | -13.26 | 97.67 | 104.30 |
| 2 | J | 431 | DG | C5-N7-C8 | -13.24 | 97.68 | 104.30 |
| 2 | K | 425 | DG | N3-C4-N9 | 13.23 | 133.94 | 126.00 |
| 1 | G | 406 | DC | C2-N3-C4 | 13.20 | 126.50 | 119.90 |
| 1 | G | 407 | DC | N3-C4-C5 | -13.15 | 116.64 | 121.90 |
| 2 | I | 424 | DG | C5-N7-C8 | -13.07 | 97.77 | 104.30 |
| 1 | H | 412 | DG | C6-N1-C2 | -13.04 | 117.28 | 125.10 |
| 1 | F | 401 | DG | C5-N7-C8 | -13.03 | 97.78 | 104.30 |
| 2 | J | 433 | DC | N3-C4-C5 | -13.03 | 116.69 | 121.90 |
| 2 | I | 425 | DG | C5-N7-C8 | -12.99 | 97.80 | 104.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | G | 401 | DG | C5-N7-C8 | -12.96 | 97.82 | 104.30 |
| 1 | F | 413 | DG | C5-N7-C8 | -12.95 | 97.83 | 104.30 |
| 2 | J | 424 | DG | C6-N1-C2 | -12.88 | 117.37 | 125.10 |
| 2 | J | 425 | DG | C5-N7-C8 | -12.87 | 97.86 | 104.30 |
| 1 | H | 408 | DT | C2-N3-C4 | -12.86 | 119.48 | 127.20 |
| 2 | K | 425 | DG | C5-N7-C8 | -12.84 | 97.88 | 104.30 |
| 1 | H | 401 | DG | C5-N7-C8 | -12.78 | 97.91 | 104.30 |
| 1 | E | 413 | DG | C6-N1-C2 | -12.74 | 117.45 | 125.10 |
| 1 | G | 413 | DG | C6-N1-C2 | -12.72 | 117.47 | 125.10 |
| 2 | L | 425 | DG | O4'-C1'-N9 | 12.72 | 116.90 | 108.00 |
| 2 | K | 431 | DG | N3-C4-N9 | 12.72 | 133.63 | 126.00 |
| 1 | H | 405 | DT | C2-N3-C4 | -12.69 | 119.59 | 127.20 |
| 1 | G | 412 | DG | C6-N1-C2 | -12.66 | 117.50 | 125.10 |
| 1 | G | 405 | DT | O4'-C1'-N1 | 12.66 | 116.86 | 108.00 |
| 2 | K | 431 | DG | C6-N1-C2 | -12.63 | 117.52 | 125.10 |
| 2 | J | 424 | DG | C5-C6-O6 | -12.62 | 121.03 | 128.60 |
| 1 | H | 401 | DG | N3-C4-N9 | 12.52 | 133.51 | 126.00 |
| 1 | E | 402 | DG | N3-C4-N9 | 12.52 | 133.51 | 126.00 |
| 1 | E | 401 | DG | C5-C6-O6 | -12.51 | 121.09 | 128.60 |
| 2 | J | 428 | DG | N3-C4-N9 | 12.47 | 133.48 | 126.00 |
| 1 | E | 404 | DT | C2-N3-C4 | -12.46 | 119.72 | 127.20 |
| 2 | K | 433 | DC | N3-C4-C5 | -12.44 | 116.92 | 121.90 |
| 1 | G | 413 | DG | N3-C4-N9 | 12.41 | 133.44 | 126.00 |
| 1 | F | 401 | DG | C5-C6-O6 | -12.39 | 121.17 | 128.60 |
| 1 | H | 401 | DG | C5-C6-N1 | 12.38 | 117.69 | 111.50 |
| 1 | H | 413 | DG | C6-N1-C2 | -12.37 | 117.68 | 125.10 |
| 1 | G | 412 | DG | N3-C4-N9 | 12.36 | 133.42 | 126.00 |
| 1 | H | 413 | DG | N3-C4-N9 | 12.36 | 133.42 | 126.00 |
| 1 | G | 406 | DC | N3-C4-C5 | -12.36 | 116.96 | 121.90 |
| 1 | F | 405 | DT | C2-N3-C4 | -12.34 | 119.80 | 127.20 |
| 2 | J | 424 | DG | C5-C6-N1 | 12.27 | 117.64 | 111.50 |
| 2 | L | 431 | DG | N3-C4-N9 | 12.24 | 133.34 | 126.00 |
| 1 | G | 404 | DT | C2-N3-C4 | -12.16 | 119.90 | 127.20 |
| 2 | J | 424 | DG | N3-C4-N9 | 12.03 | 133.22 | 126.00 |
| 1 | H | 407 | DC | N3-C4-C5 | -11.98 | 117.11 | 121.90 |
| 2 | K | 431 | DG | C5-C6-O6 | -11.97 | 121.42 | 128.60 |
| 1 | E | 412 | DG | O4'-C1'-N9 | 11.96 | 116.37 | 108.00 |
| 1 | E | 412 | DG | N3-C4-N9 | 11.94 | 133.16 | 126.00 |
| 2 | J | 428 | DG | C6-N1-C2 | -11.94 | 117.94 | 125.10 |
| 2 | L | 431 | DG | C5-C6-N1 | 11.94 | 117.47 | 111.50 |
| 2 | J | 428 | DG | C5-C6-N1 | 11.94 | 117.47 | 111.50 |
| 1 | E | 402 | DG | C6-N1-C2 | -11.93 | 117.94 | 125.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | I | 425 | DG | C6-N1-C2 | -11.89 | 117.97 | 125.10 |
| 2 | L | 431 | DG | C6-N1-C2 | -11.88 | 117.97 | 125.10 |
| 1 | G | 412 | DG | C5-C6-N1 | 11.86 | 117.43 | 111.50 |
| 2 | K | 425 | DG | C6-N1-C2 | -11.85 | 117.99 | 125.10 |
| 2 | K | 425 | DG | C5-C6-O6 | -11.83 | 121.50 | 128.60 |
| 1 | E | 402 | DG | C5-C6-N1 | 11.79 | 117.40 | 111.50 |
| 1 | G | 413 | DG | C5-C6-O6 | -11.78 | 121.53 | 128.60 |
| 2 | I | 425 | DG | N3-C4-N9 | 11.74 | 133.04 | 126.00 |
| 2 | I | 428 | DG | N3-C4-N9 | 11.73 | 133.04 | 126.00 |
| 1 | G | 402 | DG | N3-C4-N9 | 11.72 | 133.03 | 126.00 |
| 2 | I | 425 | DG | C5-C6-N1 | 11.70 | 117.35 | 111.50 |
| 1 | F | 411 | DT | O4'-C1'-N1 | 11.69 | 116.19 | 108.00 |
| 2 | I | 424 | DG | C6-N1-C2 | -11.69 | 118.09 | 125.10 |
| 1 | E | 404 | DT | C6-C5-C7 | -11.68 | 115.89 | 122.90 |
| 2 | I | 428 | DG | C5-C6-N1 | 11.68 | 117.34 | 111.50 |
| 1 | H | 402 | DG | C6-N1-C2 | -11.64 | 118.12 | 125.10 |
| 2 | I | 428 | DG | C6-N1-C2 | -11.61 | 118.13 | 125.10 |
| 1 | E | 413 | DG | C5-C6-N1 | 11.61 | 117.30 | 111.50 |
| 2 | K | 431 | DG | O4'-C1'-N9 | 11.52 | 116.06 | 108.00 |
| 1 | G | 402 | DG | C5-C6-O6 | -11.51 | 121.70 | 128.60 |
| 2 | J | 425 | DG | C5-C6-N1 | 11.50 | 117.25 | 111.50 |
| 2 | K | 431 | DG | C5-C6-N1 | 11.48 | 117.24 | 111.50 |
| 1 | E | 405 | DT | C2-N3-C4 | -11.47 | 120.32 | 127.20 |
| 1 | F | 401 | DG | C5-C6-N1 | 11.46 | 117.23 | 111.50 |
| 1 | E | 411 | DT | N3-C2-O2 | -11.45 | 115.43 | 122.30 |
| 2 | J | 431 | DG | C6-N1-C2 | -11.45 | 118.23 | 125.10 |
| 1 | G | 401 | DG | C6-N1-C2 | -11.41 | 118.25 | 125.10 |
| 2 | L | 425 | DG | C5-C6-O6 | -11.37 | 121.78 | 128.60 |
| 1 | G | 401 | DG | C5-C6-O6 | -11.35 | 121.79 | 128.60 |
| 1 | F | 402 | DG | N3-C4-N9 | 11.34 | 132.80 | 126.00 |
| 1 | G | 401 | DG | N3-C4-N9 | 11.33 | 132.80 | 126.00 |
| 1 | H | 402 | DG | N3-C4-N9 | 11.30 | 132.78 | 126.00 |
| 1 | H | 412 | DG | C5-C6-N1 | 11.27 | 117.14 | 111.50 |
| 2 | K | 428 | DG | N3-C4-N9 | 11.27 | 132.76 | 126.00 |
| 1 | E | 401 | DG | C5-C6-N1 | 11.26 | 117.13 | 111.50 |
| 1 | E | 412 | DG | C6-N1-C2 | -11.25 | 118.35 | 125.10 |
| 2 | L | 428 | DG | C6-N1-C2 | -11.22 | 118.37 | 125.10 |
| 1 | H | 412 | DG | C5-C6-O6 | -11.17 | 121.90 | 128.60 |
| 2 | K | 428 | DG | C6-N1-C2 | -11.15 | 118.41 | 125.10 |
| 1 | H | 401 | DG | O4'-C1'-N9 | 11.14 | 115.80 | 108.00 |
| 1 | F | 405 | DT | C6-C5-C7 | -11.13 | 116.22 | 122.90 |
| 1 | G | 402 | DG | C6-N1-C2 | -11.09 | 118.44 | 125.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | H | 408 | DT | C6-C5-C7 | -11.08 | 116.25 | 122.90 |
| 1 | G | 408 | DT | O4'-C1'-N1 | 11.03 | 115.72 | 108.00 |
| 2 | I | 425 | DG | C5-C6-O6 | -11.02 | 121.99 | 128.60 |
| 1 | H | 401 | DG | C6-N1-C2 | -11.02 | 118.49 | 125.10 |
| 2 | K | 428 | DG | C5-C6-N1 | 11.01 | 117.00 | 111.50 |
| 1 | F | 405 | DT | N3-C2-O2 | -10.95 | 115.73 | 122.30 |
| 2 | K | 425 | DG | C5-C6-N1 | 10.95 | 116.97 | 111.50 |
| 1 | F | 401 | DG | N3-C4-N9 | 10.94 | 132.56 | 126.00 |
| 1 | F | 413 | DG | C5-C6-N1 | 10.93 | 116.97 | 111.50 |
| 1 | H | 413 | DG | C5-C6-N1 | 10.90 | 116.95 | 111.50 |
| 1 | F | 413 | DG | C6-N1-C2 | -10.89 | 118.57 | 125.10 |
| 2 | I | 424 | DG | C5-C6-N1 | 10.82 | 116.91 | 111.50 |
| 1 | G | 411 | DT | O4'-C1'-N1 | 10.82 | 115.57 | 108.00 |
| 1 | H | 404 | DT | C2-N3-C4 | -10.80 | 120.72 | 127.20 |
| 2 | I | 431 | DG | C5-C6-N1 | 10.79 | 116.90 | 111.50 |
| 1 | G | 412 | DG | C5-C6-O6 | -10.78 | 122.13 | 128.60 |
| 2 | J | 425 | DG | N3-C4-N9 | 10.76 | 132.46 | 126.00 |
| 2 | L | 428 | DG | N3-C4-N9 | 10.73 | 132.44 | 126.00 |
| 2 | L | 428 | DG | C5-C6-N1 | 10.73 | 116.87 | 111.50 |
| 1 | G | 404 | DT | C6-C5-C7 | -10.72 | 116.47 | 122.90 |
| 1 | F | 404 | DT | C6-C5-C7 | -10.68 | 116.49 | 122.90 |
| 1 | H | 402 | DG | C5-C6-N1 | 10.68 | 116.84 | 111.50 |
| 1 | E | 405 | DT | C6-C5-C7 | -10.67 | 116.50 | 122.90 |
| 2 | I | 431 | DG | C5-N7-C8 | -10.66 | 98.97 | 104.30 |
| 2 | J | 431 | DG | N3-C4-N9 | 10.65 | 132.39 | 126.00 |
| 1 | F | 404 | DT | C2-N3-C4 | -10.62 | 120.83 | 127.20 |
| 1 | F | 402 | DG | C6-N1-C2 | -10.62 | 118.73 | 125.10 |
| 1 | F | 401 | DG | C6-N1-C2 | -10.61 | 118.73 | 125.10 |
| 2 | J | 431 | DG | C5-C6-N1 | 10.61 | 116.81 | 111.50 |
| 1 | E | 413 | DG | C5-C6-O6 | -10.56 | 122.26 | 128.60 |
| 2 | I | 431 | DG | C6-N1-C2 | -10.56 | 118.76 | 125.10 |
| 1 | F | 411 | DT | C6-C5-C7 | -10.54 | 116.58 | 122.90 |
| 2 | J | 425 | DG | C6-N1-C2 | -10.50 | 118.80 | 125.10 |
| 1 | E | 401 | DG | C6-N1-C2 | -10.50 | 118.80 | 125.10 |
| 2 | L | 424 | DG | N3-C4-N9 | 10.50 | 132.30 | 126.00 |
| 2 | K | 428 | DG | C5-C6-O6 | -10.46 | 122.32 | 128.60 |
| 2 | I | 428 | DG | C5-C6-O6 | -10.45 | 122.33 | 128.60 |
| 2 | K | 424 | DG | C6-N1-C2 | -10.45 | 118.83 | 125.10 |
| 1 | G | 402 | DG | C5-C6-N1 | 10.43 | 116.71 | 111.50 |
| 1 | F | 404 | DT | N3-C2-O2 | -10.41 | 116.06 | 122.30 |
| 1 | G | 408 | DT | C2-N3-C4 | -10.40 | 120.96 | 127.20 |
| 2 | I | 424 | DG | N3-C4-N9 | 10.38 | 132.23 | 126.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | E | 413 | DG | N3-C4-N9 | 10.34 | 132.20 | 126.00 |
| 1 | G | 401 | DG | C5-C6-N1 | 10.30 | 116.65 | 111.50 |
| 1 | H | 401 | DG | C5-C6-O6 | -10.30 | 122.42 | 128.60 |
| 2 | L | 424 | DG | C5-C6-N1 | 10.29 | 116.64 | 111.50 |
| 1 | G | 408 | DT | N3-C2-O2 | -10.27 | 116.14 | 122.30 |
| 1 | E | 411 | DT | C6-C5-C7 | -10.22 | 116.77 | 122.90 |
| 2 | K | 424 | DG | N3-C4-N9 | 10.20 | 132.12 | 126.00 |
| 1 | F | 411 | DT | N3-C2-O2 | -10.20 | 116.18 | 122.30 |
| 1 | F | 402 | DG | C5-C6-N1 | 10.17 | 116.58 | 111.50 |
| 1 | G | 411 | DT | C6-C5-C7 | -10.17 | 116.80 | 122.90 |
| 1 | F | 413 | DG | N3-C4-N9 | 10.16 | 132.10 | 126.00 |
| 2 | J | 425 | DG | C5-C6-O6 | -10.15 | 122.51 | 128.60 |
| 1 | H | 411 | DT | C2-N3-C4 | -10.14 | 121.11 | 127.20 |
| 2 | L | 425 | DG | N3-C4-N9 | 10.10 | 132.06 | 126.00 |
| 1 | F | 402 | DG | C5-C6-O6 | -10.06 | 122.56 | 128.60 |
| 1 | G | 405 | DT | C2-N3-C4 | -10.04 | 121.17 | 127.20 |
| 1 | H | 411 | DT | C6-C5-C7 | -10.03 | 116.88 | 122.90 |
| 1 | E | 412 | DG | C5-C6-N1 | 10.02 | 116.51 | 111.50 |
| 2 | L | 424 | DG | C6-N1-C2 | -10.02 | 119.09 | 125.10 |
| 1 | F | 411 | DT | N1-C2-N3 | 10.01 | 120.61 | 114.60 |
| 1 | H | 404 | DT | C6-C5-C7 | -9.99 | 116.91 | 122.90 |
| 1 | F | 408 | DT | C2-N3-C4 | -9.97 | 121.22 | 127.20 |
| 1 | F | 408 | DT | N3-C2-O2 | -9.97 | 116.32 | 122.30 |
| 1 | E | 411 | DT | C2-N3-C4 | -9.86 | 121.28 | 127.20 |
| 1 | G | 405 | DT | C6-C5-C7 | -9.78 | 117.03 | 122.90 |
| 1 | G | 411 | DT | N3-C2-O2 | -9.78 | 116.43 | 122.30 |
| 2 | K | 424 | DG | C5-C6-N1 | 9.74 | 116.37 | 111.50 |
| 1 | H | 405 | DT | C6-C5-C7 | -9.72 | 117.07 | 122.90 |
| 1 | H | 405 | DT | O4'-C1'-N1 | 9.69 | 114.78 | 108.00 |
| 2 | I | 431 | DG | N3-C4-N9 | 9.68 | 131.81 | 126.00 |
| 2 | K | 432 | DC | O4'-C1'-N1 | 9.66 | 114.77 | 108.00 |
| 1 | F | 411 | DT | C4-C5-C6 | 9.65 | 123.79 | 118.00 |
| 1 | E | 405 | DT | C4-C5-C6 | 9.62 | 123.77 | 118.00 |
| 1 | H | 413 | DG | C5-C6-O6 | -9.59 | 122.85 | 128.60 |
| 2 | J | 428 | DG | C5-C6-O6 | -9.58 | 122.85 | 128.60 |
| 1 | H | 405 | DT | N1-C2-N3 | 9.54 | 120.33 | 114.60 |
| 1 | G | 411 | DT | N1-C2-N3 | 9.53 | 120.32 | 114.60 |
| 2 | L | 425 | DG | C5-C6-N1 | 9.48 | 116.24 | 111.50 |
| 1 | E | 408 | DT | C6-C5-C7 | -9.48 | 117.21 | 122.90 |
| 2 | L | 424 | DG | C5-C6-O6 | -9.47 | 122.92 | 128.60 |
| 1 | G | 404 | DT | N3-C2-O2 | -9.45 | 116.63 | 122.30 |
| 1 | F | 410 | DC | N3-C4-N4 | 9.34 | 124.53 | 118.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | E | 404 | DT | N1-C2-N3 | 9.32 | 120.19 | 114.60 |
| 1 | G | 408 | DT | C6-C5-C7 | -9.31 | 117.31 | 122.90 |
| 1 | E | 412 | DG | C5-C6-O6 | -9.29 | 123.03 | 128.60 |
| 1 | H | 403 | DC | N3-C4-N4 | 9.21 | 124.45 | 118.00 |
| 1 | E | 408 | DT | C2-N3-C4 | -9.17 | 121.70 | 127.20 |
| 2 | J | 431 | DG | C5-C6-O6 | -9.16 | 123.11 | 128.60 |
| 2 | I | 431 | DG | O4'-C1'-N9 | 9.14 | 114.40 | 108.00 |
| 1 | H | 411 | DT | N3-C2-O2 | -9.11 | 116.83 | 122.30 |
| 2 | J | 432 | DC | N3-C4-N4 | 9.04 | 124.33 | 118.00 |
| 1 | H | 402 | DG | C5-C6-O6 | -8.99 | 123.21 | 128.60 |
| 2 | K | 425 | DG | O4'-C1'-N9 | 8.97 | 114.28 | 108.00 |
| 3 | B | 31 | ARG | CD-NE-CZ | 8.93 | 136.11 | 123.60 |
| 1 | H | 408 | DT | C4-C5-C6 | 8.91 | 123.35 | 118.00 |
| 1 | E | 402 | DG | C5-C6-O6 | -8.90 | 123.26 | 128.60 |
| 1 | H | 405 | DT | N3-C2-O2 | -8.90 | 116.96 | 122.30 |
| 1 | H | 408 | DT | N3-C2-O2 | -8.83 | 117.00 | 122.30 |
| 2 | L | 432 | DC | N3-C4-N4 | 8.83 | 124.18 | 118.00 |
| 1 | H | 408 | DT | N1-C2-N3 | 8.82 | 119.89 | 114.60 |
| 1 | E | 405 | DT | N1-C2-N3 | 8.80 | 119.88 | 114.60 |
| 1 | H | 405 | DT | C4-C5-C6 | 8.78 | 123.27 | 118.00 |
| 2 | L | 425 | DG | C6-N1-C2 | -8.77 | 119.84 | 125.10 |
| 1 | G | 402 | DG | O4'-C1'-N9 | 8.77 | 114.14 | 108.00 |
| 1 | G | 411 | DT | C4-C5-C6 | 8.71 | 123.22 | 118.00 |
| 1 | F | 412 | DG | C8-N9-C1' | 8.66 | 138.26 | 127.00 |
| 1 | F | 408 | DT | C6-C5-C7 | -8.62 | 117.73 | 122.90 |
| 1 | H | 409 | DC | N3-C4-N4 | 8.56 | 124.00 | 118.00 |
| 1 | E | 411 | DT | C4-C5-C6 | 8.51 | 123.11 | 118.00 |
| 1 | H | 404 | DT | C4-C5-C6 | 8.41 | 123.04 | 118.00 |
| 1 | G | 412 | DG | O4'-C1'-N9 | 8.40 | 113.88 | 108.00 |
| 2 | J | 422 | DC | C5-C6-N1 | 8.39 | 125.20 | 121.00 |
| 1 | G | 408 | DT | C4-C5-C6 | 8.35 | 123.01 | 118.00 |
| 1 | H | 410 | DC | C5-C6-N1 | 8.34 | 125.17 | 121.00 |
| 2 | L | 433 | DC | N3-C4-N4 | 8.31 | 123.81 | 118.00 |
| 1 | F | 412 | DG | C5-C6-N1 | 8.28 | 115.64 | 111.50 |
| 1 | F | 412 | DG | N3-C4-N9 | 8.23 | 130.94 | 126.00 |
| 2 | L | 433 | DC | C5-C6-N1 | 8.22 | 125.11 | 121.00 |
| 2 | L | 432 | DC | C5-C6-N1 | 8.20 | 125.10 | 121.00 |
| 1 | F | 413 | DG | C5-C6-O6 | -8.18 | 123.69 | 128.60 |
| 2 | J | 433 | DC | O4'-C1'-N1 | 8.18 | 113.73 | 108.00 |
| 2 | J | 426 | DA | O4'-C1'-N9 | 8.18 | 113.72 | 108.00 |
| 2 | L | 423 | DA | O4'-C1'-N9 | 8.16 | 113.71 | 108.00 |
| 1 | G | 410 | DC | N3-C4-N4 | 8.13 | 123.69 | 118.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | F | 407 | DC | O4'-C1'-N1 | 8.08 | 113.66 | 108.00 |
| 2 | J | 431 | DG | N9-C4-C5 | 8.06 | 108.62 | 105.40 |
| 1 | E | 405 | DT | N3-C2-O2 | -8.02 | 117.49 | 122.30 |
| 2 | J | 421 | DC | C5-C6-N1 | 8.01 | 125.01 | 121.00 |
| 2 | I | 422 | DC | C5-C6-N1 | 8.00 | 125.00 | 121.00 |
| 1 | F | 413 | DG | O4'-C1'-N9 | 7.97 | 113.58 | 108.00 |
| 1 | H | 403 | DC | C6-N1-C2 | -7.93 | 117.13 | 120.30 |
| 1 | E | 404 | DT | C4-C5-C6 | 7.90 | 122.74 | 118.00 |
| 2 | L | 428 | DG | C5-C6-O6 | -7.89 | 123.87 | 128.60 |
| 1 | E | 411 | DT | N1-C2-N3 | 7.86 | 119.32 | 114.60 |
| 1 | G | 404 | DT | C4-C5-C6 | 7.83 | 122.70 | 118.00 |
| 1 | H | 410 | DC | O4'-C1'-N1 | 7.83 | 113.48 | 108.00 |
| 2 | L | 430 | DA | C2-N3-C4 | 7.81 | 114.51 | 110.60 |
| 2 | J | 422 | DC | O4'-C4'-C3' | -7.79 | 101.33 | 106.00 |
| 1 | F | 406 | DC | C5-C6-N1 | 7.79 | 124.89 | 121.00 |
| 2 | I | 424 | DG | C5-C6-O6 | -7.78 | 123.93 | 128.60 |
| 1 | E | 408 | DT | C4-C5-C6 | 7.78 | 122.67 | 118.00 |
| 2 | J | 433 | DC | O4'-C4'-C3' | -7.76 | 101.35 | 106.00 |
| 1 | G | 408 | DT | N1-C2-N3 | 7.74 | 119.24 | 114.60 |
| 2 | J | 423 | DA | O4'-C1'-N9 | 7.73 | 113.41 | 108.00 |
| 2 | I | 432 | DC | C5-C6-N1 | 7.72 | 124.86 | 121.00 |
| 2 | I | 424 | DG | N9-C4-C5 | 7.68 | 108.47 | 105.40 |
| 1 | F | 412 | DG | C5-C6-O6 | -7.67 | 124.00 | 128.60 |
| 2 | K | 422 | DC | N3-C4-N4 | 7.64 | 123.35 | 118.00 |
| 2 | J | 421 | DC | N3-C4-N4 | 7.64 | 123.35 | 118.00 |
| 1 | F | 408 | DT | C4-C5-C6 | 7.61 | 122.57 | 118.00 |
| 1 | E | 403 | DC | N3-C4-N4 | 7.58 | 123.31 | 118.00 |
| 2 | J | 422 | DC | N1-C2-N3 | -7.58 | 113.89 | 119.20 |
| 1 | F | 412 | DG | C6-N1-C2 | -7.58 | 120.55 | 125.10 |
| 2 | J | 425 | DG | O4'-C1'-N9 | 7.58 | 113.30 | 108.00 |
| 1 | G | 405 | DT | N3-C2-O2 | -7.54 | 117.78 | 122.30 |
| 2 | K | 432 | DC | N3-C4-N4 | 7.49 | 123.24 | 118.00 |
| 1 | H | 404 | DT | N3-C2-O2 | -7.46 | 117.82 | 122.30 |
| 1 | E | 413 | DG | N9-C4-C5 | 7.45 | 108.38 | 105.40 |
| 1 | E | 408 | DT | N1-C2-N3 | 7.43 | 119.06 | 114.60 |
| 2 | L | 422 | DC | N3-C4-N4 | 7.41 | 123.19 | 118.00 |
| 1 | G | 413 | DG | O4'-C1'-N9 | 7.39 | 113.17 | 108.00 |
| 2 | J | 433 | DC | N3-C4-N4 | 7.37 | 123.16 | 118.00 |
| 1 | G | 405 | DT | C4-C5-C6 | 7.33 | 122.40 | 118.00 |
| 1 | G | 404 | DT | N1-C2-N3 | 7.33 | 119.00 | 114.60 |
| 2 | I | 421 | DC | C5-C6-N1 | 7.28 | 124.64 | 121.00 |
| 2 | J | 432 | DC | C5-C6-N1 | 7.28 | 124.64 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | L | 421 | DC | O4'-C1'-N1 | 7.26 | 113.08 | 108.00 |
| 1 | F | 403 | DC | C5-C6-N1 | 7.21 | 124.61 | 121.00 |
| 2 | L | 433 | DC | N1-C2-N3 | -7.18 | 114.17 | 119.20 |
| 2 | J | 421 | DC | N1-C2-N3 | -7.18 | 114.17 | 119.20 |
| 1 | F | 406 | DC | N3-C4-N4 | 7.18 | 123.02 | 118.00 |
| 1 | E | 409 | DC | N3-C4-N4 | 7.16 | 123.02 | 118.00 |
| 2 | K | 429 | DA | C5-C6-N1 | -7.16 | 114.12 | 117.70 |
| 1 | H | 403 | DC | C5-C6-N1 | 7.16 | 124.58 | 121.00 |
| 2 | J | 432 | DC | O4'-C1'-N1 | 7.12 | 112.98 | 108.00 |
| 2 | K | 429 | DA | C6-N1-C2 | 7.10 | 122.86 | 118.60 |
| 2 | K | 424 | DG | C5-C6-O6 | -7.08 | 124.35 | 128.60 |
| 1 | H | 411 | DT | C4-C5-C6 | 7.08 | 122.25 | 118.00 |
| 2 | K | 422 | DC | C5-C6-N1 | 7.04 | 124.52 | 121.00 |
| 1 | E | 410 | DC | N3-C4-N4 | 7.04 | 122.93 | 118.00 |
| 1 | H | 404 | DT | N1-C2-N3 | 7.03 | 118.82 | 114.60 |
| 1 | E | 413 | DG | O4'-C1'-N9 | 7.00 | 112.90 | 108.00 |
| 2 | I | 422 | DC | O4'-C1'-N1 | 7.00 | 112.90 | 108.00 |
| 2 | I | 433 | DC | O4'-C4'-C3' | -6.98 | 101.71 | 104.50 |
| 2 | L | 431 | DG | O4'-C1'-N9 | 6.97 | 112.88 | 108.00 |
| 2 | L | 433 | DC | O4'-C4'-C3' | -6.95 | 101.72 | 104.50 |
| 1 | F | 405 | DT | C4-C5-C6 | 6.94 | 122.16 | 118.00 |
| 1 | E | 412 | DG | N9-C4-C5 | 6.90 | 108.16 | 105.40 |
| 1 | F | 413 | DG | N9-C4-C5 | 6.89 | 108.16 | 105.40 |
| 2 | L | 432 | DC | N1-C2-N3 | -6.88 | 114.38 | 119.20 |
| 1 | F | 405 | DT | N1-C2-N3 | 6.84 | 118.71 | 114.60 |
| 2 | K | 423 | DA | C4-C5-C6 | 6.82 | 120.41 | 117.00 |
| 1 | F | 404 | DT | C4-C5-C6 | 6.82 | 122.09 | 118.00 |
| 2 | K | 424 | DG | N9-C4-C5 | 6.80 | 108.12 | 105.40 |
| 1 | F | 406 | DC | N1-C2-N3 | -6.79 | 114.45 | 119.20 |
| 2 | K | 433 | DC | C5-C6-N1 | 6.76 | 124.38 | 121.00 |
| 1 | G | 409 | DC | C5-C6-N1 | 6.73 | 124.36 | 121.00 |
| 1 | F | 404 | DT | N1-C2-N3 | 6.73 | 118.64 | 114.60 |
| 1 | H | 410 | DC | N1-C2-N3 | -6.73 | 114.49 | 119.20 |
| 2 | I | 425 | DG | O4'-C1'-N9 | 6.70 | 112.69 | 108.00 |
| 2 | I | 421 | DC | O4'-C1'-N1 | 6.68 | 112.68 | 108.00 |
| 2 | L | 424 | DG | C8-N9-C1' | 6.67 | 135.68 | 127.00 |
| 2 | I | 432 | DC | N3-C4-N4 | 6.65 | 122.66 | 118.00 |
| 2 | K | 432 | DC | C5-C6-N1 | 6.65 | 124.33 | 121.00 |
| 2 | I | 431 | DG | C8-N9-C1' | 6.64 | 135.63 | 127.00 |
| 1 | E | 410 | DC | C5-C6-N1 | 6.64 | 124.32 | 121.00 |
| 1 | E | 413 | DG | C8-N9-C1' | 6.64 | 135.63 | 127.00 |
| 1 | F | 408 | DT | O4'-C1'-N1 | 6.63 | 112.64 | 108.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | L | 426 | DA | O4'-C4'-C3' | -6.62 | 101.85 | 104.50 |
| 1 | H | 409 | DC | C5-C6-N1 | 6.61 | 124.31 | 121.00 |
| 2 | K | 421 | DC | O4'-C1'-N1 | 6.61 | 112.63 | 108.00 |
| 1 | H | 413 | DG | N9-C4-C5 | 6.60 | 108.04 | 105.40 |
| 2 | L | 421 | DC | N3-C4-N4 | 6.60 | 122.62 | 118.00 |
| 1 | F | 409 | DC | C5-C6-N1 | 6.59 | 124.30 | 121.00 |
| 2 | J | 422 | DC | P-O5'-C5' | -6.56 | 110.41 | 120.90 |
| 1 | G | 407 | DC | N1-C2-N3 | -6.56 | 114.61 | 119.20 |
| 2 | K | 428 | DG | O4'-C1'-N9 | -6.55 | 103.42 | 108.00 |
| 2 | L | 422 | DC | O4'-C1'-N1 | 6.46 | 112.52 | 108.00 |
| 1 | G | 403 | DC | N1-C2-O2 | 6.46 | 122.78 | 118.90 |
| 1 | H | 402 | DG | N9-C4-C5 | 6.45 | 107.98 | 105.40 |
| 1 | H | 411 | DT | O4'-C1'-N1 | 6.45 | 112.52 | 108.00 |
| 1 | G | 401 | DG | O4'-C1'-N9 | 6.45 | 112.51 | 108.00 |
| 2 | I | 423 | DA | O4'-C1'-N9 | 6.43 | 112.50 | 108.00 |
| 1 | G | 410 | DC | C5-C6-N1 | 6.42 | 124.21 | 121.00 |
| 2 | I | 425 | DG | N9-C4-C5 | 6.40 | 107.96 | 105.40 |
| 2 | J | 421 | DC | N1-C2-O2 | 6.39 | 122.73 | 118.90 |
| 1 | E | 406 | DC | C5-C6-N1 | 6.39 | 124.19 | 121.00 |
| 1 | H | 410 | DC | O4'-C4'-C3' | -6.38 | 101.95 | 104.50 |
| 2 | I | 431 | DG | C5-C6-O6 | -6.36 | 124.78 | 128.60 |
| 1 | E | 404 | DT | N1-C1'-C2' | 6.34 | 124.65 | 112.60 |
| 1 | F | 411 | DT | C5-C6-N1 | -6.34 | 119.90 | 123.70 |
| 1 | E | 405 | DT | O4'-C1'-N1 | 6.32 | 112.42 | 108.00 |
| 1 | F | 410 | DC | C5-C6-N1 | 6.32 | 124.16 | 121.00 |
| 1 | E | 405 | DT | C5-C6-N1 | -6.30 | 119.92 | 123.70 |
| 2 | K | 424 | DG | C8-N9-C1' | 6.30 | 135.19 | 127.00 |
| 2 | L | 421 | DC | C5-C6-N1 | 6.26 | 124.13 | 121.00 |
| 1 | F | 413 | DG | C8-N9-C1' | 6.25 | 135.13 | 127.00 |
| 2 | J | 423 | DA | O4'-C4'-C3' | -6.25 | 102.00 | 104.50 |
| 1 | G | 402 | DG | N9-C4-C5 | 6.25 | 107.90 | 105.40 |
| 2 | J | 431 | DG | C8-N9-C1' | 6.22 | 135.09 | 127.00 |
| 1 | F | 408 | DT | N1-C2-N3 | 6.22 | 118.33 | 114.60 |
| 1 | E | 403 | DC | C5-C6-N1 | 6.21 | 124.11 | 121.00 |
| 2 | I | 431 | DG | N9-C4-C5 | 6.21 | 107.89 | 105.40 |
| 2 | I | 421 | DC | N3-C4-N4 | 6.20 | 122.34 | 118.00 |
| 2 | L | 432 | DC | N3-C2-O2 | 6.20 | 126.24 | 121.90 |
| 2 | K | 433 | DC | N3-C4-N4 | 6.19 | 122.33 | 118.00 |
| 1 | E | 404 | DT | O4'-C1'-N1 | 6.19 | 112.33 | 108.00 |
| 1 | F | 412 | DG | N9-C4-C5 | 6.19 | 107.88 | 105.40 |
| 2 | K | 429 | DA | C5-C6-N6 | 6.18 | 128.65 | 123.70 |
| 1 | G | 405 | DT | N1-C2-N3 | 6.18 | 118.31 | 114.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | I | 424 | DG | C8-N9-C1' | 6.18 | 135.04 | 127.00 |
| 1 | G | 413 | DG | C8-N9-C1' | 6.17 | 135.02 | 127.00 |
| 1 | H | 407 | DC | N1-C2-N3 | -6.16 | 114.89 | 119.20 |
| 2 | L | 424 | DG | N9-C4-C5 | 6.14 | 107.86 | 105.40 |
| 1 | E | 406 | DC | O4'-C1'-N1 | 6.13 | 112.29 | 108.00 |
| 1 | G | 409 | DC | N3-C4-N4 | 6.12 | 122.28 | 118.00 |
| 1 | G | 412 | DG | N9-C4-C5 | 6.08 | 107.83 | 105.40 |
| 2 | J | 430 | DA | C4-C5-C6 | 6.05 | 120.03 | 117.00 |
| 2 | J | 424 | DG | C8-N9-C1' | 6.04 | 134.85 | 127.00 |
| 2 | I | 426 | DA | N1-C2-N3 | -6.03 | 126.28 | 129.30 |
| 2 | I | 422 | DC | N3-C4-N4 | 6.03 | 122.22 | 118.00 |
| 2 | K | 422 | DC | P-O5'-C5' | -6.02 | 111.26 | 120.90 |
| 2 | L | 430 | DA | N3-C4-C5 | -6.02 | 122.59 | 126.80 |
| 1 | H | 412 | DG | N9-C4-C5 | 6.01 | 107.80 | 105.40 |
| 1 | H | 410 | DC | N3-C4-N4 | 6.01 | 122.21 | 118.00 |
| 1 | E | 409 | DC | P-O5'-C5' | -6.00 | 111.30 | 120.90 |
| 1 | F | 409 | DC | N3-C4-N4 | 6.00 | 122.20 | 118.00 |
| 3 | A | 28 | ARG | NE-CZ-NH1 | 6.00 | 123.30 | 120.30 |
| 1 | E | 407 | DC | N1-C2-N3 | -5.99 | 115.01 | 119.20 |
| 2 | L | 422 | DC | C5-C6-N1 | 5.97 | 123.98 | 121.00 |
| 1 | H | 411 | DT | N1-C2-N3 | 5.96 | 118.18 | 114.60 |
| 1 | F | 409 | DC | N1-C2-N3 | -5.96 | 115.03 | 119.20 |
| 2 | K | 422 | DC | N1-C2-N3 | -5.96 | 115.03 | 119.20 |
| 1 | G | 413 | DG | N9-C4-C5 | 5.95 | 107.78 | 105.40 |
| 2 | K | 421 | DC | N3-C4-N4 | 5.95 | 122.16 | 118.00 |
| 2 | L | 429 | DA | O4'-C1'-C2' | -5.94 | 101.15 | 105.90 |
| 2 | J | 431 | DG | O4'-C1'-N9 | 5.93 | 112.15 | 108.00 |
| 2 | L | 430 | DA | C4-C5-C6 | 5.93 | 119.96 | 117.00 |
| 2 | K | 423 | DA | C6-C5-N7 | -5.92 | 128.16 | 132.30 |
| 1 | G | 403 | DC | P-O5'-C5' | -5.92 | 111.44 | 120.90 |
| 2 | L | 428 | DG | N9-C4-C5 | 5.90 | 107.76 | 105.40 |
| 2 | L | 425 | DG | C8-N9-C1' | 5.89 | 134.65 | 127.00 |
| 2 | K | 433 | DC | O4'-C4'-C3' | -5.88 | 102.15 | 104.50 |
| 1 | F | 402 | DG | N9-C4-C5 | 5.87 | 107.75 | 105.40 |
| 2 | K | 425 | DG | N9-C4-C5 | 5.86 | 107.74 | 105.40 |
| 1 | H | 404 | DT | C5-C6-N1 | -5.85 | 120.19 | 123.70 |
| 2 | I | 423 | DA | O4'-C4'-C3' | -5.84 | 102.16 | 104.50 |
| 2 | J | 433 | DC | C5-C6-N1 | 5.84 | 123.92 | 121.00 |
| 2 | L | 433 | DC | O4'-C1'-N1 | 5.82 | 112.08 | 108.00 |
| 1 | F | 406 | DC | O4'-C1'-N1 | 5.80 | 112.06 | 108.00 |
| 2 | J | 429 | DA | N1-C2-N3 | -5.79 | 126.41 | 129.30 |
| 2 | L | 428 | DG | C8-N9-C1' | 5.77 | 134.50 | 127.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | G | 401 | DG | C8-N9-C1' | 5.77 | 134.50 | 127.00 |
| 2 | I | 421 | DC | N1-C2-N3 | -5.75 | 115.17 | 119.20 |
| 2 | I | 422 | DC | N1-C2-O2 | 5.75 | 122.35 | 118.90 |
| 1 | G | 404 | DT | C5-C6-N1 | -5.75 | 120.25 | 123.70 |
| 1 | E | 409 | DC | C5-C6-N1 | 5.75 | 123.87 | 121.00 |
| 1 | G | 411 | DT | C5-C6-N1 | -5.75 | 120.25 | 123.70 |
| 2 | J | 426 | DA | C6-C5-N7 | -5.73 | 128.29 | 132.30 |
| 1 | H | 408 | DT | C5-C6-N1 | -5.73 | 120.26 | 123.70 |
| 2 | I | 430 | DA | C6-C5-N7 | -5.72 | 128.29 | 132.30 |
| 3 | B | 31 | ARG | NE-CZ-NH1 | -5.71 | 117.45 | 120.30 |
| 1 | E | 413 | DG | N1-C2-N3 | 5.69 | 127.31 | 123.90 |
| 1 | F | 409 | DC | P-O5'-C5' | -5.69 | 111.80 | 120.90 |
| 2 | I | 432 | DC | N1-C2-N3 | -5.67 | 115.23 | 119.20 |
| 3 | B | 31 | ARG | CG-CD-NE | 5.67 | 123.71 | 111.80 |
| 1 | E | 409 | DC | N1-C2-N3 | -5.66 | 115.24 | 119.20 |
| 2 | J | 424 | DG | N9-C4-C5 | 5.66 | 107.66 | 105.40 |
| 2 | J | 432 | DC | N1-C2-N3 | -5.66 | 115.24 | 119.20 |
| 1 | F | 405 | DT | O4'-C1'-N1 | 5.63 | 111.94 | 108.00 |
| 2 | I | 422 | DC | N1-C2-N3 | -5.62 | 115.27 | 119.20 |
| 1 | G | 410 | DC | N1-C2-N3 | -5.62 | 115.27 | 119.20 |
| 1 | E | 401 | DG | C4-C5-N7 | 5.61 | 113.04 | 110.80 |
| 2 | I | 423 | DA | P-O5'-C5' | -5.60 | 111.94 | 120.90 |
| 1 | F | 403 | DC | N1-C1'-C2' | 5.60 | 123.23 | 112.60 |
| 2 | J | 430 | DA | C6-C5-N7 | -5.60 | 128.38 | 132.30 |
| 2 | I | 433 | DC | N1-C2-N3 | -5.59 | 115.29 | 119.20 |
| 2 | J | 422 | DC | N3-C4-N4 | 5.58 | 121.91 | 118.00 |
| 2 | I | 428 | DG | C8-N9-C1' | 5.57 | 134.24 | 127.00 |
| 2 | K | 428 | DG | C8-N9-C1' | 5.56 | 134.23 | 127.00 |
| 2 | K | 433 | DC | N1-C2-N3 | -5.56 | 115.31 | 119.20 |
| 1 | G | 401 | DG | N9-C4-C5 | 5.55 | 107.62 | 105.40 |
| 2 | I | 422 | DC | P-O5'-C5' | -5.52 | 112.06 | 120.90 |
| 2 | K | 431 | DG | N1-C2-N3 | 5.52 | 127.21 | 123.90 |
| 1 | E | 413 | DG | N3-C2-N2 | -5.51 | 116.04 | 119.90 |
| 1 | H | 405 | DT | C5-C6-N1 | -5.50 | 120.40 | 123.70 |
| 1 | E | 406 | DC | N1-C2-N3 | -5.50 | 115.35 | 119.20 |
| 2 | I | 426 | DA | O4'-C1'-N9 | 5.50 | 111.85 | 108.00 |
| 1 | H | 407 | DC | O4'-C1'-N1 | 5.49 | 111.84 | 108.00 |
| 2 | J | 422 | DC | O4'-C1'-N1 | 5.49 | 111.84 | 108.00 |
| 2 | K | 430 | DA | C4-C5-C6 | 5.48 | 119.74 | 117.00 |
| 2 | L | 426 | DA | O4'-C1'-N9 | 5.46 | 111.82 | 108.00 |
| 1 | F | 403 | DC | C6-N1-C2 | -5.46 | 118.12 | 120.30 |
| 2 | I | 430 | DA | C4-C5-C6 | 5.44 | 119.72 | 117.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | I | 429 | DA | O4'-C1'-C2' | -5.44 | 101.55 | 105.90 |
| 1 | F | 405 | DT | C5-C6-N1 | -5.42 | 120.44 | 123.70 |
| 2 | J | 426 | DA | C4-C5-C6 | 5.42 | 119.71 | 117.00 |
| 2 | K | 429 | DA | O4'-C1'-C2' | -5.42 | 101.56 | 105.90 |
| 2 | J | 429 | DA | OP1-P-OP2 | -5.39 | 111.51 | 119.60 |
| 1 | E | 407 | DC | N3-C4-N4 | 5.39 | 121.77 | 118.00 |
| 2 | L | 423 | DA | C4-C5-C6 | 5.39 | 119.69 | 117.00 |
| 1 | E | 410 | DC | O4'-C1'-N1 | 5.38 | 111.76 | 108.00 |
| 1 | E | 402 | DG | N9-C4-C5 | 5.36 | 107.55 | 105.40 |
| 2 | J | 429 | DA | C2-N3-C4 | 5.36 | 113.28 | 110.60 |
| 2 | I | 433 | DC | C5-C6-N1 | 5.35 | 123.67 | 121.00 |
| 2 | J | 428 | DG | N9-C4-C5 | 5.35 | 107.54 | 105.40 |
| 2 | J | 421 | DC | O4'-C1'-N1 | 5.35 | 111.74 | 108.00 |
| 2 | J | 425 | DG | C8-N9-C1' | 5.33 | 133.93 | 127.00 |
| 2 | I | 433 | DC | O4'-C1'-N1 | 5.33 | 111.73 | 108.00 |
| 2 | K | 429 | DA | N1-C2-N3 | -5.32 | 126.64 | 129.30 |
| 2 | J | 430 | DA | C2-N3-C4 | 5.32 | 113.26 | 110.60 |
| 1 | G | 403 | DC | N1-C2-N3 | -5.31 | 115.48 | 119.20 |
| 2 | I | 422 | DC | C6-N1-C2 | -5.31 | 118.18 | 120.30 |
| 1 | H | 409 | DC | P-O5'-C5' | -5.31 | 112.41 | 120.90 |
| 2 | I | 423 | DA | C2-N3-C4 | 5.30 | 113.25 | 110.60 |
| 1 | H | 413 | DG | N1-C2-N3 | 5.29 | 127.08 | 123.90 |
| 1 | H | 407 | DC | N3-C4-N4 | 5.29 | 121.70 | 118.00 |
| 2 | L | 425 | DG | O4'-C4'-C3' | -5.28 | 102.39 | 104.50 |
| 2 | K | 430 | DA | C2-N3-C4 | 5.27 | 113.24 | 110.60 |
| 2 | L | 433 | DC | N1-C2-O2 | 5.27 | 122.06 | 118.90 |
| 2 | L | 431 | DG | C4-C5-N7 | 5.26 | 112.91 | 110.80 |
| 2 | J | 422 | DC | C4'-C3'-C2' | -5.26 | 98.37 | 103.10 |
| 1 | F | 407 | DC | N1-C2-N3 | -5.25 | 115.52 | 119.20 |
| 1 | H | 401 | DG | N9-C4-C5 | 5.25 | 107.50 | 105.40 |
| 2 | I | 430 | DA | N3-C4-C5 | -5.25 | 123.13 | 126.80 |
| 2 | I | 426 | DA | C4-C5-C6 | 5.24 | 119.62 | 117.00 |
| 1 | H | 410 | DC | C4'-C3'-C2' | -5.24 | 98.39 | 103.10 |
| 1 | F | 406 | DC | N3-C2-O2 | 5.24 | 125.56 | 121.90 |
| 2 | I | 425 | DG | C8-N9-C1' | 5.23 | 133.80 | 127.00 |
| 1 | G | 405 | DT | O4'-C1'-C2' | 5.23 | 110.08 | 105.90 |
| 1 | H | 410 | DC | N3-C2-O2 | 5.23 | 125.56 | 121.90 |
| 1 | H | 408 | DT | O4'-C1'-N1 | 5.22 | 111.66 | 108.00 |
| 2 | L | 421 | DC | N1-C2-N3 | -5.22 | 115.55 | 119.20 |
| 2 | I | 421 | DC | N1-C2-O2 | 5.21 | 122.03 | 118.90 |
| 1 | H | 409 | DC | N1-C2-N3 | -5.21 | 115.55 | 119.20 |
| 2 | L | 429 | DA | OP1-P-O3' | 5.21 | 116.66 | 105.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | J | 423 | DA | C4-C5-C6 | 5.20 | 119.60 | 117.00 |
| 1 | G | 410 | DC | P-O3'-C3' | -5.20 | 113.46 | 119.70 |
| 2 | J | 424 | DG | O4'-C1'-N9 | 5.19 | 111.64 | 108.00 |
| 2 | L | 431 | DG | C8-N9-C1' | 5.19 | 133.75 | 127.00 |
| 2 | I | 430 | DA | C2-N3-C4 | 5.19 | 113.20 | 110.60 |
| 2 | J | 426 | DA | P-O5'-C5' | -5.18 | 112.61 | 120.90 |
| 1 | F | 402 | DG | O4'-C1'-N9 | 5.17 | 111.62 | 108.00 |
| 1 | G | 406 | DC | N1-C2-N3 | -5.17 | 115.58 | 119.20 |
| 2 | K | 433 | DC | O4'-C1'-N1 | 5.16 | 111.61 | 108.00 |
| 2 | J | 426 | DA | C5-C6-N1 | -5.15 | 115.13 | 117.70 |
| 1 | E | 403 | DC | C6-N1-C2 | -5.13 | 118.25 | 120.30 |
| 1 | F | 408 | DT | C5-C6-N1 | -5.12 | 120.63 | 123.70 |
| 2 | K | 428 | DG | N9-C4-C5 | 5.12 | 107.45 | 105.40 |
| 2 | J | 428 | DG | C8-N9-C1' | 5.10 | 133.63 | 127.00 |
| 1 | H | 407 | DC | N3-C2-O2 | 5.10 | 125.47 | 121.90 |
| 2 | I | 432 | DC | N3-C2-O2 | 5.10 | 125.47 | 121.90 |
| 2 | K | 423 | DA | N3-C4-C5 | -5.09 | 123.23 | 126.80 |
| 1 | H | 406 | DC | O4'-C1'-N1 | 5.09 | 111.56 | 108.00 |
| 2 | K | 430 | DA | P-O5'-C5' | -5.09 | 112.76 | 120.90 |
| 1 | E | 408 | DT | O4'-C1'-N1 | 5.08 | 111.56 | 108.00 |
| 2 | K | 430 | DA | N3-C4-C5 | -5.08 | 123.24 | 126.80 |
| 1 | G | 410 | DC | P-O5'-C5' | -5.08 | 112.78 | 120.90 |
| 1 | F | 410 | DC | O4'-C1'-N1 | 5.08 | 111.55 | 108.00 |
| 2 | K | 421 | DC | OP1-P-O3' | 5.06 | 116.32 | 105.20 |
| 1 | F | 409 | DC | N1-C2-O2 | 5.05 | 121.93 | 118.90 |
| 2 | L | 423 | DA | C2-N3-C4 | 5.05 | 113.13 | 110.60 |
| 1 | H | 412 | DG | N1-C2-N3 | 5.05 | 126.93 | 123.90 |
| 1 | H | 411 | DT | C5-C6-N1 | -5.05 | 120.67 | 123.70 |
| 2 | J | 421 | DC | OP1-P-O3' | 5.03 | 116.27 | 105.20 |
| 2 | J | 424 | DG | N1-C2-N3 | 5.03 | 126.92 | 123.90 |
| 2 | L | 422 | DC | C6-N1-C2 | -5.02 | 118.29 | 120.30 |
| 2 | L | 426 | DA | C2-N3-C4 | 5.02 | 113.11 | 110.60 |
| 1 | G | 401 | DG | N1-C2-N3 | 5.01 | 126.90 | 123.90 |
| 2 | I | 424 | DG | N1-C2-N3 | 5.00 | 126.90 | 123.90 |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | E | 260 | 0 | 149 | 9 | 0 |
| 1 | F | 260 | 0 | 149 | 5 | 0 |
| 1 | G | 260 | 0 | 149 | 2 | 0 |
| 1 | H | 260 | 0 | 149 | 9 | 0 |
| 2 | I | 256 | 0 | 142 | 6 | 0 |
| 2 | J | 256 | 0 | 142 | 5 | 0 |
| 2 | K | 256 | 0 | 142 | 3 | 0 |
| 2 | L | 256 | 0 | 142 | 6 | 0 |
| 3 | A | 2038 | 0 | 2058 | 42 | 0 |
| 3 | B | 2030 | 0 | 2048 | 53 | 0 |
| 3 | C | 2042 | 0 | 2062 | 53 | 0 |
| 3 | D | 2039 | 0 | 2059 | 40 | 0 |
| 4 | A | 1 | 0 | 0 | 0 | 0 |
| 4 | B | 1 | 0 | 0 | 0 | 0 |
| 4 | C | 1 | 0 | 0 | 0 | 0 |
| 4 | D | 1 | 0 | 0 | 0 | 0 |
| 5 | A | 93 | 0 | 0 | 1 | 0 |
| 5 | B | 82 | 0 | 0 | 2 | 0 |
| 5 | C | 77 | 0 | 0 | 1 | 0 |
| 5 | D | 92 | 0 | 0 | 1 | 0 |
| 5 | E | 15 | 0 | 0 | 0 | 0 |
| 5 | F | 16 | 0 | 0 | 0 | 0 |
| 5 | G | 18 | 0 | 0 | 1 | 0 |
| 5 | H | 18 | 0 | 0 | 0 | 0 |
| 5 | I | 23 | 0 | 0 | 0 | 0 |
| 5 | J | 24 | 0 | 0 | 0 | 0 |
| 5 | K | 20 | 0 | 0 | 1 | 0 |
| 5 | L | 21 | 0 | 0 | 1 | 0 |
| All | All | 10716 | 0 | 9391 | 229 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (229) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:122:HIS:ND1 | 3:C:123:ASN:O | 1.76 | 1.16 |
| 3:D:211:GLN:OE1 | 3:D:232:GLU:OE2 | 1.76 | 1.03 |
| 3:A:80:LEU:HD13 | 3:A:84:LEU:HD23 | 1.45 | 0.99 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:122:HIS:CE1 | 3:C:123:ASN:O | 2.17 | 0.98 |
| 3:D:122:HIS:O | 3:D:126:THR:OG1 | 1.82 | 0.96 |
| 3:C:123:ASN:O | 3:C:124:VAL:HG13 | 1.68 | 0.94 |
| 3:D:122:HIS:C | 3:D:126:THR:OG1 | 2.07 | 0.92 |
| 3:C:181:HIS:HD2 | 3:C:183:ASP:H | 1.22 | 0.84 |
| 3:B:169:ILE:HD11 | 3:B:216:LEU:HD11 | 1.58 | 0.83 |
| 3:D:122:HIS:C | 3:D:126:THR:HG1 | 1.80 | 0.82 |
| 3:B:122:HIS:CE1 | 3:B:124:VAL:HG22 | 2.17 | 0.80 |
| 3:D:169:ILE:HD11 | 3:D:216:LEU:HD11 | 1.62 | 0.80 |
| 3:C:240:GLY:O | 3:C:249:PRO:HB3 | 1.84 | 0.77 |
| 3:B:122:HIS:O | 3:B:123:ASN:HB2 | 1.85 | 0.75 |
| 3:B:154:LYS:HE3 | 3:B:260:THR:HB | 1.71 | 0.72 |
| 3:D:228:TYR:O | 3:D:231:GLN:HG2 | 1.90 | 0.71 |
| 3:B:240:GLY:O | 3:B:249:PRO:HB3 | 1.90 | 0.71 |
| 3:C:190:SER:OG | 3:C:193:GLU:HG3 | 1.90 | 0.70 |
| 3:C:154:LYS:HZ2 | 3:C:260:THR:HG22 | 1.56 | 0.70 |
| 2:K:422:DC:H2" | 2:K:423:DA:N7 | 2.07 | 0.69 |
| 3:C:216:LEU:HD21 | 3:C:236:TYR:HE2 | 1.56 | 0.69 |
| 2:J:421:DC:H4' | 2:J:422:DC:OP1 | 1.93 | 0.69 |
| 3:D:154:LYS:HZ1 | 3:D:260:THR:HG22 | 1.57 | 0.69 |
| 3:B:184:ARG:HD3 | 3:B:268:LYS:O | 1.93 | 0.68 |
| 3:D:154:LYS:HE3 | 3:D:260:THR:HB | 1.74 | 0.68 |
| 3:A:154:LYS:HE3 | 3:A:260:THR:HB | 1.75 | 0.68 |
| 2:I:423:DA:H1' | 2:I:424:DG:H5' | 1.76 | 0.67 |
| 3:A:80:LEU:HD11 | 3:A:103:ARG:HD2 | 1.74 | 0.67 |
| 3:B:154:LYS:HZ1 | 3:B:260:THR:HG22 | 1.59 | 0.67 |
| 3:C:154:LYS:HE3 | 3:C:260:THR:HB | 1.77 | 0.67 |
| 3:B:255:HIS:ND1 | 3:B:260:THR:HG21 | 2.10 | 0.66 |
| 3:D:255:HIS:ND1 | 3:D:260:THR:HG21 | 2.10 | 0.66 |
| 3:C:215:THR:OG1 | 3:C:226:PRO:HB3 | 1.95 | 0.66 |
| 3:B:238:ARG:O | 3:B:250:ILE:HB | 1.96 | 0.65 |
| 3:C:169:ILE:HD11 | 3:C:216:LEU:HD11 | 1.79 | 0.65 |
| 2:L:422:DC:H2" | 2:L:423:DA:H5' | 1.78 | 0.65 |
| 3:C:255:HIS:ND1 | 3:C:260:THR:HG21 | 2.12 | 0.65 |
| 3:B:149:LYS:HE2 | 3:B:156:TRP:CD2 | 2.33 | 0.64 |
| 3:C:123:ASN:C | 3:C:124:VAL:HG13 | 2.18 | 0.64 |
| 3:B:37:SER:OG | 3:B:114:LEU:HA | 1.98 | 0.63 |
| 1:E:409:DC:H2" | 1:E:410:DC:O5' | 1.99 | 0.63 |
| 3:C:95:VAL:HA | 3:C:101:VAL:HG22 | 1.78 | 0.63 |
| 3:A:215:THR:OG1 | 3:A:226:PRO:HB3 | 1.98 | 0.63 |
| 3:B:84:LEU:HG | 3:B:85:PRO:HD2 | 1.80 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:409:DC:H2" | 1:G:410:DC:O5' | 1.99 | 0.63 |
| 3:D:122:HIS:CA | 3:D:126:THR:OG1 | 2.47 | 0.62 |
| 3:C:178:ALA:HB2 | 3:C:200:VAL:HG21 | 1.81 | 0.62 |
| 3:A:154:LYS:HZ2 | 3:A:260:THR:HG22 | 1.64 | 0.61 |
| 1:H:412:DG:H2" | 1:H:413:DG:O4' | 2.00 | 0.60 |
| 3:A:255:HIS:ND1 | 3:A:260:THR:HG21 | 2.16 | 0.60 |
| 3:B:178:ALA:HB2 | 3:B:200:VAL:HG21 | 1.83 | 0.60 |
| 1:E:413:DG:H1 | 2:I:421:DC:H42 | 1.51 | 0.59 |
| 3:C:46:GLN:HB3 | 3:C:62:LEU:HD13 | 1.83 | 0.59 |
| 1:F:411:DT:H4' | 1:F:412:DG:OP1 | 2.02 | 0.58 |
| 3:C:122:HIS:O | 3:C:126:THR:OG1 | 2.16 | 0.58 |
| 3:D:62:LEU:HD12 | 3:D:115:TRP:HZ3 | 1.68 | 0.58 |
| 3:C:123:ASN:O | 3:C:124:VAL:CG1 | 2.49 | 0.58 |
| 3:D:122:HIS:HA | 3:D:126:THR:OG1 | 2.04 | 0.58 |
| 1:E:411:DT:H2" | 1:E:412:DG:N7 | 2.19 | 0.58 |
| 3:A:98:ASN:ND2 | 3:A:100:LYS:HD2 | 2.19 | 0.58 |
| 3:A:149:LYS:HE2 | 3:A:156:TRP:CD2 | 2.39 | 0.58 |
| 3:B:208:SER:OG | 3:B:213:GLY:HA2 | 2.03 | 0.58 |
| 3:D:62:LEU:HD12 | 3:D:115:TRP:CZ3 | 2.39 | 0.58 |
| 1:H:412:DG:H2' | 1:H:413:DG:C8 | 2.39 | 0.57 |
| 2:K:422:DC:H2" | 2:K:423:DA:C5 | 2.39 | 0.57 |
| 2:L:422:DC:C2' | 2:L:423:DA:H5' | 2.34 | 0.57 |
| 1:E:413:DG:H1 | 2:I:421:DC:N4 | 2.02 | 0.57 |
| 3:C:181:HIS:CD2 | 3:C:182:PRO:HD2 | 2.39 | 0.57 |
| 1:H:412:DG:H2" | 1:H:413:DG:O5' | 2.05 | 0.56 |
| 1:H:412:DG:H4' | 1:H:412:DG:OP1 | 2.01 | 0.56 |
| 3:B:122:HIS:HE1 | 3:B:124:VAL:HG22 | 1.67 | 0.56 |
| 3:C:88:LYS:HD2 | 3:C:89:HIS:CE1 | 2.40 | 0.56 |
| 2:I:423:DA:C1' | 2:I:424:DG:H5' | 2.35 | 0.56 |
| 3:A:181:HIS:HB3 | 3:A:184:ARG:HG2 | 1.87 | 0.56 |
| 3:B:122:HIS:CE1 | 3:B:124:VAL:H | 2.24 | 0.56 |
| 3:B:215:THR:HG21 | 3:B:226:PRO:HB3 | 1.87 | 0.56 |
| 3:A:178:ALA:HB2 | 3:A:200:VAL:HG21 | 1.88 | 0.55 |
| 3:C:169:ILE:HG12 | 3:C:236:TYR:CD2 | 2.42 | 0.55 |
| 1:H:411:DT:H2" | 1:H:412:DG:O4' | 2.06 | 0.55 |
| 2:L:423:DA:H2" | 2:L:424:DG:N7 | 2.21 | 0.55 |
| 3:B:134:SER:OG | 3:B:136:ASP:HB2 | 2.06 | 0.55 |
| 3:D:64:GLU:OE1 | 3:D:64:GLU:HA | 2.07 | 0.55 |
| 3:D:65:GLY:HA3 | 3:D:115:TRP:CZ2 | 2.42 | 0.55 |
| 3:A:169:ILE:HD11 | 3:A:216:LEU:HD11 | 1.88 | 0.55 |
| 3:C:26:VAL:HG11 | 3:C:28:ARG:NH1 | 2.22 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:131:GLU:HB3 | 5:C:641:HOH:O | 2.08 | 0.54 |
| 1:E:410:DC:H4' | 1:E:410:DC:OP1 | 2.08 | 0.54 |
| 3:A:94:LEU:HB2 | 3:A:102:LEU:HB3 | 1.90 | 0.54 |
| 3:D:214:THR:HG23 | 3:D:230:ALA:HB2 | 1.89 | 0.54 |
| 3:B:241:GLU:O | 3:B:249:PRO:HA | 2.08 | 0.53 |
| 3:A:77:LEU:HD22 | 3:A:102:LEU:HD11 | 1.91 | 0.53 |
| 3:A:94:LEU:HD22 | 3:A:102:LEU:HD23 | 1.90 | 0.53 |
| 5:L:744:HOH:O | 3:D:128:LEU:HD21 | 2.07 | 0.53 |
| 3:C:26:VAL:HG11 | 3:C:28:ARG:HH11 | 1.73 | 0.53 |
| 3:D:84:LEU:HG | 3:D:85:PRO:HD2 | 1.90 | 0.53 |
| 3:A:200:VAL:O | 3:A:204:VAL:HG23 | 2.08 | 0.53 |
| 3:C:64:GLU:OE1 | 3:C:64:GLU:HA | 2.09 | 0.53 |
| 3:B:149:LYS:HE2 | 3:B:156:TRP:CE3 | 2.44 | 0.53 |
| 3:A:3:LEU:HB3 | 3:A:4:PRO:HD3 | 1.91 | 0.52 |
| 3:C:123:ASN:O | 3:C:124:VAL:HG22 | 2.09 | 0.52 |
| 3:B:180:ILE:HA | 3:B:268:LYS:OXT | 2.09 | 0.52 |
| 3:D:3:LEU:HB3 | 3:D:4:PRO:HD3 | 1.90 | 0.52 |
| 3:D:122:HIS:O | 3:D:123:ASN:HB2 | 2.10 | 0.52 |
| 2:J:421:DC:H2" | 2:J:422:DC:C5 | 2.45 | 0.52 |
| 1:H:410:DC:H4' | 1:H:410:DC:OP1 | 2.09 | 0.52 |
| 3:A:79:ILE:HA | 3:A:101:VAL:O | 2.10 | 0.52 |
| 3:D:139:GLY:HA3 | 3:D:195:GLU:HG2 | 1.91 | 0.52 |
| 1:H:411:DT:H2" | 1:H:412:DG:H5" | 1.92 | 0.51 |
| 3:B:215:THR:CB | 3:B:226:PRO:HB3 | 2.40 | 0.51 |
| 3:C:241:GLU:O | 3:C:249:PRO:HA | 2.10 | 0.51 |
| 2:I:422:DC:H2" | 2:I:423:DA:N7 | 2.25 | 0.51 |
| 3:D:154:LYS:NZ | 3:D:260:THR:HG22 | 2.24 | 0.51 |
| 1:H:412:DG:H2" | 1:H:413:DG:C5' | 2.40 | 0.51 |
| 3:D:141:TYR:CE1 | 3:D:145:LYS:HE2 | 2.46 | 0.51 |
| 3:D:169:ILE:CD1 | 3:D:216:LEU:HD11 | 2.37 | 0.51 |
| 2:L:421:DC:H2' | 2:L:422:DC:C6 | 2.46 | 0.51 |
| 3:C:140:GLU:HG3 | 3:C:144:GLN:NE2 | 2.24 | 0.51 |
| 3:C:215:THR:CB | 3:C:226:PRO:HB3 | 2.41 | 0.51 |
| 5:G:649:HOH:O | 3:C:151:THR:HB | 2.09 | 0.50 |
| 3:A:149:LYS:HE2 | 3:A:156:TRP:CE3 | 2.47 | 0.50 |
| 3:B:215:THR:OG1 | 3:B:226:PRO:HB3 | 2.12 | 0.50 |
| 3:C:139:GLY:HA3 | 3:C:195:GLU:HG3 | 1.94 | 0.50 |
| 3:D:80:LEU:HD11 | 3:D:103:ARG:HD2 | 1.92 | 0.50 |
| 1:E:411:DT:H4' | 1:E:412:DG:OP1 | 2.12 | 0.50 |
| 5:K:707:HOH:O | 3:D:161:LYS:HE2 | 2.11 | 0.50 |
| 3:B:246:CYS:HB2 | 3:B:265:GLN:NE2 | 2.27 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:D:181:HIS:HB3 | 3:D:184:ARG:HG2 | 1.94 | 0.50 |
| 3:A:125:LEU:HA | 3:A:128:LEU:CD1 | 2.42 | 0.50 |
| 3:C:180:ILE:HA | 3:C:268:LYS:OXT | 2.12 | 0.50 |
| 3:A:96:MET:HB2 | 3:A:98:ASN:OD1 | 2.12 | 0.49 |
| 3:C:134:SER:OG | 3:C:136:ASP:HB2 | 2.12 | 0.49 |
| 3:C:216:LEU:HD21 | 3:C:236:TYR:CE2 | 2.41 | 0.49 |
| 3:D:95:VAL:HG22 | 3:D:101:VAL:HG22 | 1.94 | 0.49 |
| 3:A:65:GLY:HA3 | 3:A:115:TRP:CZ2 | 2.47 | 0.49 |
| 1:F:409:DC:H2" | 1:F:410:DC:O5' | 2.13 | 0.49 |
| 3:A:23:LEU:HD21 | 3:A:97:SER:HB3 | 1.95 | 0.49 |
| 1:G:411:DT:H2" | 1:G:412:DG:N7 | 2.28 | 0.48 |
| 3:A:225:LYS:O | 3:A:226:PRO:O | 2.32 | 0.48 |
| 1:H:410:DC:H2" | 1:H:411:DT:C6 | 2.49 | 0.48 |
| 3:C:28:ARG:NH2 | 3:C:86:PRO:HB3 | 2.28 | 0.48 |
| 3:A:215:THR:O | 3:A:215:THR:HG22 | 2.13 | 0.48 |
| 3:B:84:LEU:HG | 3:B:85:PRO:CD | 2.43 | 0.48 |
| 3:C:181:HIS:CD2 | 3:C:183:ASP:HB2 | 2.49 | 0.48 |
| 3:C:211:GLN:NE2 | 3:C:232:GLU:OE2 | 2.47 | 0.48 |
| 3:B:3:LEU:HB3 | 3:B:4:PRO:HD3 | 1.94 | 0.47 |
| 3:C:32:LEU:HB3 | 3:C:111:GLY:O | 2.14 | 0.47 |
| 3:B:122:HIS:HE1 | 3:B:124:VAL:HG13 | 1.79 | 0.47 |
| 2:K:423:DA:H2" | 2:K:424:DG:OP2 | 2.13 | 0.47 |
| 3:C:3:LEU:HB3 | 3:C:4:PRO:HD3 | 1.95 | 0.47 |
| 3:C:181:HIS:CD2 | 3:C:183:ASP:H | 2.14 | 0.47 |
| 3:B:131:GLU:HG2 | 5:B:611:HOH:O | 2.15 | 0.47 |
| 3:B:262:TYR:HB2 | 3:B:267:GLN:OE1 | 2.15 | 0.47 |
| 3:A:139:GLY:HA3 | 3:A:195:GLU:HG2 | 1.98 | 0.46 |
| 3:B:141:TYR:CE1 | 3:B:145:LYS:HE3 | 2.50 | 0.46 |
| 2:J:424:DG:H2" | 2:J:425:DG:OP2 | 2.16 | 0.46 |
| 3:A:122:HIS:O | 3:A:126:THR:OG1 | 2.28 | 0.46 |
| 3:C:21:THR:HA | 3:C:47:PRO:HA | 1.97 | 0.46 |
| 3:B:181:HIS:CE1 | 3:B:183:ASP:HB2 | 2.50 | 0.46 |
| 3:B:214:THR:HG23 | 3:B:230:ALA:HB2 | 1.97 | 0.46 |
| 3:A:240:GLY:O | 3:A:249:PRO:HB3 | 2.16 | 0.46 |
| 3:D:178:ALA:HB2 | 3:D:200:VAL:HG21 | 1.98 | 0.45 |
| 2:I:423:DA:H2" | 2:I:424:DG:OP2 | 2.15 | 0.45 |
| 2:L:423:DA:H4' | 2:L:424:DG:OP1 | 2.14 | 0.45 |
| 3:B:81:PRO:HA | 3:B:100:LYS:HG2 | 1.98 | 0.45 |
| 3:B:200:VAL:O | 3:B:204:VAL:HG23 | 2.17 | 0.45 |
| 1:F:410:DC:H4' | 1:F:410:DC:OP1 | 2.17 | 0.45 |
| 2:J:422:DC:H2" | 2:J:423:DA:N7 | 2.32 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:A:131:GLU:HB3 | 5:A:512:HOH:O | 2.16 | 0.45 |
| 3:A:211:GLN:NE2 | 3:A:232:GLU:OE2 | 2.50 | 0.45 |
| 3:C:120:GLU:H | 3:C:120:GLU:HG2 | 1.43 | 0.45 |
| 3:B:228:TYR:O | 3:B:231:GLN:HG2 | 2.16 | 0.45 |
| 3:C:183:ASP:OD1 | 3:C:255:HIS:NE2 | 2.50 | 0.45 |
| 3:A:10:ARG:HB2 | 3:A:58:LEU:CD2 | 2.47 | 0.45 |
| 3:A:228:TYR:HA | 3:A:231:GLN:HE22 | 1.82 | 0.45 |
| 3:B:95:VAL:HA | 3:B:101:VAL:HG22 | 1.99 | 0.45 |
| 3:B:131:GLU:HB3 | 5:B:578:HOH:O | 2.17 | 0.44 |
| 3:C:33:ARG:HD3 | 3:C:34:TRP:CH2 | 2.51 | 0.44 |
| 3:D:61:GLU:HG3 | 3:D:66:TRP:CH2 | 2.52 | 0.44 |
| 1:E:410:DC:H2' | 1:E:411:DT:H72 | 2.00 | 0.44 |
| 3:A:238:ARG:HD2 | 3:A:244:ARG:HH21 | 1.83 | 0.44 |
| 2:L:424:DG:H1' | 2:L:425:DG:H5" | 2.00 | 0.44 |
| 3:B:80:LEU:O | 3:B:100:LYS:HB3 | 2.17 | 0.44 |
| 3:D:46:GLN:HB3 | 3:D:62:LEU:HD13 | 2.00 | 0.44 |
| 3:C:38:GLU:OE2 | 3:C:42:ARG:NE | 2.50 | 0.44 |
| 3:A:238:ARG:O | 3:A:250:ILE:HB | 2.18 | 0.44 |
| 3:B:210:GLU:O | 3:B:210:GLU:HG3 | 2.18 | 0.44 |
| 3:C:80:LEU:HD11 | 3:C:103:ARG:HD2 | 2.00 | 0.44 |
| 3:D:27:VAL:HG11 | 3:D:41:TYR:CZ | 2.54 | 0.43 |
| 3:B:61:GLU:OE1 | 3:D:61:GLU:OE1 | 2.37 | 0.43 |
| 3:A:23:LEU:HD21 | 3:A:97:SER:HA | 2.00 | 0.43 |
| 3:B:169:ILE:HG12 | 3:B:236:TYR:CE2 | 2.52 | 0.43 |
| 3:C:234:GLN:OE1 | 3:C:244:ARG:HD2 | 2.19 | 0.43 |
| 3:D:122:HIS:CD2 | 3:D:126:THR:HG21 | 2.53 | 0.43 |
| 3:D:61:GLU:HG3 | 3:D:66:TRP:CZ2 | 2.54 | 0.43 |
| 3:C:207:ARG:NH1 | 3:C:210:GLU:HG2 | 2.33 | 0.43 |
| 3:B:207:ARG:NH1 | 3:B:210:GLU:HG2 | 2.34 | 0.43 |
| 1:F:412:DG:O5' | 1:F:412:DG:H2' | 2.19 | 0.43 |
| 3:B:199:ARG:HH11 | 3:B:199:ARG:HG2 | 1.84 | 0.43 |
| 3:B:198:ALA:O | 3:B:202:LYS:HG3 | 2.19 | 0.42 |
| 3:B:248:THR:HA | 3:B:249:PRO:HD3 | 1.95 | 0.42 |
| 3:C:123:ASN:C | 3:C:124:VAL:CG1 | 2.88 | 0.42 |
| 3:D:131:GLU:HB3 | 5:D:704:HOH:O | 2.19 | 0.42 |
| 3:C:80:LEU:HA | 3:C:81:PRO:HD3 | 1.91 | 0.42 |
| 1:E:412:DG:H2" | 1:E:413:DG:C8 | 2.54 | 0.42 |
| 3:C:262:TYR:HB2 | 3:C:267:GLN:OE1 | 2.20 | 0.42 |
| 3:D:106:ASP:OD2 | 3:D:109:ARG:HA | 2.19 | 0.42 |
| 3:D:75:GLY:HA2 | 3:D:105:THR:O | 2.20 | 0.42 |
| 3:A:262:TYR:HB2 | 3:A:267:GLN:OE1 | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:D:134:SER:OG | 3:D:136:ASP:HB2 | 2.20 | 0.42 |
| 3:A:61:GLU:C | 3:A:62:LEU:HD23 | 2.41 | 0.41 |
| 3:A:208:SER:OG | 3:A:213:GLY:HA2 | 2.20 | 0.41 |
| 3:A:238:ARG:HD2 | 3:A:244:ARG:NH2 | 2.36 | 0.41 |
| 3:B:106:ASP:OD2 | 3:B:109:ARG:HA | 2.20 | 0.41 |
| 3:B:215:THR:CG2 | 3:B:226:PRO:HB3 | 2.49 | 0.41 |
| 3:D:181:HIS:CE1 | 3:D:183:ASP:HB2 | 2.56 | 0.41 |
| 3:A:238:ARG:NE | 3:A:244:ARG:NH2 | 2.68 | 0.41 |
| 3:B:122:HIS:CE1 | 3:B:124:VAL:HG13 | 2.55 | 0.41 |
| 3:A:62:LEU:HD23 | 3:A:62:LEU:N | 2.36 | 0.41 |
| 3:B:40:ILE:O | 3:B:43:LEU:HG | 2.21 | 0.41 |
| 3:C:207:ARG:NE | 3:C:232:GLU:OE2 | 2.54 | 0.41 |
| 1:F:410:DC:N4 | 2:J:423:DA:N6 | 2.69 | 0.40 |
| 3:A:10:ARG:HB2 | 3:A:58:LEU:HD21 | 2.03 | 0.40 |
| 3:A:125:LEU:HA | 3:A:128:LEU:HD12 | 2.04 | 0.40 |
| 3:B:184:ARG:HH22 | 3:B:193:GLU:CD | 2.25 | 0.40 |
| 3:B:225:LYS:HA | 3:B:226:PRO:HD3 | 1.92 | 0.40 |
| 1:E:411:DT:H2" | 1:E:412:DG:C8 | 2.56 | 0.40 |
| 3:B:208:SER:O | 3:B:213:GLY:N | 2.50 | 0.40 |
| 3:B:242:PRO:HA | 3:B:249:PRO:HA | 2.03 | 0.40 |
| 3:C:207:ARG:O | 3:C:210:GLU:HB3 | 2.21 | 0.40 |

There are no symmetry-related clashes.

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 3 | A | 256/268 (96%) | 243 (95%) | 10 (4%) | 3 (1%) | 13 8 |
| 3 | B | 256/268 (96%) | 244 (95%) | 11 (4%) | 1 (0%) | 34 32 |
| 3 | C | 256/268 (96%) | 249 (97%) | 5 (2%) | 2 (1%) | 19 15 |
| 3 | D | 256/268 (96%) | 240 (94%) | 15 (6%) | 1 (0%) | 34 32 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| All | All | 1024/1072 (96%) | 976 (95%) | 41 (4%) | 7 (1%) | 22 18 |

All (7) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | A | 226 | PRO |
| 3 | B | 123 | ASN |
| 3 | C | 124 | VAL |
| 3 | A | 82 | GLU |
| 3 | A | 123 | ASN |
| 3 | D | 126 | THR |
| 3 | C | 226 | PRO |

### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 3 | A | 218/230 (95%) | 206 (94%) | 12 (6%) | 21 19 |
| 3 | B | 216/230 (94%) | 204 (94%) | 12 (6%) | 21 18 |
| 3 | C | 219/230 (95%) | 204 (93%) | 15 (7%) | 16 13 |
| 3 | D | 218/230 (95%) | 210 (96%) | 8 (4%) | 34 35 |
| All | All | 871/920 (95%) | 824 (95%) | 47 (5%) | 22 20 |

All (47) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | A | 31 | ARG |
| 3 | A | 32 | LEU |
| 3 | A | 33 | ARG |
| 3 | A | 38 | GLU |
| 3 | A | 44 | SER |
| 3 | A | 94 | LEU |
| 3 | A | 122 | HIS |
| 3 | A | 210 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | A | 211 | GLN |
| 3 | A | 215 | THR |
| 3 | A | 260 | THR |
| 3 | A | 268 | LYS |
| 3 | B | 31 | ARG |
| 3 | B | 32 | LEU |
| 3 | B | 33 | ARG |
| 3 | B | 42 | ARG |
| 3 | B | 120 | GLU |
| 3 | B | 144 | GLN |
| 3 | B | 161 | LYS |
| 3 | B | 199 | ARG |
| 3 | B | 210 | GLU |
| 3 | B | 216 | LEU |
| 3 | B | 260 | THR |
| 3 | B | 268 | LYS |
| 3 | C | 31 | ARG |
| 3 | C | 32 | LEU |
| 3 | C | 38 | GLU |
| 3 | C | 82 | GLU |
| 3 | C | 84 | LEU |
| 3 | C | 88 | LYS |
| 3 | C | 120 | GLU |
| 3 | C | 124 | VAL |
| 3 | C | 144 | GLN |
| 3 | C | 207 | ARG |
| 3 | C | 210 | GLU |
| 3 | C | 215 | THR |
| 3 | C | 216 | LEU |
| 3 | C | 260 | THR |
| 3 | C | 265 | GLN |
| 3 | D | 32 | LEU |
| 3 | D | 33 | ARG |
| 3 | D | 38 | GLU |
| 3 | D | 88 | LYS |
| 3 | D | 122 | HIS |
| 3 | D | 127 | HIS |
| 3 | D | 260 | THR |
| 3 | D | 268 | LYS |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | A | 24 | HIS |
| 3 | A | 127 | HIS |
| 3 | B | 122 | HIS |
| 3 | B | 265 | GLN |
| 3 | C | 144 | GLN |
| 3 | C | 181 | HIS |
| 3 | C | 211 | GLN |
| 3 | D | 122 | HIS |
| 3 | D | 211 | GLN |

#### 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)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

# 6 Fit of model and data

## 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

## 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

## 6.4 Ligands

EDS was not executed - this section is therefore empty.

## 6.5 Other polymers

EDS was not executed - this section is therefore empty.