



Full wwPDB NMR Structure Validation Report ⓘ

Jul 6, 2017 – 09:58 AM EDT

PDB ID : 1LCD
Title : STRUCTURE OF THE COMPLEX OF LAC REPRESSOR HEAD-PIECE AND AN 11 BASE-PAIR HALF-OPERATOR DETERMINED BY NUCLEAR MAGNETIC RESONANCE SPECTROSCOPY AND RESTRAINED MOLECULAR DYNAMICS
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Deposited on : unknown

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A user guide is available at

<http://wwpdb.org/validation/2016/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

| | | |
|--------------------------------|---|--|
| Cyrange | : | Kirchner and Güntert (2011) |
| NmrClust | : | Kelley et al. (1996) |
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20161228.v01 (using entries in the PDB archive December 28th 2016) |
| RCI | : | v_1n_11_5_13_A (Berjanski et al., 2005) |
| PANAV | : | Wang et al. (2010) |
| ShiftChecker | : | rb-20029824 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | rb-20029824 |

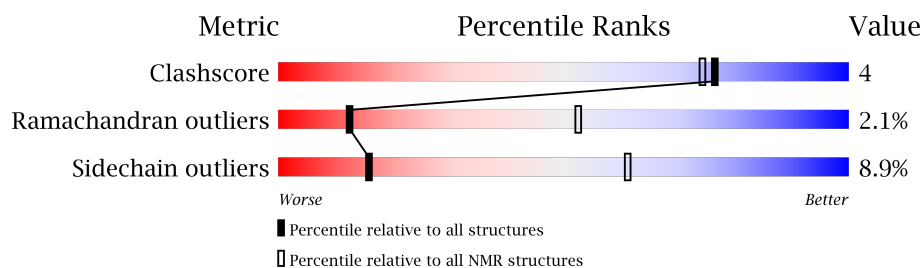
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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) | NMR archive (#Entries) |
|-----------------------|-----------------------------|---------------------------|
| Clashscore | 125131 | 11601 |
| Ramachandran outliers | 121729 | 10391 |
| Sidechain outliers | 121581 | 10367 |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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 $\leq 5\%$

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | B | 11 | 100% |
| 2 | C | 11 | 91% 9% |
| 3 | A | 51 | 69% 20% 6% . . |

2 Ensemble composition and analysis ⓘ

This entry contains 3 models. The atoms present in the NMR models are not consistent. Some calculations may have failed as a result. All residues are included in the validation scores. Model 2 is the overall representative, medoid model (most similar to other models).

The following residues are included in the computation of the global validation metrics.

| Well-defined (core) protein residues | | | |
|--------------------------------------|-----------------------|-------------------|--------------|
| Well-defined core | Residue range (total) | Backbone RMSD (Å) | Medoid model |
| 1 | A:3-A:51 (49) | 0.39 | 2 |

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 1 clusters. No single-model clusters were found.

| Cluster number | Models |
|----------------|---------|
| 1 | 1, 2, 3 |

3 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 1137 atoms, of which 243 are hydrogens and 0 are deuteriums.

- Molecule 1 is a DNA chain called DNA (5'-D(*AP*AP*TP*TP*GP*TP*GP*AP*GP*CP*G)-3').

| Mol | Chain | Residues | Atoms | | | | | | Trace |
|-----|-------|----------|-------|-----|----|----|----|----|-------|
| 1 | B | 11 | Total | C | H | N | O | P | 0 |
| | | | 252 | 109 | 25 | 44 | 64 | 10 | |

- Molecule 2 is a DNA chain called DNA (5'-D(*CP*GP*CP*TP*CP*AP*CP*AP*AP*TP*T)-3').

| Mol | Chain | Residues | Atoms | | | | | | Trace |
|-----|-------|----------|-------|-----|----|----|----|----|-------|
| 2 | C | 11 | Total | C | H | N | O | P | 0 |
| | | | 240 | 106 | 22 | 38 | 64 | 10 | |

- Molecule 3 is a protein called Lac Repressor.

| Mol | Chain | Residues | Atoms | | | | | | Trace |
|-----|-------|----------|-------|-----|----|----|----|---|-------|
| 3 | A | 51 | Total | C | H | N | O | S | 0 |
| | | | 497 | 249 | 98 | 70 | 78 | 2 | |

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

| Mol | Chain | Residues | Atoms | |
|-----|-------|----------|-------|----|
| 4 | C | 1 | Total | Na |
| | | | 1 | 1 |

- Molecule 5 is water.

| Mol | Chain | Residues | Atoms | | |
|-----|-------|----------|-------|----|----|
| 5 | B | 12 | Total | H | O |
| | | | 36 | 24 | 12 |
| 5 | C | 11 | Total | H | O |
| | | | 33 | 22 | 11 |
| 5 | A | 26 | Total | H | O |
| | | | 78 | 52 | 26 |

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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 outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

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

Chain B:  100%

A1
A2
T3
T4
G5
T6
G7
A8
G9
C10
G11

- Molecule 2: DNA (5'-D(*CP*GP*CP*TP*CP*AP*CP*AP*AP*TP*T)-3')

Chain C:  91% 9%

C1
G2
C3
T4
C5
A6
C7
A8
A9
T10
T11

- Molecule 3: Lac Repressor

Chain A:  69% 20% 6% . .

M1
R2
Y7
D8
V9
Y12
V15
S16
Y17
Q18
T19
S21
R22
Q26
R35
E36
R37
V38
Y47
R51

4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

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

Chain B:  18% 82%

A1
A2
T3
T4
G5
T6
G7
A8
G9
C10
G11

- Molecule 2: DNA (5'-D(*CP*GP*CP*TP*CP*AP*CP*AP*AP*TP*T)-3')

Chain C: 18% 82%

G1 G2 C3 T4 C5 A6 C7 A8 T10 T11

- Molecule 3: Lac Repressor

Chain A: 69% 20% 6% . .

M1 R2 P3 Y7 D8 V9 Y12 V15 S16 Y17 R22 Q26 S31 T34 R35 V38 Y47 I48 R51

4.2.2 Score per residue for model 2 (medoid)

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

Chain B: 100%

A1 A2 T3 T4 G5 T6 C7 A8 G9 C10 G11

- Molecule 2: DNA (5'-D(*CP*GP*CP*TP*CP*AP*CP*AP*AP*TP*T)-3')

Chain C: 9% 73% 18%

G1 G2 C3 T4 C5 A6 C7 A8 T10 T11

- Molecule 3: Lac Repressor

Chain A: 59% 31% 6% .

M1 R2 L6 Y7 D8 V9 A10 E11 Y12 V15 S16 Y17 Q18 T19 V20 V23 Q26 A27 S28 H29 R35 V38 E44 Y47 I48 P49 N50 R51

4.2.3 Score per residue for model 3

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

Chain B: 27% 73%

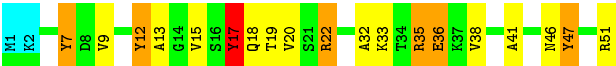
A1 A2 T3 T4 G5 T6 C7 A8 G9 C10 G11

- Molecule 2: DNA (5'-D(*CP*GP*CP*TP*CP*AP*CP*AP*AP*TP*T)-3')

Chain C: 18% 64% 18%



● Molecule 3: Lac Repressor



5 Refinement protocol and experimental data overview ⓘ

Of the ? calculated structures, 3 were deposited, based on the following criterion: ?.

The authors did not provide any information on software used for structure solution, optimization or refinement.

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality i

6.1 Standard geometry i

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

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 (average) 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 | B | 3.04±0.02 | 34±1/255 (13.5±0.5%) | 5.69±0.05 | 104±0/393 (26.5±0.1%) |
| 2 | C | 2.85±0.02 | 28±1/243 (11.4±0.5%) | 4.79±0.10 | 81±4/372 (21.9±1.0%) |
| 3 | A | 0.78±0.01 | 0±0/388 (0.0±0.0%) | 1.57±0.08 | 7±2/526 (1.3±0.3%) |
| All | All | 2.27 | 186/2658 (7.0%) | 4.18 | 578/3873 (14.9%) |

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 | Planarity |
|-----|-------|-----------|-----------|
| 1 | B | 0.0±0.0 | 9.3±1.2 |
| 2 | C | 0.0±0.0 | 9.3±0.5 |
| 3 | A | 0.0±0.0 | 5.3±1.2 |
| All | All | 0 | 72 |

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|-------|--------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | B | 8 | DA | N7-C5 | -11.68 | 1.32 | 1.39 | 1 | 3 |
| 1 | B | 7 | DG | N7-C5 | -11.33 | 1.32 | 1.39 | 3 | 3 |
| 2 | C | 8 | DA | N7-C5 | -10.94 | 1.32 | 1.39 | 2 | 3 |
| 2 | C | 9 | DA | N7-C5 | -10.64 | 1.32 | 1.39 | 2 | 3 |
| 1 | B | 1 | DA | N9-C4 | -10.55 | 1.31 | 1.37 | 3 | 3 |
| 1 | B | 9 | DG | N7-C5 | -10.54 | 1.32 | 1.39 | 1 | 3 |
| 2 | C | 6 | DA | N7-C5 | -10.11 | 1.33 | 1.39 | 3 | 3 |
| 2 | C | 4 | DT | C5-C6 | 10.11 | 1.41 | 1.34 | 3 | 3 |
| 1 | B | 2 | DA | N7-C5 | -10.07 | 1.33 | 1.39 | 1 | 3 |
| 2 | C | 2 | DG | N7-C5 | -9.31 | 1.33 | 1.39 | 3 | 3 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|-------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | B | 5 | DG | N7-C5 | -9.20 | 1.33 | 1.39 | 2 | 3 |
| 1 | B | 1 | DA | N7-C5 | -9.13 | 1.33 | 1.39 | 3 | 3 |
| 1 | B | 6 | DT | C5-C6 | 9.03 | 1.40 | 1.34 | 2 | 3 |
| 2 | C | 8 | DA | N9-C4 | -8.97 | 1.32 | 1.37 | 3 | 3 |
| 1 | B | 2 | DA | N9-C4 | -8.93 | 1.32 | 1.37 | 2 | 3 |
| 1 | B | 4 | DT | C5-C6 | 8.82 | 1.40 | 1.34 | 1 | 3 |
| 1 | B | 3 | DT | C5-C6 | 8.80 | 1.40 | 1.34 | 3 | 3 |
| 2 | C | 6 | DA | N9-C4 | -8.77 | 1.32 | 1.37 | 3 | 3 |
| 1 | B | 11 | DG | N7-C5 | -8.69 | 1.34 | 1.39 | 2 | 3 |
| 1 | B | 5 | DG | N9-C8 | -8.44 | 1.31 | 1.37 | 3 | 3 |
| 2 | C | 7 | DC | C5-C6 | 8.28 | 1.41 | 1.34 | 2 | 3 |
| 1 | B | 8 | DA | N9-C4 | -8.24 | 1.32 | 1.37 | 2 | 3 |
| 2 | C | 5 | DC | N1-C6 | 8.08 | 1.42 | 1.37 | 1 | 3 |
| 1 | B | 10 | DC | C5-C6 | 8.00 | 1.40 | 1.34 | 1 | 2 |
| 2 | C | 10 | DT | C5-C6 | 7.78 | 1.39 | 1.34 | 2 | 3 |
| 2 | C | 11 | DT | C5-C6 | 7.78 | 1.39 | 1.34 | 2 | 3 |
| 2 | C | 9 | DA | N9-C4 | -7.73 | 1.33 | 1.37 | 1 | 3 |
| 2 | C | 7 | DC | N1-C6 | 7.61 | 1.41 | 1.37 | 3 | 3 |
| 1 | B | 1 | DA | N9-C8 | -7.51 | 1.31 | 1.37 | 2 | 3 |
| 1 | B | 9 | DG | N9-C8 | -7.48 | 1.32 | 1.37 | 1 | 3 |
| 2 | C | 5 | DC | C5-C6 | 7.43 | 1.40 | 1.34 | 3 | 3 |
| 1 | B | 7 | DG | N9-C8 | -7.43 | 1.32 | 1.37 | 2 | 3 |
| 2 | C | 3 | DC | N1-C6 | 7.31 | 1.41 | 1.37 | 3 | 3 |
| 2 | C | 3 | DC | C5-C6 | 7.21 | 1.40 | 1.34 | 3 | 2 |
| 1 | B | 11 | DG | N9-C4 | -7.14 | 1.32 | 1.38 | 2 | 3 |
| 2 | C | 11 | DT | C5-C7 | 7.13 | 1.54 | 1.50 | 2 | 3 |
| 1 | B | 5 | DG | N9-C4 | -6.96 | 1.32 | 1.38 | 1 | 3 |
| 2 | C | 1 | DC | N1-C6 | 6.86 | 1.41 | 1.37 | 1 | 3 |
| 1 | B | 7 | DG | N9-C4 | -6.85 | 1.32 | 1.38 | 1 | 3 |
| 1 | B | 6 | DT | C5-C7 | 6.83 | 1.54 | 1.50 | 3 | 2 |
| 1 | B | 11 | DG | N9-C8 | -6.82 | 1.33 | 1.37 | 2 | 3 |
| 2 | C | 6 | DA | N9-C8 | -6.69 | 1.32 | 1.37 | 1 | 3 |
| 1 | B | 3 | DT | C5-C7 | 6.67 | 1.54 | 1.50 | 3 | 3 |
| 1 | B | 10 | DC | N1-C6 | 6.65 | 1.41 | 1.37 | 3 | 2 |
| 1 | B | 5 | DG | C8-N7 | 6.64 | 1.34 | 1.30 | 1 | 2 |
| 2 | C | 2 | DG | N9-C4 | -6.64 | 1.32 | 1.38 | 2 | 3 |
| 2 | C | 8 | DA | N9-C8 | -6.61 | 1.32 | 1.37 | 3 | 3 |
| 1 | B | 2 | DA | N9-C8 | -6.57 | 1.32 | 1.37 | 2 | 1 |
| 2 | C | 1 | DC | C5-C6 | 6.45 | 1.39 | 1.34 | 1 | 3 |
| 1 | B | 8 | DA | N9-C8 | -6.33 | 1.32 | 1.37 | 2 | 3 |
| 2 | C | 9 | DA | N9-C8 | -6.33 | 1.32 | 1.37 | 2 | 2 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|-------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | B | 9 | DG | N9-C4 | -6.17 | 1.33 | 1.38 | 3 | 2 |
| 1 | B | 3 | DT | N1-C6 | 6.07 | 1.42 | 1.38 | 1 | 2 |
| 2 | C | 10 | DT | C5-C7 | 6.06 | 1.53 | 1.50 | 1 | 2 |
| 1 | B | 11 | DG | C8-N7 | 5.96 | 1.34 | 1.30 | 2 | 3 |
| 2 | C | 2 | DG | N9-C8 | -5.94 | 1.33 | 1.37 | 3 | 3 |
| 2 | C | 4 | DT | C5-C7 | 5.94 | 1.53 | 1.50 | 3 | 2 |
| 1 | B | 7 | DG | C8-N7 | 5.89 | 1.34 | 1.30 | 1 | 1 |
| 2 | C | 2 | DG | C8-N7 | 5.86 | 1.34 | 1.30 | 3 | 2 |
| 1 | B | 4 | DT | C5-C7 | 5.78 | 1.53 | 1.50 | 3 | 3 |
| 1 | B | 4 | DT | N1-C6 | 5.75 | 1.42 | 1.38 | 3 | 1 |
| 2 | C | 11 | DT | C4-C5 | -5.74 | 1.39 | 1.45 | 1 | 3 |
| 1 | B | 3 | DT | N1-C2 | 5.56 | 1.42 | 1.38 | 1 | 2 |
| 2 | C | 10 | DT | C4-C5 | -5.50 | 1.40 | 1.45 | 1 | 1 |
| 2 | C | 4 | DT | C4-C5 | -5.47 | 1.40 | 1.45 | 1 | 1 |
| 2 | C | 11 | DT | N1-C6 | 5.38 | 1.42 | 1.38 | 3 | 1 |
| 1 | B | 6 | DT | C4-C5 | -5.35 | 1.40 | 1.45 | 2 | 2 |
| 1 | B | 4 | DT | C4-C5 | -5.33 | 1.40 | 1.45 | 1 | 2 |
| 1 | B | 6 | DT | N1-C2 | 5.21 | 1.42 | 1.38 | 1 | 1 |
| 2 | C | 10 | DT | N1-C6 | 5.20 | 1.41 | 1.38 | 1 | 1 |
| 1 | B | 9 | DG | C8-N7 | 5.17 | 1.34 | 1.30 | 3 | 1 |
| 1 | B | 6 | DT | N1-C6 | 5.16 | 1.41 | 1.38 | 3 | 1 |
| 1 | B | 3 | DT | C4-C5 | -5.12 | 1.40 | 1.45 | 3 | 3 |
| 1 | B | 4 | DT | N1-C2 | 5.01 | 1.42 | 1.38 | 2 | 1 |

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|----------|--------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | B | 2 | DA | C2-N3-C4 | 24.08 | 122.64 | 110.60 | 3 | 3 |
| 1 | B | 1 | DA | C2-N3-C4 | 23.57 | 122.39 | 110.60 | 1 | 3 |
| 2 | C | 6 | DA | C2-N3-C4 | 23.53 | 122.36 | 110.60 | 1 | 3 |
| 2 | C | 8 | DA | C2-N3-C4 | 23.43 | 122.32 | 110.60 | 2 | 3 |
| 2 | C | 9 | DA | C2-N3-C4 | 22.84 | 122.02 | 110.60 | 3 | 3 |
| 1 | B | 8 | DA | C2-N3-C4 | 22.53 | 121.86 | 110.60 | 1 | 3 |
| 2 | C | 8 | DA | N1-C2-N3 | -21.73 | 118.43 | 129.30 | 3 | 3 |
| 1 | B | 8 | DA | N1-C2-N3 | -21.07 | 118.77 | 129.30 | 2 | 3 |
| 1 | B | 1 | DA | N1-C2-N3 | -20.71 | 118.95 | 129.30 | 3 | 3 |
| 2 | C | 6 | DA | N1-C2-N3 | -19.87 | 119.36 | 129.30 | 1 | 3 |
| 2 | C | 2 | DG | C2-N3-C4 | 19.67 | 121.73 | 111.90 | 1 | 3 |
| 1 | B | 2 | DA | N1-C2-N3 | -19.67 | 119.47 | 129.30 | 3 | 3 |
| 1 | B | 5 | DG | C2-N3-C4 | 19.39 | 121.60 | 111.90 | 3 | 3 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|--------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | B | 9 | DG | C2-N3-C4 | 19.27 | 121.53 | 111.90 | 1 | 3 |
| 1 | B | 11 | DG | C2-N3-C4 | 19.12 | 121.46 | 111.90 | 3 | 3 |
| 1 | B | 7 | DG | C2-N3-C4 | 18.99 | 121.39 | 111.90 | 1 | 3 |
| 2 | C | 9 | DA | N1-C2-N3 | -18.75 | 119.93 | 129.30 | 3 | 3 |
| 2 | C | 2 | DG | C5-C6-N1 | 17.53 | 120.27 | 111.50 | 2 | 3 |
| 1 | B | 9 | DG | C5-C6-N1 | 17.18 | 120.09 | 111.50 | 1 | 3 |
| 1 | B | 11 | DG | C5-C6-N1 | 16.91 | 119.95 | 111.50 | 2 | 3 |
| 1 | B | 5 | DG | C5-C6-N1 | 16.48 | 119.74 | 111.50 | 3 | 3 |
| 1 | B | 5 | DG | N3-C4-C5 | -16.39 | 120.40 | 128.60 | 3 | 3 |
| 1 | B | 7 | DG | C5-C6-N1 | 16.27 | 119.64 | 111.50 | 1 | 3 |
| 1 | B | 7 | DG | N3-C4-C5 | -15.42 | 120.89 | 128.60 | 2 | 3 |
| 1 | B | 11 | DG | N3-C4-C5 | -15.30 | 120.95 | 128.60 | 3 | 3 |
| 2 | C | 2 | DG | N3-C4-C5 | -14.96 | 121.12 | 128.60 | 1 | 3 |
| 1 | B | 9 | DG | N3-C4-C5 | -13.77 | 121.72 | 128.60 | 2 | 3 |
| 1 | B | 7 | DG | C5-C6-O6 | -13.12 | 120.73 | 128.60 | 2 | 3 |
| 1 | B | 3 | DT | C2-N3-C4 | -12.93 | 119.44 | 127.20 | 3 | 3 |
| 1 | B | 6 | DT | C2-N3-C4 | -12.44 | 119.74 | 127.20 | 2 | 3 |
| 1 | B | 9 | DG | C5-C6-O6 | -12.40 | 121.16 | 128.60 | 1 | 3 |
| 1 | B | 5 | DG | C5-C6-O6 | -12.38 | 121.17 | 128.60 | 3 | 3 |
| 2 | C | 10 | DT | C2-N3-C4 | -12.32 | 119.81 | 127.20 | 2 | 3 |
| 1 | B | 3 | DT | N3-C4-C5 | 11.78 | 122.27 | 115.20 | 3 | 3 |
| 1 | B | 3 | DT | C1'-O4'-C4' | -11.78 | 98.32 | 110.10 | 2 | 2 |
| 1 | B | 11 | DG | C5-C6-O6 | -11.76 | 121.54 | 128.60 | 1 | 3 |
| 2 | C | 2 | DG | C4-C5-N7 | -11.72 | 106.11 | 110.80 | 1 | 3 |
| 1 | B | 9 | DG | N3-C4-N9 | 11.69 | 133.01 | 126.00 | 1 | 3 |
| 1 | B | 3 | DT | N3-C2-O2 | -11.66 | 115.31 | 122.30 | 1 | 3 |
| 1 | B | 2 | DA | N1-C6-N6 | -11.59 | 111.65 | 118.60 | 3 | 2 |
| 2 | C | 8 | DA | N3-C4-C5 | -11.53 | 118.73 | 126.80 | 2 | 3 |
| 1 | B | 6 | DT | N3-C4-C5 | 11.52 | 122.11 | 115.20 | 1 | 3 |
| 1 | B | 5 | DG | N3-C4-N9 | 11.41 | 132.85 | 126.00 | 3 | 3 |
| 1 | B | 4 | DT | N3-C4-C5 | 11.28 | 121.97 | 115.20 | 3 | 3 |
| 1 | B | 1 | DA | N3-C4-C5 | -11.27 | 118.91 | 126.80 | 1 | 3 |
| 1 | B | 5 | DG | C4-C5-N7 | -11.25 | 106.30 | 110.80 | 1 | 3 |
| 1 | B | 4 | DT | C2-N3-C4 | -11.19 | 120.49 | 127.20 | 3 | 3 |
| 1 | B | 6 | DT | C6-C5-C7 | -11.16 | 116.21 | 122.90 | 1 | 2 |
| 1 | B | 7 | DG | N3-C4-N9 | 10.86 | 132.52 | 126.00 | 2 | 3 |
| 2 | C | 4 | DT | C2-N3-C4 | -10.74 | 120.76 | 127.20 | 1 | 3 |
| 2 | C | 11 | DT | C2-N3-C4 | -10.70 | 120.78 | 127.20 | 1 | 3 |
| 1 | B | 9 | DG | C6-N1-C2 | -10.67 | 118.70 | 125.10 | 3 | 3 |
| 2 | C | 2 | DG | C6-N1-C2 | -10.58 | 118.75 | 125.10 | 2 | 3 |
| 3 | A | 51 | ARG | NE-CZ-NH1 | 10.56 | 125.58 | 120.30 | 3 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|--------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 2 | C | 11 | DT | N3-C2-O2 | -10.48 | 116.01 | 122.30 | 1 | 2 |
| 2 | C | 6 | DA | N3-C4-C5 | -10.31 | 119.59 | 126.80 | 1 | 3 |
| 1 | B | 9 | DG | C1'-O4'-C4' | -10.28 | 99.82 | 110.10 | 1 | 1 |
| 2 | C | 11 | DT | N3-C4-O4 | -10.24 | 113.76 | 119.90 | 1 | 3 |
| 2 | C | 8 | DA | O4'-C1'-N9 | -10.19 | 100.86 | 108.00 | 3 | 3 |
| 1 | B | 7 | DG | C4-C5-N7 | -10.12 | 106.75 | 110.80 | 1 | 3 |
| 2 | C | 9 | DA | N3-C4-C5 | -10.11 | 119.72 | 126.80 | 2 | 3 |
| 2 | C | 4 | DT | N3-C4-C5 | 10.11 | 121.27 | 115.20 | 1 | 3 |
| 1 | B | 7 | DG | C6-N1-C2 | -10.11 | 119.03 | 125.10 | 1 | 3 |
| 1 | B | 5 | DG | C6-N1-C2 | -10.11 | 119.04 | 125.10 | 1 | 3 |
| 2 | C | 6 | DA | N1-C6-N6 | -10.10 | 112.54 | 118.60 | 2 | 2 |
| 1 | B | 8 | DA | O4'-C1'-N9 | 9.98 | 114.99 | 108.00 | 1 | 1 |
| 2 | C | 9 | DA | C5-C6-N1 | 9.97 | 122.69 | 117.70 | 2 | 3 |
| 1 | B | 1 | DA | C1'-O4'-C4' | -9.97 | 100.13 | 110.10 | 3 | 2 |
| 1 | B | 11 | DG | N3-C4-N9 | 9.94 | 131.97 | 126.00 | 1 | 3 |
| 2 | C | 10 | DT | C6-C5-C7 | -9.92 | 116.95 | 122.90 | 1 | 3 |
| 1 | B | 2 | DA | N3-C4-C5 | -9.83 | 119.92 | 126.80 | 3 | 3 |
| 2 | C | 2 | DG | C5-C6-O6 | -9.77 | 122.74 | 128.60 | 2 | 3 |
| 2 | C | 10 | DT | C1'-O4'-C4' | -9.69 | 100.42 | 110.10 | 2 | 3 |
| 1 | B | 8 | DA | N3-C4-C5 | -9.60 | 120.08 | 126.80 | 3 | 3 |
| 1 | B | 11 | DG | C6-N1-C2 | -9.60 | 119.34 | 125.10 | 2 | 3 |
| 2 | C | 10 | DT | N3-C4-C5 | 9.57 | 120.94 | 115.20 | 2 | 3 |
| 1 | B | 6 | DT | N3-C4-O4 | -9.56 | 114.16 | 119.90 | 2 | 3 |
| 2 | C | 11 | DT | N3-C4-C5 | 9.56 | 120.93 | 115.20 | 2 | 3 |
| 1 | B | 2 | DA | C1'-O4'-C4' | -9.53 | 100.57 | 110.10 | 2 | 1 |
| 1 | B | 4 | DT | N1-C2-N3 | 9.48 | 120.29 | 114.60 | 1 | 3 |
| 2 | C | 8 | DA | N3-C4-N9 | 9.46 | 134.97 | 127.40 | 2 | 3 |
| 3 | A | 17 | TYR | CB-CG-CD1 | -9.46 | 115.33 | 121.00 | 1 | 1 |
| 3 | A | 12 | TYR | CB-CG-CD1 | -9.44 | 115.34 | 121.00 | 3 | 2 |
| 1 | B | 4 | DT | N3-C2-O2 | -9.42 | 116.65 | 122.30 | 1 | 3 |
| 3 | A | 47 | TYR | CB-CG-CD1 | -9.42 | 115.35 | 121.00 | 2 | 1 |
| 3 | A | 47 | TYR | CB-CG-CD2 | -9.40 | 115.36 | 121.00 | 1 | 2 |
| 1 | B | 1 | DA | C8-N9-C4 | 9.37 | 109.55 | 105.80 | 3 | 2 |
| 1 | B | 1 | DA | N7-C8-N9 | -9.31 | 109.14 | 113.80 | 3 | 3 |
| 1 | B | 5 | DG | C6-C5-N7 | 9.30 | 135.98 | 130.40 | 1 | 2 |
| 1 | B | 1 | DA | N3-C4-N9 | 9.22 | 134.78 | 127.40 | 1 | 3 |
| 2 | C | 4 | DT | N3-C2-O2 | -9.12 | 116.83 | 122.30 | 3 | 3 |
| 2 | C | 11 | DT | C1'-O4'-C4' | -9.11 | 100.99 | 110.10 | 2 | 3 |
| 1 | B | 3 | DT | N1-C2-N3 | 9.10 | 120.06 | 114.60 | 3 | 3 |
| 1 | B | 4 | DT | N3-C4-O4 | -8.99 | 114.51 | 119.90 | 3 | 3 |
| 2 | C | 2 | DG | C6-C5-N7 | 8.97 | 135.78 | 130.40 | 1 | 3 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 2 | C | 8 | DA | C5-C6-N1 | 8.95 | 122.18 | 117.70 | 2 | 3 |
| 1 | B | 6 | DT | N1-C2-N3 | 8.83 | 119.90 | 114.60 | 2 | 3 |
| 1 | B | 2 | DA | C5-C6-N1 | 8.79 | 122.10 | 117.70 | 3 | 3 |
| 1 | B | 11 | DG | C1'-O4'-C4' | -8.76 | 101.34 | 110.10 | 1 | 3 |
| 1 | B | 11 | DG | C4-C5-N7 | -8.76 | 107.30 | 110.80 | 2 | 3 |
| 1 | B | 7 | DG | C6-C5-N7 | 8.68 | 135.61 | 130.40 | 1 | 2 |
| 2 | C | 9 | DA | N1-C6-N6 | -8.66 | 113.41 | 118.60 | 1 | 1 |
| 1 | B | 6 | DT | N3-C2-O2 | -8.58 | 117.15 | 122.30 | 2 | 3 |
| 1 | B | 3 | DT | O4'-C1'-N1 | 8.55 | 113.99 | 108.00 | 2 | 2 |
| 2 | C | 2 | DG | N3-C4-N9 | 8.46 | 131.08 | 126.00 | 2 | 3 |
| 2 | C | 6 | DA | C5-C6-N1 | 8.40 | 121.90 | 117.70 | 1 | 3 |
| 3 | A | 17 | TYR | CB-CG-CD2 | -8.40 | 115.96 | 121.00 | 3 | 2 |
| 2 | C | 9 | DA | N3-C4-N9 | 8.35 | 134.08 | 127.40 | 2 | 3 |
| 1 | B | 2 | DA | N7-C8-N9 | -8.34 | 109.63 | 113.80 | 2 | 3 |
| 1 | B | 7 | DG | C3'-C2'-C1' | -8.32 | 92.51 | 102.50 | 3 | 1 |
| 1 | B | 2 | DA | C5-N7-C8 | 8.29 | 108.04 | 103.90 | 3 | 3 |
| 2 | C | 4 | DT | O4'-C1'-N1 | -8.29 | 102.20 | 108.00 | 1 | 1 |
| 1 | B | 2 | DA | C8-N9-C4 | 8.27 | 109.11 | 105.80 | 2 | 2 |
| 2 | C | 10 | DT | N1-C2-N3 | 8.20 | 119.52 | 114.60 | 2 | 3 |
| 1 | B | 2 | DA | C4-C5-N7 | -8.17 | 106.61 | 110.70 | 3 | 2 |
| 2 | C | 1 | DC | C1'-O4'-C4' | -8.14 | 101.96 | 110.10 | 1 | 2 |
| 2 | C | 10 | DT | N3-C4-O4 | -8.13 | 115.02 | 119.90 | 1 | 3 |
| 1 | B | 9 | DG | C4-C5-N7 | -8.13 | 107.55 | 110.80 | 3 | 2 |
| 1 | B | 2 | DA | C6-C5-N7 | 8.09 | 137.96 | 132.30 | 3 | 3 |
| 3 | A | 35 | ARG | NE-CZ-NH1 | 8.07 | 124.33 | 120.30 | 1 | 3 |
| 2 | C | 2 | DG | N3-C2-N2 | -8.02 | 114.28 | 119.90 | 1 | 1 |
| 1 | B | 3 | DT | N3-C4-O4 | -8.02 | 115.09 | 119.90 | 1 | 2 |
| 2 | C | 5 | DC | N3-C2-O2 | -7.97 | 116.32 | 121.90 | 1 | 1 |
| 2 | C | 2 | DG | C1'-O4'-C4' | -7.96 | 102.14 | 110.10 | 2 | 3 |
| 1 | B | 1 | DA | C5-C6-N1 | 7.90 | 121.65 | 117.70 | 1 | 3 |
| 2 | C | 10 | DT | N3-C2-O2 | -7.86 | 117.58 | 122.30 | 2 | 3 |
| 1 | B | 8 | DA | N3-C4-N9 | 7.86 | 133.69 | 127.40 | 1 | 3 |
| 2 | C | 1 | DC | N3-C4-N4 | -7.73 | 112.59 | 118.00 | 2 | 2 |
| 2 | C | 9 | DA | N7-C8-N9 | -7.72 | 109.94 | 113.80 | 3 | 3 |
| 2 | C | 2 | DG | C5-N7-C8 | 7.71 | 108.16 | 104.30 | 1 | 3 |
| 2 | C | 6 | DA | C6-C5-N7 | 7.69 | 137.68 | 132.30 | 2 | 1 |
| 2 | C | 2 | DG | N7-C8-N9 | -7.67 | 109.27 | 113.10 | 2 | 3 |
| 1 | B | 11 | DG | N7-C8-N9 | -7.59 | 109.30 | 113.10 | 2 | 2 |
| 3 | A | 22 | ARG | NE-CZ-NH2 | -7.51 | 116.54 | 120.30 | 3 | 2 |
| 2 | C | 4 | DT | N1-C2-N3 | 7.51 | 119.11 | 114.60 | 3 | 3 |
| 1 | B | 9 | DG | N1-C2-N3 | -7.44 | 119.44 | 123.90 | 1 | 2 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 2 | C | 6 | DA | N3-C4-N9 | 7.43 | 133.34 | 127.40 | 1 | 2 |
| 2 | C | 6 | DA | C4-C5-N7 | -7.41 | 106.99 | 110.70 | 2 | 1 |
| 1 | B | 11 | DG | O4'-C1'-N9 | 7.41 | 113.18 | 108.00 | 2 | 1 |
| 2 | C | 11 | DT | N1-C2-N3 | 7.40 | 119.04 | 114.60 | 1 | 3 |
| 2 | C | 5 | DC | N3-C4-N4 | -7.40 | 112.82 | 118.00 | 3 | 2 |
| 2 | C | 10 | DT | C4-C5-C7 | 7.39 | 123.43 | 119.00 | 2 | 3 |
| 2 | C | 8 | DA | N1-C6-N6 | -7.37 | 114.18 | 118.60 | 3 | 1 |
| 1 | B | 10 | DC | O4'-C1'-N1 | -7.36 | 102.85 | 108.00 | 3 | 1 |
| 1 | B | 9 | DG | C8-N9-C4 | 7.34 | 109.34 | 106.40 | 1 | 3 |
| 1 | B | 3 | DT | C5'-C4'-O4' | 7.33 | 123.23 | 109.30 | 2 | 1 |
| 2 | C | 9 | DA | C6-C5-N7 | 7.29 | 137.40 | 132.30 | 1 | 1 |
| 2 | C | 3 | DC | N3-C4-N4 | -7.28 | 112.91 | 118.00 | 3 | 1 |
| 1 | B | 7 | DG | N7-C8-N9 | -7.27 | 109.47 | 113.10 | 3 | 3 |
| 3 | A | 22 | ARG | NE-CZ-NH1 | 7.25 | 123.92 | 120.30 | 3 | 1 |
| 2 | C | 4 | DT | N3-C4-O4 | -7.21 | 115.57 | 119.90 | 2 | 3 |
| 1 | B | 11 | DG | C6-C5-N7 | 7.21 | 134.72 | 130.40 | 2 | 3 |
| 2 | C | 2 | DG | N1-C2-N3 | -7.20 | 119.58 | 123.90 | 1 | 2 |
| 2 | C | 5 | DC | C1'-O4'-C4' | -7.17 | 102.94 | 110.10 | 1 | 3 |
| 2 | C | 2 | DG | N9-C4-C5 | 7.16 | 108.26 | 105.40 | 1 | 1 |
| 2 | C | 7 | DC | N1-C2-O2 | 7.16 | 123.19 | 118.90 | 3 | 2 |
| 2 | C | 9 | DA | C1'-O4'-C4' | -7.09 | 103.01 | 110.10 | 1 | 1 |
| 1 | B | 10 | DC | N3-C4-N4 | -7.08 | 113.05 | 118.00 | 1 | 1 |
| 2 | C | 8 | DA | C1'-O4'-C4' | -7.06 | 103.04 | 110.10 | 1 | 2 |
| 3 | A | 51 | ARG | NE-CZ-NH2 | -7.03 | 116.78 | 120.30 | 2 | 2 |
| 2 | C | 1 | DC | N3-C2-O2 | -7.00 | 117.00 | 121.90 | 2 | 3 |
| 1 | B | 9 | DG | O4'-C1'-C2' | -6.97 | 100.32 | 105.90 | 1 | 1 |
| 2 | C | 2 | DG | N1-C2-N2 | 6.96 | 122.46 | 116.20 | 1 | 1 |
| 1 | B | 8 | DA | C5-C6-N1 | 6.93 | 121.17 | 117.70 | 2 | 3 |
| 2 | C | 9 | DA | C5-C6-N6 | -6.92 | 118.16 | 123.70 | 3 | 2 |
| 1 | B | 1 | DA | O4'-C1'-N9 | 6.92 | 112.84 | 108.00 | 2 | 1 |
| 2 | C | 11 | DT | C4-C5-C7 | 6.87 | 123.12 | 119.00 | 3 | 2 |
| 2 | C | 3 | DC | N3-C2-O2 | -6.86 | 117.10 | 121.90 | 1 | 3 |
| 1 | B | 7 | DG | O4'-C1'-C2' | -6.84 | 100.43 | 105.90 | 1 | 2 |
| 2 | C | 8 | DA | C5-C6-N6 | -6.84 | 118.23 | 123.70 | 2 | 1 |
| 1 | B | 7 | DG | N3-C2-N2 | -6.83 | 115.12 | 119.90 | 3 | 1 |
| 1 | B | 9 | DG | N7-C8-N9 | -6.80 | 109.70 | 113.10 | 3 | 3 |
| 2 | C | 8 | DA | O4'-C1'-C2' | -6.75 | 100.50 | 105.90 | 3 | 3 |
| 2 | C | 11 | DT | C6-C5-C7 | -6.75 | 118.85 | 122.90 | 1 | 3 |
| 1 | B | 7 | DG | C1'-O4'-C4' | -6.75 | 103.35 | 110.10 | 3 | 2 |
| 2 | C | 7 | DC | N3-C2-O2 | -6.73 | 117.19 | 121.90 | 3 | 2 |
| 3 | A | 7 | TYR | CB-CG-CD1 | -6.71 | 116.97 | 121.00 | 1 | 3 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 2 | C | 4 | DT | C4-C5-C7 | 6.70 | 123.02 | 119.00 | 1 | 2 |
| 2 | C | 9 | DA | C5'-C4'-O4' | 6.69 | 122.00 | 109.30 | 1 | 1 |
| 1 | B | 5 | DG | C5-N7-C8 | 6.66 | 107.63 | 104.30 | 1 | 2 |
| 1 | B | 9 | DG | C6-C5-N7 | 6.66 | 134.40 | 130.40 | 3 | 3 |
| 1 | B | 11 | DG | C8-N9-C4 | 6.63 | 109.05 | 106.40 | 2 | 2 |
| 2 | C | 8 | DA | C6-N1-C2 | 6.61 | 122.57 | 118.60 | 3 | 1 |
| 1 | B | 6 | DT | C1'-O4'-C4' | -6.61 | 103.49 | 110.10 | 3 | 1 |
| 1 | B | 9 | DG | O4'-C1'-N9 | 6.58 | 112.61 | 108.00 | 1 | 1 |
| 2 | C | 6 | DA | C5-N7-C8 | 6.58 | 107.19 | 103.90 | 2 | 1 |
| 1 | B | 2 | DA | N9-C4-C5 | 6.57 | 108.43 | 105.80 | 3 | 1 |
| 1 | B | 8 | DA | C4-C5-N7 | -6.54 | 107.43 | 110.70 | 3 | 1 |
| 2 | C | 8 | DA | N7-C8-N9 | -6.53 | 110.53 | 113.80 | 3 | 2 |
| 2 | C | 9 | DA | C8-N9-C4 | 6.52 | 108.41 | 105.80 | 3 | 2 |
| 2 | C | 4 | DT | C6-C5-C7 | -6.50 | 119.00 | 122.90 | 1 | 1 |
| 2 | C | 9 | DA | C5-N7-C8 | 6.49 | 107.14 | 103.90 | 3 | 2 |
| 2 | C | 3 | DC | N1-C2-O2 | 6.48 | 122.79 | 118.90 | 3 | 3 |
| 1 | B | 3 | DT | C5-C4-O4 | -6.45 | 120.38 | 124.90 | 3 | 1 |
| 2 | C | 6 | DA | N7-C8-N9 | -6.43 | 110.58 | 113.80 | 2 | 3 |
| 1 | B | 4 | DT | C5-C4-O4 | -6.42 | 120.41 | 124.90 | 1 | 1 |
| 2 | C | 6 | DA | C1'-O4'-C4' | -6.35 | 103.75 | 110.10 | 2 | 3 |
| 1 | B | 10 | DC | N3-C2-O2 | -6.34 | 117.46 | 121.90 | 3 | 1 |
| 1 | B | 5 | DG | N7-C8-N9 | -6.33 | 109.93 | 113.10 | 1 | 2 |
| 1 | B | 7 | DG | N1-C2-N2 | 6.32 | 121.89 | 116.20 | 3 | 1 |
| 1 | B | 7 | DG | C8-N9-C4 | 6.31 | 108.92 | 106.40 | 3 | 1 |
| 1 | B | 3 | DT | C6-C5-C7 | -6.29 | 119.12 | 122.90 | 2 | 2 |
| 1 | B | 2 | DA | N3-C4-N9 | 6.25 | 132.40 | 127.40 | 2 | 3 |
| 1 | B | 11 | DG | N1-C2-N3 | -6.24 | 120.16 | 123.90 | 1 | 3 |
| 1 | B | 11 | DG | C5-N7-C8 | 6.23 | 107.41 | 104.30 | 2 | 1 |
| 1 | B | 5 | DG | N9-C4-C5 | 6.20 | 107.88 | 105.40 | 1 | 1 |
| 2 | C | 2 | DG | C8-N9-C4 | 6.15 | 108.86 | 106.40 | 2 | 2 |
| 1 | B | 8 | DA | N7-C8-N9 | -6.12 | 110.74 | 113.80 | 2 | 3 |
| 2 | C | 8 | DA | C8-N9-C4 | 6.11 | 108.24 | 105.80 | 3 | 2 |
| 2 | C | 3 | DC | C1'-O4'-C4' | -6.07 | 104.03 | 110.10 | 2 | 2 |
| 1 | B | 11 | DG | N1-C6-O6 | -6.06 | 116.26 | 119.90 | 1 | 2 |
| 1 | B | 6 | DT | C4-C5-C7 | 6.04 | 122.62 | 119.00 | 2 | 1 |
| 2 | C | 6 | DA | C3'-C2'-C1' | -6.03 | 95.26 | 102.50 | 1 | 1 |
| 1 | B | 5 | DG | N1-C2-N3 | -6.02 | 120.29 | 123.90 | 3 | 1 |
| 1 | B | 7 | DG | N9-C4-C5 | 5.96 | 107.78 | 105.40 | 1 | 1 |
| 2 | C | 5 | DC | N3-C4-C5 | 5.94 | 124.28 | 121.90 | 1 | 2 |
| 1 | B | 1 | DA | C3'-C2'-C1' | -5.94 | 95.38 | 102.50 | 3 | 1 |
| 1 | B | 7 | DG | C5-N7-C8 | 5.92 | 107.26 | 104.30 | 1 | 2 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | B | 8 | DA | C5-N7-C8 | 5.89 | 106.84 | 103.90 | 3 | 2 |
| 1 | B | 3 | DT | C5-C6-N1 | -5.88 | 120.17 | 123.70 | 3 | 1 |
| 1 | B | 1 | DA | O4'-C1'-C2' | -5.87 | 101.21 | 105.90 | 1 | 1 |
| 1 | B | 7 | DG | N1-C2-N3 | -5.85 | 120.39 | 123.90 | 3 | 2 |
| 2 | C | 5 | DC | N1-C2-O2 | 5.85 | 122.41 | 118.90 | 3 | 1 |
| 2 | C | 2 | DG | N1-C6-O6 | -5.82 | 116.41 | 119.90 | 1 | 2 |
| 2 | C | 3 | DC | O4'-C1'-C2' | -5.80 | 101.26 | 105.90 | 3 | 1 |
| 2 | C | 11 | DT | C5-C4-O4 | -5.80 | 120.84 | 124.90 | 1 | 2 |
| 2 | C | 9 | DA | C4-C5-N7 | -5.79 | 107.81 | 110.70 | 1 | 1 |
| 1 | B | 9 | DG | C5-N7-C8 | 5.75 | 107.17 | 104.30 | 3 | 3 |
| 2 | C | 2 | DG | P-O3'-C3' | 5.73 | 126.58 | 119.70 | 2 | 1 |
| 2 | C | 8 | DA | C4-C5-N7 | -5.73 | 107.83 | 110.70 | 3 | 1 |
| 1 | B | 1 | DA | C6-C5-N7 | 5.72 | 136.30 | 132.30 | 2 | 2 |
| 2 | C | 1 | DC | N3-C4-C5 | 5.72 | 124.19 | 121.90 | 2 | 1 |
| 2 | C | 7 | DC | N3-C4-N4 | -5.68 | 114.03 | 118.00 | 3 | 1 |
| 1 | B | 5 | DG | C1'-O4'-C4' | -5.67 | 104.43 | 110.10 | 2 | 1 |
| 1 | B | 8 | DA | C1'-O4'-C4' | -5.65 | 104.45 | 110.10 | 3 | 2 |
| 1 | B | 4 | DT | C6-C5-C7 | -5.65 | 119.51 | 122.90 | 2 | 2 |
| 2 | C | 10 | DT | C5-C4-O4 | -5.64 | 120.95 | 124.90 | 2 | 1 |
| 1 | B | 10 | DC | C5-C4-N4 | 5.64 | 124.15 | 120.20 | 1 | 1 |
| 2 | C | 6 | DA | C8-N9-C4 | 5.64 | 108.06 | 105.80 | 3 | 2 |
| 1 | B | 3 | DT | C4-C5-C7 | 5.63 | 122.38 | 119.00 | 2 | 1 |
| 2 | C | 8 | DA | C6-C5-N7 | 5.62 | 136.24 | 132.30 | 3 | 1 |
| 1 | B | 5 | DG | P-O3'-C3' | 5.59 | 126.41 | 119.70 | 1 | 1 |
| 2 | C | 10 | DT | C5-C6-N1 | -5.55 | 120.37 | 123.70 | 3 | 1 |
| 2 | C | 4 | DT | C3'-C2'-C1' | -5.50 | 95.91 | 102.50 | 2 | 1 |
| 1 | B | 8 | DA | C6-N1-C2 | 5.49 | 121.89 | 118.60 | 2 | 1 |
| 1 | B | 3 | DT | P-O3'-C3' | 5.47 | 126.27 | 119.70 | 2 | 1 |
| 1 | B | 5 | DG | C8-N9-C4 | 5.47 | 108.59 | 106.40 | 3 | 1 |
| 1 | B | 10 | DC | O4'-C4'-C3' | 5.44 | 109.26 | 106.00 | 2 | 1 |
| 3 | A | 35 | ARG | NE-CZ-NH2 | -5.42 | 117.59 | 120.30 | 1 | 1 |
| 1 | B | 1 | DA | C5-N7-C8 | 5.42 | 106.61 | 103.90 | 3 | 1 |
| 1 | B | 9 | DG | N1-C6-O6 | -5.42 | 116.65 | 119.90 | 3 | 1 |
| 1 | B | 8 | DA | C6-C5-N7 | 5.39 | 136.08 | 132.30 | 3 | 2 |
| 2 | C | 7 | DC | C5'-C4'-O4' | 5.37 | 119.50 | 109.30 | 2 | 1 |
| 1 | B | 4 | DT | C5-C6-N1 | -5.37 | 120.48 | 123.70 | 3 | 1 |
| 1 | B | 8 | DA | O4'-C1'-C2' | -5.36 | 101.61 | 105.90 | 1 | 1 |
| 1 | B | 1 | DA | C4-C5-N7 | -5.33 | 108.03 | 110.70 | 2 | 1 |
| 2 | C | 9 | DA | P-O3'-C3' | 5.32 | 126.09 | 119.70 | 2 | 1 |
| 1 | B | 5 | DG | N1-C2-N2 | 5.31 | 120.98 | 116.20 | 2 | 1 |
| 2 | C | 7 | DC | O4'-C1'-N1 | 5.28 | 111.70 | 108.00 | 2 | 2 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | B | 2 | DA | C5-C6-N6 | -5.27 | 119.48 | 123.70 | 1 | 1 |
| 1 | B | 3 | DT | C6-N1-C2 | -5.26 | 118.67 | 121.30 | 1 | 1 |
| 1 | B | 4 | DT | C6-N1-C2 | -5.24 | 118.68 | 121.30 | 1 | 1 |
| 1 | B | 6 | DT | C5-C4-O4 | -5.18 | 121.28 | 124.90 | 1 | 1 |
| 2 | C | 3 | DC | O4'-C1'-N1 | 5.15 | 111.61 | 108.00 | 2 | 1 |
| 2 | C | 8 | DA | C5-N7-C8 | 5.15 | 106.48 | 103.90 | 3 | 1 |
| 2 | C | 8 | DA | P-O3'-C3' | 5.14 | 125.86 | 119.70 | 2 | 2 |
| 1 | B | 8 | DA | C8-N9-C4 | 5.12 | 107.85 | 105.80 | 2 | 1 |
| 2 | C | 1 | DC | C5-C4-N4 | 5.09 | 123.77 | 120.20 | 1 | 1 |
| 2 | C | 5 | DC | C5-C6-N1 | -5.09 | 118.45 | 121.00 | 1 | 1 |
| 1 | B | 10 | DC | C1'-O4'-C4' | -5.04 | 105.06 | 110.10 | 3 | 1 |
| 1 | B | 6 | DT | C5-C6-N1 | -5.01 | 120.69 | 123.70 | 3 | 1 |
| 1 | B | 9 | DG | N1-C2-N2 | 5.01 | 120.71 | 116.20 | 1 | 1 |

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Group | Models (Total) |
|-----|-------|-----|------|---------------------|----------------|
| 1 | B | 4 | DT | Sidechain | 3 |
| 1 | B | 3 | DT | Sidechain | 3 |
| 2 | C | 9 | DA | Sidechain | 3 |
| 2 | C | 5 | DC | Sidechain | 3 |
| 1 | B | 11 | DG | Sidechain | 3 |
| 3 | A | 7 | TYR | Sidechain,Mainchain | 3 |
| 2 | C | 10 | DT | Sidechain | 3 |
| 2 | C | 6 | DA | Sidechain | 3 |
| 1 | B | 5 | DG | Sidechain | 3 |
| 1 | B | 6 | DT | Sidechain | 3 |
| 2 | C | 1 | DC | Sidechain | 3 |
| 2 | C | 11 | DT | Sidechain | 3 |
| 1 | B | 7 | DG | Sidechain | 3 |
| 3 | A | 12 | TYR | Sidechain | 3 |
| 1 | B | 10 | DC | Sidechain | 2 |
| 3 | A | 17 | TYR | Sidechain | 2 |
| 1 | B | 9 | DG | Sidechain | 2 |
| 2 | C | 8 | DA | Sidechain | 2 |
| 1 | B | 1 | DA | Sidechain | 2 |
| 3 | A | 47 | TYR | Sidechain | 2 |
| 1 | B | 2 | DA | Sidechain | 2 |
| 2 | C | 2 | DG | Sidechain | 2 |

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| Mol | Chain | Res | Type | Group | Models (Total) |
|-----|-------|-----|------|-----------|----------------|
| 2 | C | 3 | DC | Sidechain | 2 |
| 2 | C | 7 | DC | Sidechain | 2 |
| 1 | B | 8 | DA | Sidechain | 2 |
| 2 | C | 4 | DT | Sidechain | 2 |
| 3 | A | 49 | PRO | Mainchain | 1 |
| 3 | A | 27 | ALA | Mainchain | 1 |
| 3 | A | 29 | HIS | Mainchain | 1 |
| 3 | A | 19 | THR | Mainchain | 1 |
| 3 | A | 11 | GLU | Mainchain | 1 |

6.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each 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 averaged over the ensemble.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 2 | C | 218 | 22 | 126 | 2±1 |
| 3 | A | 382 | 91 | 377 | 4±2 |
| 5 | A | 26 | 52 | 0 | 1±0 |
| 5 | C | 8 | 16 | 0 | 1±0 |
| All | All | 2622 | 690 | 1887 | 16 |

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 4.

All unique clashes are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 3:A:18:GLN:HG3 | 5:A:53:HOH:O | 0.68 | 1.89 | 2 | 1 |
| 2:C:4:DT:H2' | 5:A:60:HOH:O | 0.60 | 1.95 | 3 | 1 |
| 3:A:15:VAL:HG21 | 3:A:38:VAL:HG22 | 0.59 | 1.73 | 3 | 1 |
| 3:A:13:ALA:HB2 | 3:A:41:ALA:HB2 | 0.59 | 1.74 | 3 | 1 |
| 3:A:3:PRO:HA | 3:A:48:ILE:HD12 | 0.57 | 1.76 | 1 | 1 |
| 2:C:1:DC:H2' | 5:C:1958:HOH:O | 0.56 | 2.00 | 2 | 1 |
| 2:C:5:DC:H6 | 3:A:26:GLN:HE22 | 0.56 | 1.43 | 2 | 1 |
| 3:A:6:LEU:HD22 | 3:A:20:VAL:HG12 | 0.53 | 1.80 | 2 | 1 |
| 3:A:32:ALA:HA | 3:A:35:ARG:NH2 | 0.51 | 2.20 | 3 | 1 |
| 2:C:5:DC:N4 | 3:A:18:GLN:HE22 | 0.51 | 2.04 | 2 | 1 |
| 2:C:1:DC:H2' | 5:C:1817:HOH:O | 0.48 | 2.08 | 3 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 3:A:18:GLN:O | 3:A:22:ARG:HG2 | 0.47 | 2.10 | 3 | 1 |
| 3:A:33:LYS:O | 3:A:36:GLU:HB3 | 0.47 | 2.09 | 3 | 1 |
| 3:A:23:VAL:HG11 | 3:A:38:VAL:HG11 | 0.45 | 1.88 | 2 | 1 |
| 3:A:34:THR:O | 3:A:38:VAL:HG23 | 0.41 | 2.16 | 1 | 1 |
| 3:A:20:VAL:HG22 | 3:A:38:VAL:CG1 | 0.41 | 2.45 | 3 | 1 |

6.3 Torsion angles

6.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|--------------|-------------|------------|-------------|----|
| 3 | A | 48/51 (94%) | 39±1 (81±2%) | 8±1 (17±2%) | 1±1 (2±3%) | 12 | 52 |
| All | All | 144/153 (94%) | 117 (81%) | 24 (17%) | 3 (2%) | 12 | 52 |

All 3 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 3 | A | 47 | TYR | 1 |
| 3 | A | 17 | TYR | 1 |
| 3 | A | 46 | ASN | 1 |

6.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|--------------|------------|-------------|----|
| 3 | A | 41/43 (95%) | 37±1 (91±3%) | 4±1 (9±3%) | 16 | 61 |
| All | All | 123/129 (95%) | 112 (91%) | 11 (9%) | 16 | 61 |

All 7 unique residues with a non-rotameric sidechain are listed below. They are sorted by the

frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 3 | A | 9 | VAL | 3 |
| 3 | A | 15 | VAL | 2 |
| 3 | A | 17 | TYR | 2 |
| 3 | A | 36 | GLU | 1 |
| 3 | A | 26 | GLN | 1 |
| 3 | A | 31 | SER | 1 |
| 3 | A | 44 | GLU | 1 |

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided