



Full wwPDB NMR Structure Validation Report ⓘ

Mar 12, 2026 – 02:09 PM UTC

PDB ID : 149D / pdb_0000149d
Title : SOLUTION STRUCTURE OF A PYRIMIDINE(DOT)PURINE(DOT)
) PYRIMIDINE DNA TRIPLEX CONTAINING T(DOT)AT, C+(DOT)GC
 AND G(DOT)TA TRIPLES
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Deposited on : 1993-11-15

This is a Full wwPDB NMR 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/NMRValidationReportHelp>

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>.

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

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

2 Ensemble composition and analysis

This entry contains 14 models. This entry does not contain polypeptide chains, therefore identification of well-defined residues and clustering analysis are not possible. All residues are included in the validation scores.

3 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 664 atoms, of which 247 are hydrogens and 0 are deuteriums.

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

| Mol | Chain | Residues | Atoms | | | | | Trace | |
|-----|-------|----------|-------|----|----|----|----|-------|---|
| | | | Total | C | H | N | O | | P |
| 1 | A | 7 | 217 | 67 | 82 | 20 | 42 | 6 | 0 |

- Molecule 2 is a DNA chain called 5'-D(*GP*AP*AP*TP*AP*GP*G)-3'.

| Mol | Chain | Residues | Atoms | | | | | Trace | |
|-----|-------|----------|-------|----|----|----|----|-------|---|
| | | | Total | C | H | N | O | | P |
| 2 | B | 7 | 226 | 70 | 80 | 32 | 38 | 6 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | Trace | |
|-----|-------|----------|-------|----|----|----|----|-------|---|
| | | | Total | C | H | N | O | | P |
| 3 | C | 7 | 221 | 67 | 85 | 20 | 43 | 6 | 0 |

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide 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: 5'-D(*CP*CP*TP*AP*TP*TP*C)-3'



- Molecule 2: 5'-D(*GP*AP*AP*TP*AP*GP*G)-3'



- Molecule 3: 5'-D(*CP*TP*TP*GP*TP*CP*C)-3'



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: 5'-D(*CP*CP*TP*AP*TP*TP*C)-3'




- Molecule 2: 5'-D(*GP*AP*AP*TP*AP*GP*G)-3'

Chain B:  100%

G8
A9
A10
T11
A12
G13
G14

- Molecule 3: 5'-D(*CP*TP*TP*GP*TP*CP*C)-3'

Chain C:  100%

C15
T16
T17
G18
T19
C20
C21


4.2.2 Score per residue for model 2

- Molecule 1: 5'-D(*CP*CP*TP*AP*TP*TP*C)-3'

Chain A:  14% 86%


C1
C2
T3
A4
T5
T6
C7

- Molecule 2: 5'-D(*GP*AP*AP*TP*AP*GP*G)-3'

Chain B:  14% 86%

G8
A9
A10
T11
A12
G13
G14

- Molecule 3: 5'-D(*CP*TP*TP*GP*TP*CP*C)-3'

Chain C:  100%

C15
T16
T17
G18
T19
C20
C21


4.2.3 Score per residue for model 3

- Molecule 1: 5'-D(*CP*CP*TP*AP*TP*TP*C)-3'

Chain A:  14% 86%

C1
C2
T3
A4
T5
T6
C7

- Molecule 2: 5'-D(*GP*AP*AP*TP*AP*GP*G)-3'

Chain B:  14% 86%

G8
A9
A10
T11
A12
G13
G14

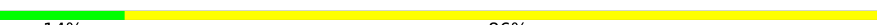
- Molecule 3: 5'-D(*CP*TP*TP*GP*TP*CP*C)-3'

Chain C:  100%

G15
T16
T17
G18
T19
C20
C21

4.2.4 Score per residue for model 4

- Molecule 1: 5'-D(*CP*CP*TP*AP*TP*TP*C)-3'

Chain A:  14% 86%


G1
C2
T3
A4
T5
T6
G7

- Molecule 2: 5'-D(*GP*AP*AP*TP*AP*GP*G)-3'

Chain B:  100%

G8
A9
A10
T11
A12
G13
G14

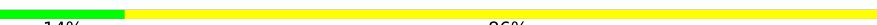
- Molecule 3: 5'-D(*CP*TP*TP*GP*TP*CP*C)-3'

Chain C:  86% 14%

G15
T16
T17
G18
T19
C20
C21

4.2.5 Score per residue for model 5

- Molecule 1: 5'-D(*CP*CP*TP*AP*TP*TP*C)-3'

Chain A:  14% 86%

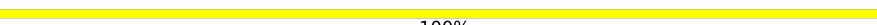
G1
C2
T3
A4
T5
T6
G7

- Molecule 2: 5'-D(*GP*AP*AP*TP*AP*GP*G)-3'

Chain B:  14% 86%

G8
A9
A10
T11
A12
G13
G14

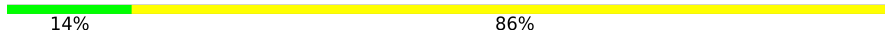
- Molecule 3: 5'-D(*CP*TP*TP*GP*TP*CP*C)-3'

Chain C:  100%

G15
T16
T17
G18
T19
C20
C21

4.2.6 Score per residue for model 6

- Molecule 1: 5'-D(*CP*CP*TP*AP*TP*TP*C)-3'

Chain A:  14% 86%

G1
C2
T3
A4
T5
T6
G7

- Molecule 2: 5'-D(*GP*AP*AP*TP*AP*GP*G)-3'

Chain B:  14% 86%

G8
A9
A10
T11
A12
G13
G14

- Molecule 3: 5'-D(*CP*TP*TP*GP*TP*CP*C)-3'

Chain C:  100%

G15
T16
T17
G18
T19
C20
C21

4.2.7 Score per residue for model 7

- Molecule 1: 5'-D(*CP*CP*TP*AP*TP*TP*C)-3'

Chain A:  14% 86%

G1
C2
T3
A4
T5
T6
G7

- Molecule 2: 5'-D(*GP*AP*AP*TP*AP*GP*G)-3'

Chain B:  14% 86%

G8
A9
A10
T11
A12
G13
G14


- Molecule 3: 5'-D(*CP*TP*TP*GP*TP*CP*C)-3'

Chain C:  14% 86%

G15
T16
T17
G18
T19
C20
C21


4.2.8 Score per residue for model 8

- Molecule 1: 5'-D(*CP*CP*TP*AP*TP*TP*C)-3'

Chain A:  14% 86%

C1 C2 T3 A4 T5 T6 C7

- Molecule 2: 5'-D(*GP*AP*AP*TP*AP*GP*G)-3'

Chain B:  14% 86%

G8 A9 A10 T11 A12 G13 G14


- Molecule 3: 5'-D(*CP*TP*TP*GP*TP*CP*C)-3'

Chain C:  14% 86%

C15 T16 T17 G18 T19 C20 C21

4.2.9 Score per residue for model 9

- Molecule 1: 5'-D(*CP*CP*TP*AP*TP*TP*C)-3'

Chain A:  14% 86%

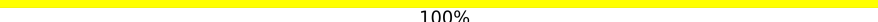
C1 C2 T3 A4 T5 T6 C7

- Molecule 2: 5'-D(*GP*AP*AP*TP*AP*GP*G)-3'

Chain B:  100%

G8 A9 A10 T11 A12 G13 G14

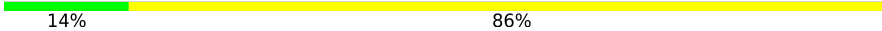
- Molecule 3: 5'-D(*CP*TP*TP*GP*TP*CP*C)-3'

Chain C:  100%

C15 T16 T17 G18 T19 C20 C21

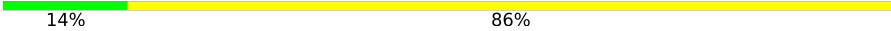
4.2.10 Score per residue for model 10

- Molecule 1: 5'-D(*CP*CP*TP*AP*TP*TP*C)-3'

Chain A:  14% 86%

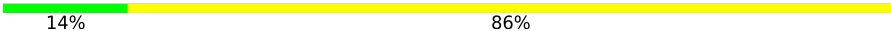
C1 C2 T3 A4 T5 T6 C7

- Molecule 2: 5'-D(*GP*AP*AP*TP*AP*GP*G)-3'

Chain B:  14% 86%

G8 A9 A10 T11 A12 G13 G14

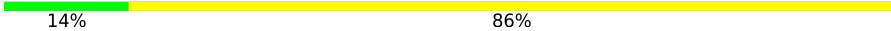
- Molecule 3: 5'-D(*CP*TP*TP*GP*TP*CP*C)-3'

Chain C:  14% 86%

G15 T16 T17 G18 T19 C20 C21

4.2.11 Score per residue for model 11

- Molecule 1: 5'-D(*CP*CP*TP*AP*TP*TP*C)-3'

Chain A:  14% 86%

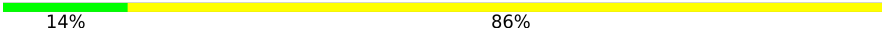
C1 C2 T3 A4 T5 T6 C7

- Molecule 2: 5'-D(*GP*AP*AP*TP*AP*GP*G)-3'

Chain B:  100%

G8 A9 A10 T11 A12 G13 G14

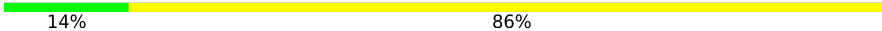
- Molecule 3: 5'-D(*CP*TP*TP*GP*TP*CP*C)-3'

Chain C:  14% 86%

G15 T16 T17 G18 T19 C20 C21

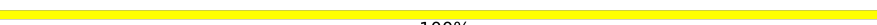
4.2.12 Score per residue for model 12

- Molecule 1: 5'-D(*CP*CP*TP*AP*TP*TP*C)-3'

Chain A:  14% 86%

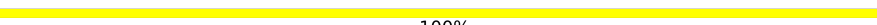
C1 C2 T3 A4 T5 T6 C7

- Molecule 2: 5'-D(*GP*AP*AP*TP*AP*GP*G)-3'

Chain B:  100%

G8
A9
A10
T11
A12
G13
G14

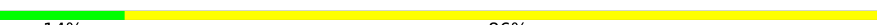
- Molecule 3: 5'-D(*CP*TP*TP*GP*TP*CP*C)-3'

Chain C:  100%

G15
T16
T17
G18
T19
C20
C21

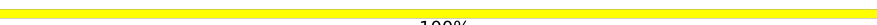
4.2.13 Score per residue for model 13

- Molecule 1: 5'-D(*CP*CP*TP*AP*TP*TP*C)-3'

Chain A:  14% 86%

G1
C2
T3
A4
T5
T6
C7

- Molecule 2: 5'-D(*GP*AP*AP*TP*AP*GP*G)-3'

Chain B:  100%

G8
A9
A10
T11
A12
G13
G14

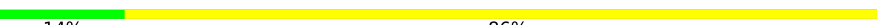
- Molecule 3: 5'-D(*CP*TP*TP*GP*TP*CP*C)-3'

Chain C:  100%

G15
T16
T17
G18
T19
C20
C21

4.2.14 Score per residue for model 14

- Molecule 1: 5'-D(*CP*CP*TP*AP*TP*TP*C)-3'

Chain A:  14% 86%

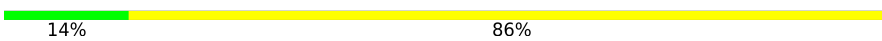
G1
C2
T3
A4
T5
T6
C7

- Molecule 2: 5'-D(*GP*AP*AP*TP*AP*GP*G)-3'

Chain B:  100%

G8
A9
A10
T11
A12
G13
G14

- Molecule 3: 5'-D(*CP*TP*TP*GP*TP*CP*C)-3'

Chain C:  14% 86%

G15
T16
T17
G18
T19
C20
G21

5 Refinement protocol and experimental data overview

The models were refined using the following method: ?.

Of the ? calculated structures, 14 were deposited, based on the following criterion: ?.

The following table shows the software used for structure solution, optimisation and refinement.

| Software name | Classification | Version |
|---------------|----------------|---------|
| X-PLOR | refinement | |

No chemical shift data was provided.

6 Model quality i

6.1 Standard geometry i

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (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 | A | 1.80±0.04 | 0±1/149 (0.3± 0.6%) | 2.14±0.07 | 8±1/227 (3.7± 0.4%) |
| 2 | B | 1.76±0.04 | 2±1/165 (1.1± 0.5%) | 2.47±0.07 | 15±3/254 (6.0± 1.0%) |
| 3 | C | 1.87±0.06 | 2±1/150 (1.2± 0.7%) | 2.37±0.07 | 11±2/229 (4.9± 0.7%) |
| All | All | 1.81 | 57/6496 (0.9%) | 2.34 | 486/9940 (4.9%) |

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 |
| 3 | C | 18 | DG | N1-C2 | -6.48 | 1.25 | 1.38 | 13 | 13 |
| 2 | B | 11 | DT | C4-C5 | 6.23 | 1.56 | 1.44 | 10 | 2 |
| 1 | A | 5 | DT | N3-C4 | -5.74 | 1.27 | 1.38 | 4 | 1 |
| 1 | A | 5 | DT | O3'-P | -5.59 | 1.52 | 1.61 | 14 | 1 |
| 3 | C | 17 | DT | N3-C4 | -5.51 | 1.27 | 1.38 | 14 | 1 |
| 2 | B | 13 | DG | N1-C2 | -5.50 | 1.26 | 1.38 | 13 | 11 |
| 3 | C | 16 | DT | C4-C5 | 5.50 | 1.55 | 1.44 | 9 | 3 |
| 3 | C | 18 | DG | C5-C4 | 5.48 | 1.49 | 1.38 | 14 | 3 |
| 3 | C | 17 | DT | C4-C5 | 5.47 | 1.55 | 1.44 | 4 | 2 |
| 3 | C | 16 | DT | N3-C4 | -5.47 | 1.27 | 1.38 | 4 | 1 |
| 3 | C | 19 | DT | C4-C5 | 5.35 | 1.55 | 1.44 | 10 | 2 |
| 3 | C | 19 | DT | N3-C4 | -5.33 | 1.28 | 1.38 | 9 | 1 |
| 1 | A | 6 | DT | N3-C4 | -5.29 | 1.28 | 1.38 | 9 | 1 |
| 2 | B | 8 | DG | N1-C2 | -5.26 | 1.27 | 1.38 | 14 | 8 |
| 2 | B | 14 | DG | N1-C2 | -5.25 | 1.27 | 1.38 | 4 | 3 |
| 1 | A | 6 | DT | C4-C5 | 5.17 | 1.54 | 1.44 | 14 | 1 |
| 2 | B | 11 | DT | N3-C4 | -5.15 | 1.28 | 1.38 | 10 | 1 |
| 1 | A | 3 | DT | C4-C5 | 5.13 | 1.54 | 1.44 | 2 | 1 |
| 1 | A | 5 | DT | C4-C5 | 5.12 | 1.54 | 1.44 | 14 | 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 |
| 3 | C | 16 | DT | O3'-P-O5' | 11.54 | 121.31 | 104.00 | 3 | 14 |
| 3 | C | 20 | DC | O3'-P-O5' | 11.06 | 120.58 | 104.00 | 5 | 14 |
| 1 | A | 2 | DC | O3'-P-O5' | 9.99 | 118.99 | 104.00 | 14 | 14 |
| 2 | B | 12 | DA | O3'-P-O5' | 9.47 | 118.21 | 104.00 | 3 | 14 |
| 2 | B | 13 | DG | O3'-P-O5' | 9.42 | 118.13 | 104.00 | 7 | 14 |
| 3 | C | 18 | DG | O3'-P-O5' | 9.35 | 118.03 | 104.00 | 1 | 14 |
| 3 | C | 17 | DT | O3'-P-O5' | 9.32 | 117.99 | 104.00 | 9 | 14 |
| 1 | A | 4 | DA | O3'-P-O5' | 9.02 | 117.53 | 104.00 | 3 | 14 |
| 2 | B | 9 | DA | O3'-P-O5' | 9.01 | 117.51 | 104.00 | 9 | 14 |
| 1 | A | 3 | DT | O3'-P-O5' | 8.75 | 117.13 | 104.00 | 3 | 14 |
| 3 | C | 19 | DT | O3'-P-O5' | 8.56 | 116.84 | 104.00 | 1 | 13 |
| 3 | C | 15 | DC | O3'-P-O5' | 8.52 | 116.77 | 104.00 | 7 | 14 |
| 2 | B | 8 | DG | O3'-P-O5' | 8.43 | 116.64 | 104.00 | 14 | 14 |
| 2 | B | 10 | DA | O3'-P-O5' | 8.14 | 116.20 | 104.00 | 3 | 14 |
| 2 | B | 11 | DT | O3'-P-O5' | 8.02 | 116.03 | 104.00 | 13 | 14 |
| 1 | A | 1 | DC | O3'-P-O5' | 7.74 | 115.61 | 104.00 | 9 | 14 |
| 1 | A | 5 | DT | O3'-P-O5' | 7.51 | 115.26 | 104.00 | 6 | 14 |
| 2 | B | 10 | DA | N1-C6-N6 | -7.45 | 107.83 | 119.00 | 14 | 14 |
| 1 | A | 6 | DT | O3'-P-O5' | 7.33 | 115.00 | 104.00 | 2 | 14 |
| 3 | C | 17 | DT | N1-C1'-C2' | 7.25 | 124.38 | 113.50 | 4 | 11 |
| 3 | C | 19 | DT | C6-C5-C7 | -7.22 | 113.17 | 124.00 | 9 | 13 |
| 2 | B | 10 | DA | O4'-C1'-N9 | 6.64 | 118.35 | 108.40 | 3 | 3 |
| 1 | A | 6 | DT | N3-C4-O4 | -6.62 | 112.68 | 122.60 | 9 | 4 |
| 2 | B | 12 | DA | N1-C6-N6 | -6.37 | 109.45 | 119.00 | 10 | 14 |
| 3 | C | 17 | DT | O4'-C1'-N1 | -6.29 | 98.96 | 108.40 | 6 | 3 |
| 3 | C | 18 | DG | N3-C4-N9 | 6.11 | 135.17 | 126.00 | 10 | 8 |
| 1 | A | 4 | DA | N1-C6-N6 | -6.06 | 109.91 | 119.00 | 13 | 5 |
| 1 | A | 5 | DT | N3-C4-O4 | -6.01 | 113.59 | 122.60 | 14 | 3 |
| 1 | A | 4 | DA | C5-C6-N1 | 6.01 | 126.61 | 117.60 | 5 | 13 |
| 2 | B | 10 | DA | C6-C5-N7 | 5.97 | 141.25 | 132.30 | 9 | 3 |
| 2 | B | 10 | DA | C5-C6-N1 | 5.92 | 126.47 | 117.60 | 4 | 9 |
| 3 | C | 19 | DT | N3-C4-O4 | -5.91 | 113.73 | 122.60 | 14 | 9 |
| 2 | B | 14 | DG | N3-C4-N9 | 5.88 | 134.83 | 126.00 | 14 | 6 |
| 2 | B | 11 | DT | N3-C4-O4 | -5.87 | 113.79 | 122.60 | 10 | 7 |
| 3 | C | 18 | DG | N3-C4-C5 | -5.80 | 119.70 | 128.40 | 10 | 7 |
| 2 | B | 8 | DG | N3-C4-N9 | 5.76 | 134.63 | 126.00 | 3 | 2 |
| 3 | C | 20 | DC | N1-C2-O2 | 5.74 | 127.82 | 119.20 | 3 | 7 |
| 2 | B | 10 | DA | C2-N3-C4 | 5.74 | 119.40 | 110.80 | 9 | 6 |
| 2 | B | 13 | DG | N3-C4-N9 | 5.68 | 134.51 | 126.00 | 11 | 3 |
| 2 | B | 12 | DA | C5-C6-N1 | 5.62 | 126.03 | 117.60 | 9 | 10 |
| 2 | B | 12 | DA | C6-C5-N7 | 5.61 | 140.71 | 132.30 | 14 | 6 |
| 2 | B | 9 | DA | N1-C6-N6 | -5.59 | 110.62 | 119.00 | 1 | 7 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | A | 4 | DA | C2-N3-C4 | 5.58 | 119.16 | 110.80 | 5 | 5 |
| 2 | B | 9 | DA | C5-C6-N1 | 5.57 | 125.95 | 117.60 | 14 | 11 |
| 3 | C | 21 | DC | N1-C2-O2 | 5.47 | 127.41 | 119.20 | 2 | 6 |
| 2 | B | 12 | DA | C2-N3-C4 | 5.47 | 119.00 | 110.80 | 9 | 8 |
| 2 | B | 9 | DA | C5'-C4'-C3' | 5.47 | 123.11 | 114.90 | 10 | 1 |
| 2 | B | 11 | DT | N1-C2-N3 | 5.45 | 122.98 | 114.80 | 10 | 1 |
| 3 | C | 20 | DC | N3-C2-O2 | -5.44 | 113.74 | 121.90 | 10 | 1 |
| 2 | B | 14 | DG | O4'-C1'-N9 | 5.44 | 116.56 | 108.40 | 14 | 1 |
| 3 | C | 16 | DT | N3-C4-O4 | -5.42 | 114.48 | 122.60 | 10 | 4 |
| 3 | C | 21 | DC | O4'-C1'-N1 | -5.39 | 100.32 | 108.40 | 13 | 1 |
| 3 | C | 21 | DC | O5'-C5'-C4' | 5.36 | 118.84 | 110.80 | 1 | 1 |
| 2 | B | 9 | DA | C6-C5-N7 | 5.26 | 140.19 | 132.30 | 5 | 2 |
| 2 | B | 14 | DG | N3-C4-C5 | -5.24 | 120.54 | 128.40 | 11 | 4 |
| 1 | A | 4 | DA | C6-C5-N7 | 5.22 | 140.12 | 132.30 | 14 | 1 |
| 2 | B | 9 | DA | C2-N3-C4 | 5.21 | 118.62 | 110.80 | 14 | 6 |
| 3 | C | 17 | DT | N3-C4-O4 | -5.11 | 114.94 | 122.60 | 9 | 1 |
| 2 | B | 8 | DG | N3-C4-C5 | -5.10 | 120.75 | 128.40 | 3 | 3 |
| 2 | B | 13 | DG | N3-C4-C5 | -5.07 | 120.80 | 128.40 | 9 | 2 |
| 1 | A | 3 | DT | N3-C4-O4 | -5.06 | 115.01 | 122.60 | 10 | 1 |
| 3 | C | 16 | DT | P-O3'-C3' | 5.01 | 127.72 | 120.20 | 6 | 1 |
| 2 | B | 8 | DG | C3'-C2'-C1' | 5.01 | 109.11 | 101.60 | 10 | 1 |

There are no chirality outliers.

There are no planarity outliers.

6.2 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 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 |
|-----|-------|-------|----------|----------|---------|
| 3 | C | 136 | 85 | 79 | 0±0 |
| All | All | 5838 | 3458 | 3269 | 1 |

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 0.

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

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|----------------|----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 3:C:20:DC:H2'' | 3:C:21:DC:H5'' | 0.41 | 1.92 | 4 | 1 |

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

6.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

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 oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

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