



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 01:48 AM UTC

PDB ID : 2CHK / pdb_00002chk
Title : NMR structure of TLLLLT quadruplex
Authors : Nielsen, J.T.; Petersen, M.
Deposited on : 2006-03-15

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
Mogul	:	2022.3.0, CSD as543be (2022)
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

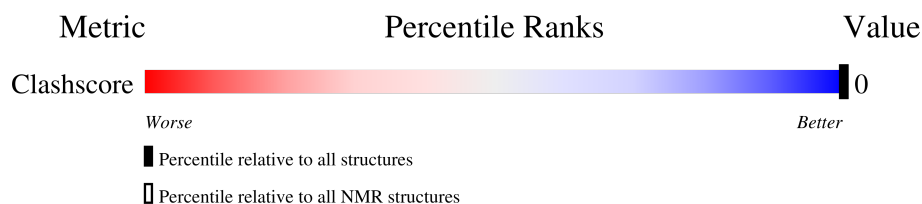
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

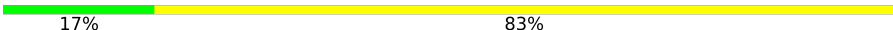
The overall completeness of chemical shifts assignment was not calculated.

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	229148	14424

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	A	6	 17% 83%
1	B	6	 17% 83%
1	C	6	 17% 83%
1	D	6	 17% 83%

2 Ensemble composition and analysis ⓘ

This entry contains 20 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 is only 1 type of molecule in this entry. The entry contains 812 atoms, of which 280 are hydrogens and 0 are deuteriums.

- Molecule 1 is a DNA chain called 5'-D(*T LCG LCG LCG LCGP*TP)-3'.

Mol	Chain	Residues	Atoms						Trace
1	A	6	Total	C	H	N	O	P	0
			203	64	70	24	40	5	
1	B	6	Total	C	H	N	O	P	0
			203	64	70	24	40	5	
1	C	6	Total	C	H	N	O	P	0
			203	64	70	24	40	5	
1	D	6	Total	C	H	N	O	P	0
			203	64	70	24	40	5	

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(*T LCG LCG LCG LCGP*TP)-3'



- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'



- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'



- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

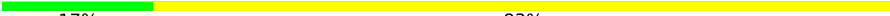


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain A:  17% 83%

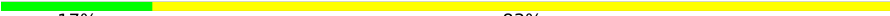
T1
G2
G3
G4
G5
T6

- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain B:  100%

T7
G8
G9
G10
G11
T12

- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain C:  17% 83%

T13
G14
G15
G16
G17
T18

- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain D:  33% 67%

T19
G20
G21
G22
G23
T24

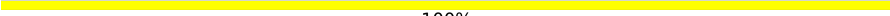
4.2.2 Score per residue for model 2

- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain A:  17% 83%

T1
G2
G3
G4
G5
T6

- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain B:  100%

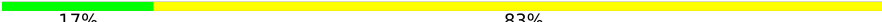
T7
G8
G9
G10
G11
T12

- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain C:  100%

T13
G14
G15
G16
G17
T18

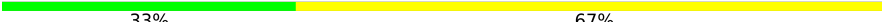
- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain D:  17% 83%

T19
G20
G21
G22
G23
T24

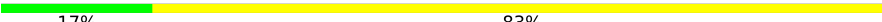
4.2.3 Score per residue for model 3

- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain A:  33% 67%

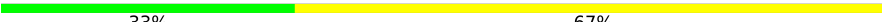
T1
G2
G3
G4
G5
T6

- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain B:  17% 83%

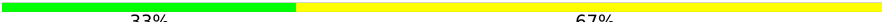
T7
G8
G9
G10
G11
T12

- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain C:  33% 67%

T13
G14
G15
G16
G17
T18

- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain D:  33% 67%

T19
G20
G21
G22
G23
T24

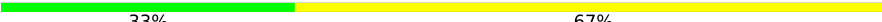
4.2.4 Score per residue for model 4

- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain A:  17% 83%

T1
G2
G3
G4
G5
T6

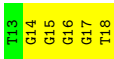
- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain B:  33% 67%

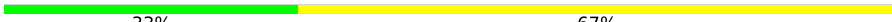
T7
G8
G9
G10
G11
T12

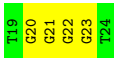
- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain C:  17% 83%

 T13 G14 G15 G16 G17 T18

- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

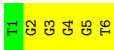
Chain D:  33% 67%

 T19 G20 G21 G22 G23 T24

4.2.5 Score per residue for model 5

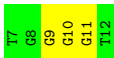
- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain A:  17% 83%

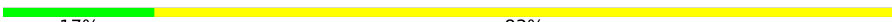
 T1 G2 G3 G4 G5 T6

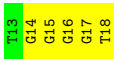
- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain B:  50% 50%

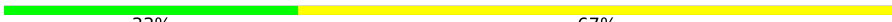
 T7 G8 G9 G10 G11 T12

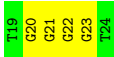
- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain C:  17% 83%

 T13 G14 G15 G16 G17 T18

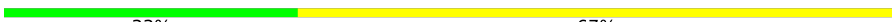
- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

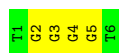
Chain D:  33% 67%

 T19 G20 G21 G22 G23 T24

4.2.6 Score per residue for model 6

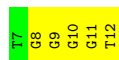
- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain A:  33% 67%



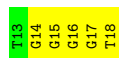
- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain B: 17% 83%



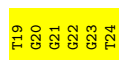
- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain C: 17% 83%



- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

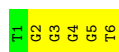
Chain D: 100%



4.2.7 Score per residue for model 7

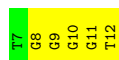
- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain A: 17% 83%



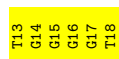
- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain B: 17% 83%



- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain C: 100%



- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain D: 33% 67%

T19
G20
G21
G22
G23
T24

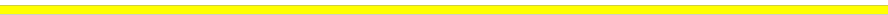
4.2.8 Score per residue for model 8

- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain A:  100%

T1
G2
G3
G4
G5
T6

- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain B:  100%

T7
G8
G9
G10
G11
T12

- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain C:  17%  83%

T13
G14
G15
G16
G17
T18

- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain D:  100%

T19
G20
G21
G22
G23
T24

4.2.9 Score per residue for model 9

- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain A:  17%  83%

T1
G2
G3
G4
G5
T6

- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain B:  17%  83%

T7
G8
G9
G10
G11
T12

- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain C:  100%

T13
G14
G15
G16
G17
T18

- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain D:  33% 67%

T19
G20
G21
G22
G23
T24

4.2.10 Score per residue for model 10

- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain A:  33% 67%

T1
G2
G3
G4
G5
T6

- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain B:  17% 83%

T7
G8
G9
G10
G11
T12

- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain C:  33% 67%

T13
G14
G15
G16
G17
T18

- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain D:  17% 83%

T19
G20
G21
G22
G23
T24

4.2.11 Score per residue for model 11

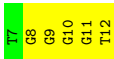
- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain A:  17% 83%

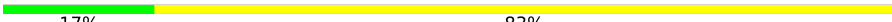
T1
G2
G3
G4
G5
T6

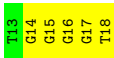
- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain B:  17% 83%

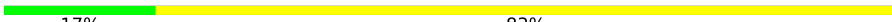
 T7 G8 G9 G10 G11 T12

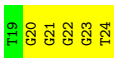
- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain C:  17% 83%

 T13 G14 G15 G16 G17 T18

- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

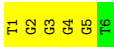
Chain D:  17% 83%

 T19 G20 G21 G22 G23 T24

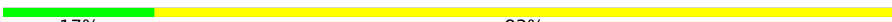
4.2.12 Score per residue for model 12

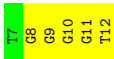
- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain A:  17% 83%

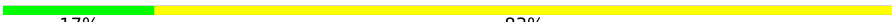
 T1 G2 G3 G4 G5 T6

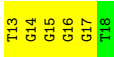
- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain B:  17% 83%

 T7 G8 G9 G10 G11 T12

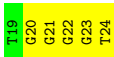
- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain C:  17% 83%

 T13 G14 G15 G16 G17 T18

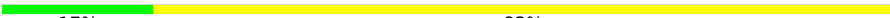
- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

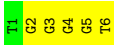
Chain D:  17% 83%

 T19 G20 G21 G22 G23 T24

4.2.13 Score per residue for model 13

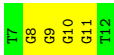
- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain A:  17% 83%

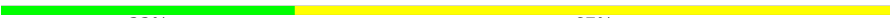
 T1 G2 G3 G4 G5 T6

- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain B:  33% 67%

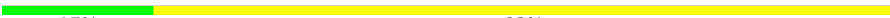
 T7 G8 G9 G10 G11 T12

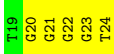
- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain C:  33% 67%

 T13 G14 G15 G16 G17 T18

- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

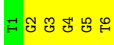
Chain D:  17% 83%

 T19 G20 G21 G22 G23 T24

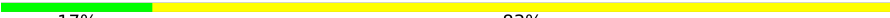
4.2.14 Score per residue for model 14

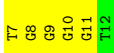
- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain A:  17% 83%

 T1 G2 G3 G4 G5 T6

- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain B:  17% 83%

 T7 G8 G9 G10 G11 T12

- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain C:  100%

T13
G14
G15
G16
G17
T18

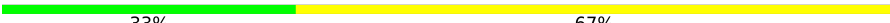
- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain D:  50% 50%

T19
G20
G21
G22
G23
T24

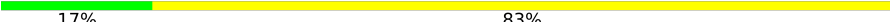
4.2.15 Score per residue for model 15

- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain A:  33% 67%

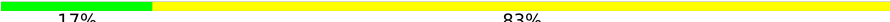
T1
G2
G3
G4
G5
T6

- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain B:  17% 83%

T7
G8
G9
G10
G11
T12

- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain C:  17% 83%

T13
G14
G15
G16
G17
T18

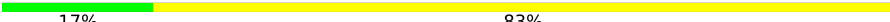
- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain D:  33% 67%

T19
G20
G21
G22
G23
T24

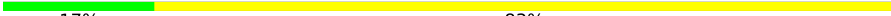
4.2.16 Score per residue for model 16

- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain A:  17% 83%

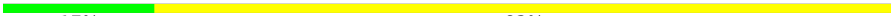
T1
G2
G3
G4
G5
T6

- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain B:  17% 83%

T7 G8 G9 G10 G11 T12

- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain C:  17% 83%

T13 G14 G15 G16 G17 T18

- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain D:  100%

T19 G20 G21 G22 G23 T24

4.2.17 Score per residue for model 17

- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain A:  17% 83%

T1 G2 G3 G4 G5 T6

- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain B:  100%

T7 G8 G9 G10 G11 T12

- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain C:  33% 67%

T13 G14 G15 G16 G17 T18

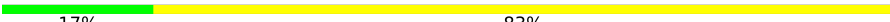
- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain D:  33% 67%

T19 G20 G21 G22 G23 T24

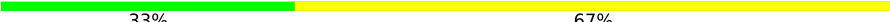
4.2.18 Score per residue for model 18

- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain A:  17% 83%

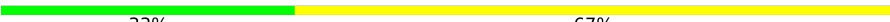
T1 G2 G3 G4 G5 T6

- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain B:  33% 67%

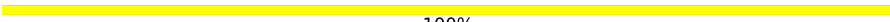
T7 G8 G9 G10 G11 T12

- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain C:  33% 67%

T13 G14 G15 G16 G17 T18

- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain D:  100%

T19 G20 G21 G22 G23 T24

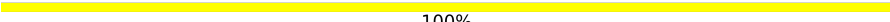
4.2.19 Score per residue for model 19

- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain A:  50% 50%

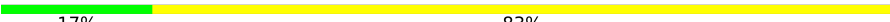
T1 G2 G3 G4 G5 T6

- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain B:  100%

T7 G8 G9 G10 G11 T12

- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain C:  17% 83%

T13
G14
G15
G16
G17
T18

- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain D:  17% 83%

T19
G20
G21
G22
G23
T24

4.2.20 Score per residue for model 20

- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain A:  17% 83%

T1
G2
G3
G4
G5
T6

- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain B:  17% 83%

T7
G8
G9
G10
G11
T12

- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain C:  17% 83%

T13
G14
G15
G16
G17
T18

- Molecule 1: 5'-D(*T LCG LCG LCG LCGP*TP)-3'

Chain D:  17% 83%

T19
G20
G21
G22
G23
T24

5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 20 calculated structures, 20 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	3.1
X-PLOR	structure solution	

No chemical shift data was provided.

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: LCG

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	0.82±0.04	0±0/39 (0.0± 0.0%)	1.60±0.17	0±0/56 (0.3± 0.6%)
1	B	0.82±0.04	0±0/39 (0.0± 0.0%)	1.69±0.15	0±1/56 (0.8± 1.1%)
1	C	0.82±0.04	0±0/39 (0.0± 0.0%)	1.63±0.16	0±1/56 (0.5± 1.1%)
1	D	0.81±0.04	0±0/39 (0.0± 0.0%)	1.65±0.16	0±0/56 (0.4± 0.8%)
All	All	0.82	0/3120 (0.0%)	1.65	23/4480 (0.5%)

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	A	0.0±0.0	0.7±0.5
1	B	0.0±0.0	0.7±0.7
1	C	0.0±0.0	0.8±0.6
1	D	0.0±0.0	0.6±0.7
All	All	0	52

There are no bond-length outliers.

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	12	DT	C5'-C4'-C3'	-5.25	107.03	114.90	15	7
1	C	18	DT	C5'-C4'-C3'	-5.22	107.07	114.90	7	4
1	D	24	DT	C5'-C4'-C3'	-5.19	107.12	114.90	16	5
1	A	6	DT	C5'-C4'-C3'	-5.16	107.16	114.90	8	3
1	C	13	DT	C4'-C3'-O3'	5.16	117.74	110.00	9	2
1	B	7	DT	C4'-C3'-O3'	5.10	117.66	110.00	14	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	12	DT	O4'-C4'-C3'	5.03	112.94	105.40	15	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	C	18	DT	Sidechain	11
1	A	6	DT	Sidechain	10
1	B	12	DT	Sidechain	8
1	D	24	DT	Sidechain	7
1	B	7	DT	Sidechain	5
1	C	13	DT	Sidechain	4
1	D	19	DT	Sidechain	4
1	A	1	DT	Sidechain	3

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
All	All	10640	5600	5600	-

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 -.

There are no clashes.

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 ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

16 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
1	LCG	A	2	1	24,27,28	0.63±0.01	0±0 (1±1%)
1	LCG	C	15	1	24,27,28	0.93±0.07	1±0 (5±2%)
1	LCG	B	10	1	24,27,28	0.76±0.01	1±0 (4±0%)
1	LCG	B	8	1	24,27,28	0.63±0.01	0±0 (0±1%)
1	LCG	A	4	1	24,27,28	0.77±0.01	1±0 (4±0%)
1	LCG	A	3	1	24,27,28	0.95±0.09	1±0 (6±2%)
1	LCG	C	17	1	24,27,28	0.76±0.02	0±1 (1±2%)
1	LCG	C	16	1	24,27,28	0.76±0.01	1±0 (4±0%)
1	LCG	B	9	1	24,27,28	0.91±0.07	1±0 (5±1%)
1	LCG	D	21	1	24,27,28	0.93±0.07	1±0 (6±2%)
1	LCG	D	23	1	24,27,28	0.74±0.03	0±1 (1±2%)
1	LCG	B	11	1	24,27,28	0.75±0.03	0±0 (0±1%)
1	LCG	A	5	1	24,27,28	0.74±0.02	0±0 (0±1%)
1	LCG	D	20	1	24,27,28	0.64±0.02	0±0 (1±1%)
1	LCG	C	14	1	24,27,28	0.66±0.02	0±0 (1±1%)
1	LCG	D	22	1	24,27,28	0.76±0.01	1±0 (4±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of

the bond angles.

Mol	Type	Chain	Res	Link	Counts	Bond angles	
						RMSZ	#Z>2
1	LCG	A	2	1	35,42,45	0.84±0.05	1±0 (2±1%)
1	LCG	C	15	1	35,42,45	1.03±0.09	2±0 (7±1%)
1	LCG	B	10	1	35,42,45	0.86±0.02	1±0 (2±0%)
1	LCG	B	8	1	35,42,45	0.85±0.04	1±0 (2±0%)
1	LCG	A	4	1	35,42,45	0.86±0.01	1±0 (2±0%)
1	LCG	A	3	1	35,42,45	0.97±0.04	3±1 (7±2%)
1	LCG	C	17	1	35,42,45	1.35±0.09	4±1 (10±4%)
1	LCG	C	16	1	35,42,45	0.86±0.01	1±0 (2±0%)
1	LCG	B	9	1	35,42,45	1.05±0.07	3±1 (7±1%)
1	LCG	D	21	1	35,42,45	1.02±0.07	2±0 (6±1%)
1	LCG	D	23	1	35,42,45	1.36±0.10	4±1 (11±3%)
1	LCG	B	11	1	35,42,45	1.31±0.10	3±1 (9±3%)
1	LCG	A	5	1	35,42,45	1.37±0.09	5±1 (13±3%)
1	LCG	D	20	1	35,42,45	0.86±0.05	1±0 (2±1%)
1	LCG	C	14	1	35,42,45	0.81±0.05	1±0 (2±1%)
1	LCG	D	22	1	35,42,45	0.87±0.02	1±0 (2±0%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LCG	B	11	1	-	0±0,8,35,36	0±0,5,4,4
1	LCG	B	10	1	-	0±0,8,35,36	0±0,5,4,4
1	LCG	B	8	1	-	0±0,8,35,36	0±0,5,4,4
1	LCG	D	21	1	-	0±0,8,35,36	0±0,5,4,4
1	LCG	C	16	1	-	0±0,8,35,36	0±0,5,4,4
1	LCG	C	15	1	-	0±0,8,35,36	0±0,5,4,4
1	LCG	A	3	1	-	0±0,8,35,36	0±0,5,4,4
1	LCG	C	17	1	-	0±0,8,35,36	0±0,5,4,4
1	LCG	A	5	1	-	0±0,8,35,36	0±0,5,4,4
1	LCG	B	9	1	-	0±0,8,35,36	0±0,5,4,4
1	LCG	A	4	1	-	0±0,8,35,36	0±0,5,4,4
1	LCG	D	23	1	-	0±0,8,35,36	0±0,5,4,4
1	LCG	C	14	1	-	0±0,8,35,36	0±0,5,4,4
1	LCG	D	22	1	-	0±0,8,35,36	0±0,5,4,4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LCG	D	20	1	-	0±0,8,35,36	0±0,5,4,4
1	LCG	A	2	1	-	0±0,8,35,36	0±0,5,4,4

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	A	3	LCG	O4'-C4'	3.91	1.40	1.45	12	20
1	B	9	LCG	O4'-C4'	3.78	1.40	1.45	11	20
1	C	15	LCG	O4'-C4'	3.65	1.40	1.45	10	20
1	D	21	LCG	O4'-C4'	3.61	1.40	1.45	6	20
1	C	16	LCG	O4'-C4'	2.85	1.41	1.45	15	20
1	D	22	LCG	O4'-C4'	2.84	1.41	1.45	12	20
1	B	10	LCG	O4'-C4'	2.83	1.41	1.45	12	20
1	A	4	LCG	O4'-C4'	2.82	1.41	1.45	6	20
1	A	3	LCG	O4'-C1'	2.55	1.38	1.42	7	9
1	C	15	LCG	O4'-C1'	2.50	1.39	1.42	10	8
1	B	9	LCG	O4'-C1'	2.41	1.39	1.42	10	5
1	D	21	LCG	O4'-C1'	2.40	1.39	1.42	1	9
1	D	20	LCG	O4'-C4'	2.21	1.42	1.45	7	7
1	C	14	LCG	O4'-C4'	2.17	1.42	1.45	5	5
1	D	23	LCG	C5'-C4'	2.16	1.55	1.51	7	4
1	A	5	LCG	C5'-C4'	2.15	1.55	1.51	14	3
1	B	8	LCG	O4'-C4'	2.13	1.42	1.45	9	4
1	B	11	LCG	O4'-C4'	2.10	1.42	1.45	12	2
1	A	2	LCG	O4'-C4'	2.09	1.42	1.45	7	6
1	C	17	LCG	C5'-C4'	2.08	1.55	1.51	20	4
1	C	17	LCG	O4'-C4'	2.08	1.42	1.45	13	3
1	D	23	LCG	O4'-C4'	2.03	1.42	1.45	10	4
1	A	5	LCG	O4'-C4'	2.02	1.42	1.45	17	1
1	B	11	LCG	C5'-C4'	2.02	1.55	1.51	18	2

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	11	LCG	O4'-C4'-C3'	4.83	109.07	102.32	9	20
1	C	17	LCG	O4'-C4'-C3'	4.81	109.03	102.32	13	20
1	D	23	LCG	O4'-C4'-C3'	4.68	108.85	102.32	9	20
1	A	5	LCG	O4'-C4'-C3'	4.67	108.84	102.32	20	20
1	C	15	LCG	O4'-C1'-N9	4.08	114.18	108.82	1	12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	D	21	LCG	O4'-C1'-N9	3.91	113.97	108.82	3	11
1	B	9	LCG	O4'-C1'-N9	3.88	113.92	108.82	6	15
1	C	17	LCG	O3'-C3'-C4'	3.76	122.48	112.41	12	12
1	B	11	LCG	O3'-C3'-C4'	3.73	122.41	112.41	4	8
1	D	23	LCG	O3'-C3'-C4'	3.63	122.14	112.41	12	9
1	A	5	LCG	O3'-C3'-C4'	3.59	122.03	112.41	14	13
1	D	20	LCG	O4'-C4'-C3'	3.40	107.06	102.32	7	2
1	C	16	LCG	O4'-C4'-C3'	3.37	107.03	102.32	5	20
1	A	4	LCG	O4'-C4'-C3'	3.34	106.98	102.32	7	20
1	D	23	LCG	O4'-C1'-N9	3.33	104.44	108.82	10	17
1	D	22	LCG	O4'-C4'-C3'	3.32	106.96	102.32	10	20
1	B	10	LCG	O4'-C4'-C3'	3.30	106.93	102.32	10	20
1	A	5	LCG	O4'-C1'-N9	3.30	104.49	108.82	17	17
1	C	17	LCG	O4'-C1'-N9	3.18	104.64	108.82	13	10
1	B	11	LCG	O4'-C1'-N9	3.14	104.69	108.82	7	14
1	C	14	LCG	O4'-C1'-N9	3.14	112.95	108.82	12	15
1	B	8	LCG	O4'-C1'-N9	3.11	112.91	108.82	1	17
1	A	2	LCG	O4'-C1'-N9	3.06	112.85	108.82	12	15
1	D	20	LCG	O4'-C1'-N9	3.00	112.77	108.82	6	15
1	A	2	LCG	O4'-C4'-C3'	2.97	106.47	102.32	5	1
1	B	8	LCG	O4'-C4'-C3'	2.89	106.35	102.32	7	1
1	A	3	LCG	C4'-O4'-C1'	2.68	102.85	107.77	1	12
1	A	3	LCG	O4'-C1'-N9	2.66	112.32	108.82	5	11
1	D	21	LCG	C4'-O4'-C1'	2.66	102.89	107.77	8	9
1	D	21	LCG	O4'-C4'-C6'	2.65	111.59	105.97	18	20
1	A	5	LCG	O4'-C4'-C6'	2.65	100.37	105.97	14	18
1	C	15	LCG	C4'-O4'-C1'	2.64	102.92	107.77	4	9
1	D	23	LCG	O4'-C4'-C6'	2.63	100.41	105.97	3	14
1	B	9	LCG	C4'-O4'-C1'	2.60	103.00	107.77	17	7
1	C	15	LCG	O4'-C4'-C6'	2.54	111.35	105.97	16	20
1	B	11	LCG	O3'-C3'-C2'	2.49	104.82	112.58	18	4
1	B	9	LCG	O4'-C4'-C6'	2.49	111.24	105.97	17	20
1	C	17	LCG	O3'-C3'-C2'	2.45	104.96	112.58	20	6
1	D	23	LCG	O3'-C3'-C2'	2.42	105.04	112.58	3	3
1	A	3	LCG	C6'-O2'-C2'	2.40	103.39	107.72	5	11
1	A	5	LCG	O3'-C3'-C2'	2.37	105.21	112.58	15	3
1	D	23	LCG	O4'-C1'-C2'	2.34	99.62	104.64	17	11
1	C	17	LCG	C3'-C2'-C1'	2.33	105.14	100.29	18	5
1	A	5	LCG	O4'-C1'-C2'	2.33	99.65	104.64	19	16
1	D	23	LCG	C3'-C2'-C1'	2.31	105.10	100.29	15	4
1	A	3	LCG	O4'-C4'-C3'	2.29	105.52	102.32	12	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	11	LCG	O4'-C1'-C2'	2.26	99.80	104.64	5	7
1	A	3	LCG	O4'-C4'-C6'	2.26	110.75	105.97	10	7
1	C	17	LCG	O4'-C1'-C2'	2.26	99.81	104.64	3	8
1	B	11	LCG	O4'-C4'-C6'	2.24	101.24	105.97	18	6
1	C	17	LCG	O4'-C4'-C6'	2.22	101.27	105.97	20	6
1	A	3	LCG	C3'-C2'-C1'	2.20	104.87	100.29	5	1
1	A	5	LCG	C3'-C2'-C1'	2.19	104.84	100.29	10	7
1	A	3	LCG	C5'-C4'-C3'	2.18	123.61	114.53	5	5
1	C	17	LCG	O4'-C4'-C5'	2.13	115.05	108.82	4	4
1	B	11	LCG	O4'-C4'-C5'	2.12	115.02	108.82	7	5
1	B	11	LCG	C3'-C2'-C1'	2.10	104.67	100.29	5	3
1	B	9	LCG	C6'-O2'-C2'	2.06	104.00	107.72	3	11
1	D	23	LCG	O4'-C4'-C5'	2.06	114.84	108.82	18	1
1	C	15	LCG	C6'-O2'-C2'	2.06	104.01	107.72	20	8
1	D	21	LCG	C6'-O2'-C2'	2.05	104.02	107.72	9	8
1	A	5	LCG	O4'-C4'-C5'	2.03	114.75	108.82	1	1

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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