



Full wwPDB NMR Structure Validation Report ⓘ

Feb 19, 2022 – 03:22 PM EST

PDB ID : 1S9L
Title : NMR Solution Structure of a Parallel LNA Quadruplex
Authors : Randazzo, A.; Esposito, V.; Ohlenschlager, O.; Ramachandran, R.; Mayola, L.
Deposited on : 2004-02-05

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : 2.26
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.26

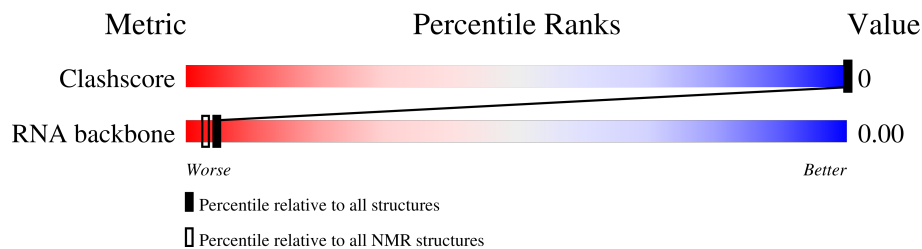
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

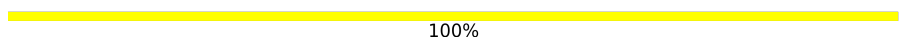
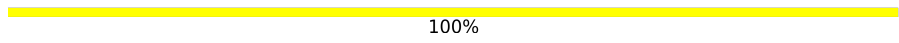
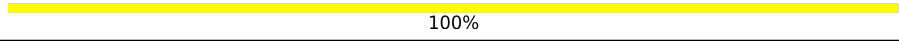
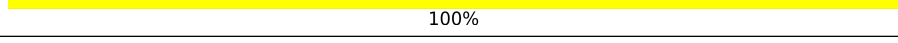
The overall completeness of chemical shifts assignment was not calculated.

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)
Clashescore	158937	12864
RNA backbone	4643	676

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	5	 100%
1	B	5	 100%
1	C	5	 100%
1	D	5	 100%

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

There is only 1 type of molecule in this entry. The entry contains 688 atoms, of which 236 are hydrogens and 0 are deuteriums.

- Molecule 1 is a RNA chain called 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'.

Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		P
1	A	5	Total 172	C 55	H 59	N 19	O 35	P 4	0
1	B	5	Total 172	C 55	H 59	N 19	O 35	P 4	0
1	C	5	Total 172	C 55	H 59	N 19	O 35	P 4	0
1	D	5	Total 172	C 55	H 59	N 19	O 35	P 4	0

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

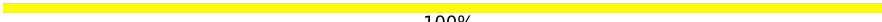
These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for 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'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain A:  100%

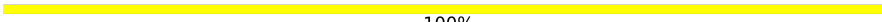
 U1 G2 G3 G4 U5

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain B:  100%

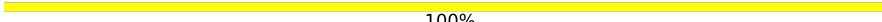
 U6 G7 G8 G9 U10

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain C:  100%

 U11 G12 G13 G14 U15

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain D:  100%

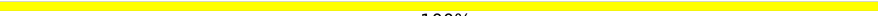
 U16 G17 G18 G19 U20

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'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain A:  100%

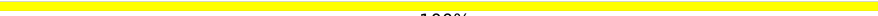
U1
G2
G3
G4
U5

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain B:  100%


U6
G7
G8
G9
U10

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain C:  100%

U11
G12
G13
G14
U15


- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain D:  100%

U16
G17
G18
G19
U20


4.2.2 Score per residue for model 2

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain A:  100%


U1
G2
G3
G4
U5

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain B:  100%


U6
G7
G8
G9
U10

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain C:  100%

U11
G12
G13
G14
U15


- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain D:  100%

U16
G17
G18
G19
U20


4.2.3 Score per residue for model 3

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain A:  100%

U1
G2
G3
G4
U5

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain B:  100%


U6
G7
G8
G9
U10

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain C:  100%

U11
G12
G13
G14
U15

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain D:  100%

U16
G17
G18
G19
U20

4.2.4 Score per residue for model 4

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain A:  100%

U1
G2
G3
G4
U5

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain B:  100%

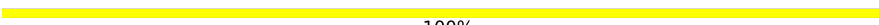
U6
G7
G8
G9
U10

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain C:  100%

U1
G12
G13
G14
U15

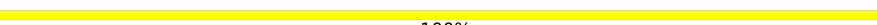
- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain D:  100%

U16
G17
G18
G19
U20

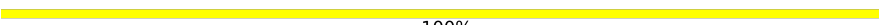
4.2.5 Score per residue for model 5

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain A:  100%

U1
G2
G3
G4
U5

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain B:  100%

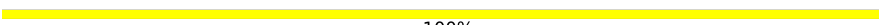
U6
G7
G8
G9
U10

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain C:  100%

U11
G12
G13
G14
U15

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain D:  100%

U16
G17
G18
G19
U20


4.2.6 Score per residue for model 6

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain A:  100%

U1
G2
G3
G4
U5

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain B:  100%


U6
G7
G8
G9
U10

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain C:  100%

U11
G12
G13
G14
U15


- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain D:  100%

U16
G17
G18
G19
U20


4.2.7 Score per residue for model 7

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain A:  100%


U1
G2
G3
G4
U5

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain B:  100%


U6
G7
G8
G9
U10

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain C:  100%

U11
G12
G13
G14
U15


- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain D:  100%

U16
G17
G18
G19
U20

4.2.8 Score per residue for model 8

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain A:  100%

U1
G2
G3
G4
U5

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain B:  100%


U6
G7
G8
G9
U10

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain C:  100%

U11
G12
G13
G14
U15


- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain D:  100%

U16
G17
G18
G19
U20

4.2.9 Score per residue for model 9

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain A:  100%

U1
G2
G3
G4
U5

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain B:  100%

U6
G7
G8
G9
U10

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain C:  100%

U11
G12
G13
G14
U15

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain D:  100%

U16
G17
G18
G19
U20


4.2.10 Score per residue for model 10

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain A:  100%

U1
G2
G3
G4
U5

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain B:  100%

U6
G7
G8
G9
U10

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain C:  100%

U11
G12
G13
G14
U15

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain D:  100%

U16
G17
G18
G19
U20

4.2.11 Score per residue for model 11

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain A:  100%

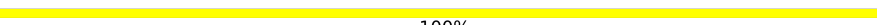
U1
G2
G3
G4
U5

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain B:  100%

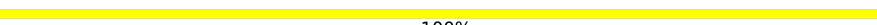
U6
G7
G8
G9
U10

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain C:  100%

U11
G12
G13
G14
U15

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain D:  100%

U16
G17
G18
G19
U20

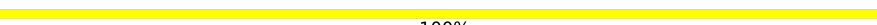
4.2.12 Score per residue for model 12

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain A:  100%

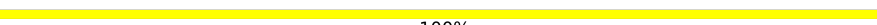
U1
G2
G3
G4
U5

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain B:  100%

U6
G7
G8
G9
U10

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain C:  100%

U11
G12
G13
G14
U15


- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain D:  100%

U16
G17
G18
G19
U20


4.2.13 Score per residue for model 13

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain A:  100%

U1
G2
G3
G4
U5

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain B:  100%

U6
G7
G8
G9
U10

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain C:  100%

U11
G12
G13
G14
U15

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain D:  100%

U16
G17
G18
G19
U20


4.2.14 Score per residue for model 14

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain A:  100%


U1
G2
G3
G4
U5

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain B:  100%

U6
G7
G8
G9
U10

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain C:  100%

U11
G12
G13
G14
U15

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain D:  100%U16
G17
G18
G19
U20

4.2.15 Score per residue for model 15

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain A:  100%U1
G2
G3
G4
U5

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain B:  100%U6
G7
G8
G9
U10

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'


Chain C:  100%U11
G12
G13
G14
U15

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'


Chain D:  100%U16
G17
G18
G19
U20

4.2.16 Score per residue for model 16

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'


Chain A:  100%U1
G2
G3
G4
U5

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain B:  100%

U6
G7
G8
G9
U10

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain C:  100%

U11
G12
G13
G14
U15

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain D:  100%

U16
G17
G18
G19
U20


4.2.17 Score per residue for model 17

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain A:  100%

U1
G2
G3
G4
U5

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain B:  100%

U6
G7
G8
G9
U10

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain C:  100%

U11
G12
G13
G14
U15

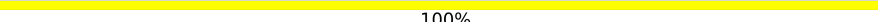
- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain D:  100%

U16
G17
G18
G19
U20


4.2.18 Score per residue for model 18

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain A:  100%

U1
G2
G3
G4
U5

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain B:  100%

U6
G7
G8
G9
U10

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain C:  100%

U11
G12
G13
G14
U15

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain D:  100%

U16
G17
G18
G19
U20


4.2.19 Score per residue for model 19

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain A:  100%

U1
G2
G3
G4
U5

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain B:  100%


U6
G7
G8
G9
U10

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain C:  100%

U11
G12
G13
G14
U15

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain D:  100%

U16
G17
G18
G19
U20

4.2.20 Score per residue for model 20

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain A:  100%

U1
G2
G3
G4
U5

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain B:  100%


U6
G7
G8
G9
U10

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain C:  100%

U11
G12
G13
G14
U15

- Molecule 1: 5'-((TLN)P*(LCG)P*(LCG)P*(LCG)P*(TLN))-3'

Chain D:  100%

U16
G17
G18
G19
U20

5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics*.

Of the 20 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CYANA	structure solution	1.0.6
Discover	refinement	98

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: TLN, LCG

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

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
All	All	9040	4720	4640	-

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 [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers	Suiteness
1	A	0/5 (0%)	-	-	0.00±0.00
1	B	0/5 (0%)	-	-	0.00±0.00
1	C	0/5 (0%)	-	-	0.00±0.00
1	D	0/5 (0%)	-	-	0.00±0.00
All	All	0/400 (0%)	-	-	0.00

The overall RNA backbone suiteness is 0.00.

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

20 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	Counts	Bond lengths	
						RMSZ	#Z>2
1	LCG	B	9	1	19,27,28	3.18±0.02	5±0 (26±0%)
1	LCG	A	4	1	19,27,28	3.18±0.02	5±0 (26±0%)
1	TLN	B	6	1	16,21,25	2.05±0.01	3±0 (18±0%)
1	TLN	C	11	1	16,21,25	2.05±0.01	3±0 (18±0%)
1	LCG	D	19	1	19,27,28	3.19±0.02	5±0 (26±0%)
1	LCG	B	8	1	19,27,28	3.16±0.01	5±0 (26±0%)
1	LCG	C	12	1	19,27,28	3.19±0.01	5±0 (26±0%)
1	LCG	C	13	1	19,27,28	3.16±0.01	5±0 (26±0%)
1	LCG	D	18	1	19,27,28	3.16±0.01	5±0 (26±0%)
1	TLN	A	1	1	16,21,25	2.05±0.01	3±0 (18±0%)
1	TLN	D	20	1	16,24,25	2.05±0.01	3±0 (18±0%)
1	TLN	A	5	1	16,24,25	2.04±0.01	3±0 (18±0%)
1	LCG	A	3	1	19,27,28	3.16±0.01	5±0 (26±0%)
1	LCG	A	2	1	19,27,28	3.19±0.01	5±0 (26±0%)
1	LCG	D	17	1	19,27,28	3.19±0.01	5±0 (26±0%)

Mol	Type	Chain	Res	Link	Counts	Bond lengths	
						RMSZ	#Z>2
1	TLN	C	15	1	16,24,25	2.05±0.01	3±0 (18±0%)
1	TLN	D	16	1	16,21,25	2.06±0.01	3±0 (18±0%)
1	LCG	C	14	1	19,27,28	3.18±0.02	5±0 (26±0%)
1	TLN	B	10	1	16,24,25	2.05±0.01	3±0 (18±0%)
1	LCG	B	7	1	19,27,28	3.19±0.01	5±0 (26±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	B	9	1	23,42,45	2.70±0.02	8±1 (36±2%)
1	LCG	A	4	1	23,42,45	2.69±0.02	8±1 (34±3%)
1	TLN	B	6	1	21,33,40	2.59±0.02	2±0 (9±0%)
1	TLN	C	11	1	21,33,40	2.60±0.01	2±0 (9±0%)
1	LCG	D	19	1	23,42,45	2.69±0.02	8±1 (36±2%)
1	LCG	B	8	1	23,42,45	2.80±0.02	9±0 (40±2%)
1	LCG	C	12	1	23,42,45	2.78±0.02	9±0 (39±0%)
1	LCG	C	13	1	23,42,45	2.81±0.03	10±0 (41±2%)
1	LCG	D	18	1	23,42,45	2.80±0.03	10±0 (41±2%)
1	TLN	A	1	1	21,33,40	2.60±0.02	2±0 (9±0%)
1	TLN	D	20	1	19,37,40	2.70±0.02	2±0 (10±0%)
1	TLN	A	5	1	19,37,40	2.71±0.03	2±0 (10±0%)
1	LCG	A	3	1	23,42,45	2.79±0.03	9±0 (40±1%)
1	LCG	A	2	1	23,42,45	2.77±0.02	9±0 (39±0%)
1	LCG	D	17	1	23,42,45	2.77±0.01	9±0 (39±0%)
1	TLN	C	15	1	19,37,40	2.71±0.02	2±0 (10±1%)
1	TLN	D	16	1	21,33,40	2.60±0.01	2±0 (9±0%)
1	LCG	C	14	1	23,42,45	2.69±0.01	8±1 (35±2%)
1	TLN	B	10	1	19,37,40	2.70±0.03	2±0 (10±0%)
1	LCG	B	7	1	23,42,45	2.77±0.01	9±0 (39±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	TLN	D	20	1	-	0±0,6,35,36	0±0,4,3,3
1	TLN	A	5	1	-	0±0,6,35,36	0±0,4,3,3
1	LCG	A	4	1	-	0±0,4,35,36	0±0,5,4,4
1	LCG	C	12	1	-	0±0,4,35,36	0±0,5,4,4
1	TLN	C	11	1	-	0±0,5,32,36	0±0,4,3,3
1	LCG	B	9	1	-	0±0,4,35,36	0±0,5,4,4
1	TLN	D	16	1	-	0±0,5,32,36	0±0,4,3,3
1	LCG	D	18	1	-	0±0,4,35,36	0±0,5,4,4
1	LCG	C	13	1	-	0±0,4,35,36	0±0,5,4,4
1	TLN	A	1	1	-	0±0,5,32,36	0±0,4,3,3
1	LCG	A	3	1	-	0±0,4,35,36	0±0,5,4,4
1	LCG	C	14	1	-	0±0,4,35,36	0±0,5,4,4
1	TLN	B	6	1	-	0±0,5,32,36	0±0,4,3,3
1	TLN	C	15	1	-	0±0,6,35,36	0±0,4,3,3
1	TLN	B	10	1	-	0±0,6,35,36	0±0,4,3,3
1	LCG	B	8	1	-	0±0,4,35,36	0±0,5,4,4
1	LCG	B	7	1	-	0±0,4,35,36	0±0,5,4,4
1	LCG	D	17	1	-	0±0,4,35,36	0±0,5,4,4
1	LCG	A	2	1	-	0±0,4,35,36	0±0,5,4,4
1	LCG	D	19	1	-	0±0,4,35,36	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	B	7	LCG	C2-N1	8.50	1.50	1.35	3	20
1	C	12	LCG	C2-N1	8.49	1.50	1.35	15	20
1	D	17	LCG	C2-N1	8.47	1.50	1.35	4	20
1	A	2	LCG	C2-N1	8.47	1.50	1.35	20	20
1	D	19	LCG	C2-N1	8.47	1.50	1.35	11	20
1	B	9	LCG	C2-N1	8.45	1.50	1.35	9	20
1	B	8	LCG	C2-N1	8.43	1.50	1.35	2	20
1	A	4	LCG	C2-N1	8.43	1.50	1.35	4	20
1	C	14	LCG	C2-N1	8.42	1.50	1.35	7	20
1	A	3	LCG	C2-N1	8.41	1.50	1.35	8	20
1	C	13	LCG	C2-N1	8.41	1.50	1.35	2	20
1	D	18	LCG	C2-N1	8.39	1.50	1.35	3	20
1	A	4	LCG	C5-C6	8.06	1.55	1.41	13	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	D	19	LCG	C5-C6	8.05	1.55	1.41	5	20
1	C	14	LCG	C5-C6	8.05	1.55	1.41	1	20
1	B	9	LCG	C5-C6	8.04	1.55	1.41	7	20
1	A	3	LCG	C5-C6	7.98	1.55	1.41	17	20
1	D	18	LCG	C5-C6	7.95	1.55	1.41	3	20
1	C	13	LCG	C5-C6	7.95	1.55	1.41	9	20
1	B	8	LCG	C5-C6	7.91	1.55	1.41	7	20
1	C	12	LCG	C5-C6	7.88	1.54	1.41	9	20
1	A	2	LCG	C5-C6	7.85	1.54	1.41	13	20
1	B	7	LCG	C5-C6	7.83	1.54	1.41	16	20
1	D	17	LCG	C5-C6	7.82	1.54	1.41	3	20
1	D	16	TLN	C5-C4	7.05	1.56	1.41	20	20
1	B	10	TLN	C5-C4	7.04	1.56	1.41	4	20
1	C	11	TLN	C5-C4	7.03	1.56	1.41	16	20
1	B	6	TLN	C5-C4	7.03	1.56	1.41	14	20
1	A	1	TLN	C5-C4	7.00	1.56	1.41	1	20
1	C	15	TLN	C5-C4	7.00	1.56	1.41	3	20
1	D	20	TLN	C5-C4	6.99	1.56	1.41	7	20
1	A	5	TLN	C5-C4	6.96	1.56	1.41	15	20
1	A	4	LCG	C4-N3	5.77	1.44	1.35	1	20
1	B	9	LCG	C4-N3	5.76	1.44	1.35	16	20
1	D	19	LCG	C4-N3	5.74	1.44	1.35	12	20
1	C	14	LCG	C4-N3	5.73	1.44	1.35	20	20
1	D	18	LCG	C4-N3	5.68	1.44	1.35	7	20
1	C	13	LCG	C4-N3	5.65	1.44	1.35	4	20
1	A	3	LCG	C4-N3	5.63	1.44	1.35	10	20
1	B	8	LCG	C4-N3	5.61	1.44	1.35	10	20
1	C	12	LCG	C4-N3	5.60	1.44	1.35	18	20
1	B	7	LCG	C4-N3	5.59	1.44	1.35	9	20
1	A	2	LCG	C4-N3	5.58	1.44	1.35	20	20
1	D	17	LCG	C4-N3	5.58	1.44	1.35	15	20
1	B	9	LCG	C2-N2	3.64	1.41	1.33	13	20
1	C	14	LCG	C2-N2	3.64	1.41	1.33	5	20
1	D	17	LCG	C2-N2	3.62	1.41	1.33	13	20
1	C	13	LCG	C2-N2	3.62	1.41	1.33	5	20
1	D	18	LCG	C2-N2	3.62	1.41	1.33	12	20
1	A	3	LCG	C2-N2	3.61	1.41	1.33	12	20
1	B	7	LCG	C2-N2	3.61	1.41	1.33	10	20
1	D	19	LCG	C2-N2	3.61	1.41	1.33	12	20
1	A	4	LCG	C2-N2	3.61	1.41	1.33	16	20
1	B	8	LCG	C2-N2	3.60	1.41	1.33	20	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	C	12	LCG	C2-N2	3.60	1.41	1.33	1	20
1	A	2	LCG	C2-N2	3.56	1.41	1.33	10	20
1	B	7	LCG	C6-N1	2.59	1.37	1.33	5	20
1	A	3	LCG	C6-N1	2.56	1.37	1.33	19	20
1	D	20	TLN	O4'-C1'	2.54	1.46	1.42	16	20
1	C	12	LCG	C6-N1	2.54	1.37	1.33	5	20
1	A	2	LCG	C6-N1	2.54	1.37	1.33	10	20
1	D	19	LCG	C6-N1	2.54	1.37	1.33	16	20
1	D	17	LCG	C6-N1	2.52	1.37	1.33	12	20
1	B	8	LCG	C6-N1	2.52	1.37	1.33	19	20
1	C	14	LCG	C6-N1	2.52	1.37	1.33	12	20
1	A	4	LCG	C6-N1	2.51	1.37	1.33	16	20
1	C	13	LCG	C6-N1	2.51	1.37	1.33	9	20
1	D	18	LCG	C6-N1	2.51	1.37	1.33	12	20
1	A	5	TLN	O4'-C1'	2.50	1.46	1.42	16	20
1	B	9	LCG	C6-N1	2.50	1.37	1.33	10	20
1	B	10	TLN	O4'-C1'	2.48	1.46	1.42	15	20
1	C	15	TLN	C4-N3	2.48	1.37	1.33	6	20
1	B	10	TLN	C4-N3	2.47	1.37	1.33	16	20
1	D	20	TLN	C4-N3	2.46	1.37	1.33	2	20
1	A	5	TLN	C4-N3	2.46	1.37	1.33	2	20
1	C	15	TLN	O4'-C1'	2.45	1.46	1.42	10	20
1	C	11	TLN	C4-N3	2.42	1.37	1.33	6	20
1	D	16	TLN	C4-N3	2.42	1.37	1.33	6	20
1	A	1	TLN	C4-N3	2.39	1.37	1.33	3	20
1	B	6	TLN	C4-N3	2.38	1.37	1.33	3	20
1	D	16	TLN	O4'-C1'	2.33	1.46	1.42	12	20
1	B	6	TLN	O4'-C1'	2.33	1.46	1.42	13	20
1	A	1	TLN	O4'-C1'	2.32	1.46	1.42	11	20
1	C	11	TLN	O4'-C1'	2.29	1.46	1.42	13	20

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	A	1	TLN	C2-N3-C4	11.11	124.53	115.14	10	20
1	A	5	TLN	C2-N3-C4	11.06	124.48	115.14	19	20
1	B	10	TLN	C2-N3-C4	11.05	124.47	115.14	7	20
1	C	15	TLN	C2-N3-C4	11.04	124.46	115.14	18	20
1	C	11	TLN	C2-N3-C4	11.01	124.44	115.14	1	20
1	B	6	TLN	C2-N3-C4	11.00	124.43	115.14	17	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	D	20	TLN	C2-N3-C4	11.00	124.43	115.14	6	20
1	D	16	TLN	C2-N3-C4	11.00	124.43	115.14	12	20
1	D	18	LCG	C2-N3-C4	7.23	123.61	115.36	3	20
1	A	3	LCG	C2-N3-C4	7.22	123.61	115.36	17	20
1	D	17	LCG	C2-N3-C4	7.21	123.60	115.36	3	20
1	A	4	LCG	C2-N3-C4	7.20	123.58	115.36	4	20
1	D	19	LCG	C2-N3-C4	7.20	123.58	115.36	19	20
1	C	13	LCG	C2-N3-C4	7.19	123.57	115.36	7	20
1	A	2	LCG	C2-N3-C4	7.19	123.57	115.36	20	20
1	B	7	LCG	C2-N3-C4	7.19	123.57	115.36	16	20
1	B	8	LCG	C2-N3-C4	7.18	123.55	115.36	7	20
1	C	14	LCG	C2-N3-C4	7.18	123.55	115.36	10	20
1	B	9	LCG	C2-N3-C4	7.17	123.55	115.36	1	20
1	C	12	LCG	C2-N3-C4	7.17	123.55	115.36	12	20
1	B	9	LCG	C5-C6-N1	6.32	114.79	123.43	19	20
1	D	18	LCG	C5-C6-N1	6.30	114.81	123.43	9	20
1	A	3	LCG	C5-C6-N1	6.30	114.82	123.43	7	20
1	B	8	LCG	C5-C6-N1	6.30	114.82	123.43	3	20
1	D	19	LCG	C5-C6-N1	6.30	114.82	123.43	7	20
1	C	14	LCG	C5-C6-N1	6.29	114.82	123.43	17	20
1	C	12	LCG	C5-C6-N1	6.29	114.83	123.43	11	20
1	C	13	LCG	C5-C6-N1	6.29	114.83	123.43	17	20
1	B	7	LCG	C5-C6-N1	6.28	114.84	123.43	15	20
1	D	17	LCG	C5-C6-N1	6.27	114.85	123.43	16	20
1	A	4	LCG	C5-C6-N1	6.26	114.87	123.43	9	20
1	A	2	LCG	C5-C6-N1	6.26	114.87	123.43	10	20
1	C	14	LCG	N3-C2-N1	4.78	120.85	127.22	13	20
1	D	19	LCG	N3-C2-N1	4.78	120.85	127.22	9	20
1	B	9	LCG	N3-C2-N1	4.76	120.87	127.22	19	20
1	B	8	LCG	N3-C2-N1	4.74	120.89	127.22	20	20
1	A	4	LCG	N3-C2-N1	4.74	120.90	127.22	7	20
1	C	13	LCG	N3-C2-N1	4.74	120.91	127.22	5	20
1	A	3	LCG	N3-C2-N1	4.73	120.91	127.22	5	20
1	A	2	LCG	N3-C2-N1	4.72	120.92	127.22	9	20
1	D	18	LCG	N3-C2-N1	4.71	120.93	127.22	10	20
1	B	7	LCG	N3-C2-N1	4.71	120.94	127.22	15	20
1	C	12	LCG	N3-C2-N1	4.69	120.96	127.22	3	20
1	D	17	LCG	N3-C2-N1	4.69	120.97	127.22	17	20
1	B	9	LCG	C2-N1-C6	4.07	122.40	115.93	19	20
1	C	14	LCG	C2-N1-C6	4.05	122.36	115.93	11	20
1	D	19	LCG	C2-N1-C6	4.04	122.35	115.93	14	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	4	LCG	C2-N1-C6	4.03	122.33	115.93	18	20
1	C	13	LCG	C2-N1-C6	4.00	122.29	115.93	20	20
1	B	8	LCG	C2-N1-C6	3.99	122.27	115.93	13	20
1	A	3	LCG	C2-N1-C6	3.99	122.27	115.93	4	20
1	B	7	LCG	C2-N1-C6	3.98	122.26	115.93	15	20
1	C	12	LCG	C2-N1-C6	3.97	122.25	115.93	3	20
1	D	18	LCG	C2-N1-C6	3.97	122.24	115.93	1	20
1	D	17	LCG	C2-N1-C6	3.94	122.19	115.93	7	20
1	A	2	LCG	C2-N1-C6	3.94	122.19	115.93	10	20
1	A	2	LCG	C4-C5-N7	3.81	113.37	109.40	18	20
1	D	17	LCG	C4-C5-N7	3.80	113.36	109.40	11	20
1	A	4	LCG	C4-C5-N7	3.80	113.36	109.40	8	20
1	B	8	LCG	C4-C5-N7	3.80	113.36	109.40	19	20
1	C	12	LCG	C4-C5-N7	3.79	113.35	109.40	2	20
1	A	3	LCG	C4-C5-N7	3.78	113.34	109.40	9	20
1	C	14	LCG	C4-C5-N7	3.78	113.34	109.40	18	20
1	B	7	LCG	C4-C5-N7	3.76	113.32	109.40	19	20
1	D	19	LCG	C4-C5-N7	3.75	113.30	109.40	18	20
1	C	13	LCG	C4-C5-N7	3.74	113.30	109.40	3	20
1	B	9	LCG	C4-C5-N7	3.74	113.30	109.40	6	20
1	D	18	LCG	C4-C5-N7	3.73	113.29	109.40	1	20
1	D	18	LCG	O4'-C4'-C3'	3.34	106.64	102.22	11	20
1	A	3	LCG	O4'-C4'-C3'	3.33	106.63	102.22	18	20
1	C	13	LCG	O4'-C4'-C3'	3.32	106.61	102.22	6	20
1	B	8	LCG	O4'-C4'-C3'	3.31	106.61	102.22	14	20
1	D	17	LCG	O4'-C4'-C3'	3.11	106.34	102.22	9	20
1	B	7	LCG	O4'-C4'-C3'	3.11	106.34	102.22	3	20
1	C	12	LCG	O4'-C4'-C3'	3.09	106.31	102.22	11	20
1	D	17	LCG	C1'-N9-C4	3.06	132.02	126.64	15	20
1	A	2	LCG	O4'-C4'-C3'	3.06	106.27	102.22	7	20
1	B	7	LCG	C1'-N9-C4	3.04	131.99	126.64	9	20
1	C	12	LCG	C1'-N9-C4	3.00	131.91	126.64	13	20
1	A	3	LCG	C1'-N9-C4	2.99	131.90	126.64	7	20
1	A	2	LCG	C1'-N9-C4	2.98	131.88	126.64	7	20
1	B	8	LCG	C1'-N9-C4	2.98	131.88	126.64	3	20
1	C	13	LCG	C1'-N9-C4	2.97	131.86	126.64	13	20
1	D	18	LCG	C1'-N9-C4	2.95	131.83	126.64	9	20
1	A	3	LCG	N2-C2-N1	2.69	121.44	117.25	11	20
1	D	18	LCG	O4'-C1'-C2'	2.67	98.66	104.50	17	20
1	D	18	LCG	N2-C2-N1	2.67	121.40	117.25	3	20
1	D	19	LCG	N2-C2-N1	2.66	121.38	117.25	17	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	9	LCG	N2-C2-N1	2.65	121.37	117.25	9	20
1	C	14	LCG	N2-C2-N1	2.65	121.37	117.25	7	20
1	C	13	LCG	O4'-C1'-C2'	2.65	98.70	104.50	7	20
1	A	4	LCG	N2-C2-N1	2.63	121.34	117.25	3	20
1	A	3	LCG	O4'-C1'-C2'	2.62	98.76	104.50	3	20
1	B	8	LCG	N2-C2-N1	2.62	121.32	117.25	7	20
1	B	8	LCG	O4'-C1'-C2'	2.61	98.77	104.50	9	20
1	C	13	LCG	N2-C2-N1	2.61	121.31	117.25	9	20
1	B	9	LCG	C1'-N9-C4	2.59	131.20	126.64	11	13
1	A	4	LCG	C1'-N9-C4	2.59	131.20	126.64	9	9
1	C	14	LCG	C1'-N9-C4	2.59	131.18	126.64	3	9
1	C	12	LCG	N2-C2-N1	2.58	121.27	117.25	20	20
1	D	17	LCG	N2-C2-N1	2.55	121.22	117.25	1	20
1	D	19	LCG	C1'-N9-C4	2.54	131.10	126.64	7	12
1	A	2	LCG	N2-C2-N1	2.53	121.19	117.25	13	20
1	B	7	LCG	N2-C2-N1	2.51	121.16	117.25	5	20
1	D	16	TLN	O4'-C1'-C2'	2.51	99.01	104.50	15	20
1	A	1	TLN	O4'-C1'-C2'	2.48	99.07	104.50	17	20
1	C	11	TLN	O4'-C1'-C2'	2.48	99.06	104.50	9	20
1	B	6	TLN	O4'-C1'-C2'	2.48	99.08	104.50	14	20
1	D	17	LCG	O4'-C1'-C2'	2.41	99.22	104.50	19	20
1	A	2	LCG	O4'-C1'-C2'	2.41	99.22	104.50	11	20
1	C	12	LCG	O4'-C1'-C2'	2.41	99.23	104.50	7	20
1	B	7	LCG	O4'-C1'-C2'	2.40	99.25	104.50	9	20
1	D	19	LCG	O4'-C1'-C2'	2.39	99.27	104.50	16	20
1	C	14	LCG	O4'-C1'-C2'	2.38	99.28	104.50	16	20
1	B	9	LCG	O4'-C1'-C2'	2.37	99.31	104.50	9	20
1	A	4	LCG	O4'-C1'-C2'	2.35	99.36	104.50	3	20
1	D	19	LCG	O4'-C4'-C3'	2.22	105.16	102.22	18	15
1	C	14	LCG	O4'-C4'-C3'	2.20	105.13	102.22	3	12
1	D	20	TLN	O4'-C1'-C2'	2.20	99.69	104.50	15	20
1	B	9	LCG	O4'-C4'-C3'	2.19	105.12	102.22	11	16
1	B	10	TLN	O4'-C1'-C2'	2.19	99.71	104.50	9	20
1	C	15	TLN	O4'-C1'-C2'	2.18	99.72	104.50	7	20
1	A	5	TLN	O4'-C1'-C2'	2.16	99.77	104.50	3	20
1	A	4	LCG	O4'-C4'-C3'	2.15	105.07	102.22	9	11
1	D	18	LCG	O2'-C6'-C4'	2.06	99.78	103.78	19	13
1	B	8	LCG	O2'-C6'-C4'	2.04	99.83	103.78	6	8
1	A	3	LCG	O2'-C6'-C4'	2.03	99.84	103.78	7	6
1	C	13	LCG	O2'-C6'-C4'	2.03	99.84	103.78	8	11
1	C	15	TLN	O4'-C4'-C3'	2.00	104.87	102.22	19	1

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6.5 Carbohydrates [i](#)

There are no monosaccharides 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