



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 04:06 am BST

PDB ID : 2X2Q  
Title : Crystal structure of an 'all locked' LNA duplex at 1.9 angstrom resolution  
Authors : Eichert, A.; Behling, K.; Fuerste, J.P.; Betzel, C.; Erdmann, V.A.; Foerster, C.  
Deposited on : 2010-01-15  
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

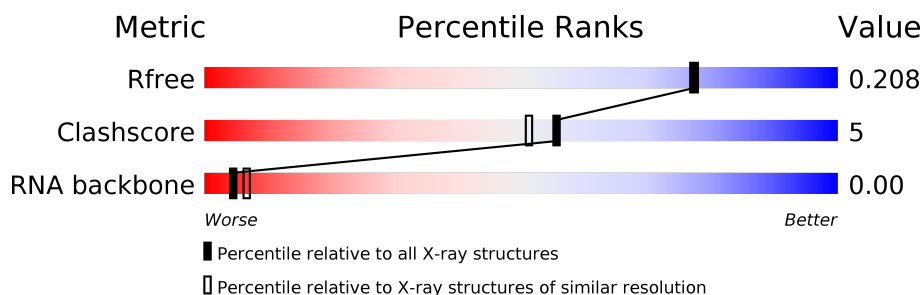
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
RNA backbone	3102	1013 (2.42-1.38)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	7	<div> <div>71%</div> <div>29%</div> </div>
1	C	7	<div> <div>86%</div> <div>14%</div> </div>
2	B	7	<div> <div>100%</div> </div>
2	D	7	<div> <div>86%</div> <div>14%</div> </div>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 741 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

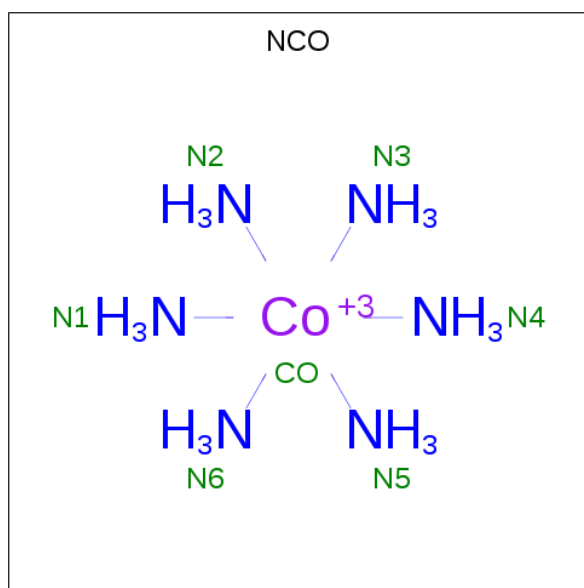
- Molecule 1 is a RNA chain called LOCKED NUCLEIC ACID DERIVED FROM TRNA SER ACCEPTOR STEM MICROHELIX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	7	Total	C	N	O	P	0	0	0
			152	77	22	47	6			
1	C	7	Total	C	N	O	P	0	0	0
			152	77	22	47	6			

- Molecule 2 is a RNA chain called LOCKED NUCLEIC ACID DERIVED FROM TRNA SER ACCEPTOR STEM MICROHELIX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	7	Total	C	N	O	P	0	0	0
			162	77	32	47	6			
2	D	7	Total	C	N	O	P	0	0	0
			162	77	32	47	6			

- Molecule 3 is COBALT HEXAMMINE(III) (three-letter code: NCO) (formula:  $\text{CoH}_{18}\text{N}_6$ ).

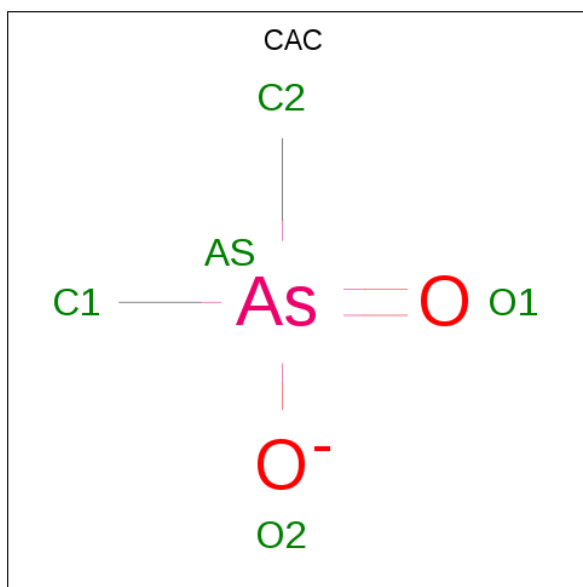


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	Co	N	0	0
			7	1	6		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	Mg	0	0
			1	1		

- Molecule 5 is CACODYLATE ION (three-letter code: CAC) (formula: C<sub>2</sub>H<sub>6</sub>AsO<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total	As	C	O	0	0
			5	1	2	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	20	Total	O	0	0
			20	20		
6	B	30	Total	O	0	0
			30	30		
6	C	17	Total	O	0	0
			17	17		
6	D	33	Total	O	0	0
			33	33		

### 3 Residue-property plots


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

- Molecule 1: LOCKED NUCLEIC ACID DERIVED FROM TRNA SER ACCEPTOR STEM MICROHELIX

Chain A: 



- Molecule 1: LOCKED NUCLEIC ACID DERIVED FROM TRNA SER ACCEPTOR STEM MICROHELIX

Chain C: 



- Molecule 2: LOCKED NUCLEIC ACID DERIVED FROM TRNA SER ACCEPTOR STEM MICROHELIX

Chain B: 

There are no outlier residues recorded for this chain.

- Molecule 2: LOCKED NUCLEIC ACID DERIVED FROM TRNA SER ACCEPTOR STEM MICROHELIX

Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.91Å 40.74Å 30.06Å 90.00° 91.02° 90.00°	Depositor
Resolution (Å)	38.95 – 1.90 36.10 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.0 (38.95-1.90) 98.1 (36.10-1.90)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.45 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.224 , 0.264 0.230 , 0.208	Depositor DCC
$R_{free}$ test set	341 reflections (4.62%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.5	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 55.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.047 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	741	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.26% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, NCO, LCG, LCC, LCA, CAC, TLN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	152	0	89	2	0
1	C	152	0	89	2	0
2	B	162	0	79	0	0
2	D	162	0	79	1	0
3	B	7	0	0	0	0
4	C	1	0	0	0	0
5	D	5	0	0	0	0
6	A	20	0	0	1	0
6	B	30	0	0	0	0
6	C	17	0	0	0	0
6	D	33	0	0	3	0
All	All	741	0	336	5	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (5) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1:LCG:N2	6:D:201:HOH:O	1.86	1.09
1:C:72:LCC:O2	6:D:201:HOH:O	1.98	0.81
1:A:67:LCC:H5M1	6:A:103:HOH:O	2.09	0.52
1:C:72:LCC:C2	6:D:201:HOH:O	2.58	0.46
1:A:67:LCC:H2'1	1:A:68:TLN:H5'	2.01	0.43

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

### 5.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	0/7	-	-
1	C	0/7	-	-
2	B	0/7	-	-
2	D	0/7	-	-
All	All	0/28	-	-

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or 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 length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	LCC	A	66	1	16,21,25	1.37	4 (25%)	24,33,40	2.36	6 (25%)
2	LCG	B	7	2	19,27,28	1.77	4 (21%)	23,42,45	2.80	9 (39%)
1	LCC	A	67	1	16,24,25	1.29	3 (18%)	22,37,40	2.17	3 (13%)
1	LCA	C	70	1,2	19,26,27	1.26	3 (15%)	21,40,43	1.54	5 (23%)
1	LCC	C	66	1	16,21,25	1.41	3 (18%)	24,33,40	2.60	7 (29%)
2	LCA	D	5	1,2	19,26,27	1.16	1 (5%)	21,40,43	1.46	3 (14%)
1	LCC	A	69	1	16,24,25	1.33	3 (18%)	22,37,40	2.42	5 (22%)
2	LCG	D	4	2	19,27,28	1.65	3 (15%)	23,42,45	2.90	10 (43%)
1	LCC	C	67	1	16,24,25	1.17	2 (12%)	22,37,40	2.47	7 (31%)
1	TLN	A	68	1,2	16,24,25	1.39	2 (12%)	19,37,40	3.86	4 (21%)
2	LCG	B	2	2	19,27,28	1.41	3 (15%)	23,42,45	2.66	9 (39%)
2	LCG	D	6	2	19,27,28	1.54	5 (26%)	23,42,45	2.33	3 (13%)
2	LCG	B	6	2	19,27,28	1.68	5 (26%)	23,42,45	2.45	7 (30%)
2	TLN	B	3	1,2	16,24,25	1.84	5 (31%)	19,37,40	3.79	2 (10%)
1	LCC	A	71	1	16,24,25	1.31	2 (12%)	22,37,40	2.49	5 (22%)
1	LCC	C	72	1,4	16,24,25	1.65	4 (25%)	22,37,40	2.49	6 (27%)
2	LCG	B	4	2	19,27,28	1.61	4 (21%)	23,42,45	2.62	5 (21%)
1	TLN	C	68	1,2	16,24,25	1.55	5 (31%)	19,37,40	3.57	3 (15%)
1	LCC	C	71	1	16,24,25	1.54	3 (18%)	22,37,40	2.46	9 (40%)
1	LCA	A	70	1,2	19,26,27	1.23	2 (10%)	21,40,43	1.43	3 (14%)
2	LCG	D	7	2	19,27,28	1.64	3 (15%)	23,42,45	2.85	10 (43%)
2	TLN	D	3	1,2	16,24,25	1.90	5 (31%)	19,37,40	3.50	4 (21%)
2	LCA	B	5	1,2	19,26,27	0.92	1 (5%)	21,40,43	1.37	4 (19%)
2	LCG	B	1	2	19,24,28	1.73	3 (15%)	25,38,45	2.57	8 (32%)
2	LCG	D	1	2	19,24,28	1.30	3 (15%)	25,38,45	2.77	9 (36%)
1	LCC	A	72	1	16,24,25	1.73	5 (31%)	22,37,40	2.75	7 (31%)
2	LCG	D	2	2	19,27,28	1.47	4 (21%)	23,42,45	3.31	8 (34%)
1	LCC	C	69	1	16,24,25	1.40	3 (18%)	22,37,40	1.90	1 (4%)

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	LCC	A	66	1	-	0/5/32/36	0/4/3/3
2	LCG	B	7	2	-	0/4/35/36	0/5/4/4
1	LCC	A	67	1	-	1/6/35/36	0/4/3/3
1	LCA	C	70	1,2	-	0/4/35/36	0/5/4/4
1	LCC	C	66	1	-	0/5/32/36	0/4/3/3
2	LCA	D	5	1,2	-	0/4/35/36	0/5/4/4
1	LCC	A	69	1	-	0/6/35/36	0/4/3/3
2	LCG	D	4	2	-	0/4/35/36	0/5/4/4
1	LCC	C	67	1	-	0/6/35/36	0/4/3/3
1	TLN	A	68	1,2	-	0/6/35/36	0/4/3/3
2	LCG	B	2	2	-	0/4/35/36	0/5/4/4
2	LCG	D	6	2	-	0/4/35/36	0/5/4/4
2	LCG	B	6	2	-	0/4/35/36	0/5/4/4
2	TLN	B	3	1,2	-	0/6/35/36	0/4/3/3
1	LCC	A	71	1	-	0/6/35/36	0/4/3/3
1	LCC	C	72	1,4	-	0/6/35/36	0/4/3/3
2	LCG	B	4	2	-	0/4/35/36	0/5/4/4
1	TLN	C	68	1,2	-	0/6/35/36	0/4/3/3
1	LCC	C	71	1	-	0/6/35/36	0/4/3/3
1	LCA	A	70	1,2	-	0/4/35/36	0/5/4/4
2	LCG	D	7	2	-	0/4/35/36	0/5/4/4
2	TLN	D	3	1,2	-	0/6/35/36	0/4/3/3
2	LCA	B	5	1,2	-	0/4/35/36	0/5/4/4
2	LCG	B	1	2	-	0/3/32/36	0/5/4/4
2	LCG	D	1	2	-	0/3/32/36	0/5/4/4
1	LCC	A	72	1	-	0/6/35/36	0/4/3/3
2	LCG	D	2	2	-	0/4/35/36	0/5/4/4
1	LCC	C	69	1	-	1/6/35/36	0/4/3/3

All (93) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	LCG	C6-N1	5.48	1.42	1.33
2	D	3	TLN	C4-N3	4.85	1.41	1.33
2	B	3	TLN	C4-N3	4.72	1.41	1.33
2	D	7	LCG	C6-N1	4.42	1.40	1.33
2	B	7	LCG	C6-N1	4.38	1.40	1.33
2	B	6	LCG	C6-N1	4.34	1.40	1.33
2	D	4	LCG	C6-N1	4.19	1.40	1.33
1	C	71	LCC	O2'-C6'	3.90	1.51	1.43
1	A	72	LCC	O2'-C6'	3.72	1.50	1.43
1	C	68	TLN	C4-N3	3.67	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	LCG	C4-N3	3.67	1.41	1.35
2	B	4	LCG	O2'-C6'	3.60	1.50	1.43
1	A	68	TLN	C4-N3	3.60	1.39	1.33
2	B	4	LCG	C6-N1	3.52	1.39	1.33
1	C	72	LCC	O2'-C6'	3.44	1.50	1.43
1	A	70	LCA	O2'-C6'	3.37	1.50	1.43
2	B	1	LCG	O2'-C6'	3.21	1.49	1.43
2	B	7	LCG	O2'-C6'	3.09	1.49	1.43
2	B	3	TLN	O2'-C6'	3.06	1.49	1.43
1	A	72	LCC	C5'-C4'	3.06	1.56	1.51
2	D	4	LCG	O4'-C1'	-3.05	1.38	1.42
1	C	66	LCC	O2'-C6'	3.03	1.49	1.43
2	D	6	LCG	C6-N1	3.00	1.38	1.33
1	C	72	LCC	C5'-C4'	2.96	1.56	1.51
2	D	6	LCG	O2'-C6'	2.87	1.49	1.43
1	C	71	LCC	C6-C5	-2.87	1.32	1.40
2	D	1	LCG	O2'-C2'	2.85	1.50	1.43
2	D	4	LCG	O2'-C6'	2.80	1.49	1.43
2	B	6	LCG	O2'-C6'	2.78	1.48	1.43
2	D	3	TLN	C4'-C3'	-2.75	1.50	1.53
2	D	1	LCG	C6-N1	2.73	1.37	1.33
1	C	68	TLN	C4'-C3'	-2.73	1.50	1.53
1	A	72	LCC	C6-C5	-2.73	1.32	1.40
1	C	69	LCC	C6-C5	-2.73	1.32	1.40
2	D	7	LCG	O2'-C6'	2.68	1.48	1.43
2	D	5	LCA	O2'-C6'	2.67	1.48	1.43
2	D	2	LCG	C6-N1	2.65	1.37	1.33
1	C	67	LCC	O2'-C6'	2.62	1.48	1.43
2	B	7	LCG	C8-N7	-2.61	1.30	1.34
2	D	6	LCG	C4'-C3'	-2.60	1.50	1.53
1	C	66	LCC	C5-C4	2.55	1.45	1.41
2	B	7	LCG	O2'-C2'	2.54	1.49	1.43
1	A	69	LCC	O2'-C6'	2.54	1.48	1.43
1	C	67	LCC	C6-C5	-2.50	1.33	1.40
2	B	2	LCG	C5-C4	-2.49	1.34	1.40
1	A	71	LCC	O2'-C6'	2.43	1.48	1.43
2	B	6	LCG	C2-N1	2.42	1.39	1.35
2	D	2	LCG	C4'-C3'	-2.41	1.50	1.53
1	A	69	LCC	C6-C5	-2.41	1.33	1.40
2	D	3	TLN	O2'-C6'	2.41	1.48	1.43
2	B	1	LCG	O2'-C2'	2.40	1.49	1.43
2	D	3	TLN	C2-N3	-2.39	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66	LCC	C6-C5	-2.38	1.33	1.40
1	A	67	LCC	C6-C5	-2.37	1.33	1.40
1	A	70	LCA	C4'-C3'	-2.36	1.51	1.53
1	C	70	LCA	O2'-C6'	2.35	1.48	1.43
2	B	4	LCG	C4'-C3'	-2.35	1.51	1.53
1	C	70	LCA	C2-N3	2.35	1.35	1.32
1	C	72	LCC	C2-N3	-2.34	1.33	1.38
1	A	69	LCC	O5'-C5'	-2.33	1.39	1.44
2	B	6	LCG	C8-N7	-2.30	1.30	1.34
2	D	1	LCG	C4'-C3'	-2.29	1.51	1.53
2	B	4	LCG	C8-N7	-2.28	1.30	1.34
2	D	7	LCG	O4'-C1'	2.28	1.46	1.42
2	D	3	TLN	C6-C5	-2.28	1.33	1.40
1	C	70	LCA	C8-N7	-2.27	1.30	1.34
1	C	68	TLN	C6-C5	-2.26	1.33	1.40
2	D	6	LCG	O2'-C2'	2.25	1.48	1.43
1	C	69	LCC	O2'-C6'	2.25	1.48	1.43
1	C	71	LCC	C4'-C3'	-2.24	1.51	1.53
2	B	2	LCG	C6-N1	2.23	1.36	1.33
1	A	66	LCC	O2'-C6'	2.23	1.47	1.43
2	B	2	LCG	O2'-C2'	2.22	1.48	1.43
2	B	3	TLN	C4-C5	2.21	1.46	1.41
1	A	66	LCC	C5-C4	2.21	1.44	1.41
1	A	66	LCC	C2-N3	-2.19	1.33	1.38
1	C	69	LCC	C4'-C3'	-2.18	1.51	1.53
2	B	5	LCA	O2'-C6'	2.18	1.47	1.43
1	A	72	LCC	C2-N3	-2.15	1.33	1.38
2	B	3	TLN	O5'-C5'	-2.14	1.39	1.44
2	B	3	TLN	C4'-C3'	-2.14	1.51	1.53
1	C	66	LCC	C2-N3	-2.14	1.33	1.38
1	C	72	LCC	C6-C5	-2.13	1.34	1.40
1	A	68	TLN	O5'-C5'	-2.12	1.39	1.44
1	A	72	LCC	O3'-C3'	2.12	1.47	1.42
2	D	6	LCG	O4'-C4'	-2.11	1.42	1.45
1	C	68	TLN	O2'-C6'	2.10	1.47	1.43
1	C	68	TLN	O2'-C2'	2.10	1.48	1.43
2	D	2	LCG	O2'-C6'	2.09	1.47	1.43
2	B	6	LCG	C4'-C3'	-2.09	1.51	1.53
1	A	67	LCC	O2'-C6'	2.07	1.47	1.43
1	A	71	LCC	O2'-C2'	2.04	1.48	1.43
1	A	67	LCC	O5'-C5'	-2.03	1.39	1.44

All (162) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3	TLN	C4-N3-C2	15.98	128.63	115.14
1	A	68	TLN	C4-N3-C2	15.24	128.01	115.14
1	C	68	TLN	C4-N3-C2	14.66	127.52	115.14
2	D	3	TLN	C4-N3-C2	14.15	127.09	115.14
1	A	72	LCC	C2-N3-C4	10.65	128.88	116.02
1	C	66	LCC	C2-N3-C4	10.09	128.21	116.02
1	A	71	LCC	C2-N3-C4	9.98	128.06	116.02
1	A	69	LCC	C2-N3-C4	9.54	127.54	116.02
2	D	2	LCG	C5-C6-N1	-9.51	110.42	123.43
1	A	66	LCC	C2-N3-C4	9.17	127.09	116.02
1	C	72	LCC	C2-N3-C4	8.60	126.40	116.02
2	B	7	LCG	C5-C6-N1	-8.55	111.73	123.43
2	B	4	LCG	C5-C6-N1	-8.19	112.23	123.43
1	C	67	LCC	C2-N3-C4	8.14	125.85	116.02
1	C	71	LCC	C2-N3-C4	8.09	125.79	116.02
2	B	1	LCG	C5-C6-N1	-8.09	112.36	123.43
1	A	67	LCC	C2-N3-C4	7.89	125.54	116.02
2	D	1	LCG	C5-C6-N1	-7.81	112.75	123.43
2	D	2	LCG	C6-N1-C2	7.69	128.15	115.93
1	C	69	LCC	C2-N3-C4	7.68	125.29	116.02
2	D	6	LCG	C5-C6-N1	-7.68	112.93	123.43
2	D	7	LCG	C5-C6-N1	-7.46	113.22	123.43
2	B	6	LCG	C5-C6-N1	-7.41	113.29	123.43
2	D	4	LCG	C5-C6-N1	-7.26	113.50	123.43
2	D	2	LCG	C2-N3-C4	-6.67	107.74	115.36
2	B	7	LCG	C6-N1-C2	6.59	126.40	115.93
2	B	4	LCG	C6-N1-C2	6.45	126.18	115.93
2	B	2	LCG	C5-C6-N1	-6.05	115.15	123.43
2	B	1	LCG	C6-N1-C2	5.91	125.33	115.93
2	D	7	LCG	C6-N1-C2	5.90	125.31	115.93
2	B	2	LCG	O4'-C4'-C3'	-5.71	94.66	102.22
2	D	1	LCG	C6-N1-C2	5.61	124.85	115.93
2	D	4	LCG	C6-N1-C2	5.55	124.74	115.93
2	D	6	LCG	C6-N1-C2	5.44	124.58	115.93
2	B	6	LCG	C6-N1-C2	5.23	124.24	115.93
2	D	4	LCG	O4'-C4'-C3'	-5.22	95.31	102.22
2	D	1	LCG	C2-N3-C4	-5.15	109.48	115.36
2	B	2	LCG	C6-N1-C2	4.94	123.78	115.93
2	D	1	LCG	O4'-C4'-C3'	-4.70	96.00	102.22
1	C	71	LCC	C5M-C5-C4	-4.54	117.13	121.72
2	B	2	LCG	C6-C5-C4	-4.48	116.52	120.80
1	C	72	LCC	O4'-C4'-C3'	-4.43	96.36	102.22
1	A	68	TLN	C5-C6-N1	4.26	126.79	122.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	7	LCG	N3-C2-N1	-4.24	121.57	127.22
1	C	67	LCC	C5M-C5-C4	-3.94	117.73	121.72
2	D	7	LCG	N3-C2-N1	-3.90	122.01	127.22
2	D	7	LCG	O2'-C2'-C1'	-3.84	93.93	105.66
2	D	5	LCA	C5-C6-N6	3.83	126.18	120.35
1	A	67	LCC	O4'-C4'-C3'	-3.83	97.15	102.22
2	D	4	LCG	O2'-C6'-C4'	-3.81	96.39	103.78
1	A	66	LCC	O5'-C5'-C4'	-3.73	104.18	111.71
2	D	4	LCG	N3-C2-N1	-3.64	122.36	127.22
2	D	1	LCG	C6-C5-C4	-3.64	117.32	120.80
2	B	1	LCG	C6-C5-C4	-3.54	117.42	120.80
2	B	4	LCG	C6-C5-C4	-3.50	117.45	120.80
2	D	6	LCG	N3-C2-N1	-3.43	122.65	127.22
1	C	70	LCA	C6'-O2'-C2'	-3.41	101.41	107.65
2	D	7	LCG	N2-C2-N3	3.39	123.32	117.79
2	B	4	LCG	N3-C2-N1	-3.35	122.75	127.22
1	A	67	LCC	C3'-C2'-C1'	-3.32	92.75	100.22
2	D	1	LCG	C6'-O2'-C2'	-3.32	101.58	107.65
2	D	7	LCG	C6-C5-C4	-3.27	117.67	120.80
2	B	7	LCG	C6-C5-C4	-3.26	117.69	120.80
2	B	6	LCG	N3-C2-N1	-3.25	122.89	127.22
2	D	4	LCG	C6-C5-C4	-3.24	117.71	120.80
1	C	72	LCC	C5M-C5-C6	3.16	125.35	118.68
2	D	7	LCG	C4-C5-N7	3.15	112.68	109.40
2	D	3	TLN	O4'-C4'-C3'	-3.13	98.08	102.22
2	B	2	LCG	N3-C2-N1	-3.06	123.14	127.22
1	C	67	LCC	O2'-C2'-C3'	3.00	109.32	103.42
1	C	67	LCC	C5-C4-N3	-2.97	116.56	121.26
2	B	6	LCG	C6-C5-C4	-2.96	117.97	120.80
2	D	5	LCA	O4'-C4'-C3'	-2.96	98.30	102.22
2	D	2	LCG	C6'-O2'-C2'	-2.95	102.25	107.65
1	A	70	LCA	C5-C6-N6	2.93	124.81	120.35
2	D	2	LCG	C4-C5-N7	2.92	112.45	109.40
1	A	68	TLN	C5M-C5-C6	2.92	124.85	118.68
2	B	6	LCG	O2'-C6'-C4'	-2.92	98.12	103.78
2	B	4	LCG	C2-N3-C4	-2.92	112.03	115.36
2	D	4	LCG	C4'-O4'-C1'	2.91	112.66	107.58
2	B	1	LCG	C2-N3-C4	-2.89	112.06	115.36
2	B	2	LCG	O2'-C2'-C3'	2.81	108.95	103.42
1	C	66	LCC	O4'-C4'-C3'	-2.80	98.51	102.22
2	B	5	LCA	O2'-C6'-C4'	-2.79	98.37	103.78
2	D	4	LCG	O3'-C3'-C4'	-2.78	105.08	112.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	68	TLN	O4'-C4'-C3'	-2.77	98.55	102.22
1	C	72	LCC	O2'-C2'-C3'	-2.77	97.98	103.42
2	D	2	LCG	O4'-C4'-C3'	-2.76	98.57	102.22
1	C	67	LCC	C3'-C2'-C1'	-2.76	94.02	100.22
2	D	4	LCG	C6'-O2'-C2'	2.75	112.68	107.65
1	A	72	LCC	C5M-C5-C6	2.74	124.47	118.68
1	A	69	LCC	C5-C6-N1	2.73	125.14	122.19
1	C	66	LCC	C5-C4-N3	-2.71	116.98	121.26
2	D	7	LCG	C3'-C2'-C1'	-2.67	94.22	100.22
1	C	71	LCC	N4-C4-N3	2.66	120.79	117.03
2	D	2	LCG	C6-C5-C4	-2.62	118.29	120.80
1	C	66	LCC	C6'-C4'-C5'	2.61	123.36	116.17
2	D	2	LCG	O4'-C1'-C2'	-2.60	98.80	104.50
1	A	71	LCC	C5-C4-N3	-2.60	117.16	121.26
1	C	68	TLN	C3'-C2'-C1'	-2.60	94.38	100.22
2	B	7	LCG	C3'-C2'-C1'	-2.59	94.40	100.22
1	C	71	LCC	C5-C4-N3	-2.57	117.20	121.26
2	B	1	LCG	O4'-C4'-C6'	-2.56	100.55	105.97
1	A	66	LCC	C6'-O2'-C2'	-2.54	103.00	107.65
2	B	5	LCA	O4'-C4'-C3'	-2.54	98.86	102.22
1	C	71	LCC	C6-N1-C1'	2.50	124.86	119.24
2	B	1	LCG	N3-C2-N1	-2.48	123.91	127.22
1	C	66	LCC	C6'-O2'-C2'	-2.47	103.12	107.65
1	A	66	LCC	C5-C4-N3	-2.47	117.35	121.26
1	A	70	LCA	C6'-O2'-C2'	-2.46	103.15	107.65
2	B	1	LCG	O4'-C1'-C2'	-2.46	99.12	104.50
2	D	1	LCG	C4-C5-N7	2.45	111.95	109.40
2	B	2	LCG	O4'-C1'-C2'	-2.43	99.18	104.50
1	C	66	LCC	C4'-O4'-C1'	-2.41	103.37	107.58
2	B	2	LCG	C6'-O2'-C2'	-2.40	103.25	107.65
1	C	71	LCC	C5M-C5-C6	2.35	123.65	118.68
1	C	66	LCC	O5'-C5'-C4'	-2.33	107.02	111.71
2	B	1	LCG	C6'-O2'-C2'	-2.32	103.40	107.65
1	A	69	LCC	C6-N1-C1'	2.31	124.42	119.24
1	C	70	LCA	C2-N1-C6	2.30	122.68	118.75
2	D	1	LCG	O4'-C1'-C2'	-2.29	99.48	104.50
2	B	5	LCA	C6'-O2'-C2'	2.29	111.84	107.65
1	A	72	LCC	O2'-C2'-C3'	-2.29	98.92	103.42
2	B	3	TLN	O4'-C4'-C3'	-2.28	99.20	102.22
1	A	66	LCC	O4'-C4'-C3'	-2.28	99.20	102.22
1	A	66	LCC	C4'-O4'-C1'	-2.28	103.61	107.58
1	A	70	LCA	O2'-C2'-C1'	2.28	112.61	105.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	69	LCC	C5M-C5-C6	2.27	123.47	118.68
1	C	72	LCC	C5M-C5-C4	-2.27	119.43	121.72
2	D	4	LCG	C4-C5-N7	2.26	111.75	109.40
1	A	72	LCC	O4'-C4'-C6'	-2.25	101.22	105.97
1	C	70	LCA	O3'-C3'-C4'	-2.24	106.52	112.52
1	A	72	LCC	N4-C4-N3	2.24	120.20	117.03
1	C	70	LCA	C4'-O4'-C1'	-2.23	103.68	107.58
1	A	72	LCC	C5M-C5-C4	-2.23	119.47	121.72
1	C	72	LCC	N4-C4-N3	2.23	120.18	117.03
2	B	7	LCG	C2-N3-C4	-2.22	112.82	115.36
1	A	71	LCC	O2'-C6'-C4'	-2.20	99.52	103.78
1	C	70	LCA	C4-C5-N7	2.20	111.69	109.40
1	C	71	LCC	O2'-C2'-C1'	-2.20	98.95	105.66
2	D	3	TLN	C5M-C5-C6	2.19	123.30	118.68
1	A	69	LCC	C4'-O4'-C1'	-2.18	103.77	107.58
1	C	67	LCC	C5M-C5-C6	2.17	123.26	118.68
2	D	1	LCG	O4'-C4'-C5'	2.16	112.89	108.97
1	A	71	LCC	C6-N1-C1'	2.16	124.09	119.24
1	C	71	LCC	C6'-O2'-C2'	-2.16	103.70	107.65
2	B	5	LCA	O2'-C2'-C3'	-2.15	99.20	103.42
2	D	7	LCG	O4'-C1'-C2'	2.14	109.21	104.50
1	A	68	TLN	C6'-O2'-C2'	-2.14	103.73	107.65
1	A	71	LCC	C5M-C5-C6	2.13	123.17	118.68
2	B	6	LCG	C4'-O4'-C1'	2.12	111.29	107.58
2	D	5	LCA	O2'-C6'-C4'	-2.12	99.67	103.78
2	B	2	LCG	N2-C2-N3	2.10	121.21	117.79
2	B	6	LCG	O4'-C4'-C3'	-2.09	99.45	102.22
1	C	67	LCC	C6-N1-C1'	2.08	123.91	119.24
2	B	7	LCG	N2-C2-N3	2.07	121.17	117.79
2	B	7	LCG	C5'-C4'-C3'	2.07	123.17	114.53
1	C	71	LCC	O2'-C2'-C3'	2.04	107.43	103.42
2	B	7	LCG	O4'-C4'-C3'	-2.03	99.54	102.22
2	D	7	LCG	C2-N3-C4	-2.02	113.05	115.36
2	D	3	TLN	C5M-C5-C4	-2.02	117.76	121.37
1	A	72	LCC	C3'-C2'-C1'	2.01	104.75	100.22

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	69	LCC	O4'-C4'-C5'-O5'
1	A	67	LCC	O4'-C4'-C5'-O5'



There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	67	LCC	2	0
1	A	68	TLN	1	0
1	C	72	LCC	2	0
2	D	1	LCG	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or 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 length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	NCO	B	101	-	6,6,6	0.70	0	-		
5	CAC	D	101	-	0,4,4	0.00	-	0,6,6	0.00	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	0/7	-	-	-	-
1	C	0/7	-	-	-	-
2	B	0/7	-	-	-	-
2	D	0/7	-	-	-	-
All	All	0/28	-	-	-	-

There are no RSRZ outliers to report.

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	LCC	A	66	19/23	0.93	0.10	32,39,46,46	0
1	LCC	C	67	22/23	0.93	0.10	31,42,46,48	0
1	LCC	A	67	22/23	0.93	0.12	32,42,45,48	0
1	TLN	C	68	22/23	0.93	0.12	36,39,45,46	0
1	LCA	C	70	23/24	0.94	0.12	23,30,41,45	0
1	TLN	A	68	22/23	0.94	0.11	35,39,45,47	0
1	LCC	C	66	19/23	0.94	0.11	32,39,45,46	0
1	LCC	A	69	22/23	0.94	0.12	30,38,42,45	0
1	LCC	C	71	22/23	0.95	0.09	21,27,32,35	0
2	LCG	B	1	21/25	0.95	0.09	19,24,28,33	0
2	LCG	D	1	21/25	0.95	0.10	19,24,28,32	0
1	LCC	C	69	22/23	0.95	0.11	31,38,44,46	0
2	LCA	D	5	23/24	0.96	0.10	27,31,34,35	0
2	LCG	B	7	24/25	0.96	0.10	28,30,33,35	0
1	LCA	A	70	23/24	0.96	0.12	22,30,40,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	LCG	D	7	24/25	0.96	0.08	28,30,33,35	0
2	LCG	D	6	24/25	0.96	0.10	26,30,32,33	0
2	LCG	B	6	24/25	0.96	0.10	27,30,31,33	0
2	LCG	D	4	24/25	0.96	0.11	25,29,32,32	0
1	LCC	A	71	22/23	0.97	0.11	22,25,32,34	0
2	TLN	D	3	22/23	0.97	0.10	20,24,26,27	0
1	LCC	A	72	22/23	0.97	0.11	19,23,27,28	0
2	LCA	B	5	23/24	0.97	0.10	25,31,34,35	0
1	LCC	C	72	22/23	0.98	0.10	20,24,27,29	0
2	LCG	B	4	24/25	0.98	0.11	24,28,31,31	0
2	TLN	B	3	22/23	0.98	0.11	18,24,25,26	0
2	LCG	D	2	24/25	0.98	0.10	19,21,24,26	0
2	LCG	B	2	24/25	0.98	0.10	19,22,25,25	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	CAC	D	101	5/5	0.91	0.14	84,86,86,87	0
3	NCO	B	101	7/7	0.99	0.15	26,27,29,30	0
4	MG	C	101	1/1	0.99	0.13	18,18,18,18	1

### 6.5 Other polymers [i](#)

There are no such residues in this entry.