



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 22, 2022 – 02:04 PM EDT

PDB ID : 7U3X  
Title : [F233] Self-assembling tensegrity triangle with two turns, three turns and three turns of DNA per axis by extension with P1 symmetry  
Authors : Woloszyn, K.; Vecchioni, S.; Seeman, N.C.; Sha, R.; Ohayon, Y.P.  
Deposited on : 2022-02-28  
Resolution : 5.68 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.

The types of validation reports are described at <http://www.wwpdb.org/validation/2017/FAQs#types>.

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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
Xtriage (Phenix)	:	1.13
EDS	:	2.29
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)	:	2.29

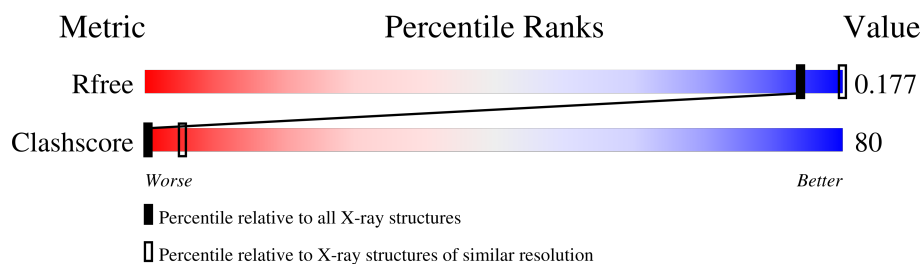
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*








The reported resolution of this entry is 5.68 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 <sub>free</sub>	130704	1001 (7.50-3.86)
Clashscore	141614	1018 (7.40-3.90)

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 of 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	31	 23% 74%
2	E	14	 14% 86%
3	D	24	 50% 46%
4	B	31	 29% 71%
5	F	24	 21% 79%
6	C	21	 14% 86%
7	M	21	 5% 95%

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 3385 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 DNA chain called DNA (31-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	31	Total	C	N	O	P	0	0	0
			633	300	123	180	30			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	14	Total	C	N	O	P	0	0	0
			285	137	49	86	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	24	Total	C	N	O	P	0	0	0
			491	234	87	147	23			

- Molecule 4 is a DNA chain called DNA (31-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	31	Total	C	N	O	P	0	0	0
			633	302	118	183	30			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	24	Total	C	N	O	P	0	0	0
			496	237	93	143	23			

- Molecule 6 is a DNA chain called DNA (5'-D(\*AP\*AP\*CP\*CP\*TP\*AP\*CP\*CP\*TP\*GP\*GP\*CP\*AP\*GP\*GP\*AP\*CP\*GP\*AP\*CP\*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	C	21	Total 426	C 203	N 82	O 121	P 20	0	0	0

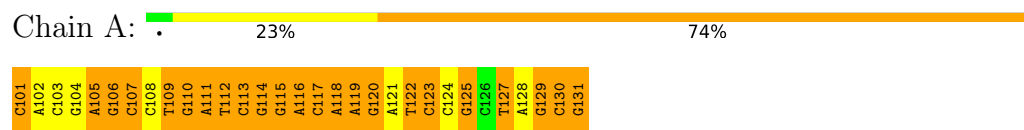
- Molecule 7 is a DNA chain called DNA (5'-D(P\*TP\*CP\*AP\*CP\*CP\*TP\*GP\*CP\*CP\*AP\*CP\*CP\*GP\*TP\*AP\*CP\*AP\*CP\*CP\*GP\*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	M	21	Total 421	C 200	N 76	O 124	P 21	0	0	0

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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. 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. 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: DNA (31-MER)



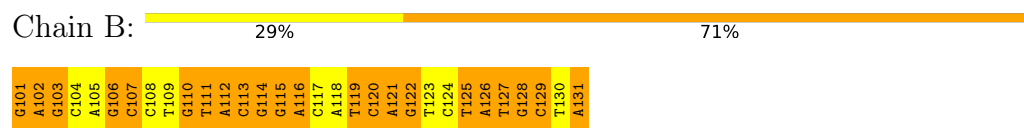
- Molecule 2: DNA (5'-D(\*TP\*TP\*AP\*GP\*TP\*CP\*GP\*TP\*GP\*GP\*CP\*TP\*CP\*G)-3')



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



- Molecule 4: DNA (31-MER)



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



- Molecule 6: DNA (5'-D(\*AP\*AP\*CP\*CP\*TP\*AP\*CP\*CP\*TP\*GP\*GP\*CP\*AP\*GP\*GP\*AP\*CP\*GP\*AP\*CP\*T)-3')



A101	A102	C103	C104	T105	A106	C107	C108	T109	G110	G111	C112	A113	G114	G115	A116	C117	G118	A119	C120	T121
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● Molecule 7: DNA (5'-D(P\*TP\*CP\*AP\*CP\*CP\*TP\*GP\*CP\*CP\*AP\*CP\*CP\*GP\*TP\*AP\*CP\*AP\*CP\*CP\*GP\*A)-3')



T101	C102	A103	C104	C105	T106	G107	C108	C109	A110	C111	C112	G113	T114	A115	C116	A117	C118	C119	G120	A121
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.96Å 100.28Å 102.06Å 100.58° 100.81° 102.39°	Depositor
Resolution (Å)	41.05 – 5.68 97.49 – 5.68	Depositor EDS
% Data completeness (in resolution range)	68.8 (41.05-5.68) 62.4 (97.49-5.68)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.03 (at 5.76Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, $R_{free}$	0.124 , 0.179 0.121 , 0.177	Depositor DCC
$R_{free}$ test set	273 reflections (5.33%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	334.3	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.10 , 999.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.030 for -h,-l,-k	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	3385	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	441.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.06% 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 ⓘ

### 5.1 Standard geometry ⓘ

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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	2.84	53/711 (7.5%)	2.33	44/1095 (4.0%)
2	E	3.40	50/318 (15.7%)	2.59	33/490 (6.7%)
3	D	2.14	17/549 (3.1%)	1.81	13/847 (1.5%)
4	B	2.56	40/710 (5.6%)	2.14	41/1094 (3.7%)
5	F	2.56	30/557 (5.4%)	1.92	17/860 (2.0%)
6	C	3.08	48/478 (10.0%)	2.21	31/735 (4.2%)
7	M	3.64	54/470 (11.5%)	2.75	57/720 (7.9%)
All	All	2.86	292/3793 (7.7%)	2.24	236/5841 (4.0%)

All (292) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	113	DG	C3'-O3'	21.95	1.72	1.44
6	C	117	DC	C3'-O3'	18.64	1.68	1.44
2	E	107	DG	C3'-O3'	18.16	1.67	1.44
1	A	112	DT	C3'-O3'	16.75	1.65	1.44
7	M	101	DT	C1'-N1	16.08	1.70	1.49
7	M	102	DC	C3'-O3'	15.40	1.64	1.44
5	F	103	DT	C1'-N1	15.17	1.69	1.49
7	M	118	DC	C3'-O3'	14.59	1.62	1.44
6	C	115	DG	C3'-O3'	14.42	1.62	1.44
1	A	115	DG	C3'-O3'	14.08	1.62	1.44
1	A	119	DA	N9-C4	-14.04	1.29	1.37
4	B	111	DT	C3'-O3'	13.91	1.62	1.44
3	D	117	DG	C3'-O3'	13.90	1.62	1.44
5	F	123	DG	C3'-O3'	-12.99	1.27	1.44
7	M	101	DT	C3'-O3'	12.76	1.60	1.44
1	A	113	DC	C1'-N1	12.66	1.65	1.49
5	F	109	DA	C3'-O3'	-12.54	1.27	1.44
7	M	112	DC	C1'-N1	12.45	1.65	1.49
7	M	102	DC	C1'-N1	12.45	1.65	1.49
1	A	103	DC	C3'-O3'	11.93	1.59	1.44
5	F	115	DA	N9-C4	-11.93	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	112	DA	N9-C4	11.88	1.45	1.37
7	M	114	DT	C1'-N1	-11.62	1.30	1.47
4	B	113	DC	C1'-N1	11.55	1.64	1.49
2	E	104	DG	C5-C4	-11.55	1.30	1.38
1	A	111	DA	N9-C4	11.48	1.44	1.37
7	M	111	DC	C3'-O3'	-11.32	1.29	1.44
4	B	119	DT	C3'-O3'	11.09	1.58	1.44
7	M	115	DA	N9-C4	11.02	1.44	1.37
7	M	104	DC	C3'-O3'	10.77	1.57	1.44
2	E	103	DA	N9-C4	-10.33	1.31	1.37
5	F	112	DC	C1'-N1	10.22	1.62	1.49
7	M	105	DC	C3'-O3'	9.96	1.56	1.44
6	C	108	DC	C3'-O3'	9.86	1.56	1.44
5	F	116	DT	C1'-N1	-9.75	1.33	1.47
4	B	111	DT	C1'-N1	9.35	1.61	1.49
7	M	109	DC	C1'-N1	9.30	1.61	1.49
7	M	115	DA	N3-C4	9.23	1.40	1.34
1	A	129	DG	C3'-O3'	9.06	1.55	1.44
5	F	111	DA	P-O5'	9.05	1.68	1.59
7	M	102	DC	P-O5'	9.04	1.68	1.59
7	M	110	DA	N9-C4	8.97	1.43	1.37
6	C	111	DG	P-O5'	8.92	1.68	1.59
7	M	118	DC	N3-C4	-8.90	1.27	1.33
6	C	113	DA	C3'-O3'	-8.81	1.32	1.44
4	B	131	DA	C6-N1	8.76	1.41	1.35
1	A	103	DC	C1'-N1	8.67	1.60	1.49
4	B	127	DT	C1'-N1	8.61	1.60	1.49
1	A	105	DA	C3'-O3'	8.60	1.55	1.44
4	B	129	DC	C3'-O3'	8.59	1.55	1.44
4	B	131	DA	C5-C6	8.57	1.48	1.41
3	D	121	DC	C3'-O3'	8.55	1.55	1.44
6	C	117	DC	P-O5'	8.54	1.68	1.59
5	F	111	DA	O5'-C5'	8.53	1.63	1.42
6	C	108	DC	P-O5'	8.47	1.68	1.59
6	C	120	DC	N3-C4	-8.45	1.28	1.33
2	E	108	DT	C5'-C4'	8.45	1.60	1.51
6	C	111	DG	C8-N7	8.42	1.36	1.30
4	B	129	DC	C1'-N1	8.38	1.60	1.49
1	A	113	DC	C3'-O3'	8.29	1.54	1.44
6	C	120	DC	N1-C6	-8.27	1.32	1.37
7	M	120	DG	C5-C6	8.25	1.50	1.42
2	E	104	DG	N9-C4	-8.12	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	101	DA	C5-C6	8.11	1.48	1.41
2	E	114	DG	N9-C4	8.11	1.44	1.38
4	B	121	DA	N9-C4	8.10	1.42	1.37
1	A	103	DC	P-O5'	8.09	1.67	1.59
7	M	119	DC	C1'-N1	8.05	1.59	1.49
4	B	112	DA	C5'-C4'	8.04	1.60	1.51
5	F	111	DA	C5'-C4'	7.99	1.60	1.51
6	C	110	DG	N9-C4	-7.84	1.31	1.38
7	M	121	DA	N9-C4	7.81	1.42	1.37
6	C	101	DA	C3'-O3'	7.77	1.54	1.44
3	D	101	DT	C1'-N1	7.76	1.59	1.49
7	M	114	DT	C5-C6	-7.67	1.28	1.34
2	E	114	DG	P-O5'	7.63	1.67	1.59
2	E	108	DT	C1'-N1	7.55	1.59	1.49
2	E	102	DT	P-O5'	7.54	1.67	1.59
4	B	124	DC	C3'-O3'	-7.52	1.34	1.44
5	F	114	DG	N9-C4	-7.50	1.31	1.38
2	E	108	DT	N3-C4	-7.49	1.32	1.38
6	C	110	DG	C3'-O3'	7.45	1.53	1.44
1	A	105	DA	C5-C6	7.45	1.47	1.41
4	B	117	DC	C3'-O3'	-7.43	1.34	1.44
2	E	108	DT	O5'-C5'	7.39	1.60	1.42
5	F	103	DT	C2-N3	7.38	1.43	1.37
4	B	111	DT	C4'-O4'	7.35	1.52	1.45
5	F	121	DT	C3'-O3'	7.35	1.53	1.44
2	E	109	DG	C3'-O3'	-7.33	1.34	1.44
1	A	105	DA	N9-C4	7.32	1.42	1.37
3	D	110	DG	C3'-O3'	7.31	1.53	1.44
1	A	112	DT	C1'-N1	7.30	1.58	1.49
1	A	115	DG	P-O5'	7.25	1.67	1.59
1	A	106	DG	C5-C6	7.22	1.49	1.42
3	D	115	DT	C2-N3	-7.22	1.31	1.37
2	E	108	DT	C4-C5	-7.22	1.38	1.45
1	A	118	DA	C3'-O3'	7.20	1.53	1.44
1	A	119	DA	N3-C4	-7.19	1.30	1.34
1	A	127	DT	C3'-O3'	7.17	1.53	1.44
7	M	113	DG	C5-C6	7.17	1.49	1.42
2	E	104	DG	C2-N3	-7.16	1.27	1.32
4	B	114	DG	C3'-O3'	7.12	1.53	1.44
1	A	123	DC	N1-C6	-7.12	1.32	1.37
1	A	107	DC	C3'-O3'	-7.10	1.34	1.44
1	A	117	DC	C1'-N1	-7.10	1.37	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	113	DG	C2'-C1'	7.08	1.59	1.52
1	A	116	DA	C3'-O3'	-7.08	1.34	1.44
6	C	107	DC	P-O5'	7.07	1.66	1.59
2	E	108	DT	P-O5'	7.06	1.66	1.59
7	M	121	DA	C5-C6	7.03	1.47	1.41
7	M	104	DC	C1'-N1	7.02	1.58	1.49
5	F	103	DT	N1-C2	7.01	1.43	1.38
7	M	107	DG	N9-C4	-6.97	1.32	1.38
2	E	105	DT	N1-C2	-6.96	1.32	1.38
5	F	113	DT	C1'-N1	6.91	1.58	1.49
3	D	124	DC	C1'-N1	6.89	1.58	1.49
2	E	103	DA	N7-C5	-6.85	1.35	1.39
6	C	117	DC	O3'-P	6.84	1.69	1.61
2	E	103	DA	C5-C4	-6.83	1.33	1.38
1	A	107	DC	C1'-N1	6.82	1.58	1.49
7	M	103	DA	C3'-O3'	6.82	1.52	1.44
6	C	107	DC	C3'-O3'	6.82	1.52	1.44
5	F	113	DT	C5'-C4'	6.81	1.58	1.51
1	A	111	DA	C3'-O3'	-6.79	1.35	1.44
6	C	117	DC	N1-C2	6.78	1.47	1.40
2	E	104	DG	C3'-O3'	-6.77	1.35	1.44
6	C	105	DT	C3'-O3'	6.75	1.52	1.44
7	M	118	DC	C2-O2	-6.72	1.18	1.24
6	C	120	DC	P-O5'	6.69	1.66	1.59
1	A	131	DG	P-O5'	6.68	1.66	1.59
7	M	117	DA	C3'-O3'	-6.67	1.35	1.44
7	M	113	DG	C8-N7	6.64	1.34	1.30
4	B	131	DA	C8-N7	6.64	1.36	1.31
2	E	110	DG	C8-N7	6.63	1.34	1.30
2	E	104	DG	C5-C6	-6.62	1.35	1.42
5	F	120	DG	C3'-O3'	6.62	1.52	1.44
2	E	102	DT	C5-C6	-6.58	1.29	1.34
2	E	114	DG	C5'-C4'	6.55	1.58	1.51
2	E	109	DG	C4'-C3'	-6.55	1.46	1.52
4	B	131	DA	N7-C5	6.52	1.43	1.39
5	F	115	DA	N3-C4	-6.51	1.30	1.34
7	M	114	DT	N1-C2	-6.51	1.32	1.38
7	M	101	DT	C5-C6	6.50	1.39	1.34
4	B	130	DT	P-O5'	6.48	1.66	1.59
5	F	101	DT	C1'-N1	6.47	1.57	1.49
4	B	130	DT	C5'-C4'	6.43	1.58	1.51
1	A	106	DG	N7-C5	6.41	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	103	DA	C5-C6	-6.39	1.35	1.41
3	D	120	DG	C6-O6	6.35	1.29	1.24
2	E	102	DT	C3'-O3'	6.35	1.52	1.44
4	B	110	DG	C2'-C1'	-6.34	1.46	1.52
3	D	124	DC	C5'-C4'	6.33	1.58	1.51
7	M	113	DG	C5-C4	6.33	1.42	1.38
2	E	104	DG	C6-O6	-6.31	1.18	1.24
4	B	101	DG	N9-C4	6.28	1.43	1.38
2	E	108	DT	C4'-O4'	6.27	1.51	1.45
6	C	109	DT	C1'-N1	6.26	1.57	1.49
7	M	113	DG	C4'-C3'	6.24	1.59	1.53
4	B	122	DG	C3'-O3'	6.23	1.52	1.44
4	B	106	DG	C3'-O3'	6.22	1.52	1.44
7	M	115	DA	N7-C5	6.21	1.43	1.39
7	M	116	DC	P-O5'	6.20	1.66	1.59
6	C	111	DG	C1'-N9	6.18	1.57	1.49
6	C	101	DA	N7-C5	6.17	1.43	1.39
2	E	107	DG	N9-C4	6.14	1.42	1.38
6	C	117	DC	O5'-C5'	6.14	1.57	1.42
7	M	114	DT	O5'-C5'	6.14	1.57	1.42
2	E	110	DG	C5-C4	6.13	1.42	1.38
1	A	116	DA	N9-C4	6.12	1.41	1.37
5	F	108	DT	C3'-O3'	-6.12	1.35	1.44
3	D	124	DC	N1-C2	6.11	1.46	1.40
7	M	102	DC	O5'-C5'	6.10	1.57	1.42
1	A	120	DG	C3'-O3'	-6.08	1.36	1.44
6	C	114	DG	C3'-O3'	-6.08	1.36	1.44
2	E	105	DT	N3-C4	-6.08	1.33	1.38
6	C	109	DT	P-O5'	6.07	1.65	1.59
7	M	120	DG	C6-O6	6.07	1.29	1.24
4	B	126	DA	C3'-O3'	6.07	1.51	1.44
1	A	106	DG	C8-N7	6.05	1.34	1.30
6	C	110	DG	N3-C4	-6.05	1.31	1.35
1	A	129	DG	C5'-C4'	6.04	1.57	1.51
7	M	115	DA	C3'-O3'	6.03	1.51	1.44
1	A	109	DT	C1'-N1	6.02	1.57	1.49
1	A	123	DC	C5-C6	-6.01	1.29	1.34
5	F	121	DT	C5'-C4'	6.01	1.57	1.51
4	B	111	DT	P-O5'	6.00	1.65	1.59
4	B	125	DT	C3'-O3'	5.97	1.51	1.44
3	D	102	DG	C3'-O3'	5.96	1.51	1.44
4	B	107	DC	C1'-N1	5.96	1.57	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	104	DG	N1-C2	-5.96	1.32	1.37
6	C	108	DC	O5'-C5'	5.95	1.57	1.42
1	A	114	DG	C5-C6	5.94	1.48	1.42
4	B	110	DG	C3'-O3'	-5.94	1.36	1.44
1	A	129	DG	P-O5'	5.92	1.65	1.59
1	A	111	DA	C5-C4	5.89	1.42	1.38
7	M	105	DC	O4'-C1'	-5.89	1.35	1.42
6	C	101	DA	N9-C4	5.85	1.41	1.37
2	E	114	DG	O5'-C5'	5.84	1.56	1.42
6	C	108	DC	C5'-C4'	5.82	1.57	1.51
3	D	119	DG	N3-C4	5.80	1.39	1.35
7	M	106	DT	C1'-N1	5.80	1.56	1.49
6	C	119	DA	C3'-O3'	5.79	1.51	1.44
4	B	113	DC	C5-C6	5.77	1.39	1.34
1	A	119	DA	C3'-O3'	5.77	1.51	1.44
5	F	118	DT	C1'-N1	-5.77	1.39	1.47
5	F	111	DA	C4'-C3'	5.76	1.59	1.53
7	M	101	DT	C3'-C2'	5.71	1.59	1.52
5	F	105	DG	P-O5'	5.71	1.65	1.59
2	E	107	DG	C3'-C2'	5.68	1.59	1.52
2	E	103	DA	C8-N7	-5.66	1.27	1.31
1	A	103	DC	C5'-C4'	5.66	1.57	1.51
1	A	116	DA	C5-C4	5.65	1.42	1.38
4	B	120	DC	C3'-O3'	-5.65	1.36	1.44
4	B	111	DT	C4-C5	-5.65	1.39	1.45
5	F	113	DT	C3'-O3'	5.62	1.51	1.44
7	M	104	DC	P-O5'	5.61	1.65	1.59
6	C	111	DG	O5'-C5'	5.54	1.56	1.42
1	A	117	DC	C4'-O4'	-5.54	1.39	1.45
7	M	102	DC	C4'-C3'	5.54	1.58	1.53
2	E	111	DC	C1'-N1	-5.53	1.39	1.47
7	M	118	DC	O3'-P	5.53	1.67	1.61
2	E	103	DA	C6-N6	-5.52	1.29	1.33
4	B	130	DT	O5'-C5'	5.50	1.55	1.42
7	M	115	DA	C6-N1	5.50	1.39	1.35
5	F	112	DC	C3'-O3'	5.49	1.51	1.44
2	E	103	DA	C6-N1	-5.46	1.31	1.35
6	C	102	DA	P-O5'	5.45	1.65	1.59
1	A	117	DC	C4-C5	5.45	1.47	1.43
6	C	119	DA	C6-N1	-5.44	1.31	1.35
4	B	111	DT	C5'-C4'	5.42	1.57	1.51
6	C	113	DA	N9-C4	-5.42	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	118	DC	N1-C6	-5.42	1.33	1.37
5	F	103	DT	C5-C6	5.41	1.38	1.34
1	A	131	DG	C5'-C4'	5.39	1.57	1.51
1	A	130	DC	P-O5'	5.37	1.65	1.59
4	B	124	DC	C1'-N1	-5.37	1.39	1.47
2	E	105	DT	N1-C6	-5.36	1.34	1.38
3	D	118	DT	C5-C7	-5.35	1.46	1.50
6	C	109	DT	O5'-C5'	5.34	1.55	1.42
6	C	120	DC	C2-O2	-5.34	1.19	1.24
4	B	113	DC	N3-C4	-5.34	1.30	1.33
6	C	116	DA	P-O5'	5.33	1.65	1.59
1	A	115	DG	O5'-C5'	5.33	1.55	1.42
6	C	107	DC	C1'-N1	5.32	1.56	1.49
1	A	115	DG	C5'-C4'	5.32	1.57	1.51
1	A	115	DG	C8-N7	5.30	1.34	1.30
4	B	128	DG	P-O5'	5.30	1.65	1.59
1	A	106	DG	C6-N1	5.29	1.43	1.39
2	E	111	DC	N1-C6	-5.29	1.33	1.37
3	D	118	DT	C4-C5	-5.29	1.40	1.45
5	F	121	DT	P-O5'	5.27	1.65	1.59
7	M	115	DA	C5-C6	5.26	1.45	1.41
6	C	119	DA	N9-C8	-5.24	1.33	1.37
3	D	119	DG	C6-N1	5.22	1.43	1.39
5	F	115	DA	C1'-N9	-5.22	1.40	1.47
2	E	110	DG	C6-N1	5.21	1.43	1.39
6	C	114	DG	C4'-C3'	-5.21	1.47	1.52
1	A	122	DT	C3'-O3'	-5.20	1.37	1.44
1	A	113	DC	C3'-C2'	5.19	1.58	1.52
4	B	113	DC	C2-N3	5.18	1.39	1.35
6	C	117	DC	C5'-C4'	5.18	1.57	1.51
7	M	120	DG	N7-C5	5.17	1.42	1.39
2	E	109	DG	N7-C5	5.15	1.42	1.39
4	B	113	DC	P-O5'	5.15	1.64	1.59
2	E	103	DA	C1'-N9	-5.14	1.40	1.47
2	E	112	DT	C3'-O3'	5.14	1.50	1.44
5	F	116	DT	N1-C2	-5.13	1.33	1.38
1	A	119	DA	N7-C5	-5.13	1.36	1.39
3	D	119	DG	N7-C5	5.12	1.42	1.39
2	E	107	DG	C5'-C4'	5.11	1.56	1.51
6	C	117	DC	C1'-N1	5.10	1.55	1.49
7	M	106	DT	C3'-O3'	5.09	1.50	1.44
7	M	113	DG	N3-C4	-5.08	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	107	DC	C4-N4	5.08	1.38	1.33
7	M	105	DC	C1'-N1	-5.08	1.40	1.47
2	E	102	DT	O5'-C5'	5.08	1.54	1.42
2	E	109	DG	N3-C4	5.06	1.39	1.35
6	C	112	DC	C1'-N1	5.06	1.55	1.49
5	F	123	DG	O3'-P	-5.05	1.55	1.61
4	B	112	DA	C1'-N9	5.04	1.55	1.49
6	C	118	DG	C5'-C4'	5.04	1.56	1.51
6	C	116	DA	N9-C4	5.04	1.40	1.37
2	E	101	DT	C3'-O3'	5.04	1.50	1.44
7	M	104	DC	C2-O2	-5.03	1.20	1.24
6	C	120	DC	C3'-O3'	-5.03	1.37	1.44
3	D	120	DG	C5-C6	5.02	1.47	1.42
6	C	111	DG	N9-C8	5.02	1.41	1.37
2	E	103	DA	C2'-C1'	-5.01	1.47	1.52
1	A	122	DT	N1-C2	-5.01	1.34	1.38
1	A	123	DC	C3'-O3'	5.01	1.50	1.44
2	E	109	DG	N9-C8	5.01	1.41	1.37
3	D	115	DT	N1-C2	-5.00	1.34	1.38

All (236) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	112	DT	O5'-P-OP1	-17.77	89.37	110.70
4	B	112	DA	O5'-P-OP1	-17.34	89.89	110.70
1	A	119	DA	O5'-P-OP1	-15.89	91.40	105.70
4	B	127	DT	O4'-C1'-N1	15.52	118.86	108.00
7	M	107	DG	O4'-C1'-N9	14.30	118.01	108.00
5	F	113	DT	O5'-P-OP1	-13.58	93.48	105.70
3	D	101	DT	O4'-C4'-C3'	-13.15	98.11	106.00
1	A	114	DG	O5'-P-OP2	-12.78	94.20	105.70
4	B	102	DA	O4'-C1'-N9	12.39	116.68	108.00
2	E	104	DG	N3-C4-N9	-11.60	119.04	126.00
7	M	101	DT	O4'-C1'-N1	11.49	116.04	108.00
6	C	109	DT	OP1-P-OP2	-11.36	102.57	119.60
1	A	130	DC	O4'-C4'-C3'	-11.28	99.23	106.00
7	M	109	DC	O5'-P-OP1	-10.84	95.95	105.70
7	M	103	DA	OP1-P-OP2	-10.74	103.49	119.60
7	M	107	DG	O5'-P-OP2	-10.66	96.11	105.70
7	M	105	DC	C1'-O4'-C4'	-10.09	100.01	110.10
1	A	120	DG	O4'-C4'-C3'	-10.07	99.96	106.00
1	A	106	DG	O4'-C1'-N9	10.03	115.02	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	103	DA	O5'-P-OP2	9.89	122.57	110.70
6	C	117	DC	O4'-C4'-C3'	-9.76	100.14	106.00
7	M	113	DG	P-O3'-C3'	9.71	131.36	119.70
3	D	116	DT	O4'-C4'-C3'	-9.53	100.28	106.00
4	B	125	DT	O4'-C4'-C3'	-9.42	100.35	106.00
2	E	108	DT	O4'-C1'-N1	9.39	114.57	108.00
1	A	118	DA	O4'-C4'-C3'	-9.21	100.48	106.00
7	M	111	DC	O4'-C4'-C3'	-9.14	100.52	106.00
1	A	130	DC	C3'-C2'-C1'	-9.12	91.55	102.50
2	E	109	DG	O4'-C4'-C3'	-9.03	100.58	106.00
3	D	119	DG	O4'-C1'-N9	8.98	114.28	108.00
3	D	101	DT	O4'-C1'-N1	8.97	114.28	108.00
6	C	112	DC	O5'-P-OP2	-8.94	97.66	105.70
1	A	115	DG	P-O3'-C3'	8.92	130.40	119.70
6	C	117	DC	P-O3'-C3'	8.80	130.26	119.70
2	E	105	DT	OP1-P-OP2	-8.64	106.64	119.60
7	M	118	DC	P-O3'-C3'	8.63	130.06	119.70
4	B	124	DC	O4'-C4'-C3'	-8.62	100.83	106.00
1	A	103	DC	O4'-C1'-N1	8.56	113.99	108.00
2	E	104	DG	N9-C4-C5	8.40	108.76	105.40
7	M	115	DA	O4'-C1'-N9	8.35	113.85	108.00
5	F	108	DT	O5'-P-OP2	-8.35	98.19	105.70
4	B	116	DA	O4'-C1'-N9	8.34	113.84	108.00
6	C	114	DG	O5'-P-OP1	8.33	120.70	110.70
5	F	104	DA	C3'-C2'-C1'	-8.22	92.64	102.50
7	M	107	DG	OP2-P-O3'	8.19	123.22	105.20
6	C	101	DA	O4'-C1'-N9	8.18	113.73	108.00
1	A	130	DC	C4'-C3'-C2'	-8.08	95.83	103.10
7	M	119	DC	O4'-C1'-N1	8.04	113.63	108.00
7	M	113	DG	C5-C6-O6	7.97	133.38	128.60
2	E	108	DT	N3-C4-O4	7.96	124.67	119.90
4	B	125	DT	C4'-C3'-C2'	-7.87	96.02	103.10
4	B	102	DA	C1'-O4'-C4'	-7.78	102.32	110.10
6	C	107	DC	O4'-C1'-N1	7.65	113.36	108.00
6	C	102	DA	O4'-C1'-N9	7.63	113.34	108.00
7	M	116	DC	C3'-C2'-C1'	-7.62	93.35	102.50
6	C	111	DG	N9-C4-C5	7.54	108.41	105.40
6	C	111	DG	C8-N9-C4	-7.52	103.39	106.40
1	A	118	DA	C4'-C3'-C2'	-7.50	96.35	103.10
6	C	110	DG	P-O3'-C3'	7.48	128.67	119.70
1	A	112	DT	OP1-P-OP2	7.47	130.81	119.60
1	A	103	DC	P-O3'-C3'	7.43	128.62	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	101	DT	C4'-C3'-C2'	-7.40	96.44	103.10
2	E	102	DT	OP1-P-OP2	-7.39	108.51	119.60
6	C	109	DT	O4'-C1'-N1	7.36	113.15	108.00
2	E	104	DG	C8-N9-C4	-7.32	103.47	106.40
2	E	107	DG	C8-N9-C4	-7.31	103.48	106.40
2	E	104	DG	C2-N3-C4	-7.26	108.27	111.90
7	M	113	DG	N9-C4-C5	7.24	108.29	105.40
7	M	110	DA	O4'-C1'-N9	7.22	113.06	108.00
3	D	117	DG	C4'-C3'-C2'	-7.21	96.61	103.10
1	A	115	DG	OP1-P-O3'	7.07	120.76	105.20
7	M	112	DC	O4'-C4'-C3'	-7.06	101.68	104.50
1	A	112	DT	P-O3'-C3'	7.02	128.13	119.70
2	E	105	DT	C1'-O4'-C4'	-7.02	103.08	110.10
6	C	116	DA	O4'-C1'-N9	7.02	112.91	108.00
3	D	111	DG	O4'-C4'-C3'	-6.96	101.72	104.50
2	E	103	DA	C3'-C2'-C1'	-6.95	94.16	102.50
2	E	106	DC	OP1-P-O3'	6.95	120.49	105.20
2	E	104	DG	N3-C4-C5	6.95	132.07	128.60
7	M	102	DC	P-O3'-C3'	6.94	128.02	119.70
2	E	114	DG	C8-N9-C4	-6.92	103.63	106.40
2	E	109	DG	O4'-C1'-N9	6.89	112.82	108.00
6	C	107	DC	OP1-P-OP2	-6.89	109.27	119.60
6	C	117	DC	C3'-C2'-C1'	-6.89	94.24	102.50
4	B	112	DA	C8-N9-C4	-6.86	103.06	105.80
1	A	106	DG	N9-C4-C5	6.85	108.14	105.40
4	B	127	DT	C3'-C2'-C1'	-6.83	94.30	102.50
4	B	120	DC	O5'-P-OP1	-6.81	99.57	105.70
1	A	122	DT	O5'-P-OP1	6.80	118.86	110.70
4	B	117	DC	O4'-C1'-N1	6.79	112.76	108.00
2	E	102	DT	O4'-C1'-N1	6.77	112.74	108.00
4	B	107	DC	O4'-C1'-N1	6.76	112.73	108.00
7	M	118	DC	O4'-C1'-N1	6.75	112.73	108.00
4	B	112	DA	O4'-C1'-N9	6.75	112.72	108.00
3	D	118	DT	N3-C4-O4	6.74	123.94	119.90
4	B	119	DT	P-O3'-C3'	6.73	127.78	119.70
6	C	117	DC	OP1-P-O3'	6.73	120.00	105.20
6	C	111	DG	O4'-C1'-N9	6.71	112.70	108.00
7	M	112	DC	OP1-P-OP2	6.68	129.62	119.60
7	M	114	DT	C6-N1-C2	6.67	124.64	121.30
7	M	120	DG	C4'-C3'-C2'	-6.67	97.10	103.10
1	A	101	DC	O4'-C1'-N1	6.63	112.64	108.00
7	M	117	DA	O4'-C4'-C3'	-6.63	101.85	104.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	125	DG	O4'-C1'-N9	6.62	112.63	108.00
7	M	114	DT	C4-C5-C7	6.62	122.97	119.00
1	A	115	DG	O4'-C1'-N9	6.61	112.62	108.00
2	E	107	DG	OP1-P-OP2	-6.59	109.72	119.60
1	A	117	DC	C6-N1-C2	6.57	122.93	120.30
4	B	117	DC	C3'-C2'-C1'	-6.57	94.62	102.50
1	A	107	DC	O4'-C1'-N1	6.55	112.58	108.00
1	A	117	DC	C1'-O4'-C4'	-6.55	103.55	110.10
7	M	107	DG	C3'-C2'-C1'	-6.55	94.64	102.50
4	B	111	DT	OP2-P-O3'	6.52	119.54	105.20
1	A	110	DG	O4'-C1'-N9	6.51	112.56	108.00
4	B	129	DC	P-O3'-C3'	6.48	127.48	119.70
4	B	131	DA	O5'-P-OP1	-6.42	99.92	105.70
4	B	111	DT	C5-C4-O4	-6.41	120.42	124.90
7	M	107	DG	C1'-O4'-C4'	-6.40	103.70	110.10
1	A	117	DC	C3'-C2'-C1'	-6.39	94.83	102.50
1	A	127	DT	O4'-C1'-N1	6.37	112.46	108.00
7	M	107	DG	N3-C4-N9	-6.37	122.18	126.00
5	F	106	DC	O4'-C1'-N1	6.36	112.45	108.00
4	B	113	DC	C6-N1-C2	-6.34	117.77	120.30
4	B	121	DA	O4'-C1'-N9	6.33	112.43	108.00
5	F	116	DT	OP1-P-OP2	-6.29	110.16	119.60
7	M	104	DC	P-O3'-C3'	6.29	127.25	119.70
7	M	102	DC	C6-N1-C2	-6.28	117.79	120.30
6	C	108	DC	OP1-P-O3'	6.27	118.99	105.20
6	C	106	DA	O4'-C1'-N9	6.24	112.36	108.00
1	A	118	DA	C3'-C2'-C1'	-6.23	95.02	102.50
6	C	117	DC	C4'-C3'-C2'	-6.20	97.52	103.10
6	C	108	DC	OP1-P-OP2	-6.17	110.34	119.60
2	E	110	DG	O5'-P-OP1	6.16	118.09	110.70
2	E	110	DG	O4'-C1'-N9	6.14	112.30	108.00
7	M	113	DG	O4'-C1'-N9	6.13	112.29	108.00
7	M	107	DG	P-O3'-C3'	6.12	127.05	119.70
2	E	103	DA	O4'-C4'-C3'	-6.11	102.06	104.50
1	A	114	DG	C3'-C2'-C1'	-6.10	95.19	102.50
7	M	104	DC	OP1-P-OP2	-6.07	110.49	119.60
2	E	105	DT	O4'-C1'-N1	6.01	112.21	108.00
2	E	107	DG	O5'-P-OP2	5.98	117.88	110.70
7	M	103	DA	C1'-O4'-C4'	-5.98	104.12	110.10
6	C	115	DG	P-O3'-C3'	5.93	126.81	119.70
4	B	115	DG	C3'-C2'-C1'	-5.92	95.39	102.50
1	A	111	DA	C8-N9-C4	-5.89	103.44	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	116	DT	C4'-C3'-C2'	-5.88	97.81	103.10
7	M	111	DC	C3'-C2'-C1'	-5.87	95.45	102.50
1	A	112	DT	O5'-P-OP2	5.85	117.72	110.70
4	B	111	DT	N3-C4-O4	5.84	123.41	119.90
3	D	101	DT	C3'-C2'-C1'	-5.83	95.50	102.50
6	C	110	DG	N3-C4-N9	-5.83	122.50	126.00
2	E	104	DG	C5-N7-C8	-5.83	101.39	104.30
7	M	105	DC	OP1-P-OP2	-5.81	110.88	119.60
7	M	113	DG	C4-C5-N7	-5.80	108.48	110.80
5	F	108	DT	N3-C4-O4	5.79	123.37	119.90
5	F	119	DG	P-O3'-C3'	5.76	126.62	119.70
7	M	113	DG	C8-N9-C4	-5.75	104.10	106.40
5	F	113	DT	OP1-P-OP2	5.74	128.20	119.60
3	D	120	DG	OP1-P-O3'	5.69	117.73	105.20
2	E	104	DG	N3-C2-N2	-5.68	115.92	119.90
1	A	106	DG	C6-C5-N7	5.67	133.80	130.40
1	A	120	DG	C4'-C3'-C2'	-5.66	98.00	103.10
1	A	107	DC	C1'-O4'-C4'	-5.64	104.46	110.10
5	F	117	DG	OP1-P-O3'	5.62	117.57	105.20
4	B	120	DC	O5'-P-OP2	5.61	117.44	110.70
2	E	108	DT	O4'-C1'-C2'	-5.61	101.42	105.90
5	F	116	DT	C1'-O4'-C4'	-5.61	104.50	110.10
5	F	120	DG	C4'-C3'-C2'	-5.60	98.06	103.10
6	C	114	DG	O4'-C1'-N9	-5.58	104.09	108.00
5	F	111	DA	O4'-C1'-C2'	-5.56	101.45	105.90
7	M	107	DG	N9-C1'-C2'	5.55	123.15	112.60
5	F	111	DA	O4'-C4'-C3'	-5.54	102.28	104.50
6	C	105	DT	O4'-C1'-N1	-5.54	104.12	108.00
7	M	107	DG	OP1-P-OP2	5.54	127.91	119.60
5	F	104	DA	P-O3'-C3'	5.54	126.35	119.70
4	B	127	DT	O4'-C1'-C2'	-5.50	101.50	105.90
7	M	120	DG	C5-C6-O6	5.49	131.90	128.60
2	E	102	DT	OP2-P-O3'	5.49	117.28	105.20
7	M	120	DG	O4'-C4'-C3'	-5.48	102.31	104.50
1	A	129	DG	P-O3'-C3'	5.48	126.28	119.70
7	M	103	DA	O4'-C1'-N9	5.48	111.83	108.00
5	F	106	DC	C1'-O4'-C4'	-5.46	104.64	110.10
1	A	118	DA	OP1-P-O3'	5.45	117.19	105.20
1	A	109	DT	O4'-C1'-N1	5.45	111.81	108.00
4	B	130	DT	C3'-C2'-C1'	-5.44	95.97	102.50
4	B	103	DG	O5'-P-OP2	-5.42	100.82	105.70
7	M	116	DC	O4'-C4'-C3'	-5.41	102.34	104.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	126	DA	O4'-C1'-N9	5.40	111.78	108.00
6	C	121	DT	C1'-O4'-C4'	-5.39	104.71	110.10
2	E	107	DG	P-O3'-C3'	5.39	126.16	119.70
2	E	102	DT	C4'-C3'-C2'	-5.38	98.26	103.10
6	C	118	DG	OP1-P-O3'	5.36	116.99	105.20
4	B	109	DT	N3-C4-O4	5.36	123.11	119.90
7	M	117	DA	C1'-O4'-C4'	-5.34	104.76	110.10
3	D	121	DC	P-O3'-C3'	5.32	126.09	119.70
1	A	112	DT	OP1-P-O3'	5.31	116.88	105.20
6	C	119	DA	C1'-O4'-C4'	-5.31	104.79	110.10
1	A	118	DA	P-O3'-C3'	5.31	126.07	119.70
1	A	117	DC	C2-N1-C1'	-5.31	112.96	118.80
4	B	102	DA	C3'-C2'-C1'	-5.30	96.14	102.50
4	B	123	DT	N3-C4-O4	5.29	123.07	119.90
4	B	130	DT	N3-C4-O4	5.28	123.07	119.90
1	A	130	DC	OP1-P-OP2	-5.27	111.69	119.60
2	E	108	DT	C6-N1-C2	-5.26	118.67	121.30
7	M	120	DG	C3'-C2'-C1'	-5.26	96.18	102.50
7	M	111	DC	N1-C2-O2	5.24	122.05	118.90
3	D	117	DG	P-O3'-C3'	5.24	125.99	119.70
4	B	121	DA	C1'-O4'-C4'	-5.23	104.87	110.10
5	F	104	DA	O4'-C4'-C3'	-5.22	102.41	104.50
1	A	106	DG	N3-C4-N9	-5.21	122.87	126.00
5	F	108	DT	C5-C4-O4	-5.21	121.25	124.90
4	B	131	DA	N9-C4-C5	5.20	107.88	105.80
7	M	107	DG	C6-C5-N7	5.20	133.52	130.40
7	M	117	DA	C4'-C3'-C2'	-5.20	98.42	103.10
1	A	113	DC	C6-N1-C2	-5.19	118.22	120.30
6	C	107	DC	O5'-P-OP2	5.17	116.91	110.70
4	B	125	DT	C1'-O4'-C4'	-5.16	104.94	110.10
7	M	118	DC	N1-C1'-C2'	5.16	122.39	112.60
1	A	105	DA	O4'-C1'-N9	5.15	111.61	108.00
7	M	114	DT	N3-C2-O2	5.15	125.39	122.30
7	M	107	DG	N9-C4-C5	5.14	107.46	105.40
7	M	109	DC	OP1-P-OP2	5.13	127.30	119.60
4	B	130	DT	C5-C4-O4	-5.13	121.31	124.90
2	E	110	DG	N3-C4-N9	-5.13	122.92	126.00
2	E	103	DA	O5'-P-OP2	-5.12	101.09	105.70
7	M	115	DA	P-O3'-C3'	5.12	125.84	119.70
7	M	101	DT	P-O3'-C3'	5.11	125.83	119.70
7	M	107	DG	C4-N9-C1'	-5.07	119.91	126.50
4	B	131	DA	O5'-P-OP2	5.06	116.77	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	125	DT	O4'-C1'-N1	5.04	111.53	108.00
4	B	117	DC	OP2-P-O3'	-5.04	94.11	105.20
6	C	119	DA	O5'-P-OP2	-5.04	101.17	105.70
4	B	121	DA	O4'-C1'-C2'	-5.03	101.88	105.90
6	C	118	DG	O5'-P-OP1	-5.02	101.18	105.70
2	E	110	DG	N9-C4-C5	5.01	107.40	105.40
7	M	101	DT	C1'-O4'-C4'	-5.00	105.10	110.10

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in 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	633	0	347	90	0
2	E	285	0	160	63	0
3	D	491	0	272	70	0
4	B	633	0	350	60	0
5	F	496	0	273	57	0
6	C	426	0	236	52	0
7	M	421	0	235	80	0
All	All	3385	0	1873	402	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 80.

All (402) 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)
7:M:101:DT:N1	7:M:101:DT:C1'	1.70	1.54
5:F:103:DT:N1	5:F:103:DT:C1'	1.69	1.51
7:M:102:DC:O3'	7:M:102:DC:C3'	1.64	1.45
5:F:111:DA:O5'	5:F:111:DA:C5'	1.63	1.45
1:A:112:DT:O3'	1:A:112:DT:C3'	1.65	1.43
2:E:107:DG:C3'	2:E:107:DG:O3'	1.67	1.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:117:DC:O3'	6:C:117:DC:C3'	1.68	1.41
7:M:113:DG:O3'	7:M:113:DG:C3'	1.72	1.37
1:A:129:DG:N2	3:D:105:DC:O2	1.78	1.17
4:B:125:DT:H2'	4:B:126:DA:C8	1.93	1.02
5:F:119:DG:H5'	7:M:111:DC:H5''	1.42	0.99
4:B:125:DT:H2'	4:B:126:DA:H8	1.24	0.97
6:C:109:DT:N3	7:M:110:DA:N1	2.11	0.96
2:E:104:DG:H2''	2:E:105:DT:H6	1.29	0.95
5:F:122:DA:H2'	5:F:123:DG:C8	2.03	0.94
4:B:122:DG:N2	5:F:112:DC:O2	2.02	0.93
7:M:108:DC:H2''	7:M:109:DC:C5	2.06	0.90
2:E:112:DT:H2'	2:E:113:DC:C6	2.08	0.88
3:D:105:DC:H2''	3:D:106:DT:H72	1.56	0.88
3:D:120:DG:N2	4:B:108:DC:C2	2.42	0.87
1:A:122:DT:H2''	1:A:123:DC:H5	1.41	0.85
3:D:118:DT:H3'	7:M:117:DA:H2''	1.60	0.84
1:A:113:DC:H1'	1:A:114:DG:C5	2.13	0.84
2:E:109:DG:H1'	7:M:103:DA:H2''	1.59	0.84
1:A:113:DC:H2''	1:A:114:DG:N7	1.93	0.84
3:D:119:DG:H2'	3:D:120:DG:C8	2.13	0.84
2:E:104:DG:H2''	2:E:105:DT:C6	2.12	0.82
5:F:107:DA:H2''	5:F:108:DT:H71	1.60	0.82
1:A:129:DG:N1	3:D:105:DC:N3	2.29	0.81
1:A:118:DA:N6	3:D:115:DT:O4	2.13	0.80
7:M:101:DT:C1'	7:M:101:DT:C2	2.64	0.80
4:B:111:DT:H2''	4:B:112:DA:OP1	1.82	0.79
1:A:109:DT:H3'	1:A:110:DG:H8	1.48	0.79
1:A:110:DG:N2	7:M:102:DC:O2	2.14	0.79
3:D:110:DG:H2'	3:D:111:DG:C8	2.18	0.79
3:D:117:DG:H2''	3:D:118:DT:O4'	1.84	0.78
5:F:103:DT:C1'	5:F:103:DT:C6	2.67	0.77
6:C:111:DG:N2	7:M:108:DC:O2	2.19	0.75
6:C:114:DG:H2''	6:C:115:DG:C8	2.20	0.75
3:D:122:DT:H2'	3:D:123:DG:H8	1.49	0.75
3:D:116:DT:H2''	3:D:117:DG:N7	2.02	0.75
2:E:109:DG:H4'	7:M:104:DC:H5'	1.69	0.74
1:A:109:DT:H3'	1:A:110:DG:C8	2.22	0.74
3:D:120:DG:N2	4:B:108:DC:N3	2.35	0.74
1:A:118:DA:H1'	1:A:119:DA:C8	2.22	0.74
1:A:118:DA:N6	3:D:115:DT:C4	2.56	0.73
5:F:103:DT:C1'	5:F:103:DT:C2	2.72	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:122:DT:H2'	3:D:123:DG:C8	2.24	0.73
2:E:107:DG:C6	2:E:108:DT:C4	2.77	0.72
5:F:118:DT:H2''	7:M:111:DC:O4'	1.90	0.72
7:M:101:DT:H2''	7:M:102:DC:C5	2.24	0.72
2:E:106:DC:H1'	2:E:107:DG:C8	2.26	0.71
4:B:110:DG:H2'	4:B:111:DT:C6	2.25	0.71
1:A:122:DT:C2'	1:A:123:DC:H5	2.03	0.71
4:B:110:DG:H2'	4:B:111:DT:C5	2.26	0.71
1:A:104:DG:H2''	1:A:105:DA:C8	2.27	0.70
1:A:122:DT:O2	1:A:123:DC:N4	2.24	0.70
3:D:122:DT:H2''	3:D:123:DG:H5'	1.74	0.70
1:A:114:DG:N2	7:M:120:DG:N2	2.40	0.69
4:B:111:DT:H2''	4:B:112:DA:H8	1.55	0.69
6:C:113:DA:H1'	6:C:114:DG:C5	2.27	0.69
7:M:105:DC:H2'	7:M:106:DT:C4	2.28	0.69
3:D:118:DT:H2''	7:M:118:DC:O4'	1.92	0.68
6:C:118:DG:H4'	6:C:119:DA:OP1	1.93	0.68
7:M:116:DC:N4	7:M:117:DA:N6	2.42	0.68
7:M:101:DT:C1'	7:M:101:DT:C6	2.74	0.68
1:A:114:DG:H22	7:M:120:DG:N2	1.91	0.68
1:A:117:DC:C4	1:A:118:DA:N6	2.62	0.68
1:A:122:DT:H2''	1:A:123:DC:C5	2.27	0.68
4:B:113:DC:H1'	4:B:114:DG:C5	2.28	0.67
6:C:120:DC:H2'	6:C:121:DT:C6	2.28	0.67
6:C:114:DG:C2'	6:C:115:DG:C8	2.78	0.67
7:M:107:DG:H1'	7:M:108:DC:P	2.35	0.67
2:E:104:DG:OP2	2:E:104:DG:H8	1.77	0.66
7:M:112:DC:H2''	7:M:113:DG:N7	2.09	0.66
5:F:122:DA:H2''	5:F:123:DG:H5'	1.77	0.66
4:B:111:DT:H2''	4:B:112:DA:C8	2.31	0.66
7:M:101:DT:N1	7:M:101:DT:H1'	1.99	0.66
6:C:104:DC:H2''	6:C:105:DT:H5'	1.78	0.66
2:E:112:DT:H2''	2:E:113:DC:C5'	2.25	0.66
4:B:114:DG:H4'	4:B:115:DG:H5'	1.78	0.65
4:B:119:DT:H2''	4:B:120:DC:O5'	1.97	0.65
1:A:105:DA:H1'	1:A:106:DG:O4'	1.96	0.65
5:F:112:DC:H2''	5:F:113:DT:OP1	1.97	0.65
5:F:114:DG:H1'	5:F:115:DA:C8	2.33	0.65
1:A:113:DC:H1'	1:A:114:DG:C6	2.33	0.64
4:B:115:DG:C6	4:B:116:DA:C6	2.85	0.64
3:D:113:DT:H2''	3:D:114:DC:H2'	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:108:DT:C2	5:F:109:DA:C8	2.85	0.64
1:A:110:DG:H2'	1:A:111:DA:C8	2.33	0.63
3:D:118:DT:C2'	7:M:118:DC:C6	2.81	0.63
1:A:121:DA:H2''	1:A:122:DT:O4'	1.99	0.63
1:A:121:DA:C6	3:D:112:DA:N1	2.67	0.63
5:F:117:DG:H2'	5:F:118:DT:H71	1.80	0.63
4:B:111:DT:C2	4:B:112:DA:N7	2.67	0.62
2:E:112:DT:H2''	2:E:113:DC:H5'	1.80	0.62
2:E:107:DG:C2	2:E:108:DT:C2	2.88	0.62
3:D:112:DA:H2'	3:D:113:DT:C4	2.35	0.62
1:A:123:DC:C4	1:A:124:DC:C4	2.88	0.61
7:M:116:DC:C4	7:M:117:DA:N6	2.68	0.61
1:A:112:DT:H2''	1:A:113:DC:C6	2.35	0.61
6:C:119:DA:H2''	6:C:120:DC:O5'	2.00	0.61
4:B:102:DA:H1'	4:B:103:DG:OP2	2.01	0.60
3:D:117:DG:C5	3:D:118:DT:C4	2.89	0.60
3:D:104:DG:H2''	3:D:105:DC:OP2	2.01	0.60
7:M:105:DC:H2'	7:M:106:DT:N3	2.15	0.60
3:D:118:DT:H2'	7:M:118:DC:C6	2.36	0.59
7:M:105:DC:H2'	7:M:106:DT:C2	2.36	0.59
6:C:118:DG:C6	6:C:119:DA:C6	2.91	0.59
4:B:131:DA:OP2	4:B:131:DA:H2'	2.03	0.59
7:M:101:DT:C2	7:M:121:DA:N6	2.70	0.59
3:D:122:DT:H2''	3:D:123:DG:C5'	2.32	0.59
7:M:114:DT:H1'	7:M:115:DA:H5'	1.85	0.59
2:E:107:DG:H2''	2:E:108:DT:O4'	2.03	0.59
3:D:118:DT:H2''	7:M:118:DC:C6	2.38	0.59
5:F:120:DG:H2''	5:F:121:DT:OP2	2.03	0.58
1:A:118:DA:C5	1:A:119:DA:C6	2.90	0.58
3:D:118:DT:H2''	7:M:118:DC:C1'	2.34	0.58
1:A:110:DG:C6	1:A:111:DA:C6	2.91	0.58
6:C:113:DA:H1'	6:C:114:DG:C6	2.37	0.58
4:B:114:DG:H2''	4:B:115:DG:C8	2.39	0.58
1:A:118:DA:C4	1:A:119:DA:C5	2.92	0.57
1:A:121:DA:N6	3:D:112:DA:C6	2.72	0.57
2:E:103:DA:C4	2:E:104:DG:N7	2.72	0.57
5:F:103:DT:H2''	5:F:104:DA:H2'	1.86	0.57
4:B:102:DA:H1'	4:B:103:DG:P	2.45	0.57
4:B:114:DG:C4'	4:B:115:DG:H5'	2.35	0.57
5:F:107:DA:C2'	5:F:108:DT:H71	2.32	0.57
2:E:102:DT:H2''	2:E:103:DA:OP2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:106:DC:C2	2:E:107:DG:N7	2.72	0.56
2:E:109:DG:N3	2:E:109:DG:H2'	2.19	0.56
2:E:111:DC:H1'	2:E:112:DT:OP1	2.06	0.56
4:B:125:DT:C2	4:B:126:DA:N7	2.74	0.56
6:C:112:DC:H2''	6:C:113:DA:H5'	1.86	0.56
2:E:104:DG:C4	2:E:105:DT:C5	2.93	0.56
4:B:125:DT:C2	4:B:126:DA:C8	2.94	0.56
1:A:111:DA:H2''	1:A:112:DT:OP1	2.05	0.55
1:A:129:DG:N2	3:D:105:DC:C2	2.55	0.55
2:E:102:DT:C4	2:E:103:DA:N6	2.74	0.55
2:E:107:DG:C5	2:E:108:DT:C5	2.94	0.55
6:C:113:DA:C5	7:M:105:DC:N4	2.74	0.55
1:A:113:DC:H2''	1:A:114:DG:C5	2.42	0.55
5:F:101:DT:O4	5:F:102:DC:C4	2.60	0.55
7:M:101:DT:C2	7:M:101:DT:H1'	2.40	0.55
4:B:127:DT:H2''	4:B:128:DG:OP2	2.07	0.55
1:A:122:DT:H4'	1:A:123:DC:OP1	2.06	0.55
3:D:103:DC:H1'	3:D:104:DG:H5'	1.89	0.55
5:F:108:DT:H6	5:F:108:DT:OP2	1.89	0.55
4:B:104:DC:H2''	4:B:105:DA:H8	1.71	0.55
4:B:121:DA:H2''	4:B:122:DG:O5'	2.07	0.55
5:F:103:DT:O4'	5:F:103:DT:OP2	2.25	0.55
4:B:126:DA:N3	4:B:127:DT:O4'	2.41	0.54
1:A:107:DC:H2'	1:A:108:DC:C6	2.42	0.54
2:E:108:DT:N3	6:C:116:DA:C2	2.75	0.54
6:C:106:DA:H1'	6:C:107:DC:H5'	1.89	0.54
2:E:108:DT:H2''	7:M:104:DC:O4'	2.07	0.54
1:A:113:DC:H1'	1:A:114:DG:C4	2.41	0.54
4:B:104:DC:H2''	4:B:105:DA:C8	2.42	0.54
7:M:114:DT:H2''	7:M:115:DA:OP2	2.06	0.54
4:B:113:DC:H1'	4:B:114:DG:C6	2.41	0.54
2:E:102:DT:C7	2:E:103:DA:H62	2.20	0.54
4:B:122:DG:N1	5:F:112:DC:N3	2.46	0.54
2:E:104:DG:C2	2:E:105:DT:C4	2.96	0.54
6:C:118:DG:C5	6:C:119:DA:C5	2.95	0.54
7:M:111:DC:H2'	7:M:111:DC:O5'	2.08	0.54
1:A:122:DT:O2	1:A:123:DC:C4	2.61	0.54
4:B:112:DA:OP1	4:B:112:DA:O4'	2.26	0.54
5:F:119:DG:N2	6:C:108:DC:N3	2.56	0.54
7:M:112:DC:H2''	7:M:113:DG:C5	2.43	0.54
7:M:118:DC:H2'	7:M:119:DC:C6	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:DC:H2'	1:A:108:DC:C5	2.43	0.53
3:D:117:DG:C3'	3:D:118:DT:H5''	2.38	0.53
6:C:117:DC:C4	6:C:118:DG:C6	2.97	0.53
2:E:102:DT:O4	2:E:103:DA:N6	2.42	0.53
5:F:119:DG:N2	6:C:108:DC:C2	2.71	0.52
7:M:107:DG:H1'	7:M:108:DC:OP2	2.09	0.52
1:A:128:DA:C6	1:A:129:DG:C6	2.97	0.52
5:F:119:DG:H1	6:C:108:DC:N4	2.07	0.52
5:F:123:DG:C4	5:F:124:DG:N7	2.78	0.52
7:M:106:DT:H1'	7:M:107:DG:O4'	2.11	0.51
2:E:103:DA:C6	2:E:104:DG:C6	2.98	0.51
3:D:122:DT:H2''	3:D:123:DG:H2'	1.91	0.51
1:A:117:DC:H4'	1:A:118:DA:C5'	2.40	0.51
2:E:109:DG:C6	2:E:110:DG:C5	2.99	0.51
5:F:111:DA:C5'	5:F:111:DA:P	2.95	0.51
5:F:114:DG:H4'	5:F:115:DA:OP1	2.10	0.51
5:F:119:DG:C5'	7:M:111:DC:H5''	2.28	0.51
6:C:105:DT:C2	6:C:106:DA:C5	2.99	0.51
7:M:112:DC:H4'	7:M:113:DG:OP1	2.09	0.51
4:B:120:DC:H2''	4:B:121:DA:H5'	1.92	0.51
3:D:123:DG:H1'	3:D:124:DC:C5	2.46	0.50
7:M:101:DT:H2''	7:M:102:DC:C6	2.45	0.50
2:E:105:DT:H2''	2:E:106:DC:C5	2.46	0.50
5:F:110:DG:N3	5:F:111:DA:N6	2.59	0.50
6:C:110:DG:O6	7:M:108:DC:C4	2.65	0.50
1:A:119:DA:H2	3:D:115:DT:O2	1.94	0.50
1:A:129:DG:H2''	1:A:130:DC:OP1	2.10	0.50
5:F:106:DC:C2	5:F:107:DA:N7	2.79	0.50
6:C:119:DA:N3	6:C:120:DC:H1'	2.27	0.50
2:E:103:DA:C4	2:E:104:DG:C5	2.99	0.50
2:E:108:DT:C4	6:C:116:DA:N1	2.80	0.50
3:D:106:DT:H2''	3:D:107:DA:C8	2.46	0.50
5:F:101:DT:H2'	5:F:102:DC:H5'	1.94	0.50
2:E:107:DG:C2'	2:E:108:DT:H5''	2.42	0.50
5:F:122:DA:H2''	5:F:123:DG:C5'	2.41	0.50
1:A:123:DC:N4	1:A:124:DC:N4	2.59	0.49
1:A:114:DG:N2	7:M:120:DG:H21	2.10	0.49
1:A:121:DA:H2'	1:A:122:DT:C6	2.47	0.49
6:C:102:DA:C2	6:C:103:DC:N4	2.80	0.49
2:E:109:DG:H4'	7:M:104:DC:C5'	2.40	0.49
2:E:112:DT:H2'	2:E:113:DC:H6	1.74	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:101:DT:H5'	7:M:121:DA:H2'	1.95	0.49
3:D:123:DG:C4	3:D:124:DC:N4	2.81	0.49
4:B:106:DG:H1'	4:B:107:DC:H5'	1.95	0.49
6:C:117:DC:H2''	6:C:118:DG:H2'	1.93	0.49
2:E:104:DG:N2	2:E:105:DT:C2	2.80	0.49
4:B:110:DG:C4	4:B:111:DT:C4	3.00	0.49
1:A:128:DA:C5	1:A:129:DG:C6	3.01	0.49
3:D:116:DT:C2	3:D:117:DG:C6	3.01	0.49
4:B:126:DA:C2	5:F:109:DA:N3	2.80	0.49
6:C:108:DC:H2''	6:C:109:DT:H5'	1.95	0.49
7:M:105:DC:H4'	7:M:105:DC:OP1	2.13	0.49
1:A:121:DA:H2'	1:A:122:DT:H6	1.77	0.48
1:A:114:DG:H22	7:M:120:DG:H22	1.57	0.48
2:E:108:DT:H4'	2:E:109:DG:OP2	2.13	0.48
4:B:125:DT:H2''	4:B:126:DA:H5'	1.95	0.48
5:F:112:DC:H6	5:F:112:DC:OP2	1.95	0.48
7:M:120:DG:H2''	7:M:121:DA:OP2	2.12	0.48
1:A:117:DC:N4	1:A:118:DA:N6	2.61	0.48
5:F:117:DG:C6	5:F:118:DT:O4	2.66	0.48
1:A:118:DA:C6	1:A:119:DA:C6	3.02	0.48
1:A:128:DA:C4	1:A:129:DG:C5	3.02	0.48
2:E:103:DA:C6	2:E:104:DG:O6	2.67	0.48
4:B:110:DG:O6	7:M:115:DA:N6	2.46	0.48
7:M:102:DC:C3'	7:M:103:DA:P	2.96	0.48
2:E:102:DT:H72	2:E:103:DA:H62	1.78	0.48
2:E:107:DG:C3'	2:E:108:DT:P	2.97	0.48
5:F:101:DT:C4	5:F:102:DC:C4	3.02	0.48
2:E:103:DA:OP2	2:E:103:DA:H8	1.97	0.48
4:B:115:DG:C6	4:B:116:DA:N6	2.82	0.48
7:M:105:DC:H3'	7:M:106:DT:C5	2.49	0.48
1:A:109:DT:H6	1:A:109:DT:O5'	1.96	0.47
1:A:124:DC:C2	1:A:125:DG:C8	3.02	0.47
1:A:114:DG:N2	7:M:120:DG:H22	2.11	0.47
1:A:119:DA:N6	3:D:114:DC:N4	2.61	0.47
4:B:110:DG:C6	7:M:115:DA:N6	2.82	0.47
6:C:119:DA:C6	6:C:120:DC:C2	3.02	0.47
1:A:130:DC:H42	3:D:103:DC:N4	2.12	0.47
1:A:101:DC:C2	1:A:102:DA:N7	2.82	0.47
1:A:123:DC:N4	1:A:124:DC:C4	2.82	0.47
1:A:118:DA:C2	1:A:119:DA:C2	3.03	0.47
1:A:130:DC:H5''	1:A:130:DC:H2'	1.66	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:101:DT:O4	5:F:102:DC:N4	2.48	0.47
3:D:116:DT:C2	3:D:117:DG:O6	2.68	0.47
5:F:111:DA:C5'	5:F:111:DA:C8	2.98	0.47
3:D:120:DG:C2	4:B:108:DC:N3	2.82	0.46
4:B:126:DA:H2''	4:B:127:DT:H5'	1.97	0.46
1:A:119:DA:H1'	1:A:120:DG:OP1	2.15	0.46
3:D:121:DC:H2''	3:D:122:DT:O5'	2.15	0.46
4:B:102:DA:H2''	4:B:103:DG:OP1	2.15	0.46
1:A:114:DG:H4'	1:A:115:DG:OP1	2.13	0.46
5:F:114:DG:C5	5:F:115:DA:N6	2.83	0.46
6:C:105:DT:C2'	6:C:106:DA:C8	2.99	0.46
1:A:111:DA:C2'	1:A:112:DT:OP1	2.62	0.46
5:F:114:DG:C4	5:F:115:DA:C5	3.04	0.46
3:D:110:DG:C2'	3:D:111:DG:C8	2.95	0.46
2:E:109:DG:O5'	7:M:104:DC:H4'	2.16	0.46
6:C:109:DT:C4	7:M:110:DA:N1	2.84	0.46
6:C:114:DG:H5''	6:C:114:DG:H8	1.80	0.46
2:E:103:DA:C5	2:E:104:DG:O6	2.69	0.46
2:E:107:DG:C5	2:E:108:DT:C4	3.02	0.46
6:C:104:DC:C2'	6:C:105:DT:H5'	2.44	0.46
6:C:114:DG:C5	6:C:115:DG:C6	3.04	0.46
7:M:105:DC:H2'	7:M:106:DT:C5	2.51	0.46
1:A:121:DA:N1	3:D:112:DA:C2	2.84	0.45
5:F:119:DG:N2	6:C:109:DT:O2	2.50	0.45
1:A:117:DC:C4	1:A:118:DA:C6	3.05	0.45
4:B:118:DA:N6	5:F:115:DA:N6	2.64	0.45
1:A:110:DG:C2	1:A:111:DA:C2	3.04	0.45
5:F:103:DT:H2''	5:F:104:DA:C8	2.52	0.45
6:C:102:DA:H2''	6:C:103:DC:OP1	2.15	0.45
1:A:113:DC:C4	7:M:119:DC:N4	2.84	0.45
2:E:103:DA:N3	2:E:104:DG:C5	2.84	0.45
2:E:103:DA:H2''	2:E:104:DG:C8	2.52	0.45
3:D:103:DC:C2'	3:D:104:DG:H5'	2.46	0.45
4:B:114:DG:H8	4:B:114:DG:H2'	1.67	0.45
5:F:105:DG:H2''	5:F:106:DC:C6	2.52	0.45
3:D:110:DG:H3'	3:D:111:DG:H8	1.81	0.45
1:A:112:DT:O2	1:A:113:DC:H5'	2.17	0.45
1:A:120:DG:H2''	1:A:121:DA:O5'	2.17	0.45
4:B:101:DG:H2'	4:B:102:DA:C8	2.52	0.45
4:B:103:DG:H2''	4:B:104:DC:C5	2.52	0.45
2:E:102:DT:C6	2:E:103:DA:N7	2.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:110:DG:C6	3:D:111:DG:C6	3.04	0.45
3:D:113:DT:C6	3:D:113:DT:H5''	2.52	0.45
7:M:118:DC:OP2	7:M:118:DC:H6	1.99	0.45
2:E:102:DT:C5	2:E:103:DA:N7	2.85	0.44
3:D:118:DT:C7	7:M:118:DC:N4	2.80	0.44
4:B:128:DG:C5	4:B:129:DC:C4	3.05	0.44
1:A:112:DT:C3'	1:A:113:DC:P	2.98	0.44
2:E:104:DG:N3	2:E:105:DT:C6	2.86	0.44
3:D:113:DT:C4	3:D:114:DC:N4	2.85	0.44
7:M:106:DT:C2	7:M:107:DG:C4	3.05	0.44
6:C:113:DA:H1'	6:C:114:DG:N7	2.33	0.44
5:F:119:DG:H2''	5:F:120:DG:O5'	2.18	0.44
6:C:106:DA:N3	6:C:107:DC:O4'	2.50	0.44
1:A:113:DC:C1'	1:A:114:DG:C5	2.95	0.44
3:D:118:DT:C5	7:M:118:DC:C4	3.04	0.44
3:D:109:DC:H3'	3:D:110:DG:O4'	2.17	0.44
3:D:121:DC:C4	3:D:122:DT:C4	3.05	0.44
3:D:122:DT:C2'	3:D:123:DG:H2'	2.48	0.44
1:A:123:DC:N4	3:D:111:DG:H1	2.15	0.44
2:E:103:DA:C2	2:E:104:DG:C5	3.06	0.44
2:E:113:DC:C4	2:E:114:DG:O6	2.70	0.44
7:M:110:DA:H4'	7:M:111:DC:OP1	2.18	0.44
1:A:121:DA:C2'	1:A:122:DT:H5''	2.48	0.44
2:E:108:DT:H2''	7:M:104:DC:C6	2.53	0.44
6:C:107:DC:N3	6:C:108:DC:N4	2.65	0.44
1:A:117:DC:OP2	1:A:117:DC:H2'	2.18	0.43
4:B:128:DG:C4	4:B:129:DC:C4	3.06	0.43
4:B:128:DG:N3	4:B:129:DC:C2	2.86	0.43
7:M:102:DC:H2'	7:M:103:DA:C8	2.52	0.43
7:M:114:DT:H6	7:M:114:DT:H2'	1.14	0.43
5:F:118:DT:H2''	7:M:111:DC:H5'	1.99	0.43
1:A:114:DG:C4	1:A:115:DG:C6	3.06	0.43
4:B:115:DG:O6	4:B:116:DA:N6	2.52	0.43
1:A:131:DG:O6	3:D:102:DG:N1	2.51	0.43
1:A:121:DA:C8	1:A:122:DT:H71	2.54	0.43
6:C:117:DC:O2	6:C:118:DG:H5'	2.18	0.43
5:F:114:DG:C5	5:F:115:DA:C6	3.06	0.43
1:A:122:DT:H1'	1:A:123:DC:C5	2.54	0.43
7:M:108:DC:C2'	7:M:109:DC:C5	2.92	0.43
5:F:101:DT:H2'	5:F:102:DC:C5'	2.48	0.43
6:C:113:DA:C6	7:M:105:DC:C4	3.07	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:120:DG:H1'	7:M:121:DA:H8	1.84	0.43
3:D:103:DC:H2''	3:D:104:DG:H5'	2.00	0.43
5:F:113:DT:H4'	5:F:114:DG:OP1	2.19	0.43
6:C:102:DA:H1'	6:C:103:DC:OP2	2.18	0.43
1:A:127:DT:H2''	1:A:128:DA:OP2	2.19	0.42
4:B:103:DG:H4'	4:B:104:DC:OP1	2.17	0.42
5:F:117:DG:H2'	5:F:118:DT:C6	2.54	0.42
2:E:113:DC:N3	2:E:114:DG:C6	2.88	0.42
4:B:126:DA:C2	5:F:109:DA:C2	3.07	0.42
4:B:128:DG:N2	5:F:107:DA:C4	2.87	0.42
7:M:119:DC:H4'	7:M:120:DG:OP1	2.19	0.42
1:A:116:DA:N1	3:D:118:DT:C4	2.87	0.42
3:D:122:DT:N3	3:D:123:DG:C5	2.88	0.42
7:M:117:DA:H2'	7:M:117:DA:H5'	1.79	0.42
2:E:108:DT:O3'	7:M:104:DC:O4'	2.38	0.42
6:C:114:DG:C5'	6:C:114:DG:C8	3.02	0.42
5:F:121:DT:H2''	5:F:122:DA:OP1	2.19	0.42
1:A:110:DG:C6	1:A:111:DA:N6	2.87	0.42
3:D:104:DG:C4	3:D:105:DC:N3	2.87	0.42
3:D:109:DC:H2'	3:D:110:DG:H1'	2.01	0.42
4:B:119:DT:H2''	4:B:120:DC:O4'	2.19	0.42
6:C:117:DC:H2''	6:C:118:DG:C8	2.54	0.42
1:A:118:DA:C5	1:A:119:DA:C5	3.08	0.42
2:E:104:DG:C2	2:E:105:DT:N3	2.88	0.42
3:D:114:DC:H2''	3:D:115:DT:H71	2.01	0.42
3:D:122:DT:C2'	3:D:123:DG:C8	2.98	0.42
4:B:125:DT:H2''	4:B:126:DA:C5'	2.48	0.42
6:C:113:DA:N7	7:M:105:DC:N4	2.68	0.42
2:E:106:DC:H1'	2:E:107:DG:H8	1.80	0.42
3:D:122:DT:C2	3:D:123:DG:C8	3.08	0.42
4:B:105:DA:C6	4:B:106:DG:C6	3.08	0.42
6:C:102:DA:N1	6:C:103:DC:N4	2.68	0.42
5:F:116:DT:C4	5:F:117:DG:C6	3.08	0.41
1:A:117:DC:C3'	1:A:117:DC:P	3.08	0.41
2:E:113:DC:C2	2:E:114:DG:N7	2.89	0.41
4:B:126:DA:C2'	4:B:127:DT:H5'	2.50	0.41
1:A:110:DG:N1	1:A:111:DA:N1	2.68	0.41
1:A:111:DA:H2'	1:A:112:DT:H72	2.02	0.41
3:D:104:DG:C4	3:D:105:DC:C4	3.07	0.41
3:D:113:DT:C6	3:D:114:DC:C5	3.08	0.41
6:C:110:DG:H8	6:C:110:DG:C5'	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:114:DG:H5''	6:C:114:DG:C8	2.56	0.41
6:C:119:DA:C6	6:C:120:DC:N3	2.88	0.41
4:B:126:DA:N1	5:F:109:DA:C2	2.88	0.41
7:M:118:DC:C6	7:M:118:DC:OP2	2.74	0.41
1:A:125:DG:C2	3:D:110:DG:C2	3.09	0.41
6:C:109:DT:N3	7:M:110:DA:C2	2.86	0.41
2:E:104:DG:C2'	2:E:105:DT:C6	2.97	0.41
3:D:118:DT:C6	7:M:118:DC:C5	3.09	0.41
2:E:107:DG:C4	2:E:108:DT:C6	3.09	0.41
3:D:104:DG:C2	3:D:105:DC:C2	3.09	0.41
4:B:126:DA:H2''	4:B:127:DT:C5'	2.50	0.41
2:E:103:DA:C5	2:E:104:DG:C6	3.09	0.41
1:A:111:DA:H2	7:M:121:DA:H61	1.69	0.40
4:B:115:DG:C2	4:B:116:DA:C4	3.09	0.40
5:F:110:DG:H2''	5:F:111:DA:N7	2.36	0.40
6:C:111:DG:H1'	6:C:112:DC:OP2	2.21	0.40
1:A:123:DC:H42	3:D:111:DG:H1	1.70	0.40
2:E:103:DA:OP2	2:E:103:DA:C8	2.73	0.40
2:E:107:DG:H2''	2:E:108:DT:H5''	2.02	0.40
2:E:109:DG:C5	2:E:110:DG:N7	2.90	0.40
2:E:113:DC:C2	2:E:114:DG:C5	3.10	0.40
3:D:102:DG:H2''	3:D:103:DC:OP2	2.21	0.40
1:A:118:DA:C1'	1:A:119:DA:C8	3.00	0.40
1:A:121:DA:H2''	1:A:122:DT:C5'	2.52	0.40
4:B:112:DA:H2''	4:B:113:DC:OP1	2.21	0.40
5:F:105:DG:H2''	5:F:106:DC:H6	1.87	0.40
6:C:107:DC:C2	6:C:108:DC:C4	3.10	0.40

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](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



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

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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.