Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2023 – 03:47 PM EDT

PDB ID	:	7U3W
Title	:	[L224] Self-assembling tensegrity triangle with two turns, two turns and four turns of DNA per axis by linker addition with P1 symmetry
Authors	:	Woloszyn, K.; Vecchioni, S.; Seeman, N.C.; Sha, R.; Ohayon, Y.P.
Deposited on	:	2022-02-28
Resolution	:	6.33 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*
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.

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

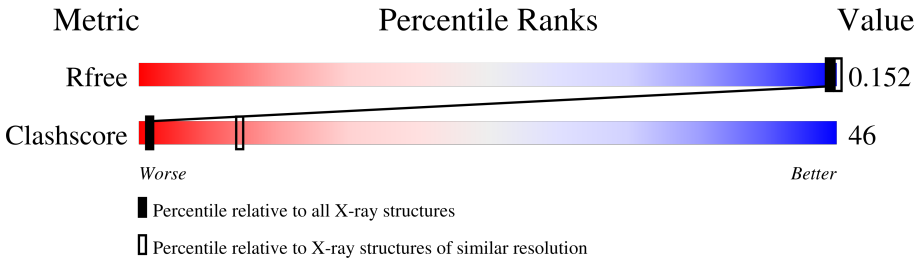
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 6.33 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	1009 (8.70-3.88)
Clashscore	141614	1058 (8.70-3.90)

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 >=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 <=5%

Mol	Chain	Length	Quality of chain
1	A	21	10% 67% 24%
2	E	14	7% 71% 21%
3	D	14	50% 50%
4	B	21	10% 62% 29%
5	F	14	64% 36%
6	C	21	10% 52% 38%
7	M	21	5% 57% 38%
8	X	21	14% 76% 10%
9	Y	21	19% 81%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 3420 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 (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
			Total	C	N	O	P			
1	A	21	426	203	82	121	20	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	E	14	290	139	53	85	13	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	D	14	288	137	55	83	13	0	0	0

- Molecule 4 is a DNA chain called DNA (5'-D(*CP*AP*CP*GP*AP*GP*CP*CP*TP*GP*AP*TP*CP*GP*GP*AP*CP*AP*AP*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
4	B	21	430	204	87	119	20	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
5	F	14	284	137	46	88	13	0	0	0

- Molecule 6 is a DNA chain called DNA (5'-D(*GP*AP*GP*CP*GP*AP*CP*CP*TP*GP*TP*AP*CP*GP*GP*AP*CP*AP*TP*CP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	C	21	Total	C	N	O	P	0	0	0
			429	204	84	121	20			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	M	21	Total	C	N	O	P	0	0	0
			418	200	76	122	20			

- Molecule 8 is a DNA chain called DNA (5'-D(*CP*TP*CP*TP*GP*CP*AP*CP*TP*AP*CP*TP*AP*CP*GP*TP*CP*AP*GP*CP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	X	21	Total	C	N	O	P	0	0	0
			420	202	74	124	20			

- Molecule 9 is a DNA chain called DNA (5'-D(P*TP*TP*TP*GP*CP*TP*GP*AP*CP*GP*TP*AP*GP*TP*AP*GP*TP*GP*CP*AP*G)-3').

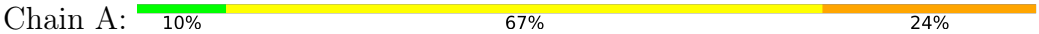
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	Y	21	Total	C	N	O	P	0	0	0
			435	207	78	129	21			

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.

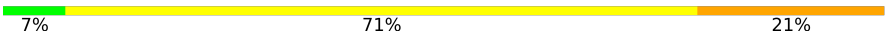
• Molecule 1: DNA (5'-D(*AP*AP*CP*CP*TP*AP*CP*CP*TP*GP*GP*CP*AP*GP*GP*AP*CP*GP*AP*CP*T)-3')

Chain A:



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

Chain E:

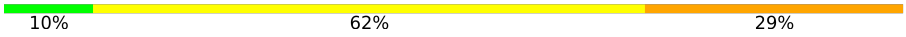


• Molecule 3: DNA (5'-D(*AP*GP*AP*GP*TP*CP*GP*TP*GP*GP*CP*TP*CP*G)-3')

Chain D:

• Molecule 4: DNA (5'-D(*CP*AP*CP*GP*AP*GP*CP*CP*TP*GP*AP*TP*CP*GP*GP*AP*CP*AP*AP*GP*A)-3')

Chain B:



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

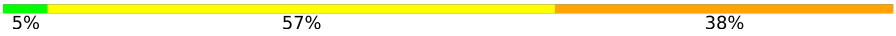
Chain F:

• Molecule 6: DNA (5'-D(*GP*AP*GP*CP*GP*AP*CP*CP*TP*GP*TP*AP*CP*GP*GP*AP*CP*AP*TP*CP*A)-3')

Chain C:

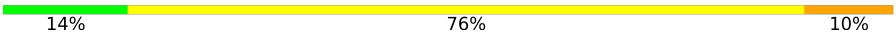
• Molecule 7: DNA (5'-D(*TP*AP*CP*AP*CP*CP*GP*AP*TP*CP*AP*CP*CP*TP*GP*CP*CP*AP*CP*CP*G)-3')

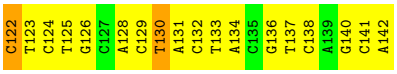
Chain M:



• Molecule 8: DNA (5'-D(*CP*TP*CP*TP*GP*CP*AP*CP*TP*AP*CP*TP*AP*CP*GP*TP*CP*AP*GP*CP*A)-3')

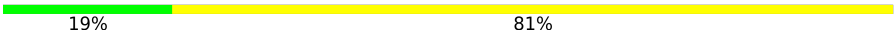
Chain X:

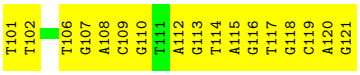




• Molecule 9: DNA (5'-D(P*TP*TP*TP*TP*GP*CP*TP*GP*AP*CP*GP*TP*AP*GP*TP*AP*GP*TP*GP*CP*AP*G)-3')

Chain Y:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	67.47Å 68.56Å 131.42Å 77.89° 79.65° 83.53°	Depositor
Resolution (Å)	36.49 – 6.33 66.83 – 6.33	Depositor EDS
% Data completeness (in resolution range)	62.8 (36.49-6.33) 54.3 (66.83-6.33)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.83 (at 6.18Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.137 , 0.152 0.137 , 0.152	Depositor DCC
R_{free} test set	191 reflections (6.32%)	wwPDB-VP
Wilson B-factor (Å^2)	128.7	Xtriage
Anisotropy	0.804	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.04 , 78.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.089 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	3420	wwPDB-VP
Average B, all atoms (Å^2)	572.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.29% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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)

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	1.41	3/478 (0.6%)	1.26	2/735 (0.3%)
2	E	1.30	2/325 (0.6%)	1.46	3/502 (0.6%)
3	D	1.54	2/323 (0.6%)	1.55	7/498 (1.4%)
4	B	1.56	5/484 (1.0%)	1.45	9/745 (1.2%)
5	F	1.45	2/316 (0.6%)	1.58	6/487 (1.2%)
6	C	1.96	10/482 (2.1%)	1.57	10/742 (1.3%)
7	M	1.97	15/467 (3.2%)	1.43	4/716 (0.6%)
8	X	1.06	0/469	1.17	2/720 (0.3%)
9	Y	1.05	1/487 (0.2%)	1.11	0/751
All	All	1.52	40/3831 (1.0%)	1.39	43/5896 (0.7%)

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	112	DA	N9-C4	13.06	1.45	1.37
6	C	111	DT	C1'-N1	11.55	1.64	1.49
7	M	120	DC	C1'-N1	11.54	1.64	1.49
4	B	111	DA	C3'-O3'	9.18	1.55	1.44
4	B	107	DC	C1'-N1	8.61	1.60	1.49
1	A	112	DC	C1'-N1	8.32	1.60	1.49
7	M	121	DG	N9-C4	8.02	1.44	1.38
6	C	115	DG	C3'-O3'	7.92	1.54	1.44
2	E	101	DT	C1'-N1	7.79	1.59	1.49
5	F	111	DT	C5'-C4'	7.35	1.59	1.51
7	M	101	DT	C1'-N1	7.30	1.58	1.49
7	M	111	DA	C3'-O3'	6.99	1.53	1.44
6	C	103	DG	C3'-O3'	6.73	1.52	1.44
6	C	116	DA	N9-C4	6.69	1.41	1.37
7	M	121	DG	C2-N3	6.46	1.38	1.32
4	B	110	DG	C3'-O3'	6.39	1.52	1.44
6	C	102	DA	N9-C4	6.33	1.41	1.37
7	M	109	DT	C5-C7	-6.31	1.46	1.50
7	M	101	DT	N1-C2	6.27	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	101	DT	C4-C5	6.25	1.50	1.45
6	C	112	DA	C5'-C4'	6.17	1.58	1.51
4	B	120	DG	C3'-O3'	-6.11	1.36	1.44
6	C	117	DC	C1'-N1	6.07	1.57	1.49
6	C	103	DG	C5'-C4'	6.05	1.58	1.51
7	M	105	DC	C3'-O3'	6.05	1.51	1.44
6	C	112	DA	C5-C6	5.87	1.46	1.41
7	M	120	DC	C3'-O3'	5.80	1.51	1.44
7	M	114	DT	C5-C6	5.72	1.38	1.34
1	A	113	DA	N9-C4	5.68	1.41	1.37
7	M	109	DT	P-O5'	5.66	1.65	1.59
3	D	132	DC	C5'-C4'	5.64	1.57	1.51
5	F	110	DG	N9-C4	5.48	1.42	1.38
7	M	121	DG	N3-C4	5.47	1.39	1.35
4	B	109	DT	C3'-O3'	-5.42	1.36	1.44
9	Y	106	DT	C1'-N1	5.35	1.56	1.49
3	D	128	DG	N3-C4	-5.34	1.31	1.35
2	E	103	DT	C1'-N1	5.33	1.56	1.49
1	A	107	DC	C1'-N1	5.29	1.56	1.49
7	M	103	DC	N3-C4	-5.24	1.30	1.33
7	M	101	DT	C3'-O3'	-5.21	1.37	1.44

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	107	DC	O4'-C1'-N1	13.27	117.29	108.00
3	D	132	DC	O5'-P-OP1	-9.56	97.10	105.70
2	E	103	DT	O4'-C1'-N1	8.73	114.11	108.00
1	A	109	DT	O4'-C4'-C3'	-7.68	101.39	106.00
6	C	116	DA	O4'-C1'-N9	7.33	113.13	108.00
6	C	111	DT	O4'-C1'-N1	7.11	112.98	108.00
4	B	107	DC	C1'-O4'-C4'	-7.04	103.06	110.10
8	X	130	DT	O4'-C1'-N1	6.64	112.65	108.00
7	M	108	DA	O4'-C1'-N9	6.30	112.41	108.00
6	C	112	DA	O4'-C1'-N9	6.25	112.38	108.00
6	C	112	DA	OP1-P-OP2	6.15	128.83	119.60
4	B	112	DT	O4'-C4'-C3'	-6.10	102.06	104.50
6	C	111	DT	C1'-O4'-C4'	-6.08	104.02	110.10
5	F	110	DG	C8-N9-C4	-6.05	103.98	106.40
5	F	104	DC	O5'-P-OP1	-6.03	100.28	105.70
7	M	105	DC	O5'-P-OP2	-5.96	100.34	105.70
3	D	133	DT	O4'-C4'-C3'	-5.90	102.14	104.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	103	DT	O4'-C1'-N1	5.87	112.11	108.00
4	B	111	DA	O4'-C1'-N9	5.84	112.09	108.00
4	B	112	DT	C5-C4-O4	-5.81	120.83	124.90
5	F	106	DT	N3-C4-O4	5.77	123.36	119.90
6	C	103	DG	OP1-P-OP2	5.77	128.25	119.60
7	M	108	DA	C1'-O4'-C4'	-5.75	104.35	110.10
6	C	103	DG	O5'-P-OP2	-5.73	100.54	105.70
3	D	124	DA	O4'-C1'-N9	5.59	111.91	108.00
1	A	106	DA	P-O3'-C3'	5.54	126.34	119.70
4	B	112	DT	N3-C4-O4	5.50	123.20	119.90
5	F	110	DG	O4'-C1'-N9	5.43	111.80	108.00
4	B	121	DA	O4'-C4'-C3'	-5.41	102.33	104.50
4	B	115	DG	O4'-C1'-N9	5.40	111.78	108.00
3	D	133	DT	O5'-P-OP2	-5.33	100.90	105.70
6	C	111	DT	N3-C4-O4	5.33	123.10	119.90
6	C	107	DC	C1'-O4'-C4'	-5.32	104.78	110.10
5	F	103	DT	N3-C4-O4	5.26	123.06	119.90
2	E	108	DT	N3-C4-O4	5.25	123.05	119.90
7	M	121	DG	O4'-C1'-N9	5.25	111.67	108.00
2	E	106	DT	C3'-C2'-C1'	-5.17	96.30	102.50
3	D	125	DG	P-O3'-C3'	5.16	125.89	119.70
3	D	131	DG	O4'-C1'-N9	5.13	111.59	108.00
8	X	122	DC	O4'-C4'-C3'	-5.10	102.46	104.50
3	D	126	DT	N3-C4-O4	5.07	122.94	119.90
4	B	110	DG	P-O3'-C3'	5.05	125.76	119.70
6	C	115	DG	P-O3'-C3'	5.03	125.73	119.70

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	426	0	236	26	0
2	E	290	0	161	20	0
3	D	288	0	159	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	430	0	235	37	0
5	F	284	0	162	30	0
6	C	429	0	236	42	0
7	M	418	0	236	29	0
8	X	420	0	238	21	0
9	Y	435	0	239	23	0
All	All	3420	0	1902	243	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 46.

All (243) 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:117:DC:H2"	7:M:118:DA:H5'	1.45	0.96
4:B:115:DG:H2'	4:B:116:DA:H8	1.32	0.94
2:E:112:DA:H2'	2:E:113:DG:C8	2.03	0.94
2:E:107:DG:H2"	2:E:108:DT:H5"	1.49	0.92
4:B:110:DG:H2'	4:B:111:DA:C8	2.04	0.91
9:Y:119:DC:H2'	9:Y:120:DA:H8	1.37	0.87
6:C:109:DT:H2'	6:C:110:DG:C8	2.12	0.85
3:D:127:DC:H2"	3:D:128:DG:C8	2.13	0.83
7:M:115:DG:H1'	7:M:116:DC:H5'	1.63	0.79
3:D:133:DT:H2'	3:D:134:DC:C6	2.17	0.79
6:C:102:DA:H2"	6:C:103:DG:H8	1.47	0.79
4:B:115:DG:H2'	4:B:116:DA:C8	2.18	0.79
8:X:136:DG:H2'	8:X:137:DT:H71	1.64	0.78
9:Y:119:DC:H2'	9:Y:120:DA:C8	2.18	0.77
4:B:101:DC:H2'	4:B:102:DA:C8	2.22	0.75
6:C:110:DG:H2'	6:C:111:DT:C6	2.21	0.74
3:D:127:DC:H2"	3:D:128:DG:H8	1.53	0.73
7:M:115:DG:H2'	7:M:115:DG:OP2	1.89	0.72
8:X:130:DT:H2"	8:X:131:DA:N7	2.04	0.72
9:Y:113:DG:H2"	9:Y:114:DT:C6	2.24	0.72
2:E:107:DG:H1'	2:E:108:DT:O4'	1.90	0.72
6:C:113:DC:H1'	6:C:114:DG:C5	2.25	0.72
1:A:110:DG:H2"	1:A:111:DG:C8	2.25	0.71
6:C:115:DG:H2'	6:C:116:DA:C8	2.26	0.71
3:D:133:DT:H2"	3:D:134:DC:H5'	1.73	0.70
1:A:107:DC:H2"	1:A:108:DC:H6	1.55	0.70
2:E:106:DT:O4	6:C:117:DC:N4	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:114:DG:H2”	6:C:115:DG:C8	2.26	0.70
6:C:102:DA:H2”	6:C:103:DG:C8	2.28	0.69
7:M:101:DT:O4’	7:M:121:DG:H1’	1.92	0.69
6:C:111:DT:H2”	6:C:112:DA:H8	1.56	0.68
5:F:112:DC:H2’	5:F:113:DG:C8	2.28	0.68
3:D:130:DG:H2’	3:D:131:DG:C8	2.29	0.68
1:A:107:DC:H2”	1:A:108:DC:C6	2.29	0.67
1:A:118:DG:H2”	1:A:119:DA:C8	2.30	0.66
4:B:112:DT:H2’	4:B:113:DC:C6	2.31	0.66
9:Y:112:DA:H1’	9:Y:113:DG:H5’	1.78	0.66
1:A:104:DC:H2’	1:A:105:DT:C6	2.30	0.65
4:B:114:DG:H2”	4:B:115:DG:N7	2.11	0.65
4:B:111:DA:H2”	4:B:112:DT:H71	1.77	0.65
6:C:115:DG:H2’	6:C:116:DA:H8	1.63	0.64
9:Y:101:DT:H1’	9:Y:102:DT:C5	2.33	0.64
3:D:133:DT:H2’	3:D:134:DC:H6	1.63	0.64
2:E:105:DA:H1’	2:E:106:DT:H5’	1.80	0.63
5:F:109:DG:C6	5:F:110:DG:C6	2.87	0.63
4:B:112:DT:H2’	4:B:113:DC:C5	2.33	0.63
1:A:108:DC:H2’	1:A:109:DT:C6	2.34	0.63
3:D:123:DG:H2”	3:D:124:DA:OP1	1.98	0.62
9:Y:108:DA:H2’	9:Y:109:DC:H4’	1.80	0.62
7:M:112:DC:H6	7:M:112:DC:H5’	1.64	0.62
4:B:106:DG:H2”	4:B:107:DC:O5’	2.00	0.61
3:D:131:DG:H2”	3:D:132:DC:OP1	2.00	0.61
4:B:115:DG:H2”	4:B:116:DA:O5’	2.01	0.61
1:A:111:DG:H2”	1:A:112:DC:C6	2.36	0.60
5:F:107:DG:H2”	5:F:108:DT:O4’	2.01	0.60
7:M:106:DC:H2”	7:M:107:DG:N7	2.16	0.60
5:F:113:DG:C5	5:F:114:DC:C4	2.90	0.60
4:B:105:DA:C6	4:B:106:DG:C6	2.89	0.60
3:D:132:DC:H2”	3:D:133:DT:O5’	2.01	0.60
5:F:102:DG:H1’	5:F:103:DT:OP2	2.02	0.60
6:C:112:DA:H2”	6:C:113:DC:O5’	2.02	0.60
9:Y:101:DT:H1’	9:Y:102:DT:C4	2.37	0.60
6:C:115:DG:H2”	6:C:116:DA:C5’	2.32	0.59
9:Y:109:DC:H2”	9:Y:110:DG:H5’	1.82	0.59
4:B:112:DT:H2”	4:B:113:DC:O5’	2.02	0.59
8:X:122:DC:H2’	8:X:123:DT:C6	2.36	0.59
1:A:115:DG:H4’	1:A:116:DA:OP1	2.01	0.59
5:F:109:DG:H3’	5:F:110:DG:H8	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:109:DT:H2"	7:M:110:DC:C6	2.38	0.59
4:B:110:DG:H2'	4:B:111:DA:N7	2.18	0.58
5:F:108:DT:H4'	5:F:109:DG:OP2	2.04	0.58
6:C:107:DC:C2	6:C:108:DC:C5	2.92	0.58
2:E:112:DA:H2'	2:E:113:DG:H8	1.62	0.58
6:C:111:DT:H2"	6:C:112:DA:C8	2.39	0.58
4:B:111:DA:C2'	4:B:112:DT:H71	2.33	0.57
6:C:114:DG:H2"	6:C:115:DG:H8	1.69	0.57
2:E:111:DT:H2"	2:E:112:DA:O5'	2.04	0.57
6:C:101:DG:N3	6:C:101:DG:H2'	2.19	0.57
7:M:108:DA:N3	7:M:109:DT:H5'	2.19	0.57
7:M:117:DC:C2'	7:M:118:DA:H5'	2.27	0.55
8:X:136:DG:H4'	8:X:137:DT:OP1	2.06	0.55
6:C:103:DG:H2'	6:C:103:DG:OP1	2.06	0.55
8:X:128:DA:H2"	8:X:129:DC:H5	1.71	0.55
5:F:108:DT:H5'	7:M:104:DA:H2"	1.88	0.55
5:F:112:DC:H2"	5:F:113:DG:H5'	1.89	0.55
8:X:141:DC:H2"	8:X:142:DA:H5'	1.87	0.55
9:Y:107:DG:H2"	9:Y:108:DA:H5'	1.89	0.55
9:Y:108:DA:H5'	9:Y:108:DA:H8	1.72	0.55
5:F:111:DT:H2"	5:F:112:DC:O5'	2.07	0.55
3:D:123:DG:H1'	3:D:124:DA:OP2	2.08	0.54
9:Y:118:DG:H8	9:Y:118:DG:OP1	1.91	0.54
4:B:110:DG:C2'	4:B:111:DA:C8	2.86	0.54
5:F:107:DG:C2	5:F:108:DT:C2	2.96	0.53
7:M:114:DT:H2"	7:M:115:DG:OP2	2.07	0.53
2:E:107:DG:C2'	2:E:108:DT:H5"	2.31	0.53
3:D:128:DG:H2"	3:D:129:DT:H5"	1.90	0.53
5:F:107:DG:H2"	5:F:108:DT:H5"	1.89	0.53
6:C:116:DA:H2"	6:C:117:DC:C6	2.44	0.53
5:F:104:DC:C6	5:F:105:DT:H72	2.43	0.53
2:E:105:DA:C8	2:E:106:DT:H72	2.44	0.53
9:Y:109:DC:H2"	9:Y:110:DG:C8	2.43	0.53
8:X:137:DT:C4	8:X:138:DC:C4	2.97	0.52
4:B:110:DG:C6	4:B:111:DA:N6	2.77	0.52
6:C:114:DG:H5"	6:C:114:DG:H8	1.74	0.52
3:D:130:DG:C6	7:M:111:DA:N6	2.78	0.52
1:A:113:DA:H2"	1:A:114:DG:C5	2.45	0.52
3:D:133:DT:C4	3:D:134:DC:C4	2.98	0.52
1:A:112:DC:O4'	1:A:112:DC:P	2.68	0.51
4:B:105:DA:H2"	4:B:106:DG:H8	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:106:DT:H4'	2:E:107:DG:OP1	2.09	0.51
6:C:112:DA:O4'	6:C:112:DA:P	2.67	0.51
3:D:133:DT:H2"	3:D:134:DC:C5'	2.39	0.51
5:F:101:DT:H2"	5:F:102:DG:OP1	2.10	0.51
8:X:123:DT:H2'	8:X:124:DC:H6	1.75	0.51
5:F:105:DT:C6	5:F:106:DT:H72	2.46	0.51
8:X:126:DG:C2	9:Y:120:DA:C2	2.98	0.51
7:M:114:DT:H1'	7:M:115:DG:C8	2.46	0.50
5:F:113:DG:C2	5:F:114:DC:C2	3.00	0.50
6:C:103:DG:C2	6:C:104:DC:C4	2.99	0.50
8:X:123:DT:H2'	8:X:124:DC:C6	2.47	0.50
1:A:112:DC:H2"	1:A:113:DA:O5'	2.11	0.49
9:Y:114:DT:C4	9:Y:115:DA:C6	3.00	0.49
1:A:113:DA:H2"	1:A:114:DG:N7	2.26	0.49
2:E:109:DG:H1'	7:M:118:DA:H1'	1.94	0.49
5:F:109:DG:H2'	5:F:110:DG:C8	2.47	0.49
1:A:110:DG:O5'	1:A:110:DG:H8	1.95	0.49
6:C:108:DC:H2'	6:C:109:DT:C6	2.48	0.49
7:M:116:DC:C2	7:M:117:DC:C2	3.00	0.49
2:E:113:DG:C6	2:E:114:DG:C6	3.00	0.49
6:C:104:DC:C2'	6:C:105:DG:H8	2.26	0.49
7:M:101:DT:H1'	7:M:102:DA:H5"	1.95	0.48
3:D:130:DG:C2	3:D:131:DG:C4	3.01	0.48
9:Y:119:DC:C2	9:Y:120:DA:C8	3.00	0.48
1:A:102:DA:H1'	1:A:103:DC:OP2	2.13	0.48
4:B:110:DG:C2	4:B:111:DA:C6	3.02	0.48
8:X:133:DT:C4	8:X:134:DA:C6	3.02	0.48
3:D:123:DG:C4	3:D:124:DA:N7	2.81	0.48
9:Y:119:DC:H2"	9:Y:120:DA:C5'	2.44	0.48
5:F:112:DC:H2'	5:F:113:DG:H8	1.76	0.48
6:C:115:DG:H2"	6:C:116:DA:H5'	1.95	0.48
6:C:103:DG:O4'	6:C:103:DG:OP2	2.32	0.47
8:X:136:DG:H2"	8:X:137:DT:O5'	2.12	0.47
3:D:127:DC:C2	3:D:128:DG:C5	3.01	0.47
4:B:113:DC:H1'	4:B:114:DG:C5	2.50	0.47
7:M:102:DA:H2"	7:M:103:DC:C6	2.50	0.47
1:A:106:DA:C5	1:A:107:DC:C4	3.02	0.47
2:E:103:DT:C2	2:E:104:DG:C8	3.02	0.47
6:C:105:DG:H2"	6:C:106:DA:O5'	2.15	0.47
3:D:129:DT:H2"	7:M:112:DC:O4'	2.14	0.47
3:D:134:DC:H2"	3:D:135:DG:O4'	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:DC:H2”	1:A:118:DG:C8	2.50	0.47
4:B:101:DC:C4	4:B:102:DA:N6	2.82	0.47
4:B:115:DG:H4’	4:B:116:DA:OP1	2.15	0.47
6:C:104:DC:C2	6:C:105:DG:N7	2.83	0.46
6:C:113:DC:N4	7:M:120:DC:C4	2.83	0.46
7:M:108:DA:H1’	7:M:109:DT:H5’	1.97	0.46
5:F:113:DG:C6	5:F:114:DC:C4	3.03	0.46
6:C:118:DA:H8	6:C:118:DA:OP2	1.98	0.46
8:X:125:DT:H2”	8:X:126:DG:H8	1.80	0.46
5:F:112:DC:H2”	5:F:113:DG:OP1	2.14	0.46
2:E:110:DG:OP2	2:E:110:DG:H8	1.98	0.46
3:D:126:DT:H2”	3:D:127:DC:C5	2.51	0.46
6:C:113:DC:H1’	6:C:114:DG:N7	2.30	0.46
6:C:101:DG:H3’	6:C:102:DA:C8	2.50	0.46
3:D:123:DG:N2	8:X:123:DT:O2	2.49	0.46
6:C:104:DC:C2’	6:C:105:DG:C8	2.99	0.46
2:E:106:DT:C2	2:E:107:DG:C6	3.04	0.46
6:C:103:DG:C6	6:C:104:DC:N4	2.84	0.46
6:C:106:DA:H2”	6:C:107:DC:OP2	2.15	0.46
4:B:105:DA:H2”	4:B:106:DG:C8	2.50	0.46
4:B:113:DC:H4’	4:B:114:DG:OP1	2.13	0.46
1:A:111:DG:N2	7:M:117:DC:O2	2.49	0.45
3:D:133:DT:O2	4:B:106:DG:N2	2.50	0.45
5:F:104:DC:H1’	5:F:105:DT:C6	2.51	0.45
9:Y:101:DT:H2’	9:Y:101:DT:OP2	2.17	0.45
8:X:140:DG:H2”	8:X:141:DC:O5’	2.15	0.45
2:E:109:DG:N3	2:E:109:DG:H2’	2.31	0.45
5:F:102:DG:C2’	5:F:103:DT:H72	2.46	0.45
8:X:131:DA:H2’	8:X:132:DC:H1’	1.97	0.45
1:A:117:DC:H2”	1:A:118:DG:OP2	2.16	0.45
6:C:113:DC:C2	6:C:114:DG:C6	3.05	0.45
8:X:125:DT:C2	8:X:126:DG:N7	2.85	0.45
1:A:115:DG:H8	1:A:115:DG:OP2	2.00	0.45
4:B:114:DG:H2”	4:B:115:DG:C8	2.52	0.45
4:B:116:DA:H2”	4:B:117:DC:H5’	2.00	0.44
4:B:110:DG:C5	4:B:111:DA:N6	2.85	0.44
3:D:124:DA:O4’	3:D:124:DA:P	2.76	0.44
2:E:103:DT:O4’	2:E:103:DT:P	2.75	0.44
3:D:133:DT:H2’	3:D:134:DC:O4’	2.18	0.44
6:C:114:DG:C2’	6:C:115:DG:C8	2.99	0.44
9:Y:120:DA:H2”	9:Y:121:DG:H8	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:X:124:DC:H2”	8:X:125:DT:O5’	2.17	0.44
4:B:113:DC:H1’	4:B:114:DG:N7	2.33	0.44
4:B:105:DA:C4	4:B:106:DG:C5	3.06	0.44
5:F:113:DG:C2	6:C:105:DG:C2	3.05	0.44
6:C:111:DT:H2”	6:C:112:DA:OP1	2.18	0.44
1:A:121:DT:C2	3:D:125:DG:N2	2.86	0.43
5:F:108:DT:H5’	7:M:104:DA:C2’	2.49	0.43
5:F:109:DG:C8	7:M:104:DA:C8	3.06	0.43
8:X:125:DT:C2	8:X:126:DG:C8	3.07	0.43
1:A:111:DG:H2”	1:A:112:DC:H6	1.82	0.43
9:Y:107:DG:C2	9:Y:108:DA:C5	3.06	0.43
9:Y:115:DA:H2”	9:Y:116:DG:C8	2.54	0.43
2:E:112:DA:H2”	2:E:113:DG:H5’	2.01	0.43
7:M:113:DC:H2”	7:M:114:DT:C4	2.54	0.43
1:A:105:DT:H2”	1:A:106:DA:O5’	2.19	0.42
4:B:110:DG:C2	4:B:111:DA:N1	2.87	0.42
6:C:101:DG:O5’	6:C:102:DA:N7	2.41	0.42
6:C:108:DC:H2’	6:C:109:DT:H71	2.02	0.42
3:D:122:DA:H2’	3:D:123:DG:C8	2.54	0.42
3:D:128:DG:H2”	3:D:129:DT:O4’	2.20	0.42
4:B:113:DC:H6	4:B:113:DC:H2’	1.69	0.42
4:B:109:DT:H3’	4:B:110:DG:H8	1.84	0.42
5:F:107:DG:H2”	5:F:108:DT:H6	1.84	0.42
5:F:113:DG:C5	5:F:114:DC:C5	3.08	0.42
7:M:102:DA:C4	7:M:103:DC:C4	3.08	0.42
4:B:105:DA:C5	4:B:106:DG:C5	3.07	0.41
3:D:124:DA:OP1	3:D:124:DA:H8	2.03	0.41
8:X:123:DT:H6	8:X:123:DT:O5’	2.03	0.41
3:D:130:DG:C6	7:M:111:DA:C6	3.09	0.41
4:B:118:DA:C2	4:B:119:DA:C4	3.08	0.41
9:Y:108:DA:C2’	9:Y:109:DC:H4’	2.50	0.41
8:X:128:DA:H2”	8:X:129:DC:C5	2.52	0.41
3:D:133:DT:C4	3:D:134:DC:N4	2.88	0.41
4:B:104:DG:N1	4:B:105:DA:C6	2.89	0.41
4:B:104:DG:C2	4:B:105:DA:C5	3.08	0.41
7:M:102:DA:N3	7:M:103:DC:C2	2.89	0.41
1:A:109:DT:H2’	1:A:110:DG:C8	2.55	0.41
2:E:106:DT:H1’	2:E:107:DG:N7	2.36	0.41
3:D:123:DG:H2”	3:D:124:DA:H8	1.86	0.41
3:D:130:DG:C5	7:M:111:DA:C6	3.09	0.41
5:F:113:DG:C4	5:F:114:DC:C6	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:118:DA:C2	6:C:119:DT:C2	3.09	0.41
9:Y:109:DC:C2'	9:Y:110:DG:C8	3.04	0.41
1:A:110:DG:O5'	1:A:110:DG:C8	2.73	0.40
4:B:118:DA:C2	5:F:107:DG:C2	3.09	0.40
7:M:109:DT:C2	7:M:110:DC:C2	3.09	0.40
9:Y:116:DG:H2"	9:Y:117:DT:O4'	2.21	0.40
2:E:106:DT:H1'	2:E:107:DG:C8	2.56	0.40
5:F:109:DG:C2	5:F:110:DG:C4	3.10	0.40
6:C:118:DA:C6	6:C:119:DT:C4	3.10	0.40
1:A:111:DG:H8	1:A:111:DG:OP2	2.05	0.40
1:A:113:DA:O3'	1:A:114:DG:C8	2.75	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

There are no ligands in this entry.

5.7 Other polymers

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

6.1 Protein, DNA and RNA chains

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

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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