Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2023 – 04:01 PM EDT

PDB ID	:	7U44
Title	:	[F344] Self-assembling tensegrity triangle with three turns, four turns and four 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	:	8.46 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:

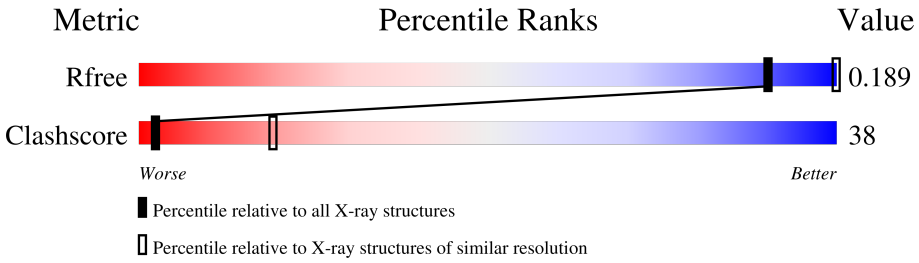
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 8.46 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	1005 (11.50-3.90)
Clashscore	141614	1070 (11.50-3.90)

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	42	5% 74% 21%
2	E	24	21% 58% 21%
3	D	35	29% 66% 6%
4	B	42	33% 57% 10%
5	F	35	23% 66% 11%
6	C	31	6% 68% 26%
7	M	21	57% 43%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 4712 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 (42-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	42	863	408	165	248	42	0	0	0

- Molecule 2 is a DNA chain called DNA (5'-D(P*TP*TP*TP*AP*GP*CP*AP*TP*AP*GP *GP*CP*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			
2	E	24	495	235	89	147	24	0	0	0

- Molecule 3 is a DNA chain called DNA (35-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	D	35	718	341	127	215	35	0	0	0

- Molecule 4 is a DNA chain called DNA (42-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
4	B	42	860	408	159	251	42	0	0	0

- Molecule 5 is a DNA chain called DNA (35-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
5	F	35	726	344	136	211	35	0	0	0

- Molecule 6 is a DNA chain called DNA (31-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	C	31	Total	C	N	O	P	0	0	0
			629	300	117	182	30			

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

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

3 Residue-property plots (i)

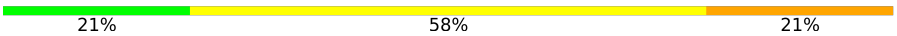
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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 (42-MER)

Chain A:

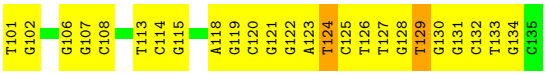
• Molecule 2: DNA (5'-D(P*TP*TP*TP*AP*GP*CP*AP*TP*AP*GP*GP*CP*AP*GP*TP*CP*GP*TP*GP*GP*CP*TP*CP*G)-3')

Chain E:



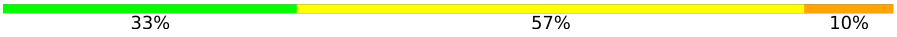
• Molecule 3: DNA (35-MER)

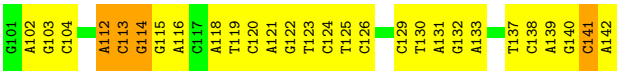
Chain D:



• Molecule 4: DNA (42-MER)

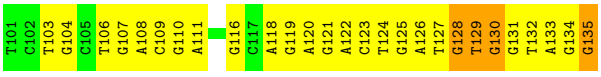
Chain B:





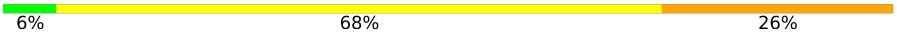
• Molecule 5: DNA (35-MER)

Chain F:



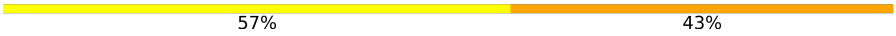
• Molecule 6: DNA (31-MER)

Chain C:



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

Chain M:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	100.42Å 135.34Å 135.19Å 99.31° 95.66° 106.50°	Depositor
Resolution (Å)	38.27 – 8.46 95.15 – 8.46	Depositor EDS
% Data completeness (in resolution range)	58.4 (38.27-8.46) 49.5 (95.15-8.46)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.54 (at 8.42Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.160 , 0.192 0.160 , 0.189	Depositor DCC
R_{free} test set	185 reflections (5.32%)	wwPDB-VP
Wilson B-factor (Å^2)	337.7	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.75 , 303.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.75	EDS
Total number of atoms	4712	wwPDB-VP
Average B, all atoms (Å^2)	1274.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.04 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.5549e-04.*

[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

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	1.17	7/969 (0.7%)	1.22	6/1493 (0.4%)
2	E	1.36	5/554 (0.9%)	1.34	5/854 (0.6%)
3	D	1.01	1/803 (0.1%)	1.16	1/1238 (0.1%)
4	B	1.09	5/964 (0.5%)	1.20	4/1485 (0.3%)
5	F	1.29	9/815 (1.1%)	1.35	8/1258 (0.6%)
6	C	1.29	5/705 (0.7%)	1.40	7/1085 (0.6%)
7	M	1.73	7/470 (1.5%)	1.74	14/720 (1.9%)
All	All	1.25	39/5280 (0.7%)	1.32	45/8133 (0.6%)

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	114	DG	N9-C4	10.55	1.46	1.38
5	F	129	DT	C3'-O3'	10.09	1.57	1.44
5	F	130	DG	C5'-C4'	9.25	1.61	1.51
7	M	118	DC	C1'-N1	9.14	1.61	1.49
5	F	130	DG	P-O5'	8.84	1.68	1.59
6	C	112	DC	C1'-N1	8.61	1.60	1.49
5	F	130	DG	N3-C4	8.60	1.41	1.35
2	E	118	DT	C1'-N1	8.51	1.60	1.49
4	B	114	DG	C2-N3	8.51	1.39	1.32
2	E	108	DT	C1'-N1	8.27	1.60	1.49
5	F	130	DG	N9-C4	7.68	1.44	1.38
7	M	118	DC	C3'-O3'	7.62	1.53	1.44
7	M	118	DC	N1-C2	7.27	1.47	1.40
5	F	130	DG	O5'-C5'	7.17	1.60	1.42
7	M	118	DC	C2-N3	6.97	1.41	1.35
5	F	130	DG	C2-N3	6.96	1.38	1.32
3	D	129	DT	C1'-N1	6.94	1.58	1.49
7	M	118	DC	C4'-C3'	6.20	1.59	1.53
1	A	115	DG	N9-C4	6.02	1.42	1.38
6	C	112	DC	N1-C2	6.01	1.46	1.40
7	M	112	DT	C1'-N1	5.98	1.57	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	107	DA	C3'-O3'	5.98	1.51	1.44
5	F	129	DT	C5-C7	5.92	1.53	1.50
4	B	112	DA	N9-C4	5.72	1.41	1.37
1	A	114	DG	C3'-O3'	-5.71	1.36	1.44
2	E	112	DC	C3'-O3'	5.66	1.51	1.44
4	B	114	DG	N1-C2	5.63	1.42	1.37
1	A	114	DG	C2-N3	5.54	1.37	1.32
1	A	108	DC	C1'-N1	5.51	1.56	1.49
1	A	114	DG	N9-C4	5.47	1.42	1.38
1	A	112	DT	C1'-N1	5.38	1.56	1.49
4	B	113	DC	N1-C2	5.37	1.45	1.40
6	C	113	DA	N9-C4	5.30	1.41	1.37
2	E	109	DA	N9-C4	5.25	1.41	1.37
7	M	109	DA	C5-C4	-5.24	1.35	1.38
5	F	129	DT	C4'-C3'	5.20	1.58	1.53
1	A	130	DC	C1'-N1	5.20	1.56	1.49
6	C	124	DC	C3'-O3'	5.12	1.50	1.44
6	C	126	DA	N9-C4	5.00	1.40	1.37

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	M	118	DC	O4'-C1'-N1	10.64	115.45	108.00
7	M	110	DC	O4'-C4'-C3'	-10.34	99.79	106.00
5	F	129	DT	O5'-P-OP2	-10.05	96.65	105.70
6	C	121	DT	P-O3'-C3'	-9.82	107.92	119.70
7	M	109	DA	C3'-C2'-C1'	-8.17	92.69	102.50
5	F	128	DG	O4'-C1'-N9	7.66	113.36	108.00
5	F	130	DG	O4'-C4'-C3'	-7.62	101.43	106.00
4	B	141	DC	O4'-C4'-C3'	-7.40	101.54	104.50
6	C	123	DC	O4'-C1'-N1	6.95	112.86	108.00
6	C	116	DA	O4'-C1'-N9	6.92	112.84	108.00
7	M	118	DC	C1'-O4'-C4'	-6.78	103.32	110.10
7	M	101	DC	O4'-C1'-N1	6.73	112.71	108.00
7	M	116	DA	O4'-C1'-N9	6.49	112.54	108.00
2	E	118	DT	N3-C4-O4	6.41	123.75	119.90
5	F	128	DG	C3'-C2'-C1'	-6.39	94.83	102.50
4	B	114	DG	N3-C4-N9	6.36	129.81	126.00
2	E	118	DT	C5-C4-O4	-6.20	120.56	124.90
2	E	112	DC	O4'-C1'-N1	6.01	112.21	108.00
5	F	135	DG	O4'-C1'-N9	5.95	112.16	108.00
1	A	114	DG	O4'-C1'-N9	-5.91	103.87	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	M	121	DA	O4'-C1'-N9	5.74	112.02	108.00
6	C	112	DC	N1-C2-O2	5.67	122.30	118.90
4	B	114	DG	N3-C4-C5	-5.64	125.78	128.60
7	M	120	DT	O4'-C1'-N1	5.62	111.93	108.00
2	E	107	DA	P-O3'-C3'	5.55	126.36	119.70
6	C	121	DT	O3'-P-O5'	5.54	114.53	104.00
7	M	103	DC	O5'-P-OP2	-5.50	100.75	105.70
7	M	118	DC	C4-C5-C6	5.49	120.14	117.40
1	A	111	DA	O4'-C1'-N9	5.46	111.82	108.00
7	M	120	DT	N3-C4-O4	5.46	123.17	119.90
6	C	114	DG	O4'-C4'-C3'	-5.43	102.33	104.50
1	A	106	DG	O4'-C1'-N9	5.33	111.73	108.00
7	M	120	DT	C5-C4-O4	-5.30	121.19	124.90
6	C	112	DC	O4'-C4'-C3'	-5.27	102.39	104.50
1	A	107	DC	O4'-C1'-N1	5.19	111.63	108.00
1	A	112	DT	N3-C4-O4	5.15	122.99	119.90
3	D	124	DT	O4'-C1'-N1	5.08	111.56	108.00
7	M	111	DC	N1-C2-O2	5.07	121.94	118.90
1	A	131	DG	C1'-O4'-C4'	-5.04	105.06	110.10
2	E	107	DA	O4'-C1'-N9	5.04	111.53	108.00
5	F	130	DG	N3-C4-N9	5.03	129.02	126.00
5	F	129	DT	OP1-P-OP2	5.01	127.12	119.60
7	M	121	DA	C1'-O4'-C4'	-5.01	105.09	110.10
4	B	114	DG	C8-N9-C4	-5.01	104.40	106.40
5	F	129	DT	C5-C4-O4	-5.00	121.40	124.90

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	863	0	470	61	1
2	E	495	0	272	35	0
3	D	718	0	396	33	0
4	B	860	0	472	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	726	0	395	54	0
6	C	629	0	349	47	0
7	M	421	0	235	45	0
All	All	4712	0	2589	275	1

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 38.

All (275) 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:E:118:DT:H2'	7:M:111:DC:H4'	1.42	1.01
5:F:107:DG:H2"	5:F:108:DA:H5"	1.55	0.88
5:F:130:DG:C8	7:M:117:DC:H5"	2.09	0.87
1:A:114:DG:H2"	1:A:115:DG:C8	2.10	0.86
6:C:110:DG:H2'	6:C:111:DG:H4'	1.57	0.85
7:M:113:DG:H1'	7:M:114:DC:H5'	1.60	0.83
1:A:112:DT:H2'	1:A:113:DC:C6	2.18	0.79
5:F:133:DA:H2'	5:F:134:DG:H8	1.47	0.78
6:C:111:DG:H2"	6:C:112:DC:OP1	1.80	0.78
6:C:112:DC:H2'	6:C:113:DA:C8	2.20	0.76
5:F:119:DG:H2'	5:F:120:DA:C8	2.21	0.76
3:D:130:DG:H3'	3:D:131:DG:C8	2.22	0.75
3:D:130:DG:H3'	3:D:131:DG:H8	1.52	0.75
6:C:103:DC:H2"	6:C:104:DC:H5"	1.68	0.74
2:E:107:DA:N1	6:C:128:DG:N2	2.36	0.74
5:F:130:DG:P	7:M:118:DC:H2"	2.29	0.72
4:B:112:DA:H2"	4:B:113:DC:H5'	1.71	0.72
7:M:102:DA:H4'	7:M:103:DC:OP2	1.90	0.72
1:A:140:DT:O2	3:D:106:DG:N2	2.24	0.70
2:E:108:DT:H2'	2:E:109:DA:H8	1.56	0.70
5:F:129:DT:H3'	7:M:118:DC:C2	2.26	0.70
6:C:124:DC:H2"	6:C:125:DT:H5"	1.74	0.70
1:A:112:DT:H2'	1:A:113:DC:H6	1.57	0.69
6:C:117:DC:H2"	6:C:118:DG:C8	2.26	0.69
3:D:128:DG:H2"	3:D:129:DT:H5"	1.73	0.69
3:D:133:DT:H2'	3:D:134:DG:H8	1.57	0.69
4:B:115:DG:H4'	4:B:116:DA:O5'	1.92	0.69
5:F:129:DT:O3'	7:M:118:DC:H2"	1.92	0.69
2:E:117:DG:H2"	2:E:118:DT:H5"	1.74	0.69
2:E:108:DT:H2"	2:E:109:DA:H5'	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:130:DT:H2”	4:B:131:DA:C8	2.29	0.67
4:B:103:DG:H2”	4:B:104:DC:H5”	1.74	0.67
2:E:103:DT:H2”	2:E:104:DA:C8	2.30	0.67
4:B:123:DT:H2”	4:B:124:DC:H2’	1.77	0.67
1:A:115:DG:H4’	1:A:116:DA:H5’	1.77	0.66
5:F:129:DT:H2”	7:M:119:DG:O4’	1.95	0.66
3:D:133:DT:H2’	3:D:134:DG:C8	2.30	0.66
7:M:114:DC:H2”	7:M:115:DC:O4’	1.96	0.65
6:C:110:DG:H5’	6:C:110:DG:H8	1.61	0.65
1:A:104:DG:H2”	1:A:105:DA:C8	2.31	0.65
2:E:109:DA:H1’	2:E:110:DG:H5’	1.79	0.64
5:F:108:DA:H3’	5:F:109:DC:H4’	1.79	0.64
1:A:101:DC:H3’	1:A:102:DA:H4’	1.80	0.64
1:A:115:DG:H1’	1:A:116:DA:C8	2.33	0.63
1:A:129:DG:H2”	1:A:130:DC:O4’	2.00	0.62
5:F:133:DA:H2’	5:F:134:DG:C8	2.32	0.62
5:F:129:DT:H3’	7:M:118:DC:O2	1.99	0.61
3:D:130:DG:N3	3:D:130:DG:H2’	2.16	0.61
7:M:116:DA:H2”	7:M:117:DC:O5’	2.01	0.61
2:E:107:DA:C6	6:C:128:DG:N2	2.69	0.60
5:F:129:DT:H3’	7:M:118:DC:H1’	1.83	0.60
7:M:116:DA:H2”	7:M:117:DC:C5’	2.30	0.60
1:A:109:DT:H2”	1:A:110:DG:N7	2.16	0.60
5:F:110:DG:H2”	5:F:111:DA:C8	2.36	0.60
6:C:110:DG:H5’	6:C:110:DG:C8	2.36	0.60
7:M:120:DT:C2	7:M:121:DA:H1’	2.37	0.60
5:F:130:DG:O5’	7:M:118:DC:H2”	2.01	0.60
1:A:131:DG:H2’	1:A:132:DA:C8	2.37	0.59
2:E:108:DT:H2’	2:E:109:DA:C8	2.36	0.59
3:D:129:DT:H3’	7:M:104:DC:OP1	2.02	0.59
4:B:129:DC:H5”	4:B:129:DC:H6	1.68	0.59
1:A:123:DC:H42	3:D:122:DG:H22	1.51	0.58
1:A:139:DC:N3	3:D:107:DG:N2	2.51	0.58
3:D:107:DG:H2”	3:D:108:DC:H5”	1.85	0.58
5:F:122:DA:H2’	5:F:123:DC:C6	2.38	0.58
6:C:115:DG:H4’	6:C:116:DA:H5’	1.85	0.58
6:C:128:DG:H1’	6:C:129:DC:O4’	2.03	0.58
1:A:125:DG:H2”	1:A:126:DC:C6	2.39	0.58
6:C:102:DA:H1’	6:C:103:DC:OP2	2.04	0.58
1:A:106:DG:OP2	1:A:106:DG:H3’	2.03	0.58
2:E:107:DA:C2	2:E:108:DT:H1’	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:129:DT:H4'	7:M:118:DC:O3'	2.04	0.57
1:A:104:DG:H2"	1:A:105:DA:H8	1.68	0.57
2:E:110:DG:H2"	2:E:111:DG:C8	2.40	0.57
2:E:104:DA:H2"	2:E:105:DG:O5'	2.05	0.56
6:C:108:DC:H2'	6:C:109:DT:O4'	2.04	0.56
6:C:123:DC:H1'	6:C:124:DC:OP2	2.05	0.56
4:B:133:DA:H8	4:B:133:DA:OP1	1.88	0.56
7:M:104:DC:H5"	7:M:104:DC:C6	2.40	0.56
1:A:111:DA:H2"	1:A:112:DT:OP2	2.06	0.56
2:E:108:DT:H2"	2:E:109:DA:C5'	2.35	0.56
4:B:141:DC:H1'	4:B:142:DA:H5'	1.88	0.56
2:E:105:DG:H8	2:E:105:DG:H5"	1.71	0.55
3:D:122:DG:H2"	3:D:123:DA:N7	2.22	0.55
4:B:113:DC:H2"	4:B:114:DG:N7	2.20	0.55
5:F:119:DG:H2'	5:F:120:DA:H8	1.66	0.55
5:F:129:DT:H5'	7:M:118:DC:O2	2.05	0.55
2:E:103:DT:H2"	2:E:104:DA:N7	2.20	0.55
4:B:121:DA:H2"	4:B:122:DG:C8	2.41	0.55
1:A:117:DC:H2"	1:A:118:DA:C8	2.41	0.55
2:E:122:DT:H2"	2:E:123:DC:O5'	2.07	0.55
5:F:124:DT:H2"	5:F:125:DG:H8	1.73	0.54
2:E:112:DC:H1'	2:E:113:DA:OP2	2.07	0.54
2:E:109:DA:C2	6:C:126:DA:C2	2.95	0.54
1:A:112:DT:H2"	1:A:113:DC:H5'	1.89	0.53
4:B:130:DT:H2"	4:B:131:DA:N7	2.23	0.53
5:F:129:DT:OP1	7:M:118:DC:H4'	2.08	0.53
7:M:104:DC:OP1	7:M:104:DC:H4'	2.09	0.53
5:F:130:DG:H8	7:M:117:DC:H5"	1.67	0.53
1:A:107:DC:H2"	1:A:108:DC:H6	1.73	0.53
7:M:120:DT:N3	7:M:121:DA:H1'	2.25	0.52
5:F:133:DA:H2"	5:F:134:DG:C5'	2.39	0.52
1:A:103:DC:H2"	1:A:104:DG:H5"	1.91	0.52
4:B:119:DT:H2"	4:B:120:DC:O5'	2.08	0.52
5:F:129:DT:C3'	7:M:118:DC:H1'	2.39	0.52
7:M:104:DC:H5"	7:M:104:DC:H6	1.74	0.52
2:E:112:DC:H2"	2:E:113:DA:OP1	2.09	0.52
5:F:127:DT:H2"	5:F:128:DG:H8	1.75	0.52
1:A:112:DT:H2"	1:A:113:DC:C5'	2.38	0.52
1:A:130:DC:C2	1:A:131:DG:C8	2.98	0.52
4:B:112:DA:H2"	4:B:113:DC:C5'	2.38	0.52
5:F:123:DC:H1'	5:F:124:DT:OP2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:DA:H2”	1:A:119:DA:C8	2.45	0.51
5:F:118:DA:H2”	5:F:119:DG:O4’	2.11	0.51
5:F:132:DT:H2”	5:F:133:DA:O5’	2.09	0.51
1:A:111:DA:C4	1:A:112:DT:H72	2.45	0.51
2:E:114:DG:H1’	2:E:115:DT:C5	2.45	0.51
3:D:124:DT:H2”	3:D:125:DC:C5	2.45	0.51
4:B:139:DA:H2”	4:B:140:DG:C8	2.46	0.51
5:F:134:DG:H1’	5:F:135:DG:H5’	1.93	0.51
1:A:134:DT:H2”	1:A:135:DT:H72	1.92	0.51
1:A:131:DG:C2	3:D:115:DG:C2	2.98	0.50
3:D:124:DT:H2”	3:D:125:DC:C6	2.46	0.50
1:A:128:DA:H2”	1:A:129:DG:C8	2.46	0.50
3:D:113:DT:H2”	3:D:114:DC:C5	2.46	0.50
3:D:128:DG:H2”	3:D:129:DT:H6	1.76	0.50
4:B:133:DA:H8	4:B:133:DA:P	2.35	0.50
1:A:112:DT:P	1:A:112:DT:O4’	2.70	0.50
5:F:131:DG:N2	5:F:132:DT:C4	2.79	0.50
1:A:121:DA:H2’	1:A:122:DT:H72	1.93	0.50
6:C:122:DG:H2”	6:C:123:DC:O4’	2.12	0.49
6:C:113:DA:H1’	6:C:114:DG:N7	2.27	0.49
6:C:120:DC:H2”	6:C:121:DT:H72	1.93	0.49
1:A:118:DA:H2”	1:A:119:DA:H8	1.76	0.49
2:E:116:DC:H1’	2:E:117:DG:C5	2.48	0.49
6:C:127:DT:H2”	6:C:128:DG:H2’	1.94	0.49
7:M:115:DC:H2”	7:M:116:DA:H5’	1.94	0.49
2:E:112:DC:H1’	2:E:113:DA:P	2.52	0.49
4:B:137:DT:C4	4:B:138:DC:C4	3.00	0.49
3:D:127:DT:H1’	3:D:128:DG:O4’	2.13	0.49
6:C:101:DA:N3	6:C:101:DA:H2’	2.28	0.49
2:E:116:DC:H1’	2:E:117:DG:N7	2.28	0.48
3:D:118:DA:H4’	3:D:119:DG:OP1	2.12	0.48
3:D:130:DG:O4’	7:M:104:DC:O5’	2.32	0.48
6:C:126:DA:H2”	6:C:127:DT:O4’	2.13	0.48
6:C:104:DC:H2”	6:C:105:DT:H5’	1.96	0.48
7:M:105:DG:C2	7:M:106:DA:C4	3.02	0.48
3:D:129:DT:H72	7:M:103:DC:C2	2.48	0.48
4:B:132:DG:H2”	4:B:133:DA:C8	2.49	0.48
3:D:128:DG:H2’	3:D:129:DT:H71	1.95	0.48
3:D:122:DG:H2”	3:D:123:DA:C8	2.49	0.47
1:A:135:DT:C2	1:A:136:DA:C8	3.02	0.47
1:A:106:DG:C2	1:A:107:DC:C2	3.03	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:DG:C2	1:A:130:DC:C2	3.02	0.47
4:B:113:DC:H1'	4:B:114:DG:C8	2.49	0.47
5:F:129:DT:P	7:M:118:DC:H4'	2.54	0.47
6:C:118:DG:C2	6:C:119:DA:C2	3.03	0.47
7:M:113:DG:N3	7:M:114:DC:O4'	2.47	0.47
1:A:108:DC:C6	1:A:109:DT:H72	2.49	0.47
2:E:107:DA:H2"	2:E:108:DT:O5'	2.15	0.47
1:A:103:DC:H2'	1:A:104:DG:C8	2.50	0.47
5:F:125:DG:H4'	5:F:126:DA:OP1	2.14	0.47
6:C:116:DA:C5	6:C:117:DC:C4	3.03	0.47
3:D:121:DG:O6	3:D:122:DG:N2	2.48	0.47
4:B:125:DT:H2"	4:B:126:DC:H5'	1.96	0.47
1:A:120:DG:H2"	1:A:121:DA:C8	2.50	0.47
5:F:132:DT:H2'	5:F:132:DT:OP1	2.15	0.46
5:F:129:DT:N1	5:F:129:DT:H5"	2.30	0.46
5:F:134:DG:N2	6:C:105:DT:C2	2.83	0.46
4:B:118:DA:C4	5:F:128:DG:N2	2.83	0.46
5:F:134:DG:N2	6:C:105:DT:O2	2.49	0.46
5:F:134:DG:C6	5:F:135:DG:C5	3.04	0.46
7:M:106:DA:H1'	7:M:107:DT:O5'	2.16	0.46
1:A:108:DC:H2'	1:A:109:DT:C7	2.46	0.46
5:F:116:DG:C8	5:F:116:DG:H5"	2.51	0.46
6:C:106:DA:H1'	6:C:107:DC:H5'	1.98	0.46
1:A:112:DT:H2"	1:A:113:DC:O5'	2.15	0.46
4:B:138:DC:C2	4:B:139:DA:C8	3.04	0.45
2:E:117:DG:C8	2:E:118:DT:H72	2.51	0.45
6:C:115:DG:N2	6:C:116:DA:C6	2.85	0.45
2:E:105:DG:H5"	2:E:105:DG:C8	2.51	0.45
2:E:113:DA:H2"	2:E:114:DG:C8	2.51	0.45
1:A:114:DG:N2	1:A:115:DG:C2	2.84	0.45
3:D:119:DG:H2"	3:D:120:DC:O5'	2.17	0.45
6:C:124:DC:H2"	6:C:125:DT:O4'	2.16	0.45
6:C:126:DA:C2	6:C:127:DT:C2	3.05	0.45
1:A:106:DG:C4	1:A:107:DC:C6	3.05	0.45
4:B:114:DG:C2	7:M:119:DG:N2	2.85	0.45
4:B:124:DC:H2"	4:B:125:DT:H71	1.98	0.45
7:M:101:DC:H1'	7:M:102:DA:H5'	1.99	0.45
5:F:127:DT:H2"	5:F:128:DG:C8	2.51	0.45
1:A:103:DC:H2"	1:A:104:DG:O4'	2.17	0.44
5:F:133:DA:H2"	5:F:134:DG:H5'	1.99	0.44
6:C:110:DG:H8	6:C:110:DG:C5'	2.28	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:DC:C2	1:A:108:DC:C6	3.05	0.44
1:A:118:DA:C6	1:A:119:DA:C6	3.05	0.44
4:B:112:DA:C2'	4:B:113:DC:H5'	2.44	0.44
4:B:102:DA:H2"	4:B:103:DG:OP2	2.17	0.44
5:F:120:DA:C6	5:F:121:DG:C6	3.05	0.44
6:C:117:DC:C2	6:C:118:DG:C2	3.05	0.44
1:A:129:DG:C4	1:A:130:DC:C6	3.05	0.44
4:B:114:DG:N2	7:M:119:DG:H21	2.15	0.44
4:B:123:DT:C4	4:B:124:DC:C5	3.06	0.44
2:E:114:DG:H2"	2:E:115:DT:C7	2.48	0.44
5:F:120:DA:H2"	5:F:121:DG:H8	1.82	0.44
6:C:116:DA:C2	6:C:117:DC:C2	3.05	0.44
5:F:108:DA:C3'	5:F:109:DC:H4'	2.47	0.44
1:A:112:DT:C2	1:A:113:DC:C5	3.06	0.44
4:B:125:DT:C2	4:B:126:DC:C5	3.06	0.44
5:F:124:DT:H2"	5:F:125:DG:C8	2.51	0.43
7:M:120:DT:C4	7:M:121:DA:H1'	2.53	0.43
1:A:123:DC:C2	1:A:124:DC:N4	2.86	0.43
5:F:120:DA:H2"	5:F:121:DG:C8	2.53	0.43
1:A:123:DC:H42	3:D:122:DG:N2	2.15	0.43
3:D:101:DT:H2'	3:D:102:DG:C8	2.54	0.43
3:D:132:DC:H2"	3:D:133:DT:O5'	2.19	0.43
4:B:118:DA:C2	5:F:128:DG:C2	3.07	0.43
5:F:116:DG:H5"	5:F:116:DG:H8	1.82	0.43
6:C:128:DG:C2	6:C:129:DC:C2	3.07	0.43
7:M:111:DC:H2"	7:M:112:DT:O4'	2.19	0.43
3:D:119:DG:H2"	3:D:120:DC:C5'	2.47	0.43
4:B:114:DG:H2"	4:B:115:DG:O4'	2.18	0.43
2:E:121:DC:H4'	2:E:122:DT:OP1	2.18	0.42
6:C:127:DT:H2"	6:C:128:DG:O5'	2.19	0.42
7:M:110:DC:H2"	7:M:111:DC:OP1	2.17	0.42
1:A:119:DA:C6	1:A:120:DG:C6	3.07	0.42
5:F:130:DG:H3'	5:F:131:DG:H5"	2.01	0.42
7:M:107:DT:C2	7:M:108:DC:C6	3.07	0.42
1:A:110:DG:H8	1:A:110:DG:P	2.41	0.42
1:A:115:DG:C2'	1:A:116:DA:H8	2.32	0.42
6:C:105:DT:C2	6:C:106:DA:C2	3.07	0.42
1:A:108:DC:N1	1:A:109:DT:H72	2.34	0.42
1:A:132:DA:H1'	1:A:133:DG:OP2	2.19	0.42
6:C:103:DC:C2	6:C:104:DC:C5	3.08	0.42
1:A:118:DA:C2	3:D:128:DG:N2	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:122:DG:H5"	6:C:122:DG:H8	1.85	0.42
7:M:103:DC:H2"	7:M:104:DC:C5	2.54	0.42
4:B:123:DT:C5	4:B:124:DC:H5	2.37	0.42
4:B:139:DA:H2"	4:B:140:DG:H8	1.84	0.42
4:B:140:DG:N2	5:F:106:DT:O2	2.53	0.42
5:F:129:DT:H2"	7:M:119:DG:C1'	2.50	0.42
6:C:105:DT:H2"	6:C:106:DA:C8	2.54	0.42
4:B:112:DA:N6	7:M:121:DA:C2	2.88	0.42
6:C:107:DC:H2"	6:C:108:DC:O4'	2.20	0.42
5:F:130:DG:C2	5:F:131:DG:C4	3.08	0.41
3:D:125:DC:H4'	3:D:126:DT:OP1	2.18	0.41
2:E:113:DA:H2"	2:E:114:DG:H8	1.85	0.41
2:E:117:DG:N2	6:C:118:DG:H21	2.18	0.41
3:D:133:DT:H2"	3:D:134:DG:C5'	2.50	0.41
3:D:133:DT:H2"	3:D:134:DG:H5'	2.03	0.41
4:B:113:DC:H2"	4:B:114:DG:C8	2.56	0.41
1:A:114:DG:C2'	1:A:115:DG:C8	2.95	0.41
4:B:114:DG:N2	7:M:119:DG:N2	2.69	0.41
4:B:137:DT:C2	4:B:138:DC:C6	3.08	0.41
2:E:117:DG:N2	6:C:118:DG:N2	2.68	0.41
4:B:115:DG:C2	4:B:116:DA:C6	3.08	0.41
1:A:105:DA:C6	1:A:106:DG:C6	3.09	0.41
1:A:127:DT:C4	1:A:128:DA:C6	3.09	0.41
2:E:116:DC:H6	2:E:116:DC:H2'	1.73	0.41
4:B:115:DG:N2	4:B:116:DA:C6	2.88	0.41
4:B:139:DA:C6	4:B:140:DG:C6	3.09	0.41
6:C:113:DA:H1'	6:C:114:DG:C5	2.56	0.41
6:C:114:DG:H8	6:C:114:DG:O5'	2.03	0.41
6:C:124:DC:H4'	6:C:125:DT:OP1	2.21	0.41
2:E:107:DA:H1'	2:E:108:DT:P	2.61	0.41
5:F:118:DA:H2"	5:F:119:DG:O5'	2.19	0.41
1:A:115:DG:H2"	1:A:116:DA:H8	1.85	0.40
1:A:136:DA:H2'	1:A:137:DG:C8	2.56	0.40
5:F:103:DT:H1'	5:F:104:DG:OP1	2.22	0.40
7:M:104:DC:H2"	7:M:105:DG:O4'	2.20	0.40
1:A:108:DC:C2	2:E:120:DG:N2	2.90	0.40
7:M:103:DC:H2"	7:M:104:DC:C6	2.56	0.40
1:A:116:DA:C6	1:A:117:DC:N3	2.89	0.40
5:F:103:DT:H2"	5:F:104:DG:O5'	2.21	0.40
6:C:113:DA:O3'	6:C:114:DG:C8	2.75	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:DC:OP1	1:A:142:DG:N2[1_556]	2.14	0.06

5.3 Torsion angles

5.3.1 Protein backbone

There are no protein molecules in this entry.

5.3.2 Protein sidechains

There are no protein molecules in this entry.

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

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.