



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 21, 2022 – 06:08 PM EDT

PDB ID : 7U42
Title : [F334] Self-assembling tensegrity triangle with three turns, three 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 : 7.71 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	:	2.29
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

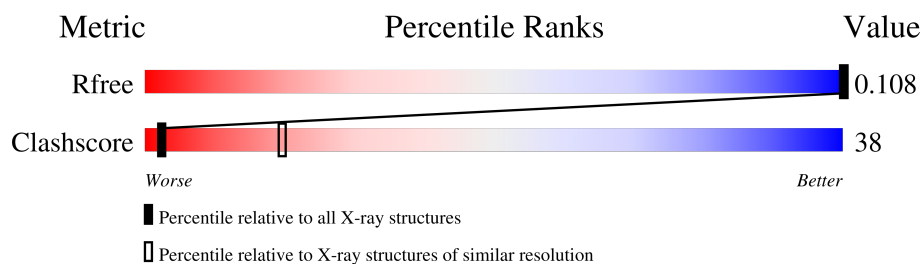
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 7.71 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	31	74% 26%
2	E	24	67% 33%
3	D	24	12% 63% 25%
4	B	42	12% 76% 12%
5	F	35	20% 66% 14%
6	C	31	16% 55% 29%
7	M	21	5% 67% 29%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 4258 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
			640	301	131	177	31			

- Molecule 2 is a DNA chain called DNA (5'-D(P*TP*TP*TP*AP*GP*CP*AP*TP*AP*GP*TP*GP*AP*GP*TP*CP*GP*TP*GP*GP*CP*TP*CP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	24	Total	C	N	O	P	0	0	0
			494	236	85	149	24			

- Molecule 3 is a DNA chain called DNA (5'-D(P*TP*GP*TP*GP*CP*TP*TP*GP*CP*GP*TP*CP*GP*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
			492	234	81	153	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	42	Total	C	N	O	P	0	0	0
			857	407	157	251	42			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	35	Total	C	N	O	P	0	0	0
			729	345	138	211	35			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	C	31	Total 628	C 300	N 117	O 181	P 30	0	0	0

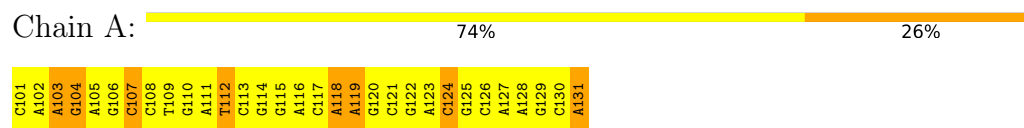
- Molecule 7 is a DNA chain called DNA (5'-D(*TP*AP*CP*AP*CP*CP*GP*AP*TP*CP*AP*CP*CP*TP*GP*CP*CP*AP*CP*CP*G)-3').

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

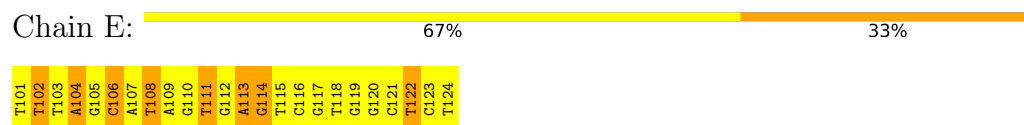
3 Residue-property plots [i](#)

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.

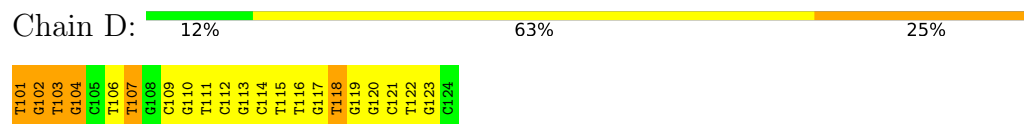
- Molecule 1: DNA (31-MER)



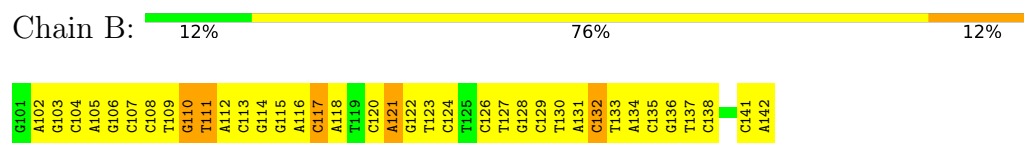
- Molecule 2: DNA (5'-D(P*TP*TP*TP*AP*GP*CP*AP*TP*AP*GP*TP*GP*AP*GP*TP*C P*GP*TP*GP*GP*CP*TP*CP*T)-3')



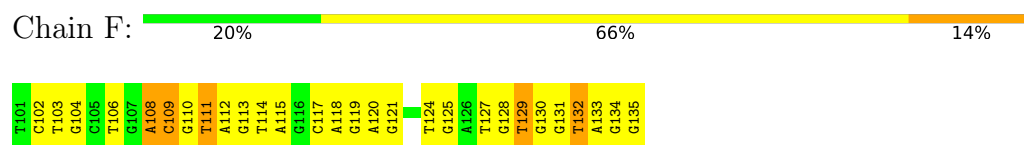
- Molecule 3: DNA (5'-D(P*TP*GP*TP*GP*CP*TP*TP*GP*CP*GP*TP*CP*GP*CP*TP*T P*GP*TP*GP*GP*CP*TP*GP*C)-3')



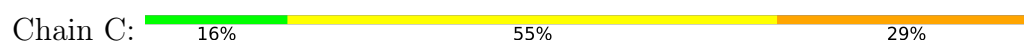
- Molecule 4: DNA (42-MER)



- Molecule 5: DNA (35-MER)



- Molecule 6: DNA (31-MER)





● 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')



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	99.72Å 101.83Å 135.72Å 99.19° 106.43° 101.55°	Depositor
Resolution (Å)	39.01 – 7.71 97.10 – 7.71	Depositor EDS
% Data completeness (in resolution range)	63.2 (39.01-7.71) 56.4 (97.10-7.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.10 (at 7.43Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.097 , 0.108 0.096 , 0.108	Depositor DCC
R_{free} test set	181 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	192.1	Xtriage
Anisotropy	0.482	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.70 , -10.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	4258	wwPDB-VP
Average B, all atoms (Å ²)	991.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.66% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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	1.55	8/721 (1.1%)	1.33	11/1110 (1.0%)
2	E	1.65	11/552 (2.0%)	1.45	6/851 (0.7%)
3	D	1.47	7/548 (1.3%)	1.29	0/845
4	B	1.28	5/960 (0.5%)	1.34	10/1478 (0.7%)
5	F	1.30	5/819 (0.6%)	1.18	3/1265 (0.2%)
6	C	1.42	7/704 (1.0%)	1.35	4/1083 (0.4%)
7	M	1.41	6/467 (1.3%)	2.40	9/716 (1.3%)
All	All	1.43	49/4771 (1.0%)	1.46	43/7348 (0.6%)

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	112	DA	N9-C4	10.80	1.44	1.37
2	E	102	DT	C3'-O3'	10.04	1.57	1.44
6	C	125	DT	C1'-N1	8.92	1.60	1.49
7	M	102	DA	P-O5'	8.16	1.68	1.59
1	A	119	DA	C3'-O3'	8.09	1.54	1.44
6	C	115	DG	C3'-O3'	7.96	1.54	1.44
7	M	101	DT	C1'-N1	7.29	1.58	1.49
6	C	101	DA	N9-C4	7.23	1.42	1.37
2	E	104	DA	C3'-O3'	7.15	1.53	1.44
4	B	111	DT	C3'-O3'	7.11	1.53	1.44
3	D	103	DT	C1'-N1	6.97	1.58	1.49
6	C	103	DC	C3'-O3'	6.95	1.52	1.44
2	E	102	DT	C1'-N1	6.70	1.57	1.49
5	F	108	DA	N9-C4	6.66	1.41	1.37
7	M	116	DC	C1'-N1	6.64	1.57	1.49
1	A	112	DT	C3'-O3'	6.61	1.52	1.44
1	A	103	DA	C3'-O3'	6.47	1.52	1.44
1	A	107	DC	C1'-N1	6.43	1.57	1.49
2	E	106	DC	C3'-O3'	6.42	1.52	1.44
4	B	111	DT	C1'-N1	6.39	1.57	1.49
1	A	104	DG	C3'-O3'	-6.33	1.35	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	106	DG	C3'-O3'	6.27	1.52	1.44
2	E	104	DA	C5'-C4'	6.25	1.58	1.51
3	D	118	DT	C1'-N1	6.23	1.57	1.49
2	E	121	DC	C1'-N1	6.19	1.57	1.49
3	D	101	DT	C1'-N1	6.04	1.57	1.49
3	D	104	DG	C5'-C4'	6.00	1.57	1.51
1	A	103	DA	C5'-C4'	5.96	1.57	1.51
5	F	109	DC	C1'-N1	5.92	1.56	1.49
5	F	111	DT	C1'-N1	5.92	1.56	1.49
4	B	112	DA	C3'-O3'	5.92	1.51	1.44
7	M	106	DC	C1'-N1	5.91	1.56	1.49
6	C	103	DC	C5'-C4'	5.68	1.57	1.51
6	C	103	DC	C1'-N1	5.50	1.56	1.49
3	D	107	DT	C3'-O3'	5.39	1.50	1.44
1	A	131	DA	N9-C4	5.37	1.41	1.37
7	M	102	DA	O5'-C5'	5.36	1.55	1.42
2	E	108	DT	C3'-O3'	5.33	1.50	1.44
2	E	111	DT	C1'-N1	5.31	1.56	1.49
5	F	106	DT	C1'-N1	5.28	1.56	1.49
3	D	102	DG	C3'-O3'	5.26	1.50	1.44
3	D	104	DG	C3'-O3'	5.25	1.50	1.44
2	E	111	DT	C3'-O3'	5.19	1.50	1.44
5	F	132	DT	C1'-N1	5.12	1.55	1.49
7	M	106	DC	C3'-O3'	5.11	1.50	1.44
4	B	112	DA	C5'-C4'	5.08	1.56	1.51
2	E	112	DG	C3'-O3'	5.08	1.50	1.44
2	E	104	DA	P-O5'	5.05	1.64	1.59
6	C	105	DT	C3'-O3'	5.03	1.50	1.44

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	108	DA	P-O3'-C3'	-43.64	67.33	119.70
7	M	108	DA	OP1-P-O3'	-25.21	49.73	105.20
7	M	108	DA	OP2-P-O3'	14.50	137.11	105.20
4	B	121	DA	O3'-P-O5'	13.91	130.43	104.00
7	M	101	DT	O4'-C1'-N1	12.45	116.71	108.00
4	B	121	DA	OP2-P-O3'	-11.24	80.47	105.20
1	A	101	DC	O4'-C1'-N1	9.84	114.89	108.00
7	M	108	DA	O3'-P-O5'	8.98	121.06	104.00
1	A	104	DG	O4'-C4'-C3'	-7.01	101.69	104.50
6	C	121	DT	C1'-O4'-C4'	-7.00	103.11	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	132	DC	O4'-C1'-N1	6.97	112.88	108.00
2	E	113	DA	O4'-C4'-C3'	-6.96	101.72	104.50
4	B	110	DG	C1'-O4'-C4'	-6.45	103.65	110.10
4	B	110	DG	O4'-C1'-N9	6.11	112.28	108.00
6	C	112	DC	O4'-C4'-C3'	-6.02	102.09	104.50
5	F	132	DT	O4'-C1'-N1	6.01	112.20	108.00
7	M	101	DT	C3'-C2'-C1'	-5.87	95.46	102.50
1	A	106	DG	O4'-C1'-N9	5.82	112.07	108.00
1	A	101	DC	C3'-C2'-C1'	-5.71	95.65	102.50
1	A	107	DC	O4'-C1'-N1	5.71	111.99	108.00
7	M	109	DT	O4'-C1'-N1	5.69	111.99	108.00
7	M	109	DT	C1'-O4'-C4'	-5.68	104.42	110.10
5	F	129	DT	O4'-C4'-C3'	-5.66	102.24	104.50
2	E	108	DT	O4'-C1'-N1	5.65	111.96	108.00
6	C	111	DG	O4'-C1'-N9	5.63	111.94	108.00
1	A	101	DC	C1'-O4'-C4'	-5.54	104.56	110.10
2	E	122	DT	N3-C4-O4	5.53	123.22	119.90
2	E	124	DT	N3-C4-O4	5.43	123.16	119.90
1	A	112	DT	P-O3'-C3'	5.40	126.18	119.70
1	A	118	DA	C3'-C2'-C1'	-5.38	96.04	102.50
4	B	117	DC	O4'-C1'-N1	5.37	111.76	108.00
4	B	132	DC	C1'-O4'-C4'	-5.35	104.75	110.10
2	E	114	DG	C4'-C3'-C2'	-5.34	98.30	103.10
4	B	111	DT	O4'-C1'-N1	5.30	111.71	108.00
7	M	101	DT	O4'-C1'-C2'	-5.25	101.70	105.90
1	A	119	DA	P-O3'-C3'	5.22	125.97	119.70
1	A	124	DC	OP1-P-O3'	5.22	116.69	105.20
4	B	117	DC	C3'-C2'-C1'	-5.20	96.26	102.50
5	F	135	DG	O4'-C1'-N9	5.18	111.63	108.00
4	B	112	DA	C8-N9-C4	-5.07	103.77	105.80
2	E	114	DG	O4'-C4'-C3'	-5.05	102.48	104.50
6	C	116	DA	O4'-C1'-N9	5.05	111.53	108.00
1	A	112	DT	N3-C4-O4	5.04	122.93	119.90

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	640	0	344	56	0
2	E	494	0	274	32	0
3	D	492	0	274	30	0
4	B	857	0	472	44	0
5	F	729	0	395	34	0
6	C	628	0	349	32	0
7	M	418	0	236	41	0
All	All	4258	0	2344	242	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 38.

All (242) 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)
1:A:102:DA:H2	1:A:103:DA:H62	1.05	0.92
1:A:120:DG:H2''	1:A:121:DC:H5'	1.48	0.91
1:A:121:DC:N3	3:D:113:DG:N1	2.20	0.88
1:A:121:DC:O2	3:D:113:DG:N2	2.06	0.87
2:E:106:DC:O2	6:C:128:DG:N2	2.10	0.84
6:C:103:DC:H2''	6:C:104:DC:H5''	1.59	0.84
5:F:109:DC:H2'	5:F:110:DG:C8	2.14	0.83
1:A:103:DA:H2''	1:A:104:DG:H5''	1.58	0.83
4:B:110:DG:H2'	4:B:111:DT:C6	2.15	0.82
1:A:102:DA:H2	1:A:103:DA:N6	1.81	0.78
4:B:133:DT:H2'	4:B:134:DA:C8	2.19	0.77
7:M:110:DC:H2''	7:M:111:DA:C8	2.20	0.76
7:M:108:DA:H8	7:M:108:DA:H5''	1.50	0.76
6:C:109:DT:H2'	6:C:110:DG:O4'	1.87	0.75
5:F:111:DT:H2''	5:F:112:DA:N7	2.03	0.74
2:E:117:DG:H2''	2:E:118:DT:H5''	1.69	0.74
5:F:119:DG:H2'	5:F:120:DA:C8	2.23	0.74
3:D:117:DG:H2''	3:D:118:DT:H5''	1.72	0.71
5:F:130:DG:H3'	5:F:131:DG:H8	1.57	0.70
6:C:101:DA:H2'	6:C:102:DA:N7	2.08	0.69
7:M:114:DT:H1'	7:M:115:DG:C8	2.28	0.69
1:A:112:DT:H2''	1:A:113:DC:H5'	1.73	0.69
4:B:129:DC:H2''	4:B:130:DT:O4'	1.93	0.68
6:C:117:DC:H2''	6:C:118:DG:C8	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:120:DA:H2''	5:F:121:DG:C8	2.29	0.67
7:M:110:DC:H2''	7:M:111:DA:H8	1.58	0.67
7:M:108:DA:N6	7:M:109:DT:C4	2.63	0.67
6:C:102:DA:H1'	6:C:103:DC:OP2	1.96	0.66
5:F:130:DG:H3'	5:F:131:DG:C8	2.30	0.66
5:F:112:DA:H1'	5:F:113:DG:H5'	1.78	0.65
2:E:115:DT:H4'	2:E:116:DC:OP1	1.96	0.65
4:B:110:DG:H2'	4:B:111:DT:C5	2.31	0.65
4:B:102:DA:H2''	4:B:103:DG:C8	2.32	0.65
6:C:111:DG:H2''	6:C:112:DC:OP1	1.96	0.65
5:F:131:DG:H2''	5:F:132:DT:OP1	1.96	0.64
5:F:119:DG:H2'	5:F:120:DA:H8	1.61	0.63
6:C:122:DC:H1'	6:C:123:DA:C8	2.33	0.63
1:A:113:DC:H1'	1:A:114:DG:C5	2.33	0.63
6:C:112:DC:H2'	6:C:113:DA:C8	2.35	0.62
2:E:109:DA:H2''	2:E:110:DG:H5'	1.82	0.62
5:F:117:DC:H2''	5:F:118:DA:C8	2.34	0.62
3:D:116:DT:H2''	3:D:117:DG:C8	2.34	0.61
2:E:117:DG:H2''	2:E:118:DT:C5'	2.30	0.61
2:E:101:DT:C6	2:E:102:DT:H72	2.35	0.61
2:E:116:DC:H1'	2:E:117:DG:N7	2.16	0.61
3:D:116:DT:H2''	3:D:117:DG:H8	1.66	0.61
6:C:118:DG:H2''	6:C:119:DA:H5'	1.81	0.61
5:F:108:DA:H3'	5:F:109:DC:H4'	1.83	0.60
1:A:112:DT:H2''	1:A:113:DC:C5'	2.31	0.60
1:A:121:DC:O2	3:D:113:DG:C2	2.55	0.59
6:C:125:DT:H2''	6:C:126:DA:H5''	1.85	0.59
2:E:106:DC:C2	6:C:128:DG:N2	2.70	0.59
2:E:102:DT:H2''	2:E:103:DT:H5'	1.85	0.59
1:A:111:DA:H1'	1:A:112:DT:OP2	2.03	0.59
1:A:114:DG:H2''	1:A:115:DG:C8	2.38	0.58
4:B:104:DC:H2''	4:B:105:DA:H5'	1.85	0.58
4:B:114:DG:H2''	4:B:115:DG:N7	2.17	0.58
7:M:115:DG:H8	7:M:115:DG:OP2	1.86	0.58
3:D:117:DG:H2''	3:D:118:DT:O4'	2.04	0.58
7:M:115:DG:H1'	7:M:116:DC:H5'	1.86	0.57
2:E:101:DT:N1	2:E:102:DT:H72	2.19	0.57
2:E:119:DG:H1'	7:M:111:DA:H1'	1.85	0.57
5:F:130:DG:H2'	5:F:130:DG:N3	2.20	0.57
1:A:121:DC:C2	3:D:113:DG:N2	2.73	0.57
6:C:110:DG:H3'	6:C:111:DG:C8	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:120:DC:H1'	7:M:121:DG:C5	2.40	0.57
4:B:108:DC:H2'	4:B:109:DT:C6	2.40	0.56
7:M:121:DG:P	7:M:121:DG:C8	2.98	0.56
6:C:115:DG:C6	6:C:116:DA:C6	2.94	0.56
7:M:111:DA:OP2	7:M:111:DA:H2'	2.05	0.56
2:E:110:DG:H2'	2:E:111:DT:C6	2.42	0.55
4:B:107:DC:H2''	4:B:108:DC:H5''	1.88	0.55
4:B:123:DT:H2''	4:B:124:DC:H5'	1.88	0.55
1:A:120:DG:N2	3:D:115:DT:O2	2.40	0.55
4:B:117:DC:H2''	4:B:118:DA:N7	2.22	0.55
3:D:117:DG:H2''	3:D:118:DT:C5'	2.37	0.55
5:F:128:DG:H2''	5:F:129:DT:H5''	1.89	0.55
7:M:103:DC:H2''	7:M:104:DA:C8	2.42	0.54
7:M:109:DT:H2'	7:M:110:DC:C6	2.42	0.54
1:A:124:DC:H2''	1:A:125:DG:H5''	1.89	0.54
1:A:110:DG:H2''	1:A:111:DA:C8	2.43	0.54
7:M:112:DC:H2'	7:M:113:DC:C6	2.43	0.54
4:B:102:DA:H2''	4:B:103:DG:H8	1.72	0.54
1:A:102:DA:N3	1:A:103:DA:N7	2.56	0.53
5:F:109:DC:H2'	5:F:110:DG:H8	1.69	0.53
6:C:114:DG:H5''	6:C:114:DG:H8	1.73	0.53
4:B:133:DT:H2''	4:B:134:DA:O5'	2.08	0.53
5:F:113:DG:H2''	5:F:114:DT:C6	2.44	0.53
1:A:126:DC:H2''	1:A:127:DA:C8	2.44	0.53
1:A:107:DC:H2''	1:A:108:DC:H5''	1.91	0.52
2:E:118:DT:H2'	7:M:111:DA:OP2	2.08	0.52
4:B:131:DA:C6	5:F:115:DA:C2	2.98	0.52
7:M:114:DT:C2	7:M:115:DG:C5	2.97	0.52
5:F:114:DT:H2'	5:F:115:DA:H8	1.74	0.52
3:D:111:DT:H1'	3:D:112:DC:O5'	2.10	0.52
4:B:107:DC:C2'	4:B:108:DC:H5''	2.40	0.51
6:C:114:DG:H2''	6:C:115:DG:C8	2.44	0.51
3:D:101:DT:C2	3:D:102:DG:N7	2.77	0.51
7:M:101:DT:O4'	7:M:121:DG:H1'	2.10	0.51
4:B:127:DT:C2	4:B:128:DG:C8	2.99	0.51
6:C:110:DG:H2'	6:C:111:DG:C4	2.46	0.51
2:E:108:DT:H2''	2:E:109:DA:O5'	2.10	0.51
1:A:119:DA:C6	1:A:120:DG:C6	3.00	0.51
1:A:109:DT:H2'	1:A:110:DG:C8	2.46	0.50
4:B:128:DG:H2''	4:B:129:DC:H5''	1.92	0.50
1:A:121:DC:C2	3:D:113:DG:N1	2.79	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:106:DG:H1'	4:B:107:DC:O4'	2.12	0.50
6:C:113:DA:C2	7:M:115:DG:C2	3.00	0.50
4:B:120:DC:H2''	4:B:121:DA:H8	1.78	0.49
6:C:124:DC:H2''	6:C:125:DT:H5''	1.95	0.49
4:B:120:DC:H2''	4:B:121:DA:H5''	1.95	0.49
3:D:111:DT:C4	3:D:112:DC:N4	2.80	0.49
7:M:101:DT:H5'	7:M:121:DG:H2''	1.95	0.49
7:M:102:DA:H2''	7:M:103:DC:C6	2.48	0.49
1:A:111:DA:N9	1:A:112:DT:H72	2.28	0.48
1:A:125:DG:H2''	1:A:126:DC:C6	2.47	0.48
2:E:122:DT:H2''	2:E:123:DC:O5'	2.13	0.48
4:B:115:DG:C4	4:B:116:DA:N7	2.81	0.48
1:A:120:DG:N2	3:D:115:DT:C2	2.81	0.48
2:E:115:DT:C2	2:E:116:DC:C4	3.00	0.48
1:A:123:DA:H2''	1:A:124:DC:OP1	2.12	0.48
4:B:122:DG:H2''	4:B:123:DT:C5	2.49	0.48
1:A:124:DC:H4'	1:A:125:DG:OP1	2.13	0.48
7:M:114:DT:C2	7:M:115:DG:N7	2.82	0.48
3:D:118:DT:H2''	3:D:119:DG:OP1	2.12	0.48
5:F:128:DG:H2''	5:F:129:DT:O4'	2.13	0.48
2:E:104:DA:H2''	2:E:105:DG:C8	2.49	0.48
7:M:106:DC:C2	7:M:107:DG:C2	3.02	0.48
1:A:129:DG:H2''	1:A:130:DC:C5	2.48	0.48
4:B:130:DT:H2'	4:B:132:DC:C5	2.49	0.48
1:A:113:DC:H2''	1:A:114:DG:N7	2.29	0.47
5:F:130:DG:C2	5:F:131:DG:C5	3.01	0.47
1:A:131:DA:H5''	1:A:131:DA:H8	1.79	0.47
3:D:112:DC:C5	3:D:113:DG:C6	3.02	0.47
7:M:112:DC:P	7:M:113:DC:H5	2.38	0.47
2:E:101:DT:C2	2:E:102:DT:H72	2.49	0.47
3:D:101:DT:H2'	3:D:102:DG:H8	1.79	0.47
3:D:119:DG:N3	3:D:119:DG:H2'	2.30	0.47
2:E:118:DT:H2''	7:M:112:DC:C6	2.49	0.47
5:F:120:DA:H2''	5:F:121:DG:H8	1.77	0.47
7:M:119:DC:H2''	7:M:120:DC:C6	2.49	0.47
1:A:113:DC:C4	7:M:106:DC:N4	2.83	0.47
3:D:121:DC:H2''	3:D:122:DT:O5'	2.14	0.47
1:A:120:DG:C2	1:A:121:DC:C2	3.02	0.47
5:F:118:DA:H2''	5:F:119:DG:O5'	2.15	0.46
6:C:122:DC:C2	6:C:123:DA:C5	3.03	0.46
3:D:123:DG:N1	4:B:105:DA:C6	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:103:DG:C5	4:B:104:DC:C4	3.04	0.46
3:D:106:DT:H2''	3:D:107:DT:OP1	2.16	0.46
4:B:110:DG:C6	7:M:102:DA:N6	2.83	0.46
1:A:124:DC:C2	1:A:125:DG:C8	3.04	0.46
1:A:111:DA:C4	1:A:112:DT:H72	2.51	0.45
1:A:122:DG:H2''	1:A:123:DA:C8	2.51	0.45
1:A:130:DC:N3	1:A:131:DA:N6	2.64	0.45
2:E:116:DC:C2	2:E:117:DG:O6	2.70	0.45
3:D:109:DC:H2'	3:D:110:DG:C8	2.51	0.45
7:M:121:DG:P	7:M:121:DG:H8	2.39	0.45
2:E:109:DA:C4	2:E:110:DG:N7	2.85	0.45
4:B:113:DC:H2''	4:B:114:DG:N7	2.32	0.45
4:B:114:DG:N2	7:M:121:DG:N2	2.64	0.45
4:B:134:DA:H2''	4:B:135:DC:C5	2.52	0.45
5:F:114:DT:C2	5:F:115:DA:C8	3.04	0.45
1:A:114:DG:N2	7:M:107:DG:N2	2.65	0.45
4:B:136:DG:C2'	4:B:137:DT:H71	2.47	0.45
5:F:124:DT:H1'	5:F:125:DG:H5'	1.97	0.45
6:C:122:DC:H4'	6:C:123:DA:O5'	2.16	0.45
1:A:112:DT:H2''	1:A:113:DC:O5'	2.17	0.45
7:M:101:DT:N3	7:M:121:DG:C6	2.84	0.45
2:E:113:DA:O4'	2:E:113:DA:OP2	2.35	0.44
1:A:125:DG:H2''	1:A:126:DC:C5	2.52	0.44
1:A:128:DA:H2''	1:A:129:DG:N7	2.32	0.44
1:A:128:DA:H2''	1:A:129:DG:C8	2.51	0.44
2:E:119:DG:C5	7:M:111:DA:C5	3.05	0.44
6:C:102:DA:H2''	6:C:103:DC:OP1	2.17	0.44
6:C:106:DA:C4	6:C:107:DC:C5	3.06	0.44
2:E:107:DA:H2''	2:E:108:DT:O5'	2.17	0.44
3:D:111:DT:C2	3:D:112:DC:C5	3.05	0.44
7:M:109:DT:H2'	7:M:110:DC:C5	2.53	0.44
7:M:107:DG:H2''	7:M:108:DA:C8	2.53	0.44
4:B:115:DG:C4	4:B:116:DA:C8	3.05	0.44
3:D:120:DG:N2	4:B:108:DC:C2	2.86	0.44
4:B:116:DA:C5	4:B:117:DC:C4	3.05	0.44
2:E:119:DG:C6	7:M:111:DA:C6	3.06	0.43
3:D:120:DG:C2	4:B:108:DC:C2	3.06	0.43
4:B:126:DC:H2''	4:B:127:DT:C6	2.53	0.43
7:M:121:DG:H8	7:M:121:DG:O5'	2.01	0.43
5:F:102:DC:H2''	5:F:103:DT:OP1	2.18	0.43
5:F:133:DA:C4	5:F:134:DG:C8	3.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:DG:H5''	1:A:104:DG:H8	1.84	0.43
4:B:103:DG:C4	4:B:104:DC:C4	3.06	0.43
4:B:137:DT:C4	4:B:138:DC:C4	3.07	0.43
1:A:118:DA:C2	1:A:119:DA:C2	3.07	0.43
5:F:114:DT:C4	5:F:115:DA:C5	3.07	0.43
7:M:108:DA:H5''	7:M:108:DA:C8	2.41	0.43
1:A:118:DA:H2''	1:A:119:DA:C8	2.54	0.43
2:E:108:DT:C2	2:E:109:DA:C8	3.07	0.43
6:C:112:DC:OP1	6:C:112:DC:H6	2.02	0.43
6:C:118:DG:C6	6:C:119:DA:C6	3.07	0.43
1:A:119:DA:C5	1:A:120:DG:C5	3.07	0.43
7:M:117:DC:H2''	7:M:118:DA:H5'	1.99	0.43
7:M:106:DC:H2''	7:M:107:DG:C5	2.54	0.43
5:F:118:DA:H8	5:F:118:DA:OP1	2.02	0.42
5:F:119:DG:C6	5:F:120:DA:C6	3.07	0.42
3:D:113:DG:C5	3:D:114:DC:C4	3.07	0.42
4:B:115:DG:C2	4:B:116:DA:C5	3.07	0.42
6:C:115:DG:C5	6:C:116:DA:C5	3.07	0.42
1:A:131:DA:C2	3:D:104:DG:N2	2.87	0.42
5:F:103:DT:H2''	5:F:104:DG:O5'	2.19	0.42
4:B:141:DC:C2	4:B:142:DA:N7	2.88	0.42
1:A:125:DG:N3	1:A:126:DC:C4	2.88	0.42
2:E:114:DG:H1'	2:E:115:DT:C6	2.55	0.42
3:D:111:DT:C4	3:D:112:DC:C4	3.08	0.42
5:F:109:DC:H2''	5:F:110:DG:H5'	2.02	0.42
2:E:118:DT:H2''	7:M:112:DC:H6	1.82	0.42
4:B:102:DA:C2	4:B:103:DG:O6	2.73	0.41
2:E:105:DG:C5	6:C:128:DG:C6	3.08	0.41
5:F:102:DC:H1'	5:F:103:DT:OP2	2.19	0.41
7:M:121:DG:C8	7:M:121:DG:O5'	2.73	0.41
2:E:109:DA:H2''	2:E:110:DG:H8	1.85	0.41
4:B:104:DC:H2''	4:B:105:DA:C5'	2.48	0.41
5:F:118:DA:C6	5:F:119:DG:C6	3.09	0.41
1:A:115:DG:C4	1:A:116:DA:C8	3.08	0.41
6:C:121:DT:H2'	6:C:122:DC:H2'	2.01	0.41
6:C:108:DC:H2'	6:C:109:DT:C6	2.55	0.41
6:C:113:DA:H2''	6:C:114:DG:C5	2.56	0.41
1:A:104:DG:H2''	1:A:105:DA:H8	1.86	0.41
1:A:108:DC:C2	2:E:120:DG:N2	2.88	0.41
2:E:113:DA:N3	2:E:114:DG:N7	2.68	0.41
5:F:127:DT:H2'	5:F:128:DG:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:DA:C2	1:A:120:DG:C2	3.09	0.41
4:B:134:DA:H2''	4:B:135:DC:H5	1.85	0.41
1:A:129:DG:C4	1:A:130:DC:C4	3.09	0.41
6:C:102:DA:H8	6:C:102:DA:OP2	2.04	0.41
4:B:103:DG:C5	4:B:104:DC:N4	2.89	0.40
1:A:104:DG:H2'	1:A:104:DG:H5'	1.91	0.40
3:D:103:DT:C4	3:D:104:DG:C6	3.09	0.40
1:A:116:DA:C4	1:A:117:DC:C5	3.09	0.40
4:B:132:DC:H2''	4:B:133:DT:OP1	2.20	0.40
1:A:123:DA:H1'	1:A:124:DC:OP2	2.22	0.40
1:A:129:DG:H2''	1:A:130:DC:C6	2.57	0.40
5:F:114:DT:H2'	5:F:115:DA:C8	2.53	0.40
6:C:105:DT:H2''	6:C:106:DA:C1'	2.51	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 [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.