



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 22, 2022 – 02:06 PM EDT

PDB ID : 7U3Y  
Title : [L233] Self-assembling tensegrity triangle with two turns, three turns and three 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 : 6.06 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

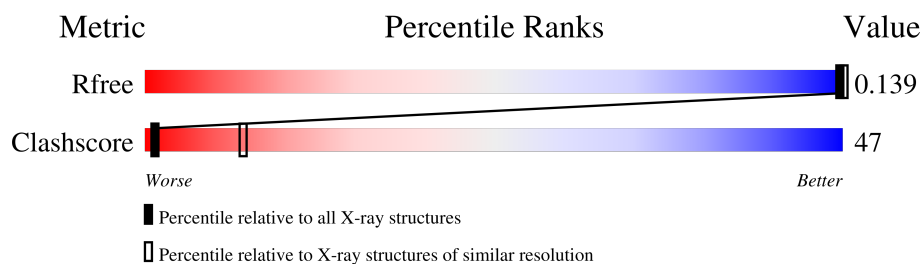
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*





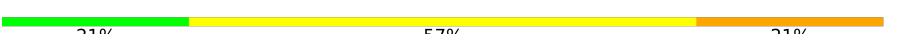




The reported resolution of this entry is 6.06 Å.

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 (8.20-3.88)
Clashscore	141614	1050 (8.20-3.90)

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	21	
2	E	14	
3	D	14	
4	B	21	
5	F	14	
6	C	21	
7	M	21	
8	U	10	
9	V	10	

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Mol	Chain	Length	Quality of chain
10	X	10	 60%40%
11	Y	10	 20%80%

## 2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 3379 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(\*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
1	A	21	Total	C	N	O	P	0	0	0
			430	204	87	119	20			

- 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(\*GP\*AP\*TP\*CP\*TP\*TP\*GP\*TP\*GP\*GP\*CP\*TP\*GP\*C)-3').

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	14	Total	C	N	O	P	0	0	0
			291	139	56	83	13			

- 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	C	N	O	P	0	0	0
			426	203	82	121	20			

- 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	C	N	O	P	0	0	0
			421	200	76	124	21			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	U	10	Total	C	N	O	P	0	0	0
			203	96	36	61	10			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	V	10	Total	C	N	O	P	0	0	0
			203	97	38	59	9			

- Molecule 10 is a DNA chain called DNA (5'-D(P\*GP\*TP\*CP\*TP\*AP\*TP\*GP\*CP\*TP\*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	10	Total	C	N	O	P	0	0	0
			204	98	34	62	10			

- Molecule 11 is a DNA chain called DNA (5'-D(\*CP\*TP\*TP\*AP\*GP\*CP\*AP\*TP\*AP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	Y	10	Total	C	N	O	P	0	0	0
			202	98	37	58	9			

### 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.

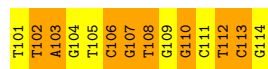
- Molecule 1: DNA (5'-D(\*CP\*AP\*CP\*GP\*AP\*GP\*CP\*CP\*TP\*GP\*AP\*TP\*CP\*GP\*GP\*AP\*CP\*AP\*AP\*GP\*A)-3')

Chain A: 




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

Chain E: 




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

Chain D: 



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

Chain B: 



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

Chain F: 




- 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')

Chain C:  10% 48% 43%

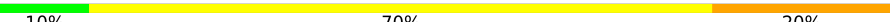
A101  
A102  
C103  
C104  
T105  
A106  
C107  
C108  
T109  
G110  
G111  
C112  
A113  
G114  
G115  
A116  
C117  
G118  
A119  
C120  
T121

- 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')

Chain M:  10% 62% 29%

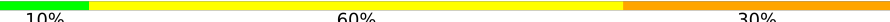
T101  
C102  
A103  
C104  
C105  
T106  
G107  
C108  
C109  
A110  
C111  
G112  
G113  
T114  
A115  
G116  
A117  
C118  
C119  
G120  
A121

- Molecule 8: DNA (5'-D(P\*TP\*CP\*CP\*GP\*CP\*TP\*AP\*GP\*CP\*G)-3')

Chain U:  10% 70% 20%


T112  
C113  
G114  
G115  
C116  
T117  
A118  
G119  
C120  
G121

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

Chain V:  10% 60% 30%

T103  
G102  
C103  
G104  
G105  
T106  
A107  
G108  
C109  
G110

- Molecule 10: DNA (5'-D(P\*GP\*TP\*CP\*TP\*AP\*TP\*GP\*CP\*TP\*A)-3')

Chain X:  60% 40%

G112  
T113  
C114  
T115  
A116  
T117  
G118  
C119  
T120  
A121

- Molecule 11: DNA (5'-D(\*CP\*TP\*TP\*AP\*GP\*CP\*AP\*TP\*AP\*G)-3')

Chain Y:  20% 80%

C101  
T102  
T103  
A104  
G105  
C106  
A107  
T108  
A109  
G110

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.14Å 99.59Å 100.16Å 104.30° 103.01° 98.11°	Depositor
Resolution (Å)	37.92 – 6.06 94.39 – 5.93	Depositor EDS
% Data completeness (in resolution range)	61.3 (37.92-6.06) 51.7 (94.39-5.93)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.41 (at 5.76Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, $R_{free}$	0.091 , 0.138 0.090 , 0.139	Depositor DCC
$R_{free}$ test set	182 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	310.4	Xtriage
Anisotropy	0.432	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.88 , -10.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.78	EDS
Total number of atoms	3379	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	628.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.79% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality [i](#)

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

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	1.87	13/484 (2.7%)	1.53	8/745 (1.1%)
2	E	1.66	4/318 (1.3%)	1.66	9/490 (1.8%)
3	D	1.64	5/318 (1.6%)	1.65	10/490 (2.0%)
4	B	1.40	5/482 (1.0%)	1.28	6/742 (0.8%)
5	F	1.40	3/327 (0.9%)	1.40	1/505 (0.2%)
6	C	1.67	7/478 (1.5%)	1.52	12/735 (1.6%)
7	M	1.57	3/470 (0.6%)	1.52	9/720 (1.2%)
8	U	1.32	0/226	1.39	3/346 (0.9%)
9	V	1.29	2/227 (0.9%)	1.35	2/349 (0.6%)
10	X	1.52	2/227 (0.9%)	1.43	3/348 (0.9%)
11	Y	1.02	0/226	1.17	0/347
All	All	1.55	44/3783 (1.2%)	1.46	63/5817 (1.1%)

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	108	DC	C1'-N1	12.12	1.65	1.49
1	A	112	DT	C1'-N1	11.30	1.64	1.49
1	A	109	DT	C1'-N1	10.43	1.62	1.49
7	M	113	DG	C3'-O3'	10.06	1.57	1.44
10	X	113	DT	C1'-N1	8.73	1.60	1.49
6	C	107	DC	C1'-N1	8.31	1.60	1.49
1	A	111	DA	C3'-O3'	8.12	1.54	1.44
5	F	111	DT	C3'-O3'	7.63	1.53	1.44
7	M	120	DG	C3'-O3'	7.56	1.53	1.44
3	D	108	DT	C3'-O3'	7.44	1.53	1.44
1	A	112	DT	C5'-C4'	7.28	1.59	1.51
1	A	111	DA	N9-C4	7.25	1.42	1.37
4	B	107	DC	C1'-N1	7.14	1.58	1.49
3	D	108	DT	C1'-N1	7.07	1.58	1.49
1	A	108	DC	C3'-O3'	6.95	1.52	1.44
4	B	109	DT	C3'-O3'	-6.74	1.35	1.44
4	B	117	DC	C3'-O3'	-6.68	1.35	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	120	DC	C3'-O3'	-6.66	1.35	1.44
3	D	103	DT	C3'-O3'	6.65	1.52	1.44
2	E	108	DT	C1'-N1	6.63	1.57	1.49
2	E	112	DT	C3'-O3'	6.59	1.52	1.44
1	A	115	DG	C3'-O3'	6.48	1.52	1.44
1	A	107	DC	C1'-N1	6.39	1.57	1.49
10	X	115	DT	C3'-O3'	6.36	1.52	1.44
6	C	117	DC	C3'-O3'	-6.35	1.35	1.44
1	A	112	DT	C3'-O3'	6.33	1.52	1.44
1	A	105	DA	C3'-O3'	6.30	1.52	1.44
9	V	108	DG	C3'-O3'	6.30	1.52	1.44
4	B	111	DT	C1'-N1	6.27	1.57	1.49
9	V	107	DA	N9-C4	-6.25	1.34	1.37
6	C	111	DG	N9-C4	6.24	1.43	1.38
2	E	113	DC	C3'-O3'	-5.98	1.36	1.44
2	E	106	DC	C3'-O3'	5.69	1.51	1.44
6	C	115	DG	C3'-O3'	5.61	1.51	1.44
1	A	104	DG	C3'-O3'	-5.24	1.37	1.44
6	C	112	DC	C5'-C4'	5.23	1.57	1.51
3	D	113	DG	C3'-O3'	-5.21	1.37	1.44
4	B	104	DC	C3'-O3'	-5.20	1.37	1.44
5	F	112	DA	C2'-C1'	-5.19	1.47	1.52
3	D	111	DC	C5'-C4'	5.19	1.57	1.51
1	A	119	DA	C3'-O3'	5.15	1.50	1.44
5	F	113	DG	C3'-O3'	-5.15	1.37	1.44
1	A	120	DG	C3'-O3'	-5.07	1.37	1.44
6	C	116	DA	C3'-O3'	-5.00	1.37	1.44

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	112	DT	O5'-P-OP1	-11.03	95.78	105.70
3	D	111	DC	O5'-P-OP1	-8.92	97.67	105.70
7	M	114	DT	O4'-C1'-N1	8.75	114.13	108.00
6	C	107	DC	O4'-C1'-N1	8.18	113.72	108.00
2	E	103	DA	O5'-P-OP2	-8.08	98.43	105.70
10	X	114	DC	O4'-C4'-C3'	-7.95	101.23	106.00
7	M	108	DC	O4'-C1'-N1	7.94	113.56	108.00
1	A	111	DA	O4'-C1'-N9	7.90	113.53	108.00
2	E	107	DG	OP1-P-OP2	-7.89	107.76	119.60
6	C	109	DT	O4'-C4'-C3'	-7.06	101.68	104.50
6	C	109	DT	C3'-C2'-C1'	-6.64	94.53	102.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	112	DT	O4'-C1'-N1	6.61	112.63	108.00
7	M	113	DG	P-O3'-C3'	6.56	127.58	119.70
7	M	110	DA	O4'-C1'-N9	6.44	112.51	108.00
8	U	115	DG	O4'-C1'-N9	6.42	112.50	108.00
6	C	114	DG	O5'-P-OP2	-6.42	99.92	105.70
3	D	104	DC	OP1-P-O3'	6.26	118.97	105.20
2	E	108	DT	O4'-C1'-N1	5.98	112.19	108.00
9	V	103	DC	O4'-C4'-C3'	-5.98	102.11	104.50
3	D	110	DG	O5'-P-OP1	-5.97	100.33	105.70
1	A	112	DT	OP1-P-OP2	5.95	128.53	119.60
3	D	108	DT	O4'-C1'-N1	5.93	112.15	108.00
3	D	103	DT	OP1-P-O3'	5.88	118.14	105.20
3	D	103	DT	P-O3'-C3'	5.76	126.62	119.70
6	C	107	DC	C1'-O4'-C4'	-5.73	104.37	110.10
4	B	112	DA	O5'-P-OP1	-5.71	100.56	105.70
8	U	115	DG	OP1-P-OP2	-5.69	111.06	119.60
2	E	107	DG	O5'-P-OP2	5.67	117.50	110.70
6	C	111	DG	C8-N9-C4	-5.63	104.15	106.40
2	E	104	DG	P-O3'-C3'	5.62	126.44	119.70
8	U	114	DC	OP2-P-O3'	5.55	117.42	105.20
10	X	113	DT	O4'-C1'-N1	5.47	111.83	108.00
4	B	117	DC	C3'-C2'-C1'	-5.46	95.94	102.50
4	B	107	DC	O4'-C1'-N1	5.43	111.80	108.00
2	E	110	DG	OP1-P-OP2	-5.42	111.47	119.60
7	M	117	DA	O4'-C4'-C3'	-5.42	102.33	104.50
2	E	112	DT	P-O3'-C3'	5.34	126.11	119.70
6	C	117	DC	C3'-C2'-C1'	-5.33	96.10	102.50
7	M	117	DA	C4'-C3'-C2'	-5.33	98.30	103.10
7	M	101	DT	C1'-O4'-C4'	-5.32	104.78	110.10
4	B	106	DG	O4'-C1'-N9	5.32	111.72	108.00
3	D	112	DT	O5'-P-OP2	-5.30	100.93	105.70
1	A	102	DA	O4'-C1'-N9	5.29	111.70	108.00
5	F	113	DG	O5'-P-OP2	-5.29	100.94	105.70
4	B	111	DT	N3-C4-O4	5.28	123.07	119.90
2	E	103	DA	OP1-P-OP2	5.24	127.46	119.60
3	D	108	DT	P-O3'-C3'	5.24	125.98	119.70
7	M	120	DG	P-O3'-C3'	5.24	125.98	119.70
1	A	107	DC	O4'-C1'-N1	5.21	111.65	108.00
4	B	112	DA	OP1-P-OP2	5.20	127.39	119.60
1	A	111	DA	O3'-P-O5'	5.19	113.87	104.00
9	V	105	DC	O4'-C1'-N1	5.19	111.63	108.00
6	C	113	DA	O4'-C4'-C3'	-5.15	102.44	104.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	114	DG	O5'-P-OP1	5.14	116.87	110.70
1	A	112	DT	P-O3'-C3'	5.12	125.84	119.70
6	C	109	DT	C4'-C3'-C2'	-5.09	98.52	103.10
6	C	109	DT	N3-C4-O4	5.08	122.95	119.90
2	E	102	DT	C5-C4-O4	-5.07	121.35	124.90
6	C	105	DT	C5-C4-O4	-5.04	121.37	124.90
3	D	113	DG	O5'-P-OP1	5.04	116.74	110.70
10	X	121	DA	O4'-C1'-N9	5.03	111.52	108.00
7	M	108	DC	O4'-C1'-C2'	-5.01	101.89	105.90
3	D	113	DG	O5'-P-OP2	-5.01	101.19	105.70

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	430	0	235	35	0
2	E	285	0	161	32	1
3	D	285	0	161	21	0
4	B	429	0	236	41	0
5	F	291	0	160	31	0
6	C	426	0	236	32	1
7	M	421	0	235	35	0
8	U	203	0	113	11	0
9	V	203	0	114	12	0
10	X	204	0	115	9	0
11	Y	202	0	115	11	0
All	All	3379	0	1881	246	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 47.

All (246) 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)
5:F:109:DG:H5'	7:M:111:DC:H5''	1.40	1.01
8:U:113:DC:H1'	8:U:114:DC:H5	1.32	0.95
7:M:108:DC:H2''	7:M:109:DC:C5	2.10	0.86
9:V:109:DC:H2'	9:V:110:DG:C8	2.12	0.85
1:A:113:DC:H2''	1:A:114:DG:C5	2.11	0.84
8:U:113:DC:H1'	8:U:114:DC:C5	2.11	0.84
6:C:113:DA:H1'	6:C:114:DG:N7	1.93	0.84
10:X:115:DT:H2'	10:X:116:DA:C8	2.16	0.80
9:V:108:DG:H2''	9:V:109:DC:H5'	1.64	0.80
2:E:105:DT:H1'	2:E:106:DC:H5'	1.64	0.79
4:B:114:DG:H2''	4:B:115:DG:N7	1.98	0.79
6:C:113:DA:H1'	6:C:114:DG:C5	2.18	0.79
6:C:101:DA:N6	6:C:102:DA:N1	2.32	0.78
5:F:109:DG:H5'	7:M:111:DC:C5'	2.13	0.77
9:V:108:DG:H2'	9:V:109:DC:C6	2.19	0.77
5:F:101:DA:H5''	5:F:102:DC:H5	1.50	0.76
4:B:110:DG:H2'	4:B:111:DT:C6	2.21	0.76
4:B:118:DA:H8	4:B:118:DA:OP2	1.70	0.75
6:C:104:DC:H6	6:C:104:DC:H5''	1.51	0.74
11:Y:108:DT:H2'	11:Y:109:DA:C8	2.23	0.74
3:D:104:DC:H4'	3:D:105:DT:OP1	1.89	0.72
7:M:112:DC:H2''	7:M:113:DG:N7	2.05	0.72
1:A:104:DG:H2''	1:A:105:DA:C8	2.25	0.71
6:C:118:DG:H8	6:C:118:DG:OP2	1.72	0.71
4:B:120:DC:H2''	4:B:121:DA:C8	2.26	0.71
11:Y:101:DC:H3'	11:Y:102:DT:H72	1.74	0.70
1:A:115:DG:H2''	1:A:116:DA:O5'	1.91	0.70
2:E:107:DG:H2''	2:E:108:DT:H5''	1.73	0.69
4:B:110:DG:H2'	4:B:111:DT:C5	2.26	0.69
11:Y:103:DT:H2''	11:Y:104:DA:C8	2.27	0.68
2:E:102:DT:H2''	2:E:103:DA:OP1	1.92	0.68
7:M:114:DT:H2''	7:M:115:DA:OP2	1.94	0.67
2:E:112:DT:H2''	2:E:113:DC:H5'	1.77	0.67
4:B:102:DG:H8	4:B:102:DG:OP2	1.78	0.67
5:F:108:DT:H2'	7:M:111:DC:O4'	1.95	0.67
8:U:114:DC:H2''	8:U:115:DG:OP2	1.93	0.66
9:V:104:DG:H1'	9:V:105:DC:H5'	1.77	0.66
9:V:105:DC:H2''	9:V:106:DT:H71	1.79	0.65
4:B:112:DA:H8	4:B:112:DA:P	2.19	0.65
4:B:103:DG:H2''	4:B:104:DC:H5''	1.79	0.65
7:M:119:DC:H2''	7:M:120:DG:C6	2.32	0.64
1:A:108:DC:H6	1:A:108:DC:H5''	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:118:DG:OP2	6:C:118:DG:H2'	1.98	0.64
2:E:106:DC:C2'	2:E:107:DG:C8	2.82	0.63
4:B:111:DT:H2''	4:B:112:DA:C8	2.34	0.63
4:B:101:DA:C8	10:X:121:DA:H1'	2.35	0.62
5:F:113:DG:H2''	5:F:114:DG:H8	1.64	0.62
6:C:109:DT:H2'	6:C:110:DG:O4'	2.00	0.62
1:A:114:DG:H1'	1:A:115:DG:N7	2.15	0.62
3:D:112:DT:H3'	3:D:113:DG:C8	2.35	0.62
4:B:114:DG:H2''	4:B:115:DG:C8	2.34	0.61
1:A:104:DG:H2''	1:A:105:DA:H8	1.63	0.61
3:D:110:DG:H2'	3:D:110:DG:OP2	1.99	0.61
5:F:112:DA:H3'	5:F:113:DG:H8	1.66	0.61
2:E:110:DG:OP2	2:E:110:DG:H8	1.84	0.60
5:F:112:DA:C2'	5:F:113:DG:H5'	2.32	0.60
5:F:112:DA:H2''	5:F:113:DG:OP1	2.00	0.60
1:A:108:DC:H5''	1:A:108:DC:C6	2.36	0.60
3:D:108:DT:H2'	7:M:118:DC:C6	2.35	0.60
3:D:110:DG:H1'	3:D:111:DC:OP1	2.02	0.60
6:C:110:DG:H5''	6:C:111:DG:N7	2.16	0.60
5:F:108:DT:H4'	5:F:109:DG:OP2	2.02	0.60
11:Y:107:DA:H2''	11:Y:108:DT:H71	1.83	0.59
2:E:102:DT:H1'	2:E:103:DA:OP2	2.03	0.59
8:U:117:DT:H2''	8:U:118:DA:C8	2.38	0.59
4:B:107:DC:H2''	4:B:108:DC:C6	2.37	0.59
7:M:112:DC:H2''	7:M:113:DG:C5	2.37	0.58
5:F:109:DG:C5'	7:M:111:DC:H5''	2.26	0.58
7:M:106:DT:H2''	7:M:107:DG:OP2	2.02	0.58
5:F:112:DA:H3'	5:F:113:DG:C8	2.37	0.58
4:B:112:DA:H2''	4:B:113:DC:O5'	2.03	0.57
5:F:107:DG:H2''	5:F:108:DT:O4'	2.04	0.57
2:E:105:DT:H1'	2:E:106:DC:C5'	2.33	0.57
9:V:108:DG:H2'	9:V:109:DC:H6	1.68	0.57
4:B:113:DC:H2''	4:B:114:DG:C5	2.39	0.57
4:B:112:DA:H8	4:B:112:DA:OP1	1.88	0.56
2:E:106:DC:H5'	2:E:106:DC:C6	2.41	0.56
4:B:105:DA:C6	4:B:106:DG:C6	2.94	0.56
4:B:105:DA:C8	4:B:105:DA:H5'	2.40	0.56
7:M:113:DG:H1'	7:M:114:DT:O5'	2.05	0.56
5:F:111:DT:H2''	5:F:112:DA:O5'	2.06	0.56
10:X:119:DC:H2''	10:X:120:DT:O5'	2.07	0.55
1:A:107:DC:H2'	1:A:108:DC:C5	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:102:DT:H1'	11:Y:103:DT:OP2	2.07	0.55
1:A:112:DT:H2''	1:A:113:DC:O5'	2.07	0.55
4:B:115:DG:H1'	4:B:116:DA:N7	2.22	0.55
9:V:108:DG:H2''	9:V:109:DC:C5'	2.36	0.54
4:B:115:DG:H1'	4:B:116:DA:C8	2.42	0.54
2:E:113:DC:H2''	2:E:114:DG:H8	1.72	0.54
6:C:111:DG:H2''	6:C:112:DC:OP1	2.05	0.54
7:M:104:DC:H2''	7:M:105:DC:C6	2.43	0.54
2:E:101:DT:H2''	2:E:102:DT:O5'	2.08	0.54
3:D:108:DT:H5'	7:M:117:DA:H2''	1.90	0.54
4:B:120:DC:H2''	4:B:121:DA:H8	1.70	0.54
5:F:101:DA:H5''	5:F:102:DC:C5	2.37	0.53
2:E:110:DG:OP2	2:E:110:DG:H2'	2.08	0.53
4:B:104:DC:H2''	4:B:105:DA:C8	2.43	0.53
7:M:107:DG:H1'	7:M:108:DC:H5'	1.91	0.53
1:A:110:DG:H2'	1:A:111:DA:C8	2.43	0.53
6:C:104:DC:H5''	6:C:104:DC:C6	2.39	0.53
2:E:108:DT:H2''	7:M:104:DC:O4'	2.09	0.53
5:F:107:DG:C2	5:F:108:DT:C2	2.97	0.53
3:D:110:DG:H1'	3:D:111:DC:P	2.49	0.52
11:Y:101:DC:H3'	11:Y:102:DT:C7	2.38	0.52
8:U:115:DG:H4'	8:U:116:DC:OP1	2.10	0.52
1:A:101:DC:N4	1:A:102:DA:H62	2.08	0.52
2:E:110:DG:OP2	2:E:110:DG:C8	2.62	0.52
1:A:110:DG:H3'	1:A:111:DA:C8	2.45	0.51
5:F:112:DA:H2''	5:F:113:DG:H5'	1.92	0.51
5:F:113:DG:H2''	5:F:114:DG:C8	2.44	0.51
9:V:107:DA:C6	9:V:108:DG:C6	2.99	0.51
9:V:108:DG:C2	9:V:109:DC:C2	2.99	0.51
5:F:112:DA:H2'	5:F:113:DG:H5'	1.93	0.51
1:A:110:DG:H3'	1:A:111:DA:H8	1.76	0.50
2:E:105:DT:C1'	2:E:106:DC:H5'	2.38	0.50
4:B:115:DG:C2	4:B:116:DA:C6	2.98	0.50
11:Y:101:DC:H2'	11:Y:102:DT:C6	2.46	0.50
7:M:114:DT:H1'	7:M:115:DA:O5'	2.11	0.50
2:E:107:DG:C2	6:C:118:DG:N2	2.79	0.49
1:A:107:DC:H2'	1:A:108:DC:H5	1.76	0.49
2:E:109:DG:O5'	7:M:104:DC:H5'	2.12	0.49
4:B:102:DG:OP2	4:B:102:DG:C8	2.62	0.49
8:U:118:DA:H2''	8:U:119:DG:C8	2.48	0.49
3:D:111:DC:H2''	3:D:112:DT:O4'	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:101:DA:N6	6:C:102:DA:C2	2.80	0.49
7:M:102:DC:N4	7:M:103:DA:N6	2.60	0.49
4:B:111:DT:H2''	4:B:112:DA:H8	1.75	0.49
10:X:120:DT:H2'	10:X:121:DA:C8	2.48	0.49
2:E:103:DA:O4'	2:E:103:DA:P	2.72	0.48
2:E:107:DG:C2'	2:E:108:DT:H5''	2.43	0.48
9:V:102:DG:OP2	9:V:102:DG:H8	1.96	0.48
6:C:104:DC:H2''	6:C:105:DT:H5'	1.95	0.48
6:C:110:DG:H3'	6:C:111:DG:C8	2.48	0.48
5:F:113:DG:C6	5:F:114:DG:C6	3.01	0.48
2:E:106:DC:H2'	2:E:107:DG:C8	2.49	0.48
9:V:105:DC:H2''	9:V:106:DT:C7	2.42	0.48
1:A:102:DA:H2''	1:A:103:DC:OP2	2.13	0.48
1:A:113:DC:H2''	1:A:114:DG:N7	2.28	0.48
6:C:101:DA:N6	6:C:102:DA:C6	2.80	0.48
6:C:113:DA:C2	6:C:114:DG:C2	3.02	0.48
7:M:118:DC:OP2	7:M:119:DC:N4	2.47	0.48
5:F:111:DT:C2	5:F:112:DA:C8	3.02	0.48
10:X:113:DT:H1'	10:X:114:DC:C5	2.49	0.47
3:D:110:DG:N2	4:B:108:DC:C2	2.83	0.47
8:U:115:DG:C4	8:U:116:DC:C5	3.01	0.47
6:C:119:DA:C2	6:C:120:DC:C2	3.03	0.47
3:D:108:DT:H3'	7:M:117:DA:H2''	1.96	0.47
4:B:115:DG:H4'	4:B:116:DA:OP1	2.14	0.47
2:E:112:DT:H2'	2:E:113:DC:O4'	2.14	0.47
1:A:112:DT:H2''	1:A:113:DC:C5'	2.45	0.47
3:D:104:DC:H2''	3:D:105:DT:H71	1.97	0.47
4:B:113:DC:H2''	4:B:114:DG:N7	2.29	0.47
1:A:119:DA:H2''	1:A:120:DG:C8	2.50	0.47
4:B:102:DG:H2''	4:B:103:DG:OP1	2.14	0.47
5:F:106:DT:N3	5:F:107:DG:C5	2.83	0.47
7:M:107:DG:H1'	7:M:108:DC:O4'	2.14	0.46
5:F:101:DA:N3	5:F:101:DA:H2'	2.30	0.46
4:B:112:DA:C8	4:B:112:DA:OP1	2.68	0.46
6:C:108:DC:H5''	6:C:108:DC:H6	1.80	0.46
7:M:118:DC:H2'	7:M:119:DC:C4	2.51	0.46
2:E:113:DC:H2''	2:E:114:DG:C8	2.51	0.45
1:A:106:DG:H2''	1:A:107:DC:O5'	2.15	0.45
5:F:110:DG:C2'	5:F:111:DT:H71	2.47	0.45
6:C:112:DC:H2''	6:C:113:DA:C8	2.50	0.45
2:E:108:DT:O3'	7:M:104:DC:H5'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:107:DG:H2''	3:D:108:DT:O4'	2.17	0.45
4:B:104:DC:H2''	4:B:105:DA:H5'	1.99	0.45
1:A:112:DT:H2''	1:A:113:DC:H5'	1.99	0.45
2:E:106:DC:H2''	2:E:107:DG:C8	2.52	0.45
6:C:109:DT:H3'	6:C:109:DT:C6	2.52	0.45
5:F:101:DA:H3'	5:F:102:DC:C6	2.51	0.45
7:M:119:DC:H2''	7:M:120:DG:C5	2.50	0.45
8:U:115:DG:C2	8:U:116:DC:C2	3.05	0.45
1:A:108:DC:C2	2:E:110:DG:N2	2.85	0.45
1:A:108:DC:C4	2:E:110:DG:N2	2.85	0.45
6:C:118:DG:C2	6:C:119:DA:C2	3.05	0.45
4:B:119:DT:C4	4:B:120:DC:N4	2.86	0.44
1:A:111:DA:H2'	1:A:112:DT:H71	1.99	0.44
1:A:109:DT:H2'	1:A:110:DG:H1'	2.00	0.44
1:A:111:DA:C5	1:A:112:DT:H73	2.52	0.44
2:E:109:DG:N7	7:M:103:DA:C4	2.86	0.44
3:D:114:DC:H2''	11:Y:101:DC:O4'	2.17	0.44
4:B:103:DG:C5	4:B:104:DC:C4	3.05	0.44
1:A:106:DG:N3	1:A:107:DC:H1'	2.33	0.44
1:A:108:DC:N3	2:E:110:DG:N2	2.65	0.44
5:F:107:DG:C6	5:F:108:DT:C4	3.05	0.44
5:F:113:DG:C4	5:F:114:DG:N7	2.85	0.43
6:C:118:DG:H2'	6:C:118:DG:P	2.58	0.43
6:C:119:DA:H2''	6:C:120:DC:O5'	2.18	0.43
4:B:102:DG:N2	11:Y:102:DT:C2	2.86	0.43
6:C:102:DA:H2''	6:C:103:DC:OP1	2.18	0.43
7:M:118:DC:H2'	7:M:119:DC:C5	2.53	0.43
7:M:101:DT:O2	7:M:102:DC:C2	2.72	0.43
3:D:113:DG:H1'	3:D:114:DC:C6	2.53	0.43
10:X:112:DG:H2''	10:X:113:DT:O4'	2.19	0.43
3:D:112:DT:H2''	3:D:113:DG:OP1	2.16	0.43
6:C:112:DC:OP1	6:C:112:DC:H6	2.02	0.43
6:C:113:DA:C4	6:C:114:DG:C6	3.06	0.43
8:U:112:DT:H6	8:U:112:DT:H2'	1.73	0.43
10:X:118:DG:H2''	10:X:119:DC:C6	2.54	0.43
5:F:107:DG:C5	5:F:108:DT:C4	3.06	0.43
3:D:113:DG:H4'	3:D:114:DC:OP1	2.18	0.42
6:C:116:DA:C5	6:C:117:DC:C4	3.07	0.42
1:A:107:DC:C2	1:A:108:DC:C5	3.07	0.42
1:A:117:DC:C2	1:A:118:DA:C5	3.08	0.42
4:B:107:DC:H2''	4:B:108:DC:H6	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:110:DG:H2''	5:F:111:DT:H71	2.00	0.42
6:C:103:DC:C4	6:C:104:DC:N4	2.87	0.42
11:Y:104:DA:H4'	11:Y:105:DG:H5'	2.00	0.42
7:M:108:DC:H2''	7:M:109:DC:C6	2.50	0.42
3:D:103:DT:O4'	3:D:103:DT:OP1	2.38	0.42
4:B:118:DA:OP2	4:B:118:DA:C8	2.61	0.42
6:C:105:DT:H6	6:C:105:DT:H2'	1.72	0.42
7:M:106:DT:H6	7:M:106:DT:H2'	1.62	0.42
10:X:116:DA:H2''	10:X:117:DT:O5'	2.19	0.42
2:E:105:DT:H2''	2:E:106:DC:H5'	2.02	0.42
2:E:111:DC:H2''	2:E:112:DT:O5'	2.20	0.42
6:C:113:DA:C6	7:M:105:DC:C4	3.08	0.42
1:A:106:DG:N2	2:E:112:DT:O2	2.53	0.42
4:B:119:DT:C2	4:B:120:DC:C4	3.08	0.42
8:U:119:DG:H4'	8:U:120:DC:OP1	2.19	0.42
11:Y:104:DA:H1'	11:Y:105:DG:C8	2.55	0.42
1:A:117:DC:H2''	1:A:118:DA:C8	2.55	0.42
2:E:105:DT:C2'	2:E:106:DC:H5'	2.49	0.42
3:D:103:DT:C6	3:D:103:DT:H5''	2.54	0.42
4:B:115:DG:N3	4:B:116:DA:C5	2.88	0.42
1:A:118:DA:C6	1:A:119:DA:C6	3.08	0.41
4:B:103:DG:H2''	4:B:104:DC:C5'	2.49	0.41
1:A:105:DA:C6	1:A:106:DG:C6	3.07	0.41
1:A:102:DA:H2'	1:A:102:DA:P	2.60	0.41
3:D:110:DG:N2	4:B:108:DC:O2	2.53	0.41
4:B:111:DT:H2''	4:B:112:DA:OP1	2.20	0.41
3:D:113:DG:H1'	3:D:114:DC:C5	2.56	0.41
6:C:113:DA:C5	7:M:105:DC:N4	2.89	0.41
6:C:110:DG:O5'	6:C:110:DG:C8	2.74	0.41
3:D:108:DT:C4	7:M:118:DC:N4	2.88	0.41
5:F:113:DG:C2'	5:F:114:DG:H8	2.32	0.41
8:U:119:DG:H2''	8:U:120:DC:O5'	2.21	0.41
9:V:107:DA:C4	9:V:108:DG:C5	3.09	0.41
7:M:101:DT:H2''	7:M:102:DC:C6	2.56	0.41
1:A:102:DA:OP2	1:A:102:DA:H8	2.04	0.40
5:F:106:DT:C4	5:F:107:DG:C6	3.09	0.40
5:F:113:DG:C2'	5:F:114:DG:C8	3.04	0.40
4:B:103:DG:H2''	4:B:104:DC:O4'	2.22	0.40
7:M:102:DC:H2''	7:M:103:DA:OP2	2.20	0.40
10:X:113:DT:H2''	10:X:114:DC:H5	1.87	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)
2:E:102:DT:O4	6:C:101:DA:N6[1_655]	1.98	0.22

## 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.