



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 21, 2022 – 06:07 PM EDT

PDB ID : 7U3Q
Title : [4T7] Self-assembling tensegrity triangle with four turns of DNA per axis with R3 symmetry
Authors : Woloszyn, K.; Vecchioni, S.; Lu, B.; Ma, Y.; Seeman, N.C.; Sha, R.; Ohayon, Y.P.; Huang, Q.
Deposited on : 2022-02-28
Resolution : 9.32 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

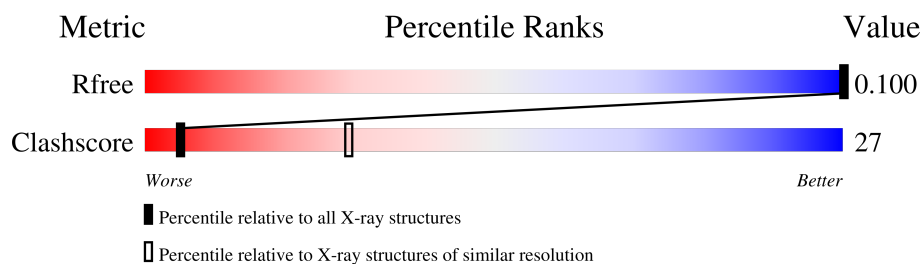
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 9.32 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	B	4	 75% 25%
2	C	29	 28% 59% 14%
3	A	42	 26% 48% 26%
4	D	6	 50% 50%
5	E	3	 100%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 1722 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(P*CP*CP*GP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	4	Total	C	N	O	P	0	0	0
			80	38	13	25	4			

- Molecule 2 is a DNA chain called DNA (29-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	29	Total	C	N	O	P	0	0	0
			586	281	97	179	29			

- Molecule 3 is a DNA chain called DNA (42-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	42	Total	C	N	O	P	0	0	0
			871	411	171	247	42			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	6	Total	C	N	O	P	0	0	0
			124	58	23	37	6			

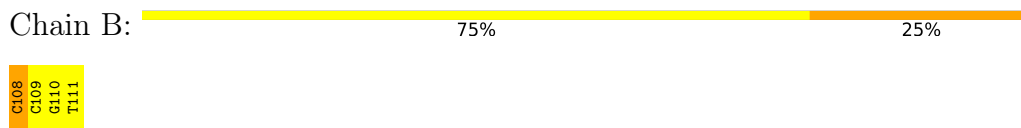
- Molecule 5 is a DNA chain called DNA (5'-D(P*AP*CP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	3	Total	C	N	O	P	0	0	0
			61	29	13	16	3			

3 Residue-property plots

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.

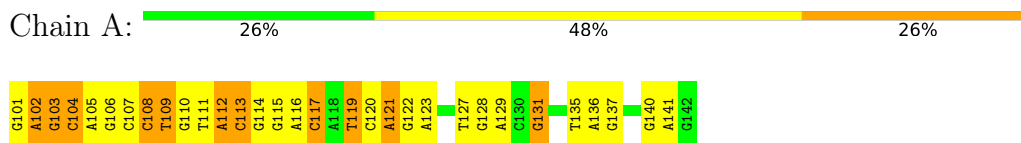
- Molecule 1: DNA (5'-D(P*CP*CP*GP*T)-3')



- Molecule 2: DNA (29-MER)



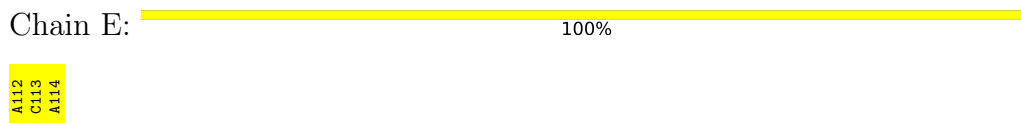
- Molecule 3: DNA (42-MER)



- Molecule 4: DNA (5'-D(P*GP*GP*CP*TP*GP*C)-3')



- Molecule 5: DNA (5'-D(P*AP*CP*A)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	205.70Å 205.70Å 197.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.06 – 9.32 86.27 – 9.32	Depositor EDS
% Data completeness (in resolution range)	79.4 (44.06-9.32) 68.6 (86.27-9.32)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.71 (at 9.93Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.095 , 0.100 0.096 , 0.100	Depositor DCC
R_{free} test set	87 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	229.1	Xtriage
Anisotropy	0.723	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	3.16 , 100.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.30$, $\langle L^2 \rangle = 0.12$	Xtriage
Estimated twinning fraction	0.230 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.74	EDS
Total number of atoms	1722	wwPDB-VP
Average B, all atoms (Å ²)	1190.0	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 34.88 % 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 6.3620e-04.*

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	B	1.55	1/88 (1.1%)	1.48	1/133 (0.8%)
2	C	1.30	4/653 (0.6%)	1.26	2/1004 (0.2%)
3	A	1.31	9/980 (0.9%)	1.54	10/1512 (0.7%)
4	D	1.47	2/138 (1.4%)	1.23	1/211 (0.5%)
5	E	1.32	0/68	1.22	0/102
All	All	1.33	16/1927 (0.8%)	1.42	14/2962 (0.5%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	119	DT	C1'-N1	7.30	1.58	1.49
1	B	108	DC	C1'-N1	6.95	1.58	1.49
3	A	104	DC	C1'-N1	6.72	1.57	1.49
3	A	117	DC	C1'-N1	6.50	1.57	1.49
2	C	127	DT	C1'-N1	6.46	1.57	1.49
3	A	103	DG	C3'-O3'	6.38	1.52	1.44
3	A	110	DG	C3'-O3'	5.87	1.51	1.44
3	A	103	DG	C5'-C4'	5.78	1.57	1.51
3	A	108	DC	C1'-N1	5.57	1.56	1.49
4	D	133	DT	C3'-O3'	5.54	1.51	1.44
3	A	111	DT	C1'-N1	5.33	1.56	1.49
3	A	131	DG	N9-C4	5.32	1.42	1.38
2	C	108	DC	C1'-N1	5.24	1.56	1.49
4	D	132	DC	C1'-N1	5.13	1.55	1.49
2	C	126	DA	C3'-O3'	5.12	1.50	1.44
2	C	122	DT	C3'-O3'	5.01	1.50	1.44

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	121	DA	OP1-P-O3'	24.05	158.11	105.20
3	A	121	DA	OP2-P-O3'	-19.86	61.50	105.20
3	A	121	DA	P-O3'-C3'	18.69	142.13	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	121	DA	O3'-P-O5'	-7.89	89.00	104.00
3	A	103	DG	O4'-C1'-N9	6.96	112.87	108.00
3	A	113	DC	P-O3'-C3'	-6.88	111.44	119.70
3	A	102	DA	O4'-C1'-N9	6.80	112.76	108.00
1	B	108	DC	O4'-C1'-N1	6.53	112.57	108.00
3	A	112	DA	P-O3'-C3'	6.44	127.42	119.70
2	C	126	DA	P-O3'-C3'	6.25	127.20	119.70
4	D	135	DC	O4'-C1'-N1	5.66	111.96	108.00
3	A	109	DT	N3-C4-O4	5.29	123.08	119.90
3	A	109	DT	C5-C4-O4	-5.10	121.33	124.90
2	C	106	DT	N3-C4-O4	5.02	122.91	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	B	80	0	46	8	0
2	C	586	0	330	23	0
3	A	871	0	470	37	0
4	D	124	0	68	5	0
5	E	61	0	34	4	0
All	All	1722	0	948	71	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 27.

All (71) 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)
3:A:104:DC:H2'	3:A:105:DA:C8	1.98	0.99
3:A:103:DG:H2''	3:A:104:DC:H5''	1.63	0.80
3:A:122:DG:H2''	3:A:123:DA:C8	2.17	0.80
3:A:107:DC:H2''	3:A:108:DC:H5''	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:133:DT:H2'	4:D:134:DG:C8	2.22	0.73
2:C:109:DT:H1'	2:C:110:DA:H5'	1.74	0.70
2:C:127:DT:H1'	2:C:128:DG:C8	2.28	0.69
3:A:113:DC:H2''	3:A:114:DG:N7	2.07	0.68
1:B:108:DC:H3'	1:B:109:DC:H5''	1.77	0.67
2:C:111:DC:H2''	2:C:112:DT:C6	2.32	0.65
4:D:132:DC:H2'	4:D:133:DT:H71	1.78	0.64
3:A:121:DA:H4'	3:A:122:DG:H5'	1.81	0.63
4:D:133:DT:H2'	4:D:134:DG:H8	1.62	0.63
3:A:101:DG:H2''	3:A:102:DA:H8	1.66	0.60
2:C:106:DT:H2''	2:C:107:DG:H8	1.67	0.58
3:A:122:DG:H2''	3:A:123:DA:N7	2.19	0.57
1:B:108:DC:H1'	2:C:129:DT:H2''	1.88	0.56
3:A:114:DG:H2''	3:A:115:DG:C8	2.43	0.54
3:A:112:DA:H1'	3:A:113:DC:H5'	1.92	0.52
3:A:112:DA:H1'	3:A:113:DC:C5'	2.39	0.52
3:A:135:DT:H2''	3:A:136:DA:C8	2.45	0.52
1:B:108:DC:H1'	2:C:129:DT:C1'	2.40	0.51
3:A:108:DC:H2''	3:A:109:DT:C6	2.45	0.51
2:C:112:DT:H2''	2:C:113:DA:C8	2.45	0.51
2:C:115:DG:C2	3:A:131:DG:C2	2.99	0.50
2:C:113:DA:H2''	2:C:114:DC:H5'	1.93	0.50
3:A:103:DG:H2''	3:A:104:DC:C5'	2.40	0.49
2:C:128:DG:C4	2:C:129:DT:C5	3.01	0.49
3:A:101:DG:N2	3:A:102:DA:N6	2.60	0.49
3:A:136:DA:H2''	3:A:137:DG:H8	1.78	0.49
3:A:106:DG:C2	3:A:107:DC:C2	3.01	0.48
3:A:135:DT:H2''	3:A:136:DA:H8	1.79	0.47
2:C:126:DA:H4'	2:C:127:DT:OP1	2.14	0.47
5:E:113:DC:H1'	5:E:114:DA:H5'	1.96	0.47
2:C:106:DT:H2''	2:C:107:DG:C8	2.49	0.47
3:A:112:DA:O4'	3:A:112:DA:P	2.73	0.47
3:A:113:DC:H2''	3:A:114:DG:C8	2.49	0.47
3:A:119:DT:H2''	3:A:120:DC:O5'	2.15	0.47
2:C:120:DC:H2''	2:C:121:DA:H8	1.79	0.47
3:A:102:DA:H2''	3:A:103:DG:OP1	2.16	0.46
2:C:109:DT:C2	2:C:110:DA:C8	3.05	0.45
2:C:120:DC:H2''	2:C:121:DA:C8	2.51	0.45
3:A:115:DG:H2'	3:A:116:DA:C8	2.51	0.45
3:A:112:DA:H4'	3:A:113:DC:OP1	2.17	0.45
1:B:108:DC:H1'	2:C:129:DT:C2'	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:DC:H1'	2:C:129:DT:H1'	1.98	0.44
3:A:127:DT:H2''	3:A:128:DG:C8	2.52	0.44
2:C:117:DC:H2''	2:C:118:DA:C8	2.53	0.44
3:A:101:DG:H2''	3:A:102:DA:C8	2.51	0.43
4:D:134:DG:H2''	4:D:135:DC:O4'	2.19	0.43
2:C:118:DA:H2''	2:C:119:DG:O4'	2.19	0.43
3:A:120:DC:H1'	3:A:121:DA:OP1	2.17	0.43
3:A:128:DG:H2''	3:A:129:DA:N7	2.34	0.43
5:E:113:DC:H2''	5:E:114:DA:H5'	2.00	0.43
5:E:113:DC:C2'	5:E:114:DA:H5'	2.49	0.43
3:A:114:DG:H2''	3:A:115:DG:N7	2.34	0.43
2:C:122:DT:H2''	2:C:123:DC:H5''	2.00	0.42
4:D:130:DG:H2'	4:D:131:DG:C8	2.54	0.42
3:A:115:DG:H2''	3:A:116:DA:O5'	2.19	0.42
3:A:136:DA:H2''	3:A:137:DG:C8	2.56	0.41
3:A:116:DA:H2''	3:A:117:DC:O5'	2.21	0.41
3:A:135:DT:C2	3:A:136:DA:C5	3.09	0.41
3:A:114:DG:C2	3:A:115:DG:C2	3.09	0.41
2:C:122:DT:H2''	2:C:123:DC:C5'	2.51	0.41
1:B:110:DG:C4	1:B:111:DT:C5	3.08	0.41
1:B:108:DC:C5	2:C:129:DT:H72	2.56	0.40
1:B:108:DC:H2'	1:B:109:DC:C6	2.56	0.40
3:A:121:DA:C2	3:A:122:DG:C5	3.10	0.40
5:E:112:DA:H2'	5:E:113:DC:C6	2.56	0.40
3:A:140:DG:H2''	3:A:141:DA:H8	1.86	0.40
2:C:123:DC:H5''	2:C:123:DC:H6	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

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

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

6.3 Carbohydrates [i](#)

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

6.4 Ligands [i](#)

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

6.5 Other polymers [i](#)

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