Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2023 – 03:45 PM EDT

PDB ID	:	8D31
Title	:	[AG/TC] Self-Assembled 3D DNA Cubic Tensegrity Triangle with 24 bp Arm Length
Authors	:	Lu, B.; Vecchioni, S.; Ohayon, Y.P.; Seeman, N.C.; Mao, C.; Sha, R.
Deposited on	:	2022-05-31
Resolution	:	7.45 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:

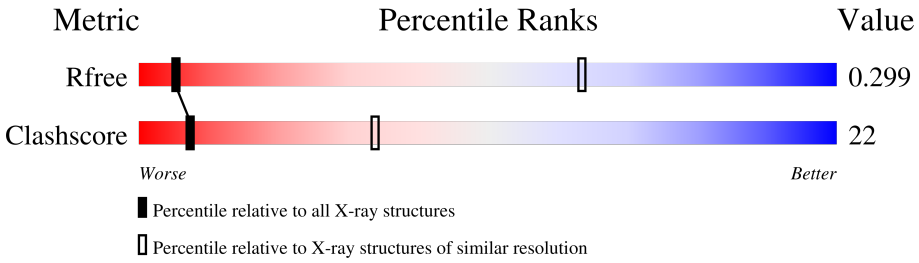
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 7.45 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	1004 (10.00-3.90)
Clashscore	141614	1069 (10.00-3.90)

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	E	24	29% 67% .
2	B	7	14% 86%
2	F	7	14% 86%
3	G	8	38% 62%
4	D	9	11% 89%
4	H	9	33% 56% 11%
5	A	24	46% 50% .
6	C	8	100%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 1952 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a DNA chain called DNA (5'-D(*AP*GP*GP*CP*CP*TP*AP*CP*CP*CP*TP*GP*TP*AP*CP*GP*GP*AP*CP*AP*TP*CP*AP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	E	24	487	232	92	140	23	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	F	7	141	67	26	41	7	0	0	0
			Total	C	N	O	P			
2	B	7	141	67	26	41	7	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	G	8	166	78	33	47	8	0	0	0

- Molecule 4 is a DNA chain called DNA (5'-D(*TP*CP*CP*TP*GP*AP*TP*GP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
4	H	9	180	88	29	55	8	0	0	0
			Total	C	N	O	P			
4	D	9	180	88	29	55	8	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
5	A	24	490	233	94	140	23	0	0	0

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

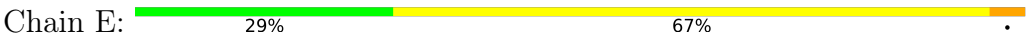
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
6	C	8	167	78	33	48	8	0	0	0

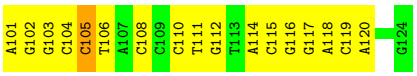
3 Residue-property plots (i)

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 (5'-D(*AP*GP*GP*CP*CP*TP*AP*CP*CP*CP*TP*GP*TP*AP*CP*GP*GP*AP*CP*AP*TP*CP*AP*G)-3')

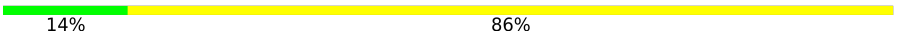
Chain E:

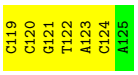




• Molecule 2: DNA (5'-D(P*CP*CP*GP*TP*AP*CP*A)-3')

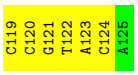
Chain F:





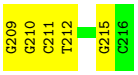
• Molecule 2: DNA (5'-D(P*CP*CP*GP*TP*AP*CP*A)-3')

Chain B:



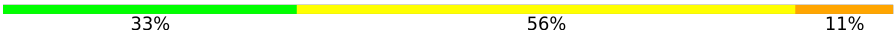
• Molecule 3: DNA (5'-D(P*GP*GP*CP*TP*AP*AP*GP*C)-3')

Chain G:



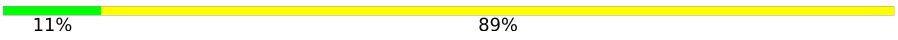
• Molecule 4: DNA (5'-D(*TP*CP*CP*TP*GP*AP*TP*GP*T)-3')

Chain H:



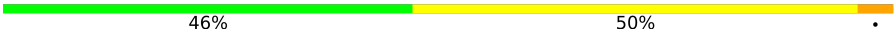
• Molecule 4: DNA (5'-D(*TP*CP*CP*TP*GP*AP*TP*GP*T)-3')

Chain D:



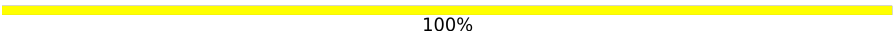
• Molecule 5: DNA (5'-D(*AP*GP*GP*CP*CP*TP*AP*GP*CP*CP*TP*GP*TP*AP*CP*GP*GP*AP*CP*AP*TP*CP*AP*G)-3')

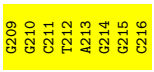
Chain A:



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

Chain C:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 3 2	Depositor
Cell constants a, b, c, α, β, γ	187.50Å 187.50Å 187.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.19 – 7.45 83.85 – 7.45	Depositor EDS
% Data completeness (in resolution range)	92.8 (44.19-7.45) 85.7 (83.85-7.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.74 (at 7.42Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.274 , 0.316 0.278 , 0.299	Depositor DCC
R_{free} test set	78 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	431.5	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.09 , 999.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.75	EDS
Total number of atoms	1952	wwPDB-VP
Average B, all atoms (Å^2)	467.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.45% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

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	E	0.74	0/546	1.08	1/840 (0.1%)
2	B	0.58	0/157	0.90	0/239
2	F	0.58	0/157	0.90	0/239
3	G	0.78	0/186	1.01	0/285
4	D	0.71	0/200	1.29	0/307
4	H	0.64	0/200	1.30	1/307 (0.3%)
5	A	0.76	0/550	1.09	1/847 (0.1%)
6	C	0.73	0/187	1.07	0/287
All	All	0.71	0/2183	1.09	3/3351 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	105	DC	O5'-P-OP2	-7.50	98.95	105.70
4	H	101	DT	O4'-C1'-N1	7.13	112.99	108.00
1	E	105	DC	O4'-C1'-N1	7.04	112.93	108.00

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	E	487	0	270	19	0
2	B	141	0	79	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	141	0	79	6	0
3	G	166	0	90	5	0
4	D	180	0	105	6	0
4	H	180	0	105	7	0
5	A	490	0	270	15	0
6	C	167	0	90	12	0
All	All	1952	0	1088	67	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 22.

All (67) 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:E:102:DG:H2"	1:E:103:DG:H5"	1.59	0.83
6:C:212:DT:H2'	6:C:213:DA:C8	2.18	0.78
5:A:117:DG:H2'	5:A:118:DA:C8	2.20	0.76
1:E:104:DC:H41	3:G:215:DG:H1	1.31	0.76
5:A:117:DG:H2'	5:A:118:DA:H8	1.51	0.76
5:A:119:DC:H2"	5:A:120:DA:C8	2.27	0.70
4:D:101:DT:H2'	4:D:102:DC:C6	2.32	0.65
2:F:120:DC:H2"	2:F:121:DG:C5	2.35	0.61
2:B:120:DC:H2"	2:B:121:DG:C5	2.35	0.61
1:E:117:DG:H2'	1:E:118:DA:H8	1.66	0.60
1:E:117:DG:H2"	1:E:118:DA:O5'	2.03	0.59
4:H:101:DT:H1'	6:C:216:DC:C6	2.40	0.57
5:A:117:DG:H2"	5:A:118:DA:O5'	2.03	0.56
1:E:119:DC:H2"	1:E:120:DA:C8	2.41	0.56
6:C:209:DG:H2'	6:C:210:DG:C8	2.42	0.55
1:E:117:DG:H2'	1:E:118:DA:C8	2.42	0.54
2:B:119:DC:H2'	2:B:120:DC:C5	2.43	0.54
6:C:211:DC:H2"	6:C:212:DT:O5'	2.07	0.53
6:C:214:DG:H1'	6:C:215:DG:H5'	1.90	0.53
1:E:101:DA:C5	1:E:102:DG:C6	2.96	0.53
2:F:119:DC:H2'	2:F:120:DC:C5	2.43	0.53
4:H:103:DC:H1'	4:H:104:DT:OP2	2.08	0.52
6:C:214:DG:H2"	6:C:215:DG:H5'	1.92	0.52
3:G:209:DG:H2'	3:G:210:DG:C8	2.45	0.52
3:G:211:DC:H2"	3:G:212:DT:O5'	2.08	0.52
4:D:101:DT:H2"	4:D:102:DC:H5'	1.92	0.51
1:E:104:DC:H2"	1:E:105:DC:C6	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:102:DG:C6	1:E:103:DG:C6	3.00	0.49
6:C:215:DG:H4'	6:C:216:DC:H5'	1.94	0.49
5:A:108:DG:H1	6:C:211:DC:H42	1.61	0.49
4:D:103:DC:H1'	4:D:104:DT:OP2	2.12	0.49
1:E:110:DC:H2'	1:E:111:DT:H6	1.77	0.48
2:F:119:DC:C4	4:H:109:DT:C4	3.01	0.48
4:H:101:DT:H2"	6:C:216:DC:H2"	1.94	0.48
6:C:214:DG:C2'	6:C:215:DG:H5'	2.43	0.48
5:A:114:DA:H4'	5:A:115:DC:OP1	2.14	0.47
2:F:121:DG:H2"	2:F:122:DT:OP2	2.15	0.47
1:E:108:DC:H42	3:G:211:DC:N4	2.13	0.47
5:A:104:DC:H1'	5:A:105:DC:OP2	2.14	0.47
5:A:116:DG:C2'	5:A:117:DG:C8	2.98	0.46
4:D:106:DA:H2"	4:D:107:DT:H71	1.97	0.46
1:E:110:DC:H2'	1:E:111:DT:C6	2.51	0.46
2:F:122:DT:H1'	2:F:123:DA:H5'	1.97	0.46
2:F:123:DA:H2"	2:F:124:DC:C5	2.50	0.46
5:A:117:DG:C2'	5:A:118:DA:C8	2.96	0.46
5:A:114:DA:OP1	5:A:114:DA:H8	1.99	0.46
1:E:114:DA:OP1	1:E:114:DA:H8	2.00	0.45
2:B:121:DG:H2"	2:B:122:DT:OP2	2.15	0.45
1:E:105:DC:H1'	1:E:106:DT:H5'	1.98	0.45
2:B:123:DA:H2"	2:B:124:DC:C5	2.51	0.45
1:E:102:DG:H4'	1:E:102:DG:OP1	2.16	0.45
5:A:116:DG:H2"	5:A:117:DG:C8	2.51	0.45
6:C:212:DT:H2"	6:C:213:DA:OP1	2.16	0.45
5:A:115:DC:H2"	5:A:116:DG:N7	2.32	0.45
4:H:106:DA:H2"	4:H:107:DT:H71	1.99	0.44
1:E:111:DT:H3'	1:E:112:DG:H8	1.83	0.43
5:A:123:DA:C2	4:D:105:DG:C2	3.07	0.43
2:B:119:DC:C4	4:D:109:DT:C4	3.06	0.43
3:G:209:DG:H3'	3:G:210:DG:C8	2.53	0.43
1:E:116:DG:C2'	1:E:117:DG:C8	3.02	0.43
1:E:104:DC:H2"	1:E:105:DC:N1	2.33	0.42
5:A:119:DC:H2"	5:A:120:DA:N7	2.34	0.42
4:H:101:DT:H6	4:H:101:DT:H2'	1.63	0.41
2:B:122:DT:H1'	2:B:123:DA:H5'	2.01	0.41
5:A:102:DG:H2"	5:A:103:DG:C8	2.55	0.41
1:E:114:DA:H4'	1:E:115:DC:OP1	2.21	0.40
4:H:101:DT:H2"	6:C:216:DC:C2'	2.51	0.40

There are no symmetry-related clashes.

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.