



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:35 PM UTC

PDB ID : 8D31 / pdb_00008d31
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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

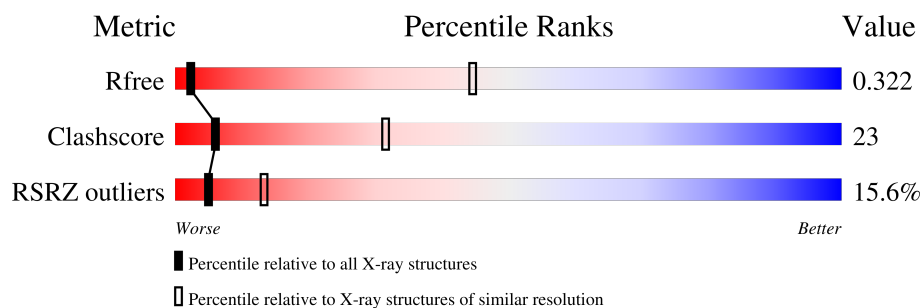
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 7.45 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}	180053	1167 (10.00-4.00)
Clashscore	190562	1000 (10.00-4.06)
RSRZ outliers	180081	1161 (10.00-4.00)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	E	24	12% 29% 71%
2	B	7	14% 86%
2	F	7	29% 14% 86%
3	G	8	12% 38% 62%
4	D	9	11% 89%
4	H	9	11% 33% 67%
5	A	24	33% 42% 58%

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Mol	Chain	Length	Quality of chain
6	C	8	 100%

2 Entry composition

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
1	E	24	Total	C	N	O	P	0	0	0
			487	232	92	140	23			

- 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
2	F	7	Total	C	N	O	P	0	0	0
			141	67	26	41	7			
2	B	7	Total	C	N	O	P	0	0	0
			141	67	26	41	7			

- 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
3	G	8	Total	C	N	O	P	0	0	0
			166	78	33	47	8			

- 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
4	H	9	Total	C	N	O	P	0	0	0
			180	88	29	55	8			
4	D	9	Total	C	N	O	P	0	0	0
			180	88	29	55	8			

- 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
5	A	24	Total	C	N	O	P	0	0	0
			490	233	94	140	23			

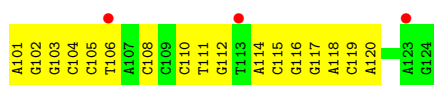
- Molecule 6 is a DNA chain called DNA (5'-D(P*GP*GP*CP*TP*AP*GP*GP*C)-3').

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

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

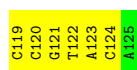
- Molecule 1: DNA (5'-D(*AP*GP*GP*CP*CP*TP*AP*CP*CP*CP*TP*GP*TP*AP*CP*GP*GP*AP*CP*AP*TP*CP*AP*G)-3')



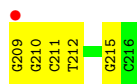
- Molecule 2: DNA (5'-D(P*CP*CP*GP*TP*AP*CP*A)-3')



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



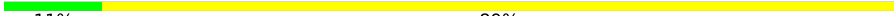
- Molecule 3: DNA (5'-D(P*GP*GP*CP*TP*AP*AP*GP*C)-3')



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



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

Chain D:  11% 89%

T101
C102
C103
T104
G105
A106
T107
G108
T109

- 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:  33% 42% 58%

A101
G102
C103
C104
C105
T106
A107
G108
A114
C115
G116
G117
A118
C119
A120
T121
C122
A123
G124

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

Chain C:  100%

G209
G210
C211
T212
A213
G214
C215
C216

4 Data and refinement statistics

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 44.19 – 7.45	Depositor EDS
% Data completeness (in resolution range)	92.8 (44.19-7.45) 85.4 (44.19-7.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.74 (at 7.42Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.274 , 0.316 0.275 , 0.322	Depositor DCC
R_{free} test set	78 reflections (4.60%)	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)	0.14 , 999.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	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.*

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 [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	E	0.30	0/546	0.61	0/840
2	B	0.25	0/157	0.44	0/239
2	F	0.26	0/157	0.44	0/239
3	G	0.33	0/186	0.60	0/285
4	D	0.32	0/200	0.74	0/307
4	H	0.27	0/200	0.70	0/307
5	A	0.32	0/550	0.63	0/847
6	C	0.31	0/187	0.60	0/287
All	All	0.30	0/2183	0.62	0/3351

There are no bond length outliers.

There are no bond angle outliers.

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	E	487	0	270	19	0
2	B	141	0	79	6	0
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	16	0
6	C	167	0	90	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	1952	0	1088	68	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 23.

All (68) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:A:120:DA:H2''	5:A:121:DT:H71	2.01	0.42
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 [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 oligosaccharides 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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	E	24/24 (100%)	0.66	3 (12%) 8 16	180, 349, 696, 731	0
2	B	7/7 (100%)	0.20	0 100 100	187, 291, 501, 529	0
2	F	7/7 (100%)	1.65	2 (28%) 1 7	368, 522, 616, 672	0
3	G	8/8 (100%)	1.13	1 (12%) 8 16	220, 400, 651, 692	0
4	D	9/9 (100%)	0.16	0 100 100	334, 551, 626, 962	0
4	H	9/9 (100%)	0.78	1 (11%) 10 18	450, 539, 732, 886	0
5	A	24/24 (100%)	1.48	8 (33%) 1 6	269, 400, 707, 1137	0
6	C	8/8 (100%)	0.69	0 100 100	194, 411, 626, 679	0
All	All	96/96 (100%)	0.91	15 (15%) 5 13	180, 434, 731, 1137	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	A	114	DA	4.3
5	A	104	DC	3.7
1	E	113	DT	3.6
5	A	103	DG	3.4
1	E	123	DA	3.3
2	F	122	DT	3.0
5	A	106	DT	2.6
5	A	107	DA	2.6
3	G	209	DG	2.6
4	H	107	DT	2.4
5	A	122	DC	2.4
5	A	117	DG	2.2
5	A	116	DG	2.1
1	E	106	DT	2.1
2	F	123	DA	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.