



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 04:50 AM UTC

PDB ID : 7U43 / pdb_00007u43
Title : [L334] Self-assembling tensegrity triangle with three turns, three turns and four turns of DNA per axis by extension and linker addition with P1 symmetry
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Deposited on : 2022-02-28
Resolution : 7.55 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

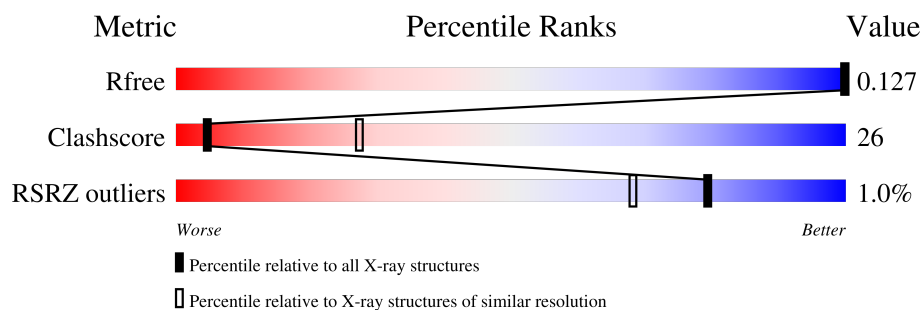
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 7.55 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.



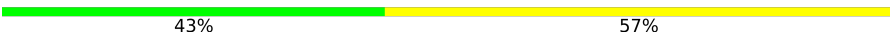
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1167 (10.00-4.00)
Clashscore	190562	1000 (10.00-4.06)
RSRZ outliers	180081	1161 (10.00-4.00)

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	A	31	3% 10% 90%
2	E	24	8% 92%
3	D	24	38% 63%
4	B	21	5% 43% 57%
5	F	14	14% 86%
6	C	31	26% 74%
7	M	21	67% 33%

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Mol	Chain	Length	Quality of chain
8	X	21	 29% 71%
9	Y	21	 43% 57%

2 Entry composition

There are 9 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 (5'-D(P*GP*AP*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
			432	204	84	123	21			

- Molecule 5 is a DNA chain called DNA (5'-D(P*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
			294	139	56	85	14			

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

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

- 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	C	N	O	P	0	0	0
			418	200	76	122	20			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	X	21	Total	C	N	O	P	0	0	0
			425	203	73	128	21			

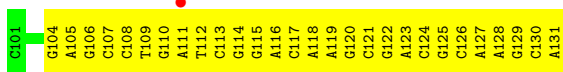
- Molecule 9 is a DNA chain called DNA (5'-D(P*TP*CP*TP*GP*CP*TP*GP*AP*CP*GP*TP*AP*GP*TP*AP*GP*CP*AP*GP*AP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	Y	21	Total	C	N	O	P	0	0	0
			435	206	82	126	21			

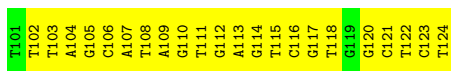
3 Residue-property plots [i](#)

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 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 (31-MER)



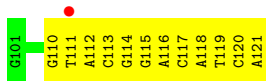
- Molecule 2: DNA (5'-D(P*TP*TP*TP*AP*GP*CP*AP*TP*AP*GP*TP*GP*AP*GP*TP*C
P*GP*TP*GP*GP*CP*TP*CP*T)-3')



- 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')

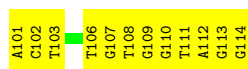


- Molecule 4: DNA (5'-D(P*GP*AP*GP*CP*AP*GP*CP*CP*TP*GP*TP*AP*CP*GP*GP*A
P*CP*AP*TP*CP*A)-3')



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





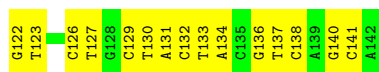
● Molecule 6: DNA (31-MER)



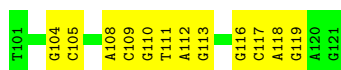
● Molecule 7: DNA (5'-D(*TP*AP*CP*AP*CP*CP*GP*AP*TP*CP*AP*CP*CP*TP*GP*CP*CP*AP*CP*CP*G)-3')



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	99.59Å 101.71Å 134.34Å 98.64° 109.49° 101.44°	Depositor
Resolution (Å)	42.78 – 7.55 42.78 – 7.55	Depositor EDS
% Data completeness (in resolution range)	60.5 (42.78-7.55) 53.5 (42.78-7.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.30 (at 7.43Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.115 , 0.124 0.116 , 0.127	Depositor DCC
R_{free} test set	185 reflections (3.11%)	wwPDB-VP
Wilson B-factor (Å ²)	292.2	Xtriage
Anisotropy	0.538	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.15 , 771.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.99	EDS
Total number of atoms	4258	wwPDB-VP
Average B, all atoms (Å ²)	738.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.74% 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	A	0.34	0/721	0.61	0/1110
2	E	0.38	0/552	0.72	0/851
3	D	0.33	0/548	0.64	0/845
4	B	0.31	0/485	0.62	0/746
5	F	0.31	0/330	0.60	0/509
6	C	0.36	0/704	0.62	0/1083
7	M	0.30	0/467	0.55	0/716
8	X	0.28	0/474	0.59	0/728
9	Y	0.25	0/488	0.50	0/752
All	All	0.32	0/4769	0.61	0/7340

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	A	640	0	344	47	0
2	E	494	0	274	35	0
3	D	492	0	274	14	0
4	B	432	0	235	14	0
5	F	294	0	159	12	0
6	C	628	0	349	23	0
7	M	418	0	236	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	X	425	0	238	13	0
9	Y	435	0	237	14	0
All	All	4258	0	2346	170	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 26.

The worst 5 of 170 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)
2:E:102:DT:H2''	2:E:103:DT:H5''	1.56	0.87
8:X:132:DC:H2''	8:X:133:DT:H71	1.58	0.85
1:A:113:DC:H1'	1:A:114:DG:C6	2.17	0.79
2:E:122:DT:H2'	2:E:123:DC:C6	2.18	0.79
2:E:106:DC:O2	6:C:128:DG:N2	2.16	0.78

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 [i](#)

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

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	A	31/31 (100%)	-0.75	1 (3%) 50 45	507, 712, 799, 843	0
2	E	24/24 (100%)	-0.83	0 100 100	575, 742, 805, 839	0
3	D	24/24 (100%)	-0.89	0 100 100	650, 748, 839, 875	0
4	B	21/21 (100%)	-0.46	1 (4%) 35 37	548, 659, 771, 807	0
5	F	14/14 (100%)	-1.00	0 100 100	609, 658, 807, 858	0
6	C	31/31 (100%)	-0.68	0 100 100	556, 664, 739, 787	0
7	M	21/21 (100%)	-0.78	0 100 100	522, 581, 625, 633	0
8	X	21/21 (100%)	-0.78	0 100 100	851, 941, 1071, 1091	0
9	Y	21/21 (100%)	-0.54	0 100 100	788, 943, 1028, 1034	0
All	All	208/208 (100%)	-0.74	2 (0%) 79 68	507, 726, 1013, 1091	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	B	111	DT	3.0
1	A	111	DA	2.4

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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.