



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 21, 2022 – 06:10 PM EDT

PDB ID : 7U45
Title : [L344] Self-assembling tensegrity triangle with three turns, four 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 : 8.05 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	:	4.02b-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

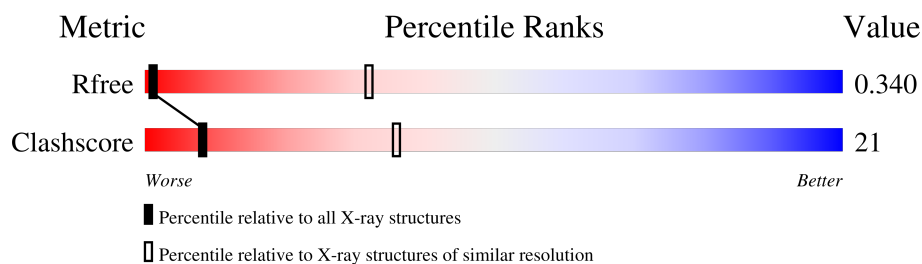
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 8.05 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	A	21	14% 76% 10%
2	E	24	17% 83%
3	D	14	29% 64% 7%
4	B	21	52% 48%
5	F	14	14% 86%
6	C	31	35% 61% .
7	M	21	38% 48% 14%
8	X	21	19% 81%
9	Y	21	76% 24%

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Mol	Chain	Length	Quality of chain
10	U	21	 43% 57%
11	V	21	 10% 90%

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 4712 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*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
			433	204	87	121	21			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	24	Total	C	N	O	P	0	0	0
			495	235	89	147	24			

- Molecule 3 is a DNA chain called DNA (5'-D(P*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
			288	137	49	88	14			

- Molecule 4 is a DNA chain called DNA (5'-D(P*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
			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
			629	300	117	182	30			

- Molecule 7 is a DNA chain called DNA (5'-D(P*CP*AP*CP*CP*GP*AP*TP*CP*AP*CP*CP*TP*GP*CP*CP*AP*CP*CP*GP*TP*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*GP*CP*TP*AP*GP*GP*CP*TP*AP*AP*CP*TP*CP*GP*CP*TP*AP*GP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	X	21	Total	C	N	O	P	0	0	0
			430	204	78	127	21			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	Y	21	Total	C	N	O	P	0	0	0
			430	204	78	127	21			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	U	21	Total	C	N	O	P	0	0	0
			432	205	80	126	21			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	V	21	Total	C	N	O	P	0	0	0
			428	204	75	128	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. 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.

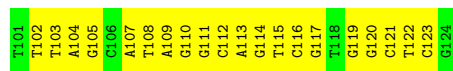
- Molecule 1: DNA (5'-D(P*CP*AP*CP*GP*AP*GP*CP*CP*TP*GP*AP*TP*CP*GP*GP*AP*CP*AP*AP*GP*A)-3')

Chain A: 



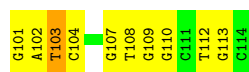
- Molecule 2: DNA (5'-D(P*TP*TP*TP*AP*GP*CP*AP*TP*AP*GP*GP*CP*AP*GP*TP*CP*GP*TP*GP*GP*CP*TP*CP*G)-3')

Chain E: 



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

Chain D: 



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

Chain F: 



- Molecule 6: DNA (31-MER)

Chain C:  35% 61% .



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

Chain M:  38% 48% 14%




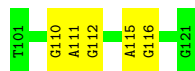
- Molecule 8: DNA (5'-D(P*TP*GP*CP*TP*AP*GP*GP*CP*TP*AP*AP*CP*TP*CP*GP*C P*TP*AP*GP*CP*G)-3')

Chain X:  19% 81%



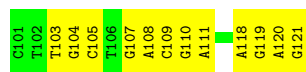
- Molecule 9: DNA (5'-D(P*TP*CP*CP*GP*CP*TP*AP*GP*CP*GP*AP*GP*TP*TP*AP*G P*CP*CP*TP*AP*G)-3')

Chain Y:  76% 24%



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

Chain U:  43% 57%



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

Chain V:  10% 90%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	100.16Å 135.05Å 135.92Å 102.92° 96.91° 108.05°	Depositor
Resolution (Å)	54.05 – 8.05 93.21 – 8.05	Depositor EDS
% Data completeness (in resolution range)	56.3 (54.05-8.05) 49.1 (93.21-8.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.92 (at 8.42Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.233 , 0.285 0.273 , 0.340	Depositor DCC
R_{free} test set	208 reflections (5.45%)	wwPDB-VP
Wilson B-factor (Å ²)	189.9	Xtriage
Anisotropy	0.681	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.80 , 0.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.68	EDS
Total number of atoms	4712	wwPDB-VP
Average B, all atoms (Å ²)	1187.0	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 27.43 % 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 2.2042e-03.*

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	A	0.77	1/487 (0.2%)	1.02	1/749 (0.1%)
2	E	0.69	0/554	1.05	0/854
3	D	0.64	0/321	1.18	1/494 (0.2%)
4	B	0.57	0/485	0.88	0/746
5	F	0.82	0/330	1.20	1/509 (0.2%)
6	C	0.68	0/705	1.04	1/1085 (0.1%)
7	M	0.70	0/470	1.07	3/720 (0.4%)
8	X	0.58	0/481	0.98	0/740
9	Y	0.61	0/481	0.94	0/740
10	U	0.58	0/484	0.89	0/745
11	V	0.59	0/478	1.00	0/735
All	All	0.66	1/5276 (0.0%)	1.02	7/8117 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	101	DC	C1'-N1	5.27	1.56	1.49

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	118	DC	O4'-C1'-N1	6.88	112.81	108.00
5	F	107	DG	O4'-C1'-N9	6.71	112.69	108.00
7	M	116	DA	O4'-C1'-N9	6.45	112.51	108.00
6	C	114	DG	O4'-C4'-C3'	-6.14	102.05	104.50
1	A	112	DT	N3-C4-O4	5.14	122.98	119.90

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	433	0	234	19	0
2	E	495	0	272	17	0
3	D	288	0	160	9	0
4	B	432	0	235	10	0
5	F	294	0	159	15	0
6	C	629	0	349	25	0
7	M	421	0	235	21	0
8	X	430	0	237	17	0
9	Y	430	0	237	6	0
10	U	432	0	237	12	0
11	V	428	0	238	15	0
All	All	4712	0	2593	152	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 21.

The worst 5 of 152 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:107:DA:N1	6:C:128:DG:N2	2.19	0.91
10:U:108:DA:H3'	10:U:109:DC:H4'	1.60	0.83
7:M:115:DC:H2'	7:M:116:DA:H8	1.49	0.78
6:C:113:DA:H1'	6:C:114:DG:N7	2.02	0.74
4:B:113:DC:O2	4:B:114:DG:N2	2.19	0.74

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 ⓘ

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.