



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 07:39 AM UTC

PDB ID : 7U3Y / pdb_00007u3y
Title : [L233] Self-assembling tensegrity triangle with two turns, three turns and three turns of DNA per axis by linker addition with P1 symmetry
Authors : Woloszyn, K.; Vecchioni, S.; Seeman, N.C.; Sha, R.; Ohayon, Y.P.
Deposited on : 2022-02-28
Resolution : 6.06 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

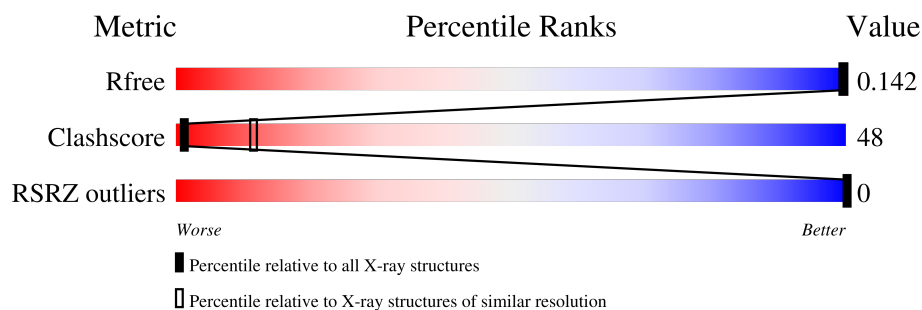
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.06 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.



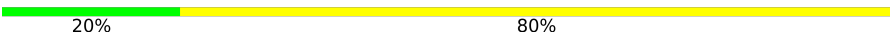
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1145 (8.08-4.00)
Clashscore	190562	1006 (8.08-4.02)
RSRZ outliers	180081	1138 (8.08-4.00)

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	21	5% 86% 10%
2	E	14	7% 93%
3	D	14	29% 71%
4	B	21	10% 90%
5	F	14	21% 79%
6	C	21	19% 81%
7	M	21	14% 81% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	U	10	 10%90%
9	V	10	 20%80%
10	X	10	 100%
11	Y	10	 20%80%

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 3379 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(*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
			430	204	87	119	20			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	14	Total	C	N	O	P	0	0	0
			285	137	49	86	13			

- Molecule 3 is a DNA chain called DNA (5'-D(*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
			285	137	49	86	13			

- Molecule 4 is a DNA chain called DNA (5'-D(*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
			429	204	84	121	20			

- Molecule 5 is a DNA chain called DNA (5'-D(*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
			291	139	56	83	13			

- Molecule 6 is a DNA chain called DNA (5'-D(*AP*AP*CP*CP*TP*AP*CP*CP*TP*GP*GP*CP*AP*GP*GP*AP*CP*GP*AP*CP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	C	21	Total	C	N	O	P	0	0	0
			426	203	82	121	20			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	U	10	Total	C	N	O	P	0	0	0
			203	96	36	61	10			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	V	10	Total	C	N	O	P	0	0	0
			203	97	38	59	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	10	Total	C	N	O	P	0	0	0
			204	98	34	62	10			

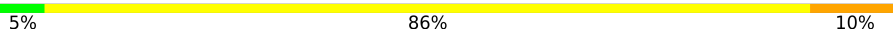
- Molecule 11 is a DNA chain called DNA (5'-D(*CP*TP*TP*AP*GP*CP*AP*TP*AP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	Y	10	Total	C	N	O	P	0	0	0
			202	98	37	58	9			

3 Residue-property plots

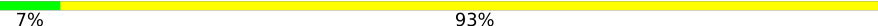
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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(*CP*AP*CP*GP*AP*GP*CP*CP*TP*GP*AP*TP*CP*GP*GP*AP*CP*AP*AP*GP*A)-3')

Chain A: 

G101	A102	G103	G104	A105	G106	G107	C108	T109	G110	A111	T112	C113	G114	A115	G116	C117	A118	A119	G120	A121
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

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

Chain E: 

T101	T102	A103	G104	T105	G106	G107	T108	G109	G110	C111	T112	C113	G114
------	------	------	------	------	------	------	------	------	------	------	------	------	------

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

Chain D: 

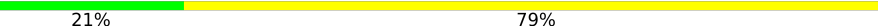
G101	A102	T103	C104	T105	G106	G107	T108	G109	G110	C111	T112	G113	C114
------	------	------	------	------	------	------	------	------	------	------	------	------	------

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

Chain B: 

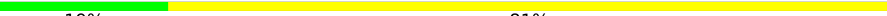
A101	G102	G103	G104	A105	G106	C107	C108	T109	G110	T111	A112	C113	G114	G115	A116	C117	A118	T119	G120	A121
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

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

Chain F: 

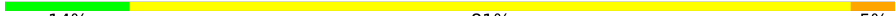
A101	C102	T106	G107	T108	G109	G110	A112	G113	G114
------	------	------	------	------	------	------	------	------	------

- Molecule 6: DNA (5'-D(*AP*AP*CP*CP*TP*AP*CP*CP*TP*GP*GP*CP*AP*GP*GP*AP*CP*GP*AP*CP*T)-3')

Chain C:  19% 81%

A101	C108	G115	A116	C117	G118	A119	C120	T121
A102	T109	G110	G111	A113	G114	A115	A117	A121
C103	G112	A114	A116	A118	A119	A120	A121	
C104	A113	A114	A115	A116	A117	A118	A119	A120
T105	G115	A116	A117	A118	A119	A120	A121	

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

Chain M:  14% 81% 5%

T101	A110	G116	A117	C118	G119	A121
C102	G111	G112	A113	A114	A115	A116
A103	G113	T114	A115	A116	A117	A118
C104	T106	G107	C108	C109	G110	A111
T105	G108	A110	G111	G112	A113	A114

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

Chain U:  10% 90%

T112	G121
C113	
C114	
G115	
C116	
T117	
A118	
G119	
C120	

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

Chain V:  20% 80%

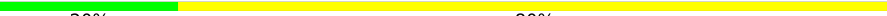
T103	G109	G110
G102	C103	G104
C105	T106	A107
C106	A108	C109

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

Chain X:  100%

G112	A121
T113	
C114	
T115	
A116	
T117	
G118	
C119	
T120	

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

Chain Y:  20% 80%

C101	G106	A107	T108	A109	G110
T102	A104	G105	A106	A107	A108
T103	G104	G105	A106	A107	A108

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	67.14Å 99.59Å 100.16Å 104.30° 103.01° 98.11°	Depositor
Resolution (Å)	37.92 – 6.06 37.92 – 6.06	Depositor EDS
% Data completeness (in resolution range)	61.3 (37.92-6.06) 55.0 (37.92-6.06)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.41 (at 5.76Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.091 , 0.138 0.091 , 0.142	Depositor DCC
R_{free} test set	182 reflections (2.94%)	wwPDB-VP
Wilson B-factor (Å ²)	310.4	Xtriage
Anisotropy	0.432	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.09 , 346.7	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	1.00	EDS
Total number of atoms	3379	wwPDB-VP
Average B, all atoms (Å ²)	628.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.79% 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	0.90	0/484	1.04	2/745 (0.3%)
2	E	0.83	0/318	1.10	0/490
3	D	0.80	0/318	1.05	0/490
4	B	0.64	0/482	0.82	0/742
5	F	0.71	0/327	0.89	0/505
6	C	0.81	0/478	0.97	0/735
7	M	0.75	1/470 (0.2%)	0.94	0/720
8	U	0.64	0/226	0.86	0/346
9	V	0.58	0/227	0.81	0/349
10	X	0.69	0/227	0.92	0/348
11	Y	0.46	0/226	0.70	0/347
All	All	0.74	1/3783 (0.0%)	0.94	2/5817 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	108	DC	C1'-N1	5.18	1.65	1.49

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111	DA	O3'-P-O5'	6.58	113.87	104.00
1	A	110	DG	N9-C1'-C2'	5.44	121.67	113.50

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	430	0	235	35	0
2	E	285	0	161	32	1
3	D	285	0	161	21	0
4	B	429	0	236	41	0
5	F	291	0	160	31	0
6	C	426	0	236	34	1
7	M	421	0	235	35	0
8	U	203	0	113	11	0
9	V	203	0	114	12	0
10	X	204	0	115	9	0
11	Y	202	0	115	11	0
All	All	3379	0	1881	248	1

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 48.

The worst 5 of 248 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)
5:F:109:DG:H5'	7:M:111:DC:H5''	1.40	1.01
8:U:113:DC:H1'	8:U:114:DC:H5	1.32	0.95
7:M:108:DC:H2''	7:M:109:DC:C5	2.10	0.86
9:V:109:DC:H2'	9:V:110:DG:C8	2.12	0.85
1:A:113:DC:H2''	1:A:114:DG:C5	2.11	0.84

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:102:DT:O4	6:C:101:DA:N6[1_655]	1.98	0.22

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	21/21 (100%)	-0.85	0 100 100	581, 611, 698, 724	0
2	E	14/14 (100%)	-1.03	0 100 100	553, 616, 659, 663	0
3	D	14/14 (100%)	-0.87	0 100 100	623, 655, 698, 735	0
4	B	21/21 (100%)	-0.85	0 100 100	523, 600, 689, 699	0
5	F	14/14 (100%)	-0.91	0 100 100	522, 581, 735, 745	0
6	C	21/21 (100%)	-0.89	0 100 100	443, 553, 586, 593	0
7	M	21/21 (100%)	-0.85	0 100 100	515, 553, 597, 615	0
8	U	10/10 (100%)	-0.91	0 100 100	679, 723, 755, 757	0
9	V	10/10 (100%)	-0.95	0 100 100	652, 703, 723, 747	0
10	X	10/10 (100%)	-0.95	0 100 100	692, 719, 766, 782	0
11	Y	10/10 (100%)	-1.06	0 100 100	648, 670, 702, 740	0
All	All	166/166 (100%)	-0.90	0 100 100	443, 620, 739, 782	0

There are no RSRZ outliers to report.

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.