

# wwPDB X-ray Structure Validation Summary Report (i)

#### Oct 14, 2023 – 01:52 PM EDT

PDB ID	:	7U3P
Title	:	[3T7] Self-assembling tensegrity triangle with three turns of DNA per axis with
		R3 symmetry
Authors	:	Woloszyn, K.; Vecchioni, S.; Lu, B.; Ma, Y.; 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 (i) 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 (1)) were used in the production of this report:

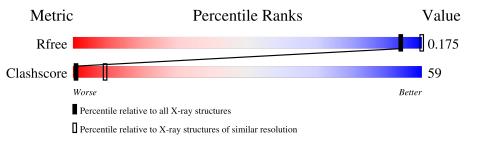
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

## 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	130704	1001 (8.20-3.88)
Clashscore	141614	1050 (8.20-3.90)

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		Q	uality of chain	
1	С	18	17%		83%	
2	А	31	6%	42%	52%	
3	В	7	14%		86%	
4	D	6			100%	



#### 7U3P

## 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 1268 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\*GP\*TP\*AP\*CP\*TP\*CP\*AP\*GP\*CP\*AP \*TP\*CP\*TP\*GP\*AP\*TP\*GP\*T)-3').

Mol	Chain	Residues		At	$\mathbf{oms}$			ZeroOcc	AltConf	Trace
1	С	18	Total 368	C 176	N 64	O 110	Р 18	0	0	0

• Molecule 2 is a DNA chain called DNA (31-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	А	31	Total 635	C 302	N 121	0 182	Р 30	0	0	0

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

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
3	В	7	Total 141	C 67	N 26	0 41	Р 7	0	0	0

• Molecule 4 is a DNA chain called DNA (5'-D(P\*GP\*GP\*CP\*TP\*GP\*C)-3').

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
4	D	6	Total 124	C 58	N 23	O 37	Р 6	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(P\*GP\*TP\*AP\*CP\*TP\*CP\*AP\*GP\*CP\*AP\*TP\*CP\*TP\*GP\*AP\*T P\*GP\*T)-3')

Chain C: 1	7%	83%
G101           T102           C104           C104           C106           C106           G107           G108           G108           G109           G109           T111	C112 7113 7114 7115 7116 7116 7118	
• Molecule 2: 1	DNA (31-MER)	
Chain A: 6%	42%	52%
A101 C102 C102 C104 A105 C104 C106 C106 C107 C108 T110 T111	0,112 0,113 0,114 0,115 0,115 0,115 0,119 0,120 0,120 0,120 0,120 0,120 0,120 0,120 0,120 0,120 0,120 0,120 0,120 0,120 0,120 0,120 0,112 0,113 0,113 0,113 0,113 0,114 0,115 0,115 0,115 0,115 0,115 0,115 0,115 0,115 0,115 0,115 0,115 0,116 0,116 0,116 0,116 0,116 0,116 0,116 0,116 0,116 0,116 0,116 0,116 0,117 0,112 0,120000000000	
• Molecule 3: 1	DNA (5'-D(P*CP*CP*GP*'	TP*AP*CP*A)-3')
Chain B: 14	%	86%
C101 C102 C102 C104 A105 C106 A107		
• Molecule 4: ]	DNA (5'-D(P*GP*GP*CP*	TP*GP*C)-3')
Chain D:	10'	0%
6109 6110 7111 7112 6113 6113 6114		



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants	159.21Å 159.21Å 127.74Å	Denesiton
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$	Depositor
Resolution (Å)	37.55 - 6.06	Depositor
Resolution (A)	93.71 - 6.06	EDS
% Data completeness	64.3 (37.55-6.06)	Depositor
(in resolution range)	59.0(93.71-6.06)	EDS
R <sub>merge</sub>	(Not available)	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	0.43 (at 6.19 Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
D D	0.128 , $0.174$	Depositor
$R, R_{free}$	0.125 , $0.175$	DCC
$R_{free}$ test set	118 reflections $(5.78\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	440.9	Xtriage
Anisotropy	0.906	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.14, 999.0	EDS
L-test for twinning <sup>2</sup>	$< L >=0.46, < L^2>=0.28$	Xtriage
Estimated twinning fraction	0.044 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	1268	wwPDB-VP
Average B, all atoms $(Å^2)$	638.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 10.34% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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	Bo	nd lengths	Bond angles		
	Ullaili	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	С	2.34	21/411~(5.1%)	2.02	20/632~(3.2%)	
2	А	2.23	23/713~(3.2%)	1.85	24/1099~(2.2%)	
3	В	2.30	9/157~(5.7%)	2.16	10/239~(4.2%)	
4	D	1.64	0/138	1.44	0/211	
All	All	2.22	53/1419~(3.7%)	1.90	54/2181~(2.5%)	

The worst 5 of 53 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\mathrm{Ideal}(\mathrm{\AA})$
2	А	112	DA	C3'-O3'	18.64	1.68	1.44
1	С	117	DG	C3'-O3'	12.20	1.59	1.44
2	А	113	DC	P-O5'	11.51	1.71	1.59
2	А	124	DT	C1'-N1	10.52	1.62	1.49
2	А	113	DC	C5'-C4'	9.75	1.62	1.51

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
2	А	113	DC	O5'-P-OP2	12.74	125.99	110.70
2	А	113	DC	OP1-P-OP2	-10.80	103.41	119.60
1	С	108	DG	O4'-C4'-C3'	-10.64	99.62	106.00
1	С	108	DG	O4'-C1'-N9	10.31	115.22	108.00
2	А	112	DA	P-O3'-C3'	9.41	130.99	119.70

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



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	С	368	0	205	30	1
2	А	635	0	349	64	0
3	В	141	0	79	21	0
4	D	124	0	68	17	1
All	All	1268	0	701	113	1

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.

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 59.

The worst 5 of 113 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:A:112:DA:C3'	2:A:112:DA:O3'	1.68	1.39
1:C:117:DG:H2'	1:C:118:DT:H71	1.37	1.02
1:C:108:DG:H2'	1:C:109:DC:C6	1.95	1.01
1:C:118:DT:H2'	3:B:101:DC:H1'	1.53	0.90
2:A:106:DG:H1	4:D:111:DC:H42	1.22	0.86

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-1 Atom-2		Clash overlap (Å)
1:C:101:DG:O6	4:D:114:DC:N4[7_444]	2.12	0.08

### 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 (i)

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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

## 6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

## 6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

