

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

#### Oct 14, 2023 – 05:45 PM EDT

PDB ID	:	8D93
Title	:	[2T7] Self-assembling tensegrity triangle with R3 symmetry at 2.96 A resolu-
		tion, update and junction cut for entry 3GBI
Authors	:	Vecchioni, S.; Woloszyn, K.; Lu, B.; Sha, R.; Ohayon, Y.P.; Seeman, N.C.
Deposited on		
Resolution	:	2.96  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:

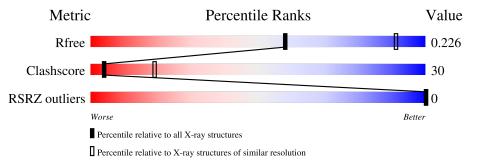
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)		
Ideal geometry (DNA, RNA)		
Validation Pipeline (wwPDB-VP)	:	2.36

# 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 2.96 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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% 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	А	12	42%	58%					
2	В	7	14%	86%					
3	С	14	7%	79%	14%				
4	D	9	33%	67%					



## 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 855 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(\*GP\*AP\*GP\*CP\*AP\*GP\*CP\*CP\*TP\*GP\* TP\*A)-3').

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	А	12	Total 245	C 117	N 48	O 69	Р 11	0	0	0

• Molecule 2 is a DNA chain called DNA (5'-D(P\*AP\*CP\*AP\*CP\*CP\*GP\*T)-3').

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	В	7	Total	C 67	11	O 41	P 7	0	0	0
			141	07	26	41	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	С	14	Total 285	C 137	N 49	O 86	Р 13	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	9	Total 184	C 87	N 36	O 52	Р 9	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 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(\*GP\*AP\*GP\*CP\*AP\*GP\*CP\*CP\*TP\*GP\*TP\*A)-3')

Chain A:		42%		58%	-
G101 A102 G103 G104 A105 G106 C107 C107	T109 G110 T111 A112				
• Molecule	2: DNA	(5'-D(P*AP*CP*	AP*CP*CP*GF	<b>P*</b> T)-3')	
Chain B:	14%		86%		-
A105 A106 A107 C111 C112 C112 C112 C113 T114					
• Molecule	3: DNA	(5'-D(*TP*CP*T	P*GP*AP*TP*	GP*TP*GP*GP*CI	P*TP*GP*C)-3')
Chain C:	7%		79%	14%	-
T101 C102 T103 G104 A105 T106 G107 T108	6109 6110 7111 61112 6113 C114				
• Molecule	4: DNA	(5'-D(P*CP*GP*	GP*AP*CP*AF	D*TP*CP*A)-3')	
Chain D:	33	3%	679	%	-
C113 G114 G115 A116 T119 C120 A121					



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants	105.55Å $105.55$ Å $96.27$ Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.29 - 2.96	Depositor
Resolution (A)	66.29 - 2.96	EDS
% Data completeness	40.0 (41.29-2.96)	Depositor
(in resolution range)	$36.1 \ (66.29 - 2.96)$	EDS
R <sub>merge</sub>	(Not available)	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$0.04 (at 2.96 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
D D	0.185 , $0.226$	Depositor
$R, R_{free}$	0.185 , $0.226$	DCC
$R_{free}$ test set	176 reflections $(5.27\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	39.5	Xtriage
Anisotropy	0.591	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.04 , -10.0	EDS
L-test for $twinning^2$	$<  L  > = 0.46, < L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.067 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	855	wwPDB-VP
Average B, all atoms $(Å^2)$	119.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 8.61% 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	Bon	d lengths	Bond angles		
	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	1.12	0/275	1.39	8/423~(1.9%)	
2	В	1.05	1/157~(0.6%)	2.54	4/239~(1.7%)	
3	С	1.07	0/318	1.51	5/490~(1.0%)	
4	D	0.90	0/206	1.05	0/315	
All	All	1.05	1/956~(0.1%)	1.61	17/1467~(1.2%)	

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	В	106	DC	C3'-O3'	-5.01	1.37	1.44

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
2	В	107	DA	OP2-P-O3'	22.46	154.61	105.20
2	В	107	DA	P-O3'-C3'	20.23	143.97	119.70
2	В	107	DA	O3'-P-O5'	-13.83	77.73	104.00
2	В	107	DA	OP1-P-O3'	-11.60	79.69	105.20
3	С	103	DT	O4'-C1'-N1	11.12	115.79	108.00

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	А	245	0	136	12	1
2	В	141	0	79	7	0
3	С	285	0	161	16	2
4	D	184	0	101	7	0
All	All	855	0	477	40	2

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 30.

The worst 5 of 40 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:B:112:DC:H2"	2:B:113:DG:N7	1.89	0.88
1:A:109:DT:H2'	1:A:110:DG:C8	2.16	0.79
4:D:114:DG:H2"	4:D:115:DG:C8	2.24	0.73
1:A:104:DC:H2'	1:A:105:DA:C8	2.24	0.73
3:C:101:DT:H2'	3:C:102:DC:C5	2.26	0.71

All (2) 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)
1:A:101:DG:O6	3:C:102:DC:N4[6_555]	2.11	0.09
3:C:101:DT:O5'	3:C:114:DC:O3'[8_544]	2.16	0.04

### 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)

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,  $95^{th}$  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		RZ>2	$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q < 0.9
1	А	12/12~(100%)	-1.55	0	100	100	91, 140, 153, 165	0
2	В	7/7~(100%)	-1.46	0	100	100	90, 97, 110, 123	0
3	С	14/14~(100%)	-1.40	0	100	100	93, 124, 161, 165	0
4	D	9/9~(100%)	-1.53	0	100	100	93, 99, 103, 113	0
All	All	42/42 (100%)	-1.48	0	100	100	90, 111, 159, 165	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 monosaccharides 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.

