



# wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 7U3P  
Title : [3T7] Self-assembling tensegrity triangle with three turns of DNA per axis with R3 symmetry  
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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](mailto: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>.

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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

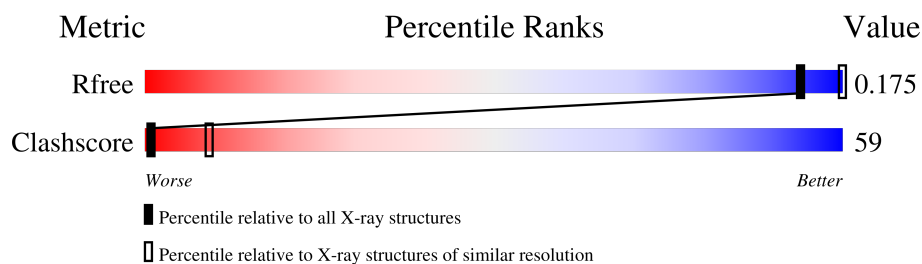
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	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  $\geq 3$ , 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	C	18	17% 83%
2	A	31	6% 42% 52%
3	B	7	14% 86%
4	D	6	100%

## 2 Entry composition

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	Atoms					ZeroOcc	AltConf	Trace
1	C	18	Total	C	N	O	P	0	0	0
			368	176	64	110	18			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	31	Total	C	N	O	P	0	0	0
			635	302	121	182	30			

- 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	B	7	Total	C	N	O	P	0	0	0
			141	67	26	41	7			

- 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	C	N	O	P	0	0	0
			124	58	23	37	6			

### 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. 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\*TP\*GP\*T)-3')

Chain C: 

G101	T102	A103	C104	T105	G106	A107	G108	C109	A110	T111	G112	T113	G114	A115	T116	G117	T118
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- Molecule 2: DNA (31-MER)

Chain A: 

A101	C102	G103	C104	A105	G106	C107	G108	T109	G110	T111	A112	C113	G114	A115	G116	C117	A118	T119	C120	A121	G122	T123	G124	A125	C126	T127	G128	A129	G130	T131
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- Molecule 3: DNA (5'-D(P\*CP\*CP\*GP\*TP\*AP\*CP\*A)-3')

Chain B: 

C101	C102	G103	T104	A105	C106	A107
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- Molecule 4: DNA (5'-D(P\*GP\*GP\*CP\*TP\*GP\*C)-3')

Chain D: 

G109	G110	C111	T112	G113	C114
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## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	159.21Å 159.21Å 127.74Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	37.55 – 6.06 93.71 – 6.06	Depositor EDS
% Data completeness (in resolution range)	64.3 (37.55-6.06) 59.0 (93.71-6.06)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.43 (at 6.19Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, $R_{free}$	0.128 , 0.174 0.125 , 0.175	Depositor DCC
$R_{free}$ test set	118 reflections (5.78%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	440.9	Xtriage
Anisotropy	0.906	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.14 , 999.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	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 <sup>2</sup> )	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>1</sup>Intensities estimated from amplitudes.

<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.

## 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	C	2.34	21/411 (5.1%)	2.02	20/632 (3.2%)
2	A	2.23	23/713 (3.2%)	1.85	24/1099 (2.2%)
3	B	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	Observed(Å)	Ideal(Å)
2	A	112	DA	C3'-O3'	18.64	1.68	1.44
1	C	117	DG	C3'-O3'	12.20	1.59	1.44
2	A	113	DC	P-O5'	11.51	1.71	1.59
2	A	124	DT	C1'-N1	10.52	1.62	1.49
2	A	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	Observed(°)	Ideal(°)
2	A	113	DC	O5'-P-OP2	12.74	125.99	110.70
2	A	113	DC	OP1-P-OP2	-10.80	103.41	119.60
1	C	108	DG	O4'-C4'-C3'	-10.64	99.62	106.00
1	C	108	DG	O4'-C1'-N9	10.31	115.22	108.00
2	A	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

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	C	368	0	205	30	1
2	A	635	0	349	64	0
3	B	141	0	79	21	0
4	D	124	0	68	17	1
All	All	1268	0	701	113	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 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-2	Interatomic distance (Å)	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 ⓘ

### 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.