



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 15, 2023 – 01:50 PM EDT

PDB ID : 8DAG  
Title : [8 bp center] Self-Assembled 3D DNA Hexagonal Tensegrity Triangle  
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Deposited on : 2022-06-13  
Resolution : 6.16 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 : 2.36  
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



## 2 Entry composition

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\*TP\*GP\*TP\*GP\*AP\*CP\*GP\*GP\*AP\*CP\*AP\*TP\*CP\*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	21	432	205	86	121	20	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	8	160	76	29	47	8	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	C	5	102	48	18	31	5	0	0	0

- Molecule 4 is a DNA chain called DNA (5'-D(\*TP\*CP\*TP\*GP\*AP\*TP\*GP\*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
4	D	8	161	79	26	49	7	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(\*GP\*AP\*GP\*CP\*AP\*GP\*CP\*TP\*GP\*TP\*GP\*AP\*CP\*GP\*GP\*AP\*CP\*AP\*TP\*CP\*A)-3')

Chain A:  71% 29%

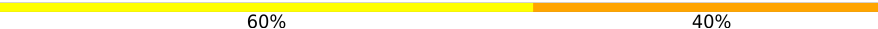


- Molecule 2: DNA (5'-D(P\*CP\*CP\*GP\*TP\*CP\*AP\*CP\*A)-3')

Chain B:  12% 62% 25%



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

Chain C:  60% 40%



- Molecule 4: DNA (5'-D(\*TP\*CP\*TP\*GP\*AP\*TP\*GP\*T)-3')

Chain D:  12% 12% 75%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	130.43Å 130.43Å 53.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.69 – 6.16 65.21 – 6.16	Depositor EDS
% Data completeness (in resolution range)	81.5 (42.69-6.16) 72.6 (65.21-6.16)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.58 (at 6.17Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.120 , 0.127 0.121 , 0.126	Depositor DCC
$R_{free}$ test set	36 reflections (3.42%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	374.3	Xtrriage
Anisotropy	0.995	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.95 , -10.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	0.125 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	855	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	684.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.05% 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	A	1.51	5/486 (1.0%)	1.48	7/749 (0.9%)
2	B	1.33	1/178 (0.6%)	1.34	2/271 (0.7%)
3	C	1.39	1/113 (0.9%)	1.51	1/172 (0.6%)
4	D	1.42	2/179 (1.1%)	1.61	6/275 (2.2%)
All	All	1.45	9/956 (0.9%)	1.49	16/1467 (1.1%)

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	104	DC	C3'-O3'	7.87	1.54	1.44
1	A	104	DC	C1'-N1	7.68	1.59	1.49
1	A	106	DG	N9-C4	6.10	1.42	1.38
1	A	107	DC	C1'-N1	5.92	1.56	1.49
2	B	125	DC	C3'-O3'	-5.91	1.36	1.44

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	102	DA	O5'-P-OP1	-8.17	98.35	105.70
1	A	101	DG	O4'-C1'-N9	7.54	113.28	108.00
1	A	118	DA	O4'-C1'-N9	-6.44	103.49	108.00
1	A	109	DG	O4'-C1'-N9	6.42	112.49	108.00
4	D	206	DT	C1'-O4'-C4'	-5.81	104.29	110.10

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	432	0	236	40	1
2	B	160	0	90	14	0
3	C	102	0	57	22	0
4	D	161	0	94	12	1
All	All	855	0	477	80	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 61.

The worst 5 of 80 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)
1:A:109:DG:H2'	1:A:110:DT:C6	2.03	0.94
3:C:210:DG:H2'	3:C:211:DC:C6	2.05	0.92
2:B:119:DC:H2'	2:B:120:DC:C6	2.14	0.82
1:A:108:DT:H2'	1:A:109:DG:H8	1.46	0.80
4:D:207:DG:H2'	4:D:208:DT:H71	1.64	0.79

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:A:101:DG:O6	4:D:202:DC:N4[6_554]	2.19	0.01

## 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.