



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 22, 2026 – 11:24 AM EDT

PDB ID : 8CS2 / pdb\_00008cs2  
Title : [(1AP)G/TC] Self-Assembled 3D DNA Hexagonal Tensegrity Triangle  
Authors : Lu, B.; Vecchioni, S.; Ohayon, Y.P.; Seeman, N.C.; Mao, C.; Sha, R.  
Deposited on : 2022-05-12  
Resolution : 6.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 2.0  
EDS : **FAILED**  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

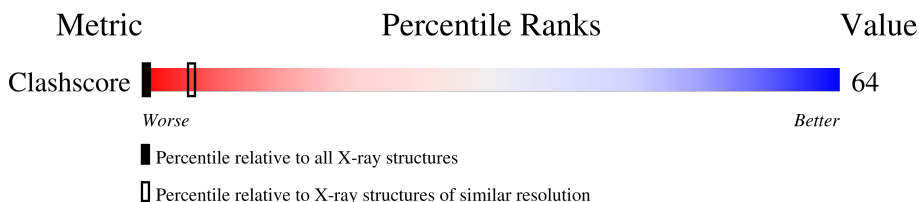
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 6.00 Å.


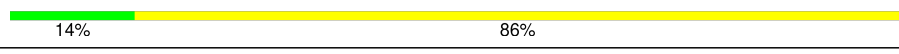
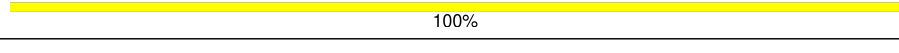
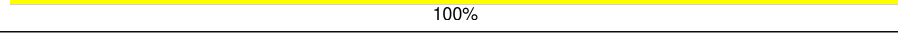
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1210 (8.00-4.00)

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  $\geq 3$ , 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  $\leq 5\%$

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	21	 86% 14%
2	B	7	 14% 86%
3	C	6	 100%
4	D	8	 100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	1AP	A	101	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 856 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>(\* (1AP)P\*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
			Total	C	N	O	P			
1	A	21	430	204	85	121	20	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	7	141	67	26	41	7	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	C	6	124	58	23	37	6	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

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.

Note EDS failed to run properly.

- Molecule 1: DNA (5'-D(\*(1AP)P\*GP\*GP\*CP\*AP\*GP\*CP\*CP\*TP\*GP\*TP\*AP\*CP\*GP\*GP\*AP\*CP\*AP\*TP\*CP\*A)-3')

Chain A: 

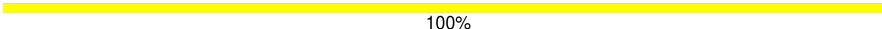
A101	G102	G103	C104	A105	G106	C107	C108	T109	G110	T111	A112	C113	G114	G115	A116	C117	A118	T119	C120	A121
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

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

Chain B: 

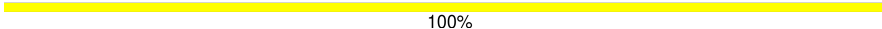
C119	C120	G121	T122	A123	C124	A125
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- Molecule 3: DNA (5'-D(P\*GP\*GP\*CP\*TP\*GP\*C)-3')

Chain C: 

G209	G210	C211	T212	G213	C214
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- Molecule 4: DNA (5'-D(\*TP\*CP\*TP\*GP\*AP\*TP\*GP\*T)-3')

Chain D: 

T201	C202	T203	G204	A205	T206	G207	T208
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## 4 Data and refinement statistics i

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	123.97Å 123.97Å 64.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.17 – 6.00	Depositor
% Data completeness (in resolution range)	76.3 (41.17-6.00)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	-0.04 (at 6.17Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.111 , 0.200	Depositor
Wilson B-factor (Å <sup>2</sup> )	361.6	Xtrriage
Anisotropy	0.920	Xtrriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.111 for h,-h-k,-l	Xtrriage
Total number of atoms	856	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	627.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.56% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 1AP

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	0.96	1/461 (0.2%)	1.04	1/709 (0.1%)
2	B	0.89	0/157	0.95	0/239
3	C	0.76	0/138	1.01	0/211
4	D	0.98	0/179	1.25	0/275
All	All	0.92	1/935 (0.1%)	1.07	1/1434 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	113	DC	C1'-N1	-5.02	1.34	1.49

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	120	DC	C3'-C2'-C1'	-5.09	93.96	101.60

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	236	45	1
2	B	141	0	79	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	124	0	68	16	0
4	D	161	0	94	17	1
All	All	856	0	477	75	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 64.

All (75) 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:108:DC:H42	3:C:209:DG:H1	1.22	0.85
1:A:101:1AP:H31	1:A:102:DG:H5''	1.62	0.82
1:A:107:DC:O2	1:A:108:DC:N4	2.15	0.80
1:A:111:DT:H2''	1:A:112:DA:C8	2.23	0.73
1:A:107:DC:O2	3:C:210:DG:N2	2.22	0.73
4:D:201:DT:H1'	4:D:202:DC:C6	2.25	0.71
1:A:102:DG:H5''	1:A:102:DG:H8	1.56	0.71
1:A:102:DG:H2'	1:A:103:DG:C8	2.27	0.69
1:A:113:DC:H1'	1:A:114:DG:C8	2.34	0.63
1:A:115:DG:C4	1:A:116:DA:N7	2.67	0.63
1:A:104:DC:H1'	1:A:105:DA:C8	2.35	0.61
2:B:119:DC:OP2	2:B:120:DC:H5	1.84	0.61
4:D:205:DA:H4'	4:D:206:DT:H5'	1.83	0.60
1:A:112:DA:H1'	1:A:113:DC:H5'	1.84	0.59
3:C:210:DG:H2'	3:C:211:DC:C6	2.37	0.59
4:D:201:DT:C6	4:D:202:DC:C4	2.91	0.58
1:A:110:DG:H2''	1:A:111:DT:C6	2.40	0.56
1:A:118:DA:C6	1:A:119:DT:C4	2.93	0.56
1:A:104:DC:H2''	1:A:105:DA:C8	2.40	0.56
1:A:113:DC:H1'	1:A:114:DG:N7	2.21	0.56
1:A:101:1AP:H51	1:A:102:DG:C8	2.41	0.56
1:A:115:DG:C2	1:A:116:DA:C5	2.95	0.55
1:A:115:DG:N3	1:A:116:DA:C8	2.74	0.55
1:A:112:DA:H2''	1:A:113:DC:O5'	2.07	0.54
4:D:201:DT:H1'	4:D:202:DC:N1	2.22	0.54
1:A:105:DA:C2	3:C:213:DG:N2	2.76	0.53
2:B:125:DA:H2'	2:B:125:DA:OP2	2.09	0.53
1:A:110:DG:H2''	1:A:111:DT:H5''	1.91	0.52
4:D:201:DT:H2''	4:D:202:DC:C5	2.44	0.52
4:D:205:DA:H4'	4:D:206:DT:C5'	2.39	0.52
1:A:105:DA:C4	1:A:106:DG:C8	2.97	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:201:DT:C4'	4:D:202:DC:H5'	2.40	0.52
1:A:102:DG:H5''	1:A:102:DG:C8	2.42	0.51
4:D:204:DG:H2''	4:D:205:DA:C8	2.45	0.51
3:C:212:DT:H3'	3:C:213:DG:C8	2.46	0.51
1:A:115:DG:N3	1:A:116:DA:N7	2.59	0.50
1:A:101:1AP:H31	1:A:102:DG:C5'	2.37	0.49
1:A:110:DG:C3'	1:A:111:DT:H5''	2.43	0.48
1:A:108:DC:N4	3:C:209:DG:H22	2.10	0.48
1:A:108:DC:N4	3:C:209:DG:H1	2.02	0.48
2:B:125:DA:H1'	3:C:209:DG:O4'	2.13	0.48
4:D:207:DG:C8	4:D:208:DT:H72	2.49	0.47
4:D:204:DG:C6	4:D:205:DA:C6	3.02	0.47
1:A:115:DG:H1'	1:A:116:DA:C8	2.49	0.47
1:A:118:DA:C2	1:A:119:DT:C2	3.03	0.47
4:D:201:DT:C2	4:D:202:DC:C2	3.02	0.47
1:A:106:DG:H2''	1:A:107:DC:O5'	2.16	0.46
1:A:109:DT:C4	3:C:209:DG:N2	2.84	0.46
1:A:113:DC:C2	1:A:114:DG:C6	3.04	0.46
2:B:124:DC:C4	2:B:125:DA:N6	2.84	0.46
4:D:204:DG:C5	4:D:205:DA:C6	3.04	0.45
4:D:204:DG:C5	4:D:205:DA:C5	3.05	0.45
1:A:119:DT:C2	1:A:120:DC:C4	3.05	0.45
1:A:120:DC:N4	1:A:121:DA:N6	2.65	0.45
4:D:203:DT:O4'	4:D:203:DT:OP2	2.36	0.44
4:D:203:DT:H6	4:D:203:DT:H2'	1.47	0.44
1:A:104:DC:H4'	1:A:105:DA:OP1	2.15	0.44
2:B:121:DG:H1'	2:B:122:DT:H5'	2.00	0.43
4:D:201:DT:O4'	4:D:202:DC:H5'	2.17	0.43
4:D:204:DG:C8	4:D:205:DA:N7	2.86	0.43
2:B:119:DC:OP2	2:B:120:DC:C5	2.68	0.43
1:A:111:DT:H2''	1:A:112:DA:N7	2.34	0.43
3:C:210:DG:C6	3:C:211:DC:N4	2.87	0.42
1:A:101:1AP:C4	1:A:102:DG:C8	3.03	0.42
1:A:114:DG:N1	2:B:121:DG:N2	2.68	0.42
1:A:110:DG:C2'	1:A:111:DT:H5''	2.49	0.41
1:A:108:DC:H42	3:C:209:DG:H22	1.68	0.41
1:A:101:1AP:C4	1:A:102:DG:N7	2.83	0.41
3:C:213:DG:O5'	3:C:213:DG:H8	2.04	0.41
1:A:101:1AP:C5	1:A:102:DG:C5	3.04	0.41
3:C:211:DC:H2'	3:C:212:DT:C6	2.56	0.41
3:C:212:DT:C5'	3:C:212:DT:H6	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:DT:N3	3:C:209:DG:N2	2.68	0.40
1:A:116:DA:C6	1:A:117:DC:N3	2.89	0.40
3:C:213:DG:C4	3:C:214:DC:C6	3.09	0.40

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:101:1AP:N6	4:D:202:DC:C2[6_554]	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](#)

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	1AP	A	101	1,4	21,21,25	3.58	8 (38%)	31,31,38	4.89	12 (38%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	1AP	A	101	1,4	-	2/6/18/22	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	101	1AP	O4'-C4'	8.21	1.63	1.45
1	A	101	1AP	C3'-C4'	-7.47	1.33	1.53
1	A	101	1AP	C2-N2	6.49	1.46	1.33
1	A	101	1AP	O3'-C3'	5.38	1.54	1.43
1	A	101	1AP	C6-N6	5.21	1.47	1.34
1	A	101	1AP	O4'-C1'	-4.51	1.32	1.42
1	A	101	1AP	C5-C4	-2.13	1.35	1.39
1	A	101	1AP	C8-N7	2.08	1.35	1.31

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	1AP	N2-C2-N3	17.00	142.71	117.22
1	A	101	1AP	N2-C2-N1	-13.25	97.35	117.22
1	A	101	1AP	C1'-N9-C8	-9.89	92.37	126.95
1	A	101	1AP	C4-N9-C1'	7.79	157.74	126.50
1	A	101	1AP	N9-C8-N7	-4.97	106.89	113.94
1	A	101	1AP	C5-C4-N3	-3.95	123.02	127.18
1	A	101	1AP	C4-N9-C8	3.92	109.86	105.74
1	A	101	1AP	C2-N1-C6	3.74	121.77	117.28
1	A	101	1AP	N3-C2-N1	-3.62	119.94	125.48
1	A	101	1AP	C5-N7-C8	2.75	107.78	103.45
1	A	101	1AP	N3-C4-N9	2.52	130.19	126.99
1	A	101	1AP	C2'-C1'-N9	-2.36	109.08	114.63

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	101	1AP	C2'-C1'-N9-C4
1	A	101	1AP	C2'-C1'-N9-C8

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	101	1AP	6	1

## 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](#)

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

EDS failed to run properly - this section is therefore empty.

### 6.4 Ligands [i](#)

EDS failed to run properly - this section is therefore empty.

### 6.5 Other polymers [i](#)

EDS failed to run properly - this section is therefore empty.