



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:39 PM UTC

PDB ID : 8SJU / pdb_00008sju
Title : [4T17] Self-assembling right-handed four-turn tensegrity triangle with 17 interjunction base pairs and R3 symmetry
Authors : Janowski, J.; Vecchioni, S.; Sha, R.; Ohayon, Y.P.
Deposited on : 2023-04-18
Resolution : 7.14 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

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>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

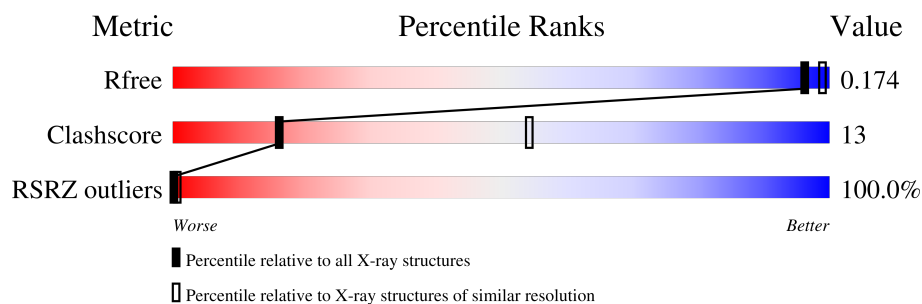
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 7.14 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}	180053	1167 (10.00-4.00)
Clashscore	190562	1000 (10.00-4.06)
RSRZ outliers	180081	1161 (10.00-4.00)

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 ≥ 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 $\leq 5\%$. 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	A	24	100% 21% 79%
2	B	17	100% 53% 47%
3	C	25	100% 24% 76%
4	D	18	100% 89% 11%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 1716 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*AP*AP*AP*AP*CP*AP*CP*TP*GP*CP*CP*TP*GP*AP*AP*TP*AP*CP*CP*GP*CP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	24	Total	C	N	O	P	0	0	0
			488	233	97	135	23			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	17	Total	C	N	O	P	0	0	0
			347	165	63	102	17			

- Molecule 3 is a DNA chain called DNA (25-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	25	Total	C	N	O	P	0	0	0
			511	247	83	157	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	18	Total	C	N	O	P	0	0	0
			370	176	70	106	18			

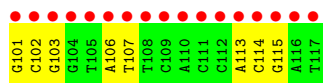
3 Residue-property plots

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



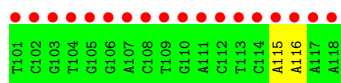
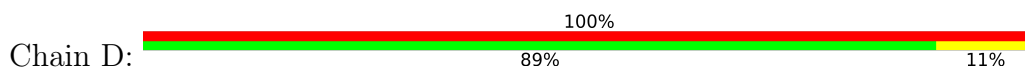
- Molecule 2: DNA (5'-D(P*GP*CP*GP*GP*TP*AP*TP*TP*CP*AP*CP*CP*AP*CP*GP*A P*T)-3')



- Molecule 3: DNA (25-MER)



- Molecule 4: DNA (5'-D(P*TP*CP*GP*TP*GP*GP*AP*CP*TP*GP*AP*CP*TP*CP*AP*A P*AP*A)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	224.53Å 224.53Å 126.52Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	37.17 – 7.14 37.17 – 7.14	Depositor EDS
% Data completeness (in resolution range)	68.2 (37.17-7.14) 62.2 (37.17-7.14)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	-0.12 (at 6.72Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.111 , 0.177 0.113 , 0.174	Depositor DCC
R_{free} test set	117 reflections (3.10%)	wwPDB-VP
Wilson B-factor (Å ²)	272.6	Xtriage
Anisotropy	1.236	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	3.59 , 999.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.057 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	1716	wwPDB-VP
Average B, all atoms (Å ²)	912.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.17	0/549	0.37	0/844
2	B	0.16	0/388	0.34	0/596
3	C	0.21	0/570	0.44	0/880
4	D	0.18	0/415	0.37	0/638
All	All	0.18	0/1922	0.39	0/2958

There are no bond length outliers.

There are no bond angle outliers.

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	488	0	269	15	0
2	B	347	0	192	6	0
3	C	511	0	289	13	0
4	D	370	0	203	1	0
All	All	1716	0	953	35	0

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 13.

All (35) 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)
3:C:117:DC:H2'	3:C:118:DA:C8	2.24	0.72
1:A:108:DA:H2''	1:A:109:DC:H5''	1.70	0.72
1:A:117:DA:H2''	1:A:118:DT:H5''	1.72	0.71
1:A:114:DT:H2'	1:A:115:DG:C8	2.35	0.62
3:C:107:DG:H2''	3:C:108:DA:C8	2.35	0.61
3:C:115:DG:H2'	3:C:116:DG:C8	2.35	0.60
3:C:110:DT:H2'	3:C:111:DC:C6	2.37	0.60
3:C:108:DA:H2''	3:C:109:DG:H5''	1.84	0.60
2:B:102:DC:H2''	2:B:103:DG:C8	2.37	0.59
2:B:106:DA:H2''	2:B:107:DT:H5''	1.85	0.58
1:A:105:DA:H2''	1:A:106:DA:C8	2.39	0.58
2:B:101:DG:H2''	2:B:102:DC:H5''	1.87	0.56
1:A:115:DG:H2'	1:A:116:DA:C8	2.41	0.56
3:C:113:DG:H2''	3:C:114:DT:H5'	1.87	0.56
3:C:122:DT:H2''	3:C:123:DT:C6	2.41	0.56
1:A:118:DT:H2''	1:A:119:DA:H5''	1.87	0.55
1:A:102:DA:H2''	1:A:103:DA:H5''	1.90	0.54
3:C:102:DC:H2''	3:C:103:DT:H5''	1.90	0.53
4:D:115:DA:H2''	4:D:116:DA:C8	2.44	0.52
1:A:112:DC:H2''	1:A:113:DC:H5'	1.92	0.51
1:A:121:DC:H2''	1:A:122:DG:H5''	1.92	0.50
3:C:120:DT:H2'	3:C:121:DG:O4'	2.12	0.50
3:C:117:DC:H2'	3:C:118:DA:H8	1.72	0.48
1:A:122:DG:H2''	1:A:123:DC:C2	2.49	0.47
1:A:104:DA:H2''	1:A:105:DA:C8	2.50	0.47
3:C:119:DG:H2'	3:C:120:DT:H71	1.96	0.47
1:A:101:DG:C2	1:A:102:DA:C5	3.04	0.45
2:B:113:DA:H2''	2:B:114:DC:C5	2.51	0.44
1:A:116:DA:H2''	1:A:117:DA:C8	2.52	0.44
3:C:116:DG:H2''	3:C:117:DC:H6	1.84	0.42
2:B:114:DC:H2''	2:B:115:DG:H5''	2.01	0.42
1:A:114:DT:H2'	1:A:115:DG:O4'	2.21	0.41
2:B:103:DG:C8	2:B:103:DG:H5'	2.55	0.41
1:A:114:DT:C2	1:A:115:DG:C8	3.09	0.41
3:C:112:DA:C2	3:C:113:DG:C5	3.09	0.41

There are no symmetry-related clashes.

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 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

6.1 Protein, DNA and RNA chains

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, 95th 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	OWAB(Å ²)	Q<0.9
1	A	24/24 (100%)	4.66	24 (100%) 0 1	720, 935, 1058, 1071	0
2	B	17/17 (100%)	4.18	17 (100%) 0 1	787, 925, 1003, 1021	0
3	C	25/25 (100%)	4.65	25 (100%) 0 1	694, 874, 1051, 1099	0
4	D	18/18 (100%)	4.58	18 (100%) 0 1	689, 953, 1070, 1113	0
All	All	84/84 (100%)	4.54	84 (100%) 0 1	689, 927, 1058, 1113	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	112	DA	7.2
1	A	107	DC	6.9
3	C	108	DA	6.4
1	A	117	DA	6.4
4	D	109	DT	6.2
2	B	108	DT	6.2
3	C	121	DG	6.0
3	C	111	DC	6.0
3	C	118	DA	6.0
4	D	116	DA	6.0
2	B	109	DC	5.9
2	B	106	DA	5.9
4	D	115	DA	5.8
1	A	108	DA	5.8
3	C	125	DT	5.8
1	A	116	DA	5.7
1	A	105	DA	5.7
3	C	102	DC	5.5
1	A	106	DA	5.5
3	C	117	DC	5.4
3	C	123	DT	5.4

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Mol	Chain	Res	Type	RSRZ
4	D	117	DA	5.2
1	A	104	DA	5.2
3	C	116	DG	5.1
1	A	123	DC	5.0
1	A	102	DA	4.9
4	D	106	DG	4.9
4	D	104	DT	4.9
4	D	105	DG	4.8
4	D	114	DC	4.8
1	A	118	DT	4.8
1	A	119	DA	4.8
2	B	114	DC	4.6
1	A	120	DC	4.6
2	B	107	DT	4.6
3	C	124	DT	4.6
3	C	104	DT	4.5
4	D	113	DT	4.5
3	C	113	DG	4.5
4	D	118	DA	4.5
1	A	124	DA	4.5
3	C	109	DG	4.5
3	C	103	DT	4.3
4	D	111	DA	4.3
3	C	120	DT	4.3
1	A	103	DA	4.3
4	D	103	DG	4.2
1	A	113	DC	4.2
4	D	101	DT	4.2
1	A	110	DT	4.1
2	B	102	DC	4.1
1	A	112	DC	4.1
2	B	112	DC	4.1
4	D	110	DG	4.1
1	A	122	DG	4.0
2	B	110	DA	3.9
2	B	105	DT	3.9
4	D	112	DC	3.9
1	A	111	DG	3.9
2	B	115	DG	3.9
1	A	115	DG	3.8
3	C	122	DT	3.8
4	D	108	DC	3.8

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Mol	Chain	Res	Type	RSRZ
3	C	107	DG	3.8
2	B	113	DA	3.7
1	A	109	DC	3.7
2	B	117	DT	3.7
3	C	101	DT	3.7
2	B	103	DG	3.5
3	C	119	DG	3.5
1	A	101	DG	3.4
3	C	115	DG	3.4
3	C	106	DT	3.4
1	A	121	DC	3.4
2	B	111	DC	3.4
4	D	107	DA	3.4
2	B	104	DG	3.3
1	A	114	DT	3.3
3	C	110	DT	3.2
3	C	105	DT	3.2
2	B	116	DA	3.2
2	B	101	DG	3.1
3	C	114	DT	3.0
4	D	102	DC	3.0

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 oligosaccharides 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.