



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:00 PM UTC

PDB ID : 9Q5K / pdb_00009q5k
Title : [23-7B C|A] 23 bp tensegrity triangle that propagates via blunt-end stacking with C stacking on A at the interface
Authors : Horvath, A.; Woloszyn, K.; Vecchioni, S.; Ohayon, Y.P.; Sha, R.
Deposited on : 2025-08-20
Resolution : 9.96 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

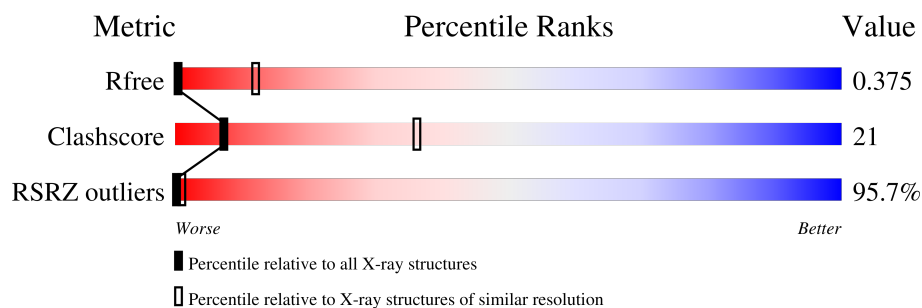
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 9.96 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1168 (11.50-4.00)
Clashscore	190562	1002 (15.00-4.06)
RSRZ outliers	180081	1162 (11.50-4.00)

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	23	83% 22% 78%
1	E	23	100% 17% 83%
2	B	7	100% 29% 71%
2	F	7	100% 71% 29%
3	C	8	100% 38% 62%
3	G	8	100% 12% 88%
4	D	8	100% 38% 62%

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Mol	Chain	Length	Quality of chain
4	H	8	 A horizontal bar chart showing the quality of chain H. The bar is divided into three segments: green (25%), yellow (75%), and red (100%). The segments are labeled with their respective percentages: 25%, 75%, and 100%.

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 1865 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(*CP*GP*AP*CP*TP*GP*CP*CP*TP*GP*TP*AP*CP*GP*GP*AP*CP*AP*GP*AP*TP*CP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	23	Total	C	N	O	P	0	0	0
			468	223	89	134	22			
1	E	23	Total	C	N	O	P	0	0	0
			468	223	89	134	22			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	7	Total	C	N	O	P	0	0	0
			138	67	26	39	6			
2	F	7	Total	C	N	O	P	0	0	0
			138	67	26	39	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	8	Total	C	N	O	P	0	0	0
			167	78	33	48	8			
3	G	8	Total	C	N	O	P	0	0	0
			164	78	33	46	7			

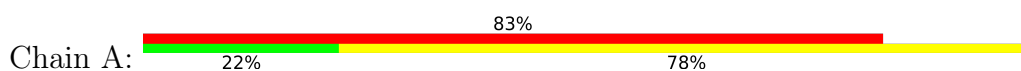
- Molecule 4 is a DNA chain called DNA (5'-D(*TP*GP*AP*TP*CP*TP*GP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	8	Total	C	N	O	P	0	0	0
			161	79	26	49	7			
4	H	8	Total	C	N	O	P	0	0	0
			161	79	26	49	7			

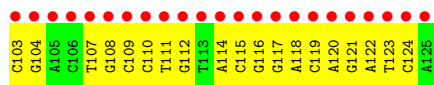
3 Residue-property plots

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.

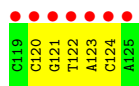
- Molecule 1: DNA (5'-D(*CP*GP*AP*CP*TP*GP*CP*CP*TP*GP*TP*AP*CP*GP*GP*AP*CP*AP*GP*AP*TP*CP*A)-3')



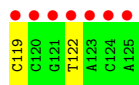
- Molecule 1: DNA (5'-D(*CP*GP*AP*CP*TP*GP*CP*CP*TP*GP*TP*AP*CP*GP*GP*AP*CP*AP*GP*AP*TP*CP*A)-3')



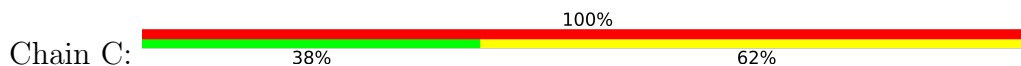
- Molecule 2: DNA (5'-D(*CP*CP*GP*TP*AP*CP*A)-3')



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



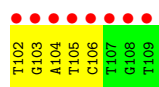
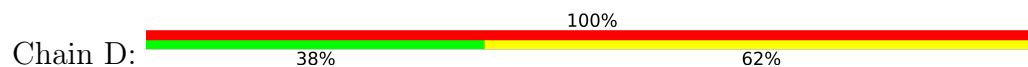
- Molecule 3: DNA (5'-D(P*GP*GP*CP*AP*GP*TP*CP*G)-3')



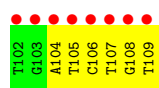
- Molecule 3: DNA (5'-D(P*GP*GP*CP*AP*GP*TP*CP*G)-3')



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 3 2	Depositor
Cell constants a, b, c, α , β , γ	183.14Å 183.14Å 183.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	64.75 – 9.96 64.75 – 9.96	Depositor EDS
% Data completeness (in resolution range)	91.0 (64.75-9.96) 79.9 (64.75-9.96)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.282 , 0.355 0.300 , 0.375	Depositor DCC
R_{free} test set	30 reflections (4.28%)	wwPDB-VP
Wilson B-factor (Å ²)	(Not available)	Xtriage
Anisotropy	(Not available)	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.59 , 0.0	EDS
L-test for twinning ¹	$\langle L \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.51	EDS
Total number of atoms	1865	wwPDB-VP
Average B, all atoms (Å ²)	1238.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *(Not available)*

¹Theoretical 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	0.35	0/525	0.59	0/808
1	E	0.33	0/525	0.61	0/808
2	B	0.33	0/154	0.62	0/235
2	F	0.37	0/154	0.64	0/235
3	C	0.29	0/187	0.55	0/287
3	G	0.32	0/184	0.67	0/283
4	D	0.35	0/179	0.67	0/275
4	H	0.29	0/179	0.61	0/275
All	All	0.33	0/2087	0.61	0/3206

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	468	0	259	16	0
1	E	468	0	259	21	0
2	B	138	0	80	5	0
2	F	138	0	80	2	0
3	C	167	0	90	4	0
3	G	164	0	91	5	0
4	D	161	0	94	4	0
4	H	161	0	94	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	1865	0	1047	60	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 21.

All (60) 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:E:107:DT:H2''	1:E:108:DG:C8	2.20	0.77
2:B:122:DT:H2''	2:B:123:DA:C8	2.23	0.73
2:B:123:DA:H2''	2:B:124:DC:C5	2.25	0.71
4:D:104:DA:H2'	4:D:105:DT:H71	1.72	0.70
3:G:211:DC:H2''	3:G:212:DA:N7	2.06	0.69
1:A:111:DT:H2''	1:A:112:DG:C8	2.30	0.67
1:E:119:DC:H2''	1:E:120:DA:N7	2.10	0.67
3:G:211:DC:H2''	3:G:212:DA:C8	2.31	0.65
2:B:120:DC:H2''	2:B:121:DG:N7	2.11	0.65
1:E:119:DC:H2''	1:E:120:DA:C8	2.32	0.64
1:A:113:DT:H2''	1:A:114:DA:N7	2.14	0.63
1:E:107:DT:H2''	1:E:108:DG:N7	2.15	0.61
1:A:118:DA:H2''	1:A:119:DC:H5'	1.83	0.61
1:A:121:DG:H2''	1:A:122:DA:C8	2.36	0.60
3:G:214:DT:H2''	3:G:215:DC:C6	2.37	0.60
1:E:103:DC:H2''	1:E:104:DG:C8	2.37	0.60
3:C:209:DG:H3'	3:C:210:DG:H8	1.67	0.58
4:H:107:DT:H2''	4:H:108:DG:N7	2.20	0.56
4:D:104:DA:H2''	4:D:105:DT:H2'	1.88	0.56
4:D:105:DT:H2''	4:D:106:DC:C5	2.42	0.55
2:B:122:DT:H2''	2:B:123:DA:N7	2.22	0.55
1:A:122:DA:H2'	1:A:123:DT:H71	1.88	0.54
1:E:117:DG:H2''	1:E:118:DA:C8	2.44	0.53
1:A:117:DG:H2''	1:A:118:DA:C8	2.44	0.53
1:A:123:DT:H2''	1:A:124:DC:C6	2.44	0.52
1:E:123:DT:H2''	1:E:124:DC:C6	2.44	0.52
2:B:123:DA:H2''	2:B:124:DC:C6	2.45	0.52
1:A:115:DC:H2''	1:A:116:DG:N7	2.26	0.51
1:E:109:DC:C2	1:E:110:DC:C5	2.99	0.51
1:E:118:DA:H2''	1:E:119:DC:H6	1.75	0.51
1:E:117:DG:H2''	1:E:118:DA:O5'	2.10	0.50
1:E:114:DA:H61	2:F:122:DT:H3	1.60	0.49
1:E:116:DG:H2''	1:E:117:DG:N7	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:122:DA:C8	1:E:123:DT:H72	2.50	0.47
1:E:118:DA:C4	1:E:119:DC:C5	3.03	0.47
1:E:120:DA:H2''	1:E:121:DG:C8	2.50	0.47
1:E:121:DG:H2''	1:E:122:DA:C8	2.50	0.47
2:F:119:DC:O4'	4:H:109:DT:H2''	2.14	0.46
1:E:118:DA:H2''	1:E:119:DC:C6	2.50	0.46
1:E:115:DC:H2''	1:E:116:DG:N7	2.31	0.46
1:E:120:DA:C4	1:E:121:DG:C5	3.04	0.46
4:H:108:DG:H1'	4:H:109:DT:H5'	1.97	0.45
3:C:212:DA:H2''	3:C:213:DG:H8	1.80	0.45
1:A:109:DC:H2''	1:A:110:DC:O5'	2.17	0.44
1:E:111:DT:H2''	1:E:112:DG:C8	2.53	0.44
1:A:117:DG:H2''	1:A:118:DA:H8	1.81	0.43
1:A:112:DG:H2''	1:A:113:DT:C5	2.53	0.43
4:H:106:DC:H2'	4:H:107:DT:H71	2.01	0.43
1:A:118:DA:H2''	1:A:119:DC:C6	2.53	0.43
4:H:104:DA:H2''	4:H:105:DT:O5'	2.19	0.43
1:A:111:DT:H2''	1:A:112:DG:H8	1.82	0.42
1:A:124:DC:C2	1:A:125:DA:C8	3.08	0.42
3:C:213:DG:H2''	3:C:214:DT:OP1	2.19	0.42
3:G:209:DG:O5'	3:G:210:DG:H8	2.02	0.42
4:D:102:DT:H2''	4:D:103:DG:H5'	2.02	0.42
3:C:212:DA:H2''	3:C:213:DG:C8	2.54	0.42
3:G:212:DA:C2	3:G:213:DG:C6	3.08	0.41
1:A:104:DG:H2''	1:A:105:DA:C8	2.56	0.41
1:E:120:DA:C6	1:E:121:DG:C6	3.09	0.41
1:A:112:DG:H2''	1:A:113:DT:C7	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

There are no protein molecules in this entry.

5.3.2 Protein sidechains ⓘ

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	23/23 (100%)	3.53	19 (82%) 0 1	1053, 1223, 1436, 1529	0
1	E	23/23 (100%)	5.31	23 (100%) 0 1	1109, 1198, 1504, 1601	0
2	B	7/7 (100%)	4.80	7 (100%) 0 1	1174, 1280, 1407, 1419	0
2	F	7/7 (100%)	5.16	7 (100%) 0 1	1064, 1124, 1257, 1265	0
3	C	8/8 (100%)	3.75	8 (100%) 0 1	1132, 1192, 1245, 1354	0
3	G	8/8 (100%)	6.13	8 (100%) 0 1	1060, 1164, 1177, 1228	0
4	D	8/8 (100%)	7.34	8 (100%) 0 1	1066, 1190, 1402, 1572	0
4	H	8/8 (100%)	5.59	8 (100%) 0 1	1008, 1110, 1278, 1395	0
All	All	92/92 (100%)	4.95	88 (95%) 0 1	1008, 1198, 1498, 1601	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	106	DC	11.3
4	H	109	DT	10.7
4	D	107	DT	8.9
4	D	104	DA	8.6
4	D	103	DG	8.6
3	G	213	DG	8.4
1	E	125	DA	8.1
1	E	103	DC	8.0
1	E	111	DT	7.9
3	G	212	DA	7.7
3	G	214	DT	7.6
1	E	112	DG	7.4
1	E	113	DT	7.2
4	D	105	DT	7.1
1	E	118	DA	7.0
2	F	121	DG	7.0

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Mol	Chain	Res	Type	RSRZ
4	H	107	DT	6.7
1	E	104	DG	6.7
2	B	124	DC	6.7
3	G	209	DG	6.2
2	B	121	DG	6.2
1	A	103	DC	6.1
1	A	110	DC	6.1
4	H	106	DC	6.1
4	H	108	DG	6.0
2	F	120	DC	6.0
3	G	210	DG	6.0
1	E	124	DC	5.9
1	E	117	DG	5.8
3	C	213	DG	5.7
4	D	108	DG	5.6
2	F	122	DT	5.6
3	C	216	DG	5.5
1	E	109	DC	5.3
3	G	215	DC	5.3
1	E	120	DA	5.2
1	A	108	DG	5.2
1	A	109	DC	5.0
4	D	102	DT	5.0
2	F	125	DA	5.0
1	E	110	DC	4.9
1	A	104	DG	4.9
1	A	125	DA	4.8
4	H	104	DA	4.8
2	B	122	DT	4.7
1	E	105	DA	4.6
1	A	120	DA	4.6
1	E	119	DC	4.5
2	F	124	DC	4.5
2	B	119	DC	4.5
2	F	119	DC	4.5
1	A	117	DG	4.4
2	B	123	DA	4.3
1	E	106	DC	4.2
1	A	118	DA	4.2
1	E	108	DG	4.2
2	B	125	DA	4.2
3	G	211	DC	4.1

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Mol	Chain	Res	Type	RSRZ
1	E	114	DA	4.1
3	C	210	DG	4.1
4	H	105	DT	4.0
3	C	209	DG	4.0
1	E	123	DT	3.8
1	E	121	DG	3.8
1	E	107	DT	3.7
1	A	124	DC	3.7
1	E	122	DA	3.7
1	A	123	DT	3.6
1	A	121	DG	3.6
3	G	216	DG	3.6
2	F	123	DA	3.6
4	D	109	DT	3.5
4	H	103	DG	3.5
1	A	111	DT	3.4
2	B	120	DC	3.2
1	A	122	DA	3.1
1	E	116	DG	3.0
3	C	215	DC	2.9
4	H	102	DT	2.9
1	E	115	DC	2.9
3	C	214	DT	2.8
1	A	105	DA	2.7
1	A	116	DG	2.7
1	A	119	DC	2.6
3	C	212	DA	2.5
3	C	211	DC	2.4
1	A	114	DA	2.4
1	A	112	DG	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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.