



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 11, 2025 – 04:28 PM EDT

PDB ID : 9PF6 / pdb\_00009pf6  
Title : [A4M] Asymmetric tensegrity triangle with a 4 nucleotide single stranded region on one side  
Authors : Horvath, A.; Wang, M.; Woloszyn, K.; Vecchioni, S.; Ohayon, Y.P.; Sha, R.  
Deposited on : 2025-07-03  
Resolution : 6.83 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 Phenix2.0rc1  
Xtriage (Phenix) : 2.0rc1  
EDS : **FAILED**  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

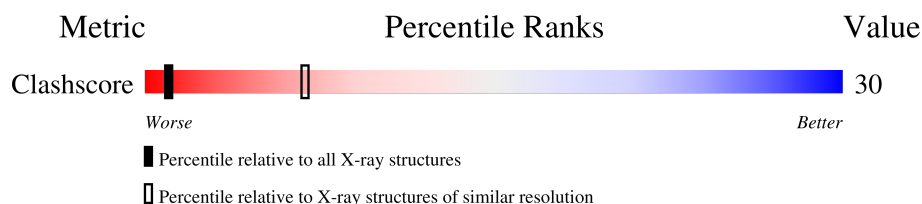
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 6.83 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	180529	1145 (9.50-4.00)

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  $\geq 3$ , 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	
2	E	14	
3	D	14	
4	B	21	
5	F	14	
6	C	21	
7	M	17	

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 2480 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\*GP\*AP\*CP\*CP\*TP\*GP\*TP\*AP\*CP\*GP\*GP\*AP\*CP\*AP\*TP\*CP\*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	21	Total	C	N	O	P	0	0	0
			429	204	84	121	20			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	14	Total	C	N	O	P	0	0	0
			287	137	52	85	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	14	Total	C	N	O	P	0	0	0
			290	139	53	85	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	21	Total	C	N	O	P	0	0	0
			426	203	82	121	20			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	14	Total	C	N	O	P	0	0	0
			285	138	48	86	13			

- Molecule 6 is a DNA chain called DNA (5'-D(\*CP\*AP\*GP\*AP\*TP\*AP\*CP\*CP\*TP\*GP\*AP\*TP\*CP\*GP\*GP\*AP\*CP\*TP\*AP\*CP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	C	21	Total	C	N	O	P	0	0	0
			427	204	81	122	20			

- Molecule 7 is a DNA chain called DNA (5'-D(\*CP\*AP\*CP\*CP\*GP\*AP\*TP\*CP\*AP\*CP\*CP\*TP\*GP\*CP\*CP\*AP\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	M	17	Total	C	N	O	P	0	0	0
			336	161	61	98	16			

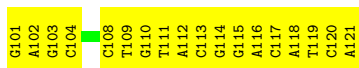
### 3 Residue-property plots

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

Chain A: 



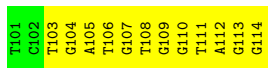
- Molecule 2: DNA (5'-D(\*TP\*GP\*CP\*GP\*TP\*AP\*GP\*TP\*GP\*GP\*TP\*CP\*GP\*C)-3')

Chain E: 



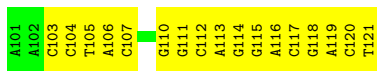
- Molecule 3: DNA (5'-D(\*TP\*CP\*TP\*GP\*AP\*TP\*GP\*TP\*GP\*GP\*TP\*AP\*GP\*G)-3')

Chain D: 



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

Chain B: 

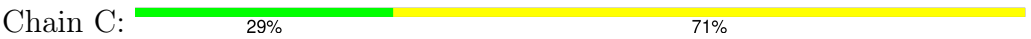


- Molecule 5: DNA (5'-D(\*TP\*TP\*AP\*GP\*TP\*CP\*GP\*TP\*GP\*GP\*TP\*AP\*TP\*C)-3')

Chain F: 



- Molecule 6: DNA (5'-D(\*CP\*AP\*GP\*AP\*TP\*AP\*CP\*CP\*TP\*GP\*AP\*TP\*CP\*GP\*GP\*AP\*CP\*TP\*AP\*CP\*G)-3')



G101	A102	G103	A104	G108	T109	G110	A111	T112	C113	G114	G115	A116	C117	T118	A119	C120	G121
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● Molecule 7: DNA (5'-D(\*CP\*AP\*CP\*CP\*GP\*AP\*TP\*CP\*AP\*CP\*CP\*TP\*GP\*CP\*CP\*AP\*C)-3')



G102	A103	A107	T108	C109	A110	C111	T112	C113	C118
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## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.85Å 68.85Å 69.17Å 105.48° 96.06° 95.90°	Depositor
Resolution (Å)	65.73 – 6.83	Depositor
% Data completeness (in resolution range)	70.4 (65.73-6.83)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.72 (at 6.71Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, $R_{free}$	0.200 , 0.206	Depositor
Wilson B-factor (Å <sup>2</sup> )	112.2	Xtriage
Anisotropy	0.580	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.059 for -h,-l,-k	Xtriage
Total number of atoms	2480	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	593.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.08% 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	0.41	0/482	0.64	0/742
2	E	0.36	0/321	0.65	0/495
3	D	0.37	0/325	0.70	0/502
4	B	0.37	0/478	0.66	0/735
5	F	0.31	0/318	0.66	0/490
6	C	0.35	0/479	0.53	0/737
7	M	0.35	0/375	0.55	0/574
All	All	0.36	0/2778	0.63	0/4275

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	429	0	236	28	0
2	E	287	0	160	8	0
3	D	290	0	161	12	0
4	B	426	0	236	20	0
5	F	285	0	162	17	0
6	C	427	0	237	22	0
7	M	336	0	191	10	0
All	All	2480	0	1383	113	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 30.

All (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)
1:A:103:DG:H2''	1:A:104:DC:H5''	1.56	0.88
1:A:114:DG:H22	7:M:118:DC:H2'	1.41	0.86
5:F:101:DT:H3'	5:F:102:DT:H71	1.63	0.77
1:A:111:DT:H2''	1:A:112:DA:C5'	2.19	0.72
6:C:110:DG:H2'	6:C:111:DA:C8	2.29	0.67
3:D:109:DG:H2'	3:D:110:DG:C8	2.31	0.66
5:F:107:DG:H2''	5:F:108:DT:H5''	1.77	0.66
7:M:108:DT:H2''	7:M:109:DC:C5	2.31	0.66
4:B:114:DG:H2'	4:B:115:DG:C8	2.32	0.65
2:E:109:DG:H2''	2:E:110:DG:H8	1.61	0.65
6:C:112:DT:H2'	6:C:113:DC:C5	2.34	0.63
6:C:111:DA:H2''	6:C:112:DT:H71	1.79	0.63
1:A:103:DG:H2''	1:A:104:DC:C5'	2.29	0.62
5:F:109:DG:H2'	5:F:110:DG:C8	2.35	0.62
6:C:120:DC:H2''	6:C:121:DG:H5''	1.82	0.62
4:B:117:DC:H2''	4:B:118:DG:C8	2.36	0.61
4:B:118:DG:H1'	4:B:119:DA:H5'	1.82	0.61
1:A:112:DA:H1'	1:A:113:DC:H2'	1.83	0.59
3:D:106:DT:C2	3:D:107:DG:C8	2.90	0.59
7:M:108:DT:H2''	7:M:109:DC:H5	1.68	0.58
2:E:109:DG:H2''	2:E:110:DG:C8	2.37	0.58
1:A:115:DG:H2''	1:A:116:DA:O5'	2.02	0.57
2:E:106:DA:H1'	2:E:107:DG:C8	2.40	0.56
1:A:120:DC:H2''	1:A:121:DA:H5''	1.87	0.56
1:A:117:DC:H2'	1:A:118:DA:C8	2.40	0.56
4:B:119:DA:H4'	4:B:120:DC:OP1	2.05	0.56
4:B:112:DC:H2''	4:B:113:DA:C8	2.40	0.56
1:A:113:DC:H2''	1:A:114:DG:C4	2.41	0.55
5:F:104:DG:H4'	5:F:105:DT:H5'	1.89	0.55
1:A:112:DA:H4'	1:A:113:DC:OP1	2.06	0.55
6:C:108:DC:H2'	6:C:109:DT:C6	2.42	0.55
7:M:109:DC:H1'	7:M:110:DA:H5'	1.88	0.54
1:A:101:DG:N3	1:A:101:DG:H2'	2.21	0.54
7:M:107:DA:H1'	7:M:108:DT:H5'	1.88	0.54
6:C:112:DT:H2'	6:C:113:DC:C6	2.43	0.54
1:A:113:DC:H2''	1:A:114:DG:N3	2.23	0.53
5:F:110:DG:H1'	5:F:111:DT:OP1	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:112:DA:H2'	3:D:113:DG:C8	2.44	0.52
5:F:111:DT:H2''	5:F:112:DA:C8	2.44	0.52
2:E:111:DT:H2''	2:E:112:DC:O5'	2.10	0.51
2:E:110:DG:H1'	2:E:111:DT:OP2	2.11	0.51
1:A:113:DC:H4'	1:A:114:DG:O5'	2.10	0.51
1:A:110:DG:H2'	1:A:111:DT:C6	2.46	0.50
1:A:113:DC:H2''	1:A:114:DG:C2	2.46	0.50
6:C:111:DA:H1'	6:C:112:DT:OP2	2.11	0.50
1:A:110:DG:H2'	1:A:111:DT:N1	2.26	0.50
3:D:111:DT:H2''	3:D:112:DA:O5'	2.11	0.50
2:E:104:DG:H2''	2:E:105:DT:H71	1.93	0.50
7:M:111:DC:H3'	7:M:112:DC:O4'	2.12	0.50
5:F:103:DA:H2''	5:F:104:DG:C8	2.47	0.49
1:A:111:DT:H2''	1:A:112:DA:H5''	1.92	0.49
6:C:103:DG:OP1	6:C:103:DG:H8	1.95	0.49
4:B:120:DC:H2''	4:B:121:DT:C5	2.49	0.48
1:A:111:DT:H2''	1:A:112:DA:O5'	2.11	0.48
6:C:116:DA:H2''	6:C:117:DC:C5	2.49	0.48
5:F:110:DG:N2	6:C:108:DC:O2	2.47	0.48
4:B:103:DC:H1'	4:B:104:DC:OP1	2.14	0.48
1:A:112:DA:O3'	1:A:113:DC:H3'	2.15	0.47
1:A:101:DG:H5''	1:A:102:DA:H8	1.80	0.46
6:C:109:DT:H3'	6:C:110:DG:H8	1.81	0.46
2:E:103:DC:C2	2:E:104:DG:C8	3.03	0.46
6:C:115:DG:H4'	6:C:116:DA:OP1	2.16	0.46
1:A:103:DG:H1'	1:A:104:DC:OP1	2.16	0.46
4:B:114:DG:H2''	4:B:115:DG:O4'	2.16	0.46
1:A:102:DA:H1'	1:A:103:DG:P	2.56	0.46
4:B:105:DT:H2''	4:B:106:DA:OP2	2.15	0.46
6:C:103:DG:H2''	6:C:104:DA:H5''	1.98	0.46
3:D:108:DT:H4'	3:D:109:DG:OP2	2.15	0.46
3:D:106:DT:H2''	3:D:107:DG:H8	1.81	0.46
4:B:115:DG:H4'	4:B:116:DA:OP1	2.16	0.46
6:C:109:DT:C2	6:C:110:DG:C8	3.03	0.46
4:B:112:DC:OP1	4:B:112:DC:H6	1.99	0.46
5:F:108:DT:C4	7:M:111:DC:C2	3.04	0.46
4:B:103:DC:H2'	4:B:103:DC:OP1	2.16	0.45
1:A:102:DA:C2	1:A:103:DG:C5	3.04	0.45
5:F:110:DG:H4'	5:F:111:DT:OP2	2.17	0.45
3:D:106:DT:C2'	3:D:107:DG:H8	2.30	0.45
1:A:114:DG:H2''	1:A:115:DG:O4'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:111:DA:H2''	6:C:112:DT:OP1	2.16	0.44
1:A:102:DA:H2''	1:A:103:DG:OP1	2.17	0.44
4:B:110:DG:H8	4:B:110:DG:O5'	2.01	0.44
5:F:109:DG:H2'	5:F:109:DG:N3	2.33	0.44
2:E:105:DT:H2''	2:E:106:DA:N7	2.33	0.44
4:B:118:DG:N1	5:F:107:DG:C2	2.86	0.44
3:D:109:DG:H2'	3:D:110:DG:H8	1.81	0.43
7:M:112:DC:H2'	7:M:113:DT:C5	2.54	0.43
3:D:103:DT:H1'	3:D:104:DG:C8	2.54	0.43
5:F:112:DA:H2'	5:F:113:DT:C6	2.53	0.43
4:B:103:DC:OP1	4:B:103:DC:H6	2.01	0.43
4:B:106:DA:H4'	4:B:107:DC:OP1	2.19	0.43
6:C:117:DC:H5'	6:C:117:DC:C6	2.54	0.43
5:F:103:DA:H4'	5:F:104:DG:OP1	2.19	0.43
1:A:108:DC:H3'	1:A:109:DT:H72	2.00	0.42
1:A:118:DA:H1'	1:A:119:DT:H5'	2.00	0.42
6:C:103:DG:H8	6:C:103:DG:P	2.42	0.42
6:C:109:DT:H2'	6:C:110:DG:C8	2.55	0.42
5:F:104:DG:C4'	5:F:105:DT:H5'	2.49	0.42
6:C:102:DA:H2''	6:C:103:DG:C8	2.55	0.41
6:C:102:DA:H2''	6:C:103:DG:H8	1.85	0.41
4:B:111:DG:H1'	4:B:112:DC:OP2	2.20	0.41
5:F:101:DT:H2''	5:F:102:DT:OP1	2.19	0.41
6:C:111:DA:C2'	6:C:112:DT:H71	2.48	0.41
4:B:115:DG:H1'	4:B:116:DA:C8	2.55	0.41
3:D:106:DT:C2	3:D:107:DG:N7	2.89	0.41
3:D:113:DG:C6	3:D:114:DG:C6	3.09	0.41
5:F:102:DT:H1'	5:F:103:DA:OP2	2.21	0.41
7:M:103:DA:C8	7:M:103:DA:H5'	2.56	0.41
4:B:104:DC:H2''	4:B:105:DT:H71	2.03	0.41
4:B:120:DC:H1'	4:B:121:DT:C2	2.55	0.41
7:M:110:DA:OP1	7:M:111:DC:H5	2.04	0.41
1:A:108:DC:H2'	1:A:109:DT:C5	2.55	0.40
3:D:105:DA:C8	3:D:106:DT:H72	2.57	0.40
6:C:117:DC:H2''	6:C:118:DT:C6	2.56	0.40

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

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

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

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

### 6.3 Carbohydrates

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

### 6.4 Ligands

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

### 6.5 Other polymers

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