



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2017 – 07:14 pm GMT

PDB ID : 4B8D
Title : TENSEGRITY TRIANGLE FROM ENZYMATICALLY MANUFACTURED DNA
Authors : Ducani, C.; Kaul, C.D.; Moche, M.; Shih, W.M.; Hogberg, B.
Deposited on : 2012-08-26
Resolution : 4.79 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

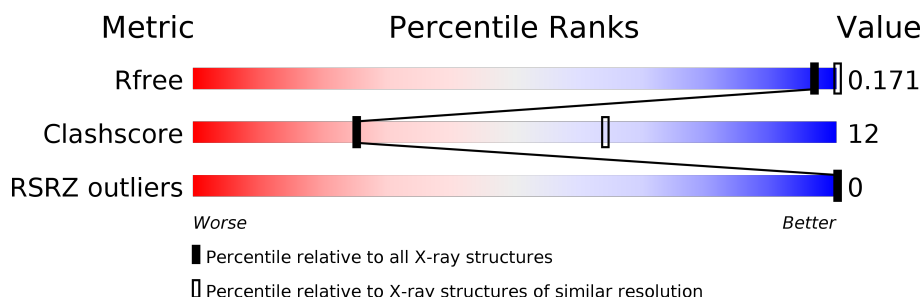
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.79 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}	100719	1019 (5.94-3.66)
Clashscore	112137	1067 (5.90-3.70)
RSRZ outliers	101464	1028 (5.94-3.66)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	21	
2	B	7	
3	C	6	
4	D	8	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 863 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 5'-D(*GP*AP*GP*CP*AP*GP*CP*CP*TP*GP*TP*AP*CP*DGP *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
			433	204	84	124	21			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	6	Total	C	N	O	P	0	0	0
			124	58	23	37	6			

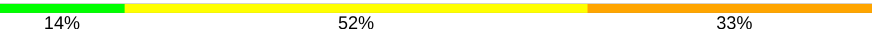
- Molecule 4 is a DNA chain called 5'-D(*TP*CP*TP*GP*AP*TP*GP*TP)-3'.

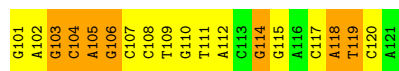
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	8	Total	C	N	O	P	0	0	0
			165	79	26	52	8			

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: 5'-D(*GP*AP*GP*CP*AP*GP*CP*CP*TP*GP*TP*AP*CP*DGP *GP*AP*CP*AP*TP*CP*A)-3'

Chain A: 




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

Chain B: 

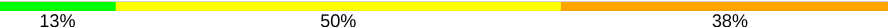


- Molecule 3: 5'-D(*GP*GP*CP*TP*GP*CP)-3'

Chain C: 



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

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	106.44Å 106.44Å 95.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.28 – 4.79 42.28 – 4.79	Depositor EDS
% Data completeness (in resolution range)	99.6 (42.28-4.79) 100.0 (42.28-4.79)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 4.85Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.185 , 0.205 0.181 , 0.171	Depositor DCC
R_{free} test set	185 reflections (10.32%)	DCC
Wilson B-factor (Å ²)	231.8	Xtriage
Anisotropy	0.689	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	-0.18 , 7721.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.125 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	863	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.06% 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	1.18	1/486 (0.2%)	2.47	32/746 (4.3%)
2	B	1.03	0/157	2.23	10/239 (4.2%)
3	C	1.27	0/138	2.67	7/211 (3.3%)
4	D	1.25	1/183 (0.5%)	2.67	14/279 (5.0%)
All	All	1.18	2/964 (0.2%)	2.50	63/1475 (4.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	101	DG	OP3-P	-10.30	1.48	1.61
4	D	101	DT	OP3-P	-9.77	1.49	1.61

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	102	DC	O4'-C1'-N1	19.82	121.88	108.00
1	A	111	DT	O4'-C1'-N1	17.24	120.07	108.00
3	C	213	DG	O4'-C1'-N9	16.18	119.33	108.00
1	A	102	DA	O4'-C1'-N9	13.82	117.67	108.00
4	D	106	DT	O4'-C1'-N1	12.43	116.70	108.00
1	A	103	DG	O4'-C1'-N9	11.86	116.30	108.00
1	A	106	DG	P-O3'-C3'	11.75	133.79	119.70
2	B	121	DG	P-O3'-C3'	11.53	133.54	119.70
4	D	104	DG	P-O3'-C3'	11.41	133.39	119.70
1	A	117	DC	O4'-C1'-N1	11.25	115.87	108.00
1	A	101	DG	O4'-C4'-C3'	-11.19	99.28	106.00
1	A	112	DA	P-O3'-C3'	11.02	132.92	119.70
1	A	107	DC	O4'-C1'-N1	10.57	115.40	108.00
3	C	211	DC	O4'-C1'-N1	10.14	115.10	108.00
1	A	115	DG	P-O3'-C3'	9.92	131.60	119.70
3	C	211	DC	P-O3'-C3'	9.47	131.06	119.70
3	C	210	DG	O4'-C1'-N9	9.29	114.50	108.00
4	D	104	DG	O4'-C1'-N9	9.28	114.49	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	212	DT	P-O3'-C3'	9.03	130.54	119.70
1	A	119	DT	P-O3'-C3'	9.02	130.53	119.70
4	D	103	DT	P-O3'-C3'	8.92	130.40	119.70
2	B	119	DC	P-O3'-C3'	8.91	130.40	119.70
1	A	103	DG	P-O3'-C3'	8.54	129.95	119.70
3	C	213	DG	P-O3'-C3'	8.07	129.38	119.70
1	A	118	DA	P-O3'-C3'	7.88	129.16	119.70
1	A	108	DC	O4'-C1'-N1	7.70	113.39	108.00
1	A	104	DC	O4'-C1'-N1	7.67	113.37	108.00
4	D	102	DC	P-O3'-C3'	7.19	128.33	119.70
1	A	108	DC	O4'-C4'-C3'	-7.16	101.64	104.50
1	A	101	DG	OP1-P-OP2	-7.04	109.04	119.60
1	A	104	DC	P-O3'-C3'	7.04	128.15	119.70
1	A	110	DG	P-O3'-C3'	7.04	128.15	119.70
4	D	101	DT	P-O3'-C3'	7.03	128.14	119.70
4	D	101	DT	OP1-P-OP2	-7.01	109.08	119.60
1	A	106	DG	O4'-C1'-N9	6.76	112.73	108.00
4	D	103	DT	O4'-C1'-N1	6.64	112.65	108.00
1	A	108	DC	N1-C2-O2	6.64	122.88	118.90
1	A	109	DT	O4'-C1'-N1	6.51	112.56	108.00
4	D	106	DT	C1'-O4'-C4'	-6.47	103.63	110.10
1	A	101	DG	C4'-C3'-C2'	-6.42	97.32	103.10
2	B	124	DC	P-O3'-C3'	6.29	127.24	119.70
1	A	109	DT	N3-C2-O2	-6.25	118.55	122.30
1	A	105	DA	C8-N9-C4	-5.98	103.41	105.80
2	B	122	DT	C6-C5-C7	-5.97	119.32	122.90
1	A	109	DT	C6-C5-C7	-5.97	119.32	122.90
1	A	101	DG	O4'-C1'-N9	5.91	112.14	108.00
4	D	101	DT	O4'-C1'-N1	5.80	112.06	108.00
4	D	105	DA	P-O3'-C3'	5.77	126.62	119.70
4	D	108	DT	O4'-C1'-N1	5.77	112.04	108.00
2	B	122	DT	C4-C5-C7	5.75	122.45	119.00
2	B	122	DT	P-O3'-C3'	5.73	126.57	119.70
2	B	124	DC	C1'-O4'-C4'	-5.72	104.38	110.10
1	A	105	DA	N7-C8-N9	5.72	116.66	113.80
3	C	212	DT	P-O5'-C5'	5.63	129.90	120.90
1	A	119	DT	O4'-C1'-C2'	5.54	110.33	105.90
1	A	108	DC	N3-C2-O2	-5.30	118.19	121.90
1	A	108	DC	C2-N1-C1'	5.28	124.61	118.80
2	B	122	DT	C1'-O4'-C4'	-5.20	104.90	110.10
2	B	123	DA	O4'-C1'-N9	-5.13	104.41	108.00
2	B	124	DC	N1-C1'-C2'	5.12	122.32	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	102	DC	N1-C2-O2	5.03	121.92	118.90
1	A	114	DG	P-O3'-C3'	5.01	125.72	119.70
1	A	109	DT	C4-C5-C7	5.01	122.00	119.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	433	0	235	8	0
2	B	141	0	79	3	0
3	C	124	0	68	2	0
4	D	165	0	93	3	0
All	All	863	0	475	13	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 12.

All (13) 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:104:DC:H2''	1:A:105:DA:H5''	1.39	1.04
4:D:104:DG:H1'	4:D:105:DA:H5'	1.79	0.64
1:A:114:DG:H21	2:B:121:DG:H22	1.60	0.48
4:D:104:DG:H4'	4:D:105:DA:OP1	2.16	0.46
4:D:105:DA:H1'	4:D:106:DT:O4'	2.16	0.46
1:A:114:DG:H21	2:B:121:DG:H1	1.65	0.45
3:C:211:DC:H2''	3:C:212:DT:O5'	2.17	0.44
1:A:105:DA:C5	1:A:106:DG:N7	2.85	0.44
3:C:210:DG:H1'	3:C:211:DC:OP2	2.17	0.44
1:A:103:DG:H1'	1:A:104:DC:OP1	2.19	0.43
1:A:114:DG:N2	2:B:121:DG:H1	2.16	0.43
1:A:118:DA:C2	1:A:119:DT:C2	3.08	0.42
1:A:119:DT:H2''	1:A:120:DC:O5'	2.20	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 carbohydrates 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](#)

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	21/21 (100%)	-1.18	0 100 100	20, 20, 20, 20	0
2	B	7/7 (100%)	-1.16	0 100 100	20, 20, 20, 20	0
3	C	6/6 (100%)	-1.17	0 100 100	20, 20, 20, 20	0
4	D	8/8 (100%)	-1.40	0 100 100	20, 20, 20, 20	0
All	All	42/42 (100%)	-1.22	0 100 100	20, 20, 20, 20	0

There are no RSRZ outliers to report.

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 carbohydrates 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.