



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 21, 2022 – 06:11 PM EDT

PDB ID : 7U44
Title : [F344] Self-assembling tensegrity triangle with three turns, four turns and four turns of DNA per axis by extension with P1 symmetry
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Deposited on : 2022-02-28
Resolution : 8.46 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.29
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

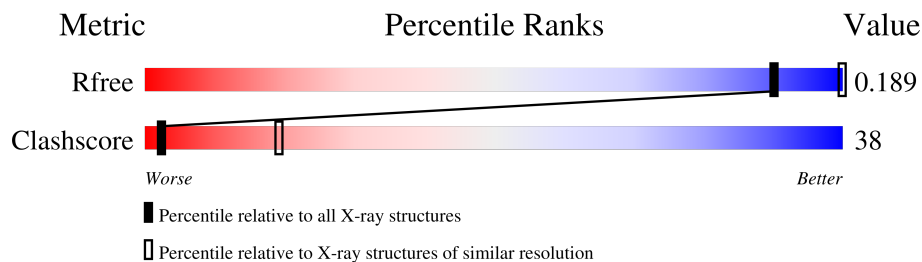
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 8.46 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}	130704	1005 (11.50-3.90)
Clashscore	141614	1070 (11.50-3.90)

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	42	
2	E	24	
3	D	35	
4	B	42	
5	F	35	
6	C	31	
7	M	21	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 4712 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 (42-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	42	Total	C	N	O	P	0	0	0
			863	408	165	248	42			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	24	Total	C	N	O	P	0	0	0
			495	235	89	147	24			

- Molecule 3 is a DNA chain called DNA (35-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	35	Total	C	N	O	P	0	0	0
			718	341	127	215	35			

- Molecule 4 is a DNA chain called DNA (42-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	42	Total	C	N	O	P	0	0	0
			860	408	159	251	42			

- Molecule 5 is a DNA chain called DNA (35-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	35	Total	C	N	O	P	0	0	0
			726	344	136	211	35			

- Molecule 6 is a DNA chain called DNA (31-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	C	31	Total 629	C 300	N 117	O 182	P 30	0	0	0

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

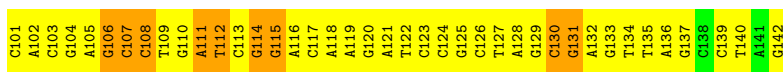
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	M	21	Total 421	C 200	N 76	O 124	P 21	0	0	0

3 Residue-property plots [i](#)

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.

- Molecule 1: DNA (42-MER)

Chain A: 5% 74% 21%



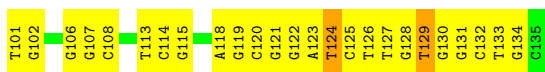
- Molecule 2: DNA (5'-D(P*TP*TP*TP*AP*GP*CP*AP*TP*AP*GP*GP*CP*AP*GP*TP*C P*GP*TP*GP*GP*CP*TP*CP*G)-3')

Chain E: 21% 58% 21%



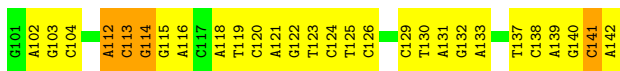
- Molecule 3: DNA (35-MER)

Chain D: 29% 66% 6%



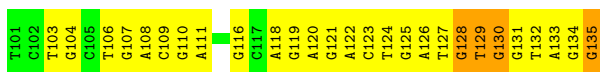
- Molecule 4: DNA (42-MER)

Chain B: 33% 57% 10%



- Molecule 5: DNA (35-MER)

Chain F: 23% 66% 11%



- Molecule 6: DNA (31-MER)

Chain C: 6% 68% 26%

A101	A102	C103	C104	T105	A106	C107	C108	T109	G110	G111	C112	A113	G114	G115	A116	C117	G118	A119	C120	T121	G122	C123	C124	T125	A126	T127	G128	C129	T130	A131
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● Molecule 7: DNA (5'-D(P*CP*AP*CP*CP*GP*AP*TP*CP*AP*CP*CP*TP*GP*CP*CP*AP*CP*CP*GP*TP*A)-3')



C101	A102	C103	C104	G105	A106	T107	C108	A109	C110	C111	T112	G113	C114	C115	A116	C117	C118	G119	T120	A121
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	100.42Å 135.34Å 135.19Å 99.31° 95.66° 106.50°	Depositor
Resolution (Å)	38.27 – 8.46 95.15 – 8.46	Depositor EDS
% Data completeness (in resolution range)	58.4 (38.27-8.46) 49.5 (95.15-8.46)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.54 (at 8.42Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.160 , 0.192 0.160 , 0.189	Depositor DCC
R_{free} test set	185 reflections (5.32%)	wwPDB-VP
Wilson B-factor (Å ²)	337.7	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.75 , 303.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.75	EDS
Total number of atoms	4712	wwPDB-VP
Average B, all atoms (Å ²)	1274.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.04 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.5549e-04.*

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	1.17	7/969 (0.7%)	1.22	6/1493 (0.4%)
2	E	1.36	5/554 (0.9%)	1.34	5/854 (0.6%)
3	D	1.01	1/803 (0.1%)	1.16	1/1238 (0.1%)
4	B	1.09	5/964 (0.5%)	1.20	4/1485 (0.3%)
5	F	1.29	9/815 (1.1%)	1.35	8/1258 (0.6%)
6	C	1.29	5/705 (0.7%)	1.40	7/1085 (0.6%)
7	M	1.73	7/470 (1.5%)	1.74	14/720 (1.9%)
All	All	1.25	39/5280 (0.7%)	1.32	45/8133 (0.6%)

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	114	DG	N9-C4	10.55	1.46	1.38
5	F	129	DT	C3'-O3'	10.09	1.57	1.44
5	F	130	DG	C5'-C4'	9.25	1.61	1.51
7	M	118	DC	C1'-N1	9.14	1.61	1.49
5	F	130	DG	P-O5'	8.84	1.68	1.59

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	118	DC	O4'-C1'-N1	10.64	115.45	108.00
7	M	110	DC	O4'-C4'-C3'	-10.34	99.79	106.00
5	F	129	DT	O5'-P-OP2	-10.05	96.65	105.70
6	C	121	DT	P-O3'-C3'	-9.82	107.92	119.70
7	M	109	DA	C3'-C2'-C1'	-8.17	92.69	102.50

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	863	0	470	61	1
2	E	495	0	272	35	0
3	D	718	0	396	33	0
4	B	860	0	472	40	0
5	F	726	0	395	54	0
6	C	629	0	349	47	0
7	M	421	0	235	45	0
All	All	4712	0	2589	275	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 38.

The worst 5 of 275 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)
2:E:118:DT:H2'	7:M:111:DC:H4'	1.42	1.01
5:F:107:DG:H2''	5:F:108:DA:H5''	1.55	0.88
5:F:130:DG:C8	7:M:117:DC:H5''	2.09	0.87
1:A:114:DG:H2''	1:A:115:DG:C8	2.10	0.86
6:C:110:DG:H2'	6:C:111:DG:H4'	1.57	0.85

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:DC:OP1	1:A:142:DG:N2[1_556]	2.14	0.06

5.3 Torsion angles

5.3.1 Protein backbone

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 monosaccharides 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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.