

Full wwPDB X-ray Structure Validation Report (i)

May 24, 2020 – 11:46 am BST

PDB ID : 1XBR

Title : T DOMAIN FROM XENOPUS LAEVIS BOUND TO DNA

Authors : Muller, C.W. Deposited on : 1997-07-16

Resolution : 2.50 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity: 4.02b-467

Xtriage (Phenix) : NOT EXECUTED EDS : NOT EXECUTED

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

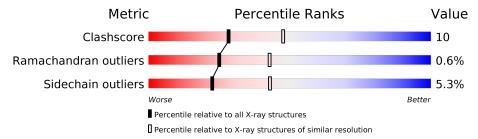
Validation Pipeline (wwPDB-VP) : 2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{resolution range}(ext{Å}))$
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain					
1	С	24	54%	38%	8%			
1	D	24	63%	33%	•			
2	A	184	75%	20%	5%			
2	В	184	78%	20%				



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4075 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(*AP*AP*TP*TP*TP*CP*AP*CP*AP*CP* CP*TP*AP*GP*GP*TP*G P*TP*GP*AP*AP*AP* TP*T)-3').

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	С	24	Total	С	N	О	Р	0	0	0
1		24	489	236	88	142	23	U	U	0
1	D	24	Total	С	N	О	Р	0	0	0
1	ש		489	236	88	142	23	0		U

• Molecule 2 is a protein called PROTEIN (T PROTEIN).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	Λ.	184	Total	С	N	О	S	0	0	0
	A	104	1481	947	261	264	9	0	U	0
9	D	183	Total	С	N	О	S	0	0	0
	Б	100	1473	943	259	262	9		U	U

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	С	23	Total O 23 23	0	0
3	D	25	Total O 25 25	0	0
3	A	50	Total O 50 50	0	0
3	В	45	Total O 45 45	0	0



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. 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 was not executed.

• Molecule 1: DNA (5'-D(*AP*AP*TP*TP*TP*CP*AP*CP*AP*CP*CP*TP*AP*GP*GP*TP*GP*AP*AP*AP*AP*TP*T)-3')

Chain C: 54% 38% 8%

• Molecule 1: DNA (5'-D(*AP*AP*TP*TP*TP*CP*AP*CP*AP*CP*CP*TP*AP*GP*GP*TP*GP*AP*AP*AP*AP*TP*T)-3')

Chain D: 63% 33% .

• Molecule 2: PROTEIN (T PROTEIN)

• Molecule 2: PROTEIN (T PROTEIN)

Chain B: 78% 20% ...



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	37.90Å 113.90Å 149.00Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 - 2.50	Depositor
% Data completeness	98.9 (20.00-2.50)	Depositor
(in resolution range)	,	Беровног
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.215 , 0.283	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4075	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP



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	Bo	nd angles
MIOI	I Chain	RMSZ	# Z >5	RMSZ	# Z > 5
1	С	0.60	0/548	0.91	1/844 (0.1%)
1	D	0.57	0/548	0.88	0/844
2	A	0.49	0/1521	0.69	0/2058
2	В	0.47	0/1513	0.67	0/2047
All	All	0.51	0/4130	0.75	$1/5793 \ (0.0\%)$

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	С	0	2
1	D	0	2
All	All	0	4

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$Ideal(^{o})$
1	С	514	DG	C1'-O4'-C4'	-5.01	105.09	110.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	С	513	DA	Sidechain
1	С	516	DT	Sidechain
1	D	516	DT	Sidechain
1	D	521	DA	Sidechain



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)	$\mathbf{H}(\mathbf{added})$	Clashes	Symm-Clashes
1	С	489	0	274	12	0
1	D	489	0	274	8	0
2	A	1481	0	1475	33	0
2	В	1473	0	1469	23	0
3	A	50	0	0	0	0
3	В	45	0	0	0	0
3	С	23	0	0	0	0
3	D	25	0	0	0	0
All	All	4075	0	3492	73	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 10.

All (73) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} ({\rm \AA}) \end{array}$	Clash overlap (Å)
1:C:512:DT:H2"	1:C:513:DA:H5'	1.36	1.07
2:A:95:ALA:HB3	2:A:163:LYS:HB3	1.54	0.90
1:D:516:DT:H2"	1:D:517:DG:C8	2.07	0.89
1:C:516:DT:H2"	1:C:517:DG:C8	2.23	0.73
2:B:141:PHE:O	2:B:144:VAL:HG12	1.93	0.69
2:A:169:HIS:HD2	2:A:182:SER:OG	1.77	0.67
2:A:52:ARG:HG3	2:A:204:LEU:HD11	1.76	0.65
2:A:112:LYS:H	2:A:112:LYS:HD2	1.62	0.65
2:B:74:LYS:HG2	2:B:140:SER:HB2	1.80	0.64
1:C:516:DT:C2'	1:C:517:DG:C8	2.81	0.63
1:C:512:DT:C2'	1:C:513:DA:H5'	2.22	0.62
2:A:166:PRO:HD2	2:A:188:THR:OG1	2.03	0.59
1:D:516:DT:C2'	1:D:517:DG:C8	2.85	0.56
2:B:50:TRP:CE2	2:B:71:PRO:HG2	2.42	0.55
2:B:68:ARG:HD3	2:B:142:SER:O	2.07	0.55
1:D:523:DT:H2"	1:D:524:DT:H5'	1.87	0.55
2:B:52:ARG:NH2	2:B:56:LEU:HD21	2.22	0.54
2:A:171:VAL:HG22	2:A:180:ILE:HG23	1.90	0.54
1:D:511:DC:H6	1:D:511:DC:C5'	2.21	0.53

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Atom-1	Atom-2	${\rm distance}({\rm \AA})$	overlap (Å)	
2:A:149:LYS:O	2:A:157:MET:HG3	2.10	0.52	
2:B:169:HIS:CD2	2:B:182:SER:OG	2.64	0.50	
2:A:172:ARG:HG3	2:A:172:ARG:HH11	1.76	0.50	
1:D:507:DA:H1'	1:D:508:DC:H5'	1.93	0.50	
2:B:52:ARG:HG3	2:B:204:LEU:HD11	1.94	0.49	
2:A:91:ASP:HB3	2:A:121:VAL:HG23	1.95	0.49	
2:B:169:HIS:HD2	2:B:182:SER:OG	1.97	0.48	
2:A:40:LEU:CD1	2:A:80:LEU:HD23	2.43	0.48	
2:B:97:ASN:N	2:B:97:ASN:OD1	2.47	0.48	
2:A:70:PHE:HA	2:A:71:PRO:C	2.34	0.48	
2:A:178:ARG:HA	2:A:178:ARG:HD3	1.64	0.48	
2:A:172:ARG:NH1	2:A:173:VAL:O	2.48	0.47	
2:B:95:ALA:HB3	2:B:163:LYS:HB3	1.96	0.47	
2:A:52:ARG:NH2	2:A:56:LEU:HD21	2.29	0.47	
1:C:516:DT:H2'	1:C:517:DG:N7	2.30	0.47	
2:A:201:ILE:HG22	2:A:202:THR:N	2.29	0.46	
2:B:176:THR:H	2:B:179:MET:HE2	1.80	0.46	
2:B:166:PRO:HD2	2:B:188:THR:OG1	2.15	0.46	
2:A:146:LEU:HD22	2:A:158:LEU:HD11	1.97	0.46	
2:A:81:ASP:HB3	2:A:84:ALA:CB	2.45	0.46	
2:A:81:ASP:HB3	2:A:84:ALA:HB2	1.98	0.46	
2:B:176:THR:N	2:B:179:MET:HE2	2.31	0.45	
2:A:129:ASN:ND2	2:B:128:PRO:HD2	2.31	0.45	
2:A:163:LYS:HG3	2:A:191:ILE:HG12	1.97	0.45	
2:A:102:TYR:CE2	2:A:105:GLY:HA2	2.52	0.45	
1:C:512:DT:H2"	1:C:513:DA:C5'	2.25	0.45	
1:C:516:DT:H2'	1:C:517:DG:C8	2.51	0.45	
2:A:169:HIS:CD2	2:A:182:SER:OG	2.62	0.45	
2:A:56:LEU:O	2:A:57:THR:HB	2.18	0.44	
2:A:40:LEU:HA	2:A:78:SER:O	2.17	0.44	
2:B:39:GLU:O	2:B:41:LYS:HG2	2.18	0.44	
2:B:176:THR:H	2:B:179:MET:HG3	1.83	0.43	
1:C:523:DT:H2"	1:C:524:DT:H5'	1.99	0.43	
2:A:116:GLN:HE22	2:A:162:HIS:HB3	1.84	0.43	
2:A:178:ARG:O	2:A:179:MET:HG3	2.18	0.42	
2:B:40:LEU:HA	2:B:78:SER:O	2.19	0.42	
2:A:40:LEU:CD2	2:A:181:THR:HG21	2.49	0.42	
2:B:51:THR:O	2:B:55:GLU:HG3	2.19	0.42	
1:C:511:DC:H5"	1:C:511:DC:H6	1.84	0.42	
2:B:70:PHE:HA	2:B:71:PRO:C	2.40	0.42	
1:C:504:DT:O2	1:D:522:DA:C2	2.73	0.42	

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Atom-1	Atom-2	$egin{array}{c} ext{Interatomic} \ ext{distance } (ext{Å}) \end{array}$	Clash overlap (Å)
2:B:126:ASP:O	2:B:129:ASN:HB2	2.20	0.42
2:B:116:GLN:NE2	2:B:159:ASN:HB2	2.35	0.42
2:B:122:TYR:HB2	2:B:156:ILE:HD11	2.01	0.42
2:A:207:LYS:O	2:A:207:LYS:HG3	2.19	0.41
1:D:516:DT:H2'	2:A:67:ARG:NH2	2.35	0.41
2:A:52:ARG:HD2	2:A:52:ARG:HA	1.76	0.41
2:B:126:ASP:OD2	2:B:133:HIS:HE1	2.03	0.41
1:D:511:DC:H6	1:D:511:DC:H5"	1.85	0.41
1:C:524:DT:H2'	1:C:524:DT:H6	1.71	0.41
2:A:97:ASN:HB2	2:A:114:GLU:O	2.20	0.40
2:A:97:ASN:OD1	2:A:97:ASN:N	2.53	0.40
1:C:518:DT:H2'	1:C:519:DG:C8	2.56	0.40
2:A:112:LYS:HA	2:A:113:PRO:HD2	1.99	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
2	A	182/184 (99%)	174 (96%)	7 (4%)	1 (0%)	29	48
2	В	181/184 (98%)	171 (94%)	9 (5%)	1 (1%)	25	43
All	All	363/368 (99%)	345 (95%)	16 (4%)	2 (1%)	25	43

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	В	177	GLN
2	A	40	LEU



5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percen	tiles
2	A	162/162 (100%)	152 (94%)	10 (6%)	18	35
2	В	161/162 (99%)	154 (96%)	7 (4%)	29	53
All	All	323/324 (100%)	306 (95%)	17 (5%)	22	43

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	77	MET
2	A	112	LYS
2	A	121	VAL
2	A	129	ASN
2	A	172	ARG
2	A	178	ARG
2	A	189	GLN
2	A	201	ILE
2	A	204	LEU
2	A	207	LYS
2	В	47	ARG
2	В	97	ASN
2	В	114	GLU
2	В	159	ASN
2	В	177	GLN
2	В	189	GLN
2	В	201	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	116	GLN
2	A	133	HIS
2	A	151	ASN
2	A	169	HIS
2	В	116	GLN

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Mol	Chain	Res	Type
2	В	133	HIS
2	В	151	ASN
2	В	169	HIS

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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

