

Full wwPDB X-ray Structure Validation Report (i)

#### May 22, 2020 - 03:12 am BST

PDB ID	:	10CT
Title	:	CRYSTAL STRUCTURE OF THE OCT-1 POU DOMAIN BOUND TO
		AN OCTAMER SITE: DNA RECOGNITION WITH TETHERED DNA-
		BINDING MODULES
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Deposited on		
Resolution	:	3.00  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:

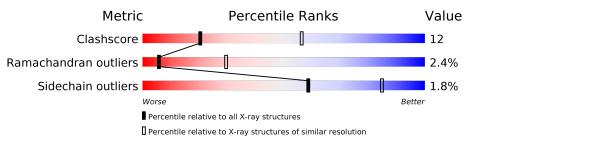
MolProbity : 4.02b-467	
Xtriage (Phenix) : NOT EXECUTED	
$\mathbf{EDS}$ : <b>NOT EXECUTED</b>	
$ \begin{tabular}{lllllllllllllllllllllllllllllllllll$	25 th 2019
Ideal geometry (proteins) : Engh & Huber (2001)	
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)	
Validation Pipeline (wwPDB-VP) : 2.11	

# 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 3.00 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries},{ m resolution\ range}({ m \AA}))$
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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 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	А	15	20%	60%		20%			
2	В	15	13%	40%	47%				
3	С	156		57%	26%	• 16%			



# 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 1670 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(\*TP\*GP\*TP\*AP\*TP\*GP\*CP\*AP\*AP\*AP\* TP\*AP\*AP\*GP\*G)-3').

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	А	15	Total 310	C 149	N 61	O 86	Р 14	0	0	0

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

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	В	15	Total 299	C 146	N 49	O 90	Р 14	0	0	0

• Molecule 3 is a protein called PROTEIN (OCT-1 POU DOMAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	С	131	Total 1061	C 668	N 188	O 199	S 6	0	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 colorcoded 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	(*TP*GP*TF	P*AP*TP*G	P*CP*AF	P*AP*AP*7	$\Gamma P^* A P^* A$	∿P*GP*G)-3
Chain A:	20%		60%		20%	•	
1201 6202 1203 1205 6205 6206 6206 1208 1208 1208 1208	211 2211 2215 215						
• Molecule 2 )	: DNA (5'-D	(*AP*CP*CI	P*TP*TP*Al	P*TP*TF	P*TP*GP*(	CP*AP*7	[P*AP*C)-3
Chain B:	13%	40%		47%		•	
A216 C217 C217 T219 T220 T222 T223 T223 T223	C220 A227 A227 A229 C230 C230						
• Molecule 3:	: PROTEIN	(OCT-1 POU	DOMAIN)				
Chain C:		57%		26%	• 16%		
15 16 19 11 12 12 12 12 12 12	123 126 126 126 126	137 138 843 843 147 160 160 061	E63 1663 1665 1665 1669 171 171 171	ASN LEU SER SER SER SER	LEU SER PRO SER ALA ALA ASN SER	PRO GLY ILE GLU GLY	
LEU SER ARG ARG ARG R102 R105 T110	1111 1112 1114 1115 1116 1116 1123 126	1131 1132 1132 1134 1134 1135 0135 0137 1138 1138	1145 R146 K155 R155 N160 N160				



# 4 Data and refinement statistics (i)

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

Property	Value	Source	
Space group	C 2 2 21	Depositor	
Cell constants	97.50Å $89.80$ Å $80.00$ Å	Depositor	
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor	
Resolution (Å)	20.00 - 3.00	Depositor	
% Data completeness	(Not available) (20.00-3.00)	Depositor	
(in resolution range)	(1007 available) (20.00-5.00)		
$R_{merge}$	(Not available)	Depositor	
R <sub>sym</sub>	(Not available)	Depositor	
Refinement program	X-PLOR, TNT	Depositor	
$R, R_{free}$	0.237 , (Not available)	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	1670	wwPDB-VP	
Average B, all atoms $(Å^2)$	31.0	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	Boı	nd lengths	Bond angles		
	Ullalli	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	1.45	2/349~(0.6%)	2.17	19/538~(3.5%)	
2	В	1.29	0/333	2.47	25/511~(4.9%)	
3	С	0.38	0/1075	0.56	0/1441	
All	All	0.90	2/1757~(0.1%)	1.56	44/2490~(1.8%)	

All (2) bond length outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
1	А	209	DA	C3'-O3'	-5.70	1.36	1.44
1	А	208	DA	C3'-O3'	-5.59	1.36	1.44

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
2	В	217	DC	O4'-C4'-C3'	-14.00	97.60	106.00
2	В	217	DC	C1'-O4'-C4'	-9.32	100.78	110.10
1	А	209	DA	O4'-C1'-N9	8.16	113.71	108.00
2	В	217	DC	O4'-C1'-N1	8.12	113.69	108.00
2	В	219	DT	P-O5'-C5'	-8.07	107.98	120.90
1	А	208	DA	O4'-C1'-C2'	-8.02	99.48	105.90
2	В	230	DC	O4'-C4'-C3'	-8.02	101.19	106.00
2	В	227	DA	O4'-C1'-N9	-7.69	102.62	108.00
2	В	223	DT	O4'-C1'-N1	-7.39	102.83	108.00
2	В	216	DA	O4'-C1'-C2'	7.33	111.76	105.90
2	В	224	DT	C1'-O4'-C4'	-7.32	102.78	110.10
2	В	216	DA	P-O3'-C3'	-7.28	110.96	119.70
2	В	225	DG	P-O5'-C5'	-7.15	109.46	120.90
2	В	222	DT	N3-C2-O2	-7.09	118.04	122.30
1	А	202	DG	O4'-C4'-C3'	-6.87	101.75	104.50
1	А	201	DT	C4'-C3'-C2'	-6.62	97.14	103.10
1	А	202	DG	C4'-C3'-C2'	6.55	109.00	103.10
1	А	202	DG	P-O3'-C3'	-6.48	111.92	119.70
1	А	212	DA	O4'-C1'-N9	-6.40	103.52	108.00

All (44) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	В	224	DT	C4-C5-C7	-6.35	115.19	119.00
2	В	218	DC	P-O5'-C5'	-6.34	110.75	120.90
2	В	216	DA	O3'-P-O5'	-6.33	91.98	104.00
2	В	225	DG	O4'-C1'-N9	-6.31	103.58	108.00
1	А	204	DA	P-O5'-C5'	-6.30	110.82	120.90
1	А	210	DA	P-O5'-C5'	-6.30	110.82	120.90
2	В	224	DT	N3-C4-O4	6.22	123.63	119.90
1	А	205	DT	C6-C5-C7	-6.14	119.21	122.90
1	А	204	DA	O4'-C1'-N9	-6.01	103.79	108.00
1	А	207	DC	P-O5'-C5'	-6.01	111.29	120.90
2	В	224	DT	C5-C4-O4	-5.71	120.91	124.90
1	А	202	DG	N1-C6-O6	5.66	123.30	119.90
1	А	212	DA	P-O5'-C5'	-5.62	111.90	120.90
1	А	211	DT	N1-C2-O2	-5.56	118.65	123.10
2	В	227	DA	O4'-C1'-C2'	-5.54	101.47	105.90
2	В	227	DA	P-O5'-C5'	-5.53	112.06	120.90
2	В	222	DT	P-O3'-C3'	5.52	126.33	119.70
1	А	201	DT	P-O3'-C3'	-5.52	113.08	119.70
1	А	206	DG	C5-C6-O6	-5.52	125.29	128.60
1	А	206	DG	C4-C5-N7	5.50	113.00	110.80
2	В	222	DT	O4'-C1'-C2'	-5.47	101.53	105.90
2	В	219	DT	N3-C4-O4	-5.29	116.73	119.90
2	В	220	DT	O4'-C4'-C3'	-5.20	102.42	104.50
2	В	219	DT	O4'-C1'-N1	-5.06	104.46	108.00
1	А	208	DA	O4'-C4'-C3'	-5.05	102.48	104.50

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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	А	310	0	171	3	0
2	В	299	0	173	10	0
3	С	1061	0	1053	27	0
All	All	1670	0	1397	38	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 (38) 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)
3:C:9:LEU:HD21	3:C:60:MET:HB3	1.32	1.10
3:C:26:THR:O	3:C:30:VAL:HG23	1.97	0.65
3:C:146:ARG:HH11	3:C:146:ARG:HB3	1.63	0.63
3:C:7:GLU:O	3:C:10:GLU:HB3	2.00	0.61
3:C:64:LYS:HB3	3:C:65:PRO:HD3	1.84	0.60
3:C:112:ILE:O	3:C:116:LEU:HG	2.01	0.60
1:A:211:DT:H2'	1:A:212:DA:C8	2.38	0.59
3:C:12:PHE:CD2	3:C:64:LYS:HG3	2.41	0.55
3:C:38:TYR:OH	3:C:69:LYS:HD2	2.06	0.55
2:B:217:DC:H2"	2:B:218:DC:O5'	2.06	0.54
3:C:19:ARG:HD2	3:C:71:LEU:HD21	1.91	0.53
2:B:224:DT:OP1	3:C:62:LYS:NZ	2.42	0.53
3:C:19:ARG:O	3:C:23:LEU:HD13	2.09	0.53
3:C:20:ARG:NH2	3:C:27:GLN:HG3	2.25	0.51
3:C:7:GLU:HA	3:C:10:GLU:HB3	1.93	0.51
2:B:223:DT:H2"	2:B:224:DT:O5'	2.13	0.49
3:C:123:ASN:ND2	3:C:126:PRO:HA	2.28	0.48
3:C:69:LYS:C	3:C:69:LYS:HD3	2.34	0.48
3:C:131:ILE:HG23	3:C:145:ILE:HG22	1.96	0.47
2:B:217:DC:H2"	2:B:218:DC:C6	2.49	0.47
2:B:216:DA:N3	2:B:216:DA:H2'	2.31	0.45
3:C:131:ILE:HG23	3:C:145:ILE:CG2	2.47	0.44
3:C:135:ALA:HB1	3:C:140:MET:O	2.17	0.44
2:B:219:DT:C5	2:B:220:DT:H73	2.53	0.44
1:A:211:DT:C2'	1:A:212:DA:C8	3.01	0.43
2:B:217:DC:H2"	2:B:218:DC:H6	1.82	0.43
2:B:226:DC:H5'	3:C:105:ARG:HB3	2.01	0.43
3:C:133:MET:O	3:C:136:ASP:HB3	2.18	0.43
3:C:155:LYS:O	3:C:159:ILE:HG13	2.19	0.42
3:C:110:THR:O	3:C:114:VAL:HG23	2.19	0.42
1:A:202:DG:H2"	1:A:203:DT:O5'	2.18	0.42
3:C:112:ILE:HD12	3:C:138:LEU:HD22	2.02	0.41
3:C:37:LEU:HD23	3:C:38:TYR:CE2	2.56	0.41
3:C:43:SER:O	3:C:47:ILE:HG12	2.21	0.41
2:B:229:DA:H2'	2:B:229:DA:OP2	2.19	0.41
3:C:12:PHE:CE2	3:C:64:LYS:HG3	2.55	0.41
3:C:160:ASN:HA	3:C:161:PRO:HD2	1.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:217:DC:C2'	2:B:218:DC:C6	3.04	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	Percentiles
3	С	127/156~(81%)	108~(85%)	16 (13%)	3(2%)	6 29

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	С	6	LEU
3	С	139	ASN
3	С	65	PRO

#### 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	Percentiles
3	С	114/142~(80%)	112 (98%)	2(2%)	59 85

All (2) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
3	С	59	ASN
3	С	146	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
3	С	40	ASN
3	С	123	ASN

#### 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.

