

Full wwPDB X-ray Structure Validation Report (i)

Dec 3, 2023 – 06:19 am GMT

PDB ID	:	1E3O
Title	:	Crystal structure of Oct-1 POU dimer bound to MORE
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Deposited on	:	2000-06-20
Resolution	:	1.90 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 types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

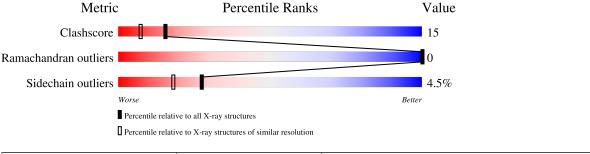
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 1.90 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	$(\# {\rm Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length		Quality of chain	
1	А	11	27%	73%	
2	В	11	55%	45%	
3	С	160	59%	21% • 18%	,



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 1631 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(*AP*TP*GP*CP*AP*TP*GP*AP*GP*GP*A)-3'.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	А	11	Total	C	N	0	Р	0	0	0
			224	109	47	59	9			

• Molecule 2 is a DNA chain called 5'-D(*TP*CP*CP*TP*CP*AP*TP*GP*CP*AP*T)-3'.

Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf	Trace
2	В	11	Total 217	C 106	N 35	O 66	Р 10	0	0	0

• Molecule 3 is a protein called OCTAMER-BINDING TRANSCRIPTION FACTOR 1.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
3	С	132	Total 1052	C 660	N 186	O 203	${ m S} { m 3}$	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
С	61	SER	CYS	engineered mutation	UNP P14859
С	76	ALA	ASN	conflict	UNP P14859
С	77	ASN	-	insertion	UNP P14859
С	121	MET	LEU	conflict	UNP P14859
С	130	ASP	GLU	conflict	UNP P14859
С	133	LEU	MET	conflict	UNP P14859
С	136	GLU	ASP	conflict	UNP P14859
С	150	SER	CYS	engineered mutation	UNP P14859

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	23	TotalO2323	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	В	33	Total O 33 33	0	0
4	С	82	TotalO8282	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.

Note EDS was not executed.

• Molecule 1: 5'-D(*AP*TP*GP*CP*AP*TP*GP*AP*GP*GP*A)-3'

Chain A:	27%		73%	
A201 T202 G203 G203 C204 A205 G207 G210 A211 A211				
• Molecule 2:	5'-D(*TP*CP*CI	P*TP*CP*AP*T	P*GP*CP*AP	*T)-3'
Chain B:	55%		45%	
T201 C202 C203 T204 T207 C203 C209 C209 C209 T211				
• Molecule 3:	OCTAMER-BIN	DING TRANSCI	RIPTION FAC	TOR 1
Chain C:	59%		21% •	18%
E B B B B B B B B B B B B B B B B B B B	K14 K17 K19 K19 R20 M34 M34 M40 M40	E51 N59 N62 K62 F65 L63 V64 V70 V70 L71	E75 ALA ASLA ASLA SER SER SER SER SER SER SER	SER SER PRO PRO SER ALA ALA ASN ASN CLU CLU CLU CLU CLU
SER ARG ARG ARG LYS LYS R105 1108 E108	T110 N111 N112 N113 V114 V124 126 127 128 129 129 1213 1235 124 1235 1235 1235 1235 1235 1235	L138 N139 N140 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 1 2 1	Depositor
Cell constants	93.30Å 52.40Å 69.00Å	Depositor
a, b, c, α , β , γ	90.00° 127.60° 90.00°	Depositor
Resolution (Å)	20.00 - 1.90	Depositor
% Data completeness	95.3 (20.00-1.90)	Depositor
(in resolution range)	55.5 (20.00-1.50)	Depositor
R_{merge}	0.04	Depositor
R _{sym}	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.220 , 0.242	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1631	wwPDB-VP
Average B, all atoms $(Å^2)$	47.0	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	Boi	Bond lengths		nd angles
	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.89	0/252	1.00	1/387~(0.3%)
2	В	1.21	1/241~(0.4%)	1.16	2/369~(0.5%)
3	С	0.71	0/1066	0.72	$1/1431 \ (0.1\%)$
All	All	0.83	1/1559~(0.1%)	0.86	4/2187~(0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	В	209	DC	C4-N4	5.84	1.39	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	А	201	DA	OP2-P-O3'	8.46	123.81	105.20
3	С	9	LEU	CA-CB-CG	6.17	129.50	115.30
2	В	207	DT	OP2-P-O3'	6.07	118.55	105.20
2	В	210	DA	OP2-P-O3'	5.67	117.67	105.20

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	224	0	124	6	0
2	В	217	0	127	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	С	1052	0	1025	35	0
4	А	23	0	0	1	0
4	В	33	0	0	0	0
4	С	82	0	0	1	0
All	All	1631	0	1276	40	0

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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 15.

All (40) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:C:19:ARG:O	3:C:23:LEU:HD13	1.82	0.79
3:C:17:LYS:HG3	3:C:20:ARG:HH12	1.58	0.68
3:C:71:LEU:O	3:C:75:GLU:HG2	1.94	0.68
3:C:2:GLU:H	3:C:3:PRO:HD2	1.59	0.67
3:C:20:ARG:NH1	3:C:51:GLU:OE2	2.29	0.66
3:C:14:LYS:HE3	3:C:14:LYS:HA	1.81	0.63
3:C:5:ASP:OD1	3:C:8:GLU:HG3	2.00	0.62
3:C:9:LEU:HD12	3:C:64:LYS:HD2	1.84	0.59
2:B:203:DC:H2'	2:B:204:DT:H72	1.83	0.59
3:C:109:GLU:HB3	3:C:112:ILE:HG13	1.90	0.54
3:C:64:LYS:HB3	3:C:65:PRO:HD3	1.89	0.53
3:C:111:ASN:O	3:C:114:VAL:CG2	2.57	0.53
3:C:120:PHE:CZ	3:C:124:GLN:HG2	2.44	0.53
3:C:2:GLU:N	3:C:3:PRO:HD2	2.23	0.51
1:A:206:DT:H2"	1:A:207:DG:C8	2.46	0.51
3:C:111:ASN:O	3:C:114:VAL:HG23	2.10	0.50
3:C:120:PHE:CE1	3:C:124:GLN:HG2	2.45	0.50
3:C:20:ARG:HB3	3:C:20:ARG:HH11	1.77	0.50
3:C:112:ILE:HG21	3:C:140:MET:HE2	1.94	0.49
1:A:205:DA:C5'	3:C:105:ARG:HG3	2.42	0.49
1:A:210:DG:H1'	1:A:211:DA:O5'	2.13	0.49
3:C:19:ARG:NE	3:C:23:LEU:HD11	2.28	0.48
3:C:112:ILE:HD12	4:C:2059:HOH:O	2.13	0.48
3:C:112:ILE:HG21	3:C:140:MET:CE	2.45	0.47
3:C:4:SER:OG	3:C:8:GLU:HB2	2.14	0.47
3:C:19:ARG:NE	3:C:75:GLU:OE1	2.48	0.46
3:C:105:ARG:HH11	3:C:105:ARG:HG2	1.81	0.46
3:C:135:ALA:O	3:C:139:ASN:N	2.49	0.45
3:C:137:GLN:HG3	3:C:138:LEU:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:6:LEU:O	3:C:6:LEU:HD23	2.16	0.45
3:C:34:MET:SD	3:C:70:TRP:HB2	2.57	0.45
3:C:62:LYS:O	3:C:66:LEU:CD2	2.65	0.45
3:C:6:LEU:HD23	3:C:6:LEU:C	2.36	0.45
3:C:17:LYS:HA	3:C:20:ARG:NH1	2.32	0.45
3:C:105:ARG:HD3	3:C:105:ARG:N	2.33	0.44
1:A:203:DG:H1'	4:A:2009:HOH:O	2.18	0.42
3:C:5:ASP:OD1	3:C:5:ASP:C	2.57	0.41
1:A:210:DG:H1'	1:A:211:DA:HO5'	1.87	0.40
3:C:109:GLU:O	3:C:113:ARG:HG3	2.21	0.40
1:A:204:DC:OP2	3:C:108:ILE:HD12	2.22	0.40

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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	128/160~(80%)	124 (97%)	4 (3%)	0	100 100

There are no Ramachandran outliers to report.

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	111/145~(77%)	106 (96%)	5(4%)	27 18

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	С	14	LYS
3	С	40	ASN
3	С	59	ASN
3	С	105	ARG
3	С	137	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	С	137	GLN

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 (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.

