

wwPDB X-ray Structure Validation Summary Report (i)

Jan 7, 2024 – 04:55 pm GMT

PDB ID	:	5MLO
Title	:	Crystal structure of human PCNA in complex with ZRANB3 PIP box peptide
Authors	:	Ariza, A.
Deposited on		
Resolution	:	1.96 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 (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:

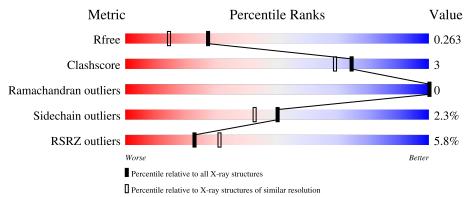
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.96 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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% 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
			3%	
1	А	261	92%	6% ·
			4%	
1	С	261	89%	8% ••
			7%	
1	Ε	261	91%	6% •
			13%	
2	В	15	67%	33%
			33%	
2	D	15	67%	7% 27%

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Mol	Chain	Length	Qua	lity of chain	
	Б		7%		
2	F,	15	47%	27%	27%



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6705 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.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Δ	A 077	Total	С	Ν	0	S	0	4	0
	А	255	1987	1248	323	400	16	0		
1	С	255	Total	С	Ν	0	S	0	10	0
	C	200	2023	1270	334	402	17	0	10	0
1	E	255	Total	С	Ν	0	S	0	0	0
		255	2015	1265	332	401	17	0	9	0

• Molecule 1 is a protein called Proliferating cell nuclear antigen.

• Molecule 2 is a protein called ZRANB3 PIP box peptide.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	В	10	Total C N O 90 59 17 14	0	0	0
2	D	11	Total C N O 99 64 18 17	0	0	0
2	F	11	Total C N O 97 64 18 15	0	0	0

• Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	2	Total Na 2 2	0	0
3	С	1	Total Na 1 1	0	0
3	Ε	1	Total Na 1 1	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	124	Total O 126 126	0	2

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	В	2	Total O 2 2	0	0
4	С	145	Total O 146 146	0	1
4	Е	112	Total O 114 114	0	2
4	F	2	Total O 2 2	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 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.

- Chain A: 92% 6% • • Molecule 1: Proliferating cell nuclear antigen Chain C: 89% 8% GLU GLU SER • Molecule 1: Proliferating cell nuclear antigen Chain E: 6% · 91% ASP GLU GLU GLY SER • Molecule 2: ZRANB3 PIP box peptide 13% Chain B: 67% 33% • Molecule 2: ZRANB3 PIP box peptide 33% Chain D: 67% 7% 27%
- Molecule 1: Proliferating cell nuclear antigen





• Molecule 2: ZRANB3 PIP box peptide





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	68.14Å 86.80Å 156.68Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	78.34 - 1.96	Depositor
	78.34 - 1.96	EDS
% Data completeness	$100.0\ (78.34-1.96)$	Depositor
(in resolution range)	$100.0\ (78.34-1.96)$	EDS
R_{merge}	0.08	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.84 (at 1.95 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.211 , 0.259	Depositor
It, Itfree	0.217 , 0.263	DCC
R_{free} test set	3325 reflections $(4.93%)$	wwPDB-VP
Wilson B-factor ($Å^2$)	35.7	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.33 , 49.2	EDS
L-test for twinning ²	$ \langle L \rangle = 0.45, \langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6705	wwPDB-VP
Average B, all atoms $(Å^2)$	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.24% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NA

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	
MOI	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.54	0/2024	0.68	1/2735~(0.0%)
1	С	0.61	0/2076	0.72	1/2803~(0.0%)
1	Е	0.53	0/2065	0.69	1/2788~(0.0%)
2	В	0.35	0/92	0.41	0/121
2	D	0.34	0/101	0.39	0/133
2	F	0.40	0/100	0.60	0/133
All	All	0.55	0/6458	0.69	3/8713~(0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
1	С	16	LEU	CA-CB-CG	-7.92	97.08	115.30
1	Е	16	LEU	CA-CB-CG	-7.75	97.48	115.30
1	А	16	LEU	CA-CB-CG	-7.40	98.27	115.30

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	1987	0	1995	9	0
1	С	2023	0	2049	20	0

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Mol	Chain	Non-H	${ m H}({ m model})$	H(added)	Clashes	Symm-Clashes			
1	Ε	2015	0	2040	10	0			
2	В	90	0	87	0	0			
2	D	99	0	93	0	0			
2	F	97	0	94	5	0			
3	А	2	0	0	0	0			
3	С	1	0	0	0	0			
3	Ε	1	0	0	0	0			
4	А	126	0	0	2	0			
4	В	2	0	0	0	0			
4	С	146	0	0	4	0			
4	Е	114	0	0	0	0			
4	F	2	0	0	0	0			
All	All	6705	0	6358	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 3.

The worst 5 of 40 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:C:149[B]:ARG:HG2	1:C:149[B]:ARG:HH11	1.04	1.18
1:C:210[A]:ARG:HB2	1:C:210[A]:ARG:NH1	1.78	0.98
1:C:113[A]:ASP:OD1	4:C:401:HOH:O	1.83	0.95
1:C:149[B]:ARG:HG2		1.73	0.90
1:C:210[A]:ARG:HB2	1:C:210[A]:ARG:HH11	1.39	0.86

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
1	А	257/261~(98%)	252~(98%)	5(2%)	0	100	100
1	С	263/261~(101%)	259~(98%)	4(2%)	0	100	100
1	Ε	262/261~(100%)	258~(98%)	4 (2%)	0	100	100
2	В	8/15~(53%)	8 (100%)	0	0	100	100
2	D	9/15~(60%)	9 (100%)	0	0	100	100
2	F	9/15~(60%)	8 (89%)	1 (11%)	0	100	100
All	All	808/828~(98%)	794 (98%)	14 (2%)	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 side chain 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	Perce	ntiles
1	А	227/228~(100%)	224~(99%)	3~(1%)	69	65
1	С	233/228~(102%)	225~(97%)	8 (3%)	37	25
1	Ε	232/228~(102%)	226~(97%)	6 (3%)	46	36
2	В	10/15~(67%)	10 (100%)	0	100	100
2	D	11/15~(73%)	$10 \ (91\%)$	1 (9%)	9	2
2	F	11/15~(73%)	11 (100%)	0	100	100
All	All	724/729~(99%)	706~(98%)	18 (2%)	50	38

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Ε	97	ASP
1	Е	184	GLN
1	Е	113[B]	ASP
1	С	113[B]	ASP
1	Е	20	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.



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)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis. There are no bond length outliers. There are no bond angle outliers. There are no chirality outliers. There are no torsion outliers. There are no ring outliers.

No monomer is involved in short contacts.

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, 95^{th} 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	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(A^2)$	Q < 0.9
1	А	255/261~(97%)	0.35	9 (3%) 44 53	29, 43, 73, 117	0
1	С	255/261~(97%)	0.38	11 (4%) 35 45	24, 34, 74, 97	0
1	Ε	255/261~(97%)	0.61	18 (7%) 16 24	27, 41, 101, 126	0
2	В	10/15~(66%)	0.70	2(20%) 1 1	51, 57, 80, 92	0
2	D	11/15~(73%)	1.52	5~(45%) 0 0	42, 56, 81, 89	0
2	F	11/15~(73%)	0.85	1 (9%) 9 15	39, 52, 69, 73	0
All	All	797/828~(96%)	0.47	46 (5%) 23 31	24, 40, 77, 126	0

The worst 5 of 46 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Е	96	ALA	9.2
1	С	189	ASP	6.5
1	С	107	ASN	5.8
2	F	526	PHE	5.6
1	Е	95	ASN	5.2

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 monosaccharides in this entry.



6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
3	NA	Ε	301	1/1	0.73	0.11	$63,\!63,\!63,\!63$	0
3	NA	А	301	1/1	0.76	0.18	48,48,48,48	0
3	NA	С	301	1/1	0.91	0.15	81,81,81,81	0
3	NA	А	302	1/1	0.97	0.14	32,32,32,32	0

6.5 Other polymers (i)

There are no such residues in this entry.

