



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 11:37 am GMT

PDB ID : 3JA9
EMDB ID: : EMD-6339
Title : Structure of native human PCNA
Authors : Lau, W.C.Y.; Li, Y.; Zhang, Q.; Huen, M.S.Y.
Deposited on : 2015-05-19
Resolution : 22.00 Å(reported)
Based on PDB ID : 1VYM

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : recalc29047

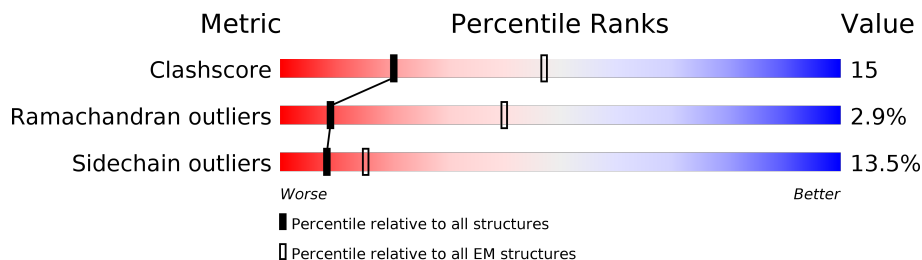
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 22.00 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	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	261	
1	B	261	
1	C	261	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6033 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 protein called Proliferating cell nuclear antigen.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	256	Total 1964	C 1233	N 323	O 392	S 16	0	1
1	B	256	Total 1964	C 1233	N 323	O 392	S 16	0	1
1	C	256	Total 1964	C 1233	N 323	O 392	S 16	0	1

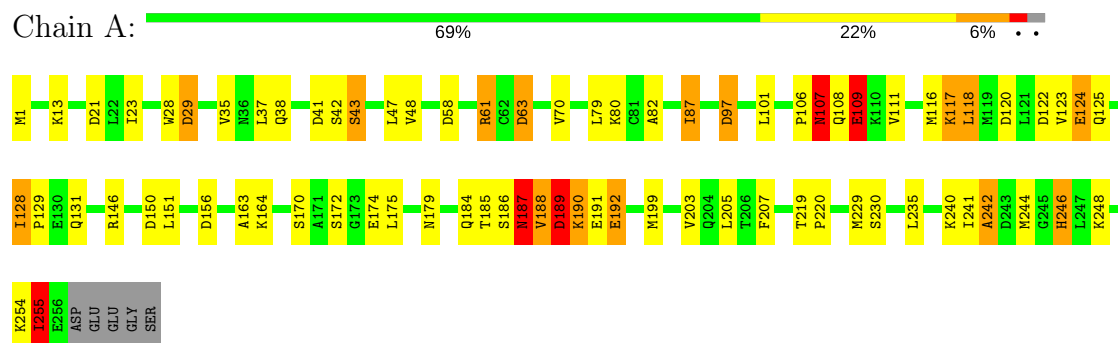
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		AltConf
2	A	39	Total 39	O 39	0
2	B	44	Total 44	O 44	0
2	C	58	Total 58	O 58	0

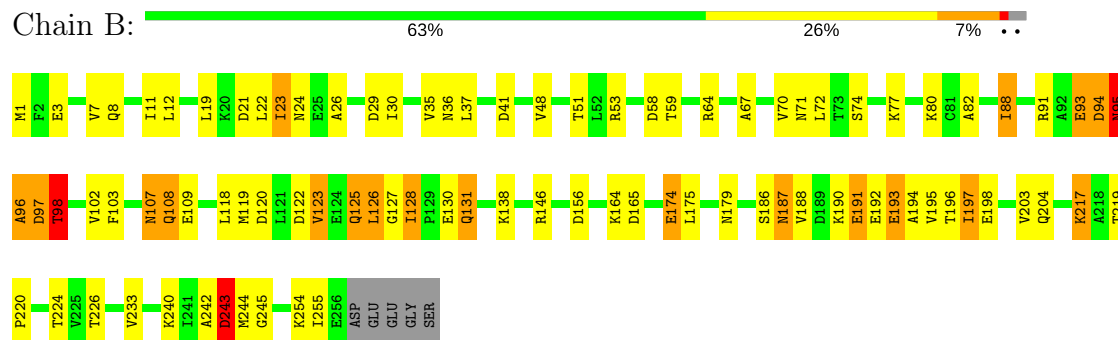
3 Residue-property plots

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.

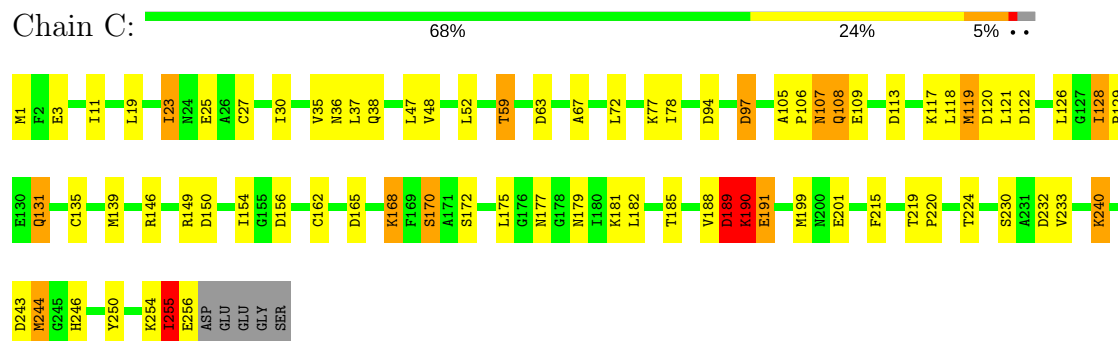
- Molecule 1: Proliferating cell nuclear antigen



- Molecule 1: Proliferating cell nuclear antigen



- Molecule 1: Proliferating cell nuclear antigen



4 Experimental information

Property	Value	Source
Reconstruction method	Not provided	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images used	7330	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	Particles	Depositor
Microscope	JEOL 2010	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	18	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	50000	Depositor
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	Depositor

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.57	0/1990	0.95	10/2689 (0.4%)
1	B	0.61	0/1990	1.00	10/2689 (0.4%)
1	C	0.67	0/1990	1.01	12/2689 (0.4%)
All	All	0.62	0/5970	0.99	32/8067 (0.4%)

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	A	0	3
1	B	0	2
All	All	0	5

There are no bond length outliers.

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	63	ASP	CB-CG-OD2	8.31	125.78	118.30
1	B	243	ASP	CB-CG-OD2	7.21	124.79	118.30
1	C	150	ASP	CB-CG-OD2	7.14	124.73	118.30
1	C	156	ASP	CB-CG-OD2	6.96	124.57	118.30
1	B	156	ASP	CB-CG-OD2	6.68	124.31	118.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	ASN	Peptide
1	A	109	GLU	Peptide
1	A	192	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	B	95	ASN	Mainchain
1	B	98	THR	Peptide

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	A	1964	0	1973	57	0
1	B	1964	0	1973	67	0
1	C	1964	0	1973	63	0
2	A	39	0	0	3	0
2	B	44	0	0	11	0
2	C	58	0	0	7	0
All	All	6033	0	5919	181	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 15.

The worst 5 of 181 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:254:LYS:O	1:C:255:ILE:HB	1.28	1.07
1:C:128:ILE:HD13	1:C:129:PRO:HD2	1.36	1.02
1:B:187:ASN:ND2	1:B:188:VAL:HG23	1.75	1.00
1:B:187:ASN:HD22	1:B:188:VAL:HG23	1.28	0.98
1:A:187:ASN:HB3	1:A:190:LYS:NZ	1.81	0.96

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 PDB entries followed by that with respect to all EM entries.

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	
1	A	254/261 (97%)	223 (88%)	20 (8%)	11 (4%)	3	29
1	B	254/261 (97%)	229 (90%)	17 (7%)	8 (3%)	5	37
1	C	254/261 (97%)	238 (94%)	13 (5%)	3 (1%)	15	57
All	All	762/783 (97%)	690 (91%)	50 (7%)	22 (3%)	9	38

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	SER
1	A	108	GLN
1	A	118	LEU
1	A	187	ASN
1	A	188	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	
1	A	223/228 (98%)	195 (87%)	28 (13%)	5	26
1	B	223/228 (98%)	189 (85%)	34 (15%)	3	19
1	C	223/228 (98%)	195 (87%)	28 (13%)	5	26
All	All	669/684 (98%)	579 (86%)	90 (14%)	8	24

5 of 90 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	125	GLN
1	B	190	LYS
1	C	190	LYS
1	B	128	ILE
1	B	164	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	187	ASN
1	C	131	GLN
1	C	107	ASN
1	B	65	ASN
1	C	49	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 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.