

# wwPDB EM Validation Summary Report (i)

Jan 19, 2025 – 12:13 AM JST

PDB ID : 8YJS

EMDB ID : EMD-39348

Title : Structure of the human endogenous PCNA-FEN1 complex - State E

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Deposited on : 2024-03-02

Resolution : 3.55 Å(reported)

This is a wwPDB EM 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/EMValidationReportHelp
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:

EMDB validation analysis : FAILED

MolProbity : 4.02b-467

Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)

MapQ : FAILED

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

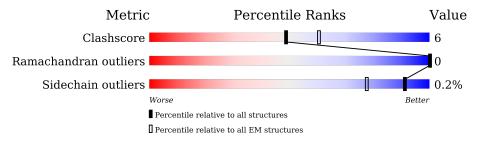
Validation Pipeline (wwPDB-VP) : 2.40

## 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $ELECTRON\ MICROSCOPY$ 

The reported resolution of this entry is 3.55 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 $(\# \mathrm{Entries})$	${ m EM\ structures} \ (\#{ m Entries})$
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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%

Mol	Chain	Length	Quality of chain	
1	A	261	80%	16%
1	В	261	85%	12% •
1	С	261	80%	16%
2	D	380	78%	14% • 8%
3	J	19	84%	16%
4	Е	29	90%	10%
5	F	11	55%	45%
6	Н	3	100%	



## 2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 9880 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	С	254	Total	С	N	О	S	0	0
1	O	204	1951	1225	321	389	16	0	0
1	В	253	Total	С	N	О	S	0	0
1	Б	293	1947	1222	320	390	15	0	U
1	А	253	Total	С	N	О	S	0	0
1	А	299	1947	1222	320	390	15	0	U

• Molecule 2 is a protein called Flap endonuclease 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	351	Total 2769	C 1742	N 485	O 527	S 15	0	0

• Molecule 3 is a DNA chain called upstream DNA.

Mol	Chain	Residues	Atoms				AltConf	Trace	
3	J	19	Total 387	C 190	N 59	O 119	P 19	0	0

• Molecule 4 is a DNA chain called parent strand DNA.

Mol	Chain	Residues		At	$\mathbf{oms}$			AltConf	Trace
4	Е	29	Total 590	C 290	N 97	O 175	P 28	0	0

• Molecule 5 is a DNA chain called downstream DNA.

Mol	Chain	Residues		Ato	oms			AltConf	Trace
5	F	11	Total	С	N	О	Р	0	0
	I.	11	229	110	49	59	11		U

• Molecule 6 is a DNA chain called 5 prime flap DNA.



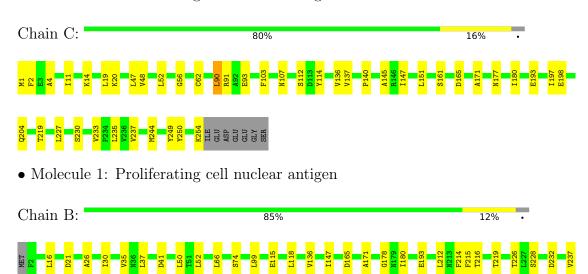
Mol	Chain	Residues	Atoms				AltConf	Trace	
6	Н	3	Total 60	C 30	N 6	O 21	P 3	0	0



## 3 Residue-property plots (i)

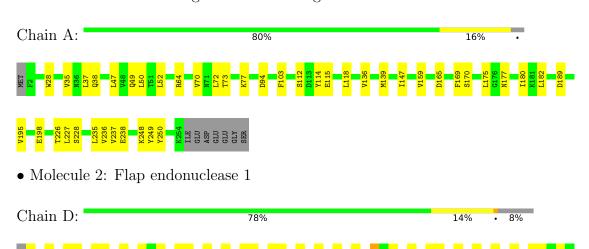
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

• Molecule 1: Proliferating cell nuclear antigen

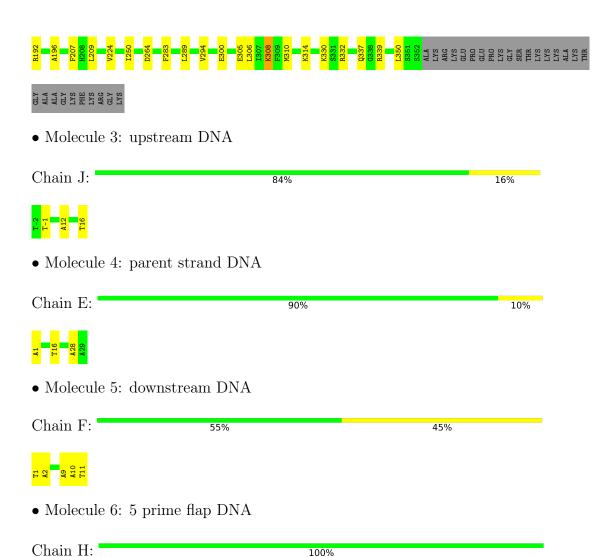




• Molecule 1: Proliferating cell nuclear antigen







100%

There are no outlier residues recorded for this chain.



# 4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	78778	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	60	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k 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			
IVIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5		
1	A	0.30	0/1973	0.62	0/2666		
1	В	0.34	0/1973	0.68	1/2666~(0.0%)		
1	С	0.34	0/1977	0.67	$1/2671 \ (0.0\%)$		
2	D	0.35	0/2816	0.71	$2/3785 \ (0.1\%)$		
3	J	0.55	0/431	1.14	0/663		
4	Е	0.54	0/660	1.01	0/1017		
5	F	0.48	0/259	0.79	0/397		
6	Н	0.56	0/65	1.29	0/98		
All	All	0.37	0/10154	0.74	4/13963 (0.0%)		

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
2	D	145	LEU	CA-CB-CG	7.15	131.74	115.30
1	С	90	LEU	CA-CB-CG	5.72	128.45	115.30
2	D	67	MET	CA-CB-CG	5.41	122.50	113.30
1	В	16	LEU	CB-CG-CD2	5.20	119.84	111.00

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	A	1947	0	1948	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	В	1947	0	1948	19	0
1	С	1951	0	1956	26	0
2	D	2769	0	2792	33	0
3	J	387	0	222	3	0
4	Е	590	0	337	3	0
5	F	229	0	124	4	0
6	Н	60	0	37	0	0
All	All	9880	0	9364	105	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 6.

The worst 5 of 105 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:145:ALA:HB2	1:C:219:THR:HG21	1.85	0.59
1:C:56:GLY:HA3	1:C:244:MET:HG3	1.86	0.57
2:D:33:ILE:HG12	2:D:176:ALA:HB3	1.87	0.57
1:A:35:VAL:HB	1:A:52:LEU:HB2	1.87	0.56
2:D:192:ARG:HH12	5:F:2:DA:H4'	1.71	0.55

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	Perce	ntiles
1	A	$251/261\ (96\%)$	235 (94%)	16 (6%)	0	100	100
1	В	$251/261\ (96\%)$	238 (95%)	13 (5%)	0	100	100
1	С	252/261 (97%)	237 (94%)	15 (6%)	0	100	100
2	D	349/380 (92%)	335 (96%)	14 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentile	$\mathbf{s}$
All	All	1103/1163 (95%)	1045 (95%)	58 (5%)	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 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	Perce	$\mathbf{ntiles}$
1	A	$221/228 \ (97\%)$	221 (100%)	0	100	100
1	В	221/228 (97%)	221 (100%)	0	100	100
1	С	221/228 (97%)	221 (100%)	0	100	100
2	D	301/322 (94%)	299 (99%)	2 (1%)	81	90
All	All	964/1006 (96%)	962 (100%)	2 (0%)	91	97

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

Mol	Chain	Res	Type
2	D	308	LYS
2	D	330	LYS

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

Mol	Chain	Res	Type
1	A	38	GLN
1	A	125	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 oligosaccharides 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.

