



Full wwPDB EM Validation Report ⓘ

Jan 19, 2025 – 12:15 AM JST

PDB ID : 8YJL
EMDB ID : EMD-39344
Title : Structure of the human endogenous PCNA-FEN1 complex - State B
Authors : Tian, Y.; Gao, N.
Deposited on : 2024-03-02
Resolution : 3.51 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) 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

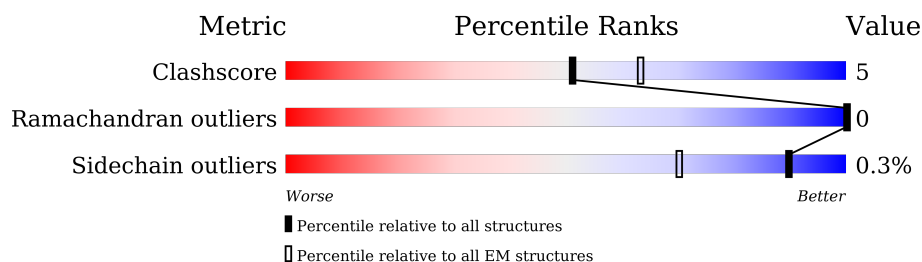
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.51 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	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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	J	17	76% 24%
2	E	28	82% 18%
3	F	11	100%
4	H	3	100%
5	A	261	82% 15% ..
5	B	261	79% 18% .
5	C	261	82% 15% ..
6	D	380	80% 12% 8%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9853 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 DNA chain called upstream DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	J	17	Total	C	N	O	P	0	0
			344	170	46	111	17		

- Molecule 2 is a DNA chain called parent strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	28	Total	C	N	O	P	0	0
			574	280	107	160	27		

- Molecule 3 is a DNA chain called downstream DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	11	Total	C	N	O	P	0	0
			227	110	43	63	11		

- Molecule 4 is a DNA chain called 5 prime DNA.

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

- Molecule 5 is a protein called Proliferating cell nuclear antigen.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	256	Total	C	N	O	S	0	0
			1968	1236	323	393	16		
5	B	254	Total	C	N	O	S	0	0
			1955	1227	321	391	16		
5	A	254	Total	C	N	O	S	0	0
			1955	1227	321	391	16		

- Molecule 6 is a protein called Flap endonuclease 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	351	Total	C	N	O	S	0	0
			2770	1743	485	527	15		

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: upstream DNA

Chain J: 



- Molecule 2: parent strand

Chain E: 



- Molecule 3: downstream DNA

Chain F: 


There are no outlier residues recorded for this chain.

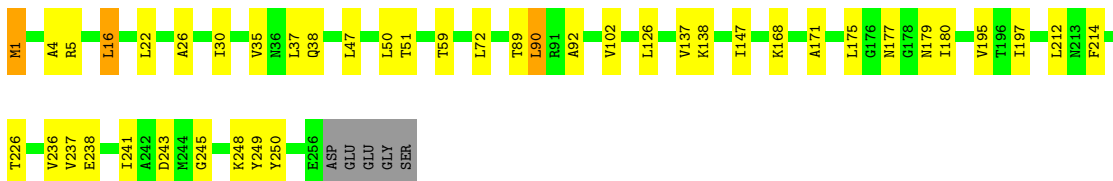
- Molecule 4: 5 prime DNA

Chain H: 


There are no outlier residues recorded for this chain.

- Molecule 5: Proliferating cell nuclear antigen

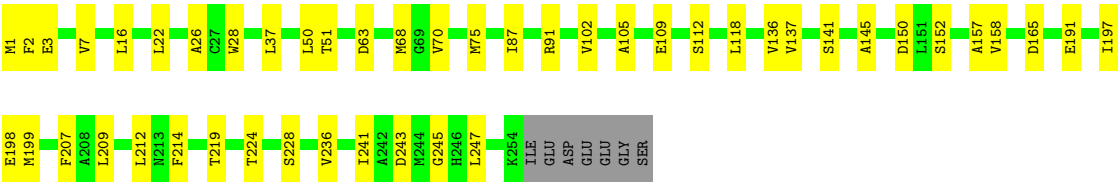
Chain C: 



- Molecule 5: Proliferating cell nuclear antigen

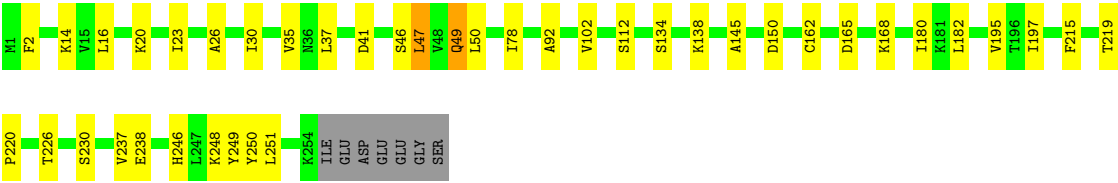
Chain B: 





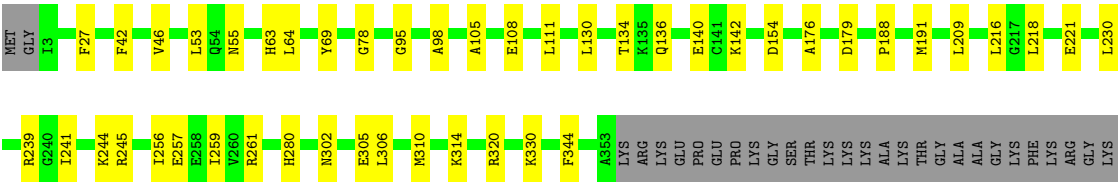
• Molecule 5: Proliferating cell nuclear antigen

Chain A: 82% 15% ..



• Molecule 6: Flap endonuclease 1

Chain D: 80% 12% 8%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	89413	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	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

5.1 Standard geometry

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	$\# Z > 5$	RMSZ	$\# Z > 5$
1	J	0.55	0/381	1.18	0/586
2	E	0.54	0/646	0.99	0/995
3	F	0.53	0/255	0.97	0/391
4	H	0.60	0/65	1.33	0/98
5	A	0.31	0/1981	0.68	2/2676 (0.1%)
5	B	0.31	0/1981	0.67	3/2676 (0.1%)
5	C	0.33	0/1994	0.66	2/2694 (0.1%)
6	D	0.32	0/2817	0.65	2/3787 (0.1%)
All	All	0.36	0/10120	0.74	9/13903 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	243	ASP	CB-CG-OD2	9.54	126.89	118.30
6	D	179	ASP	CB-CG-OD1	8.12	125.61	118.30
5	A	150	ASP	CB-CG-OD1	6.23	123.91	118.30
5	C	90	LEU	CA-CB-CG	5.93	128.93	115.30
5	B	150	ASP	CB-CG-OD1	5.84	123.56	118.30
5	A	47	LEU	CA-CB-CG	5.62	128.22	115.30
6	D	230	LEU	CA-CB-CG	5.54	128.03	115.30
5	C	16	LEU	CB-CG-CD2	5.39	120.16	111.00
5	B	199	MET	CB-CG-SD	5.15	127.86	112.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	J	344	0	201	3	0
2	E	574	0	321	4	0
3	F	227	0	126	0	0
4	H	60	0	37	0	0
5	A	1955	0	1960	22	0
5	B	1955	0	1960	25	0
5	C	1968	0	1973	25	0
6	D	2770	0	2794	25	0
All	All	9853	0	9372	99	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 5.

All (99) 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)
5:C:51:THR:O	5:C:245:GLY:HA3	1.70	0.91
5:C:138:LYS:O	5:C:195:VAL:HA	1.76	0.84
5:A:16:LEU:O	5:A:20:LYS:HB3	1.89	0.72
5:B:51:THR:O	5:B:245:GLY:HA3	1.94	0.68
6:D:306:LEU:O	6:D:310:MET:HB3	1.94	0.66
5:C:171:ALA:O	5:C:177:ASN:HA	1.95	0.66
5:B:28:TRP:HB2	5:B:68:MET:HB2	1.82	0.62
5:A:145:ALA:HB2	5:A:219:THR:HG21	1.83	0.61
6:D:176:ALA:HA	6:D:191:MET:HB2	1.83	0.61
6:D:105:ALA:O	6:D:108:GLU:HB2	2.04	0.57
5:B:145:ALA:HB2	5:B:219:THR:HG21	1.87	0.56
5:A:30:ILE:HG12	5:A:35:VAL:HG22	1.87	0.54
5:C:5:ARG:HB3	5:C:59:THR:HB	1.88	0.54
5:A:102:VAL:HA	5:A:112:SER:O	2.06	0.54
5:A:2:PHE:HB3	5:A:92:ALA:HB3	1.89	0.54
1:J:3:DT:O4	2:E:24:DA:N6	2.41	0.53
5:C:126:LEU:HD23	6:D:344:PHE:HB2	1.91	0.53
5:C:241:ILE:HG22	5:C:243:ASP:H	1.73	0.53
5:C:26:ALA:HB1	5:C:37:LEU:HD11	1.89	0.53
5:C:30:ILE:HG12	5:C:35:VAL:HG13	1.92	0.52
5:A:37:LEU:HB3	5:A:50:LEU:HB3	1.90	0.52
5:B:137:VAL:HG12	5:B:197:ILE:HG12	1.91	0.52
5:C:1:MET:N	5:C:92:ALA:O	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:226:THR:HB	5:A:238:GLU:HB3	1.92	0.51
5:C:137:VAL:HG12	5:C:197:ILE:HG12	1.91	0.51
5:B:3:GLU:OE1	5:B:91:ARG:NH1	2.44	0.51
5:A:237:VAL:HB	5:A:249:TYR:HB2	1.93	0.51
5:C:175:LEU:HD23	5:A:78:ILE:HG13	1.93	0.50
5:C:236:VAL:HG11	5:C:248:LYS:HZ2	1.75	0.50
5:B:37:LEU:HB3	5:B:50:LEU:HB3	1.92	0.50
5:B:228:SER:HB2	5:B:236:VAL:HB	1.94	0.49
1:J:10:DA:H2''	1:J:11:DT:H5''	1.93	0.49
6:D:42:PHE:HB3	6:D:63:HIS:HA	1.95	0.49
5:A:138:LYS:O	5:A:195:VAL:HA	2.13	0.49
6:D:46:VAL:HG12	6:D:53:LEU:HD13	1.96	0.48
5:C:38:GLN:NE2	5:C:126:LEU:O	2.46	0.48
5:A:49:GLN:HE21	5:A:248:LYS:HB2	1.77	0.48
5:B:2:PHE:O	5:B:91:ARG:HA	2.14	0.48
5:A:47:LEU:HB3	5:A:250:TYR:HB2	1.94	0.48
6:D:95:GLY:O	6:D:98:ALA:HB3	2.13	0.48
6:D:221:GLU:OE2	6:D:280:HIS:NE2	2.37	0.48
6:D:216:LEU:HB3	6:D:218:LEU:HG	1.96	0.48
5:C:237:VAL:HB	5:C:249:TYR:HB2	1.95	0.48
5:C:37:LEU:HB3	5:C:50:LEU:HB3	1.97	0.47
5:B:7:VAL:HA	5:B:87:ILE:HG12	1.97	0.47
5:C:147:ILE:HG23	5:C:180:ILE:HD12	1.96	0.47
5:B:22:LEU:HG	5:B:214:PHE:HB3	1.96	0.47
5:B:1:MET:N	5:B:63:ASP:OD2	2.48	0.46
1:J:2:DT:O4	2:E:25:DA:N6	2.48	0.46
6:D:55:ASN:HD22	6:D:314:LYS:HA	1.79	0.46
5:C:89:THR:HB	5:C:102:VAL:HB	1.96	0.46
5:A:41:ASP:HB2	5:A:46:SER:H	1.80	0.46
5:C:1:MET:N	5:C:1:MET:SD	2.88	0.46
5:B:26:ALA:HB1	5:B:37:LEU:HD11	1.96	0.46
5:A:215:PHE:HE2	5:A:251:LEU:HB2	1.81	0.46
5:B:105:ALA:HB3	5:B:109:GLU:H	1.82	0.45
5:C:226:THR:HB	5:C:238:GLU:HB3	1.99	0.45
5:B:136:VAL:HB	5:B:198:GLU:HG2	1.99	0.45
5:A:165:ASP:OD1	5:A:165:ASP:N	2.48	0.45
5:A:23:ILE:HG21	5:A:26:ALA:HB2	1.98	0.45
5:B:165:ASP:OD1	5:B:165:ASP:N	2.47	0.45
5:A:168:LYS:HA	5:A:180:ILE:O	2.17	0.45
6:D:257:GLU:HB3	6:D:261:ARG:HH12	1.82	0.45
5:A:182:LEU:HD23	5:A:195:VAL:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:16:LEU:HD11	5:C:72:LEU:HD22	1.99	0.44
6:D:108:GLU:O	6:D:111:LEU:HB2	2.18	0.44
6:D:306:LEU:O	6:D:310:MET:CB	2.65	0.44
5:B:16:LEU:HG	5:B:75:MET:HG2	2.01	0.43
5:C:4:ALA:HB3	5:C:90:LEU:HB2	1.99	0.43
5:C:47:LEU:HB3	5:C:250:TYR:HB2	1.98	0.43
5:B:191:GLU:O	5:B:224:THR:OG1	2.35	0.43
6:D:302:ASN:ND2	6:D:305:GLU:OE1	2.51	0.43
5:A:14:LYS:HD2	5:A:220:PRO:HB2	2.00	0.43
6:D:142:LYS:NZ	6:D:154:ASP:OD1	2.46	0.43
5:B:158:VAL:HG23	5:B:209:LEU:HD11	2.00	0.43
6:D:27:PHE:HA	6:D:78:GLY:HA3	2.00	0.43
5:B:209:LEU:HA	5:B:212:LEU:HB2	2.01	0.42
5:B:157:ALA:HA	5:B:207:PHE:O	2.19	0.42
5:C:212:LEU:HD23	5:C:212:LEU:HA	1.92	0.42
6:D:134:THR:HG22	6:D:136:GLN:H	1.84	0.42
6:D:241:ILE:HG23	6:D:245:ARG:HB3	2.01	0.42
5:A:162:CYS:HB2	5:A:197:ILE:HD11	2.01	0.42
2:E:6:DT:OP1	6:D:239:ARG:NH1	2.51	0.42
5:A:134:SER:H	5:A:230:SER:HG	1.63	0.42
5:B:152:SER:HA	5:B:209:LEU:HD13	2.02	0.42
5:B:102:VAL:HA	5:B:112:SER:O	2.20	0.41
6:D:244:LYS:HB3	6:D:244:LYS:HE2	1.85	0.41
6:D:64:LEU:HD21	6:D:140:GLU:HB3	2.01	0.41
2:E:14:DA:N6	2:E:15:DA:N1	2.69	0.41
6:D:188:PRO:HA	6:D:209:LEU:HB3	2.02	0.41
5:A:49:GLN:HE22	5:A:246:HIS:CD2	2.39	0.41
5:B:70:VAL:HG22	5:B:118:LEU:HD22	2.02	0.41
5:B:241:ILE:HD11	5:B:247:LEU:HB2	2.02	0.41
6:D:69:TYR:OH	6:D:320:ARG:NH1	2.53	0.40
6:D:256:ILE:HA	6:D:259:ILE:HG22	2.03	0.40
5:C:22:LEU:HB2	5:C:214:PHE:HB3	2.02	0.40
5:C:168:LYS:HE2	5:C:179:ASN:HB3	2.03	0.40
5:B:141:SER:HB2	5:B:219:THR:HG22	2.03	0.40
6:D:108:GLU:HG2	6:D:130:LEU:HD11	2.04	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 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	
5	A	252/261 (97%)	243 (96%)	9 (4%)	0	100	100
5	B	252/261 (97%)	243 (96%)	9 (4%)	0	100	100
5	C	254/261 (97%)	245 (96%)	9 (4%)	0	100	100
6	D	349/380 (92%)	335 (96%)	14 (4%)	0	100	100
All	All	1107/1163 (95%)	1066 (96%)	41 (4%)	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	Percentiles	
5	A	222/228 (97%)	221 (100%)	1 (0%)	86	92
5	B	222/228 (97%)	222 (100%)	0	100	100
5	C	223/228 (98%)	222 (100%)	1 (0%)	89	94
6	D	301/322 (94%)	300 (100%)	1 (0%)	91	96
All	All	968/1006 (96%)	965 (100%)	3 (0%)	90	96

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	C	1	MET
5	A	49	GLN
6	D	330	LYS

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

Mol	Chain	Res	Type
5	A	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 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.