



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 02:42 AM UTC

PDB ID : 3HI8 / pdb_00003hi8
Title : Crystal structure of proliferating cell nuclear antigen (PCNA) from *Haloferax volcanii*
Authors : Morgunova, E.; Gray, F.C.; MacNeill, S.A.; Ladenstein, R.
Deposited on : 2009-05-19
Resolution : 3.20 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 ⓘ 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:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

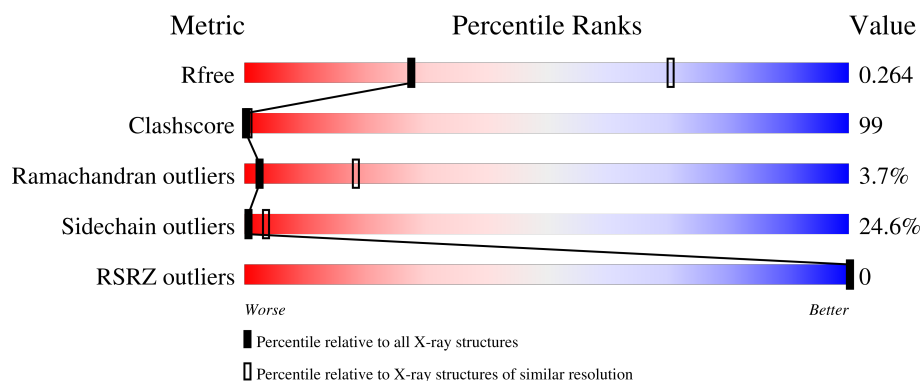
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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.



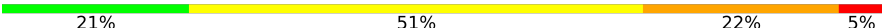
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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 $\leq 5\%$. 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
1	A	247	22% 51% 22% 5%
1	B	247	21% 52% 22% 5%
1	C	247	21% 52% 22% 5%
1	D	247	21% 52% 22% 5%
1	E	247	21% 51% 22% 5%

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Mol	Chain	Length	Quality of chain
1	F	247	 A horizontal bar chart showing the quality of chain F. The bar is divided into four segments: green (21%), yellow (51%), orange (22%), and red (5%). The percentages are labeled below the bar.

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11245 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 protein called Proliferating cell nuclear antigen PcnA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	247	Total	C	N	O	S	0	0	0
			1869	1167	308	386	8			
1	B	247	Total	C	N	O	S	0	0	0
			1869	1167	308	386	8			
1	C	247	Total	C	N	O	S	0	0	0
			1869	1167	308	386	8			
1	D	247	Total	C	N	O	S	0	0	0
			1869	1167	308	386	8			
1	E	247	Total	C	N	O	S	0	0	0
			1869	1167	308	386	8			
1	F	247	Total	C	N	O	S	0	0	0
			1869	1167	308	386	8			

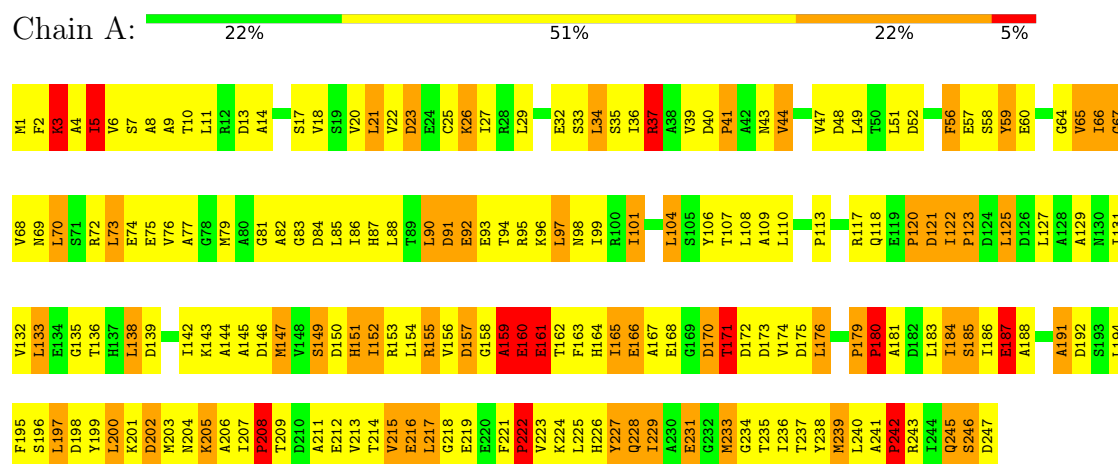
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	5	Total	O	0	0
			5	5		
2	B	3	Total	O	0	0
			3	3		
2	C	2	Total	O	0	0
			2	2		
2	D	7	Total	O	0	0
			7	7		
2	E	5	Total	O	0	0
			5	5		
2	F	9	Total	O	0	0
			9	9		

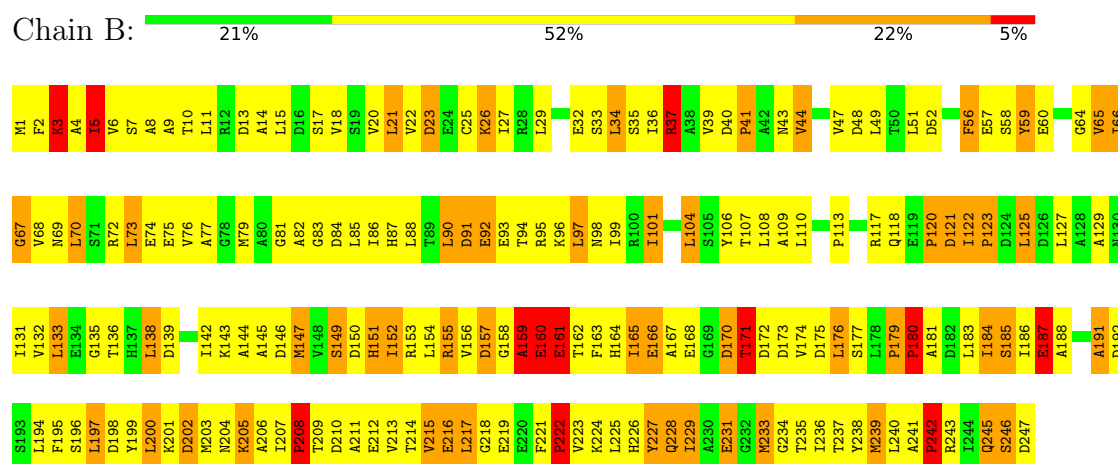
3 Residue-property plots

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.

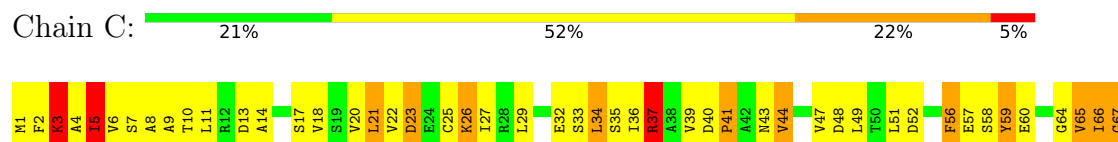
• Molecule 1: Proliferating cell nuclear antigen PcnA

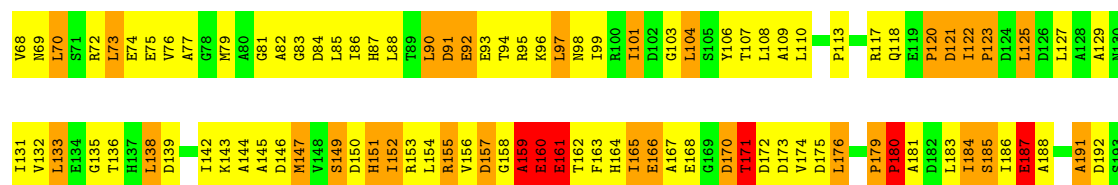


• Molecule 1: Proliferating cell nuclear antigen PcnA

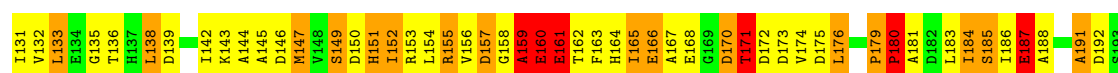


• Molecule 1: Proliferating cell nuclear antigen PcnA

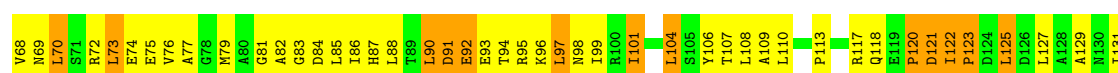
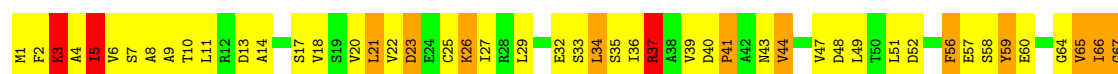




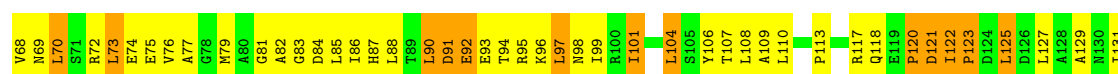
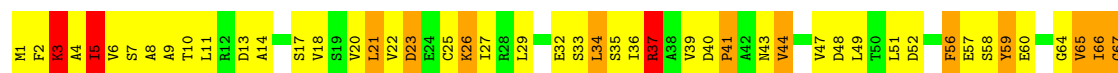
• Molecule 1: Proliferating cell nuclear antigen PcnA



• Molecule 1: Proliferating cell nuclear antigen PcnA



• Molecule 1: Proliferating cell nuclear antigen PcnA



V132	L133	E134	G135	T136	H137	L138	D139		I142	K143	A144	A145	D146	M147	V148	S149	D150	H151	I152	R153	L154	R155	V156	D157	G158	A159	E160	E161	T162	F163	H164	I165	E166	A167	E168	G169	D170	T171	D172	D173	V174	D175	L176		P179	P180	A181	D182	L183	I184	S185	I186	E187	A188		A191	D192	S193	L194
F195	S196	L197	D198	Y199	L200	K201	D202	M203	N204	K205	A206	L207	P208	T209	D210	A211	E212	V213	T214	V215	E216	L217	G218	E219	E220	F221	P222	V223	K224	L225	H226	Y227	Q228	I229	A230	E231	G232	M233	G234	T235	I236	T237	Y238	M239	L240	A241	P242	R243	T244	Q245	S246	D247							

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	174.44Å 123.24Å 123.26Å 90.00° 135.00° 90.00°	Depositor
Resolution (Å)	32.95 – 3.20 32.95 – 3.20	Depositor EDS
% Data completeness (in resolution range)	86.6 (32.95-3.20) 86.5 (32.95-3.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.19 (at 3.18Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.237 , 0.250 0.230 , 0.264	Depositor DCC
R_{free} test set	1323 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	138.1	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 316.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.34$, $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	0.357 for -h-2*k,l,h+1 0.348 for k+1,h+1,-l 0.357 for -k+1,-h-l,-l 0.349 for -h-k-l,l,k 0.349 for -h+k-l,-l,-k 0.347 for -h-k-l,-l,h+1 0.347 for k+1,-h-l,-k 0.348 for -h+k-l,l,h+1 0.349 for -k+1,h+1,k 0.357 for -h,-k,h+1 0.358 for -h-2*k,-k,l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	11245	wwPDB-VP
Average B, all atoms (Å ²)	139.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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.

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	A	1.04	1/1893 (0.1%)	1.68	44/2572 (1.7%)
1	B	1.04	1/1893 (0.1%)	1.68	44/2572 (1.7%)
1	C	1.04	1/1893 (0.1%)	1.68	44/2572 (1.7%)
1	D	1.04	1/1893 (0.1%)	1.68	44/2572 (1.7%)
1	E	1.04	1/1893 (0.1%)	1.68	44/2572 (1.7%)
1	F	1.04	1/1893 (0.1%)	1.68	44/2572 (1.7%)
All	All	1.04	6/11358 (0.1%)	1.68	264/15432 (1.7%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	161	GLU	N-CA	7.42	1.55	1.46
1	A	161	GLU	N-CA	7.34	1.55	1.46
1	F	161	GLU	N-CA	7.34	1.55	1.46
1	B	161	GLU	N-CA	7.32	1.55	1.46
1	C	161	GLU	N-CA	7.32	1.55	1.46

The worst 5 of 264 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	180	PRO	CA-N-CD	-14.75	91.35	112.00
1	F	180	PRO	CA-N-CD	-14.73	91.38	112.00
1	C	180	PRO	CA-N-CD	-14.72	91.39	112.00
1	A	180	PRO	CA-N-CD	-14.72	91.39	112.00
1	E	180	PRO	CA-N-CD	-14.71	91.41	112.00

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	A	1869	0	1847	386	0
1	B	1869	0	1847	391	0
1	C	1869	0	1847	385	0
1	D	1869	0	1847	390	0
1	E	1869	0	1847	380	0
1	F	1869	0	1847	375	0
2	A	5	0	0	0	0
2	B	3	0	0	0	0
2	C	2	0	0	0	0
2	D	7	0	0	0	0
2	E	5	0	0	0	0
2	F	9	0	0	0	0
All	All	11245	0	11082	2202	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 99.

The worst 5 of 2202 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:A:149:SER:CB	1:A:167:ALA:HB1	1.53	1.38
1:B:149:SER:CB	1:B:167:ALA:HB1	1.53	1.37
1:C:149:SER:CB	1:C:167:ALA:HB1	1.53	1.36
1:F:149:SER:CB	1:F:167:ALA:HB1	1.53	1.35
1:E:149:SER:CB	1:E:167:ALA:HB1	1.53	1.35

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	
1	A	245/247 (99%)	206 (84%)	30 (12%)	9 (4%)	2	18
1	B	245/247 (99%)	206 (84%)	30 (12%)	9 (4%)	2	18
1	C	245/247 (99%)	206 (84%)	30 (12%)	9 (4%)	2	18
1	D	245/247 (99%)	206 (84%)	30 (12%)	9 (4%)	2	18
1	E	245/247 (99%)	206 (84%)	30 (12%)	9 (4%)	2	18
1	F	245/247 (99%)	206 (84%)	30 (12%)	9 (4%)	2	18
All	All	1470/1482 (99%)	1236 (84%)	180 (12%)	54 (4%)	2	18

5 of 54 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	184	ILE
1	A	208	PRO
1	B	184	ILE
1	B	208	PRO
1	C	184	ILE

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 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	
1	A	203/203 (100%)	153 (75%)	50 (25%)	1	3
1	B	203/203 (100%)	153 (75%)	50 (25%)	1	3
1	C	203/203 (100%)	153 (75%)	50 (25%)	1	3
1	D	203/203 (100%)	153 (75%)	50 (25%)	1	3
1	E	203/203 (100%)	153 (75%)	50 (25%)	1	3
1	F	203/203 (100%)	153 (75%)	50 (25%)	1	3
All	All	1218/1218 (100%)	918 (75%)	300 (25%)	1	3

5 of 300 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	161	GLU
1	F	176	LEU
1	E	185	SER
1	F	65	VAL
1	B	233	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	43	ASN
1	D	130	ASN
1	F	130	ASN
1	E	130	ASN
1	F	43	ASN

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.

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, 95th 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	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	247/247 (100%)	-1.49	0 100 100	93, 138, 172, 203	0
1	B	247/247 (100%)	-1.57	0 100 100	94, 139, 172, 204	0
1	C	247/247 (100%)	-1.58	0 100 100	94, 139, 172, 203	0
1	D	247/247 (100%)	-1.51	0 100 100	94, 138, 173, 204	0
1	E	247/247 (100%)	-1.50	0 100 100	94, 139, 172, 203	0
1	F	247/247 (100%)	-1.51	0 100 100	94, 139, 172, 205	0
All	All	1482/1482 (100%)	-1.53	0 100 100	93, 139, 175, 205	0

There are no RSRZ outliers to report.

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.