



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 21, 2020 – 07:55 pm BST

PDB ID : 6O09  
Title : Structure of AtPCNA in complex with the PIP motif of ATXR6  
Authors : Couture, J.F.; Davarinejad, H.  
Deposited on : 2019-02-15  
Resolution : 2.06 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](mailto: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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

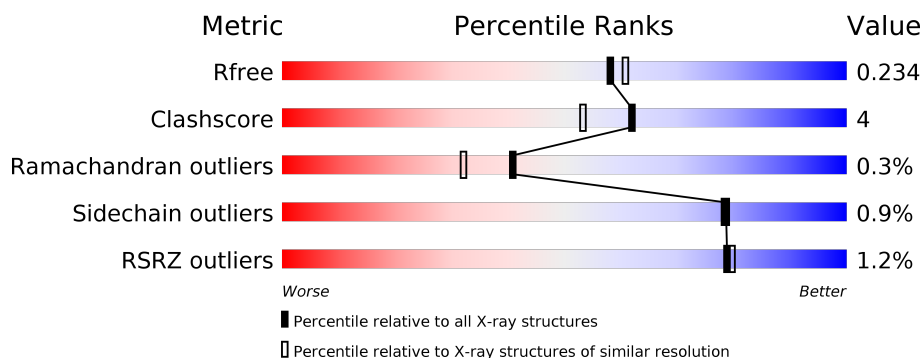
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.06 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))
$R_{free}$	130704	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	312	<div> <div>%</div> <div> <div></div> <div>73%</div> <div>10%</div> <div>16%</div> </div> </div>
1	C	312	<div> <div></div> <div>74%</div> <div>9%</div> <div>16%</div> </div>
1	D	312	<div> <div>%</div> <div> <div></div> <div>75%</div> <div>9%</div> <div>16%</div> </div> </div>
1	F	312	<div> <div>%</div> <div> <div></div> <div>75%</div> <div>8%</div> <div>16%</div> </div> </div>
1	H	312	<div> <div>2%</div> <div> <div></div> <div>71%</div> <div>7%</div> <div>21%</div> </div> </div>
1	K	312	<div> <div>%</div> <div> <div></div> <div>74%</div> <div>5%</div> <div>20%</div> </div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	B	20	<div><div></div><div>65%35%</div></div>
2	E	20	<div><div></div><div>65%35%</div></div>
2	G	20	<div><div></div><div>55%5%40%</div></div>
2	I	20	<div><div>5%</div><div></div><div>70%30%</div></div>
2	J	20	<div><div></div><div>65%5%30%</div></div>
2	L	20	<div><div>5%</div><div></div><div>65%35%</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12307 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 cellular nuclear antigen 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	261	Total	C	N	O	S	0	0	0
			1926	1219	315	375	17			
1	A	261	Total	C	N	O	S	0	0	0
			1916	1217	309	374	16			
1	D	261	Total	C	N	O	S	0	0	0
			1904	1205	308	376	15			
1	F	262	Total	C	N	O	S	0	0	0
			1919	1210	310	384	15			
1	H	246	Total	C	N	O	S	0	0	0
			1795	1148	290	340	17			
1	K	249	Total	C	N	O	S	0	0	0
			1786	1143	285	342	16			

There are 294 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-48	MET	-	initiating methionine	UNP Q9M7Q7
C	-47	GLY	-	expression tag	UNP Q9M7Q7
C	-46	SER	-	expression tag	UNP Q9M7Q7
C	-45	SER	-	expression tag	UNP Q9M7Q7
C	-44	HIS	-	expression tag	UNP Q9M7Q7
C	-43	HIS	-	expression tag	UNP Q9M7Q7
C	-42	HIS	-	expression tag	UNP Q9M7Q7
C	-41	HIS	-	expression tag	UNP Q9M7Q7
C	-40	HIS	-	expression tag	UNP Q9M7Q7
C	-39	HIS	-	expression tag	UNP Q9M7Q7
C	-38	SER	-	expression tag	UNP Q9M7Q7
C	-37	SER	-	expression tag	UNP Q9M7Q7
C	-36	GLY	-	expression tag	UNP Q9M7Q7
C	-35	LEU	-	expression tag	UNP Q9M7Q7
C	-34	VAL	-	expression tag	UNP Q9M7Q7
C	-33	PRO	-	expression tag	UNP Q9M7Q7
C	-32	ARG	-	expression tag	UNP Q9M7Q7

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
C	-31	GLY	-	expression tag	UNP Q9M7Q7
C	-30	SER	-	expression tag	UNP Q9M7Q7
C	-29	HIS	-	expression tag	UNP Q9M7Q7
C	-28	MET	-	expression tag	UNP Q9M7Q7
C	-27	ALA	-	expression tag	UNP Q9M7Q7
C	-26	SER	-	expression tag	UNP Q9M7Q7
C	-25	MET	-	expression tag	UNP Q9M7Q7
C	-24	THR	-	expression tag	UNP Q9M7Q7
C	-23	GLY	-	expression tag	UNP Q9M7Q7
C	-22	GLY	-	expression tag	UNP Q9M7Q7
C	-21	GLN	-	expression tag	UNP Q9M7Q7
C	-20	GLN	-	expression tag	UNP Q9M7Q7
C	-19	MET	-	expression tag	UNP Q9M7Q7
C	-18	GLY	-	expression tag	UNP Q9M7Q7
C	-17	ARG	-	expression tag	UNP Q9M7Q7
C	-16	GLY	-	expression tag	UNP Q9M7Q7
C	-15	SER	-	expression tag	UNP Q9M7Q7
C	-14	MET	-	expression tag	UNP Q9M7Q7
C	-13	GLY	-	expression tag	UNP Q9M7Q7
C	-12	HIS	-	expression tag	UNP Q9M7Q7
C	-11	HIS	-	expression tag	UNP Q9M7Q7
C	-10	HIS	-	expression tag	UNP Q9M7Q7
C	-9	HIS	-	expression tag	UNP Q9M7Q7
C	-8	HIS	-	expression tag	UNP Q9M7Q7
C	-7	HIS	-	expression tag	UNP Q9M7Q7
C	-6	GLU	-	expression tag	UNP Q9M7Q7
C	-5	ASN	-	expression tag	UNP Q9M7Q7
C	-4	LEU	-	expression tag	UNP Q9M7Q7
C	-3	TYR	-	expression tag	UNP Q9M7Q7
C	-2	PHE	-	expression tag	UNP Q9M7Q7
C	-1	GLN	-	expression tag	UNP Q9M7Q7
C	0	GLY	-	expression tag	UNP Q9M7Q7
A	-48	MET	-	initiating methionine	UNP Q9M7Q7
A	-47	GLY	-	expression tag	UNP Q9M7Q7
A	-46	SER	-	expression tag	UNP Q9M7Q7
A	-45	SER	-	expression tag	UNP Q9M7Q7
A	-44	HIS	-	expression tag	UNP Q9M7Q7
A	-43	HIS	-	expression tag	UNP Q9M7Q7
A	-42	HIS	-	expression tag	UNP Q9M7Q7
A	-41	HIS	-	expression tag	UNP Q9M7Q7
A	-40	HIS	-	expression tag	UNP Q9M7Q7
A	-39	HIS	-	expression tag	UNP Q9M7Q7

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	-38	SER	-	expression tag	UNP Q9M7Q7
A	-37	SER	-	expression tag	UNP Q9M7Q7
A	-36	GLY	-	expression tag	UNP Q9M7Q7
A	-35	LEU	-	expression tag	UNP Q9M7Q7
A	-34	VAL	-	expression tag	UNP Q9M7Q7
A	-33	PRO	-	expression tag	UNP Q9M7Q7
A	-32	ARG	-	expression tag	UNP Q9M7Q7
A	-31	GLY	-	expression tag	UNP Q9M7Q7
A	-30	SER	-	expression tag	UNP Q9M7Q7
A	-29	HIS	-	expression tag	UNP Q9M7Q7
A	-28	MET	-	expression tag	UNP Q9M7Q7
A	-27	ALA	-	expression tag	UNP Q9M7Q7
A	-26	SER	-	expression tag	UNP Q9M7Q7
A	-25	MET	-	expression tag	UNP Q9M7Q7
A	-24	THR	-	expression tag	UNP Q9M7Q7
A	-23	GLY	-	expression tag	UNP Q9M7Q7
A	-22	GLY	-	expression tag	UNP Q9M7Q7
A	-21	GLN	-	expression tag	UNP Q9M7Q7
A	-20	GLN	-	expression tag	UNP Q9M7Q7
A	-19	MET	-	expression tag	UNP Q9M7Q7
A	-18	GLY	-	expression tag	UNP Q9M7Q7
A	-17	ARG	-	expression tag	UNP Q9M7Q7
A	-16	GLY	-	expression tag	UNP Q9M7Q7
A	-15	SER	-	expression tag	UNP Q9M7Q7
A	-14	MET	-	expression tag	UNP Q9M7Q7
A	-13	GLY	-	expression tag	UNP Q9M7Q7
A	-12	HIS	-	expression tag	UNP Q9M7Q7
A	-11	HIS	-	expression tag	UNP Q9M7Q7
A	-10	HIS	-	expression tag	UNP Q9M7Q7
A	-9	HIS	-	expression tag	UNP Q9M7Q7
A	-8	HIS	-	expression tag	UNP Q9M7Q7
A	-7	HIS	-	expression tag	UNP Q9M7Q7
A	-6	GLU	-	expression tag	UNP Q9M7Q7
A	-5	ASN	-	expression tag	UNP Q9M7Q7
A	-4	LEU	-	expression tag	UNP Q9M7Q7
A	-3	TYR	-	expression tag	UNP Q9M7Q7
A	-2	PHE	-	expression tag	UNP Q9M7Q7
A	-1	GLN	-	expression tag	UNP Q9M7Q7
A	0	GLY	-	expression tag	UNP Q9M7Q7
D	-48	MET	-	initiating methionine	UNP Q9M7Q7
D	-47	GLY	-	expression tag	UNP Q9M7Q7
D	-46	SER	-	expression tag	UNP Q9M7Q7

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
D	-45	SER	-	expression tag	UNP Q9M7Q7
D	-44	HIS	-	expression tag	UNP Q9M7Q7
D	-43	HIS	-	expression tag	UNP Q9M7Q7
D	-42	HIS	-	expression tag	UNP Q9M7Q7
D	-41	HIS	-	expression tag	UNP Q9M7Q7
D	-40	HIS	-	expression tag	UNP Q9M7Q7
D	-39	HIS	-	expression tag	UNP Q9M7Q7
D	-38	SER	-	expression tag	UNP Q9M7Q7
D	-37	SER	-	expression tag	UNP Q9M7Q7
D	-36	GLY	-	expression tag	UNP Q9M7Q7
D	-35	LEU	-	expression tag	UNP Q9M7Q7
D	-34	VAL	-	expression tag	UNP Q9M7Q7
D	-33	PRO	-	expression tag	UNP Q9M7Q7
D	-32	ARG	-	expression tag	UNP Q9M7Q7
D	-31	GLY	-	expression tag	UNP Q9M7Q7
D	-30	SER	-	expression tag	UNP Q9M7Q7
D	-29	HIS	-	expression tag	UNP Q9M7Q7
D	-28	MET	-	expression tag	UNP Q9M7Q7
D	-27	ALA	-	expression tag	UNP Q9M7Q7
D	-26	SER	-	expression tag	UNP Q9M7Q7
D	-25	MET	-	expression tag	UNP Q9M7Q7
D	-24	THR	-	expression tag	UNP Q9M7Q7
D	-23	GLY	-	expression tag	UNP Q9M7Q7
D	-22	GLY	-	expression tag	UNP Q9M7Q7
D	-21	GLN	-	expression tag	UNP Q9M7Q7
D	-20	GLN	-	expression tag	UNP Q9M7Q7
D	-19	MET	-	expression tag	UNP Q9M7Q7
D	-18	GLY	-	expression tag	UNP Q9M7Q7
D	-17	ARG	-	expression tag	UNP Q9M7Q7
D	-16	GLY	-	expression tag	UNP Q9M7Q7
D	-15	SER	-	expression tag	UNP Q9M7Q7
D	-14	MET	-	expression tag	UNP Q9M7Q7
D	-13	GLY	-	expression tag	UNP Q9M7Q7
D	-12	HIS	-	expression tag	UNP Q9M7Q7
D	-11	HIS	-	expression tag	UNP Q9M7Q7
D	-10	HIS	-	expression tag	UNP Q9M7Q7
D	-9	HIS	-	expression tag	UNP Q9M7Q7
D	-8	HIS	-	expression tag	UNP Q9M7Q7
D	-7	HIS	-	expression tag	UNP Q9M7Q7
D	-6	GLU	-	expression tag	UNP Q9M7Q7
D	-5	ASN	-	expression tag	UNP Q9M7Q7
D	-4	LEU	-	expression tag	UNP Q9M7Q7

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	TYR	-	expression tag	UNP Q9M7Q7
D	-2	PHE	-	expression tag	UNP Q9M7Q7
D	-1	GLN	-	expression tag	UNP Q9M7Q7
D	0	GLY	-	expression tag	UNP Q9M7Q7
F	-48	MET	-	initiating methionine	UNP Q9M7Q7
F	-47	GLY	-	expression tag	UNP Q9M7Q7
F	-46	SER	-	expression tag	UNP Q9M7Q7
F	-45	SER	-	expression tag	UNP Q9M7Q7
F	-44	HIS	-	expression tag	UNP Q9M7Q7
F	-43	HIS	-	expression tag	UNP Q9M7Q7
F	-42	HIS	-	expression tag	UNP Q9M7Q7
F	-41	HIS	-	expression tag	UNP Q9M7Q7
F	-40	HIS	-	expression tag	UNP Q9M7Q7
F	-39	HIS	-	expression tag	UNP Q9M7Q7
F	-38	SER	-	expression tag	UNP Q9M7Q7
F	-37	SER	-	expression tag	UNP Q9M7Q7
F	-36	GLY	-	expression tag	UNP Q9M7Q7
F	-35	LEU	-	expression tag	UNP Q9M7Q7
F	-34	VAL	-	expression tag	UNP Q9M7Q7
F	-33	PRO	-	expression tag	UNP Q9M7Q7
F	-32	ARG	-	expression tag	UNP Q9M7Q7
F	-31	GLY	-	expression tag	UNP Q9M7Q7
F	-30	SER	-	expression tag	UNP Q9M7Q7
F	-29	HIS	-	expression tag	UNP Q9M7Q7
F	-28	MET	-	expression tag	UNP Q9M7Q7
F	-27	ALA	-	expression tag	UNP Q9M7Q7
F	-26	SER	-	expression tag	UNP Q9M7Q7
F	-25	MET	-	expression tag	UNP Q9M7Q7
F	-24	THR	-	expression tag	UNP Q9M7Q7
F	-23	GLY	-	expression tag	UNP Q9M7Q7
F	-22	GLY	-	expression tag	UNP Q9M7Q7
F	-21	GLN	-	expression tag	UNP Q9M7Q7
F	-20	GLN	-	expression tag	UNP Q9M7Q7
F	-19	MET	-	expression tag	UNP Q9M7Q7
F	-18	GLY	-	expression tag	UNP Q9M7Q7
F	-17	ARG	-	expression tag	UNP Q9M7Q7
F	-16	GLY	-	expression tag	UNP Q9M7Q7
F	-15	SER	-	expression tag	UNP Q9M7Q7
F	-14	MET	-	expression tag	UNP Q9M7Q7
F	-13	GLY	-	expression tag	UNP Q9M7Q7
F	-12	HIS	-	expression tag	UNP Q9M7Q7
F	-11	HIS	-	expression tag	UNP Q9M7Q7

*Continued on next page...*



*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
F	-10	HIS	-	expression tag	UNP Q9M7Q7
F	-9	HIS	-	expression tag	UNP Q9M7Q7
F	-8	HIS	-	expression tag	UNP Q9M7Q7
F	-7	HIS	-	expression tag	UNP Q9M7Q7
F	-6	GLU	-	expression tag	UNP Q9M7Q7
F	-5	ASN	-	expression tag	UNP Q9M7Q7
F	-4	LEU	-	expression tag	UNP Q9M7Q7
F	-3	TYR	-	expression tag	UNP Q9M7Q7
F	-2	PHE	-	expression tag	UNP Q9M7Q7
F	-1	GLN	-	expression tag	UNP Q9M7Q7
F	0	GLY	-	expression tag	UNP Q9M7Q7
H	-48	MET	-	initiating methionine	UNP Q9M7Q7
H	-47	GLY	-	expression tag	UNP Q9M7Q7
H	-46	SER	-	expression tag	UNP Q9M7Q7
H	-45	SER	-	expression tag	UNP Q9M7Q7
H	-44	HIS	-	expression tag	UNP Q9M7Q7
H	-43	HIS	-	expression tag	UNP Q9M7Q7
H	-42	HIS	-	expression tag	UNP Q9M7Q7
H	-41	HIS	-	expression tag	UNP Q9M7Q7
H	-40	HIS	-	expression tag	UNP Q9M7Q7
H	-39	HIS	-	expression tag	UNP Q9M7Q7
H	-38	SER	-	expression tag	UNP Q9M7Q7
H	-37	SER	-	expression tag	UNP Q9M7Q7
H	-36	GLY	-	expression tag	UNP Q9M7Q7
H	-35	LEU	-	expression tag	UNP Q9M7Q7
H	-34	VAL	-	expression tag	UNP Q9M7Q7
H	-33	PRO	-	expression tag	UNP Q9M7Q7
H	-32	ARG	-	expression tag	UNP Q9M7Q7
H	-31	GLY	-	expression tag	UNP Q9M7Q7
H	-30	SER	-	expression tag	UNP Q9M7Q7
H	-29	HIS	-	expression tag	UNP Q9M7Q7
H	-28	MET	-	expression tag	UNP Q9M7Q7
H	-27	ALA	-	expression tag	UNP Q9M7Q7
H	-26	SER	-	expression tag	UNP Q9M7Q7
H	-25	MET	-	expression tag	UNP Q9M7Q7
H	-24	THR	-	expression tag	UNP Q9M7Q7
H	-23	GLY	-	expression tag	UNP Q9M7Q7
H	-22	GLY	-	expression tag	UNP Q9M7Q7
H	-21	GLN	-	expression tag	UNP Q9M7Q7
H	-20	GLN	-	expression tag	UNP Q9M7Q7
H	-19	MET	-	expression tag	UNP Q9M7Q7
H	-18	GLY	-	expression tag	UNP Q9M7Q7

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
H	-17	ARG	-	expression tag	UNP Q9M7Q7
H	-16	GLY	-	expression tag	UNP Q9M7Q7
H	-15	SER	-	expression tag	UNP Q9M7Q7
H	-14	MET	-	expression tag	UNP Q9M7Q7
H	-13	GLY	-	expression tag	UNP Q9M7Q7
H	-12	HIS	-	expression tag	UNP Q9M7Q7
H	-11	HIS	-	expression tag	UNP Q9M7Q7
H	-10	HIS	-	expression tag	UNP Q9M7Q7
H	-9	HIS	-	expression tag	UNP Q9M7Q7
H	-8	HIS	-	expression tag	UNP Q9M7Q7
H	-7	HIS	-	expression tag	UNP Q9M7Q7
H	-6	GLU	-	expression tag	UNP Q9M7Q7
H	-5	ASN	-	expression tag	UNP Q9M7Q7
H	-4	LEU	-	expression tag	UNP Q9M7Q7
H	-3	TYR	-	expression tag	UNP Q9M7Q7
H	-2	PHE	-	expression tag	UNP Q9M7Q7
H	-1	GLN	-	expression tag	UNP Q9M7Q7
H	0	GLY	-	expression tag	UNP Q9M7Q7
K	-48	MET	-	initiating methionine	UNP Q9M7Q7
K	-47	GLY	-	expression tag	UNP Q9M7Q7
K	-46	SER	-	expression tag	UNP Q9M7Q7
K	-45	SER	-	expression tag	UNP Q9M7Q7
K	-44	HIS	-	expression tag	UNP Q9M7Q7
K	-43	HIS	-	expression tag	UNP Q9M7Q7
K	-42	HIS	-	expression tag	UNP Q9M7Q7
K	-41	HIS	-	expression tag	UNP Q9M7Q7
K	-40	HIS	-	expression tag	UNP Q9M7Q7
K	-39	HIS	-	expression tag	UNP Q9M7Q7
K	-38	SER	-	expression tag	UNP Q9M7Q7
K	-37	SER	-	expression tag	UNP Q9M7Q7
K	-36	GLY	-	expression tag	UNP Q9M7Q7
K	-35	LEU	-	expression tag	UNP Q9M7Q7
K	-34	VAL	-	expression tag	UNP Q9M7Q7
K	-33	PRO	-	expression tag	UNP Q9M7Q7
K	-32	ARG	-	expression tag	UNP Q9M7Q7
K	-31	GLY	-	expression tag	UNP Q9M7Q7
K	-30	SER	-	expression tag	UNP Q9M7Q7
K	-29	HIS	-	expression tag	UNP Q9M7Q7
K	-28	MET	-	expression tag	UNP Q9M7Q7
K	-27	ALA	-	expression tag	UNP Q9M7Q7
K	-26	SER	-	expression tag	UNP Q9M7Q7
K	-25	MET	-	expression tag	UNP Q9M7Q7

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
K	-24	THR	-	expression tag	UNP Q9M7Q7
K	-23	GLY	-	expression tag	UNP Q9M7Q7
K	-22	GLY	-	expression tag	UNP Q9M7Q7
K	-21	GLN	-	expression tag	UNP Q9M7Q7
K	-20	GLN	-	expression tag	UNP Q9M7Q7
K	-19	MET	-	expression tag	UNP Q9M7Q7
K	-18	GLY	-	expression tag	UNP Q9M7Q7
K	-17	ARG	-	expression tag	UNP Q9M7Q7
K	-16	GLY	-	expression tag	UNP Q9M7Q7
K	-15	SER	-	expression tag	UNP Q9M7Q7
K	-14	MET	-	expression tag	UNP Q9M7Q7
K	-13	GLY	-	expression tag	UNP Q9M7Q7
K	-12	HIS	-	expression tag	UNP Q9M7Q7
K	-11	HIS	-	expression tag	UNP Q9M7Q7
K	-10	HIS	-	expression tag	UNP Q9M7Q7
K	-9	HIS	-	expression tag	UNP Q9M7Q7
K	-8	HIS	-	expression tag	UNP Q9M7Q7
K	-7	HIS	-	expression tag	UNP Q9M7Q7
K	-6	GLU	-	expression tag	UNP Q9M7Q7
K	-5	ASN	-	expression tag	UNP Q9M7Q7
K	-4	LEU	-	expression tag	UNP Q9M7Q7
K	-3	TYR	-	expression tag	UNP Q9M7Q7
K	-2	PHE	-	expression tag	UNP Q9M7Q7
K	-1	GLN	-	expression tag	UNP Q9M7Q7
K	0	GLY	-	expression tag	UNP Q9M7Q7

- Molecule 2 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	14	Total	C	N	O	0	0	0
			121	82	20	19			
2	B	13	Total	C	N	O	0	0	0
			106	74	15	17			
2	E	13	Total	C	N	O	0	0	0
			106	72	17	17			
2	G	12	Total	C	N	O	0	0	0
			105	72	17	16			
2	J	14	Total	C	N	O	0	0	0
			111	77	16	18			
2	L	13	Total	C	N	O	0	0	0
			110	75	18	17			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	77	TYR	-	insertion	UNP K7MRE7
B	77	TYR	-	insertion	UNP K7MRE7
E	77	TYR	-	insertion	UNP K7MRE7
G	77	TYR	-	insertion	UNP K7MRE7
J	77	TYR	-	insertion	UNP K7MRE7
L	77	TYR	-	insertion	UNP K7MRE7

- Molecule 3 is water.

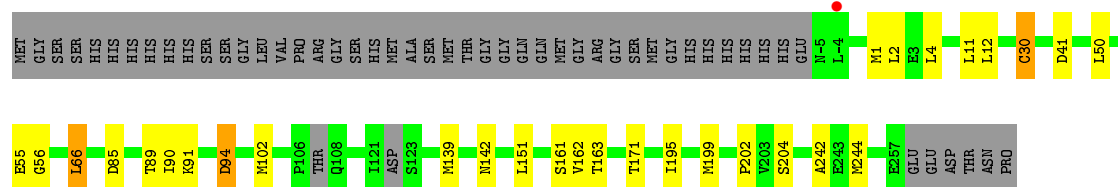
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	68	Total O 68 68	0	0
3	I	8	Total O 8 8	0	0
3	A	63	Total O 63 63	0	0
3	B	10	Total O 10 10	0	0
3	D	80	Total O 80 80	0	0
3	E	2	Total O 2 2	0	0
3	F	91	Total O 91 91	0	0
3	G	3	Total O 3 3	0	0
3	H	38	Total O 38 38	0	0
3	J	1	Total O 1 1	0	0
3	K	37	Total O 37 37	0	0
3	L	1	Total O 1 1	0	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 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.

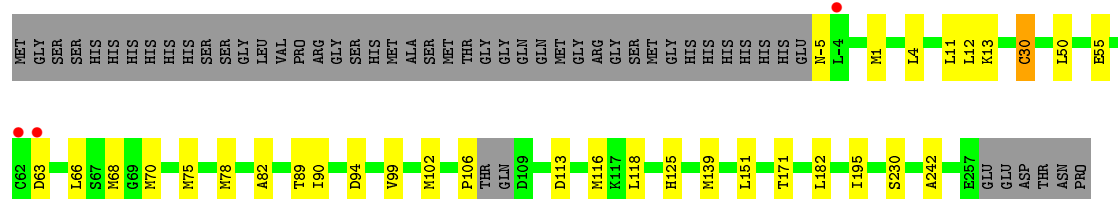
- Molecule 1: Proliferating cellular nuclear antigen 1

Chain C: 




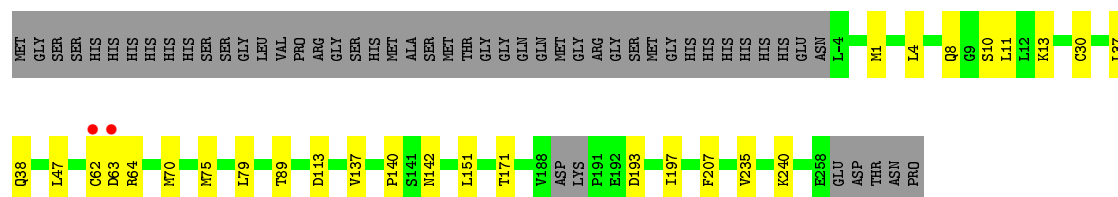
- Molecule 1: Proliferating cellular nuclear antigen 1

Chain A: 




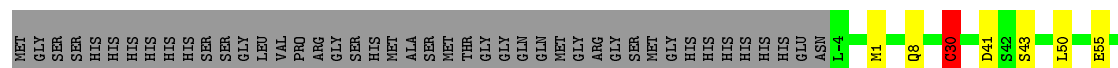
- Molecule 1: Proliferating cellular nuclear antigen 1

Chain D: 



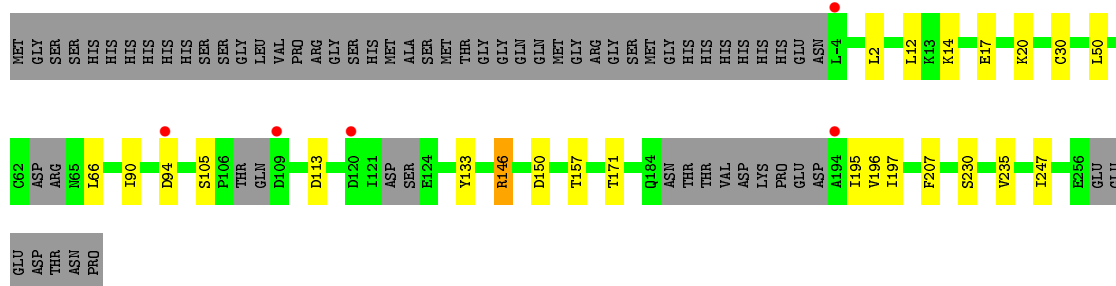
- Molecule 1: Proliferating cellular nuclear antigen 1

Chain F: 

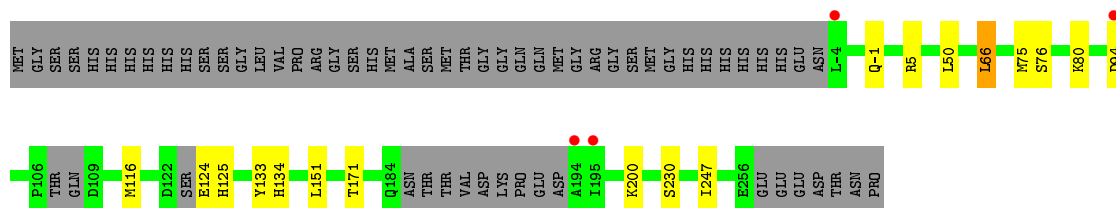




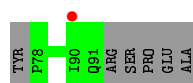
- Molecule 1: Proliferating cellular nuclear antigen 1



- Molecule 1: Proliferating cellular nuclear antigen 1



- Molecule 2: Uncharacterized protein



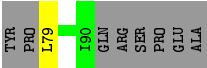
- Molecule 2: Uncharacterized protein



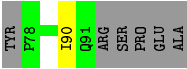
- Molecule 2: Uncharacterized protein



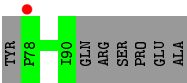
- Molecule 2: Uncharacterized protein



• Molecule 2: Uncharacterized protein



• Molecule 2: Uncharacterized protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.90Å 90.55Å 90.51Å 60.05° 73.46° 73.59°	Depositor
Resolution (Å)	29.65 – 2.06 29.65 – 2.06	Depositor EDS
% Data completeness (in resolution range)	94.3 (29.65-2.06) 93.7 (29.65-2.06)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.90 (at 2.06Å)	Xtriage
Refinement program	PHENIX (1.13_2998)	Depositor
R, $R_{free}$	0.197 , 0.234 0.197 , 0.234	Depositor DCC
$R_{free}$ test set	2006 reflections (1.82%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.8	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 36.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.53$ , $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.477 for -h,-l,-k	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	12307	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.44% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [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  >5	RMSZ	# Z  >5
1	A	0.41	1/1945 (0.1%)	0.63	3/2642 (0.1%)
1	C	0.44	1/1953 (0.1%)	0.64	2/2647 (0.1%)
1	D	0.42	2/1932 (0.1%)	0.63	0/2625
1	F	0.44	2/1947 (0.1%)	0.61	0/2647
1	H	0.36	0/1819	0.56	0/2460
1	K	0.37	0/1811	0.56	0/2459
2	B	0.39	0/108	0.53	0/145
2	E	0.37	0/107	0.53	0/144
2	G	0.40	0/106	0.49	0/141
2	I	0.34	0/123	0.54	0/164
2	J	0.34	0/113	0.50	0/152
2	L	0.40	0/111	0.47	0/148
All	All	0.41	6/12075 (0.0%)	0.60	5/16374 (0.0%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	30	CYS	CB-SG	-6.39	1.71	1.82
1	F	30	CYS	CB-SG	-6.35	1.71	1.82
1	D	30	CYS	CB-SG	-5.82	1.72	1.81
1	D	62	CYS	CB-SG	-5.46	1.73	1.81
1	A	30	CYS	CB-SG	-5.33	1.73	1.81

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66	LEU	CA-CB-CG	6.13	129.39	115.30
1	C	50	LEU	CA-CB-CG	5.58	128.13	115.30
1	A	50	LEU	CA-CB-CG	5.47	127.88	115.30
1	C	66	LEU	CB-CG-CD2	-5.42	101.78	111.00
1	A	50	LEU	CB-CG-CD1	-5.22	102.12	111.00

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	1916	0	1840	16	0
1	C	1926	0	1874	26	0
1	D	1904	0	1814	16	0
1	F	1919	0	1821	16	0
1	H	1795	0	1755	17	0
1	K	1786	0	1711	12	0
2	B	106	0	112	0	0
2	E	106	0	106	0	0
2	G	105	0	115	1	0
2	I	121	0	131	0	0
2	J	111	0	114	1	0
2	L	110	0	117	0	0
3	A	63	0	0	2	0
3	B	10	0	0	0	0
3	C	68	0	0	2	0
3	D	80	0	0	3	0
3	E	2	0	0	0	0
3	F	91	0	0	2	0
3	G	3	0	0	0	0
3	H	38	0	0	1	0
3	I	8	0	0	0	0
3	J	1	0	0	0	0
3	K	37	0	0	2	0
3	L	1	0	0	0	0
All	All	12307	0	11510	104	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 4.

The worst 5 of 104 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:D:70:MET:HE1	1:D:75:MET:SD	2.08	0.93

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1:MET:H	1:F:63:ASP:HB2	1.36	0.90
1:C:66:LEU:CD2	1:C:94:ASP:HA	2.02	0.89
1:C:142:ASN:ND2	3:C:301:HOH:O	2.07	0.86
1:C:66:LEU:HD23	1:C:94:ASP:HA	1.55	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	Percentiles	
1	A	257/312 (82%)	252 (98%)	3 (1%)	2 (1%)	19	9
1	C	255/312 (82%)	247 (97%)	7 (3%)	1 (0%)	34	25
1	D	257/312 (82%)	253 (98%)	4 (2%)	0	100	100
1	F	258/312 (83%)	245 (95%)	12 (5%)	1 (0%)	34	25
1	H	236/312 (76%)	235 (100%)	1 (0%)	0	100	100
1	K	241/312 (77%)	235 (98%)	6 (2%)	0	100	100
2	B	11/20 (55%)	11 (100%)	0	0	100	100
2	E	11/20 (55%)	11 (100%)	0	0	100	100
2	G	10/20 (50%)	10 (100%)	0	0	100	100
2	I	12/20 (60%)	12 (100%)	0	0	100	100
2	J	12/20 (60%)	11 (92%)	1 (8%)	0	100	100
2	L	11/20 (55%)	11 (100%)	0	0	100	100
All	All	1571/1992 (79%)	1533 (98%)	34 (2%)	4 (0%)	41	32

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	125	HIS
1	F	125	HIS
1	C	94	ASP
1	A	94	ASP

### 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	204/274 (74%)	201 (98%)	3 (2%)	65	62
1	C	209/274 (76%)	208 (100%)	1 (0%)	88	89
1	D	201/274 (73%)	200 (100%)	1 (0%)	88	89
1	F	205/274 (75%)	202 (98%)	3 (2%)	65	62
1	H	190/274 (69%)	188 (99%)	2 (1%)	73	72
1	K	185/274 (68%)	184 (100%)	1 (0%)	88	89
2	B	12/19 (63%)	12 (100%)	0	100	100
2	E	11/19 (58%)	11 (100%)	0	100	100
2	G	12/19 (63%)	12 (100%)	0	100	100
2	I	14/19 (74%)	14 (100%)	0	100	100
2	J	12/19 (63%)	12 (100%)	0	100	100
2	L	12/19 (63%)	12 (100%)	0	100	100
All	All	1267/1758 (72%)	1256 (99%)	11 (1%)	78	78

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	113	ASP
1	F	30	CYS
1	H	105	SER
1	A	230	SER
1	F	230	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such

sidechains are listed below:

Mol	Chain	Res	Type
1	C	142	ASN
1	A	44	HIS
1	H	179	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 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.

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	261/312 (83%)	-0.31	3 (1%) 80 81	26, 41, 65, 105	0
1	C	261/312 (83%)	-0.30	1 (0%) 92 93	26, 41, 73, 96	0
1	D	261/312 (83%)	-0.34	2 (0%) 86 87	24, 41, 66, 94	0
1	F	262/312 (83%)	-0.27	2 (0%) 86 87	25, 41, 72, 102	0
1	H	246/312 (78%)	-0.18	5 (2%) 65 67	34, 50, 76, 110	0
1	K	249/312 (79%)	-0.17	4 (1%) 72 73	35, 50, 75, 107	0
2	B	13/20 (65%)	-0.03	0 100 100	34, 42, 66, 91	0
2	E	13/20 (65%)	-0.28	0 100 100	32, 38, 63, 82	0
2	G	12/20 (60%)	-0.41	0 100 100	31, 42, 57, 62	0
2	I	14/20 (70%)	0.16	1 (7%) 16 16	35, 43, 83, 86	0
2	J	14/20 (70%)	0.01	0 100 100	46, 59, 96, 98	0
2	L	13/20 (65%)	0.20	1 (7%) 13 13	46, 56, 88, 89	0
All	All	1619/1992 (81%)	-0.25	19 (1%) 79 80	24, 44, 75, 110	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	194	ALA	4.5
1	K	-4	LEU	3.7
2	I	90	ILE	3.4
1	A	-4	LEU	3.4
2	L	78	PRO	3.3

### 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 carbohydrates 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.