



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 10:17 PM GMT

PDB ID : 1SXJ  
Title : Crystal Structure of the Eukaryotic Clamp Loader (Replication Factor C, RFC) Bound to the DNA Sliding Clamp (Proliferating Cell Nuclear Antigen, PCNA)  
Authors : Bowman, G.D.; O'Donnell, M.; Kuriyan, J.  
Deposited on : 2004-03-30  
Resolution : 2.85 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

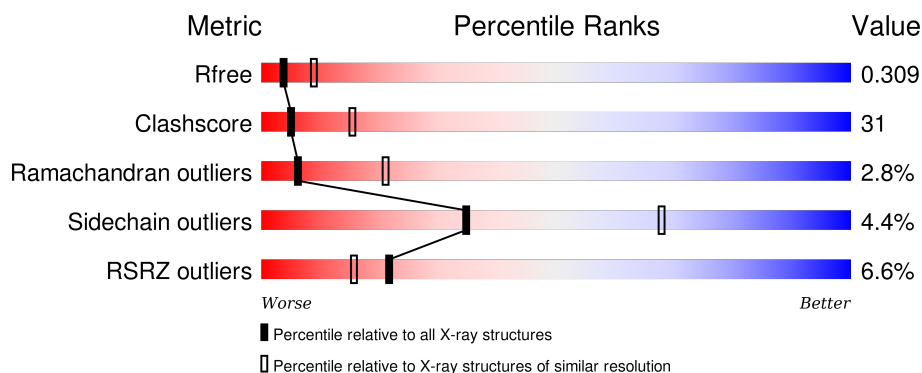
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 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))
$R_{free}$	91344	2228 (2.90-2.82)
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)
RSRZ outliers	91569	2236 (2.90-2.82)

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. 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	516	<div> <div>3%</div> <div>44%</div> <div>39%</div> <div>15%</div> </div>
2	B	323	<div> <div>%</div> <div>59%</div> <div>36%</div> <div>••</div> </div>
3	C	340	<div> <div>2%</div> <div>43%</div> <div>47%</div> <div>• 5%</div> </div>
4	D	353	<div> <div>9%</div> <div>43%</div> <div>46%</div> <div>•• 7%</div> </div>
5	E	354	<div> <div>11%</div> <div>39%</div> <div>47%</div> <div>• 10%</div> </div>

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Mol	Chain	Length	Quality of chain
6	F	283	
6	G	283	
6	H	283	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	MG	A	811	-	-	-	X
7	MG	B	812	-	-	-	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 19740 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 Activator 1 95 kDa subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	441	Total	C	N	O	S	0	0	0
			3345	2110	603	617	15			

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	270	MET	-	EXPRESSION TAG	UNP P38630
A	271	GLY	-	EXPRESSION TAG	UNP P38630
A	272	SER	-	EXPRESSION TAG	UNP P38630
A	273	SER	-	EXPRESSION TAG	UNP P38630
A	274	HIS	-	EXPRESSION TAG	UNP P38630
A	275	HIS	-	EXPRESSION TAG	UNP P38630
A	276	HIS	-	EXPRESSION TAG	UNP P38630
A	277	HIS	-	EXPRESSION TAG	UNP P38630
A	278	HIS	-	EXPRESSION TAG	UNP P38630
A	279	HIS	-	EXPRESSION TAG	UNP P38630
A	280	SER	-	EXPRESSION TAG	UNP P38630
A	281	SER	-	EXPRESSION TAG	UNP P38630
A	282	GLY	-	EXPRESSION TAG	UNP P38630
A	283	LEU	-	EXPRESSION TAG	UNP P38630
A	284	GLU	-	EXPRESSION TAG	UNP P38630
A	285	VAL	-	EXPRESSION TAG	UNP P38630
A	286	LEU	-	EXPRESSION TAG	UNP P38630
A	287	PHE	-	EXPRESSION TAG	UNP P38630
A	288	GLN	-	EXPRESSION TAG	UNP P38630
A	289	GLY	-	EXPRESSION TAG	UNP P38630
A	290	PRO	-	EXPRESSION TAG	UNP P38630
A	291	HIS	-	EXPRESSION TAG	UNP P38630
A	292	MET	-	EXPRESSION TAG	UNP P38630
A	293	ALA	-	EXPRESSION TAG	UNP P38630
A	294	SER	-	EXPRESSION TAG	UNP P38630

- Molecule 2 is a protein called Activator 1 37 kDa subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	316	Total	C	N	O	S	0	0	0
			2482	1566	441	462	13			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	157	GLN	ARG	ENGINEERED	UNP P40339

- Molecule 3 is a protein called Activator 1 40 kDa subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	322	Total	C	N	O	S	0	0	0
			2544	1604	443	489	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	160	GLN	ARG	ENGINEERED	UNP P38629

- Molecule 4 is a protein called Activator 1 41 kDa subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	328	Total	C	N	O	S	0	0	0
			2597	1642	446	499	10			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	183	GLN	ARG	ENGINEERED	UNP P40348

- Molecule 5 is a protein called Activator 1 40 kDa subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	317	Total	C	N	O	S	0	0	0
			2495	1582	428	468	17			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	184	GLN	ARG	ENGINEERED	UNP P38251

- Molecule 6 is a protein called Proliferating cell nuclear antigen.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
6	F	258	Total 2021	C 1291	N 319	O 401	S 4	Se 6	0	0	0
6	G	258	Total 2022	C 1292	N 319	O 400	S 4	Se 7	5	0	0
6	H	267	Total 2079	C 1329	N 330	O 409	S 4	Se 7	0	0	0

There are 93 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-24	MSE	-	EXPRESSION TAG	UNP P15873
F	-23	GLY	-	EXPRESSION TAG	UNP P15873
F	-22	SER	-	EXPRESSION TAG	UNP P15873
F	-21	SER	-	EXPRESSION TAG	UNP P15873
F	-20	HIS	-	EXPRESSION TAG	UNP P15873
F	-19	HIS	-	EXPRESSION TAG	UNP P15873
F	-18	HIS	-	EXPRESSION TAG	UNP P15873
F	-17	HIS	-	EXPRESSION TAG	UNP P15873
F	-16	HIS	-	EXPRESSION TAG	UNP P15873
F	-15	HIS	-	EXPRESSION TAG	UNP P15873
F	-14	SER	-	EXPRESSION TAG	UNP P15873
F	-13	SER	-	EXPRESSION TAG	UNP P15873
F	-12	GLY	-	EXPRESSION TAG	UNP P15873
F	-11	LEU	-	EXPRESSION TAG	UNP P15873
F	-10	GLU	-	EXPRESSION TAG	UNP P15873
F	-9	VAL	-	EXPRESSION TAG	UNP P15873
F	-8	LEU	-	EXPRESSION TAG	UNP P15873
F	-7	PHE	-	EXPRESSION TAG	UNP P15873
F	-6	GLN	-	EXPRESSION TAG	UNP P15873
F	-5	GLY	-	EXPRESSION TAG	UNP P15873
F	-4	PRO	-	EXPRESSION TAG	UNP P15873
F	-3	HIS	-	EXPRESSION TAG	UNP P15873
F	-2	MSE	-	EXPRESSION TAG	UNP P15873
F	-1	ALA	-	EXPRESSION TAG	UNP P15873
F	0	SER	-	EXPRESSION TAG	UNP P15873
F	1	MSE	MET	MODIFIED RESIDUE	UNP P15873
F	70	MSE	MET	MODIFIED RESIDUE	UNP P15873
F	119	MSE	MET	MODIFIED RESIDUE	UNP P15873
F	161	MSE	MET	MODIFIED RESIDUE	UNP P15873
F	188	MSE	MET	MODIFIED RESIDUE	UNP P15873
F	199	MSE	MET	MODIFIED RESIDUE	UNP P15873
G	-24	MSE	-	EXPRESSION TAG	UNP P15873
G	-23	GLY	-	EXPRESSION TAG	UNP P15873

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-22	SER	-	EXPRESSION TAG	UNP P15873
G	-21	SER	-	EXPRESSION TAG	UNP P15873
G	-20	HIS	-	EXPRESSION TAG	UNP P15873
G	-19	HIS	-	EXPRESSION TAG	UNP P15873
G	-18	HIS	-	EXPRESSION TAG	UNP P15873
G	-17	HIS	-	EXPRESSION TAG	UNP P15873
G	-16	HIS	-	EXPRESSION TAG	UNP P15873
G	-15	HIS	-	EXPRESSION TAG	UNP P15873
G	-14	SER	-	EXPRESSION TAG	UNP P15873
G	-13	SER	-	EXPRESSION TAG	UNP P15873
G	-12	GLY	-	EXPRESSION TAG	UNP P15873
G	-11	LEU	-	EXPRESSION TAG	UNP P15873
G	-10	GLU	-	EXPRESSION TAG	UNP P15873
G	-9	VAL	-	EXPRESSION TAG	UNP P15873
G	-8	LEU	-	EXPRESSION TAG	UNP P15873
G	-7	PHE	-	EXPRESSION TAG	UNP P15873
G	-6	GLN	-	EXPRESSION TAG	UNP P15873
G	-5	GLY	-	EXPRESSION TAG	UNP P15873
G	-4	PRO	-	EXPRESSION TAG	UNP P15873
G	-3	HIS	-	EXPRESSION TAG	UNP P15873
G	-2	MSE	-	EXPRESSION TAG	UNP P15873
G	-1	ALA	-	EXPRESSION TAG	UNP P15873
G	0	SER	-	EXPRESSION TAG	UNP P15873
G	1	MSE	MET	MODIFIED RESIDUE	UNP P15873
G	70	MSE	MET	MODIFIED RESIDUE	UNP P15873
G	119	MSE	MET	MODIFIED RESIDUE	UNP P15873
G	161	MSE	MET	MODIFIED RESIDUE	UNP P15873
G	188	MSE	MET	MODIFIED RESIDUE	UNP P15873
G	199	MSE	MET	MODIFIED RESIDUE	UNP P15873
H	-24	MSE	-	EXPRESSION TAG	UNP P15873
H	-23	GLY	-	EXPRESSION TAG	UNP P15873
H	-22	SER	-	EXPRESSION TAG	UNP P15873
H	-21	SER	-	EXPRESSION TAG	UNP P15873
H	-20	HIS	-	EXPRESSION TAG	UNP P15873
H	-19	HIS	-	EXPRESSION TAG	UNP P15873
H	-18	HIS	-	EXPRESSION TAG	UNP P15873
H	-17	HIS	-	EXPRESSION TAG	UNP P15873
H	-16	HIS	-	EXPRESSION TAG	UNP P15873
H	-15	HIS	-	EXPRESSION TAG	UNP P15873
H	-14	SER	-	EXPRESSION TAG	UNP P15873
H	-13	SER	-	EXPRESSION TAG	UNP P15873
H	-12	GLY	-	EXPRESSION TAG	UNP P15873

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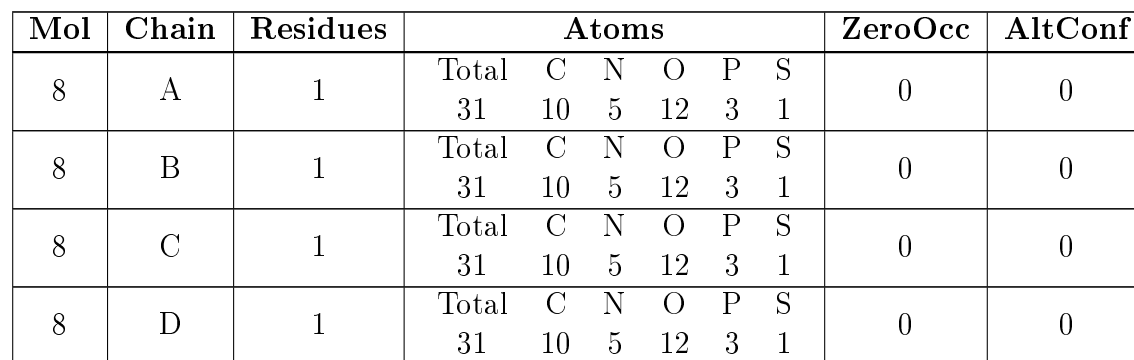
Chain	Residue	Modelled	Actual	Comment	Reference
H	-11	LEU	-	EXPRESSION TAG	UNP P15873
H	-10	GLU	-	EXPRESSION TAG	UNP P15873
H	-9	VAL	-	EXPRESSION TAG	UNP P15873
H	-8	LEU	-	EXPRESSION TAG	UNP P15873
H	-7	PHE	-	EXPRESSION TAG	UNP P15873
H	-6	GLN	-	EXPRESSION TAG	UNP P15873
H	-5	GLY	-	EXPRESSION TAG	UNP P15873
H	-4	PRO	-	EXPRESSION TAG	UNP P15873
H	-3	HIS	-	EXPRESSION TAG	UNP P15873
H	-2	MSE	-	EXPRESSION TAG	UNP P15873
H	-1	ALA	-	EXPRESSION TAG	UNP P15873
H	0	SER	-	EXPRESSION TAG	UNP P15873
H	1	MSE	MET	MODIFIED RESIDUE	UNP P15873
H	70	MSE	MET	MODIFIED RESIDUE	UNP P15873
H	119	MSE	MET	MODIFIED RESIDUE	UNP P15873
H	161	MSE	MET	MODIFIED RESIDUE	UNP P15873
H	188	MSE	MET	MODIFIED RESIDUE	UNP P15873
H	199	MSE	MET	MODIFIED RESIDUE	UNP P15873

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total Mg 1 1	0	0
7	A	1	Total Mg 1 1	0	0
7	D	1	Total Mg 1 1	0	0
7	C	1	Total Mg 1 1	0	0

- Molecule 8 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>S).



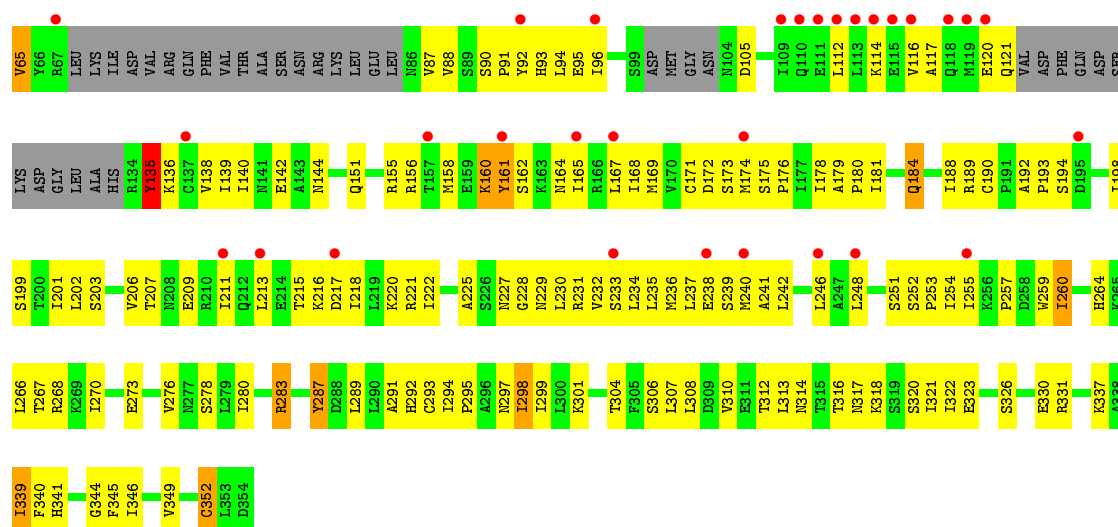


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- The chemical structure of ADP (Adenosine Diphosphate) is shown. It consists of an adenine base (a purine ring system with an amino group at N6) attached to a ribose sugar (a five-membered ring with hydroxyl groups at C2' and C3'). The ribose sugar is linked to a diphosphate group (two phosphate groups connected by an oxygen atom). The phosphate groups are labeled with oxygen atoms O1A, O2A, O3A, O4A, O5A, O6A, O7A, O8A, O9A, O10A, O11A, O12A, O13A, O14A, O15A, O16A, O17A, O18A, O19A, O20A, O21A, O22A, O23A, O24A, O25A, O26A, O27A, O28A, O29A, O30A, O31A, O32A, O33A, O34A, O35A, O36A, O37A, O38A, O39A, O40A, O41A, O42A, O43A, O44A, O45A, O46A, O47A, O48A, O49A, O50A, O51A, O52A, O53A, O54A, O55A, O56A, O57A, O58A, O59A, O60A, O61A, O62A, O63A, O64A, O65A, O66A, O67A, O68A, O69A, O70A, O71A, O72A, O73A, O74A, O75A, O76A, O77A, O78A, O79A, O80A, O81A, O82A, O83A, O84A, O85A, O86A, O87A, O88A, O89A, O90A, O91A, O92A, O93A, O94A, O95A, O96A, O97A, O98A, O99A, O100A, O101A, O102A, O103A, O104A, O105A, O106A, O107A, O108A, O109A, O110A, O111A, O112A, O113A, O114A, O115A, O116A, O117A, O118A, O119A, O120A, O121A, O122A, O123A, O124A, O125A, O126A, O127A, O128A, O129A, O130A, O131A, O132A, O133A, O134A, O135A, O136A, O137A, O138A, O139A, O140A, O141A, O142A, O143A, O144A, O145A, O146A, O147A, O148A, O149A, O150A, O151A, O152A, O153A, O154A, O155A, O156A, O157A, O158A, O159A, O160A, O161A, O162A, O163A, O164A, O165A, O166A, O167A, O168A, O169A, O170A, O171A, O172A, O173A, O174A, O175A, O176A, O177A, O178A, O179A, O180A, O181A, O182A, O183A, O184A, O185A, O186A, O187A, O188A, O189A, O190A, O191A, O192A, O193A, O194A, O195A, O196A, O197A, O198A, O199A, O200A, O201A, O202A, O203A, O204A, O205A, O206A, O207A, O208A, O209A, O210A, O211A, O212A, O213A, O214A, O215A, O216A, O217A, O218A, O219A, O220A, O221A, O222A, O223A, O224A, O225A, O226A, O227A, O228A, O229A, O230A, O231A, O232A, O233A, O234A, O235A, O236A, O237A, O238A, O239A, O240A, O241A, O242A, O243A, O244A, O245A, O246A, O247A, O248A, O249A, O250A, O251A, O252A, O253A, O254A, O255A, O256A, O257A, O258A, O259A, O260A, O261A, O262A, O263A, O264A, O265A, O266A, O267A, O268A, O269A, O270A, O271A, O272A, O273A, O274A, O275A, O276A, O277A, O278A, O279A, O280A, O281A, O282A, O283A, O284A, O285A, O286A, O287A, O288A, O289A, O290A, O291A, O292A, O293A, O294A, O295A, O296A, O297A, O298A, O299A, O300A, O301A, O302A, O303A, O304A, O305A, O306A, O307A, O308A, O309A, O310A, O311A, O312A, O313A, O314A, O315A, O316A, O317A, O318A, O319A, O320A, O321A, O322A, O323A, O324A, O325A, O326A, O327A, O328A, O329A, O330A, O331A, O332A, O333A, O334A, O335A, O336A, O337A, O338A, O339A, O340A, O341A, O342A, O343A, O344A, O345A, O346A, O347A, O348A, O349A, O350A, O351A, O352A, O353A, O354A, O355A, O356A, O357A, O358A, O359A, O360A, O361A, O362A, O363A, O364A, O365A, O366A, O367A, O368A, O369A, O370A, O371A, O372A, O373A, O374A, O375A, O376A, O377A, O378A, O379A, O380A, O381A, O382A, O383A, O384A, O385A, O386A, O387A, O388A, O389A, O390A, O391A, O392A, O393A, O394A, O395A, O396A, O397A, O398A, O399A, O400A, O401A, O402A, O403A, O404A, O405A, O406A, O407A, O408A, O409A, O410A, O411A, O412A, O413A, O414A, O415A, O416A, O417A, O418A, O419A, O420A, O421A, O422A, O423A, O424A, O425A, O426A, O427A, O428A, O429A, O430A, O431A, O432A, O433A, O434A, O435A, O436A, O437A, O438A, O439A, O440A, O441A, O442A, O443A, O444A, O445A, O446A, O447A, O448A, O449A, O450A, O451A, O452A, O453A, O454A, O455A, O456A, O457A, O458A, O459A, O460A, O461A, O462A, O463A, O464A, O465A, O466A, O467A, O468A, O469A, O470A, O471A, O472A, O473A, O474A, O475A, O476A, O477A, O478A, O479A, O480A, O481A, O482A, O483A, O484A, O485A, O486A, O487A, O488A, O489A, O490A, O491A, O492A, O493A, O494A, O495A, O496A, O497A, O498A, O499A, O500A, O501A, O502A, O503A, O504A, O505A, O506A, O507A, O508A, O509A, O510A, O511A, O512A, O513A, O514A, O515A, O516A, O517A, O518A, O519A, O520A, O521A, O522A, O523A, O524A, O525A, O526A, O527A, O528A, O529A, O530A, O531A, O532A, O533A, O534A, O535A, O536A, O537A, O538A, O539A, O540A, O541A, O542A, O543A, O544A, O545A, O546A, O547A, O548A, O549A, O550A, O551A, O552A, O553A, O554A, O555A, O556A, O557A, O558A, O559A, O560A, O561A, O562A, O563A, O564A, O565A, O566A, O567A, O568A, O569A, O570A, O571A, O572A, O573A, O574A, O575A, O576A, O577A, O578A, O579A, O580A, O581A, O582A, O583A, O584A, O585A, O586A, O587A, O588A, O589A, O590A, O591A, O592A, O593A, O594A, O595A, O596A, O597A, O598A, O599A, O600A, O601A, O602A, O603A, O604A, O605A, O606A, O607A, O608A, O609A, O610A, O611A, O612A, O613A, O614A, O615A, O616A, O617A, O618A, O619A, O620A, O621A, O622A, O623A, O624A, O625A, O626A, O627A, O628A, O629A, O630A, O631A, O632A, O633A, O634A, O635A, O636A, O637A, O638A, O639A, O640A, O641A, O642A, O643A, O644A, O645A, O646A, O647A, O648A, O649A, O650A, O651A, O652A, O653A, O654A, O655A, O656A, O657A, O658A, O659A, O660A, O661A, O662A, O663A, O664A, O665A, O666A, O667A, O668A, O669A, O670A, O671A, O672A, O673A, O674A, O675A, O676A, O677A, O678A, O679A, O6

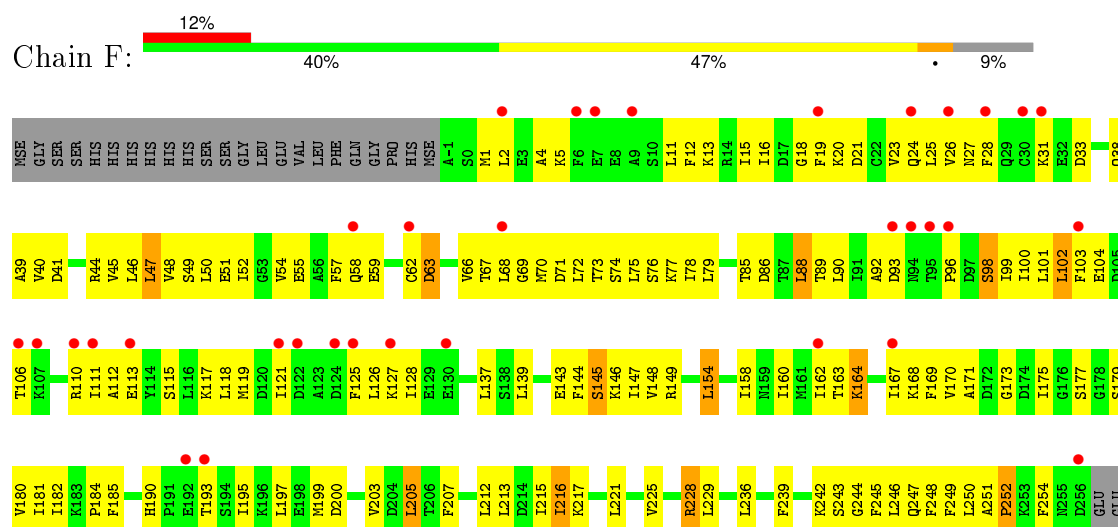
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		



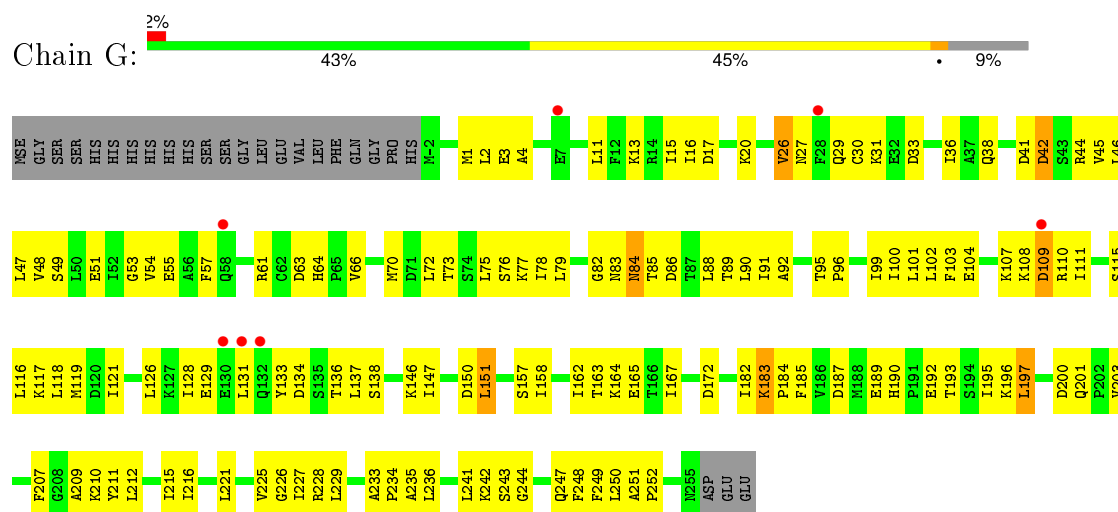




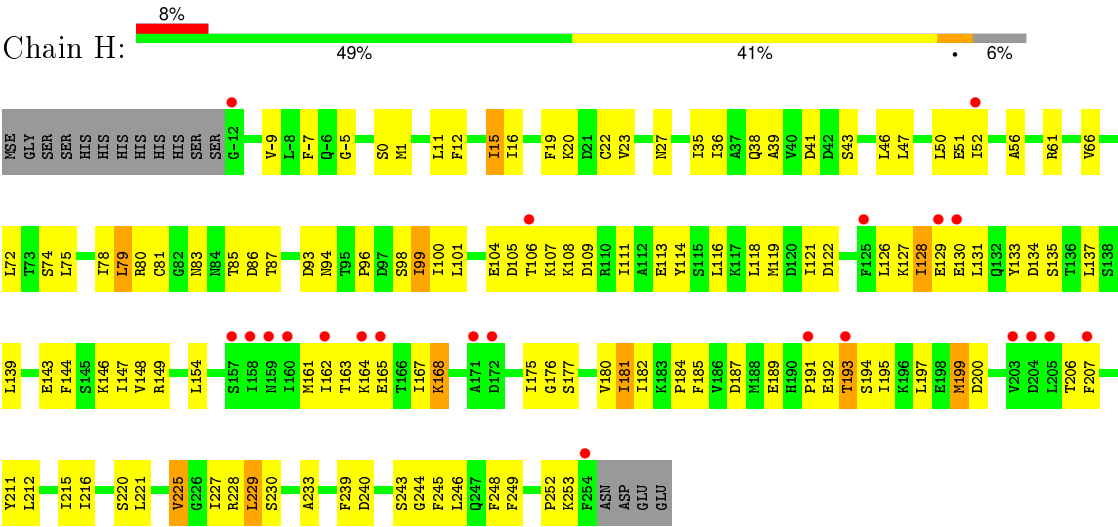
• Molecule 6: Proliferating cell nuclear antigen



• Molecule 6: Proliferating cell nuclear antigen



• Molecule 6: Proliferating cell nuclear antigen



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.21Å 110.48Å 268.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.81 – 2.85 48.81 – 2.80	Depositor EDS
% Data completeness (in resolution range)	95.1 (48.81-2.85) 94.8 (48.81-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.00 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.251 , 0.306 0.255 , 0.309	Depositor DCC
$R_{free}$ test set	3169 reflections (4.56%)	DCC
Wilson B-factor (Å <sup>2</sup> )	72.9	Xtriage
Anisotropy	0.491	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 51.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 147308 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	19740	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, AGS, ADP

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	0.31	0/3173	0.59	0/4283
2	B	0.32	0/2517	0.58	0/3394
3	C	0.30	0/2584	0.56	0/3497
4	D	0.27	0/2642	0.53	0/3573
5	E	0.27	0/2529	0.52	0/3416
6	F	0.30	0/2045	0.55	0/2749
6	G	0.31	0/2046	0.56	0/2749
6	H	0.31	0/2105	0.56	0/2828
All	All	0.30	0/19641	0.56	0/26489

There are no bond length outliers.

There are no bond angle outliers.

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	3345	0	3207	210	0
2	B	2482	0	2572	132	0
3	C	2544	0	2573	171	0
4	D	2597	0	2627	183	0
5	E	2495	0	2598	216	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	2021	0	2036	159	0
6	G	2022	0	2044	122	0
6	H	2079	0	2083	126	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	A	31	0	12	1	0
8	B	31	0	12	2	0
8	C	31	0	12	2	0
8	D	31	0	12	2	0
9	E	27	0	12	3	0
All	All	19740	0	19800	1225	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 31.

The worst 5 of 1225 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:523:THR:HG21	1:A:547:ILE:HG21	1.30	1.09
4:D:138:ILE:HG22	4:D:167:CYS:HB3	1.39	1.04
3:C:221:ASN:HB2	3:C:222:PRO:HD3	1.33	1.03
5:E:39:LEU:HD21	5:E:41:LEU:HG	1.41	1.01
4:D:41:ALA:HB1	4:D:192:LEU:HD22	1.41	1.01

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	391/516 (76%)	324 (83%)	55 (14%)	12 (3%)	5	18
2	B	314/323 (97%)	279 (89%)	32 (10%)	3 (1%)	19	49
3	C	320/340 (94%)	257 (80%)	53 (17%)	10 (3%)	5	18
4	D	326/353 (92%)	268 (82%)	43 (13%)	15 (5%)	3	10
5	E	309/354 (87%)	244 (79%)	57 (18%)	8 (3%)	7	23
6	F	256/283 (90%)	216 (84%)	32 (12%)	8 (3%)	5	18
6	G	256/283 (90%)	219 (86%)	31 (12%)	6 (2%)	8	26
6	H	265/283 (94%)	224 (84%)	34 (13%)	7 (3%)	7	23
All	All	2437/2735 (89%)	2031 (83%)	337 (14%)	69 (3%)	6	21

5 of 69 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	467	ASP
1	A	584	ASP
2	B	25	GLY
2	B	27	LYS
4	D	41	ALA

### 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	340/400 (85%)	320 (94%)	20 (6%)	24	54
2	B	277/283 (98%)	263 (95%)	14 (5%)	29	62
3	C	279/296 (94%)	266 (95%)	13 (5%)	32	66
4	D	292/312 (94%)	282 (97%)	10 (3%)	44	77
5	E	290/324 (90%)	280 (97%)	10 (3%)	44	77
6	F	231/246 (94%)	224 (97%)	7 (3%)	48	80
6	G	232/246 (94%)	221 (95%)	11 (5%)	32	66
6	H	235/246 (96%)	224 (95%)	11 (5%)	32	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2176/2353 (92%)	2080 (96%)	96 (4%)	35 68

5 of 96 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	197	LEU
4	D	284	LYS
6	H	168	LYS
3	C	220	ASP
4	D	94	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	96	ASN
4	D	303	GLN
6	G	247	GLN
4	D	112	ASN
4	D	183	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link

column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	AGS	A	801	7	24,33,33	2.32	4 (16%)	28,52,52	1.37	1 (3%)
8	AGS	B	802	7	24,33,33	2.20	4 (16%)	28,52,52	1.22	1 (3%)
8	AGS	C	803	7	24,33,33	2.42	4 (16%)	28,52,52	1.27	1 (3%)
8	AGS	D	804	7	24,33,33	2.20	4 (16%)	28,52,52	1.37	2 (7%)
9	ADP	E	805	-	22,29,29	1.66	5 (22%)	27,45,45	1.40	2 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	AGS	A	801	7	-	0/15/38/38	0/3/3/3
8	AGS	B	802	7	-	0/15/38/38	0/3/3/3
8	AGS	C	803	7	-	0/15/38/38	0/3/3/3
8	AGS	D	804	7	-	0/15/38/38	0/3/3/3
9	ADP	E	805	-	-	0/12/32/32	0/3/3/3

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	803	AGS	PG-S1G	-10.54	1.70	1.90
8	A	801	AGS	PG-S1G	-10.02	1.71	1.90
8	B	802	AGS	PG-S1G	-9.43	1.72	1.90
8	D	804	AGS	PG-S1G	-8.86	1.73	1.90
9	E	805	ADP	PB-O2B	-2.20	1.46	1.54

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	E	805	ADP	N3-C2-N1	-2.87	126.70	128.89
8	D	804	AGS	C4'-O4'-C1'	2.42	112.38	109.72
8	B	802	AGS	C1'-N9-C4	4.41	133.59	126.94
8	C	803	AGS	C1'-N9-C4	4.67	133.98	126.94
9	E	805	ADP	C1'-N9-C4	4.91	134.34	126.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	801	AGS	1	0
8	B	802	AGS	2	0
8	C	803	AGS	2	0
8	D	804	AGS	2	0
9	E	805	ADP	3	0

## 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	395/516 (76%)	0.07	15 (3%) 44 37	37, 72, 130, 181	0
2	B	316/323 (97%)	-0.08	3 (0%) 85 84	32, 60, 99, 142	0
3	C	322/340 (94%)	0.07	8 (2%) 61 56	33, 76, 126, 178	0
4	D	328/353 (92%)	0.46	32 (9%) 10 5	53, 105, 167, 187	0
5	E	317/354 (89%)	0.67	40 (12%) 5 3	45, 113, 154, 181	0
6	F	252/283 (89%)	0.62	34 (13%) 4 2	48, 107, 154, 179	0
6	G	251/283 (88%)	0.10	7 (2%) 56 51	42, 77, 136, 165	0
6	H	260/283 (91%)	0.41	22 (8%) 13 8	44, 92, 148, 169	0
All	All	2441/2735 (89%)	0.28	161 (6%) 22 16	32, 85, 149, 187	0

The worst 5 of 161 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	F	122	ASP	12.2
6	H	158	ILE	8.4
1	A	533	HIS	6.0
6	F	193	THR	6.0
4	D	216	VAL	5.7

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
7	MG	A	811	1/1	0.89	0.43	9.94	56,56,56,56	0
7	MG	B	812	1/1	0.82	0.30	3.18	48,48,48,48	0
8	AGS	C	803	31/31	0.96	0.18	0.05	50,50,50,50	0
8	AGS	B	802	31/31	0.94	0.18	-0.27	51,51,51,51	0
8	AGS	A	801	31/31	0.96	0.17	-0.31	51,51,51,51	0
8	AGS	D	804	31/31	0.93	0.16	-1.07	86,86,86,86	0
9	ADP	E	805	27/27	0.93	0.15	-1.18	93,93,93,93	0
7	MG	D	814	1/1	0.93	0.17	-1.19	66,66,66,66	0
7	MG	C	813	1/1	0.94	0.30	-	40,40,40,40	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.