wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 14, 2023 – 05:16 PM JST

PDB ID	:	5ZUT
Title	:	Crystal Structure of Yeast PCNA in Complex with N24 Peptide
Authors	:	Cheng, X.Y.; Kuang, X.L.; Zhou, Y.; Xia, X.M.; SU, Z.D.
Deposited on	:	2018-05-08
Resolution	:	2.82 Å(reported)

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

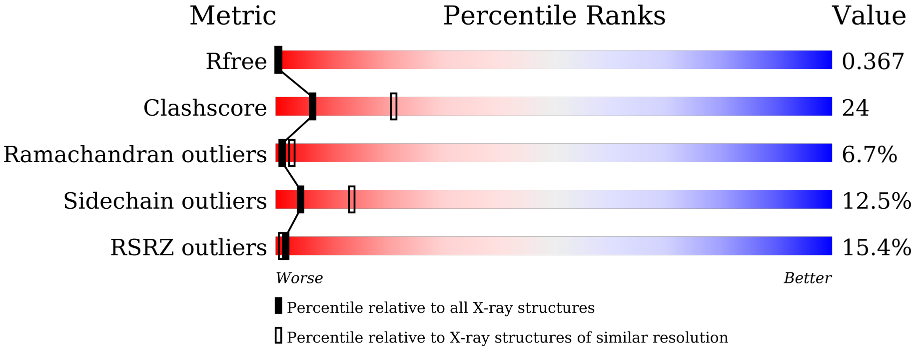
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

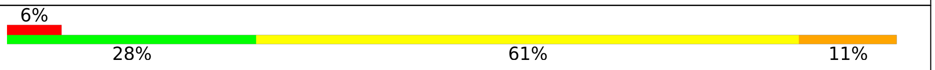
The reported resolution of this entry is 2.82 Å.

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	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (2.84-2.80)

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 <=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	289	
2	E	18	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2155 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	255	2003	1281	316	396	10	0	0	0

There are 31 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	259	GLY	-	expression tag	UNP P15873
A	260	GLY	-	expression tag	UNP P15873
A	261	GLY	-	expression tag	UNP P15873
A	262	MET	-	expression tag	UNP P15873
A	263	ASP	-	expression tag	UNP P15873
A	264	ARG	-	expression tag	UNP P15873
A	265	ASP	-	expression tag	UNP P15873
A	266	ASP	-	expression tag	UNP P15873
A	267	ALA	-	expression tag	UNP P15873
A	268	ASP	-	expression tag	UNP P15873
A	269	TRP	-	expression tag	UNP P15873
A	270	ARG	-	expression tag	UNP P15873
A	271	GLU	-	expression tag	UNP P15873
A	272	VAL	-	expression tag	UNP P15873
A	273	MET	-	expression tag	UNP P15873
A	274	MET	-	expression tag	UNP P15873
A	275	PRO	-	expression tag	UNP P15873
A	276	TYR	-	expression tag	UNP P15873
A	277	SER	-	expression tag	UNP P15873
A	278	THR	-	expression tag	UNP P15873
A	279	GLU	-	expression tag	UNP P15873
A	280	LEU	-	expression tag	UNP P15873
A	281	ILE	-	expression tag	UNP P15873
A	282	PHE	-	expression tag	UNP P15873
A	283	TYR	-	expression tag	UNP P15873
A	284	ILE	-	expression tag	UNP P15873
A	285	GLU	-	expression tag	UNP P15873

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Chain	Residue	Modelled	Actual	Comment	Reference
A	286	MET	-	expression tag	UNP P15873
A	287	ASP	-	expression tag	UNP P15873
A	288	PRO	-	expression tag	UNP P15873
A	289	CYS	-	expression tag	UNP P15873

- Molecule 2 is a protein called N24.

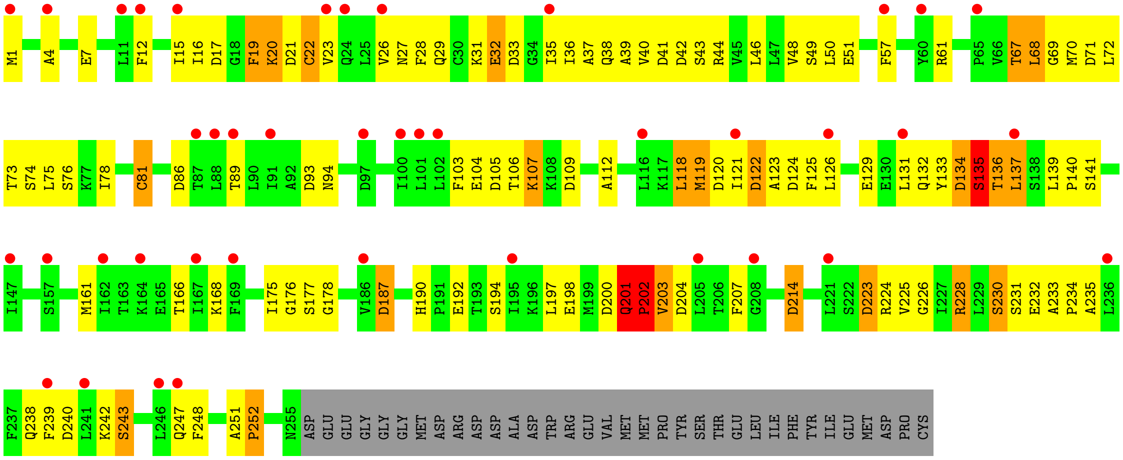
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	E	18	152	101	18	30	3	0	0	0

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.

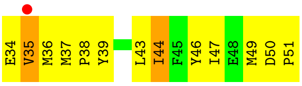
- Molecule 1: Proliferating cell nuclear antigen

Chain A:



- Molecule 2: N24

Chain E:



4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	80.35Å 84.03Å 58.15Å 90.00° 93.62° 90.00°	Depositor
Resolution (Å)	58.03 – 2.82 58.03 – 2.83	Depositor EDS
% Data completeness (in resolution range)	98.4 (58.03-2.82) 97.9 (58.03-2.83)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.76 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.326 , 0.397 0.320 , 0.367	Depositor DCC
R_{free} test set	471 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å^2)	86.7	Xtriage
Anisotropy	0.568	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 96.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.417 for -1/2*h+1/2*k-l,1/2*h-1/2*k-l,-1/2 *h-1/2*k 0.378 for -1/2*h-1/2*k-l,-1/2*h-1/2*k+l,-1/ 2*h+1/2*k	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	2155	wwPDB-VP
Average B, all atoms (Å^2)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.39% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.35	0/2033	0.62	1/2742 (0.0%)
2	E	0.38	0/156	0.56	0/211
All	All	0.35	0/2189	0.61	1/2953 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	202	PRO	N-CA-C	5.02	125.16	112.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	135	SER	Peptide

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	2003	0	2025	96	4
2	E	152	0	143	16	0
All	All	2155	0	2168	102	4

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 24.

The worst 5 of 102 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:134:ASP:HB2	1:A:230:SER:HA	1.22	1.08
1:A:44:ARG:O	2:E:35:VAL:HG13	1.51	1.08
1:A:192:GLU:O	1:A:224:ARG:NH1	1.93	1.01
1:A:19:PHE:O	1:A:22:CYS:SG	2.36	0.84
1:A:134:ASP:HB2	1:A:230:SER:CA	2.08	0.82

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:ASP:OD1	1:A:198:GLU:C[2_556]	1.81	0.39
1:A:134:ASP:OD1	1:A:198:GLU:CA[2_556]	1.84	0.36
1:A:134:ASP:OD1	1:A:198:GLU:CB[2_556]	2.00	0.20
1:A:136:THR:N	1:A:200:ASP:OD1[2_556]	2.13	0.07

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	253/289 (88%)	183 (72%)	54 (21%)	16 (6%)	1 3
2	E	16/18 (89%)	11 (69%)	3 (19%)	2 (12%)	0 1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	269/307 (88%)	194 (72%)	57 (21%)	18 (7%)	1 3

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	LYS
1	A	32	GLU
1	A	134	ASP
1	A	202	PRO
1	A	252	PRO

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	230/260 (88%)	201 (87%)	29 (13%)	4 13
2	E	18/18 (100%)	16 (89%)	2 (11%)	6 18
All	All	248/278 (89%)	217 (88%)	31 (12%)	4 14

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	132	GLN
1	A	230	SER
1	A	137	LEU
2	E	43	LEU
1	A	214	ASP

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

Mol	Chain	Res	Type
1	A	29	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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, 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	255/289 (88%)	0.84	41 (16%)	1	1	59, 101, 120, 120	0
2	E	18/18 (100%)	0.73	1 (5%)	24	16	116, 120, 120, 120	0
All	All	273/307 (88%)	0.83	42 (15%)	2	1	59, 102, 120, 120	0

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	101	LEU	6.0
1	A	126	LEU	5.2
1	A	121	ILE	5.0
1	A	205	LEU	4.6
1	A	89	THR	4.6

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 monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.