

wwPDB X-ray Structure Validation Summary Report (i)

Aug 14, 2023 – 06:15 PM EDT

PDB ID	:	1RXZ
Title	:	C-terminal region of A. fulgidus FEN-1 complexed with A. fulgidus PCNA
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		J.A.
Deposited on		
Resolution	:	2.00 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 (i) 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 (1)) were used in the production of this report:

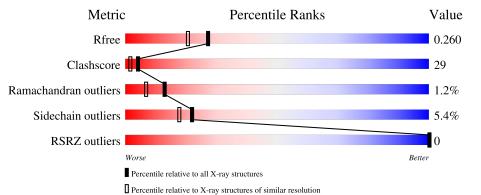
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)		
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.00 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	А	245	529	%	44%	•					
2	В	11	27%		73%						



$1\mathrm{RXZ}$

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2102 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 DNA polymerase sliding clamp.

Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf	Trace
1	А	245	Total 1916	C 1225	N 313	O 370	S 8	0	0	0

• Molecule 2 is a protein called Flap structure-specific endonuclease.

Mol	Chain	Residues	L	Ator	ns		ZeroOcc	AltConf	Trace
2	В	11	Total 97	C 62	N 17	0 18	0	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	86	Total O 86 86	0	0
3	В	3	Total O 3 3	0	0



Chain B:

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 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.

73%

Cł	nai	n	A:	-									5	2%	6																	44	%								•	-			
M1	V4 TE	9W	T7 G8	E3	L10	K13	T13	V14	T15	415 417	118 118	V19	A 20	L21	777	A25	R26	127 1100	H28 F29	L30	E31	K32	ЦЗБ	S36	R37	A38 V20	039 D40	P41	A42	N43	M46	V47	148 	V49	151	-	F56 F57	V58	-	D62	E63	I67	G68	V69	M71
D72 R73	174	177	S78	S82	T83	K84 D85		E88	L89	FQ7	D93	E94	S95	T96	K100	F101	G102	1100	¥106 K107	V108	A109	L110		P113	S114	A115	K118	E119	P120	D103	F124	L125	E126	L12/ D138	0.71 1	I131	V132	G136		K139	K140	1148	S149	D150	V152
1153	E159 C160	F161	R162 1163	E164		V169 V169		V173	F174	6/ 1H M1 76		E180	L181	1182 7160	E183 F184	N185	G186	11 11 11	5194 S194	V195		C202	K203	107A	H214	L215	1210 T017	N218	Y219	P220 V221	R222		F226	E226		V234	E235 V236		A239	P240	R241 1242	E243	S244	E245	
•]	Мс	ole	cu	le	2	:	Fl	a	р	st	rı	ıc	tı	ır	e-	sp	e	ci	fic	: e	en	do	on	u	cl	ea	se	è																	

• Molecule 1: DNA polymerase sliding clamp

27%

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants	86.53Å 86.53 Å 96.73 Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	60.00 - 2.00	Depositor
Resolution (A)	27.18 - 2.00	EDS
% Data completeness	99.4 (60.00-2.00)	Depositor
(in resolution range)	99.8 (27.18 - 2.00)	EDS
R _{merge}	(Not available)	Depositor
R _{sym}	0.08	Depositor
$< I/\sigma(I) > 1$	$1.86 (at 1.99 \text{\AA})$	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.180 , 0.262	Depositor
n, nfree	0.177 , 0.260	DCC
R_{free} test set	3472 reflections $(9.54%)$	wwPDB-VP
Wilson B-factor ($Å^2$)	37.9	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.33 , 43.7	EDS
L-test for twinning ²	$< L > = 0.39, < L^2 > = 0.21$	Xtriage
Estimated twinning fraction	0.366 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2102	wwPDB-VP
Average B, all atoms $(Å^2)$	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.48% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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		lengths	Bond angles					
	Ullaill	RMSZ	# Z > 5	RMSZ	# Z > 5				
1	А	0.36	0/1944	0.64	0/2620				
2	В	0.41	0/99	0.55	0/131				
All	All	0.36	0/2043	0.64	0/2751				

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	А	1916	0	1964	118	0
2	В	97	0	96	17	0
3	А	86	0	0	3	0
3	В	3	0	0	1	0
All	All	2102	0	2060	120	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 29.

The worst 5 of 120 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:39:VAL:HG13	1:A:120:PRO:HG3	1.41	1.03



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:PRO:HB2	2:B:11:PHE:HE1	1.25	0.98
1:A:16:ARG:HG2	1:A:204:VAL:HG23	1.48	0.96
1:A:241:ARG:HB3	1:A:241:ARG:HH11	1.36	0.91
1:A:17:ALA:HB2	1:A:204:VAL:HG21	1.53	0.88

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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	А	243/245~(99%)	216 (89%)	24 (10%)	3~(1%)	13 7
2	В	9/11~(82%)	9 (100%)	0	0	100 100
All	All	252/256~(98%)	225~(89%)	24 (10%)	3 (1%)	13 7

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	58	VAL
1	А	63	GLU
1	А	19	VAL

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 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	А	212/212 (100%)	200~(94%)	12~(6%)	20 16	
2	В	10/10 (100%)	10 (100%)	0	100 100	
All	All	222/222 (100%)	210~(95%)	12~(5%)	22 18	

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	119	GLU
1	А	150	ASP
1	А	245	GLU
1	А	168	ASP
1	А	71	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	151	GLN
1	А	218	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 monosaccharides 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^{th} 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	$\langle RSRZ \rangle$	#RSRZ>2		Z>2	$OWAB(Å^2)$	Q < 0.9
1	А	245/245~(100%)	-0.54	0	100	100	24, 43, 62, 73	0
2	В	11/11 (100%)	-0.17	0	100	100	37, 45, 59, 71	0
All	All	256/256~(100%)	-0.53	0	100	100	24, 43, 63, 73	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 monosaccharides 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.

