WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 19, 2023 – 11:35 PM EDT

PDB ID : 8F5Q
Title : Crystal structure of human PCNA in complex with the PIP box of FBH1
Authors : Liu, J.; Chaves-Arquero, B.; Wei, P.; Tencer, H.; Zhang, G.; Blanco, F.; Kutateladze, T.
Deposited on : 2022-11-15
Resolution : 1.90 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:

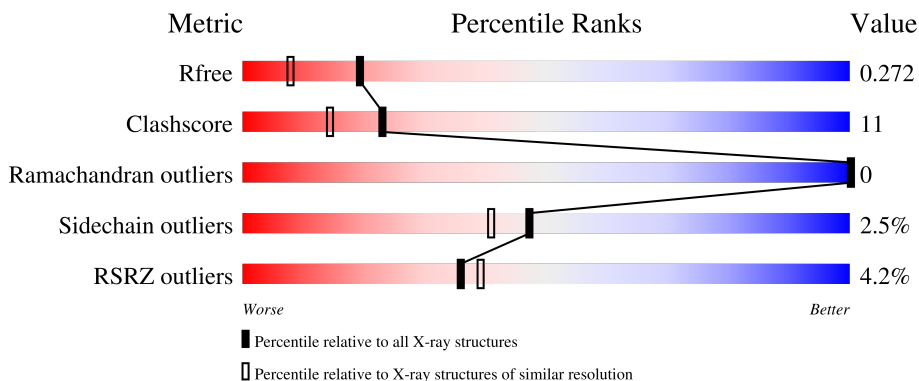|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 1.90 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	Percentile Ranks	Value
Rfree		0.272
Clashscore		11
Ramachandran outliers		0
Sidechain outliers		2.5%
RSRZ outliers		4.2%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	259	4% 73% 17% • 8%
1	C	259	4% 69% 24% • 6%
1	E	259	3% 68% 23% • 7%
2	B	9	11% 56% 33% 11%
2	D	9	44% 44% 11%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	9	78%　　11%　11%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 6055 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
1	A	237	Total	C	N	O	S	0	3	0
			1840	1161	302	359	18			
1	C	244	Total	C	N	O	S	0	2	0
			1891	1192	310	372	17			
1	E	240	Total	C	N	O	S	0	1	0
			1849	1168	304	361	16			

- Molecule 2 is a protein called F-box DNA helicase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	8	Total	C	N	O	S	0	0	0
			72	48	12	11	1			
2	D	8	Total	C	N	O	S	0	0	0
			72	48	12	11	1			
2	F	9	Total	C	N	O	S	0	0	0
			78	51	13	13	1			

- Molecule 3 is water.

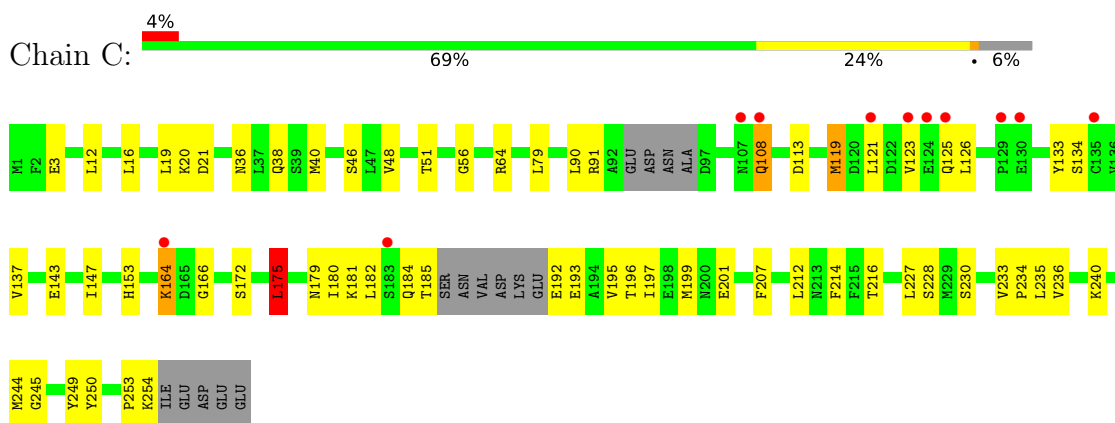| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	100	Total	O	0	0
			100	100		
3	B	5	Total	O	0	0
			5	5		
3	C	73	Total	O	0	0
			73	73		
3	D	2	Total	O	0	0
			2	2		
3	E	72	Total	O	0	0
			72	72		
3	F	1	Total	O	0	0
			1	1		

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.
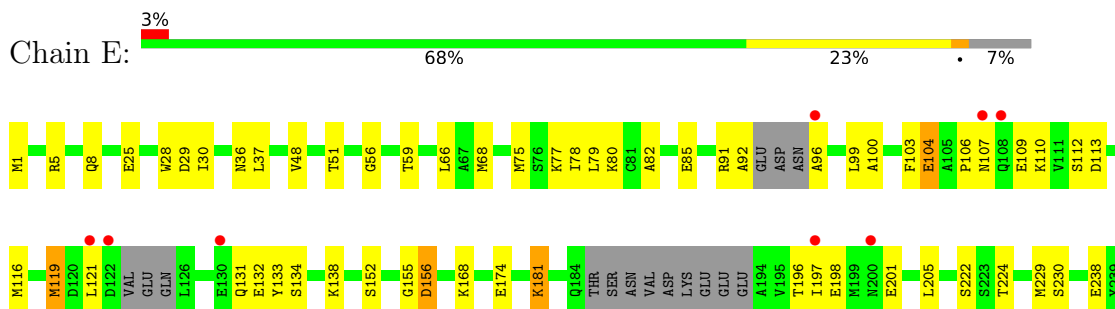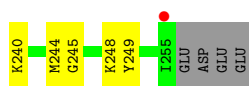
• Molecule 1: Proliferating cell nuclear antigen
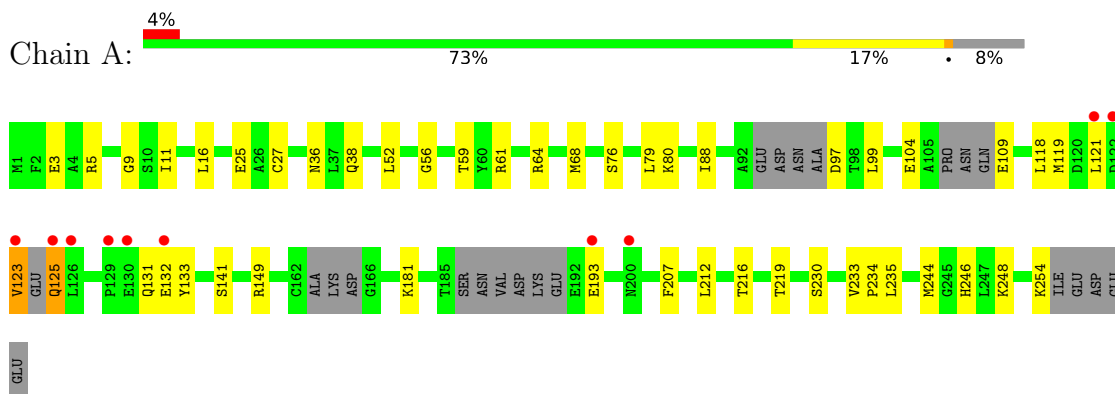
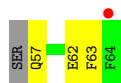• Molecule 1: Proliferating cell nuclear antigen

• Molecule 1: Proliferating cell nuclear antigen

K240 M244 G245 K248 Y249 I255 GLU ASP GLU GLU

• Molecule 2: F-box DNA helicase 1

Chain B:

11%

56%   33%   11%

SER Q57 E62 F63 F64

• Molecule 2: F-box DNA helicase 1

Chain D:

44%   44%   11%

SER Q57 R58 C59 E62 F63 F64

• Molecule 2: F-box DNA helicase 1

Chain F:

78%   11%   11%

S56 Q57 R58 E62 F63 F64
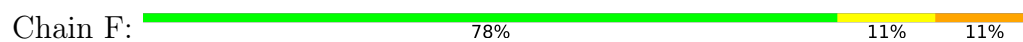
4   Data and refinement statistics   ⓘ

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	81.95Å 82.21Å 118.56Å 90.00° 91.26° 90.00°	Depositor
Resolution (Å)	41.79 – 1.90 41.79 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.3 (41.79-1.90) 98.3 (41.79-1.90)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.98 (at 1.89Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.224 , 0.266 0.226 , 0.272	Depositor DCC
R_{free} test set	1997 reflections (3.28%)	wwPDB-VP
Wilson B-factor (Å^2)	25.3	Xtriage
Anisotropy	0.508	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 35.9	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.004 for -1/2*h+1/2*k-1/2*l,-1/2*h+1/2*k+1/2*l,h+k 0.000 for -1/2*h+1/2*k+1/2*l,-1/2*h+1/2*k-1/2*l,-h-k 0.000 for -1/2*h-1/2*k-1/2*l,1/2*h+1/2*k-1/2*l,h-k 0.011 for -1/2*h-1/2*k+1/2*l,1/2*h+1/2*k+1/2*l,-h+k 0.002 for k,h,-l 0.015 for -k,-h,-l 0.024 for -1/2*h+1/2*k-1/2*l,1/2*h-1/2*k-1/2*l,-h-k 0.001 for -1/2*h-1/2*k-1/2*l,-1/2*h-1/2*k+1/2*l,-h+k 0.084 for -1/2*h+1/2*k+1/2*l,1/2*h-1/2*k+1/2*l,h+k 0.168 for -1/2*h-1/2*k+1/2*l,-1/2*h-1/2*k-1/2*l,h-k 0.019 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6055	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

---

[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.

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.60% of the height of the origin peak. No significant pseudotranslation is detected.*

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	0.37	0/1860	0.69	2/2503 (0.1%)
1	C	0.49	0/1915	0.76	4/2584 (0.2%)
1	E	0.45	0/1872	1.16	5/2524 (0.2%)
2	B	0.59	0/74	0.56	0/98
2	D	0.51	0/74	0.63	0/98
2	F	0.60	0/80	0.53	0/106
All	All	0.44	0/5875	0.88	11/7913 (0.1%)

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	E	0	3

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($°$)	Ideal($°$)
1	E	104	GLU	OE1-CD-OE2	-38.83	76.71	123.30
1	E	104	GLU	CG-CD-OE1	19.25	156.79	118.30
1	E	104	GLU	CG-CD-OE2	-18.81	80.68	118.30
1	C	119	MET	CG-SD-CE	-8.15	87.16	100.20
1	A	64	ARG	CG-CD-NE	7.55	127.65	111.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	155	GLY	Mainchain
1	E	156[A]	ASP	Mainchain

Continued on next page...

WORLDWIDE PDB

PROTEIN DATA BANK

Continued from previous page...

Mol	Chain	Res	Type	Group
1	E	156[B]	ASP	Mainchain

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	1840	0	1856	38	0
1	C	1891	0	1906	54	3
1	E	1849	0	1870	42	10
2	B	72	0	67	4	0
2	D	72	0	67	5	0
2	F	78	0	72	1	0
3	A	100	0	0	6	0
3	B	5	0	0	1	0
3	C	73	0	0	10	0
3	D	2	0	0	2	0
3	E	72	0	0	5	0
3	F	1	0	0	0	0
All	All	6055	0	5838	133	10

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 11.

The worst 5 of 133 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:E:229:MET:SD	3:E:369:HOH:O	2.15	1.04
1:A:254:LYS:NZ	3:A:301:HOH:O	1.91	1.03
1:A:3:GLU:OE1	1:A:61:ARG:NH2	1.97	0.98
1:C:36:ASN:OD1	3:C:301:HOH:O	1.91	0.88
1:A:56:GLY:HA3	1:A:244[B]:MET:HG2	1.58	0.84

The worst 5 of 10 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:E:174:GLU:CD	1:E:174:GLU:OE2[2_555]	0.62	1.58
1:E:174:GLU:OE2	1:E:174:GLU:OE2[2_555]	0.67	1.53
1:C:64:ARG:NH2	1:E:29:ASP:OD1[3_454]	1.66	0.54
1:E:174:GLU:OE1	1:E:174:GLU:OE2[2_555]	1.73	0.47
1:E:174:GLU:CG	1:E:174:GLU:OE2[2_555]	1.80	0.40

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	228/259 (88%)	227 (100%)	1 (0%)	0	100	100
1	C	240/259 (93%)	232 (97%)	8 (3%)	0	100	100
1	E	233/259 (90%)	228 (98%)	5 (2%)	0	100	100
2	B	6/9 (67%)	6 (100%)	0	0	100	100
2	D	6/9 (67%)	6 (100%)	0	0	100	100
2	F	7/9 (78%)	7 (100%)	0	0	100	100
All	All	720/804 (90%)	706 (98%)	14 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	209/227 (92%)	204 (98%)	5 (2%)	49	43

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	215/227 (95%)	210 (98%)	5 (2%)	50	45
1	E	209/227 (92%)	202 (97%)	7 (3%)	38	29
2	B	8/9 (89%)	8 (100%)	0	100	100
2	D	8/9 (89%)	8 (100%)	0	100	100
2	F	9/9 (100%)	8 (89%)	1 (11%)	6	2
All	All	658/708 (93%)	640 (97%)	18 (3%)	47	38

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	196	THR
2	F	58	ARG
1	E	198	GLU
1	C	172	SER
1	E	181	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	GLN
1	A	131	GLN
1	C	108	GLN
1	C	179	ASN
1	E	213	ASN

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(Å²)	Q<0.9
1	A	237/259 (91%)	0.29	10 (4%)	36	39	17, 31, 56, 74	0
1	C	244/259 (94%)	0.33	11 (4%)	33	36	20, 33, 62, 82	0
1	E	240/259 (92%)	0.33	9 (3%)	40	43	19, 35, 61, 78	0
2	B	8/9 (88%)	0.69	1 (12%)	3	4	34, 44, 54, 59	0
2	D	8/9 (88%)	0.77	0	100	100	40, 47, 61, 62	0
2	F	9/9 (100%)	0.43	0	100	100	36, 46, 59, 61	0
All	All	746/804 (92%)	0.33	31 (4%)	36	39	17, 34, 61, 82	0

The worst 5 of 31 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	123	VAL	8.3
1	A	123	VAL	7.3
1	C	108	GLN	6.2
1	A	125	GLN	4.1
1	E	122	ASP	4.0

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 (i)

There are no such residues in this entry.