



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 04:35 am GMT

PDB ID : 5BZ0  
Title : Crystal structure of IBV papain-like protease PLpro C101S mutant in complex with ubiquitin  
Authors : Kong, L.Y.; Yan, L.M.; Zhang, Y.; Rao, Z.H.  
Deposited on : 2015-06-11  
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

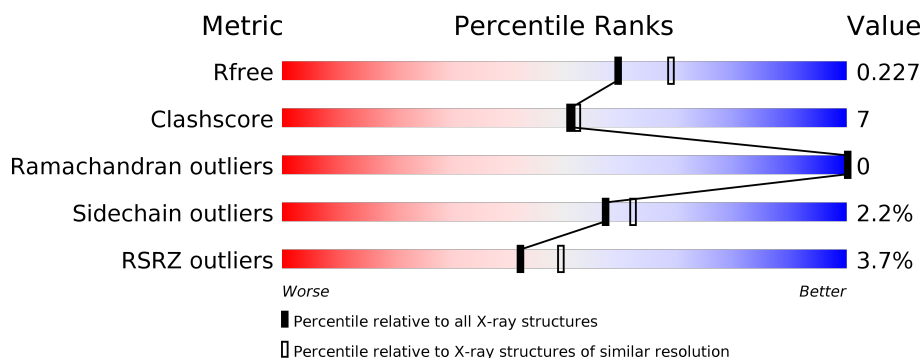
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
$R_{free}$	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

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	313	<div> <div>4%</div> <div> <div></div> <div>70%</div> <div>8%</div> <div>21%</div> </div> </div>
2	B	76	<div> <div>88%</div> <div>12%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2854 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 Replicase polypeptide 1ab.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	248	Total	C	N	O	S	Se	0	0	0
			1952	1249	323	370	9	1			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	LEU	-	expression tag	UNP P0C6Y1
A	-1	GLY	-	expression tag	UNP P0C6Y1
A	0	SER	-	expression tag	UNP P0C6Y1
A	101	SER	CYS	engineered mutation	UNP P0C6Y1

- Molecule 2 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	76	Total	C	N	O	S	0	0	0
			601	378	105	117	1			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

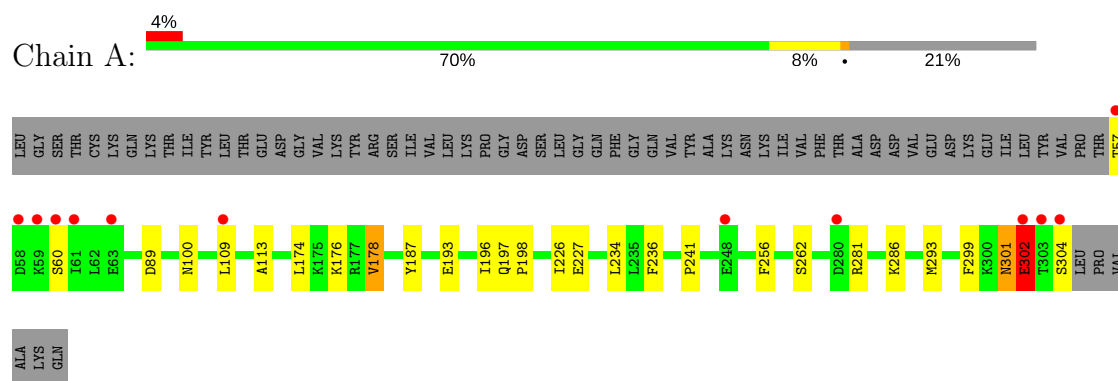
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	229	Total	O	0	0
			229	229		
4	B	71	Total	O	0	0
			71	71		

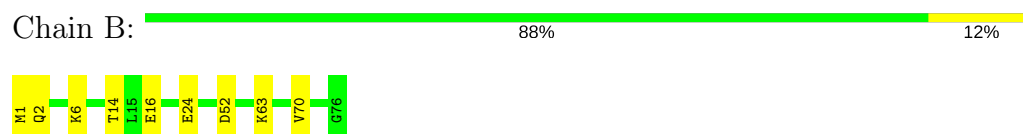
### 3 Residue-property plots [i](#)

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: Replicase polypeptide 1ab



- Molecule 2: Ubiquitin-40S ribosomal protein S27a



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.06Å 74.81Å 95.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.68 – 2.10 26.68 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (26.68-2.10) 99.9 (26.68-2.10)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	11.51 (at 2.10Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.191 , 0.228 0.191 , 0.227	Depositor DCC
$R_{free}$ test set	1348 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.2	Xtriage
Anisotropy	0.583	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 46.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	2854	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.81% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.48	0/1998	0.74	4/2713 (0.1%)
2	B	0.46	0/607	0.60	0/816
All	All	0.48	0/2605	0.71	4/3529 (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	A	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	302	GLU	N-CA-C	-14.50	71.86	111.00
1	A	302	GLU	CB-CA-C	12.90	136.21	110.40
1	A	302	GLU	C-N-CA	11.01	149.23	121.70
1	A	109	LEU	CB-CG-CD1	-6.83	99.39	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	301	ASN	Peptide
1	A	302	GLU	Peptide

## 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	1952	0	1882	26	0
2	B	601	0	629	8	0
3	A	1	0	0	0	0
4	A	229	0	0	5	1
4	B	71	0	0	4	0
All	All	2854	0	2511	33	1

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 7.

All (33) 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:234:LEU:HD13	1:A:293:MSE:HE3	1.41	1.02
1:A:234:LEU:HD13	1:A:293:MSE:CE	1.93	0.98
2:B:52:ASP:O	4:B:201:HOH:O	1.93	0.85
1:A:234:LEU:CD1	1:A:293:MSE:HE3	2.10	0.80
2:B:1:MET:HE2	2:B:63:LYS:HB3	1.67	0.77
1:A:302:GLU:O	4:A:501:HOH:O	2.03	0.75
1:A:234:LEU:HD13	1:A:293:MSE:HE2	1.76	0.66
1:A:193:GLU:OE2	4:A:502:HOH:O	2.14	0.65
1:A:89:ASP:O	4:A:503:HOH:O	2.14	0.64
2:B:16:GLU:OE1	4:B:202:HOH:O	2.14	0.64
1:A:174:LEU:HD23	1:A:176:LYS:HE2	1.80	0.63
1:A:299:PHE:CZ	1:A:301:ASN:OD1	2.51	0.63
1:A:226:ILE:O	1:A:301:ASN:HB2	1.98	0.62
2:B:24:GLU:HB2	4:B:201:HOH:O	2.01	0.60
1:A:301:ASN:ND2	1:A:302:GLU:O	2.36	0.59
2:B:6:LYS:NZ	4:B:204:HOH:O	2.35	0.58
1:A:227:GLU:OE2	4:A:504:HOH:O	2.17	0.57
1:A:113:ALA:HB2	1:A:293:MSE:SE	2.57	0.54
1:A:113:ALA:CB	1:A:293:MSE:SE	3.08	0.52
1:A:241:PRO:HG3	1:A:256:PHE:HB3	1.94	0.49
2:B:1:MET:HE2	2:B:63:LYS:CB	2.41	0.48
1:A:301:ASN:CG	1:A:302:GLU:O	2.54	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:LYS:NZ	4:A:505:HOH:O	2.21	0.46
1:A:236:PHE:HE2	2:B:70:VAL:HG21	1.82	0.44
1:A:304:SER:OG	1:A:304:SER:O	2.34	0.44
1:A:178:VAL:HG22	1:A:187:TYR:HE1	1.82	0.44
1:A:196:ILE:HG22	1:A:236:PHE:CE1	2.53	0.43
1:A:299:PHE:HZ	1:A:301:ASN:OD1	1.98	0.43
1:A:301:ASN:CB	1:A:302:GLU:O	2.67	0.42
1:A:301:ASN:HB3	1:A:302:GLU:O	2.19	0.42
2:B:2:GLN:HG3	2:B:14:THR:HG23	2.02	0.42
1:A:196:ILE:HG22	1:A:236:PHE:HE1	1.84	0.42
1:A:197:GLN:HA	1:A:198:PRO:HD2	1.96	0.40

All (1) 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)
4:A:605:HOH:O	4:A:607:HOH:O[4_555]	2.11	0.09

## 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	246/313 (79%)	235 (96%)	11 (4%)	0	100	100
2	B	74/76 (97%)	74 (100%)	0	0	100	100
All	All	320/389 (82%)	309 (97%)	11 (3%)	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	205/261 (78%)	199 (97%)	6 (3%)	48	51
2	B	68/68 (100%)	68 (100%)	0	100	100
All	All	273/329 (83%)	267 (98%)	6 (2%)	57	62

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	THR
1	A	60	SER
1	A	100	ASN
1	A	178	VAL
1	A	262	SER
1	A	281	ARG

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

Mol	Chain	Res	Type
1	A	77	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 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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 [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	247/313 (78%)	0.06	12 (4%) 30 37	14, 23, 50, 92	0
2	B	76/76 (100%)	-0.33	0 100 100	20, 26, 38, 40	0
All	All	323/389 (83%)	-0.03	12 (3%) 42 49	14, 24, 47, 92	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	304	SER	11.8
1	A	303	THR	10.5
1	A	302	GLU	9.4
1	A	57	THR	7.0
1	A	60	SER	4.5
1	A	61	ILE	3.8
1	A	58	ASP	3.2
1	A	59	LYS	2.8
1	A	280	ASP	2.3
1	A	63	GLU	2.2
1	A	248	GLU	2.1
1	A	109	LEU	2.0

### 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](#)

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
3	ZN	A	400	1/1	0.99	0.03	-2.16	21,21,21,21	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.