



# wwPDB X-ray Structure Validation Summary Report

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PDB ID : 3UIU  
Title : Crystal structure of Apo-PKR kinase domain  
Authors : Li, F.; Li, S.; Yang, X.; Shen, Y.; Zhang, T.  
Deposited on : 2011-11-06  
Resolution : 2.90 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](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

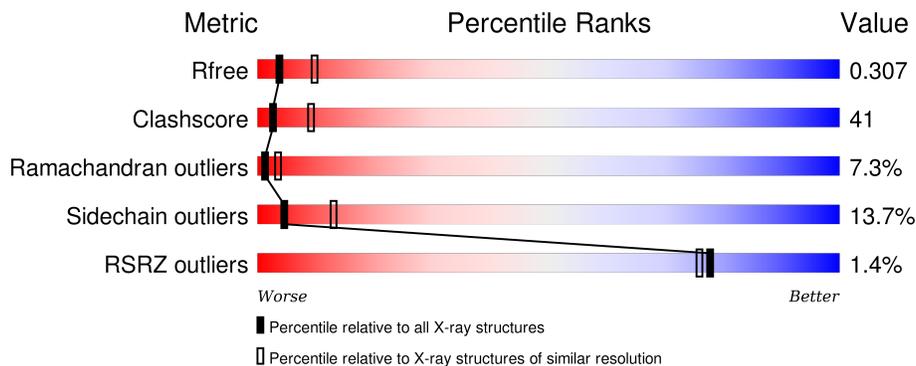
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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 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	306	
1	B	306	

## 2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 4102 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 Interferon-induced, double-stranded RNA-activated protein kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	255	2039	1311	350	372	6	0	0	0
1	B	255	2039	1311	350	372	6	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	296	ARG	LYS	SEE REMARK 999	UNP P19525
A	552	VAL	-	EXPRESSION TAG	UNP P19525
A	553	LEU	-	EXPRESSION TAG	UNP P19525
A	554	HIS	-	EXPRESSION TAG	UNP P19525
A	555	HIS	-	EXPRESSION TAG	UNP P19525
A	556	HIS	-	EXPRESSION TAG	UNP P19525
A	557	HIS	-	EXPRESSION TAG	UNP P19525
A	558	HIS	-	EXPRESSION TAG	UNP P19525
A	559	HIS	-	EXPRESSION TAG	UNP P19525
B	296	ARG	LYS	SEE REMARK 999	UNP P19525
B	552	VAL	-	EXPRESSION TAG	UNP P19525
B	553	LEU	-	EXPRESSION TAG	UNP P19525
B	554	HIS	-	EXPRESSION TAG	UNP P19525
B	555	HIS	-	EXPRESSION TAG	UNP P19525
B	556	HIS	-	EXPRESSION TAG	UNP P19525
B	557	HIS	-	EXPRESSION TAG	UNP P19525
B	558	HIS	-	EXPRESSION TAG	UNP P19525
B	559	HIS	-	EXPRESSION TAG	UNP P19525

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	13	Total	O	0	0
			13	13		

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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
2	B	11	Total	O	0	0
			11	11		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 1 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	95.41Å 95.41Å 122.02Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	27.80 – 2.90 28.98 – 2.90	Depositor EDS
% Data completeness (in resolution range)	95.7 (27.80-2.90) 95.3 (28.98-2.90)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.61 (at 2.90Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, $R_{free}$	0.240 , 0.305 0.251 , 0.307	Depositor DCC
$R_{free}$ test set	1370 reflections (10.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	88.0	Xtrriage
Anisotropy	0.005	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 63.1	EDS
Estimated twinning fraction	0.490 for -h,-k,l	Xtrriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Outliers	0 of 14174 reflections	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	4102	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	97.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.54	0/2074	0.71	0/2784
1	B	0.54	0/2074	0.71	0/2784
All	All	0.54	0/4148	0.71	0/5568

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	2039	0	2033	166	0
1	B	2039	0	2033	168	0
2	A	13	0	0	0	0
2	B	11	0	0	0	0
All	All	4102	0	4066	333	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 41.

The worst 5 of 333 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:B:412:HIS:NE2	1:B:432:ASP:HB3	1.30	1.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:HIS:NE2	1:A:432:ASP:HB3	1.30	1.40
1:B:453:ARG:HG2	1:B:454:TYR:H	1.12	1.08
1:A:453:ARG:HG2	1:A:454:TYR:H	1.13	1.03
1:A:412:HIS:NE2	1:A:432:ASP:CB	2.26	0.98

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	247/306 (81%)	175 (71%)	54 (22%)	18 (7%)	1	3
1	B	247/306 (81%)	175 (71%)	54 (22%)	18 (7%)	1	3
All	All	494/612 (81%)	350 (71%)	108 (22%)	36 (7%)	1	3

5 of 36 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	504	SER
1	A	540	LYS
1	B	504	SER
1	B	540	LYS
1	A	261	LYS

### 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	A	215/280 (77%)	185 (86%)	30 (14%)	4	12
1	B	215/280 (77%)	186 (86%)	29 (14%)	5	13
All	All	430/560 (77%)	371 (86%)	59 (14%)	4	13

5 of 59 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	502	ILE
1	B	266	ASP
1	B	487	THR
1	A	510	LYS
1	A	534	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	483	HIS
1	B	301	ASN
1	B	406	HIS
1	A	427	GLN
1	B	322	HIS

### 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 carbohydrates 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<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	255/306 (83%)	-0.18	3 (1%) 81 78	40, 98, 133, 146	0
1	B	255/306 (83%)	-0.15	4 (1%) 74 72	40, 98, 133, 146	0
All	All	510/612 (83%)	-0.16	7 (1%) 78 76	40, 98, 133, 146	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	439	LEU	3.4
1	A	359	THR	3.1
1	B	391	ALA	3.0
1	A	439	LEU	2.8
1	B	359	THR	2.4

### 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](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.