



# wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 03:17 PM GMT

PDB ID : 3W3U  
Title : Crystal structure of Kap121p mutant R349A/Q350A/D353A/E396A/N430K/D438A/N477A  
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Deposited on : 2012-12-28  
Resolution : 2.60 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

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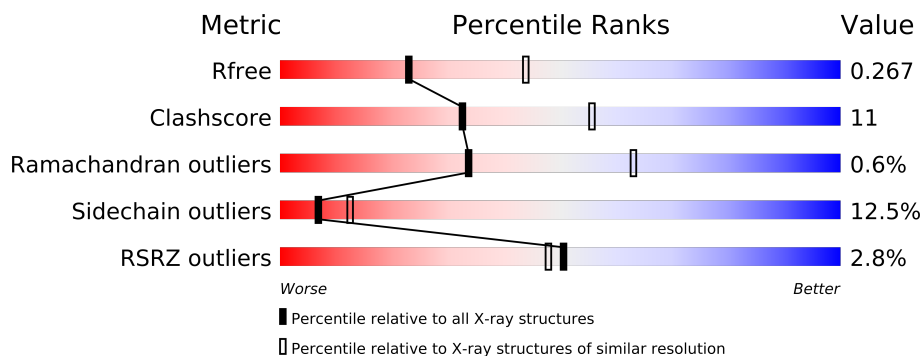
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.60 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))
$R_{free}$	66092	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	1078	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7849 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Importin subunit beta-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1030	7849	5043	1260	1510	36	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	PRO	DELETION	UNP P32337
A	?	-	SER	DELETION	UNP P32337
A	?	-	SER	DELETION	UNP P32337
A	?	-	LYS	DELETION	UNP P32337
A	?	-	LEU	DELETION	UNP P32337
A	?	-	MET	DELETION	UNP P32337
A	?	-	ILE	DELETION	UNP P32337
A	?	-	MET	DELETION	UNP P32337
A	?	-	SER	DELETION	UNP P32337
A	?	-	LYS	DELETION	UNP P32337
A	?	-	ASN	DELETION	UNP P32337
A	349	ALA	ARG	ENGINEERED MUTATION	UNP P32337
A	350	ALA	GLN	ENGINEERED MUTATION	UNP P32337
A	353	ALA	ASP	ENGINEERED MUTATION	UNP P32337
A	396	ALA	GLU	ENGINEERED MUTATION	UNP P32337
A	430	LYS	ASN	ENGINEERED MUTATION	UNP P32337
A	438	ALA	ASP	ENGINEERED MUTATION	UNP P32337
A	477	ALA	ASN	ENGINEERED MUTATION	UNP P32337



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.38Å 124.20Å 85.03Å 90.00° 116.73° 90.00°	Depositor
Resolution (Å)	26.54 – 2.60 26.53 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.5 (26.54-2.60) 97.7 (26.53-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.92 (at 2.60Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.222 , 0.267 0.222 , 0.267	Depositor DCC
$R_{free}$ test set	2165 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	65.7	Xtriage
Anisotropy	0.430	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 44.4	EDS
Estimated twinning fraction	0.022 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 43079 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7849	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.54% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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	0.66	0/7988	0.86	8/10884 (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	1

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	300	CYS	N-CA-CB	-13.87	85.64	110.60
1	A	1075	ARG	N-CA-CB	-9.18	94.08	110.60
1	A	646	ALA	N-CA-C	6.99	129.86	111.00
1	A	646	ALA	CB-CA-C	-6.89	99.77	110.10
1	A	936	ALA	N-CA-CB	-6.76	100.63	110.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	79	PRO	Mainchain

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit,

and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7849	0	7756	177	0
All	All	7849	0	7756	177	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 11.

The worst 5 of 177 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:898:LYS:NZ	1:A:937:ASP:OD2	1.83	1.10
1:A:1058:LYS:HD3	1:A:1089:ALA:HB3	1.34	1.05
1:A:406:ILE:HG23	1:A:407:PRO:HD3	1.40	1.04
1:A:892:GLU:HG2	1:A:934:THR:CG2	1.90	1.00
1:A:890:GLY:O	1:A:893:GLN:HB3	1.63	0.97

There are no symmetry-related clashes.

## 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	1008/1078 (94%)	955 (95%)	47 (5%)	6 (1%)	33 63

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	ILE
1	A	1074	ASN
1	A	8	VAL
1	A	336	ASP
1	A	591	ASP

### 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	841/931 (90%)	736 (88%)	105 (12%)	7 12

5 of 105 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	435	ILE
1	A	571	GLU
1	A	989	THR
1	A	437	THR
1	A	535	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	550	ASN
1	A	661	GLN
1	A	888	GLN
1	A	541	ASN
1	A	893	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

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, 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	1030/1078 (95%)	-0.02	29 (2%)	50 48	46, 73, 112, 212	0

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	26	ILE	8.6
1	A	593	ASP	6.3
1	A	592	ILE	4.7
1	A	594	GLU	4.6
1	A	829	PHE	4.4

### 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 carbohydrates 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.