

# Full wwPDB NMR Structure Validation Report (i)

### May 28, 2020 – 11:35 pm BST

PDB ID	:	2MA6
$\operatorname{Title}$	:	Solution NMR Structure of the RING finger domain from the Kip1 ubiquitin
		ation-promoting E3 complex protein 1 (KPC1/RNF123) from Homo sapiens,
		Northeast Structural Genomics Consortium (NESG) Target HR8700A
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		Genomics Consortium (NESG)
Deposited on	:	2013-06-28

This is a Full wwPDB NMR Structure Validation 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/NMRValidationReportHelp with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

Cyrange	:	Kirchner and Güntert (2011)
$\operatorname{NmrClust}$	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	$v_1n_11_5_13_A$ (Berjanski et al., 2005)
PANAV	:	Wang et al. $(2010)$
${ m ShiftChecker}$	:	2.11
Ideal geometry (proteins)	:	Engh & Huber $(2001)$
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

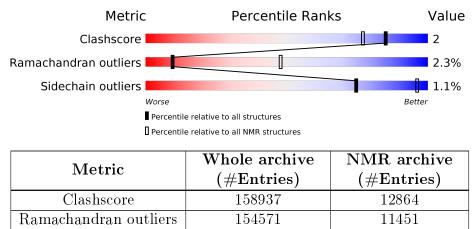
Sidechain outliers

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $SOLUTION \ NMR$ 

The overall completeness of chemical shifts assignment is 96%.

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.



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The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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%

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Mol	Chain	Length	Quality of chain		
1	А	61	79%	•	20%



# 2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 9 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues							
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model				
1	A:10-A:58 (49)	0.34	9				

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 3 clusters and 4 single-model clusters were found.

Cluster number	Models
1	1, 2, 7, 9, 10, 11, 12, 17
2	3, 4, 13, 18, 20
3	5, 14, 15
Single-model clusters	6; 8; 16; 19



## 3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 924 atoms, of which 446 are hydrogens and 0 are deuteriums.

• Molecule 1 is a protein called E3 ubiquitin-protein ligase RNF123.

Mol	Chain	Residues	Atoms					Trace	
1	٨	61	Total	С	Η	Ν	Ο	S	0
	61	922	297	446	80	90	9	0	

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	EXPRESSION TAG	UNP Q5XPI4
А	2	HIS	-	EXPRESSION TAG	UNP Q5XPI4
А	3	MET	-	EXPRESSION TAG	UNP Q5XPI4

• Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		
2	А	2	Total Zn 2 2		



## 4 Residue-property plots (i)

## 4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: E3 ubiquitin-protein ligase RNF123

Chain A:	79%	•	20%
S1 H2 P4 F4 E7 E8 E8 E8 E8 E8 E8 E8 E8	888 660 661		

## 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

• Molecule 1: E3 ubiquitin-protein ligase RNF123



#### 4.2.2 Score per residue for model 2





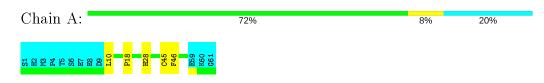
#### 4.2.3 Score per residue for model 3

• Molecule 1: E3 ubiquitin-protein ligase RNF123

Chain A:	72%	8%	20%
S1 H2 F4 F5 F5 F1 D9 F1 D9 F1	H28 S30 F46 F46 G61 G61		

#### 4.2.4 Score per residue for model 4

• Molecule 1: E3 ubiquitin-protein ligase RNF123



#### 4.2.5 Score per residue for model 5

• Molecule 1: E3 ubiquitin-protein ligase RNF123

Chain A:					72%	8%	20%
81 10 10 10 10 10 10 10 10 10 10 10 10 10	P18	H28	C45 F46	E59 K60 G61			

#### 4.2.6 Score per residue for model 6

• Molecule 1: E3 ubiquitin-protein ligase RNF123

Chain A: 70% 10% 20%

#### 4.2.7 Score per residue for model 7





#### 4.2.8 Score per residue for model 8

• Molecule 1: E3 ubiquitin-protein ligase RNF123

Chain A:					72%	8%	20%
S1 M3 P4 P4 F5 S6 F3 F8 K3 K32 K32	135 135	K49	V55 E56	E59 K60 G61			

#### 4.2.9 Score per residue for model 9 (medoid)

• Molecule 1: E3 ubiquitin-protein ligase RNF123

Chain A:						ī	75%					5%		20%	
23日 23日 23日 23日 23日 23日 23日 23日 23日 23日	135	139	F46	E59 K60 G61											

#### 4.2.10 Score per residue for model 10

 $\bullet$  Molecule 1: E3 ubiquitin-protein ligase RNF123

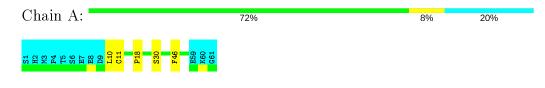
Chain A:			70	0%	10%	20%
81 83 10 10 10 10 10 10 10 10 10 10 10 10 10	H28	C45 F46 C48 C48	E59 K60 G61			

### 4.2.11 Score per residue for model 11

 $\bullet$  Molecule 1: E3 ubiquitin-protein ligase RNF123

Chain A:	74%	7%	20%
2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2	P18 P25 P46 061 061		

### 4.2.12 Score per residue for model 12





#### 4.2.13 Score per residue for model 13

• Molecule 1: E3 ubiquitin-protein ligase RNF123

Chain A:	79%	• 20%
81 H2 F46 D9 F46 D9	R 60 6 6 1 6 6 1	

#### 4.2.14 Score per residue for model 14

• Molecule 1: E3 ubiquitin-protein ligase RNF123

Chain A:		_		_	_	74%	7%	20%
2	H28	K32	C45 F46	653	K60 G61			

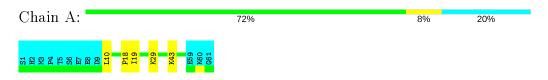
#### 4.2.15 Score per residue for model 15

 $\bullet$  Molecule 1: E3 ubiquitin-protein ligase RNF123

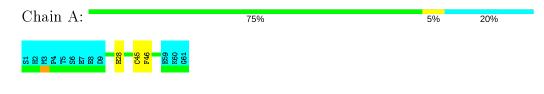
Chain A:	77%	• 20%
81 H2 M3 P4 F4 S6 S6 E7 E8 E8 E8 E8 E8 E8	<mark>F 46</mark> 1559 1661 1661	

#### 4.2.16 Score per residue for model 16

• Molecule 1: E3 ubiquitin-protein ligase RNF123



### 4.2.17 Score per residue for model 17





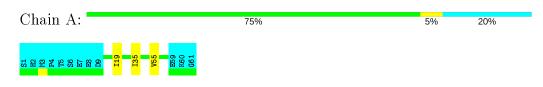
## 4.2.18 Score per residue for model 18

• Molecule 1: E3 ubiquitin-protein ligase RNF123

Chain A:	79%	• 20%
81 81 83 83 83 83 83 83 83 83 83 83 84 99 99	E 20 E 20 E 20 E 20 E 20 E 20 E 20 E 20	

#### 4.2.19 Score per residue for model 19

• Molecule 1: E3 ubiquitin-protein ligase RNF123



#### 4.2.20 Score per residue for model 20

Chain A:					66%			15%	20%	-
S1 M3 M3 M3 M3 M3 M3 M3 M3 M3 M3 M3 M3 M3	P18	H28 K29 S30	135	L39	C45 F46	E59 K60 G61				



## 5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: simulated annealing, null.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures* with the lowest energy.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
TALOS+	geometry optimization	Version 1.2009.0721.18
FMCGUI	refinement	fmcgui2.5_linux
CNS	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	$input\_cs.cif$
Number of chemical shift lists	1
Total number of shifts	745
Number of shifts mapped to atoms	745
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	96%

No validations of the models with respect to experimental NMR restraints is performed at this time.



# 6 Model quality (i)

## 6.1 Standard geometry (i)

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

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 6.2 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	А	383	366	365	$2\pm1$
All	All	7700	7320	7300	33

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 2.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models		
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total	
1:A:28:HIS:HB2	1:A:45:CYS:SG	0.57	2.40	5	10	
1:A:11:CYS:SG	1:A:30:SER:HB2	0.51	2.45	20	4	
1:A:10:LEU:HA	1:A:18:PRO:HA	0.50	1.82	16	10	
1:A:35:ILE:HG12	1:A:55:VAL:HG21	0.49	1.83	1	3	
1:A:35:ILE:HG21	1:A:55:VAL:HG11	0.49	1.83	8	2	
1:A:45:CYS:O	1:A:45:CYS:SG	0.43	2.77	10	1	
1:A:19:ILE:HG21	1:A:29:LYS:HB3	0.42	1.91	16	1	
1:A:35:ILE:O	1:A:39:LEU:HG	0.41	2.16	9	2	

All unique clashes are listed below, sorted by their clash magnitude.



## 6.3 Torsion angles (i)

## 6.3.1 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 PDB entries followed by that with respect to all NMR entries. 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	Perc	entiles
1	А	49/61~(80%)	$41\pm2~(83\pm3\%)$	$7 \pm 1 \ (15 \pm 3\%)$	$1 \pm 1 \ (2 \pm 1\%)$	9	48
All	All	980/1220~(80%)	814 (83%)	143~(15%)	23~(2%)	9	48

All 4 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	$\mathbf{Res}$	Type	Models (Total)
1	А	46	PHE	17
1	А	19	ILE	3
1	А	25	PRO	2
1	А	48	CYS	1

### 6.3.2 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 PDB entries followed by that with respect to all NMR entries. 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	45/56~(80%)	$45 \pm 1 \ (99 \pm 2\%)$	$1\pm1~(1\pm2\%)$	74 96
All	All	900/1120~(80%)	890 (99%)	10 (1%)	74 96

All 5 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	$\mathbf{Res}$	Type	Models (Total)
1	А	32	LYS	4
1	А	49	LYS	3
1	А	24	GLN	1
1	А	56	GLU	1
1	А	43	LYS	1



## 6.3.3 RNA (i)

There are no RNA molecules in this entry.

## 6.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.5 Carbohydrates (i)

There are no carbohydrates in this entry.

## 6.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

## 6.7 Other polymers (i)

There are no such molecules in this entry.

## 6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



## 7 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 96% for the well-defined parts and 94% for the entire structure.

## 7.1 Chemical shift list 1

File name: input\_cs.cif

Chemical shift list name: <code>assigned\_chem\_shift\_list\_1</code>

## 7.1.1 Bookkeeping (i)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	745
Number of shifts mapped to atoms	745
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

## 7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	${\bf Correction}\pm{\bf precision},ppm$	Suggested action
$^{13}C_{\alpha}$	60	$-0.49 \pm 0.22$	None needed ( $< 0.5$ ppm)
$^{13}C_{\beta}$	58	$0.28 \pm 0.44$	None needed ( $< 0.5$ ppm)
$^{13}C'$	55	$-0.04 \pm 0.19$	None needed ( $< 0.5$ ppm)
<sup>15</sup> N	55	$-0.12 \pm 0.78$	None needed ( $< 0.5$ ppm)

### 7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 96%, i.e. 571 atoms were assigned a chemical shift out of a possible 592. 5 out of 5 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^{1}\mathrm{H}$	$^{13}\mathrm{C}$	$^{15}\mathbf{N}$
Backbone	236/239~(99%)	95/95~(100%)	95/98~(97%)	46/46~(100%)
Sidechain	271/283~(96%)	167/169~(99%)	99/105~(94%)	5/9~(56%)

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	Total	$^{1}\mathrm{H}$	$^{13}\mathrm{C}$	$^{15}\mathbf{N}$
Aromatic	64/70~(91%)	31/37~(84%)	27/27~(100%)	6/6~(100%)
Overall	571/592~(96%)	293/301~(97%)	221/230~(96%)	57/61~(93%)

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The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 94%, i.e. 682 atoms were assigned a chemical shift out of a possible 726. 5 out of 5 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^{1}\mathrm{H}$	$^{13}\mathrm{C}$	$^{15}$ N
Backbone	285/297~(96%)	115/118~(97%)	115/122~(94%)	55/57~(96%)
Sidechain	327/351~(93%)	204/210~(97%)	118/131~(90%)	5/10~(50%)
Aromatic	70/78~(90%)	33/41~(80%)	29/29~(100%)	8/8 (100%)
Overall	682/726~(94%)	352/369~(95%)	262/282~(93%)	68/75~(91%)

### 7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

### 7.1.5 Random Coil Index (RCI) plots (1)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:

