



# wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 1SVJ  
Title : The solution structure of the nucleotide binding domain of KdpB  
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Deposited on : 2004-03-29

This is a wwPDB NMR 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/NMRValidationReportHelp>

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:

Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	trunk28760
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

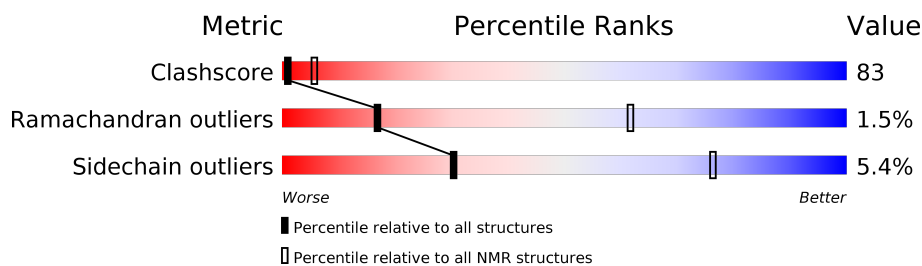
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 88%.

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)	NMR archive (#Entries)
Clashscore	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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  $\geq 3$ , 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	156	

## 2 Ensemble composition and analysis ⓘ

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2098 atoms, of which 1057 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Potassium-transporting ATPase B chain.

Mol	Chain	Residues	Atoms						Trace
1	A	136	Total	C	H	N	O	S	0
			2098	642	1057	198	199	2	

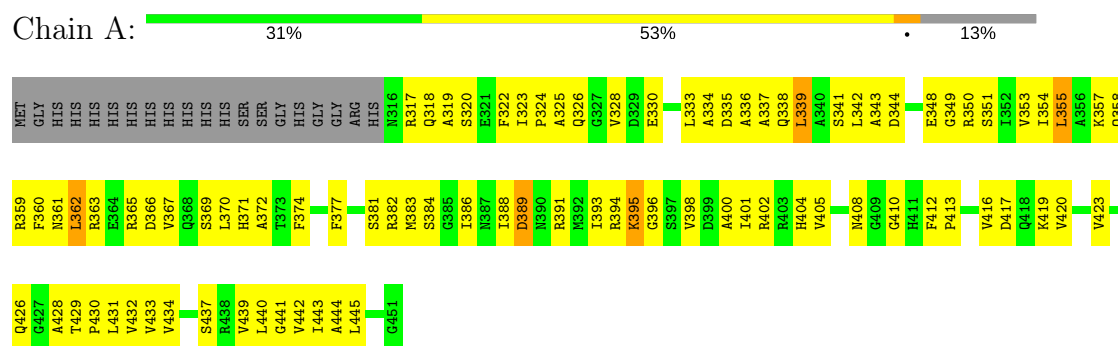
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	296	MET	-	EXPRESSION TAG	UNP P03960
A	297	GLY	-	EXPRESSION TAG	UNP P03960
A	298	HIS	-	EXPRESSION TAG	UNP P03960
A	299	HIS	-	EXPRESSION TAG	UNP P03960
A	300	HIS	-	EXPRESSION TAG	UNP P03960
A	301	HIS	-	EXPRESSION TAG	UNP P03960
A	302	HIS	-	EXPRESSION TAG	UNP P03960
A	303	HIS	-	EXPRESSION TAG	UNP P03960
A	304	HIS	-	EXPRESSION TAG	UNP P03960
A	305	HIS	-	EXPRESSION TAG	UNP P03960
A	306	HIS	-	EXPRESSION TAG	UNP P03960
A	307	HIS	-	EXPRESSION TAG	UNP P03960
A	308	SER	-	EXPRESSION TAG	UNP P03960
A	309	SER	-	EXPRESSION TAG	UNP P03960
A	310	GLY	-	EXPRESSION TAG	UNP P03960
A	311	HIS	-	EXPRESSION TAG	UNP P03960
A	312	GLY	-	EXPRESSION TAG	UNP P03960
A	313	GLY	-	EXPRESSION TAG	UNP P03960
A	314	ARG	-	EXPRESSION TAG	UNP P03960
A	315	HIS	-	EXPRESSION TAG	UNP P03960

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

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: Potassium-transporting ATPase B chain



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *SIMULATED ANNEALING*.

Of the ? calculated structures, 1 were deposited, based on the following criterion: ?.

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

Software name	Classification	Version
X-PLOR NIH-2.9.3	refinement	NIH-2.9.3
XWINNMR	structure solution	3.5
X-PLOR NIH-2.9.3	structure solution	NIH-2.9.3

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)	BMRB entry 6029
Number of chemical shift lists	1
Total number of shifts	1656
Number of shifts mapped to atoms	1656
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	88%

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

## 6 Model quality

### 6.1 Standard geometry

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

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	A	1041	1057	1056	175
All	All	1041	1057	1056	175

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 83.

5 of 175 clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:322:PHE:CD1	1:A:355:LEU:HD21	1.03	1.88
1:A:339:LEU:HD11	1:A:393:ILE:HD12	1.00	1.33
1:A:420:VAL:HG23	1:A:442:VAL:HG21	0.97	1.35
1:A:398:VAL:HG21	1:A:420:VAL:HG11	0.90	1.44
1:A:398:VAL:HG21	1:A:420:VAL:CG1	0.88	1.98

### 6.3 Torsion angles

#### 6.3.1 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 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	Percentiles	
1	A	134/156 (86%)	129 (96%)	3 (2%)	2 (1%)	17	62
All	All	134/156 (86%)	129 (96%)	3 (2%)	2 (1%)	17	62

All 2 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	389	ASP
1	A	362	LEU

### 6.3.2 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 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	A	111/127 (87%)	105 (95%)	6 (5%)	30	76
All	All	111/127 (87%)	105 (95%)	6 (5%)	30	76

5 of 6 residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	326	GLN
1	A	395	LYS
1	A	369	SER
1	A	339	LEU
1	A	437	SER

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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](#)

There are no ligands in this entry.

## 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

The completeness of assignment taking into account all chemical shift lists is 88% for the well-defined parts and 88% for the entire structure.

### 7.1 Chemical shift list 1

File name: BMRB entry 6029

Chemical shift list name: *assigned\_chem\_shift\_list\_1*

#### 7.1.1 Bookkeeping

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	1656
Number of shifts mapped to atoms	1656
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	10

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	136	$-0.16 \pm 0.09$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	126	$0.03 \pm 0.11$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	130	$0.04 \pm 0.11$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	130	$-0.20 \pm 0.33$	None needed ( $< 0.5$ ppm)

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 88%, i.e. 1456 atoms were assigned a chemical shift out of a possible 1659. 24 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	662/670 (99%)	266/267 (100%)	266/272 (98%)	130/131 (99%)
Sidechain	766/923 (83%)	467/536 (87%)	282/331 (85%)	17/56 (30%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	28/66 (42%)	28/37 (76%)	0/26 (0%)	0/3 (0%)
Overall	1456/1659 (88%)	761/840 (91%)	548/629 (87%)	147/190 (77%)

#### 7.1.4 Statistically unusual chemical shifts ⓘ

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	425	ARG	NE	128.40	92.63 – 76.73	27.5
1	A	403	ARG	NE	128.35	92.63 – 76.73	27.5
1	A	438	ARG	NE	127.94	92.63 – 76.73	27.2
1	A	350	ARG	NE	127.86	92.63 – 76.73	27.2
1	A	391	ARG	NE	127.84	92.63 – 76.73	27.1
1	A	363	ARG	NE	127.69	92.63 – 76.73	27.1
1	A	359	ARG	NE	126.43	92.63 – 76.73	26.3
1	A	365	ARG	NE	126.29	92.63 – 76.73	26.2
1	A	402	ARG	NE	124.40	92.63 – 76.73	25.0
1	A	427	GLY	N	129.40	129.07 – 90.27	5.1

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

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:

