



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 2A29
Title : The solution structure of the AMP-PNP bound nucleotide binding domain of KdpB
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This is a wwPDB NMR Structure Validation Summary 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 ⓘ symbol.

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
Mogul	:	1.7.3 (157068), CSD as539be (2018)
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	trunk30686
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk30686

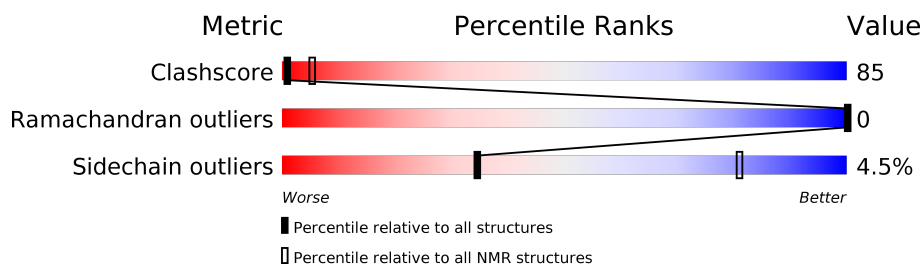
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 77%.

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	136279	12091
Ramachandran outliers	132675	10835
Sidechain outliers	132484	10811

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 $\leq 5\%$

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 are 2 unique types of molecules in this entry. The entry contains 2142 atoms, of which 1070 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

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).

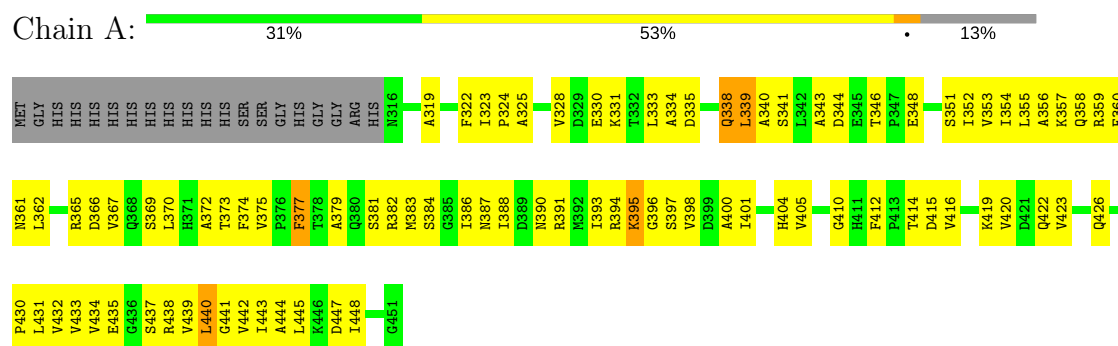


Mol	Chain	Residues	Atoms					
2	A	1	Total	C	H	N	O	P
			44	10	13	6	12	3

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	refinement	NIH-2.9.3
XWINNMR	structure solution	3.5
X-PLOR	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 6030
Number of chemical shift lists	1
Total number of shifts	1455
Number of shifts mapped to atoms	1455
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	77%

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: ANP

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	A	1041	1057	1056	182
2	A	31	13	13	13
All	All	1072	1070	1069	183

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 85.

5 of 183 clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:375:VAL:HG11	1:A:394:ARG:NH1	0.91	1.81
1:A:416:VAL:HG11	1:A:439:VAL:HG11	0.91	1.41
1:A:319:ALA:HB1	1:A:355:LEU:HD22	0.90	1.38
1:A:419:LYS:O	1:A:423:VAL:HG23	0.87	1.69
1:A:398:VAL:HG21	1:A:420:VAL:CG1	0.84	2.02

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%)	128 (96%)	6 (4%)	0 (0%)	100	100
All	All	134/156 (86%)	128 (96%)	6 (4%)	0 (0%)	100	100

There are no Ramachandran outliers.

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%)	106 (95%)	5 (5%)	34	81
All	All	111/127 (87%)	106 (95%)	5 (5%)	34	81

All 5 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	377	PHE
1	A	395	LYS
1	A	440	LEU
1	A	338	GLN
1	A	339	LEU

6.3.3 RNA

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](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	ANP	A	1001	-	29,33,33	1.83	0 (0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	ANP	A	1001	-	29,52,52	2.89	2 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ANP	A	1001	-	-	0,13,38,38	0,3,3,3

There are no bond-length outliers.

All angle outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	ANP	N3-C2-N1	12.73	117.97	128.86
2	A	1001	ANP	C4'-O4'-C1'	5.18	104.42	109.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 77% for the well-defined parts and 77% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 6030

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	1455
Number of shifts mapped to atoms	1455
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	8

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	135	0.04 ± 0.22	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	125	0.41 ± 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	130	-0.22 ± 0.29	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 77%, i.e. 1275 atoms were assigned a chemical shift out of a possible 1659. 21 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	527/670 (79%)	262/267 (98%)	135/272 (50%)	130/131 (99%)
Sidechain	727/923 (79%)	440/536 (82%)	273/331 (82%)	14/56 (25%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	21/66 (32%)	21/37 (57%)	0/26 (0%)	0/3 (0%)
Overall	1275/1659 (77%)	723/840 (86%)	408/629 (65%)	144/190 (76%)

7.1.4 Statistically unusual chemical shifts [i](#)

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	128.50	92.63 – 76.73	27.6
1	A	359	ARG	NE	126.50	92.63 – 76.73	26.3
1	A	365	ARG	NE	126.30	92.63 – 76.73	26.2
1	A	402	ARG	NE	124.60	92.63 – 76.73	25.1
1	A	357	LYS	HE2	1.62	3.87 – 1.97	-6.8
1	A	357	LYS	HE3	1.62	3.86 – 1.96	-6.8
1	A	427	GLY	N	129.30	129.07 – 90.27	5.1
1	A	396	GLY	N	129.20	129.07 – 90.27	5.0

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

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:

