



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 2A00
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
<http://wwpdb.org/validation/2016/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 : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

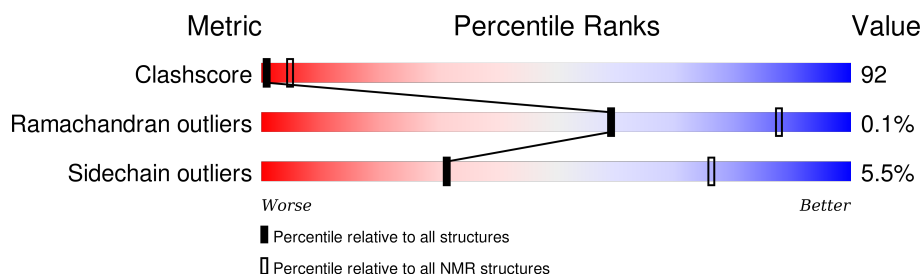
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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	<div> <div>24%</div> <div>49%</div> <div>•</div> <div>12%</div> <div>13%</div> </div>

2 Ensemble composition and analysis ⓘ

This entry contains 19 models. Model 10 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 violations*.

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:318-A:344, A:348-A:356, A:365-A:446 (118)	0.14	10

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 1 single-model cluster was found.

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

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.

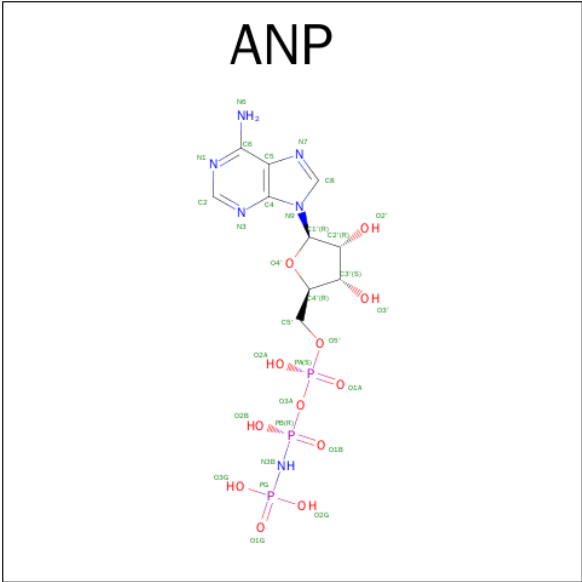
- Molecule 1 is a protein called Potassium-transporting ATPase B chain.

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					
			Total	C	H	N	O	P
2	A	1	44	10	13	6	12	3

5 Refinement protocol and experimental data overview

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

Of the 50 calculated structures, 19 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality

6.1 Standard geometry

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

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	886	899	899	167±8
2	A	31	13	13	9±3
All	All	17423	17328	17328	3187

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 92.

5 of 514 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:319:ALA:HB1	1:A:355:LEU:HD12	1.10	1.18	7	7
1:A:416:VAL:HG11	1:A:439:VAL:HG11	1.05	1.29	1	19
1:A:319:ALA:CB	1:A:355:LEU:HD12	1.01	1.84	15	7
1:A:433:VAL:HG12	1:A:440:LEU:HD21	0.99	1.27	16	18
1:A:322:PHE:CD1	1:A:355:LEU:HD21	0.98	1.94	10	2

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	Percentiles	
1	A	118/156 (76%)	112±1 (95±1%)	6±1 (5±1%)	0±0 (0±0%)	59	88
All	All	2242/2964 (76%)	2129 (95%)	111 (5%)	2 (0%)	59	88

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

Mol	Chain	Res	Type	Models (Total)
1	A	390	ASN	1
1	A	389	ASP	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	A	94/127 (74%)	89±1 (94±1%)	5±1 (6±1%)	31	76
All	All	1786/2413 (74%)	1687 (94%)	99 (6%)	31	76

5 of 18 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	440	LEU	19
1	A	395	LYS	18
1	A	339	LEU	17
1	A	338	GLN	14
1	A	377	PHE	8

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 ⓘ

There are no carbohydrates in this entry.

6.6 Ligand geometry ⓘ

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	1.82±0.01	0±0 (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	-	26,52,52	3.08±0.02	1±0 (3±0%)

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±0,13,38,38	0±0,3,3,3

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	A	1001	ANP	N3-C2-N1	13.95	117.91	128.87	4	19

There are no chirality outliers.

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

Mol	Chain	Res	Type	Atoms	Models (Total)
2	A	1001	ANP	O1B-PB-N3B-PG	5
2	A	1001	ANP	O1G-PG-N3B-PB	2

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

No chemical shift data were provided