

Full wwPDB NMR Structure Validation Report (i)

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PDB ID : 20FH

Title : Solution structure of the n-terminal domain of the zinc(II) ATPase ziaa in its

apo form

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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.

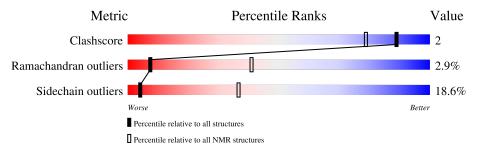
The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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 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 $(\# \mathrm{Entries})$	$ m NMR~archive \ (\#Entries)$	
Clashscore	158937	12864	
Ramachandran outliers	154571	11451	
Sidechain outliers	154315	11428	

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%

Mol	Chain	Length	Quality of chain		
1	X	111	50%	11%	36%



2 Ensemble composition and analysis (i)

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



3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1084 atoms, of which 554 are hydrogens and 0 are deuteriums.

• Molecule 1 is a protein called Zinc-transporting ATPase.

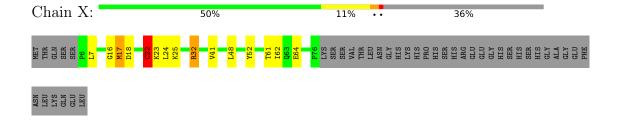
Mol	Chain	Residues	Atoms				Trace		
1	v	71	Total	С	Н	N	О	S	0
1	Λ	(1	1084	330	554	90	106	4	



4 Residue-property plots (i)

These plots are provided for all protein, RNA, DNA and oligosaccharide 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: Zinc-transporting ATPase





Refinement protocol and experimental data overview (i) 5



The models were refined using the following method: Simulated Annealing in TAD followed by Restrained Energy Minimization.

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
CYANA	structure solution	2.1
Amber	refinement	8

No chemical shift data was provided.



6 Model quality (i)

6.1 Standard geometry (i)

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 (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol Chain		Bor	nd lengths	Bond angles		
WIOI	Chain	RMSZ	#Z>5	RMSZ	#Z>5	
1	X	0.59	0/534 (0.0%)	1.07	2/720~(~0.3%)	
All	All	0.59	0/534 (0.0%)	1.07	2/720 (0.3%)	

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	Planarity
1	X	0	1
All	All	0	1

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	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	X	32	ARG	CD-NE-CZ	5.32	131.04	123.60
1	X	32	ARG	NE-CZ-NH2	-5.05	117.78	120.30

There are no chirality outliers.

All planar outliers are listed below.

Mo	1	Chain	Res	Type	Group
1		X	17	MET	Peptide

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	X	530	554	554	2
All	All	530	554	554	2

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.

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

Atom-1	Atom-2	$\operatorname{Clash}(ext{\AA})$	$\operatorname{Distance}(\text{\AA})$
1:X:41:VAL:HG12	1:X:48:LEU:CD2	0.57	2.30
1:X:22:CYS:HA	1:X:25:LYS:HE2	0.46	1.88

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	Perce	entiles
1	X	69/111 (62%)	50 (72%)	17 (25%)	2 (3%)	7	41
All	All	69/111 (62%)	50 (72%)	17 (25%)	2 (3%)	7	41

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

Mol	Chain	Res	Type
1	X	16	GLY
1	X	22	CYS

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	X	59/94 (63%)	48 (81%)	11 (19%)	4 37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	59/94 (63%)	48 (81%)	11 (19%)	4 37

All 11 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	X	7	LEU
1	X	17	MET
1	X	18	ASP
1	X	22	CYS
1	X	23	LYS
1	X	24	LEU
1	X	32	ARG
1	X	52	TYR
1	X	61	THR
1	X	62	ILE
1	X	64	GLU

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 monosaccharides 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 (i)

No chemical shift data were provided

