



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 2GA7
Title : Solution structure of the copper(I) form of the third metal-binding domain of ATP7A protein (menkes disease protein)
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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 : unknown
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

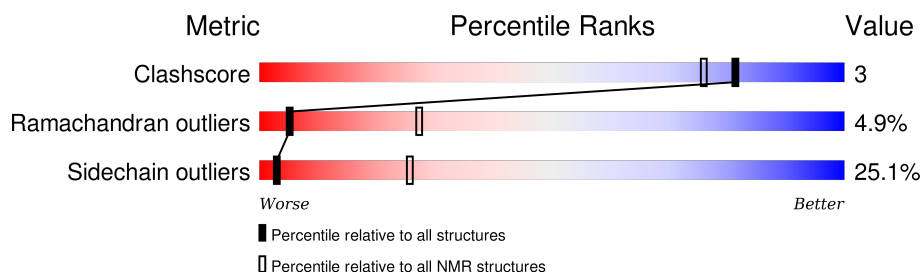
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment 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	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	90	

2 Ensemble composition and analysis ⓘ

This entry contains 30 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest 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:2-A:49, A:54-A:74 (69)	0.41	3

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 2 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28
2	2, 29, 30

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1151 atoms, of which 577 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Copper-transporting ATPase 1.

Mol	Chain	Residues	Atoms						Trace
1	A	77	Total	C	H	N	O	S	0
			1150	356	577	95	119	3	

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	46	VAL	LYS	ENGINEERED	UNP Q04656
A	79	ILE	-	CLONING ARTIFACT	UNP Q04656
A	80	GLU	-	CLONING ARTIFACT	UNP Q04656
A	81	GLY	-	CLONING ARTIFACT	UNP Q04656
A	82	ARG	-	CLONING ARTIFACT	UNP Q04656
A	83	LEU	-	CLONING ARTIFACT	UNP Q04656
A	84	GLU	-	CLONING ARTIFACT	UNP Q04656
A	85	HIS	-	EXPRESSION TAG	UNP Q04656
A	86	HIS	-	EXPRESSION TAG	UNP Q04656
A	87	HIS	-	EXPRESSION TAG	UNP Q04656
A	88	HIS	-	EXPRESSION TAG	UNP Q04656
A	89	HIS	-	EXPRESSION TAG	UNP Q04656
A	90	HIS	-	EXPRESSION TAG	UNP Q04656

- Molecule 2 is COPPER (I) ION (three-letter code: CU1) (formula: Cu).

Mol	Chain	Residues	Atoms	
2	A	1	Total	Cu
			1	1

5 Refinement protocol and experimental data overview

The models were refined using the following method: *Torsion angle dynamics coupled with simulated annealing followed by restrained energy minimization.*

Of the 300 calculated structures, 30 were deposited, based on the following criterion: *target function.*

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

Software name	Classification	Version
CYANA	structure solution	2.1
AMBER	refinement	8.0

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 7068
Number of chemical shift lists	1
Total number of shifts	857
Number of shifts mapped to atoms	857
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

6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CU1

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	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.63±0.01	0±0/524 (0.0±0.0%)	1.29±0.06	4±2/713 (0.6±0.3%)
All	All	0.63	0/15720 (0.0%)	1.30	119/21390 (0.6%)

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	A	0.0±0.0	1.3±0.8
All	All	0	38

There are no bond-length outliers.

5 of 28 unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	35	VAL	CA-CB-CG1	9.03	124.44	110.90	9	2
1	A	18	VAL	CA-CB-CG1	8.87	124.20	110.90	11	11
1	A	58	ARG	NE-CZ-NH1	8.86	124.73	120.30	28	11
1	A	64	VAL	CG1-CB-CG2	-8.41	97.44	110.90	2	1
1	A	70	ARG	NE-CZ-NH2	-8.28	116.16	120.30	20	1

There are no chirality outliers.

5 of 6 unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	47	TYR	Sidechain	14

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	7	PHE	Sidechain	9
1	A	41	ARG	Sidechain	6
1	A	58	ARG	Sidechain	5
1	A	69	TYR	Sidechain	2

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	517	525	525	3±2
All	All	15540	15750	15749	100

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 3.

5 of 33 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:7:PHE:CD2	1:A:73:ILE:HD12	0.71	2.21	27	14
1:A:20:ASN:HD21	1:A:64:VAL:HG11	0.65	1.51	12	1
1:A:21:ILE:HG22	1:A:25:LEU:HD23	0.63	1.68	15	1
1:A:18:VAL:HG11	1:A:38:LEU:HA	0.59	1.73	26	3
1:A:15:LYS:O	1:A:18:VAL:HG13	0.57	1.99	9	6

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	69/90 (77%)	56±2 (82±3%)	9±2 (13±3%)	3±1 (5±2%)	5	27
All	All	2070/2700 (77%)	1694 (82%)	274 (13%)	102 (5%)	5	27

5 of 16 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	35	VAL	30
1	A	70	ARG	11
1	A	17	CYS	9
1	A	40	ASN	8
1	A	41	ARG	8

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	61/81 (75%)	46±3 (75±4%)	15±3 (25±4%)	3	26
All	All	1830/2430 (75%)	1371 (75%)	459 (25%)	3	26

5 of 47 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	34	ILE	30
1	A	35	VAL	29
1	A	38	LEU	29
1	A	20	ASN	28
1	A	39	GLU	25

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 1 ligands modelled in this entry, 1 is 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 77% for the well-defined parts and 75% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 7068

Chemical shift list name: *assigned_chem_shift_list_1*

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	857
Number of shifts mapped to atoms	857
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	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	78	-0.43 ± 0.24	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	75	0.16 ± 0.14	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	—
^{15}N	75	0.14 ± 0.59	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 77%, i.e. 611 atoms were assigned a chemical shift out of a possible 795. 12 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	254/341 (74%)	127/136 (93%)	65/138 (47%)	62/67 (93%)
Sidechain	341/414 (82%)	205/240 (85%)	133/159 (84%)	3/15 (20%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	16/40 (40%)	16/21 (76%)	0/18 (0%)	0/1 (0%)
Overall	611/795 (77%)	348/397 (88%)	198/315 (63%)	65/83 (78%)

7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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:

