



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 02:03 PM BST

PDB ID : 1DFS
Title : SOLUTION STRUCTURE OF THE ALPHA-DOMAIN OF MOUSE METALLOTHIONEIN-1
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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
<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

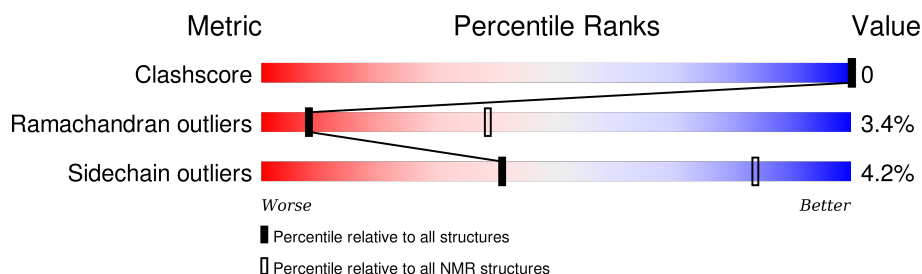
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

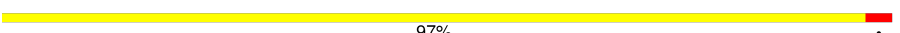
The overall completeness of chemical shifts assignment was not calculated.

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	31	 97% .

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 399 atoms, of which 197 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called METALLOTHIONEIN-1.

Mol	Chain	Residues	Atoms						Trace
1	A	31	Total	C	H	N	O	S	0
			395	112	197	36	39	11	

- Molecule 2 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	
2	A	4	Total	Cd
			4	4

4 Residue-property plots

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: METALLOTHIONEIN-1

Chain A:  97% .

K1	S2	C3	C4	S5	C6	C7	P8	V9	G10	C11	S12	K13	C14	A15	Q16	G17	C18	V19	C20	K21	G22	A23	A24	D25	K26	C27	T28	C29	C30	A31
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5 Refinement protocol and experimental data overview

The models were refined using the following method: *HYBRID DISTANCE GEOMETRY-DYNAMICAL SIMULATED ANNEALING*.

Of the 50 calculated structures, 1 were deposited, based on the following criterion: *MINIMIZED AVERAGE STRUCTURE*.

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

Software name	Classification	Version
X-PLOR	structure solution	3.851
X-PLOR	refinement	3.851

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 [i](#)

6.1 Standard geometry [i](#)

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

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	5.69	114/198 (57.6%)	1.70	0/261 (0.0%)
All	All	5.69	114/198 (57.6%)	1.70	0/261 (0.0%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	22	GLY	N-CA	10.77	1.62	1.46
1	A	11	CYS	N-CA	10.46	1.67	1.46
1	A	15	ALA	N-CA	9.78	1.66	1.46
1	A	17	GLY	N-CA	9.75	1.60	1.46
1	A	9	VAL	N-CA	9.60	1.65	1.46
1	A	22	GLY	CA-C	9.49	1.67	1.51
1	A	24	ALA	N-CA	9.35	1.65	1.46
1	A	18	CYS	N-CA	9.29	1.65	1.46
1	A	26	LYS	N-CA	9.23	1.64	1.46
1	A	25	ASP	N-CA	9.17	1.64	1.46
1	A	3	CYS	N-CA	9.08	1.64	1.46
1	A	6	CYS	N-CA	8.96	1.64	1.46
1	A	19	VAL	CA-CB	8.92	1.73	1.54
1	A	29	CYS	N-CA	8.92	1.64	1.46
1	A	10	GLY	CA-C	8.88	1.66	1.51
1	A	21	LYS	N-CA	8.84	1.64	1.46
1	A	5	SER	N-CA	8.68	1.63	1.46
1	A	16	GLN	N-CA	8.60	1.63	1.46
1	A	8	PRO	CA-C	8.49	1.69	1.52
1	A	10	GLY	N-CA	8.49	1.58	1.46
1	A	23	ALA	N-CA	8.46	1.63	1.46
1	A	19	VAL	N-CA	8.38	1.63	1.46
1	A	9	VAL	CA-CB	8.36	1.72	1.54
1	A	12	SER	N-CA	8.35	1.63	1.46
1	A	8	PRO	N-CA	8.30	1.61	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	28	THR	N-CA	8.29	1.62	1.46
1	A	2	SER	N-CA	8.28	1.62	1.46
1	A	27	CYS	N-CA	8.24	1.62	1.46
1	A	31	ALA	N-CA	8.17	1.62	1.46
1	A	20	CYS	N-CA	8.07	1.62	1.46
1	A	7	CYS	C-N	8.07	1.49	1.34
1	A	1	LYS	N-CA	8.02	1.62	1.46
1	A	4	CYS	N-CA	7.86	1.62	1.46
1	A	7	CYS	N-CA	7.77	1.61	1.46
1	A	13	LYS	N-CA	7.72	1.61	1.46
1	A	30	CYS	N-CA	7.56	1.61	1.46
1	A	14	CYS	N-CA	7.53	1.61	1.46
1	A	4	CYS	CA-CB	7.53	1.70	1.53
1	A	11	CYS	CA-CB	7.47	1.70	1.53
1	A	2	SER	CA-CB	7.39	1.64	1.52
1	A	21	LYS	C-N	7.36	1.46	1.33
1	A	1	LYS	CA-CB	7.35	1.70	1.53
1	A	3	CYS	CA-CB	7.20	1.69	1.53
1	A	19	VAL	CB-CG1	7.03	1.67	1.52
1	A	12	SER	CA-CB	6.94	1.63	1.52
1	A	11	CYS	CA-C	6.89	1.70	1.52
1	A	26	LYS	CA-CB	6.82	1.69	1.53
1	A	5	SER	CA-C	6.80	1.70	1.52
1	A	30	CYS	CA-CB	6.80	1.69	1.53
1	A	6	CYS	CA-CB	6.79	1.68	1.53
1	A	20	CYS	CA-CB	6.78	1.68	1.53
1	A	14	CYS	CA-C	6.74	1.70	1.52
1	A	14	CYS	CA-CB	6.70	1.68	1.53
1	A	5	SER	CA-CB	6.69	1.62	1.52
1	A	28	THR	CA-CB	6.53	1.70	1.53
1	A	18	CYS	CA-CB	6.41	1.68	1.53
1	A	28	THR	CA-C	6.40	1.69	1.52
1	A	18	CYS	CA-C	6.39	1.69	1.52
1	A	25	ASP	CA-CB	6.39	1.68	1.53
1	A	8	PRO	N-CD	6.34	1.56	1.47
1	A	21	LYS	CD-CE	6.30	1.67	1.51
1	A	2	SER	C-N	6.22	1.48	1.34
1	A	22	GLY	C-N	6.17	1.48	1.34
1	A	7	CYS	CA-CB	6.16	1.67	1.53
1	A	17	GLY	CA-C	6.14	1.61	1.51
1	A	8	PRO	C-N	6.11	1.48	1.34
1	A	19	VAL	CA-C	6.05	1.68	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2	SER	CA-C	5.97	1.68	1.52
1	A	28	THR	C-N	5.96	1.47	1.34
1	A	9	VAL	CB-CG2	5.95	1.65	1.52
1	A	16	GLN	C-N	5.94	1.43	1.33
1	A	5	SER	C-N	5.93	1.47	1.34
1	A	29	CYS	CA-CB	5.89	1.67	1.53
1	A	21	LYS	CA-CB	5.88	1.66	1.53
1	A	30	CYS	CA-C	5.83	1.68	1.52
1	A	1	LYS	C-N	5.80	1.47	1.34
1	A	3	CYS	CA-C	5.79	1.68	1.52
1	A	1	LYS	CD-CE	5.79	1.65	1.51
1	A	23	ALA	CA-CB	5.77	1.64	1.52
1	A	13	LYS	CA-CB	5.74	1.66	1.53
1	A	9	VAL	C-N	5.72	1.43	1.33
1	A	16	GLN	CA-CB	5.71	1.66	1.53
1	A	13	LYS	CD-CE	5.64	1.65	1.51
1	A	1	LYS	CA-C	5.63	1.67	1.52
1	A	26	LYS	CA-C	5.60	1.67	1.52
1	A	27	CYS	CA-C	5.59	1.67	1.52
1	A	14	CYS	C-N	5.58	1.46	1.34
1	A	20	CYS	CA-C	5.53	1.67	1.52
1	A	19	VAL	CB-CG2	5.50	1.64	1.52
1	A	17	GLY	C-N	5.48	1.46	1.34
1	A	25	ASP	CA-C	5.44	1.67	1.52
1	A	15	ALA	CA-C	5.44	1.67	1.52
1	A	24	ALA	CA-CB	5.43	1.63	1.52
1	A	24	ALA	C-N	5.39	1.46	1.34
1	A	26	LYS	CD-CE	5.37	1.64	1.51
1	A	7	CYS	CA-C	5.37	1.67	1.52
1	A	10	GLY	C-N	5.36	1.46	1.34
1	A	16	GLN	CA-C	5.35	1.66	1.52
1	A	29	CYS	CA-C	5.32	1.66	1.52
1	A	26	LYS	CB-CG	5.32	1.67	1.52
1	A	26	LYS	C-N	5.31	1.46	1.34
1	A	24	ALA	CA-C	5.28	1.66	1.52
1	A	13	LYS	CA-C	5.27	1.66	1.52
1	A	30	CYS	C-N	5.25	1.46	1.34
1	A	21	LYS	CB-CG	5.25	1.66	1.52
1	A	27	CYS	CA-CB	5.22	1.65	1.53
1	A	9	VAL	CB-CG1	5.22	1.63	1.52
1	A	4	CYS	C-N	5.19	1.46	1.34
1	A	12	SER	C-N	5.18	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	21	LYS	CA-C	5.13	1.66	1.52
1	A	12	SER	CA-C	5.13	1.66	1.52
1	A	3	CYS	CB-SG	5.09	1.91	1.82
1	A	13	LYS	C-N	5.08	1.45	1.34
1	A	16	GLN	CG-CD	5.02	1.62	1.51

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
All	All	202	197	186	-

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 -.

There are no clashes.

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	29/31 (94%)	21 (72%)	7 (24%)	1 (3%)	8	38
All	All	29/31 (94%)	21 (72%)	7 (24%)	1 (3%)	8	38

All 1 Ramachandran outliers are listed below.

Mol	Chain	Res	Type
1	A	11	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	A	24/24 (100%)	23 (96%)	1 (4%)	41	84
All	All	24/24 (100%)	23 (96%)	1 (4%)	41	84

All 1 residues with a non-rotameric sidechain are listed below.

Mol	Chain	Res	Type
1	A	11	CYS

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 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided