



wwPDB NMR Structure Validation Summary Report ⓘ

Mar 20, 2026 – 06:26 AM UTC

PDB ID : 1J5L / pdb_00001j5l
BMRB ID : 4754
Title : NMR STRUCTURE OF THE ISOLATED BETA_C DOMAIN OF LOBSTER METALLOTHIONEIN-1
Authors : Munoz, A.; Forsterling, F.H.; Shaw III, C.F.; Petering, D.H.
Deposited on : 2002-05-16

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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

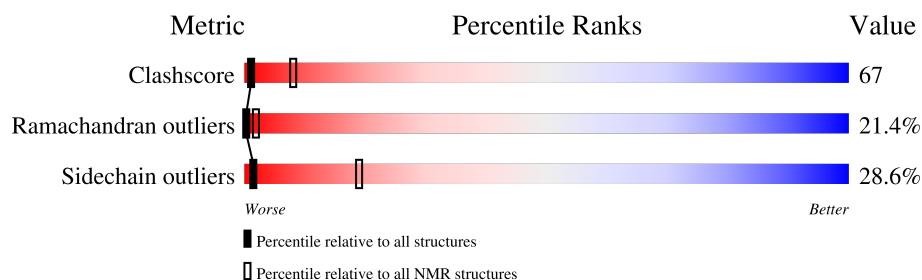
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 51%.

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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	30	

2 Ensemble composition and analysis ⓘ

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

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 407 atoms, of which 196 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called METALLOTHIONEIN-1.

Mol	Chain	Residues	Atoms						Trace
1	A	30	Total	C	H	N	O	S	0
			404	120	196	35	44	9	

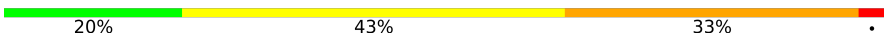
- Molecule 2 is CADMIUM ION (CCD ID: CD) (formula: Cd).

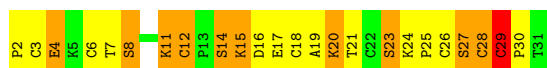
Mol	Chain	Residues	Atoms	
2	A	3	Total	Cd
			3	3

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: METALLOTHIONEIN-1

Chain A: 



5 Refinement protocol and experimental data overview

The models were refined using the following method: *ab initio 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	structure solution	3.851
X-PLOR	refinement	3.851

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)	working_cs.cif
Number of chemical shift lists	4
Total number of shifts	169
Number of shifts mapped to atoms	166
Number of unparsed shifts	0
Number of shifts with mapping errors	3
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	51%

6 Model quality

6.1 Standard geometry

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

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	208	196	194	27
All	All	211	196	194	27

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 67.

5 of 27 clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:29:CYS:CB	1:A:30:PRO:HD2	0.63	2.22
1:A:29:CYS:CB	1:A:30:PRO:CD	0.59	2.80
1:A:11:LYS:O	1:A:12:CYS:C	0.54	2.50
1:A:26:CYS:O	1:A:28:CYS:N	0.53	2.41
1:A:23:SER:O	1:A:24:LYS:CG	0.53	2.57

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	28/30 (93%)	11 (39%)	11 (39%)	6 (21%)	0	2
All	All	28/30 (93%)	11 (39%)	11 (39%)	6 (21%)	0	2

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

Mol	Chain	Res	Type
1	A	8	SER
1	A	12	CYS
1	A	15	LYS
1	A	27	SER
1	A	28	CYS

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	28/28 (100%)	20 (71%)	8 (29%)	1	19
All	All	28/28 (100%)	20 (71%)	8 (29%)	1	19

5 of 8 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	4	GLU
1	A	11	LYS
1	A	14	SER
1	A	17	GLU
1	A	20	LYS

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 oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 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 [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 51% for the well-defined parts and 51% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

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	166
Number of shifts mapped to atoms	166
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](#)

No chemical shift referencing corrections were calculated (not enough data).

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 51%, i.e. 166 atoms were assigned a chemical shift out of a possible 323. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	57/143 (40%)	57/57 (100%)	0/60 (0%)	0/26 (0%)
Sidechain	109/180 (61%)	109/115 (95%)	0/60 (0%)	0/5 (0%)
Overall	166/323 (51%)	166/172 (97%)	0/120 (0%)	0/31 (0%)

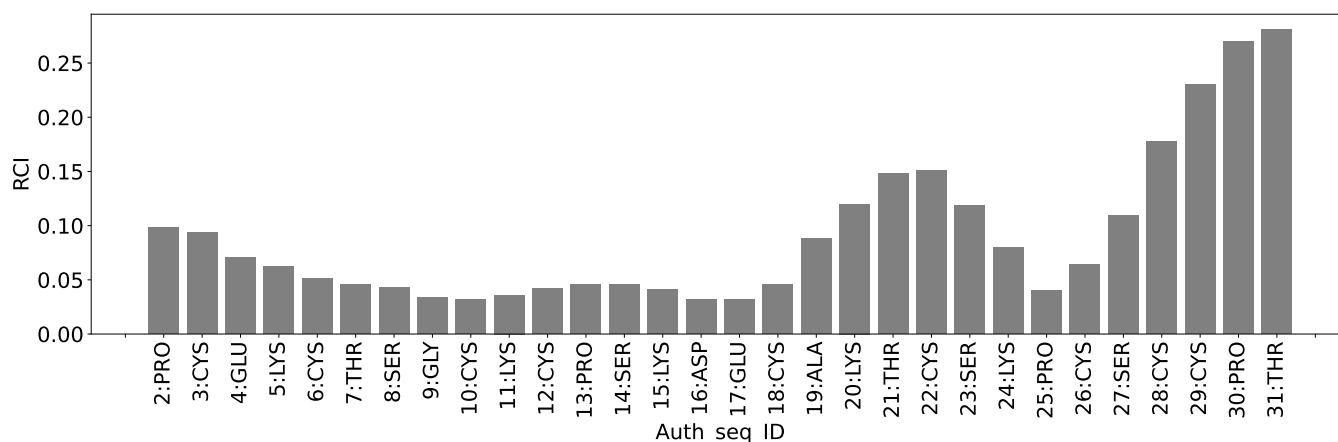
7.1.4 Statistically unusual chemical shifts [i](#)

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. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



7.2 Chemical shift list 2

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_2*

7.2.1 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	1
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	1
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 1 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2	A	1	CD	CD	659.6	?	1

7.2.2 Chemical shift referencing [i](#)

No chemical shift referencing corrections were calculated (not enough data).

7.2.3 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 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 323. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	0/143 (0%)	0/57 (0%)	0/60 (0%)	0/26 (0%)
Sidechain	0/180 (0%)	0/115 (0%)	0/60 (0%)	0/5 (0%)
Overall	0/323 (0%)	0/172 (0%)	0/120 (0%)	0/31 (0%)

7.2.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

No *random coil index*(RCI) plot could be generated from the current chemical shift list. RCI is only applicable to proteins

7.3 Chemical shift list 3

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_3*

7.3.1 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	1
Number of shifts mapped to atoms	0

Number of unparsed shifts	0
Number of shifts with mapping errors	1
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 1 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3	A	1	CD	CD	638.1	?	1

7.3.2 Chemical shift referencing [i](#)

No chemical shift referencing corrections were calculated (not enough data).

7.3.3 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 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 323. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	0/143 (0%)	0/57 (0%)	0/60 (0%)	0/26 (0%)
Sidechain	0/180 (0%)	0/115 (0%)	0/60 (0%)	0/5 (0%)
Overall	0/323 (0%)	0/172 (0%)	0/120 (0%)	0/31 (0%)

7.3.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

No *random coil index*(RCI) plot could be generated from the current chemical shift list. RCI is only applicable to proteins

7.4 Chemical shift list 4

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_4*

7.4.1 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	1
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	1
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 1 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
4	A	1	CD	CD	611.7	?	1

7.4.2 Chemical shift referencing [i](#)

No chemical shift referencing corrections were calculated (not enough data).

7.4.3 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 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 323. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	0/143 (0%)	0/57 (0%)	0/60 (0%)	0/26 (0%)
Sidechain	0/180 (0%)	0/115 (0%)	0/60 (0%)	0/5 (0%)
Overall	0/323 (0%)	0/172 (0%)	0/120 (0%)	0/31 (0%)

7.4.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.4.5 Random Coil Index (RCI) plots

No *random coil index*(RCI) plot could be generated from the current chemical shift list. RCI is only applicable to proteins