



Full wwPDB NMR Structure Validation Report ⓘ

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PDB ID : 2M30 / pdb_00002m30
BMRB ID : 7376
Title : Solution NMR refinement of a metal ion bound protein using quantum mechanical/molecular mechanical and molecular dynamics methods
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Deposited on : 2013-01-04

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 ⓘ 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 : **FAILED**
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 26%.

There are no overall percentile quality scores available for this entry.

The sequence quality summary graphics cannot be shown.

2 Ensemble composition and analysis

This entry contains 10 models. Model 8 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:10-A:73, A:78-A:101, B:10-B:72, B:78-B:100 (174)	0.52	8

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 1 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 5, 6, 7, 8, 9, 10

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 3058 atoms, of which 1546 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Repressor protein.

Mol	Chain	Residues	Atoms						Trace
1	A	95	Total	C	H	N	O	S	0
			1528	471	773	141	140	3	
1	B	95	Total	C	H	N	O	S	0
			1528	471	773	141	140	3	

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

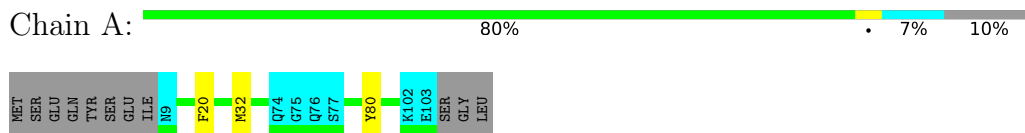
Mol	Chain	Residues	Atoms	
2	A	1	Total	Zn
			1	1
2	B	1	Total	Zn
			1	1

4 Residue-property plots [i](#)

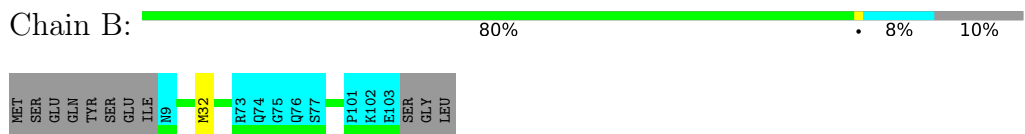
4.1 Average score per residue in the NMR ensemble

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: Repressor protein



- Molecule 1: Repressor protein

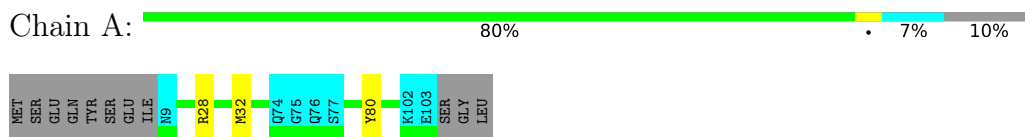


4.2 Scores per residue for each member of the ensemble

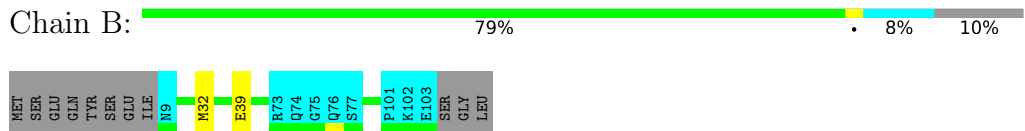
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Repressor protein

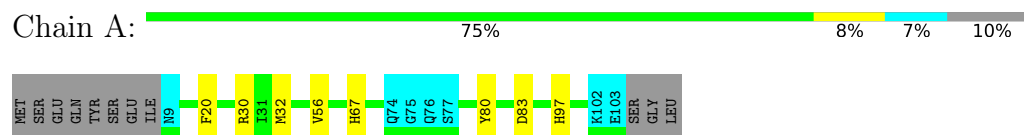


- Molecule 1: Repressor protein

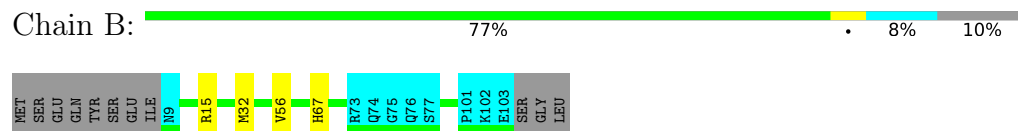


4.2.2 Score per residue for model 2

- Molecule 1: Repressor protein

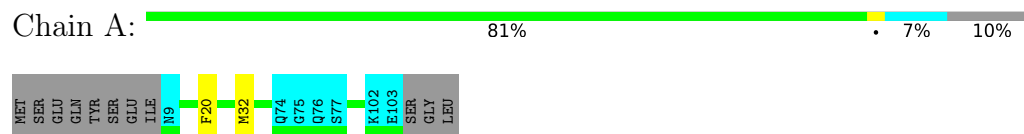


- Molecule 1: Repressor protein

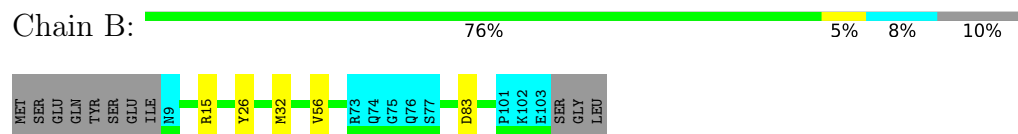


4.2.3 Score per residue for model 3

- Molecule 1: Repressor protein

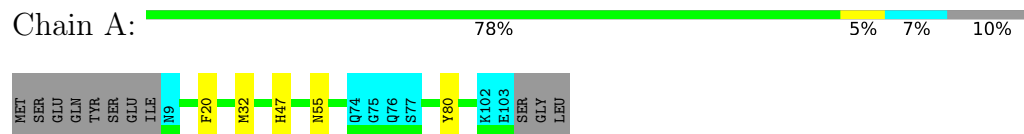


- Molecule 1: Repressor protein

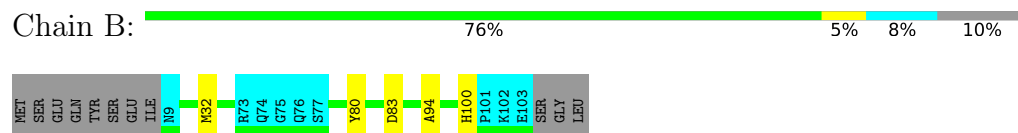


4.2.4 Score per residue for model 4

- Molecule 1: Repressor protein



- Molecule 1: Repressor protein



4.2.5 Score per residue for model 5

- Molecule 1: Repressor protein

Chain A:  82% 7% 10%



- Molecule 1: Repressor protein

Chain B:  79% 8% 10%



4.2.6 Score per residue for model 6

- Molecule 1: Repressor protein

Chain A:  76% 7% 7% 10%



- Molecule 1: Repressor protein

Chain B:  79% 8% 10%



4.2.7 Score per residue for model 7

- Molecule 1: Repressor protein

Chain A:  80% 7% 10%



- Molecule 1: Repressor protein

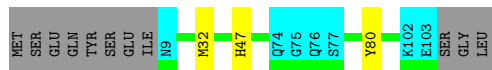
Chain B:  78% 8% 10%



4.2.8 Score per residue for model 8 (medoid)

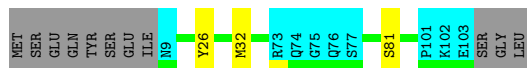
- Molecule 1: Repressor protein

Chain A:  80% 7% 10%



- Molecule 1: Repressor protein

Chain B:  78% 8% 10%



4.2.9 Score per residue for model 9

- Molecule 1: Repressor protein

Chain A:  78% 5% 7% 10%



- Molecule 1: Repressor protein

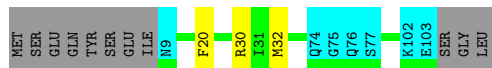
Chain B:  78% 8% 10%



4.2.10 Score per residue for model 10

- Molecule 1: Repressor protein

Chain A:  80% 7% 10%



- Molecule 1: Repressor protein

Chain B:  76% 5% 8% 10%



5 Refinement protocol and experimental data overview

The models were refined using the following method: *molecular dynamics and quantum mechanical molecular mechanical molecular dynamics*.

Of the 132000 calculated structures, 10 were deposited, based on the following criterion: *Structures from 1 ns of independent QM/MM MD sampling*.

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

Software name	Classification	Version
Amber	structure solution	11
Amber	refinement	11
Amber	geometry optimization	11

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	1
Total number of shifts	730
Number of shifts mapped to atoms	671
Number of unparsed shifts	0
Number of shifts with mapping errors	59
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	26%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.3.3 RNA [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.5 Carbohydrates [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.6 Ligand geometry [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.7 Other polymers [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 26% for the well-defined parts and 25% 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

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	730
Number of shifts mapped to atoms	671
Number of unparsed shifts	0
Number of shifts with mapping errors	59
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 59 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	2	ALA	CA	51.528	0.400	1
1	A	2	ALA	CB	18.91	0.400	1
1	A	3	GLU	H	8.66	0.020	1
1	A	3	GLU	C	176.132	0.400	1
1	A	3	GLU	CA	59.126	0.400	1
1	A	3	GLU	CB	28.842	0.400	1
1	A	3	GLU	N	120.962	0.400	1
1	A	4	GLN	H	8.442	0.020	1
1	A	4	GLN	HE21	7.414	0.020	2
1	A	4	GLN	HE22	6.798	0.020	2
1	A	4	GLN	C	175.591	0.400	1
1	A	4	GLN	CA	55.755	0.400	1
1	A	4	GLN	CB	29.475	0.400	1
1	A	4	GLN	N	122.004	0.400	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	4	GLN	NE2	111.932	0.400	1
1	A	5	TYR	H	8.305	0.020	1
1	A	5	TYR	CA	57.668	0.400	1
1	A	5	TYR	CB	38.067	0.400	1
1	A	5	TYR	N	121.338	0.400	1
1	A	6	SER	H	7.988	0.020	1
1	A	6	SER	C	173.873	0.400	1
1	A	6	SER	CA	57.59	0.400	1
1	A	6	SER	CB	63.618	0.400	1
1	A	6	SER	N	118.236	0.400	1
1	A	7	GLU	H	8.286	0.020	1
1	A	7	GLU	C	175.802	0.400	1
1	A	7	GLU	CA	56.31	0.400	1
1	A	7	GLU	CB	29.88	0.400	1
1	A	7	GLU	N	123.02	0.400	1
1	A	8	ILE	H	8.101	0.020	1
1	A	8	ILE	HD11	0.772	0.020	1
1	A	8	ILE	HD12	0.772	0.020	1
1	A	8	ILE	HD13	0.772	0.020	1
1	A	8	ILE	C	175.128	0.400	1
1	A	8	ILE	CA	60.246	0.400	1
1	A	8	ILE	CB	37.568	0.400	1
1	A	8	ILE	CD1	12.321	0.400	1
1	A	8	ILE	N	121.13	0.400	1
1	A	104	SER	H	8.367	0.020	1
1	A	104	SER	C	174.942	0.400	1
1	A	104	SER	CA	58.258	0.400	1
1	A	104	SER	CB	63.548	0.400	1
1	A	104	SER	N	116.875	0.400	1
1	A	105	GLY	H	8.381	0.020	1
1	A	105	GLY	C	173.181	0.400	1
1	A	105	GLY	CA	45.047	0.400	1
1	A	105	GLY	N	111.32	0.400	1
1	A	106	LEU	H	7.723	0.020	1
1	A	106	LEU	HD11	0.838	0.020	2
1	A	106	LEU	HD12	0.838	0.020	2
1	A	106	LEU	HD13	0.838	0.020	2
1	A	106	LEU	HD21	0.875	0.020	2
1	A	106	LEU	HD22	0.875	0.020	2
1	A	106	LEU	HD23	0.875	0.020	2
1	A	106	LEU	CA	56.233	0.400	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	106	LEU	CB	43.101	0.400	1
1	A	106	LEU	CD1	23.405	0.400	1
1	A	106	LEU	CD2	25.12	0.400	1
1	A	106	LEU	N	127.393	0.400	1

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	105	-0.37 ± 0.17	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	96	0.50 ± 0.16	None needed (< 0.5 ppm)
$^{13}\text{C}'$	100	-0.58 ± 0.14	Should be applied
^{15}N	103	0.59 ± 0.45	None needed (imprecise)

7.1.3 Completeness of resonance assignments ⓘ

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 26%, i.e. 631 atoms were assigned a chemical shift out of a possible 2465. 0 out of 38 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	348/872 (40%)	87/351 (25%)	174/348 (50%)	87/173 (50%)
Sidechain	283/1425 (20%)	150/937 (16%)	127/439 (29%)	6/49 (12%)
Aromatic	0/168 (0%)	0/90 (0%)	0/62 (0%)	0/16 (0%)
Overall	631/2465 (26%)	237/1378 (17%)	301/849 (35%)	93/238 (39%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 25%, i.e. 671 atoms were assigned a chemical shift out of a possible 2672. 0 out of 38 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	376/952 (39%)	94/384 (24%)	188/380 (49%)	94/188 (50%)
Sidechain	295/1552 (19%)	154/1014 (15%)	133/478 (28%)	8/60 (13%)
Aromatic	0/168 (0%)	0/90 (0%)	0/62 (0%)	0/16 (0%)
Overall	671/2672 (25%)	248/1488 (17%)	321/920 (35%)	102/264 (39%)

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:

