



Full wwPDB NMR Structure Validation Report ⓘ

Dec 19, 2016 – 02:59 PM EST

PDB ID : 1TTX
Title : Solution Structure of human beta parvalbumin (oncomodulin) refined with a paramagnetism based strategy
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Deposited on : 2004-06-23

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	:	NOT EXECUTED
NmrClust	:	NOT EXECUTED
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	NOT EXECUTED
PANAV	:	NOT EXECUTED
ShiftChecker	:	NOT EXECUTED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

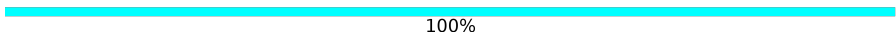
The overall completeness of chemical shifts assignment was not calculated.

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

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	109	 100%

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. The atoms present in the NMR models are not consistent. Some calculations may have failed as a result. All residues are included in the validation scores.

Cyrange was unable to find well-defined residues.

Error message: Cyrange did not run

NmrClust was unable to cluster the ensemble.

Error message: NmrClust did not run

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 1655 atoms, of which 799 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Oncomodulin.

Mol	Chain	Residues	Atoms						Trace
1	A	109	Total	C	H	N	O	S	0
			1653	528	799	137	184	5	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	ARG	GLN	ENGINEERED	UNP P32930

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

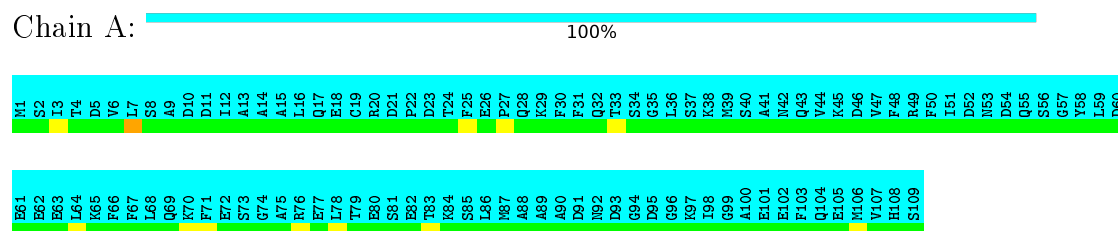
Mol	Chain	Residues	Atoms	
2	A	2	Total	Ca
			2	2

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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: Oncomodulin

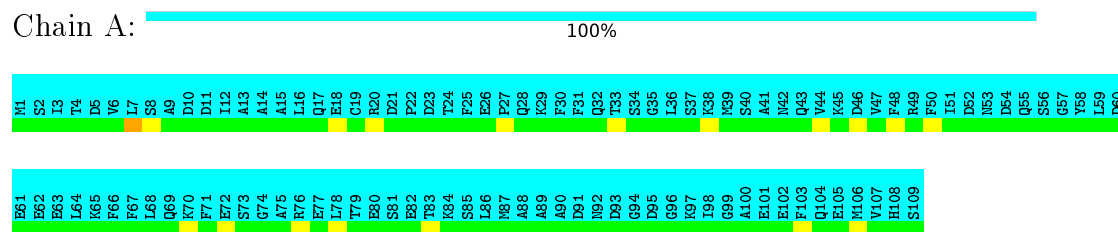


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

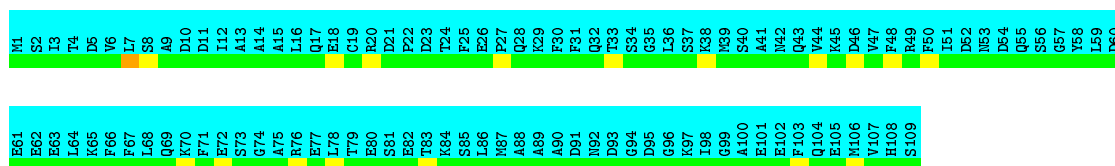
- Molecule 1: Oncomodulin



4.2.2 Score per residue for model 2

- Molecule 1: Oncomodulin

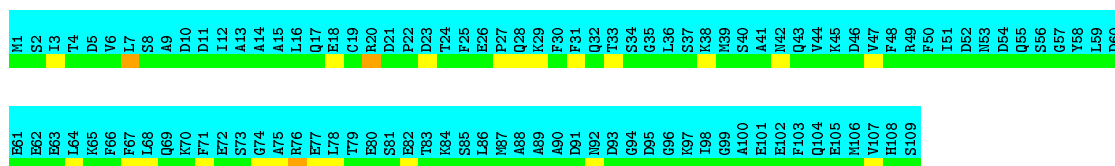




4.2.3 Score per residue for model 3

- Molecule 1: Oncomodulin

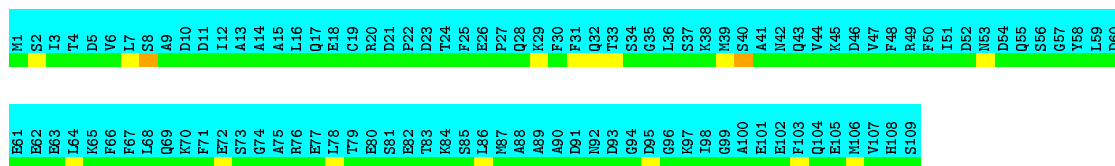
Chain A:  100%



4.2.4 Score per residue for model 4

- Molecule 1: Oncomodulin

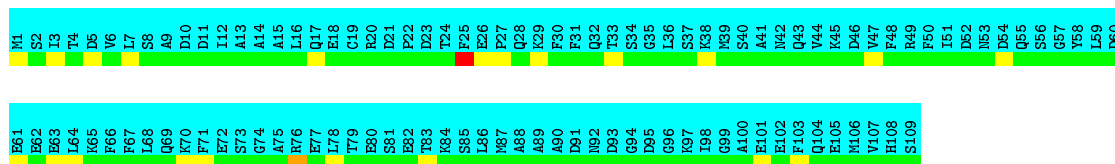
Chain A:  100%



4.2.5 Score per residue for model 5

- Molecule 1: Oncomodulin

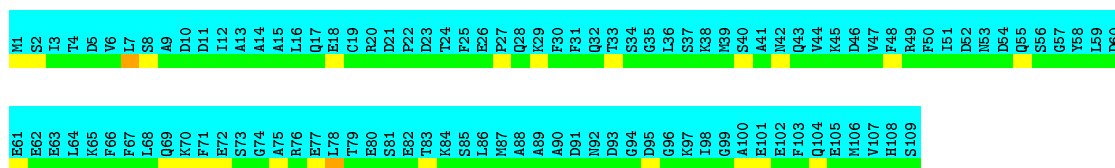
Chain A:  100%



4.2.6 Score per residue for model 6

- Molecule 1: Oncomodulin

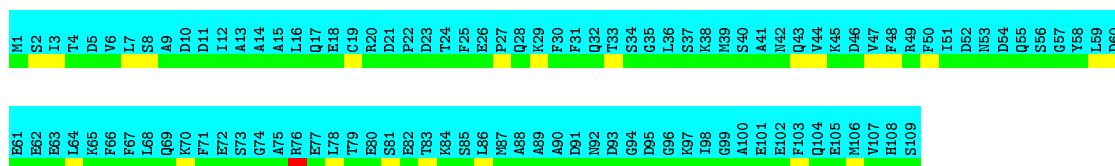
Chain A:  100%



4.2.7 Score per residue for model 7

- Molecule 1: Oncomodulin

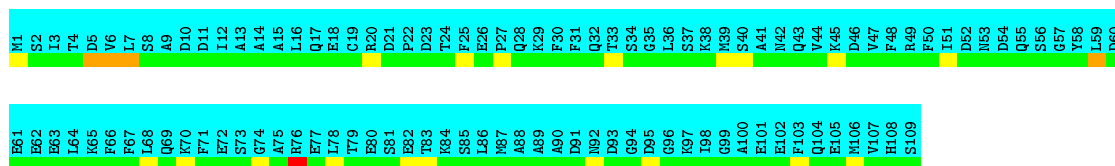
Chain A:  100%



4.2.8 Score per residue for model 8

- Molecule 1: Oncomodulin

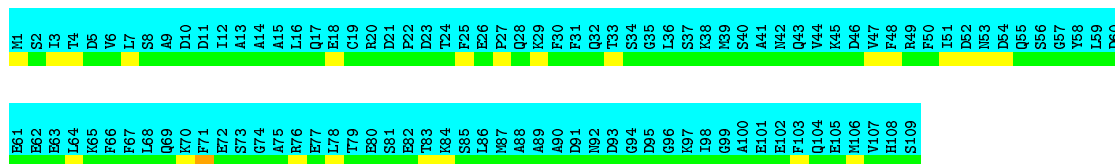
Chain A:  100%



4.2.9 Score per residue for model 9

- Molecule 1: Oncomodulin

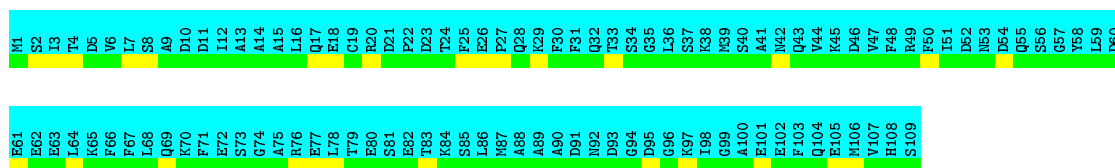
Chain A:  100%



4.2.10 Score per residue for model 10

- Molecule 1: Oncomodulin

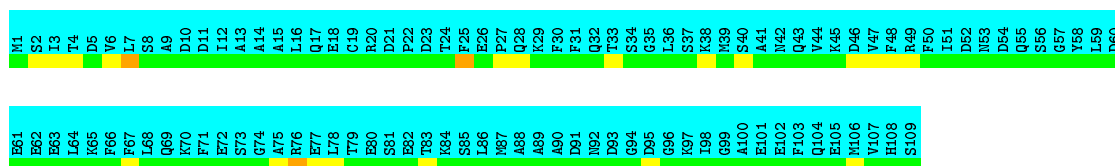
Chain A:  100%



4.2.11 Score per residue for model 11

- Molecule 1: Oncomodulin

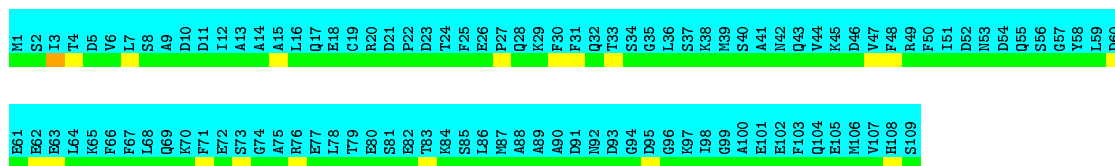
Chain A:  100%



4.2.12 Score per residue for model 12

- Molecule 1: Oncomodulin

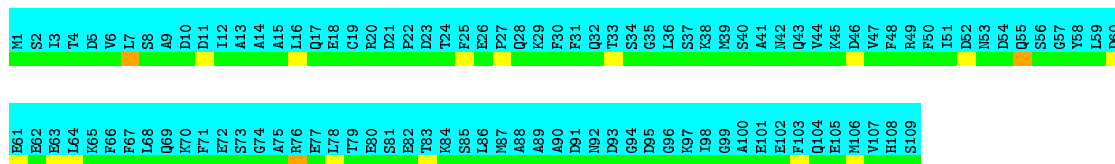
Chain A:  100%



4.2.13 Score per residue for model 13

- Molecule 1: Oncomodulin

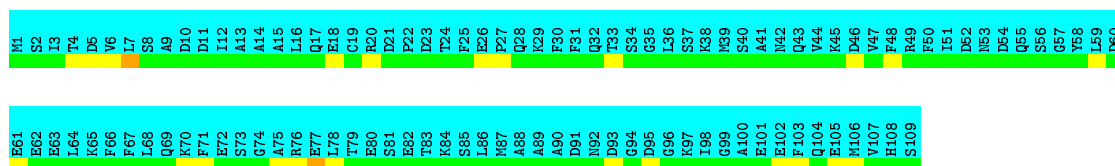
Chain A:  100%



4.2.14 Score per residue for model 14

- Molecule 1: Oncomodulin

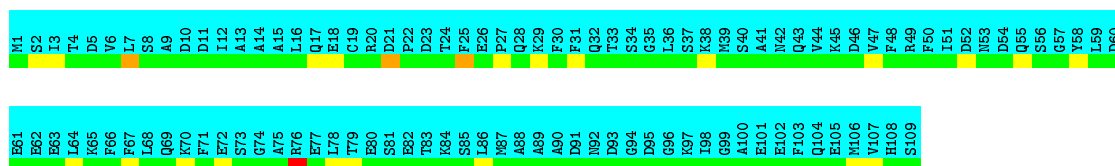
Chain A:  100%



4.2.15 Score per residue for model 15

- Molecule 1: Oncomodulin

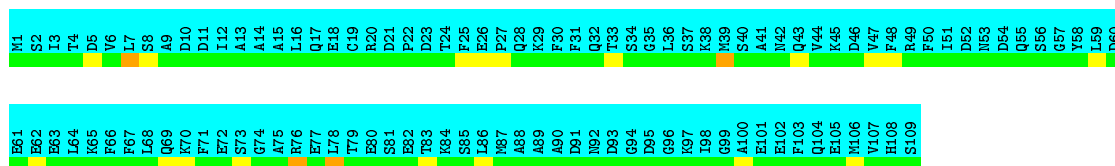
Chain A: 100%



4.2.16 Score per residue for model 16

- Molecule 1: Oncomodulin

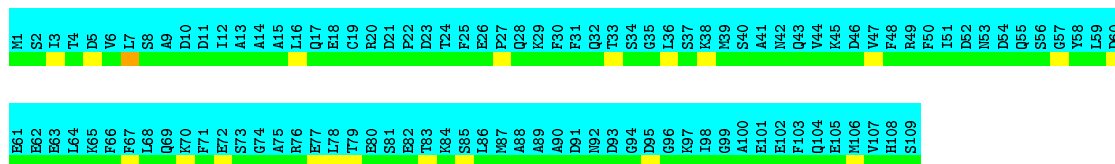
Chain A: 100%



4.2.17 Score per residue for model 17

- Molecule 1: Oncomodulin

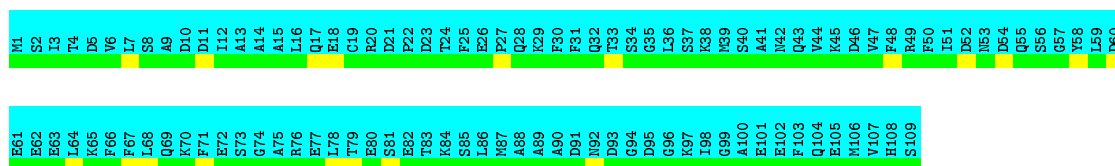
Chain A: 100%



4.2.18 Score per residue for model 18

- Molecule 1: Oncomodulin

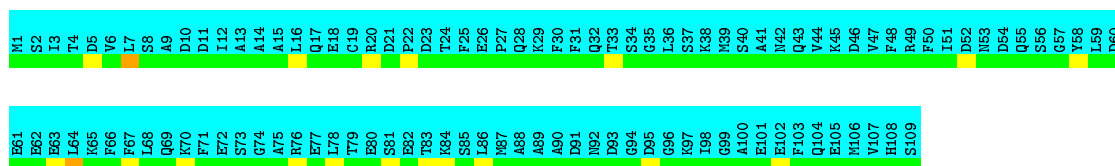
Chain A: 100%



4.2.19 Score per residue for model 19

- Molecule 1: Oncomodulin

Chain A:  100%



4.2.20 Score per residue for model 20

- Molecule 1: Oncomodulin

Chain A:  100%



5 Refinement protocol and experimental data overview

The models were refined using the following method: *distance geometry simulated annealing torsion angle dynamics; pseudocontact shifts residual dipolar couplings*;

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
DYANA	structure solution	1.5
AMBER	refinement	5

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:
CA

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 [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	0	0	0	0±0
All	All	40	0	0	-

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	0	-	-	-	-
All	All	0	-	-	-	-

There are no Ramachandran outliers.

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	0	-	-	-
All	All	0	-	-	-

There are no protein residues with a non-rotameric sidechain to report.

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

6.7 Other polymers ⓘ

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