



# wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 6GDL  
BMRB ID : 34263  
Title : Calmodulin mutant - F141L apo-form Unstructured C-domain  
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This is a wwPDB NMR Structure Validation Summary Report for a publicly released PDB entry.

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The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
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) : 2.37.1

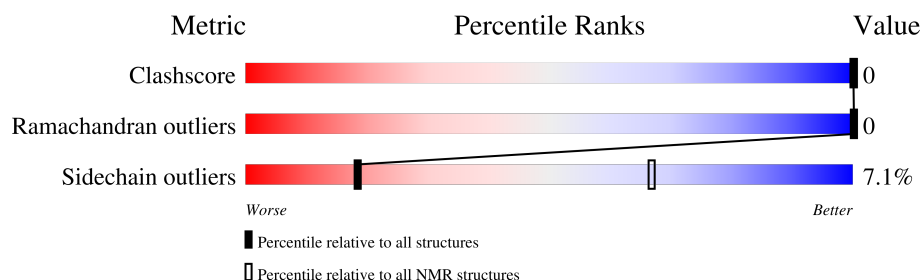
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 92%.

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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  $\geq 3$ , 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	148	

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:5-A:75 (71)	1.15	1

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 3 clusters and 3 single-model clusters were found.

Cluster number	Models
1	1, 3, 4, 5, 6, 7, 8, 13, 14, 15, 17, 20
2	2, 11, 18
3	12, 19
Single-model clusters	9; 10; 16

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1198 atoms, of which 586 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms						Trace
1	A	79	Total	C	H	N	O	S	0
			1198	377	586	97	133	5	

There is a discrepancy between the modelled and reference sequences:

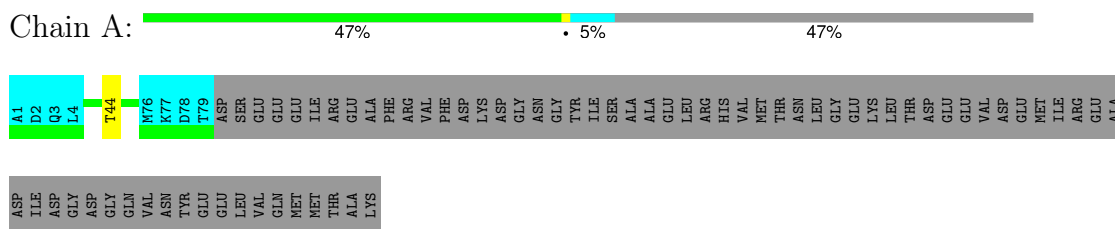
Chain	Residue	Modelled	Actual	Comment	Reference
A	141	LEU	PHE	engineered mutation	UNP P0DP23

## 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.

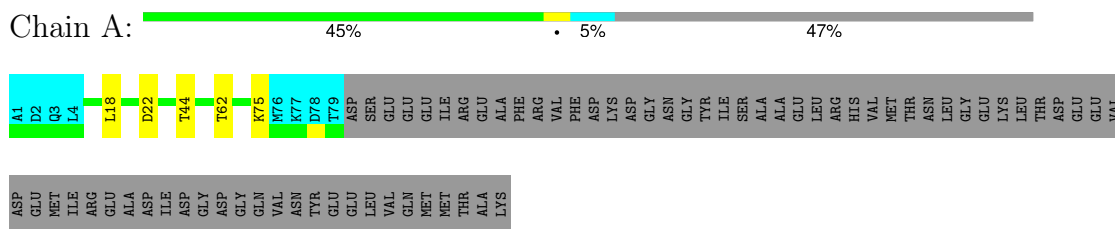
- Molecule 1: Calmodulin-1



### 4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 1. Colouring as in section 4.1 above.

- Molecule 1: Calmodulin-1



## 5 Refinement protocol and experimental data overview

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

Of the 100 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
YASARA	refinement	18.2.7
CYANA	structure calculation	3.97

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	1107
Number of shifts mapped to atoms	938
Number of unparsed shifts	0
Number of shifts with mapping errors	169
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	92%

## 6 Model quality [i](#)

### 6.1 Standard geometry [i](#)

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	550	523	523	0±0
All	All	11000	10460	10460	1

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 0.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:6:GLU:H	1:A:6:GLU:CD	0.44	2.16	15	1

### 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	71/148 (48%)	70±1 (99±1%)	1±1 (1±1%)	0±0 (0±0%)	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1420/2960 (48%)	1401 (99%)	19 (1%)	0 (0%)	100	100

There are no Ramachandran outliers.

### 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	60/126 (48%)	56±1 (93±2%)	4±1 (7±2%)	18	67
All	All	1200/2520 (48%)	1115 (93%)	85 (7%)	18	67

5 of 32 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	44	THR	19
1	A	75	LYS	6
1	A	62	THR	4
1	A	26	THR	4
1	A	34	THR	4

### 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 monosaccharides in this entry.



## 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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

The completeness of assignment taking into account all chemical shift lists is 92% for the well-defined parts and 92% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: *assigned\_chem\_shift\_list*

#### 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	1107
Number of shifts mapped to atoms	938
Number of unparsed shifts	0
Number of shifts with mapping errors	169
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. First 5 (of 169) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	80	ASP	H	8.477	0.002	1
1	A	80	ASP	N	124.597	0.032	1
1	A	134	GLY	H	8.603	0.003	1
1	A	134	GLY	N	110.635	0.025	1
1	A	131	ASP	H	8.578	0.003	1
1	A	131	ASP	N	124.784	0.049	1
1	A	129	ASP	H	8.367	0.003	1
1	A	129	ASP	N	121.341	0.052	1
1	A	114	GLU	H	8.186	0.004	1
1	A	114	GLU	N	121.384	0.052	1
1	A	132	GLY	H	8.283	0.002	1
1	A	132	GLY	N	109.312	0.034	1
1	A	81	SER	H	8.462	0.002	1
1	A	81	SER	N	118.499	0.027	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	130	ILE	H	7.919	0.003	1
1	A	130	ILE	N	122.284	0.047	1
1	A	113	GLY	H	8.179	0.004	1
1	A	113	GLY	N	109.455	0.031	1
1	A	96	GLY	H	8.051	0.005	1
1	A	96	GLY	N	111.35	0.037	1
1	A	133	ASP	H	8.354	0.003	1
1	A	133	ASP	N	120.997	0.041	1
1	A	135	GLN	H	8.337	0.005	1
1	A	135	GLN	N	121.128	0.039	1
1	A	148	LYS	H	7.773	0.004	1
1	A	148	LYS	N	127.054	0.035	1
1	A	82	GLU	H	8.459	0.003	1
1	A	82	GLU	N	123.324	0.023	1
1	A	115	LYS	H	8.258	0.003	1
1	A	115	LYS	N	121.792	0.05	1
1	A	134	GLY	C	174.173	0.004	1
1	A	81	SER	C	175.403	0.004	1
1	A	112	LEU	C	177.663	0.003	1
1	A	128	ALA	C	177.281	0.002	1
1	A	113	GLY	C	174.694	0.004	1
1	A	130	ILE	C	176.765	0.004	1
1	A	114	GLU	C	176.305	0.003	1
1	A	129	ASP	C	175.886	0.003	1
1	A	147	ALA	C	176.766	0.004	1
1	A	132	GLY	C	174.585	0.007	1
1	A	133	ASP	C	176.926	0.004	1
1	A	131	ASP	C	177.68	0.004	1
1	A	80	ASP	C	176.848	0.002	1
1	A	128	ALA	H	7.698	0.006	1
1	A	128	ALA	N	123.446	0.033	1
1	A	107	HIS	CB	29.394	0.058	1
1	A	147	ALA	H	7.695	0.006	1
1	A	147	ALA	N	127.288	0.014	1
1	A	146	THR	H	7.764	0.007	1
1	A	146	THR	N	111.883	0.046	1
1	A	95	ASP	H	8.604	0.002	1
1	A	95	ASP	N	118.035	.	1
1	A	81	SER	CA	59.835	0.061	1
1	A	81	SER	CB	63.617	0.037	1
1	A	80	ASP	CB	41.242	0.001	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	80	ASP	CA	54.779	0.047	1
1	A	147	ALA	CB	19.092	0.043	1
1	A	147	ALA	CA	52.798	0.02	1
1	A	146	THR	CB	69.825	0.046	1
1	A	146	THR	CA	62.355	0.072	1
1	A	148	LYS	CB	33.692	0.062	1
1	A	135	GLN	CA	55.083	0.001	1
1	A	133	ASP	CA	53.898	0.021	1
1	A	133	ASP	CB	41.488	0.013	1
1	A	132	GLY	CA	46.361	0.006	1
1	A	131	ASP	CB	41.34	0.01	1
1	A	131	ASP	CA	53.793	0.009	1
1	A	130	ILE	CA	61.208	0.059	1
1	A	130	ILE	CB	39.263	0.029	1
1	A	129	ASP	CB	40.699	0.038	1
1	A	129	ASP	CA	54.359	0.021	1
1	A	128	ALA	CA	52.599	0.074	1
1	A	128	ALA	CB	19.503	0.059	1
1	A	114	GLU	CB	29.661	0.02	1
1	A	114	GLU	CA	56.567	0.037	1
1	A	115	LYS	CB	32.71	.	1
1	A	115	LYS	CA	56.7	0.019	1
1	A	113	GLY	CA	46.175	0.021	1
1	A	82	GLU	CA	59.141	.	1
1	A	80	ASP	HA	4.706	0.004	1
1	A	80	ASP	HB2	2.795	0.008	2
1	A	80	ASP	HB3	2.745	0.006	2
1	A	81	SER	HA	4.418	0.007	1
1	A	81	SER	HB2	4.036	0.002	2
1	A	81	SER	HB3	3.968	0.005	2
1	A	95	ASP	HA	4.757	0.003	1
1	A	95	ASP	HB2	2.782	.	2
1	A	95	ASP	HB3	2.747	.	2
1	A	112	LEU	HA	4.35	0.005	1
1	A	112	LEU	HB2	1.75	0.005	2
1	A	112	LEU	HB3	1.602	0.003	2
1	A	113	GLY	HA2	3.96	.	2
1	A	113	GLY	HA3	3.928	0.02	2
1	A	114	GLU	HA	4.294	0.003	1
1	A	114	GLU	HB2	2.094	0.005	2
1	A	114	GLU	HB3	1.936	0.006	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	127	GLU	HA	4.206	0.007	1
1	A	128	ALA	HB1	1.417	0.006	1
1	A	128	ALA	HB2	1.417	0.006	1
1	A	128	ALA	HB3	1.417	0.006	1
1	A	128	ALA	HA	4.307	0.005	1
1	A	129	ASP	HA	4.674	0.005	1
1	A	129	ASP	HB2	2.848	0.007	2
1	A	129	ASP	HB3	2.619	0.004	2
1	A	130	ILE	HA	4.428	0.007	1
1	A	130	ILE	HB	1.857	0.006	1
1	A	131	ASP	HA	4.732	0.005	1
1	A	131	ASP	HB2	2.832	.	2
1	A	131	ASP	HB3	2.652	.	2
1	A	132	GLY	HA2	3.969	0.008	2
1	A	132	GLY	HA3	3.922	0.009	2
1	A	133	ASP	HA	4.8	0.005	1
1	A	133	ASP	HB2	2.795	.	2
1	A	133	ASP	HB3	2.683	.	2
1	A	134	GLY	HA2	4.128	0.002	2
1	A	134	GLY	HA3	3.803	0.01	2
1	A	147	ALA	HA	4.385	0.003	1
1	A	147	ALA	HB1	1.46	0.003	1
1	A	147	ALA	HB2	1.46	0.003	1
1	A	147	ALA	HB3	1.46	0.003	1
1	A	146	THR	HA	4.348	0.009	1
1	A	146	THR	HB	4.346	0.01	1
1	A	148	LYS	CA	57.595	0.016	1
1	A	134	GLY	CA	45.872	0.05	1
1	A	135	GLN	CB	30.576	.	1
1	A	112	LEU	CA	55.35	0.018	1
1	A	112	LEU	CB	42.699	0.038	1
1	A	95	ASP	CA	54.365	0.041	1
1	A	96	GLY	CA	46.838	0.012	1
1	A	95	ASP	CB	41.162	0.01	1
1	A	148	LYS	C	181.488	0.0	1
1	A	135	GLN	C	175.09	0.0	1
1	A	115	LYS	C	176.237	0.0	1
1	A	96	GLY	C	175.162	0.0	1
1	A	95	ASP	C	176.848	0.004	1
1	A	130	ILE	CG1	27.265	0.031	1
1	A	130	ILE	CG2	17.507	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	130	ILE	CD1	13.361	0.025	1
1	A	127	GLU	CB	29.736	.	1
1	A	127	GLU	CA	57.182	0.051	1
1	A	114	GLU	CG	35.941	0.039	1
1	A	114	GLU	HG2	2.269	0.0	2
1	A	114	GLU	HG3	2.283	0.005	2
1	A	130	ILE	HG12	1.138	0.01	2
1	A	130	ILE	HG13	1.542	0.005	2
1	A	130	ILE	HG22	0.956	.	1
1	A	130	ILE	HG21	0.956	.	1
1	A	130	ILE	HG23	0.956	.	1
1	A	130	ILE	HD11	0.868	0.008	1
1	A	130	ILE	HD13	0.868	0.008	1
1	A	130	ILE	HD12	0.868	0.008	1
1	A	146	THR	HG23	1.253	0.003	1
1	A	146	THR	HG22	1.253	0.003	1
1	A	146	THR	HG21	1.253	0.003	1
1	A	146	THR	CG2	21.7	0.029	1
1	A	112	LEU	HD11	0.799	0.002	2
1	A	112	LEU	HD12	0.799	0.002	2
1	A	112	LEU	HD13	0.799	0.002	2
1	A	148	LYS	HA	4.176	.	1
1	A	112	LEU	CD1	26.228	0.033	2
1	A	112	LEU	HD21	0.785	.	2
1	A	112	LEU	HD22	0.785	.	2
1	A	112	LEU	HD23	0.785	.	2
1	A	112	LEU	CD2	23.178	.	2
1	A	107	HIS	HB2	3.287	.	2
1	A	107	HIS	HB3	3.145	.	2
1	A	148	LYS	HB2	1.872	0.0	2
1	A	148	LYS	HB3	1.753	0.001	2
1	A	115	LYS	HA	4.246	.	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
$^{13}\text{C}_\alpha$	100	$-0.30 \pm 0.08$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	90	$0.13 \pm 0.07$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	97	$-0.47 \pm 0.16$	None needed ( $< 0.5$ ppm)

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Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{15}\text{N}$	95	-0.63 $\pm$ 0.27	Should be applied

### 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 92%, i.e. 847 atoms were assigned a chemical shift out of a possible 921. 0 out of 7 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	357/357 (100%)	146/146 (100%)	142/142 (100%)	69/69 (100%)
Sidechain	450/514 (88%)	306/330 (93%)	144/168 (86%)	0/16 (0%)
Aromatic	40/50 (80%)	22/25 (88%)	18/25 (72%)	0/0 (—%)
Overall	847/921 (92%)	474/501 (95%)	304/335 (91%)	69/85 (81%)

### 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:

