



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 2K0F
Title : Calmodulin complexed with calmodulin-binding peptide from smooth muscle myosin light chain kinase
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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 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
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : trunk30686
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

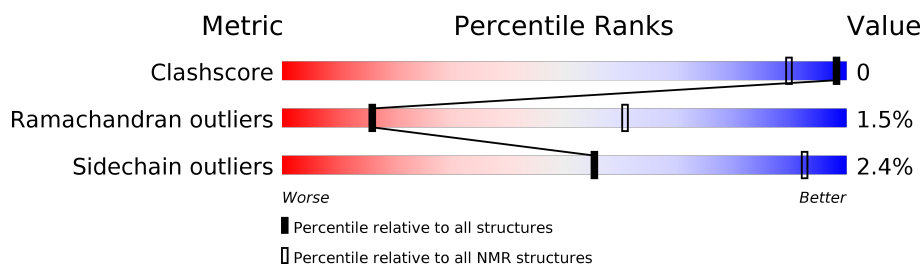
1 Overall quality at a glance

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	136279	12091
Ramachandran outliers	132675	10835
Sidechain outliers	132484	10811

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	148	 84% 11% . .
2	B	19	 63% 21% 16%

2 Ensemble composition and analysis

This entry contains 160 models. Model 54 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

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:3-A:142, B:1-B:16 (156)	0.80	54

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 13 clusters and 7 single-model clusters were found.

Cluster number	Models
1	2, 4, 6, 7, 8, 11, 12, 14, 16, 18, 20, 22, 24, 28, 29, 30, 31, 32, 34, 36, 38, 40, 42, 44, 45, 46, 50, 52, 54, 56, 60, 61, 66, 70, 74, 76, 82, 86, 88, 92, 98, 102, 104, 105, 106, 108, 114, 116, 118, 120, 121, 122, 124, 126, 130, 132, 134, 135, 136, 138, 140, 142, 148, 152, 154, 156, 158, 159
2	1, 3, 9, 15, 17, 21, 23, 25, 27, 33, 37, 39, 41, 43, 53, 57, 59, 63, 69, 72, 75, 77, 79, 85, 87, 93, 95, 101, 109, 111, 117, 119, 125, 127, 133, 141, 143, 149
3	26, 62, 78, 80, 84, 96, 100, 112, 128, 144, 160
4	35, 47, 51, 67, 83, 99, 115, 131, 147
5	49, 65, 81, 97, 113, 129, 145
6	5, 13, 19, 110
7	55, 71, 103
8	58, 90, 94
9	139, 155
10	91, 107
11	137, 153
12	48, 64
13	68, 150
Single-model clusters	10; 73; 89; 123; 146; 151; 157

3 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2494 atoms, of which 1213 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called calmodulin.

Mol	Chain	Residues	Atoms						Trace
1	A	142	Total	C	H	N	O	S	0
			2168	687	1047	180	245	9	

- Molecule 2 is a protein called 19-mer peptide from Myosin light chain kinase.

Mol	Chain	Residues	Atoms					Trace
2	B	19	Total	C	H	N	O	0
			322	95	166	37	24	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	9	HIS	ASN	ENGINEERED	UNP Q15746

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

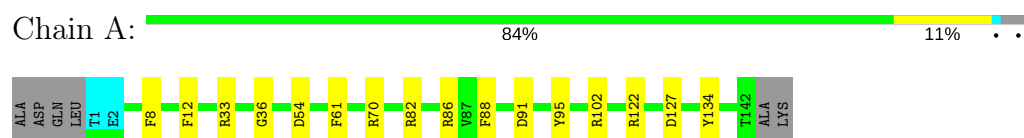
Mol	Chain	Residues	Atoms	
3	A	4	Total	Ca
			4	4

4 Residue-property plots [i](#)

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: calmodulin



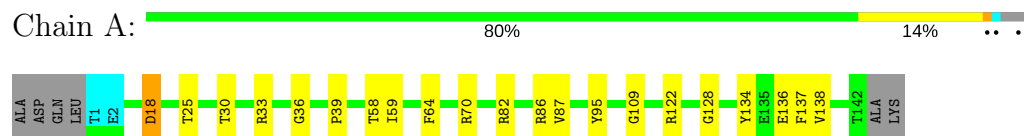
- Molecule 2: 19-mer peptide from Myosin light chain kinase



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

The representative model is number 54. Colouring as in section 4.1 above.

- Molecule 1: calmodulin



- Molecule 2: 19-mer peptide from Myosin light chain kinase



5 Refinement protocol and experimental data overview

The models were refined using the following method: *CHARMM*.

Of the 160 calculated structures, 160 were deposited, based on the following criterion: *all calculated structures submitted*.

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

Software name	Classification	Version
CHARMM	refinement	C30

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

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	0.97±0.00	0±0/1117 (0.0±0.0%)	1.97±0.07	28±5/1499 (1.9±0.4%)
2	B	1.26±0.00	0±0/138 (0.0±0.0%)	2.24±0.22	5±2/183 (3.0±1.1%)
All	All	1.00	0/200800 (0.0%)	2.00	5351/269120 (2.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	2.7±1.3
2	B	0.0±0.0	1.2±1.0
All	All	0	631

There are no bond-length outliers.

5 of 692 unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	70	ARG	NE-CZ-NH2	-26.19	107.20	120.30	152	58
1	A	33	ARG	NE-CZ-NH1	24.27	132.44	120.30	88	91
1	A	88	PHE	CB-CG-CD2	20.29	135.00	120.80	6	48
2	B	1	ARG	NE-CZ-NH2	-20.05	110.28	120.30	103	66
1	A	70	ARG	NE-CZ-NH1	18.75	129.67	120.30	7	78

There are no chirality outliers.

5 of 43 unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
2	B	12	ARG	Sidechain	52
2	B	16	ARG	Sidechain	50
2	B	2	ARG	Sidechain,Peptide	47
1	A	33	ARG	Sidechain	47
1	A	95	TYR	Sidechain	40

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	1105	1035	1035	1±1
2	B	135	145	148	0±0
All	All	199040	188800	189279	103

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.

5 of 83 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:51:VAL:HG21	1:A:59:ILE:HD12	0.71	1.62	39	1
1:A:8:PHE:CD2	1:A:65:LEU:HD22	0.60	2.31	139	1
1:A:28:LEU:HD23	1:A:44:LEU:HD13	0.57	1.76	13	1
1:A:28:LEU:HD23	1:A:44:LEU:HD11	0.56	1.76	76	1
1:A:90:LYS:HD2	1:A:103:HIS:CD2	0.56	2.36	22	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	139/148 (94%)	128±3 (92±2%)	9±3 (6±2%)	2±2 (2±1%)	15	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	15/19 (79%)	14±1 (95±6%)	1±1 (4±5%)	0±0 (0±1%)	47	81
All	All	24640/26720 (92%)	22755 (92%)	1511 (6%)	374 (2%)	16	61

5 of 35 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	36	GLY	112
1	A	128	GLY	55
1	A	109	GLY	40
1	A	21	GLY	30
1	A	127	ASP	24

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	120/126 (95%)	117±2 (98±1%)	3±2 (2±1%)	54	92
2	B	12/15 (80%)	12±0 (98±4%)	0±0 (2±4%)	63	94
All	All	21120/22560 (94%)	20609 (98%)	511 (2%)	55	92

5 of 99 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	91	ASP	36
1	A	127	ASP	33
1	A	54	ASP	31
1	A	59	ILE	27
1	A	18	ASP	24

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 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 [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided