



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 2K0E
Title : A Coupled Equilibrium Shift Mechanism in Calmodulin-Mediated Signal Transduction
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This is a wwPDB NMR Structure Validation Summary Report for a publicly released PDB entry.

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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

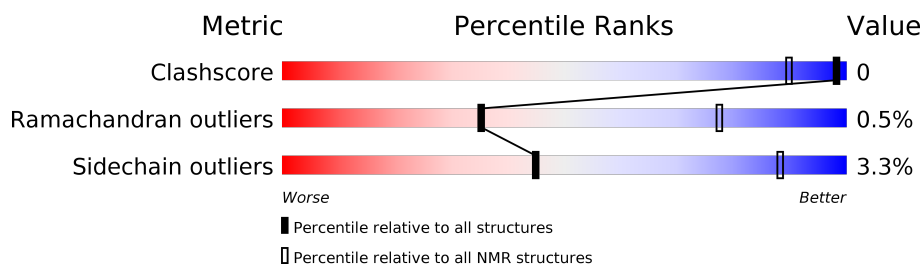
1 Overall quality at a glance

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	<div> <div></div> <div>79%</div> <div>10%</div> <div>11%</div> </div>

2 Ensemble composition and analysis

This entry contains 160 models. Model 157 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:5-A:73 (69)	0.63	157
2	A:83-A:145 (63)	0.70	2

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 24 clusters and 5 single-model clusters were found.

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

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2263 atoms, of which 1093 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Calmodulin.

Mol	Chain	Residues	Atoms						Trace
1	A	148	Total	C	H	N	O	S	0
			2259	714	1093	188	255	9	

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

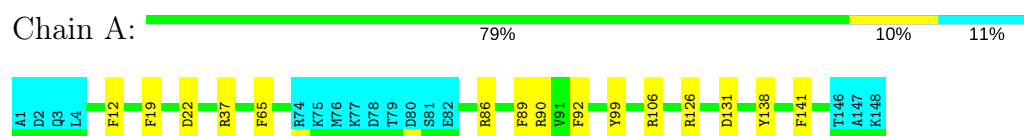
Mol	Chain	Residues	Atoms	
2	A	4	Total	Ca
			4	4

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.

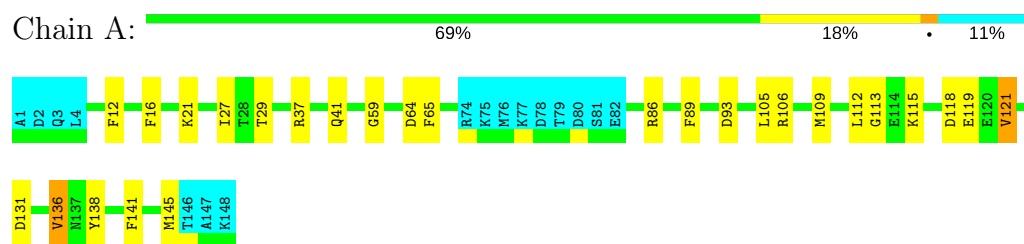
- Molecule 1: Calmodulin



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

The representative model is number 157. Colouring as in section 4.1 above.

- Molecule 1: Calmodulin



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	0.96±0.00	0±0/1052 (0.0±0.0%)	1.99±0.06	28±5/1416 (2.0±0.3%)
All	All	0.96	0/168320 (0.0%)	1.99	4451/226560 (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	2.8±1.4
All	All	0	449

There are no bond-length outliers.

5 of 577 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	37	ARG	NE-CZ-NH1	20.87	130.74	120.30	84	84
1	A	86	ARG	NE-CZ-NH1	20.51	130.56	120.30	102	76
1	A	106	ARG	NE-CZ-NH1	19.68	130.14	120.30	128	87
1	A	86	ARG	NE-CZ-NH2	-18.57	111.02	120.30	5	67
1	A	37	ARG	NE-CZ-NH2	-18.40	111.10	120.30	34	73

There are no chirality outliers.

5 of 40 unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	138	TYR	Sidechain	75

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	126	ARG	Sidechain	53
1	A	37	ARG	Sidechain	45
1	A	99	TYR	Sidechain,Mainchain	44
1	A	106	ARG	Sidechain	38

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	1039	967	967	1±1
All	All	166880	154720	154720	87

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:92:PHE:HA	1:A:108:VAL:HG21	0.70	1.63	38	2
1:A:85:ILE:HD12	1:A:142:VAL:HG13	0.62	1.68	40	1
1:A:104:GLU:O	1:A:108:VAL:HG23	0.61	1.95	131	4
1:A:138:TYR:O	1:A:142:VAL:HG23	0.59	1.98	41	13
1:A:83:GLU:CD	1:A:86:ARG:HH21	0.57	2.02	5	2

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	132/148 (89%)	127±2 (96±2%)	5±2 (3±2%)	1±1 (0±1%)	35	77
All	All	21120/23680 (89%)	20294 (96%)	730 (3%)	96 (0%)	35	77

5 of 20 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	113	GLY	47
1	A	98	GLY	9
1	A	56	ASP	7
1	A	132	GLY	6
1	A	131	ASP	4

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	112/126 (89%)	108±2 (97±2%)	4±2 (3±2%)	45 88
All	All	17920/20160 (89%)	17337 (97%)	583 (3%)	45 88

5 of 82 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	22	ASP	53
1	A	85	ILE	46
1	A	131	ASP	33
1	A	27	ILE	31
1	A	26	THR	24

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 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