



wwPDB NMR Structure Validation Summary Report ⓘ

Mar 7, 2026 – 03:50 AM UTC

PDB ID : 8DGK / pdb_00008dgk
BMRB ID : 51222
Title : NMR structure of calmodulin bound to N-terminal site in the beta-subunit of cyclic nucleotide-gated channel
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Deposited on : 2022-06-23

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 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 : 4-5-2 with Phenix2.0
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

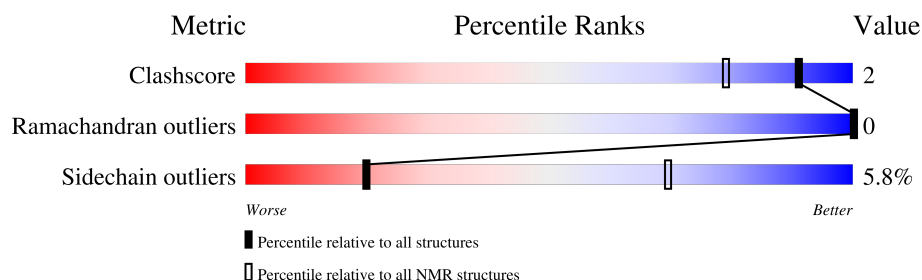
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 57%.

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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	149	
2	B	12	

2 Ensemble composition and analysis

This entry contains 10 models. Model 4 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:9-A:78, B:570-B:575 (76)	0.66	4

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 1 single-model cluster was found.

Cluster number	Models
1	1, 4, 8, 10
2	2, 3, 7
3	5, 9
Single-model clusters	6

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 1405 atoms, of which 693 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms						Trace
1	A	78	Total	C	H	N	O	S	0
			1186	374	579	96	132	5	

- Molecule 2 is a protein called Cyclic nucleotide-gated cation channel beta-1.

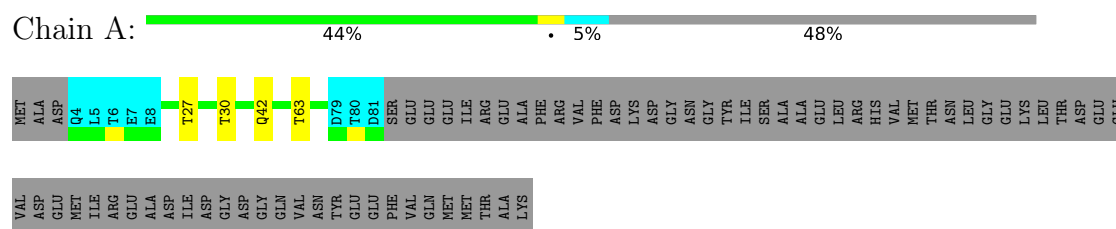
Mol	Chain	Residues	Atoms					Trace
2	B	12	Total	C	H	N	O	0
			219	68	114	19	18	

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



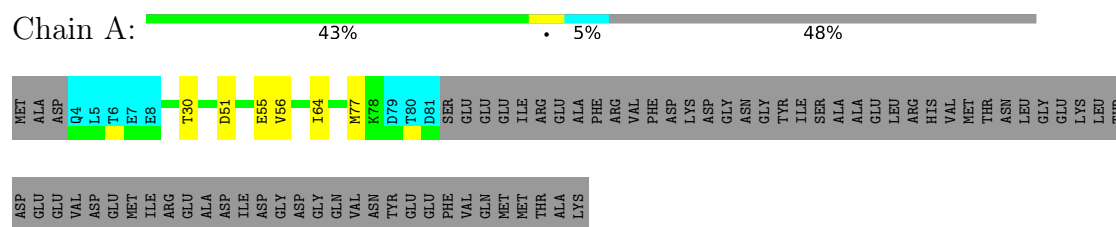
- Molecule 2: Cyclic nucleotide-gated cation channel beta-1



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

The representative model is number 4. Colouring as in section 4.1 above.

- Molecule 1: Calmodulin-1



- Molecule 2: Cyclic nucleotide-gated cation channel beta-1





5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 200 calculated structures, 10 were deposited, based on the following criterion: *structures with acceptable covalent geometry*.

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

Software name	Classification	Version
HADDOCK	refinement	
HADDOCK	structure calculation	

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	678
Number of shifts mapped to atoms	663
Number of unparsed shifts	0
Number of shifts with mapping errors	15
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	57%

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	542	526	526	2±2
2	B	52	59	59	0±0
All	All	5940	5850	5850	19

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 2.

5 of 13 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:ALA:HB2	2:B:571:LEU:HD13	0.56	1.77	3	1
1:A:65:ASP:CG	1:A:67:PRO:HD2	0.53	2.29	8	2
1:A:38:ARG:HA	1:A:42:GLN:O	0.51	2.06	8	3
1:A:27:THR:HA	1:A:64:ILE:O	0.50	2.07	6	2
1:A:42:GLN:O	1:A:44:PRO:HD3	0.46	2.11	5	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	70/149 (47%)	69±0 (99±1%)	1±0 (1±1%)	0±0 (0±0%)	100	100
2	B	6/12 (50%)	6±0 (100±0%)	0±0 (0±0%)	0±0 (0±0%)	100	100
All	All	760/1610 (47%)	753 (99%)	7 (1%)	0 (0%)	100	100

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	59/127 (46%)	55±2 (94±3%)	4±2 (6±3%)	18	67
2	B	6/12 (50%)	6±0 (98±5%)	0±0 (2±5%)	52	92
All	All	650/1390 (47%)	612 (94%)	38 (6%)	20	69

5 of 14 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	63	THR	8
1	A	30	THR	7
1	A	27	THR	5
1	A	77	MET	3
1	A	39	SER	2

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 [i](#)

There are no oligosaccharides 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 57% for the well-defined parts and 55% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chemical_shifts_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	678
Number of shifts mapped to atoms	663
Number of unparsed shifts	0
Number of shifts with mapping errors	15
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 15) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	2	ALA	HA	4.347	0.000	1
1	A	2	ALA	HB1	1.419	0.010	1
1	A	2	ALA	HB2	1.419	0.010	1
1	A	2	ALA	HB3	1.419	0.010	1
1	A	2	ALA	C	176.997	0.000	1
1	A	2	ALA	CA	52.884	0.000	1
1	A	2	ALA	CB	19.098	0.061	1
1	A	3	ASP	H	8.306	0.001	1
1	A	3	ASP	HA	4.662	0.009	1
1	A	3	ASP	HB2	2.724	0.012	2
1	A	3	ASP	HB3	2.582	0.007	2
1	A	3	ASP	C	175.627	0.000	1
1	A	3	ASP	CA	54.75	0.028	1
1	A	3	ASP	CB	41.455	0.011	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	3	ASP	N	118.473	0.068	1

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	72	-0.30 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	65	0.18 ± 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}'$	63	-0.67 ± 0.07	Should be applied
^{15}N	64	0.37 ± 0.27	None needed (< 0.5 ppm)

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 57%, i.e. 581 atoms were assigned a chemical shift out of a possible 1018. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	288/382 (75%)	117/156 (75%)	116/152 (76%)	55/74 (74%)
Sidechain	277/576 (48%)	184/372 (49%)	93/186 (50%)	0/18 (0%)
Aromatic	16/60 (27%)	16/30 (53%)	0/30 (0%)	0/0 (—%)
Overall	581/1018 (57%)	317/558 (57%)	209/368 (57%)	55/92 (60%)

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:

