

# Full wwPDB NMR Structure Validation Report (i)

#### Dec 5, 2022 - 08:02 AM EST

PDB ID	:	8DGH
BMRB ID	:	51447
Title	:	NMR Structure of calmodulin bound to C-terminal site in the beta-subunit of
		cyclic nucleotide-gated channel
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Deposited on	:	2022-06-23

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 https://www.wwpdb.org/validation/2017/NMRValidationReportHelp with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

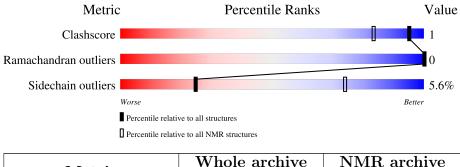
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. $(2010)$
ShiftChecker	:	2.31.2
Ideal geometry (proteins)	:	Engh & Huber $(2001)$
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $SOLUTION\ NMR$ 

The overall completeness of chemical shifts assignment is 68%.

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 $(\# Entries)$	${f NMR} \ {f archive} \ (\#{f Entries})$
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 >=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 <=5%

Mol	Chain	Length	Quality of chain				
1	А	149	44%	••	54%		-
2	В	12	67	%	8%	25%	-



# 2 Ensemble composition and analysis (i)

This entry contains 10 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:84-A:149, B:1128-B:1136	0.30	1				
	(75)						

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 2 clusters and 5 single-model clusters were found.

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



# 3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1271 atoms, of which 625 are hydrogens and 0 are deuteriums.

• Molecule 1 is a protein called Calmodulin-1.

Mol	Chain	Residues		Atoms					Trace
1	Δ	69	Total	С	Η	Ν	0	S	0
	A	68	1051	333	506	90	118	4	0

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

Mol	Chain	Residues		A	toms			Trace
0	В	19	Total	С	Н	Ν	0	0
	D	12	220	65	119	22	14	0

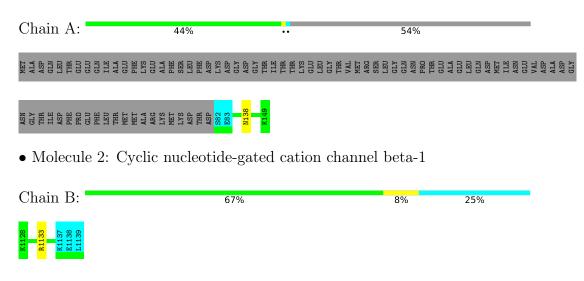


# 4 Residue-property plots (i)

### 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 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 (medoid)



# 

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



Chain I	3: 50%	25%	25%
K1128 L1129 L1132 R1133	K1137 E1138 L1139		
4.2.2	Score per residue for model 2		
• Mole	cule 1: Calmodulin-1		
Chain .	A: 42% ···	54%	
MET ALA ASP GLN LEU	CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU	GLU LEU CLEU CLEU VAL MET ARG SER CLV GLV GLV GLV ASN FIN	GLU GLU GLU CLU CLU CLU CLU CLU CLU ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP
ASN GLY THR ILE ASP	PALE PALE PHE CLU PHE CLU PHE CLU PHE ARG CLY ARG ARG ARG ARG ARG ARG ARG ARG ARG ARG		
• Mole	cule 2: Cyclic nucleotide-gated catio	on channel beta-1	
Chain 1	3: 75%		25%
K1128 K1137 E1138 E1138 L1139			
4.2.3	Score per residue for model 3		
• Mole	cule 1: Calmodulin-1		
Chain .	A: 43% ···	54%	
MET ALA ASP GLN LEU	GLU GLU GLU GLU GLU GLU GLU FHE FHE ALA ASP PHE CVS ASP ASP ASP CLV GLV THR THR THR THR THR THR THR	GLU LEU CLEU CLEU ART ARG SER CLY GLY GLN ASN FRO THR	GLU ALA GLU GLU GLU GLU GLU ASP ASN ASP ASP ASP GLY GLY
ASN GLY THR ILE ASP	Price		
• Mole	cule 2: Cyclic nucleotide-gated catio	on channel beta-1	
Chain 1	3: 75%		25%
K1128 K1137 E1138 E1138			

#### 4.2.4 Score per residue for model 4

• Molecule 1: Calmodulin-1



Chain A:	42%	••	54%		
MET ALA ASP ASP GLN CLN GLU GLU GLU ILE	ALA GLU CLU CLYS CLU CLU ALA ALA PHE CLU CLYS ASP ASP	GLY ASP ASP GLY THR THR THR CLU GLU	GLY THR VAL MET MET ARG SER LEU GLY GLY GLN ASN THR	GLU ALA GLU GLU GLN MET ASP ASP ASN GLU GLU GLU	VAL ASP ALA ASP CT V
ASN GLY THR ILE ASP PHE FRO GLU LEU	THR MET MET ALA ALA ALA LYS LYS LYS ASP ASP B83 B82	D1 19 N1 38 T1 47 A1 48 K1 49			
• Molecule 2:	Cyclic nucleotide	-gated cation	channel beta-1		
Chain B:	58%		17%	25%	
K1128 L1132 R1133 K1137 E1138 L1139					
4.2.5 Score	e per residue fo	r model 5			
• Molecule 1:	Calmodulin-1				
Chain A:	42%		54%		
MET ALA ASP ASP GLU GLU GLU GLU GLU	ALA GLU PHE LYS GLU ALA ALA PHE SER LEU PHE ASP LYS ASP	GLY ASP GLY THR THR THR THR CLU CLU	GLY THR VAL MET ARG SER LEU GLY GLY GLN THR	GLU ALA GLU GLU GLU ASP MET ASN ASN GLU GLU	ASP ASP ASP ASP CI V
ASN GLY THR ILE ASP PHE PHE GLU LEU	THR MET MET ALCA ALCA ALCA ACP LYS LYS ASP ASP SS2 SS2 SS2	L106 M110 N138 K149			
• Molecule 2:	Cyclic nucleotide	-gated cation	channel beta-1		
Chain B:	6	7%	8%	25%	
K1128 R1133 E1137 E1138 L1139					
4.2.6 Score	e per residue for	r model 6			
• Molecule 1:	Calmodulin-1				
Chain A:	40%		54%		
MET ALA ASP ASP GLN GLU GLU GLU ILE	ALA PHE LYS CLV CLYS CLV CLYS CLV CLV PHE PHE PHE PHE CLV ASP ASP	GLY ASP GLY THR THR THR THR LYS GLU LUS	GLY THR VAL MET ARG SER LEU GLY GLY GLY GLN ASN PRO THR	GLU ALA GLU GLU GLU ASP MET ASN ASN GLU GLU	ASP ASP ALA ASP
ASN GLY THR ILE ASP PHE PRO GLU PHE LEU	THR MET MET ALA ALA ARG LYS LYS ASP ASP S82 E83	L106 M110 E121 M125 V137	N138 K149		
• Molecule 2:	Cyclic nucleotide	-gated cation	channel beta-1		



Chain B:		75%		25%
K1128 K1137 E1138 L1139				
4.2.7 S	core per residue for	model 7		
• Molecul	e 1: Calmodulin-1			
Chain A:	40%	5%•	54%	
MET ALA ASP GLN LEU THR GLU	GLU GLU TILE ALA ALA CLU PHE CLU CLU CLU SER PHE SER CLU SHE SER CLU SHE SER CLU	ASP GLY THR ILE LYS GLU CLU GLU CLU GLY VAL	MET ARG SER LEU GLY GLN ASN THR THR CLU	ALA GLU CELU CELU GLU ASP ASP ASP ASP ASP ALA ASP ALA ASP CLY GLY
ASN GLY THR ILE ASP PHE PRO	GLU PHE LEU TTRR MET MET ALA ARG LYS ASP ASP ASP SS2 SS2 SS2	D94 K <mark>65</mark> G97 D123 D132 D132 M145 M145	K149	
• Molecul	e 2: Cyclic nucleotide-	gated cation chan	nel beta-1	
Chain B:	58%		17%	25%
1128 1132 1133 1133 1133 1138	1139			
X 1K XB	а 			
4.2.8 S	core per residue for	model 8		
• Molecul	e 1: Calmodulin-1			
Chain A:	40%		54%	
MET ALA ASP GLN LEU THR GLU	GLU GLN TLE GLN GLU PHE PHE CLU PHE SER ASP ASP ASP ASP	ASP ASP GLY THR THR THR THR LYS GLU CLU CLU CLU CLU VAL	ARG SER LEU GLY GLN ASN PRO FLN GLU	ALA GLU CLEU GLN GLN GLN ASP ASP ALA ASP ALA ASP ALA
ASN GLY THR ILE ASP PHE PRO	GLU THR THR MET MET MET MET LLYS ASP ASP ASP ASP S82 B32 B32	0119 0130 0130 M145 F142 M145	6 <b>7</b> 146	
	e 2: Cyclic nucleotide-	gated cation chan	nel beta-1	
Chain B:	,	75%		25%
33 33 33				2375
4.2.9 S	core per residue for	model 9		

• Molecule 1: Calmodulin-1



Chain A:	42%	••	54%		
MET ALA ALA ALA GLN CLU GLU CLU CLN CLU CLN CLU CLV CLV CLV CLV CLV CLV CLV CLV CLV CLV	ALA PHE SER LEU PHE ASP ASP ASP GLY ASP	GLY THR THR THR THR THR LEU CLU CLU CLU THR	VAL MET ARG SER LEU GLN ASN PRO	THR GLU GLU GLU GLU GLU GLN GLN MET MET ASP ASP ASP ASP	ALA ASP GLY
ASN GLY THR ILE ASP PHE PHE CLU CLU CLU CLU CLU CLU ALA ALA ALA	LYS MET LYS ASP ASP ASP B82 E83 E83 B138 N138	F1 42 F1 43 Q1 44 M1 45 M1 45 K1 49			
• Molecule 2: Cyclic	e nucleotide-ga	ted cation cha	annel beta-1		
Chain B:	50%		25%	25%	
K1128 H1131 L1132 R1133 R1137 E11139 L11139					
4.2.10 Score per	residue for	model 10			
• Molecule 1: Calmo	odulin-1				
Chain A:	40%	••	54%		
MET ALA ASP ASP CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU	ALA PHE SER SER LEU PHE ASP CLY ASP ASP ASP ASP	GLY THR THR THR THR CLY CLY CLY CLY CLY	VAL MET ARG SER LEU GLY GLN ASN	THR GLU GLU GLU GLU GLN GLN MET MET ASP GLU VAL ASP	ALA ASP GLY
ASN MET GLY ALA THR ASP TLE GLN ASP TLE GLN ASP PHE THR PHE CLU GLU CLU GLU MET ALA MET ALA ARG GLU MET PHE		V122 118 123 118 118 118 118 118 118 114 114 114 114	MET MET ARG ARG CLU GLV ASN ASN	THR THR ALM ALM ALM ALM ALM CLU CLU CLU ASN ASN ASN ASN VAL	ALA ASP GLY
	LINS MET LINS ASP ASP ASP ASP B83 B83 B83 B83	V122 D123 N138 N146 N148 X148		THR THR ALA ALA ALA ALA ALA ASN ASN ASN ASN ASN ASN ASN ASN ASN AS	ALA ASP GLY
ASN THR TLE ASP ASP ASP PHE CLU CLU CLU CLU CLU MET MET ARG	LINS MET LINS ASP ASP ASP ASP B83 B83 B83 B83	V122 D123 N138 N146 N148 X148		HHL D D D D D D D D D D D D D D D D D D D	ALA ASP GLY



# 5 Refinement protocol and experimental data overview (i)

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	1450
Number of shifts mapped to atoms	1450
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	68%



# 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	А	530	495	495	1±1
2	В	75	89	88	$0\pm 0$
All	All	6050	5840	5830	12

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 1.

Models Clash(Å) Distance(Å) Atom-1 Atom-2 Total Worst 1:A:94:ASP:OD1 1:A:97:GLY:HA2 0.472.097 1 1:A:142:PHE:O 1:A:145:MET:HG2 2.109 0.474 1:A:123:ASP:O 1:A:127:ARG:HG3 1 0.452.111 1:A:106:LEU:O 1:A:110:MET:HG2 6 20.452.121:A:107:ARG:HD3 1:A:122:VAL:HG21 10 1 0.421.91 1:A:146:MET:HA 2:B:1133:ARG:NH2 2.29100.421 1:A:85:GLU:HB3 2:B:1133:ARG:NH1 0.422.291 1 1:A:121:GLU:O 1:A:125:MET:HG3 0.412.166 1

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



### 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	А	65/149~(44%)	$64 \pm 1 (98 \pm 1\%)$	$1\pm1 (2\pm1\%)$	0±0 (0±0%)	100 100
2	В	8/12~(67%)	8±0 (100±0%)	0±0 (0±0%)	0±0 (0±0%)	100 100
All	All	730/1610~(45%)	716 (98%)	14 (2%)	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 side chain 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 side chain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	56/127~(44%)	$54\pm1$ (96 $\pm2\%$ )	$2\pm1~(4\pm2\%)$	33 81
2	В	7/10~(70%)	$6\pm1$ (84 $\pm15\%$ )	$1\pm1 (16\pm15\%)$	5 42
All	All	630/1370~(46%)	595~(94%)	35~(6%)	25 74

All 16 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	А	138	ASN	7
2	В	1132	LEU	4
1	А	123	ASP	4
2	В	1133	ARG	4
1	А	119	ASP	3
1	А	132	ASP	2
1	А	147	THR	2
2	В	1129	LEU	1
1	А	102	SER	1
1	А	84	GLU	1

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Mol	Chain	Res	Type	Models (Total)
1	А	137	VAL	1
1	А	96	ASP	1
1	А	130	ASP	1
1	А	144	GLN	1
2	В	1131	HIS	1
2	В	1136	LEU	1

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#### 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 (i)

The completeness of assignment taking into account all chemical shift lists is 68% for the well-defined parts and 65% 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 (i)

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	1450
Number of shifts mapped to atoms	1450
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

#### 7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	${\rm Correction}\pm{\rm precision},ppm$	Suggested action
$^{13}C_{\alpha}$	143	$-0.41 \pm 0.09$	None needed ( $< 0.5$ ppm)
$^{13}C_{\beta}$	132	$0.12 \pm 0.16$	None needed ( $< 0.5$ ppm)
$^{13}C'$	123	$-0.45 \pm 0.13$	None needed ( $< 0.5$ ppm)
<sup>15</sup> N	138	$0.03 \pm 0.56$	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 68%, i.e. 640 atoms were assigned a chemical shift out of a possible 940. 8 out of 11 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^{1}\mathbf{H}$	$^{13}\mathrm{C}$	$^{15}\mathbf{N}$
Backbone	325/375~(87%)	132/150~(88%)	127/150~(85%)	66/75~(88%)
Sidechain	297/508~(58%)	181/294~(62%)	116/187~(62%)	0/27~(0%)

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	Total	$^{1}\mathrm{H}$	$^{13}\mathrm{C}$	$^{15}\mathbf{N}$
Aromatic	18/57~(32%)	18/31~(58%)	0/24~(0%)	0/2~(0%)
Overall	640/940~(68%)	331/475~(70%)	243/361~(67%)	66/104~(63%)

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The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 65%, i.e. 652 atoms were assigned a chemical shift out of a possible 1004. 8 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^{1}\mathrm{H}$	$^{13}\mathrm{C}$	$^{15}$ N
Backbone	333/400~(83%)	135/160~(84%)	130/160~(81%)	68/80~(85%)
Sidechain	301/547~(55%)	183/317~(58%)	118/202~(58%)	0/28~(0%)
Aromatic	18/57~(32%)	18/31~(58%)	0/24~(0%)	0/2~(0%)
Overall	652/1004~(65%)	336/508~(66%)	248/386~(64%)	68/110~(62%)

#### 7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

#### 7.1.5 Random Coil Index (RCI) plots (1)

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.

Random coil index (RCI) for chain A:

