



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 16, 2018 – 07:34 am GMT

PDB ID : 1QX7  
Title : Crystal structure of apoCaM bound to the gating domain of small conductance  
Ca<sup>2+</sup>-activated potassium channel  
Authors : Schumacher, M.A.; Crum, M.; Miller, M.C.  
Deposited on : 2003-09-04  
Resolution : 3.09 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30686

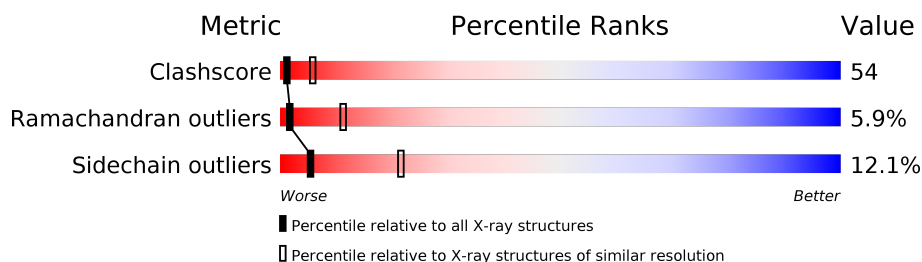
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.09 Å.

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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	122078	1042 (3.10-3.10)
Ramachandran outliers	120005	1010 (3.10-3.10)
Sidechain outliers	119972	1010 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	148	
1	B	148	
1	I	148	
1	M	148	
1	R	148	
2	D	85	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5523 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Calmodulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	I	145	Total	C	N	O	Se	0	0	0
			1146	702	184	251	9			
1	R	145	Total	C	N	O	Se	0	0	0
			1146	702	184	251	9			
1	A	145	Total	C	N	O	Se	0	0	0
			1146	702	184	251	9			
1	B	136	Total	C	N	O	Se	0	0	0
			1083	669	173	232	9			
1	M	115	Total	C	N	O	Se	0	0	0
			903	556	138	202	7			

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	36	MSE	MET	MODIFIED RESIDUE	UNP P62161
I	51	MSE	MET	MODIFIED RESIDUE	UNP P62161
I	71	MSE	MET	MODIFIED RESIDUE	UNP P62161
I	72	MSE	MET	MODIFIED RESIDUE	UNP P62161
I	76	MSE	MET	MODIFIED RESIDUE	UNP P62161
I	109	MSE	MET	MODIFIED RESIDUE	UNP P62161
I	124	MSE	MET	MODIFIED RESIDUE	UNP P62161
I	144	MSE	MET	MODIFIED RESIDUE	UNP P62161
I	145	MSE	MET	MODIFIED RESIDUE	UNP P62161
R	36	MSE	MET	MODIFIED RESIDUE	UNP P62161
R	51	MSE	MET	MODIFIED RESIDUE	UNP P62161
R	71	MSE	MET	MODIFIED RESIDUE	UNP P62161
R	72	MSE	MET	MODIFIED RESIDUE	UNP P62161
R	76	MSE	MET	MODIFIED RESIDUE	UNP P62161
R	109	MSE	MET	MODIFIED RESIDUE	UNP P62161
R	124	MSE	MET	MODIFIED RESIDUE	UNP P62161
R	144	MSE	MET	MODIFIED RESIDUE	UNP P62161
R	145	MSE	MET	MODIFIED RESIDUE	UNP P62161
B	36	MSE	MET	MODIFIED RESIDUE	UNP P62161

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Chain	Residue	Modelled	Actual	Comment	Reference
B	51	MSE	MET	MODIFIED RESIDUE	UNP P62161
B	71	MSE	MET	MODIFIED RESIDUE	UNP P62161
B	72	MSE	MET	MODIFIED RESIDUE	UNP P62161
B	76	MSE	MET	MODIFIED RESIDUE	UNP P62161
B	109	MSE	MET	MODIFIED RESIDUE	UNP P62161
B	124	MSE	MET	MODIFIED RESIDUE	UNP P62161
B	144	MSE	MET	MODIFIED RESIDUE	UNP P62161
B	145	MSE	MET	MODIFIED RESIDUE	UNP P62161
A	36	MSE	MET	MODIFIED RESIDUE	UNP P62161
A	51	MSE	MET	MODIFIED RESIDUE	UNP P62161
A	71	MSE	MET	MODIFIED RESIDUE	UNP P62161
A	72	MSE	MET	MODIFIED RESIDUE	UNP P62161
A	76	MSE	MET	MODIFIED RESIDUE	UNP P62161
A	109	MSE	MET	MODIFIED RESIDUE	UNP P62161
A	124	MSE	MET	MODIFIED RESIDUE	UNP P62161
A	144	MSE	MET	MODIFIED RESIDUE	UNP P62161
A	145	MSE	MET	MODIFIED RESIDUE	UNP P62161
M	36	MSE	MET	MODIFIED RESIDUE	UNP P62161
M	51	MSE	MET	MODIFIED RESIDUE	UNP P62161
M	71	MSE	MET	MODIFIED RESIDUE	UNP P62161
M	72	MSE	MET	MODIFIED RESIDUE	UNP P62161
M	76	MSE	MET	MODIFIED RESIDUE	UNP P62161
M	109	MSE	MET	MODIFIED RESIDUE	UNP P62161
M	124	MSE	MET	MODIFIED RESIDUE	UNP P62161
M	144	MSE	MET	MODIFIED RESIDUE	UNP P62161
M	145	MSE	MET	MODIFIED RESIDUE	UNP P62161

- Molecule 2 is a protein called Small conductance calcium-activated potassium channel protein 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	11	Total	C	N	O	0	0	0
			99	67	15	17			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	488	LEU	-	CLONING ARTIFACT	UNP P70604
D	489	GLU	-	CLONING ARTIFACT	UNP P70604
D	490	HIS	-	EXPRESSION TAG	UNP P70604
D	491	HIS	-	EXPRESSION TAG	UNP P70604
D	492	HIS	-	EXPRESSION TAG	UNP P70604

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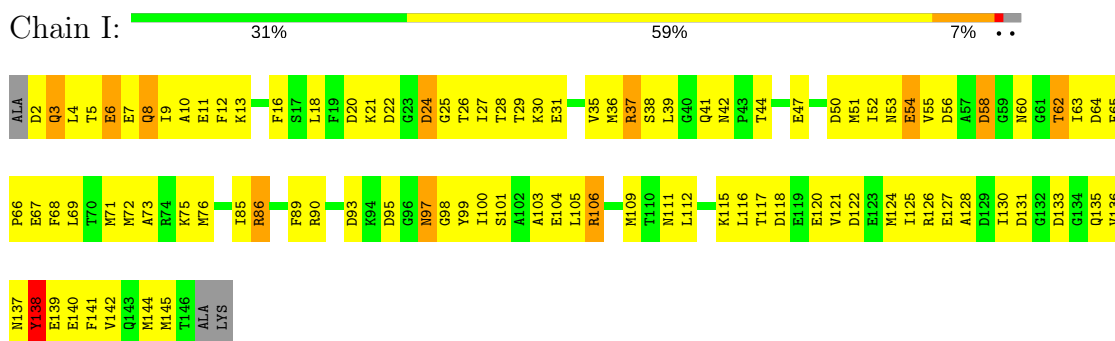
Chain	Residue	Modelled	Actual	Comment	Reference
D	493	HIS	-	EXPRESSION TAG	UNP P70604
D	494	HIS	-	EXPRESSION TAG	UNP P70604
D	495	HIS	-	EXPRESSION TAG	UNP P70604

### 3 Residue-property plots [i](#)

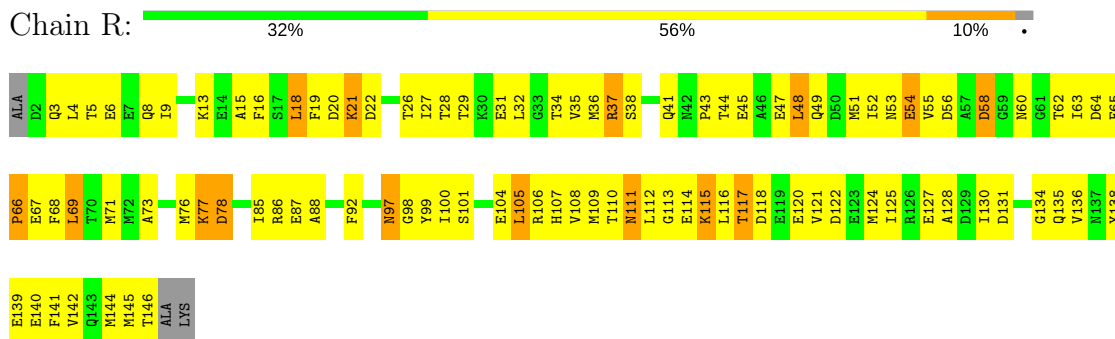
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

#### • Molecule 1: Calmodulin



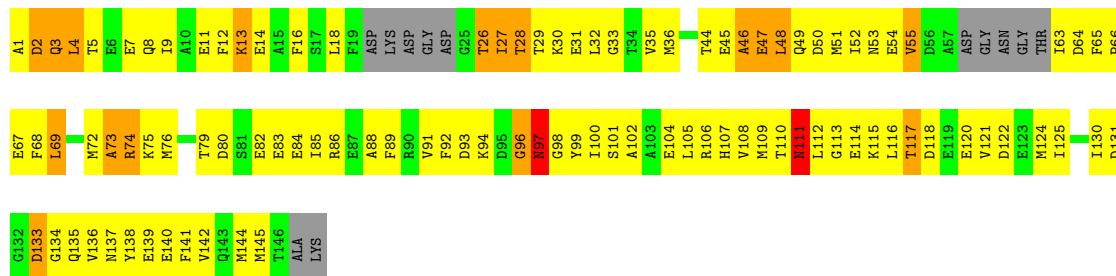
#### • Molecule 1: Calmodulin



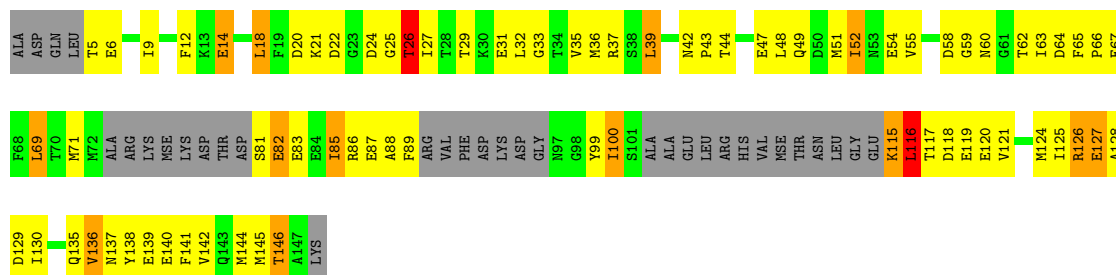
#### • Molecule 1: Calmodulin



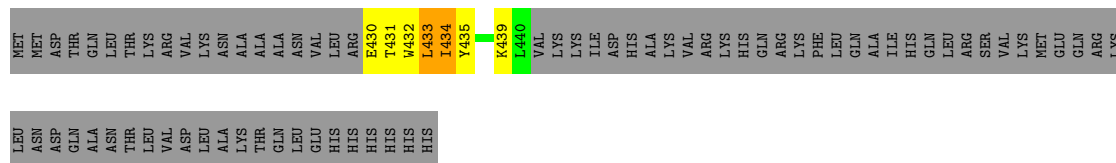
## ● Molecule 1: Calmodulin

Chain B:  23% 56% 11% 8%

## ● Molecule 1: Calmodulin

Chain M:  26% 42% 9% 22%

## ● Molecule 2: Small conductance calcium-activated potassium channel protein 2

Chain D:  5% 6% 87%

## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.93Å 79.93Å 220.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	75.16 – 3.09	Depositor
% Data completeness (in resolution range)	99.8 (75.16-3.09)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.286 , 0.308	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5523	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	wwPDB-VP



## 5 Model quality [i](#)

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

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 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	0.37	0/1149	0.55	0/1528
1	B	0.39	0/1084	0.58	0/1438
1	I	0.41	0/1149	0.61	0/1528
1	M	0.33	0/903	0.51	0/1199
1	R	0.45	0/1149	0.63	0/1528
2	D	0.75	0/101	1.01	0/136
All	All	0.40	0/5535	0.59	0/7357

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 the 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 within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1146	0	1070	125	0
1	B	1083	0	1025	153	0
1	I	1146	0	1070	118	0
1	M	903	0	828	108	0
1	R	1146	0	1070	131	0
2	D	99	0	103	25	0
All	All	5523	0	5166	574	0

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 54.

The worst 5 of 574 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:115:LYS:HD3	2:D:431:THR:HA	1.27	1.15
1:B:36:MSE:HE1	1:B:51:MSE:HE1	1.30	1.12
1:B:16:PHE:HE1	1:B:27:ILE:HD12	1.16	1.07
1:B:27:ILE:HD13	1:B:27:ILE:H	1.21	1.05
1:B:64:ASP:HB2	1:B:67:GLU:HG3	1.39	1.03

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 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 X-ray entries followed by that with respect to entries of similar resolution.

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	143/148 (97%)	116 (81%)	19 (13%)	8 (6%)	2	12
1	B	130/148 (88%)	100 (77%)	19 (15%)	11 (8%)	1	5
1	I	143/148 (97%)	107 (75%)	30 (21%)	6 (4%)	3	18
1	M	107/148 (72%)	80 (75%)	16 (15%)	11 (10%)	0	3
1	R	143/148 (97%)	117 (82%)	22 (15%)	4 (3%)	5	28
2	D	9/85 (11%)	8 (89%)	1 (11%)	0	100	100
All	All	675/825 (82%)	528 (78%)	107 (16%)	40 (6%)	2	11

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	21	LYS
1	A	82	GLU
1	B	46	ALA
1	I	54	GLU
1	R	54	GLU

### 5.3.2 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 X-ray entries followed by that with respect to entries of similar resolution.

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	125/117 (107%)	111 (89%)	14 (11%)	6	26
1	B	118/117 (101%)	104 (88%)	14 (12%)	6	22
1	I	125/117 (107%)	111 (89%)	14 (11%)	6	26
1	M	99/117 (85%)	86 (87%)	13 (13%)	4	19
1	R	125/117 (107%)	109 (87%)	16 (13%)	5	20
2	D	11/78 (14%)	9 (82%)	2 (18%)	2	8
All	All	603/663 (91%)	530 (88%)	73 (12%)	5	21

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	83	GLU
1	M	116	LEU
1	A	64	ASP
1	A	97	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	135	GLN
1	M	42	ASN
1	A	60	ASN
1	A	97	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.