



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 07:06 pm GMT

PDB ID : 1QX5
Title : Crystal structure of apoCalmodulin
Authors : Schumacher, M.A.; Crum, M.; Miller, M.C.
Deposited on : 2003-09-04
Resolution : 2.54 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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

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:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

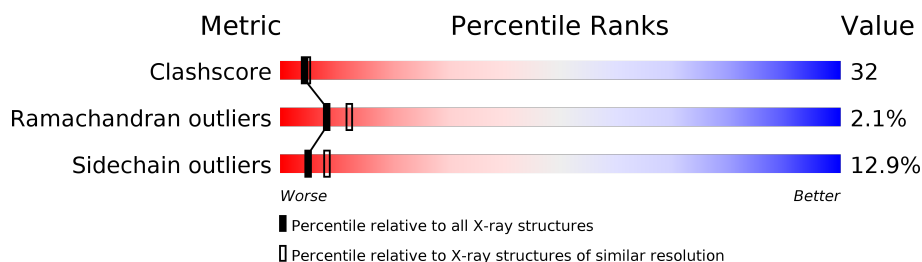
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.54 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	112137	5755 (2.58-2.50)
Ramachandran outliers	110173	5652 (2.58-2.50)
Sidechain outliers	110143	5654 (2.58-2.50)

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 ≥ 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	B	148	
1	D	148	
1	I	148	
1	J	148	
1	K	148	
1	R	148	
1	T	148	

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Mol	Chain	Length	Quality of chain
1	Y	148	<div><div></div><div>46%</div><div>43%</div><div>9%</div><div></div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9333 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	D	145	Total	C	N	O	S	0	0	0
			1146	702	184	251	9			
1	I	145	Total	C	N	O	S	0	0	0
			1146	702	184	251	9			
1	B	145	Total	C	N	O	S	0	0	0
			1146	702	184	251	9			
1	J	144	Total	C	N	O	S	0	0	0
			1138	698	183	248	9			
1	K	143	Total	C	N	O	S	0	0	0
			1129	693	181	246	9			
1	T	145	Total	C	N	O	S	0	0	0
			1146	702	184	251	9			
1	R	147	Total	C	N	O	S	0	0	0
			1161	711	187	254	9			
1	Y	145	Total	C	N	O	S	0	0	0
			1146	702	184	251	9			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	26	Total	O	0	0
			26	26		
2	D	24	Total	O	0	0
			24	24		
2	I	30	Total	O	0	0
			30	30		
2	J	15	Total	O	0	0
			15	15		
2	K	20	Total	O	0	0
			20	20		
2	R	30	Total	O	0	0
			30	30		

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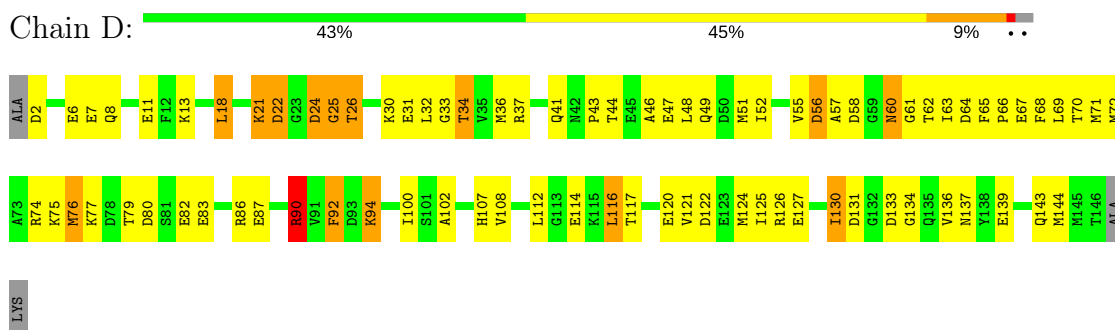
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	T	7	Total	O	0	0
			7	7		
2	Y	23	Total	O	0	0
			23	23		

3 Residue-property plots [i](#)

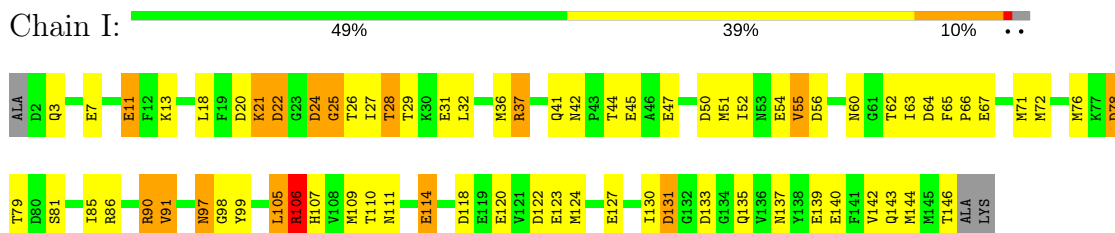
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

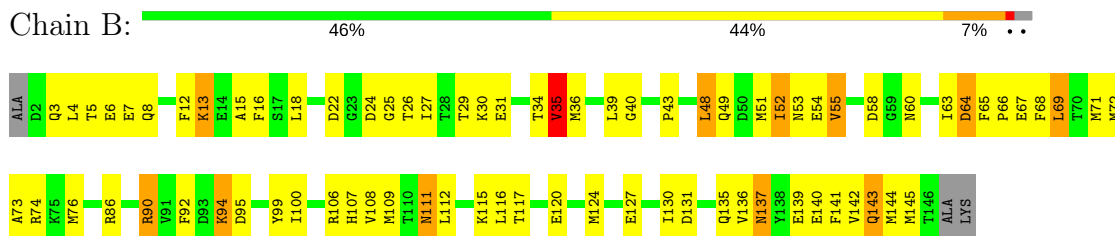
• Molecule 1: Calmodulin



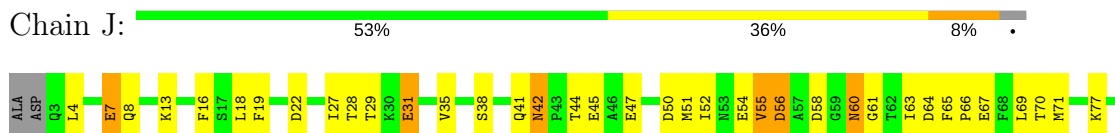
• Molecule 1: Calmodulin

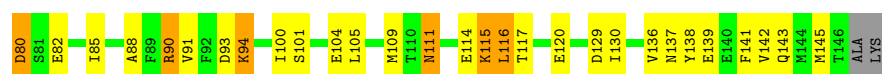


• Molecule 1: Calmodulin



• Molecule 1: Calmodulin

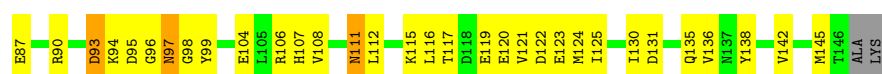
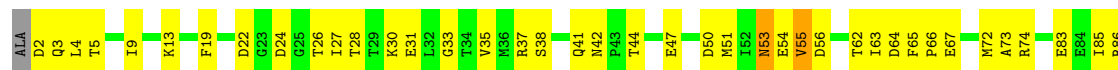




• Molecule 1: Calmodulin



• Molecule 1: Calmodulin



• Molecule 1: Calmodulin



• Molecule 1: Calmodulin



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	146.00 Å 146.00 Å 78.00 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	66.39 – 2.54	Depositor
% Data completeness (in resolution range)	98.5 (66.39-2.54)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.227 , 0.277	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9333	wwPDB-VP
Average B, all atoms (Å ²)	70.0	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	B	0.83	2/1158 (0.2%)	0.83	0/1555
1	D	0.87	1/1158 (0.1%)	0.87	2/1555 (0.1%)
1	I	1.01	0/1158	1.06	8/1555 (0.5%)
1	J	0.68	0/1150	0.73	1/1544 (0.1%)
1	K	0.82	0/1141	0.82	1/1532 (0.1%)
1	R	0.93	1/1173 (0.1%)	0.92	1/1573 (0.1%)
1	T	0.59	0/1158	0.68	1/1555 (0.1%)
1	Y	0.77	0/1158	0.87	4/1555 (0.3%)
All	All	0.82	4/9254 (0.0%)	0.85	18/12424 (0.1%)

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 outliers	#Planarity outliers
1	D	0	1
1	R	0	1
1	Y	0	1
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	83	GLU	CG-CD	6.67	1.61	1.51
1	R	83	GLU	CG-CD	5.80	1.60	1.51
1	B	35	VAL	CA-CB	5.67	1.66	1.54
1	B	15	ALA	CA-CB	5.19	1.63	1.52

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	106	ARG	NE-CZ-NH2	-7.73	116.44	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	37	ARG	NE-CZ-NH2	-7.70	116.45	120.30
1	Y	131	ASP	CB-CG-OD2	-7.38	111.66	118.30
1	I	131	ASP	CB-CG-OD1	7.36	124.93	118.30
1	R	129	ASP	CB-CG-OD1	-6.13	112.79	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	92	PHE	Sidechain
1	R	99	TYR	Sidechain
1	Y	138	TYR	Sidechain

5.2 Too-close contacts ⓘ

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	B	1146	0	1070	89	0
1	D	1146	0	1070	83	0
1	I	1146	0	1070	63	0
1	J	1138	0	1066	67	0
1	K	1129	0	1058	93	0
1	R	1161	0	1088	77	0
1	T	1146	0	1070	74	0
1	Y	1146	0	1070	66	0
2	B	26	0	0	1	0
2	D	24	0	0	2	0
2	I	30	0	0	2	0
2	J	15	0	0	2	0
2	K	20	0	0	2	0
2	R	30	0	0	1	0
2	T	7	0	0	2	0
2	Y	23	0	0	2	0
All	All	9333	0	8562	566	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 32.

The worst 5 of 566 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:B:94:LYS:HG3	1:K:94:LYS:HG2	1.39	1.04
1:K:4:LEU:HD21	1:K:73:ALA:HA	1.39	1.04
1:D:44:THR:HG21	1:I:131:ASP:OD2	1.59	1.03
1:R:124:MET:HA	1:R:144:MET:HE1	1.42	1.01
1:J:90:ARG:HG2	1:J:90:ARG:HH11	1.24	1.01

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	B	143/148 (97%)	131 (92%)	11 (8%)	1 (1%)	25	42
1	D	143/148 (97%)	131 (92%)	9 (6%)	3 (2%)	8	12
1	I	143/148 (97%)	130 (91%)	10 (7%)	3 (2%)	8	12
1	J	142/148 (96%)	125 (88%)	14 (10%)	3 (2%)	8	12
1	K	141/148 (95%)	123 (87%)	12 (8%)	6 (4%)	3	3
1	R	145/148 (98%)	135 (93%)	5 (3%)	5 (3%)	4	5
1	T	143/148 (97%)	128 (90%)	13 (9%)	2 (1%)	13	22
1	Y	143/148 (97%)	129 (90%)	13 (9%)	1 (1%)	25	42
All	All	1143/1184 (96%)	1032 (90%)	87 (8%)	24 (2%)	8	12

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	22	ASP
1	I	55	VAL
1	T	96	GLY

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Mol	Chain	Res	Type
1	R	55	VAL
1	R	147	ALA

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	B	125/126 (99%)	106 (85%)	19 (15%)	3	5
1	D	125/126 (99%)	105 (84%)	20 (16%)	3	4
1	I	125/126 (99%)	105 (84%)	20 (16%)	3	4
1	J	124/126 (98%)	106 (86%)	18 (14%)	4	6
1	K	123/126 (98%)	113 (92%)	10 (8%)	14	24
1	R	126/126 (100%)	112 (89%)	14 (11%)	7	12
1	T	125/126 (99%)	115 (92%)	10 (8%)	14	25
1	Y	125/126 (99%)	107 (86%)	18 (14%)	4	6
All	All	998/1008 (99%)	869 (87%)	129 (13%)	5	8

5 of 129 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	143	GLN
1	J	90	ARG
1	Y	77	LYS
1	J	7	GLU
1	J	42	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	137	ASN
1	K	97	ASN
1	Y	53	ASN

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Mol	Chain	Res	Type
1	K	42	ASN
1	K	53	ASN

5.3.3 RNA [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.