



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 3BYA / pdb_00003bya
Title : Structure of a Calmodulin Complex
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Deposited on : 2008-01-15
Resolution : 1.85 Å(reported)

This is a Full wwPDB X-ray 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/XrayValidationReportHelp>

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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

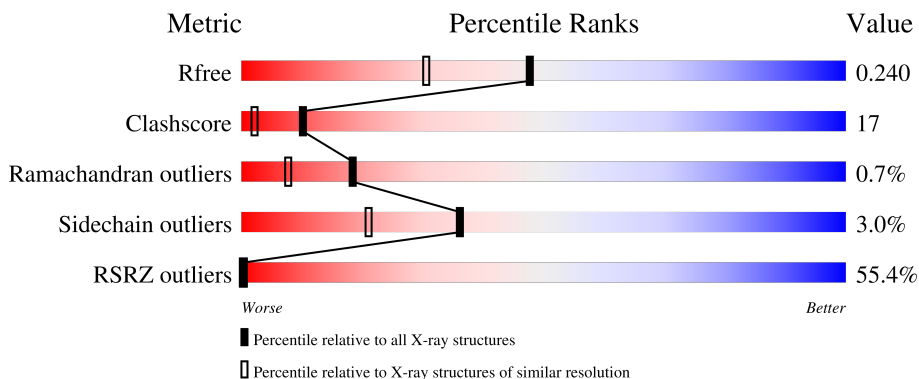
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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))
R_{free}	180053	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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.

Mol	Chain	Length	Quality of chain
1	A	148	51% 70% 22% • 7%
2	B	24	50% 46% 33% • 17%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 1352 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	A	137	Total	C	N	O	S	0	5	0
			1105	683	171	240	11			

- Molecule 2 is a protein called Glutamate [NMDA] receptor subunit zeta-1 peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	20	Total	C	N	O	0	1	0
			164	104	33	27			

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	Ca	0	0
			4	4		

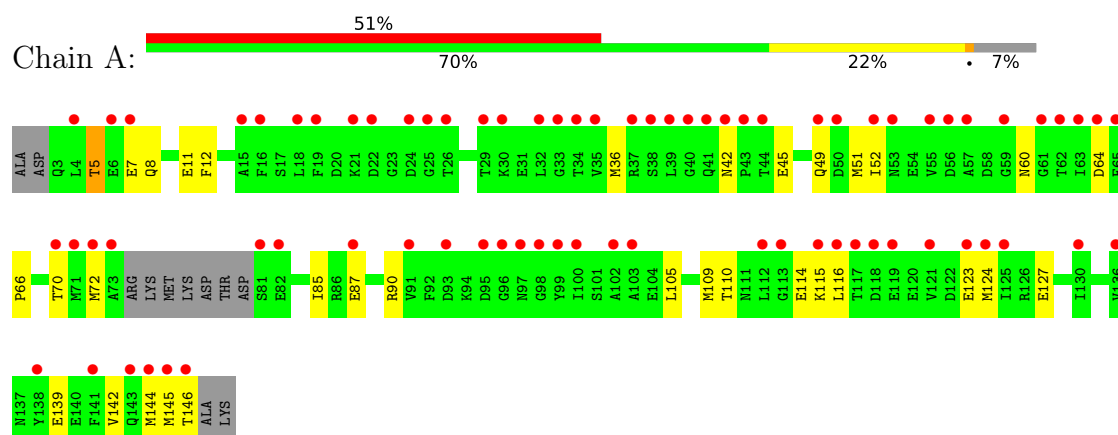
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	77	Total	O	0	0
			77	77		
4	B	2	Total	O	0	0
			2	2		

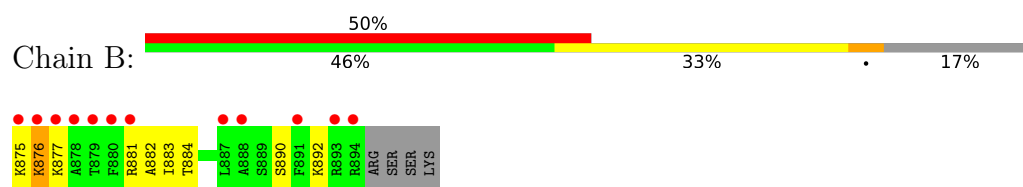
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

• Molecule 1: Calmodulin



• Molecule 2: Glutamate [NMDA] receptor subunit zeta-1 peptide



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	67.77Å 42.74Å 62.01Å 90.00° 106.92° 90.00°	Depositor
Resolution (Å)	32.74 – 1.85 32.74 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.7 (32.74-1.85) 99.8 (32.74-1.85)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.181 , 0.232 0.190 , 0.240	Depositor DCC
R_{free} test set	735 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	25.5	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 60.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	1352	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.66% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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 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	1.12	0/1131	1.06	0/1517
2	B	0.95	0/168	0.94	0/220
All	All	1.10	0/1299	1.04	0/1737

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

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	1105	0	1041	41	0
2	B	164	0	186	15	0
3	A	4	0	0	0	0
4	A	77	0	0	4	0
4	B	2	0	0	0	0
All	All	1352	0	1227	43	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 17.

All (43) 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:A:145[B]:MET:HE3	2:B:884:THR:CG2	1.60	1.32
1:A:145[B]:MET:CE	2:B:884:THR:HG21	1.86	1.05
1:A:145[B]:MET:HE3	2:B:884:THR:HG21	1.38	1.04
1:A:145[B]:MET:HE3	2:B:884:THR:HG22	1.37	1.04
1:A:109[A]:MET:HE3	1:A:124:MET:HE1	1.39	0.99
1:A:145[B]:MET:CE	2:B:884:THR:CG2	2.39	0.97
1:A:72:MET:HE1	2:B:882:ALA:HB2	1.50	0.92
1:A:145[B]:MET:SD	2:B:884:THR:HG21	2.10	0.92
1:A:109[A]:MET:CE	1:A:124:MET:HE1	2.13	0.79
1:A:42:ASN:ND2	4:A:229:HOH:O	2.17	0.77
1:A:45[B]:GLU:OE1	4:A:220:HOH:O	2.12	0.65
1:A:85:ILE:HG23	1:A:145[B]:MET:CE	2.28	0.64
1:A:139:GLU:HG3	4:A:210:HOH:O	2.00	0.61
1:A:72:MET:HE1	2:B:882:ALA:CB	2.27	0.60
1:A:85:ILE:HG23	1:A:145[B]:MET:HE1	1.84	0.59
1:A:60:ASN:ND2	4:A:226:HOH:O	2.32	0.53
1:A:110:THR:HG23	1:A:115:LYS:HD3	1.89	0.52
1:A:5:THR:HG22	1:A:8:GLN:CG	2.39	0.52
2:B:875:LYS:O	2:B:877:LYS:N	2.41	0.52
1:A:109[A]:MET:HE3	1:A:124:MET:CE	2.28	0.51
1:A:85:ILE:HG12	1:A:145[B]:MET:HE2	1.95	0.48
1:A:5:THR:HG23	1:A:7:GLU:N	2.29	0.48
1:A:124:MET:CG	2:B:876:LYS:HB2	2.46	0.46
1:A:5:THR:HG22	1:A:8:GLN:CD	2.41	0.46
1:A:5:THR:CG2	1:A:8:GLN:H	2.29	0.46
1:A:109[B]:MET:CE	1:A:114:GLU:OE1	2.65	0.45
1:A:105:LEU:O	1:A:109[B]:MET:HG2	2.17	0.44
1:A:87:GLU:HG2	1:A:90:ARG:NH2	2.32	0.44
2:B:877:LYS:O	2:B:881:ARG:HG3	2.18	0.43
1:A:114:GLU:OE1	1:A:116:LEU:HD11	2.18	0.43
1:A:5:THR:HG22	1:A:8:GLN:H	1.84	0.43
1:A:5:THR:HG22	1:A:8:GLN:HG3	2.01	0.43
1:A:142:VAL:O	1:A:146:THR:HG23	2.19	0.43
1:A:123:GLU:O	1:A:127:GLU:HG3	2.19	0.42
1:A:36:MET:HE3	1:A:36:MET:HB3	1.77	0.42
1:A:144:MET:HG3	2:B:877:LYS:HE2	2.01	0.42
1:A:12:PHE:CE1	1:A:72:MET:HE3	2.54	0.42
1:A:11:GLU:OE1	2:B:875:LYS:O	2.38	0.42
1:A:51[A]:MET:HE2	2:B:890:SER:HA	2.03	0.41
1:A:64:ASP:CG	1:A:66:PRO:HD2	2.46	0.40
1:A:109[A]:MET:HE1	2:B:883:ILE:CD1	2.50	0.40
1:A:109[B]:MET:HE2	1:A:114:GLU:OE1	2.21	0.40

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	138/148 (93%)	137 (99%)	1 (1%)	0	100	100
2	B	19/24 (79%)	17 (90%)	1 (5%)	1 (5%)	1	0
All	All	157/172 (91%)	154 (98%)	2 (1%)	1 (1%)	18	10

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	876	LYS

5.3.2 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 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	122/126 (97%)	119 (98%)	3 (2%)	42	27
2	B	18/21 (86%)	17 (94%)	1 (6%)	19	6
All	All	140/147 (95%)	136 (97%)	4 (3%)	36	22

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	52	ILE

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Mol	Chain	Res	Type
1	A	70	THR
2	B	892	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	137/148 (92%)	2.25	75 (54%) 0 0	18, 37, 52, 59	5 (3%)
2	B	20/24 (83%)	2.33	12 (60%) 0 0	31, 52, 75, 75	1 (5%)
All	All	157/172 (91%)	2.26	87 (55%) 0 0	18, 38, 59, 75	6 (3%)

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	96	GLY	5.6
1	A	34	THR	5.3
1	A	70	THR	4.3
1	A	37	ARG	4.2
1	A	40	GLY	4.1
1	A	52	ILE	4.0
1	A	38	SER	4.0
1	A	42	ASN	4.0
1	A	57	ALA	3.9
2	B	888	ALA	3.8
1	A	39	LEU	3.8
1	A	146	THR	3.7
1	A	35	VAL	3.7
1	A	121	VAL	3.7
1	A	25	GLY	3.6
1	A	73	ALA	3.6
1	A	33	GLY	3.6
1	A	71	MET	3.6
1	A	30	LYS	3.5
1	A	118	ASP	3.5
1	A	113	GLY	3.4
2	B	891	PHE	3.4
1	A	97	ASN	3.4
1	A	130	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	19	PHE	3.2
1	A	99	TYR	3.2
2	B	876	LYS	3.1
1	A	117	THR	3.1
2	B	879	THR	3.1
1	A	64	ASP	3.1
1	A	43	PRO	3.0
1	A	141	PHE	3.0
1	A	100	ILE	3.0
1	A	87	GLU	3.0
1	A	41	GLN	3.0
1	A	18	LEU	2.9
1	A	81	SER	2.9
1	A	16	PHE	2.9
1	A	138	TYR	2.8
2	B	894	ARG	2.8
2	B	878	ALA	2.7
1	A	55	VAL	2.7
1	A	50	ASP	2.7
1	A	145[A]	MET	2.7
1	A	4	LEU	2.7
1	A	53	ASN	2.7
1	A	91	VAL	2.7
1	A	115	LYS	2.6
1	A	29	THR	2.6
2	B	893	ARG	2.6
2	B	875	LYS	2.6
2	B	887	LEU	2.5
1	A	7	GLU	2.5
1	A	98	GLY	2.4
2	B	881	ARG	2.4
1	A	24	ASP	2.4
1	A	61	GLY	2.4
1	A	143	GLN	2.4
1	A	72	MET	2.4
1	A	103	ALA	2.4
1	A	124	MET	2.4
1	A	59	GLY	2.4
1	A	6	GLU	2.3
1	A	49	GLN	2.3
1	A	116	LEU	2.3
1	A	62	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	102	ALA	2.3
1	A	63	ILE	2.3
1	A	21	LYS	2.3
1	A	56	ASP	2.3
1	A	125	ILE	2.3
1	A	82	GLU	2.2
1	A	119	GLU	2.2
1	A	22	ASP	2.2
1	A	65	PHE	2.2
1	A	95	ASP	2.1
1	A	32	LEU	2.1
1	A	112	LEU	2.1
1	A	15	ALA	2.1
1	A	26	THR	2.1
2	B	877	LYS	2.1
1	A	93	ASP	2.1
1	A	123	GLU	2.0
1	A	44	THR	2.0
1	A	136	VAL	2.0
1	A	144	MET	2.0
2	B	880	PHE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CA	A	151	1/1	0.85	0.15	69,69,69,69	0
3	CA	A	152	1/1	0.96	0.14	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CA	A	149	1/1	0.98	0.16	23,23,23,23	0
3	CA	A	150	1/1	0.98	0.15	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.