



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 04:30 AM UTC

PDB ID : 7URW / pdb_00007urw
Title : Tetradecameric hub domain of CaMKII beta
Authors : Ozden, C.; Samkutty, A.; Stratton, M.M.; Garman, S.C.
Deposited on : 2022-04-22
Resolution : 3.11 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

<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

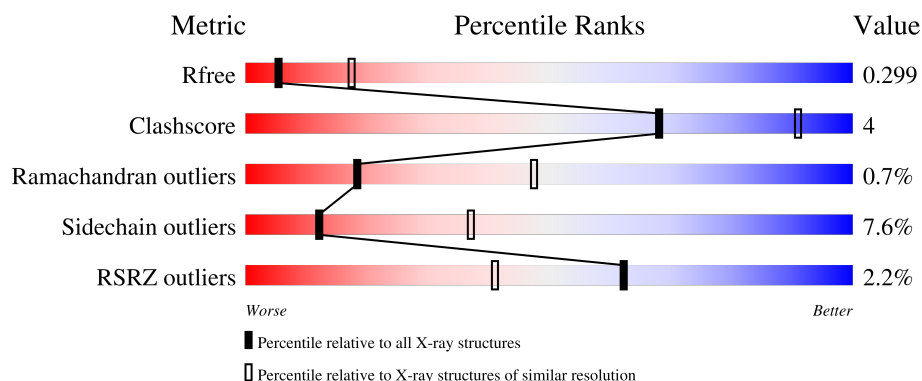
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.11 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	1816 (3.14-3.10)
Clashscore	190562	1906 (3.14-3.10)
Ramachandran outliers	187476	1802 (3.14-3.10)
Sidechain outliers	187428	1802 (3.14-3.10)
RSRZ outliers	180081	1816 (3.14-3.10)

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 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	137	 3% 74% 13% • 11%
1	B	137	 % 75% 13% • 11%
1	C	137	 2% 79% 10% •• 9%
1	D	137	 2% 78% 12% • 9%
1	E	137	 % 80% 16% ••

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Mol	Chain	Length	Quality of chain
1	F	137	% 78% 12% • 9%
1	G	137	2% 80% 12% • 7%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6789 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 Calcium/calmodulin-dependent protein kinase type II subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	127	Total	C	N	O	S	0	0	0
			963	609	169	180	5			
1	A	122	Total	C	N	O	S	0	0	0
			946	598	165	179	4			
1	B	122	Total	C	N	O	S	0	0	0
			949	599	165	181	4			
1	C	124	Total	C	N	O	S	0	0	0
			943	598	162	179	4			
1	D	125	Total	C	N	O	S	0	0	0
			972	612	170	186	4			
1	E	134	Total	C	N	O	S	0	0	0
			1040	657	183	196	4			
1	F	125	Total	C	N	O	S	0	0	0
			976	616	172	184	4			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	530	GLY	-	expression tag	UNP Q13554
G	531	PRO	-	expression tag	UNP Q13554
G	532	HIS	-	expression tag	UNP Q13554
G	533	MET	-	expression tag	UNP Q13554
A	530	GLY	-	expression tag	UNP Q13554
A	531	PRO	-	expression tag	UNP Q13554
A	532	HIS	-	expression tag	UNP Q13554
A	533	MET	-	expression tag	UNP Q13554
B	530	GLY	-	expression tag	UNP Q13554
B	531	PRO	-	expression tag	UNP Q13554
B	532	HIS	-	expression tag	UNP Q13554
B	533	MET	-	expression tag	UNP Q13554
C	530	GLY	-	expression tag	UNP Q13554
C	531	PRO	-	expression tag	UNP Q13554

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Chain	Residue	Modelled	Actual	Comment	Reference
C	532	HIS	-	expression tag	UNP Q13554
C	533	MET	-	expression tag	UNP Q13554
D	530	GLY	-	expression tag	UNP Q13554
D	531	PRO	-	expression tag	UNP Q13554
D	532	HIS	-	expression tag	UNP Q13554
D	533	MET	-	expression tag	UNP Q13554
E	530	GLY	-	expression tag	UNP Q13554
E	531	PRO	-	expression tag	UNP Q13554
E	532	HIS	-	expression tag	UNP Q13554
E	533	MET	-	expression tag	UNP Q13554
F	530	GLY	-	expression tag	UNP Q13554
F	531	PRO	-	expression tag	UNP Q13554
F	532	HIS	-	expression tag	UNP Q13554
F	533	MET	-	expression tag	UNP Q13554

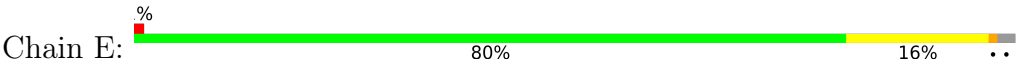
- Molecule 1: Calcium/calmodulin-dependent protein kinase type II subunit beta

[illegible][illegible]

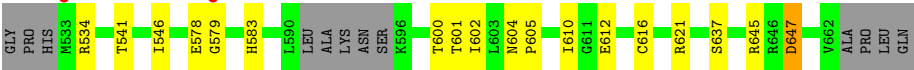
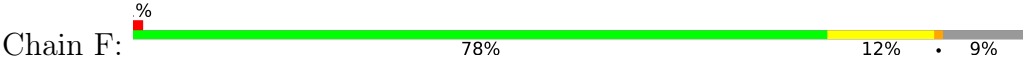
GLY	PHO	HTS	M534	TE41	I546	E578	G579	H583	L590	LEU	ALA	LYS	ASN	SER	K596	T600	T601	I602	L603	N604	P605	I610	C616	R621	S637	D647	V661	VAL	ALA	PRO	PRO	LEU	GLN
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GLY	PRO	HIS	MET	RS34	TS41	IS46	ES78	GS79	HS83	NS89	LS90	LEU	ALA	LYS	NS94	SS95	TS01	IS02	LE03	NG04	PG05	IG10	GS11	ES12	CS16	RS21	SG37	RG45	RG46	DG47	AS60	PG61	VAL	ALA	PRO	PRO	LEU	GLN
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● Molecule 1: Calcium/calmodulin-dependent protein kinase type II subunit beta



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	104.24Å 183.19Å 108.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.80 – 3.11 37.80 – 3.11	Depositor EDS
% Data completeness (in resolution range)	97.7 (37.80-3.11) 97.9 (37.80-3.11)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.55 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.255 , 0.300 0.254 , 0.299	Depositor DCC
R_{free} test set	972 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	68.4	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 36.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.55$, $\langle L^2 \rangle = 0.40$	Xtriage
Estimated twinning fraction	0.000 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.000 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	6789	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% 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

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	0.99	0/970	1.40	2/1320 (0.2%)
1	B	1.01	0/973	1.37	1/1325 (0.1%)
1	C	1.01	0/968	1.38	1/1321 (0.1%)
1	D	1.00	0/997	1.38	2/1357 (0.1%)
1	E	1.02	0/1067	1.39	0/1455
1	F	1.01	0/1001	1.35	0/1362
1	G	1.03	0/988	1.41	1/1348 (0.1%)
All	All	1.01	0/6964	1.38	7/9488 (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	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
All	All	0	7

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	647	ASP	CA-CB-CG	8.62	121.22	112.60
1	B	647	ASP	CA-CB-CG	7.08	119.68	112.60
1	G	647	ASP	CA-CB-CG	6.93	119.53	112.60
1	D	589	ASN	CA-C-N	6.03	132.55	121.70
1	D	589	ASN	C-N-CA	6.03	132.55	121.70

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	578	GLU	Peptide
1	B	578	GLU	Peptide
1	C	578	GLU	Peptide
1	D	578	GLU	Peptide
1	G	578	GLU	Peptide

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	946	0	849	7	0
1	B	949	0	854	8	1
1	C	943	0	836	6	0
1	D	972	0	879	5	0
1	E	1040	0	960	11	0
1	F	976	0	890	6	0
1	G	963	0	863	5	0
All	All	6789	0	6131	47	1

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 4.

The worst 5 of 47 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:579:GLY:O	1:A:583:HIS:ND1	2.14	0.80
1:B:579:GLY:O	1:B:583:HIS:ND1	2.14	0.79
1:F:579:GLY:O	1:F:583:HIS:ND1	2.14	0.79
1:G:579:GLY:O	1:G:583:HIS:ND1	2.14	0.79
1:C:579:GLY:O	1:C:583:HIS:ND1	2.14	0.78

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:647:ASP:OD1	1:B:647:ASP:OD1[4_555]	1.69	0.51

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	118/137 (86%)	115 (98%)	2 (2%)	1 (1%)	16	45
1	B	118/137 (86%)	116 (98%)	2 (2%)	0	100	100
1	C	120/137 (88%)	118 (98%)	2 (2%)	0	100	100
1	D	121/137 (88%)	118 (98%)	2 (2%)	1 (1%)	16	45
1	E	132/137 (96%)	126 (96%)	4 (3%)	2 (2%)	8	30
1	F	121/137 (88%)	119 (98%)	1 (1%)	1 (1%)	16	45
1	G	125/137 (91%)	122 (98%)	2 (2%)	1 (1%)	16	45
All	All	855/959 (89%)	834 (98%)	15 (2%)	6 (1%)	18	47

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	591	LEU
1	E	665	LEU
1	E	647	ASP
1	D	647	ASP
1	F	647	ASP

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	93/117 (80%)	86 (92%)	7 (8%)	12	38
1	B	95/117 (81%)	89 (94%)	6 (6%)	16	43
1	C	91/117 (78%)	83 (91%)	8 (9%)	9	31
1	D	98/117 (84%)	91 (93%)	7 (7%)	13	39
1	E	105/117 (90%)	97 (92%)	8 (8%)	12	37
1	F	98/117 (84%)	91 (93%)	7 (7%)	13	39
1	G	93/117 (80%)	85 (91%)	8 (9%)	10	32
All	All	673/819 (82%)	622 (92%)	51 (8%)	12	37

5 of 51 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	647	ASP
1	D	637	SER
1	F	621	ARG
1	D	541	THR
1	D	610	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	652	ASN
1	D	652	ASN
1	F	652	ASN
1	E	652	ASN
1	B	652	ASN

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 [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](#)

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	122/137 (89%)	0.15	4 (3%)	49	29	47, 67, 109, 137	0
1	B	122/137 (89%)	0.11	2 (1%)	70	49	48, 71, 98, 115	0
1	C	124/137 (90%)	0.25	3 (2%)	59	38	47, 75, 114, 132	0
1	D	125/137 (91%)	0.15	3 (2%)	59	38	48, 74, 112, 150	0
1	E	134/137 (97%)	0.14	2 (1%)	72	52	46, 68, 100, 140	0
1	F	125/137 (91%)	0.18	2 (1%)	70	49	44, 73, 103, 126	0
1	G	127/137 (92%)	0.27	3 (2%)	59	38	50, 81, 111, 124	0
All	All	879/959 (91%)	0.18	19 (2%)	62	41	44, 72, 111, 150	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	533	MET	4.1
1	F	533	MET	3.7
1	E	533	MET	3.6
1	C	579	GLY	3.2
1	C	533	MET	3.2

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.