Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2023 – 05:34 PM EDT

PDB ID	:	7URZ
Title	:	Hexadecameric hub domain of CaMKII beta
Authors	:	Ozden, C.; Samkutty, A.; Stratton, M.M.; Garman, S.C.
Deposited on	:	2022-04-22
Resolution	:	3.45 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:

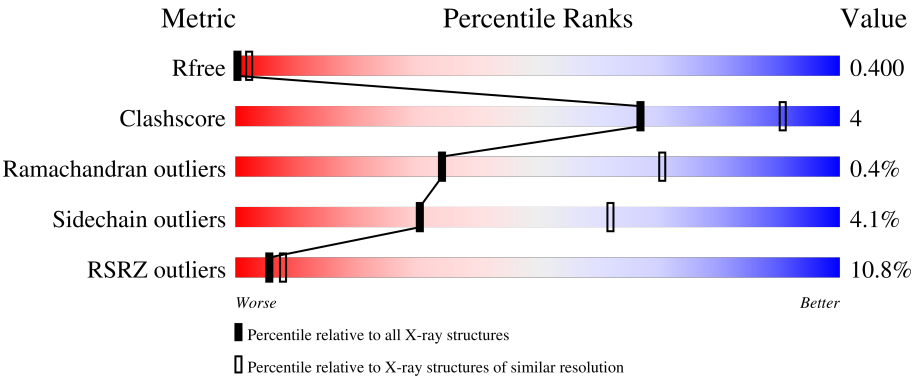
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.45 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}	130704	1291 (3.52-3.40)
Clashscore	141614	1372 (3.52-3.40)
Ramachandran outliers	138981	1337 (3.52-3.40)
Sidechain outliers	138945	1338 (3.52-3.40)
RSRZ outliers	127900	1205 (3.52-3.40)

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 <=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	12% 77% 10% 13%
1	B	137	9% 82% 14%
1	C	137	7% 85% 12%
1	G	137	12% 82% 9% 9%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3910 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	125	Total	C	N	O	S	0	0	0
			967	610	169	184	4			
1	A	119	Total	C	N	O	S	0	0	0
			932	590	160	178	4			
1	B	132	Total	C	N	O	S	0	0	0
			1007	636	175	192	4			
1	C	132	Total	C	N	O	S	0	0	0
			1004	632	175	192	5			

There are 16 discrepancies between the modelled and reference sequences:

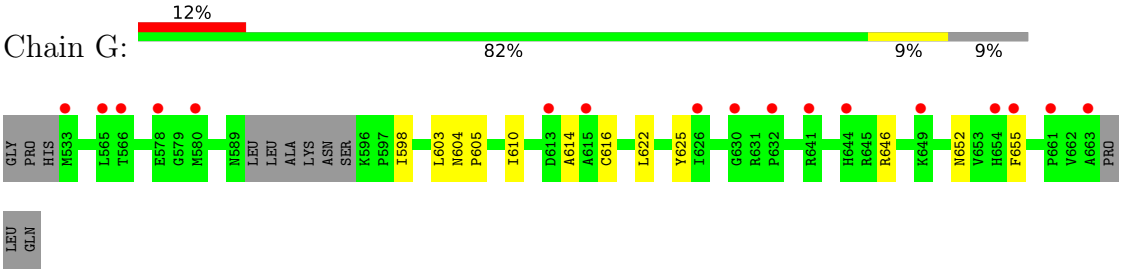
Chain	Residue	Modelled	Actual	Comment	Reference
G	530	GLY	-	expression tag	UNP Q13554
G	531	PRO	-	expression tag	UNP Q13554
G	532	HIS	-	expression tag	UNP Q13554
G	533	MET	-	expression tag	UNP Q13554
A	530	GLY	-	expression tag	UNP Q13554
A	531	PRO	-	expression tag	UNP Q13554
A	532	HIS	-	expression tag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

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.

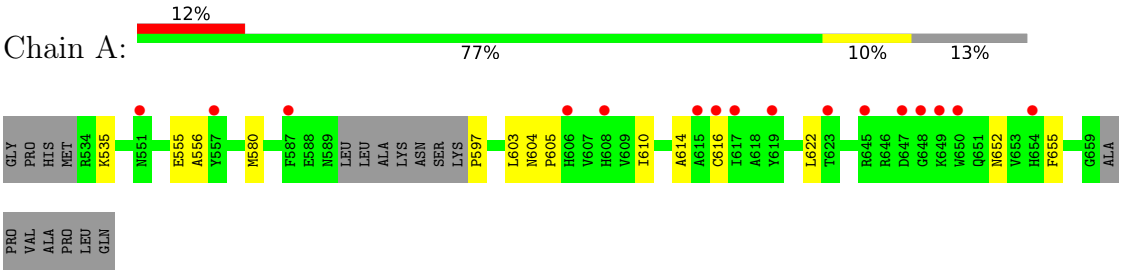
• Molecule 1: Calcium/calmodulin-dependent protein kinase type II subunit beta

Chain G:



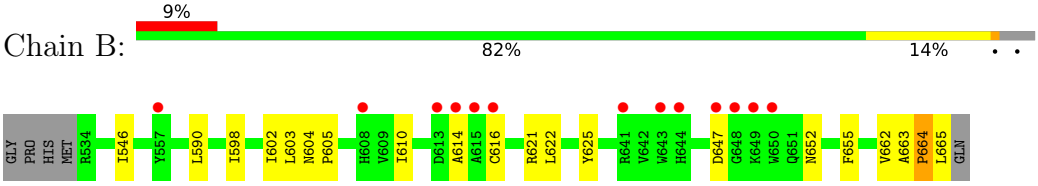
• Molecule 1: Calcium/calmodulin-dependent protein kinase type II subunit beta

Chain A:



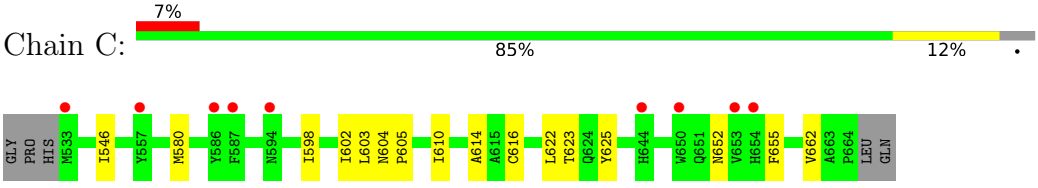
• Molecule 1: Calcium/calmodulin-dependent protein kinase type II subunit beta

Chain B:



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

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α, β, γ	81.34Å 81.34Å 180.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.09 – 3.45 37.06 – 3.45	Depositor EDS
% Data completeness (in resolution range)	97.8 (37.09-3.45) 97.9 (37.06-3.45)	Depositor EDS
R_{merge}	0.37	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.63 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.352 , 0.407 0.348 , 0.400	Depositor DCC
R_{free} test set	424 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	86.3	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 39.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.82	EDS
Total number of atoms	3910	wwPDB-VP
Average B, all atoms (Å^2)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.68% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.66	0/956	0.73	1/1299 (0.1%)
1	B	0.66	0/1034	0.71	0/1413
1	C	0.68	0/1031	0.72	0/1408
1	G	0.66	0/992	0.70	0/1351
All	All	0.67	0/4013	0.71	1/5471 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	597	PRO	CA-N-CD	-5.30	104.07	111.50

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	932	0	846	4	0
1	B	1007	0	906	8	0
1	C	1004	0	895	13	0
1	G	967	0	873	4	0
All	All	3910	0	3520	29	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 4.

All (29) 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:C:623:THR:CB	1:C:662:VAL:HG21	2.12	0.80
1:C:623:THR:HG21	1:C:662:VAL:CG2	2.26	0.66
1:C:623:THR:HG21	1:C:662:VAL:HG22	1.84	0.59
1:C:623:THR:HB	1:C:662:VAL:HG21	1.86	0.58
1:C:623:THR:OG1	1:C:662:VAL:HG21	2.06	0.54
1:G:610:ILE:O	1:G:614:ALA:HB3	2.08	0.53
1:B:610:ILE:O	1:B:614:ALA:HB3	2.08	0.53
1:A:610:ILE:O	1:A:614:ALA:HB3	2.08	0.53
1:C:610:ILE:O	1:C:614:ALA:HB3	2.08	0.53
1:C:662:VAL:HG13	1:C:662:VAL:O	2.11	0.51
1:B:598:ILE:HG22	1:B:625:TYR:CB	2.42	0.49
1:C:598:ILE:HG22	1:C:625:TYR:CB	2.42	0.49
1:B:621:ARG:HG2	1:B:662:VAL:HG21	1.97	0.47
1:G:598:ILE:HG22	1:G:625:TYR:CB	2.44	0.47
1:C:623:THR:CG2	1:C:662:VAL:HG21	2.44	0.47
1:A:603:LEU:HD11	1:A:622:LEU:HD12	1.97	0.46
1:C:623:THR:HG21	1:C:662:VAL:HG21	1.96	0.46
1:G:603:LEU:HD11	1:G:622:LEU:HD12	1.99	0.45
1:B:603:LEU:HD11	1:B:622:LEU:HD12	2.00	0.44
1:G:604:ASN:N	1:G:605:PRO:HD3	2.33	0.44
1:B:604:ASN:N	1:B:605:PRO:HD3	2.33	0.44
1:C:604:ASN:N	1:C:605:PRO:HD3	2.33	0.43
1:B:590:LEU:HD13	1:B:664:PRO:O	2.17	0.43
1:A:604:ASN:N	1:A:605:PRO:HD3	2.33	0.43
1:B:546:ILE:HD12	1:B:602:ILE:HD11	2.00	0.43
1:A:555:GLU:HG3	1:A:556:ALA:N	2.34	0.43
1:C:603:LEU:HD11	1:C:622:LEU:HD12	2.01	0.42
1:B:663:ALA:O	1:B:665:LEU:N	2.55	0.40
1:C:546:ILE:HD12	1:C:602:ILE:HD11	2.03	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	115/137 (84%)	108 (94%)	6 (5%)	1 (1%)	17 54
1	B	130/137 (95%)	121 (93%)	8 (6%)	1 (1%)	19 57
1	C	130/137 (95%)	120 (92%)	10 (8%)	0	100 100
1	G	121/137 (88%)	113 (93%)	8 (7%)	0	100 100
All	All	496/548 (90%)	462 (93%)	32 (6%)	2 (0%)	34 70

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	580	MET
1	B	664	PRO

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	94/117 (80%)	90 (96%)	4 (4%)	29 61
1	B	99/117 (85%)	95 (96%)	4 (4%)	31 63
1	C	98/117 (84%)	94 (96%)	4 (4%)	30 62
1	G	96/117 (82%)	92 (96%)	4 (4%)	30 61
All	All	387/468 (83%)	371 (96%)	16 (4%)	30 62

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	616	CYS
1	G	646	ARG
1	G	652	ASN
1	G	655	PHE
1	A	535	LYS
1	A	616	CYS

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Mol	Chain	Res	Type
1	A	652	ASN
1	A	655	PHE
1	B	616	CYS
1	B	647	ASP
1	B	652	ASN
1	B	655	PHE
1	C	580	MET
1	C	616	CYS
1	C	652	ASN
1	C	655	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	575	ASN
1	A	575	ASN
1	A	604	ASN
1	B	575	ASN
1	C	550	ASN
1	C	604	ASN
1	C	636	GLN

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 monosaccharides 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

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, 95^{th} 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	119/137 (86%)	0.96	16 (13%) 3 4	87, 112, 138, 172	0
1	B	132/137 (96%)	0.75	13 (9%) 7 9	82, 112, 139, 166	0
1	C	132/137 (96%)	0.68	9 (6%) 17 19	88, 107, 134, 158	0
1	G	125/137 (91%)	0.78	17 (13%) 3 4	86, 105, 136, 146	0
All	All	508/548 (92%)	0.79	55 (10%) 5 8	82, 109, 137, 172	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	648	GLY	8.0
1	A	649	LYS	5.9
1	B	648	GLY	4.6
1	A	615	ALA	4.5
1	A	616	CYS	4.1
1	C	653	VAL	3.9
1	A	606	HIS	3.8
1	B	615	ALA	3.7
1	C	533	MET	3.5
1	B	650	TRP	3.5
1	A	557	TYR	3.4
1	A	647	ASP	3.3
1	B	643	TRP	3.3
1	G	644	HIS	3.2
1	C	586	TYR	3.0
1	G	654	HIS	3.0
1	C	557	TYR	3.0
1	C	654	HIS	3.0
1	B	614	ALA	3.0
1	A	608	HIS	3.0
1	C	594	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	613	ASP	2.9
1	C	587	PHE	2.8
1	B	647	ASP	2.8
1	G	578	GLU	2.8
1	G	565	LEU	2.7
1	G	566	THR	2.7
1	A	650	TRP	2.7
1	A	617	ILE	2.6
1	B	649	LYS	2.5
1	C	650	TRP	2.5
1	G	663	ALA	2.5
1	A	623	THR	2.5
1	A	645	ARG	2.5
1	B	616	CYS	2.5
1	G	661	PRO	2.4
1	A	551	ASN	2.4
1	C	644	HIS	2.3
1	G	533	MET	2.3
1	A	654	HIS	2.3
1	B	608	HIS	2.2
1	G	649	LYS	2.2
1	G	632	PRO	2.2
1	B	641	ARG	2.2
1	G	613	ASP	2.2
1	A	587	PHE	2.1
1	G	626	ILE	2.1
1	B	557	TYR	2.1
1	G	580	MET	2.1
1	G	655	PHE	2.1
1	G	615	ALA	2.1
1	B	644	HIS	2.1
1	G	641	ARG	2.1
1	G	630	GLY	2.1
1	A	619	TYR	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 monosaccharides 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.