

wwPDB X-ray Structure Validation Summary Report (i)

Aug 17, 2023 – 12:03 AM EDT

PDB ID	:	2BDW
Title	:	Crystal Structure of the Auto-Inhibited Kinase Domain of Cal-
		cium/Calmodulin Activated Kinase II
Authors	:	Rosenberg, O.S.; Kuriyan, J.
Deposited on	:	2005-10-20
Resolution	:	1.80 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 (i) 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 (1)) were used in the production of this report:

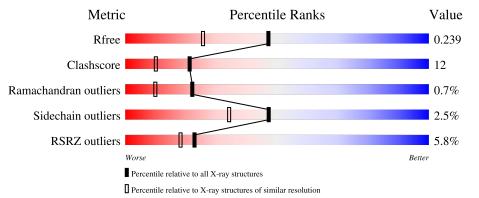
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)		
Ideal geometry (DNA, RNA)		
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 1.80 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	5950 (1.80-1.80)
Clashscore	141614	6793(1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	А	362	70%	15%	15%		
1	В	362	7%	24%	• 15%		



2BDW

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5354 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.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Δ	309	Total	С	Ν	0	S	0	0	0
	A	309	2461	1569	431	452	9	0	0	0
1	В	309	Total	С	Ν	0	S	0	0	0
	D	309	2462	1570	433	450	9	0	0	0

• Molecule 1 is a protein called Hypothetical protein K11E8.1d.

Chain	Residue	Modelled	Actual	Comment	Reference
А	-18	GLY	-	cloning artifact	UNP Q9NG91
А	-17	PRO	-	cloning artifact	UNP Q9NG91
А	-16	HIS	-	cloning artifact	UNP Q9NG91
А	-15	MET	-	cloning artifact	UNP Q9NG91
А	-14	ALA	-	cloning artifact	UNP Q9NG91
А	-13	SER	-	cloning artifact	UNP Q9NG91
А	-12	MET	-	cloning artifact	UNP Q9NG91
A	-11	THR	-	cloning artifact	UNP Q9NG91
А	-10	GLY	-	cloning artifact	UNP Q9NG91
А	-9	GLY	-	cloning artifact	UNP Q9NG91
А	-8	GLN	-	cloning artifact	UNP Q9NG91
А	-7	GLN	-	cloning artifact	UNP Q9NG91
А	-6	MET	-	cloning artifact	UNP Q9NG91
А	-5	GLY	-	cloning artifact	UNP Q9NG91
А	-4	ARG	-	cloning artifact	UNP Q9NG91
А	-3	GLY	-	cloning artifact	UNP Q9NG91
А	-2	SER	-	cloning artifact	UNP Q9NG91
А	-1	GLU	-	cloning artifact	UNP Q9NG91
А	0	PHE	-	cloning artifact	UNP Q9NG91
А	45	ASN	ASP	engineered mutation	UNP Q9NG91
В	-18	GLY	-	cloning artifact	UNP Q9NG91
В	-17	PRO	-	cloning artifact	UNP Q9NG91
В	-16	HIS	-	cloning artifact	UNP Q9NG91
В	-15	MET	-	cloning artifact	UNP Q9NG91
В	-14	ALA	-	cloning artifact	UNP Q9NG91

There are 40 discrepancies between the modelled and reference sequences:

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Chain	Residue	Modelled	Actual	Comment	Reference
В	-13	SER	-	cloning artifact	UNP Q9NG91
В	-12	MET	-	cloning artifact	UNP Q9NG91
В	-11	THR	-	cloning artifact	UNP Q9NG91
В	-10	GLY	-	cloning artifact	UNP Q9NG91
В	-9	GLY	-	cloning artifact	UNP Q9NG91
В	-8	GLN	-	cloning artifact	UNP Q9NG91
В	-7	GLN	-	cloning artifact	UNP Q9NG91
В	-6	MET	-	cloning artifact	UNP Q9NG91
В	-5	GLY	-	cloning artifact	UNP Q9NG91
В	-4	ARG	-	cloning artifact	UNP Q9NG91
В	-3	GLY	-	cloning artifact	UNP Q9NG91
В	-2	SER	-	cloning artifact	UNP Q9NG91
В	-1	GLU	-	cloning artifact	UNP Q9NG91
В	0	PHE	-	cloning artifact	UNP Q9NG91
В	45	ASN	ASP	engineered mutation	UNP Q9NG91

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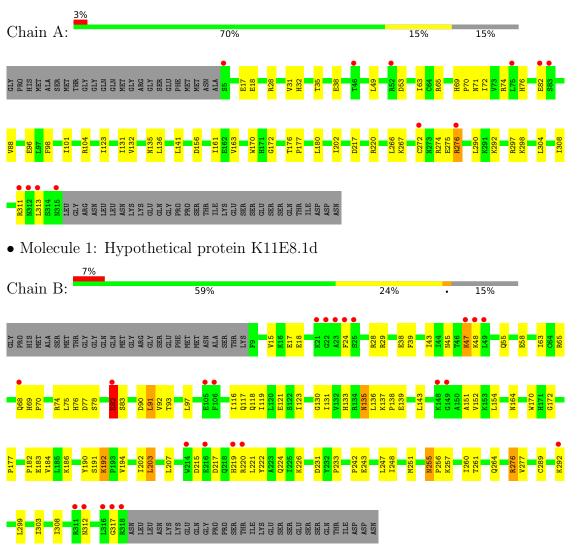
• Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	277	Total O 277 277	0	0
2	В	154	Total O 154 154	0	0



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: Hypothetical protein K11E8.1d



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	46.12Å 77.10Å 119.52Å	Depositor
a, b, c, α , β , γ	90.00° 96.74° 90.00°	Depositor
Resolution (Å)	45.80 - 1.80	Depositor
	47.03 - 1.80	EDS
% Data completeness	95.6 (45.80-1.80)	Depositor
(in resolution range)	95.8(47.03-1.80)	EDS
R _{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$4.23 (at 1.81 \text{\AA})$	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.216 , 0.236	Depositor
It, Itfree	0.218 , 0.239	DCC
R_{free} test set	7753 reflections (10.17%)	wwPDB-VP
Wilson B-factor ($Å^2$)	22.1	Xtriage
Anisotropy	0.519	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.38, 54.6	EDS
L-test for twinning ²	$ \langle L \rangle = 0.49, \langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5354	wwPDB-VP
Average B, all atoms $(Å^2)$	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.75% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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		lengths	Bond angles	
	Ullaill	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.36	0/2516	0.58	0/3406
1	В	0.29	0/2517	0.51	0/3407
All	All	0.33	0/5033	0.55	0/6813

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	А	2461	0	2469	43	0
1	В	2462	0	2471	79	0
2	А	277	0	0	10	0
2	В	154	0	0	5	0
All	All	5354	0	4940	119	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 12.

The worst 5 of 119 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1			Clash overlap (Å)
1:B:63:ILE:HG23	1:B:131:ILE:HD13	1.49	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:ILE:O	1:A:311:ARG:HG2	1.79	0.82
1:A:69:HIS:HD2	1:A:71:ASN:H	1.26	0.81
1:B:45:ASN:OD1	1:B:47:LYS:HD2	1.86	0.76
1:B:74:ARG:HB3	1:B:90:ASP:OD2	1.87	0.75

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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	Perce	ntiles
1	А	307/362~(85%)	298~(97%)	7~(2%)	2(1%)	22	10
1	В	307/362~(85%)	297~(97%)	8 (3%)	2(1%)	22	10
All	All	614/724~(85%)	595~(97%)	15~(2%)	4 (1%)	22	10

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	82	GLU
1	В	24	PHE
1	В	82	GLU
1	А	156	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	А	265/309~(86%)	262~(99%)	3~(1%)	73 68
1	В	264/309~(85%)	254 (96%)	10 (4%)	33 18
All	All	529/618~(86%)	516~(98%)	13~(2%)	47 34

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	154	LEU
1	В	192	LYS
1	В	276	ARG
1	В	224	GLN
1	В	255	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	В	85	HIS
1	В	264	GLN
1	В	114	HIS
1	В	312	ASN
1	В	164	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 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 (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, 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	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	309/362~(85%)	0.08	12 (3%) 39 33	12, 22, 43, 71	0
1	В	309/362~(85%)	0.35	24 (7%) 13 10	17, 33, 54, 69	0
All	All	618/724~(85%)	0.22	36 (5%) 23 18	12, 28, 50, 71	0

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	24	PHE	12.2
1	В	214	TRP	6.5
1	В	82	GLU	5.5
1	В	219	HIS	4.7
1	А	315	ASN	4.6

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.

