

# Full wwPDB X-ray Structure Validation Report (i)

#### Feb 17, 2024 – 09:51 PM EST

PDB ID : 3UPZ

Title : Calcium-Dependent Protein Kinase 1 from Toxoplasma gondii (TgCDPK1) in

complex with bumpless BKI analog UW1243

Authors: Merritt, E.A.; Larson, E.T.

Deposited on : 2011-11-18

Resolution : 2.20 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 (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:

 $Mol Probity \quad : \quad 4.02b\text{--}467$ 

Mogul: 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.36

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$ 

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

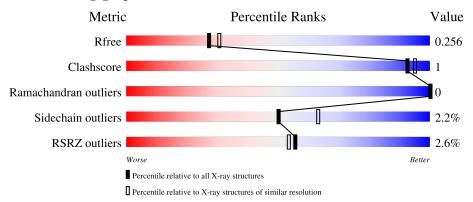
Validation Pipeline (wwPDB-VP) : 2.36

# 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 2.20 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar \ resolution} \\ (\#{\rm Entries, \ resolution \ range(\AA)}) \end{array}$
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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				
			2%				
1	A	484	89%	5% 5%			



# 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3780 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.

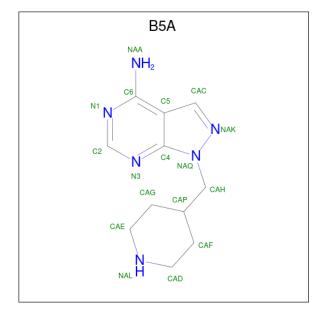
• Molecule 1 is a protein called Calmodulin-domain protein kinase 1.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	٨	458	Total	С	N	О	S	0	7	0
1	A	400	3698	2345	620	713	20	U	1	

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	GLY	-	expression tag	UNP Q9BJF5
A	25	PRO	-	expression tag	UNP Q9BJF5
A	26	GLY	-	expression tag	UNP Q9BJF5
A	27	SER	-	expression tag	UNP Q9BJF5
A	28	MET	-	expression tag	UNP Q9BJF5
A	29	MET	-	expression tag	UNP Q9BJF5

• Molecule 2 is 1-(piperidin-4-ylmethyl)-1H-pyrazolo[3,4-d]pyrimidin-4-amine (three-letter code: B5A) (formula: C<sub>11</sub>H<sub>16</sub>N<sub>6</sub>).





Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
2	A	1	Total 17	C 11	N 6	0	0

### • Molecule 3 is water.

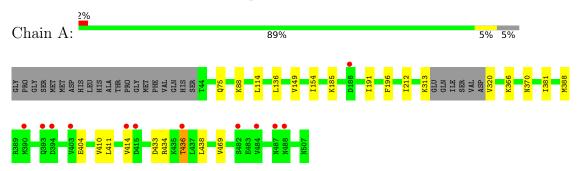
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	65	Total O 65 65	0	0



# 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: Calmodulin-domain protein kinase 1





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	48.27Å 72.79Å 67.29Å	Donositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 103.49° 90.00°	Depositor
Resolution (Å)	37.16 - 2.20	Depositor
rtesolution (A)	37.16 - 2.20	EDS
% Data completeness	99.0 (37.16-2.20)	Depositor
(in resolution range)	99.0 (37.16-2.20)	EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$< I/\sigma(I) > 1$	2.12 (at 2.20Å)	Xtriage
Refinement program	REFMAC	Depositor
D D.	0.191 , 0.251	Depositor
$R, R_{free}$	0.198 , $0.256$	DCC
$R_{free}$ test set	1171 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.6	Xtriage
Anisotropy	0.456	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.31, 35.0	EDS
L-test for twinning <sup>2</sup>	$ < L > = 0.49, < L^2> = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3780	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 7.26% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 5 Model quality (i)

## 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: B5A

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).

Mal	Chain	Bond	$\mathbf{lengths}$	Bond angles	
MIOI	Iol Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	A	0.39	0/3778	0.49	0/5075

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	A	3698	0	3706	11	0
2	A	17	0	16	0	0
3	A	65	0	0	1	0
All	All	3780	0	3722	11	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 1.

All (11) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
1:A:433:ASP:HA	1:A:436:THR:HB	1.93	0.51

Continued on next page...



Continued from previous page...

Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	${ m distance}({ m \AA})$	$\text{overlap } (\text{\AA})$
1:A:149:VAL:HG23	1:A:320:VAL:HG21	1.92	0.50
1:A:410:VAL:HG22	1:A:434:ARG:HD3	1.94	0.49
1:A:154:ILE:HG23	1:A:191:ILE:CD1	2.43	0.48
1:A:381:ILE:HD13	1:A:404:GLU:HG2	1.95	0.48
1:A:154:ILE:HG23	1:A:191:ILE:HD11	1.96	0.47
1:A:114[B]:LEU:HD11	3:A:543:HOH:O	2.15	0.47
1:A:136:LEU:HD21	1:A:154:ILE:HG21	1.97	0.46
1:A:438:LEU:C	1:A:438:LEU:HD23	2.36	0.46
1:A:212:ILE:HD12	1:A:469:VAL:HG12	1.99	0.45
1:A:411:LEU:O	1:A:414:VAL:HG12	2.20	0.41

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	461/484 (95%)	454 (98%)	7 (2%)	0	100 100

There are no Ramachandran outliers to report.

### 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	407/427 (95%)	398 (98%)	9 (2%)	52 65



All (	(9)	residues	with a	a non-rotan	eric sic	dechain	are listed	below:
-------	-----	----------	--------	-------------	----------	---------	------------	--------

Mol	Chain	Res	Type
1	A	75	GLN
1	A	88	LYS
1	A	185	LYS
1	A	196	PHE
1	A	313	LYS
1	A	366	LYS
1	A	370	ASN
1	A	388	MET
1	A	436	THR

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

#### 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)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

	Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
	MIOI		Chain		Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
Ī	2	B5A	A	1	-	17,19,19	1.78	2 (11%)	15,26,26	2.36	4 (26%)



In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

$\mathbf{N}$	<b>Iol</b>	Type	Chain	Res	Link	Chirals	Torsions	Rings
	2	B5A	A	1	-	-	0/2/12/12	0/3/3/3

#### All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(A)	$\operatorname{Ideal}(\text{\AA})$
2	A	1	B5A	C6-C5	-6.02	1.39	1.45
2	A	1	B5A	CAC-C5	-3.49	1.33	1.40

#### All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$\operatorname{Ideal}(^{o})$
2	A	1	B5A	CAC-NAK-NAQ	5.38	109.83	104.23
2	A	1	B5A	N3-C2-N1	-4.38	121.83	128.68
2	A	1	B5A	CAH-NAQ-NAK	4.07	124.70	117.08
2	A	1	B5A	C5-C6-N1	-3.32	118.48	121.93

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 (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	<RSRZ $>$	$\#\mathrm{RSRZ}{>}2$		$OWAB(A^2)$	Q < 0.9	
1	A	458/484 (94%)	-0.02	12 (2%)	56	53	31, 50, 86, 116	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	414	VAL	4.5
1	A	482	SER	4.3
1	A	393	GLN	4.0
1	A	390	MET	3.7
1	A	188	ASP	3.6
1	A	415	ASP	3.0
1	A	484	VAL	2.9
1	A	394	ASP	2.7
1	A	488	ASN	2.6
1	1 A		VAL	2.4
1	1 A		THR	2.3
1	1 A		ASN	2.1

# 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)

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,  $95^{th}$  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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
2	B5A	A	1	17/17	0.97	0.10	36,42,54,57	0

# 6.5 Other polymers (i)

There are no such residues in this entry.

