

wwPDB X-ray Structure Validation Summary Report (i)

Sep 4, 2023 – 11:06 PM EDT

PDB ID	:	3UFF
Title	:	Structural and functional characterization of an anesthetic binding site in the
		second cysteine-rich domain of protein kinase Cdelta
Authors	:	Shanmugasundararaj, S.; Stehle, T.; Miller, K.W.
Deposited on		
Resolution	:	1.30 Å(reported)
Deposited on	:	Shanmugasundararaj, S.; Stehle, T.; Miller, K.W.

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:

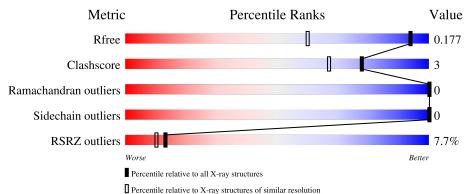
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 1.30 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	1058 (1.30-1.30)
Clashscore	141614	1101 (1.30-1.30)
Ramachandran outliers	138981	1058 (1.30-1.30)
Sidechain outliers	138945	1058 (1.30-1.30)
RSRZ outliers	127900	1029 (1.30-1.30)

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			
1	А	65	<mark>6%</mark> 97%	·	
1	В	65	9%	5%	



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 1293 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	Λ	65	Total	С	Ν	Ο	\mathbf{S}	0	1	0
	05	510	315	95	92	8	0		0	
1	D	65	Total	С	Ν	0	S	0	1	0
I D	00	510	315	95	92	8			0	

• Molecule 1 is a protein called Protein kinase C delta type.

Chain	Residue	Modelled	Actual	Comment	Reference
А	222	GLY	-	expression tag	UNP P28867
А	223	SER	-	expression tag	UNP P28867
А	224	ARG	-	expression tag	UNP P28867
А	225	ARG	-	expression tag	UNP P28867
А	226	ALA	-	expression tag	UNP P28867
А	227	SER	-	expression tag	UNP P28867
А	228	VAL	-	expression tag	UNP P28867
А	229	GLY	-	expression tag	UNP P28867
A	230	SER	-	expression tag	UNP P28867
А	236	THR	TYR	engineered mutation	UNP P28867
А	281	GLU	-	expression tag	UNP P28867
А	282	PHE	-	expression tag	UNP P28867
А	283	ILE	-	expression tag	UNP P28867
А	284	VAL	-	expression tag	UNP P28867
А	285	THR	-	expression tag	UNP P28867
А	286	ASP	-	expression tag	UNP P28867
В	222	GLY	-	expression tag	UNP P28867
В	223	SER	-	expression tag	UNP P28867
В	224	ARG	-	expression tag	UNP P28867
В	225	ARG	-	expression tag	UNP P28867
В	226	ALA	-	expression tag	UNP P28867
В	227	SER	-	expression tag	UNP P28867
В	228	VAL	-	expression tag	UNP P28867
В	229	GLY	-	expression tag	UNP P28867
В	230	SER	-	expression tag	UNP P28867

There are 32 discrepancies between the modelled and reference sequences:

Continued on next page...



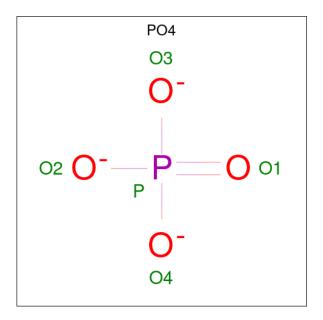
Chain	Residue	Modelled	Actual	Comment	Reference
В	236	THR	TYR	engineered mutation	UNP P28867
В	281	GLU	-	expression tag	UNP P28867
В	282	PHE	-	expression tag	UNP P28867
В	283	ILE	-	expression tag	UNP P28867
В	284	VAL	-	expression tag	UNP P28867
В	285	THR	-	expression tag	UNP P28867
В	286	ASP	-	expression tag	UNP P28867

Continued from previous page...

• Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	2	Total Zn 2 2	0	0
2	В	2	Total Zn 2 2	0	0

• Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0

Continued on next page...



Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0

• Molecule 4 is water.

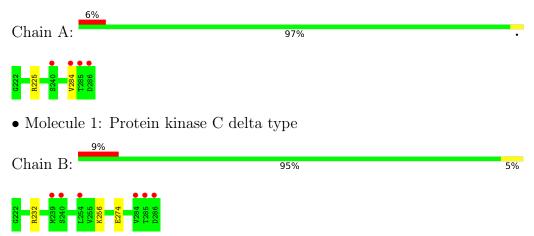
Μ	ol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	А	118	Total O 118 118	0	0
4	L	В	121	Total O 121 121	0	0



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: Protein kinase C delta type





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	44.20Å 32.33Å 49.82Å	Depositor
a, b, c, α , β , γ	90.00° 93.66° 90.00°	Depositor
Resolution (Å)	9.94 - 1.30	Depositor
	15.37 - 1.16	EDS
% Data completeness	91.3 (9.94-1.30)	Depositor
(in resolution range)	86.9(15.37-1.16)	EDS
R _{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.86 (at 1.15 \text{\AA})$	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.150 , 0.182	Depositor
II, II, <i>free</i>	0.144 , 0.177	DCC
R_{free} test set	1991 reflections (4.63%)	wwPDB-VP
Wilson B-factor $(Å^2)$	10.8	Xtriage
Anisotropy	0.414	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.48,60.8	EDS
L-test for twinning ²	$< L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	1293	wwPDB-VP
Average B, all atoms $(Å^2)$	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 12.71% 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)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, PO4

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	nd angles		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5		
1	А	0.35	0/523	0.53	0/699		
1	В	0.35	0/523	0.52	0/699		
All	All	0.35	0/1046	0.53	0/1398		

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	510	0	494	3	0
1	В	510	0	494	3	0
2	А	2	0	0	0	0
2	В	2	0	0	0	0
3	А	15	0	0	0	0
3	В	15	0	0	1	0
4	А	118	0	0	0	0
4	В	121	0	0	1	0
All	All	1293	0	988	6	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 3.



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:ARG:NE	3:B:9:PO4:O2	2.14	0.81
1:B:274:GLU:HG3	4:B:298:HOH:O	1.91	0.69
1:A:284:VAL:O	1:A:284:VAL:HG23	2.13	0.49
1:A:225:ARG:HB3	1:A:284:VAL:HG22	1.97	0.47
1:A:225:ARG:HB3	1:A:284:VAL:CG2	2.49	0.41

The worst 5 of 6 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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	64/65~(98%)	64 (100%)	0	0	100	100
1	В	64/65~(98%)	64 (100%)	0	0	100	100
All	All	128/130~(98%)	128 (100%)	0	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	А	58/57~(102%)	58 (100%)	0	100 100	

Continued on next page...



	9	Analysed	Rotameric	Outliers	Percer	ntiles
1	В	58/57~(102%)	58 (100%)	0	100	100
All	All	116/114~(102%)	116 (100%)	0	100	100

Continued from previous page...

There are no protein residues with a non-rotameric sidechain to report.

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. There are no such side chains 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)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 for Mogul analysis.

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	Turne	Chain	Res Link		Bog Link Bond		gths	Bond angles						
10101	туре	Type	туре	туре	Unain	main Res			Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
3	PO4	А	6	-	4,4,4	0.84	0	$6,\!6,\!6$	0.51	0				
3	PO4	В	9	-	4,4,4	0.92	0	$6,\!6,\!6$	0.29	0				
3	PO4	А	8	-	4,4,4	0.87	0	$6,\!6,\!6$	0.41	0				
3	PO4	В	5	-	4,4,4	0.88	0	$6,\!6,\!6$	0.48	0				
3	PO4	А	287	-	4,4,4	1.01	0	$6,\!6,\!6$	0.63	0				
3	PO4	В	1	-	4,4,4	0.93	0	$6,\!6,\!6$	0.50	0				



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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	В	9	PO4	1	0

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	65/65~(100%)	0.89	4 (6%) 20 18	8, 14, 26, 46	0
1	В	65/65~(100%)	0.94	6 (9%) 9 6	8, 14, 26, 43	0
All	All	130/130~(100%)	0.92	10 (7%) 13 10	8, 15, 26, 46	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	286	ASP	13.0
1	В	286	ASP	10.0
1	В	285	THR	5.3
1	А	285	THR	4.6
1	В	239	MET	4.1

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	$\operatorname{B-factors}(\operatorname{\AA}^2)$	$Q{<}0.9$
3	PO4	А	287	5/5	0.76	0.31	21,36,42,42	0
3	PO4	В	5	5/5	0.77	0.37	40,41,45,45	0
3	PO4	А	8	5/5	0.82	0.39	32,34,39,41	0
3	PO4	А	6	5/5	0.83	0.24	35,37,40,41	0
3	PO4	В	9	5/5	0.86	0.36	30,30,30,30	0
3	PO4	В	1	5/5	0.90	0.21	$19,\!34,\!35,\!37$	0
2	ZN	В	3	1/1	1.00	0.08	10,10,10,10	0
2	ZN	В	4	1/1	1.00	0.07	8,8,8,8	0
2	ZN	А	1	1/1	1.00	0.07	10,10,10,10	0
2	ZN	А	2	1/1	1.00	0.07	8,8,8,8	0

6.5 Other polymers (i)

There are no such residues in this entry.

