

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

#### Oct 5, 2023 – 03:48 AM EDT

PDB ID	:	6V5A
Title	:	Crystal structure of the human BK channel gating ring L390P mutant
Authors	:	Deng, Z.; Yuan, P.
Deposited on		
Resolution	:	2.00  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:

MolProbity	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
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:  $X\hbox{-}RAY\,DIFFRACTION$ 

The reported resolution of this entry is 2.00 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.



# 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4915 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-activated potassium channel subunit alpha-1.

Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace	
1	А	594	Total 4683	C 2999	N 777	0 873	S 34	0	0	0

There are 11 discrepancies between the modelled and reference sequences:

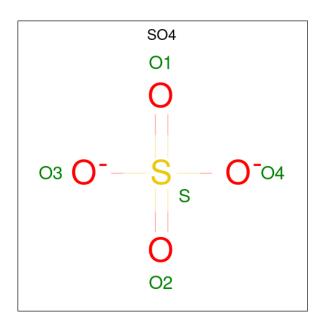
Chain	Residue	Modelled	Actual	Comment	Reference
А	340	MET	-	initiating methionine	UNP Q12791
А	390	PRO	LEU	engineered mutation	UNP Q12791
А	1057	SER	-	expression tag	UNP Q12791
А	1058	ASN	-	expression tag	UNP Q12791
A	1059	SER	-	expression tag	UNP Q12791
А	1060	LEU	-	expression tag	UNP Q12791
А	1061	GLU	-	expression tag	UNP Q12791
А	1062	VAL	-	expression tag	UNP Q12791
А	1063	LEU	-	expression tag	UNP Q12791
А	1064	PHE	-	expression tag	UNP Q12791
А	1065	GLN	-	expression tag	UNP Q12791

• Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

[	Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
	2	А	1	Total C 1 1	a	0	0

• Molecule 3 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).





Mol	Chain	Residues	Ato	$\mathbf{ms}$		ZeroOcc	AltConf
3	А	1	Total 5	0 4	S 1	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	226	Total O   226 226	0	0

MolProbity and EDS failed to run properly - this section is therefore empty.



# 3 Data and refinement statistics (i)

Property	Value	Source		
Space group	H 3 2	Depositor		
Cell constants	145.52Å 145.52Å 242.85Å	Depositor		
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$	Depositor		
Resolution (Å)	30.00 - 2.00	Depositor		
% Data completeness	99.9 (30.00-2.00)	Depositor		
(in resolution range)		-		
R <sub>merge</sub>	0.06	Depositor		
R <sub>sym</sub>	(Not available)	Depositor		
$< I/\sigma(I) > 1$	$2.25 (at 2.00 \text{\AA})$	Xtriage		
Refinement program	REFMAC 5.8.0103	Depositor		
$R, R_{free}$	0.203 , $0.226$	Depositor		
Wilson B-factor $(Å^2)$	36.5	Xtriage		
Anisotropy	0.005	Xtriage		
L-test for twinning <sup>2</sup>	$ < L >=0.49, < L^2>=0.32$	Xtriage		
Estimated twinning fraction	No twinning to report.	Xtriage		
Total number of atoms	4915	wwPDB-VP		
Average B, all atoms $(Å^2)$	45.0	wwPDB-VP		

EDS failed to run properly - this section is therefore incomplete.

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.60% of the height of the origin peak. No significant pseudotranslation is detected.

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



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

# 4 Model quality (i)

# 4.1 Standard geometry (i)

MolProbity failed to run properly - this section is therefore empty.

### 4.2 Too-close contacts (i)

MolProbity failed to run properly - this section is therefore empty.

### 4.3 Torsion angles (i)

#### 4.3.1 Protein backbone (i)

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.2 Protein sidechains (i)

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.3 RNA (i)

MolProbity failed to run properly - this section is therefore empty.

### 4.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

### 4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 4.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	Type	Chain	Res	Link	В	ond leng	gths	В	ond ang	gles
	WIOI	Type	Unam			Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
	3	SO4	А	2002	-	4,4,4	0.36	0	$6,\!6,\!6$	0.15	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.

No monomer is involved in short contacts.

### 4.7 Other polymers (i)

There are no such residues in this entry.

## 4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



# 5 Fit of model and data (i)

# 5.1 Protein, DNA and RNA chains (i)

EDS failed to run properly - this section is therefore empty.

## 5.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS failed to run properly - this section is therefore empty.

## 5.3 Carbohydrates (i)

EDS failed to run properly - this section is therefore empty.

## 5.4 Ligands (i)

EDS failed to run properly - this section is therefore empty.

### 5.5 Other polymers (i)

EDS failed to run properly - this section is therefore empty.

