

Full wwPDB X-ray Structure Validation Report (i)

Oct 4, 2023 – 10:39 PM EDT

PDB ID	:	6W0E
Title	:	Open-gate KcsA soaked in 10 mM BaCl2
Authors	:	Rohaim, A.; Gong, L.; Li, J.
Deposited on		
Resolution	:	3.51 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:

:	FAILED
:	1.13
:	FAILED
:	20191225.v01 (using entries in the PDB archive December 25th 2019)
:	Engh & Huber (2001)
:	Parkinson et al. (1996)
:	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 3.51 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.



6W0E

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 3945 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 Fab Heavy Chain.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	А	219	Total 1604	C 1019	N 267	O 312	S 6	0	0	0

• Molecule 2 is a protein called Fab Light Chain.

Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf	Trace
2	В	212	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0	0
2	D	212	1646	1022	282	337	5			

• Molecule 3 is a protein called pH-gated potassium channel KcsA.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
3	С	93	Total 688	C 455	N 111	0 121	S 1	0	0	0

• Molecule 4 is BARIUM ION (three-letter code: BA) (formula: Ba) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Aton	ns	ZeroOcc	AltConf
4	С	1	Total 1	Ba 1	0	0

• Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	С	1	Total K 1 1	0	0

• Molecule 6 is water.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	С	5	Total O 5 5	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	I 4	Depositor
Cell constants	158.28Å 158.28 Å 74.21 Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	51.22 - 3.51	Depositor
% Data completeness	98.8 (51.22-3.51)	Depositor
(in resolution range)		-
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.26 (at 3.49 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.194 , 0.250	Depositor
Wilson B-factor $(Å^2)$	109.5	Xtriage
Anisotropy	0.132	Xtriage
L-test for $twinning^2$	$< L > = 0.45, < L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.056 for -k,-h,-l	Xtriage
Total number of atoms	3945	wwPDB-VP
Average B, all atoms $(Å^2)$	123.0	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 4.30% 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.

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, 2 are monoatomic - leaving 0 for Mogul analysis.

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.

