

Full wwPDB X-ray Structure Validation Report (i)

Oct 5, 2023 – 12:54 AM EDT

PDB ID	:	6V2J
Title	:	Crystal structure of ClC-ec1 triple mutant (E113Q, E148Q, E203Q)
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Deposited on		
Resolution	:	2.62 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 2.62 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 3 unique types of molecules in this entry. The entry contains 3310 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 H(+)/Cl(-) exchange transporter ClcA.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	А	435	Total 3252	C 2141	N 544	0 547	S 20	0	1	0

Chain	Residue	Modelled	Actual	Comment	Reference
А	113	GLN	GLU	engineered mutation	UNP P37019
А	148	GLN	GLU	engineered mutation	UNP P37019
А	203	GLN	GLU	engineered mutation	UNP P37019
А	469	LYS	-	expression tag	UNP P37019
А	470	GLY	-	expression tag	UNP P37019
А	471	SER	-	expression tag	UNP P37019
А	472	GLY	-	expression tag	UNP P37019
А	473	THR	-	expression tag	UNP P37019
А	474	LEU	-	expression tag	UNP P37019
А	475	VAL	-	expression tag	UNP P37019
A	476	PRO	-	expression tag	UNP P37019
A	477	ARG	-	expression tag	UNP P37019
А	478	GLY	-	expression tag	UNP P37019
А	479	SER	-	expression tag	UNP P37019
А	480	GLY	-	expression tag	UNP P37019
A	481	GLY	-	expression tag	UNP P37019
A	482	LEU	-	expression tag	UNP P37019
A	483	GLU	-	expression tag	UNP P37019
A	484	HIS	-	expression tag	UNP P37019
А	485	HIS	-	expression tag	UNP P37019
А	486	HIS	-	expression tag	UNP P37019
А	487	HIS	-	expression tag	UNP P37019
А	488	HIS	-	expression tag	UNP P37019
А	489	HIS	-	expression tag	UNP P37019

There are 24 discrepancies between the modelled and reference sequences:

• Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	3	Total Cl 3 3	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	55	$\begin{array}{cc} \text{Total} & \text{O} \\ 55 & 55 \end{array}$	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 2 2 2	Depositor
Cell constants	80.97Å 12 0.44 Å 12 2.57 Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.65 - 2.62	Depositor
% Data completeness	97.2 (28.65-2.62)	Depositor
(in resolution range)		-
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.58 (at 2.61 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.193 , 0.262	Depositor
Wilson B-factor $(Å^2)$	57.2	Xtriage
Anisotropy	0.641	Xtriage
L-test for twinning ²	$< L > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,-l,-k	Xtriage
Total number of atoms	3310	wwPDB-VP
Average B, all atoms $(Å^2)$	64.0	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 10.75% 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.

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 3 ligands modelled in this entry, 3 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.

