

Full wwPDB X-ray Structure Validation Report (i)

Oct 5, 2023 – 08:29 AM EDT

PDB ID : 6VD9

Title : Metal-bound C-terminal domain of the CzcD transporter from Cuprividus met-

allidurans

 $\begin{array}{cccc} \text{Authors} & : & \text{Maher, M.J.} \\ \text{Deposited on} & : & 2019\text{-}12\text{-}23 \end{array}$

Resolution : 1.75 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 Xtriage (Phenix) : 1.13 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-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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 2459 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 Metal cation efflux system protein CzcD.

Mol	Chain	Residues		Ato	oms			ZeroOcc	AltConf	Trace
1	Λ	73	Total	С	N	О	S	0	1	0
1	A	19	575	370	93	110	2	U	1	
1	В	73	Total	С	N	О	S	0	2	0
1	Ъ	15	580	375	93	110	2	0	_	
1	С	68	Total	С	N	О	S	0	0	0
1		00	534	345	86	101	2	0	0	
1	D	69	Total	С	N	О	S	0	0	0
1			538	348	86	102	2			

• Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ni 1 1	0	0
2	В	1	Total Ni 1 1	0	0
2	С	1	Total Ni 1 1	0	0
2	D	1	Total Ni 1 1	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	59	Total O 59 59	0	0
3	В	62	Total O 62 62	0	0
3	С	58	Total O 58 58	0	0
3	D	49	Total O 49 49	0	0



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



3 Data and refinement statistics (i)

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

Property	Value	Source	
Space group	P 1	Depositor	
Cell constants	32.76Å 39.03Å 63.97Å	Depositor	
a, b, c, α , β , γ	98.78° 104.76° 90.09°	Depositor	
Resolution (Å)	38.57 - 1.75	Depositor	
% Data completeness	96.3 (38.57-1.75)	Depositor	
(in resolution range)		-	
R_{merge}	(Not available)	Depositor	
R_{sym}	(Not available)	Depositor	
$< I/\sigma(I) > 1$	2.79 (at 1.75Å)	Xtriage	
Refinement program	REFMAC 7.0.073	Depositor	
R, R_{free}	0.224 , 0.258	Depositor	
Wilson B-factor (A^2)	20.2	Xtriage	
Anisotropy	0.245	Xtriage	
L-test for twinning ²	$< L > = 0.49, < L^2> = 0.32$	Xtriage	
Estimated twinning fraction	0.033 for h,-k,-h-l	Xtriage	
Total number of atoms	2459	wwPDB-VP	
Average B, all atoms (\mathring{A}^2)	26.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 25.54 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.1119e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

²Theoretical 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.



 $^{^{1}}$ 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 4 ligands modelled in this entry, 4 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.

