wwPDB EM Validation Summary Report (i)

May 27, 2024 – 07:07 PM EDT

PDB ID	:	6CLA
EMDB ID	:	EMD-7493
Title	:	2.80 A MicroED structure of proteinase K at 6.0 e- / A^2
Authors	:	Hattne, J.; Shi, D.; Glynn, C.; Zee, C.-T.; Gallagher-Jones, M.; Martynowycz, M.W.; Rodriguez, J.A.; Gonen, T.
Deposited on	:	2018-03-02
Resolution	:	2.80 Å(reported)
Based on initial model	:	5I9S

This is a wwPDB EM 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/EMValidationReportHelp
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 (i)) were used in the production of this report:

EMDB validation analysis	:	FAILED
MolProbity	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON CRYSTALLOGRAPHY

The reported resolution of this entry is 2.80 Å.

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

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2029 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Proteinase K.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	279	2029	1247	357	415	10	0	0

SEQUENCE-PLOTS INFOmissingINFO

3 Experimental information (i)

Property	Value	Source
EM reconstruction method	CRYSTALLOGRAPHY	Depositor
Imposed symmetry	3D CRYSTAL, a=67.4502 Å, b=67.4502 Å, c=100.818 Å, α=90°, β=90°, γ=90°, space group=P 43 21 2	Depositor
Number of images used	Not provided	
Resolution determination method	DIFFRACTION PATTERN/LAYERLINES	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose (e^-/Å^2)	0.0357	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	TVIPS TEMCAM-F416 (4k x 4k)	Depositor

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)

validation-pack failed to run properly - this section is therefore empty.

4.5 Carbohydrates (i)

validation-pack failed to run properly - this section is therefore empty.

4.6 Ligand geometry (i)

validation-pack failed to run properly - this section is therefore empty.

4.7 Other polymers (i)

validation-pack failed to run properly - this section is therefore empty.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.