wwPDB EM Validation Summary Report

Feb 20, 2025 – 02:21 PM EST

PDB ID	:	7ULY
EMDB ID	:	EMD-26596
Title	:	MicroED structure of triclinic lysozyme
Authors	:	Clabbers, M.T.B.; Martynowycz, M.W.; Hattne, J.; Gonen, T.
Deposited on	:	2022-04-05
Resolution	:	0.87 Å(reported)

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 ⓘ 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 ⓘ) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev117
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	FAILED
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	NOT EXECUTED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

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 0.87 Å.

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

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

2 Entry composition (i)

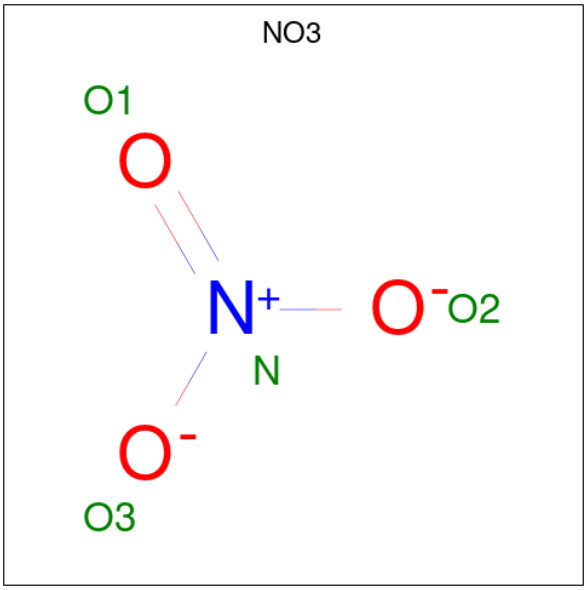
There are 3 unique types of molecules in this entry. The entry contains 2281 atoms, of which 1065 are hydrogens and 0 are deuteriums.

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 Lysozyme C.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	129	2153	672	1065	211	195	10	12	0

- Molecule 2 is NITRATE ION (three-letter code: NO3) (formula: NO_3).



Mol	Chain	Residues	Atoms				AltConf
			Total	N	O		
2	A	1	4	1	3		0
2	A	1	4	1	3		0
2	A	1	4	1	3		0
2	A	1	4	1	3		0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		AltConf
3	A	112	Total	O	0
			112	112	

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

3 Experimental information (i)

Property	Value	Source
EM reconstruction method	CRYSTALLOGRAPHY	Depositor
Imposed symmetry	3D CRYSTAL, a=26.42 Å, b=30.72 Å, c=33.01 Å, α=88.319°, β=109.095°, γ=112.075°, space group=P1	Depositor
Number of images used	Not provided	
Resolution determination method	DIFFRACTION PATTERN/LAYERLINES	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose (e^-/Å^2)	0.001	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor

4 Model quality

4.1 Standard geometry

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

4.2 Too-close contacts

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

4.3 Torsion angles

4.3.1 Protein backbone

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

4.3.2 Protein sidechains

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

4.3.3 RNA

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

4.4 Non-standard residues in protein, DNA, RNA chains

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

4.5 Carbohydrates

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

4.6 Ligand geometry

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

4.7 Other polymers

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.

5 Map visualisation

This section contains visualisations of the EMDB entry EMD-26596. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

5.1 Orthogonal projections

This section was not generated.

5.2 Central slices

This section was not generated.

5.3 Largest variance slices

This section was not generated.

5.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

5.5 Orthogonal surface views

This section was not generated.

5.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

6 Map analysis

This section contains the results of statistical analysis of the map.

6.1 Map-value distribution

This section was not generated.

6.2 Volume estimate versus contour level

This section was not generated.

6.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

7 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

8 Map-model fit

This section was not generated.