



Full wwPDB EM Validation Report ⓘ

Oct 8, 2022 – 01:08 PM EDT

PDB ID : 8E54
EMDB ID : EMD-27902
Title : MicroED structure of triclinic lysozyme recorded on K3
Authors : Clabbers, M.T.B.; Martynowycz, M.W.; Hattne, J.; Nannenga, B.L.; Gonen, T.
Deposited on : 2022-08-19
Resolution : 1.20 Å(reported)

This is a Full wwPDB EM 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/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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : **NOT EXECUTED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

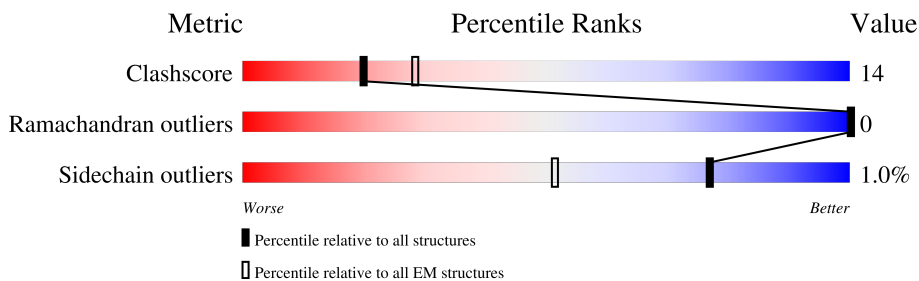
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON CRYSTALLOGRAPHY

The reported resolution of this entry is 1.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	AAA	147	 61% 27% 12%

2 Entry composition [i](#)

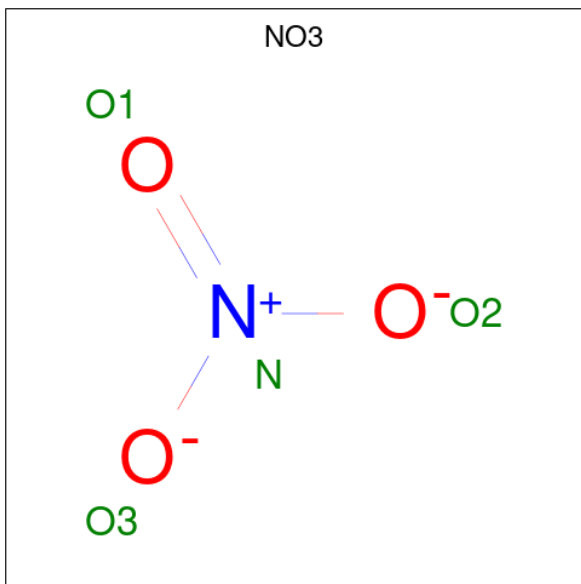
There are 3 unique types of molecules in this entry. The entry contains 1123 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Lysozyme C.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	AAA	129	1001	613	193	185	10	0	0

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



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

- Molecule 3 is water.

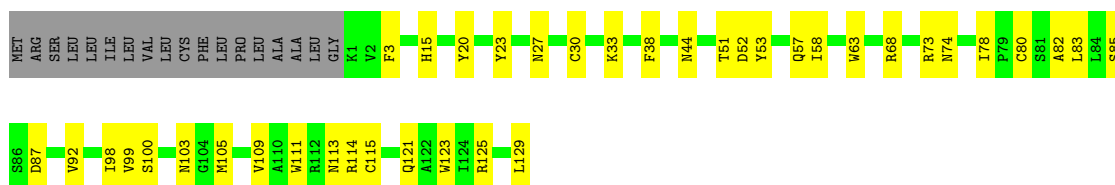
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
3	AAA	118	118	118	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Lysozyme C

Chain AAA:  61% 27% 12%



4 Experimental information

Property	Value	Source
EM reconstruction method	CRYSTALLOGRAPHY	Depositor
Imposed symmetry	3D CRYSTAL, $a=26.38 \text{ \AA}$, $b=30.76 \text{ \AA}$, $c=33 \text{ \AA}$, $\alpha=87.85^\circ$, $\beta=108.85^\circ$, $\gamma=112.60^\circ$, space group=P-1	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 ($e^-/\text{\AA}^2$)	0.001	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NO3

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	AAA	0.89	0/1021	1.10	1/1379 (0.1%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	23	TYR	CB-CG-CD1	-6.64	117.01	121.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	1001	0	959	27	0
2	AAA	4	0	0	0	0
3	AAA	118	0	0	9	0
All	All	1123	0	959	27	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (27) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:87:ASP:OD1	3:AAA:301:HOH:O	1.92	0.85
1:AAA:99:VAL:HA	1:AAA:103:ASN:O	1.88	0.73
1:AAA:44:ASN:ND2	3:AAA:303:HOH:O	2.21	0.72
1:AAA:15:HIS:HB3	1:AAA:92:VAL:HG11	1.73	0.69
1:AAA:129:LEU:OXT	3:AAA:302:HOH:O	2.10	0.68
1:AAA:85:SER:N	3:AAA:304:HOH:O	2.28	0.65
1:AAA:111:TRP:CD1	1:AAA:115:CYS:HB2	2.40	0.56
1:AAA:87:ASP:HA	3:AAA:380:HOH:O	2.07	0.54
1:AAA:33:LYS:HG2	1:AAA:123:TRP:CH2	2.47	0.50
1:AAA:63:TRP:CD2	1:AAA:98:ILE:HG12	2.47	0.50
1:AAA:58:ILE:HB	1:AAA:83:LEU:HD13	1.93	0.48
1:AAA:68:ARG:NH2	3:AAA:316:HOH:O	2.45	0.48
1:AAA:51:THR:HB	1:AAA:53:TYR:CE1	2.49	0.48
1:AAA:85:SER:HB3	3:AAA:304:HOH:O	2.13	0.47
1:AAA:121:GLN:HG2	1:AAA:125:ARG:HH21	1.80	0.46
1:AAA:73:ARG:NH1	3:AAA:324:HOH:O	2.50	0.45
1:AAA:53:TYR:CD1	1:AAA:80:CYS:HB3	2.52	0.45
1:AAA:63:TRP:CE2	1:AAA:98:ILE:HG12	2.52	0.44
1:AAA:78:ILE:HD11	1:AAA:83:LEU:HD21	1.99	0.44
1:AAA:3:PHE:HB2	1:AAA:38:PHE:HB3	2.00	0.43
1:AAA:27:ASN:HB3	1:AAA:105:MET:SD	2.59	0.43
1:AAA:109:VAL:HG22	1:AAA:113:ASN:ND2	2.33	0.43
1:AAA:82:ALA:C	3:AAA:304:HOH:O	2.57	0.43
1:AAA:73:ARG:O	1:AAA:74:ASN:C	2.57	0.42
1:AAA:20:TYR:OH	1:AAA:100:SER:OG	2.37	0.41
1:AAA:52:ASP:HB3	1:AAA:57:GLN:HB3	2.02	0.41
1:AAA:30:CYS:HB2	1:AAA:123:TRP:CD1	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AAA	127/147 (86%)	124 (98%)	3 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AAA	105/120 (88%)	104 (99%)	1 (1%)	76	47

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	114	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NO3	AAA	201	-	1,3,3	0.36	0	0,3,3	-	-

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.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-27902. 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.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal surface views

This section was not generated.

6.5 Mask visualisation

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

7 Map analysis

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

7.1 Map-value distribution

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

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

8 Fourier-Shell correlation

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

9 Map-model fit

This section was not generated.