

wwPDB EM Validation Summary Report (i)

Jan 5, 2023 – 09:21 am GMT

PDB ID : 8BQN

EMDB ID : EMD-28627

Title: Structure of empty Coxsackievirus A10 embedded in crystalline ice frozen at

-140 degree

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Deposited on : 2022-11-21

Resolution : 3.10 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB/EMDB 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 (1)) were used in the production of this report:

MolProbity: 4.02b-467

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)

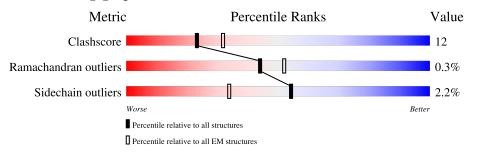
Validation Pipeline (wwPDB-VP) : 2.31.3

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $ELECTRON\ MICROSCOPY$

The reported resolution of this entry is 3.10 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 $(\# ext{Entries})$	${ m EM~structures} \ (\#{ m Entries})$		
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 <=5%

Mol	Chain	Length	Quality of chain						
1	A	298	49% 20%			31%			
2	В	255	61%		18%	•	19%	_	
3	С	240	69%			21%	• 9%	_	



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4947 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 Capsid protein VP1.

\mathbf{Mol}	Chain	Residues		\mathbf{At}	oms			AltConf	Trace
1	A	207	Total 1669	C 1072	N 288	O 298	S 11	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	VAL	ALA	variant	UNP G0YPI2
A	26	ALA	VAL	variant	UNP G0YPI2
A	141	LYS	GLU	variant	UNP G0YPI2
A	240	GLU	LYS	variant	UNP G0YPI2

• Molecule 2 is a protein called Capsid protein VP2.

Mol	Chain	Residues		Ato	oms			AltConf	Trace
2	В	207	Total 1618	C 1053	N 270	O 290	S 5	0	0

• Molecule 3 is a protein called Capsid protein VP3.

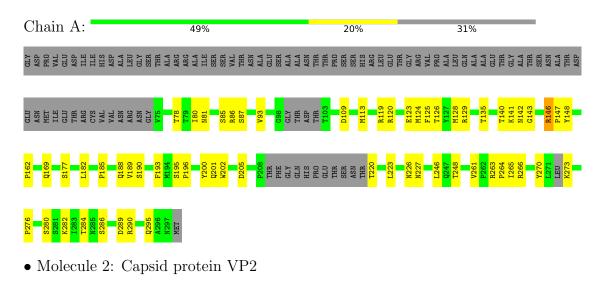
Mol	Chain	Residues		At	oms			AltConf	Trace
3	С	218	Total 1660	C 1062	N 269	O 319	S 10	0	0

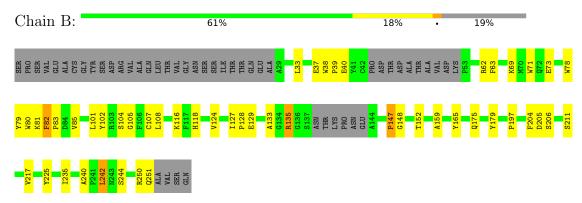


3 Residue-property plots (i)

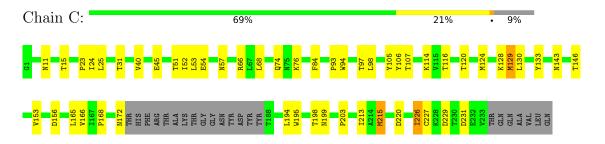
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: Capsid protein VP1





• Molecule 3: Capsid protein VP3





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	7945	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	60	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor



5 Model quality (i)

5.1 Standard geometry (i)

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		
IVIOI		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.31	0/1716	0.53	0/2329	
2	В	0.30	0/1672	0.50	0/2291	
3	С	0.30	0/1702	0.49	0/2333	
All	All	0.30	0/5090	0.51	0/6953	

There are no bond length outliers.

There are no bond angle outliers.

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	A	1669	0	1637	61	0
2	В	1618	0	1564	39	0
3	С	1660	0	1639	51	0
All	All	4947	0	4840	120	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 12.

The worst 5 of 120 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} \text{Interatomic} \\ \text{distance (Å)} \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
1:A:86:ARG:NH1	3:C:227:CYS:HB2	1.74	1.03

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Atom-1	Atom-2	$egin{aligned} & ext{Interatomic} \ & ext{distance} \ & ext{(Å)} \end{aligned}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
1:A:86:ARG:HH12	3:C:227:CYS:HB2	1.27	0.96
2:B:39:PRO:HB3	2:B:105:GLY:HA3	1.53	0.88
1:A:86:ARG:CZ	3:C:227:CYS:HB2	2.05	0.86
1:A:86:ARG:NH2	3:C:227:CYS:HB2	1.94	0.82

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	Perce	entiles
1	A	199/298 (67%)	189 (95%)	10 (5%)	0	100	100
2	В	201/255 (79%)	189 (94%)	11 (6%)	1 (0%)	29	64
3	С	214/240 (89%)	200 (94%)	13 (6%)	1 (0%)	29	64
All	All	614/793 (77%)	578 (94%)	34 (6%)	2 (0%)	44	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	В	147	PRO
3	С	226	ILE

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	A	182/255~(71%)	178 (98%)	4 (2%)	52 78
2	В	175/215 (81%)	170 (97%)	5 (3%)	42 72
3	С	184/202 (91%)	181 (98%)	3 (2%)	62 84
All	All	541/672 (80%)	529 (98%)	12 (2%)	54 78

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	В	135	ARG
2	В	242	LEU
3	С	220	ASP
3	С	129	MET
1	A	286	SER

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)

There are no ligands in this entry.

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.

