



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:00 PM BST

PDB ID : 4BIQ  
EMDB ID: : EMD-2027  
Title : Homology model of coxsackievirus A7 (CAV7) empty capsid proteins.  
Authors : Seitsonen, J.J.T.; Shakeel, S.; Susi, P.; Pandurangan, A.P.; Sinkovits, R.S.; Hyvonen, H.; Laurinmaki, P.; Yla-Pelto, J.; Topf, M.; Hyypia, T.; Butcher, S.J.  
Deposited on : 2013-04-12  
Resolution : 6.09 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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MolProbity : 4.02b-467  
Mogul : unknown  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk27241

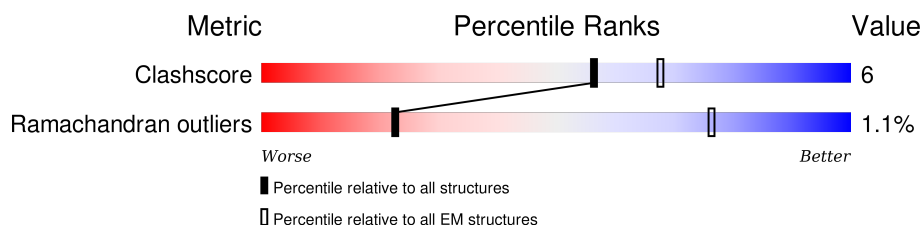
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 6.09 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	114402	924
Ramachandran outliers	111179	726

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	A	204	
2	B	254	
3	C	202	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2643 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 VP1.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	204	Total	C	N	O	0	0
			817	408	204	205		

- Molecule 2 is a protein called VP2.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	254	Total	C	N	O	0	0
			1017	508	254	255		

- Molecule 3 is a protein called VP3.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	202	Total	C	N	O	0	0
			809	404	202	203		

### 3 Residue-property plots


These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

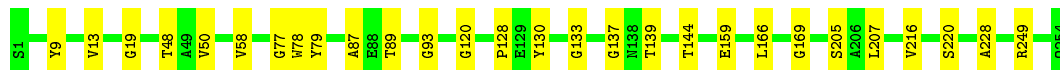
- Molecule 1: VP1

Chain A:  94% 5%



- Molecule 2: VP2

Chain B:  89% 11%



- Molecule 3: VP3

Chain C:  97% .



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	EACH MICROGRAPH	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	17	Depositor
Minimum defocus (nm)	620	Depositor
Maximum defocus (nm)	4810	Depositor
Magnification	62000	Depositor
Image detector	KODAK SO163 FILM	Depositor

## 5 Model quality

### 5.1 Standard geometry

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  >2	RMSZ	# Z  >2
1	A	1.08	0/816	0.98	0/1017
2	B	1.05	0/1016	0.93	0/1267
3	C	1.02	0/808	0.87	0/1007
All	All	1.05	0/2640	0.93	0/3291

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
2	B	0	6
All	All	0	12

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	105	PHE	Peptide
1	A	174	THR	Peptide
1	A	185	PRO	Peptide
1	A	222	GLY	Peptide
1	A	270	TYR	Peptide
1	A	275	TYR	Peptide
2	B	144	THR	Peptide
2	B	166	LEU	Peptide
2	B	228	ALA	Peptide
2	B	48	THR	Peptide

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Mol	Chain	Res	Type	Group
2	B	79	TYR	Peptide
2	B	9	TYR	Peptide

## 5.2 Too-close contacts

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	817	0	215	6	0
2	B	1017	0	272	14	0
3	C	809	0	221	4	0
All	All	2643	0	708	21	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 6.

All (21) 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)
3:C:97:GLN:CA	3:C:102:GLY:HA3	2.19	0.71
2:B:77:GLY:HA3	2:B:216:VAL:O	2.03	0.57
2:B:87:ALA:O	2:B:93:GLY:HA3	2.04	0.57
2:B:89:THR:O	2:B:93:GLY:HA3	2.06	0.55
3:C:96:TRP:O	3:C:102:GLY:HA3	2.07	0.54
2:B:205:SER:C	2:B:207:LEU:H	2.18	0.47
3:C:129:GLY:HA3	3:C:201:ASN:O	2.15	0.47
3:C:96:TRP:C	3:C:102:GLY:HA3	2.36	0.46
1:A:277:ASN:OXT	2:B:133:GLY:HA3	2.16	0.46
2:B:87:ALA:CA	2:B:93:GLY:CA	2.94	0.46
2:B:87:ALA:CA	2:B:93:GLY:HA2	2.47	0.45
2:B:137:GLY:C	2:B:139:THR:H	2.20	0.44
2:B:19:GLY:HA3	2:B:58:VAL:CA	2.49	0.43
2:B:78:TRP:CA	2:B:159:GLU:CA	2.96	0.43
1:A:277:ASN:CA	2:B:133:GLY:HA3	2.49	0.43
1:A:109:GLY:HA2	1:A:230:GLY:O	2.19	0.43
1:A:277:ASN:H	2:B:169:GLY:N	2.17	0.42
1:A:216:ASP:C	1:A:218:ASP:H	2.21	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:ASP:N	1:A:185:PRO:CA	2.85	0.40
2:B:120:GLY:HA3	2:B:220:SER:O	2.22	0.40
2:B:87:ALA:C	2:B:93:GLY:HA3	2.41	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	A	202/204 (99%)	196 (97%)	6 (3%)	0	100	100
2	B	252/254 (99%)	237 (94%)	10 (4%)	5 (2%)	9	51
3	C	200/202 (99%)	192 (96%)	6 (3%)	2 (1%)	19	64
All	All	654/660 (99%)	625 (96%)	22 (3%)	7 (1%)	23	63

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	130	TYR
2	B	249	ARG
3	C	152	GLY
2	B	13	VAL
3	C	201	ASN
2	B	50	VAL
2	B	128	PRO

### 5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

### 5.7 Other polymers ⓘ

There are no such residues in this entry.

### 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.