



wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 11:26 am GMT

PDB ID : 3J2J
EMDB ID: : EMD-5514
Title : Empty coxsackievirus A9 capsid
Authors : Shakeel, S.; Seitsonen, J.J.T.; Kajander, T.; Laurinmaki, P.; Hyypia, T.; Susi, P.; Butcher, S.J.
Deposited on : 2012-10-04
Resolution : 9.54 Å(reported)
Based on PDB ID : 1D4M

This is a wwPDB/EMDatabank EM Map/Model 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
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : recalc29047

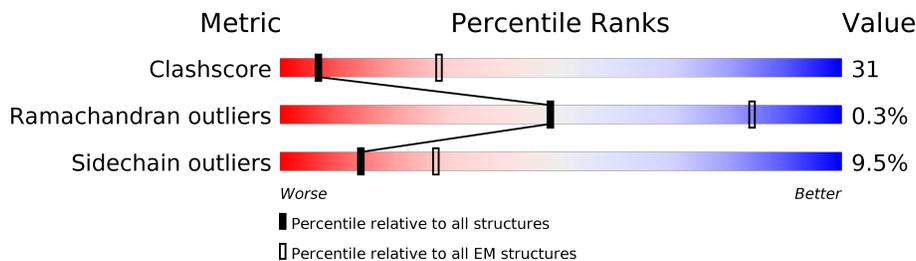
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 9.54 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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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 ≥ 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	222	
2	B	238	
3	C	252	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5601 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 Protein VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	222	1799	1152	308	329	10	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	ASN	LYS	CONFLICT	UNP P21404
A	23	ASP	HIS	CONFLICT	UNP P21404
A	80	HIS	ARG	CONFLICT	UNP P21404

- Molecule 2 is a protein called Protein VP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	238	1843	1173	302	350	18	0	0

- Molecule 3 is a protein called Protein VP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	252	1959	1239	332	372	16	0	0

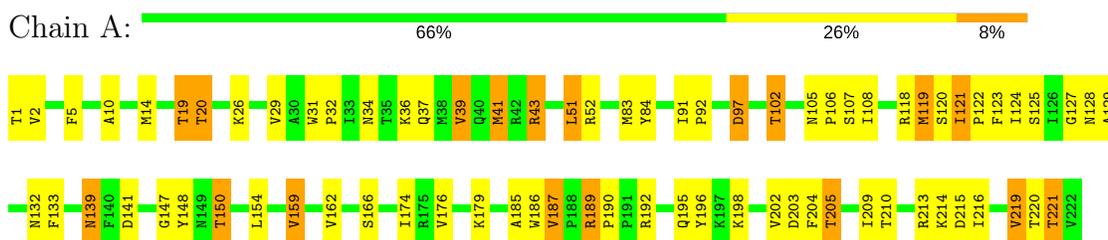
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	101	VAL	LEU	CONFLICT	UNP P21404

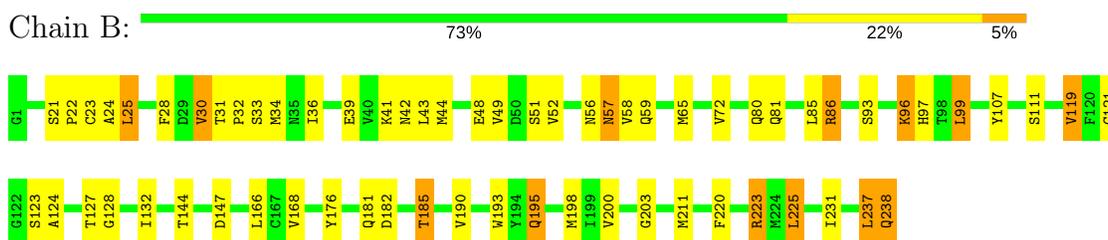
3 Residue-property plots

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

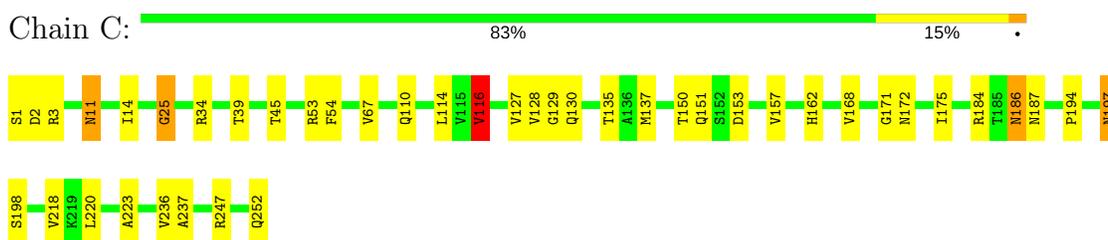
- Molecule 1: Protein VP1



- Molecule 2: Protein VP3



- Molecule 3: Protein VP2



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	1200	Depositor
Resolution determination method	FSC at 0.5 cut-off	Depositor
CTF correction method	whole micrograph	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	830	Depositor
Maximum defocus (nm)	4120	Depositor
Magnification	62000	Depositor
Image detector	Not provided	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	
		RMSZ	# Z >2	RMSZ	# Z >2
1	A	0.57	0/1855	0.81	0/2531
2	B	0.55	0/1892	0.80	0/2581
3	C	0.55	0/2009	0.81	2/2740 (0.1%)
All	All	0.56	0/5756	0.81	2/7852 (0.0%)

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
3	C	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	116	VAL	CB-CA-C	-5.86	100.27	111.40
3	C	186	ASN	CB-CA-C	-5.80	98.80	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	186	ASN	Mainchain

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	1799	0	1754	272	0
2	B	1843	0	1799	269	0
3	C	1959	0	1881	64	0
All	All	5601	0	5434	338	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 31.

The worst 5 of 338 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:A:119:MET:CE	2:B:24:ALA:CB	1.81	1.59
1:A:118:ARG:CD	2:B:21:SER:CB	1.79	1.57
1:A:118:ARG:CG	2:B:21:SER:CB	1.81	1.56
1:A:216:ILE:HB	2:B:58:VAL:CG1	1.38	1.54
1:A:118:ARG:CD	2:B:21:SER:HB3	1.30	1.51

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	220/222 (99%)	207 (94%)	12 (6%)	1 (0%)	32	74
2	B	236/238 (99%)	228 (97%)	8 (3%)	0	100	100
3	C	250/252 (99%)	227 (91%)	22 (9%)	1 (0%)	38	77
All	All	706/712 (99%)	662 (94%)	42 (6%)	2 (0%)	48	81

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	VAL
3	C	25	GLY

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	201/201 (100%)	177 (88%)	24 (12%)	6	27
2	B	211/211 (100%)	194 (92%)	17 (8%)	14	44
3	C	209/209 (100%)	191 (91%)	18 (9%)	12	42
All	All	621/621 (100%)	562 (90%)	59 (10%)	14	36

5 of 59 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	57	ASN
2	B	168	VAL
3	C	197	ASN
2	B	72	VAL
2	B	86	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	57	ASN
2	B	195	GLN
3	C	163	ASN
2	B	97	HIS
2	B	206	ASN

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 carbohydrates 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.