



wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 11:25 am GMT

PDB ID : 3J22
EMDB ID: : EMD-5465
Title : The Enterovirus 71 A-particle
Authors : Shingler, K.L.
Deposited on : 2012-08-13
Resolution : 6.30 Å(reported)
Based on PDB ID : 3VBU

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

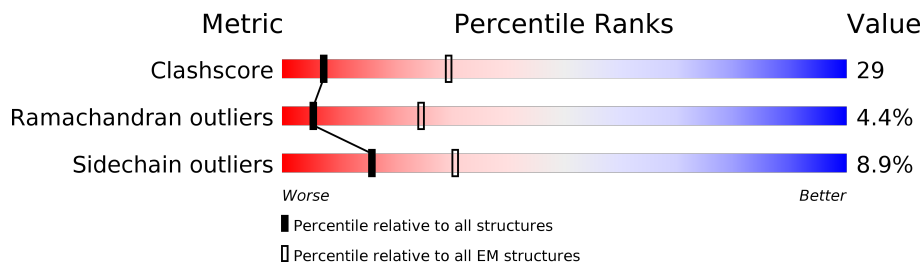
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.30 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	225	
2	B	237	
3	C	239	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5397 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	218	Total	C	N	O	S	0	0
			1724	1107	290	316	11		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	225	MET	CYS	SEE REMARK 999	UNP B2ZUN0

- Molecule 2 is a protein called capsid protein VP0.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	237	Total	C	N	O	S	0	0
			1834	1179	301	346	8		

- Molecule 3 is a protein called capsid protein VP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	239	Total	C	N	O	S	0	0
			1839	1182	306	340	11		

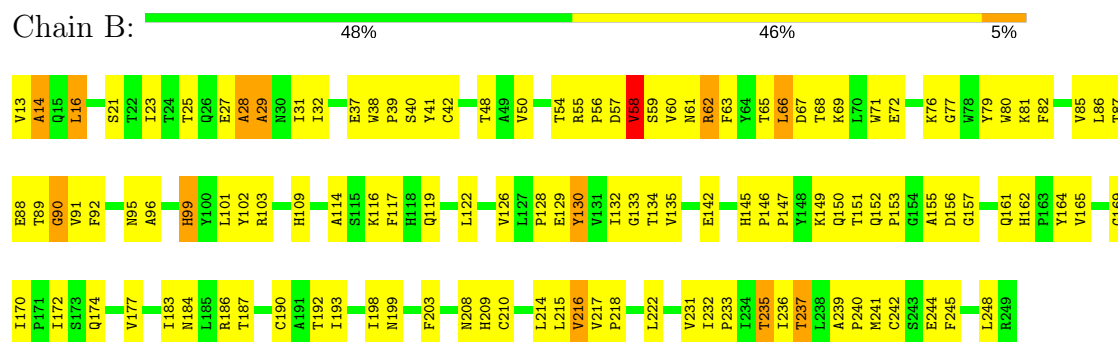
3 Residue-property plots

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.

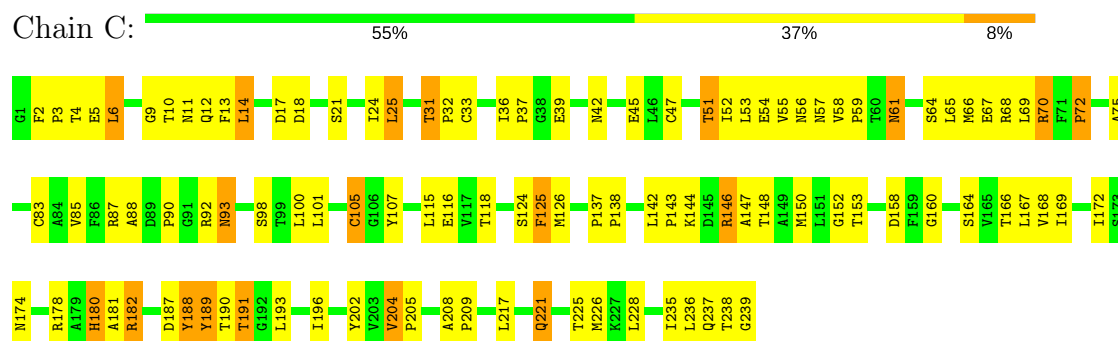
• Molecule 1: capsid protein VP1



• Molecule 2: capsid protein VP0



• Molecule 3: capsid protein VP3



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	11436	Depositor
Resolution determination method	FSC at 0.5 cut-off	Depositor
CTF correction method	auto3DEM	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	15	Depositor
Minimum defocus (nm)	1730	Depositor
Maximum defocus (nm)	4280	Depositor
Magnification	50000	Depositor
Image detector	Kodak SO-163 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	0.53	0/1776	0.78	0/2419
2	B	0.56	0/1889	0.75	1/2592 (0.0%)
3	C	0.50	0/1891	0.73	0/2586
All	All	0.53	0/5556	0.75	1/7597 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	248	LEU	CA-CB-CG	5.64	128.28	115.30

There are no chirality outliers.

There are no planarity outliers.

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	1724	0	1688	118	0
2	B	1834	0	1774	123	0
3	C	1839	0	1814	123	0
All	All	5397	0	5276	312	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 29.

The worst 5 of 312 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:281:GLY:HA3	2:B:135:VAL:HG13	1.14	1.09
1:A:229:MET:HE2	1:A:231:GLY:H	1.16	1.07
1:A:156:VAL:HG22	1:A:232:THR:HB	1.42	0.99
2:B:134:THR:HG23	2:B:146:PRO:HG3	1.47	0.96
2:B:164:TYR:HA	3:C:66:MET:HE3	1.49	0.94

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	214/225 (95%)	188 (88%)	15 (7%)	11 (5%)	2	26
2	B	235/237 (99%)	196 (83%)	31 (13%)	8 (3%)	4	34
3	C	237/239 (99%)	202 (85%)	24 (10%)	11 (5%)	3	28
All	All	686/701 (98%)	586 (85%)	70 (10%)	30 (4%)	5	29

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	85	SER
2	B	28	ALA
2	B	29	ALA
2	B	58	VAL
3	C	93	ASN

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	187/193 (97%)	170 (91%)	17 (9%)	11	38
2	B	201/201 (100%)	186 (92%)	15 (8%)	16	48
3	C	199/199 (100%)	179 (90%)	20 (10%)	9	33
All	All	587/593 (99%)	535 (91%)	52 (9%)	16	39

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	76	LYS
2	B	216	VAL
3	C	204	VAL
2	B	99	HIS
2	B	126	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	145	HIS
2	B	150	GLN
3	C	93	ASN
2	B	119	GLN
3	C	154	HIS

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.