



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:57 PM BST

PDB ID : 4C0U
EMDB ID: : EMD-2397
Title : Cryo-EM reconstruction of enterovirus 71 in complex with a neutralizing antibody E18
Authors : Plevka, P.; Perera, R.; Cardoso, J.; Suksatu, A.; Kuhn, R.J.; Rossmann, M.G.
Deposited on : 2013-08-08
Resolution : 10.00 Å(reported)
Based on PDB ID : 3ZFE

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
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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

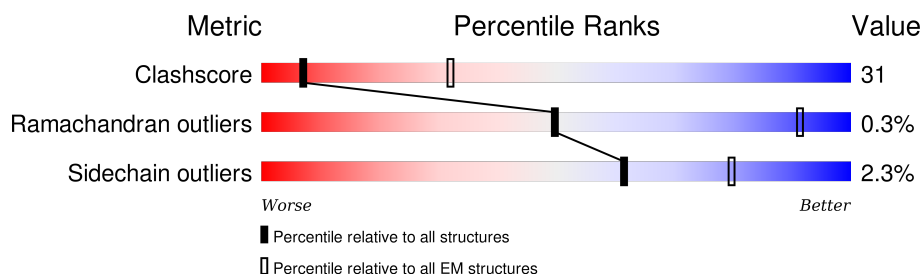
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 10.00 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
Sidechain outliers	111093	686

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	298	53% 21% . 24%
2	B	254	77% 18% . .
3	C	242	67% 32% .
4	Y	217	68% 31% .
5	Z	220	65% 35%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8074 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	225	Total	C	N	O	S	0	0
			1786	1144	302	329	11		

- Molecule 2 is a protein called VP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	244	Total	C	N	O	S	0	0
			1893	1212	313	359	9		

- Molecule 3 is a protein called VP3.

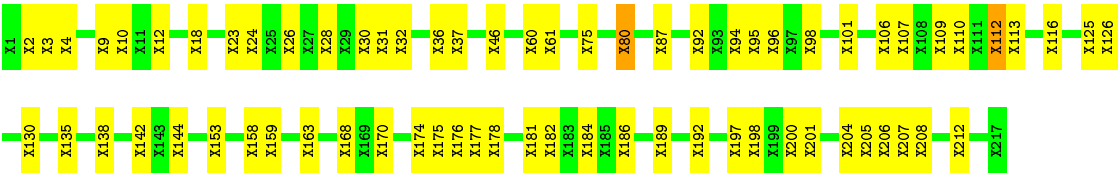
Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	242	Total	C	N	O	S	0	0
			1866	1198	311	345	12		

- Molecule 4 is a protein called FAB EV18 4 D6-1 F1 G9.

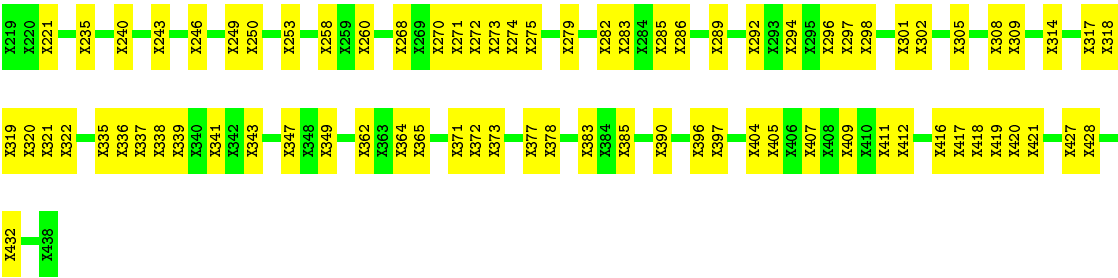
Mol	Chain	Residues	Atoms				AltConf	Trace
4	Y	217	Total	C	N	O	0	0
			1265	831	217	217		

- Molecule 5 is a protein called FAB EV18 4 D6-1 F1 G9.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	Z	220	Total	C	N	O	0	0
			1264	824	220	220		



● Molecule 5: FAB EV18 4 D6-1 F1 G9



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, 1	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	CTF DETERMINED FOR ALL PARTICLES FROM ONE FILM, PHASE FLIP	Depositor
Microscope	FEI/PHILIPS CM200FEG/UT	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	18	Depositor
Minimum defocus (nm)	0.75	Depositor
Maximum defocus (nm)	4.5	Depositor
Magnification	50000	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	0.32	0/1841	0.60	0/2509
2	B	0.32	0/1948	0.63	1/2670 (0.0%)
3	C	0.32	0/1920	0.59	0/2626
All	All	0.32	0/5709	0.61	1/7805 (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
4	Y	0	4
5	Z	0	2
All	All	0	6

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	82	PHE	N-CA-C	6.68	129.03	111.00

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	Y	112	UNK	Mainchain
4	Y	46	UNK	Peptide
4	Y	80	UNK	Peptide
4	Y	98	UNK	Peptide
5	Z	338	UNK	Mainchain

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	1786	0	1735	142	0
2	B	1893	0	1827	93	0
3	C	1866	0	1832	244	0
4	Y	1265	0	1180	92	0
5	Z	1264	0	1120	166	0
All	All	8074	0	7694	487	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 487 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)
4:Y:92:UNK:CG	4:Y:92:UNK:CB	1.77	1.63
4:Y:138:UNK:CB	4:Y:138:UNK:CG	1.78	1.59
5:Z:365:UNK:CG	5:Z:365:UNK:CB	1.78	1.59
5:Z:314:UNK:CB	5:Z:314:UNK:CG	1.77	1.59
5:Z:240:UNK:HG1	5:Z:314:UNK:CG	1.10	1.58

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	223/298 (75%)	209 (94%)	13 (6%)	1 (0%)	39 80

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	242/254 (95%)	224 (93%)	18 (7%)	0	100	100
3	C	240/242 (99%)	227 (95%)	12 (5%)	1 (0%)	39	80
All	All	705/794 (89%)	660 (94%)	43 (6%)	2 (0%)	50	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	58	VAL
1	A	262	ILE

5.3.2 Protein sidechains ⓘ

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	194/253 (77%)	189 (97%)	5 (3%)	54	80
2	B	208/215 (97%)	202 (97%)	6 (3%)	50	78
3	C	203/203 (100%)	200 (98%)	3 (2%)	72	88
All	All	605/671 (90%)	591 (98%)	14 (2%)	61	83

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	48	THR
2	B	86	LEU
3	C	70	ARG
2	B	12	ARG
2	B	111	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	270	ASN
3	C	237	GLN

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Mol	Chain	Res	Type
2	B	109	HIS
1	A	268	ASN
3	C	76	GLN

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.