wwPDB EM Map/Model Validation Report (i)

Oct 17, 2016 – 12:28 PM EDT

PDB ID	:	3JAU
EMDB ID:	:	EMD-6366
Title	:	The cryoEM map of EV71 mature viron in complex with the Fab fragment of antibody D5
Authors	:	Fan, C.; Ye, X.H.; Ku, Z.Q.; Zuo, T.; Kong, L.L.; Zhang, C.; Shi, J.P.; Liu, Q.W.; Chen, T.; Zhang, Y.Y.; Jiang, W.; Zhang, L.Q.; Huang, Z.; Cong, Y.
Deposited on	:	2015-06-24
Resolution	:	4.80 Å(reported)
Based on PDB ID	:	3VBS

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

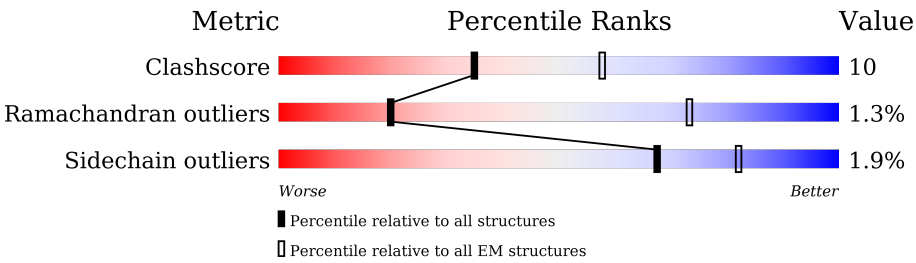
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

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 4.80 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	17	71% 29%
2	H	117	74% 18% 6% •
3	L	111	86% 14%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 1915 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
			Total	C	N	O		
1	A	17	142	90	22	30	0	0

- Molecule 2 is a protein called Heavy chain of Fab fragment variable region of antibody D5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	H	117	920	582	148	188	2	0	0

- Molecule 3 is a protein called Light chain of Fab fragment variable region of antibody D5.

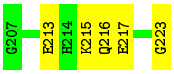
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	L	111	853	539	142	169	3	0	0

3 Residue-property plots (i)

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.

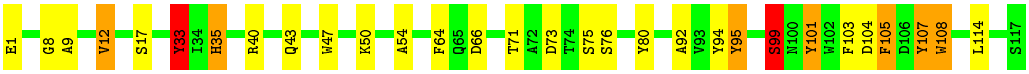
- Molecule 1: Capsid protein VP1

Chain A:



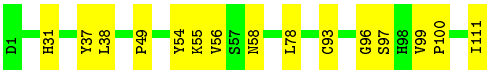
- Molecule 2: Heavy chain of Fab fragment variable region of antibody D5

Chain H:



- Molecule 3: Light chain of Fab fragment variable region of antibody D5

Chain L:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	2902	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^{-}/\text{Å}^{2})$	16	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	37000	Depositor
Image detector	FEI FALCON II (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	
		RMSZ	$\#\|Z\| >2$	RMSZ	$\#\|Z\| >2$
1	A	1.64	2/146 (1.4%)	0.80	1/193 (0.5%)
2	H	1.72	9/943 (1.0%)	1.98	25/1284 (1.9%)
3	L	0.80	2/873 (0.2%)	0.52	1/1183 (0.1%)
All	All	1.38	13/1962 (0.7%)	1.44	27/2660 (1.0%)

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
2	H	0	3

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	223	GLY	C-O	-14.52	1.00	1.23
3	L	111	ILE	C-OXT	-12.10	1.00	1.23
3	L	111	ILE	C-O	-12.04	1.00	1.23
1	A	223	GLY	C-OXT	-12.04	1.00	1.23
2	H	108	TRP	CG-CD1	7.53	1.47	1.36

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	103	PHE	CB-CG-CD1	-13.31	111.48	120.80
2	H	80	TYR	CB-CG-CD1	-13.21	113.07	121.00
2	H	80	TYR	CB-CG-CD2	11.51	127.91	121.00
2	H	107	TYR	CB-CG-CD2	9.39	126.63	121.00
2	H	107	TYR	CB-CG-CD1	-9.10	115.54	121.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	105	PHE	Sidechain
2	H	33	TYR	Peptide
2	H	95	TYR	Sidechain

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	142	0	123	3	0
2	H	920	0	868	7	0
3	L	853	0	832	31	0
All	All	1915	0	1823	39	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 10.

The worst 5 of 39 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:L:31:HIS:CE1	3:L:97:SER:OG	1.69	1.43
3:L:31:HIS:CD2	3:L:37:TYR:HD2	1.39	1.39
3:L:31:HIS:CD2	3:L:37:TYR:CD2	2.17	1.32
3:L:31:HIS:NE2	3:L:37:TYR:HB2	1.47	1.28
3:L:31:HIS:ND1	3:L:97:SER:OG	1.89	1.05

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	15/17 (88%)	14 (93%)	1 (7%)	0	100	100
2	H	115/117 (98%)	106 (92%)	6 (5%)	3 (3%)	7	46
3	L	109/111 (98%)	105 (96%)	4 (4%)	0	100	100
All	All	239/245 (98%)	225 (94%)	11 (5%)	3 (1%)	20	60

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	107	TYR
2	H	104	ASP
2	H	99	SER

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	14/14 (100%)	14 (100%)	0	100	100
2	H	100/100 (100%)	97 (97%)	3 (3%)	48	78
3	L	97/97 (100%)	96 (99%)	1 (1%)	82	92
All	All	211/211 (100%)	207 (98%)	4 (2%)	67	86

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	12	VAL
2	H	50	LYS
2	H	75	SER
3	L	78	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	98	ASN
3	L	31	HIS

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.