

wwPDB EM Validation Summary Report (i)

Nov 4, 2024 – 06:41 PM JST

PDB ID : 8Y0Q

EMDB ID : EMD-38814

Title: Complex of FMDV O/18074 and inter-serotype broadly neutralizing antibodies

pOA-2

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Resolution : 2.44 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

EMDB validation analysis : FAILED

MolProbity: 4.02b-467

Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)

MapQ : FAILED

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

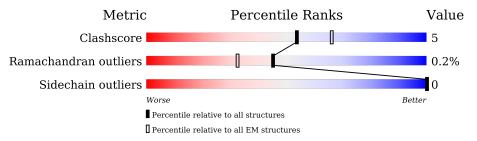
Validation Pipeline (wwPDB-VP) : 2.39

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 2.44 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 $(\# \mathrm{Entries})$	${ m EM\ structures} \ (\#{ m Entries})$
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	1	213	75% 11%	• 14%
2	2	218	83%	11% 6%
3	3	220	85%	14%
4	4	85	54% 46%	
5	Н	123	84%	16%
6	L	109	87%	13%



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6858 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 of capsid protein.

Mol	Chain	Residues	${f Atoms}$					AltConf	Trace
1	1	184	Total	С	N	О	S	0	0
1	1	101	1441	914	252	272	3		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	33	THR	ALA	conflict	UNP A0A1P8DYS7
1	47	GLU	GLN	conflict	UNP A0A1P8DYS7
1	141	THR	ALA	conflict	UNP A0A1P8DYS7
1	194	ILE	THR	conflict	UNP A0A1P8DYS7
1	199	ALA	ASP	conflict	UNP A0A1P8DYS7
1	209	VAL	ALA	conflict	UNP A0A1P8DYS7

• Molecule 2 is a protein called VP2 of capsid protein.

Mol	Chain	Residues		Ato	AltConf	Trace			
2	2	205	Total 1608	C 1025	N 276	O 301	S 6	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	182	THR	MET	conflict	UNP J9PGT1
2	190	LYS	ASN	conflict	UNP J9PGT1
2	209	TYR	HIS	conflict	UNP J9PGT1

• Molecule 3 is a protein called VP3 of capsid protein.

\mathbf{Mol}	Chain	Residues	Atoms					AltConf	Trace	
3	3	219	Total	С	N	О	S	0	0	1
9	9		1674	1073	273	320	8			

There are 5 discrepancies between the modelled and reference sequences:



Chain	Residue	Modelled	Actual	Comment	Reference
3	56	ARG	HIS	conflict	UNP A0A1C6ZW66
3	73	LYS	VAL	conflict	UNP A0A1C6ZW66
3	75	VAL	ALA	conflict	UNP A0A1C6ZW66
3	134	THR	LYS	conflict	UNP A0A1C6ZW66
3	219	ALA	THR	conflict	UNP A0A1C6ZW66

 \bullet Molecule 4 is a protein called VP4 of capsid protein.

Mol	Chain	Residues		Ato	ms	AltConf	Trace		
4	4	46	Total 356	C 224	N 58	O 72	S 2	0	0

 $\bullet\,$ Molecule 5 is a protein called pOA2 VH.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	П	123	Total	С	N	О	S	0	0
5	11	123	964	604	171	183	6	U	U

• Molecule 6 is a protein called pOA2 VL.

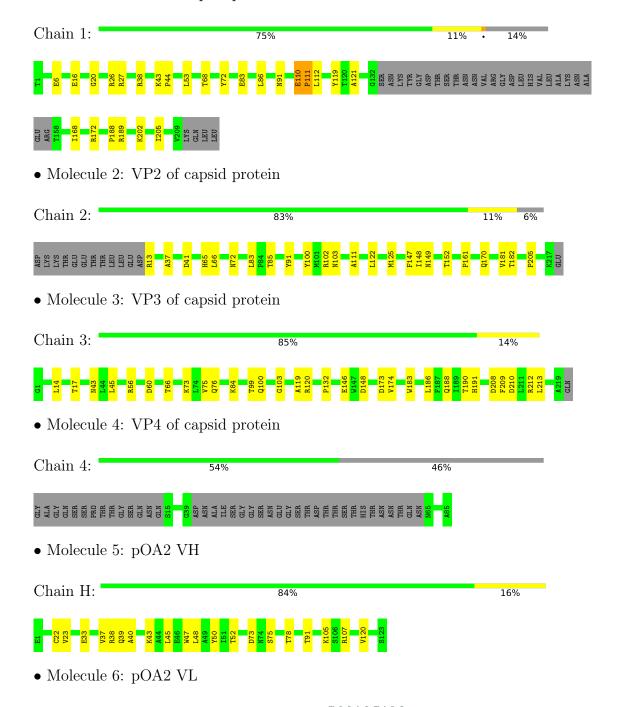
Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	109	Total 815	C 515	N 135	O 161	S 4	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: VP1 of capsid protein



Chain L: 87% 13%



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	3202	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	30	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k 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	
IVIOI		RMSZ	# Z > 5	RMSZ	# Z > 5
1	1	0.30	0/1474	0.52	0/2016
2	2	0.31	0/1650	0.52	0/2255
3	3	0.30	0/1722	0.49	0/2356
4	4	0.28	0/362	0.41	0/486
5	Н	0.30	0/985	0.52	0/1330
6	L	0.28	0/834	0.49	0/1138
All	All	0.30	0/7027	0.50	0/9581

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1	1441	0	1448	18	0
2	2	1608	0	1576	16	0
3	3	1674	0	1614	22	0
4	4	356	0	327	0	0
5	Н	964	0	928	12	0
6	L	815	0	792	9	0
All	All	6858	0	6685	67	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 5.



The worst 5 of 67 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{array}{ll} ext{Interatomic} \ ext{distance} \ (ext{Å}) \end{array}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$	
1:1:91:ASN:HD21	1:1:121:ALA:HA	1.48	0.78	
2:2:72:ASN:ND2	6:L:95:ASN:OD1	2.29	0.66	
6:L:34:PRO:HD2	6:L:52:ALA:HB2	1.78	0.66	
2:2:103:ASN:HD22	2:2:205:PRO:HB3	1.63	0.64	
1:1:110:GLU:HB3	1:1:111:PRO:HD3	1.81	0.63	

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	Percentil	les
1	1	180/213 (84%)	171 (95%)	7 (4%)	2 (1%)	12 12	2
2	2	203/218 (93%)	192 (95%)	11 (5%)	0	100 10)0
3	3	217/220~(99%)	212 (98%)	5 (2%)	0	100 10	00
4	4	42/85 (49%)	40 (95%)	2 (5%)	0	100 10)0
5	Н	121/123~(98%)	117 (97%)	4 (3%)	0	100 10)0
6	L	107/109 (98%)	104 (97%)	3 (3%)	0	100 10)0
All	All	870/968 (90%)	836 (96%)	32 (4%)	2 (0%)	45 53	}

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	110	GLU
1	1	111	PRO



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	Perce	ntiles
1	1	156/181~(86%)	156 (100%)	0	100	100
2	2	177/190 (93%)	177 (100%)	0	100	100
3	3	177/178 (99%)	177 (100%)	0	100	100
4	4	37/68 (54%)	37 (100%)	0	100	100
5	Н	102/102 (100%)	102 (100%)	0	100	100
6	L	89/89 (100%)	89 (100%)	0	100	100
All	All	738/808 (91%)	738 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	91	ASN
2	2	72	ASN
2	2	103	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 oligosaccharides 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.

