W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB EM Validation Summary Report (i)

Nov 7, 2024 – 10:07 PM JST

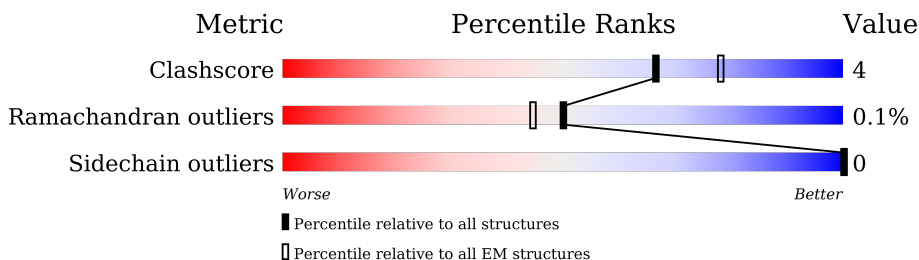|		
PDB ID	:	8Y0R
EMDB ID	:	EMD-38815
Title	:	Complex of FMDV A/WH/CHA/09 and inter-serotype broadly neutralizing antibodies pOA-2
Authors	:	Wu, S.; Lei, D.
Deposited on	:	2024-01-23
Resolution	:	2.52 Å(reported)

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 2.52 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	Percentile Ranks	Value
Clashscore		4
Ramachandran outliers		0.1%
Sidechain outliers		0

Worse   *Better*

▮ Percentile relative to all structures
❑ Percentile relative to all EM structures

Metric	Whole archive (#Entries)	EM structures (#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	212	82% 9% 8%
2	2	218	91% 5% 5%
3	3	221	89% 11%
4	4	85	51% • 46%
5	H	123	90% 10%
6	L	109	83% 17%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6998 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	Atoms					AltConf	Trace
1	1	194	Total 1522	C 962	N 277	O 278	S 5	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	133	ASN	THR	conflict	UNP D0E7R9
1	193	LYS	GLU	conflict	UNP D0E7R9

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	208	Total 1650	C 1049	N 283	O 313	S 5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	220	Total 1691	C 1077	N 277	O 328	S 9	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	121	TYR	CYS	conflict	UNP D0E7R9

- Molecule 4 is a protein called VP4 of capsid protein.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	77	THR	SER	conflict	UNP E4W502

- Molecule 5 is a protein called pOA2 VH.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	123	Total	C	N	O	S	0	0
			964	604	171	183	6		

- Molecule 6 is a protein called pOA2 VL.

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

3   Residue-property plots ⓘ

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.
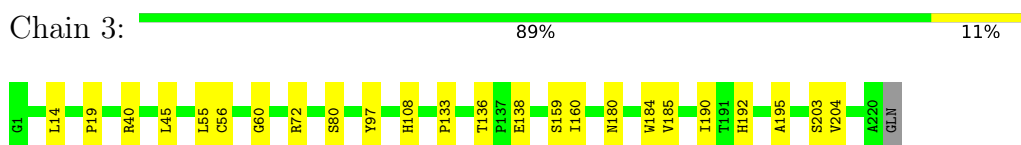
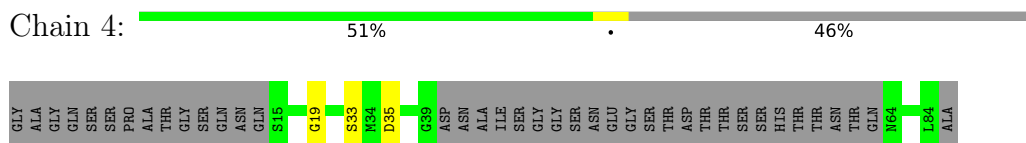• Molecule 1: VP1 of capsid protein
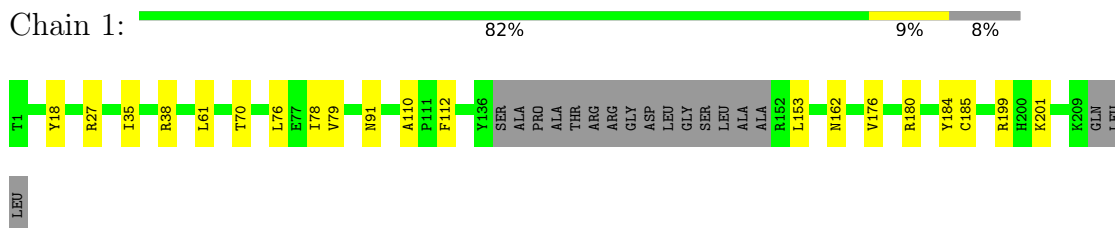
Chain 1:

• Molecule 2: VP2 of capsid protein
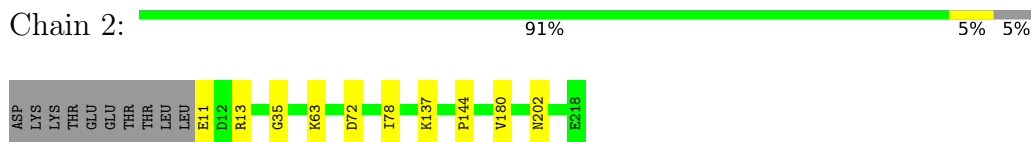
Chain 2:

• Molecule 3: VP3 of capsid protein

Chain 3:

• Molecule 4: VP4 of capsid protein

Chain 4:

• Molecule 5: pOA2 VH
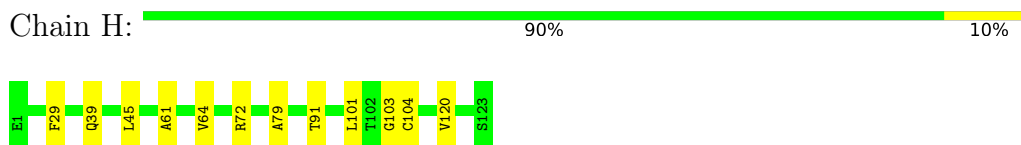
Chain H:

• Molecule 6: pOA2 VL

Chain L:

83%

17%

Q1 T2 V3 I4 Q5 T29 G30 T31 S35 Q38 L48 I49 Y50 D86 Y87 F88 C89 C90 L91 Y92 K93 T94 G101 H105 L109
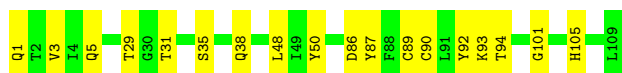
4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	7341	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
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 ⓘ

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	$\#|Z|>5$	RMSZ	$\#|Z|>5$
1	1	0.31	0/1558	0.54	0/2124
2	2	0.32	0/1695	0.50	0/2307
3	3	0.33	0/1739	0.49	0/2381
4	4	0.29	0/362	0.42	0/487
5	H	0.25	0/985	0.52	0/1330
6	L	0.26	0/834	0.46	0/1138
All	All	0.30	0/7173	0.50	0/9767

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 ⓘ

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	1522	0	1526	17	0
2	2	1650	0	1603	6	0
3	3	1691	0	1620	18	0
4	4	356	0	327	4	0
5	H	964	0	928	8	0
6	L	815	0	792	10	0
All	All	6998	0	6796	51	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 4.

The worst 5 of 51 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)
3:3:72:ARG:HH21	3:3:190:ILE:HA	1.58	0.66
3:3:19:PRO:HB2	4:4:19:GLY:H	1.65	0.61
1:1:76:LEU:HD11	1:1:176:VAL:HB	1.82	0.60
1:1:180:ARG:NH2	4:4:35:ASP:OD2	2.36	0.58
5:H:101:LEU:HG	5:H:104:CYS:HB3	1.86	0.57

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	1	190/212 (90%)	181 (95%)	8 (4%)	1 (0%)	25	42
2	2	206/218 (94%)	197 (96%)	9 (4%)	0	100	100
3	3	218/221 (99%)	212 (97%)	6 (3%)	0	100	100
4	4	42/85 (49%)	41 (98%)	1 (2%)	0	100	100
5	H	121/123 (98%)	120 (99%)	1 (1%)	0	100	100
6	L	107/109 (98%)	103 (96%)	4 (4%)	0	100	100
All	All	884/968 (91%)	854 (97%)	29 (3%)	1 (0%)	50	67

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	110	ALA

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	1	163/175 (93%)	163 (100%)	0	100	100
2	2	184/194 (95%)	184 (100%)	0	100	100
3	3	181/182 (100%)	181 (100%)	0	100	100
4	4	38/67 (57%)	38 (100%)	0	100	100
5	H	102/102 (100%)	102 (100%)	0	100	100
6	L	89/89 (100%)	89 (100%)	0	100	100
All	All	757/809 (94%)	757 (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. There are no such sidechains identified.

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 oligosaccharides 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.