



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:37 PM BST

PDB ID : 1QGC
EMDB ID: : unknown
Title : STRUCTURE OF THE COMPLEX OF A FAB FRAGMENT OF A NEUTRALIZING ANTIBODY WITH FOOT AND MOUTH DISEASE VIRUS
Authors : Fita, I.
Deposited on : 1999-04-23
Resolution : 30.00 Å(reported)
Based on PDB ID : 1FMD

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 : 1.7.1 (RC1), CSD as537be (2016)
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

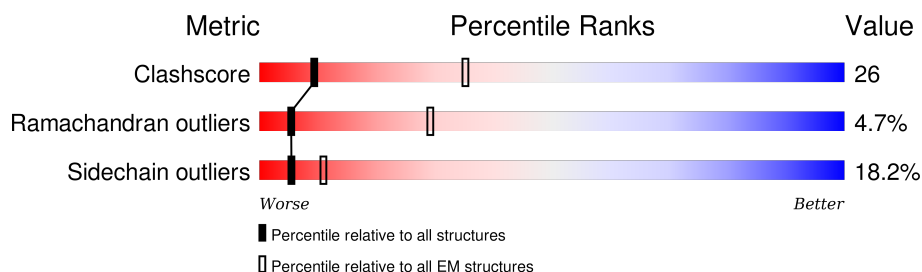
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 30.00 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	1	207	
2	2	218	
3	3	219	
4	4	218	
5	A	220	
6	5	24	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8279 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 PROTEIN (VIRUS CAPSID PROTEIN VP1).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	183	Total	C	N	O	S	0	0
			1416	893	253	267	3		

- Molecule 2 is a protein called PROTEIN (VIRUS CAPSID PROTEIN VP2).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	218	Total	C	N	O	S	0	0
			1680	1061	296	316	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	50	ALA	GLY	CONFLICT	UNP Q9QCE2

- Molecule 3 is a protein called PROTEIN (VIRUS CAPSID PROTEIN VP3).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	219	Total	C	N	O	S	0	0
			1690	1075	277	327	11		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	168	THR	ALA	CONFLICT	UNP P15072

- Molecule 4 is a protein called PROTEIN (IMMUNOGLOBULIN LIGHT CHAIN).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	218	Total	C	N	O	S	0	0
			1683	1042	287	347	7		

- Molecule 5 is a protein called PROTEIN (IMMUNOGLOBULIN HEAVY CHAIN).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	220	Total	C	N	O	S	0	0
			1644	1039	275	320	10		

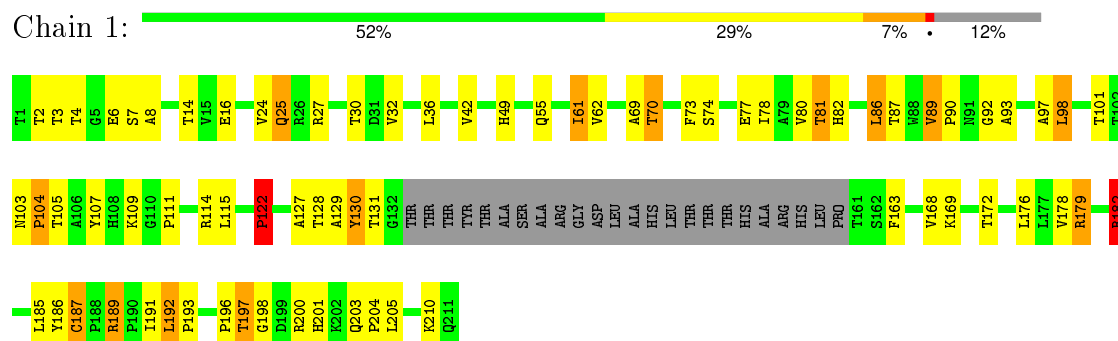
- Molecule 6 is a protein called PROTEIN (GH-LOOP FROM VIRUS CAPSID PROTEIN VP1).

Mol	Chain	Residues	Atoms				AltConf	Trace
6	5	24	Total	C	N	O	0	0
			166	102	29	35		

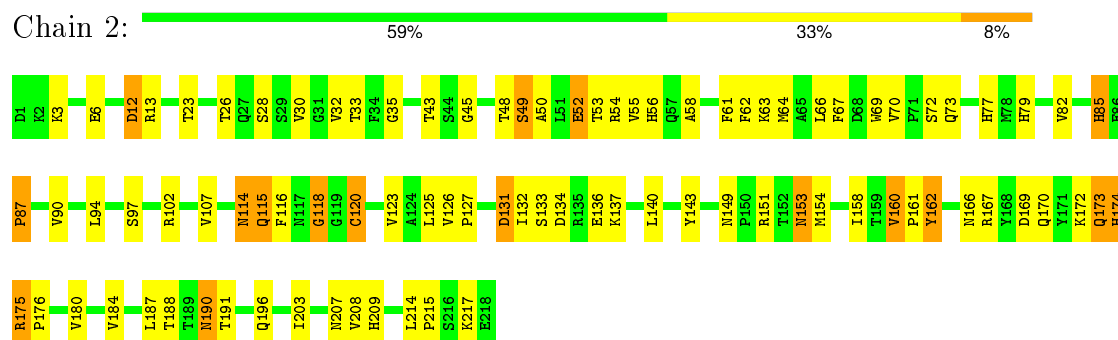
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

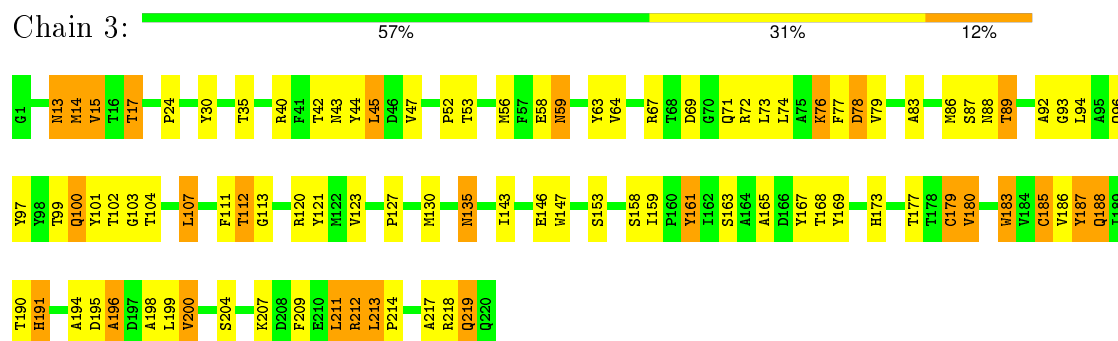
- Molecule 1: PROTEIN (VIRUS CAPSID PROTEIN VP1)



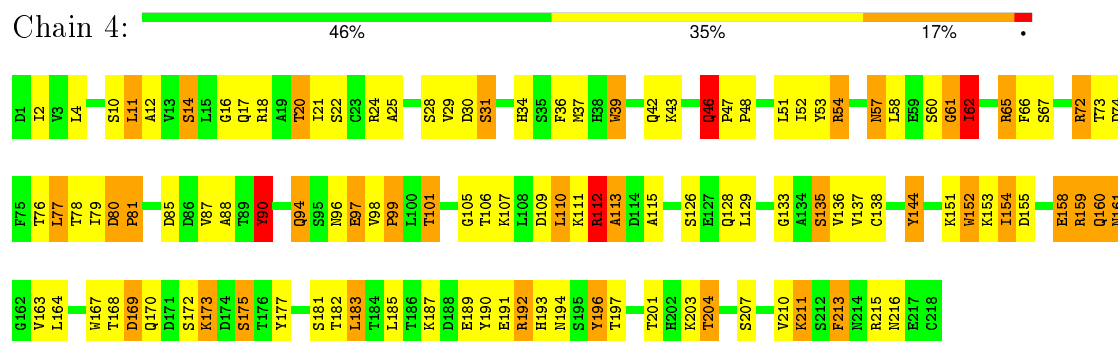
- Molecule 2: PROTEIN (VIRUS CAPSID PROTEIN VP2)



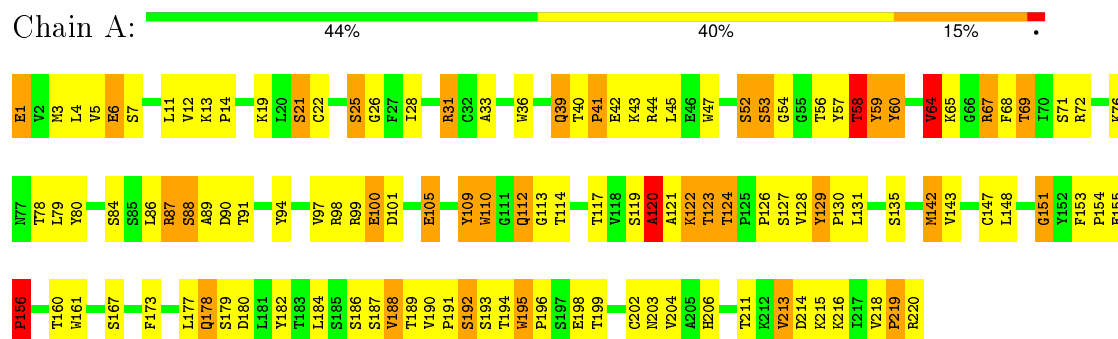
- Molecule 3: PROTEIN (VIRUS CAPSID PROTEIN VP3)



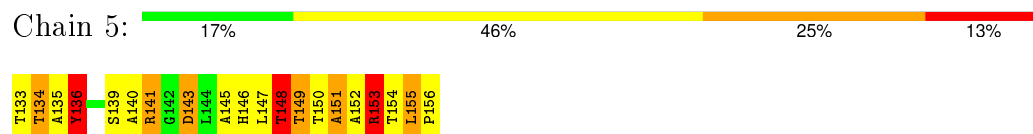
- Molecule 4: PROTEIN (IMMUNOGLOBULIN LIGHT CHAIN)



• Molecule 5: PROTEIN (IMMUNOGLOBULIN HEAVY CHAIN)



• Molecule 6: PROTEIN (GH-LOOP FROM VIRUS CAPSID PROTEIN VP1)



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	JEOL 1200 EX-II	Depositor
Voltage (kV)	100	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2000	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	30000	Depositor
Image detector	KODAK SO163 FILM	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: OCS

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	1	0.55	0/1449	0.86	4/1982 (0.2%)
2	2	0.54	0/1723	0.83	1/2352 (0.0%)
3	3	0.57	0/1739	0.88	1/2377 (0.0%)
4	4	1.18	4/1713 (0.2%)	2.07	42/2329 (1.8%)
5	A	1.11	0/1685	2.19	68/2300 (3.0%)
6	5	0.78	0/168	1.91	6/232 (2.6%)
All	All	0.84	4/8477 (0.0%)	1.52	122/11572 (1.1%)

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
3	3	0	1
4	4	0	6
5	A	0	3
All	All	0	10

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	4	112	ARG	C-N	-17.55	0.93	1.34
4	4	28	SER	CA-CB	6.39	1.62	1.52
4	4	39	TRP	CG-CD2	-5.49	1.34	1.43
4	4	54	ARG	CG-CD	5.03	1.64	1.51

The worst 5 of 122 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	120	ALA	CA-C-N	-23.53	65.44	117.20
4	4	112	ARG	CA-C-N	-22.66	67.35	117.20
4	4	112	ARG	C-N-CA	-22.41	65.67	121.70
5	A	120	ALA	C-N-CA	-22.31	65.92	121.70
5	A	120	ALA	O-C-N	18.86	152.88	122.70

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	3	30	TYR	Sidechain
4	4	46	GLN	Peptide
4	4	80	ASP	Peptide
4	4	90	TYR	Sidechain
4	4	98	VAL	Peptide

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	1416	0	1415	69	0
2	2	1680	0	1608	64	0
3	3	1690	0	1603	81	0
4	4	1683	0	1605	78	0
5	A	1644	0	1620	95	0
6	5	166	0	161	84	0
All	All	8279	0	8012	429	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 26.

The worst 5 of 429 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)
5:A:13:LYS:CE	5:A:122:LYS:HE3	1.29	1.60
5:A:13:LYS:HE3	5:A:122:LYS:CE	1.49	1.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:173:HIS:CE1	6:5:141:ARG:HH22	1.42	1.37
6:5:136:TYR:O	6:5:150:THR:CG2	1.75	1.33
6:5:148:THR:HB	6:5:152:ALA:N	1.48	1.27

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	1	179/207 (86%)	154 (86%)	17 (10%)	8 (4%)	3	33
2	2	216/218 (99%)	177 (82%)	29 (13%)	10 (5%)	3	33
3	3	217/219 (99%)	182 (84%)	25 (12%)	10 (5%)	3	33
4	4	216/218 (99%)	185 (86%)	21 (10%)	10 (5%)	3	33
5	A	218/220 (99%)	187 (86%)	24 (11%)	7 (3%)	5	41
6	5	22/24 (92%)	12 (54%)	5 (23%)	5 (23%)	0	2
All	All	1068/1106 (97%)	897 (84%)	121 (11%)	50 (5%)	5	32

5 of 50 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	2	6	GLU
2	2	35	GLY
2	2	174	HIS
3	3	87	SER
3	3	219	GLN

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	154/173 (89%)	128 (83%)	26 (17%)	2	18
2	2	177/187 (95%)	143 (81%)	34 (19%)	2	13
3	3	177/177 (100%)	141 (80%)	36 (20%)	1	11
4	4	192/192 (100%)	158 (82%)	34 (18%)	2	16
5	A	183/183 (100%)	153 (84%)	30 (16%)	3	19
6	5	16/17 (94%)	12 (75%)	4 (25%)	1	6
All	All	899/929 (97%)	735 (82%)	164 (18%)	5	15

5 of 164 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	3	100	GLN
3	3	207	LYS
5	A	122	LYS
3	3	107	LEU
3	3	179	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
3	3	13	ASN
3	3	100	GLN
4	4	38	HIS
2	2	166	ASN
4	4	57	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	OCS	4	218	4	3,6,9	4.97	1 (33%)	2,7,13	2.67	1 (50%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OCS	4	218	4	-	0/2/6/9	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	4	218	OCS	CB-CA	8.34	1.62	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	218	OCS	CA-CB-SG	3.78	123.08	114.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

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.