



wwPDB EM Validation Summary Report ⓘ

Dec 12, 2022 – 11:26 PM EST

PDB ID : 1QGC
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 initial model : 1FMD

This is a wwPDB EM Validation Summary Report for a publicly released PDB/EMDB 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

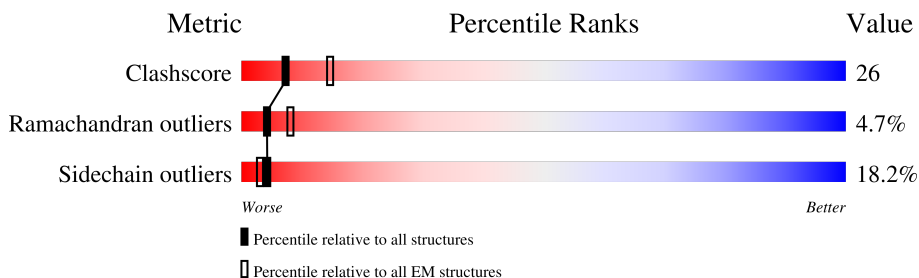
1 Overall quality at a glance

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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	1	207	52% 29% 7% • 12%
2	2	218	59% 33% 8%
3	3	219	57% 31% 12%
4	4	218	46% 36% 17% •
5	A	220	44% 40% 15% •
6	5	24	17% 46% 25% 12%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	OCS	4	218	-	X	-	-

2 Entry composition

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		

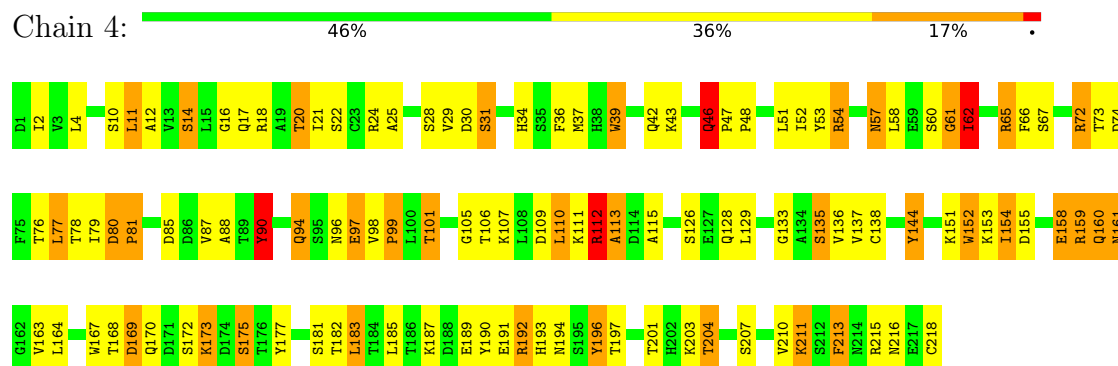
- Molecule 5 is a protein called PROTEIN (IMMUNOGLOBULIN HEAVY CHAIN).

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

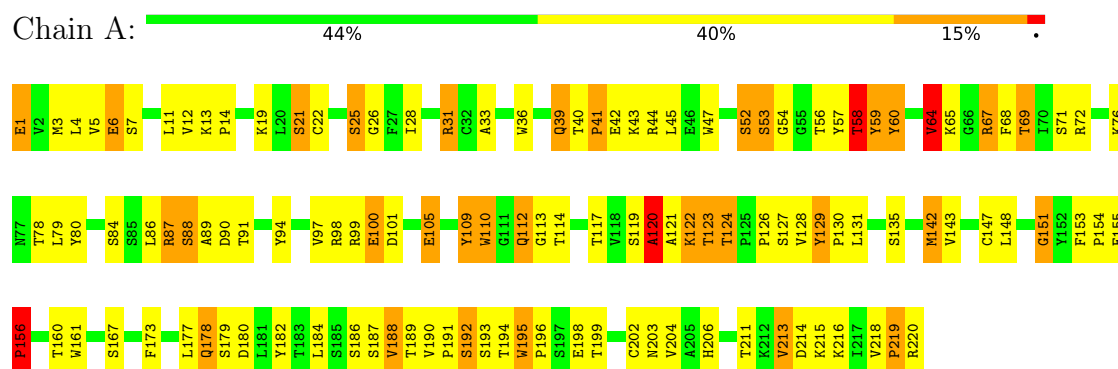
- Molecule 6 is a protein called PROTEIN (GH-LOOP FROM VIRUS CAPSID PROTEIN VP1).

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

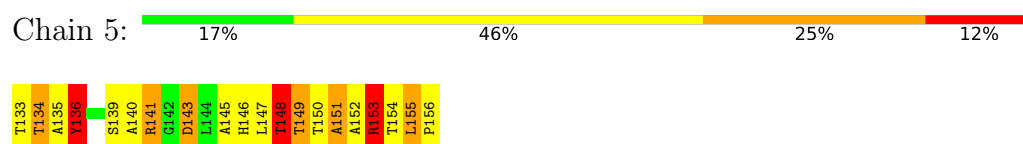
• Molecule 4: PROTEIN (IMMUNOGLOBULIN LIGHT CHAIN)



• Molecule 5: PROTEIN (IMMUNOGLOBULIN HEAVY CHAIN)



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



4 Data and refinement statistics

Xtrriage (Phenix) and EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	1.00Å 1.00Å 1.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 30.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-30.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	8279	wwPDB-VP
Average B, all atoms (Å ²)	110.0	wwPDB-VP

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	$\# Z > 5$	RMSZ	$\# Z > 5$
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 [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	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

Continued on next page...

Continued from previous page...

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%)	2	22
2	2	216/218 (99%)	177 (82%)	29 (13%)	10 (5%)	2	21
3	3	217/219 (99%)	182 (84%)	25 (12%)	10 (5%)	2	21
4	4	216/218 (99%)	185 (86%)	21 (10%)	10 (5%)	2	21
5	A	218/220 (99%)	187 (86%)	24 (11%)	7 (3%)	4	26
6	5	22/24 (92%)	12 (54%)	5 (23%)	5 (23%)	0	2
All	All	1068/1106 (97%)	897 (84%)	121 (11%)	50 (5%)	4	21

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	12
2	2	177/187 (95%)	143 (81%)	34 (19%)	1	8
3	3	177/177 (100%)	141 (80%)	36 (20%)	1	7
4	4	192/192 (100%)	158 (82%)	34 (18%)	2	10
5	A	183/183 (100%)	153 (84%)	30 (16%)	2	12
6	5	16/17 (94%)	12 (75%)	4 (25%)	0	3
All	All	899/929 (97%)	735 (82%)	164 (18%)	4	10

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

Mol	Chain	Res	Type
4	4	137	VAL
5	A	69	THR
4	4	160	GLN
5	A	4	LEU
5	A	114	THR

Sometimes 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	191	HIS
4	4	38	HIS
5	A	39	GLN
4	4	57	ASN
4	4	17	GLN

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	5,6,9	3.93	2 (40%)	5,7,13	3.12	3 (60%)

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	-	5/6/6/9	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	4	218	OCS	CB-CA	8.32	1.62	1.53
4	4	218	OCS	CB-SG	2.05	1.85	1.81

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	218	OCS	CB-CA-C	4.74	114.61	109.89
4	4	218	OCS	CA-CB-SG	4.01	123.08	114.44
4	4	218	OCS	OXT-C-CA	2.49	121.88	113.38

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	4	218	OCS	OXT-C-CA-CB
4	4	218	OCS	O-C-CA-CB
4	4	218	OCS	N-CA-CB-SG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	4	218	OCS	OXT-C-CA-N
4	4	218	OCS	C-CA-CB-SG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	4	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	4	112:ARG	C	113:ALA	N	0.93