



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:38 PM BST

PDB ID : 3IY6
EMDB ID: : EMD-5111
Title : Variable domains of the computer generated model (WAM) of Fab E fitted into the cryoEM reconstruction of the virus-Fab E complex
Authors : Hafenstein, S.; Bowman, V.D.; Sun, T.; Nelson, C.D.; Palermo, L.M.; Chipman, P.R.; Battisti, A.J.; Parrish, C.R.; Rossmann, M.G.
Deposited on : 2009-04-09
Resolution : 12.00 Å(reported)

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) : trunk27241

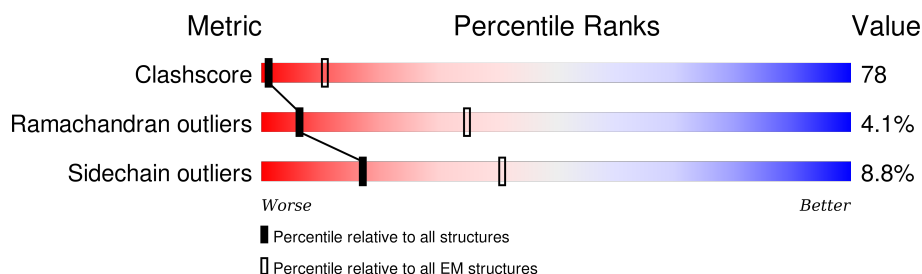
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 12.00 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	A	107	
2	B	115	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1719 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 fragment from neutralizing antibody E (light chain).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	107	Total	C	N	O	S	0	0
			820	507	139	167	7		

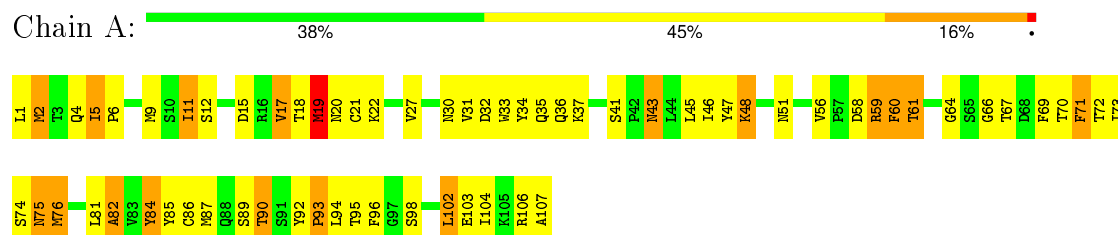
- Molecule 2 is a protein called fragment from neutralizing antibody E (heavy chain).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	115	Total	C	N	O	S	0	0
			899	575	148	172	4		

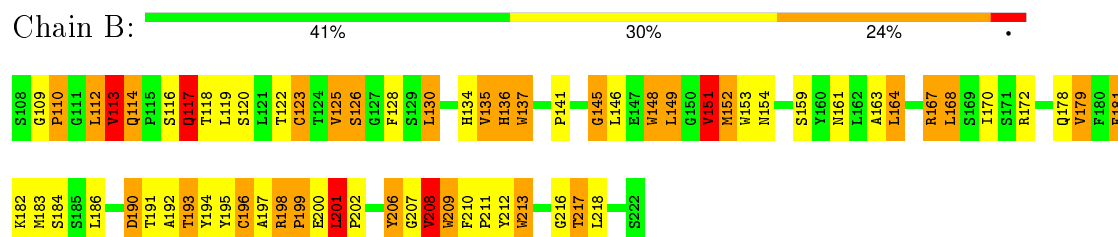
3 Residue-property plots

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: fragment from neutralizing antibody E (light chain)



- Molecule 2: fragment from neutralizing antibody E (heavy chain)



4 Experimental information ⓘ

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	1684	Depositor
Resolution determination method	FSC at 0.5 cutoff	Depositor
CTF correction method	robem	Depositor
Microscope	Not provided	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	23.8	Depositor
Minimum defocus (nm)	0.5	Depositor
Maximum defocus (nm)	5.6	Depositor
Magnification	45000	Depositor
Image detector	Kodak SO-163 film	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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	1.15	5/834 (0.6%)	1.58	16/1127 (1.4%)
2	B	1.35	9/927 (1.0%)	2.08	41/1266 (3.2%)
All	All	1.26	14/1761 (0.8%)	1.86	57/2393 (2.4%)

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
1	A	1	0
2	B	1	3
All	All	2	3

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	60	PHE	CG-CD1	-12.23	1.20	1.38
2	B	145	GLY	C-O	10.93	1.41	1.23
1	A	71	PHE	CD2-CE2	-8.47	1.22	1.39
2	B	181	PHE	CE2-CZ	-6.80	1.24	1.37
1	A	60	PHE	CD2-CE2	-6.60	1.26	1.39

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	60	PHE	CB-CG-CD1	19.22	134.25	120.80
2	B	168	LEU	CD1-CG-CD2	-14.91	65.78	110.50
2	B	117	GLN	OE1-CD-NE2	-12.64	92.82	121.90
2	B	113	VAL	CG1-CB-CG2	-11.67	92.23	110.90
2	B	113	VAL	CA-C-N	11.24	141.94	117.20

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	19	MET	CA
2	B	113	VAL	CA

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	113	VAL	Mainchain
2	B	117	GLN	Sidechain
2	B	136	HIS	Sidechain

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	A	820	0	798	113	0
2	B	899	0	860	177	0
All	All	1719	0	1658	263	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 78.

The worst 5 of 263 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)
1:A:19:MET:HE1	1:A:84:TYR:HB2	1.20	1.10
2:B:113:VAL:HG13	2:B:117:GLN:HG3	1.37	1.05
1:A:19:MET:CE	1:A:84:TYR:HB2	1.91	1.00
2:B:201:LEU:HD13	2:B:207:GLY:HA3	1.43	1.00
2:B:113:VAL:HG21	2:B:119:LEU:HD22	1.44	0.99

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	A	105/107 (98%)	95 (90%)	8 (8%)	2 (2%)	10	52
2	B	113/115 (98%)	97 (86%)	9 (8%)	7 (6%)	2	26
All	All	218/222 (98%)	192 (88%)	17 (8%)	9 (4%)	6	35

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	ALA
2	B	213	TRP
2	B	217	THR
2	B	116	SER
1	A	66	GLY

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	A	93/93 (100%)	82 (88%)	11 (12%)	6	32
2	B	101/101 (100%)	95 (94%)	6 (6%)	24	61
All	All	194/194 (100%)	177 (91%)	17 (9%)	17	45

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	THR

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Mol	Chain	Res	Type
1	A	75	ASN
2	B	193	THR
1	A	58	ASP
2	B	196	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	51	ASN
1	A	75	ASN
2	B	117	GLN
2	B	187	GLN

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.