



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Nov 9, 2017 – 05:13 PM EST

PDB ID : 6AVR  
EMDB ID: : EMD-7012  
Title : Human alpha-V beta-3 Integrin (intermediate conformation) in complex with the therapeutic antibody LM609  
Authors : Borst, A.J.; James, Z.N.; Zagotta, W.N.; Ginsberg, M.; Rey, F.A.; DiMaio, F.; Backovic, M.; Veesler, D.  
Deposited on : unknown  
Resolution : 35.00 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

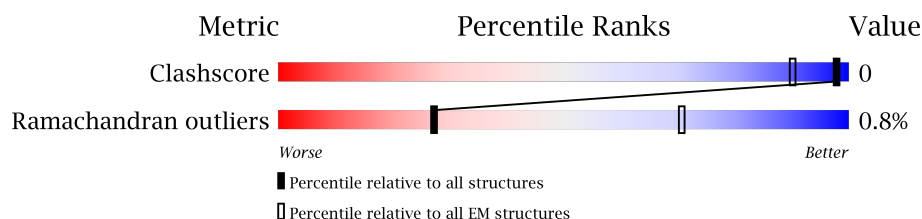
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 35.00 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	125131	1336
Ramachandran outliers	121729	1120

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  $\geq 3$ , 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	957	96% ..
2	B	692	96% ..
3	H	257	83% 17%
4	L	214	96% ..

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10016 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 Integrin alpha-V.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	924	Total	C	N	O	0	0
			4547	2699	924	924		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	753	ILE	VAL	conflict	UNP P06756

- Molecule 2 is a protein called Integrin beta-3.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	685	Total	C	N	O	0	0
			3375	2005	685	685		

- Molecule 3 is a protein called Fab LM609 heavy chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	H	214	Total	C	N	O	0	0
			1052	624	214	214		

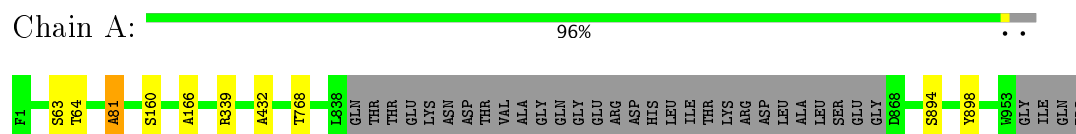
- Molecule 4 is a protein called Fab LM609 light chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	L	211	Total	C	N	O	0	0
			1042	620	211	211		

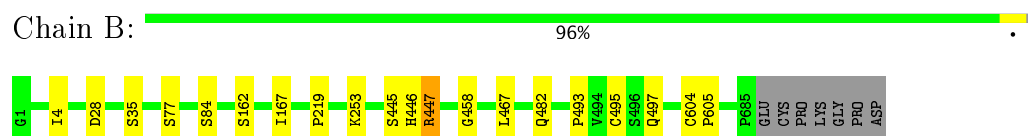
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

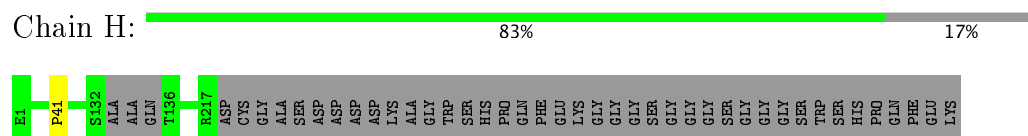
- Molecule 1: Integrin alpha-V



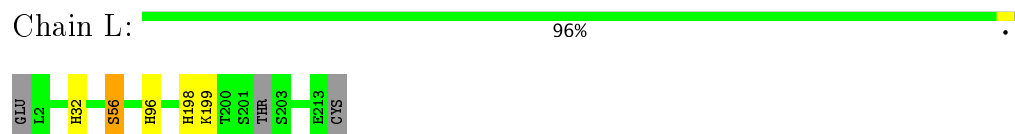
- Molecule 2: Integrin beta-3



- Molecule 3: Fab LM609 heavy chain



- Molecule 4: Fab LM609 light chain



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	650	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TECNAI 12	Depositor
Voltage (kV)	120	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	30	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN ULTRASCAN 4000 (4k 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	
		RMSZ	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	A	0.57	1/4545 (0.0%)	0.95	5/6316 (0.1%)
2	B	0.56	0/3374	0.90	1/4692 (0.0%)
3	H	0.53	0/1050	0.82	0/1456
4	L	0.50	0/1040	0.89	2/1445 (0.1%)
All	All	0.56	1/10009 (0.0%)	0.91	8/13909 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	160	SER	CA-CB	-5.32	1.45	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	894	SER	N-CA-CB	-8.12	98.31	110.50
1	A	432	ALA	N-CA-CB	6.11	118.65	110.10
1	A	81	ALA	N-CA-CB	6.07	118.59	110.10
4	L	32	HIS	CB-CA-C	-5.78	98.83	110.40
1	A	898	TYR	CB-CA-C	-5.56	99.29	110.40
1	A	81	ALA	CB-CA-C	-5.30	102.14	110.10
4	L	96	HIS	CB-CA-C	5.02	120.43	110.40
2	B	493	PRO	N-CA-C	-5.00	99.10	112.10

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	A	4547	0	2076	2	0
2	B	3375	0	1470	4	0
3	H	1052	0	476	0	0
4	L	1042	0	447	2	0
All	All	10016	0	4469	7	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 0.

All (7) 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)
4:L:198:HIS:C	4:L:199:LYS:O	2.46	0.49
1:A:81:ALA:HB2	4:L:56:SER:N	2.28	0.48
1:A:63:SER:O	1:A:64:THR:C	2.58	0.42
2:B:604:CYS:O	2:B:605:PRO:C	2.55	0.42
2:B:446:HIS:O	2:B:447:ARG:CB	2.67	0.42
2:B:28:ASP:H	2:B:458:GLY:HA3	1.84	0.42
2:B:219:PRO:HA	2:B:253:LYS:O	2.21	0.41

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	920/957 (96%)	883 (96%)	34 (4%)	3 (0%)	44 81
2	B	683/692 (99%)	637 (93%)	34 (5%)	12 (2%)	10 49
3	H	210/257 (82%)	209 (100%)	0	1 (0%)	32 74
4	L	207/214 (97%)	195 (94%)	11 (5%)	1 (0%)	32 74
All	All	2020/2120 (95%)	1924 (95%)	79 (4%)	17 (1%)	27 67

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	35	SER
2	B	167	ILE
2	B	467	LEU
1	A	339	ARG
1	A	166	ALA
1	A	768	THR
2	B	77	SER
2	B	445	SER
2	B	495	CYS
2	B	497	GLN
4	L	56	SER
2	B	84	SER
2	B	162	SER
2	B	447	ARG
2	B	482	GLN
2	B	4	ILE
3	H	41	PRO

### 5.3.2 Protein sidechains [i](#)

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

### 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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.