



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Nov 9, 2017 – 01:55 PM EST

PDB ID : 6AVU
EMDB ID: : EMD-7013
Title : Human alpha-V beta-3 Integrin (open 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 wwPDB/EMDataBank EM Map/Model 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
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

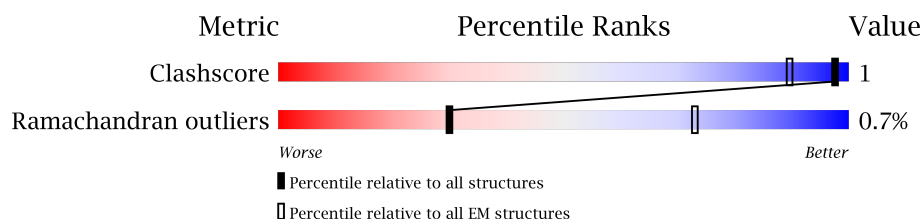
1 Overall quality at a glance

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 ≥ 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	95% . .
2	B	692	64% . 33%
3	H	257	83% 17%
4	L	214	98% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8913 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	923	Total	C	N	O	0	0
			4542	2696	923	923		

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	461	Total	C	N	O	0	0
			2277	1355	461	461		

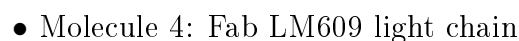
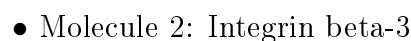
- Molecule 3 is a protein called Fab LM609 heavy chain.

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		

- Molecule 1: Integrin alpha-V



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	0.55	0/4540	0.92	2/6309 (0.0%)
2	B	0.58	0/2276	0.92	0/3168
3	H	0.52	0/1050	0.79	0/1456
4	L	0.49	0/1040	0.81	0/1445
All	All	0.55	0/8906	0.89	2/12378 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	551	LYS	C-N-CA	8.49	142.92	121.70
1	A	551	LYS	N-CA-C	5.22	125.10	111.00

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	4542	0	2074	4	0
2	B	2277	0	999	4	0
3	H	1052	0	476	0	0
4	L	1042	0	447	1	0
All	All	8913	0	3996	8	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 1.

The worst 5 of 8 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:418:GLY:H	1:A:486:VAL:H	1.36	0.72
2:B:242:ALA:C	2:B:420:GLY:HA2	2.28	0.53
2:B:243:SER:N	2:B:420:GLY:HA2	2.31	0.46
1:A:594:LEU:O	1:A:595:ASP:C	2.53	0.44
1:A:63:SER:O	1:A:64:THR:C	2.57	0.43

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	A	919/957 (96%)	883 (96%)	33 (4%)	3 (0%)	44	81
2	B	459/692 (66%)	431 (94%)	20 (4%)	8 (2%)	11	50
3	H	210/257 (82%)	209 (100%)	0	1 (0%)	32	74
4	L	207/214 (97%)	197 (95%)	10 (5%)	0	100	100
All	All	1795/2120 (85%)	1720 (96%)	63 (4%)	12 (1%)	30	68

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	35	SER
2	B	109	ASP
2	B	167	ILE
2	B	352	ARG
1	A	339	ARG

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.