



wwPDB/EMDataBank EM Map/Model Validation Summary 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 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

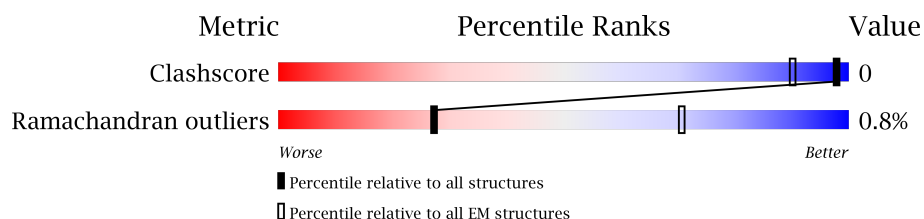
1 Overall quality at a glance

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	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.

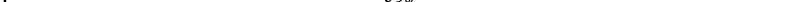
Mol	Chain	Residues	Atoms				AltConf	Trace
4	L	211	Total	C	N	O	0	0
			1042	620	211	211		

- Molecule 1: Integrin alpha-V

F1	S63	T64	A61	S160	A166	R339	A432	T768	L238	GLN	THR	THR	GLU	GLY	ASN	ASP	VAL	ALA	GLY	GLN	GLY	GLU	ARG	ASP	HIS	LEU	ILE	THR	THR	LYS	ARG	ASP	LEU	ALA	LEU	SER	SER	GLU	GLY	GLY	D668	S894	Y898	W853	GLY	GLY	LEU	GLN
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Chain B: 96% 4%

G1	I4	D28	S35	S77	S84	S162	I167	P219	K253	S445	H446	R447	G458	L467	Q482	P493	V494	C495	S496	Q497	C604	P605	P685	GLU	CYS	PRO	PRO	LYS	GLY	PRO	PRO
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Chain H:  83% 17%

E1
P41
S132
ALA ALA GLN
T136
R217
ASP CYS GLY
ALA SER ASP
ASP ASP ASP
LVS ALA ALA
GLY TRP
SER HIS PRO
GLN PHE GLU
LVS GLY GLY
GLY GLY GLY
SER SER GLY
GLY GLY GLY
SER SER GLY
HIS HIS PRO
GLN PHE GLU
CYS VAL LEU

Chain L: 96%

GLU
L2
H32
S56
H96
H198
K199
T200
S201
THR
S203
E213
CYS

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

The worst 5 of 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

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.

The worst 5 of 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

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	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

5 of 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

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.