



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:52 PM BST

PDB ID : 3JBI
EMDB ID: : EMD-6446
Title : MDFF model of the vinculin tail domain bound to F-actin
Authors : Kim, L.Y.; Thompson, P.M.; Lee, H.T.; Pershad, M.; Campbell, S.L.; Alushin, G.M.
Deposited on : 2015-09-02
Resolution : 8.50 Å(reported)
Based on PDB ID : 1QKR, 3J8A

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 : 1.7.1 (RC1), CSD as537be (2016)
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

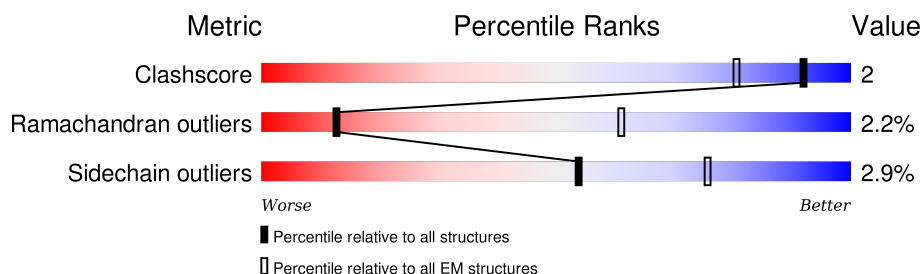
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 8.50 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	375	 87% 9% ...
1	B	375	 83% 13% ...
2	V	254	 48% . 48%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6777 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 Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	367	Total	C	N	O	S	0	0
			2861	1812	481	548	20		
1	B	367	Total	C	N	O	S	0	0
			2861	1812	481	548	20		

- Molecule 2 is a protein called Vinculin.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	V	131	Total	C	N	O	S	0	0
			999	608	187	195	9		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	808	GLY	-	EXPRESSION TAG	UNP P12003
V	809	SER	-	EXPRESSION TAG	UNP P12003

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

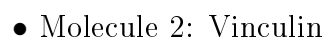
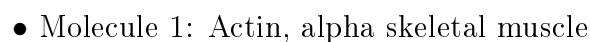
Mol	Chain	Residues	Atoms		AltConf
3	B	1	Total	Mg	0
			1	1	
3	A	1	Total	Mg	0
			1	1	

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total 27	C 10	N 5	O 10	P 2	0
4	B	1	Total 27	C 10	N 5	O 10	P 2	0

- Molecule 1: Actin, alpha skeletal muscle



4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	FREALIGN (per segment)	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	120	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	100000	Depositor
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ADP

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	0.83	0/2923	1.23	16/3963 (0.4%)
1	B	0.83	0/2923	1.22	20/3963 (0.5%)
2	V	0.71	0/1000	1.09	9/1339 (0.7%)
All	All	0.82	0/6846	1.21	45/9265 (0.5%)

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	0	5
1	B	0	9
2	V	0	1
All	All	0	15

There are no bond length outliers.

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	147	ARG	NE-CZ-NH1	9.27	124.94	120.30
1	A	39	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	B	196	ARG	NE-CZ-NH1	7.69	124.14	120.30
1	A	256	ARG	NE-CZ-NH1	7.68	124.14	120.30
1	B	196	ARG	NE-CZ-NH2	-7.52	116.54	120.30
2	V	935	ARG	NE-CZ-NH1	7.31	123.95	120.30
1	A	147	ARG	NE-CZ-NH2	-7.27	116.67	120.30
1	A	39	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	A	28	ARG	NE-CZ-NH1	7.05	123.83	120.30
1	A	196	ARG	NE-CZ-NH2	-7.04	116.78	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	1039	ARG	NE-CZ-NH1	7.03	123.81	120.30
1	B	37	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	B	147	ARG	NE-CZ-NH2	-6.85	116.88	120.30
1	B	37	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	A	290	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	A	290	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	B	62	ARG	NE-CZ-NH1	6.72	123.66	120.30
2	V	963	ARG	NE-CZ-NH2	-6.69	116.96	120.30
2	V	978	ARG	NE-CZ-NH1	6.69	123.64	120.30
1	B	256	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	A	183	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	B	116	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	B	119	MET	CG-SD-CE	-6.30	90.12	100.20
1	B	39	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	B	154	ASP	CB-CG-OD2	5.99	123.69	118.30
2	V	976	ARG	NE-CZ-NH1	5.97	123.29	120.30
1	A	154	ASP	CB-CG-OD2	5.94	123.64	118.30
1	B	206	ARG	NE-CZ-NH2	-5.91	117.34	120.30
2	V	987	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	B	116	ARG	NE-CZ-NH2	-5.79	117.41	120.30
2	V	963	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	A	16	LEU	N-CA-CB	5.72	121.84	110.40
1	A	196	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A	15	GLY	C-N-CA	5.56	135.61	121.70
2	V	938	ARG	NE-CZ-NH2	-5.54	117.53	120.30
2	V	945	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	B	15	GLY	O-C-N	-5.30	114.21	122.70
1	A	210	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	A	157	ASP	C-N-CA	5.22	133.26	122.30
1	B	206	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	B	157	ASP	C-N-CA	5.16	133.14	122.30
1	B	154	ASP	OD1-CG-OD2	-5.15	113.51	123.30
1	B	16	LEU	N-CA-CB	5.15	120.70	110.40
1	B	15	GLY	C-N-CA	5.14	134.55	121.70
1	B	266	PHE	CB-CG-CD2	-5.12	117.22	120.80

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	183	ARG	Sidechain
1	A	206	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	290	ARG	Sidechain
1	A	335	ARG	Sidechain
1	A	62	ARG	Sidechain
1	B	206	ARG	Sidechain
1	B	210	ARG	Sidechain
1	B	28	ARG	Sidechain
1	B	290	ARG	Sidechain
1	B	312	ARG	Sidechain
1	B	332	PRO	Peptide
1	B	349	LEU	Peptide
1	B	69	TYR	Sidechain
1	B	95	ARG	Sidechain
2	V	987	ARG	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	2861	0	2831	14	0
1	B	2861	0	2831	14	0
2	V	999	0	1059	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	27	0	12	0	0
4	B	27	0	12	0	0
All	All	6777	0	6745	26	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 2.

All (26) 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:B:141:SER:HA	1:B:144:ALA:HB3	1.78	0.65
1:B:295:ALA:HA	1:B:328:LYS:H	1.63	0.64
1:B:219:VAL:HG22	1:B:258:PRO:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:PRO:HA	1:A:65:LEU:HA	1.90	0.53
1:B:157:ASP:HA	1:B:182:GLY:H	1.74	0.51
1:A:295:ALA:HA	1:A:328:LYS:H	1.75	0.50
1:A:157:ASP:HA	1:A:182:GLY:H	1.76	0.50
1:B:15:GLY:HA3	1:B:16:LEU:HB2	1.92	0.50
1:A:15:GLY:HA3	1:A:16:LEU:HB2	1.96	0.48
1:A:40:HIS:CE1	1:B:173:HIS:CE1	3.02	0.47
1:A:158:GLY:HA2	1:A:183:ARG:H	1.78	0.47
1:B:295:ALA:HA	1:B:328:LYS:N	2.29	0.47
1:A:88:HIS:CE1	1:A:92:ASN:HD21	2.32	0.47
1:B:38:PRO:HA	1:B:65:LEU:HA	1.97	0.47
1:B:158:GLY:HA2	1:B:183:ARG:H	1.81	0.46
1:A:295:ALA:HA	1:A:328:LYS:N	2.33	0.44
1:A:42:GLY:HA2	1:B:169:TYR:HA	2.00	0.43
1:A:158:GLY:HA2	1:A:182:GLY:H	1.84	0.43
1:B:16:LEU:H	1:B:32:PRO:HA	1.82	0.43
1:A:91:TYR:O	1:A:95:ARG:HA	2.20	0.42
1:B:219:VAL:HG23	1:B:306:TYR:HB3	2.02	0.42
1:B:103:THR:HG22	1:B:129:VAL:HG11	2.02	0.42
1:B:253:GLU:HA	1:B:256:ARG:HB3	2.03	0.41
1:A:253:GLU:H	1:A:253:GLU:CD	2.24	0.41
1:A:253:GLU:HA	1:A:256:ARG:HB3	2.03	0.41
1:A:219:VAL:HG22	1:A:258:PRO:HB2	2.03	0.41

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	365/375 (97%)	330 (90%)	28 (8%)	7 (2%)	10	52
1	B	365/375 (97%)	317 (87%)	36 (10%)	12 (3%)	5	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	V	129/254 (51%)	128 (99%)	1 (1%)	0	100	100
All	All	859/1004 (86%)	775 (90%)	65 (8%)	19 (2%)	13	49

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	ILE
1	B	34	ILE
1	A	16	LEU
1	A	23	GLY
1	B	16	LEU
1	B	295	ALA
1	A	33	SER
1	A	180	LEU
1	A	251	GLY
1	B	167	GLU
1	B	235	SER
1	B	251	GLY
1	B	304	THR
1	B	45	VAL
1	A	269	MET
1	B	33	SER
1	B	220	ALA
1	B	271	SER
1	B	367	PRO

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	310/318 (98%)	302 (97%)	8 (3%)	54	80
1	B	310/318 (98%)	299 (96%)	11 (4%)	43	74
2	V	110/214 (51%)	108 (98%)	2 (2%)	66	87
All	All	730/850 (86%)	709 (97%)	21 (3%)	54	78

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	VAL
1	A	12	ASN
1	A	18	LYS
1	A	92	ASN
1	A	157	ASP
1	A	173	HIS
1	A	179	ASP
1	A	222	ASP
1	B	9	VAL
1	B	12	ASN
1	B	71	ILE
1	B	87	HIS
1	B	103	THR
1	B	107	GLU
1	B	147	ARG
1	B	157	ASP
1	B	162	ASN
1	B	179	ASP
1	B	253	GLU
2	V	1013	ASP
2	V	1031	MET

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	88	HIS
1	A	92	ASN
1	A	275	HIS
1	B	173	HIS
2	V	949	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	ADP	A	402	3	24,29,29	0.76	0	23,45,45	0.99	1 (4%)
4	ADP	B	402	3	24,29,29	0.78	0	23,45,45	1.01	1 (4%)

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	ADP	A	402	3	-	0/12/32/32	0/3/3/3
4	ADP	B	402	3	-	0/12/32/32	0/3/3/3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	402	ADP	C4'-O4'-C1'	-2.32	107.19	109.64
4	A	402	ADP	C2'-C3'-C4'	2.03	106.78	102.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.