



wwPDB EM Map/Model Validation Report i

Apr 10, 2016 – 01:48 PM BST

PDB ID : 3J4K
EMDB ID: : EMD-5751
Title : Cryo-EM structures of the actin:tropomyosin filament reveal the mechanism for the transition from C- to M-state
Authors : Sousa, D.R.; Stagg, S.M.; Stroupe, M.E.
Deposited on : 2013-08-26
Resolution : 8.00 Å(reported)
Based on PDB ID : 4A7F

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>

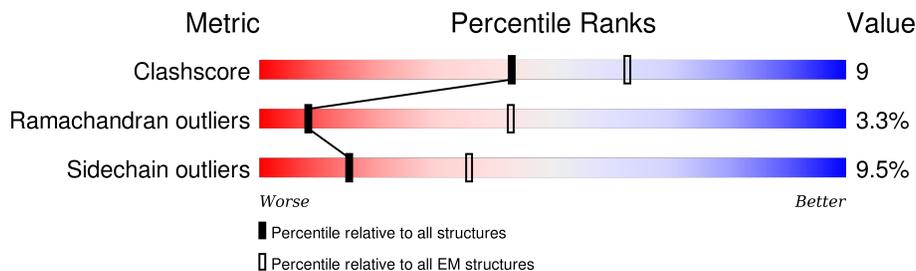
MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 8.00 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	375	67% 25% 7% .
1	B	375	64% 29% 6% .
1	C	375	68% 24% 7% .
1	D	375	62% 27% 10% .
1	E	375	63% 29% 8% .
2	F	136	100%
2	G	136	100%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16160 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
			Total	C	N	O	S		
1	A	375	2933	1854	493	565	21	0	0
1	B	375	2933	1854	493	565	21	0	0
1	C	375	2933	1854	493	565	21	0	0
1	D	375	2933	1854	493	565	21	0	0
1	E	375	2933	1854	493	565	21	0	0

- Molecule 2 is a protein called tropomyosin.

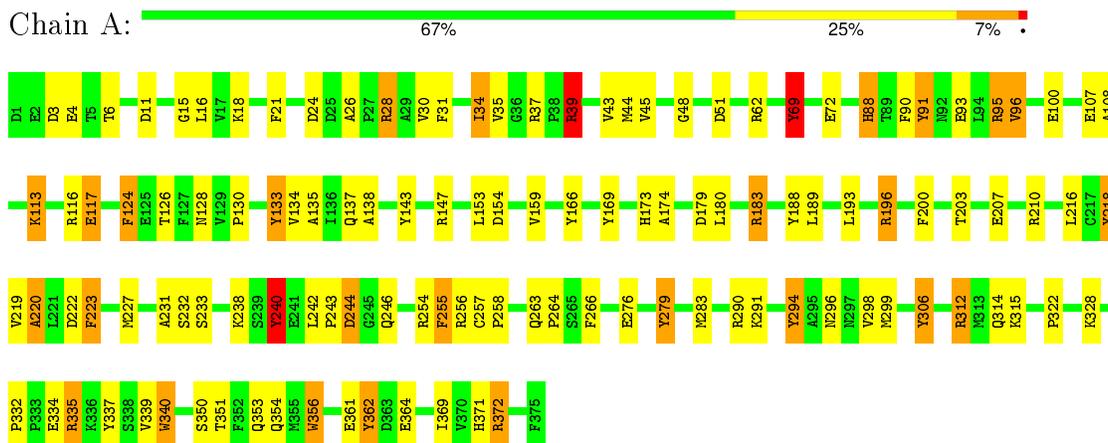
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	F	136	680	408	136	136	0	0
2	G	136	680	408	136	136	0	0

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

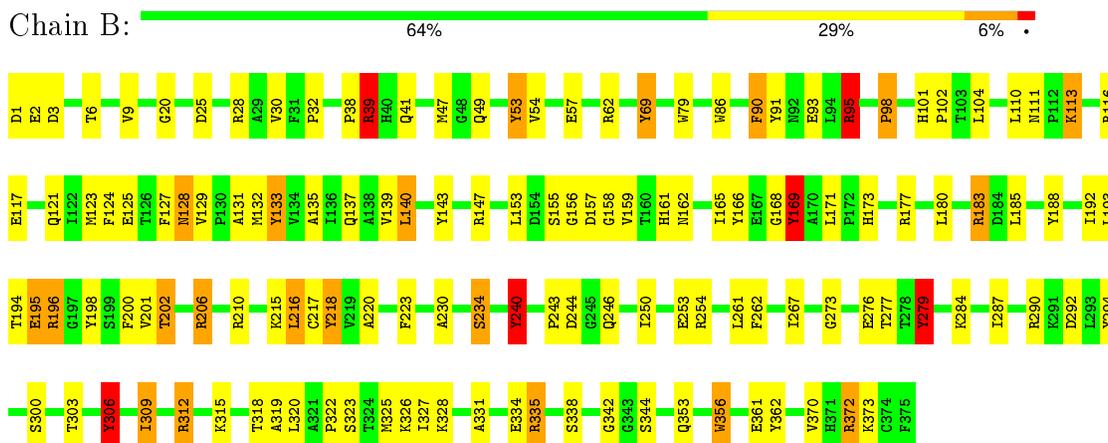
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

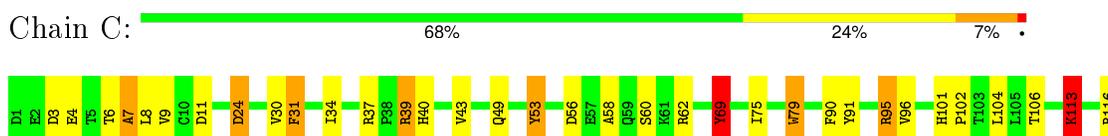
- Molecule 1: Actin, alpha skeletal muscle

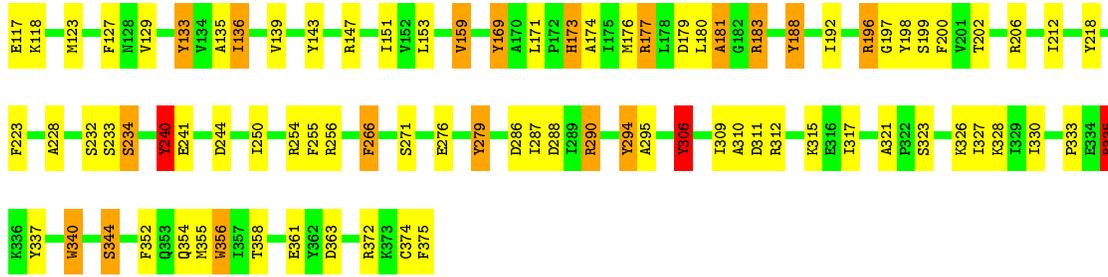


- Molecule 1: Actin, alpha skeletal muscle

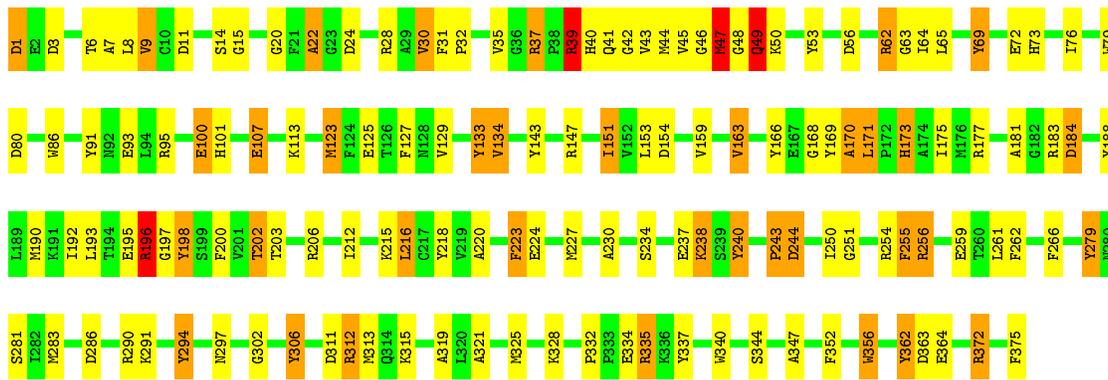


- Molecule 1: Actin, alpha skeletal muscle

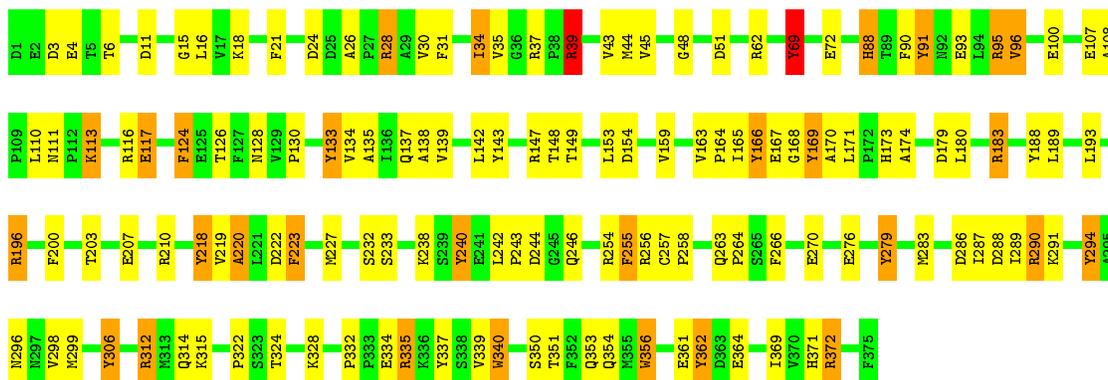




• Molecule 1: Actin, alpha skeletal muscle



• Molecule 1: Actin, alpha skeletal muscle



• Molecule 2: tropomyosin



There are no outlier residues recorded for this chain.

• Molecule 2: tropomyosin



There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	224337	Depositor
Resolution determination method	FSC at 0.5 cut-off	Depositor
CTF correction method	individual images	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	59000	Depositor
Image detector	Gatan Ultrascan 4000	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.74	25/2996 (0.8%)	1.97	78/4058 (1.9%)
1	B	1.75	35/2996 (1.2%)	2.00	80/4058 (2.0%)
1	C	1.71	21/2996 (0.7%)	1.99	86/4058 (2.1%)
1	D	1.73	29/2996 (1.0%)	2.11	108/4058 (2.7%)
1	E	1.74	26/2996 (0.9%)	1.97	77/4058 (1.9%)
All	All	1.73	136/14980 (0.9%)	2.01	429/20290 (2.1%)

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	15
1	B	0	11
1	C	0	12
1	D	0	8
1	E	0	15
All	All	0	61

The worst 5 of 136 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	37	ARG	NE-CZ	9.09	1.44	1.33
1	E	37	ARG	NE-CZ	9.08	1.44	1.33
1	B	95	ARG	CD-NE	8.06	1.60	1.46
1	C	169	TYR	CG-CD1	7.54	1.49	1.39
1	D	32	PRO	N-CD	-7.51	1.37	1.47

The worst 5 of 429 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	D	196	ARG	NE-CZ-NH2	-18.93	110.83	120.30
1	D	62	ARG	NE-CZ-NH2	-16.66	111.97	120.30
1	A	39	ARG	NE-CZ-NH2	14.71	127.66	120.30
1	E	39	ARG	NE-CZ-NH2	14.65	127.62	120.30
1	B	127	PHE	CB-CG-CD1	-14.49	110.66	120.80

There are no chirality outliers.

5 of 61 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	28	ARG	Sidechain
1	A	69	TYR	Sidechain
1	A	88	HIS	Sidechain
1	A	91	TYR	Sidechain
1	A	95	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	2933	0	2894	18	0
1	B	2933	0	2894	26	0
1	C	2933	0	2894	14	0
1	D	2933	0	2893	195	0
1	E	2933	0	2893	202	0
2	F	680	0	138	0	0
2	G	680	0	138	0	0
3	A	27	0	12	0	0
3	B	27	0	12	0	0
3	C	27	0	12	0	0
3	D	27	0	12	2	0
3	E	27	0	12	0	0
All	All	16160	0	14804	266	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 9.

The worst 5 of 266 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:D:40:HIS:CD2	1:E:166:TYR:CD1	1.88	1.62
1:D:43:VAL:CG1	1:E:139:VAL:HG22	1.35	1.54
1:D:40:HIS:CD2	1:E:166:TYR:HD1	1.17	1.53
1:D:64:ILE:HD11	1:E:289:ILE:CG2	1.38	1.51
1:D:243:PRO:C	1:E:324:THR:HG21	1.36	1.46

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	373/375 (100%)	321 (86%)	40 (11%)	12 (3%)	5	41
1	B	373/375 (100%)	326 (87%)	33 (9%)	14 (4%)	4	37
1	C	373/375 (100%)	322 (86%)	39 (10%)	12 (3%)	5	41
1	D	373/375 (100%)	325 (87%)	37 (10%)	11 (3%)	6	43
1	E	373/375 (100%)	321 (86%)	40 (11%)	12 (3%)	5	41
All	All	1865/1875 (100%)	1615 (87%)	189 (10%)	61 (3%)	8	40

5 of 61 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	THR
1	A	246	GLN
1	B	6	THR
1	B	39	ARG
1	B	128	ASN

5.3.2 Protein sidechains [i](#)

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	318/318 (100%)	293 (92%)	25 (8%)	15	51
1	B	318/318 (100%)	277 (87%)	41 (13%)	5	28
1	C	318/318 (100%)	288 (91%)	30 (9%)	11	42
1	D	318/318 (100%)	288 (91%)	30 (9%)	11	42
1	E	318/318 (100%)	293 (92%)	25 (8%)	15	51
All	All	1590/1590 (100%)	1439 (90%)	151 (10%)	15	41

5 of 151 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	31	PHE
1	C	250	ILE
1	E	203	THR
1	C	56	ASP
1	C	151	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	252	ASN
1	D	40	HIS
1	E	360	GLN
1	C	371	HIS
1	D	78	ASN

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](#)

5 ligands are modelled in this entry.

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
3	ADP	A	401	-	24,29,29	1.71	5 (20%)	23,45,45	1.81	7 (30%)
3	ADP	B	401	-	24,29,29	1.32	2 (8%)	23,45,45	1.68	4 (17%)
3	ADP	C	401	-	24,29,29	1.23	2 (8%)	23,45,45	2.10	7 (30%)
3	ADP	D	401	-	24,29,29	1.39	2 (8%)	23,45,45	2.89	8 (34%)
3	ADP	E	401	-	24,29,29	1.72	5 (20%)	23,45,45	1.81	7 (30%)

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
3	ADP	A	401	-	-	0/12/32/32	0/3/3/3
3	ADP	B	401	-	-	0/12/32/32	0/3/3/3
3	ADP	C	401	-	-	0/12/32/32	0/3/3/3
3	ADP	D	401	-	-	0/12/32/32	0/3/3/3
3	ADP	E	401	-	-	0/12/32/32	0/3/3/3

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	ADP	C2'-C1'	-4.47	1.46	1.53
3	A	401	ADP	C8-N7	-3.12	1.28	1.34
3	E	401	ADP	C8-N7	-3.09	1.28	1.34
3	E	401	ADP	C5-C4	-2.64	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	ADP	C5-C4	-2.62	1.34	1.40

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	401	ADP	N3-C2-N1	-3.83	125.86	128.87
3	A	401	ADP	N3-C2-N1	-3.80	125.89	128.87
3	C	401	ADP	C5'-C4'-C3'	-3.20	102.84	115.20
3	D	401	ADP	C5'-C4'-C3'	-2.85	104.18	115.20
3	E	401	ADP	C5'-C4'-C3'	-2.55	105.34	115.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	401	ADP	2	0

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.