



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:53 PM BST

PDB ID : 3JAX  
EMDB ID: : EMD-6370  
Title : Heavy meromyosin from Schistosoma mansoni muscle thick filament by negative stain EM  
Authors : Sulbaran, G.; Alamo, L.; Pinto, A.; Marquez, G.; Mendez, F.; Padron, R.; Craig, R.  
Deposited on : 2015-07-03  
Resolution : 23.00 Å(reported)  
Based on PDB ID : 3DTP

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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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MolProbity : 4.02b-467  
Mogul : unknown  
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

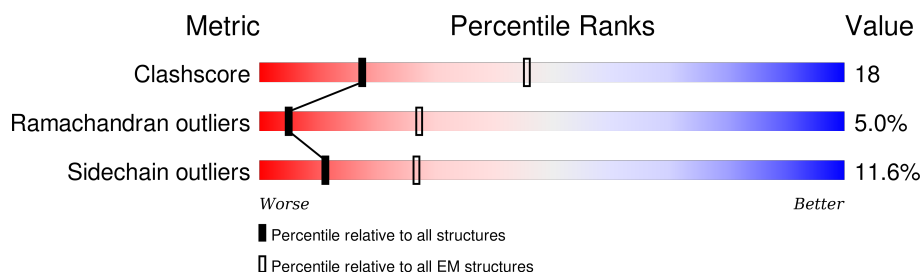
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 23.00 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  $\geq 3$ , 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	974	
1	B	974	
2	C	151	
2	D	151	
3	E	196	
3	F	196	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 25293 atoms, of which 4713 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 myosin 2 heavy chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	938	Total	C	H	N	O	S	0	0
			9360	4819	1759	1312	1432	38		
1	B	940	Total	C	H	N	O	S	0	0
			9379	4828	1764	1315	1434	38		

- Molecule 2 is a protein called smooth muscle myosin essential light chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	C	148	Total	C	H	N	O	S	0	0
			1411	722	251	193	234	11		
2	D	148	Total	C	H	N	O	S	0	0
			1411	722	251	193	234	11		

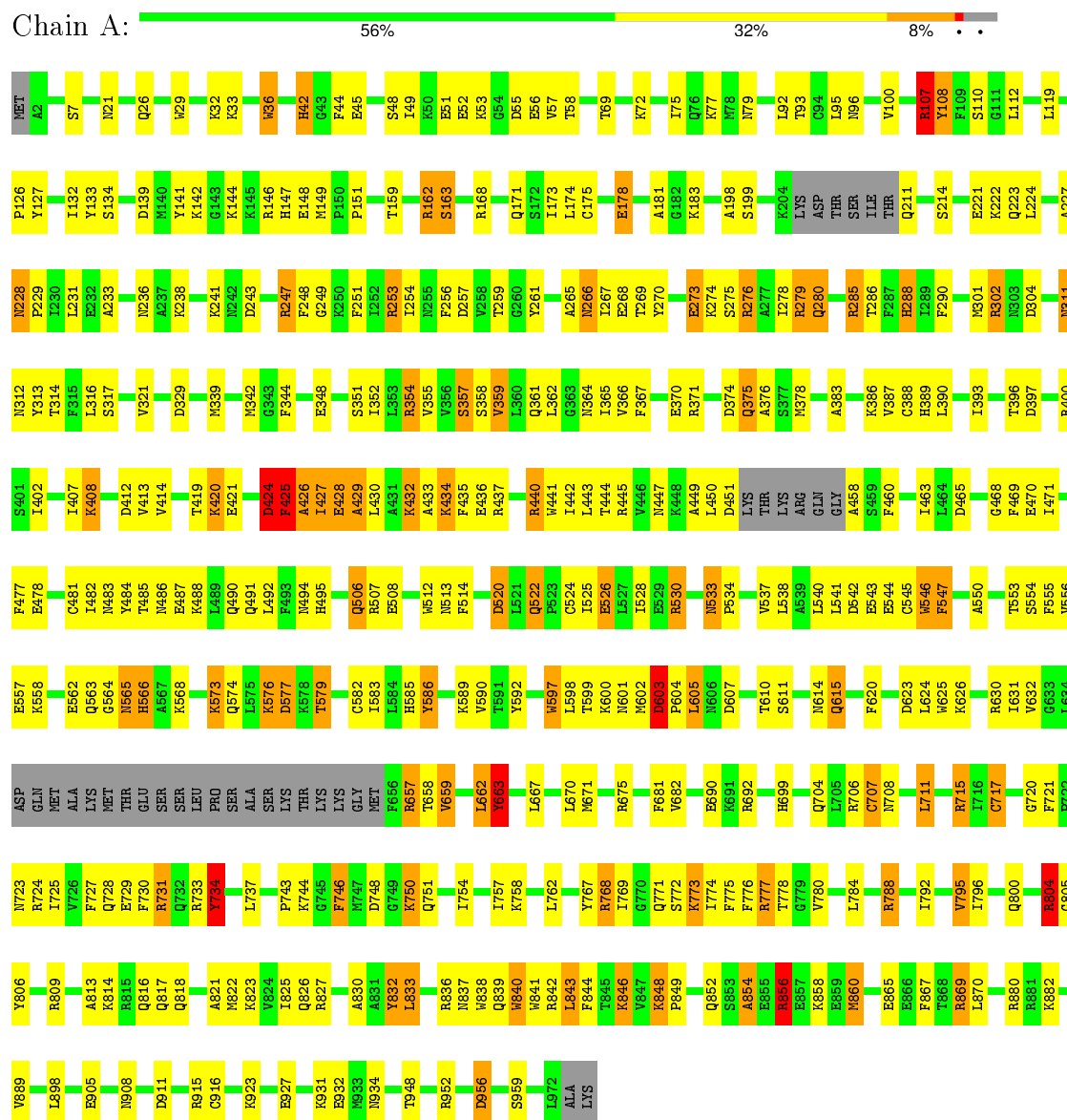
- Molecule 3 is a protein called myosin regulatory light chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	E	196	Total	C	H	N	O	S	0	0
			1866	948	344	259	309	6		
3	F	196	Total	C	H	N	O	S	0	0
			1866	948	344	259	309	6		

### 3 Residue-property plots

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.

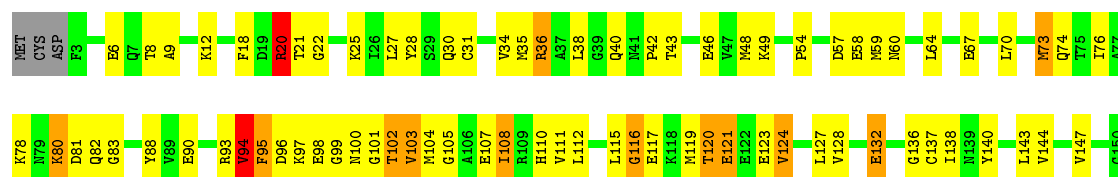
- Molecule 1: myosin 2 heavy chain



- Molecule 1: myosin 2 heavy chain

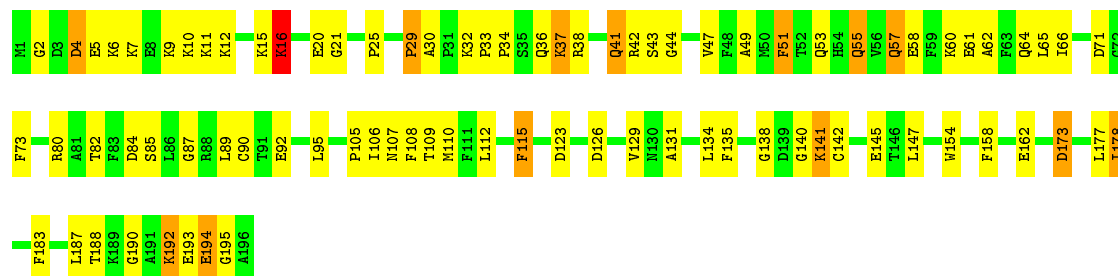






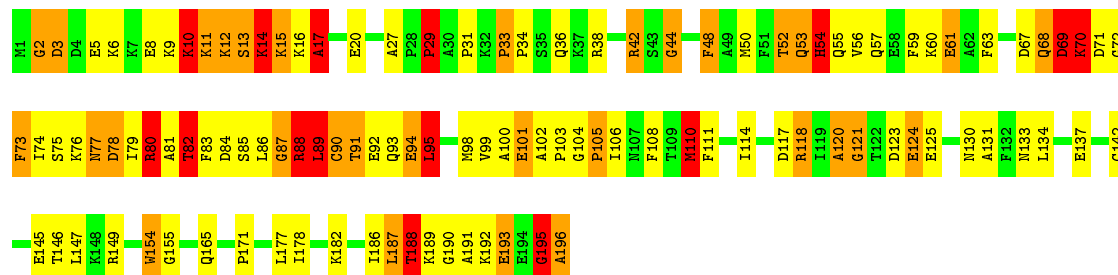
• Molecule 3: myosin regulatory light chain

Chain E: 57% 36% 7%



• Molecule 3: myosin regulatory light chain

Chain F: 43% 34% 16% 8%



## 4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	9500	Depositor
Resolution determination method	FSC 0.5	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI/PHILIPS CM120T	Depositor
Voltage (kV)	80	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	10	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	42000	Depositor
Image detector	TVIPS TEMCAM-F224 (2k x 2k)	Depositor

## 5 Model quality

### 5.1 Standard geometry

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	0.66	0/7730	1.43	80/10402 (0.8%)
1	B	0.66	0/7744	1.42	77/10420 (0.7%)
2	C	0.63	0/1175	1.19	2/1575 (0.1%)
2	D	0.65	0/1175	1.33	5/1575 (0.3%)
3	E	0.65	0/1546	1.34	10/2071 (0.5%)
3	F	0.68	0/1546	1.57	21/2071 (1.0%)
All	All	0.66	0/20916	1.41	195/28114 (0.7%)

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	22
1	B	0	31
2	D	0	7
3	E	0	3
3	F	0	16
All	All	0	79

There are no bond length outliers.

The worst 5 of 195 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	107	ARG	NE-CZ-NH2	-16.82	111.89	120.30
1	A	107	ARG	NE-CZ-NH1	11.83	126.22	120.30
2	C	36	ARG	NE-CZ-NH2	-10.39	115.10	120.30
1	A	285	ARG	NE-CZ-NH1	10.04	125.32	120.30
1	B	484	TYR	CB-CG-CD2	-9.59	115.25	121.00

There are no chirality outliers.



5 of 79 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	ARG	Sidechain
1	A	108	TYR	Sidechain
1	A	127	TYR	Sidechain
1	A	133	TYR	Sidechain
1	A	249	GLY	Peptide

## 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	7601	1759	7638	236	0
1	B	7615	1764	7656	339	0
2	C	1160	251	1126	17	0
2	D	1160	251	1126	57	0
3	E	1522	344	1492	59	0
3	F	1522	344	1492	109	0
All	All	20580	4713	20530	726	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 18.

The worst 5 of 726 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)
3:E:12:LYS:HA	3:F:68:GLN:HG3	1.41	0.99
1:B:238:LYS:HB3	1:B:285:ARG:HB2	1.43	0.98
1:B:375:GLN:HA	1:B:419:THR:HA	1.43	0.98
1:B:178:GLU:HA	1:B:469:PHE:HB3	1.42	0.98
1:A:273:GLU:HA	1:A:478:GLU:HG2	1.46	0.97

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	930/974 (96%)	739 (80%)	154 (17%)	37 (4%)	4	35
1	B	932/974 (96%)	764 (82%)	127 (14%)	41 (4%)	3	33
2	C	146/151 (97%)	127 (87%)	12 (8%)	7 (5%)	3	32
2	D	146/151 (97%)	122 (84%)	18 (12%)	6 (4%)	3	35
3	E	194/196 (99%)	159 (82%)	23 (12%)	12 (6%)	2	26
3	F	194/196 (99%)	118 (61%)	52 (27%)	24 (12%)	0	8
All	All	2542/2642 (96%)	2029 (80%)	386 (15%)	127 (5%)	5	31

5 of 127 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	181	ALA
1	A	224	LEU
1	A	429	ALA
1	A	533	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	828/859 (96%)	741 (90%)	87 (10%)	8	36
1	B	829/859 (96%)	720 (87%)	109 (13%)	5	28
2	C	127/130 (98%)	118 (93%)	9 (7%)	18	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	127/130 (98%)	113 (89%)	14 (11%)	8	34
3	E	162/162 (100%)	146 (90%)	16 (10%)	10	39
3	F	162/162 (100%)	137 (85%)	25 (15%)	3	22
All	All	2235/2302 (97%)	1975 (88%)	260 (12%)	11	32

5 of 260 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	314	THR
1	B	565	ASN
3	F	50	MET
1	B	369	LYS
1	B	412	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	326	GLN
1	B	389	HIS
3	E	57	GLN
1	B	364	ASN
1	B	494	ASN

### 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 [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.