wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 01:42 PM BST

PDB ID	:	3J04
EMDB ID:	:	EMD-5257
Title	:	EM structure of the heavy meromyosin subfragment of Chick smooth muscle Myosin with regulatory light chain in phosphorylated state
Authors	:	Baumann, B.A.J.; Taylor, D.; Huang, Z.; Tama, F.; Fagnant, P.M.; Trybus, K.; Taylor, K.
Deposited on	:	2011-02-18
Resolution	:	20.00 Å(reported)

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

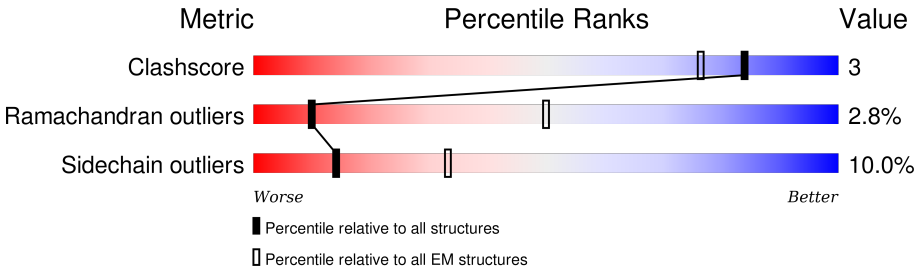
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 20.00 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	909	83% 12%
1	D	909	82% 12%
2	B	143	74% 18% 5%
2	E	143	71% 18% 8%
3	C	148	84% 14%
3	F	148	83% 15%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19065 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 Myosin-11.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	903	Total	C	N	O	S	0	0
			7214	4585	1228	1365	36		
1	D	903	Total	C	N	O	S	0	0
			7231	4596	1233	1366	36		

- Molecule 2 is a protein called Myosin regulatory light chain 2, smooth muscle major isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	143	Total	C	N	O	S	0	0
			1160	727	189	234	10		
2	E	143	Total	C	N	O	S	0	0
			1160	727	189	234	10		

- Molecule 3 is a protein called Myosin light polypeptide 6.

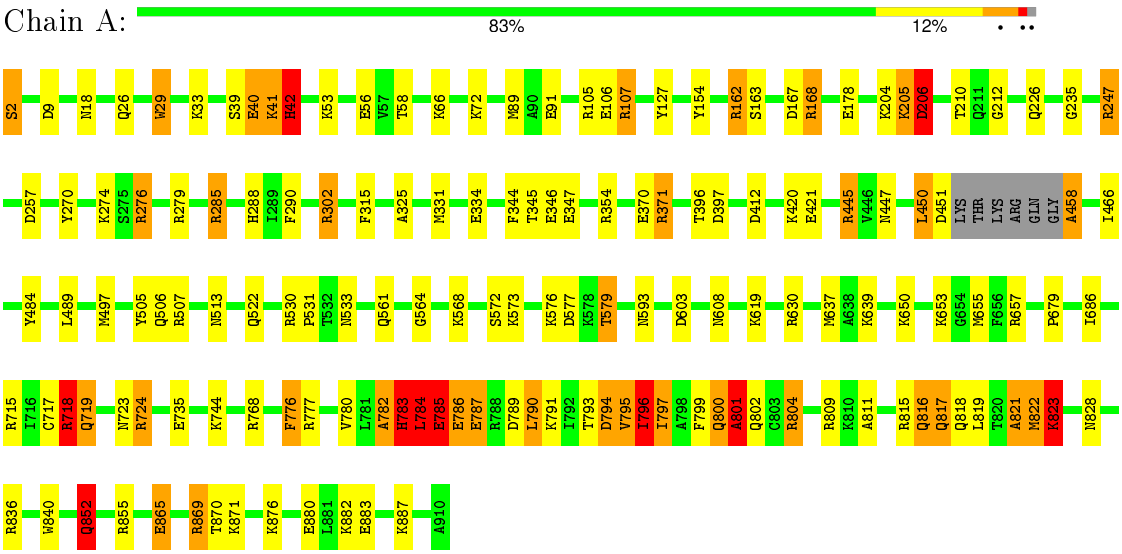
Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	148	Total	C	N	O	S	0	0
			1150	716	189	234	11		
3	F	148	Total	C	N	O	S	0	0
			1150	716	189	234	11		

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.

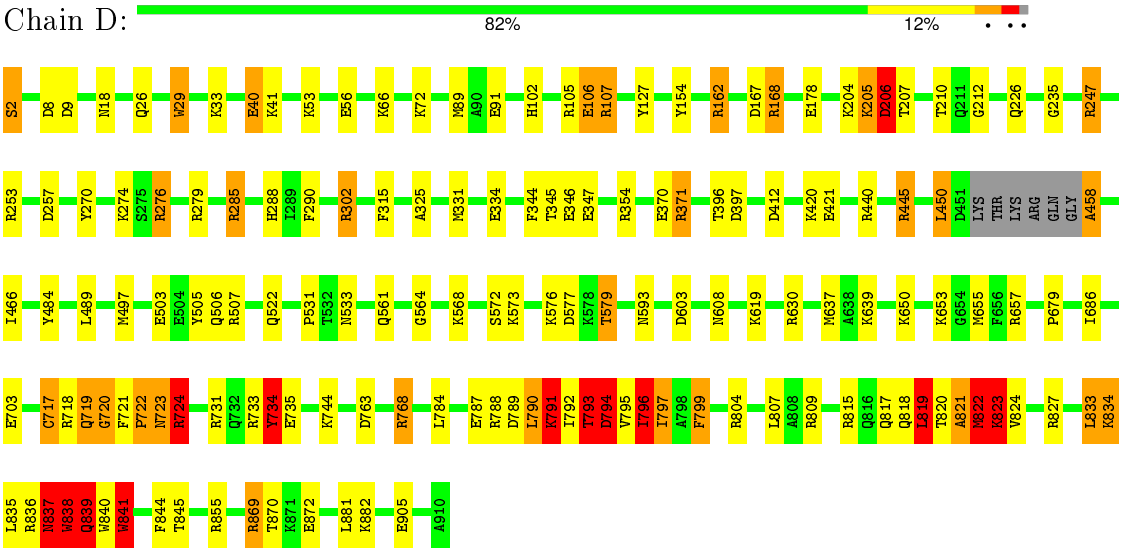
- Molecule 1: Myosin-11

Chain A:



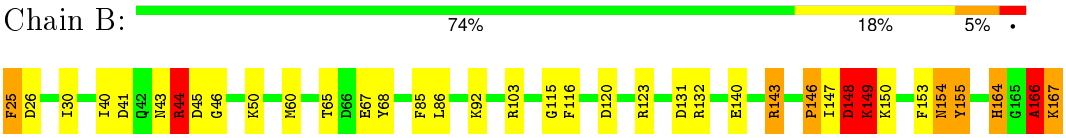
- Molecule 1: Myosin-11

Chain D:



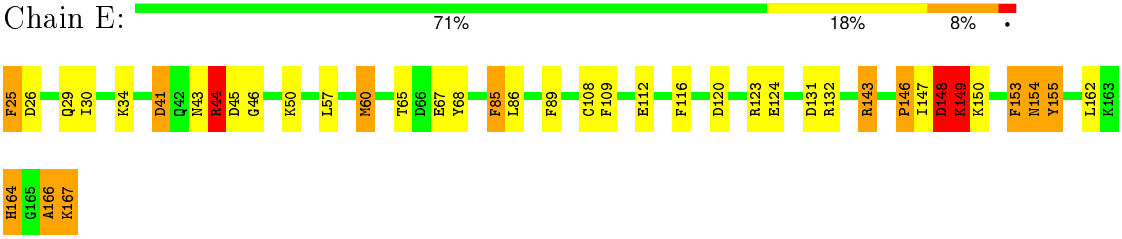
- Molecule 2: Myosin regulatory light chain 2, smooth muscle major isoform

Chain B:



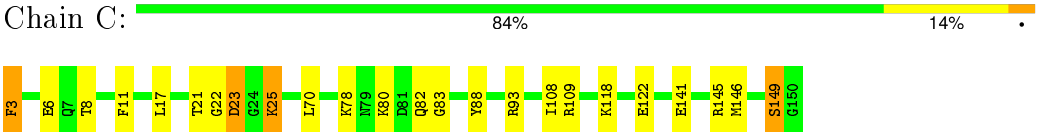
- Molecule 2: Myosin regulatory light chain 2, smooth muscle major isoform

Chain E:



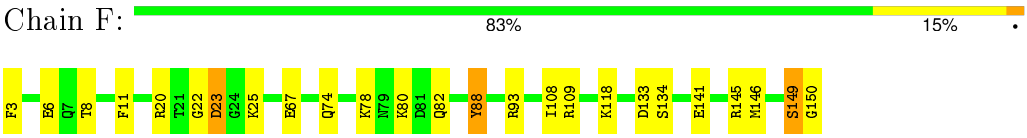
- Molecule 3: Myosin light polypeptide 6

Chain C:



- Molecule 3: Myosin light polypeptide 6

Chain F:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	CRYSTALLOGRAPHY	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	determined using ICE anc corrected with CTFAPPPLY	Depositor
Microscope	FEI/PHILIPS CM300FEG/T	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	4000	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	24000	Depositor
Image detector	Not provided	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	0.85	2/7333 (0.0%)	1.85	107/9877 (1.1%)
1	D	0.81	1/7351 (0.0%)	1.76	102/9902 (1.0%)
2	B	0.84	0/1184	1.74	22/1589 (1.4%)
2	E	0.84	0/1184	1.55	21/1589 (1.3%)
3	C	0.83	2/1163 (0.2%)	1.50	5/1559 (0.3%)
3	F	0.82	0/1163	1.30	9/1559 (0.6%)
All	All	0.83	5/19378 (0.0%)	1.74	266/26075 (1.0%)

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	46
1	D	0	48
2	B	0	11
2	E	0	13
3	C	0	5
3	F	0	5
All	All	0	128

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2	SER	C-O	-13.16	0.98	1.23
1	D	2	SER	C-O	-12.97	0.98	1.23
1	A	2	SER	N-CA	-6.24	1.33	1.46
3	C	23	ASP	C-N	5.38	1.42	1.33
3	C	83	GLY	C-N	-5.18	1.22	1.34

The worst 5 of 266 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	719	GLN	O-C-N	-53.98	31.43	123.20
1	D	837	ASN	O-C-N	-48.98	44.33	122.70
1	A	822	MET	O-C-N	-40.25	58.30	122.70
1	A	42	HIS	O-C-N	-36.58	61.01	123.20
1	D	841	TRP	O-C-N	-36.19	64.80	122.70

There are no chirality outliers.

5 of 128 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	ARG	Sidechain
1	A	127	TYR	Sidechain
1	A	168	ARG	Sidechain
1	A	41	LYS	Mainchain
1	A	42	HIS	Mainchain,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	7214	0	7236	14	0
1	D	7231	0	7262	11	0
2	B	1160	0	1076	31	0
2	E	1160	0	1076	34	0
3	C	1150	0	1116	16	0
3	F	1150	0	1114	3	0
All	All	19065	0	18880	107	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 3.

The worst 5 of 107 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)
2:E:25:PHE:CE2	2:E:86:LEU:HD11	1.15	1.63
3:C:3:PHE:CZ	3:C:70:LEU:HD11	1.15	1.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:25:PHE:CZ	2:E:30:ILE:HD11	1.34	1.60
2:B:25:PHE:CZ	2:B:30:ILE:HD11	1.29	1.59
2:E:25:PHE:CZ	2:E:86:LEU:HD11	1.36	1.59

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	899/909 (99%)	807 (90%)	69 (8%)	23 (3%)	7 45
1	D	899/909 (99%)	808 (90%)	65 (7%)	26 (3%)	6 43
2	B	141/143 (99%)	123 (87%)	11 (8%)	7 (5%)	3 31
2	E	141/143 (99%)	123 (87%)	12 (8%)	6 (4%)	3 34
3	C	146/148 (99%)	135 (92%)	9 (6%)	2 (1%)	14 58
3	F	146/148 (99%)	135 (92%)	8 (6%)	3 (2%)	9 50
All	All	2372/2400 (99%)	2131 (90%)	174 (7%)	67 (3%)	10 44

5 of 67 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	533	ASN
1	A	564	GLY
1	A	679	PRO
1	A	724	ARG
1	A	785	GLU

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	779/801 (97%)	707 (91%)	72 (9%)	11 43
1	D	782/801 (98%)	704 (90%)	78 (10%)	9 38
2	B	125/125 (100%)	108 (86%)	17 (14%)	5 27
2	E	125/125 (100%)	106 (85%)	19 (15%)	3 22
3	C	125/127 (98%)	114 (91%)	11 (9%)	12 45
3	F	125/127 (98%)	115 (92%)	10 (8%)	15 50
All	All	2061/2106 (98%)	1854 (90%)	207 (10%)	14 38

5 of 207 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	78	LYS
1	D	207	THR
2	E	148	ASP
3	C	108	ILE
1	D	40	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	751	GLN
1	D	533	ASN
1	D	223	GLN
1	A	522	GLN
3	C	16	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

There are no ligands in this entry.

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.