



wwPDB EM Map/Model Validation Report ⓘ

Sep 6, 2016 – 06:03 PM EDT

PDB ID : 5KG8
EMDB ID: : EMD-8244
Title : Rigor myosin X co-complexed with an actin filament
Authors : Sindelar, C.V.; Houdusse, A.; Sweeney, L.
Deposited on : 2016-06-12
Resolution : 9.10 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) : rb-20027939

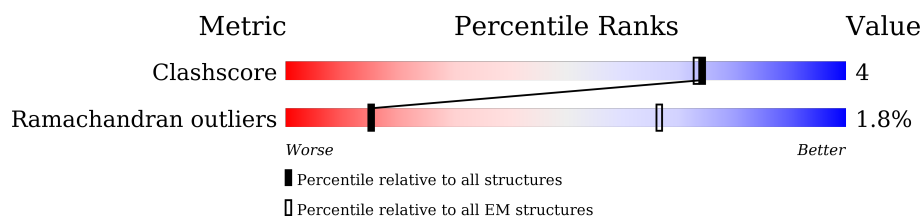
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 9.10 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

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	739	
2	B	375	
2	C	375	
2	D	375	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6464 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 Unconventional myosin-X.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	677	Total	C	N	O	0	0
			2708	1354	677	677		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	599	ALA	THR	conflict	UNP Q9HD67
A	600	ALA	LEU	conflict	UNP Q9HD67
A	601	ALA	LYS	conflict	UNP Q9HD67
A	602	ALA	CYS	conflict	UNP Q9HD67
A	603	ALA	GLY	conflict	UNP Q9HD67
A	604	ALA	SER	conflict	UNP Q9HD67
A	605	ALA	LYS	conflict	UNP Q9HD67
A	606	ALA	HIS	conflict	UNP Q9HD67

- Molecule 2 is a protein called Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	313	Total	C	N	O	0	0
			1252	626	313	313		
2	C	313	Total	C	N	O	0	0
			1252	626	313	313		
2	D	313	Total	C	N	O	0	0
			1252	626	313	313		

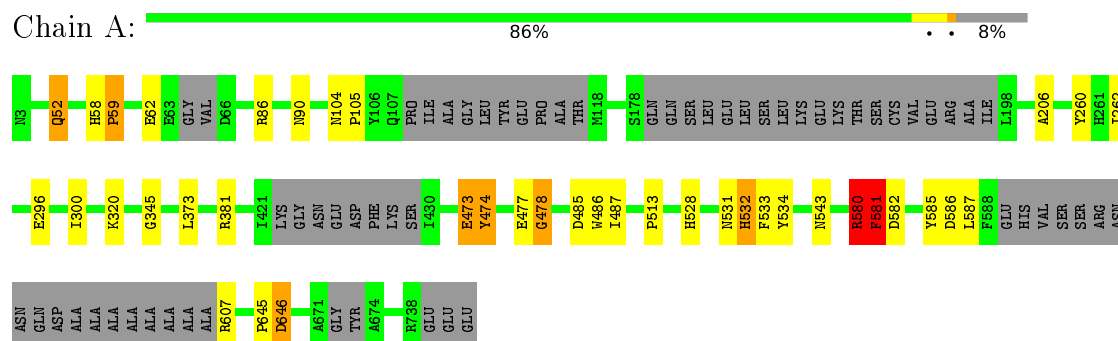
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	73	CYS	HIS	conflict	UNP P68135
C	73	CYS	HIS	conflict	UNP P68135
D	73	CYS	HIS	conflict	UNP P68135

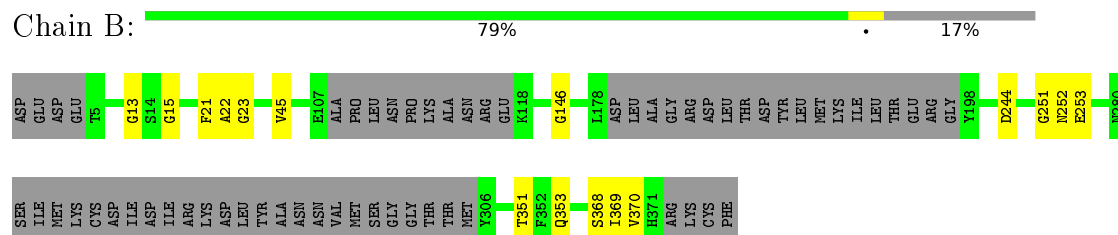
3 Residue-property plots

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.

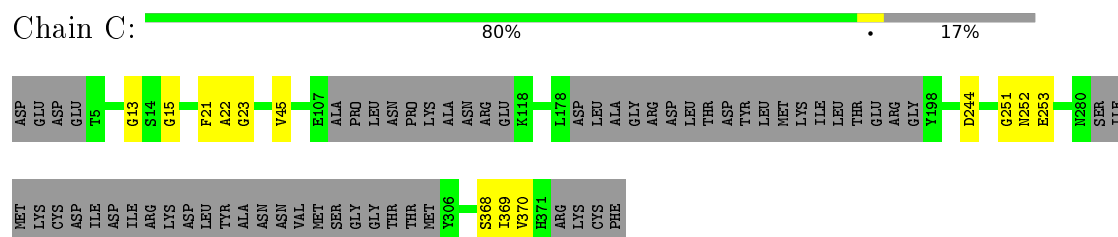
- Molecule 1: Unconventional myosin-X



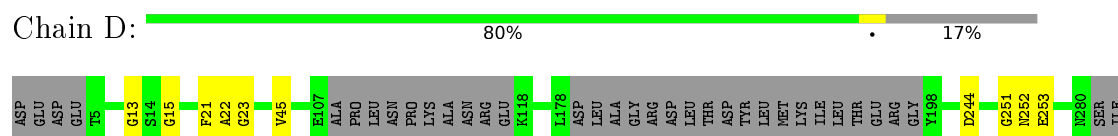
- Molecule 2: Actin, alpha skeletal muscle



- Molecule 2: Actin, alpha skeletal muscle



- Molecule 2: Actin, alpha skeletal muscle



4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of segments used	57927	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	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	0.61	5/2701 (0.2%)	0.91	11/3364 (0.3%)
2	B	0.24	0/1248	0.54	0/1553
2	C	0.25	0/1248	0.57	0/1553
2	D	0.25	0/1248	0.55	0/1553
All	All	0.44	5/6445 (0.1%)	0.72	11/8023 (0.1%)

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	8

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	474	TYR	C-O	-10.16	1.04	1.23
1	A	373	LEU	C-N	-6.92	1.18	1.34
1	A	485	ASP	CA-C	-5.98	1.37	1.52
1	A	473	GLU	C-O	-5.79	1.12	1.23
1	A	320	LYS	C-N	-5.31	1.21	1.34

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	580	ARG	CA-C-O	-15.28	88.01	120.10
1	A	580	ARG	CA-C-N	10.31	139.88	117.20
1	A	478	GLY	O-C-N	-9.78	107.05	122.70
1	A	373	LEU	C-N-CA	7.74	141.04	121.70
1	A	473	GLU	O-C-N	-7.64	110.48	122.70

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	104	ASN	Mainchain
1	A	345	GLY	Peptide
1	A	486	TRP	Peptide
1	A	532	HIS	Peptide
1	A	580	ARG	Mainchain

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	2708	0	725	18	0
2	B	1252	0	340	7	0
2	C	1252	0	340	5	0
2	D	1252	0	340	4	0
All	All	6464	0	1745	33	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 4.

The worst 5 of 33 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:A:532:HIS:C	1:A:534:TYR:H	1.78	0.87
1:A:580:ARG:O	1:A:581:PHE:C	2.23	0.76
1:A:474:TYR:O	1:A:478:GLY:O	2.05	0.74
1:A:580:ARG:O	1:A:581:PHE:O	2.13	0.65
1:A:86:ARG:O	1:A:90:ASN:O	2.13	0.65

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	663/739 (90%)	619 (93%)	30 (4%)	14 (2%)	9	50	
2	B	305/375 (81%)	267 (88%)	33 (11%)	5 (2%)	12	56	
2	C	305/375 (81%)	267 (88%)	33 (11%)	5 (2%)	12	56	
2	D	305/375 (81%)	265 (87%)	35 (12%)	5 (2%)	12	56	
All	All	1578/1864 (85%)	1418 (90%)	131 (8%)	29 (2%)	15	53	

5 of 29 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	59	PRO
1	A	105	PRO
1	A	296	GLU
1	A	300	ILE
1	A	487	ILE

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	373:LEU	C	374:THR	N	1.18