wwPDB EM Map/Model Validation Report (i)

Oct 10, 2016 – 02:29 PM EDT

PDB ID	:	5JLH
EMDB ID:	:	EMD-8164
Title	:	Cryo-EM structure of a human cytoplasmic actomyosin complex at near-atomic resolution
Authors	:	von der Ecken, J.; Heissler, S.M.; Pathan-Chhatbar, S.; Manstein, D.J.; Raunser, S.
Deposited on	:	2016-04-27
Resolution	:	3.90 Å(reported)
Based on PDB ID	:	4A7F, 3J8A, 4PD3

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

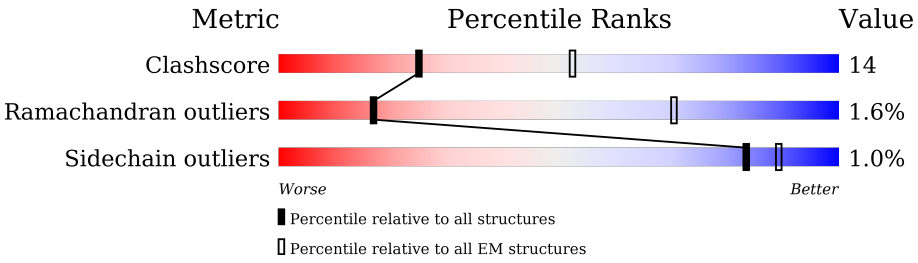
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

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 3.90 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	374	72% 27% .
1	B	374	75% 23% .
1	C	374	73% 26% .
1	D	374	73% 26% .
1	E	374	72% 27% .
2	F	1039	45% 25% . 29%
2	G	1039	46% 24% . 29%
3	H	135	100%
3	I	135	98% .

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Mol	Chain	Length	Quality of chain
3	J	135	99%
3	K	135	99%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 29177 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, cytoplasmic 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	374	Total	C	N	O	S	0	0
			2921	1849	490	560	22		
1	B	374	Total	C	N	O	S	0	0
			2921	1849	490	560	22		
1	C	374	Total	C	N	O	S	0	0
			2921	1849	490	560	22		
1	D	374	Total	C	N	O	S	0	0
			2921	1849	490	560	22		
1	E	374	Total	C	N	O	S	0	0
			2921	1849	490	560	22		

- Molecule 2 is a protein called Myosin-14,Alpha-actinin A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	737	Total	C	N	O	S	0	0
			5866	3711	1045	1083	27		
2	G	737	Total	C	N	O	S	0	0
			5866	3711	1045	1083	27		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	800	ALA	-	linker	UNP Q7Z406
F	801	SER	-	linker	UNP Q7Z406
G	800	ALA	-	linker	UNP Q7Z406
G	801	SER	-	linker	UNP Q7Z406

- Molecule 3 is a protein called Tropomyosin alpha-3 chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	H	135	Total	C	N	O	0	0
			675	405	135	135		

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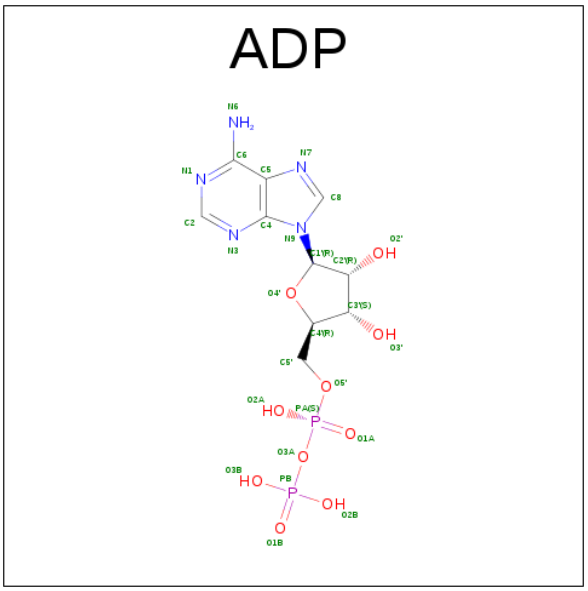
Mol	Chain	Residues	Atoms				AltConf	Trace
3	I	135	Total	C	N	O	0	0
			675	405	135	135		
3	J	135	Total	C	N	O	0	0
			675	405	135	135		
3	K	135	Total	C	N	O	0	0
			675	405	135	135		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
5	B	1	Total	Mg	0
			1	1	

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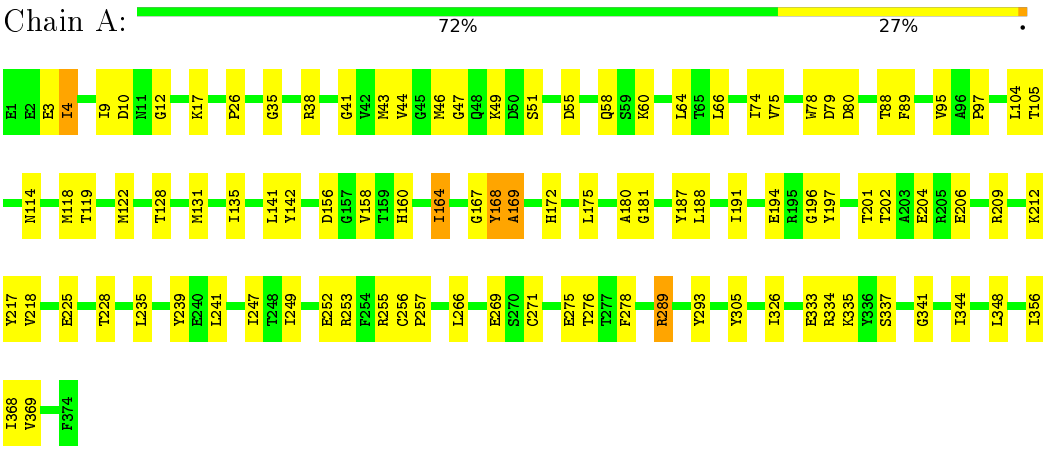
Mol	Chain	Residues	Atoms	AltConf
5	A	1	Total Mg 1 1	0
5	D	1	Total Mg 1 1	0
5	C	1	Total Mg 1 1	0
5	E	1	Total Mg 1 1	0

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.

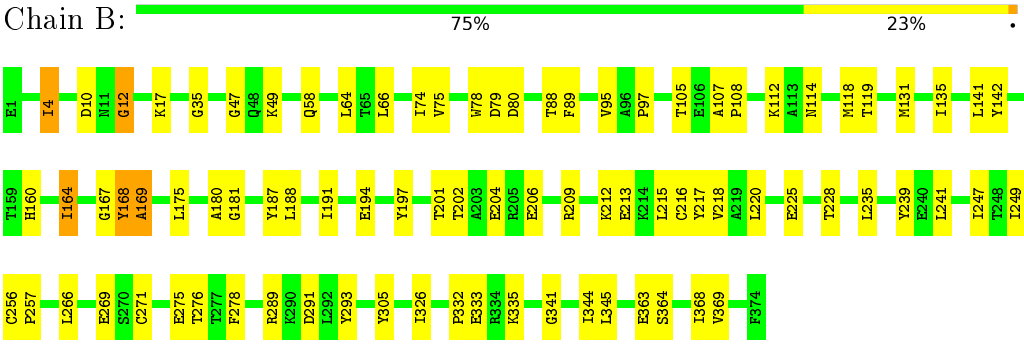
- Molecule 1: Actin, cytoplasmic 2

Chain A:



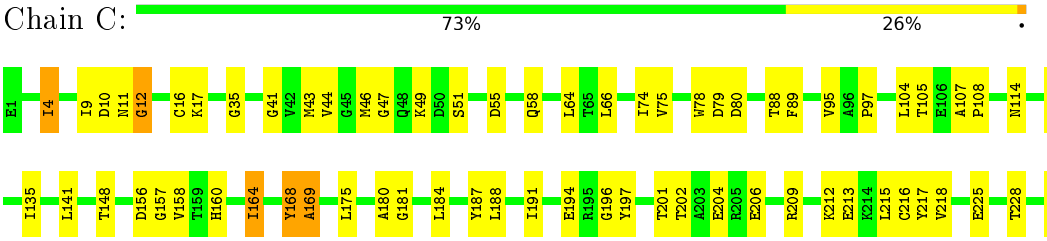
- Molecule 1: Actin, cytoplasmic 2

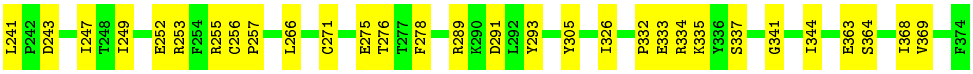
Chain B:



- Molecule 1: Actin, cytoplasmic 2

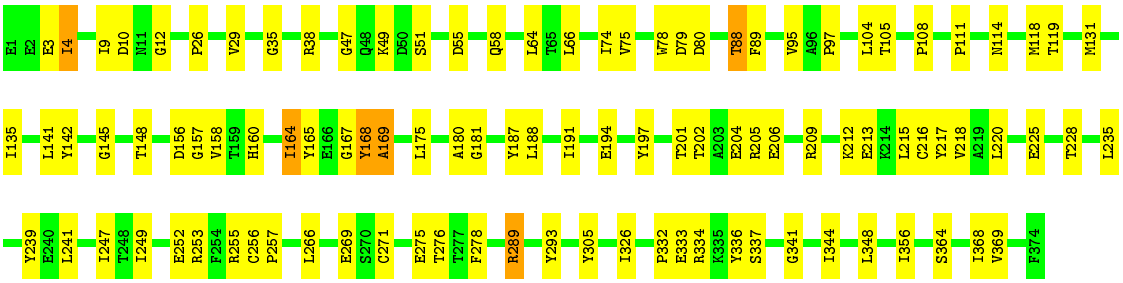
Chain C:





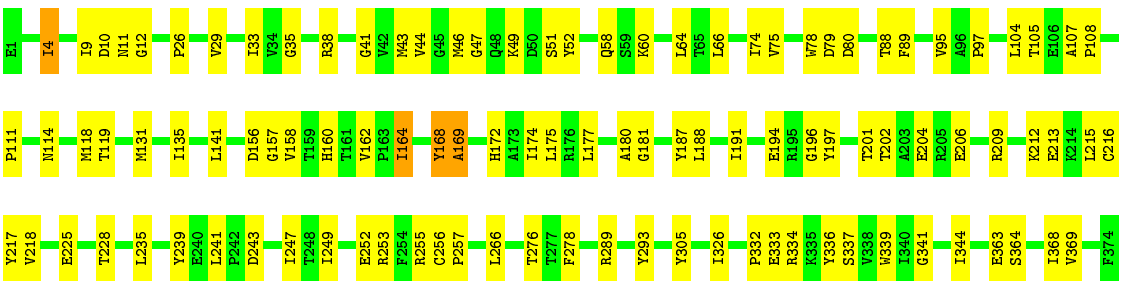
- Molecule 1: Actin, cytoplasmic 2

Chain D:



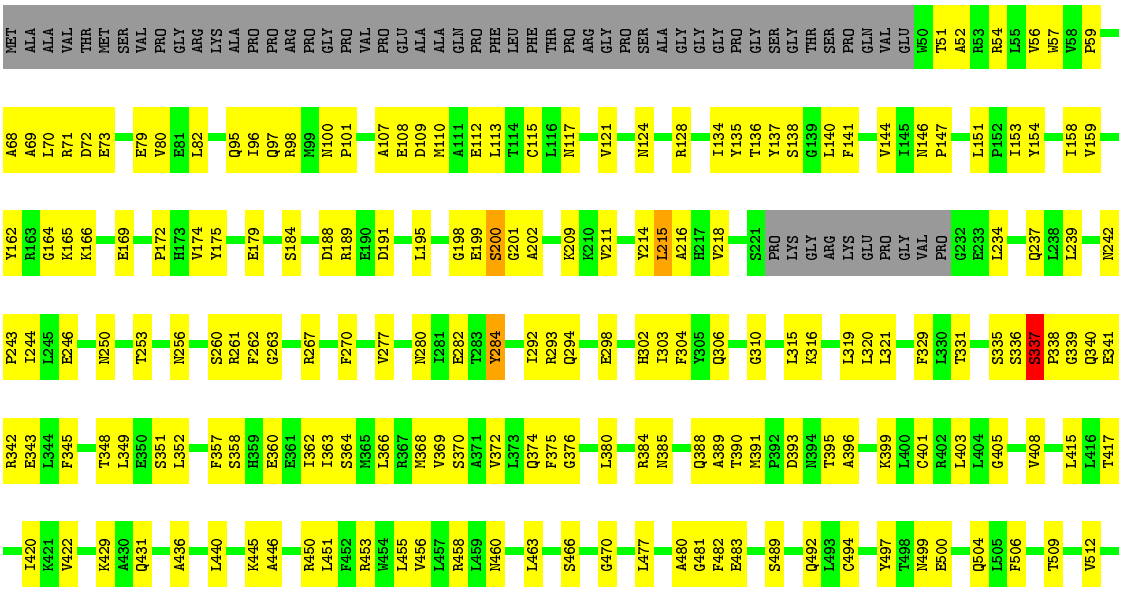
- Molecule 1: Actin, cytoplasmic 2

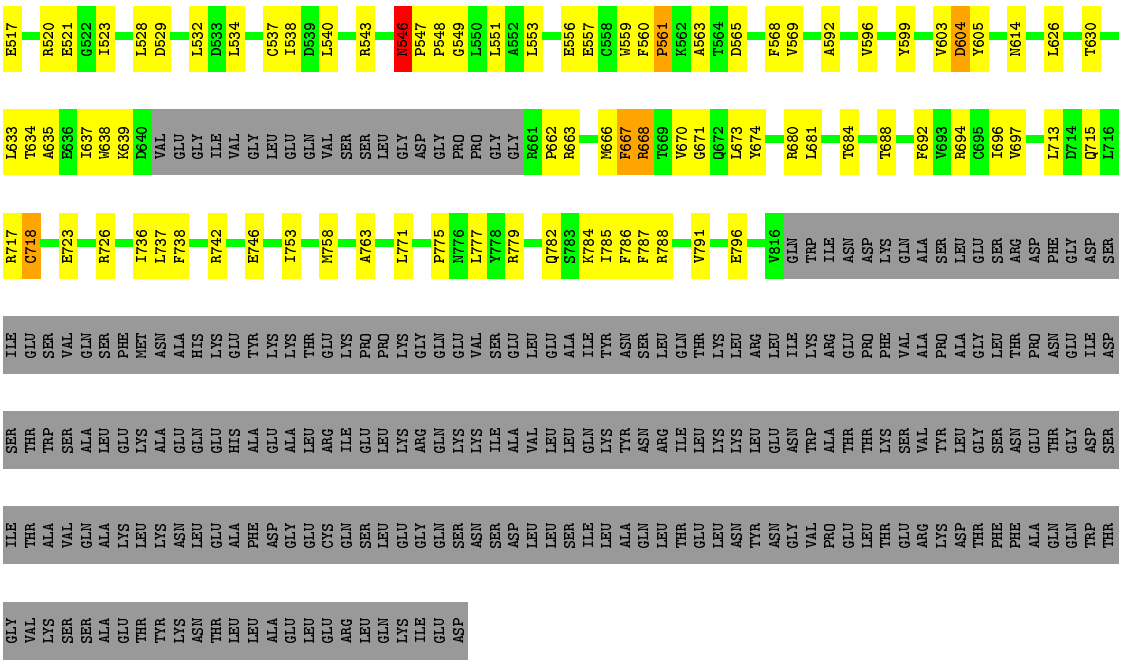
Chain E:



- Molecule 2: Myosin-14,Alpha-actinin A

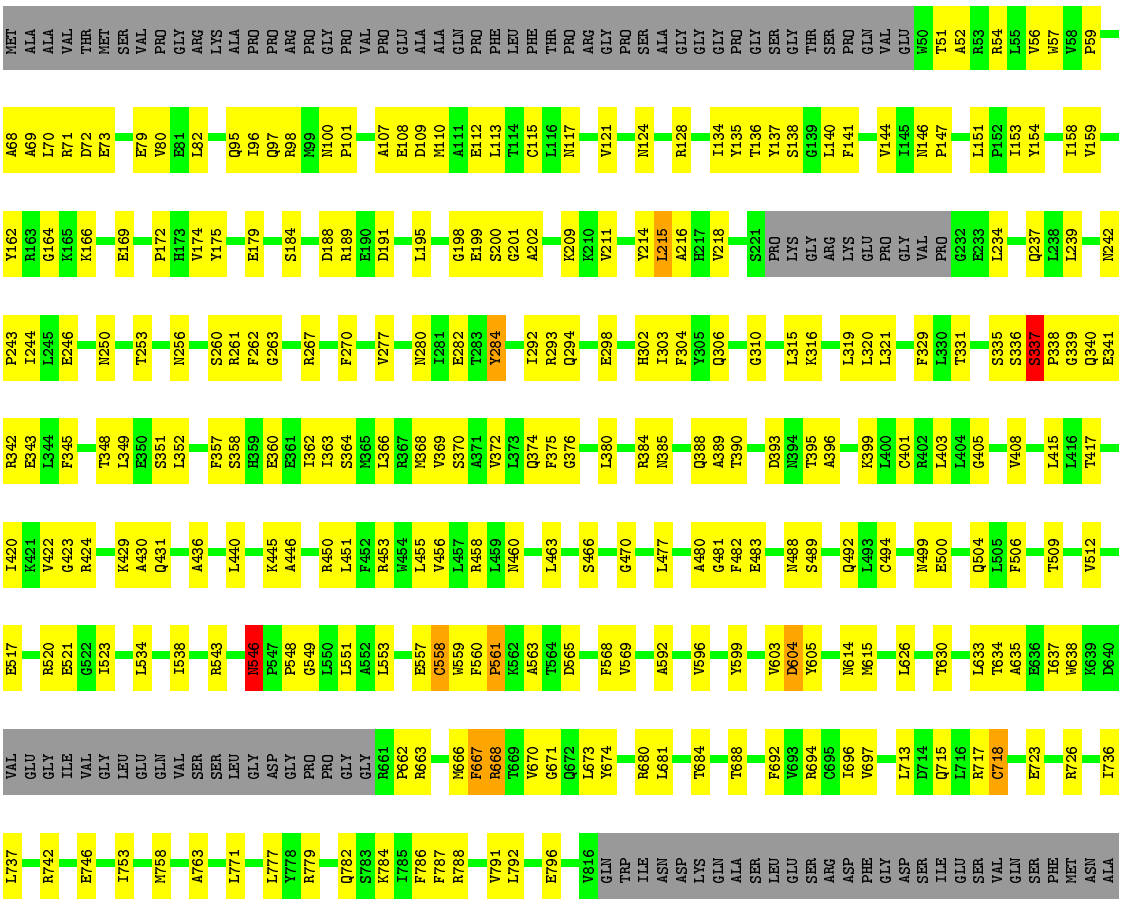
Chain F:





- Molecule 2: Myosin-14,Alpha-actinin A

Chain G:



HIS LYS GLU TYR LYS LYS THR GLU LYS PRO PRO LYS GLY GLN GLU VAL SER GLU LEU GLU ALA ILE TYR ASN SER LEU GLN THR LYS LEU ARG LEU ILE LYS ARG GLU PRO PHE VAL ALA PRO ALA GLY LEU THR PRO ASN GLU ILE ASP SER THR TRP SER ALA LEU GLU LYS ALA GLU

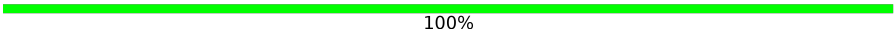
GLN GLU HIS ALA GLU ALA LEU ARG ILE GLU LEU LYS ARG GLN LYS LYS ILE ALA VAL LEU LEU GLN LYS TYR ASN ARG ILE LEU LYS LYS LEU GLU ASN TRP ALA THR THR LYS SER VAL TYR LEU GLY SER ASN GLU THR GLY ASP SER ILE THR ALA VAL GLN ALA LYS LEU LYS ASN

LEU GLU ALA PHE ASP GLY GLU CYS GLN SER LEU GLU GLY GLN SER ASN SER ASP LEU LEU SER ILE LEU ALA GLN LEU THR GLU LEU ASN TYR ASN GLY VAL PRO GLU LEU THR GLU ARG LYS ASP THR PHE PHE ALA GLN GLN TRP THR GLY VAL LYS SER SER ALA GLU THR TYR LYS

ASN THR LEU LEU ALA GLU LEU GLU ARG LEU GLN LYS ILE GLU ASP

- Molecule 3: Tropomyosin alpha-3 chain

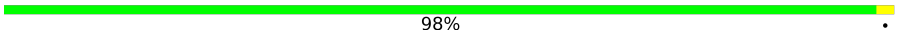
Chain H:

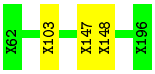


There are no outlier residues recorded for this chain.

- Molecule 3: Tropomyosin alpha-3 chain

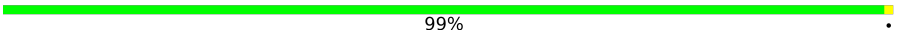
Chain I:

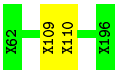




- Molecule 3: Tropomyosin alpha-3 chain

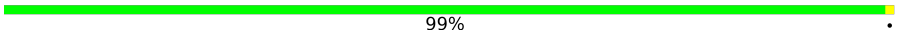
Chain J:





- Molecule 3: Tropomyosin alpha-3 chain

Chain K:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	118000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	16	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	59000	Depositor
Image detector	Not provided	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	0.80	0/2984	0.97	1/4039 (0.0%)
1	B	0.75	0/2984	0.94	2/4039 (0.0%)
1	C	0.76	0/2984	0.94	2/4039 (0.0%)
1	D	0.78	0/2984	0.97	3/4039 (0.1%)
1	E	0.79	0/2984	0.97	1/4039 (0.0%)
2	F	0.75	0/5980	0.91	3/8074 (0.0%)
2	G	0.75	0/5980	0.91	2/8074 (0.0%)
All	All	0.77	0/26880	0.93	14/36343 (0.0%)

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	D	0	1
1	E	0	2
2	F	0	2
2	G	0	1
All	All	0	6

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	289	ARG	NE-CZ-NH2	6.94	123.77	120.30
2	G	604	ASP	CB-CG-OD1	5.97	123.67	118.30
1	B	289	ARG	NE-CZ-NH2	5.92	123.26	120.30
2	F	604	ASP	CB-CG-OD1	5.65	123.39	118.30
1	E	289	ARG	NE-CZ-NH2	5.57	123.08	120.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	336	TYR	Mainchain
1	E	11	ASN	Peptide
1	E	336	TYR	Mainchain
2	F	546	ASN	Peptide
2	F	639	LYS	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	2921	0	2890	88	0
1	B	2921	0	2890	67	0
1	C	2921	0	2890	76	0
1	D	2921	0	2890	84	0
1	E	2921	0	2890	80	0
2	F	5866	0	5777	211	0
2	G	5866	0	5775	204	0
3	H	675	0	137	0	0
3	I	675	0	137	9	0
3	J	675	0	137	8	0
3	K	675	0	137	1	0
4	A	27	0	12	3	0
4	B	27	0	12	2	0
4	C	27	0	12	2	0
4	D	27	0	12	2	0
4	E	27	0	12	2	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
All	All	29177	0	26610	769	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 14.

The worst 5 of 769 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:G:384:ARG:HH12	3:J:110:UNK:CA	1.05	1.57
2:G:384:ARG:NH1	3:J:110:UNK:HA	1.29	1.39
2:G:384:ARG:HD2	3:J:109:UNK:CB	1.73	1.16
2:G:384:ARG:NH1	3:J:110:UNK:CA	1.89	1.13
2:G:384:ARG:CD	3:J:109:UNK:CB	2.32	1.05

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	372/374 (100%)	346 (93%)	21 (6%)	5 (1%)	15	59
1	B	372/374 (100%)	349 (94%)	17 (5%)	6 (2%)	12	56
1	C	372/374 (100%)	348 (94%)	18 (5%)	6 (2%)	12	56
1	D	372/374 (100%)	349 (94%)	17 (5%)	6 (2%)	12	56
1	E	372/374 (100%)	347 (93%)	19 (5%)	6 (2%)	12	56
2	F	731/1039 (70%)	680 (93%)	39 (5%)	12 (2%)	12	56
2	G	731/1039 (70%)	679 (93%)	40 (6%)	12 (2%)	12	56
All	All	3322/3948 (84%)	3098 (93%)	171 (5%)	53 (2%)	17	56

5 of 53 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	169	ALA
2	F	337	SER
2	F	466	SER
2	F	667	PHE
2	F	668	ARG

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	317/317 (100%)	314 (99%)	3 (1%)	84 92
1	B	317/317 (100%)	314 (99%)	3 (1%)	84 92
1	C	317/317 (100%)	314 (99%)	3 (1%)	84 92
1	D	317/317 (100%)	315 (99%)	2 (1%)	90 95
1	E	317/317 (100%)	314 (99%)	3 (1%)	84 92
2	F	613/888 (69%)	606 (99%)	7 (1%)	80 90
2	G	613/888 (69%)	606 (99%)	7 (1%)	80 90
All	All	2811/3361 (84%)	2783 (99%)	28 (1%)	83 91

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	278	PHE
2	F	215	LEU
2	G	569	VAL
1	E	363	GLU
2	F	140	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	295	ASN
1	E	91	ASN
2	G	302	HIS
1	E	58	GLN
1	B	87	HIS

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)

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 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	401	5	24,29,29	1.10	2 (8%)	23,45,45	1.47	3 (13%)
4	ADP	B	401	5	24,29,29	1.09	1 (4%)	23,45,45	1.50	3 (13%)
4	ADP	C	401	5	24,29,29	1.11	2 (8%)	23,45,45	1.48	3 (13%)
4	ADP	D	401	5	24,29,29	1.10	1 (4%)	23,45,45	1.48	3 (13%)
4	ADP	E	401	5	24,29,29	1.10	2 (8%)	23,45,45	1.50	3 (13%)

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	401	5	-	0/12/32/32	0/3/3/3
4	ADP	B	401	5	-	0/12/32/32	0/3/3/3
4	ADP	C	401	5	-	0/12/32/32	0/3/3/3
4	ADP	D	401	5	-	0/12/32/32	0/3/3/3
4	ADP	E	401	5	-	0/12/32/32	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	401	ADP	C2-N3	2.05	1.35	1.32
4	E	401	ADP	C2-N3	2.09	1.35	1.32
4	C	401	ADP	C2-N3	2.11	1.35	1.32
4	E	401	ADP	C5-C4	3.51	1.48	1.40
4	C	401	ADP	C5-C4	3.52	1.48	1.40

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	401	ADP	N3-C2-N1	-4.04	125.70	128.87
4	B	401	ADP	N3-C2-N1	-4.02	125.71	128.87
4	C	401	ADP	N3-C2-N1	-3.93	125.78	128.87
4	D	401	ADP	N3-C2-N1	-3.87	125.83	128.87
4	A	401	ADP	N3-C2-N1	-3.87	125.83	128.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	401	ADP	3	0
4	B	401	ADP	2	0
4	C	401	ADP	2	0
4	D	401	ADP	2	0
4	E	401	ADP	2	0

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
3	K	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	K	195:UNK	C	196:UNK	N	1.14