



# wwPDB Geometry-Only Validation Summary Report ⓘ

Mar 11, 2018 – 04:22 pm GMT

PDB ID : 3B5U  
Title : Actin filament model from extended form of acromsomal bundle in the Limulus sperm  
Authors : Cong, Y.; Topf, M.; Sali, A.; Matsudaira, P.; Dougherty, M.; Chiu, W.; Schmid, M.F.  
Deposited on : 2007-10-26  
Resolution : 9.50 Å(reported)

This is a wwPDB Geometry-Only Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk31020

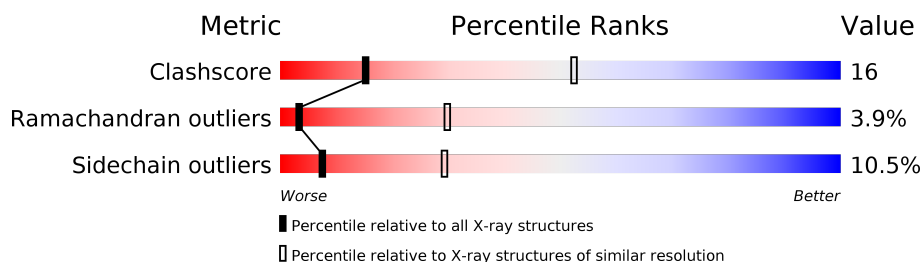
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON CRYSTALLOGRAPHY*

The reported resolution of this entry is 9.50 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	122126	1148 (15.00-3.80)
Ramachandran outliers	120053	1072 (11.50-3.80)
Sidechain outliers	120020	1039 (11.50-3.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	377	 57% 36% 5% ..
1	B	377	 58% 34% 6% ..
1	C	377	 66% 27% 6% .
1	D	377	 57% 33% 9% ..
1	E	377	 60% 29% 9% ..
1	F	377	 58% 34% 6% ..
1	G	377	 65% 29% 6% .
1	H	377	 69% 27% . ..

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Mol	Chain	Length	Quality of chain
1	I	377	<div><div></div><div>61%33%6%<div><div></div><div></div></div></div></div>
1	J	377	<div><div></div><div>60%31%6%<div><div></div><div></div></div></div></div>
1	K	377	<div><div></div><div>61%31%6%<div><div></div><div></div></div></div></div>
1	L	377	<div><div></div><div>56%36%6%<div><div></div><div></div></div></div></div>
1	M	377	<div><div></div><div>64%28%6%<div><div></div><div></div></div></div></div>
1	N	377	<div><div></div><div>57%32%9%<div><div></div><div></div></div></div></div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 41062 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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.

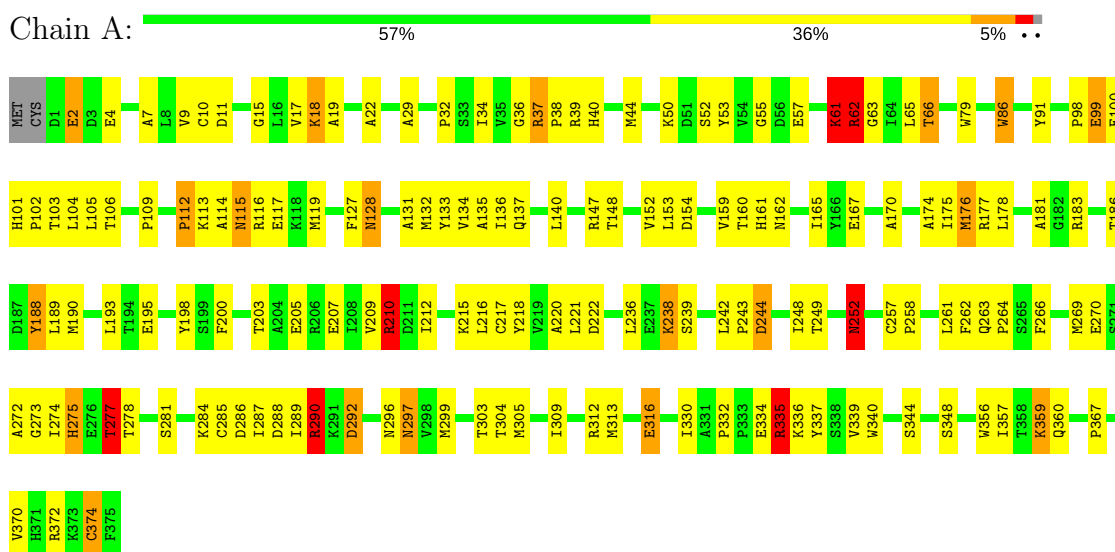
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	375	Total	C	N	O	S	0	0	0
			2933	1854	493	565	21			
1	B	375	Total	C	N	O	S	0	0	0
			2933	1854	493	565	21			
1	C	375	Total	C	N	O	S	0	0	0
			2933	1854	493	565	21			
1	D	375	Total	C	N	O	S	0	0	0
			2933	1854	493	565	21			
1	E	375	Total	C	N	O	S	0	0	0
			2933	1854	493	565	21			
1	F	375	Total	C	N	O	S	0	0	0
			2933	1854	493	565	21			
1	G	375	Total	C	N	O	S	0	0	0
			2933	1854	493	565	21			
1	H	375	Total	C	N	O	S	0	0	0
			2933	1854	493	565	21			
1	I	375	Total	C	N	O	S	0	0	0
			2933	1854	493	565	21			
1	J	375	Total	C	N	O	S	0	0	0
			2933	1854	493	565	21			
1	K	375	Total	C	N	O	S	0	0	0
			2933	1854	493	565	21			
1	L	375	Total	C	N	O	S	0	0	0
			2933	1854	493	565	21			
1	M	375	Total	C	N	O	S	0	0	0
			2933	1854	493	565	21			
1	N	375	Total	C	N	O	S	0	0	0
			2933	1854	493	565	21			

### 3 Residue-property plots

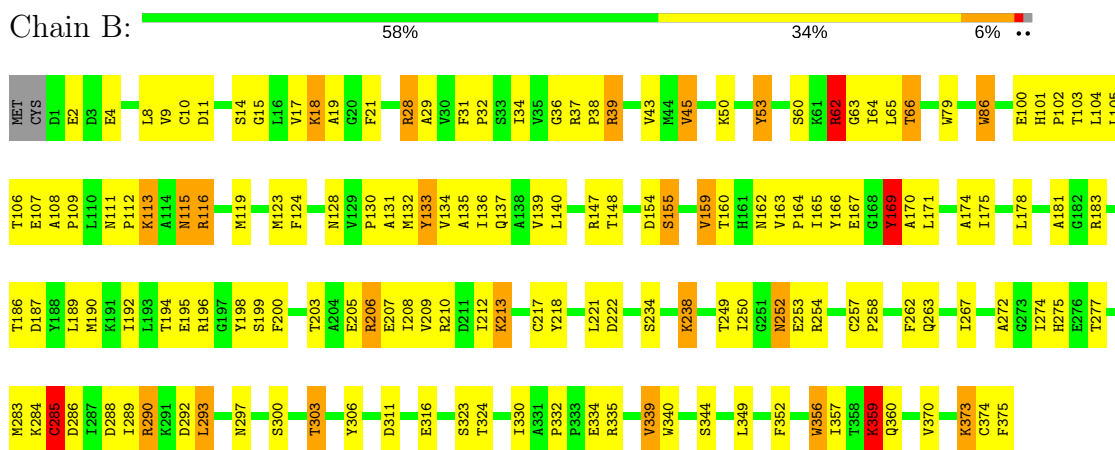
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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.

Note EDS was not executed.

- Molecule 1: Actin, alpha skeletal muscle

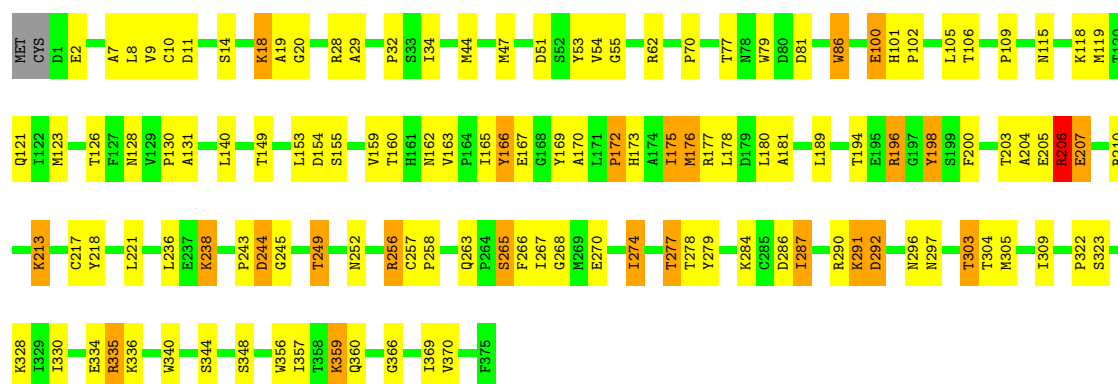


- Molecule 1: Actin, alpha skeletal muscle



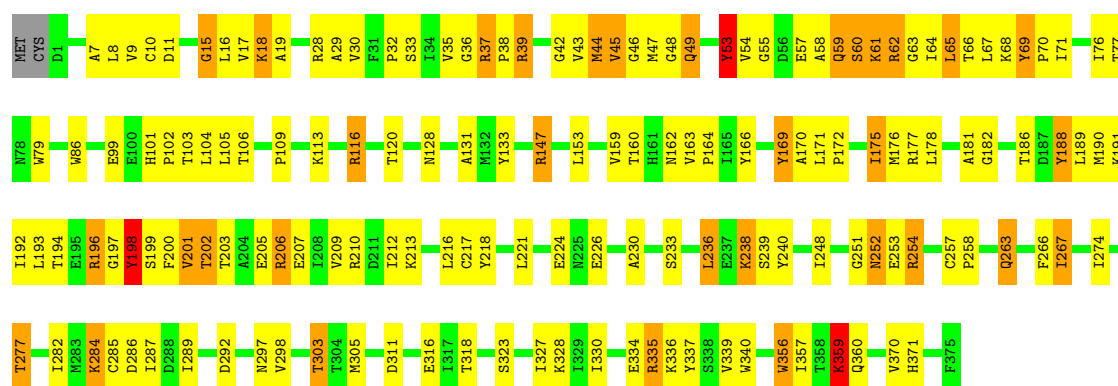
- Molecule 1: Actin, alpha skeletal muscle





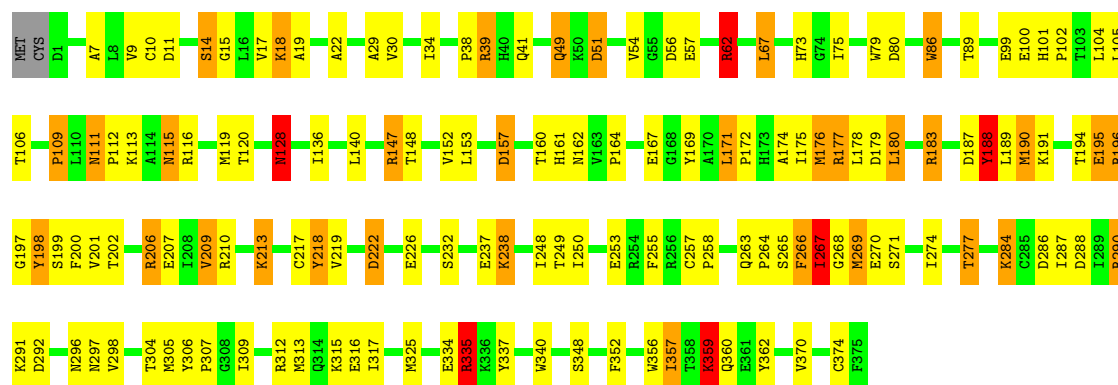
- Molecule 1: Actin, alpha skeletal muscle

Chain D: 57% 33% 9% ..



- Molecule 1: Actin, alpha skeletal muscle

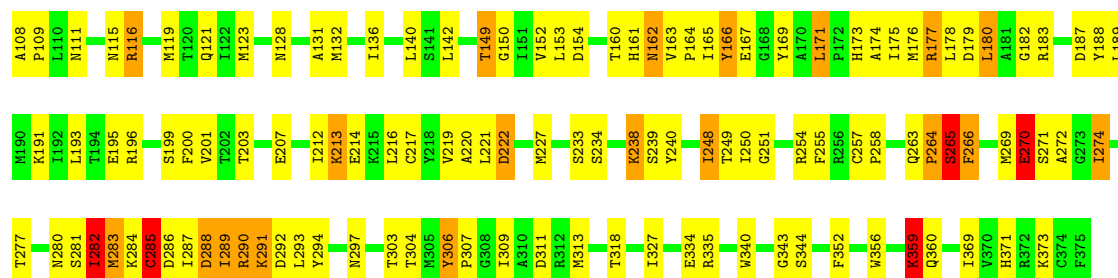
Chain E: 60% 29% 9% ..



- Molecule 1: Actin, alpha skeletal muscle

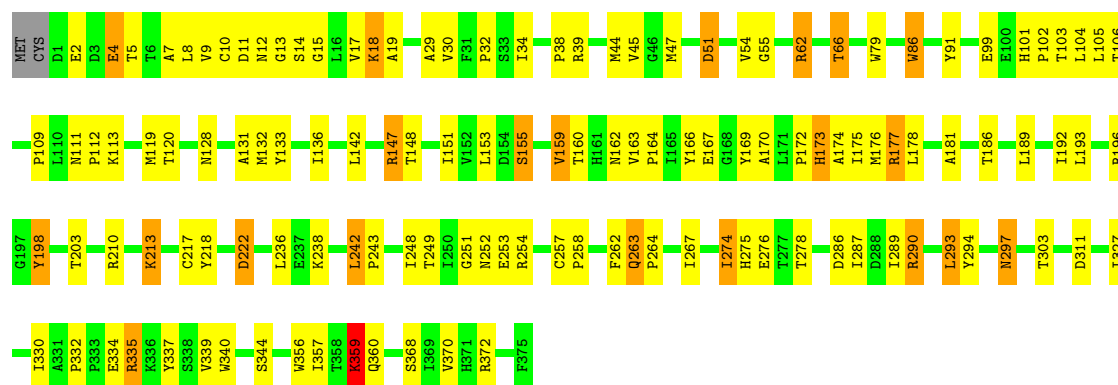
Chain F: 58% 34% 6% ..





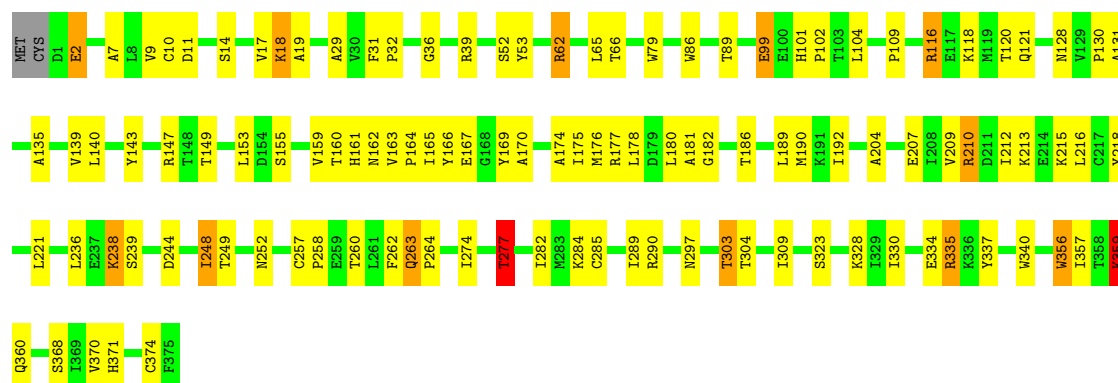
- Molecule 1: Actin, alpha skeletal muscle

Chain G: 65% 29% 6%



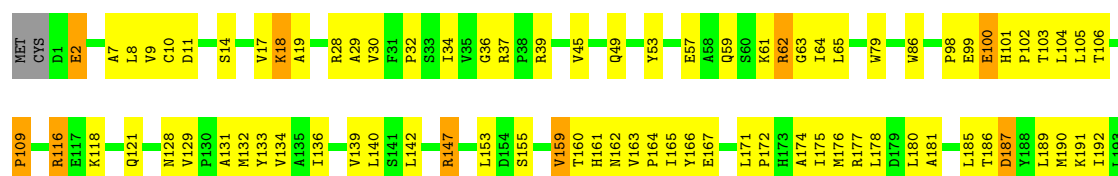
- Molecule 1: Actin, alpha skeletal muscle

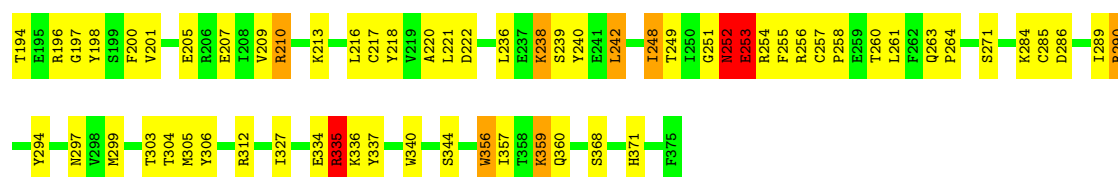
Chain H: 69% 27%



- Molecule 1: Actin, alpha skeletal muscle

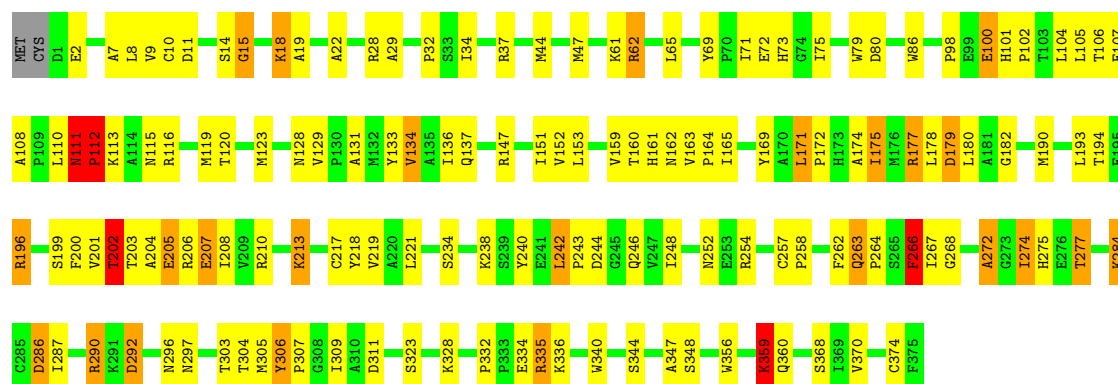
Chain I: 61% 33%





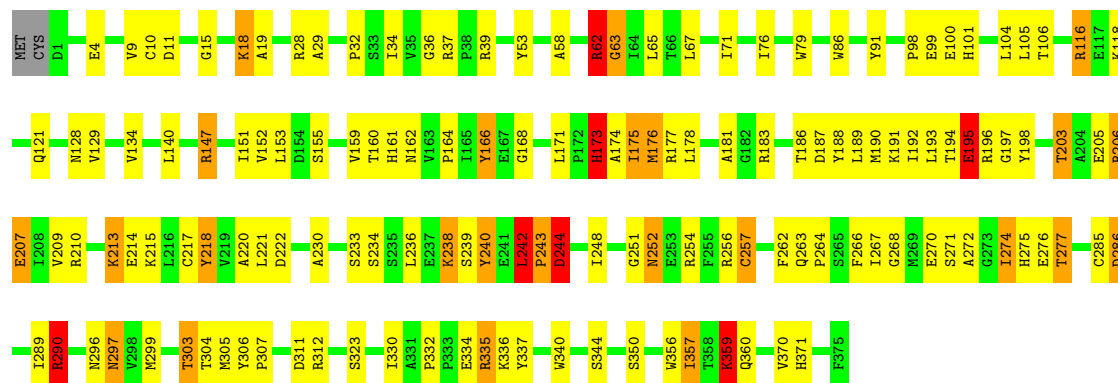
• Molecule 1: Actin, alpha skeletal muscle

Chain J: 60% 31% 6% ..



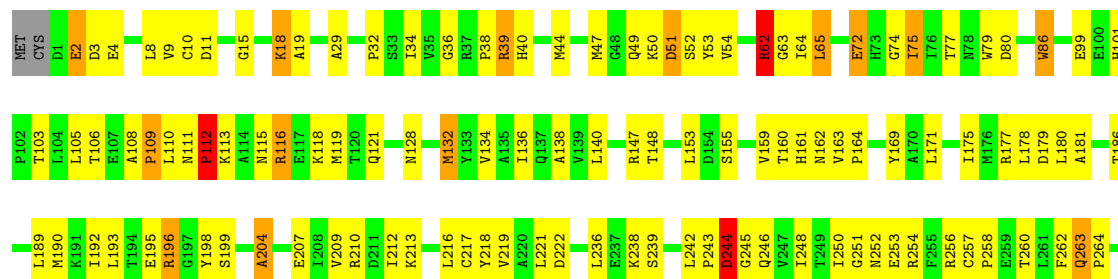
• Molecule 1: Actin, alpha skeletal muscle

Chain K: 61% 31% 6% ..

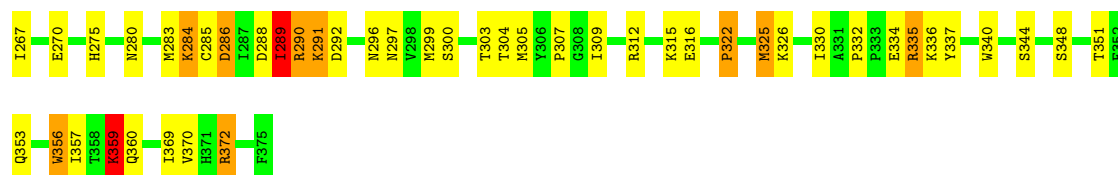


• Molecule 1: Actin, alpha skeletal muscle

Chain L: 56% 36% 6% ..

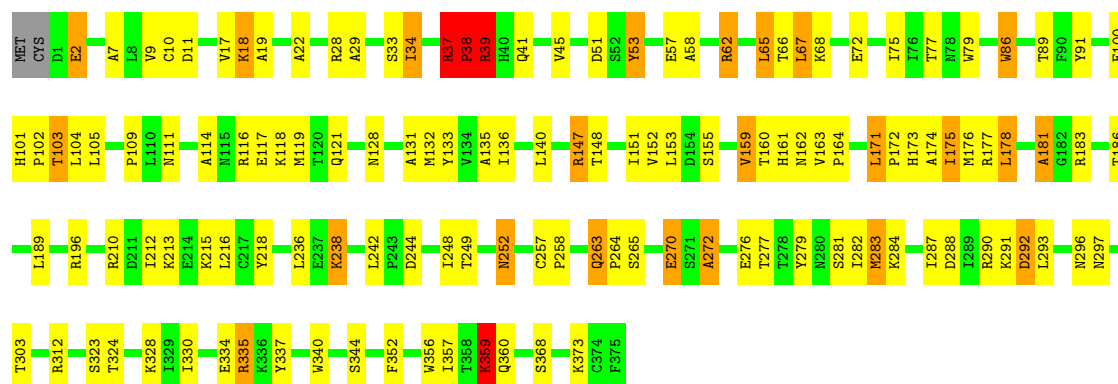






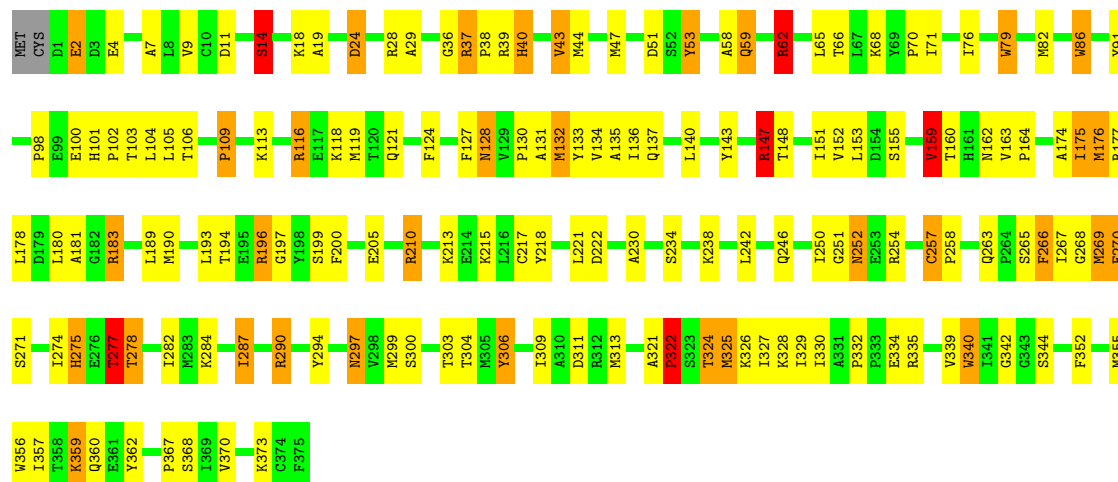
- Molecule 1: Actin, alpha skeletal muscle

Chain M: 64% 28% 6% ..



- Molecule 1: Actin, alpha skeletal muscle

Chain N: 57% 32% 9% ..



## 4 Model quality

### 4.1 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  > 5$	RMSZ	# $ Z  > 5$
1	A	0.69	0/2996	1.34	21/4058 (0.5%)
1	B	0.68	0/2996	1.35	23/4058 (0.6%)
1	C	0.64	0/2996	1.30	22/4058 (0.5%)
1	D	0.66	0/2996	1.42	33/4058 (0.8%)
1	E	0.65	0/2996	1.40	30/4058 (0.7%)
1	F	0.64	0/2996	1.34	19/4058 (0.5%)
1	G	0.65	0/2996	1.29	23/4058 (0.6%)
1	H	0.67	0/2996	1.32	20/4058 (0.5%)
1	I	0.67	0/2996	1.29	24/4058 (0.6%)
1	J	1.60	6/2996 (0.2%)	1.32	22/4058 (0.5%)
1	K	2.88	3/2996 (0.1%)	1.40	36/4058 (0.9%)
1	L	1.19	5/2996 (0.2%)	1.39	28/4058 (0.7%)
1	M	0.69	0/2996	1.40	27/4058 (0.7%)
1	N	0.69	0/2996	1.39	32/4058 (0.8%)
All	All	1.11	14/41944 (0.0%)	1.35	360/56812 (0.6%)

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
1	B	0	11
1	C	0	7
1	D	0	11
1	E	0	10
1	F	0	8
1	G	0	3
1	H	0	6
1	I	0	9
1	J	0	8
1	K	0	12

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	13
1	M	0	7
1	N	0	10
All	All	0	123

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	195	GLU	CB-CG	122.37	3.84	1.52
1	K	173	HIS	CB-CG	91.74	3.15	1.50
1	J	266	PHE	CG-CD2	38.22	1.96	1.38
1	J	266	PHE	CG-CD1	37.55	1.95	1.38
1	J	266	PHE	CE2-CZ	30.64	1.95	1.37

The worst 5 of 360 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	173	HIS	CA-CB-CG	16.70	141.98	113.60
1	E	177	ARG	NE-CZ-NH2	11.76	126.18	120.30
1	M	183	ARG	NE-CZ-NH2	-11.55	114.53	120.30
1	D	116	ARG	NE-CZ-NH1	10.44	125.52	120.30
1	N	196	ARG	NE-CZ-NH2	-10.23	115.19	120.30

There are no chirality outliers.

5 of 123 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	188	TYR	Sidechain
1	A	210	ARG	Sidechain
1	A	37	ARG	Sidechain
1	A	62	ARG	Sidechain
1	A	91	TYR	Sidechain

## 4.2 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	113	0
1	B	2933	0	2894	110	0
1	C	2933	0	2894	98	0
1	D	2933	0	2894	241	0
1	E	2933	0	2894	109	0
1	F	2933	0	2894	270	0
1	G	2933	0	2894	67	0
1	H	2933	0	2894	85	0
1	I	2933	0	2894	76	0
1	J	2933	0	2894	105	0
1	K	2933	0	2894	120	0
1	L	2933	0	2894	114	0
1	M	2933	0	2894	69	0
1	N	2933	0	2894	82	0
All	All	41062	0	40516	1305	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 16.

The worst 5 of 1305 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:44:MET:CG	1:F:293:LEU:CD2	1.79	1.58
1:J:266:PHE:CE2	1:J:266:PHE:CZ	1.95	1.52
1:J:266:PHE:CD1	1:J:266:PHE:CE1	1.94	1.52
1:J:266:PHE:CG	1:J:266:PHE:CD1	1.95	1.52
1:J:266:PHE:CD2	1:J:266:PHE:CE2	1.95	1.51

There are no symmetry-related clashes.

## 4.3 Torsion angles [i](#)

### 4.3.1 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 X-ray entries followed by that with respect to entries of similar resolution.

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	373/377 (99%)	297 (80%)	63 (17%)	13 (4%)	4	32
1	B	373/377 (99%)	298 (80%)	58 (16%)	17 (5%)	2	27
1	C	373/377 (99%)	310 (83%)	55 (15%)	8 (2%)	8	43
1	D	373/377 (99%)	310 (83%)	49 (13%)	14 (4%)	3	30
1	E	373/377 (99%)	303 (81%)	56 (15%)	14 (4%)	3	30
1	F	373/377 (99%)	291 (78%)	62 (17%)	20 (5%)	2	24
1	G	373/377 (99%)	315 (84%)	46 (12%)	12 (3%)	4	34
1	H	373/377 (99%)	308 (83%)	55 (15%)	10 (3%)	5	38
1	I	373/377 (99%)	318 (85%)	45 (12%)	10 (3%)	5	38
1	J	373/377 (99%)	308 (83%)	48 (13%)	17 (5%)	2	27
1	K	373/377 (99%)	323 (87%)	33 (9%)	17 (5%)	2	27
1	L	373/377 (99%)	311 (83%)	44 (12%)	18 (5%)	2	26
1	M	373/377 (99%)	300 (80%)	54 (14%)	19 (5%)	2	25
1	N	373/377 (99%)	307 (82%)	51 (14%)	15 (4%)	3	29
All	All	5222/5278 (99%)	4299 (82%)	719 (14%)	204 (4%)	3	30

5 of 204 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
1	A	236	LEU
1	A	252	ASN
1	A	272	ALA
1	B	113	LYS

#### 4.3.2 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 X-ray entries followed by that with respect to entries of similar resolution.

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	318/320 (99%)	284 (89%)	34 (11%)	7	28
1	B	318/320 (99%)	285 (90%)	33 (10%)	8	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	318/320 (99%)	281 (88%)	37 (12%)	6	25
1	D	318/320 (99%)	284 (89%)	34 (11%)	7	28
1	E	318/320 (99%)	282 (89%)	36 (11%)	6	26
1	F	318/320 (99%)	287 (90%)	31 (10%)	9	32
1	G	318/320 (99%)	294 (92%)	24 (8%)	15	45
1	H	318/320 (99%)	291 (92%)	27 (8%)	12	40
1	I	318/320 (99%)	288 (91%)	30 (9%)	9	33
1	J	318/320 (99%)	277 (87%)	41 (13%)	5	22
1	K	318/320 (99%)	289 (91%)	29 (9%)	10	35
1	L	318/320 (99%)	286 (90%)	32 (10%)	8	30
1	M	318/320 (99%)	286 (90%)	32 (10%)	8	30
1	N	318/320 (99%)	271 (85%)	47 (15%)	3	18
All	All	4452/4480 (99%)	3985 (90%)	467 (10%)	7	29

5 of 467 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	159	VAL
1	I	62	ARG
1	N	100	GLU
1	G	252	ASN
1	H	210	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	263	GLN
1	G	263	GLN
1	M	252	ASN
1	G	111	ASN
1	G	275	HIS

#### 4.3.3 RNA ⓘ

There are no RNA molecules in this entry.

#### 4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

#### 4.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

#### 4.6 Ligand geometry [i](#)

There are no ligands in this entry.

#### 4.7 Other polymers [i](#)

There are no such residues in this entry.

#### 4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.