



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Aug 17, 2017 – 05:05 PM EDT

PDB ID : 2W49
EMDB ID: : EMD-1561
Title : ISOMETRICALLY CONTRACTING INSECT ASYNCHRONOUS FLIGHT
MUSCLE
Authors : Wu, S.; Liu, J.; Reedy, M.C.; Tregear, R.T.; Winkler, H.; Franzini-Armstrong,
C.; Sasaki, H.; Lucaveche, C.; Goldman, Y.E.; Reedy, M.K.; Taylor, K.A.
Deposited on : unknown
Resolution : 35.00 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

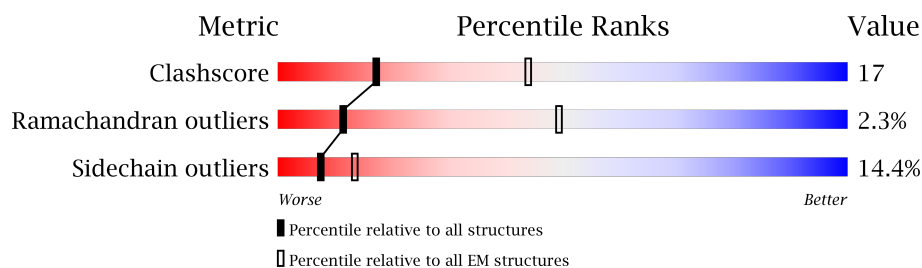
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 35.00 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.




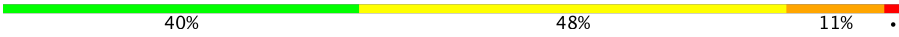






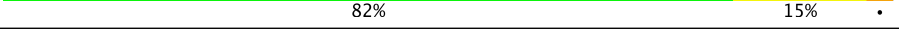

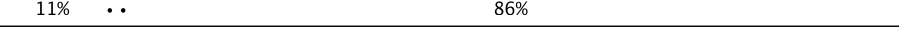
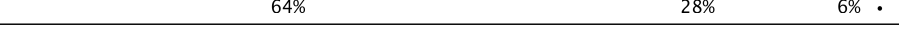

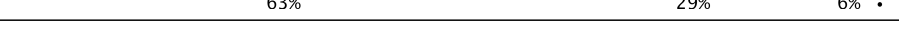


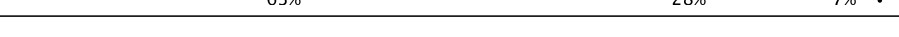

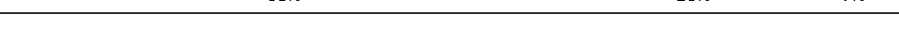






Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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	0	159	47% 44% 6% .
1	3	159	46% 45% 6% .
1	6	159	46% 45% 6% .
1	9	159	45% 46% 6% .
2	1	90	51% 37% 12%
2	4	90	51% 38% 11%
2	7	90	52% 39% 9%
2	Y	90	51% 40% 9%
3	2	141	43% 44% 11% .

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Mol	Chain	Length	Quality of chain
3	5	141	 41% 45% 13% .
3	8	141	 40% 48% 11% .
3	Z	141	 43% 44% 11% .
4	A	277	 82% 15% .
4	B	277	 81% 17% .
4	C	277	 11% . . 86%
4	T	277	 9% . . 86%
4	U	277	 81% 17% .
4	V	277	 82% 15% .
4	W	277	 9% . . 86%
4	X	277	 11% . . 86%
5	D	372	 64% 28% 6% .
5	E	372	 64% 28% 7% .
5	F	372	 63% 29% 6% .
5	G	372	 64% 28% 6% .
5	H	372	 64% 28% 7% .
5	I	372	 63% 28% 7% .
5	J	372	 64% 28% 7% .
5	K	372	 63% 29% 7% .
5	L	372	 63% 29% 6% .
5	M	372	 63% 29% 7% .
5	N	372	 63% 28% 7% .
5	O	372	 63% 29% 6% .
5	P	372	 63% 29% 7% .
5	Q	372	 64% 28% 7% .

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Mol	Chain	Length	Quality of chain
5	R	372	<div><div></div><div>64%</div><div>28%</div><div>7%</div><div></div></div>
5	S	372	<div><div></div><div>64%</div><div>28%</div><div>7%</div><div></div></div>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 69376 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 TROPONIN C, SKELETAL MUSCLE.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	159	Total	C	N	O	S	0	0
			1252	770	199	272	11		
1	3	159	Total	C	N	O	S	0	0
			1252	770	199	272	11		
1	6	159	Total	C	N	O	S	0	0
			1252	770	199	272	11		
1	9	159	Total	C	N	O	S	0	0
			1252	770	199	272	11		

- Molecule 2 is a protein called TROPONIN T, FAST SKELETAL MUSCLE ISOFORMS.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	1	90	Total	C	N	O	0	0
			774	486	146	142		
2	4	90	Total	C	N	O	0	0
			774	486	146	142		
2	7	90	Total	C	N	O	0	0
			774	486	146	142		
2	Y	90	Total	C	N	O	0	0
			774	486	146	142		

- Molecule 3 is a protein called TROPONIN I, FAST SKELETAL MUSCLE.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	141	Total	C	N	O	S	0	0
			1140	709	214	212	5		
3	5	141	Total	C	N	O	S	0	0
			1140	709	214	212	5		
3	8	141	Total	C	N	O	S	0	0
			1140	709	214	212	5		
3	Z	141	Total	C	N	O	S	0	0
			1140	709	214	212	5		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	48	SER	CYS	conflict	UNP P68246
2	64	SER	CYS	conflict	UNP P68246
2	89	ILE	ASN	conflict	UNP P68246
5	48	SER	CYS	conflict	UNP P68246
5	64	SER	CYS	conflict	UNP P68246
5	89	ILE	ASN	conflict	UNP P68246
8	48	SER	CYS	conflict	UNP P68246
8	64	SER	CYS	conflict	UNP P68246
8	89	ILE	ASN	conflict	UNP P68246
Z	48	SER	CYS	conflict	UNP P68246
Z	64	SER	CYS	conflict	UNP P68246
Z	89	ILE	ASN	conflict	UNP P68246

- Molecule 4 is a protein called TROPOMYOSIN ALPHA-1 CHAIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	277	Total	C	N	O	S	0	0
			2230	1362	378	484	6		
4	B	277	Total	C	N	O	S	0	0
			2230	1362	378	484	6		
4	C	39	Total	C	N	O	S	0	0
			316	198	48	69	1		
4	T	39	Total	C	N	O	S	0	0
			316	198	48	69	1		
4	U	277	Total	C	N	O	S	0	0
			2230	1362	378	484	6		
4	V	277	Total	C	N	O	S	0	0
			2230	1362	378	484	6		
4	W	39	Total	C	N	O	S	0	0
			316	198	48	69	1		
4	X	39	Total	C	N	O	S	0	0
			316	198	48	69	1		

- Molecule 5 is a protein called ACTIN, ALPHA SKELETAL MUSCLE.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	372	Total	C	N	O	S	0	0
			2907	1836	489	562	20		
5	E	372	Total	C	N	O	S	0	0
			2907	1836	489	562	20		
5	F	372	Total	C	N	O	S	0	0
			2907	1836	489	562	20		
5	G	372	Total	C	N	O	S	0	0
			2907	1836	489	562	20		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	372	Total	C	N	O	S	0	0
			2907	1836	489	562	20		
5	I	372	Total	C	N	O	S	0	0
			2907	1836	489	562	20		
5	J	372	Total	C	N	O	S	0	0
			2907	1836	489	562	20		
5	K	372	Total	C	N	O	S	0	0
			2907	1836	489	562	20		
5	L	372	Total	C	N	O	S	0	0
			2907	1836	489	562	20		
5	M	372	Total	C	N	O	S	0	0
			2907	1836	489	562	20		
5	N	372	Total	C	N	O	S	0	0
			2907	1836	489	562	20		
5	O	372	Total	C	N	O	S	0	0
			2907	1836	489	562	20		
5	P	372	Total	C	N	O	S	0	0
			2907	1836	489	562	20		
5	Q	372	Total	C	N	O	S	0	0
			2907	1836	489	562	20		
5	R	372	Total	C	N	O	S	0	0
			2907	1836	489	562	20		
5	S	372	Total	C	N	O	S	0	0
			2907	1836	489	562	20		

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
6	0	4	Total	Ca	0
			4	4	
6	9	4	Total	Ca	0
			4	4	
6	3	4	Total	Ca	0
			4	4	
6	6	4	Total	Ca	0
			4	4	

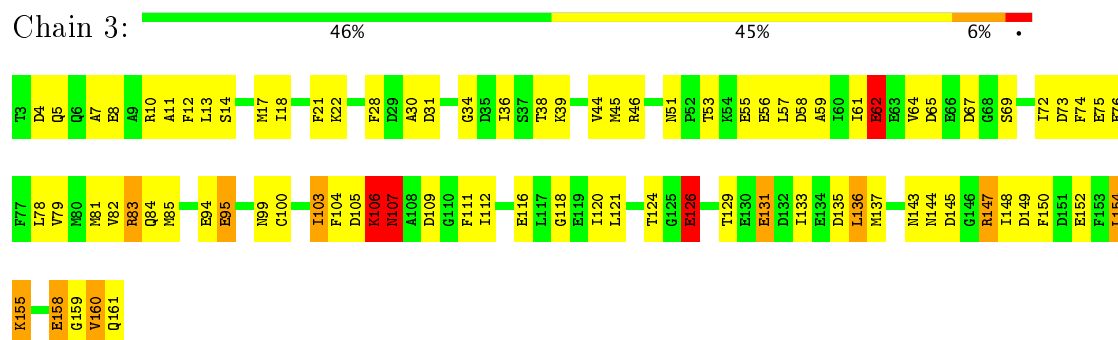
3 Residue-property plots

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.

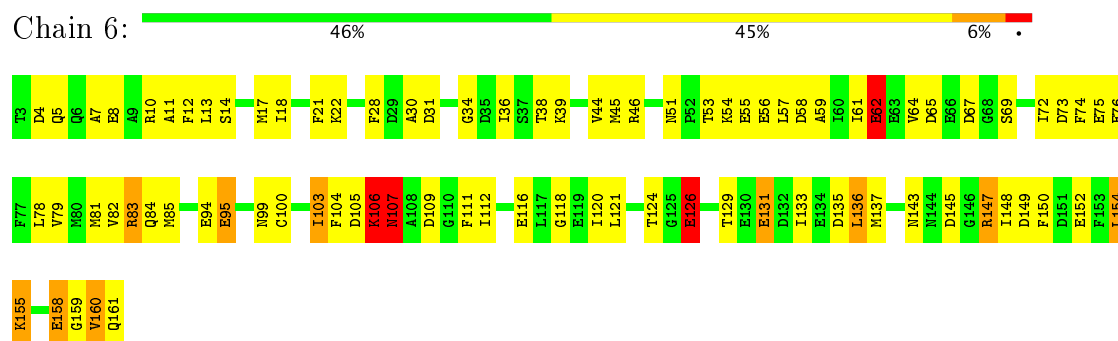
- Molecule 1: TROPONIN C, SKELETAL MUSCLE



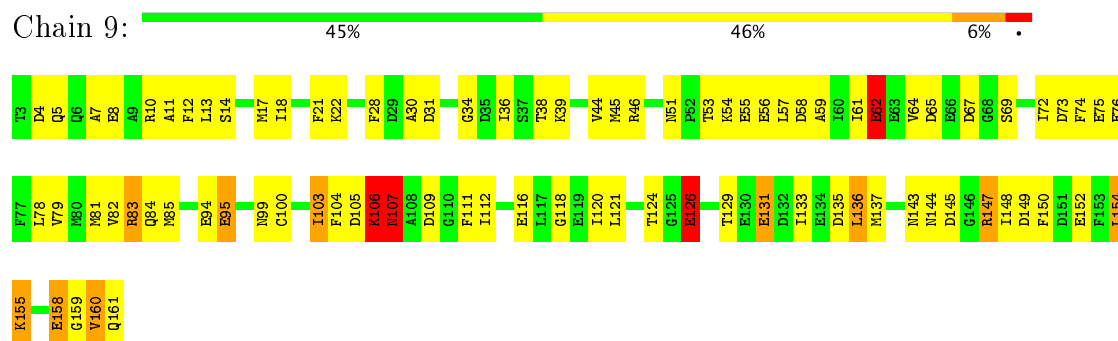
- Molecule 1: TROPONIN C, SKELETAL MUSCLE



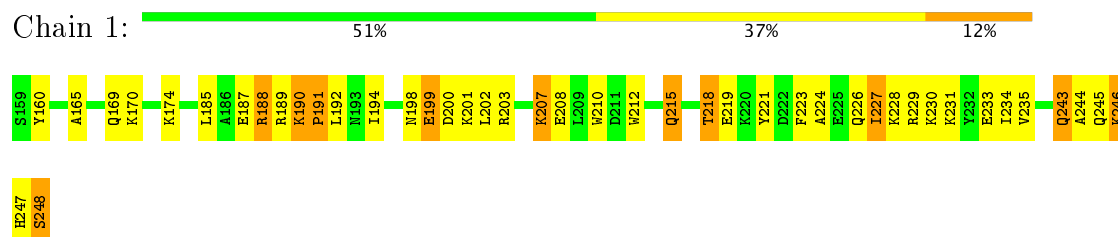
- Molecule 1: TROPONIN C, SKELETAL MUSCLE



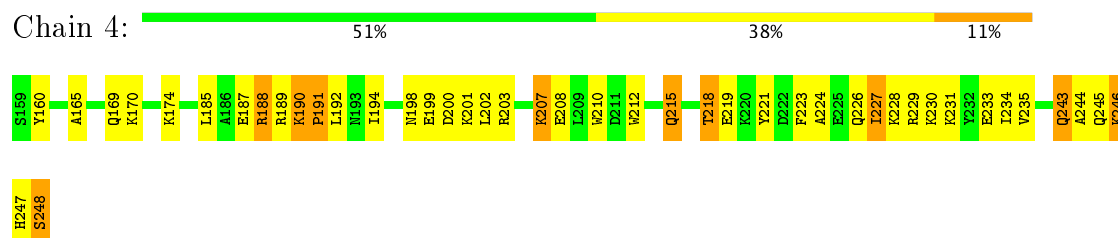
- Molecule 1: TROPONIN C, SKELETAL MUSCLE



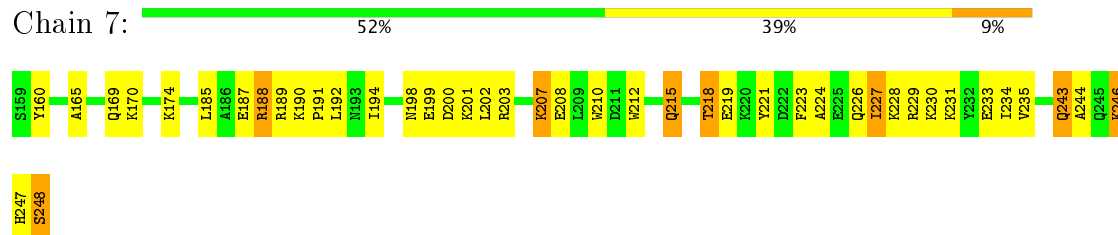
- Molecule 2: TROPONIN T, FAST SKELETAL MUSCLE ISOFORMS



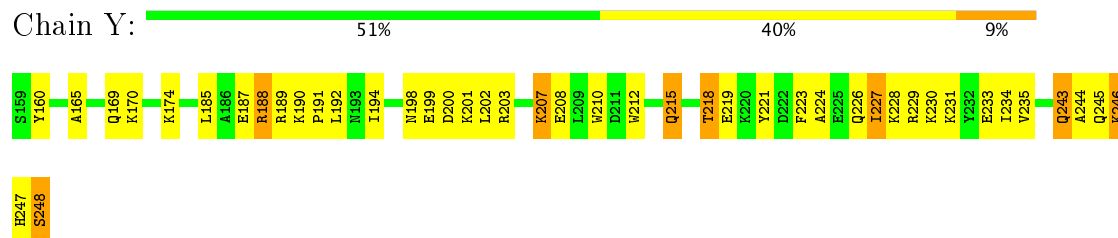
- Molecule 2: TROPONIN T, FAST SKELETAL MUSCLE ISOFORMS



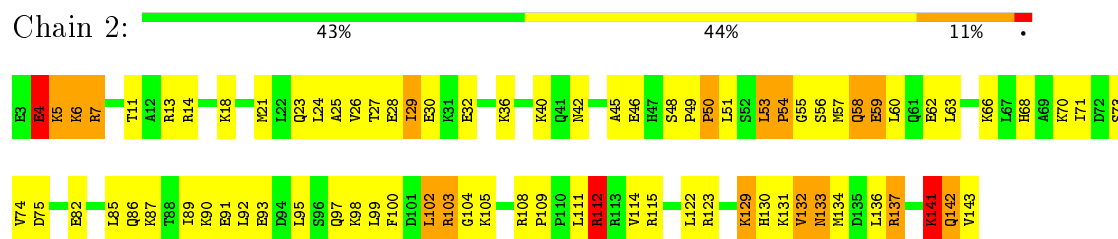
- Molecule 2: TROPONIN T, FAST SKELETAL MUSCLE ISOFORMS



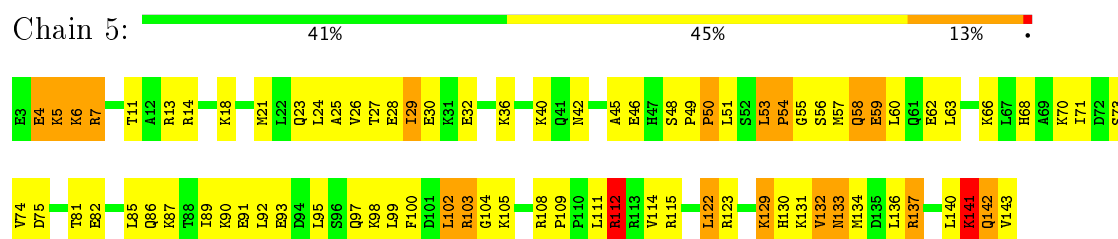
- Molecule 2: TROPONIN T, FAST SKELETAL MUSCLE ISOFORMS



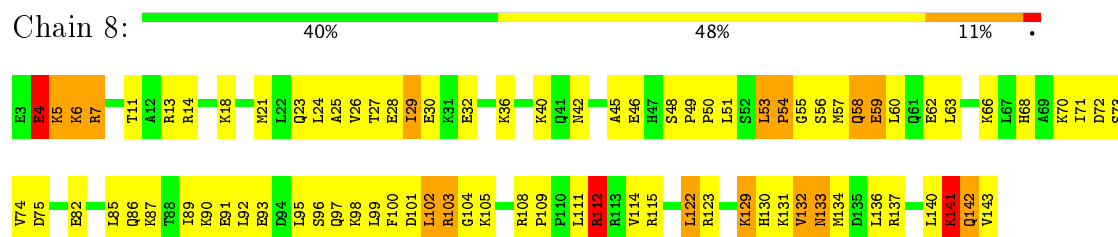
- Molecule 3: TROPONIN I, FAST SKELETAL MUSCLE



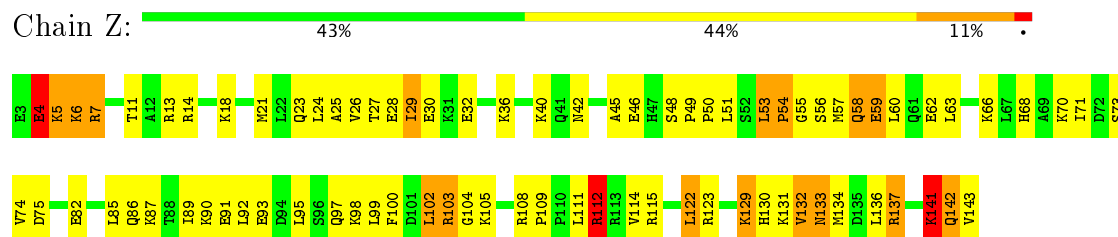
- Molecule 3: TROPONIN I, FAST SKELETAL MUSCLE



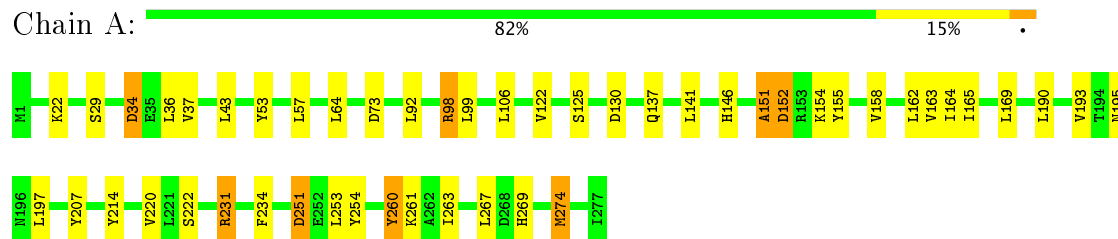
- Molecule 3: TROPONIN I, FAST SKELETAL MUSCLE




- Molecule 3: TROPONIN I, FAST SKELETAL MUSCLE

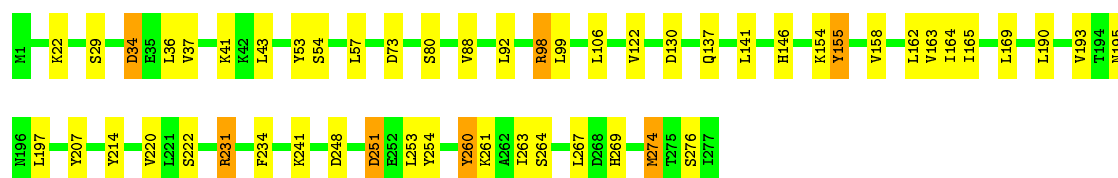


- Molecule 4: TROPOMYOSIN ALPHA-1 CHAIN



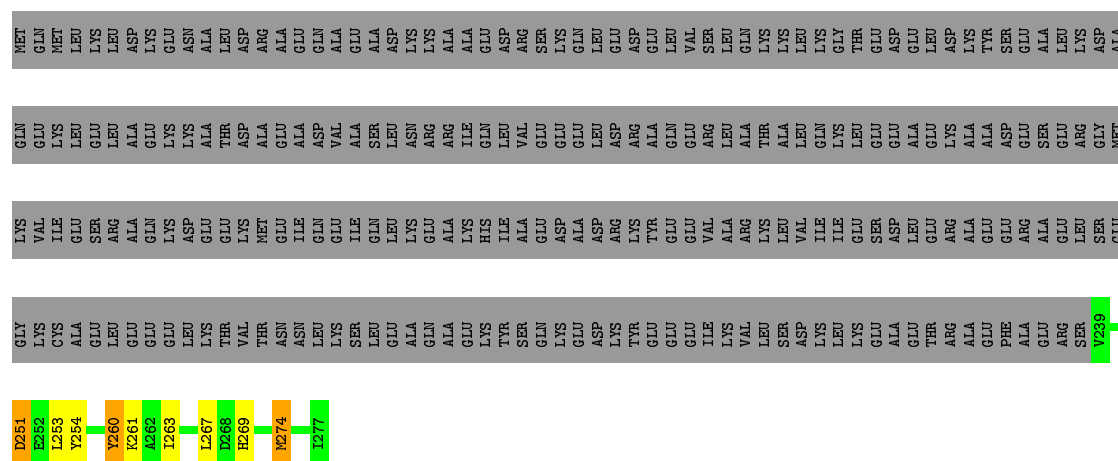
- Molecule 4: TROPOMYOSIN ALPHA-1 CHAIN

Chain B:  81% 17% .



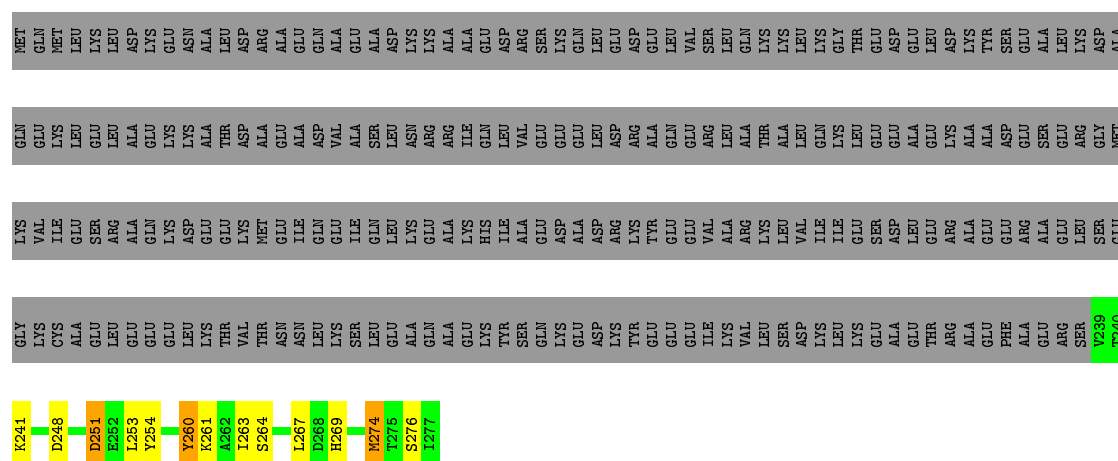
● Molecule 4: TROPOMYOSIN ALPHA-1 CHAIN

Chain C:  11% .. 86%



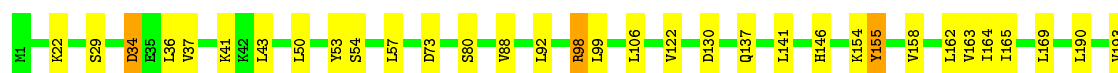
• Molecule 4: TROPOMYOSIN ALPHA-1 CHAIN

Chain T:  9% 2% 86%




• Molecule 4: TROPOMYOSIN ALPHA-1 CHAIN

Chain U: 81% 17% .





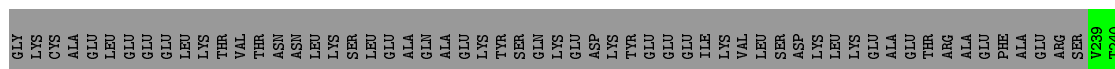
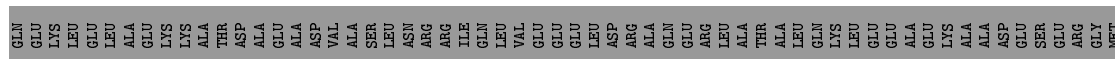
● Molecule 4: TROPOMYOSIN ALPHA-1 CHAIN

Chain V:  82% 15% 3%



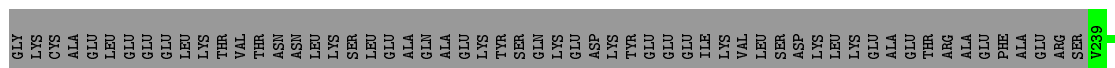
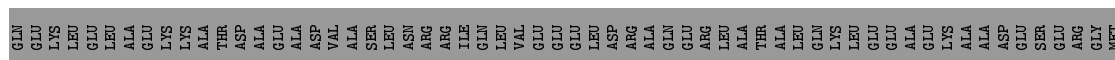
• Molecule 4: TROPOMYOSIN ALPHA-1 CHAIN

Chain W:  9% 2% 86%

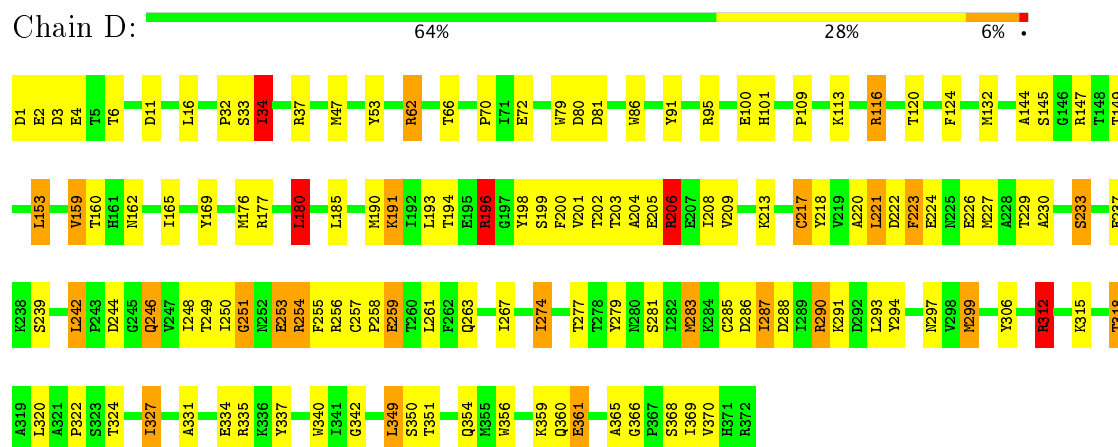


• Molecule 4: TROPOMYOSIN ALPHA-1 CHAIN

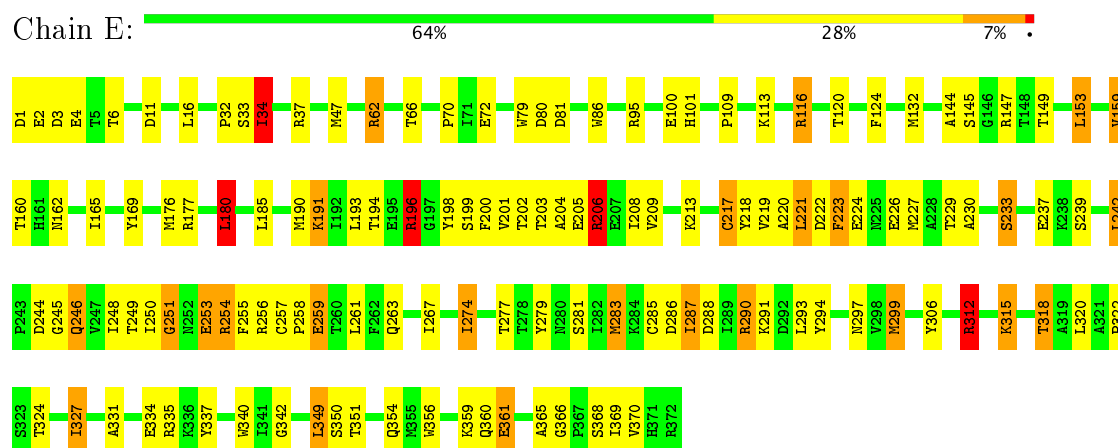
Chain X:  11% .. 86%



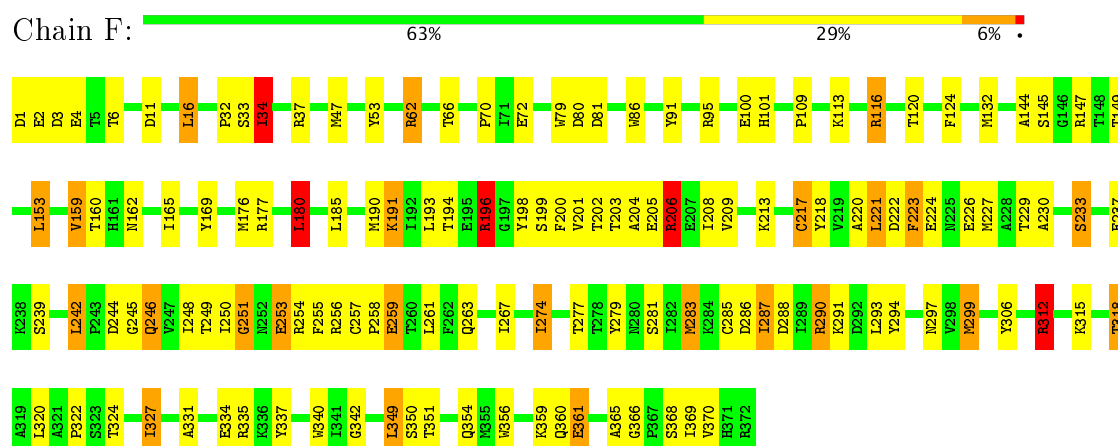
- Molecule 5: ACTIN, ALPHA SKELETAL MUSCLE



• Molecule 5: ACTIN, ALPHA SKELETAL MUSCLE

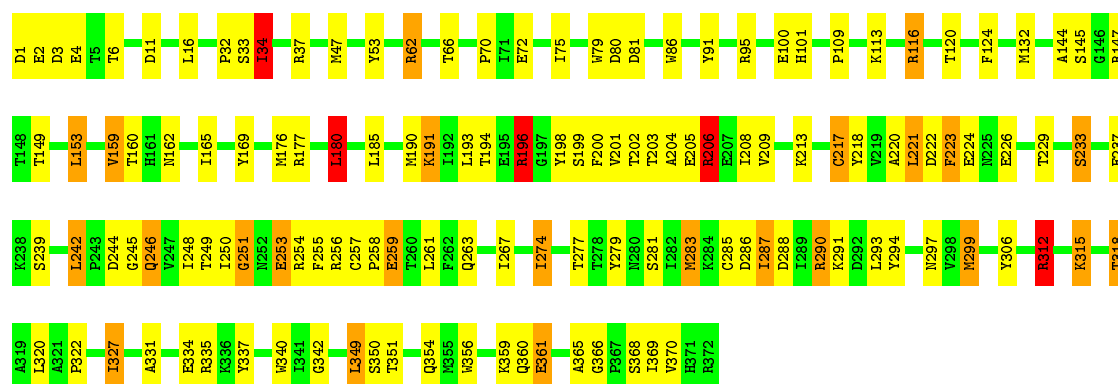


• Molecule 5: ACTIN, ALPHA SKELETAL MUSCLE



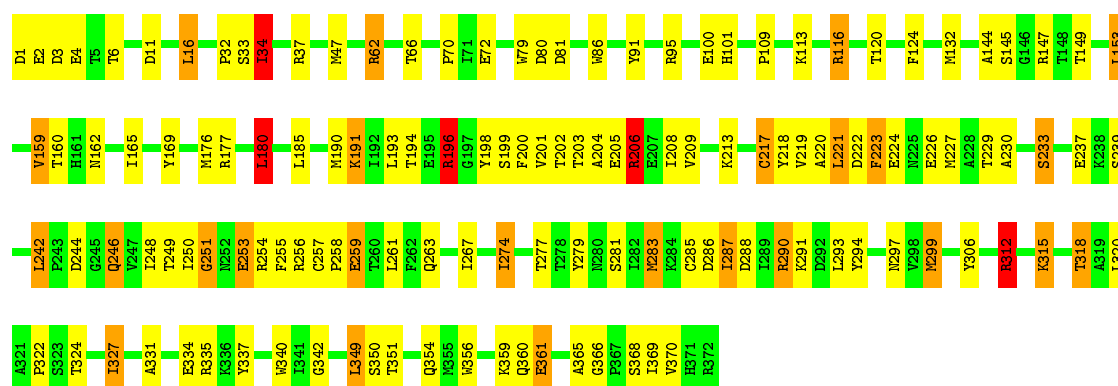
• Molecule 5: ACTIN, ALPHA SKELETAL MUSCLE





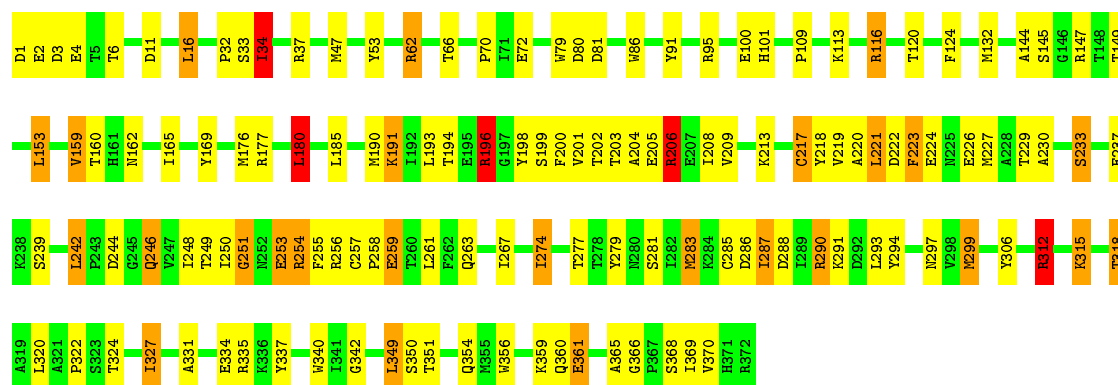
• Molecule 5: ACTIN, ALPHA SKELETAL MUSCLE

Chain H: 64% 28% 7% •



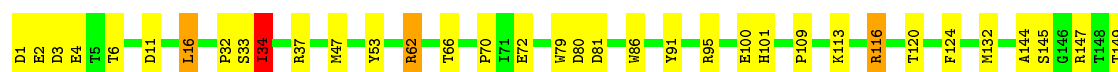
• Molecule 5: ACTIN, ALPHA SKELETAL MUSCLE

Chain I: 63% 28% 7% •



• Molecule 5: ACTIN, ALPHA SKELETAL MUSCLE

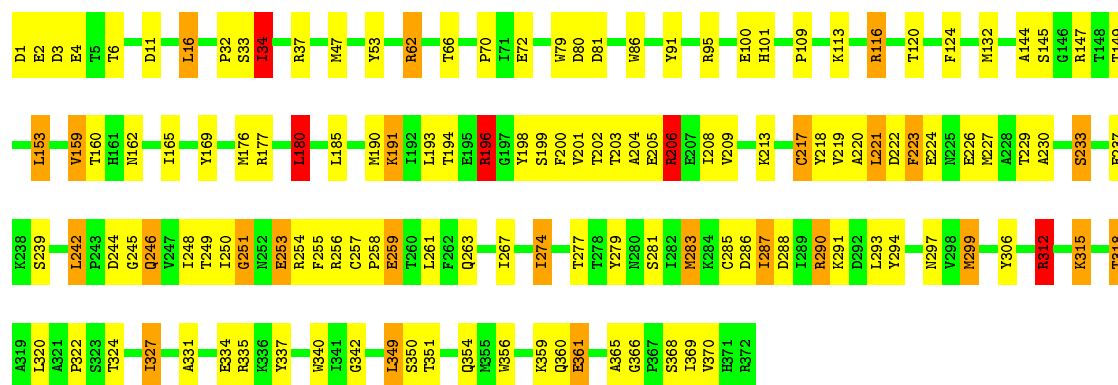
Chain J: 64% 28% 7% •





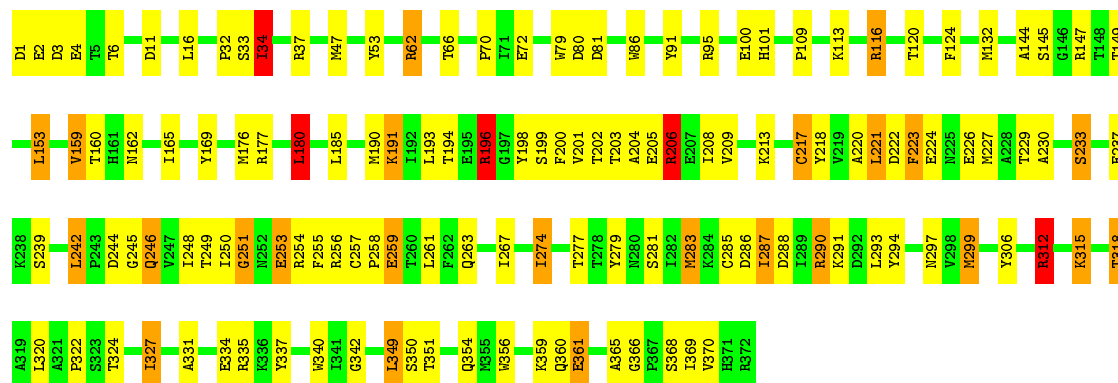
• Molecule 5: ACTIN, ALPHA SKELETAL MUSCLE

Chain K: 63% 29% 7%



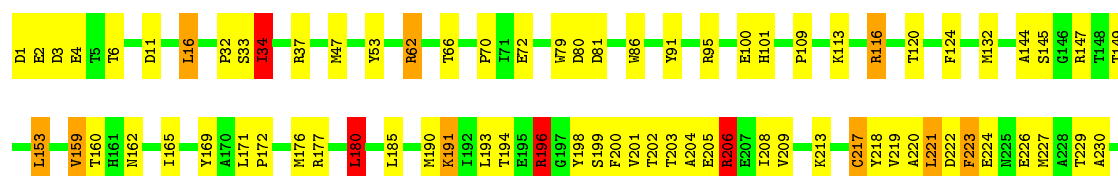
• Molecule 5: ACTIN, ALPHA SKELETAL MUSCLE

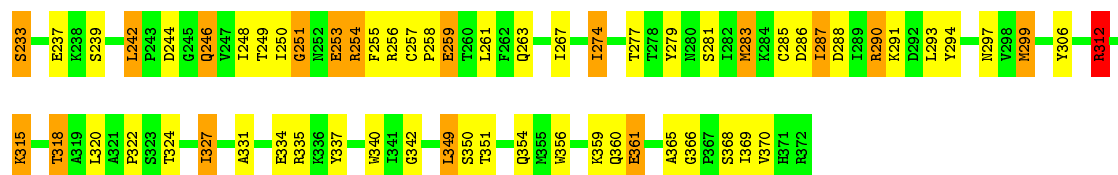
Chain L: 63% 29% 6%



• Molecule 5: ACTIN, ALPHA SKELETAL MUSCLE

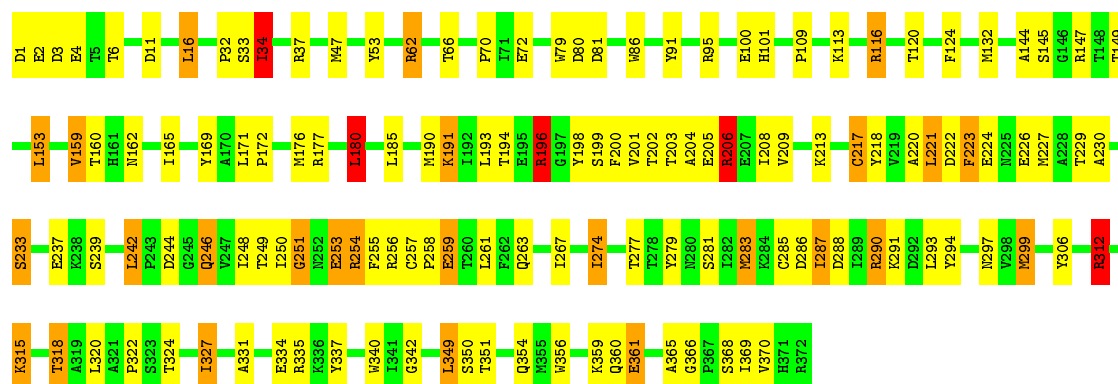
Chain M: 63% 29% 7%





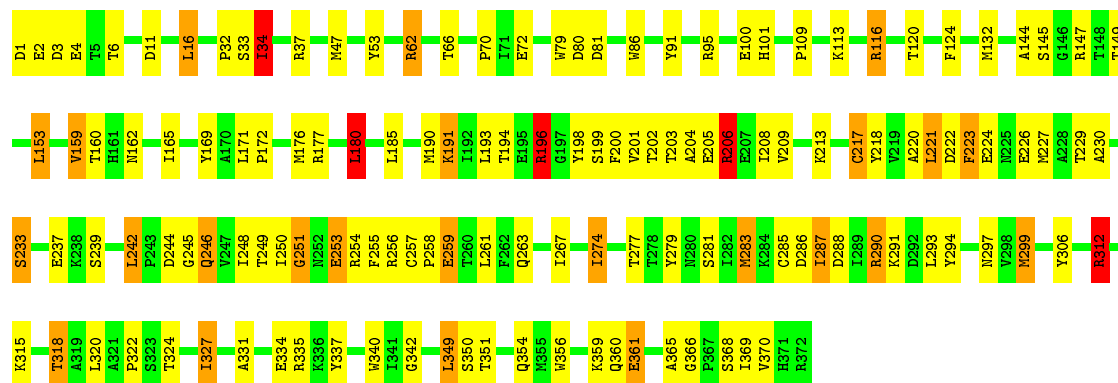
• Molecule 5: ACTIN, ALPHA SKELETAL MUSCLE

Chain N: 63% 28% 7%



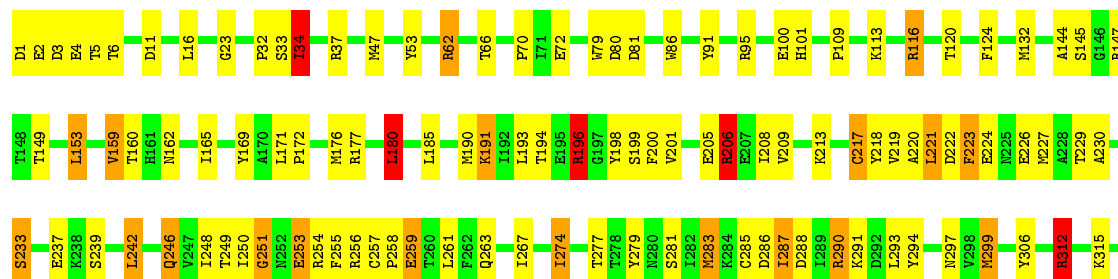
• Molecule 5: ACTIN, ALPHA SKELETAL MUSCLE

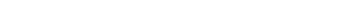
Chain O: 63% 29% 6%

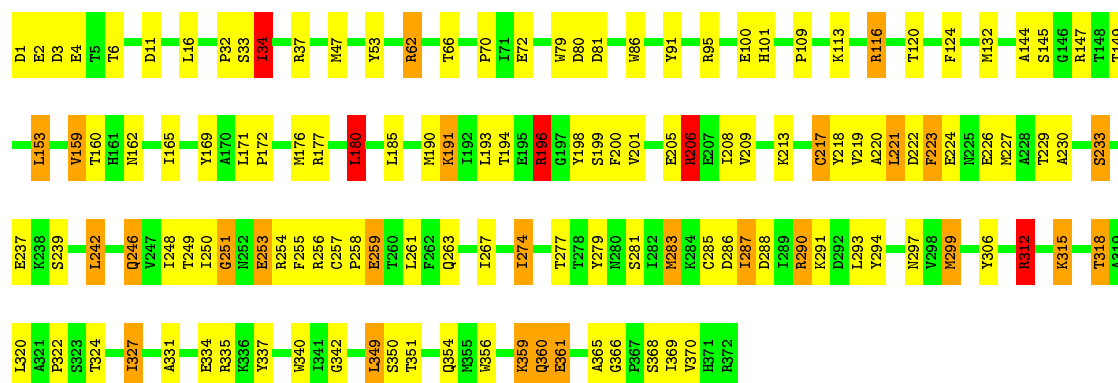


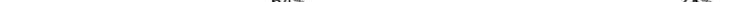
• Molecule 5: ACTIN, ALPHA SKELETAL MUSCLE

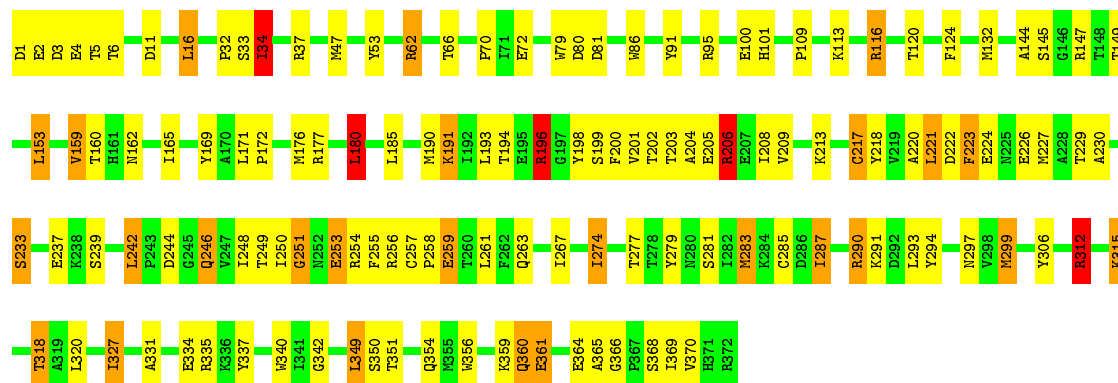
Chain P: 63% 29% 7%

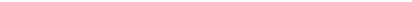


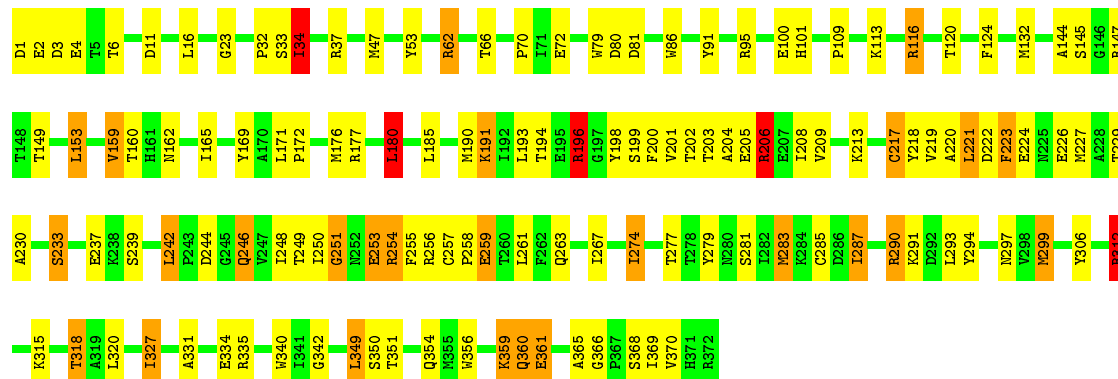
Chain Q:  64% 28% 7%



Chain R:  64% 28% 7%



Chain S:  64% 28% 7%



4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=Not provided°, rise=Not provided Å, axial sym=Not provided	Depositor
Number of segments used	Not provided	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI/PHILIPS CM300FEG/T	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	TVIPS TEMCAM-F224 (2k x 2k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section:
CA

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	0	0.55	0/1264	0.67	1/1687 (0.1%)
1	3	0.55	0/1264	0.67	1/1687 (0.1%)
1	6	0.55	0/1264	0.67	1/1687 (0.1%)
1	9	0.55	0/1264	0.67	1/1687 (0.1%)
2	1	0.57	0/786	0.59	0/1046
2	4	0.57	0/786	0.59	0/1046
2	7	0.57	0/786	0.59	0/1046
2	Y	0.57	0/786	0.59	0/1046
3	2	0.53	0/1152	0.71	0/1535
3	5	0.53	0/1152	0.70	0/1535
3	8	0.53	0/1152	0.70	0/1535
3	Z	0.53	0/1152	0.70	0/1535
4	A	3.01	15/2238 (0.7%)	1.82	48/2983 (1.6%)
4	B	3.60	9/2238 (0.4%)	1.86	45/2983 (1.5%)
4	C	7.01	7/318 (2.2%)	2.35	13/425 (3.1%)
4	T	7.04	7/318 (2.2%)	2.26	12/425 (2.8%)
4	U	3.60	9/2238 (0.4%)	1.85	46/2983 (1.5%)
4	V	3.01	15/2238 (0.7%)	1.82	48/2983 (1.6%)
4	W	7.04	7/318 (2.2%)	2.26	12/425 (2.8%)
4	X	7.01	7/318 (2.2%)	2.34	13/425 (3.1%)
5	D	0.89	2/2969 (0.1%)	1.64	51/4023 (1.3%)
5	E	0.89	2/2969 (0.1%)	1.64	49/4023 (1.2%)
5	F	0.89	2/2969 (0.1%)	1.64	52/4023 (1.3%)
5	G	0.89	2/2969 (0.1%)	1.64	52/4023 (1.3%)
5	H	0.89	2/2969 (0.1%)	1.64	51/4023 (1.3%)
5	I	0.89	2/2969 (0.1%)	1.64	51/4023 (1.3%)
5	J	0.89	2/2969 (0.1%)	1.64	51/4023 (1.3%)
5	K	0.89	2/2969 (0.1%)	1.64	50/4023 (1.2%)
5	L	0.89	2/2969 (0.1%)	1.64	50/4023 (1.2%)
5	M	0.89	2/2969 (0.1%)	1.64	50/4023 (1.2%)
5	N	0.89	2/2969 (0.1%)	1.64	52/4023 (1.3%)
5	O	0.89	1/2969 (0.0%)	1.64	52/4023 (1.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
5	P	0.89	1/2969 (0.0%)	1.64	51/4023 (1.3%)
5	Q	0.89	2/2969 (0.1%)	1.64	51/4023 (1.3%)
5	R	0.89	2/2969 (0.1%)	1.64	51/4023 (1.3%)
5	S	0.89	2/2969 (0.1%)	1.64	49/4023 (1.2%)
All	All	1.70	106/70536 (0.2%)	1.56	1054/95072 (1.1%)

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
4	A	0	4
4	B	0	5
4	C	0	2
4	T	0	2
4	U	0	5
4	V	0	4
4	W	0	2
4	X	0	2
5	D	0	1
5	E	0	1
5	F	0	1
5	G	0	1
5	H	0	1
5	I	0	1
5	J	0	1
5	K	0	1
5	L	0	1
5	M	0	1
5	N	0	1
5	O	0	1
5	P	0	1
5	Q	0	1
5	R	0	1
5	S	0	1
All	All	0	42

The worst 5 of 106 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	T	260	TYR	CA-CB	110.52	3.97	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	U	260	TYR	CA-CB	110.51	3.97	1.53
4	B	260	TYR	CA-CB	110.50	3.97	1.53
4	W	260	TYR	CA-CB	110.48	3.97	1.53
4	C	260	TYR	CA-CB	110.21	3.96	1.53

The worst 5 of 1054 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	155	TYR	CB-CG-CD1	-26.75	104.95	121.00
4	U	155	TYR	CB-CG-CD1	-26.69	104.99	121.00
4	V	260	TYR	CB-CG-CD2	-21.14	108.31	121.00
4	X	260	TYR	CB-CG-CD2	-21.11	108.33	121.00
4	C	260	TYR	CB-CG-CD2	-21.07	108.36	121.00

There are no chirality outliers.

5 of 42 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	231	ARG	Sidechain
4	A	260	TYR	Sidechain
4	A	261	LYS	Mainchain
4	A	98	ARG	Sidechain
4	B	98	ARG	Sidechain

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	0	1252	0	1172	102	0
1	3	1252	0	1172	80	0
1	6	1252	0	1172	95	0
1	9	1252	0	1172	76	0
2	1	774	0	797	48	0
2	4	774	0	796	51	0
2	7	774	0	797	48	0
2	Y	774	0	791	49	0
3	2	1140	0	1201	104	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	5	1140	0	1201	93	0
3	8	1140	0	1199	88	0
3	Z	1140	0	1201	86	0
4	A	2230	0	2227	0	0
4	B	2230	0	2227	0	0
4	C	316	0	314	0	0
4	T	316	0	312	0	0
4	U	2230	0	2227	0	0
4	V	2230	0	2227	0	0
4	W	316	0	307	0	0
4	X	316	0	314	0	0
5	D	2907	0	2862	101	0
5	E	2907	0	2862	101	0
5	F	2907	0	2864	101	0
5	G	2907	0	2864	98	0
5	H	2907	0	2864	103	0
5	I	2907	0	2864	102	0
5	J	2907	0	2864	103	0
5	K	2907	0	2864	103	0
5	L	2907	0	2864	97	0
5	M	2907	0	2864	104	0
5	N	2907	0	2864	105	0
5	O	2907	0	2864	104	0
5	P	2907	0	2860	120	0
5	Q	2907	0	2863	116	0
5	R	2907	0	2863	115	0
5	S	2907	0	2862	94	0
6	0	4	0	0	0	0
6	3	4	0	0	0	0
6	6	4	0	0	0	0
6	9	4	0	0	0	0
All	All	69376	0	68638	2028	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 17.

The worst 5 of 2028 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)
3:2:100:PHE:CG	5:R:5:THR:HG22	1.40	1.54
3:5:97:GLN:HE22	5:Q:4:GLU:CG	1.19	1.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:62:GLU:CG	5:P:360:GLN:HB2	1.52	1.40
1:0:62:GLU:CG	5:P:359:LYS:HD2	1.52	1.38
3:5:97:GLN:NE2	5:Q:4:GLU:CG	1.85	1.37

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	0	157/159 (99%)	130 (83%)	20 (13%)	7 (4%)	3	29
1	3	157/159 (99%)	130 (83%)	20 (13%)	7 (4%)	3	29
1	6	157/159 (99%)	130 (83%)	20 (13%)	7 (4%)	3	29
1	9	157/159 (99%)	130 (83%)	20 (13%)	7 (4%)	3	29
2	1	88/90 (98%)	66 (75%)	18 (20%)	4 (4%)	3	29
2	4	88/90 (98%)	66 (75%)	18 (20%)	4 (4%)	3	29
2	7	88/90 (98%)	65 (74%)	19 (22%)	4 (4%)	3	29
2	Y	88/90 (98%)	66 (75%)	18 (20%)	4 (4%)	3	29
3	2	139/141 (99%)	108 (78%)	18 (13%)	13 (9%)	1	14
3	5	139/141 (99%)	108 (78%)	18 (13%)	13 (9%)	1	14
3	8	139/141 (99%)	108 (78%)	18 (13%)	13 (9%)	1	14
3	Z	139/141 (99%)	107 (77%)	19 (14%)	13 (9%)	1	14
4	A	275/277 (99%)	266 (97%)	7 (2%)	2 (1%)	25	68
4	B	275/277 (99%)	264 (96%)	11 (4%)	0	100	100
4	C	37/277 (13%)	34 (92%)	3 (8%)	0	100	100
4	T	37/277 (13%)	34 (92%)	3 (8%)	0	100	100
4	U	275/277 (99%)	264 (96%)	11 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	V	275/277 (99%)	266 (97%)	7 (2%)	2 (1%)	25	68
4	W	37/277 (13%)	34 (92%)	3 (8%)	0	100	100
4	X	37/277 (13%)	34 (92%)	3 (8%)	0	100	100
5	D	370/372 (100%)	335 (90%)	29 (8%)	6 (2%)	11	51
5	E	370/372 (100%)	334 (90%)	30 (8%)	6 (2%)	11	51
5	F	370/372 (100%)	335 (90%)	29 (8%)	6 (2%)	11	51
5	G	370/372 (100%)	334 (90%)	30 (8%)	6 (2%)	11	51
5	H	370/372 (100%)	334 (90%)	30 (8%)	6 (2%)	11	51
5	I	370/372 (100%)	335 (90%)	29 (8%)	6 (2%)	11	51
5	J	370/372 (100%)	335 (90%)	29 (8%)	6 (2%)	11	51
5	K	370/372 (100%)	335 (90%)	29 (8%)	6 (2%)	11	51
5	L	370/372 (100%)	335 (90%)	29 (8%)	6 (2%)	11	51
5	M	370/372 (100%)	335 (90%)	29 (8%)	6 (2%)	11	51
5	N	370/372 (100%)	335 (90%)	29 (8%)	6 (2%)	11	51
5	O	370/372 (100%)	334 (90%)	30 (8%)	6 (2%)	11	51
5	P	370/372 (100%)	334 (90%)	30 (8%)	6 (2%)	11	51
5	Q	370/372 (100%)	334 (90%)	30 (8%)	6 (2%)	11	51
5	R	370/372 (100%)	335 (90%)	29 (8%)	6 (2%)	11	51
5	S	370/372 (100%)	335 (90%)	29 (8%)	6 (2%)	11	51
All	All	8704/9728 (90%)	7764 (89%)	744 (8%)	196 (2%)	11	43

5 of 196 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	0	107	ASN
1	0	126	GLU
3	2	57	MET
3	2	142	GLN
1	3	107	ASN

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	0	134/134 (100%)	115 (86%)	19 (14%)	4	22
1	3	134/134 (100%)	115 (86%)	19 (14%)	4	22
1	6	134/134 (100%)	115 (86%)	19 (14%)	4	22
1	9	134/134 (100%)	115 (86%)	19 (14%)	4	22
2	1	82/82 (100%)	70 (85%)	12 (15%)	3	21
2	4	82/82 (100%)	70 (85%)	12 (15%)	3	21
2	7	82/82 (100%)	70 (85%)	12 (15%)	3	21
2	Y	82/82 (100%)	70 (85%)	12 (15%)	3	21
3	2	124/124 (100%)	108 (87%)	16 (13%)	5	25
3	5	124/124 (100%)	108 (87%)	16 (13%)	5	25
3	8	124/124 (100%)	108 (87%)	16 (13%)	5	25
3	Z	124/124 (100%)	108 (87%)	16 (13%)	5	25
4	A	239/239 (100%)	212 (89%)	27 (11%)	7	29
4	B	239/239 (100%)	206 (86%)	33 (14%)	4	23
4	C	36/239 (15%)	31 (86%)	5 (14%)	4	23
4	T	36/239 (15%)	28 (78%)	8 (22%)	1	7
4	U	239/239 (100%)	206 (86%)	33 (14%)	4	23
4	V	239/239 (100%)	212 (89%)	27 (11%)	7	29
4	W	36/239 (15%)	28 (78%)	8 (22%)	1	7
4	X	36/239 (15%)	31 (86%)	5 (14%)	4	23
5	D	315/315 (100%)	269 (85%)	46 (15%)	3	21
5	E	315/315 (100%)	269 (85%)	46 (15%)	3	21
5	F	315/315 (100%)	268 (85%)	47 (15%)	3	20
5	G	315/315 (100%)	269 (85%)	46 (15%)	3	21
5	H	315/315 (100%)	268 (85%)	47 (15%)	3	20
5	I	315/315 (100%)	268 (85%)	47 (15%)	3	20
5	J	315/315 (100%)	268 (85%)	47 (15%)	3	20
5	K	315/315 (100%)	268 (85%)	47 (15%)	3	20
5	L	315/315 (100%)	269 (85%)	46 (15%)	3	21
5	M	315/315 (100%)	268 (85%)	47 (15%)	3	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	N	315/315 (100%)	268 (85%)	47 (15%)	3	20
5	O	315/315 (100%)	268 (85%)	47 (15%)	3	20
5	P	315/315 (100%)	269 (85%)	46 (15%)	3	21
5	Q	315/315 (100%)	269 (85%)	46 (15%)	3	21
5	R	315/315 (100%)	268 (85%)	47 (15%)	3	20
5	S	315/315 (100%)	269 (85%)	46 (15%)	3	21
All	All	7500/8312 (90%)	6421 (86%)	1079 (14%)	7	22

5 of 1079 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	I	297	ASN
5	L	80	ASP
4	U	195	ASN
5	I	361	GLU
5	J	359	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 165 such sidechains are listed below:

Mol	Chain	Res	Type
5	G	137	GLN
5	J	137	GLN
2	Y	175	GLN
5	G	263	GLN
5	H	354	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

Of 16 ligands modelled in this entry, 16 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.