



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:23 PM BST

PDB ID : 2W4G
EMDB ID: : EMD-1584
Title : ISOMETRICALLY CONTRACTING INSECT ASYNCHRONOUS FLIGHT
MUSCLE QUICK FROZEN AFTER A QUICK STRETCH STEP
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 : 2008-11-25
Resolution : 35.00 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

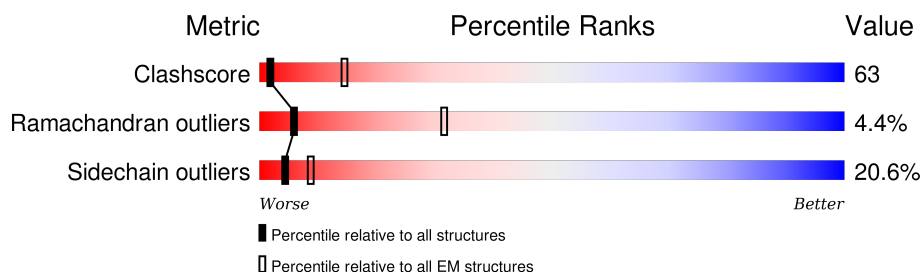
1 Overall quality at a glance

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.







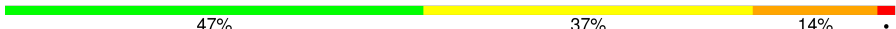





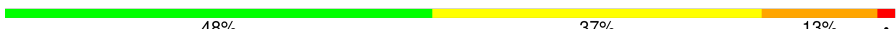
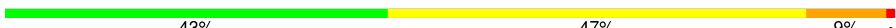




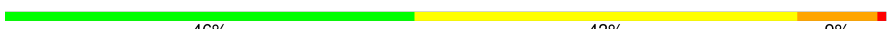



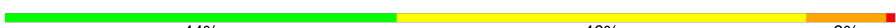

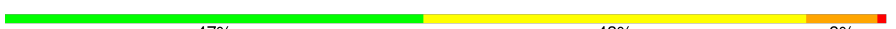


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	1-B	150	49% 35% 13% .
1	10-B	150	49% 35% 14% .
1	11-B	150	47% 37% 13% .
1	12-B	150	48% 37% 13% .
1	13-B	150	48% 37% 13% .
1	14-B	150	49% 36% 13% .
1	15-B	150	49% 36% 13% .
1	16-B	150	49% 35% 13% .
1	17-B	150	50% 35% 13% .














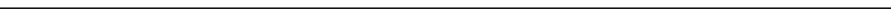

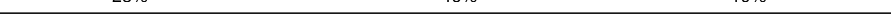
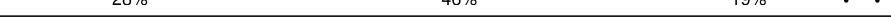
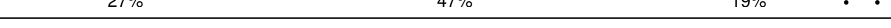
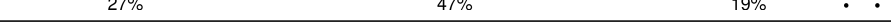
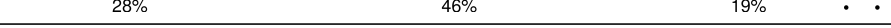
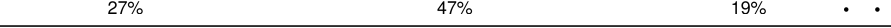
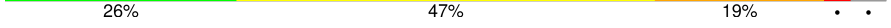
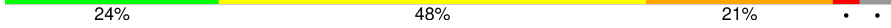
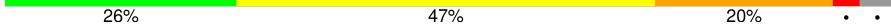
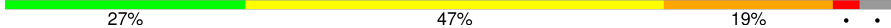
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Mol	Chain	Length	Quality of chain
1	18-B	150	 49% 36% 13% .
1	19-B	150	 50% 35% 13% .
1	2-B	150	 48% 37% 13% .
1	20-B	150	 49% 35% 14% .
1	3-B	150	 47% 37% 14% .
1	4-B	150	 49% 35% 14% .
1	5-B	150	 49% 36% 13% .
1	6-B	150	 49% 35% 13% .
1	7-B	150	 49% 35% 13% .
1	8-B	150	 50% 35% 13% .
1	9-B	150	 48% 37% 13% .
2	1-C	145	 43% 47% 9% .
2	10-C	145	 52% 39% 8% .
2	11-C	145	 46% 44% 8% .
2	12-C	145	 47% 43% 8% .
2	13-C	145	 43% 46% 9% .
2	14-C	145	 46% 43% 9% .
2	15-C	145	 52% 39% 8% .
2	16-C	145	 52% 38% 8% .
2	17-C	145	 52% 39% 8% .
2	18-C	145	 44% 46% 9% .
2	19-C	145	 52% 39% 8% .
2	2-C	145	 47% 43% 8% .
2	20-C	145	 49% 41% 8% .
2	3-C	145	 51% 39% 8% .

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Mol	Chain	Length	Quality of chain
2	4-C	145	
2	5-C	145	
2	6-C	145	
2	7-C	145	
2	8-C	145	
2	9-C	145	
3	1-M	840	
3	10-M	840	
3	11-M	840	
3	12-M	840	
3	13-M	840	
3	14-M	840	
3	15-M	840	
3	16-M	840	
3	17-M	840	
3	18-M	840	
3	19-M	840	
3	2-M	840	
3	20-M	840	
3	3-M	840	
3	4-M	840	
3	5-M	840	
3	6-M	840	
3	7-M	840	
3	8-M	840	

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Mol	Chain	Length	Quality of chain
3	9-M	840	<div><div></div><div>27%</div><div>46%</div><div>19%</div><div></div><div></div></div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 175160 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 REGULATORY LIGHT CHAIN 2, SKELETAL MUSCLE ISOFORM.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1-B	150	Total	C	N	O	S	0	0
			1177	748	187	234	8		
1	2-B	150	Total	C	N	O	S	0	0
			1177	748	187	234	8		
1	3-B	150	Total	C	N	O	S	0	0
			1177	748	187	234	8		
1	4-B	150	Total	C	N	O	S	0	0
			1177	748	187	234	8		
1	5-B	150	Total	C	N	O	S	0	0
			1177	748	187	234	8		
1	6-B	150	Total	C	N	O	S	0	0
			1177	748	187	234	8		
1	7-B	150	Total	C	N	O	S	0	0
			1177	748	187	234	8		
1	8-B	150	Total	C	N	O	S	0	0
			1177	748	187	234	8		
1	9-B	150	Total	C	N	O	S	0	0
			1177	748	187	234	8		
1	10-B	150	Total	C	N	O	S	0	0
			1177	748	187	234	8		
1	11-B	150	Total	C	N	O	S	0	0
			1177	748	187	234	8		
1	12-B	150	Total	C	N	O	S	0	0
			1177	748	187	234	8		
1	13-B	150	Total	C	N	O	S	0	0
			1177	748	187	234	8		
1	14-B	150	Total	C	N	O	S	0	0
			1177	748	187	234	8		
1	15-B	150	Total	C	N	O	S	0	0
			1177	748	187	234	8		
1	16-B	150	Total	C	N	O	S	0	0
			1177	748	187	234	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	17-B	150	Total	C	N	O	S	0	0
			1177	748	187	234	8		
1	18-B	150	Total	C	N	O	S	0	0
			1177	748	187	234	8		
1	19-B	150	Total	C	N	O	S	0	0
			1177	748	187	234	8		
1	20-B	150	Total	C	N	O	S	0	0
			1177	748	187	234	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	26	ASP	GLU	CONFLICT	UNP P02609

- Molecule 2 is a protein called MYOSIN LIGHT CHAIN 3, SKELETAL MUSCLE ISOFORM.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1-C	145	Total	C	N	O	S	0	0
			1126	701	188	230	7		
2	2-C	145	Total	C	N	O	S	0	0
			1126	701	188	230	7		
2	3-C	145	Total	C	N	O	S	0	0
			1126	701	188	230	7		
2	4-C	145	Total	C	N	O	S	0	0
			1126	701	188	230	7		
2	5-C	145	Total	C	N	O	S	0	0
			1126	701	188	230	7		
2	6-C	145	Total	C	N	O	S	0	0
			1126	701	188	230	7		
2	7-C	145	Total	C	N	O	S	0	0
			1126	701	188	230	7		
2	8-C	145	Total	C	N	O	S	0	0
			1126	701	188	230	7		
2	9-C	145	Total	C	N	O	S	0	0
			1126	701	188	230	7		
2	10-C	145	Total	C	N	O	S	0	0
			1126	701	188	230	7		
2	11-C	145	Total	C	N	O	S	0	0
			1126	701	188	230	7		
2	12-C	145	Total	C	N	O	S	0	0
			1126	701	188	230	7		
2	13-C	145	Total	C	N	O	S	0	0
			1126	701	188	230	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	14-C	145	Total	C	N	O	S	0	0
			1126	701	188	230	7		
2	15-C	145	Total	C	N	O	S	0	0
			1126	701	188	230	7		
2	16-C	145	Total	C	N	O	S	0	0
			1126	701	188	230	7		
2	17-C	145	Total	C	N	O	S	0	0
			1126	701	188	230	7		
2	18-C	145	Total	C	N	O	S	0	0
			1126	701	188	230	7		
2	19-C	145	Total	C	N	O	S	0	0
			1126	701	188	230	7		
2	20-C	145	Total	C	N	O	S	0	0
			1126	701	188	230	7		

- Molecule 3 is a protein called MYOSIN HEAVY CHAIN, SKELETAL MUSCLE, ADULT.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1-M	804	Total	C	N	O	S	0	0
			6455	4140	1089	1190	36		
3	2-M	804	Total	C	N	O	S	0	0
			6455	4140	1089	1190	36		
3	3-M	804	Total	C	N	O	S	0	0
			6455	4140	1089	1190	36		
3	4-M	804	Total	C	N	O	S	0	0
			6455	4140	1089	1190	36		
3	5-M	804	Total	C	N	O	S	0	0
			6455	4140	1089	1190	36		
3	6-M	804	Total	C	N	O	S	0	0
			6455	4140	1089	1190	36		
3	7-M	804	Total	C	N	O	S	0	0
			6455	4140	1089	1190	36		
3	8-M	804	Total	C	N	O	S	0	0
			6455	4140	1089	1190	36		
3	9-M	804	Total	C	N	O	S	0	0
			6455	4140	1089	1190	36		
3	10-M	804	Total	C	N	O	S	0	0
			6455	4140	1089	1190	36		
3	11-M	804	Total	C	N	O	S	0	0
			6455	4140	1089	1190	36		
3	12-M	804	Total	C	N	O	S	0	0
			6455	4140	1089	1190	36		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	13-M	804	Total	C	N	O	S	0	0
			6455	4140	1089	1190	36		
3	14-M	804	Total	C	N	O	S	0	0
			6455	4140	1089	1190	36		
3	15-M	804	Total	C	N	O	S	0	0
			6455	4140	1089	1190	36		
3	16-M	804	Total	C	N	O	S	0	0
			6455	4140	1089	1190	36		
3	17-M	804	Total	C	N	O	S	0	0
			6455	4140	1089	1190	36		
3	18-M	804	Total	C	N	O	S	0	0
			6455	4140	1089	1190	36		
3	19-M	804	Total	C	N	O	S	0	0
			6455	4140	1089	1190	36		
3	20-M	804	Total	C	N	O	S	0	0
			6455	4140	1089	1190	36		

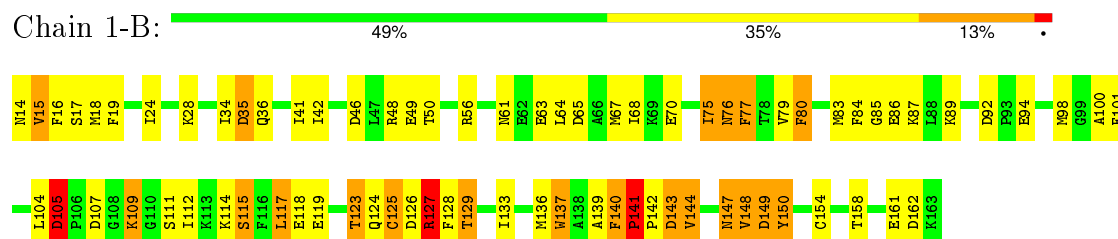
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	138	LYS	GLU	CONFLICT	UNP P02609

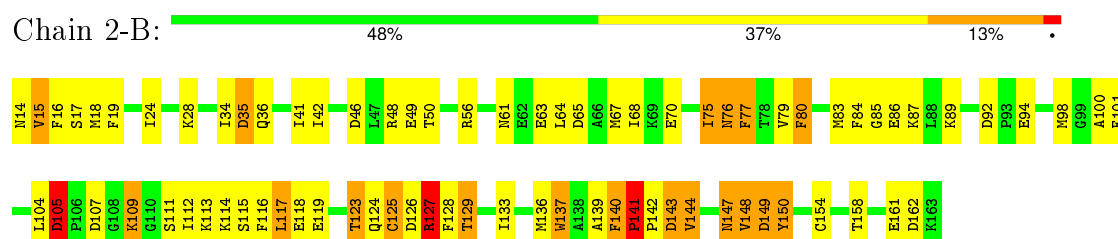
3 Residue-property plots

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.

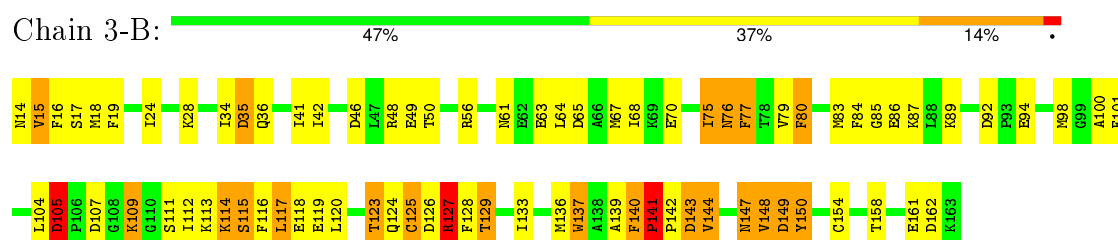
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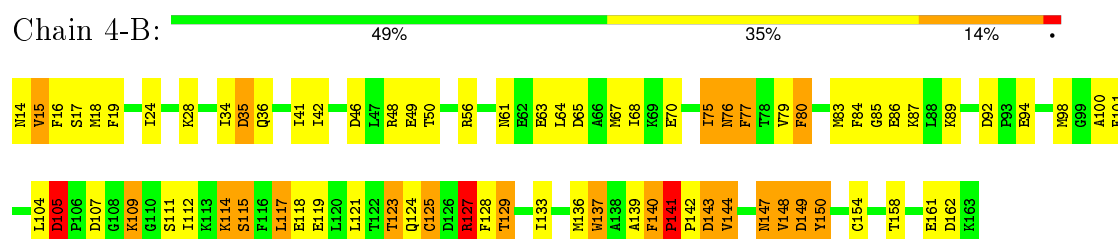
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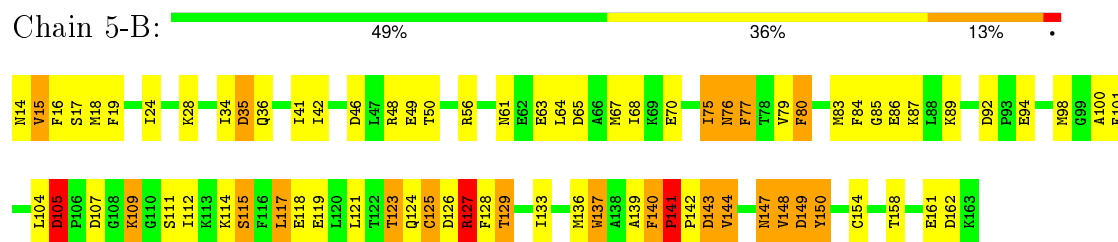
- Molecule 1: MYOSIN REGULATORY LIGHT CHAIN 2, SKELETAL MUSCLE ISOFORM



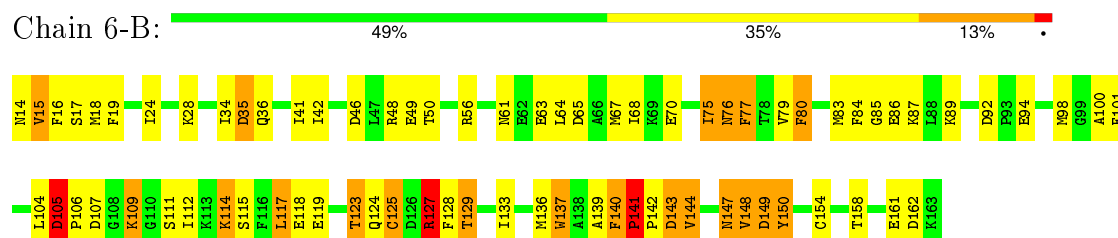
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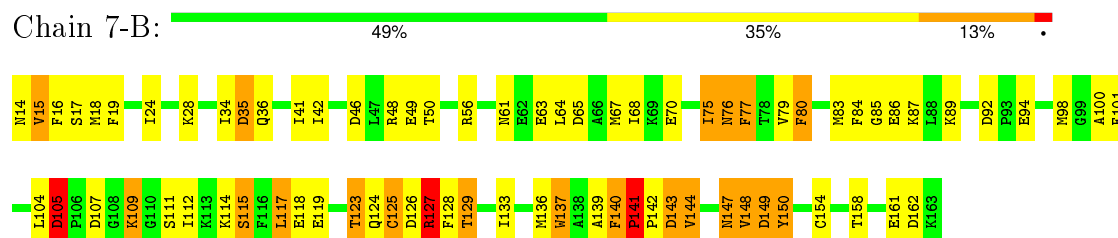
- Molecule 1: MYOSIN REGULATORY LIGHT CHAIN 2, SKELETAL MUSCLE ISOFORM



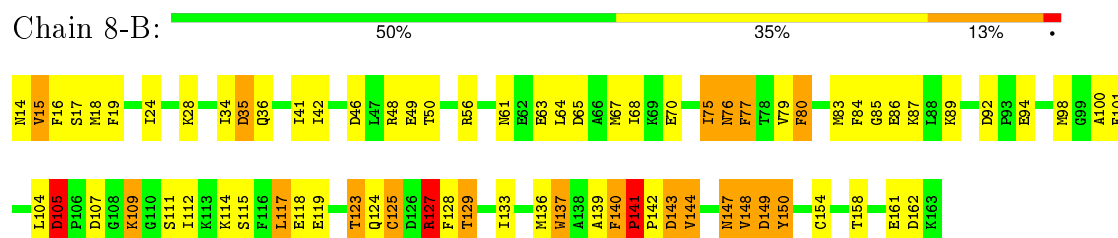
- Molecule 1: MYOSIN REGULATORY LIGHT CHAIN 2, SKELETAL MUSCLE ISOFORM



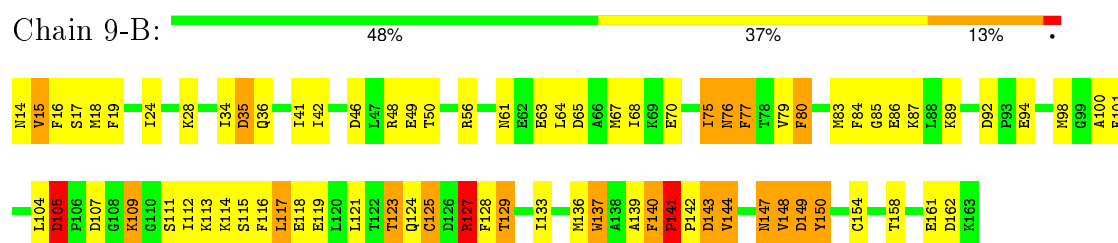
- Molecule 1: MYOSIN REGULATORY LIGHT CHAIN 2, SKELETAL MUSCLE ISOFORM



- Molecule 1: MYOSIN REGULATORY LIGHT CHAIN 2, SKELETAL MUSCLE ISOFORM

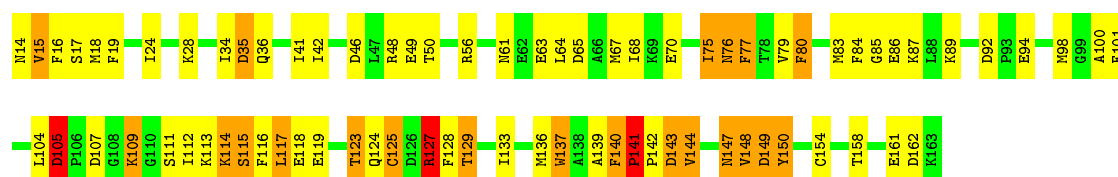


- Molecule 1: MYOSIN REGULATORY LIGHT CHAIN 2, SKELETAL MUSCLE ISOFORM

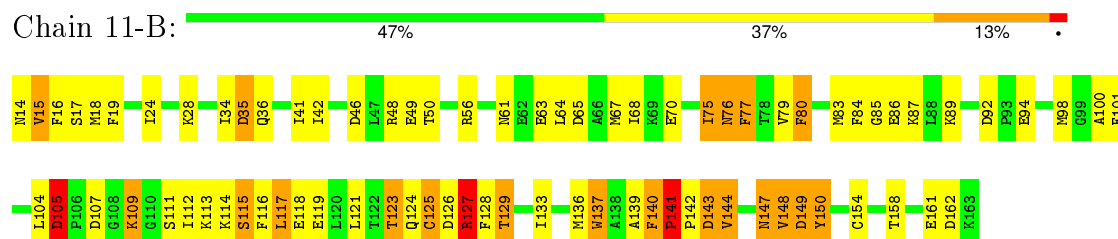


- Molecule 1: MYOSIN REGULATORY LIGHT CHAIN 2, SKELETAL MUSCLE ISOFORM

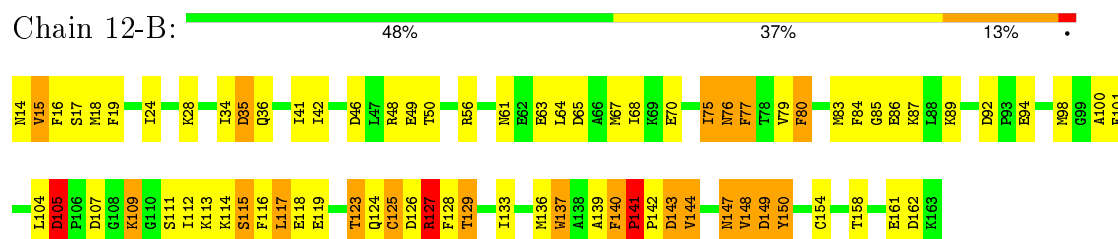




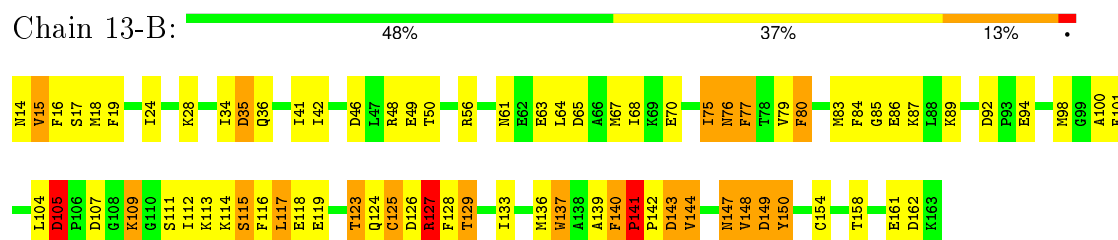
- Molecule 1: MYOSIN REGULATORY LIGHT CHAIN 2, SKELETAL MUSCLE ISOFORM



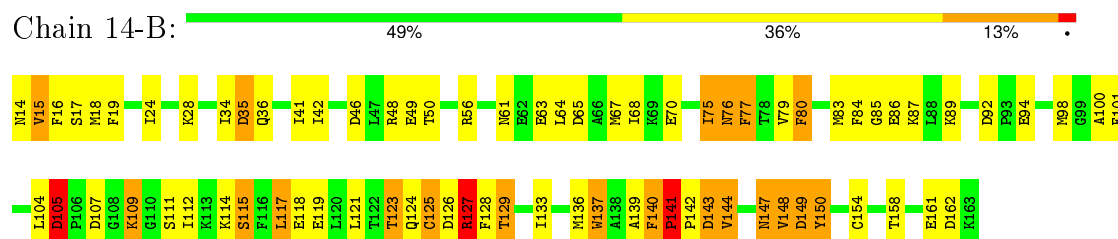
- Molecule 1: MYOSIN REGULATORY LIGHT CHAIN 2, SKELETAL MUSCLE ISOFORM



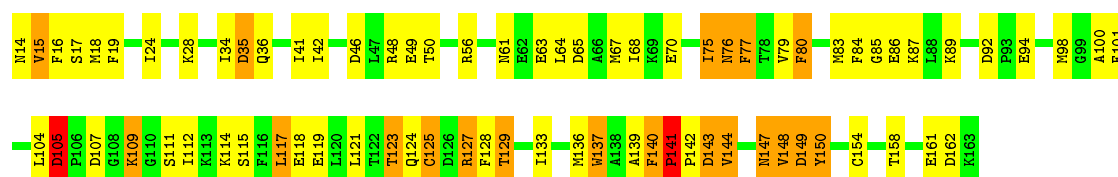
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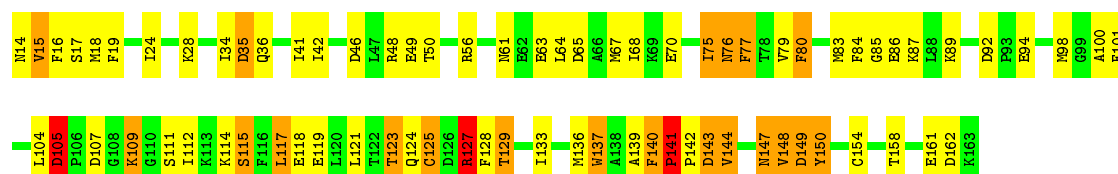


- Molecule 1: MYOSIN REGULATORY LIGHT CHAIN 2, SKELETAL MUSCLE ISOFORM



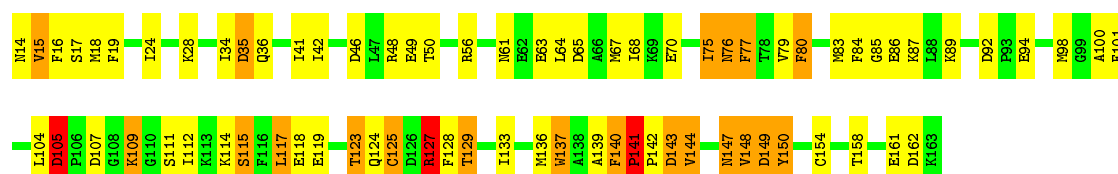
- Molecule 1: MYOSIN REGULATORY LIGHT CHAIN 2, SKELETAL MUSCLE ISOFORM

Chain 16-B: 49% 35% 13%



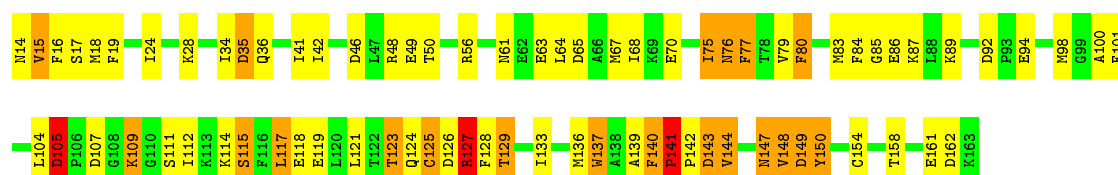
- Molecule 1: MYOSIN REGULATORY LIGHT CHAIN 2, SKELETAL MUSCLE ISOFORM

Chain 17-B: 50% 35% 13%



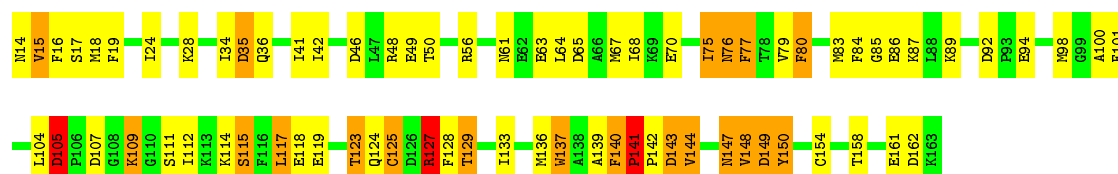
- Molecule 1: MYOSIN REGULATORY LIGHT CHAIN 2, SKELETAL MUSCLE ISOFORM

Chain 18-B: 49% 36% 13%



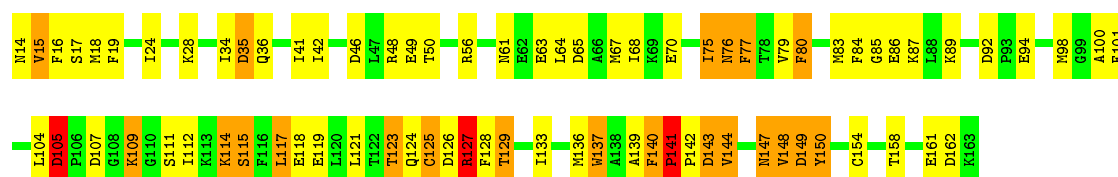
- Molecule 1: MYOSIN REGULATORY LIGHT CHAIN 2, SKELETAL MUSCLE ISOFORM

Chain 19-B: 50% 35% 13%



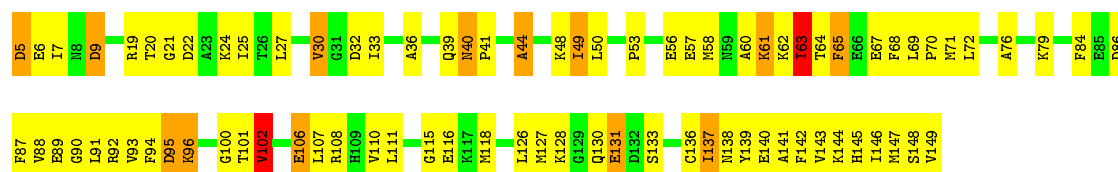
- Molecule 1: MYOSIN REGULATORY LIGHT CHAIN 2, SKELETAL MUSCLE ISOFORM

Chain 20-B: 49% 35% 14%



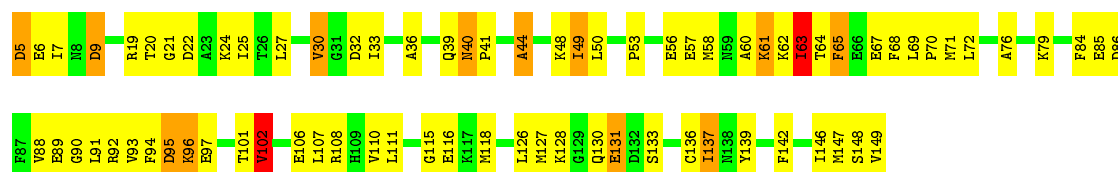
- Molecule 2: MYOSIN LIGHT CHAIN 3, SKELETAL MUSCLE ISOFORM

Chain 1-C: 43% 47% 9% .



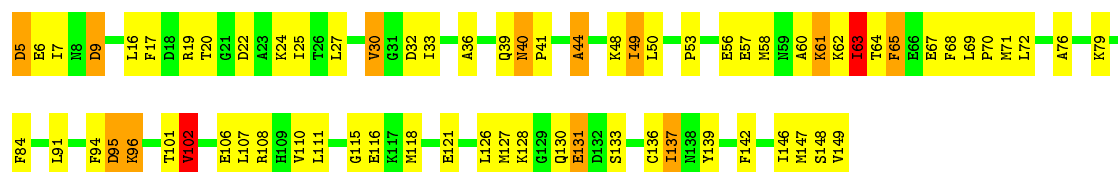
- Molecule 2: MYOSIN LIGHT CHAIN 3, SKELETAL MUSCLE ISOFORM

Chain 2-C: 47% 43% 8% .



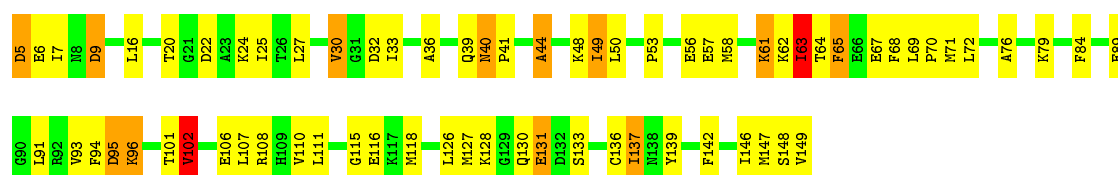
- Molecule 2: MYOSIN LIGHT CHAIN 3, SKELETAL MUSCLE ISOFORM

Chain 3-C: 51% 39% 8% .



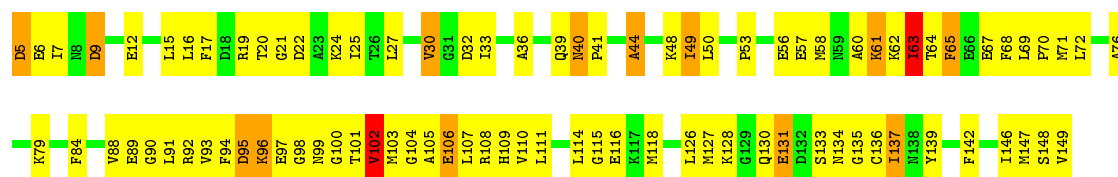
- Molecule 2: MYOSIN LIGHT CHAIN 3, SKELETAL MUSCLE ISOFORM

Chain 4-C: 52% 38% 8% .



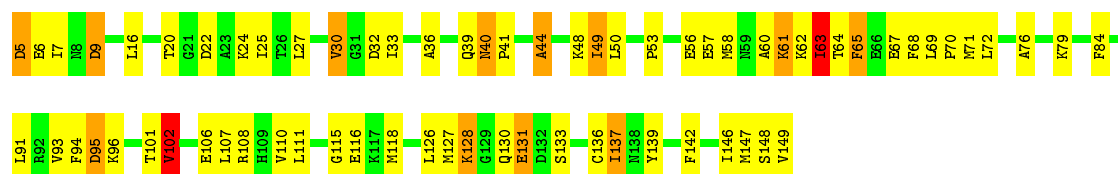
- Molecule 2: MYOSIN LIGHT CHAIN 3, SKELETAL MUSCLE ISOFORM

Chain 5-C: 39% 51% 9% .



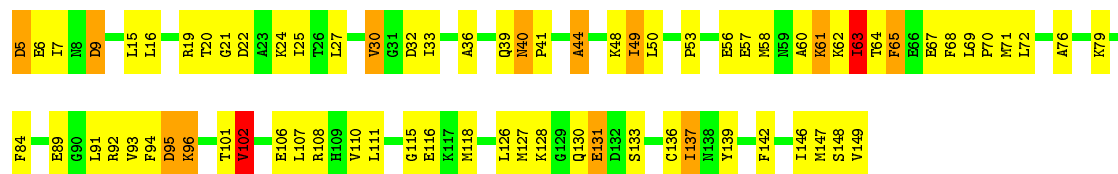
• Molecule 2: MYOSIN LIGHT CHAIN 3, SKELETAL MUSCLE ISOFORM

Chain 6-C: 52% 38% 8% .



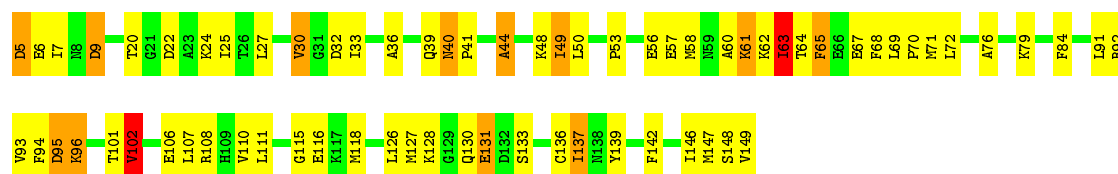
• Molecule 2: MYOSIN LIGHT CHAIN 3, SKELETAL MUSCLE ISOFORM

Chain 7-C: 49% 41% 8% .



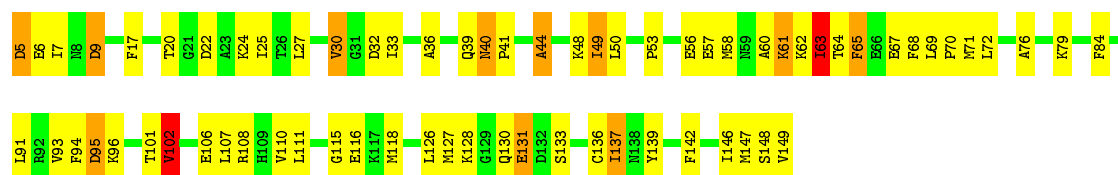
• Molecule 2: MYOSIN LIGHT CHAIN 3, SKELETAL MUSCLE ISOFORM

Chain 8-C: 52% 38% 8% .



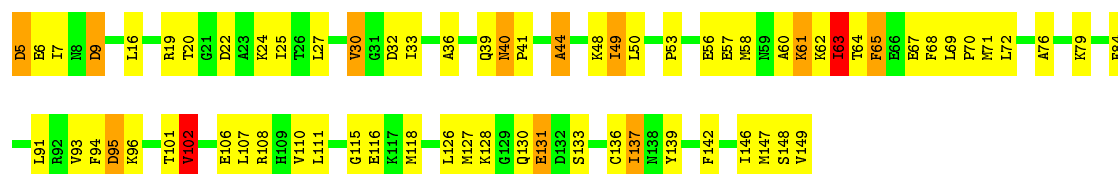
• Molecule 2: MYOSIN LIGHT CHAIN 3, SKELETAL MUSCLE ISOFORM

Chain 9-C: 52% 39% 8% .



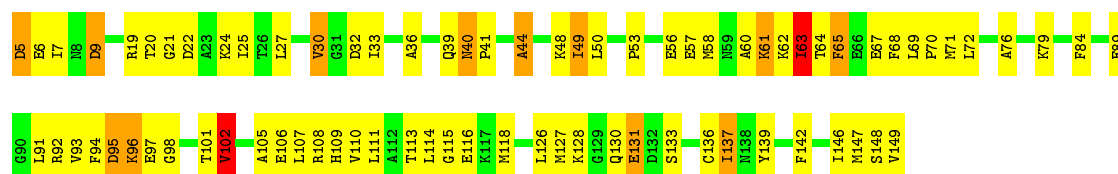
• Molecule 2: MYOSIN LIGHT CHAIN 3, SKELETAL MUSCLE ISOFORM

Chain 10-C: 52% 39% 8% .



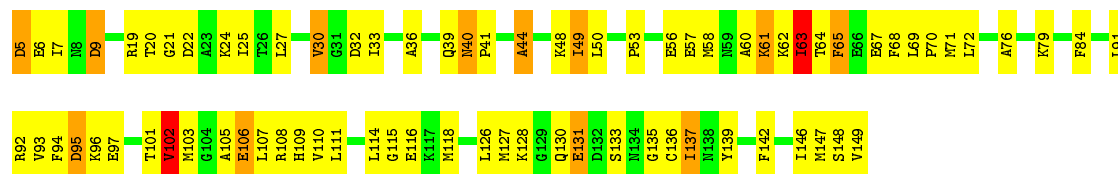
• Molecule 2: MYOSIN LIGHT CHAIN 3, SKELETAL MUSCLE ISOFORM

Chain 11-C: 46% 44% 8%



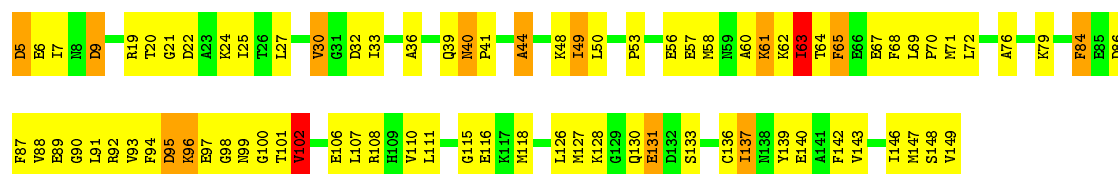
• Molecule 2: MYOSIN LIGHT CHAIN 3, SKELETAL MUSCLE ISOFORM

Chain 12-C: 47% 43% 8%



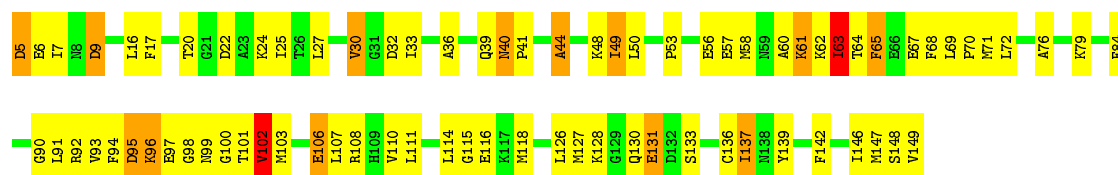
• Molecule 2: MYOSIN LIGHT CHAIN 3, SKELETAL MUSCLE ISOFORM

Chain 13-C: 43% 46% 9%



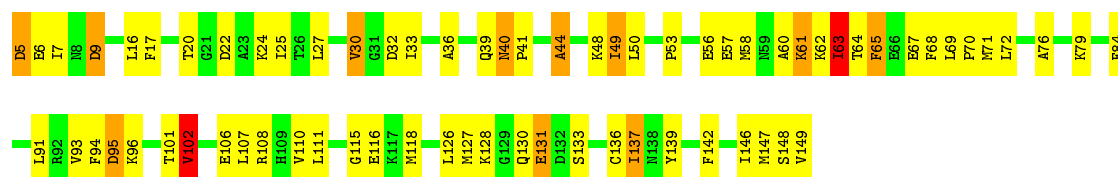
• Molecule 2: MYOSIN LIGHT CHAIN 3, SKELETAL MUSCLE ISOFORM

Chain 14-C: 46% 43% 9%



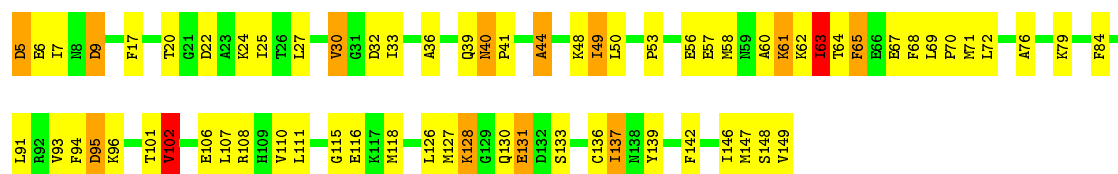
• Molecule 2: MYOSIN LIGHT CHAIN 3, SKELETAL MUSCLE ISOFORM

Chain 15-C: 52% 39% 8%



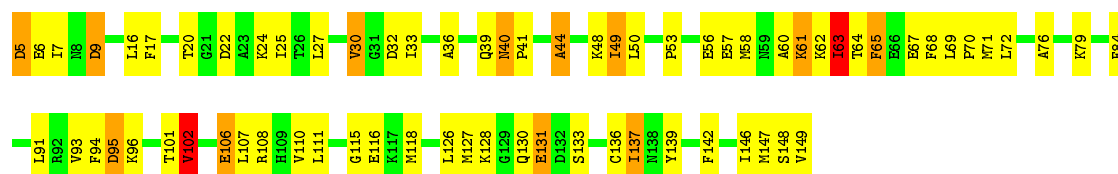
• Molecule 2: MYOSIN LIGHT CHAIN 3, SKELETAL MUSCLE ISOFORM

Chain 16-C: 52% 38% 8%



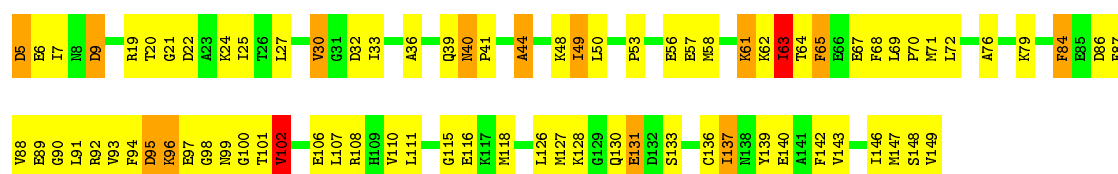
• Molecule 2: MYOSIN LIGHT CHAIN 3, SKELETAL MUSCLE ISOFORM

Chain 17-C: 52% 39% 8%



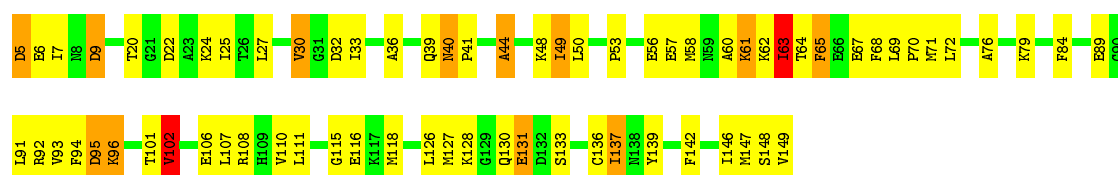
• Molecule 2: MYOSIN LIGHT CHAIN 3, SKELETAL MUSCLE ISOFORM

Chain 18-C: 44% 46% 9%



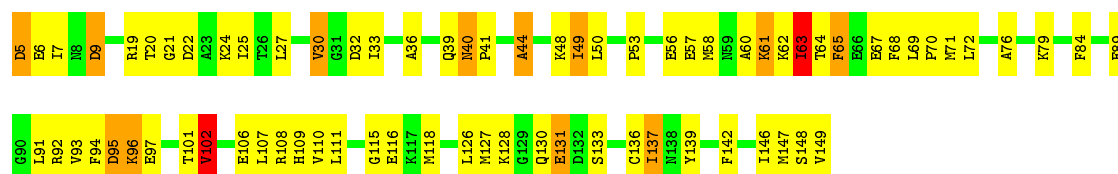
• Molecule 2: MYOSIN LIGHT CHAIN 3, SKELETAL MUSCLE ISOFORM

Chain 19-C: 52% 39% 8%



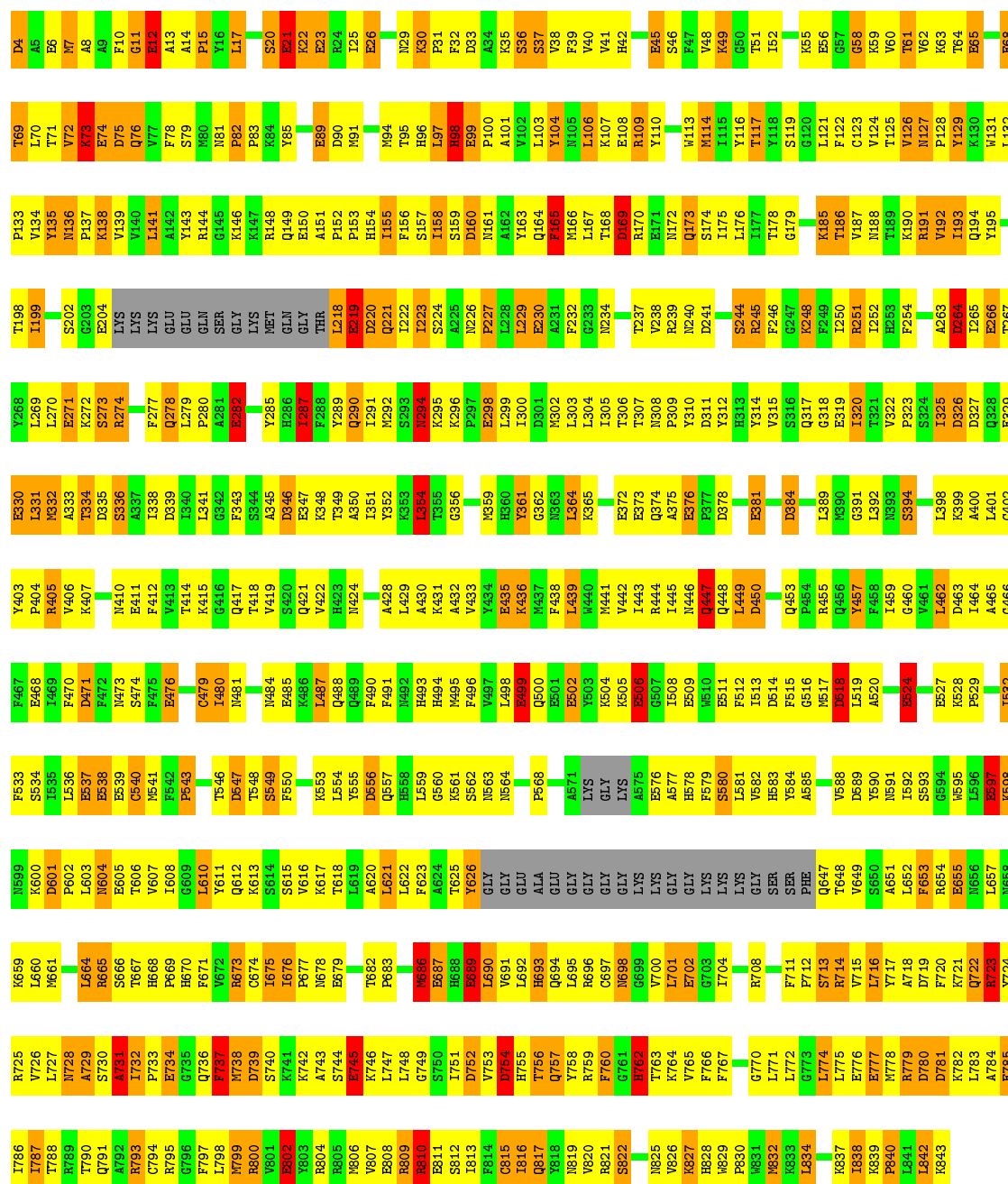
• Molecule 2: MYOSIN LIGHT CHAIN 3, SKELETAL MUSCLE ISOFORM

Chain 20-C: 49% 41% 8%



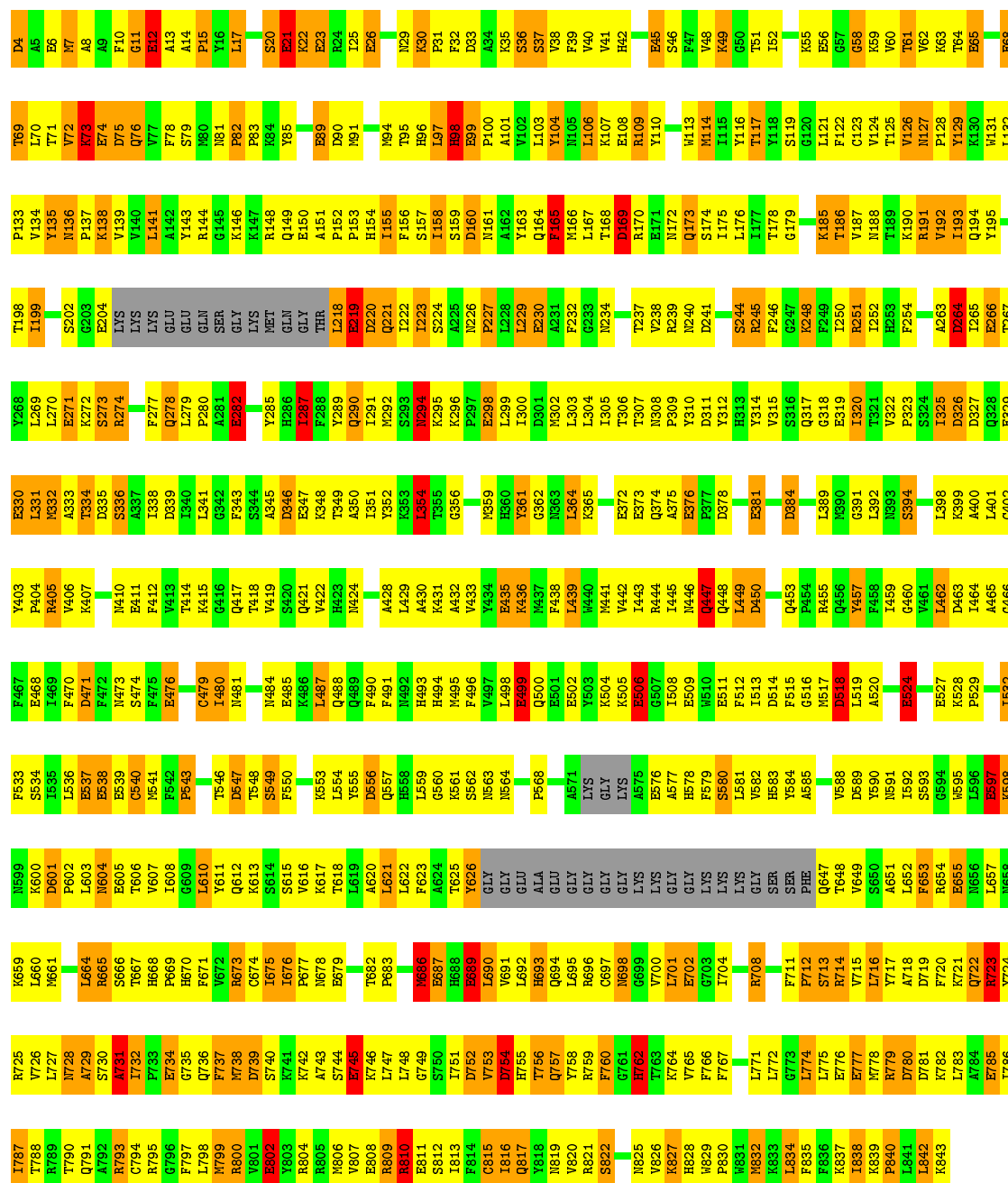
• Molecule 3: MYOSIN HEAVY CHAIN, SKELETAL MUSCLE, ADULT

Chain 1-M: 26% 47% 19%



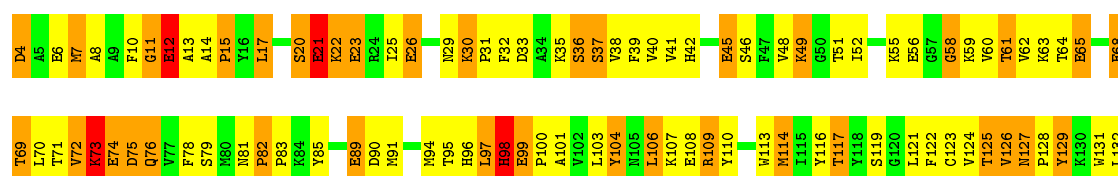
• Molecule 3: MYOSIN HEAVY CHAIN, SKELETAL MUSCLE, ADULT

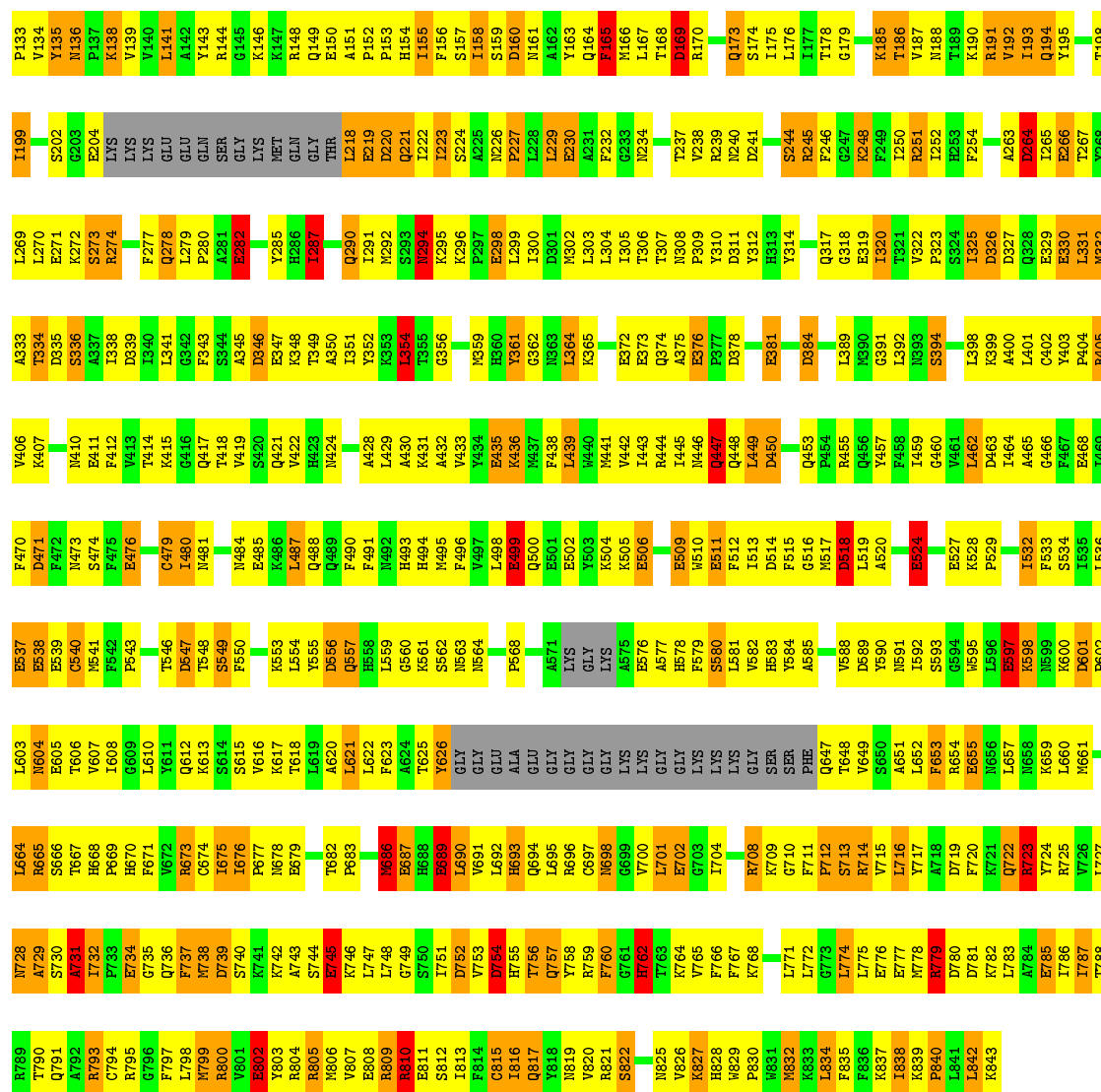
Chain 2-M: 



● Molecule 3: MYOSIN HEAVY CHAIN, SKELETAL MUSCLE, ADULT

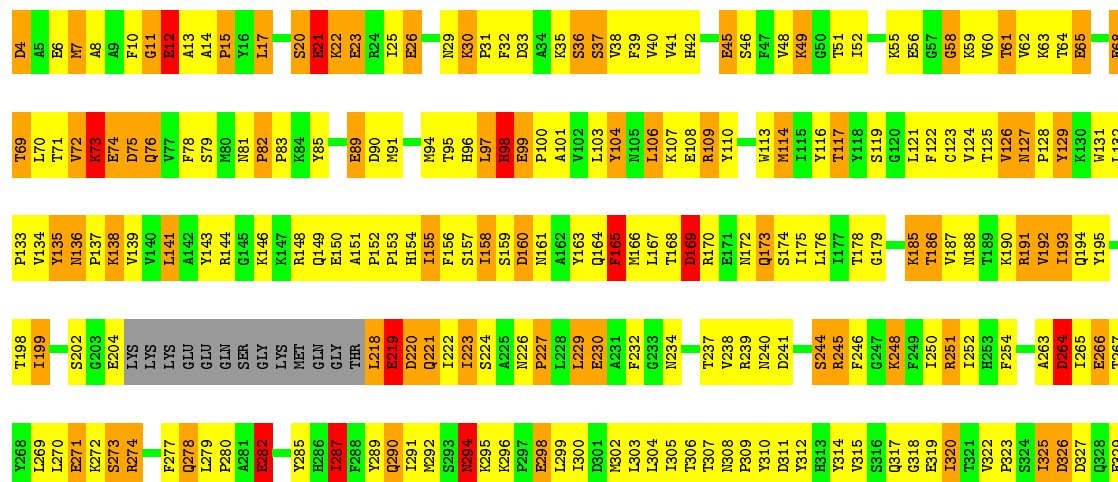
Chain 3-M: 

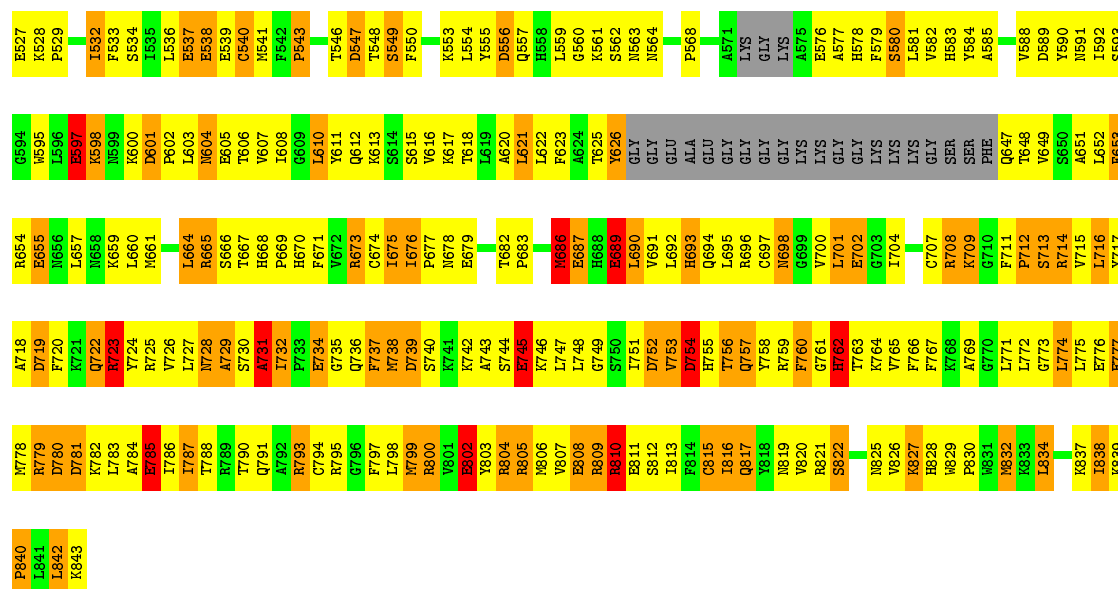




• Molecule 3: MYOSIN HEAVY CHAIN, SKELETAL MUSCLE, ADULT

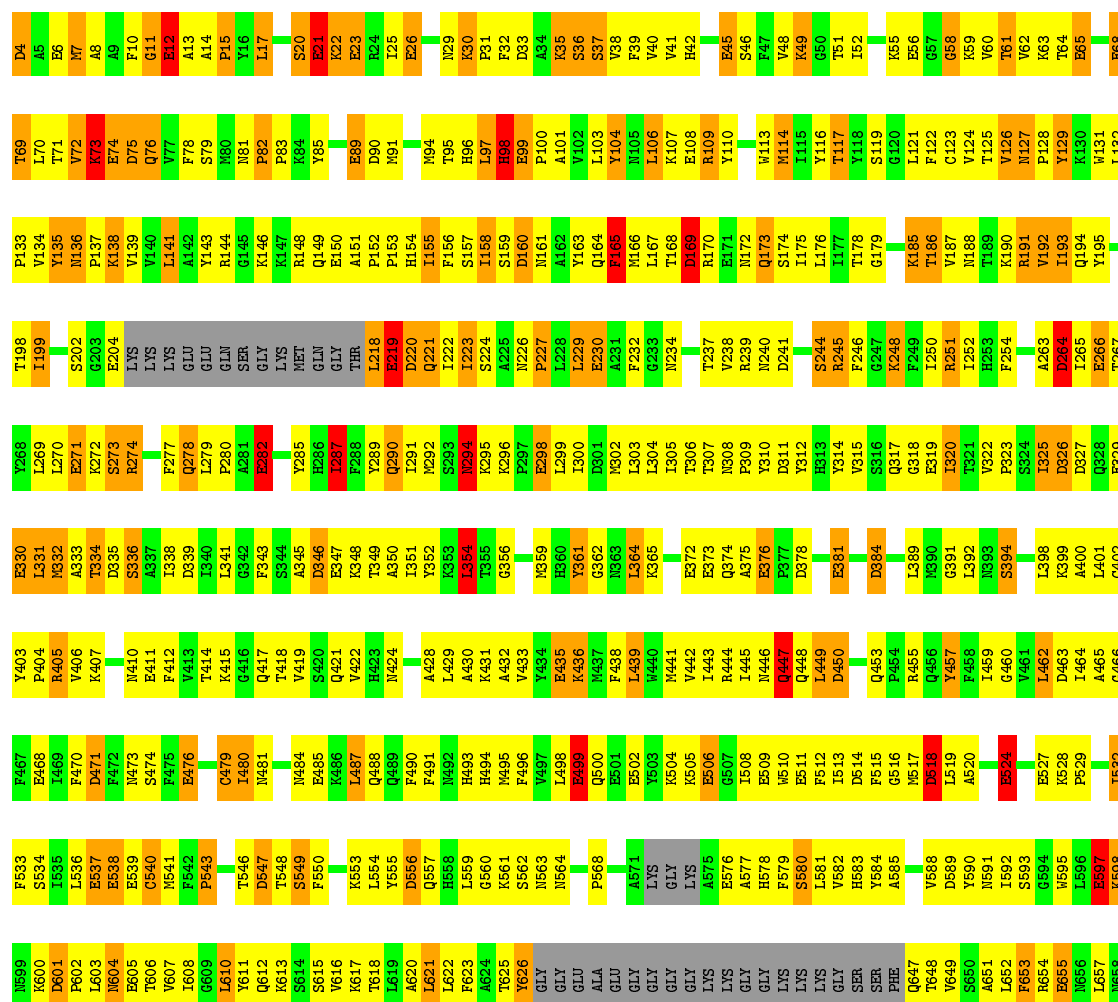
Chain 4-M: 26% 47% 19%





● Molecule 3: MYOSIN HEAVY CHAIN, SKELETAL MUSCLE, ADULT

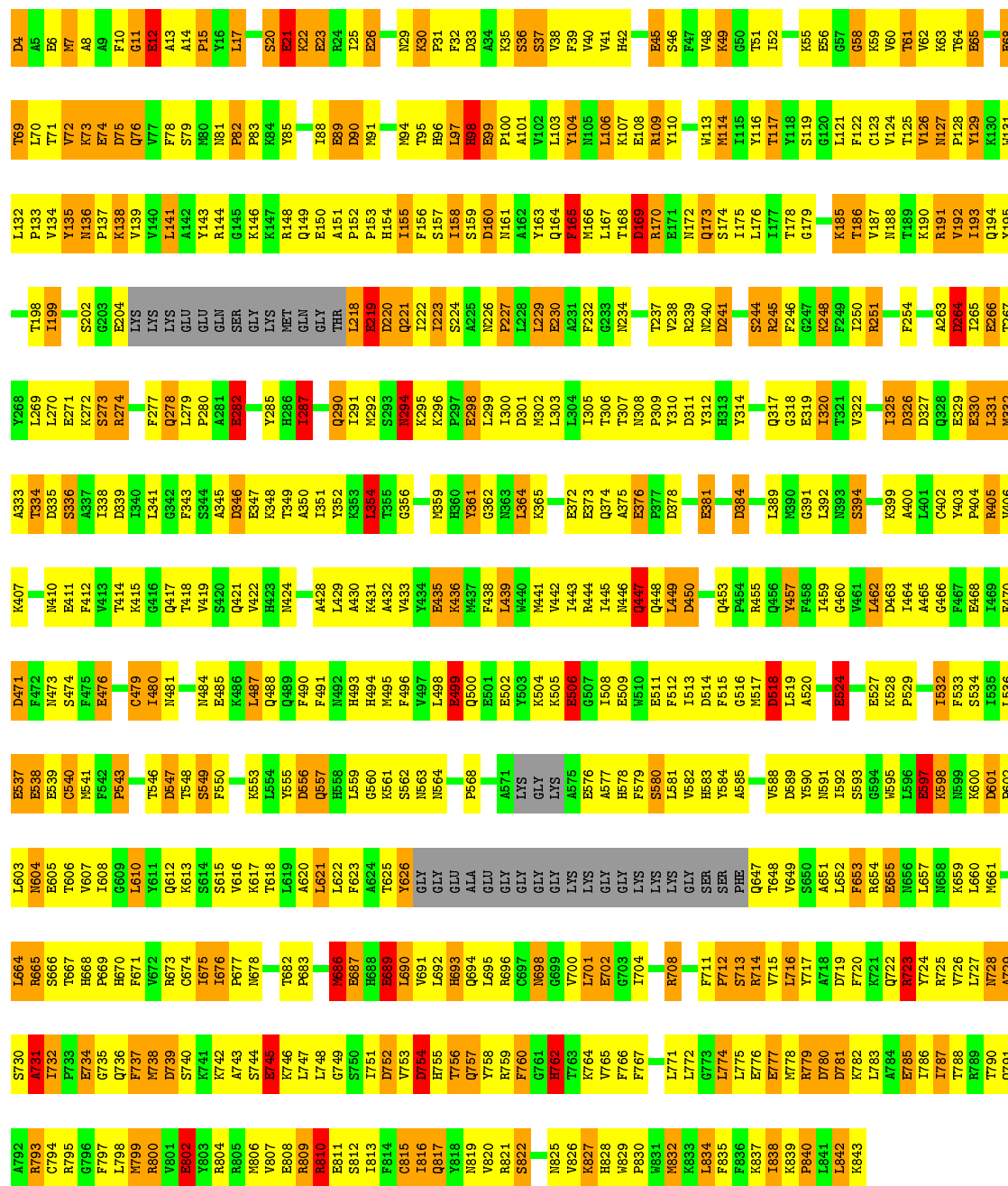
Chain 6-M: 26% 47% 20%





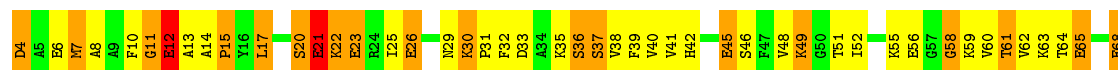
- Molecule 3: MYOSIN HEAVY CHAIN, SKELETAL MUSCLE, ADULT

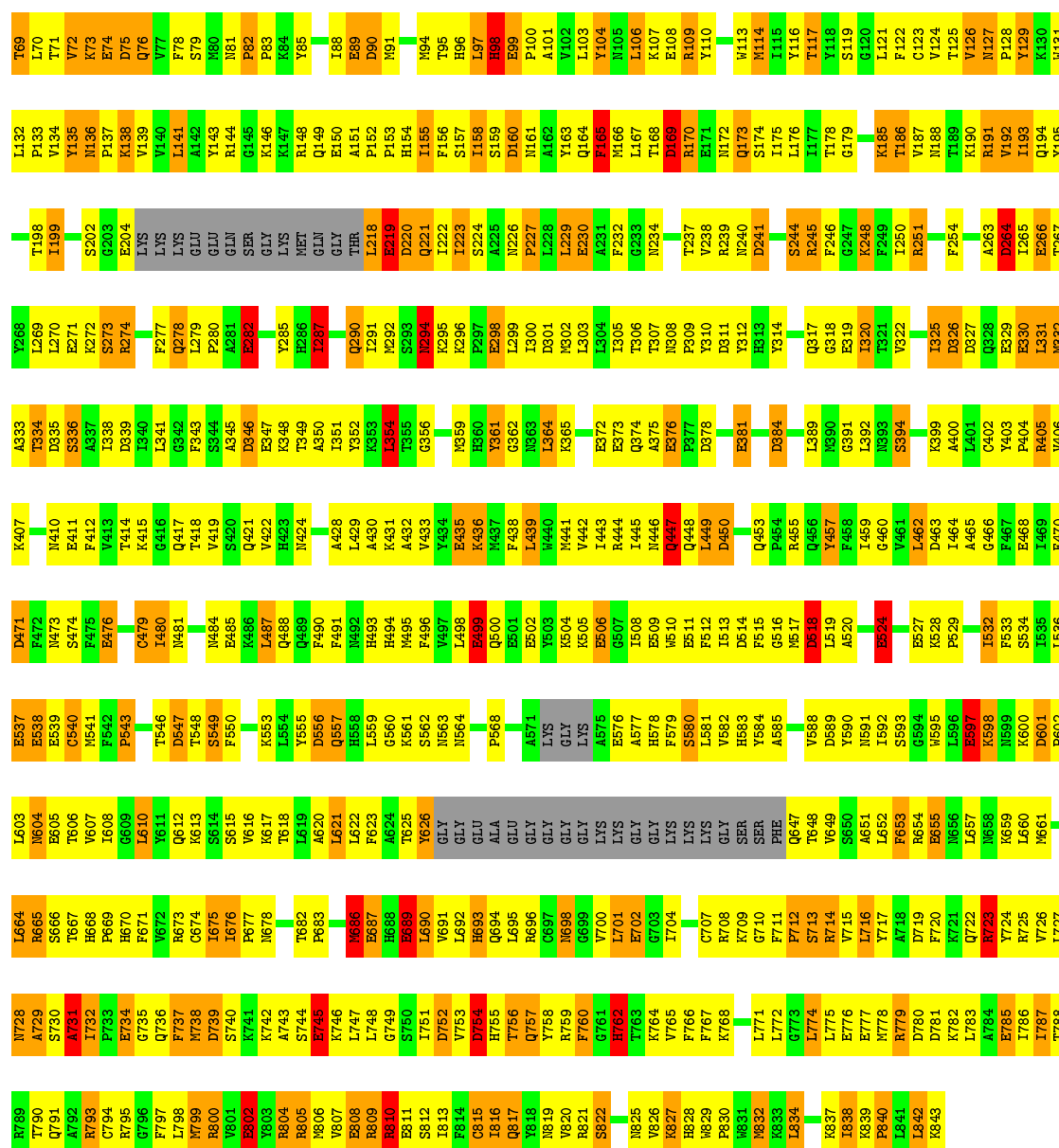
Chain 8-M:  28% 45% 19% . .

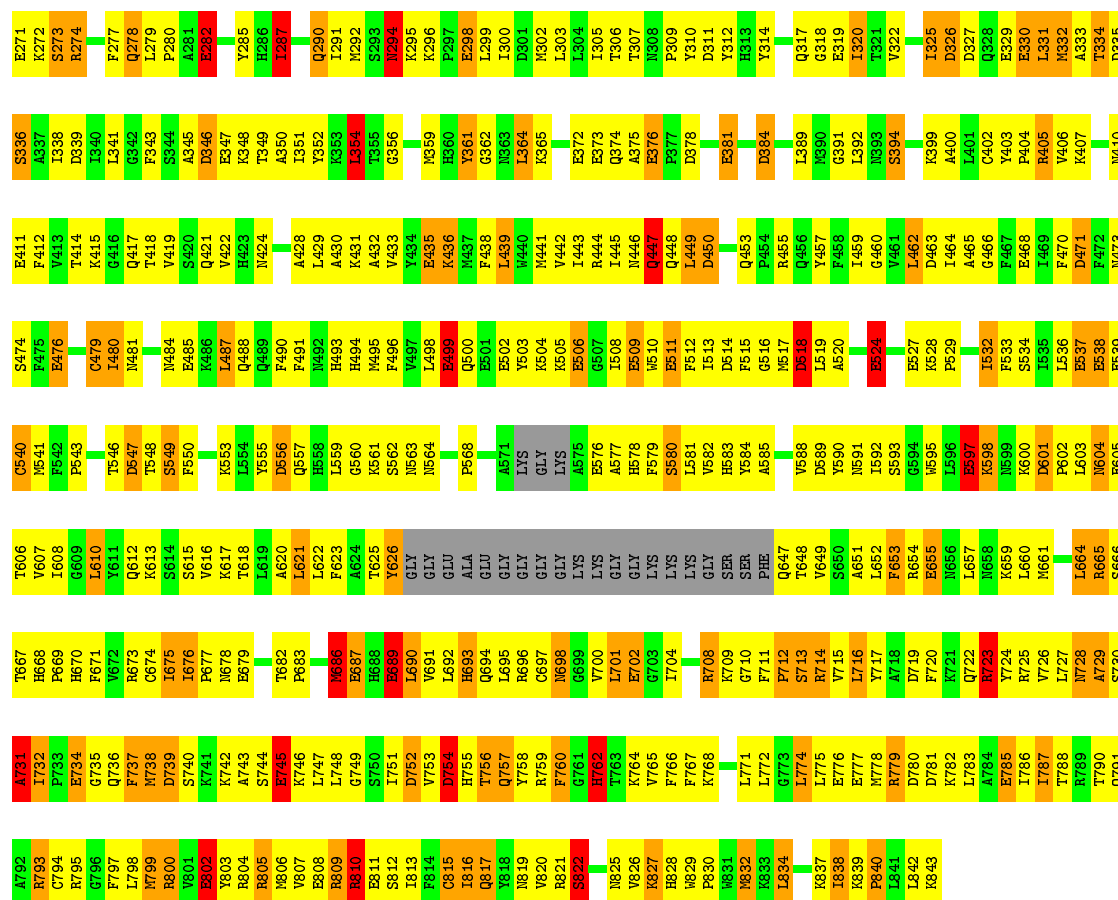


- Molecule 3: MYOSIN HEAVY CHAIN, SKELETAL MUSCLE, ADULT

Chain 9-M:  27% 46% 19% . .

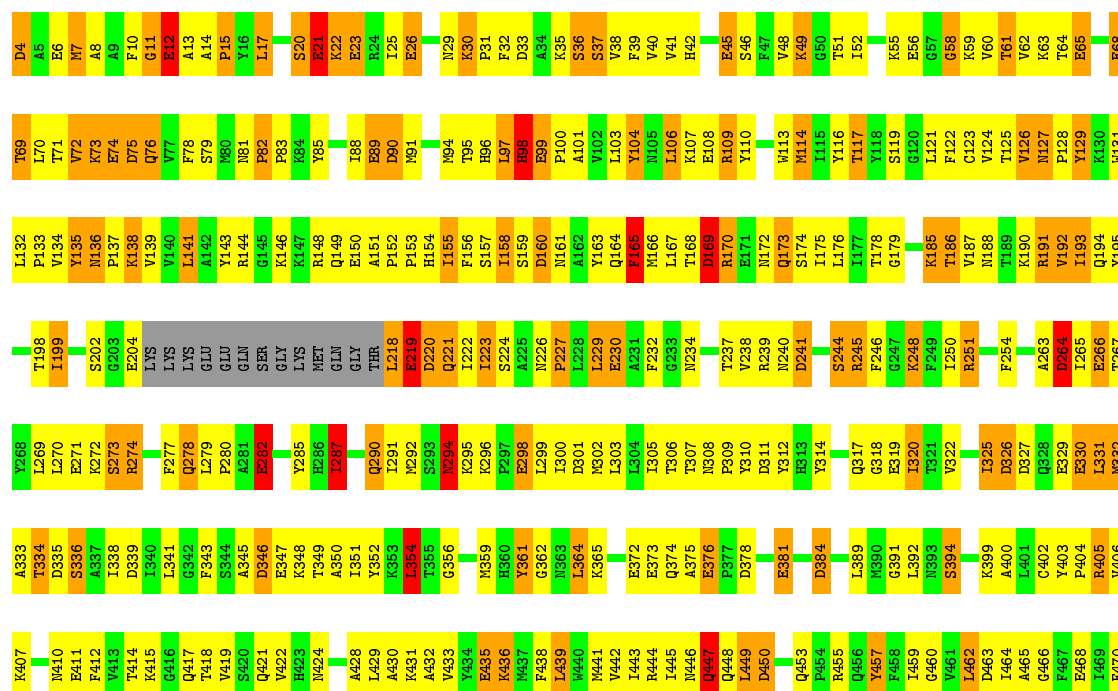






• Molecule 3: MYOSIN HEAVY CHAIN, SKELETAL MUSCLE, ADULT

Chain 11-M: 28% 45% 20%

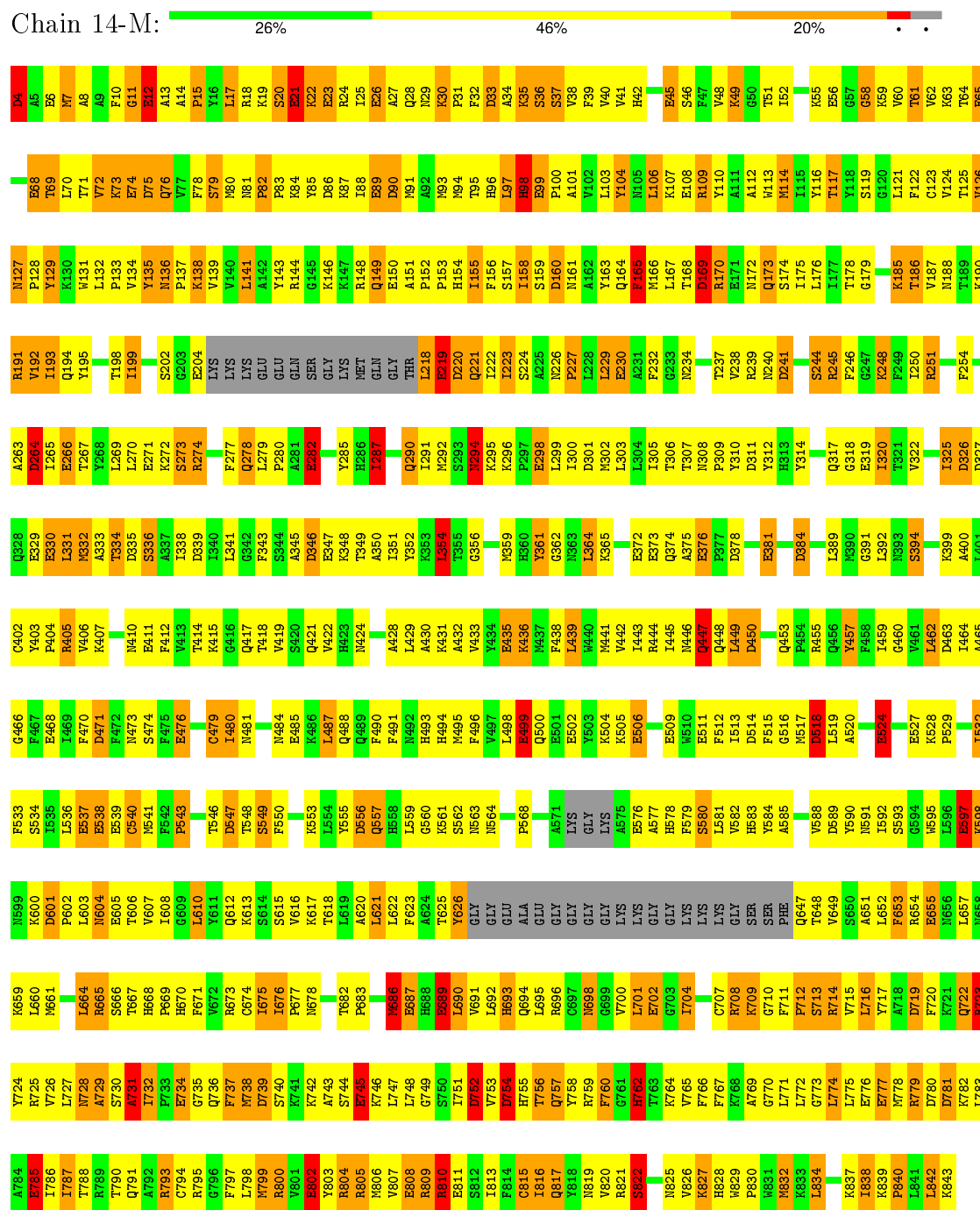




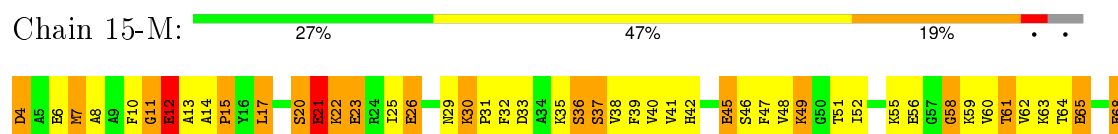


Chain 13-M:

• Molecule 3: MYOSIN HEAVY CHAIN, SKELETAL MUSCLE, ADULT



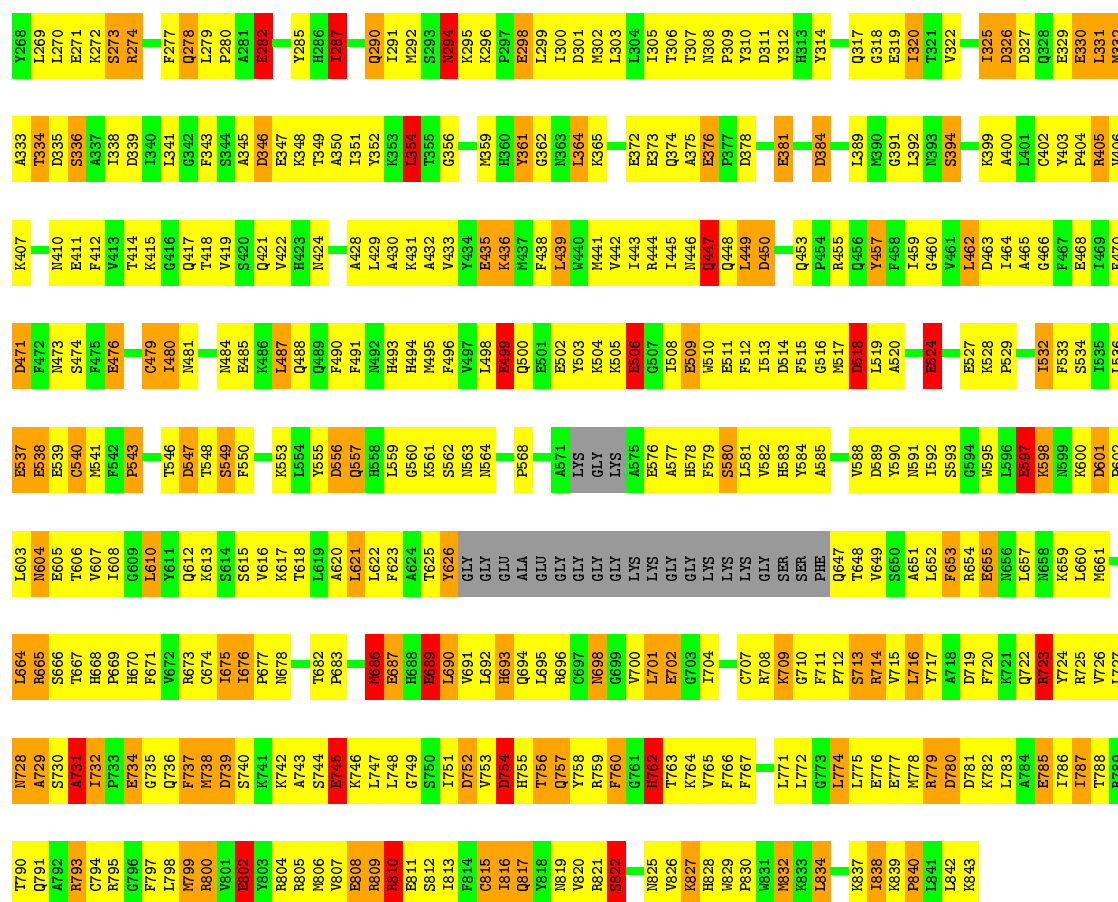
• Molecule 3: MYOSIN HEAVY CHAIN, SKELETAL MUSCLE, ADULT





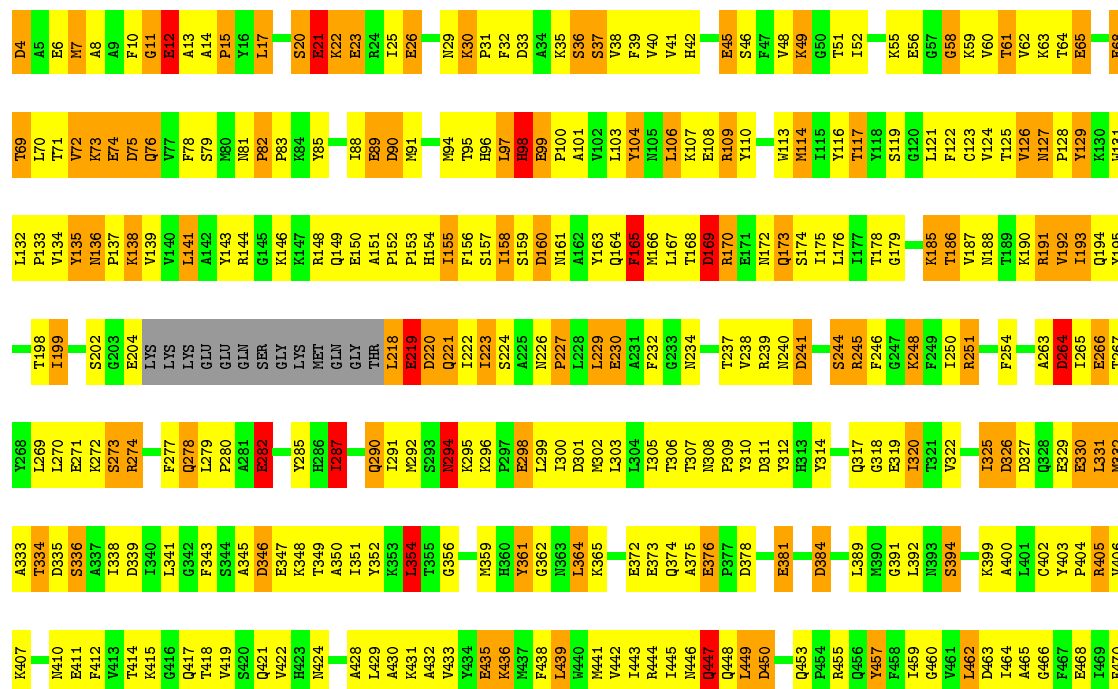
Frequency	Percentage
Daily	27%
Often	46%
Sometimes	19%
Rarely	3%
Never	5%

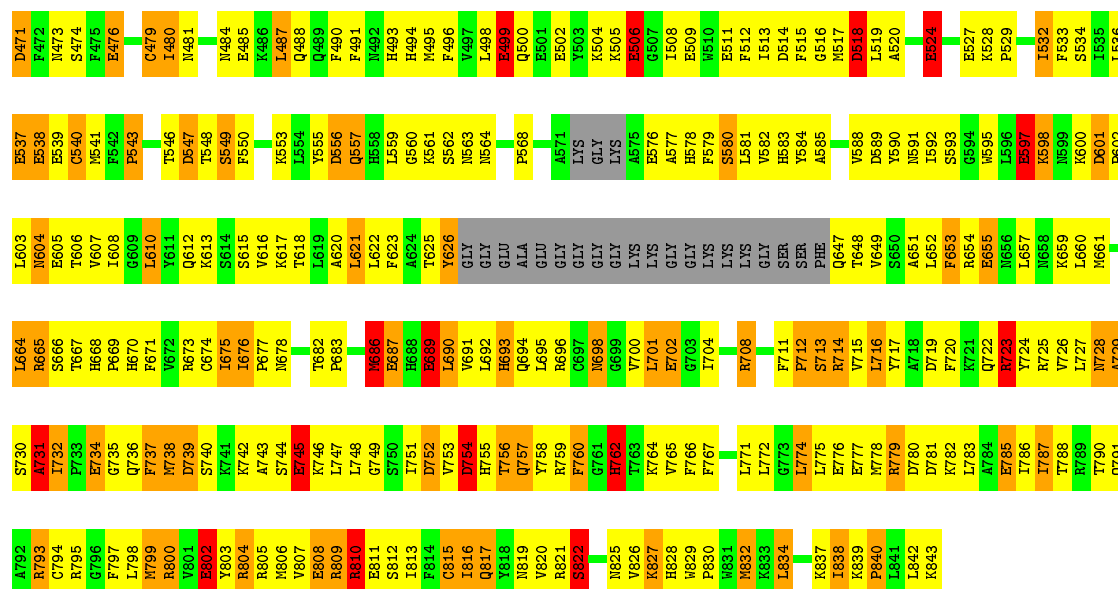




• Molecule 3: MYOSIN HEAVY CHAIN, SKELETAL MUSCLE, ADULT

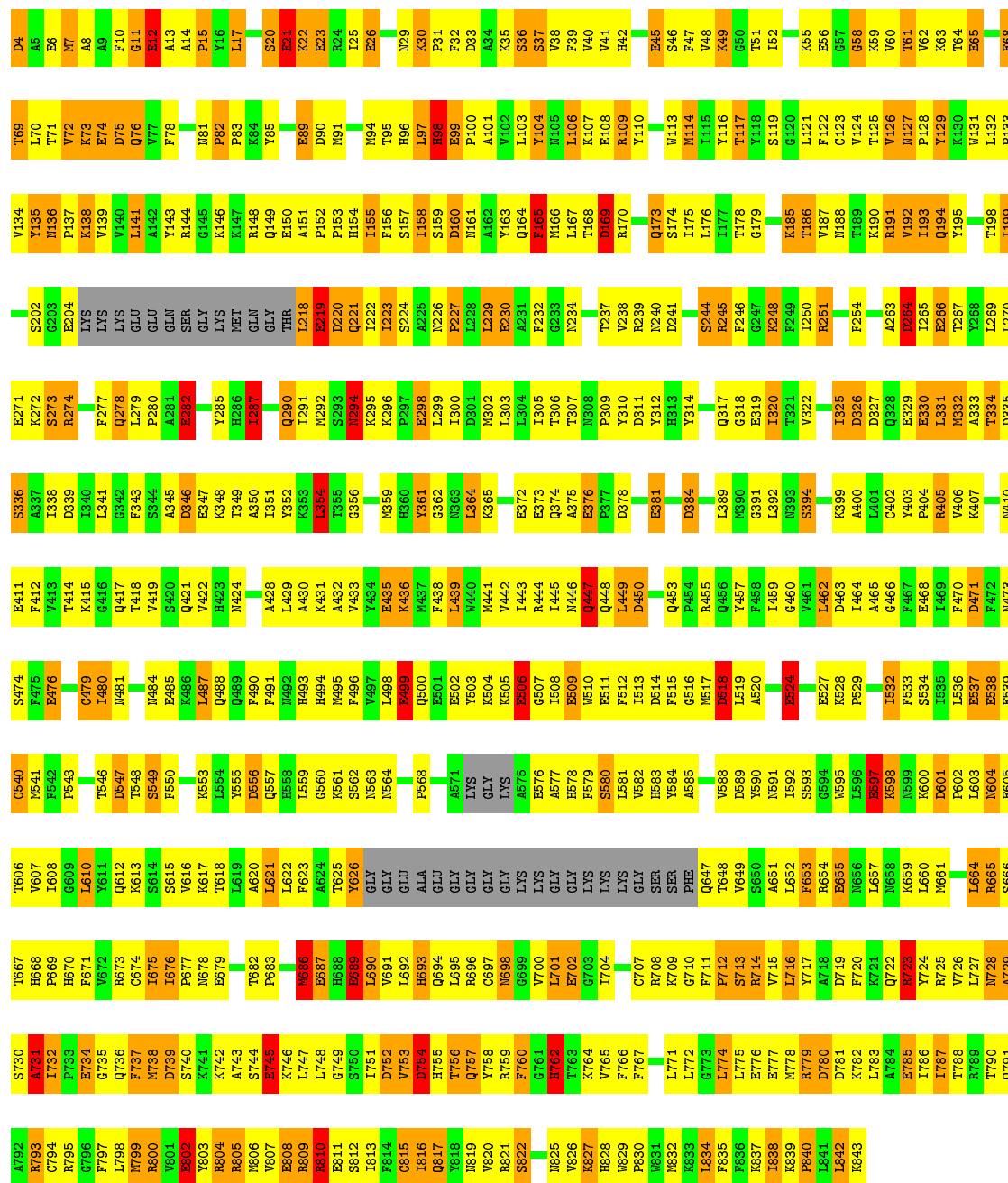
Chain 17-M: 28% 46% 19%



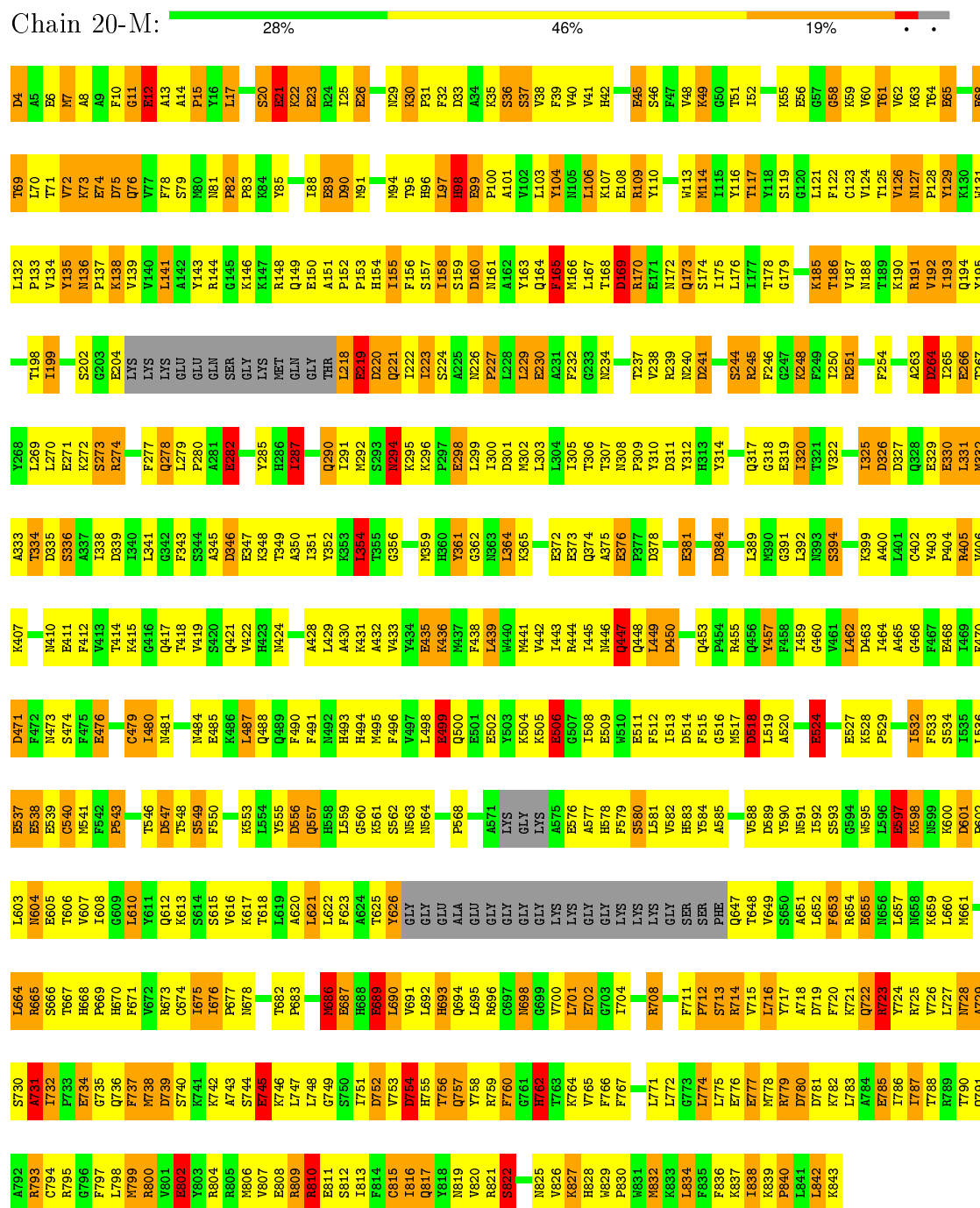




Chain 19-M: 27% 47% 19% . .



● Molecule 3: MYOSIN HEAVY CHAIN, SKELETAL MUSCLE, ADULT



4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	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	TIETZ TEM-CAM F224	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	1-B	0.70	0/1199	1.67	18/1617 (1.1%)
1	10-B	0.70	0/1199	1.67	18/1617 (1.1%)
1	11-B	0.70	0/1199	1.67	18/1617 (1.1%)
1	12-B	0.70	0/1199	1.67	18/1617 (1.1%)
1	13-B	0.70	0/1199	1.67	18/1617 (1.1%)
1	14-B	0.69	0/1199	1.67	18/1617 (1.1%)
1	15-B	0.70	0/1199	1.67	17/1617 (1.1%)
1	16-B	0.70	0/1199	1.67	18/1617 (1.1%)
1	17-B	0.69	0/1199	1.67	18/1617 (1.1%)
1	18-B	0.70	0/1199	1.67	18/1617 (1.1%)
1	19-B	0.70	0/1199	1.67	18/1617 (1.1%)
1	2-B	0.70	0/1199	1.67	18/1617 (1.1%)
1	20-B	0.70	0/1199	1.67	18/1617 (1.1%)
1	3-B	0.69	0/1199	1.67	18/1617 (1.1%)
1	4-B	0.70	0/1199	1.67	18/1617 (1.1%)
1	5-B	0.70	0/1199	1.67	18/1617 (1.1%)
1	6-B	0.70	0/1199	1.67	18/1617 (1.1%)
1	7-B	0.70	0/1199	1.67	18/1617 (1.1%)
1	8-B	0.70	0/1199	1.67	18/1617 (1.1%)
1	9-B	0.70	0/1199	1.67	18/1617 (1.1%)
2	1-C	0.74	1/1140 (0.1%)	1.58	9/1530 (0.6%)
2	10-C	0.74	1/1140 (0.1%)	1.58	9/1530 (0.6%)
2	11-C	0.74	1/1140 (0.1%)	1.59	9/1530 (0.6%)
2	12-C	0.74	1/1140 (0.1%)	1.59	9/1530 (0.6%)
2	13-C	0.74	1/1140 (0.1%)	1.58	9/1530 (0.6%)
2	14-C	0.74	1/1140 (0.1%)	1.59	9/1530 (0.6%)
2	15-C	0.74	1/1140 (0.1%)	1.59	9/1530 (0.6%)
2	16-C	0.74	1/1140 (0.1%)	1.58	9/1530 (0.6%)
2	17-C	0.74	1/1140 (0.1%)	1.59	9/1530 (0.6%)
2	18-C	0.74	1/1140 (0.1%)	1.59	9/1530 (0.6%)
2	19-C	0.74	1/1140 (0.1%)	1.58	9/1530 (0.6%)
2	2-C	0.74	1/1140 (0.1%)	1.58	9/1530 (0.6%)
2	20-C	0.74	1/1140 (0.1%)	1.59	9/1530 (0.6%)
2	3-C	0.74	1/1140 (0.1%)	1.59	9/1530 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
2	4-C	0.74	1/1140 (0.1%)	1.59	9/1530 (0.6%)
2	5-C	0.74	1/1140 (0.1%)	1.58	9/1530 (0.6%)
2	6-C	0.74	1/1140 (0.1%)	1.59	9/1530 (0.6%)
2	7-C	0.74	1/1140 (0.1%)	1.59	9/1530 (0.6%)
2	8-C	0.74	1/1140 (0.1%)	1.59	9/1530 (0.6%)
2	9-C	0.74	1/1140 (0.1%)	1.59	9/1530 (0.6%)
3	1-M	1.28	60/6593 (0.9%)	1.54	95/8881 (1.1%)
3	10-M	1.31	60/6593 (0.9%)	1.54	95/8881 (1.1%)
3	11-M	1.29	58/6594 (0.9%)	1.54	99/8884 (1.1%)
3	12-M	1.30	58/6594 (0.9%)	1.55	101/8884 (1.1%)
3	13-M	1.33	60/6593 (0.9%)	1.54	95/8881 (1.1%)
3	14-M	1.30	59/6594 (0.9%)	1.55	102/8884 (1.1%)
3	15-M	1.31	60/6593 (0.9%)	1.54	95/8881 (1.1%)
3	16-M	1.35	58/6593 (0.9%)	1.54	99/8881 (1.1%)
3	17-M	1.28	57/6594 (0.9%)	1.53	98/8884 (1.1%)
3	18-M	1.28	59/6593 (0.9%)	1.53	94/8881 (1.1%)
3	19-M	1.32	61/6593 (0.9%)	1.54	96/8881 (1.1%)
3	2-M	1.28	60/6593 (0.9%)	1.54	95/8881 (1.1%)
3	20-M	1.29	58/6594 (0.9%)	1.54	99/8884 (1.1%)
3	3-M	1.28	60/6593 (0.9%)	1.56	98/8881 (1.1%)
3	4-M	1.32	63/6594 (1.0%)	1.54	97/8884 (1.1%)
3	5-M	1.30	61/6594 (0.9%)	1.57	98/8884 (1.1%)
3	6-M	1.31	61/6593 (0.9%)	1.54	96/8881 (1.1%)
3	7-M	1.29	62/6594 (0.9%)	1.54	98/8884 (1.1%)
3	8-M	1.29	58/6594 (0.9%)	1.54	99/8884 (1.1%)
3	9-M	1.31	58/6593 (0.9%)	1.54	99/8881 (1.1%)
All	All	1.18	1211/178649 (0.7%)	1.57	2487/240587 (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	1-B	0	4
1	10-B	0	4
1	11-B	0	4
1	12-B	0	4
1	13-B	0	4
1	14-B	0	4
1	15-B	0	4
1	16-B	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	17-B	0	4
1	18-B	0	4
1	19-B	0	4
1	2-B	0	4
1	20-B	0	4
1	3-B	0	4
1	4-B	0	4
1	5-B	0	4
1	6-B	0	4
1	7-B	0	4
1	8-B	0	4
1	9-B	0	4
3	1-M	0	1
3	10-M	0	1
3	11-M	0	1
3	12-M	0	1
3	13-M	0	1
3	14-M	0	3
3	15-M	0	1
3	16-M	0	1
3	17-M	0	1
3	18-M	0	1
3	19-M	0	1
3	2-M	0	1
3	20-M	0	1
3	3-M	0	4
3	4-M	0	1
3	5-M	0	4
3	6-M	0	1
3	7-M	0	1
3	8-M	0	1
3	9-M	0	1
All	All	0	108

The worst 5 of 1211 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	16-M	709	LYS	C-N	34.79	1.95	1.33
3	13-M	709	LYS	C-N	29.52	1.86	1.33
3	10-M	805	ARG	C-N	25.22	1.92	1.34
3	15-M	731	ALA	C-N	25.18	1.92	1.34
3	19-M	731	ALA	C-N	25.17	1.92	1.34

The worst 5 of 2487 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	4-M	731	ALA	O-C-N	-28.58	76.97	122.70
3	6-M	731	ALA	O-C-N	-28.58	76.97	122.70
3	16-M	731	ALA	O-C-N	-28.58	76.97	122.70
3	2-M	731	ALA	O-C-N	-28.57	76.99	122.70
3	5-M	731	ALA	O-C-N	-28.57	76.99	122.70

There are no chirality outliers.

5 of 108 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1-B	105	ASP	Peptide
1	1-B	127	ARG	Peptide
1	1-B	140	PHE	Peptide
1	1-B	141	PRO	Peptide
3	1-M	98	HIS	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	1-B	1177	0	1134	138	0
1	2-B	1177	0	1134	136	0
1	3-B	1177	0	1133	153	0
1	4-B	1177	0	1134	133	0
1	5-B	1177	0	1134	158	0
1	6-B	1177	0	1134	138	0
1	7-B	1177	0	1134	163	0
1	8-B	1177	0	1132	129	0
1	9-B	1177	0	1134	133	0
1	10-B	1177	0	1134	134	0
1	11-B	1177	0	1134	137	0
1	12-B	1177	0	1134	134	0
1	13-B	1177	0	1134	135	0
1	14-B	1177	0	1134	133	0
1	15-B	1177	0	1134	130	0
1	16-B	1177	0	1134	134	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	17-B	1177	0	1134	129	0
1	18-B	1177	0	1134	136	0
1	19-B	1177	0	1134	131	0
1	20-B	1177	0	1134	135	0
2	1-C	1126	0	1068	409	0
2	2-C	1126	0	1078	250	0
2	3-C	1126	0	1084	133	0
2	4-C	1126	0	1083	142	0
2	5-C	1126	0	1078	432	0
2	6-C	1126	0	1084	95	0
2	7-C	1126	0	1083	192	0
2	8-C	1126	0	1081	124	0
2	9-C	1126	0	1084	88	0
2	10-C	1126	0	1084	89	0
2	11-C	1126	0	1080	215	0
2	12-C	1126	0	1079	202	0
2	13-C	1126	0	1070	241	0
2	14-C	1126	0	1077	281	0
2	15-C	1126	0	1084	89	0
2	16-C	1126	0	1084	85	0
2	17-C	1126	0	1084	100	0
2	18-C	1126	0	1070	245	0
2	19-C	1126	0	1079	111	0
2	20-C	1126	0	1084	206	0
3	1-M	6455	0	6360	1233	0
3	2-M	6455	0	6376	1018	0
3	3-M	6455	0	6376	876	0
3	4-M	6455	0	6380	919	0
3	5-M	6455	0	6344	1488	0
3	6-M	6455	0	6381	868	0
3	7-M	6455	0	6376	936	0
3	8-M	6455	0	6382	862	0
3	9-M	6455	0	6382	860	0
3	10-M	6455	0	6381	859	0
3	11-M	6455	0	6376	949	0
3	12-M	6455	0	6363	1156	0
3	13-M	6455	0	6368	1055	0
3	14-M	6455	0	6345	1358	0
3	15-M	6455	0	6382	856	0
3	16-M	6455	0	6380	874	0
3	17-M	6455	0	6384	841	0
3	18-M	6455	0	6369	1032	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	19-M	6455	0	6377	908	0
3	20-M	6455	0	6381	961	0
All	All	175160	0	171738	21980	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 63.

The worst 5 of 21980 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:C:139:TYR:CE2	3:M:725:ARG:HG3	1.24	1.71
3:M:508:ILE:HD13	3:M:766:PHE:CE2	1.26	1.70
2:C:93:VAL:CG1	3:M:724:TYR:CD1	1.76	1.65
3:M:540:CYS:CB	3:M:602:PRO:HG2	1.27	1.63
3:M:540:CYS:CB	3:M:602:PRO:HG2	1.27	1.63

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	1-B	148/150 (99%)	120 (81%)	16 (11%)	12 (8%)	1	19
1	2-B	148/150 (99%)	119 (80%)	17 (12%)	12 (8%)	1	19
1	3-B	148/150 (99%)	119 (80%)	17 (12%)	12 (8%)	1	19
1	4-B	148/150 (99%)	119 (80%)	17 (12%)	12 (8%)	1	19
1	5-B	148/150 (99%)	120 (81%)	16 (11%)	12 (8%)	1	19
1	6-B	148/150 (99%)	120 (81%)	16 (11%)	12 (8%)	1	19
1	7-B	148/150 (99%)	119 (80%)	17 (12%)	12 (8%)	1	19
1	8-B	148/150 (99%)	119 (80%)	17 (12%)	12 (8%)	1	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	9-B	148/150 (99%)	119 (80%)	17 (12%)	12 (8%)	1	19
1	10-B	148/150 (99%)	119 (80%)	17 (12%)	12 (8%)	1	19
1	11-B	148/150 (99%)	119 (80%)	17 (12%)	12 (8%)	1	19
1	12-B	148/150 (99%)	119 (80%)	17 (12%)	12 (8%)	1	19
1	13-B	148/150 (99%)	119 (80%)	17 (12%)	12 (8%)	1	19
1	14-B	148/150 (99%)	119 (80%)	17 (12%)	12 (8%)	1	19
1	15-B	148/150 (99%)	119 (80%)	17 (12%)	12 (8%)	1	19
1	16-B	148/150 (99%)	119 (80%)	17 (12%)	12 (8%)	1	19
1	17-B	148/150 (99%)	120 (81%)	16 (11%)	12 (8%)	1	19
1	18-B	148/150 (99%)	119 (80%)	17 (12%)	12 (8%)	1	19
1	19-B	148/150 (99%)	119 (80%)	17 (12%)	12 (8%)	1	19
1	20-B	148/150 (99%)	119 (80%)	17 (12%)	12 (8%)	1	19
2	1-C	143/145 (99%)	111 (78%)	20 (14%)	12 (8%)	1	18
2	2-C	143/145 (99%)	111 (78%)	20 (14%)	12 (8%)	1	18
2	3-C	143/145 (99%)	111 (78%)	20 (14%)	12 (8%)	1	18
2	4-C	143/145 (99%)	111 (78%)	20 (14%)	12 (8%)	1	18
2	5-C	143/145 (99%)	111 (78%)	20 (14%)	12 (8%)	1	18
2	6-C	143/145 (99%)	111 (78%)	20 (14%)	12 (8%)	1	18
2	7-C	143/145 (99%)	111 (78%)	20 (14%)	12 (8%)	1	18
2	8-C	143/145 (99%)	111 (78%)	20 (14%)	12 (8%)	1	18
2	9-C	143/145 (99%)	111 (78%)	20 (14%)	12 (8%)	1	18
2	10-C	143/145 (99%)	111 (78%)	20 (14%)	12 (8%)	1	18
2	11-C	143/145 (99%)	110 (77%)	21 (15%)	12 (8%)	1	18
2	12-C	143/145 (99%)	111 (78%)	20 (14%)	12 (8%)	1	18
2	13-C	143/145 (99%)	111 (78%)	20 (14%)	12 (8%)	1	18
2	14-C	143/145 (99%)	111 (78%)	20 (14%)	12 (8%)	1	18
2	15-C	143/145 (99%)	111 (78%)	20 (14%)	12 (8%)	1	18
2	16-C	143/145 (99%)	111 (78%)	20 (14%)	12 (8%)	1	18
2	17-C	143/145 (99%)	111 (78%)	20 (14%)	12 (8%)	1	18
2	18-C	143/145 (99%)	111 (78%)	20 (14%)	12 (8%)	1	18
2	19-C	143/145 (99%)	111 (78%)	20 (14%)	12 (8%)	1	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	20-C	143/145 (99%)	110 (77%)	21 (15%)	12 (8%)	1	18
3	1-M	786/840 (94%)	649 (83%)	114 (14%)	23 (3%)	6	43
3	2-M	786/840 (94%)	649 (83%)	114 (14%)	23 (3%)	6	43
3	3-M	786/840 (94%)	648 (82%)	116 (15%)	22 (3%)	6	44
3	4-M	788/840 (94%)	651 (83%)	114 (14%)	23 (3%)	6	43
3	5-M	788/840 (94%)	650 (82%)	115 (15%)	23 (3%)	6	43
3	6-M	786/840 (94%)	648 (82%)	114 (14%)	24 (3%)	5	42
3	7-M	788/840 (94%)	650 (82%)	115 (15%)	23 (3%)	6	43
3	8-M	788/840 (94%)	650 (82%)	115 (15%)	23 (3%)	6	43
3	9-M	786/840 (94%)	648 (82%)	115 (15%)	23 (3%)	6	43
3	10-M	786/840 (94%)	649 (83%)	114 (14%)	23 (3%)	6	43
3	11-M	788/840 (94%)	650 (82%)	115 (15%)	23 (3%)	6	43
3	12-M	788/840 (94%)	650 (82%)	114 (14%)	24 (3%)	5	42
3	13-M	786/840 (94%)	648 (82%)	116 (15%)	22 (3%)	6	44
3	14-M	788/840 (94%)	647 (82%)	116 (15%)	25 (3%)	5	41
3	15-M	786/840 (94%)	649 (83%)	115 (15%)	22 (3%)	6	44
3	16-M	786/840 (94%)	648 (82%)	114 (14%)	24 (3%)	5	42
3	17-M	788/840 (94%)	650 (82%)	114 (14%)	24 (3%)	5	42
3	18-M	786/840 (94%)	649 (83%)	115 (15%)	22 (3%)	6	44
3	19-M	786/840 (94%)	649 (83%)	115 (15%)	22 (3%)	6	44
3	20-M	788/840 (94%)	650 (82%)	114 (14%)	24 (3%)	5	42
All	All	21558/22700 (95%)	17584 (82%)	3032 (14%)	942 (4%)	6	33

5 of 942 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-B	76	ASN
1	1-B	109	LYS
1	1-B	115	SER
1	1-B	141	PRO
1	1-B	142	PRO

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	1-B	128 / 130 (98%)	116 (91%)	12 (9%)	11	42
1	2-B	128 / 130 (98%)	116 (91%)	12 (9%)	11	42
1	3-B	128 / 130 (98%)	116 (91%)	12 (9%)	11	42
1	4-B	128 / 130 (98%)	116 (91%)	12 (9%)	11	42
1	5-B	128 / 130 (98%)	116 (91%)	12 (9%)	11	42
1	6-B	128 / 130 (98%)	116 (91%)	12 (9%)	11	42
1	7-B	128 / 130 (98%)	116 (91%)	12 (9%)	11	42
1	8-B	128 / 130 (98%)	116 (91%)	12 (9%)	11	42
1	9-B	128 / 130 (98%)	116 (91%)	12 (9%)	11	42
1	10-B	128 / 130 (98%)	116 (91%)	12 (9%)	11	42
1	11-B	128 / 130 (98%)	116 (91%)	12 (9%)	11	42
1	12-B	128 / 130 (98%)	116 (91%)	12 (9%)	11	42
1	13-B	128 / 130 (98%)	116 (91%)	12 (9%)	11	42
1	14-B	128 / 130 (98%)	116 (91%)	12 (9%)	11	42
1	15-B	128 / 130 (98%)	116 (91%)	12 (9%)	11	42
1	16-B	128 / 130 (98%)	116 (91%)	12 (9%)	11	42
1	17-B	128 / 130 (98%)	116 (91%)	12 (9%)	11	42
1	18-B	128 / 130 (98%)	116 (91%)	12 (9%)	11	42
1	19-B	128 / 130 (98%)	116 (91%)	12 (9%)	11	42
1	20-B	128 / 130 (98%)	116 (91%)	12 (9%)	11	42
2	1-C	120 / 122 (98%)	109 (91%)	11 (9%)	11	43
2	2-C	120 / 122 (98%)	109 (91%)	11 (9%)	11	43
2	3-C	120 / 122 (98%)	109 (91%)	11 (9%)	11	43
2	4-C	120 / 122 (98%)	109 (91%)	11 (9%)	11	43
2	5-C	120 / 122 (98%)	109 (91%)	11 (9%)	11	43
2	6-C	120 / 122 (98%)	109 (91%)	11 (9%)	11	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	7-C	120/122 (98%)	109 (91%)	11 (9%)	11	43
2	8-C	120/122 (98%)	109 (91%)	11 (9%)	11	43
2	9-C	120/122 (98%)	109 (91%)	11 (9%)	11	43
2	10-C	120/122 (98%)	109 (91%)	11 (9%)	11	43
2	11-C	120/122 (98%)	109 (91%)	11 (9%)	11	43
2	12-C	120/122 (98%)	109 (91%)	11 (9%)	11	43
2	13-C	120/122 (98%)	109 (91%)	11 (9%)	11	43
2	14-C	120/122 (98%)	109 (91%)	11 (9%)	11	43
2	15-C	120/122 (98%)	109 (91%)	11 (9%)	11	43
2	16-C	120/122 (98%)	109 (91%)	11 (9%)	11	43
2	17-C	120/122 (98%)	109 (91%)	11 (9%)	11	43
2	18-C	120/122 (98%)	109 (91%)	11 (9%)	11	43
2	19-C	120/122 (98%)	109 (91%)	11 (9%)	11	43
2	20-C	120/122 (98%)	109 (91%)	11 (9%)	11	43
3	1-M	693/724 (96%)	522 (75%)	171 (25%)	1	6
3	2-M	693/724 (96%)	522 (75%)	171 (25%)	1	6
3	3-M	693/724 (96%)	523 (76%)	170 (24%)	1	6
3	4-M	693/724 (96%)	522 (75%)	171 (25%)	1	6
3	5-M	693/724 (96%)	522 (75%)	171 (25%)	1	6
3	6-M	693/724 (96%)	522 (75%)	171 (25%)	1	6
3	7-M	693/724 (96%)	522 (75%)	171 (25%)	1	6
3	8-M	693/724 (96%)	522 (75%)	171 (25%)	1	6
3	9-M	693/724 (96%)	522 (75%)	171 (25%)	1	6
3	10-M	693/724 (96%)	523 (76%)	170 (24%)	1	6
3	11-M	693/724 (96%)	522 (75%)	171 (25%)	1	6
3	12-M	693/724 (96%)	522 (75%)	171 (25%)	1	6
3	13-M	693/724 (96%)	523 (76%)	170 (24%)	1	6
3	14-M	693/724 (96%)	522 (75%)	171 (25%)	1	6
3	15-M	693/724 (96%)	523 (76%)	170 (24%)	1	6
3	16-M	693/724 (96%)	522 (75%)	171 (25%)	1	6
3	17-M	693/724 (96%)	522 (75%)	171 (25%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	18-M	693/724 (96%)	523 (76%)	170 (24%)	1	6
3	19-M	693/724 (96%)	523 (76%)	170 (24%)	1	6
3	20-M	693/724 (96%)	522 (75%)	171 (25%)	1	6
All	All	18820/19520 (96%)	14946 (79%)	3874 (21%)	4	10

5 of 3874 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	10-B	129	THR
3	12-M	55	LYS
3	19-M	325	ILE
3	10-M	158	ILE
3	11-M	22	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 562 such sidechains are listed below:

Mol	Chain	Res	Type
1	10-B	36	GLN
2	12-C	77	ASN
3	19-M	317	GLN
3	10-M	164	GLN
2	11-C	40	ASN

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 [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](#)

There are no chain breaks in this entry.