wwPDB EM Validation Summary Report (i)

Nov 20, 2022 – 03:01 pm GMT

PDB ID	:	2W4H
EMDB ID	:	EMD-1584
Title	:	Isometrically contracting insect asynchronous flight muscle quick frozen after a quick release 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 Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

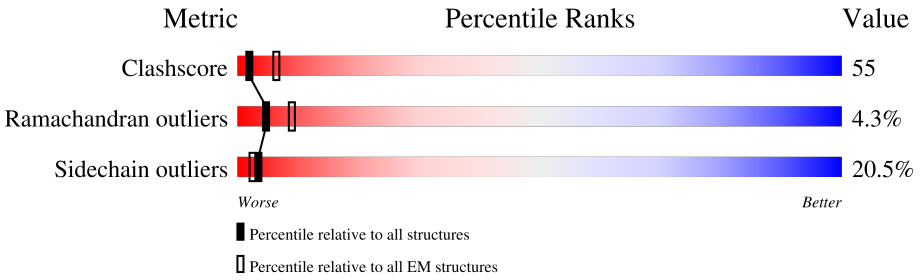
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	1-B	150	49% 35% 13% •
1	10-B	150	49% 36% 13% •
1	11-B	150	49% 35% 14% •
1	12-B	150	49% 34% 15% •
1	13-B	150	49% 36% 13% •
1	14-B	150	49% 35% 14% •
1	2-B	150	49% 35% 14% •
1	3-B	150	49% 36% 14% •
1	4-B	150	49% 35% 13% •

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Mol	Chain	Length	Quality of chain
1	5-B	150	47% 37% 14%
1	6-B	150	49% 36% 13%
1	7-B	150	49% 34% 15%
1	8-B	150	49% 34% 15%
1	9-B	150	49% 35% 15%
2	1-C	145	52% 39% 8%
2	10-C	145	52% 39% 8%
2	11-C	145	52% 39% 8%
2	12-C	145	52% 39% 8%
2	13-C	145	52% 39% 8%
2	14-C	145	52% 39% 8%
2	2-C	145	52% 39% 8%
2	3-C	145	52% 39% 8%
2	4-C	145	52% 39% 8%
2	5-C	145	52% 39% 8%
2	6-C	145	52% 39% 8%
2	7-C	145	52% 39% 8%
2	8-C	145	52% 39% 8%
2	9-C	145	52% 39% 8%
3	1-M	840	26% 47% 19%
3	10-M	840	28% 46% 19%
3	11-M	840	28% 46% 19%
3	12-M	840	28% 47% 18%
3	13-M	840	28% 46% 19%
3	14-M	840	28% 46% 18%

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Mol	Chain	Length	Quality of chain
3	2-M	840	26% 48% 19%
3	3-M	840	27% 47% 19%
3	4-M	840	26% 48% 19%
3	5-M	840	27% 47% 19%
3	6-M	840	27% 47% 19%
3	7-M	840	26% 48% 19%
3	8-M	840	27% 47% 19%
3	9-M	840	27% 47% 19%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 122612 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		

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		
2	14-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		

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Mol	Chain	Residues	Atoms					AltConf	Trace
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		
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		

There is a discrepancy between the modelled and reference sequences:

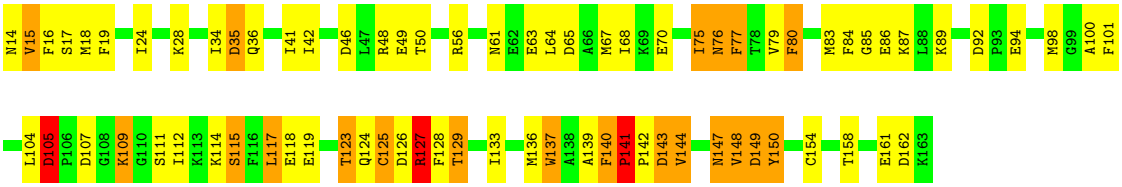
Chain	Residue	Modelled	Actual	Comment	Reference
M	138	LYS	GLU	conflict	UNP P02609

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

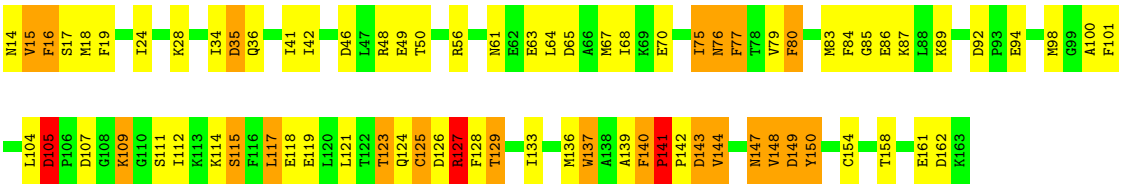
• Molecule 1: MYOSIN REGULATORY LIGHT CHAIN 2, SKELETAL MUSCLE ISOFORM

Chain 1-B:



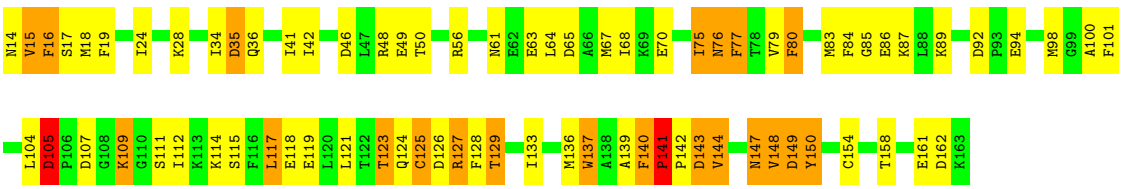
• Molecule 1: MYOSIN REGULATORY LIGHT CHAIN 2, SKELETAL MUSCLE ISOFORM

Chain 2-B:



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

Chain 3-B:

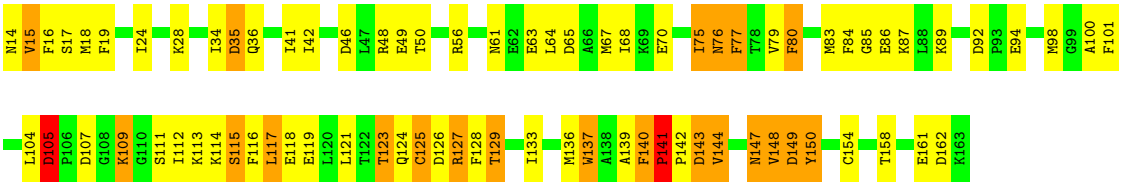


• Molecule 1: MYOSIN REGULATORY LIGHT CHAIN 2, SKELETAL MUSCLE ISOFORM

Chain 4-B:

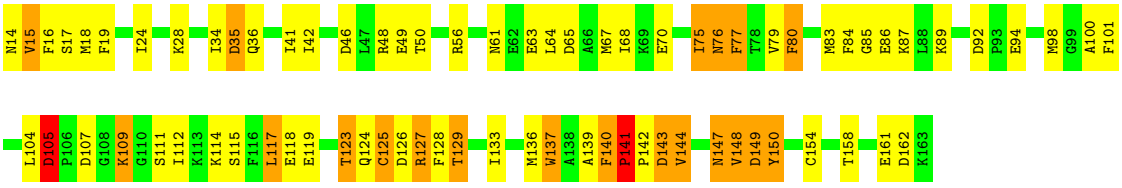
• Molecule 1: MYOSIN REGULATORY LIGHT CHAIN 2, SKELETAL MUSCLE ISOFORM

Chain 5-B:



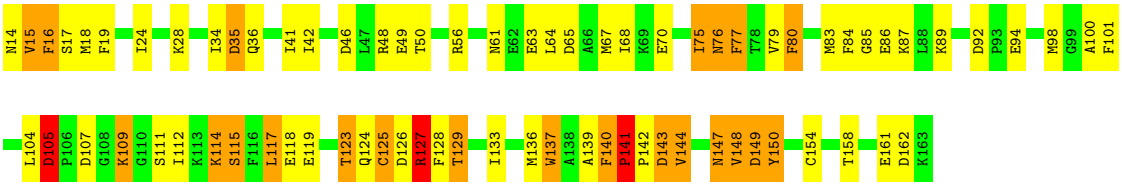
• Molecule 1: MYOSIN REGULATORY LIGHT CHAIN 2, SKELETAL MUSCLE ISOFORM

Chain 6-B:



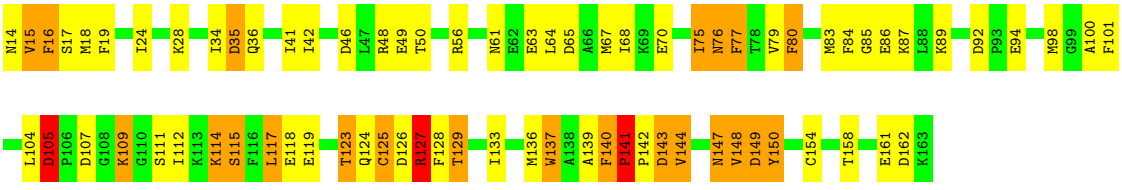
• Molecule 1: MYOSIN REGULATORY LIGHT CHAIN 2, SKELETAL MUSCLE ISOFORM

Chain 7-B:



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

Chain 8-B:

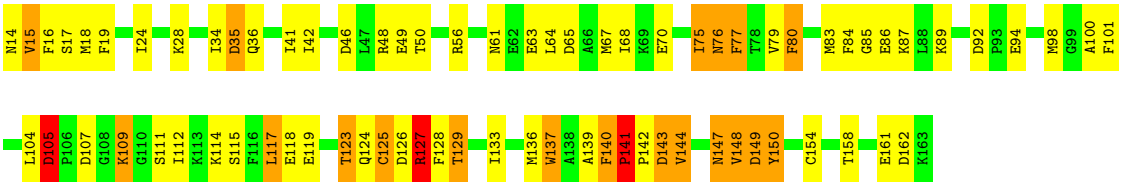


• Molecule 1: MYOSIN REGULATORY LIGHT CHAIN 2, SKELETAL MUSCLE ISOFORM

Chain 9-B:

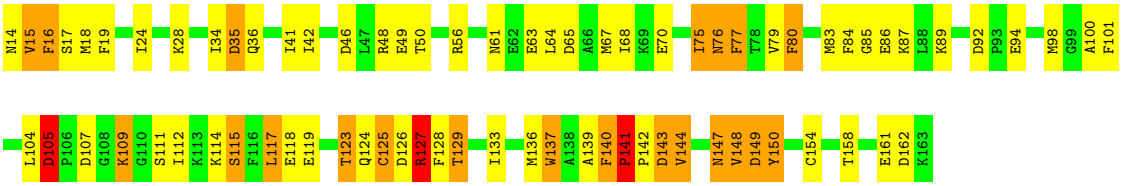
• Molecule 1: MYOSIN REGULATORY LIGHT CHAIN 2, SKELETAL MUSCLE ISOFORM

Chain 10-B:



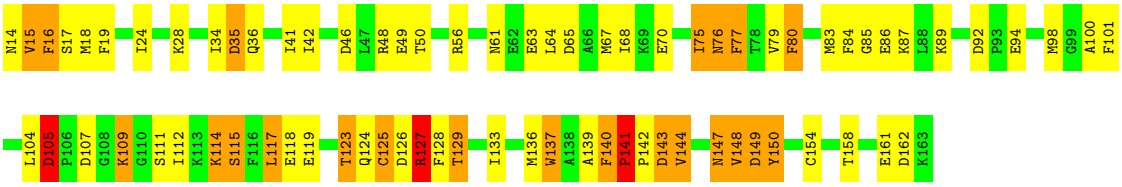
• Molecule 1: MYOSIN REGULATORY LIGHT CHAIN 2, SKELETAL MUSCLE ISOFORM

Chain 11-B:



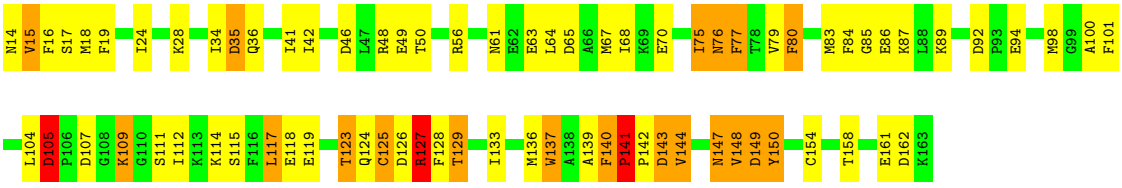
• Molecule 1: MYOSIN REGULATORY LIGHT CHAIN 2, SKELETAL MUSCLE ISOFORM

Chain 12-B:



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

Chain 13-B:

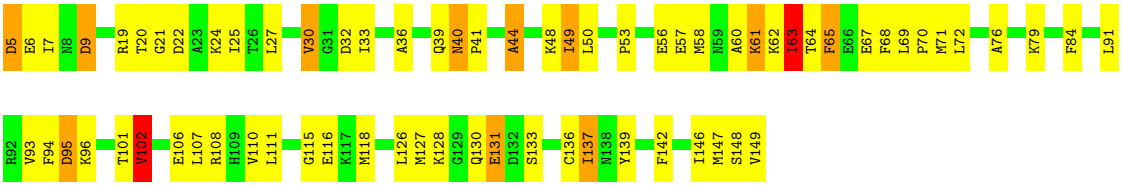


• Molecule 1: MYOSIN REGULATORY LIGHT CHAIN 2, SKELETAL MUSCLE ISOFORM

Chain 14-B:

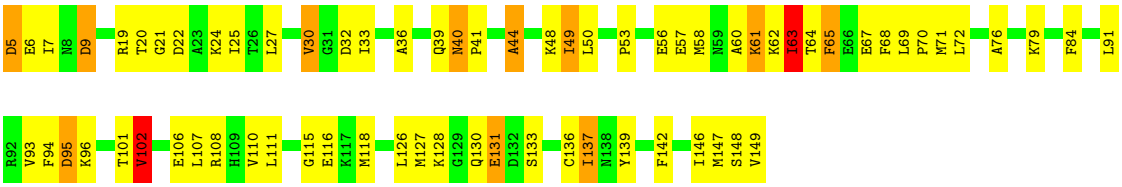
• Molecule 2: MYOSIN LIGHT CHAIN 3, SKELETAL MUSCLE ISOFORM

Chain 1-C:



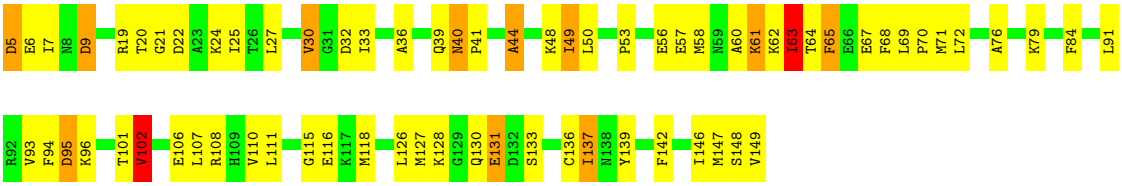
• Molecule 2: MYOSIN LIGHT CHAIN 3, SKELETAL MUSCLE ISOFORM

Chain 2-C:



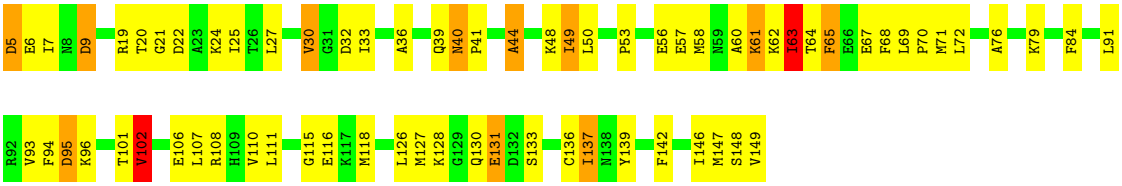
• Molecule 2: MYOSIN LIGHT CHAIN 3, SKELETAL MUSCLE ISOFORM

Chain 3-C:



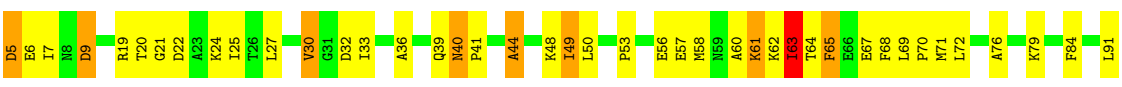
• Molecule 2: MYOSIN LIGHT CHAIN 3, SKELETAL MUSCLE ISOFORM

Chain 4-C:



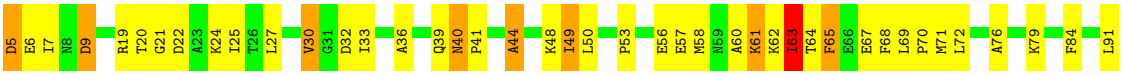
• Molecule 2: MYOSIN LIGHT CHAIN 3, SKELETAL MUSCLE ISOFORM

Chain 5-C:



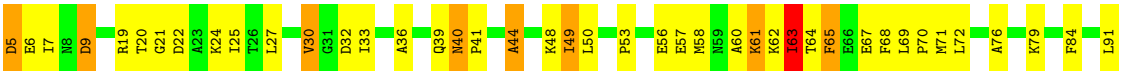
• Molecule 2: MYOSIN LIGHT CHAIN 3, SKELETAL MUSCLE ISOFORM

Chain 6-C:



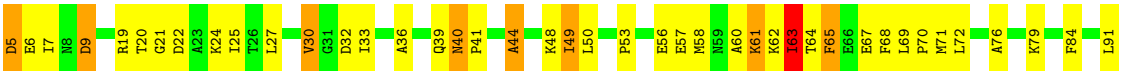
• Molecule 2: MYOSIN LIGHT CHAIN 3, SKELETAL MUSCLE ISOFORM

Chain 7-C:



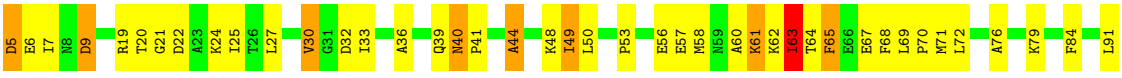
• Molecule 2: MYOSIN LIGHT CHAIN 3, SKELETAL MUSCLE ISOFORM

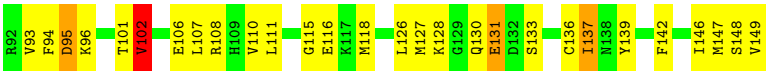
Chain 8-C:



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

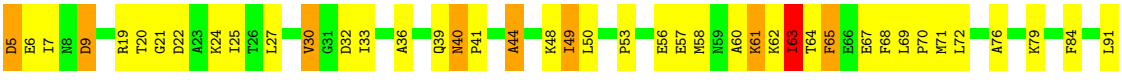
Chain 9-C:





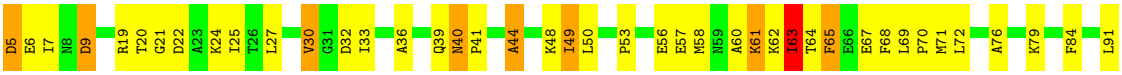
• Molecule 2: MYOSIN LIGHT CHAIN 3, SKELETAL MUSCLE ISOFORM

Chain 10-C:



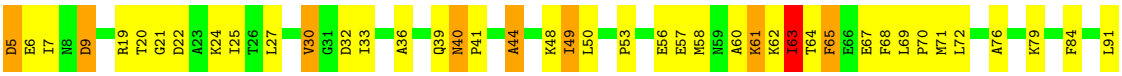
• Molecule 2: MYOSIN LIGHT CHAIN 3, SKELETAL MUSCLE ISOFORM

Chain 11-C:



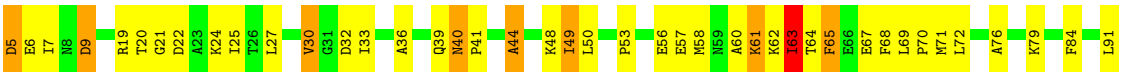
• Molecule 2: MYOSIN LIGHT CHAIN 3, SKELETAL MUSCLE ISOFORM

Chain 12-C:



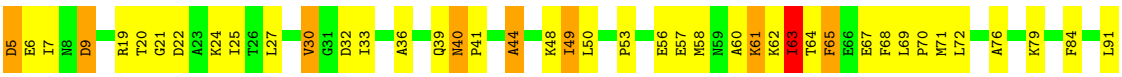
• Molecule 2: MYOSIN LIGHT CHAIN 3, SKELETAL MUSCLE ISOFORM

Chain 13-C:



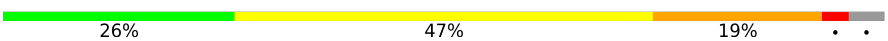
• Molecule 2: MYOSIN LIGHT CHAIN 3, SKELETAL MUSCLE ISOFORM

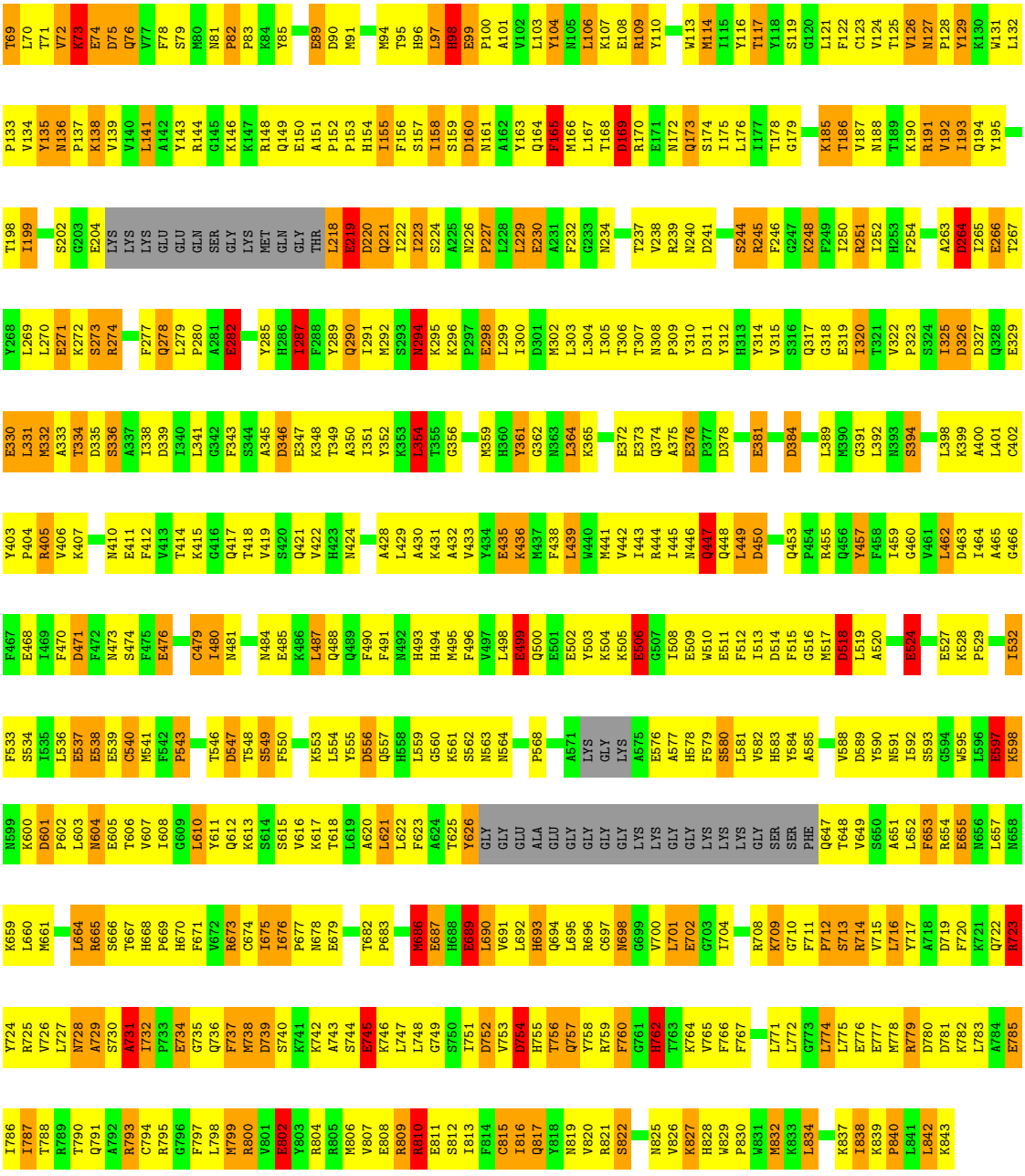
Chain 14-C:



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

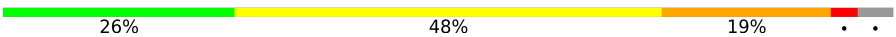
Chain 1-M:

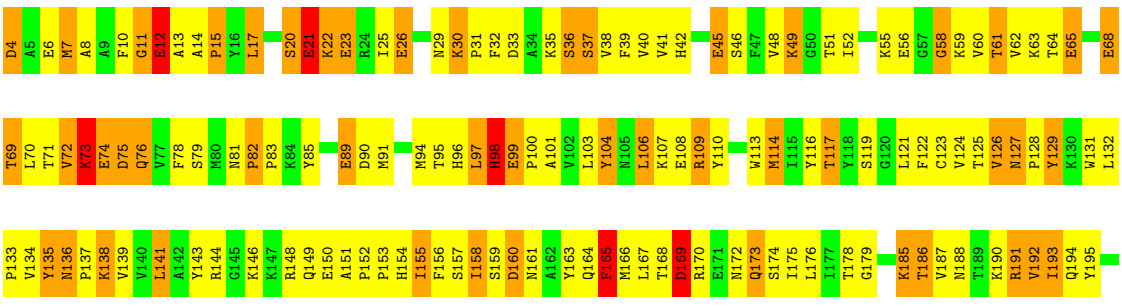


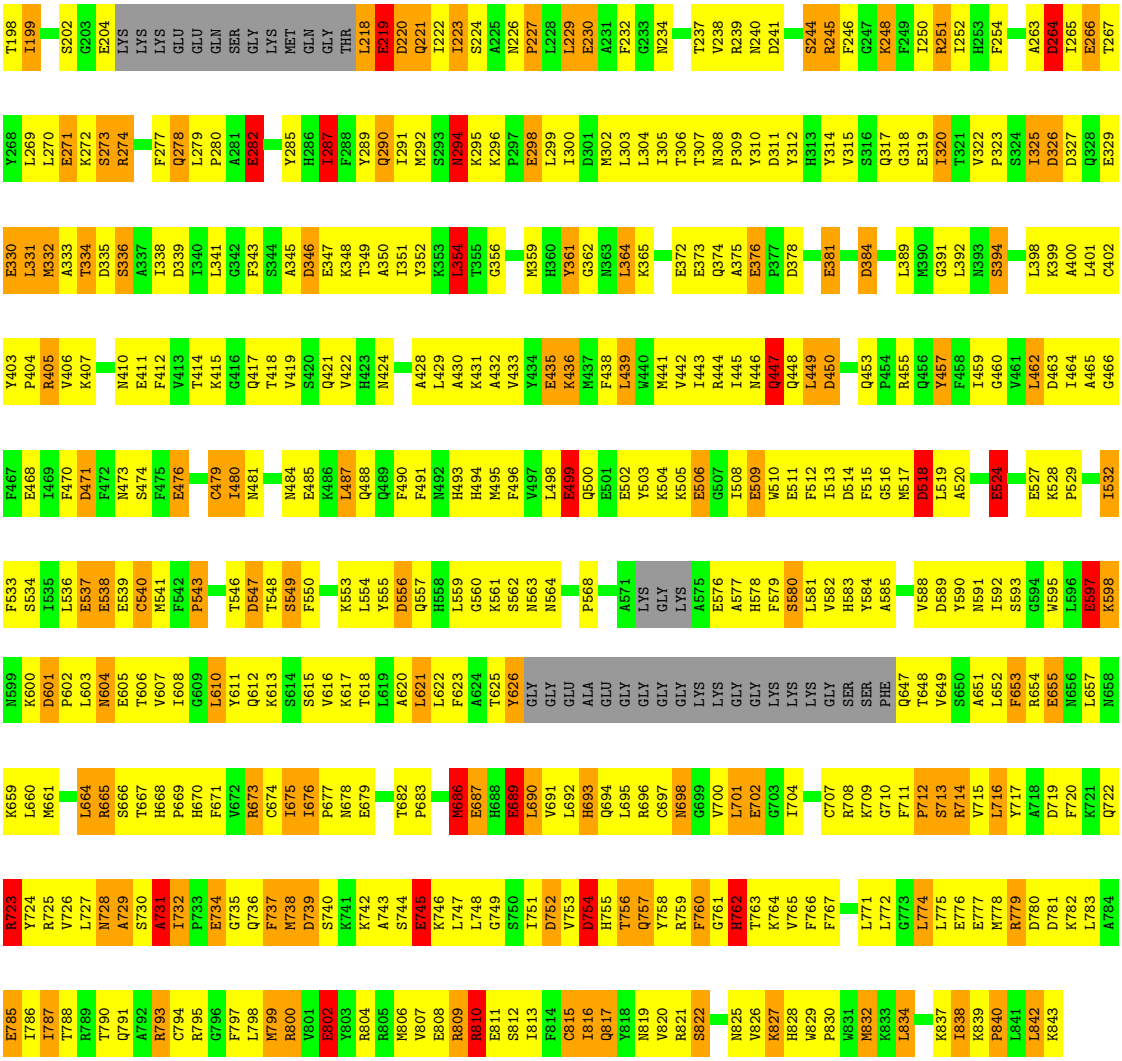


• Molecule 3: MYOSIN HEAVY CHAIN, SKELETAL MUSCLE, ADULT

Chain 2-M:

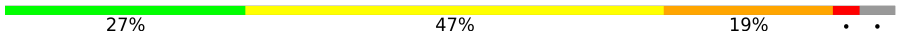


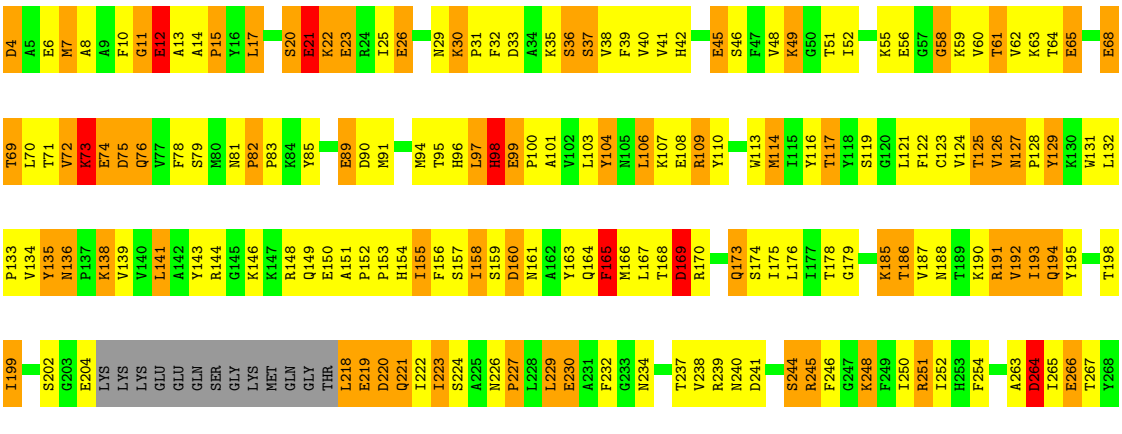


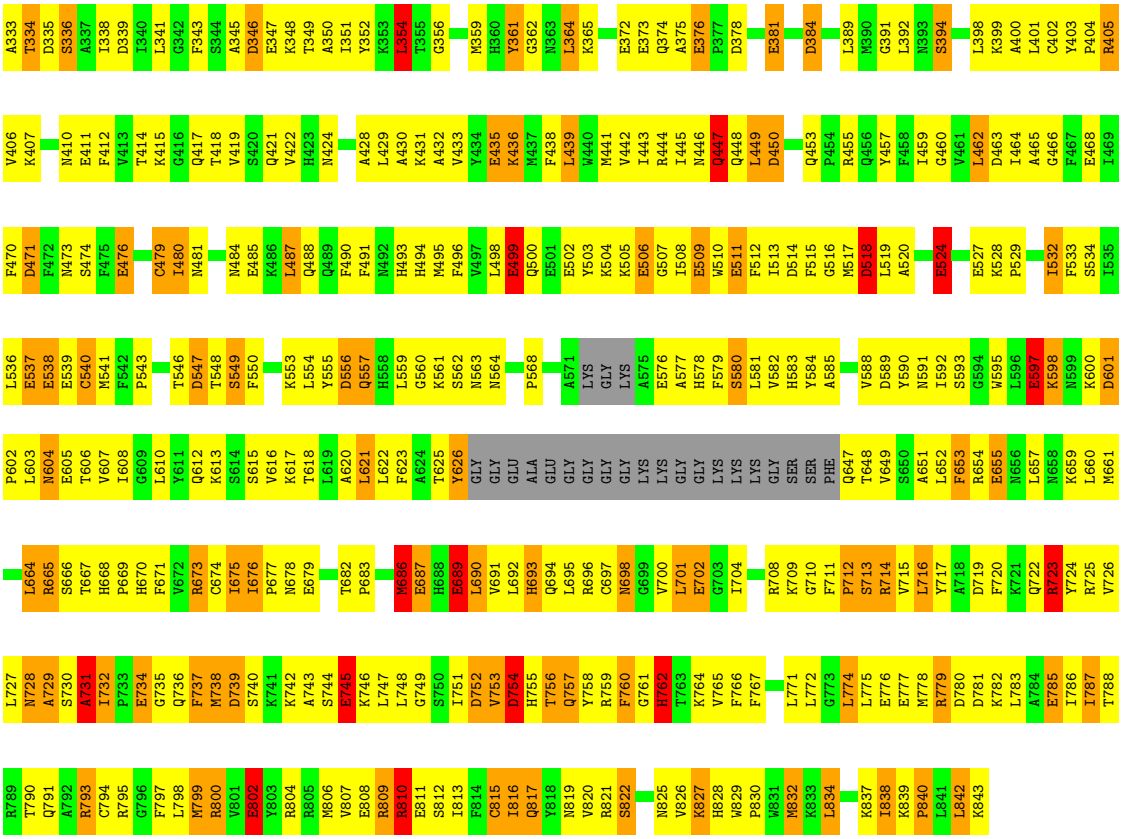


• Molecule 3: MYOSIN HEAVY CHAIN, SKELETAL MUSCLE, ADULT

Chain 3-M:

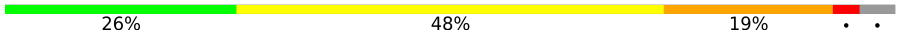


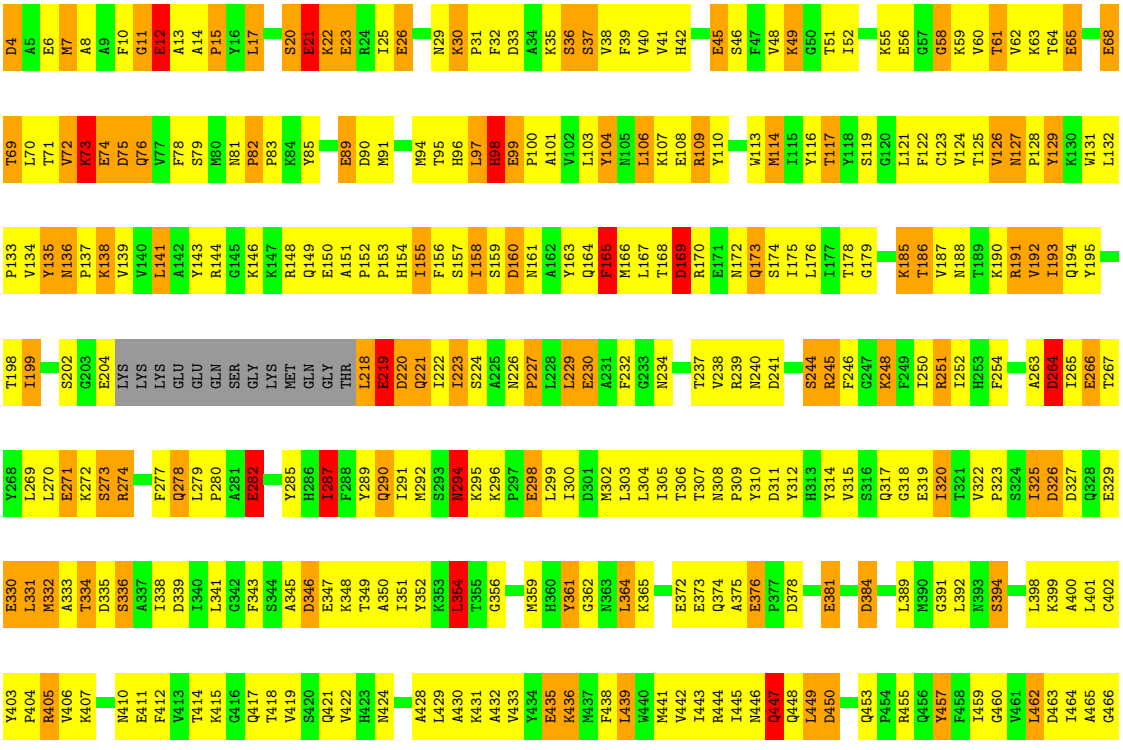


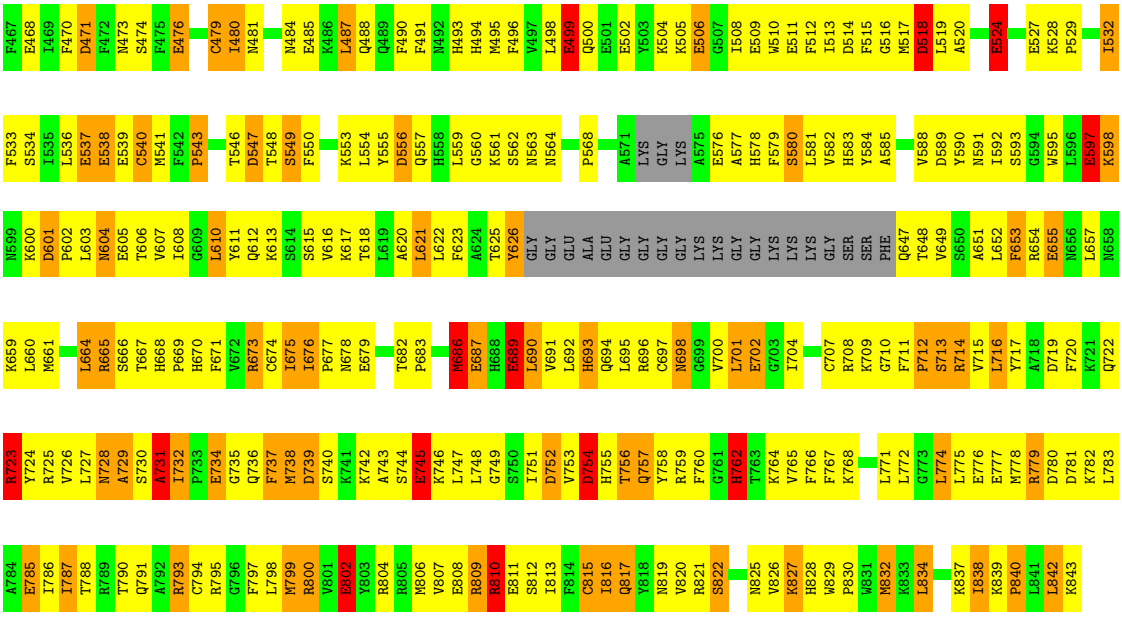


• Molecule 3: MYOSIN HEAVY CHAIN, SKELETAL MUSCLE, ADULT

Chain 4-M:

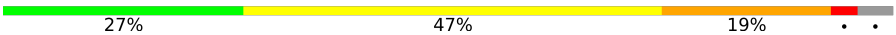


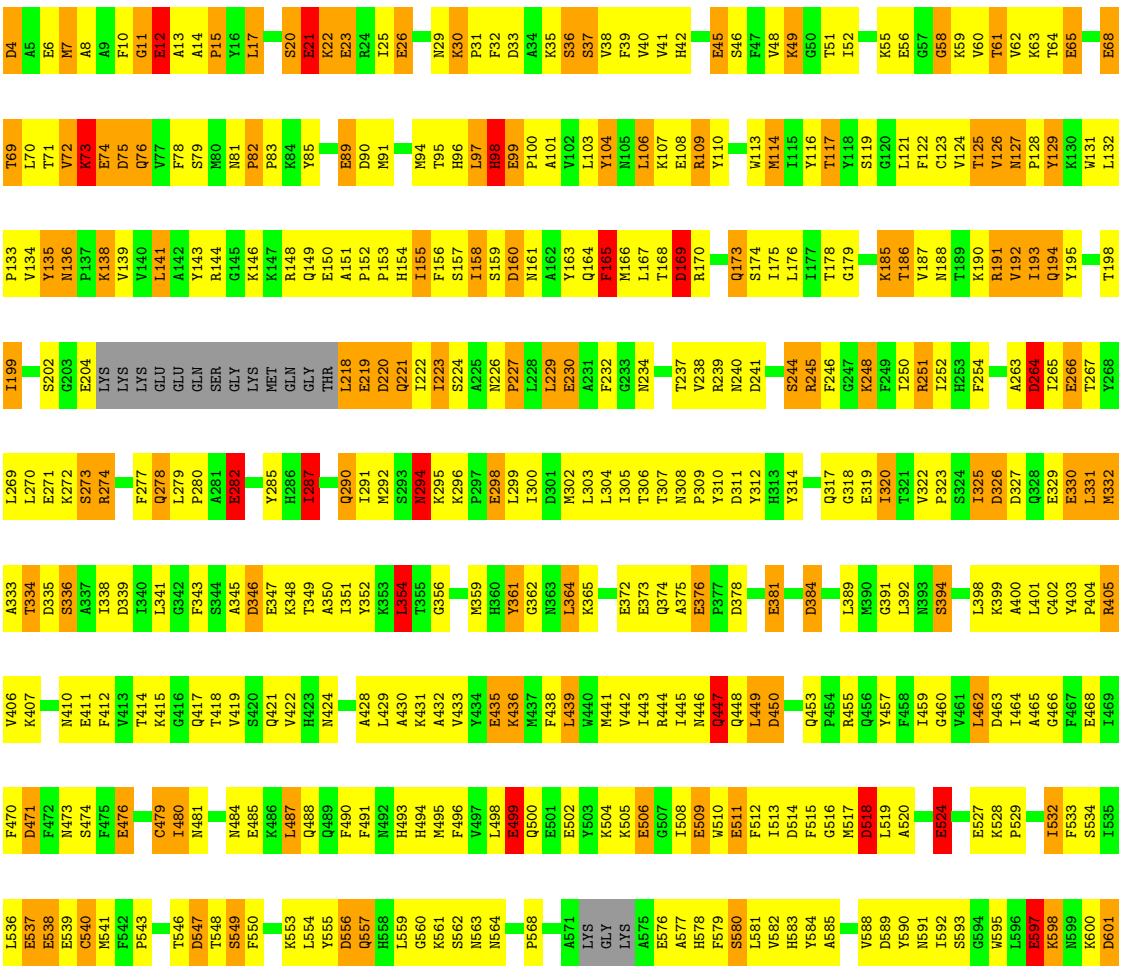


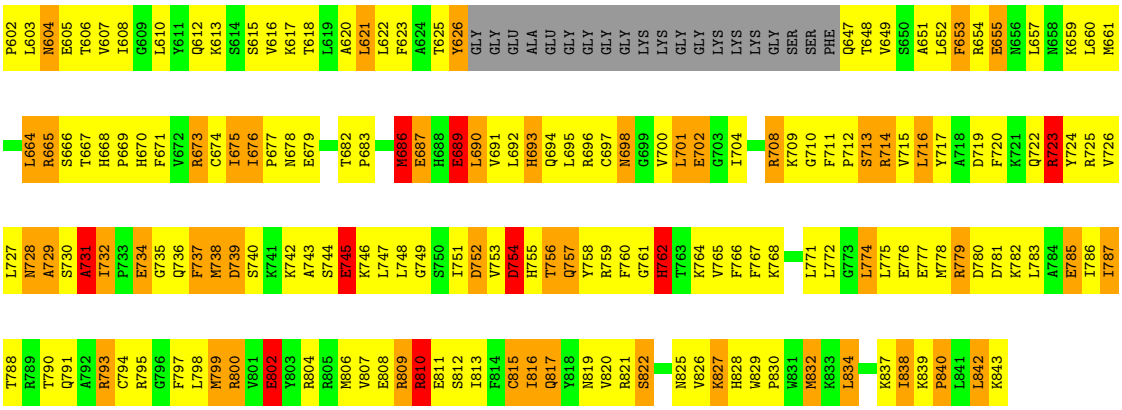


• Molecule 3: MYOSIN HEAVY CHAIN, SKELETAL MUSCLE, ADULT

Chain 5-M:

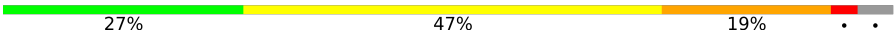


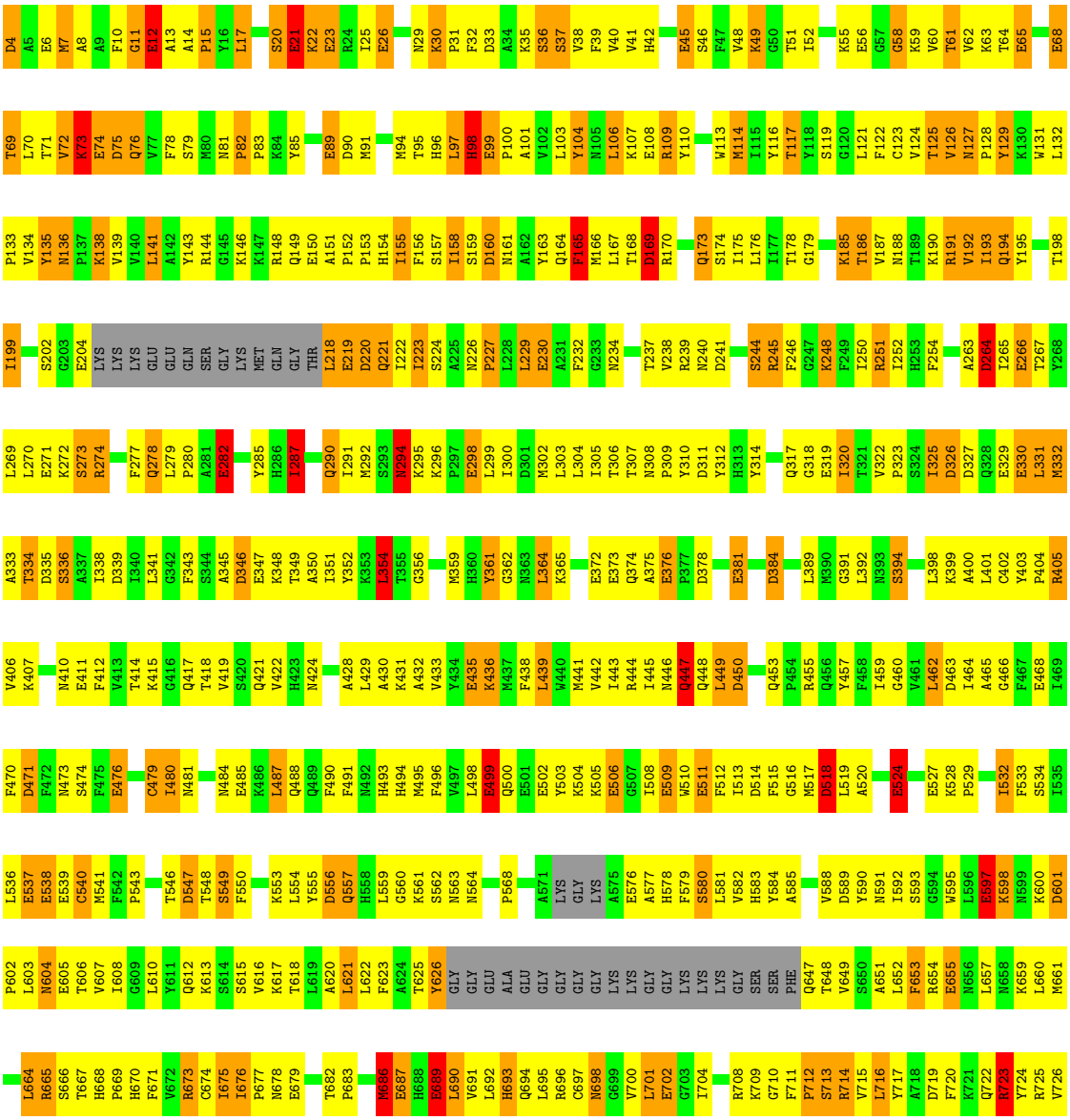


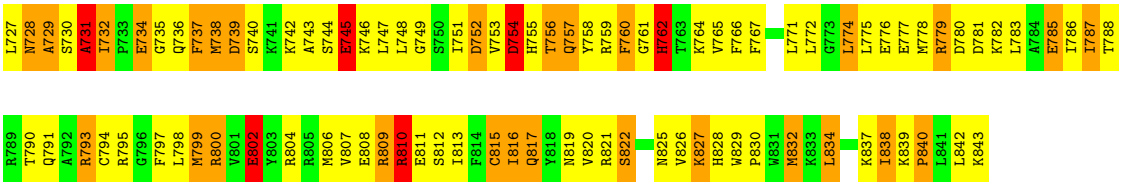


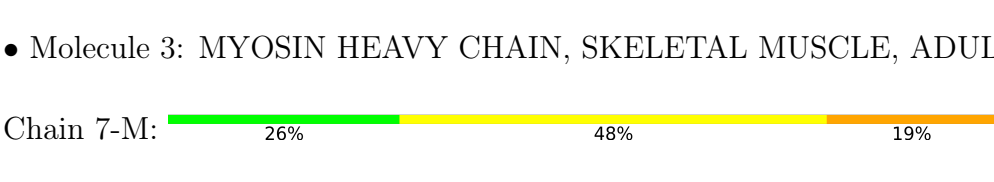
• Molecule 3: MYOSIN HEAVY CHAIN, SKELETAL MUSCLE, ADULT

Chain 6-M:



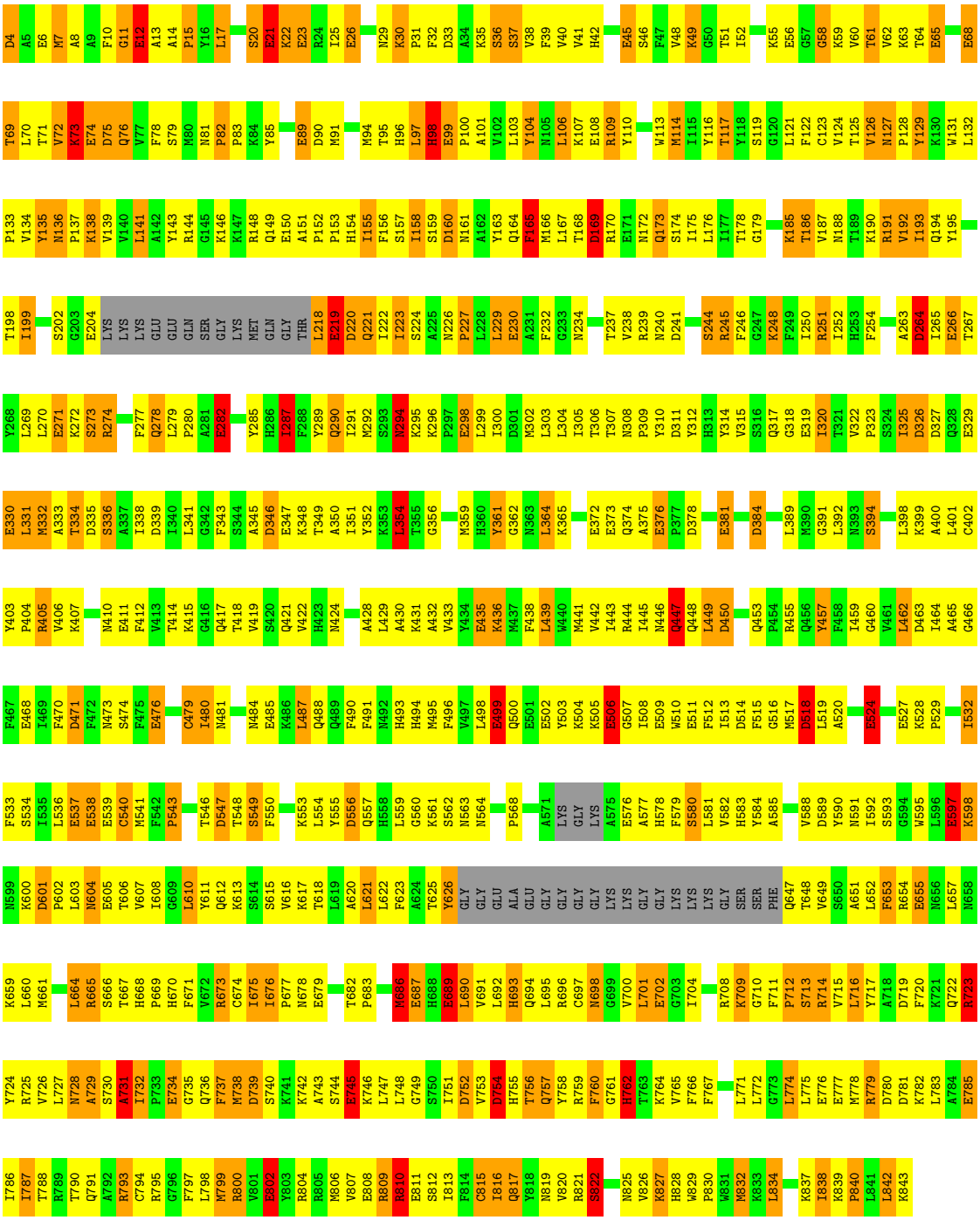






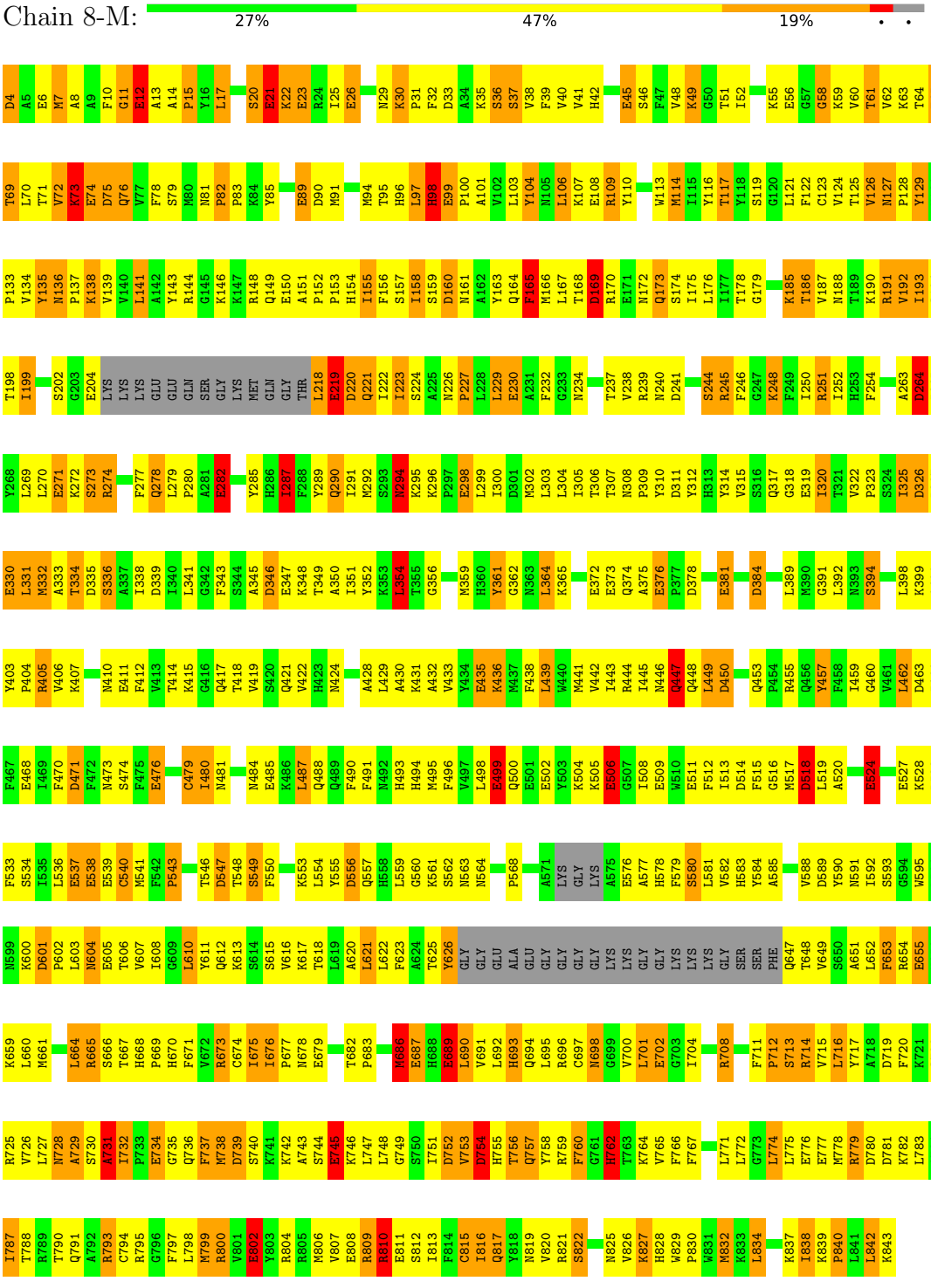
• Molecule 3: MYOSIN HEAVY CHAIN, SKELETAL MUSCLE, ADULT

Chain 7-M:



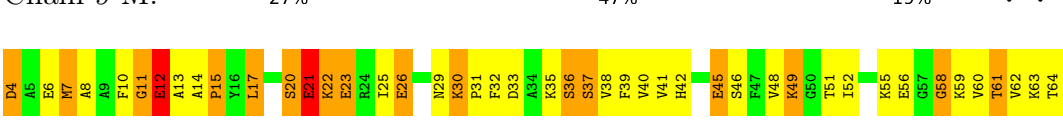
• Molecule 3: MYOSIN HEAVY CHAIN, SKELETAL MUSCLE, ADULT

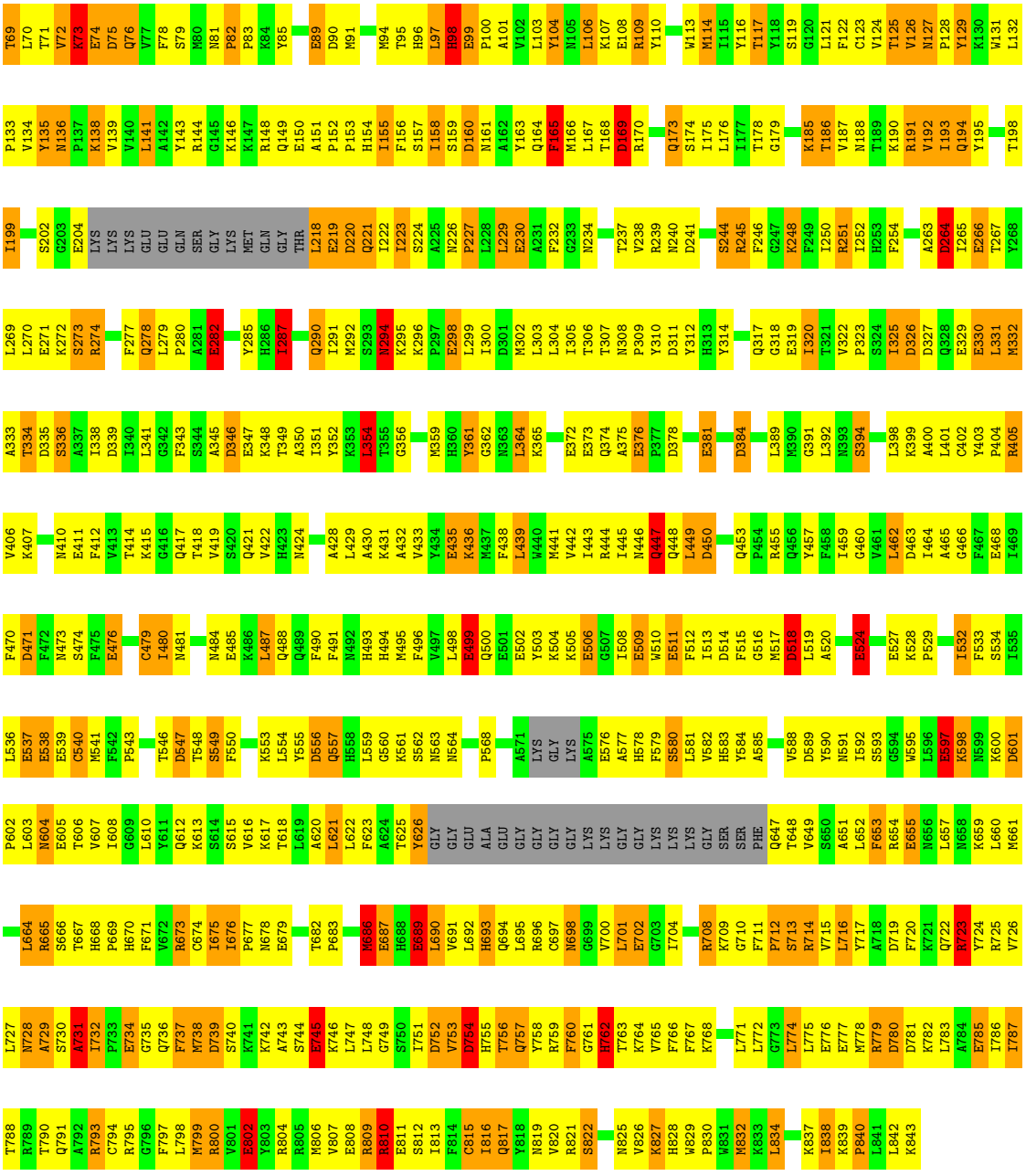
Chain 8-M:



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

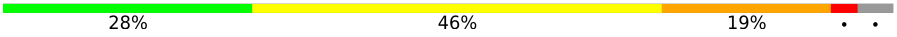
Chain 9-M:

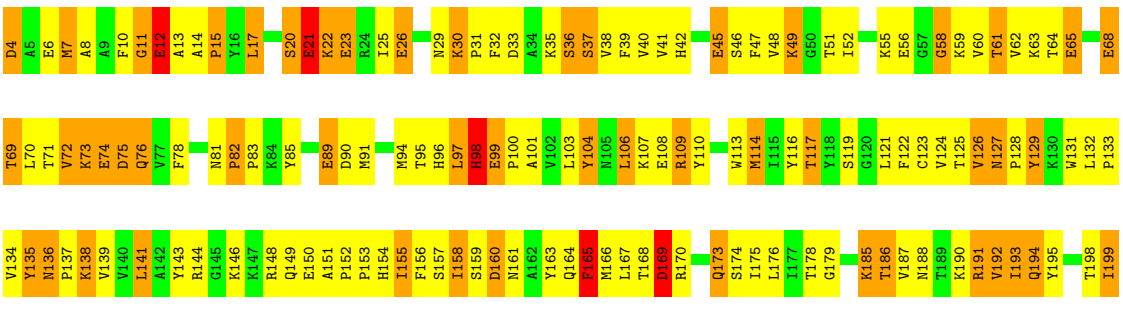


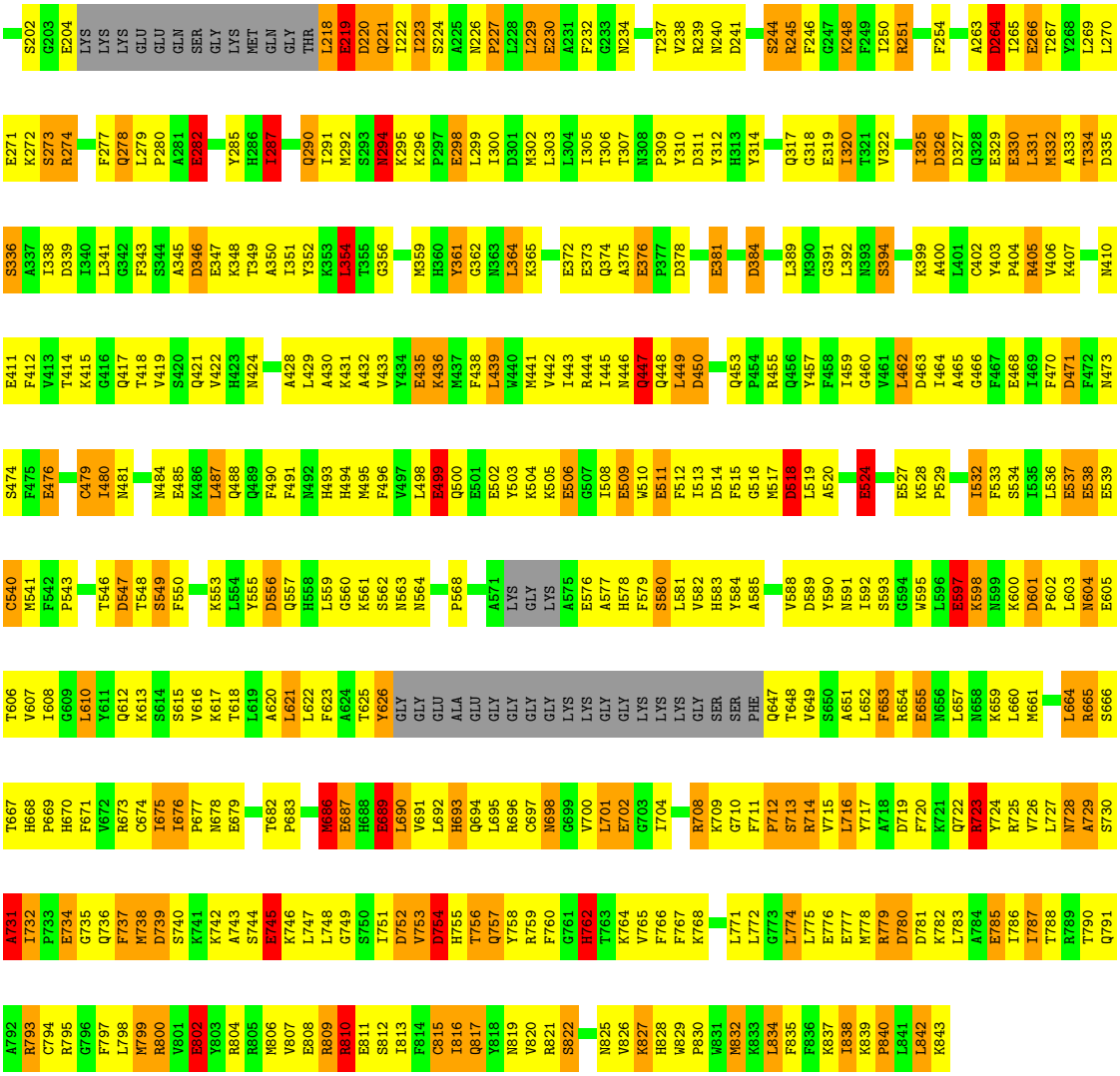


• Molecule 3: MYOSIN HEAVY CHAIN, SKELETAL MUSCLE, ADULT

Chain 10-M:

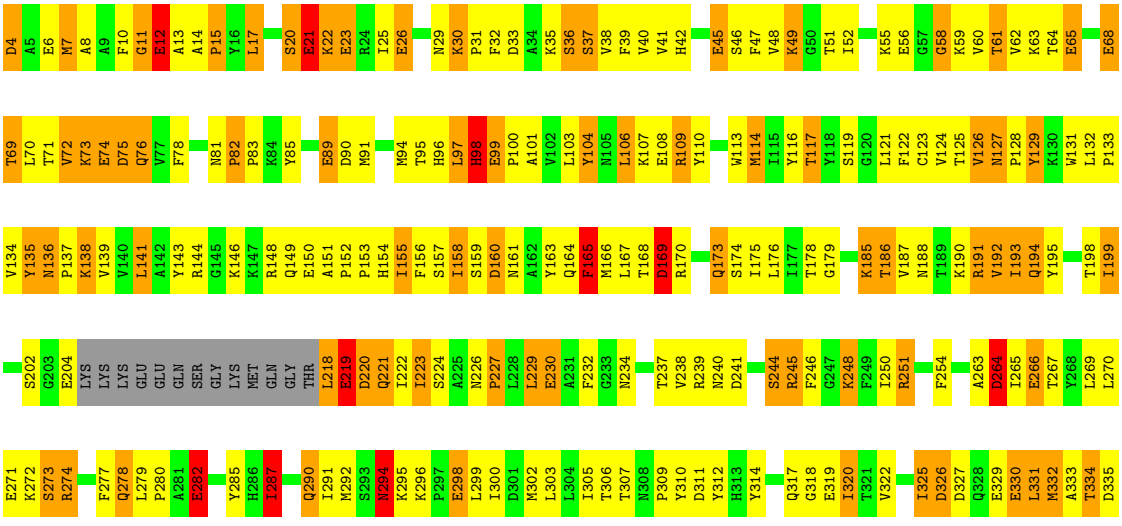


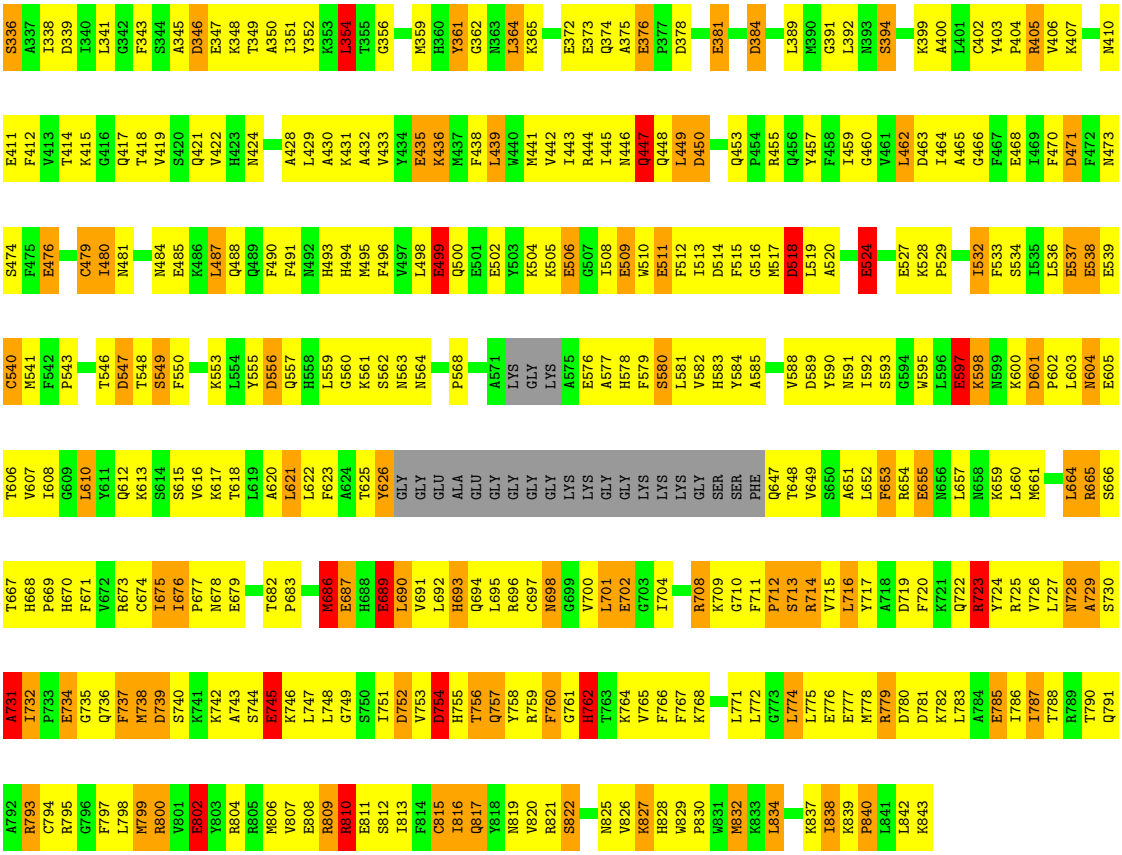




• Molecule 3: MYOSIN HEAVY CHAIN, SKELETAL MUSCLE, ADULT

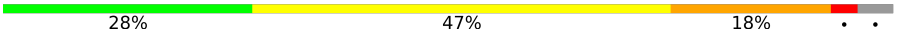
Chain 11-M:

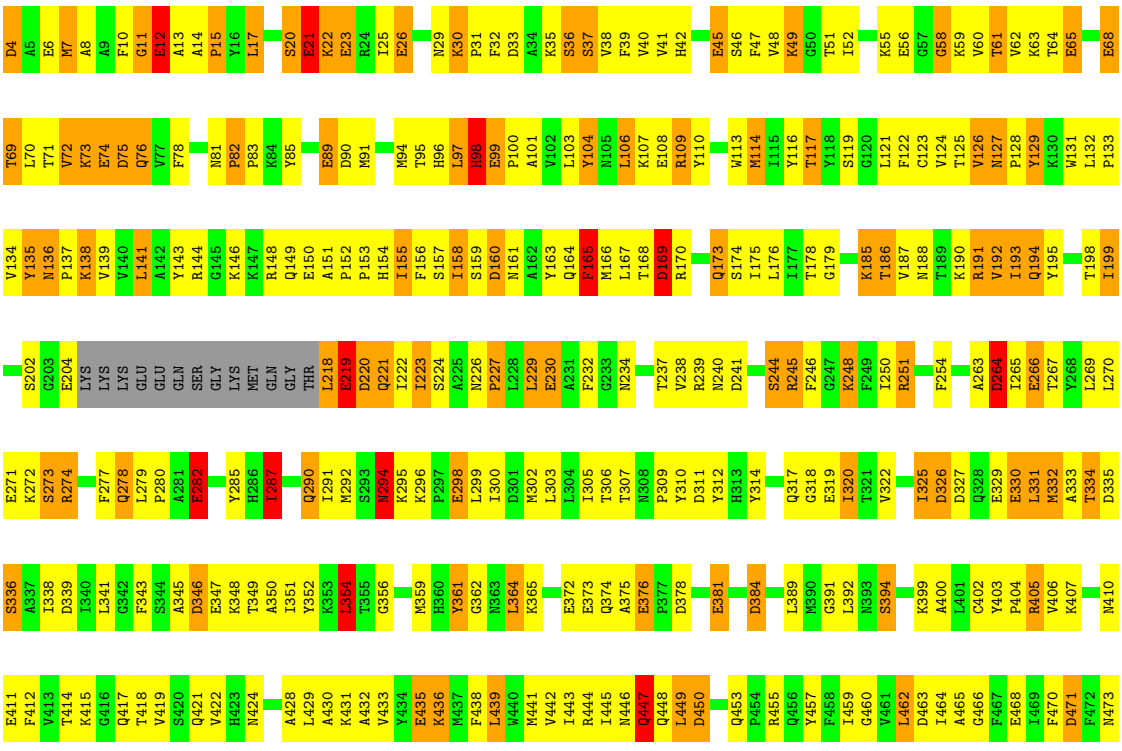


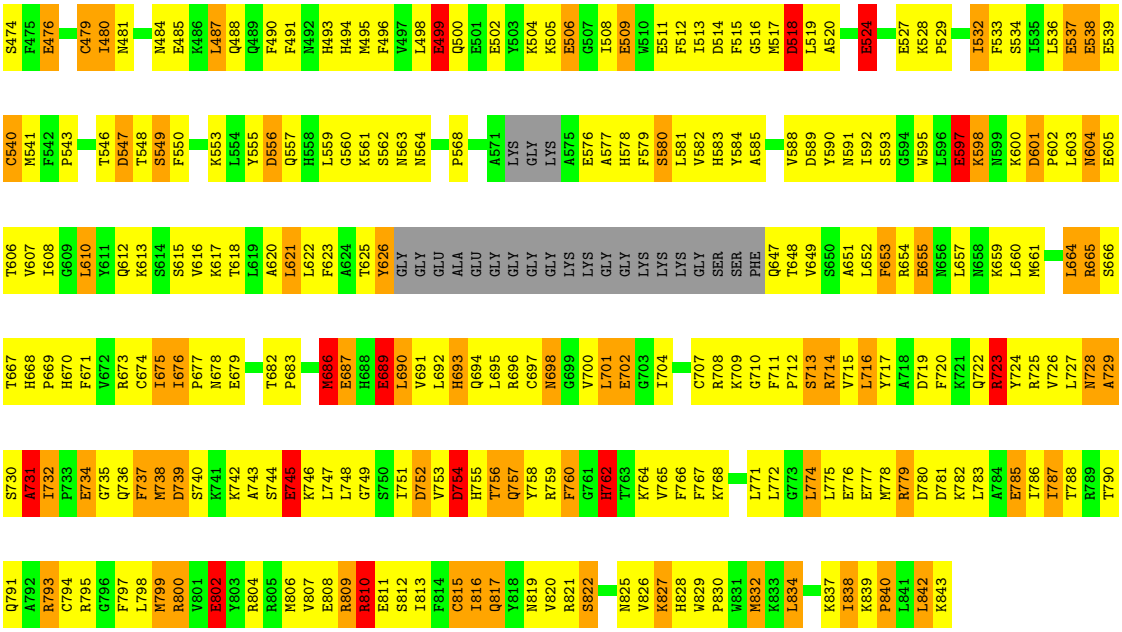


• Molecule 3: MYOSIN HEAVY CHAIN, SKELETAL MUSCLE, ADULT

Chain 12-M:

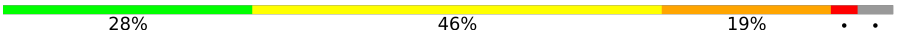


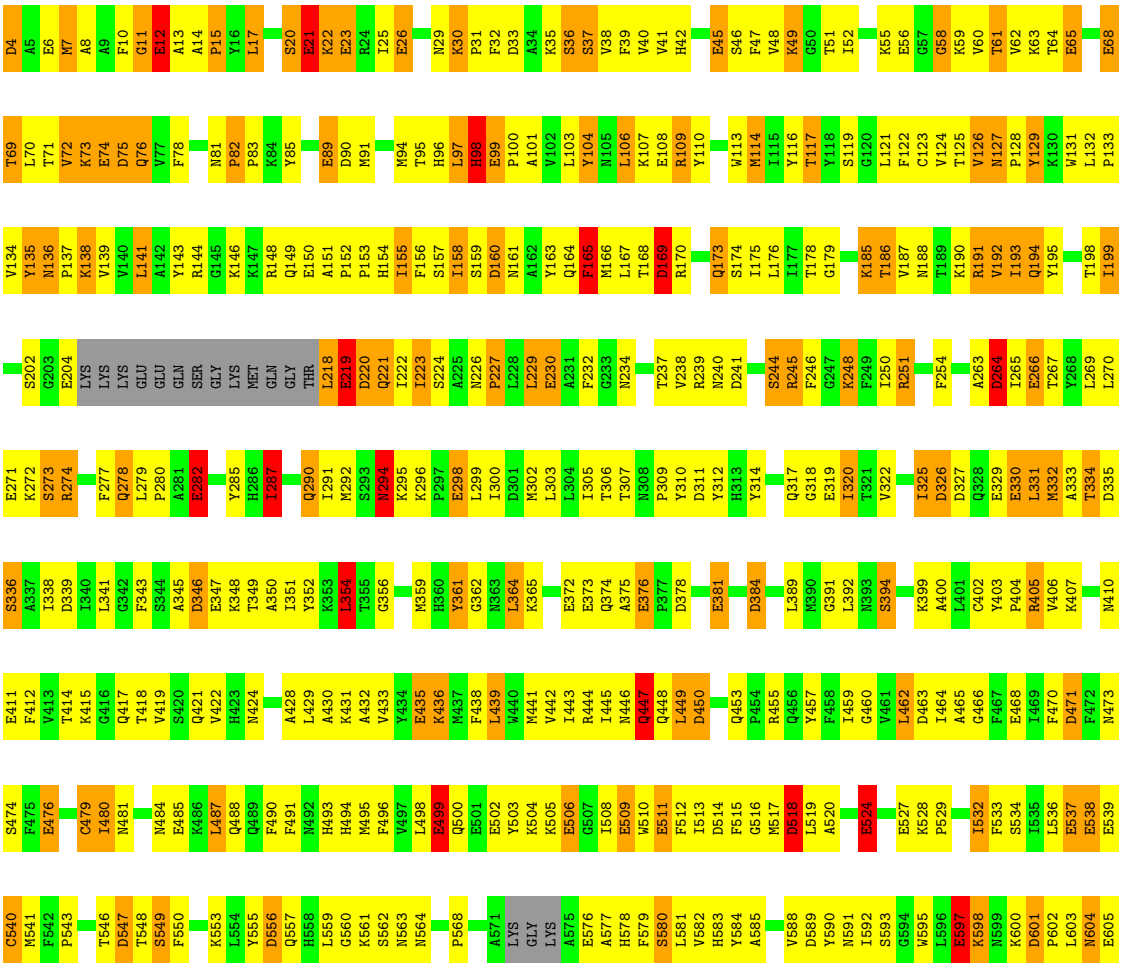


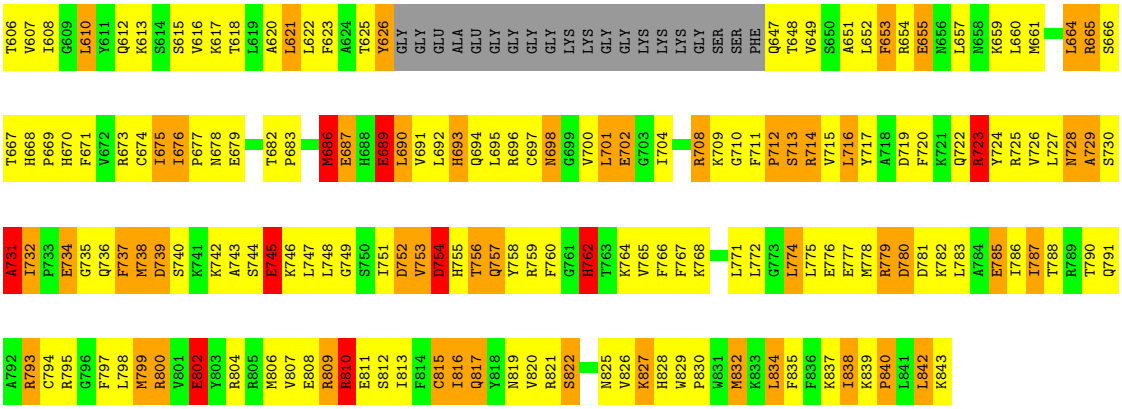


• Molecule 3: MYOSIN HEAVY CHAIN, SKELETAL MUSCLE, ADULT

Chain 13-M:

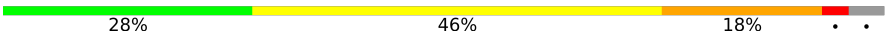


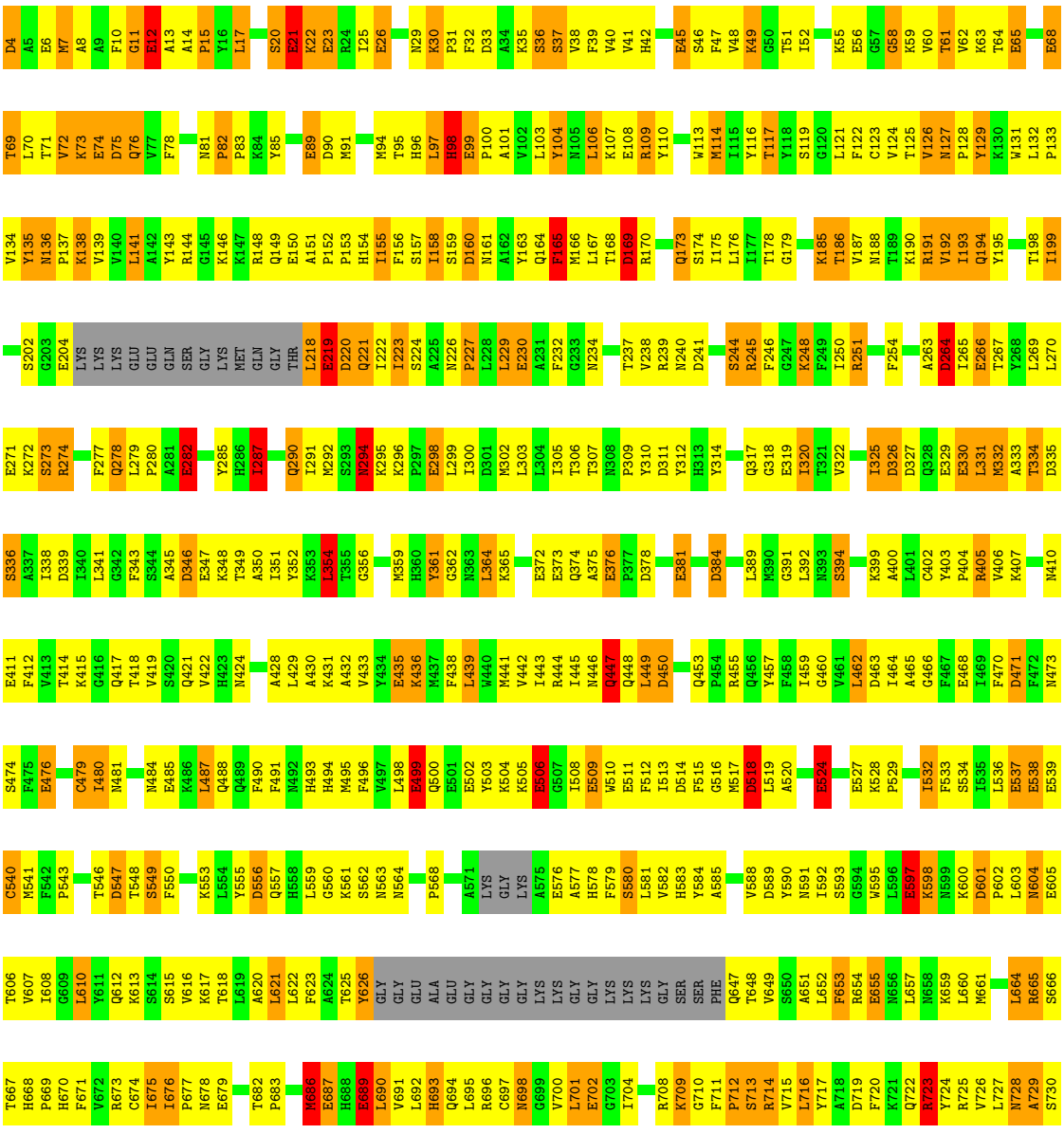


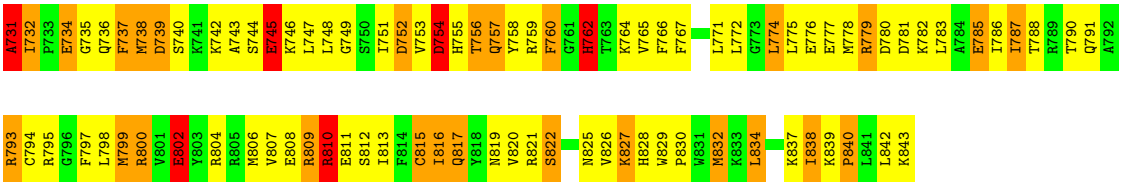


• Molecule 3: MYOSIN HEAVY CHAIN, SKELETAL MUSCLE, ADULT

Chain 14-M:






A731 I732 P733 E734 G735 Q736 F737 M738 D739 S740 K741 K742 A743 S744 E745 K746 L747 L748 G749 S750 I751 D752 V753 D754 H755 T756 Q757 Y758 R759 F760 G761 H762 T763 K764 V765 F766 F767 L771 L772 G773 L774 L775 E776 E777 M778 R779 D780 D781 K782 L783 A784 E785 I786 I787 T788 R789 T790 Q791 A792
R793 C794 R795 G796 F797 L798 M799 R800 V801 E802 Y803 R804 R805 M806 V807 E808 R809 R810 E811 S812 I813 F814 C815 I816 Q817 Y818 N819 V820 R821 S822 N825 V826 K827 H828 W829 P830 W831 M832 K833 L834 K837 I838 K839 P840 L841 L842 K843

4 Experimental information (i)

Property	Value	Source
EM 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	
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	FEI/PHILIPS CM300FEG/T	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	Not provided	
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	TVIPS TEMCAM-F224 (2k x 2k)	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	1-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	3-B	0.70	0/1199	1.67	17/1617 (1.1%)
1	4-B	0.70	0/1199	1.67	18/1617 (1.1%)
1	5-B	0.70	0/1199	1.67	17/1617 (1.1%)
1	6-B	0.69	0/1199	1.67	17/1617 (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	0.69	0/1199	1.67	17/1617 (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	0.70	0/1199	1.67	18/1617 (1.1%)
2	1-C	0.74	1/1140 (0.1%)	1.58	9/1530 (0.6%)
2	2-C	0.74	1/1140 (0.1%)	1.58	9/1530 (0.6%)
2	3-C	0.74	1/1140 (0.1%)	1.59	9/1530 (0.6%)
2	4-C	0.74	1/1140 (0.1%)	1.58	9/1530 (0.6%)
2	5-C	0.74	1/1140 (0.1%)	1.59	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%)	1.58	9/1530 (0.6%)
2	8-C	0.74	1/1140 (0.1%)	1.58	9/1530 (0.6%)
2	9-C	0.74	1/1140 (0.1%)	1.59	9/1530 (0.6%)
2	10-C	0.74	1/1140 (0.1%)	1.59	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%)	1.58	9/1530 (0.6%)
2	13-C	0.74	1/1140 (0.1%)	1.59	9/1530 (0.6%)
2	14-C	0.74	1/1140 (0.1%)	1.59	9/1530 (0.6%)
3	1-M	1.33	61/6594 (0.9%)	1.54	96/8884 (1.1%)
3	2-M	1.28	60/6593 (0.9%)	1.54	95/8881 (1.1%)
3	3-M	1.28	59/6593 (0.9%)	1.53	95/8881 (1.1%)
3	4-M	1.28	60/6593 (0.9%)	1.54	95/8881 (1.1%)
3	5-M	1.28	59/6593 (0.9%)	1.53	95/8881 (1.1%)
3	6-M	1.28	59/6593 (0.9%)	1.53	95/8881 (1.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
3	7-M	1.32	61/6594 (0.9%)	1.54	96/8884 (1.1%)
3	8-M	1.28	60/6594 (0.9%)	1.54	95/8884 (1.1%)
3	9-M	1.28	59/6593 (0.9%)	1.53	95/8881 (1.1%)
3	10-M	1.28	59/6593 (0.9%)	1.53	94/8881 (1.1%)
3	11-M	1.28	59/6593 (0.9%)	1.53	95/8881 (1.1%)
3	12-M	1.28	59/6593 (0.9%)	1.53	94/8881 (1.1%)
3	13-M	1.28	59/6593 (0.9%)	1.53	94/8881 (1.1%)
3	14-M	1.34	60/6594 (0.9%)	1.54	95/8884 (1.1%)
All	All	1.17	848/125052 (0.7%)	1.56	1703/168404 (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	2-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
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
3	1-M	0	1
3	2-M	0	1
3	3-M	0	1
3	4-M	0	1
3	5-M	0	1
3	6-M	0	1
3	7-M	0	1
3	8-M	0	1
3	9-M	0	1
3	10-M	0	1
3	11-M	0	1
3	12-M	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	13-M	0	1
3	14-M	0	1
All	All	0	70

The worst 5 of 848 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	14-M	709	LYS	C-N	34.19	1.94	1.33
3	1-M	709	LYS	C-N	30.07	1.87	1.33
3	7-M	709	LYS	C-N	27.30	1.82	1.33
3	2-M	731	ALA	C-N	25.18	1.92	1.34
3	1-M	731	ALA	C-N	25.15	1.91	1.34

The worst 5 of 1703 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	2-M	731	ALA	O-C-N	-28.58	76.97	122.70
3	1-M	731	ALA	O-C-N	-28.58	76.98	122.70
3	7-M	731	ALA	O-C-N	-28.57	76.99	122.70
3	8-M	731	ALA	O-C-N	-28.57	76.99	122.70
3	4-M	731	ALA	O-C-N	-28.55	77.02	122.70

There are no chirality outliers.

5 of 70 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 (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1-B	1177	0	1134	134	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2-B	1177	0	1134	134	0
1	3-B	1177	0	1134	134	0
1	4-B	1177	0	1134	132	0
1	5-B	1177	0	1134	135	0
1	6-B	1177	0	1134	132	0
1	7-B	1177	0	1134	139	0
1	8-B	1177	0	1134	138	0
1	9-B	1177	0	1134	135	0
1	10-B	1177	0	1134	133	0
1	11-B	1177	0	1134	134	0
1	12-B	1177	0	1134	136	0
1	13-B	1177	0	1134	133	0
1	14-B	1177	0	1134	135	0
2	1-C	1126	0	1084	88	0
2	2-C	1126	0	1084	90	0
2	3-C	1126	0	1084	87	0
2	4-C	1126	0	1084	88	0
2	5-C	1126	0	1084	89	0
2	6-C	1126	0	1084	86	0
2	7-C	1126	0	1084	89	0
2	8-C	1126	0	1084	89	0
2	9-C	1126	0	1084	87	0
2	10-C	1126	0	1084	90	0
2	11-C	1126	0	1084	91	0
2	12-C	1126	0	1084	90	0
2	13-C	1126	0	1084	90	0
2	14-C	1126	0	1084	88	0
3	1-M	6455	0	6383	855	0
3	2-M	6455	0	6377	836	0
3	3-M	6455	0	6379	877	0
3	4-M	6455	0	6383	832	0
3	5-M	6455	0	6383	887	0
3	6-M	6455	0	6382	891	0
3	7-M	6455	0	6383	849	0
3	8-M	6455	0	6384	815	0
3	9-M	6455	0	6382	863	0
3	10-M	6455	0	6383	832	0
3	11-M	6455	0	6381	835	0
3	12-M	6455	0	6381	818	0
3	13-M	6455	0	6383	832	0
3	14-M	6455	0	6383	838	0
All	All	122612	0	120399	13304	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 55.

The worst 5 of 13304 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:M:510:TRP:CE3	3:M:766:PHE:HB3	1.18	1.70
3:M:510:TRP:CH2	3:M:711:PHE:CE2	1.76	1.68
3:M:510:TRP:CZ3	3:M:766:PHE:CB	1.79	1.64
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%)	119 (80%)	17 (12%)	12 (8%)	1	12
1	2-B	148/150 (99%)	119 (80%)	17 (12%)	12 (8%)	1	12
1	3-B	148/150 (99%)	119 (80%)	17 (12%)	12 (8%)	1	12
1	4-B	148/150 (99%)	119 (80%)	17 (12%)	12 (8%)	1	12
1	5-B	148/150 (99%)	120 (81%)	16 (11%)	12 (8%)	1	12
1	6-B	148/150 (99%)	119 (80%)	17 (12%)	12 (8%)	1	12
1	7-B	148/150 (99%)	119 (80%)	17 (12%)	12 (8%)	1	12
1	8-B	148/150 (99%)	119 (80%)	17 (12%)	12 (8%)	1	12
1	9-B	148/150 (99%)	120 (81%)	16 (11%)	12 (8%)	1	12
1	10-B	148/150 (99%)	119 (80%)	17 (12%)	12 (8%)	1	12
1	11-B	148/150 (99%)	119 (80%)	17 (12%)	12 (8%)	1	12
1	12-B	148/150 (99%)	119 (80%)	17 (12%)	12 (8%)	1	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	13-B	148/150 (99%)	119 (80%)	17 (12%)	12 (8%)	1	12
1	14-B	148/150 (99%)	119 (80%)	17 (12%)	12 (8%)	1	12
2	1-C	143/145 (99%)	111 (78%)	20 (14%)	12 (8%)	1	12
2	2-C	143/145 (99%)	111 (78%)	20 (14%)	12 (8%)	1	12
2	3-C	143/145 (99%)	111 (78%)	20 (14%)	12 (8%)	1	12
2	4-C	143/145 (99%)	111 (78%)	20 (14%)	12 (8%)	1	12
2	5-C	143/145 (99%)	111 (78%)	20 (14%)	12 (8%)	1	12
2	6-C	143/145 (99%)	111 (78%)	20 (14%)	12 (8%)	1	12
2	7-C	143/145 (99%)	111 (78%)	20 (14%)	12 (8%)	1	12
2	8-C	143/145 (99%)	111 (78%)	20 (14%)	12 (8%)	1	12
2	9-C	143/145 (99%)	111 (78%)	20 (14%)	12 (8%)	1	12
2	10-C	143/145 (99%)	111 (78%)	20 (14%)	12 (8%)	1	12
2	11-C	143/145 (99%)	111 (78%)	20 (14%)	12 (8%)	1	12
2	12-C	143/145 (99%)	111 (78%)	20 (14%)	12 (8%)	1	12
2	13-C	143/145 (99%)	111 (78%)	20 (14%)	12 (8%)	1	12
2	14-C	143/145 (99%)	111 (78%)	20 (14%)	12 (8%)	1	12
3	1-M	788/840 (94%)	651 (83%)	114 (14%)	23 (3%)	4	29
3	2-M	786/840 (94%)	649 (83%)	114 (14%)	23 (3%)	4	29
3	3-M	786/840 (94%)	649 (83%)	115 (15%)	22 (3%)	5	30
3	4-M	786/840 (94%)	649 (83%)	114 (14%)	23 (3%)	4	29
3	5-M	786/840 (94%)	649 (83%)	115 (15%)	22 (3%)	5	30
3	6-M	786/840 (94%)	649 (83%)	115 (15%)	22 (3%)	5	30
3	7-M	788/840 (94%)	651 (83%)	113 (14%)	24 (3%)	4	28
3	8-M	788/840 (94%)	651 (83%)	114 (14%)	23 (3%)	4	29
3	9-M	786/840 (94%)	649 (83%)	115 (15%)	22 (3%)	5	30
3	10-M	786/840 (94%)	649 (83%)	115 (15%)	22 (3%)	5	30
3	11-M	786/840 (94%)	649 (83%)	115 (15%)	22 (3%)	5	30
3	12-M	786/840 (94%)	649 (83%)	115 (15%)	22 (3%)	5	30
3	13-M	786/840 (94%)	649 (83%)	115 (15%)	22 (3%)	5	30
3	14-M	788/840 (94%)	651 (83%)	115 (15%)	22 (3%)	5	30
All	All	15086/15890 (95%)	12316 (82%)	2120 (14%)	650 (4%)	5	22

5 of 650 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 (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1-B	128/130 (98%)	116 (91%)	12 (9%)	8	28
1	2-B	128/130 (98%)	116 (91%)	12 (9%)	8	28
1	3-B	128/130 (98%)	116 (91%)	12 (9%)	8	28
1	4-B	128/130 (98%)	116 (91%)	12 (9%)	8	28
1	5-B	128/130 (98%)	116 (91%)	12 (9%)	8	28
1	6-B	128/130 (98%)	116 (91%)	12 (9%)	8	28
1	7-B	128/130 (98%)	116 (91%)	12 (9%)	8	28
1	8-B	128/130 (98%)	116 (91%)	12 (9%)	8	28
1	9-B	128/130 (98%)	116 (91%)	12 (9%)	8	28
1	10-B	128/130 (98%)	116 (91%)	12 (9%)	8	28
1	11-B	128/130 (98%)	116 (91%)	12 (9%)	8	28
1	12-B	128/130 (98%)	116 (91%)	12 (9%)	8	28
1	13-B	128/130 (98%)	116 (91%)	12 (9%)	8	28
1	14-B	128/130 (98%)	116 (91%)	12 (9%)	8	28
2	1-C	120/122 (98%)	109 (91%)	11 (9%)	9	29
2	2-C	120/122 (98%)	109 (91%)	11 (9%)	9	29
2	3-C	120/122 (98%)	109 (91%)	11 (9%)	9	29
2	4-C	120/122 (98%)	109 (91%)	11 (9%)	9	29
2	5-C	120/122 (98%)	109 (91%)	11 (9%)	9	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	6-C	120/122 (98%)	109 (91%)	11 (9%)	9	29
2	7-C	120/122 (98%)	109 (91%)	11 (9%)	9	29
2	8-C	120/122 (98%)	109 (91%)	11 (9%)	9	29
2	9-C	120/122 (98%)	109 (91%)	11 (9%)	9	29
2	10-C	120/122 (98%)	109 (91%)	11 (9%)	9	29
2	11-C	120/122 (98%)	109 (91%)	11 (9%)	9	29
2	12-C	120/122 (98%)	109 (91%)	11 (9%)	9	29
2	13-C	120/122 (98%)	109 (91%)	11 (9%)	9	29
2	14-C	120/122 (98%)	109 (91%)	11 (9%)	9	29
3	1-M	693/724 (96%)	522 (75%)	171 (25%)	0	3
3	2-M	693/724 (96%)	522 (75%)	171 (25%)	0	3
3	3-M	693/724 (96%)	523 (76%)	170 (24%)	0	3
3	4-M	693/724 (96%)	522 (75%)	171 (25%)	0	3
3	5-M	693/724 (96%)	523 (76%)	170 (24%)	0	3
3	6-M	693/724 (96%)	523 (76%)	170 (24%)	0	3
3	7-M	693/724 (96%)	522 (75%)	171 (25%)	0	3
3	8-M	693/724 (96%)	522 (75%)	171 (25%)	0	3
3	9-M	693/724 (96%)	523 (76%)	170 (24%)	0	3
3	10-M	693/724 (96%)	523 (76%)	170 (24%)	0	3
3	11-M	693/724 (96%)	523 (76%)	170 (24%)	0	3
3	12-M	693/724 (96%)	523 (76%)	170 (24%)	0	3
3	13-M	693/724 (96%)	523 (76%)	170 (24%)	0	3
3	14-M	693/724 (96%)	523 (76%)	170 (24%)	0	3
All	All	13174/13664 (96%)	10467 (80%)	2707 (20%)	3	7

5 of 2707 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	10-M	439	LEU
3	12-M	714	ARG
3	10-M	716	LEU
3	10-M	410	ASN
3	11-M	615	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 405 such sidechains are listed below:

Mol	Chain	Res	Type
1	9-B	36	GLN
3	10-M	757	GLN
3	14-M	578	HIS
3	9-M	127	ASN
1	10-B	36	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	1-M	7
3	2-M	7
3	3-M	7
3	4-M	7
3	5-M	7

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Mol	Chain	Number of breaks
3	6-M	7
3	7-M	7
3	9-M	7
3	10-M	7
3	11-M	7
3	12-M	7
3	13-M	7
3	14-M	7
3	8-M	6

The worst 5 of 97 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	M	601:ASP	C	602:PRO	N	9.78
2	M	601:ASP	C	602:PRO	N	9.78
3	M	601:ASP	C	602:PRO	N	9.78
4	M	601:ASP	C	602:PRO	N	9.78
5	M	601:ASP	C	602:PRO	N	9.78

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-1584. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal surface views

This section was not generated.

6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.