wwPDB EM Validation Summary Report (i)

Nov 20, 2022 – 03:23 pm GMT

PDB ID	:	2W4V
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	:	2008-12-02
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:

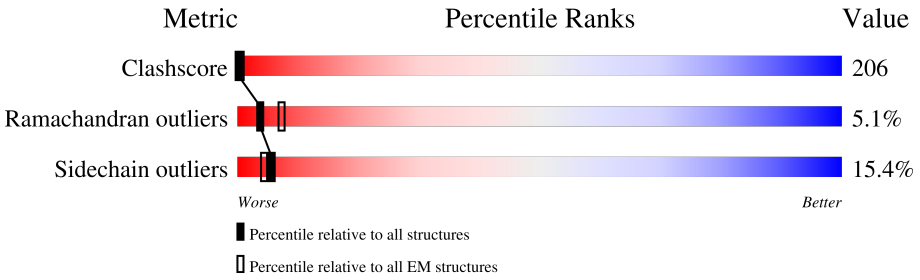
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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-C	831	13% 59% 18% • 7%
1	10-C	831	14% 59% 18% • 7%
1	11-C	831	14% 60% 17% • 7%
1	12-C	831	14% 60% 17% • 7%
1	13-C	831	13% 60% 18% • 7%
1	14-C	831	13% 59% 18% • 7%
1	15-C	831	13% 59% 18% • 7%
1	16-C	831	13% 59% 18% • 7%
1	17-C	831	13% 59% 18% • 7%

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Mol	Chain	Length	Quality of chain
1	18-C	831	13% 59% 18% • 7%
1	19-C	831	13% 59% 18% • 7%
1	2-C	831	14% 59% 18% • 7%
1	20-C	831	14% 59% 18% • 7%
1	21-C	831	12% 61% 18% • 7%
1	22-C	831	14% 59% 18% • 7%
1	23-C	831	14% 59% 18% • 7%
1	24-C	831	13% 59% 18% • 7%
1	25-C	831	13% 59% 18% • 7%
1	26-C	831	14% 59% 18% • 7%
1	27-C	831	13% 59% 18% • 7%
1	3-C	831	14% 60% 17% • 7%
1	4-C	831	13% 60% 18% • 7%
1	5-C	831	14% 59% 18% • 7%
1	6-C	831	13% 60% 18% • 7%
1	7-C	831	14% 59% 18% • 7%
1	8-C	831	13% 59% 18% • 7%
1	9-C	831	13% 59% 18% • 7%
2	1-Y	136	13% 65% 19% •
2	10-Y	136	13% 65% 20% •
2	11-Y	136	13% 65% 21% •
2	12-Y	136	13% 65% 21% •
2	13-Y	136	12% 67% 19% •
2	14-Y	136	12% 68% 18% •
2	15-Y	136	14% 65% 18% •

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Mol	Chain	Length	Quality of chain
2	16-Y	136	12% 68% 18%
2	17-Y	136	15% 65% 19%
2	18-Y	136	12% 68% 18%
2	19-Y	136	12% 67% 19%
2	2-Y	136	12% 67% 20%
2	20-Y	136	12% 67% 19%
2	21-Y	136	12% 68% 18%
2	22-Y	136	12% 66% 20%
2	23-Y	136	12% 67% 19%
2	24-Y	136	14% 66% 18%
2	25-Y	136	12% 68% 19%
2	26-Y	136	12% 67% 19%
2	27-Y	136	13% 66% 18%
2	3-Y	136	13% 65% 21%
2	4-Y	136	13% 65% 21%
2	5-Y	136	13% 65% 19%
2	6-Y	136	14% 65% 19%
2	7-Y	136	12% 67% 20%
2	8-Y	136	12% 68% 18%
2	9-Y	136	12% 67% 19%
3	1-Z	151	19% 62% 17%
3	10-Z	151	21% 61% 17%
3	11-Z	151	19% 62% 17%
3	12-Z	151	19% 62% 17%
3	13-Z	151	19% 63% 17%

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Mol	Chain	Length	Quality of chain
3	14-Z	151	19% 62% 17%
3	15-Z	151	19% 62% 17%
3	16-Z	151	19% 62% 17%
3	17-Z	151	19% 62% 17%
3	18-Z	151	19% 62% 17%
3	19-Z	151	19% 62% 17%
3	2-Z	151	19% 62% 17%
3	20-Z	151	19% 63% 17%
3	21-Z	151	17% 64% 17%
3	22-Z	151	19% 63% 17%
3	23-Z	151	19% 62% 17%
3	24-Z	151	19% 62% 17%
3	25-Z	151	19% 63% 17%
3	26-Z	151	19% 63% 17%
3	27-Z	151	19% 63% 17%
3	3-Z	151	19% 62% 17%
3	4-Z	151	18% 64% 17%
3	5-Z	151	19% 62% 17%
3	6-Z	151	19% 63% 17%
3	7-Z	151	19% 63% 17%
3	8-Z	151	19% 62% 17%
3	9-Z	151	19% 63% 17%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 229527 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 HEAVY CHAIN, STRIATED MUSCLE.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1-C	772	Total	C	N	O	S	0	0
			6215	3957	1067	1155	36		
1	2-C	772	Total	C	N	O	S	0	0
			6215	3957	1067	1155	36		
1	3-C	772	Total	C	N	O	S	0	0
			6215	3957	1067	1155	36		
1	4-C	772	Total	C	N	O	S	0	0
			6215	3957	1067	1155	36		
1	5-C	772	Total	C	N	O	S	0	0
			6215	3957	1067	1155	36		
1	6-C	772	Total	C	N	O	S	0	0
			6215	3957	1067	1155	36		
1	7-C	772	Total	C	N	O	S	0	0
			6215	3957	1067	1155	36		
1	8-C	772	Total	C	N	O	S	0	0
			6215	3957	1067	1155	36		
1	9-C	772	Total	C	N	O	S	0	0
			6215	3957	1067	1155	36		
1	10-C	772	Total	C	N	O	S	0	0
			6215	3957	1067	1155	36		
1	11-C	772	Total	C	N	O	S	0	0
			6215	3957	1067	1155	36		
1	12-C	772	Total	C	N	O	S	0	0
			6215	3957	1067	1155	36		
1	13-C	772	Total	C	N	O	S	0	0
			6215	3957	1067	1155	36		
1	14-C	772	Total	C	N	O	S	0	0
			6215	3957	1067	1155	36		
1	15-C	772	Total	C	N	O	S	0	0
			6215	3957	1067	1155	36		
1	16-C	772	Total	C	N	O	S	0	0
			6215	3957	1067	1155	36		
1	17-C	772	Total	C	N	O	S	0	0
			6215	3957	1067	1155	36		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	18-C	772	Total	C	N	O	S	0	0
			6215	3957	1067	1155	36		
1	19-C	772	Total	C	N	O	S	0	0
			6215	3957	1067	1155	36		
1	20-C	772	Total	C	N	O	S	0	0
			6215	3957	1067	1155	36		
1	21-C	772	Total	C	N	O	S	0	0
			6215	3957	1067	1155	36		
1	22-C	772	Total	C	N	O	S	0	0
			6215	3957	1067	1155	36		
1	23-C	772	Total	C	N	O	S	0	0
			6215	3957	1067	1155	36		
1	24-C	772	Total	C	N	O	S	0	0
			6215	3957	1067	1155	36		
1	25-C	772	Total	C	N	O	S	0	0
			6215	3957	1067	1155	36		
1	26-C	772	Total	C	N	O	S	0	0
			6215	3957	1067	1155	36		
1	27-C	772	Total	C	N	O	S	0	0
			6215	3957	1067	1155	36		

- Molecule 2 is a protein called MYOSIN REGULATORY LIGHT CHAIN, STRIATED ADDUCTOR MUSCLE.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1-Y	136	Total	C	N	O	S	0	0
			1088	687	173	219	9		
2	2-Y	136	Total	C	N	O	S	0	0
			1088	687	173	219	9		
2	3-Y	136	Total	C	N	O	S	0	0
			1088	687	173	219	9		
2	4-Y	136	Total	C	N	O	S	0	0
			1088	687	173	219	9		
2	5-Y	136	Total	C	N	O	S	0	0
			1088	687	173	219	9		
2	6-Y	136	Total	C	N	O	S	0	0
			1088	687	173	219	9		
2	7-Y	136	Total	C	N	O	S	0	0
			1088	687	173	219	9		
2	8-Y	136	Total	C	N	O	S	0	0
			1088	687	173	219	9		
2	9-Y	136	Total	C	N	O	S	0	0
			1088	687	173	219	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	10-Y	136	Total	C	N	O	S	0	0
			1088	687	173	219	9		
2	11-Y	136	Total	C	N	O	S	0	0
			1088	687	173	219	9		
2	12-Y	136	Total	C	N	O	S	0	0
			1088	687	173	219	9		
2	13-Y	136	Total	C	N	O	S	0	0
			1088	687	173	219	9		
2	14-Y	136	Total	C	N	O	S	0	0
			1088	687	173	219	9		
2	15-Y	136	Total	C	N	O	S	0	0
			1088	687	173	219	9		
2	16-Y	136	Total	C	N	O	S	0	0
			1088	687	173	219	9		
2	17-Y	136	Total	C	N	O	S	0	0
			1088	687	173	219	9		
2	18-Y	136	Total	C	N	O	S	0	0
			1088	687	173	219	9		
2	19-Y	136	Total	C	N	O	S	0	0
			1088	687	173	219	9		
2	20-Y	136	Total	C	N	O	S	0	0
			1088	687	173	219	9		
2	21-Y	136	Total	C	N	O	S	0	0
			1088	687	173	219	9		
2	22-Y	136	Total	C	N	O	S	0	0
			1088	687	173	219	9		
2	23-Y	136	Total	C	N	O	S	0	0
			1088	687	173	219	9		
2	24-Y	136	Total	C	N	O	S	0	0
			1088	687	173	219	9		
2	25-Y	136	Total	C	N	O	S	0	0
			1088	687	173	219	9		
2	26-Y	136	Total	C	N	O	S	0	0
			1088	687	173	219	9		
2	27-Y	136	Total	C	N	O	S	0	0
			1088	687	173	219	9		

- Molecule 3 is a protein called MYOSIN ESSENTIAL LIGHT CHAIN, STRIATED ADDUCTOR MUSCLE.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1-Z	151	Total	C	N	O	S	0	0
			1198	757	190	244	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	2-Z	151	Total	C	N	O	S	0	0
			1198	757	190	244	7		
3	3-Z	151	Total	C	N	O	S	0	0
			1198	757	190	244	7		
3	4-Z	151	Total	C	N	O	S	0	0
			1198	757	190	244	7		
3	5-Z	151	Total	C	N	O	S	0	0
			1198	757	190	244	7		
3	6-Z	151	Total	C	N	O	S	0	0
			1198	757	190	244	7		
3	7-Z	151	Total	C	N	O	S	0	0
			1198	757	190	244	7		
3	8-Z	151	Total	C	N	O	S	0	0
			1198	757	190	244	7		
3	9-Z	151	Total	C	N	O	S	0	0
			1198	757	190	244	7		
3	10-Z	151	Total	C	N	O	S	0	0
			1198	757	190	244	7		
3	11-Z	151	Total	C	N	O	S	0	0
			1198	757	190	244	7		
3	12-Z	151	Total	C	N	O	S	0	0
			1198	757	190	244	7		
3	13-Z	151	Total	C	N	O	S	0	0
			1198	757	190	244	7		
3	14-Z	151	Total	C	N	O	S	0	0
			1198	757	190	244	7		
3	15-Z	151	Total	C	N	O	S	0	0
			1198	757	190	244	7		
3	16-Z	151	Total	C	N	O	S	0	0
			1198	757	190	244	7		
3	17-Z	151	Total	C	N	O	S	0	0
			1198	757	190	244	7		
3	18-Z	151	Total	C	N	O	S	0	0
			1198	757	190	244	7		
3	19-Z	151	Total	C	N	O	S	0	0
			1198	757	190	244	7		
3	20-Z	151	Total	C	N	O	S	0	0
			1198	757	190	244	7		
3	21-Z	151	Total	C	N	O	S	0	0
			1198	757	190	244	7		
3	22-Z	151	Total	C	N	O	S	0	0
			1198	757	190	244	7		

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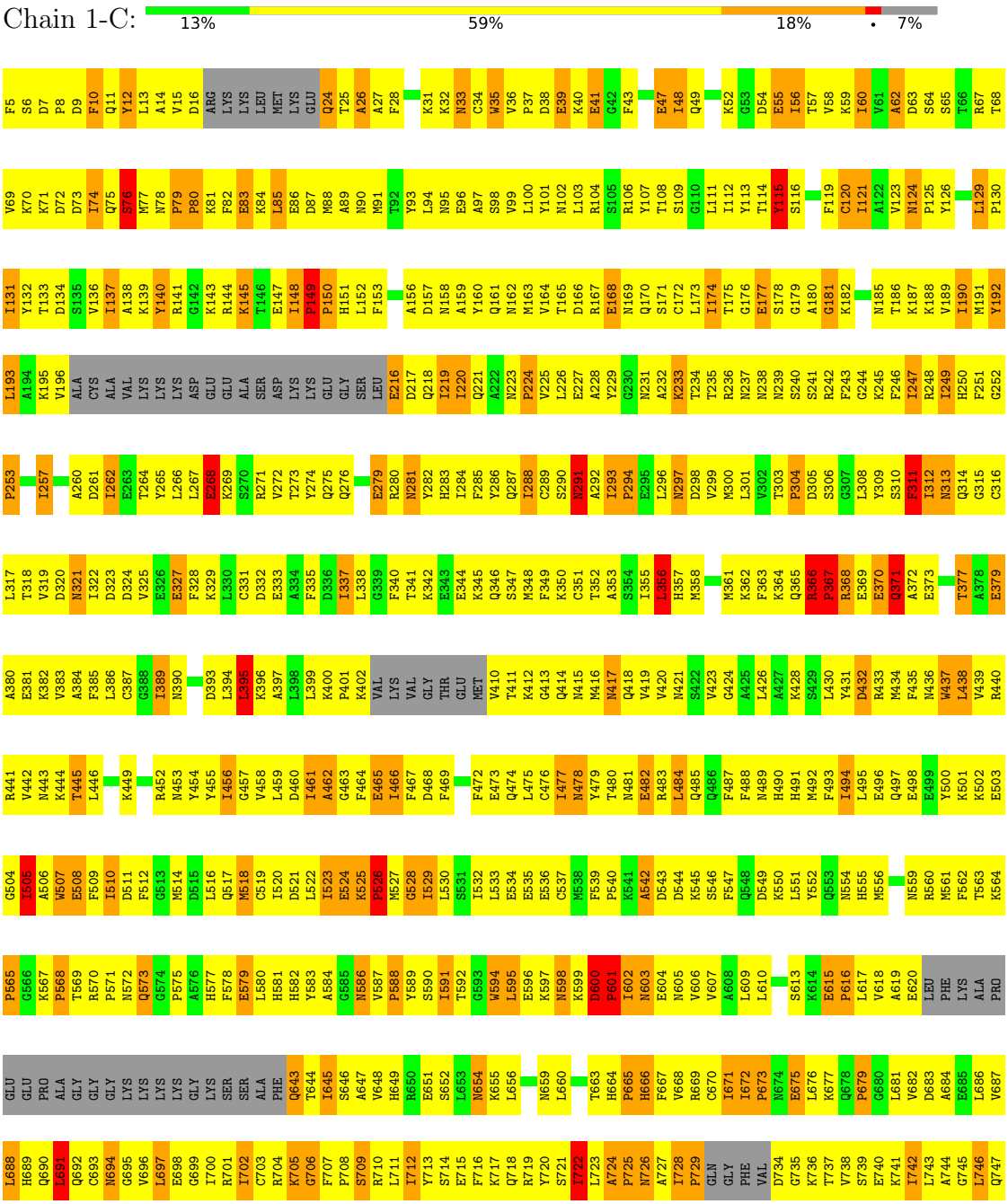
Mol	Chain	Residues	Atoms					AltConf	Trace
3	23-Z	151	Total	C	N	O	S	0	0
			1198	757	190	244	7		
3	24-Z	151	Total	C	N	O	S	0	0
			1198	757	190	244	7		
3	25-Z	151	Total	C	N	O	S	0	0
			1198	757	190	244	7		
3	26-Z	151	Total	C	N	O	S	0	0
			1198	757	190	244	7		
3	27-Z	151	Total	C	N	O	S	0	0
			1198	757	190	244	7		

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.

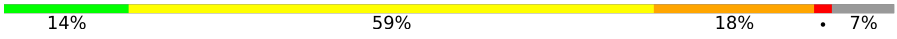
- Molecule 1: MYOSIN HEAVY CHAIN, STRIATED MUSCLE

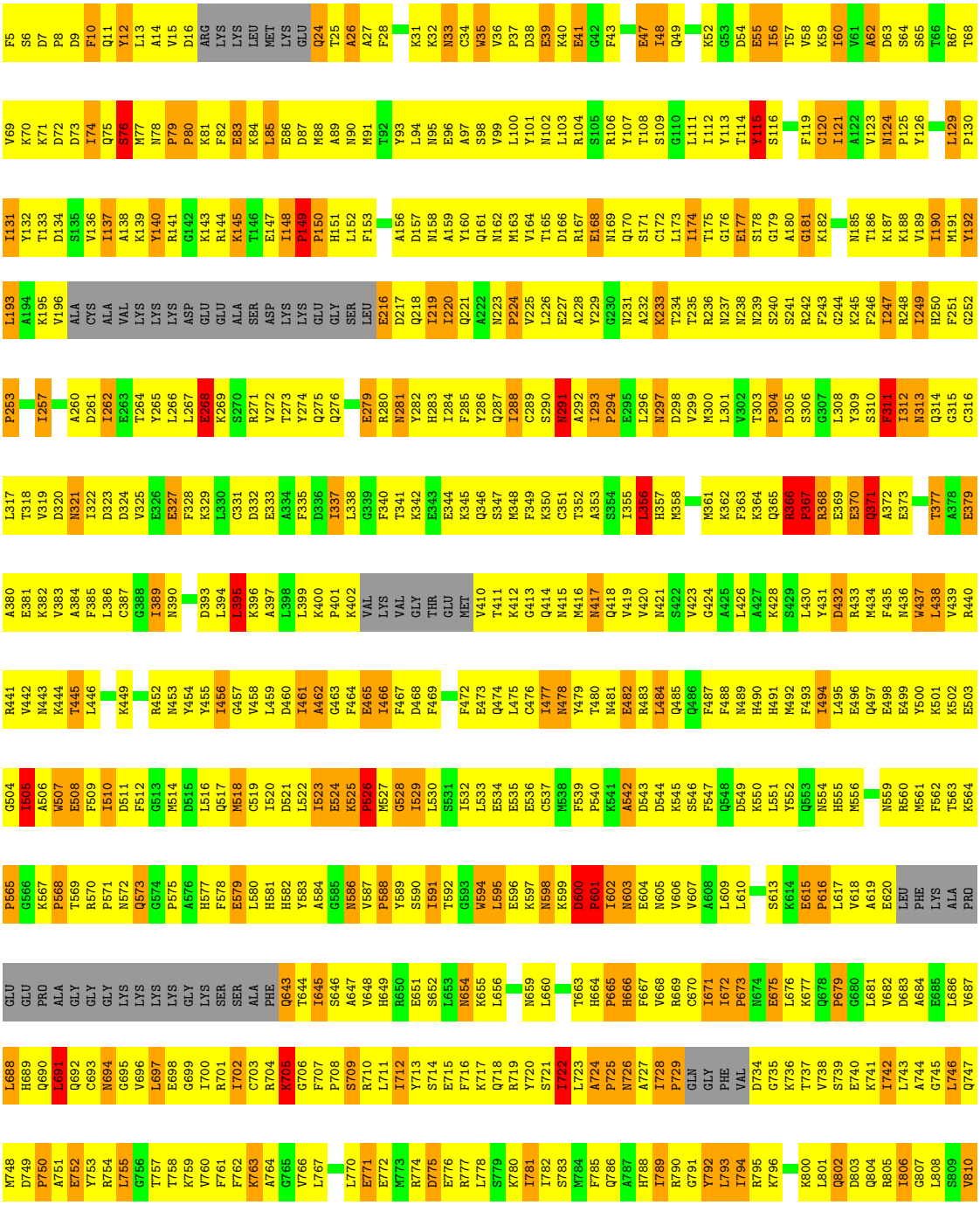
Chain 1-C:

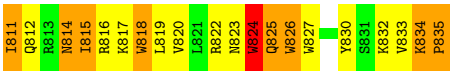


• Molecule 1: MYOSIN HEAVY CHAIN, STRIATED MUSCLE

Chain 2-C:

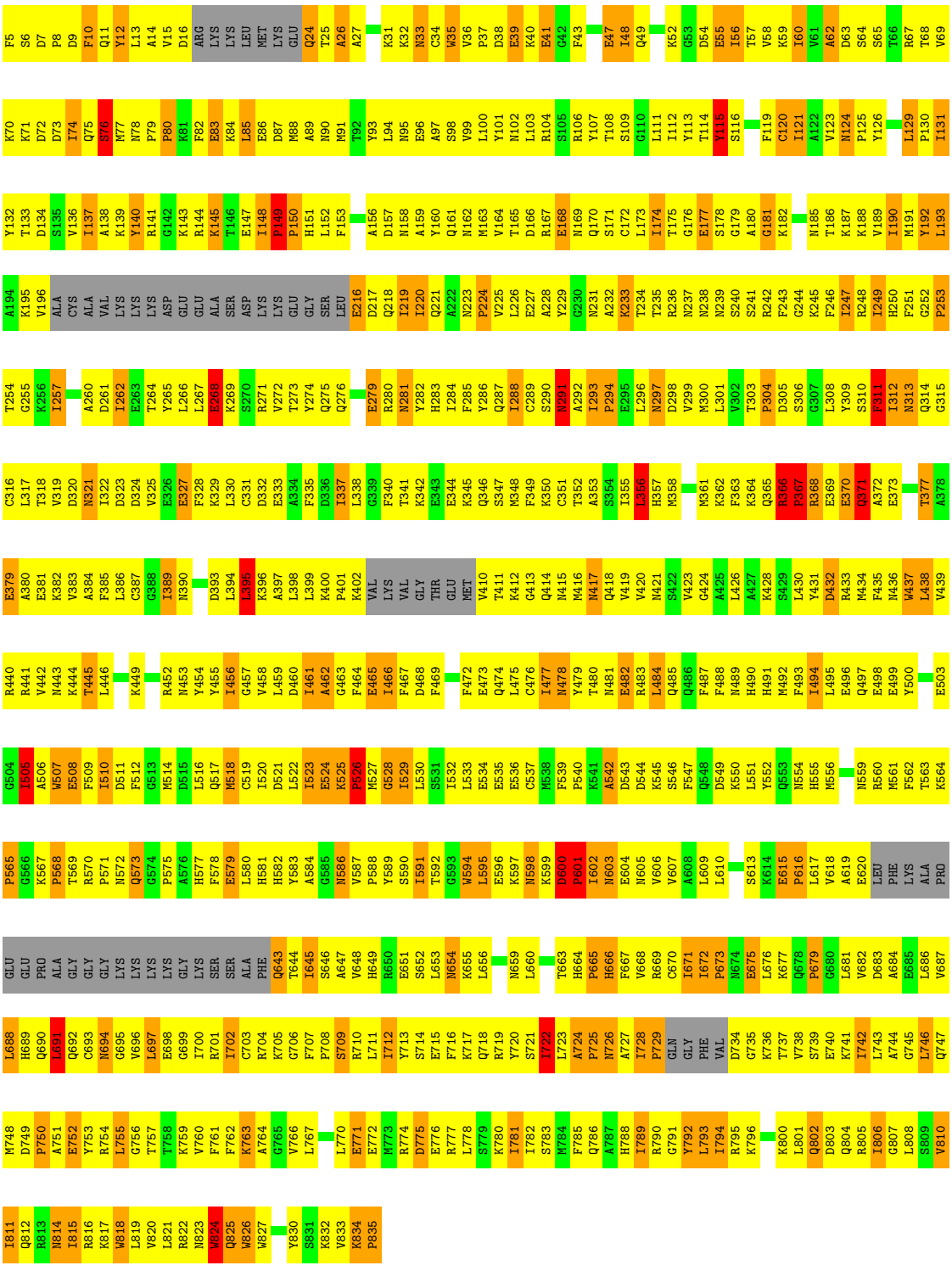






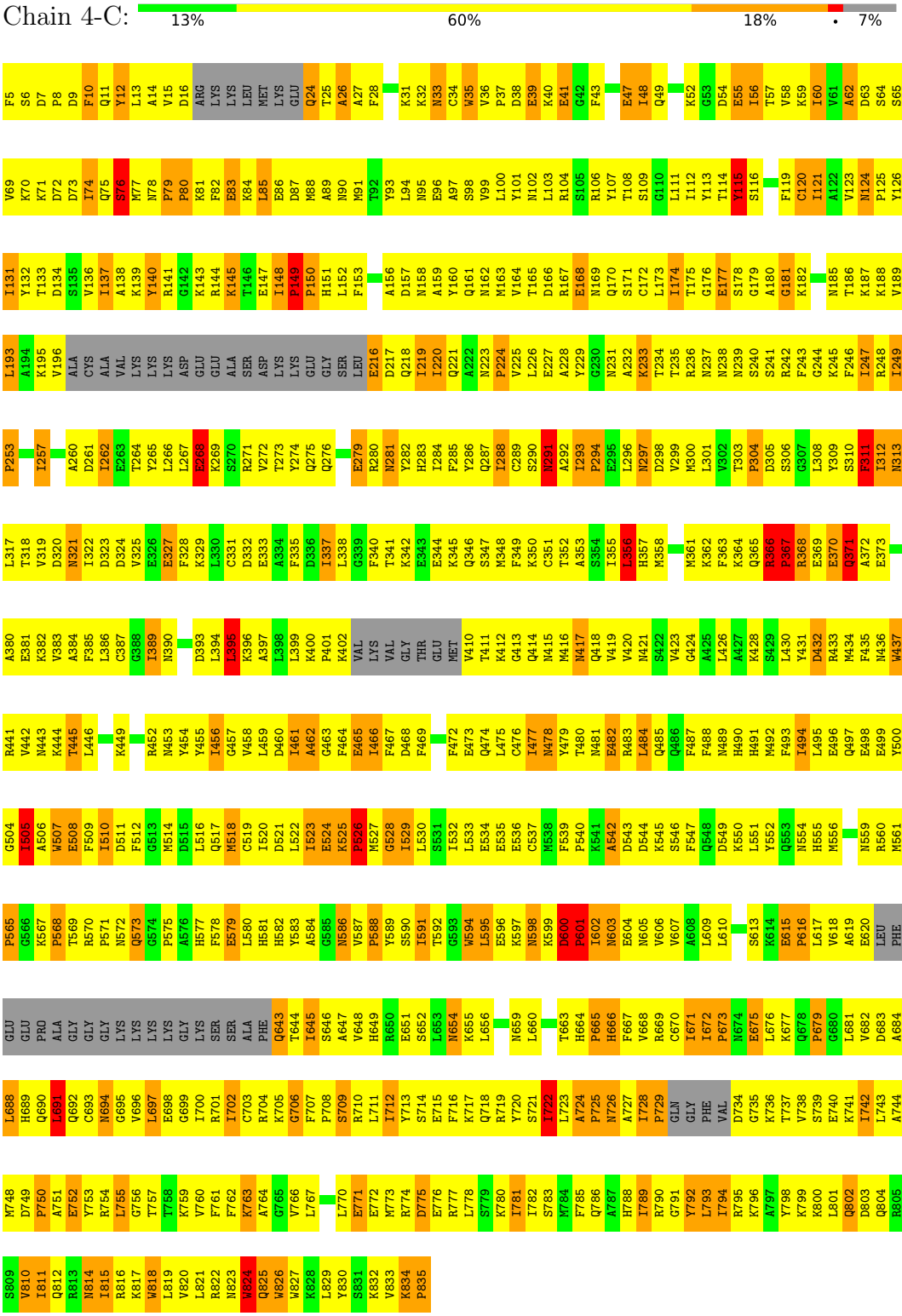
• Molecule 1: MYOSIN HEAVY CHAIN, STRIATED MUSCLE

Chain 3-C:



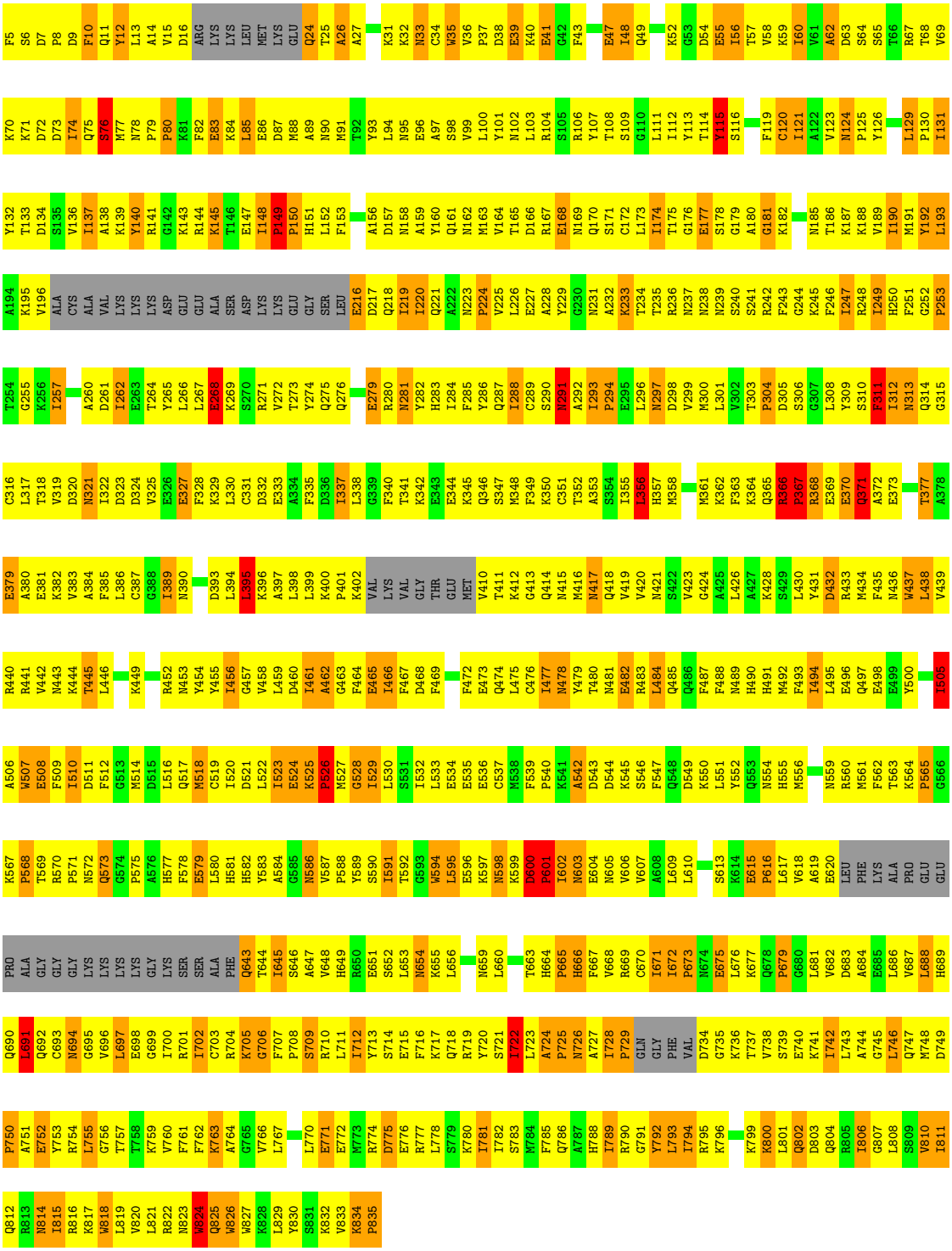
• Molecule 1: MYOSIN HEAVY CHAIN, STRIATED MUSCLE

Chain 4-C:



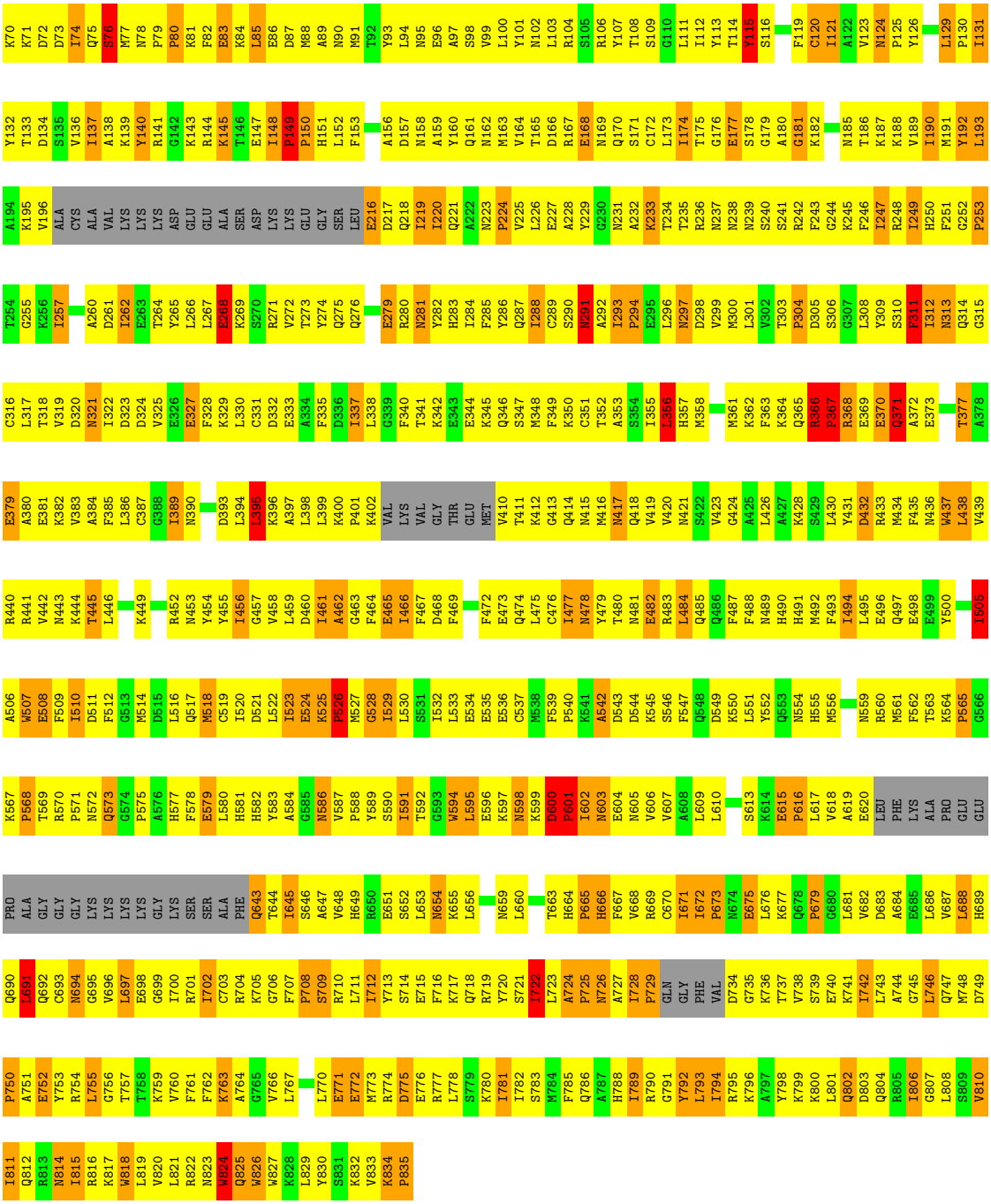
• Molecule 1: MYOSIN HEAVY CHAIN, STRIATED MUSCLE

Chain 5-C:



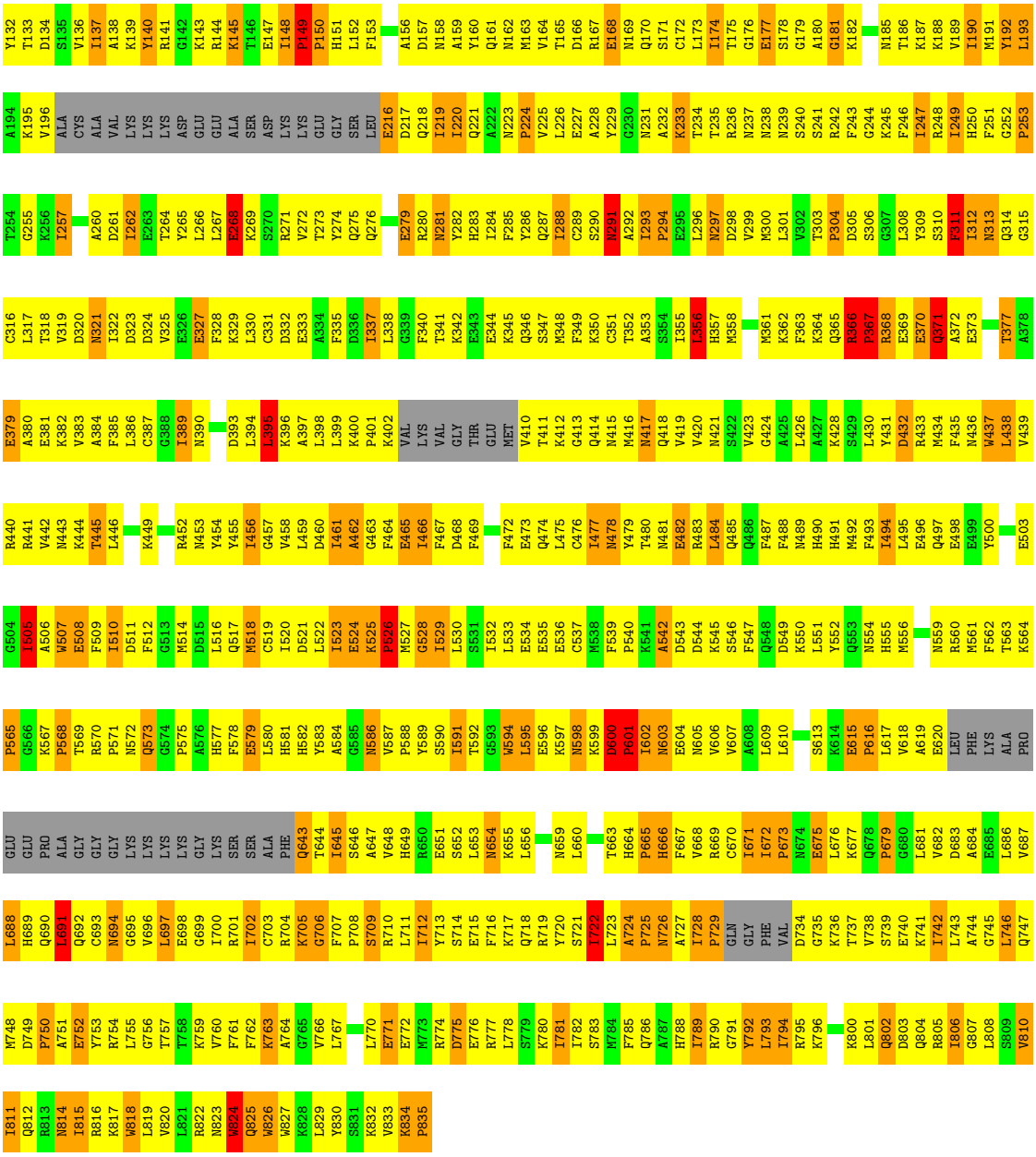
• Molecule 1: MYOSIN HEAVY CHAIN, STRIATED MUSCLE

Chain 6-C:



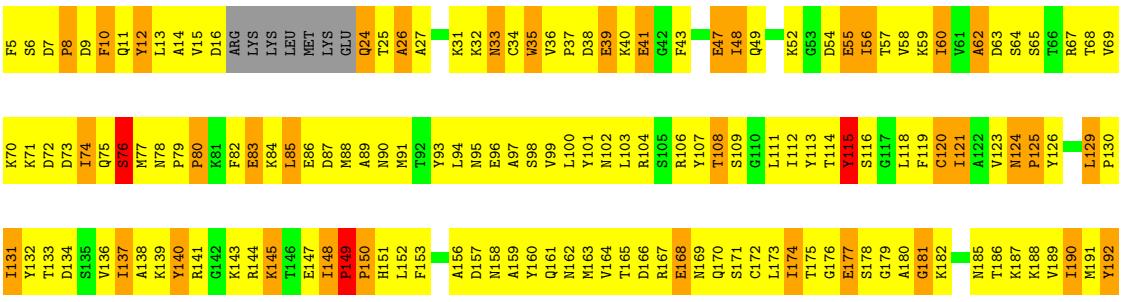
• Molecule 1: MYOSIN HEAVY CHAIN, STRIATED MUSCLE

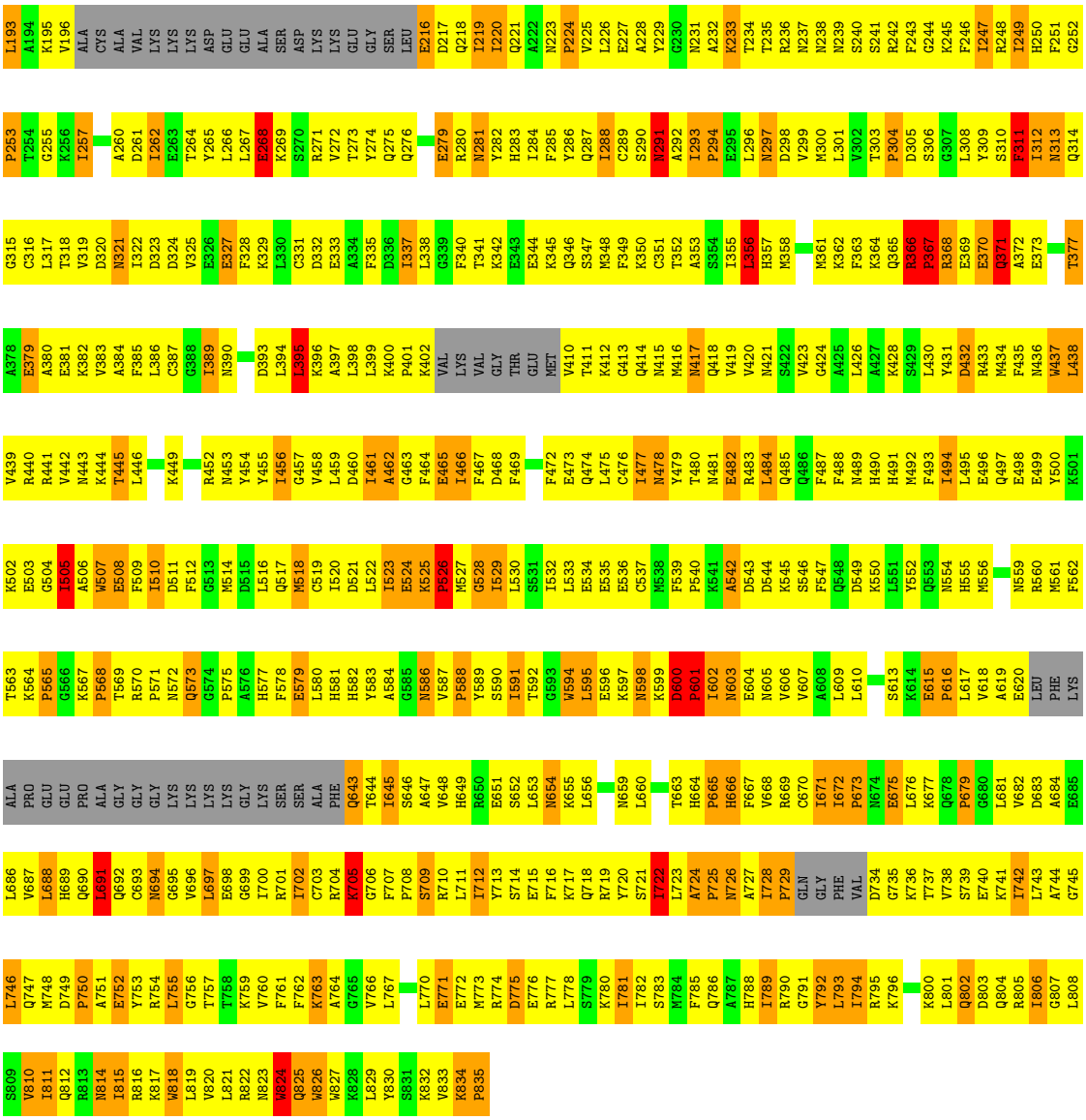
Chain 7-C:



• Molecule 1: MYOSIN HEAVY CHAIN, STRIATED MUSCLE

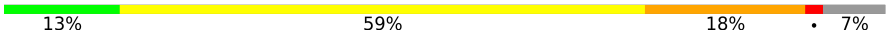
Chain 8-C:

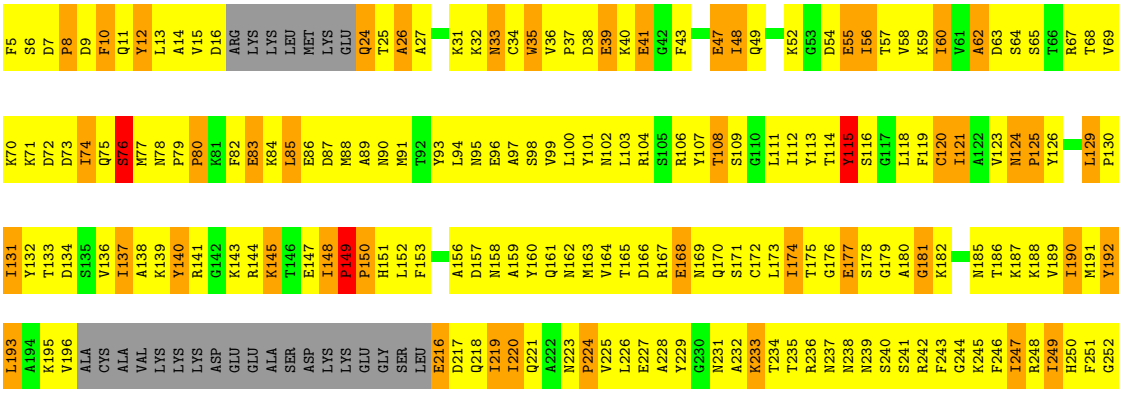


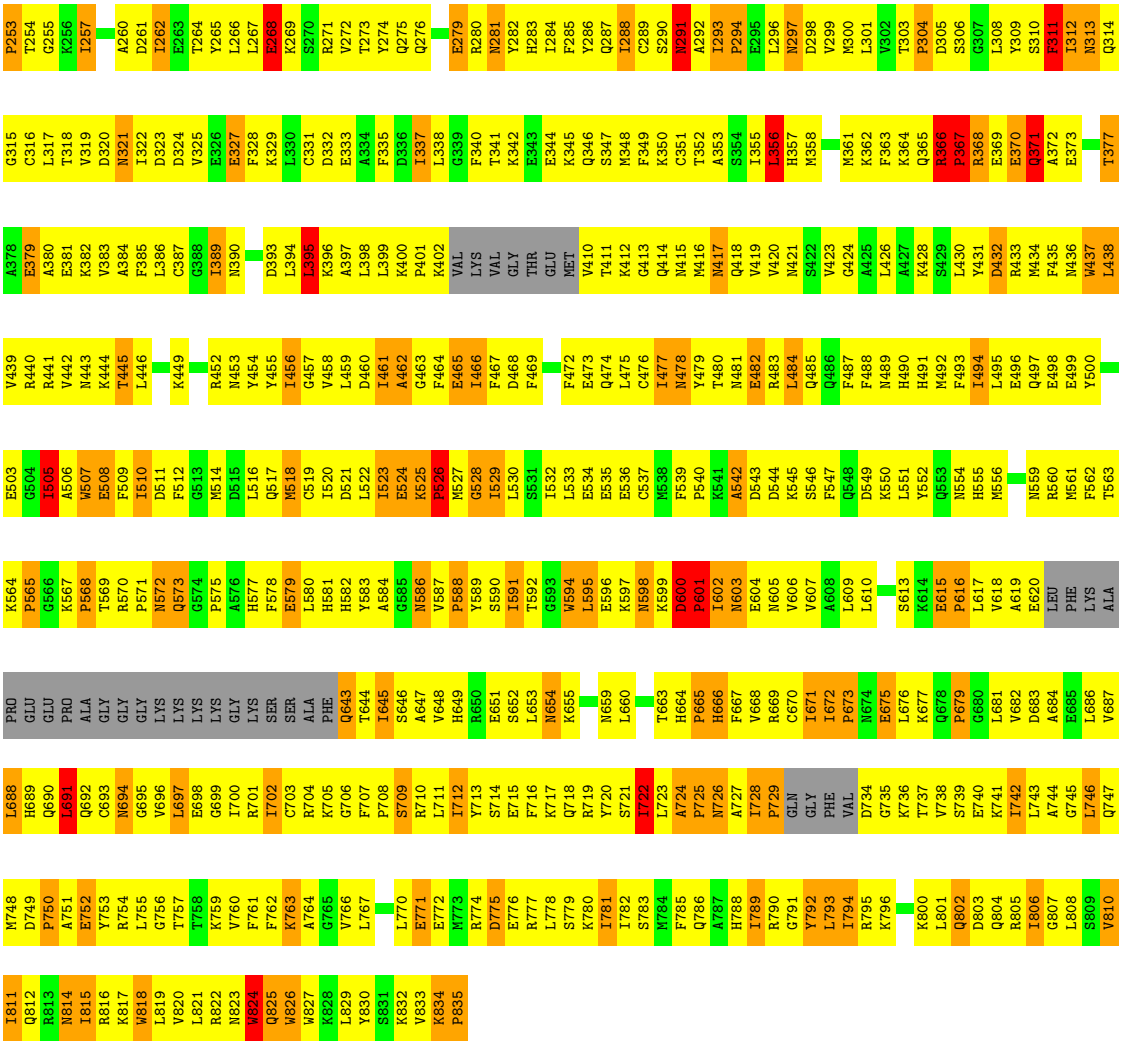


• Molecule 1: MYOSIN HEAVY CHAIN, STRIATED MUSCLE

Chain 9-C:

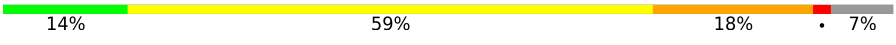


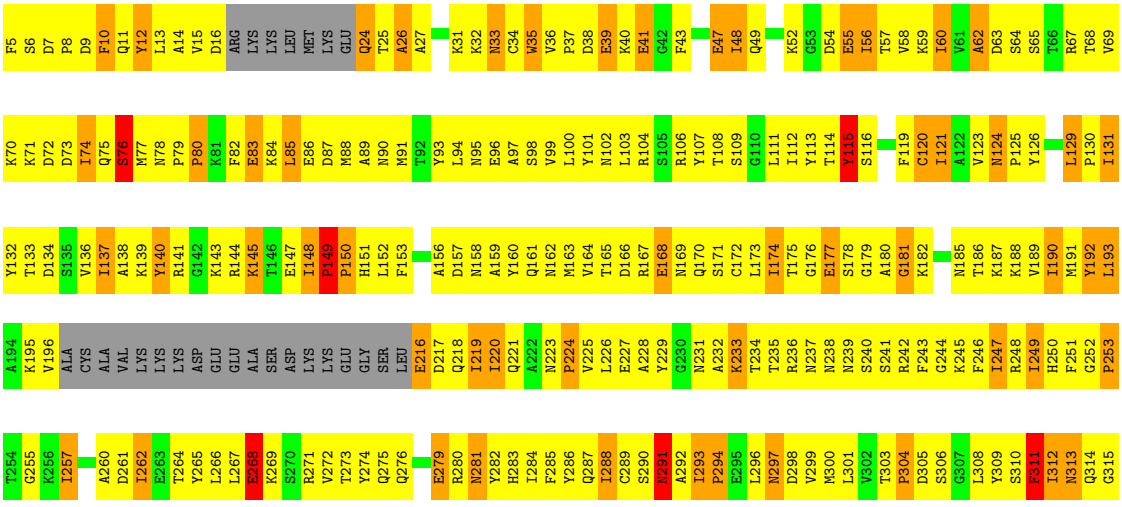


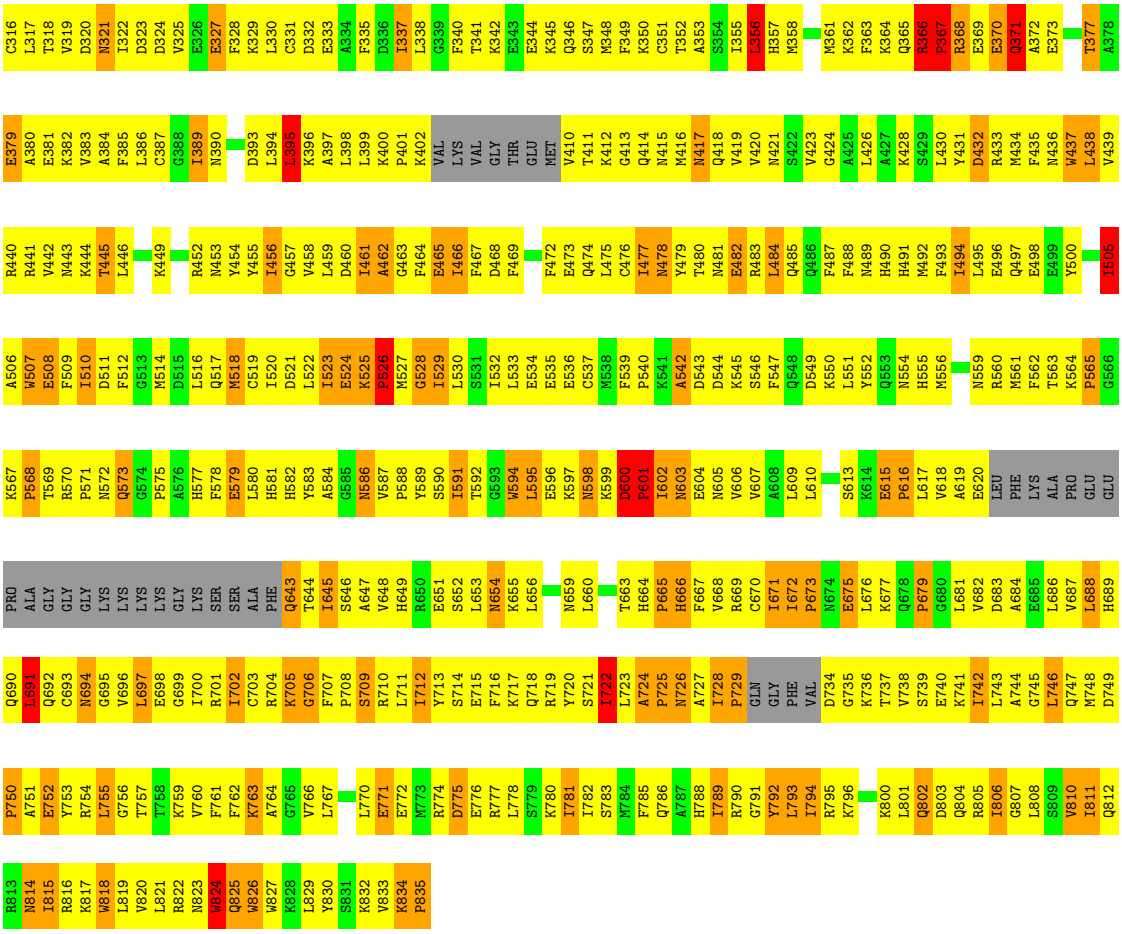


• Molecule 1: MYOSIN HEAVY CHAIN, STRIATED MUSCLE

Chain 10-C:

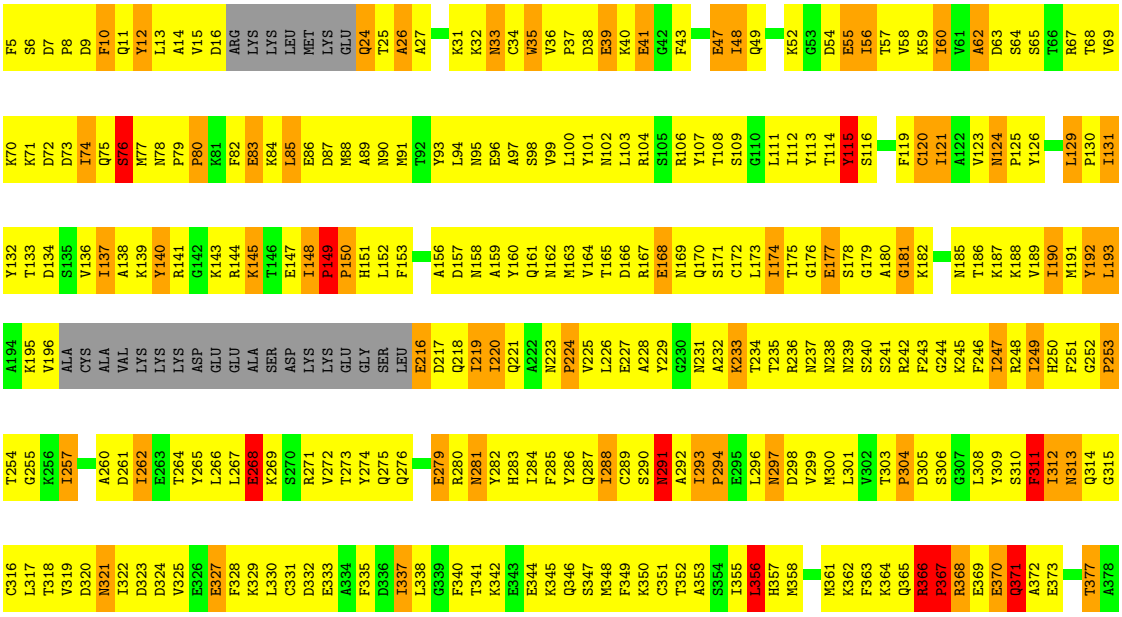


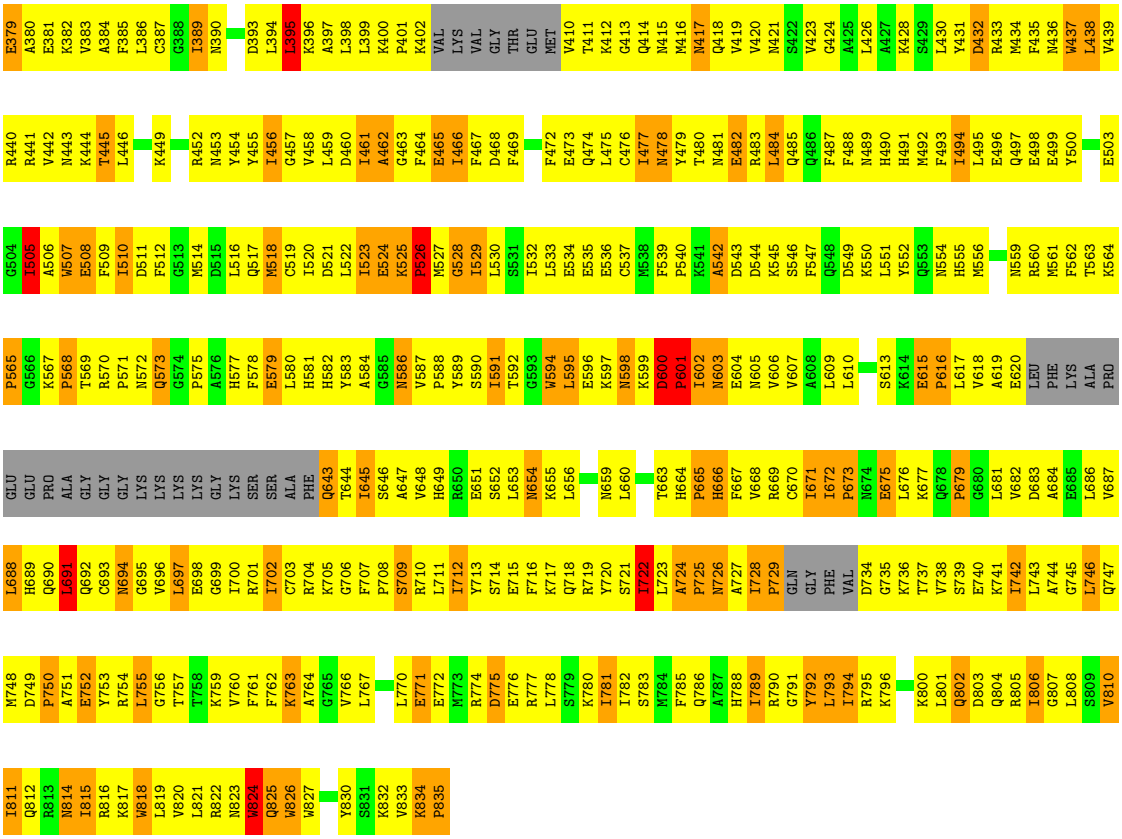




• Molecule 1: MYOSIN HEAVY CHAIN, STRIATED MUSCLE

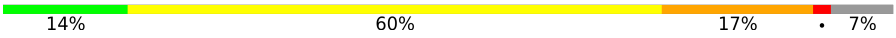
Chain 11-C:

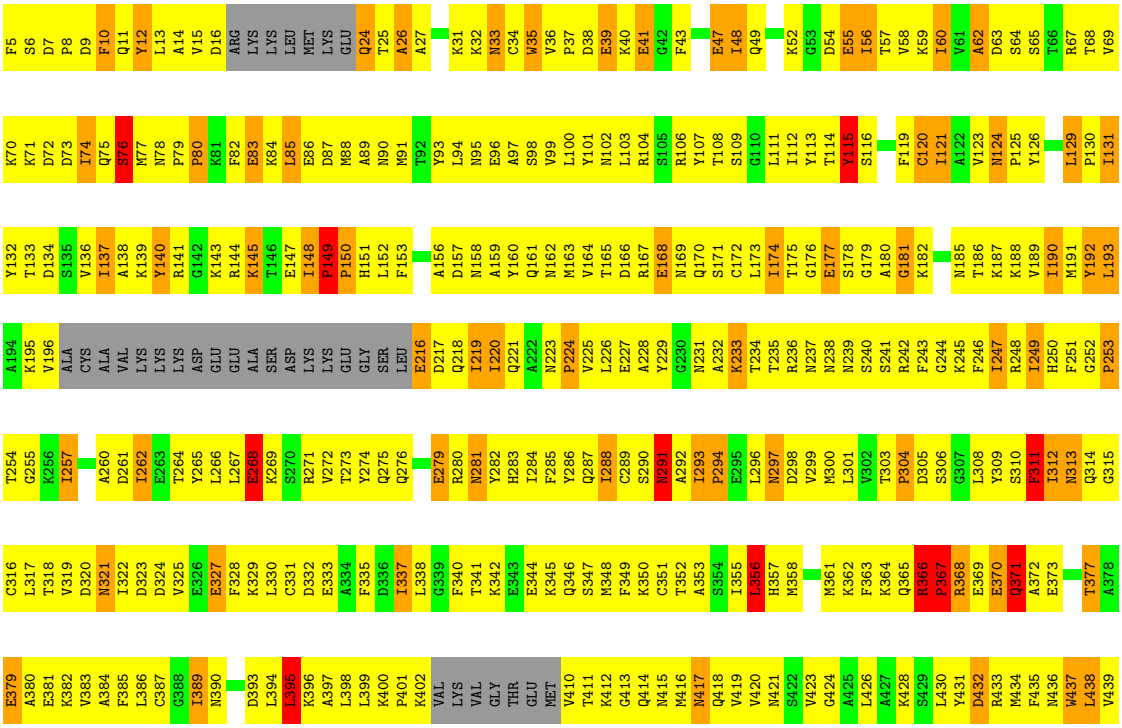


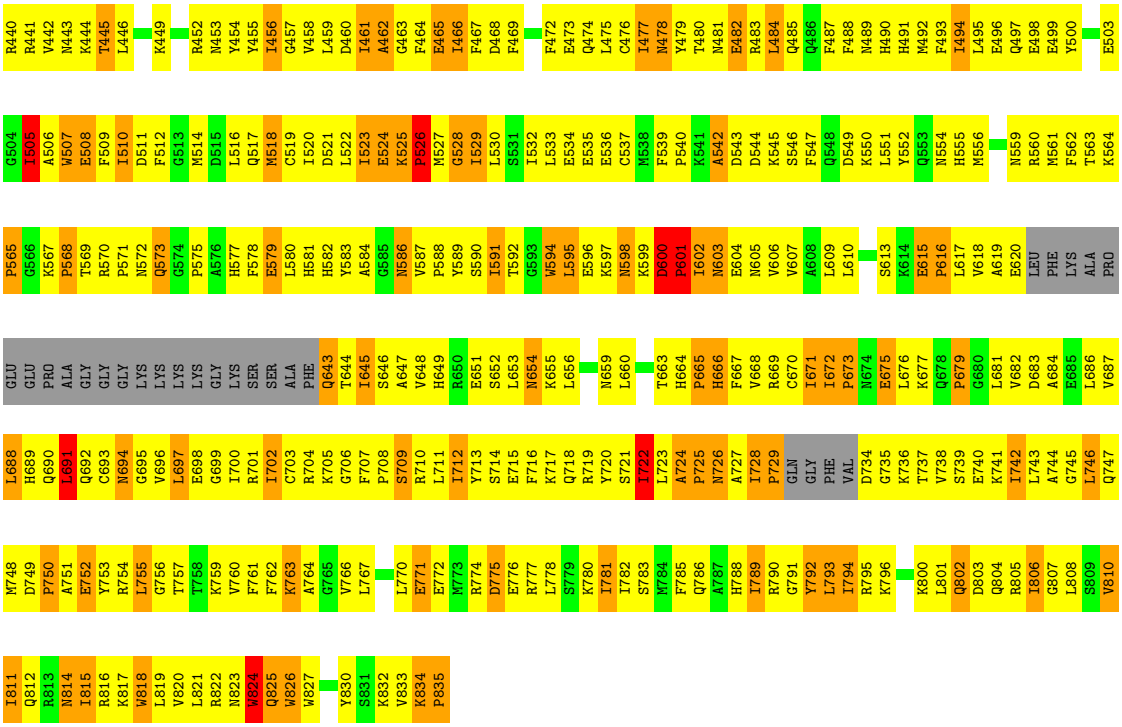


• Molecule 1: MYOSIN HEAVY CHAIN, STRIATED MUSCLE

Chain 12-C:

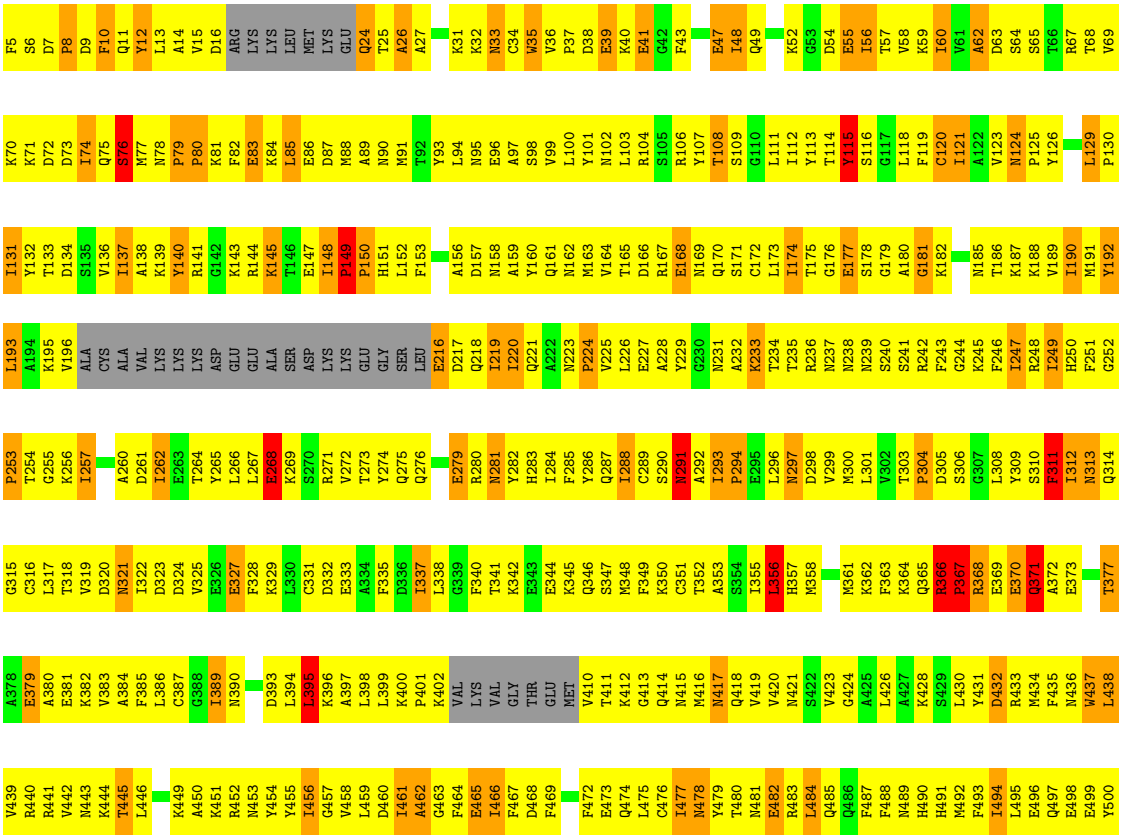


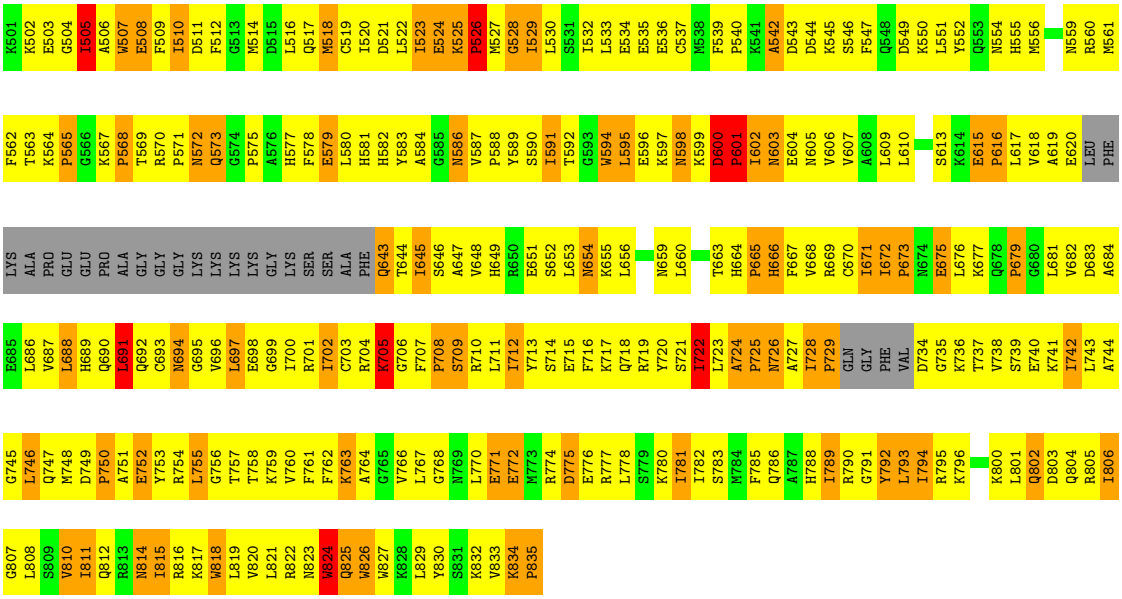




• Molecule 1: MYOSIN HEAVY CHAIN, STRIATED MUSCLE

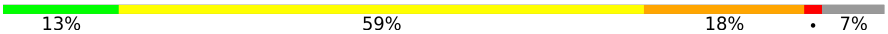
Chain 13-C:

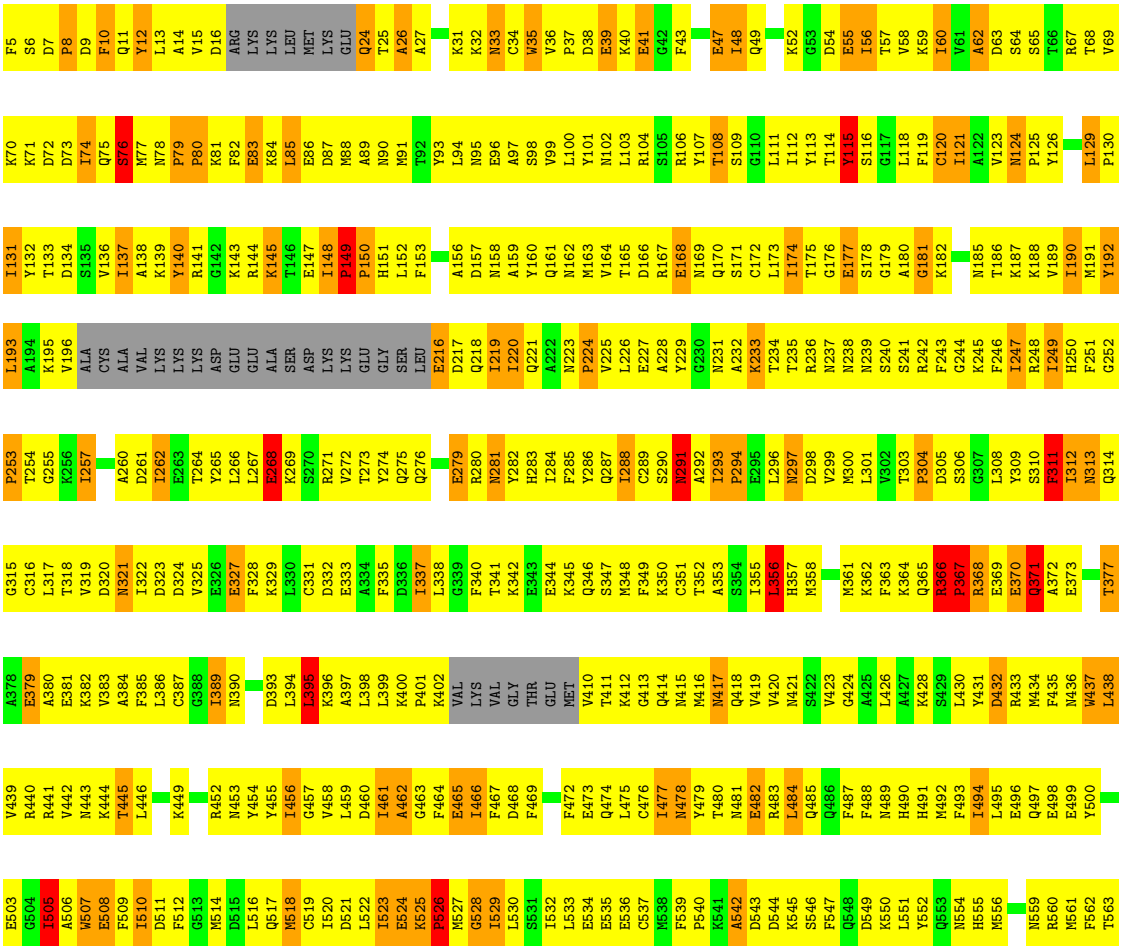


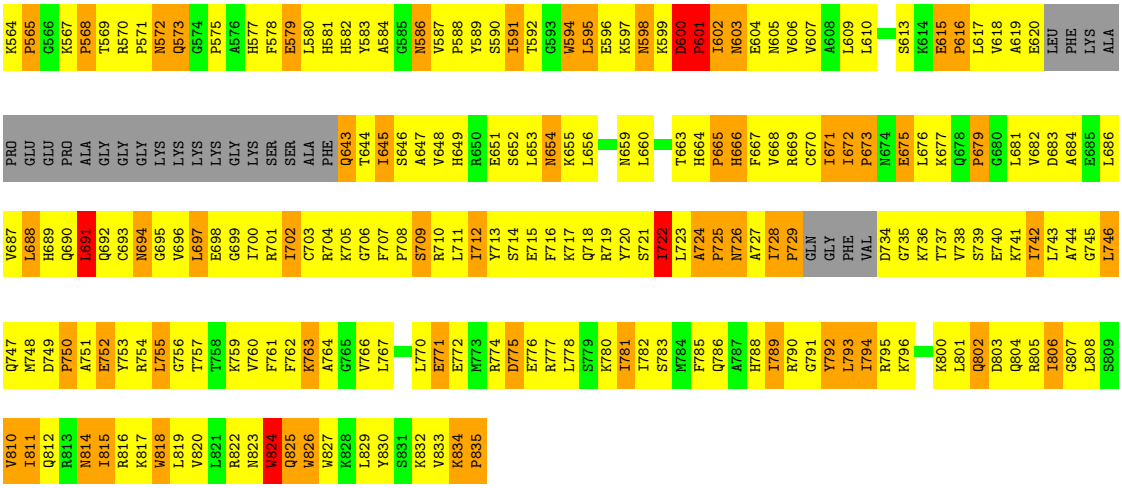


• Molecule 1: MYOSIN HEAVY CHAIN, STRIATED MUSCLE

Chain 14-C:

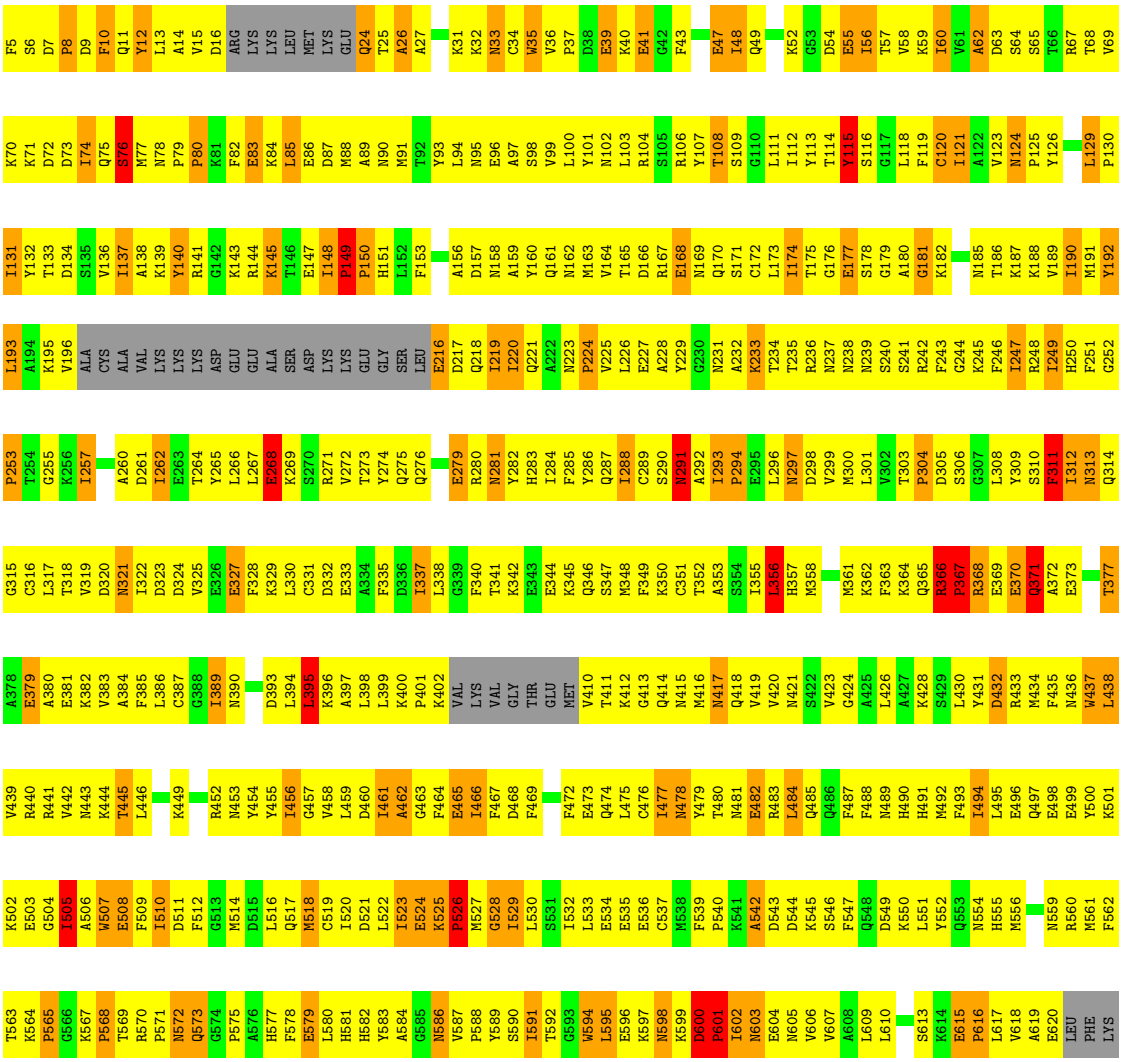


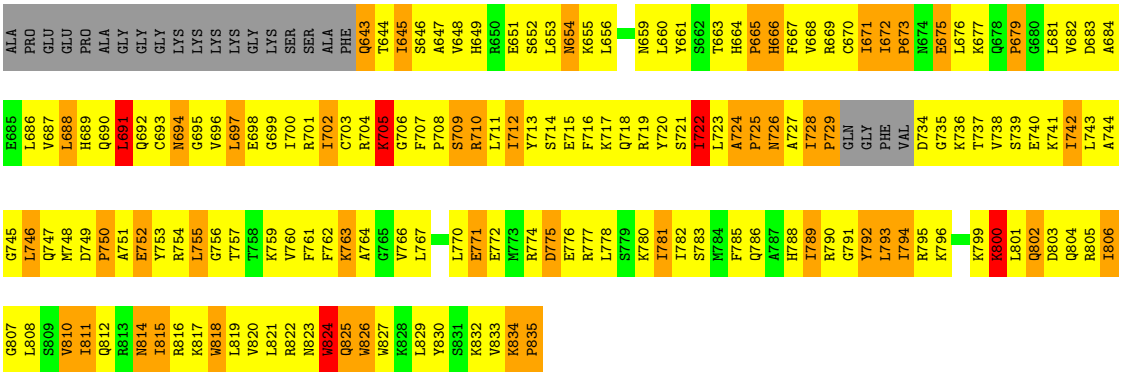




• Molecule 1: MYOSIN HEAVY CHAIN, STRIATED MUSCLE

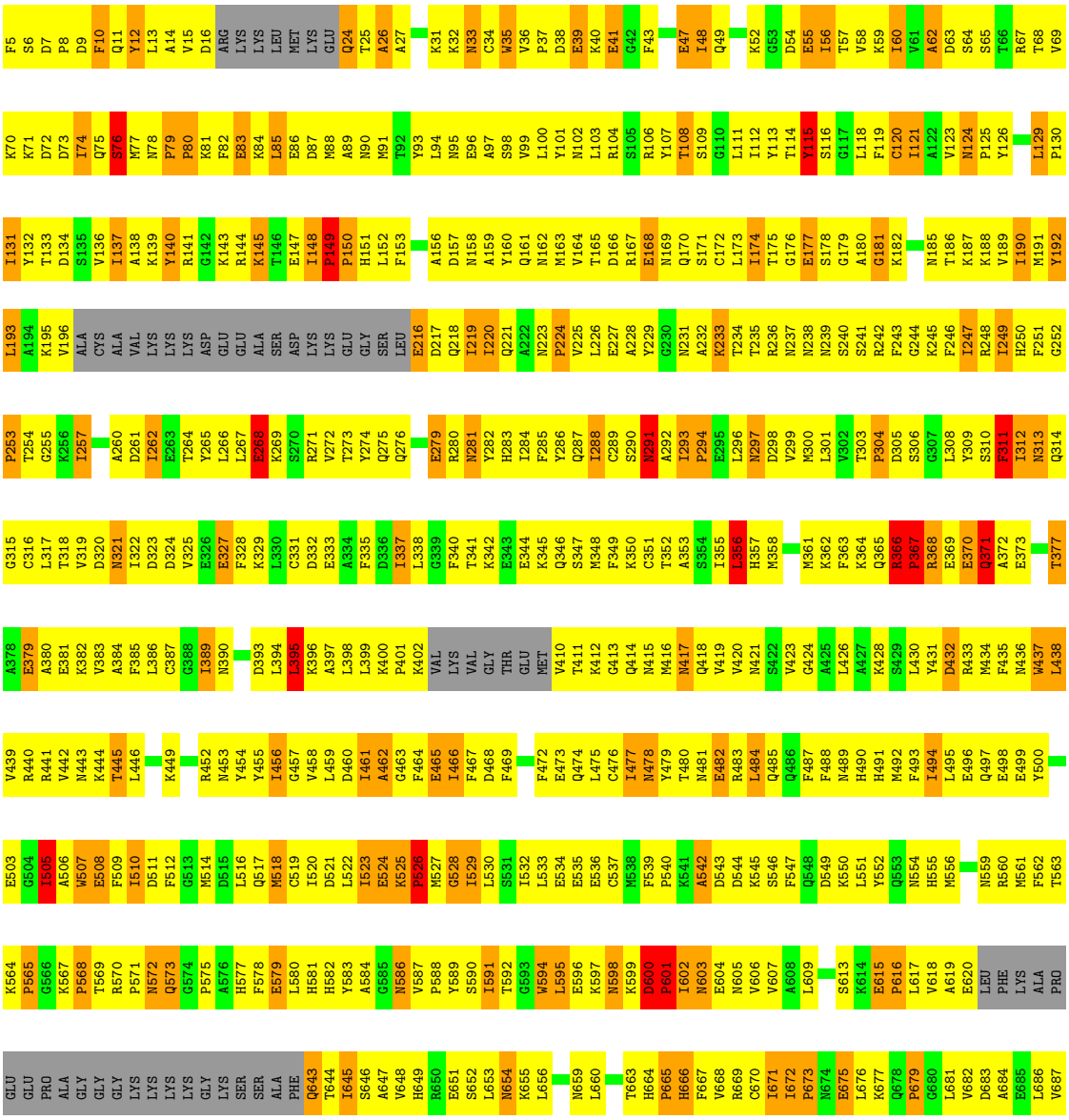
Chain 15-C:





• Molecule 1: MYOSIN HEAVY CHAIN, STRIATED MUSCLE

Chain 16-C:



L688 H689 Q690 L691 Q692 C693 N694 G695 V696 L697 E698 G699 I700 R701 I702 C703 R704 K705 G706 F707 P708 S709 R710 L711 I712 Y713 S714 E715 F716 K717 Q718 R719 Y720 S721 I722 L723 A724 P725 N726 A727 I728 P729 GLN GLY PHE VAL D734 G735 K736 T737 V738 S739 E740 K741 I742 L743 A744 G745 L746 Q747

M748 D749 P750 A751 E752 Y753 R754 L755 G756 T757 T758 K759 V760 F761 F762 K763 A764 G765 V766 L767 L770 E771 E772 M773 R774 D775 E776 R777 L778 S779 K780 I781 I782 S783 M784 F785 Q786 A787 H788 I789 R790 G791 Y792 L793 I794 R795 K796 K800 L801 Q802 D803 Q804 R805 I806 G807 L808 S809 V810

I811 Q812 R813 N814 I815 R816 K817 W818 L819 V820 L821 R822 N823 W824 Q825 W826 W827 K828 L829 Y830 S831 K832 V833 K834 P835

- Molecule 1: MYOSIN HEAVY CHAIN, STRIATED MUSCLE

Chain 17-C: 13% 59% 18% • 7%

F5 S6 D7 P8 D9 F10 Q11 Y12 L13 A14 V15 D16 ARG LYS LYS LEU MET LYS GLU Q24 T25 A26 A27 K31 K32 N33 C34 W35 V36 P37 D38 E39 K40 E41 G42 F43 E47 I48 Q49 K52 G53 D54 E55 I56 T57 V58 K59 I60 V61 A62 D63 S64 S65 T66 R67 T68 V69

K70 K71 D72 D73 I74 Q75 S76 M77 N78 P79 P80 K81 F82 E83 K84 L85 E86 D87 M88 A89 N90 M91 T92 Y93 L94 N95 E96 A97 S98 V99 L100 Y101 N102 L103 R104 S105 R106 Y107 T108 S109 G110 L111 I112 Y113 T114 Y115 S116 G117 L118 F119 C120 I121 A122 V123 N124 P125 Y126 L129 P130

I131 Y132 T133 D134 S135 V136 I137 A138 K139 Y140 R141 G142 K143 R144 K145 T146 E147 I148 P149 P150 H151 L152 F153 A156 D157 N158 A159 Y160 Q161 N162 M163 V164 T165 D166 R167 E168 N169 Q170 S171 C172 L173 I174 T175 G176 E177 S178 G179 A180 G181 K182 N185 T186 K187 K188 V189 I190 M191 Y192

L193 A194 K195 V196 ALA CYS ALA VAL LYS LYS LYS ASP GLU GLU ALA SER ASP LYS LYS GLU GLY SER LEU E216 D217 Q218 I219 I220 Q221 A222 N223 P224 V225 L226 E227 A228 Y229 G230 N231 A232 K233 T234 T235 R236 N237 N238 N239 S240 S241 R242 F243 G244 K245 F246 I247 R248 I249 H250 F251 G252

P253 T254 G255 K256 I257 A260 D261 I262 E263 T264 Y265 L266 L267 E268 K269 S270 R271 V272 T273 Y274 Q275 Q276 E279 R280 N281 Y282 H283 I284 F285 Y286 Q287 I288 C289 S290 N291 A292 I293 P294 E295 L296 N297 D298 V299 M300 L301 V302 T303 P304 D305 S306 G307 L308 Y309 S310 F311 I312 N313 Q314

G315 C316 L317 T318 V319 D320 N321 I322 D323 D324 V325 E326 E327 F328 K329 L330 C331 D332 E333 A334 F335 D336 I337 L338 G339 F340 T341 K342 E343 E344 K345 Q346 S347 M348 F349 K350 C351 T352 A353 S354 I355 L356 H357 M358 M361 K362 F363 K364 Q365 R366 P367 R368 E369 E370 Q371 A372 E373 T377

A378 E379 A380 E381 K382 V383 A384 F385 L386 C387 G388 I389 N390 D393 L394 L395 K396 A397 L398 L399 K400 P401 K402 VAL LYS VAL GLY THR GLU MET V410 T411 K412 G413 Q414 N415 M416 N417 Q418 V419 V420 N421 S422 V423 G424 A425 L426 A427 K428 S429 L430 Y431 D432 R433 M434 F435 N436 W437 L438

V439 R440 R441 V442 N443 K444 T445 L446 K449 R452 N453 Y454 Y455 I456 G457 V458 L459 D460 I461 A462 G463 F464 E465 I466 F467 D468 F469 F472 E473 Q474 L475 C476 I477 N478 Y479 T480 N481 E482 R483 L484 Q485 Q486 F487 F488 N489 H490 H491 M492 F493 I494 L495 E496 Q497 E498 E499 Y500 K501

K502 E503 G504 I505 A506 W507 E508 F509 I510 D511 F512 G513 M514 D515 L516 Q517 M518 C519 I520 D521 L522 I523 E524 K525 P526 M527 G528 I529 L530 S531 I532 L533 E534 E535 E536 C537 M538 F539 P540 K541 A542 D543 D544 K545 S546 F547 Q548 D549 K550 L551 Y552 Q553 N554 H555 M556 N559 R560 M561 F562

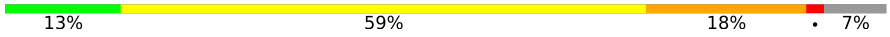
T563 K564 P565 G566 K567 P568 T569 R570 P571 N572 Q573 G574 P575 A576 H577 F578 E579 L580 H581 H582 Y583 A584 G585 N586 V587 P588 Y589 S590 I591 T592 G593 W594 L595 E596 K597 N598 K599 D600 P601 I602 N603 E604 N605 V606 V607 A608 L609 L610 S613 K614 E615 P616 L617 V618 A619 E620 LEU PHE LYS

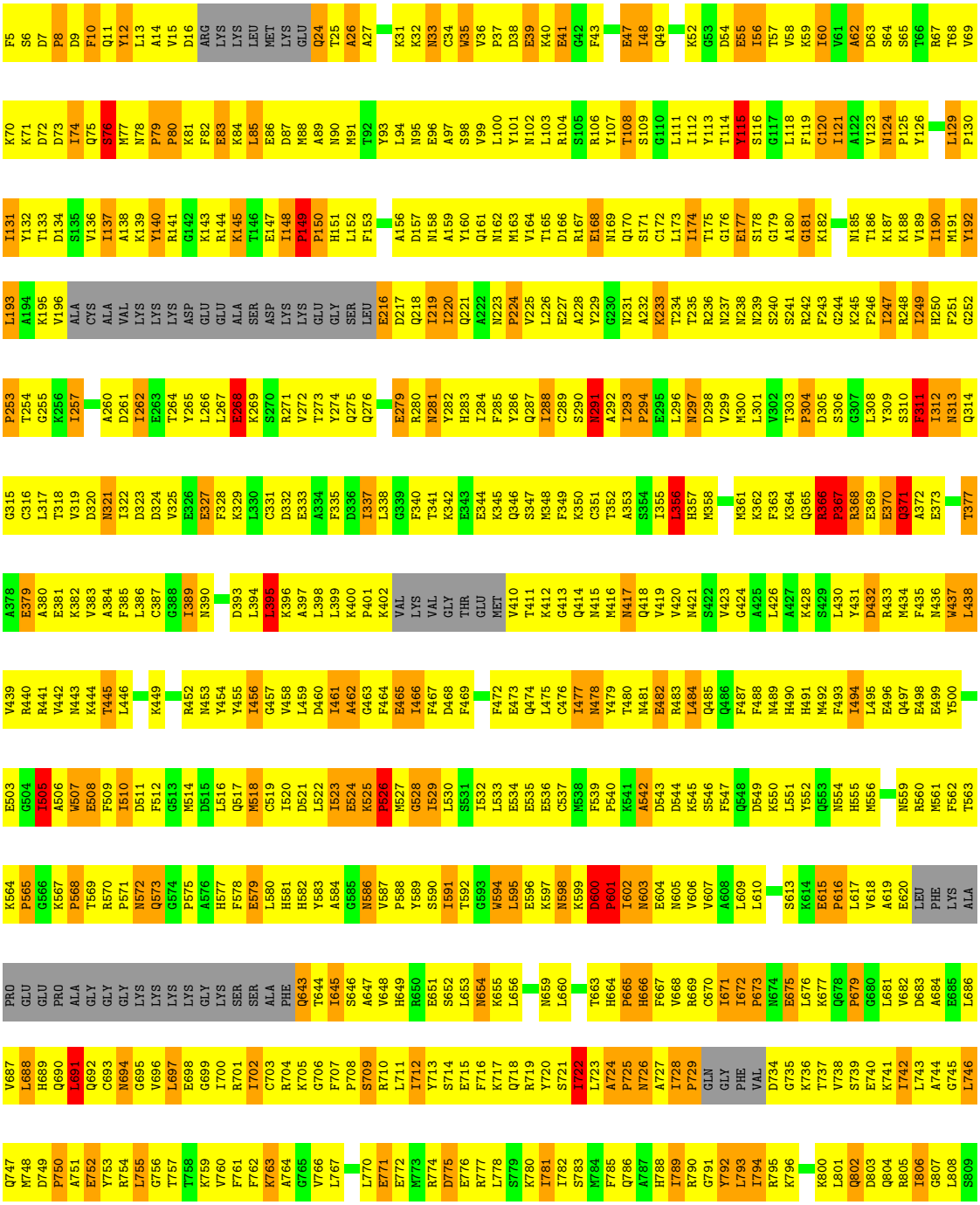
ALA PRO GLU GLU PRO ALA GLY GLY GLY LYS LYS LYS LYS GLY LYS SER SER ALA PHE Q643 T644 I645 S646 A647 V648 H649 R650 E651 S652 L653 N654 K655 L656 N659 L660 T663 H664 P665 H666 F667 V668 R669 C670 I671 I672 P673 N674 E675 L676 K677 Q678 P679 G680 L681 V682 D683 A684 E685

L686 V687 L688 H689 Q690 L691 Q692 C693 N694 G695 V696 L697 E698 G699 I700 R701 I702 C703 R704 K705 G706 F707 P708 S709 R710 L711 I712 Y713 S714 E715 F716 K717 Q718 R719 Y720 S721 I722 L723 A724 P725 N726 A727 I728 P729 GLN GLY PHE VAL D734 G735 K736 T737 V738 S739 E740 K741 I742 L743 A744 G745

• Molecule 1: MYOSIN HEAVY CHAIN, STRIATED MUSCLE

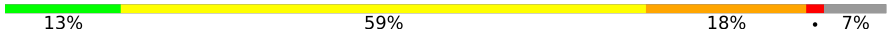
Chain 18-C:

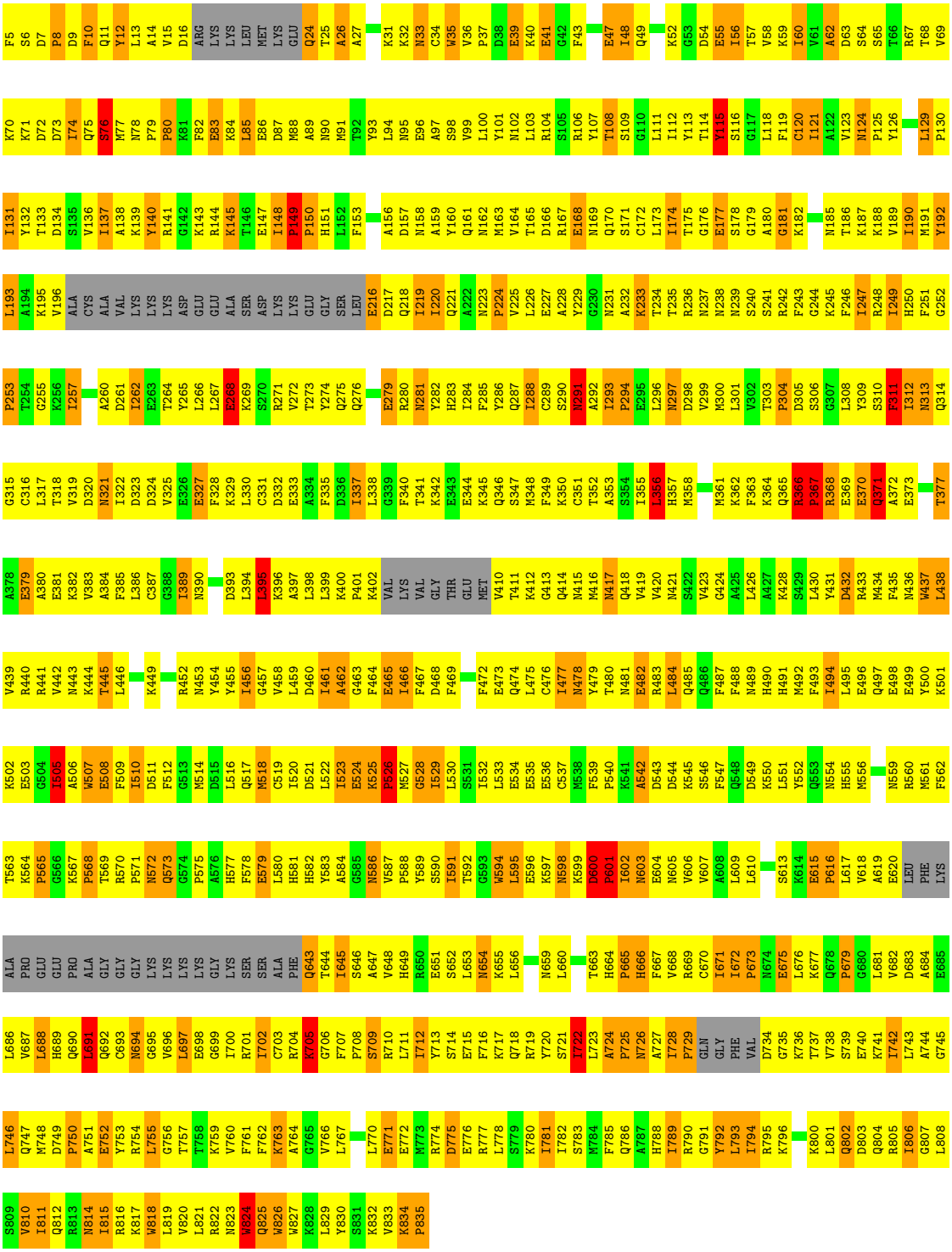




• Molecule 1: MYOSIN HEAVY CHAIN, STRIATED MUSCLE

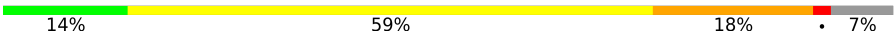
Chain 19-C:

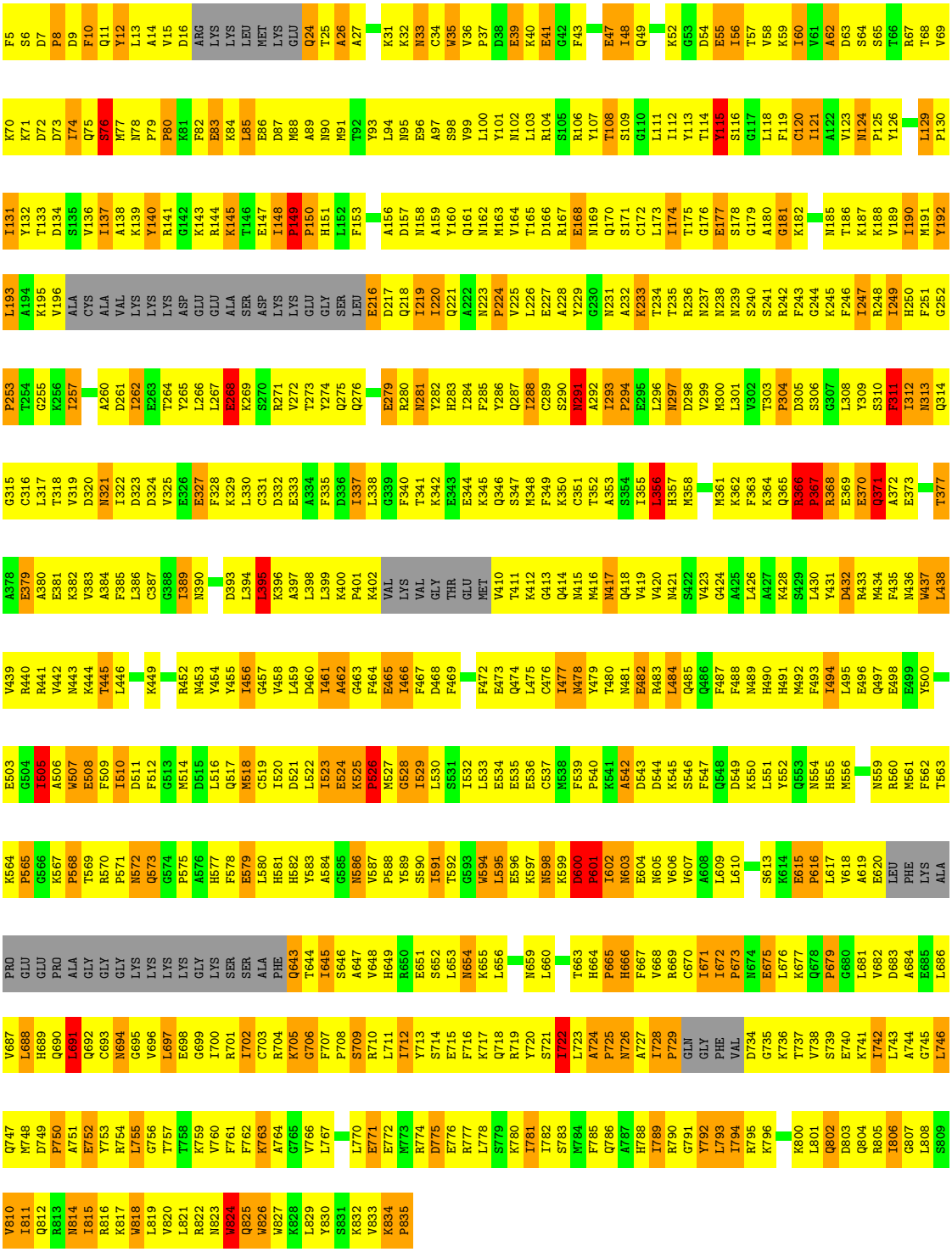




• Molecule 1: MYOSIN HEAVY CHAIN, STRIATED MUSCLE

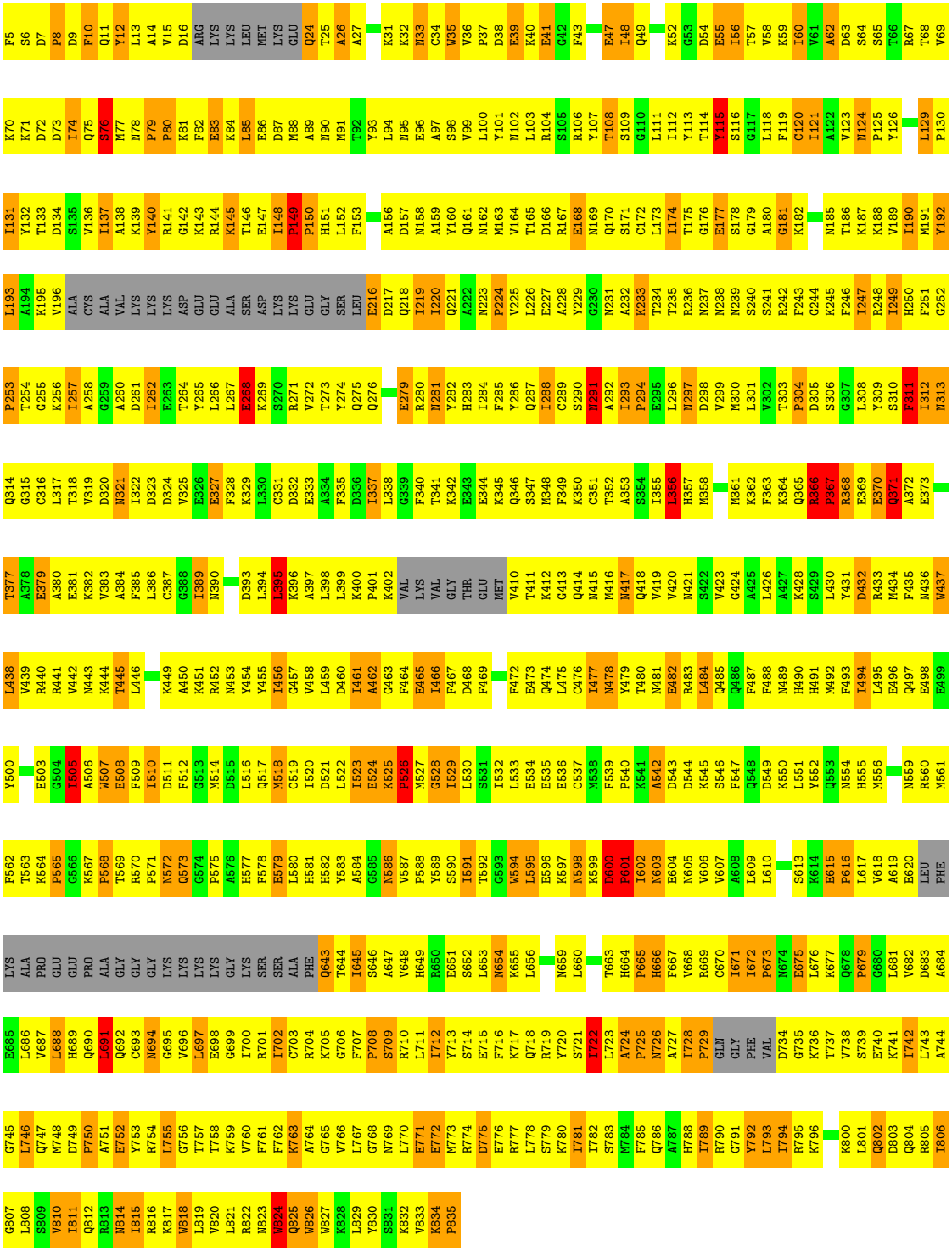
Chain 20-C:





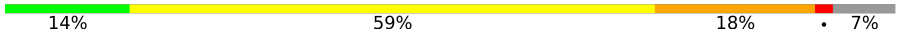
• Molecule 1: MYOSIN HEAVY CHAIN, STRIATED MUSCLE

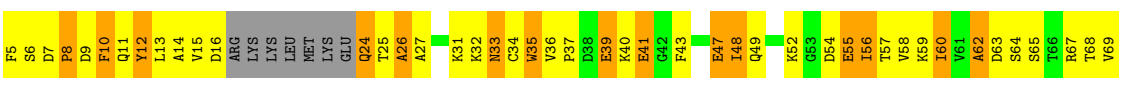
Chain 21-C:

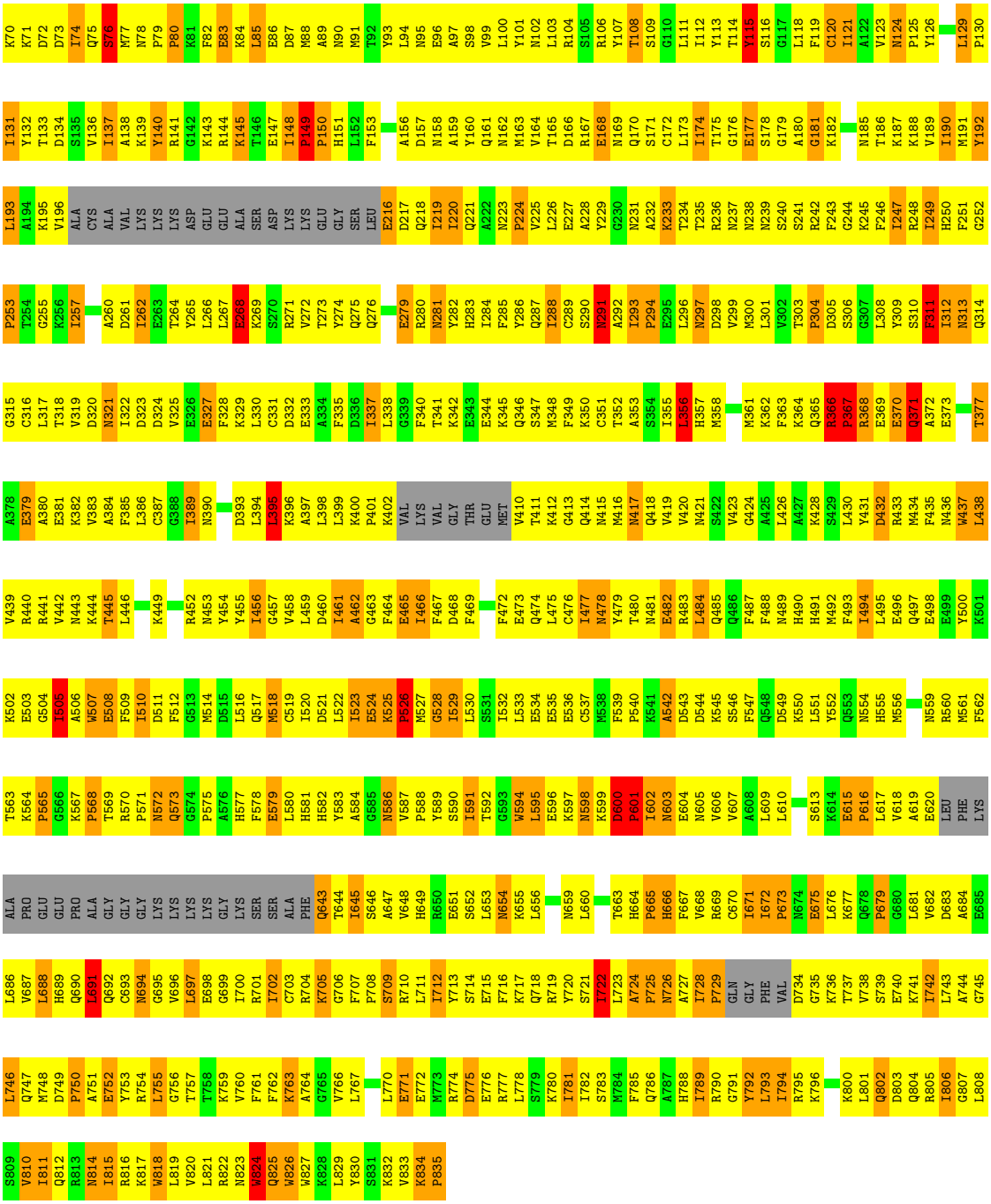


• Molecule 1: MYOSIN HEAVY CHAIN, STRIATED MUSCLE

Chain 22-C:

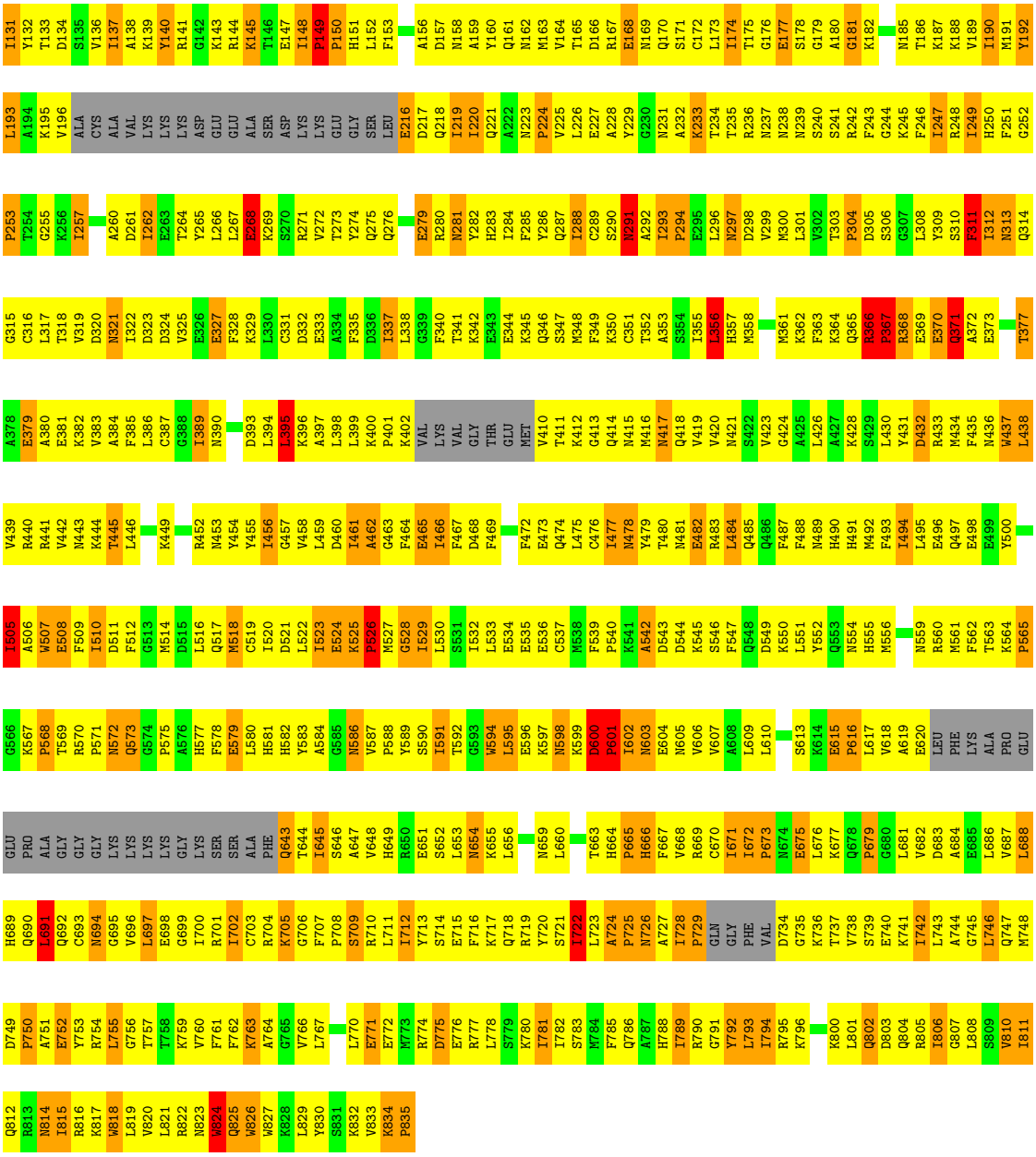






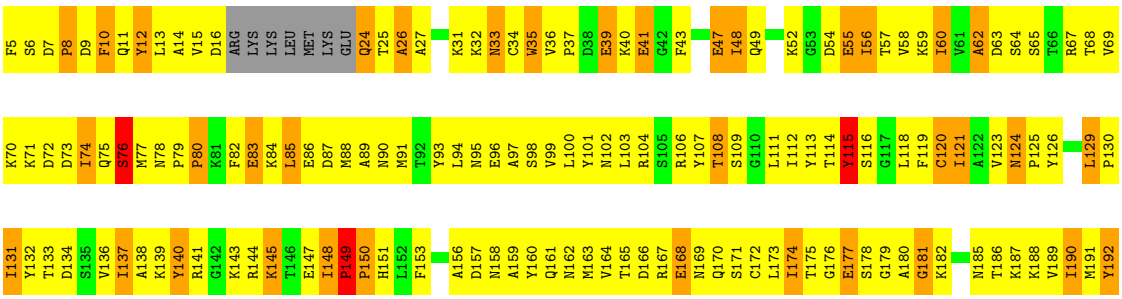
• Molecule 1: MYOSIN HEAVY CHAIN, STRIATED MUSCLE

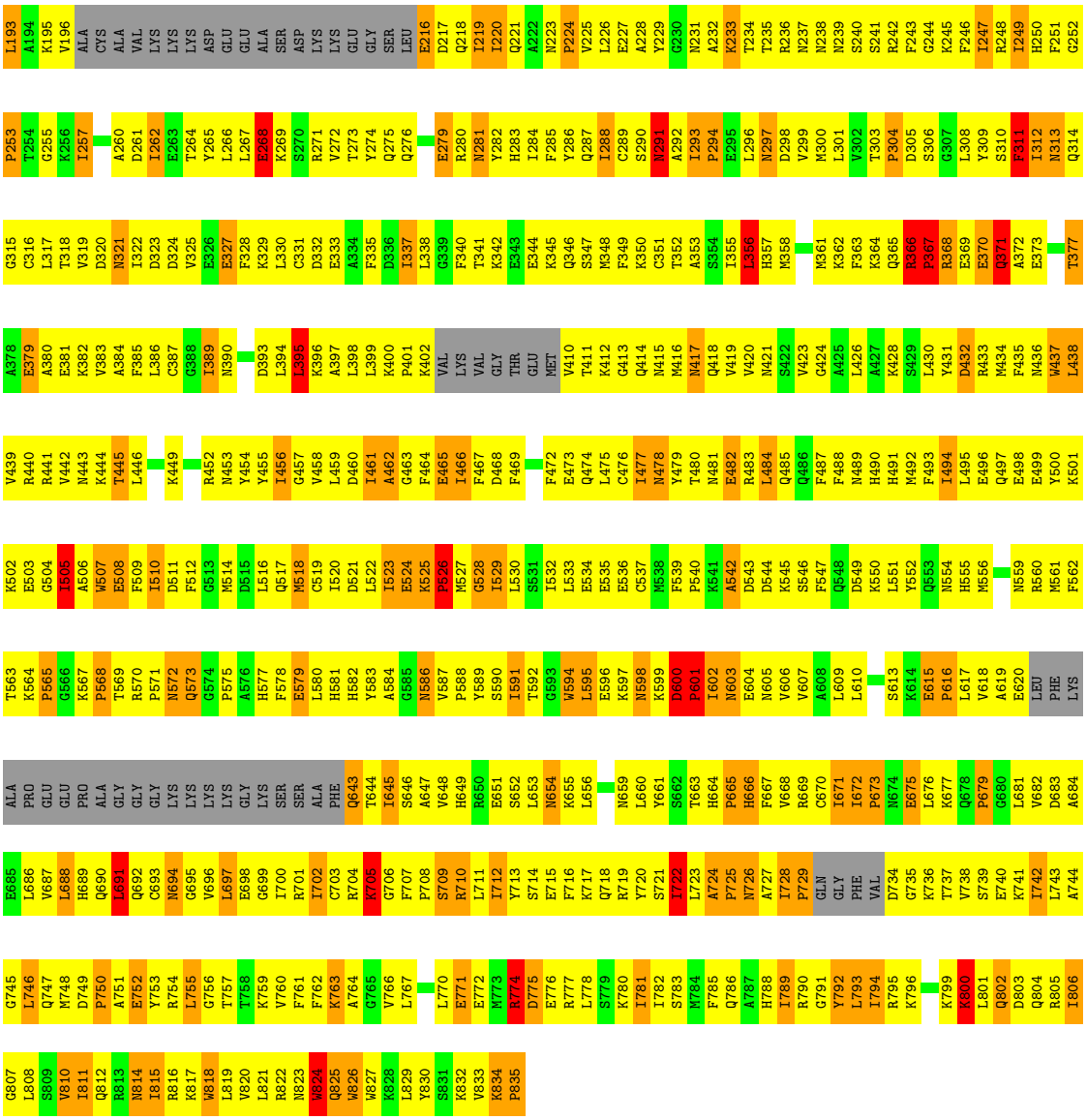
Chain 23-C:



• Molecule 1: MYOSIN HEAVY CHAIN, STRIATED MUSCLE

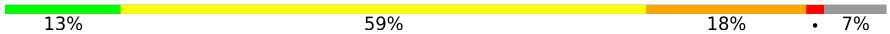
Chain 24-C: 13% 59% 18% • 7%

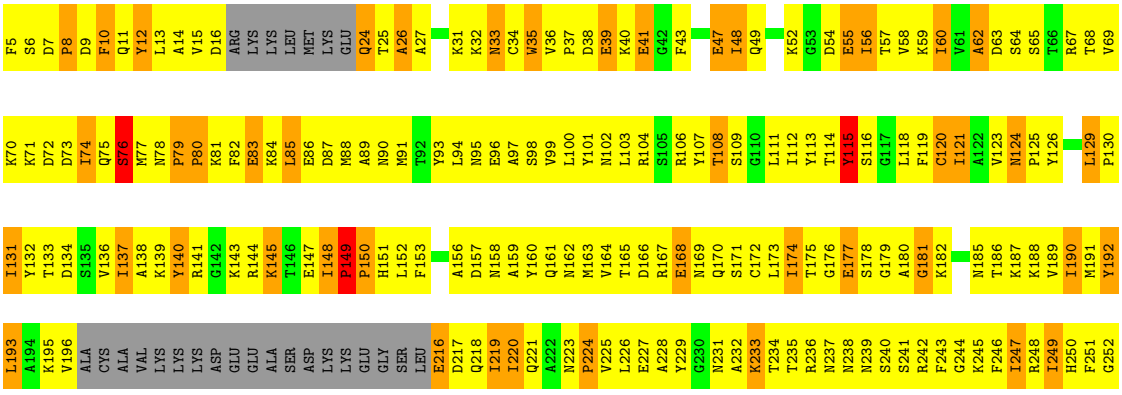


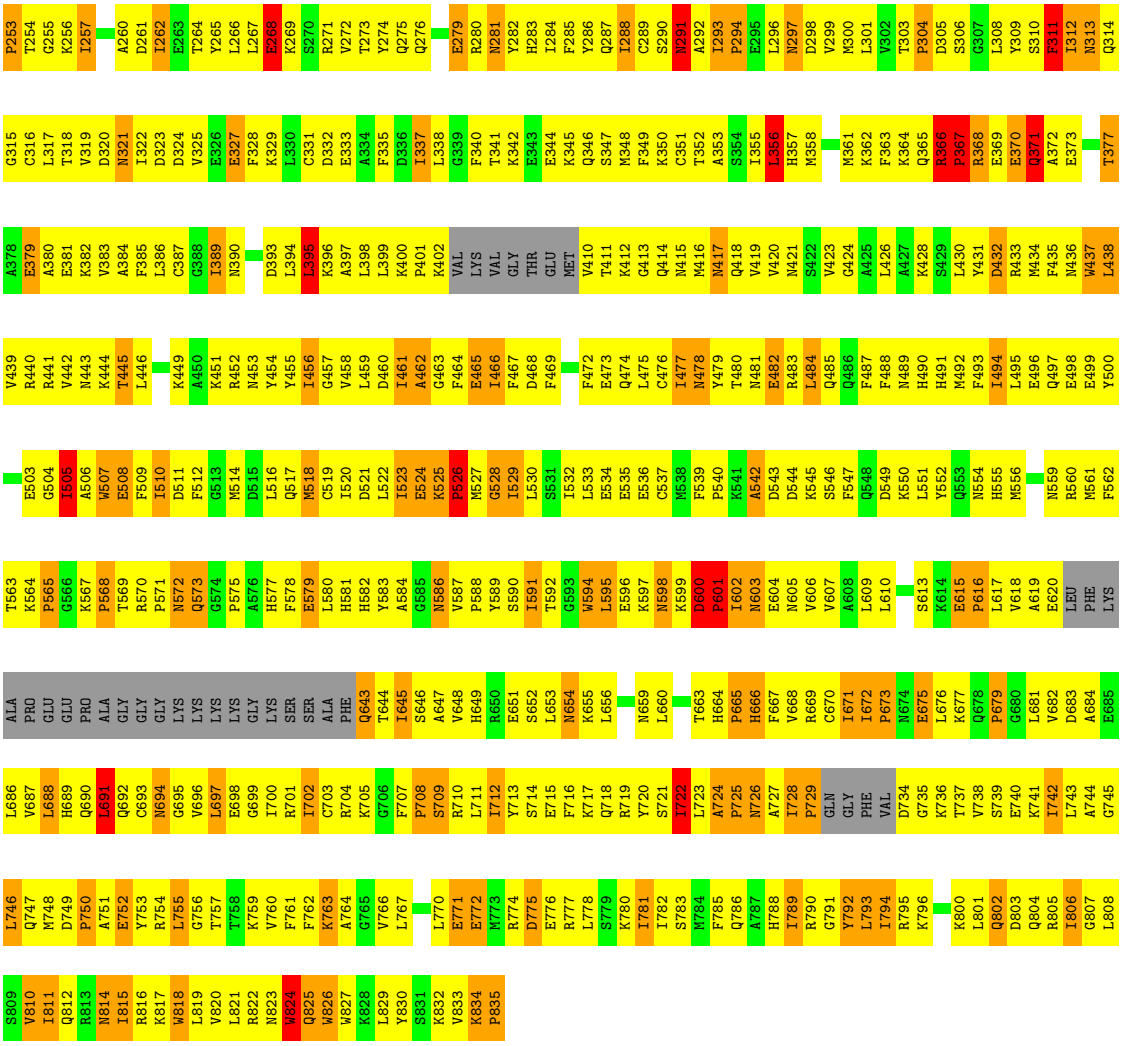


• Molecule 1: MYOSIN HEAVY CHAIN, STRIATED MUSCLE

Chain 25-C:

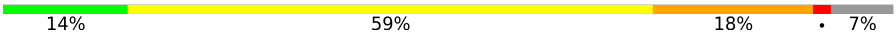


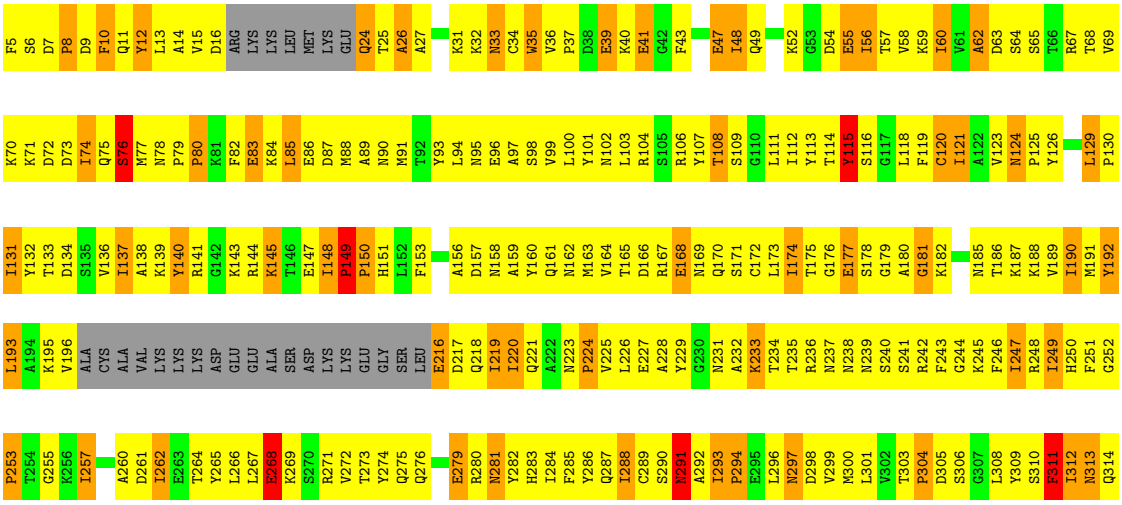


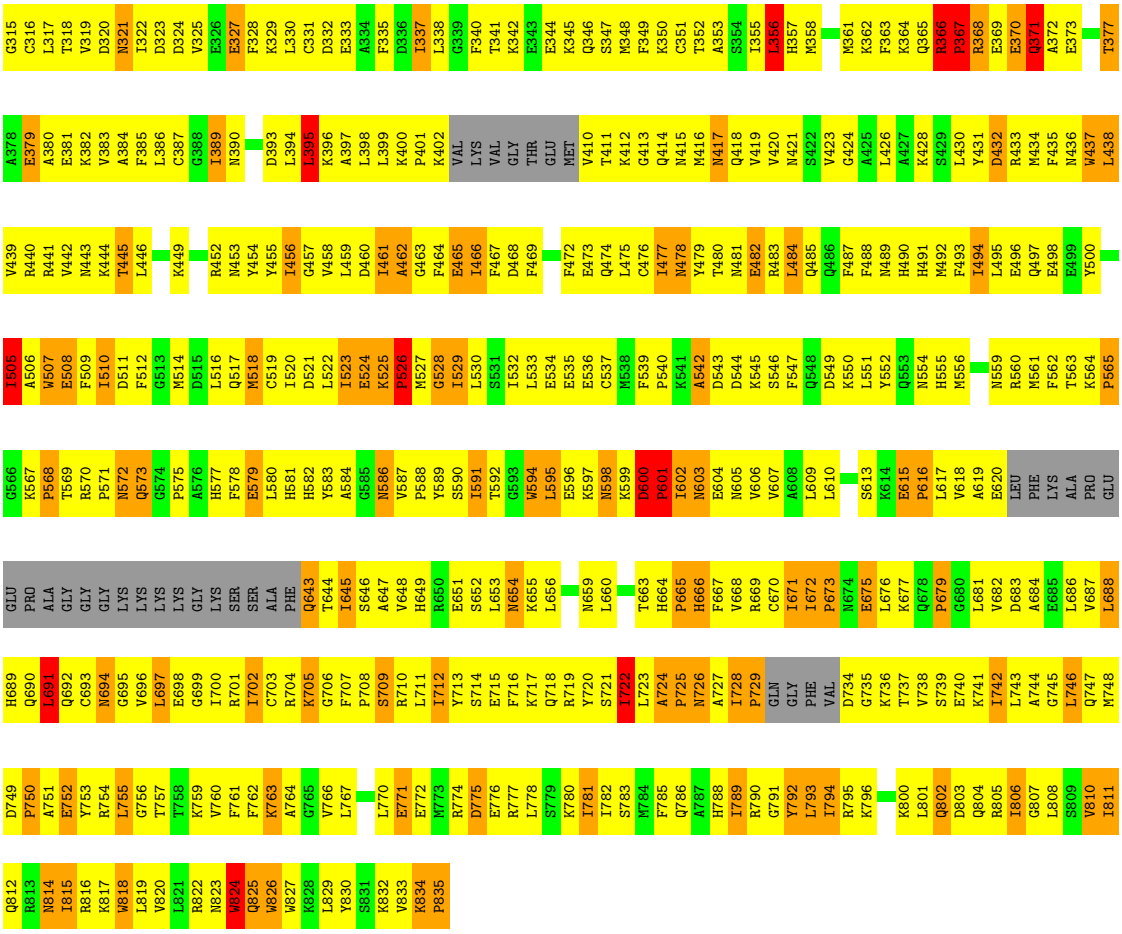


• Molecule 1: MYOSIN HEAVY CHAIN, STRIATED MUSCLE

Chain 26-C:

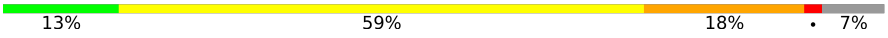


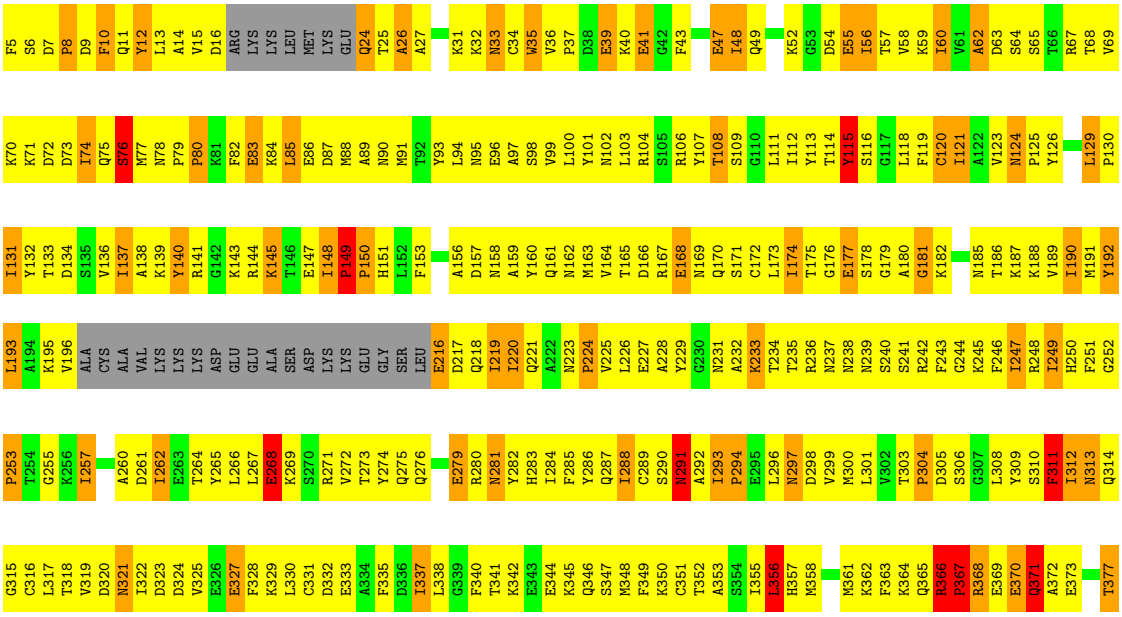


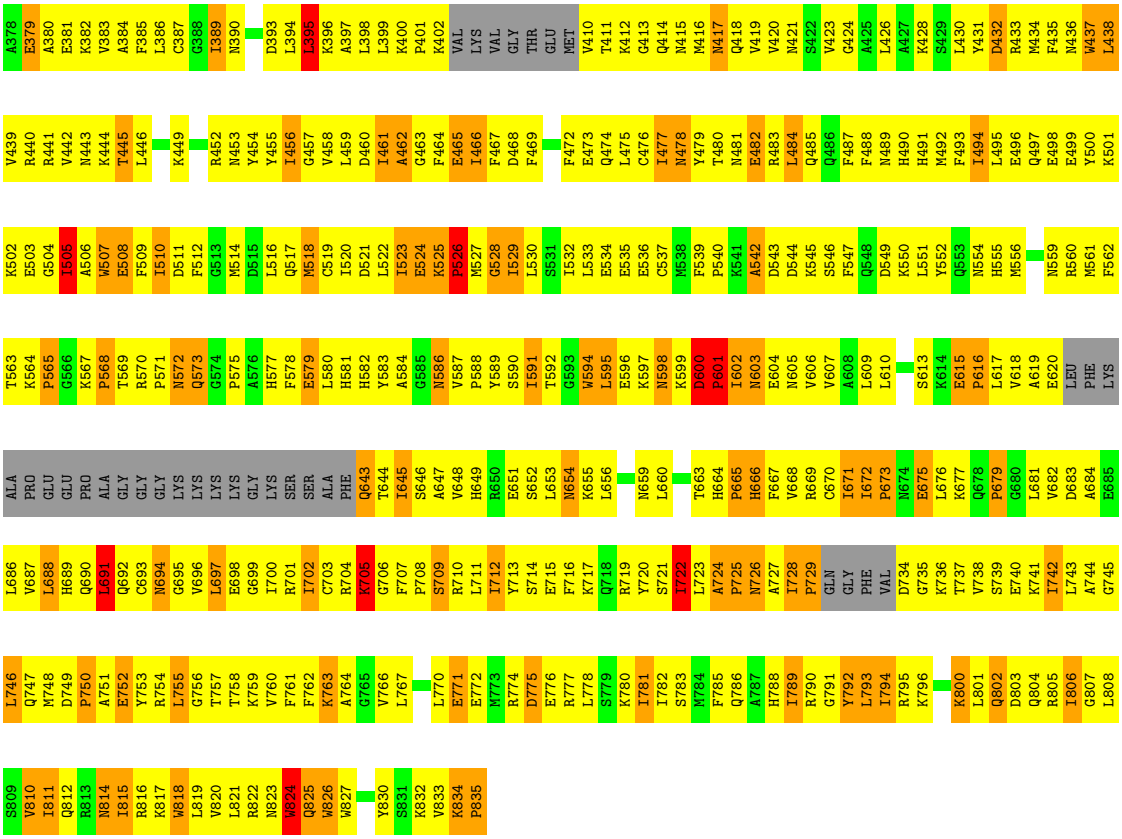


• Molecule 1: MYOSIN HEAVY CHAIN, STRIATED MUSCLE

Chain 27-C:

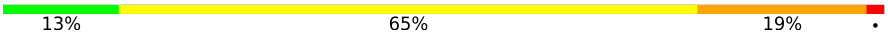


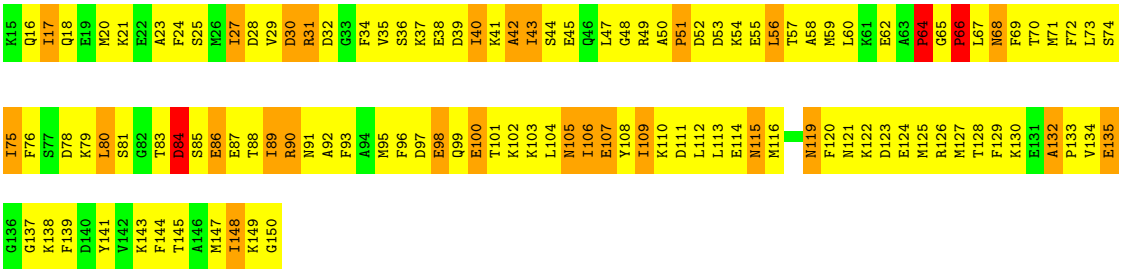




• Molecule 2: MYOSIN REGULATORY LIGHT CHAIN, STRIATED ADDUCTOR MUSCLE

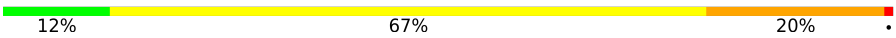
Chain 1-Y:

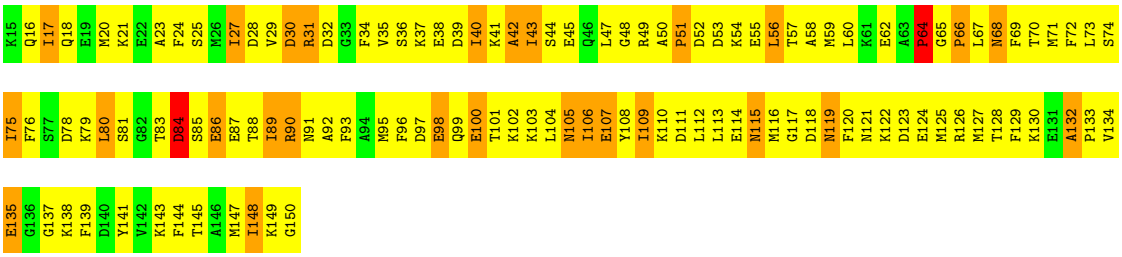




• Molecule 2: MYOSIN REGULATORY LIGHT CHAIN, STRIATED ADDUCTOR MUSCLE

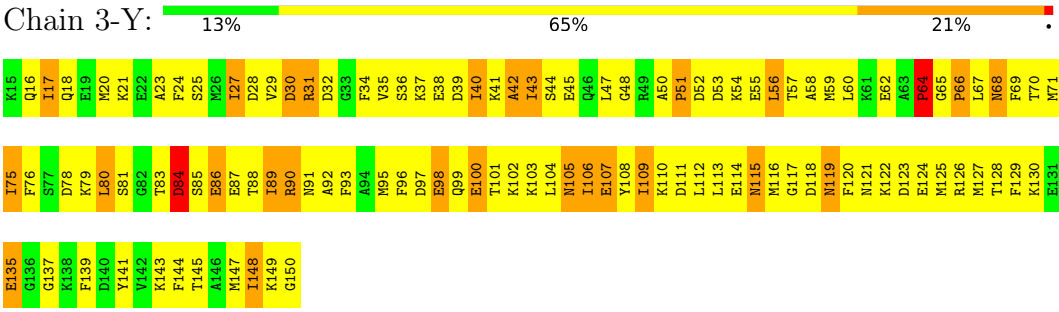
Chain 2-Y:





• Molecule 2: MYOSIN REGULATORY LIGHT CHAIN, STRIATED ADDUCTOR MUSCLE

Chain 3-Y:

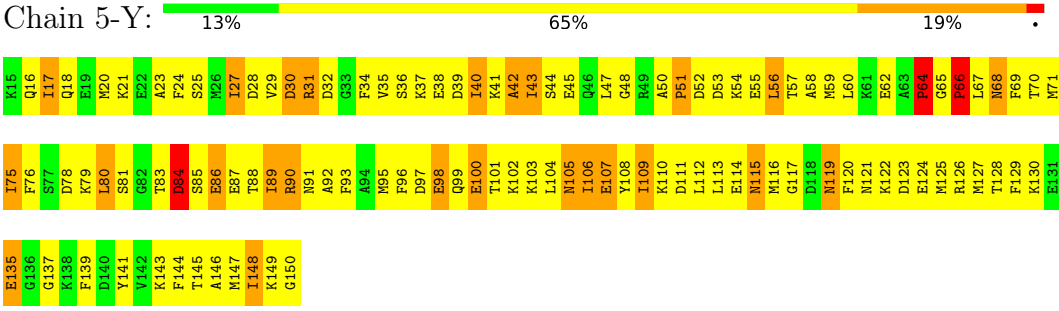


• Molecule 2: MYOSIN REGULATORY LIGHT CHAIN, STRIATED ADDUCTOR MUSCLE

Chain 4-Y:

• Molecule 2: MYOSIN REGULATORY LIGHT CHAIN, STRIATED ADDUCTOR MUSCLE

Chain 5-Y:

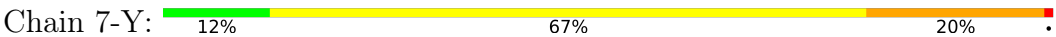


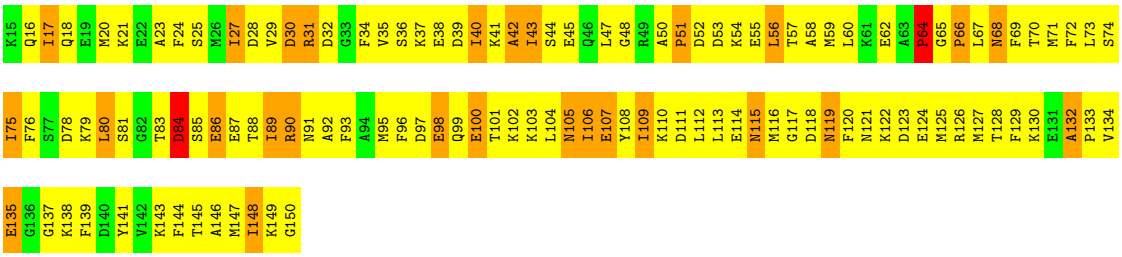
• Molecule 2: MYOSIN REGULATORY LIGHT CHAIN, STRIATED ADDUCTOR MUSCLE

Chain 6-Y:

• Molecule 2: MYOSIN REGULATORY LIGHT CHAIN, STRIATED ADDUCTOR MUSCLE

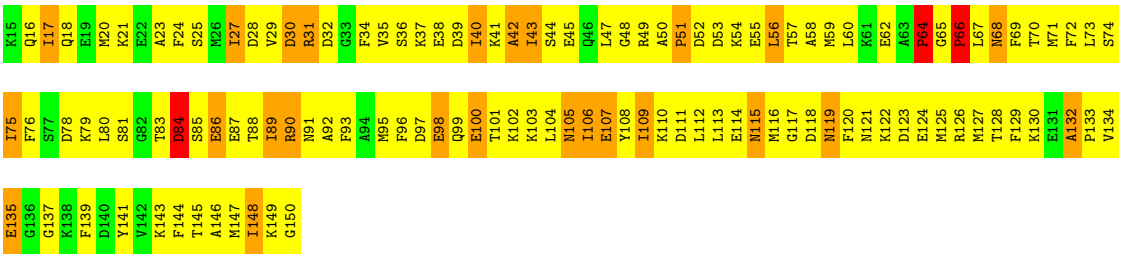
Chain 7-Y:





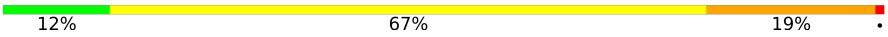
• Molecule 2: MYOSIN REGULATORY LIGHT CHAIN, STRIATED ADDUCTOR MUSCLE

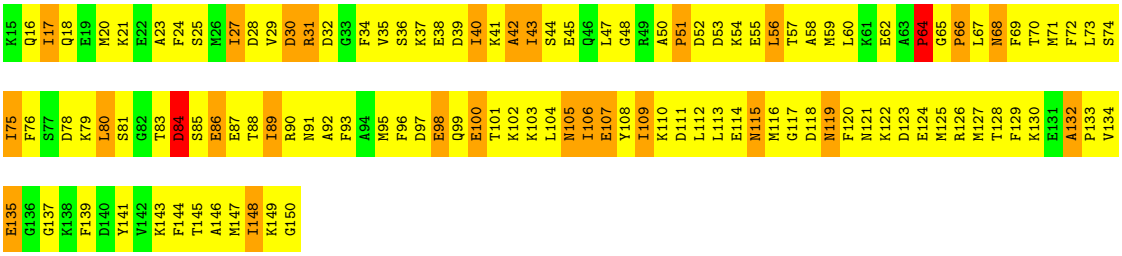
Chain 8-Y:



• Molecule 2: MYOSIN REGULATORY LIGHT CHAIN, STRIATED ADDUCTOR MUSCLE

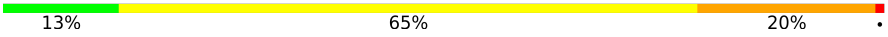
Chain 9-Y:

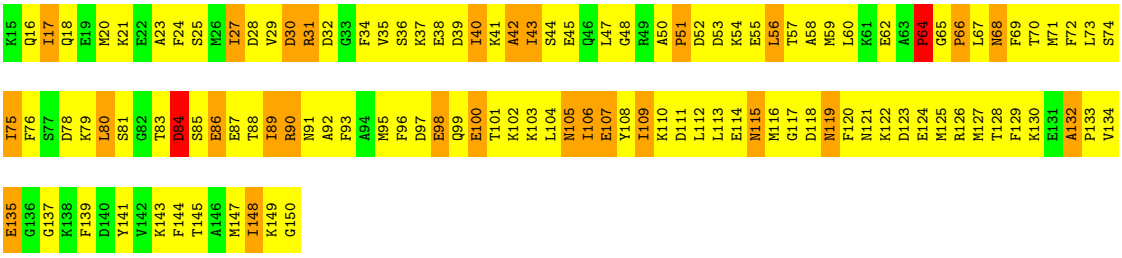




• Molecule 2: MYOSIN REGULATORY LIGHT CHAIN, STRIATED ADDUCTOR MUSCLE

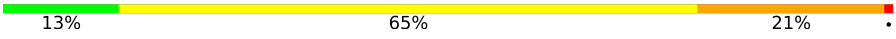
Chain 10-Y:

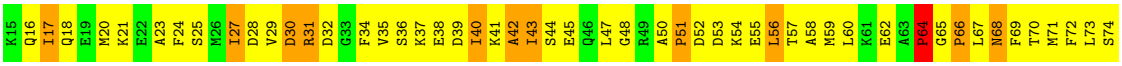




• Molecule 2: MYOSIN REGULATORY LIGHT CHAIN, STRIATED ADDUCTOR MUSCLE

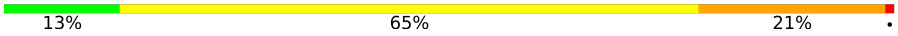
Chain 11-Y:

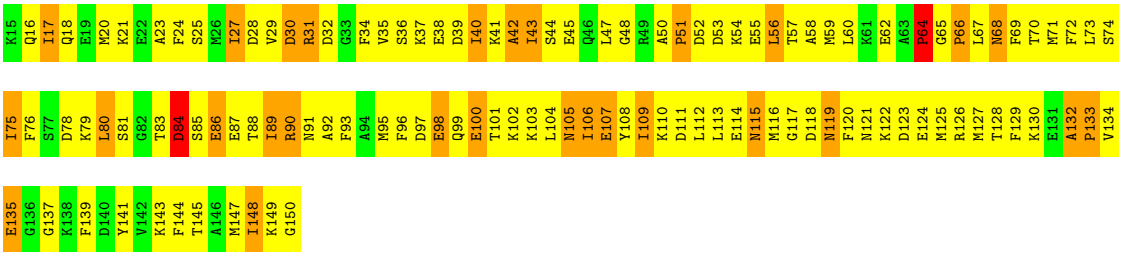




• Molecule 2: MYOSIN REGULATORY LIGHT CHAIN, STRIATED ADDUCTOR MUSCLE

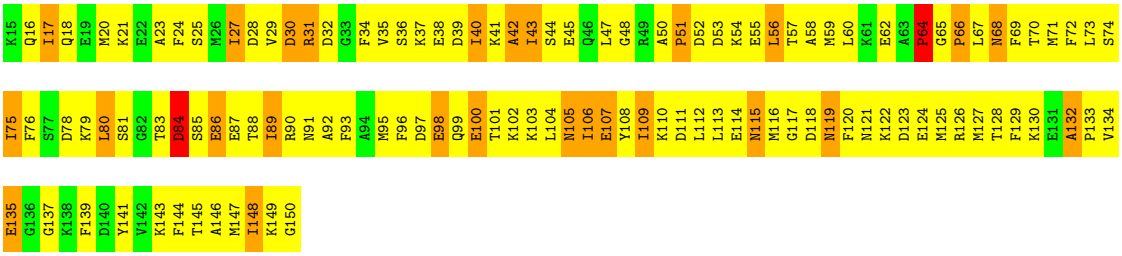
Chain 12-Y:





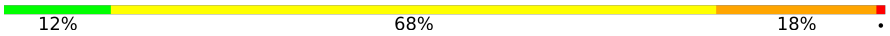
• Molecule 2: MYOSIN REGULATORY LIGHT CHAIN, STRIATED ADDUCTOR MUSCLE

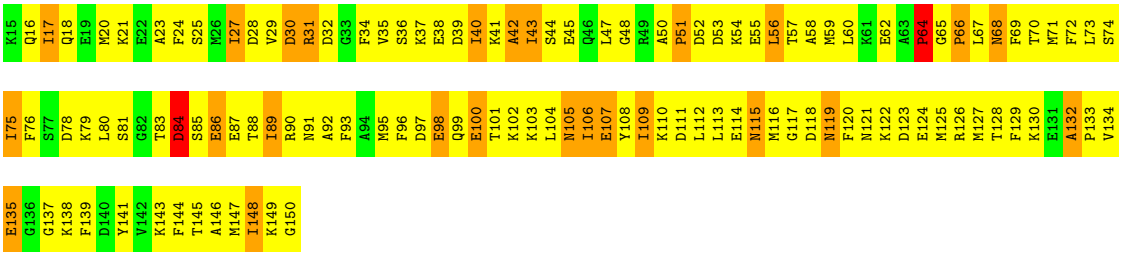
Chain 13-Y:



• Molecule 2: MYOSIN REGULATORY LIGHT CHAIN, STRIATED ADDUCTOR MUSCLE

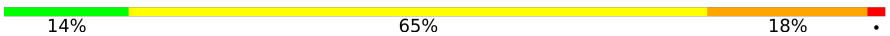
Chain 14-Y:





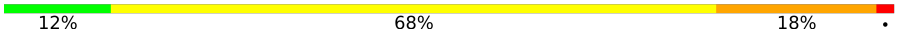
• Molecule 2: MYOSIN REGULATORY LIGHT CHAIN, STRIATED ADDUCTOR MUSCLE

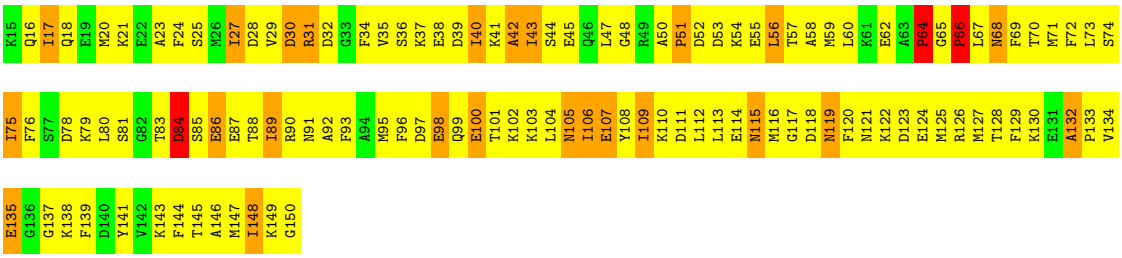
Chain 15-Y:



• Molecule 2: MYOSIN REGULATORY LIGHT CHAIN, STRIATED ADDUCTOR MUSCLE

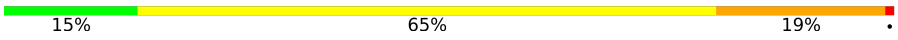
Chain 16-Y:

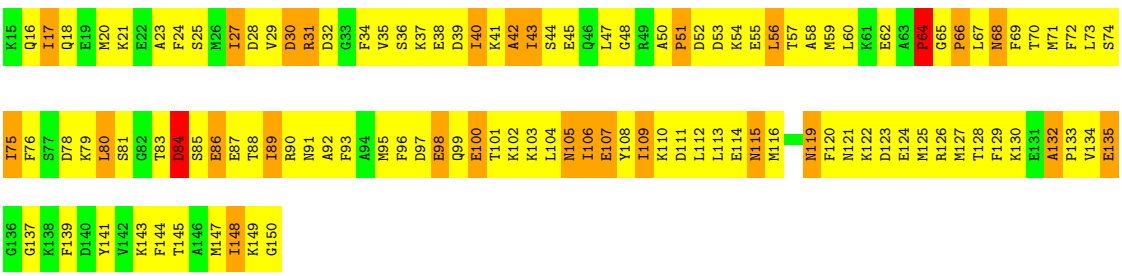




• Molecule 2: MYOSIN REGULATORY LIGHT CHAIN, STRIATED ADDUCTOR MUSCLE

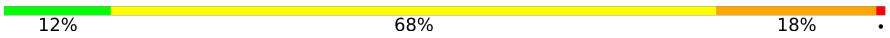
Chain 17-Y:

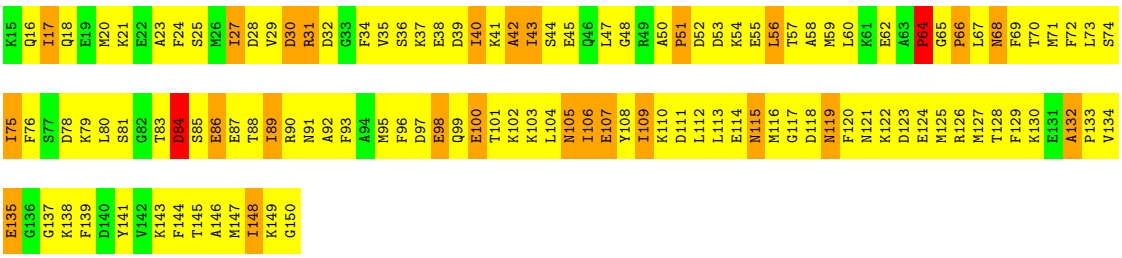




• Molecule 2: MYOSIN REGULATORY LIGHT CHAIN, STRIATED ADDUCTOR MUSCLE

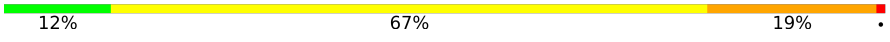
Chain 18-Y:

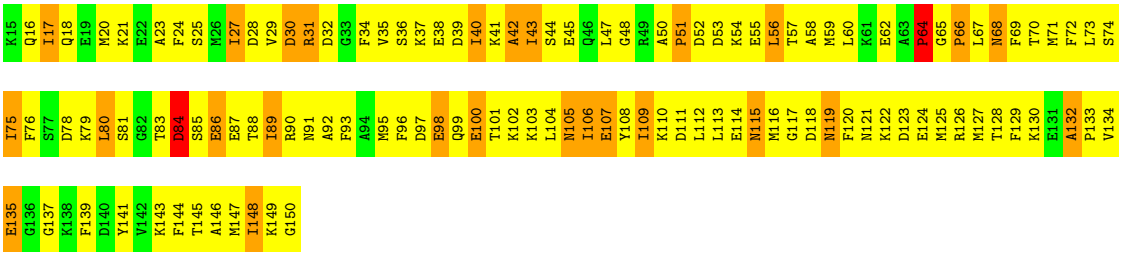




• Molecule 2: MYOSIN REGULATORY LIGHT CHAIN, STRIATED ADDUCTOR MUSCLE

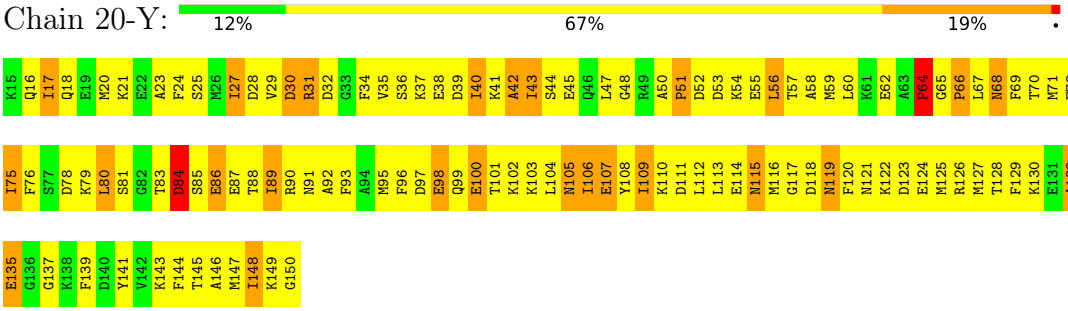
Chain 19-Y:





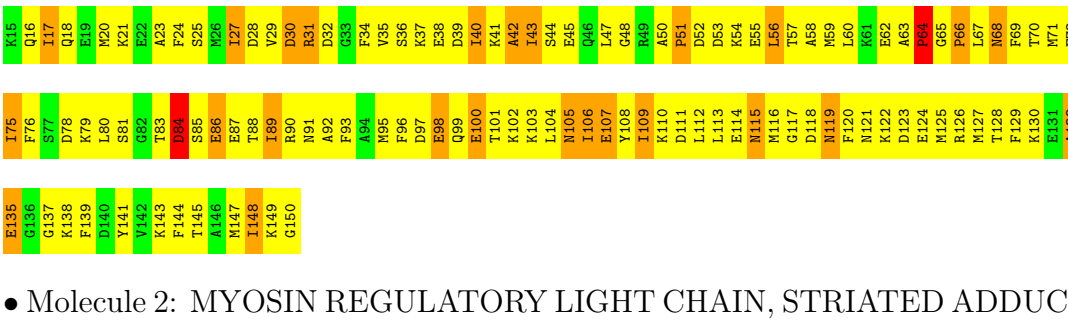
• Molecule 2: MYOSIN REGULATORY LIGHT CHAIN, STRIATED ADDUCTOR MUSCLE

Chain 20-Y:



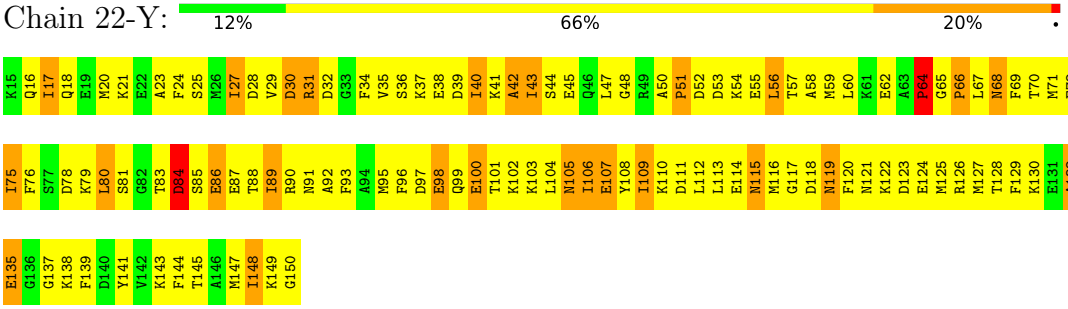
• Molecule 2: MYOSIN REGULATORY LIGHT CHAIN, STRIATED ADDUCTOR MUSCLE

Chain 21-Y:



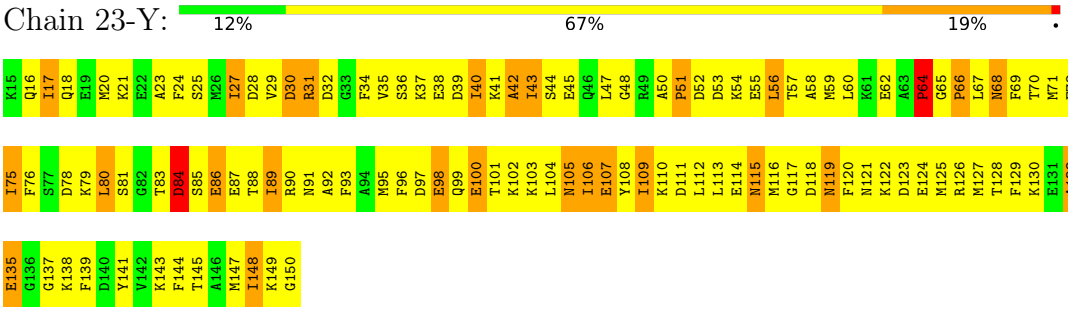
• Molecule 2: MYOSIN REGULATORY LIGHT CHAIN, STRIATED ADDUCTOR MUSCLE

Chain 22-Y:



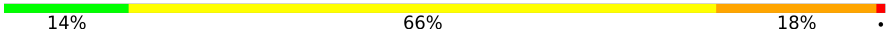
• Molecule 2: MYOSIN REGULATORY LIGHT CHAIN, STRIATED ADDUCTOR MUSCLE

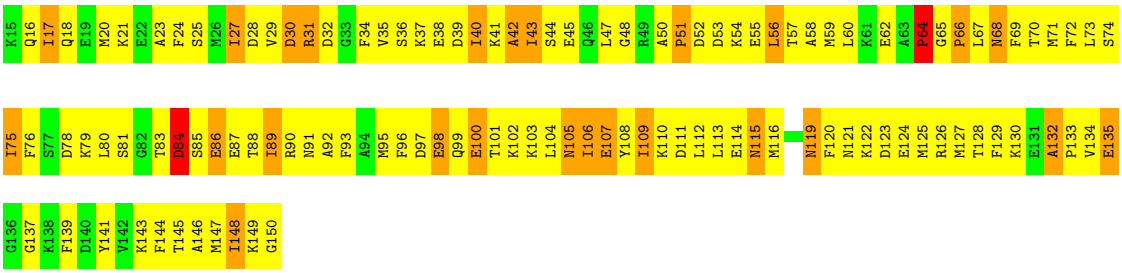
Chain 23-Y:



• Molecule 2: MYOSIN REGULATORY LIGHT CHAIN, STRIATED ADDUCTOR MUSCLE

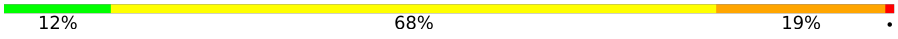
Chain 24-Y:

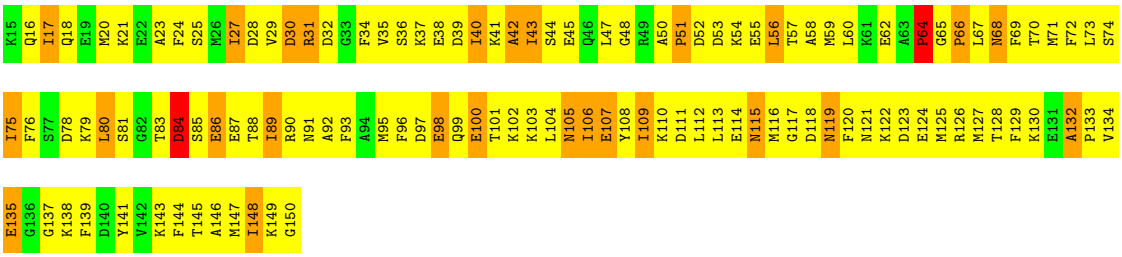




• Molecule 2: MYOSIN REGULATORY LIGHT CHAIN, STRIATED ADDUCTOR MUSCLE

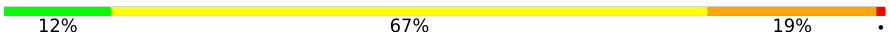
Chain 25-Y:





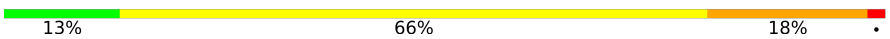
• Molecule 2: MYOSIN REGULATORY LIGHT CHAIN, STRIATED ADDUCTOR MUSCLE

Chain 26-Y:



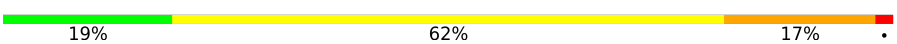
• Molecule 2: MYOSIN REGULATORY LIGHT CHAIN, STRIATED ADDUCTOR MUSCLE

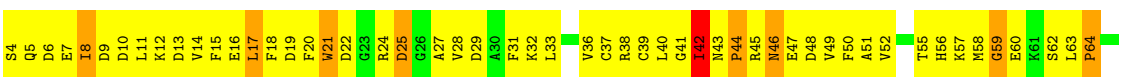
Chain 27-Y:

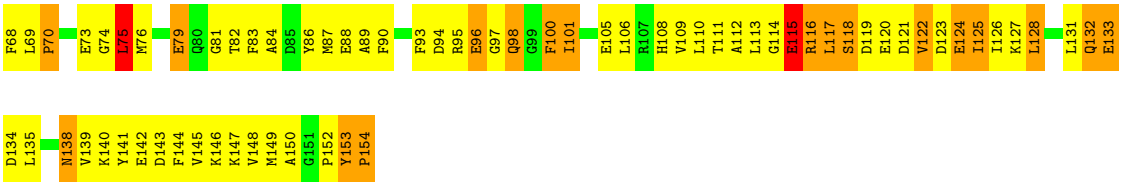


• Molecule 3: MYOSIN ESSENTIAL LIGHT CHAIN, STRIATED ADDUCTOR MUSCLE

Chain 1-Z:

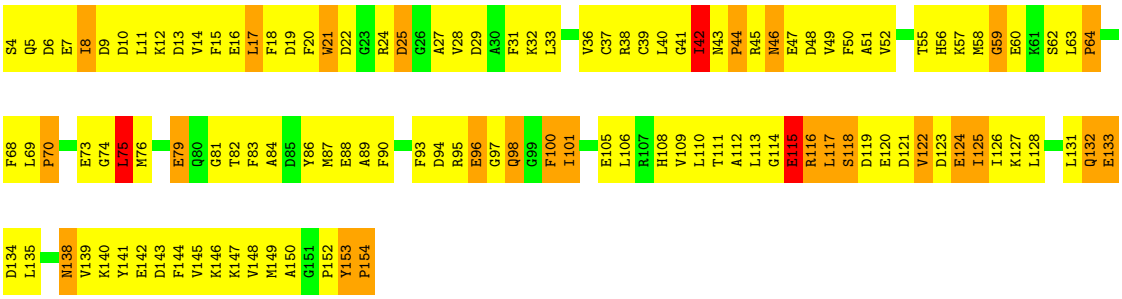






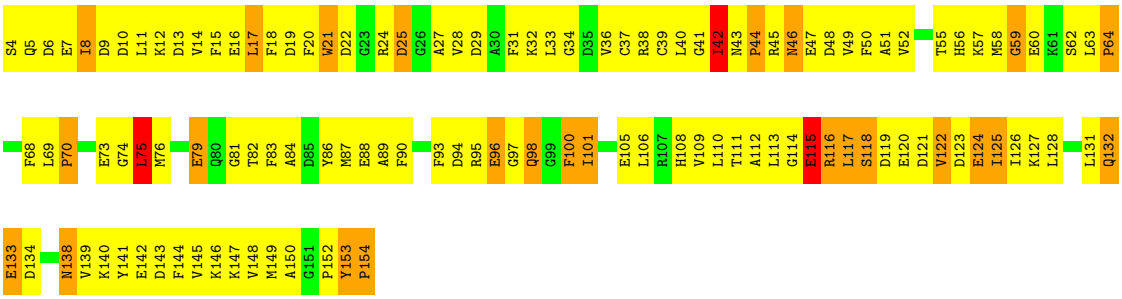
• Molecule 3: MYOSIN ESSENTIAL LIGHT CHAIN, STRIATED ADDUCTOR MUSCLE

Chain 2-Z: 19% 62% 17%



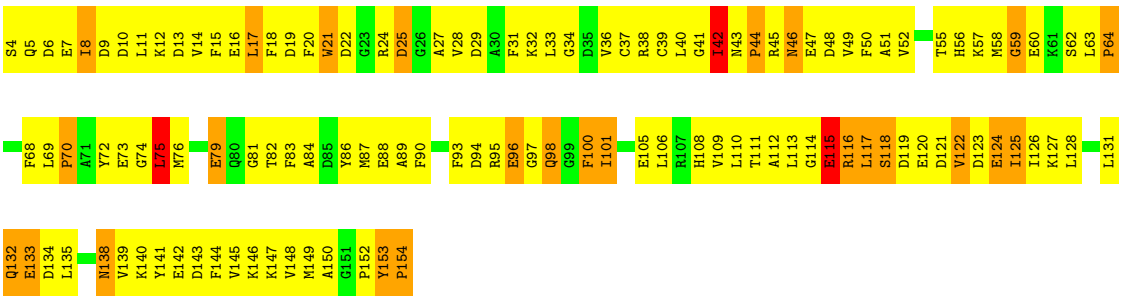
• Molecule 3: MYOSIN ESSENTIAL LIGHT CHAIN, STRIATED ADDUCTOR MUSCLE

Chain 3-Z: 19% 62% 17%



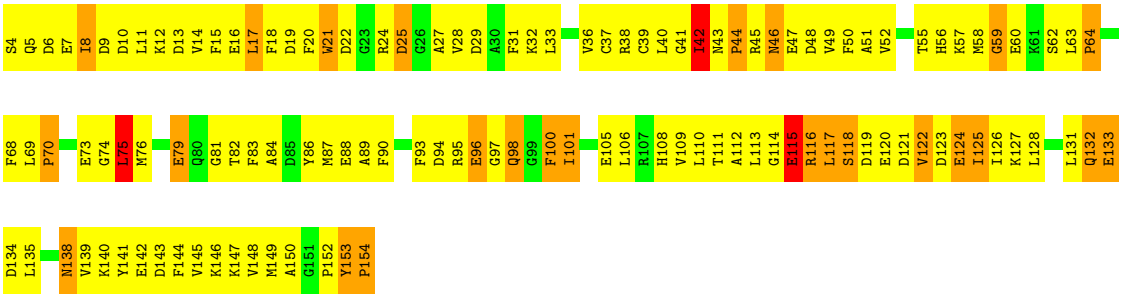
• Molecule 3: MYOSIN ESSENTIAL LIGHT CHAIN, STRIATED ADDUCTOR MUSCLE

Chain 4-Z: 18% 64% 17%



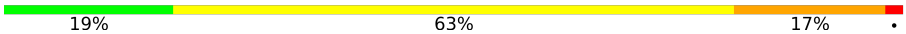
• Molecule 3: MYOSIN ESSENTIAL LIGHT CHAIN, STRIATED ADDUCTOR MUSCLE

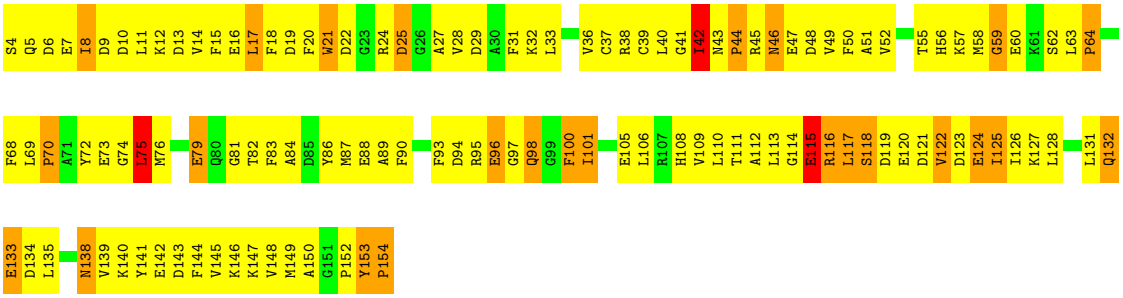
Chain 5-Z: 19% 62% 17%



• Molecule 3: MYOSIN ESSENTIAL LIGHT CHAIN, STRIATED ADDUCTOR MUSCLE

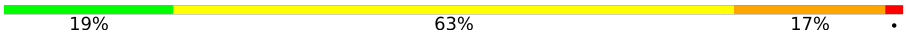
Chain 6-Z:

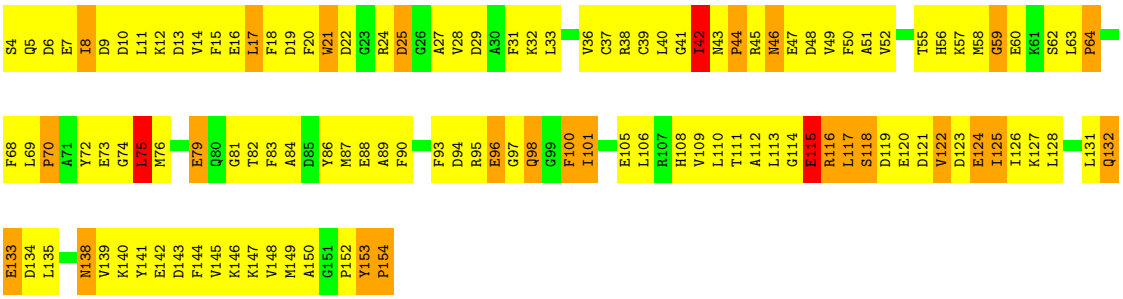




• Molecule 3: MYOSIN ESSENTIAL LIGHT CHAIN, STRIATED ADDUCTOR MUSCLE

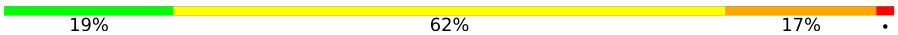
Chain 7-Z:

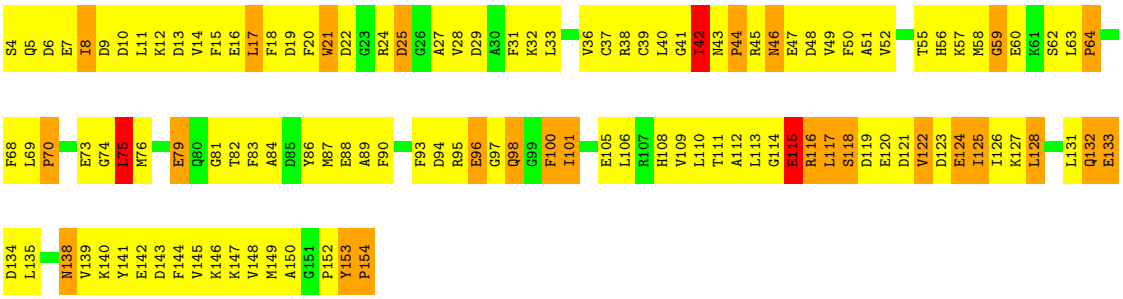




• Molecule 3: MYOSIN ESSENTIAL LIGHT CHAIN, STRIATED ADDUCTOR MUSCLE

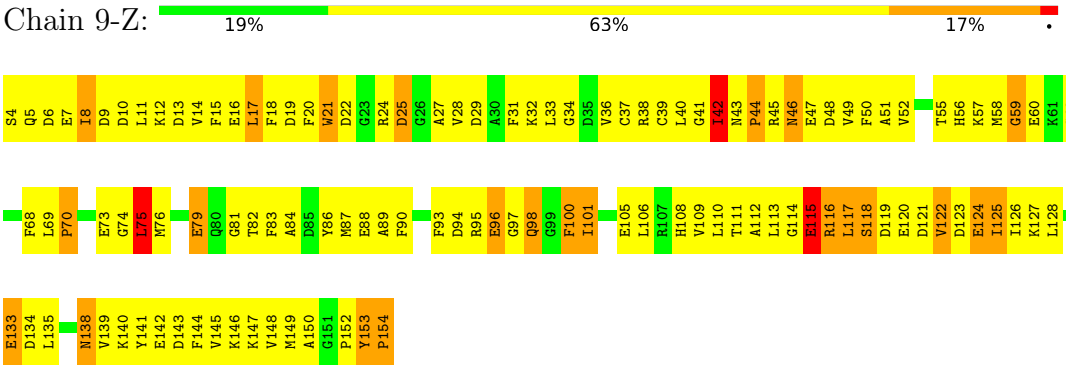
Chain 8-Z:





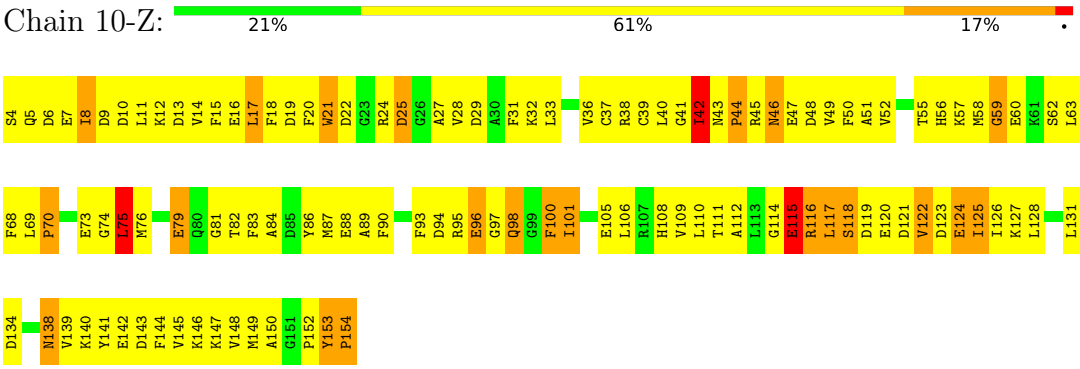
• Molecule 3: MYOSIN ESSENTIAL LIGHT CHAIN, STRIATED ADDUCTOR MUSCLE

Chain 9-Z:



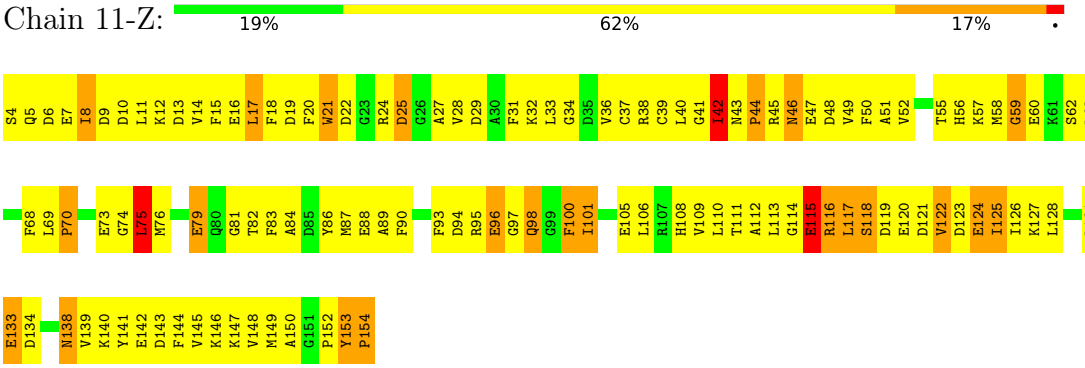
• Molecule 3: MYOSIN ESSENTIAL LIGHT CHAIN, STRIATED ADDUCTOR MUSCLE

Chain 10-Z:



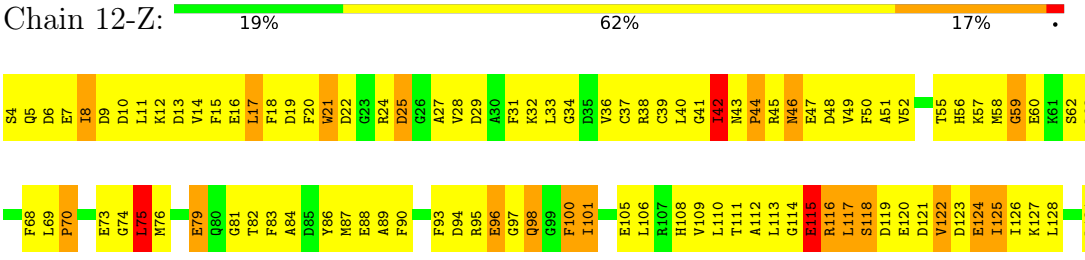
• Molecule 3: MYOSIN ESSENTIAL LIGHT CHAIN, STRIATED ADDUCTOR MUSCLE

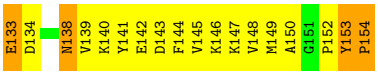
Chain 11-Z:



• Molecule 3: MYOSIN ESSENTIAL LIGHT CHAIN, STRIATED ADDUCTOR MUSCLE

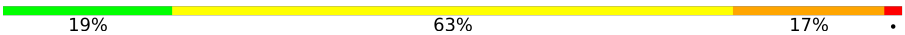
Chain 12-Z:

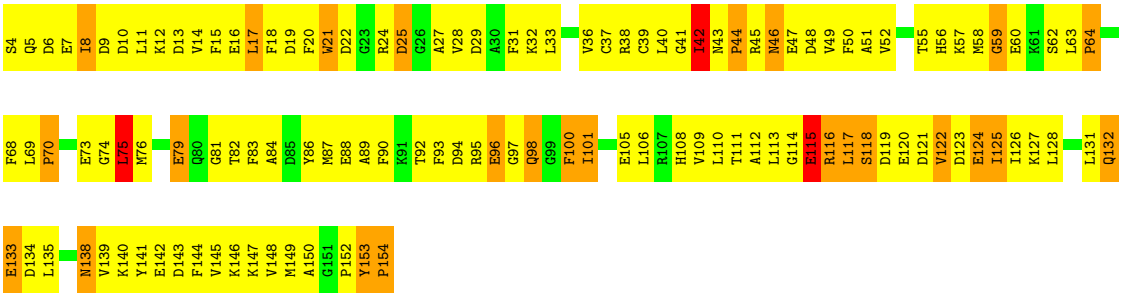




• Molecule 3: MYOSIN ESSENTIAL LIGHT CHAIN, STRIATED ADDUCTOR MUSCLE

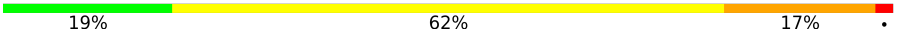
Chain 13-Z:

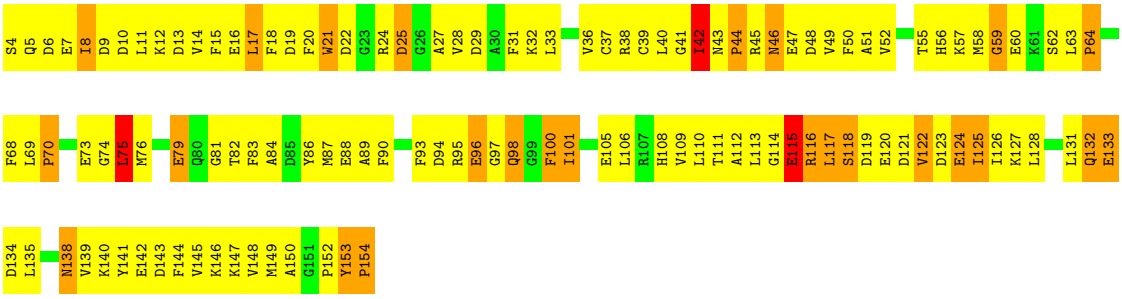




• Molecule 3: MYOSIN ESSENTIAL LIGHT CHAIN, STRIATED ADDUCTOR MUSCLE

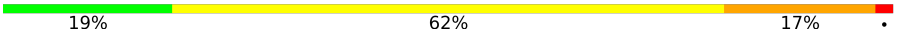
Chain 14-Z:

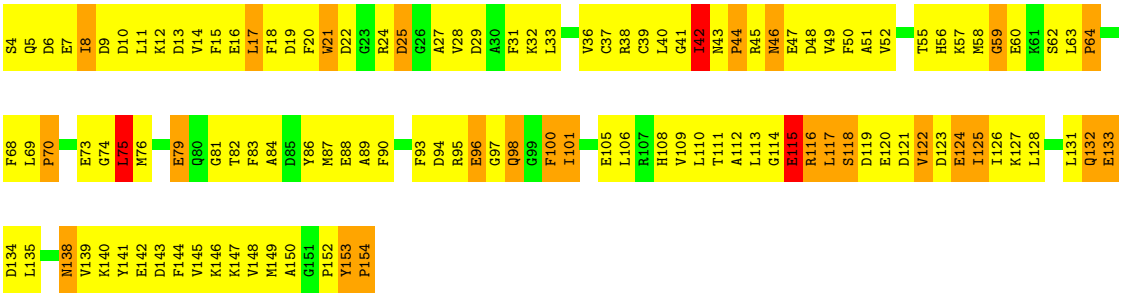




• Molecule 3: MYOSIN ESSENTIAL LIGHT CHAIN, STRIATED ADDUCTOR MUSCLE

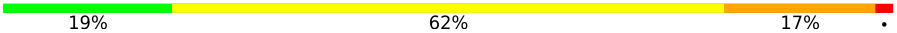
Chain 15-Z:

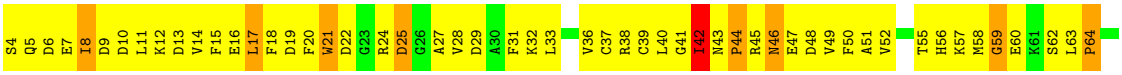


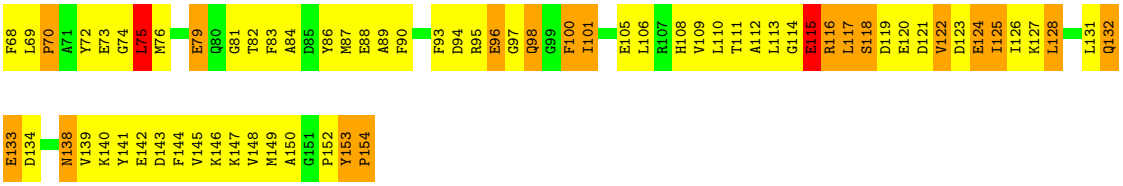


• Molecule 3: MYOSIN ESSENTIAL LIGHT CHAIN, STRIATED ADDUCTOR MUSCLE

Chain 16-Z:

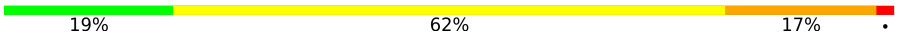


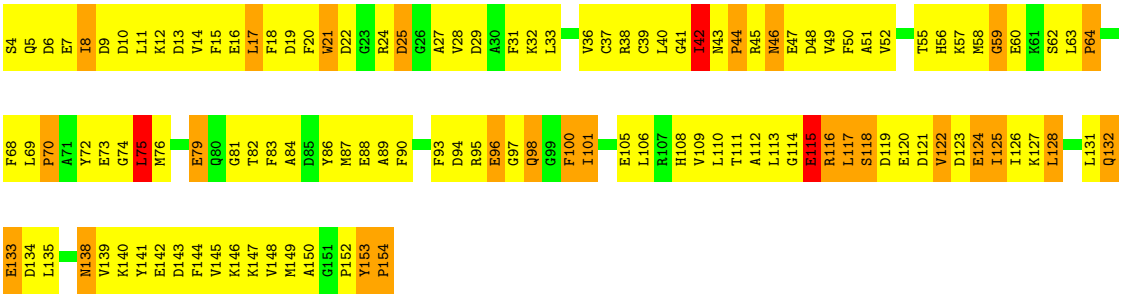




• Molecule 3: MYOSIN ESSENTIAL LIGHT CHAIN, STRIATED ADDUCTOR MUSCLE

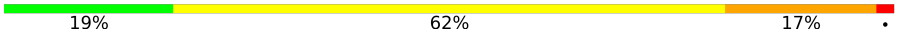
Chain 17-Z:

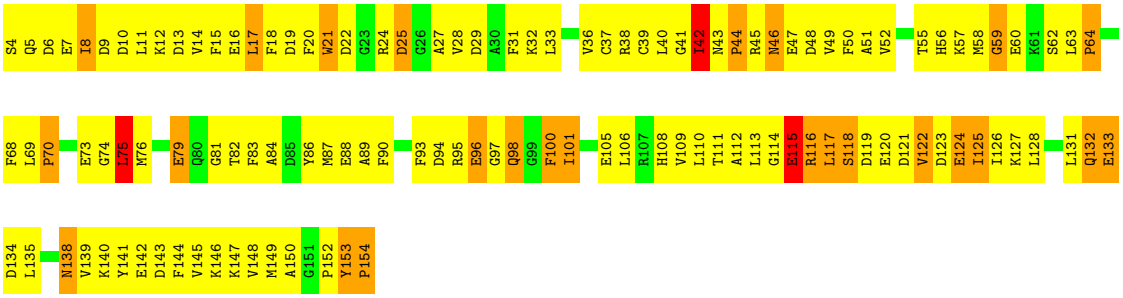




• Molecule 3: MYOSIN ESSENTIAL LIGHT CHAIN, STRIATED ADDUCTOR MUSCLE

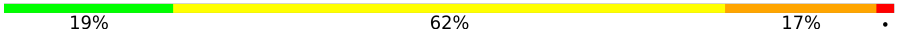
Chain 18-Z:

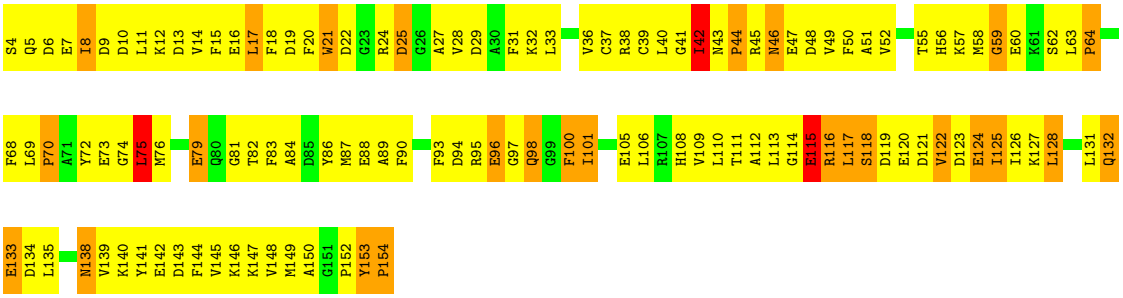




• Molecule 3: MYOSIN ESSENTIAL LIGHT CHAIN, STRIATED ADDUCTOR MUSCLE

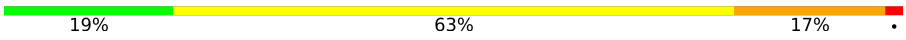
Chain 19-Z:

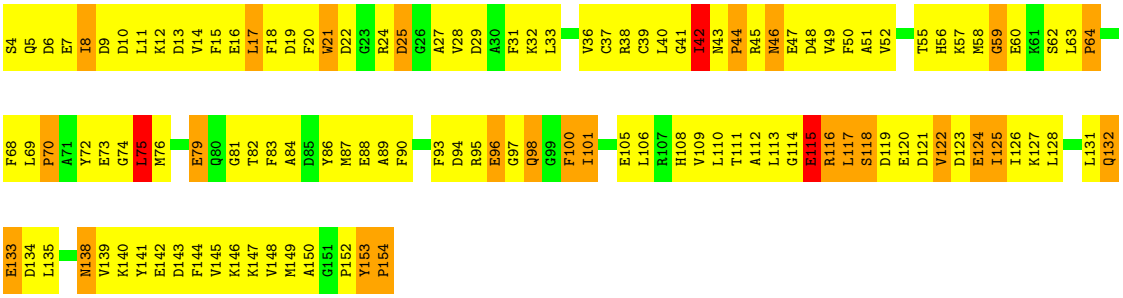




• Molecule 3: MYOSIN ESSENTIAL LIGHT CHAIN, STRIATED ADDUCTOR MUSCLE

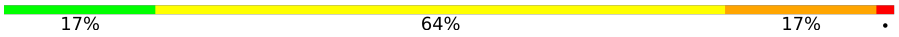
Chain 20-Z:

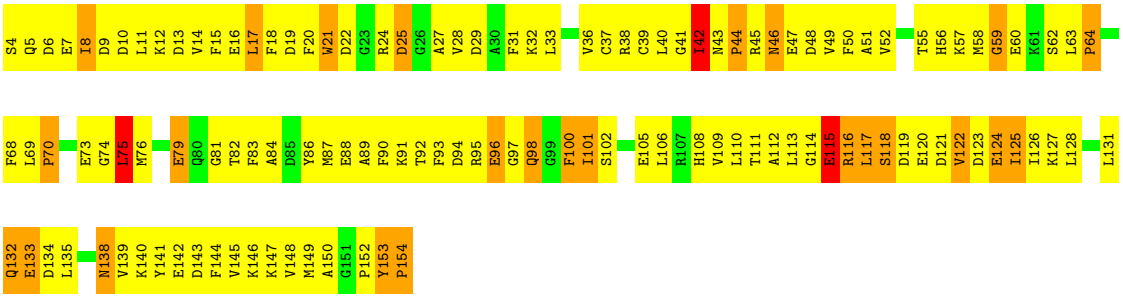




• Molecule 3: MYOSIN ESSENTIAL LIGHT CHAIN, STRIATED ADDUCTOR MUSCLE

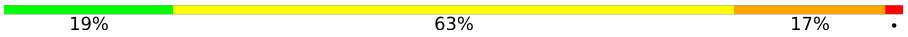
Chain 21-Z:

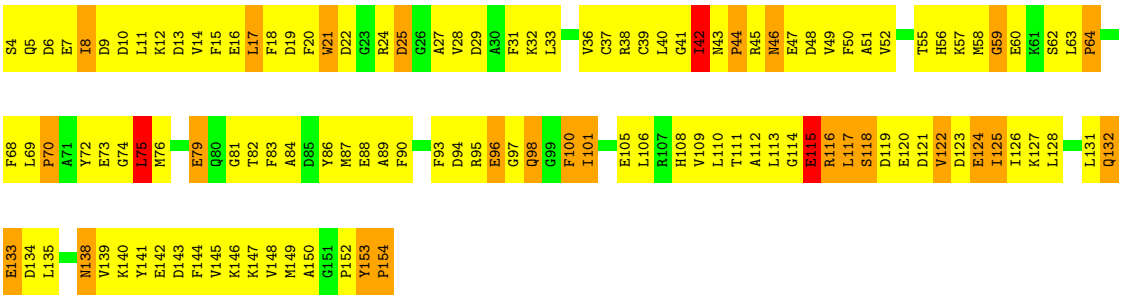




• Molecule 3: MYOSIN ESSENTIAL LIGHT CHAIN, STRIATED ADDUCTOR MUSCLE

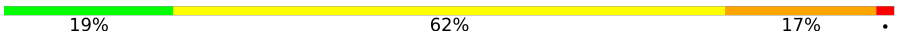
Chain 22-Z:

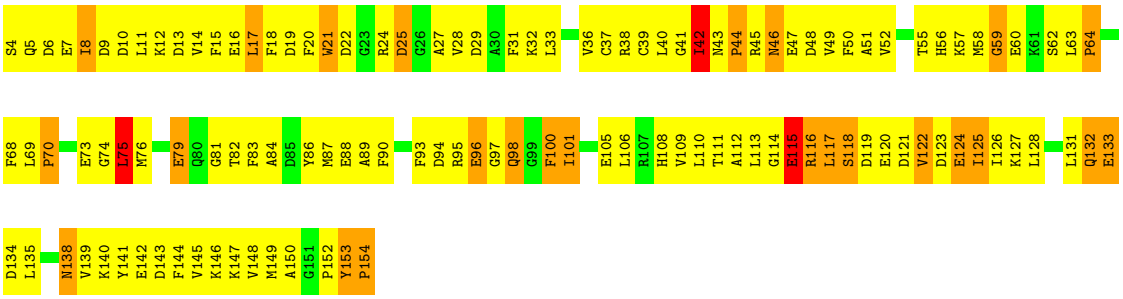




• Molecule 3: MYOSIN ESSENTIAL LIGHT CHAIN, STRIATED ADDUCTOR MUSCLE

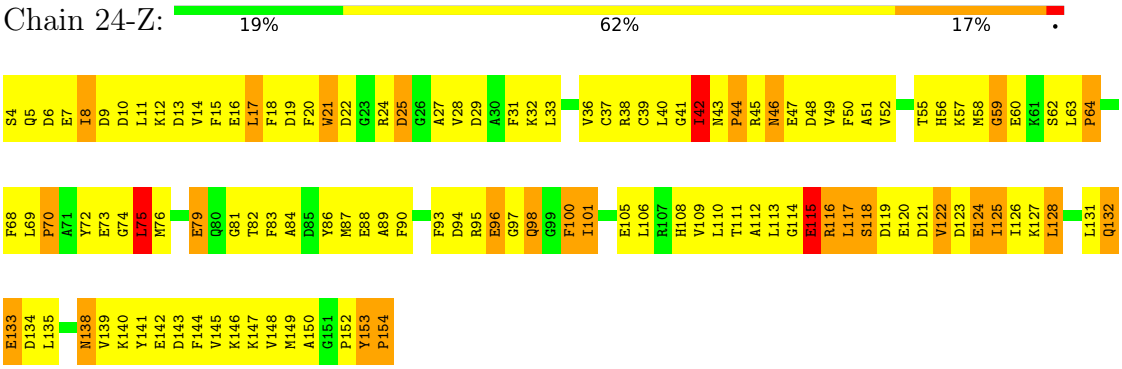
Chain 23-Z:





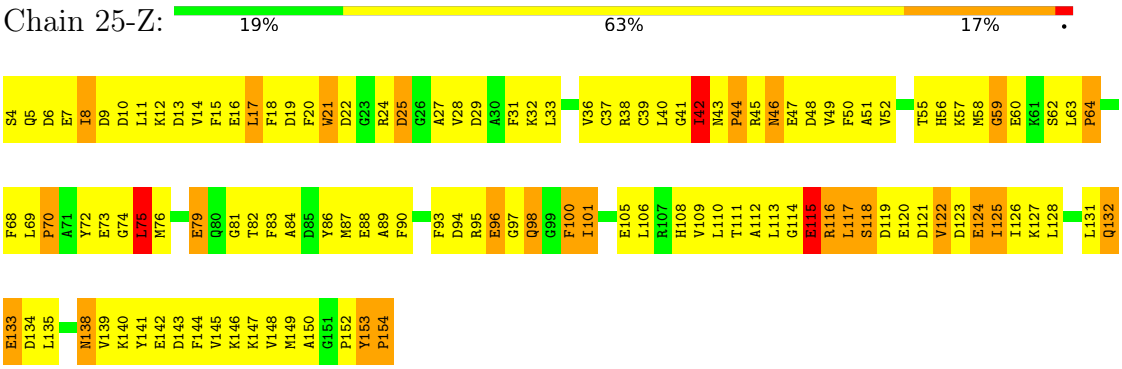
• Molecule 3: MYOSIN ESSENTIAL LIGHT CHAIN, STRIATED ADDUCTOR MUSCLE

Chain 24-Z:



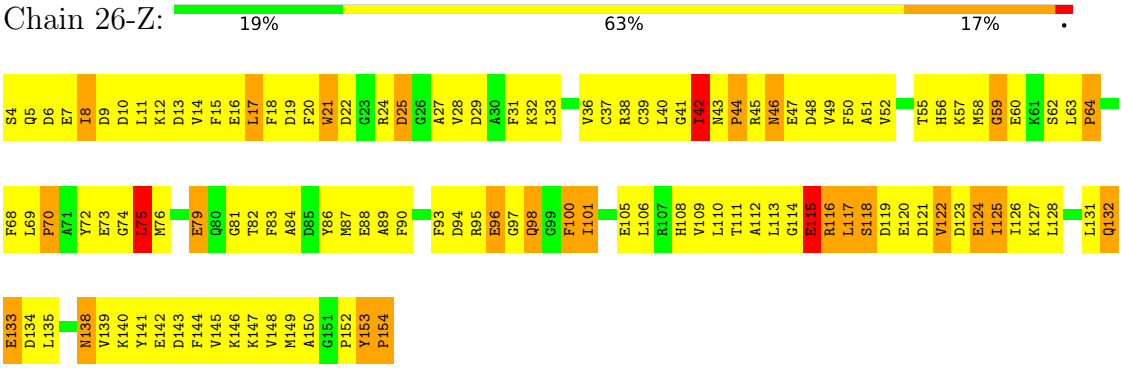
• Molecule 3: MYOSIN ESSENTIAL LIGHT CHAIN, STRIATED ADDUCTOR MUSCLE

Chain 25-Z:



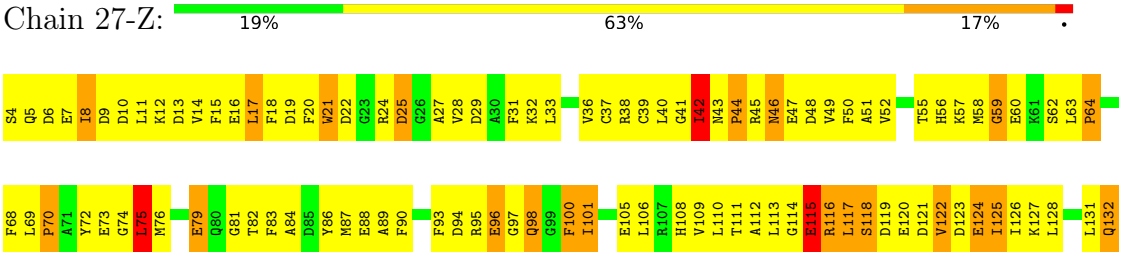
• Molecule 3: MYOSIN ESSENTIAL LIGHT CHAIN, STRIATED ADDUCTOR MUSCLE

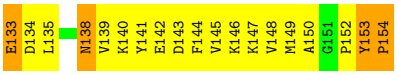
Chain 26-Z:



• Molecule 3: MYOSIN ESSENTIAL LIGHT CHAIN, STRIATED ADDUCTOR MUSCLE

Chain 27-Z:




E133
D134
L135
M138
V139
K140
Y141
E142
D143
F144
V145
K146
K147
V148
M149
A150
G151
P152
Y153
P154

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of tilted images used	Not provided	
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
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-C	1.15	82/6339 (1.3%)	1.30	31/8536 (0.4%)
1	2-C	1.15	82/6340 (1.3%)	1.31	31/8539 (0.4%)
1	3-C	1.14	81/6340 (1.3%)	1.29	29/8539 (0.3%)
1	4-C	1.14	81/6339 (1.3%)	1.29	27/8536 (0.3%)
1	5-C	1.16	83/6340 (1.3%)	1.29	30/8539 (0.4%)
1	6-C	1.14	81/6338 (1.3%)	1.29	27/8533 (0.3%)
1	7-C	1.14	82/6340 (1.3%)	1.29	29/8539 (0.3%)
1	8-C	1.14	81/6340 (1.3%)	1.29	28/8539 (0.3%)
1	9-C	1.14	80/6340 (1.3%)	1.29	28/8539 (0.3%)
1	10-C	1.14	82/6340 (1.3%)	1.29	29/8539 (0.3%)
1	11-C	1.14	81/6340 (1.3%)	1.29	29/8539 (0.3%)
1	12-C	1.14	81/6340 (1.3%)	1.29	29/8539 (0.3%)
1	13-C	1.14	82/6340 (1.3%)	1.29	30/8539 (0.4%)
1	14-C	1.14	81/6340 (1.3%)	1.29	30/8539 (0.4%)
1	15-C	1.15	82/6340 (1.3%)	1.34	33/8539 (0.4%)
1	16-C	1.14	81/6340 (1.3%)	1.29	29/8539 (0.3%)
1	17-C	1.15	82/6339 (1.3%)	1.30	33/8536 (0.4%)
1	18-C	1.14	81/6340 (1.3%)	1.29	30/8539 (0.4%)
1	19-C	1.15	82/6340 (1.3%)	1.30	33/8539 (0.4%)
1	20-C	1.14	82/6340 (1.3%)	1.29	30/8539 (0.4%)
1	21-C	1.14	81/6340 (1.3%)	1.29	29/8539 (0.3%)
1	22-C	1.14	82/6340 (1.3%)	1.29	30/8539 (0.4%)
1	23-C	1.14	82/6340 (1.3%)	1.29	30/8539 (0.4%)
1	24-C	1.15	82/6340 (1.3%)	1.34	35/8539 (0.4%)
1	25-C	1.14	81/6340 (1.3%)	1.29	30/8539 (0.4%)
1	26-C	1.16	82/6340 (1.3%)	1.29	31/8539 (0.4%)
1	27-C	1.16	83/6340 (1.3%)	1.30	32/8539 (0.4%)
2	1-Y	0.80	9/1104 (0.8%)	1.06	2/1472 (0.1%)
2	2-Y	0.80	9/1104 (0.8%)	1.06	2/1472 (0.1%)
2	3-Y	0.80	9/1104 (0.8%)	1.06	2/1472 (0.1%)
2	4-Y	0.80	9/1104 (0.8%)	1.06	2/1472 (0.1%)
2	5-Y	0.80	9/1104 (0.8%)	1.06	2/1472 (0.1%)
2	6-Y	0.80	9/1104 (0.8%)	1.06	2/1472 (0.1%)
2	7-Y	0.80	9/1104 (0.8%)	1.06	2/1472 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
2	8-Y	0.80	9/1104 (0.8%)	1.06	2/1472 (0.1%)
2	9-Y	0.80	8/1104 (0.7%)	1.06	1/1472 (0.1%)
2	10-Y	0.80	9/1104 (0.8%)	1.06	2/1472 (0.1%)
2	11-Y	0.80	9/1104 (0.8%)	1.06	2/1472 (0.1%)
2	12-Y	0.80	9/1104 (0.8%)	1.06	2/1472 (0.1%)
2	13-Y	0.80	8/1104 (0.7%)	1.06	1/1472 (0.1%)
2	14-Y	0.80	9/1104 (0.8%)	1.06	1/1472 (0.1%)
2	15-Y	0.80	9/1104 (0.8%)	1.05	1/1472 (0.1%)
2	16-Y	0.80	9/1104 (0.8%)	1.05	1/1472 (0.1%)
2	17-Y	0.80	8/1104 (0.7%)	1.06	1/1472 (0.1%)
2	18-Y	0.80	9/1104 (0.8%)	1.06	1/1472 (0.1%)
2	19-Y	0.80	9/1104 (0.8%)	1.05	1/1472 (0.1%)
2	20-Y	0.80	9/1104 (0.8%)	1.05	1/1472 (0.1%)
2	21-Y	0.80	9/1104 (0.8%)	1.06	1/1472 (0.1%)
2	22-Y	0.80	8/1104 (0.7%)	1.06	1/1472 (0.1%)
2	23-Y	0.80	8/1104 (0.7%)	1.06	1/1472 (0.1%)
2	24-Y	0.80	8/1104 (0.7%)	1.05	1/1472 (0.1%)
2	25-Y	0.80	8/1104 (0.7%)	1.06	1/1472 (0.1%)
2	26-Y	0.80	8/1104 (0.7%)	1.06	1/1472 (0.1%)
2	27-Y	0.80	9/1104 (0.8%)	1.05	1/1472 (0.1%)
3	1-Z	0.81	11/1222 (0.9%)	1.09	2/1644 (0.1%)
3	2-Z	0.81	10/1222 (0.8%)	1.09	2/1644 (0.1%)
3	3-Z	0.81	11/1222 (0.9%)	1.09	2/1644 (0.1%)
3	4-Z	0.82	11/1222 (0.9%)	1.09	2/1644 (0.1%)
3	5-Z	0.81	11/1222 (0.9%)	1.09	2/1644 (0.1%)
3	6-Z	0.81	10/1222 (0.8%)	1.09	2/1644 (0.1%)
3	7-Z	0.81	11/1222 (0.9%)	1.09	2/1644 (0.1%)
3	8-Z	0.81	10/1222 (0.8%)	1.09	2/1644 (0.1%)
3	9-Z	0.81	10/1222 (0.8%)	1.09	2/1644 (0.1%)
3	10-Z	0.81	11/1222 (0.9%)	1.09	2/1644 (0.1%)
3	11-Z	0.81	11/1222 (0.9%)	1.09	2/1644 (0.1%)
3	12-Z	0.81	11/1222 (0.9%)	1.09	2/1644 (0.1%)
3	13-Z	0.81	10/1222 (0.8%)	1.09	2/1644 (0.1%)
3	14-Z	0.81	11/1222 (0.9%)	1.09	2/1644 (0.1%)
3	15-Z	0.82	11/1222 (0.9%)	1.09	2/1644 (0.1%)
3	16-Z	0.81	10/1222 (0.8%)	1.09	2/1644 (0.1%)
3	17-Z	0.82	11/1222 (0.9%)	1.09	2/1644 (0.1%)
3	18-Z	0.81	11/1222 (0.9%)	1.09	2/1644 (0.1%)
3	19-Z	0.82	11/1222 (0.9%)	1.09	2/1644 (0.1%)
3	20-Z	0.81	11/1222 (0.9%)	1.09	2/1644 (0.1%)
3	21-Z	0.81	11/1222 (0.9%)	1.09	1/1644 (0.1%)
3	22-Z	0.81	10/1222 (0.8%)	1.09	2/1644 (0.1%)
3	23-Z	0.81	11/1222 (0.9%)	1.09	1/1644 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
3	24-Z	0.81	10/1222 (0.8%)	1.09	2/1644 (0.1%)
3	25-Z	0.81	10/1222 (0.8%)	1.09	2/1644 (0.1%)
3	26-Z	0.81	10/1222 (0.8%)	1.09	2/1644 (0.1%)
3	27-Z	0.82	11/1222 (0.9%)	1.09	2/1644 (0.1%)
All	All	1.06	2725/233977 (1.2%)	1.24	902/314670 (0.3%)

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-C	0	4
1	2-C	0	6
1	3-C	0	4
1	4-C	0	4
1	5-C	0	4
1	6-C	0	4
1	7-C	0	4
1	8-C	0	5
1	9-C	0	4
1	10-C	0	4
1	11-C	0	4
1	12-C	0	4
1	13-C	0	5
1	14-C	0	4
1	15-C	0	6
1	16-C	0	4
1	17-C	0	4
1	18-C	0	4
1	19-C	0	6
1	20-C	0	4
1	21-C	0	4
1	22-C	0	4
1	23-C	0	4
1	24-C	0	7
1	25-C	0	4
1	26-C	0	4
1	27-C	0	6
2	1-Y	0	1
2	2-Y	0	1
2	3-Y	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
2	4-Y	0	1
2	5-Y	0	1
2	6-Y	0	1
2	7-Y	0	1
2	8-Y	0	1
2	9-Y	0	1
2	10-Y	0	1
2	11-Y	0	1
2	12-Y	0	1
2	13-Y	0	1
2	14-Y	0	1
2	15-Y	0	1
2	16-Y	0	1
2	17-Y	0	1
2	18-Y	0	1
2	19-Y	0	1
2	20-Y	0	1
2	21-Y	0	1
2	22-Y	0	1
2	23-Y	0	1
2	24-Y	0	1
2	25-Y	0	1
2	26-Y	0	1
2	27-Y	0	1
All	All	0	148

The worst 5 of 2725 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16-C	462	ALA	C-N	33.23	1.92	1.33
1	15-C	462	ALA	C-N	33.21	1.92	1.33
1	17-C	462	ALA	C-N	33.21	1.92	1.33
1	19-C	462	ALA	C-N	33.21	1.92	1.33
1	20-C	462	ALA	C-N	33.21	1.92	1.33

The worst 5 of 902 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	15-C	705	LYS	O-C-N	-27.34	76.73	123.20
1	24-C	705	LYS	O-C-N	-27.34	76.73	123.20
1	23-C	709	SER	O-C-N	27.20	166.23	122.70
1	14-C	709	SER	O-C-N	27.19	166.20	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	18-C	709	SER	O-C-N	27.19	166.20	122.70

There are no chirality outliers.

5 of 148 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1-C	115	TYR	Mainchain
1	1-C	691	LEU	Mainchain
1	1-C	76	SER	Mainchain
1	1-C	824	TRP	Mainchain
2	1-Y	84	ASP	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-C	6215	0	6168	2801	0
1	2-C	6215	0	6174	2730	0
1	3-C	6215	0	6185	2593	0
1	4-C	6215	0	6176	2764	0
1	5-C	6215	0	6182	2606	0
1	6-C	6215	0	6180	2671	0
1	7-C	6215	0	6181	2610	0
1	8-C	6215	0	6179	2653	0
1	9-C	6215	0	6185	2597	0
1	10-C	6215	0	6183	2596	0
1	11-C	6215	0	6185	2593	0
1	12-C	6215	0	6185	2593	0
1	13-C	6215	0	6167	2821	0
1	14-C	6215	0	6185	2599	0
1	15-C	6215	0	6168	2778	0
1	16-C	6215	0	6185	2591	0
1	17-C	6215	0	6173	2811	0
1	18-C	6215	0	6185	2599	0
1	19-C	6215	0	6176	2664	0
1	20-C	6215	0	6184	2596	0
1	21-C	6215	0	6162	2939	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	22-C	6215	0	6182	2642	0
1	23-C	6215	0	6185	2594	0
1	24-C	6215	0	6168	2770	0
1	25-C	6215	0	6172	2712	0
1	26-C	6215	0	6185	2588	0
1	27-C	6215	0	6176	2716	0
2	1-Y	1088	0	1066	501	0
2	2-Y	1088	0	1066	474	0
2	3-Y	1088	0	1066	471	0
2	4-Y	1088	0	1066	497	0
2	5-Y	1088	0	1066	476	0
2	6-Y	1088	0	1066	475	0
2	7-Y	1088	0	1066	472	0
2	8-Y	1088	0	1066	471	0
2	9-Y	1088	0	1066	467	0
2	10-Y	1088	0	1066	474	0
2	11-Y	1088	0	1066	471	0
2	12-Y	1088	0	1066	471	0
2	13-Y	1088	0	1066	472	0
2	14-Y	1088	0	1066	474	0
2	15-Y	1088	0	1066	470	0
2	16-Y	1088	0	1066	475	0
2	17-Y	1088	0	1065	503	0
2	18-Y	1088	0	1066	474	0
2	19-Y	1088	0	1066	474	0
2	20-Y	1088	0	1066	475	0
2	21-Y	1088	0	1066	467	0
2	22-Y	1088	0	1066	475	0
2	23-Y	1088	0	1066	472	0
2	24-Y	1088	0	1066	465	0
2	25-Y	1088	0	1066	468	0
2	26-Y	1088	0	1066	471	0
2	27-Y	1088	0	1066	475	0
3	1-Z	1198	0	1119	509	0
3	2-Z	1198	0	1120	499	0
3	3-Z	1198	0	1120	496	0
3	4-Z	1198	0	1119	508	0
3	5-Z	1198	0	1120	498	0
3	6-Z	1198	0	1120	505	0
3	7-Z	1198	0	1120	505	0
3	8-Z	1198	0	1120	500	0
3	9-Z	1198	0	1120	498	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	10-Z	1198	0	1120	497	0
3	11-Z	1198	0	1120	496	0
3	12-Z	1198	0	1120	496	0
3	13-Z	1198	0	1120	541	0
3	14-Z	1198	0	1120	502	0
3	15-Z	1198	0	1120	507	0
3	16-Z	1198	0	1120	504	0
3	17-Z	1198	0	1118	538	0
3	18-Z	1198	0	1120	502	0
3	19-Z	1198	0	1120	501	0
3	20-Z	1198	0	1120	505	0
3	21-Z	1198	0	1118	619	0
3	22-Z	1198	0	1120	507	0
3	23-Z	1198	0	1120	506	0
3	24-Z	1198	0	1120	512	0
3	25-Z	1198	0	1118	526	0
3	26-Z	1198	0	1120	504	0
3	27-Z	1198	0	1120	501	0
All	All	229527	0	225829	94003	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 206.

The worst 5 of 94003 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:536:GLU:CB	1:C:547:PHE:HE1	1.04	1.67
1:C:536:GLU:CB	1:C:547:PHE:HE1	1.04	1.67
1:C:536:GLU:CB	1:C:547:PHE:HE1	1.04	1.67
1:C:536:GLU:CB	1:C:547:PHE:HE1	1.04	1.67
1:C:536:GLU:CB	1:C:547:PHE:HE1	1.04	1.67

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-C	756/831 (91%)	604 (80%)	113 (15%)	39 (5%)	2	19
1	2-C	758/831 (91%)	607 (80%)	113 (15%)	38 (5%)	2	20
1	3-C	758/831 (91%)	606 (80%)	114 (15%)	38 (5%)	2	20
1	4-C	756/831 (91%)	604 (80%)	113 (15%)	39 (5%)	2	19
1	5-C	758/831 (91%)	606 (80%)	113 (15%)	39 (5%)	2	19
1	6-C	754/831 (91%)	604 (80%)	112 (15%)	38 (5%)	2	20
1	7-C	758/831 (91%)	606 (80%)	113 (15%)	39 (5%)	2	19
1	8-C	758/831 (91%)	607 (80%)	113 (15%)	38 (5%)	2	20
1	9-C	758/831 (91%)	605 (80%)	115 (15%)	38 (5%)	2	20
1	10-C	758/831 (91%)	605 (80%)	114 (15%)	39 (5%)	2	19
1	11-C	758/831 (91%)	606 (80%)	114 (15%)	38 (5%)	2	20
1	12-C	758/831 (91%)	606 (80%)	114 (15%)	38 (5%)	2	20
1	13-C	758/831 (91%)	608 (80%)	112 (15%)	38 (5%)	2	20
1	14-C	758/831 (91%)	607 (80%)	113 (15%)	38 (5%)	2	20
1	15-C	758/831 (91%)	607 (80%)	112 (15%)	39 (5%)	2	19
1	16-C	758/831 (91%)	607 (80%)	113 (15%)	38 (5%)	2	20
1	17-C	756/831 (91%)	604 (80%)	113 (15%)	39 (5%)	2	19
1	18-C	758/831 (91%)	607 (80%)	113 (15%)	38 (5%)	2	20
1	19-C	758/831 (91%)	607 (80%)	113 (15%)	38 (5%)	2	20
1	20-C	758/831 (91%)	606 (80%)	113 (15%)	39 (5%)	2	19
1	21-C	758/831 (91%)	607 (80%)	113 (15%)	38 (5%)	2	20
1	22-C	758/831 (91%)	607 (80%)	113 (15%)	38 (5%)	2	20
1	23-C	758/831 (91%)	606 (80%)	114 (15%)	38 (5%)	2	20
1	24-C	758/831 (91%)	606 (80%)	113 (15%)	39 (5%)	2	19
1	25-C	758/831 (91%)	608 (80%)	112 (15%)	38 (5%)	2	20
1	26-C	758/831 (91%)	606 (80%)	114 (15%)	38 (5%)	2	20
1	27-C	758/831 (91%)	606 (80%)	114 (15%)	38 (5%)	2	20
2	1-Y	134/136 (98%)	95 (71%)	33 (25%)	6 (4%)	2	22
2	2-Y	134/136 (98%)	95 (71%)	33 (25%)	6 (4%)	2	22
2	3-Y	134/136 (98%)	95 (71%)	33 (25%)	6 (4%)	2	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	4-Y	134/136 (98%)	95 (71%)	33 (25%)	6 (4%)	2	22
2	5-Y	134/136 (98%)	95 (71%)	33 (25%)	6 (4%)	2	22
2	6-Y	134/136 (98%)	95 (71%)	33 (25%)	6 (4%)	2	22
2	7-Y	134/136 (98%)	95 (71%)	33 (25%)	6 (4%)	2	22
2	8-Y	134/136 (98%)	95 (71%)	33 (25%)	6 (4%)	2	22
2	9-Y	134/136 (98%)	95 (71%)	33 (25%)	6 (4%)	2	22
2	10-Y	134/136 (98%)	95 (71%)	33 (25%)	6 (4%)	2	22
2	11-Y	134/136 (98%)	95 (71%)	33 (25%)	6 (4%)	2	22
2	12-Y	134/136 (98%)	95 (71%)	33 (25%)	6 (4%)	2	22
2	13-Y	134/136 (98%)	95 (71%)	33 (25%)	6 (4%)	2	22
2	14-Y	134/136 (98%)	95 (71%)	33 (25%)	6 (4%)	2	22
2	15-Y	134/136 (98%)	95 (71%)	33 (25%)	6 (4%)	2	22
2	16-Y	134/136 (98%)	95 (71%)	33 (25%)	6 (4%)	2	22
2	17-Y	134/136 (98%)	95 (71%)	33 (25%)	6 (4%)	2	22
2	18-Y	134/136 (98%)	95 (71%)	33 (25%)	6 (4%)	2	22
2	19-Y	134/136 (98%)	95 (71%)	33 (25%)	6 (4%)	2	22
2	20-Y	134/136 (98%)	95 (71%)	33 (25%)	6 (4%)	2	22
2	21-Y	134/136 (98%)	95 (71%)	33 (25%)	6 (4%)	2	22
2	22-Y	134/136 (98%)	95 (71%)	33 (25%)	6 (4%)	2	22
2	23-Y	134/136 (98%)	95 (71%)	33 (25%)	6 (4%)	2	22
2	24-Y	134/136 (98%)	95 (71%)	33 (25%)	6 (4%)	2	22
2	25-Y	134/136 (98%)	95 (71%)	33 (25%)	6 (4%)	2	22
2	26-Y	134/136 (98%)	95 (71%)	33 (25%)	6 (4%)	2	22
2	27-Y	134/136 (98%)	95 (71%)	33 (25%)	6 (4%)	2	22
3	1-Z	149/151 (99%)	104 (70%)	35 (24%)	10 (7%)	1	15
3	2-Z	149/151 (99%)	104 (70%)	36 (24%)	9 (6%)	1	17
3	3-Z	149/151 (99%)	104 (70%)	36 (24%)	9 (6%)	1	17
3	4-Z	149/151 (99%)	104 (70%)	36 (24%)	9 (6%)	1	17
3	5-Z	149/151 (99%)	104 (70%)	36 (24%)	9 (6%)	1	17
3	6-Z	149/151 (99%)	104 (70%)	36 (24%)	9 (6%)	1	17
3	7-Z	149/151 (99%)	104 (70%)	36 (24%)	9 (6%)	1	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	8-Z	149/151 (99%)	104 (70%)	35 (24%)	10 (7%)	1	15
3	9-Z	149/151 (99%)	104 (70%)	36 (24%)	9 (6%)	1	17
3	10-Z	149/151 (99%)	104 (70%)	36 (24%)	9 (6%)	1	17
3	11-Z	149/151 (99%)	104 (70%)	36 (24%)	9 (6%)	1	17
3	12-Z	149/151 (99%)	104 (70%)	36 (24%)	9 (6%)	1	17
3	13-Z	149/151 (99%)	104 (70%)	36 (24%)	9 (6%)	1	17
3	14-Z	149/151 (99%)	104 (70%)	36 (24%)	9 (6%)	1	17
3	15-Z	149/151 (99%)	104 (70%)	36 (24%)	9 (6%)	1	17
3	16-Z	149/151 (99%)	104 (70%)	35 (24%)	10 (7%)	1	15
3	17-Z	149/151 (99%)	104 (70%)	35 (24%)	10 (7%)	1	15
3	18-Z	149/151 (99%)	104 (70%)	36 (24%)	9 (6%)	1	17
3	19-Z	149/151 (99%)	104 (70%)	35 (24%)	10 (7%)	1	15
3	20-Z	149/151 (99%)	104 (70%)	36 (24%)	9 (6%)	1	17
3	21-Z	149/151 (99%)	104 (70%)	36 (24%)	9 (6%)	1	17
3	22-Z	149/151 (99%)	104 (70%)	36 (24%)	9 (6%)	1	17
3	23-Z	149/151 (99%)	104 (70%)	36 (24%)	9 (6%)	1	17
3	24-Z	149/151 (99%)	104 (70%)	35 (24%)	10 (7%)	1	15
3	25-Z	149/151 (99%)	104 (70%)	36 (24%)	9 (6%)	1	17
3	26-Z	149/151 (99%)	104 (70%)	36 (24%)	9 (6%)	1	17
3	27-Z	149/151 (99%)	104 (70%)	36 (24%)	9 (6%)	1	17
All	All	28097/30186 (93%)	21738 (77%)	4913 (18%)	1446 (5%)	4	19

5 of 1446 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-C	27	ALA
1	1-C	366	ARG
1	1-C	368	ARG
1	1-C	371	GLN
1	1-C	542	ALA

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-C	678/724 (94%)	571 (84%)	107 (16%)	2	13
1	2-C	678/724 (94%)	571 (84%)	107 (16%)	2	13
1	3-C	678/724 (94%)	571 (84%)	107 (16%)	2	13
1	4-C	678/724 (94%)	571 (84%)	107 (16%)	2	13
1	5-C	678/724 (94%)	571 (84%)	107 (16%)	2	13
1	6-C	678/724 (94%)	571 (84%)	107 (16%)	2	13
1	7-C	678/724 (94%)	571 (84%)	107 (16%)	2	13
1	8-C	678/724 (94%)	571 (84%)	107 (16%)	2	13
1	9-C	678/724 (94%)	571 (84%)	107 (16%)	2	13
1	10-C	678/724 (94%)	571 (84%)	107 (16%)	2	13
1	11-C	678/724 (94%)	571 (84%)	107 (16%)	2	13
1	12-C	678/724 (94%)	571 (84%)	107 (16%)	2	13
1	13-C	678/724 (94%)	571 (84%)	107 (16%)	2	13
1	14-C	678/724 (94%)	571 (84%)	107 (16%)	2	13
1	15-C	678/724 (94%)	571 (84%)	107 (16%)	2	13
1	16-C	678/724 (94%)	571 (84%)	107 (16%)	2	13
1	17-C	678/724 (94%)	571 (84%)	107 (16%)	2	13
1	18-C	678/724 (94%)	571 (84%)	107 (16%)	2	13
1	19-C	678/724 (94%)	571 (84%)	107 (16%)	2	13
1	20-C	678/724 (94%)	571 (84%)	107 (16%)	2	13
1	21-C	678/724 (94%)	571 (84%)	107 (16%)	2	13
1	22-C	678/724 (94%)	571 (84%)	107 (16%)	2	13
1	23-C	678/724 (94%)	571 (84%)	107 (16%)	2	13
1	24-C	678/724 (94%)	571 (84%)	107 (16%)	2	13
1	25-C	678/724 (94%)	571 (84%)	107 (16%)	2	13
1	26-C	678/724 (94%)	571 (84%)	107 (16%)	2	13
1	27-C	678/724 (94%)	571 (84%)	107 (16%)	2	13
2	1-Y	119/119 (100%)	100 (84%)	19 (16%)	2	13
2	2-Y	119/119 (100%)	100 (84%)	19 (16%)	2	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	3-Y	119/119 (100%)	100 (84%)	19 (16%)	2	13
2	4-Y	119/119 (100%)	100 (84%)	19 (16%)	2	13
2	5-Y	119/119 (100%)	100 (84%)	19 (16%)	2	13
2	6-Y	119/119 (100%)	100 (84%)	19 (16%)	2	13
2	7-Y	119/119 (100%)	100 (84%)	19 (16%)	2	13
2	8-Y	119/119 (100%)	100 (84%)	19 (16%)	2	13
2	9-Y	119/119 (100%)	100 (84%)	19 (16%)	2	13
2	10-Y	119/119 (100%)	100 (84%)	19 (16%)	2	13
2	11-Y	119/119 (100%)	100 (84%)	19 (16%)	2	13
2	12-Y	119/119 (100%)	100 (84%)	19 (16%)	2	13
2	13-Y	119/119 (100%)	100 (84%)	19 (16%)	2	13
2	14-Y	119/119 (100%)	100 (84%)	19 (16%)	2	13
2	15-Y	119/119 (100%)	100 (84%)	19 (16%)	2	13
2	16-Y	119/119 (100%)	100 (84%)	19 (16%)	2	13
2	17-Y	119/119 (100%)	100 (84%)	19 (16%)	2	13
2	18-Y	119/119 (100%)	100 (84%)	19 (16%)	2	13
2	19-Y	119/119 (100%)	100 (84%)	19 (16%)	2	13
2	20-Y	119/119 (100%)	100 (84%)	19 (16%)	2	13
2	21-Y	119/119 (100%)	100 (84%)	19 (16%)	2	13
2	22-Y	119/119 (100%)	100 (84%)	19 (16%)	2	13
2	23-Y	119/119 (100%)	100 (84%)	19 (16%)	2	13
2	24-Y	119/119 (100%)	100 (84%)	19 (16%)	2	13
2	25-Y	119/119 (100%)	100 (84%)	19 (16%)	2	13
2	26-Y	119/119 (100%)	100 (84%)	19 (16%)	2	13
2	27-Y	119/119 (100%)	100 (84%)	19 (16%)	2	13
3	1-Z	127/127 (100%)	111 (87%)	16 (13%)	4	19
3	2-Z	127/127 (100%)	111 (87%)	16 (13%)	4	19
3	3-Z	127/127 (100%)	111 (87%)	16 (13%)	4	19
3	4-Z	127/127 (100%)	111 (87%)	16 (13%)	4	19
3	5-Z	127/127 (100%)	111 (87%)	16 (13%)	4	19
3	6-Z	127/127 (100%)	111 (87%)	16 (13%)	4	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	7-Z	127/127 (100%)	111 (87%)	16 (13%)	4	19
3	8-Z	127/127 (100%)	111 (87%)	16 (13%)	4	19
3	9-Z	127/127 (100%)	111 (87%)	16 (13%)	4	19
3	10-Z	127/127 (100%)	111 (87%)	16 (13%)	4	19
3	11-Z	127/127 (100%)	111 (87%)	16 (13%)	4	19
3	12-Z	127/127 (100%)	111 (87%)	16 (13%)	4	19
3	13-Z	127/127 (100%)	111 (87%)	16 (13%)	4	19
3	14-Z	127/127 (100%)	111 (87%)	16 (13%)	4	19
3	15-Z	127/127 (100%)	111 (87%)	16 (13%)	4	19
3	16-Z	127/127 (100%)	111 (87%)	16 (13%)	4	19
3	17-Z	127/127 (100%)	111 (87%)	16 (13%)	4	19
3	18-Z	127/127 (100%)	111 (87%)	16 (13%)	4	19
3	19-Z	127/127 (100%)	111 (87%)	16 (13%)	4	19
3	20-Z	127/127 (100%)	111 (87%)	16 (13%)	4	19
3	21-Z	127/127 (100%)	111 (87%)	16 (13%)	4	19
3	22-Z	127/127 (100%)	111 (87%)	16 (13%)	4	19
3	23-Z	127/127 (100%)	111 (87%)	16 (13%)	4	19
3	24-Z	127/127 (100%)	111 (87%)	16 (13%)	4	19
3	25-Z	127/127 (100%)	111 (87%)	16 (13%)	4	19
3	26-Z	127/127 (100%)	111 (87%)	16 (13%)	4	19
3	27-Z	127/127 (100%)	111 (87%)	16 (13%)	4	19
All	All	24948/26190 (95%)	21114 (85%)	3834 (15%)	6	14

5 of 3834 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	14-C	47	GLU
3	25-Z	125	ILE
1	17-C	140	TYR
1	25-C	793	LEU
1	27-C	726	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 1296 such sidechains are listed below:

Mol	Chain	Res	Type
1	20-C	291	ASN
3	24-Z	43	ASN
2	20-Y	91	ASN
1	20-C	283	HIS
1	22-C	689	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no 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
1	6-C	12
1	1-C	12
1	17-C	12
1	4-C	11
1	2-C	11
1	5-C	11
1	7-C	11
1	19-C	11

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Mol	Chain	Number of breaks
1	26-C	11
1	27-C	11
1	3-C	10
1	8-C	10
1	9-C	10
1	10-C	10
1	11-C	10
1	12-C	10
1	13-C	10
1	14-C	10
1	15-C	10
1	16-C	10
1	18-C	10
1	20-C	10
1	21-C	10
1	22-C	10
1	23-C	10
1	24-C	10
1	25-C	10

The worst 5 of 283 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
6	C	800:LYS	C	801:LEU	N	2.57
6	C	705:LYS	C	706:GLY	N	2.32
1	C	800:LYS	C	801:LEU	N	2.23
4	C	800:LYS	C	801:LEU	N	2.23
17	C	800:LYS	C	801:LEU	N	2.19

6 Tomogram visualisation

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

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 Mask visualisation

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

7 Tomogram analysis (i)

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

7.1 Map-value distribution (i)

This section was not generated.

8 Map-model fit

This section was not generated.