



wwPDB EM Map/Model Validation Report

Apr 10, 2016 – 02:12 PM BST

PDB ID : 2W4H
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 Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

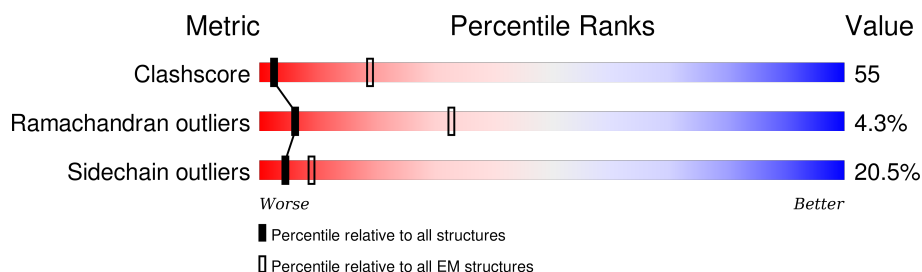
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 35.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.






















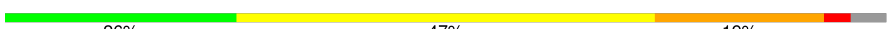
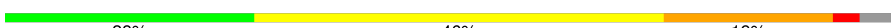
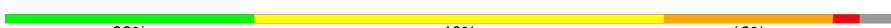
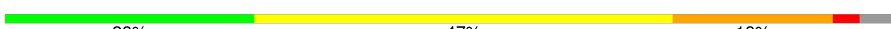
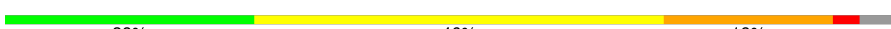

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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

Mol	Chain	Length	Quality of chain
1	1-B	150	
1	10-B	150	
1	11-B	150	
1	12-B	150	
1	13-B	150	
1	14-B	150	
1	2-B	150	
1	3-B	150	
1	4-B	150	

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Mol	Chain	Length	Quality of chain
1	5-B	150	
1	6-B	150	
1	7-B	150	
1	8-B	150	
1	9-B	150	
2	1-C	145	
2	10-C	145	
2	11-C	145	
2	12-C	145	
2	13-C	145	
2	14-C	145	
2	2-C	145	
2	3-C	145	
2	4-C	145	
2	5-C	145	
2	6-C	145	
2	7-C	145	
2	8-C	145	
2	9-C	145	
3	1-M	840	
3	10-M	840	
3	11-M	840	
3	12-M	840	
3	13-M	840	
3	14-M	840	

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

2 Entry composition

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		

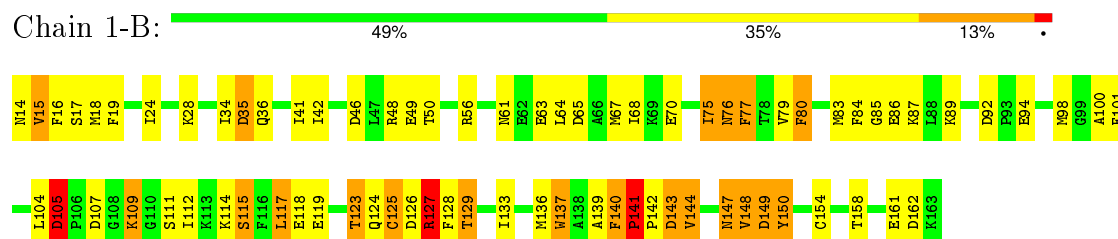
There is a discrepancy between the modelled and reference sequences:

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

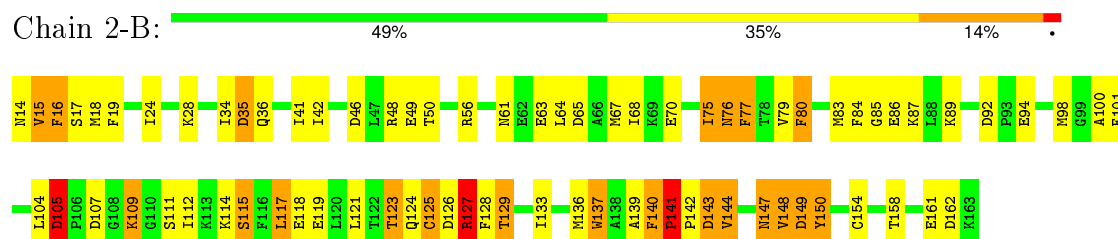
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

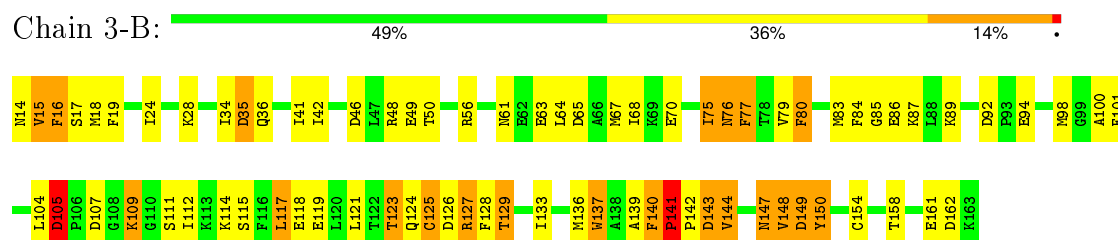
- Molecule 1: MYOSIN REGULATORY LIGHT CHAIN 2, SKELETAL MUSCLE ISOFORM



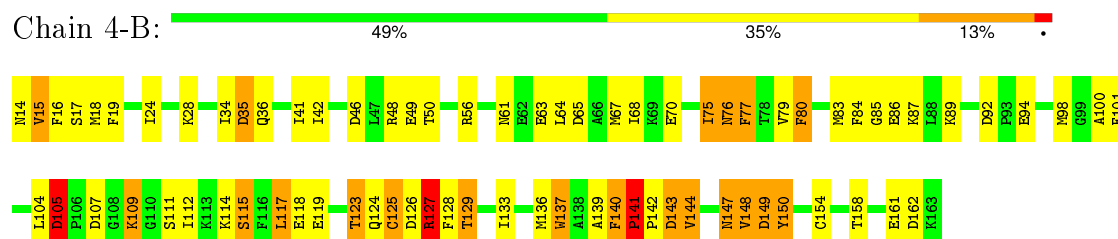
- Molecule 1: MYOSIN REGULATORY LIGHT CHAIN 2, SKELETAL MUSCLE ISOFORM



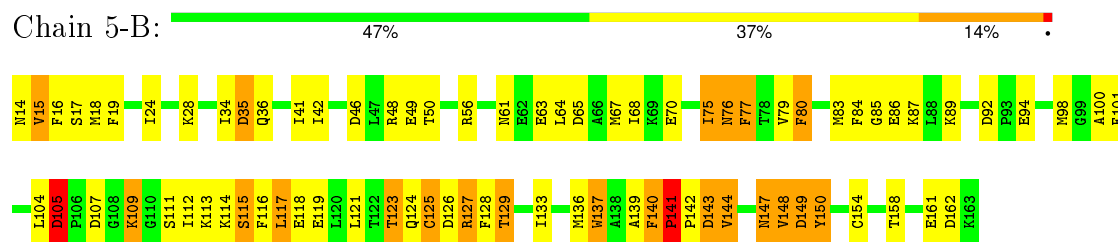
- Molecule 1: MYOSIN REGULATORY LIGHT CHAIN 2, SKELETAL MUSCLE ISOFORM



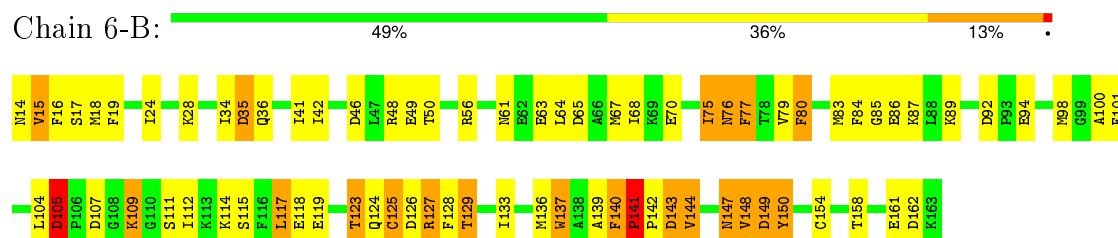
- Molecule 1: MYOSIN REGULATORY LIGHT CHAIN 2, SKELETAL MUSCLE ISOFORM



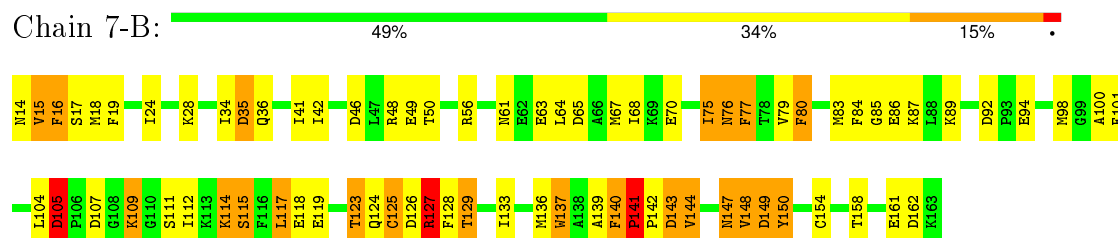
- Molecule 1: MYOSIN REGULATORY LIGHT CHAIN 2, SKELETAL MUSCLE ISOFORM



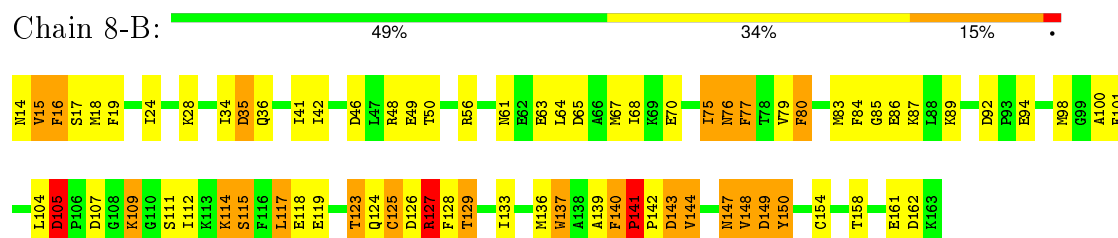
- Molecule 1: MYOSIN REGULATORY LIGHT CHAIN 2, SKELETAL MUSCLE ISOFORM



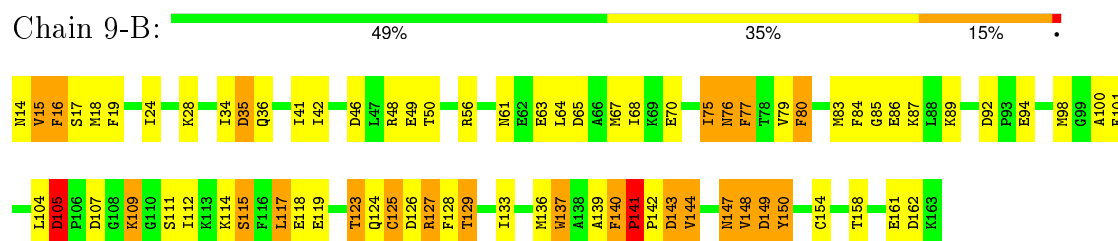
- Molecule 1: MYOSIN REGULATORY LIGHT CHAIN 2, SKELETAL MUSCLE ISOFORM



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

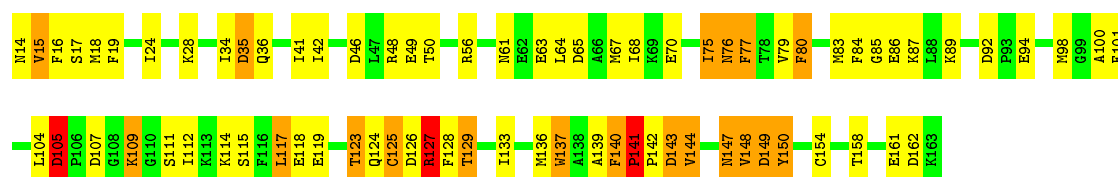


- Molecule 1: MYOSIN REGULATORY LIGHT CHAIN 2, SKELETAL MUSCLE ISOFORM



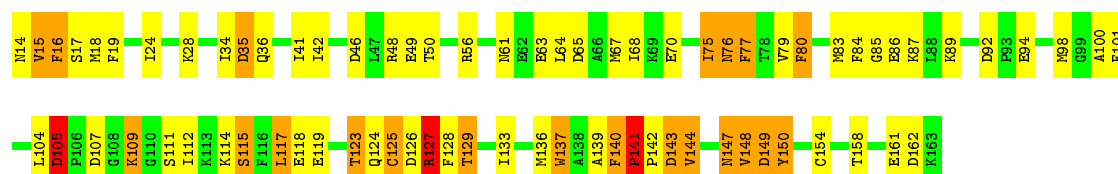
- Molecule 1: MYOSIN REGULATORY LIGHT CHAIN 2, SKELETAL MUSCLE ISOFORM





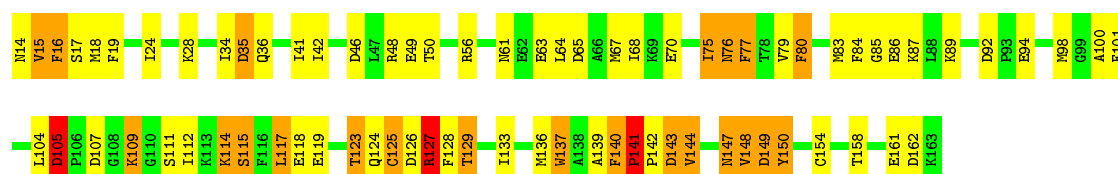
- Molecule 1: MYOSIN REGULATORY LIGHT CHAIN 2, SKELETAL MUSCLE ISOFORM

Chain 11-B: 49% 35% 14%



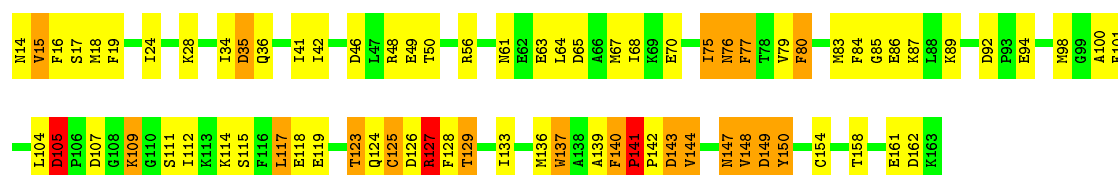
- Molecule 1: MYOSIN REGULATORY LIGHT CHAIN 2, SKELETAL MUSCLE ISOFORM

Chain 12-B: 49% 34% 15%



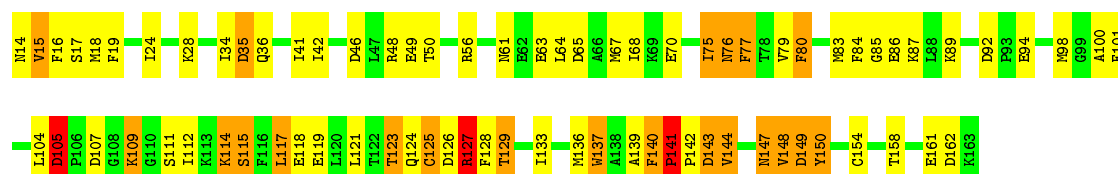
- Molecule 1: MYOSIN REGULATORY LIGHT CHAIN 2, SKELETAL MUSCLE ISOFORM

Chain 13-B: 49% 36% 13%



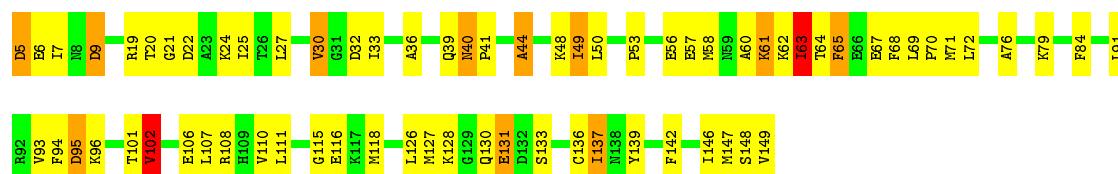
- Molecule 1: MYOSIN REGULATORY LIGHT CHAIN 2, SKELETAL MUSCLE ISOFORM

Chain 14-B: 49% 35% 14%



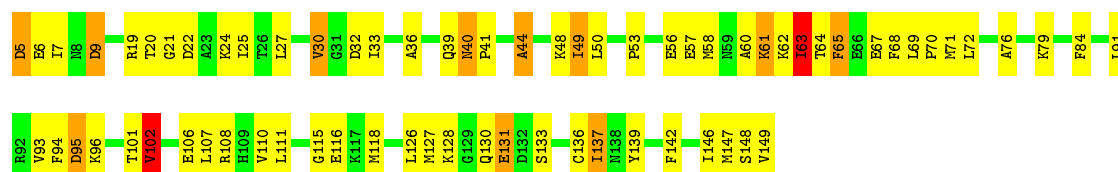
- Molecule 2: MYOSIN LIGHT CHAIN 3, SKELETAL MUSCLE ISOFORM

Chain 1-C: 52% 39% 8%



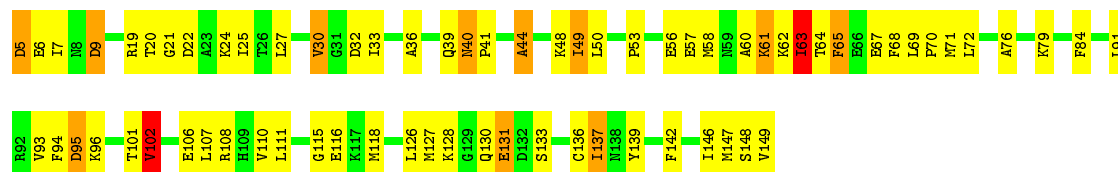
- Molecule 2: MYOSIN LIGHT CHAIN 3, SKELETAL MUSCLE ISOFORM

Chain 2-C: 52% 39% 8%



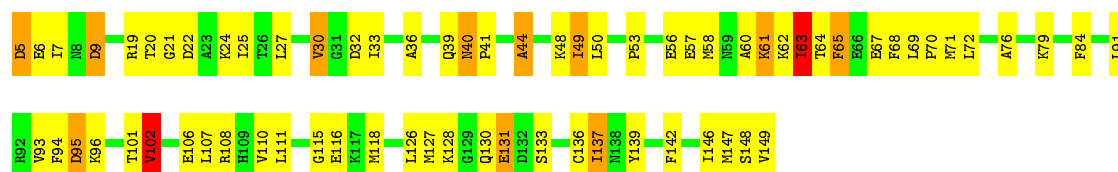
- Molecule 2: MYOSIN LIGHT CHAIN 3, SKELETAL MUSCLE ISOFORM

Chain 3-C: 52% 39% 8%



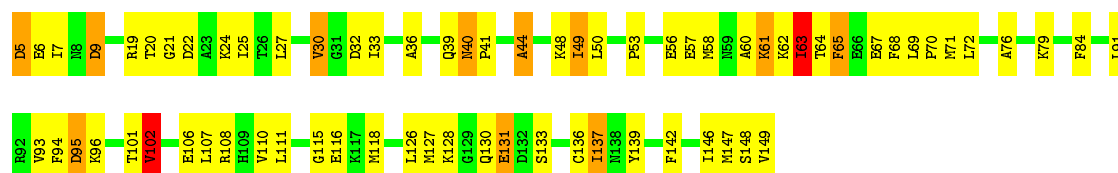
- Molecule 2: MYOSIN LIGHT CHAIN 3, SKELETAL MUSCLE ISOFORM

Chain 4-C: 52% 39% 8%



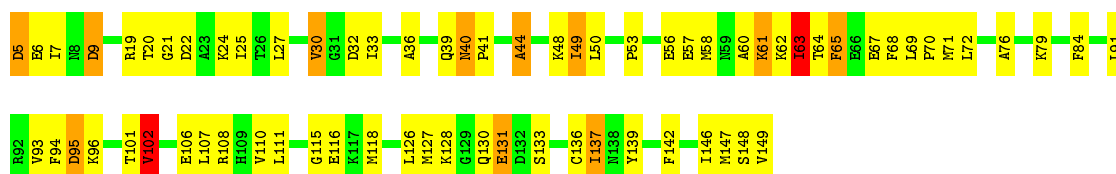
- Molecule 2: MYOSIN LIGHT CHAIN 3, SKELETAL MUSCLE ISOFORM

Chain 5-C: 52% 39% 8%



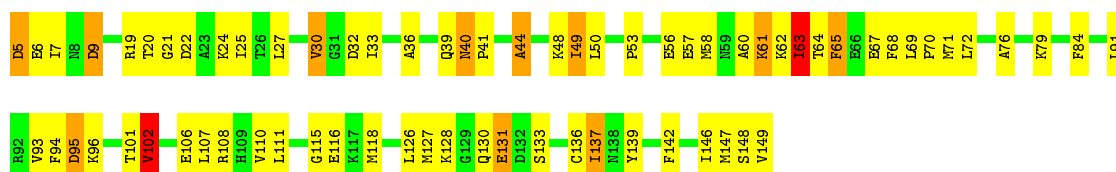
- Molecule 2: MYOSIN LIGHT CHAIN 3, SKELETAL MUSCLE ISOFORM

Chain 6-C: 52% 39% 8%



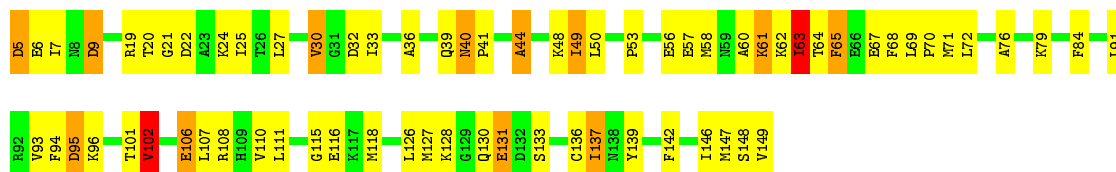
- Molecule 2: MYOSIN LIGHT CHAIN 3, SKELETAL MUSCLE ISOFORM

Chain 7-C: 52% 39% 8%



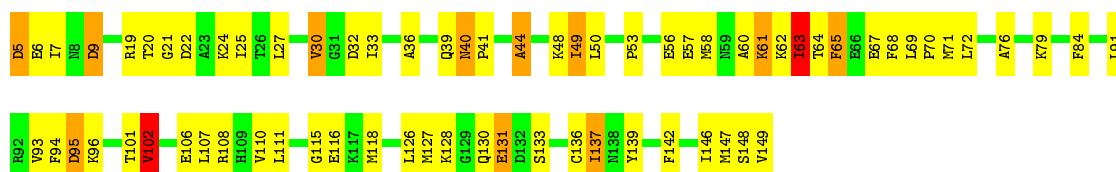
- Molecule 2: MYOSIN LIGHT CHAIN 3, SKELETAL MUSCLE ISOFORM

Chain 8-C: 52% 39% 8%



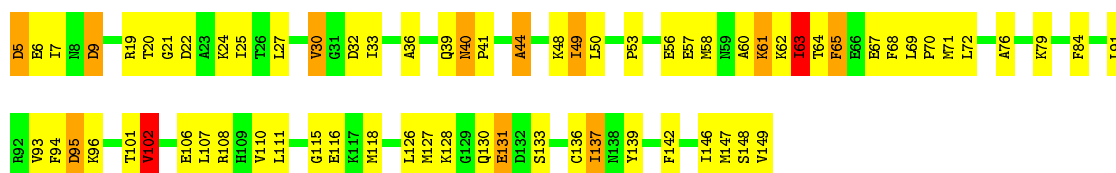
- Molecule 2: MYOSIN LIGHT CHAIN 3, SKELETAL MUSCLE ISOFORM

Chain 9-C: 52% 39% 8%



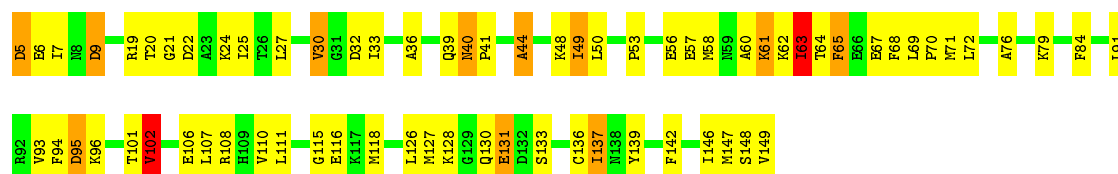
- Molecule 2: MYOSIN LIGHT CHAIN 3, SKELETAL MUSCLE ISOFORM

Chain 10-C: 52% 39% 8%



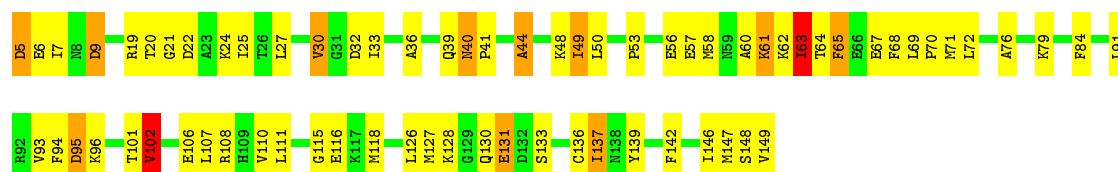
- Molecule 2: MYOSIN LIGHT CHAIN 3, SKELETAL MUSCLE ISOFORM

Chain 11-C: 52% 39% 8%



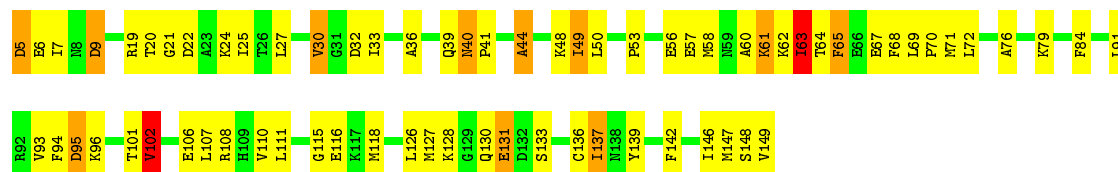
• Molecule 2: MYOSIN LIGHT CHAIN 3, SKELETAL MUSCLE ISOFORM

Chain 12-C: 52% 39% 8%



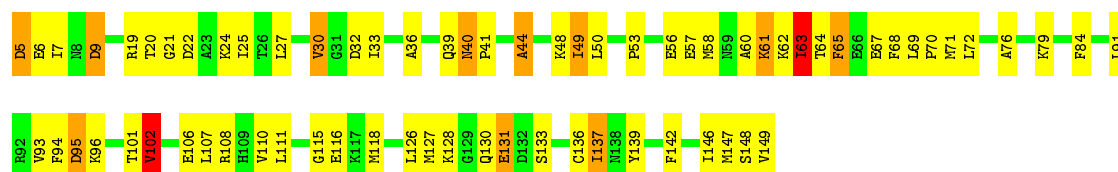
• Molecule 2: MYOSIN LIGHT CHAIN 3, SKELETAL MUSCLE ISOFORM

Chain 13-C: 52% 39% 8%



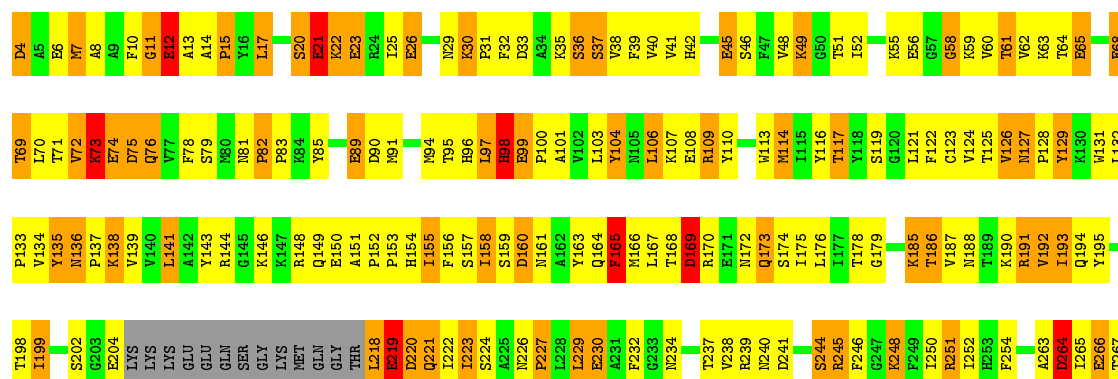
• Molecule 3: MYOSIN HEAVY CHAIN, SKELETAL MUSCLE, ADULT

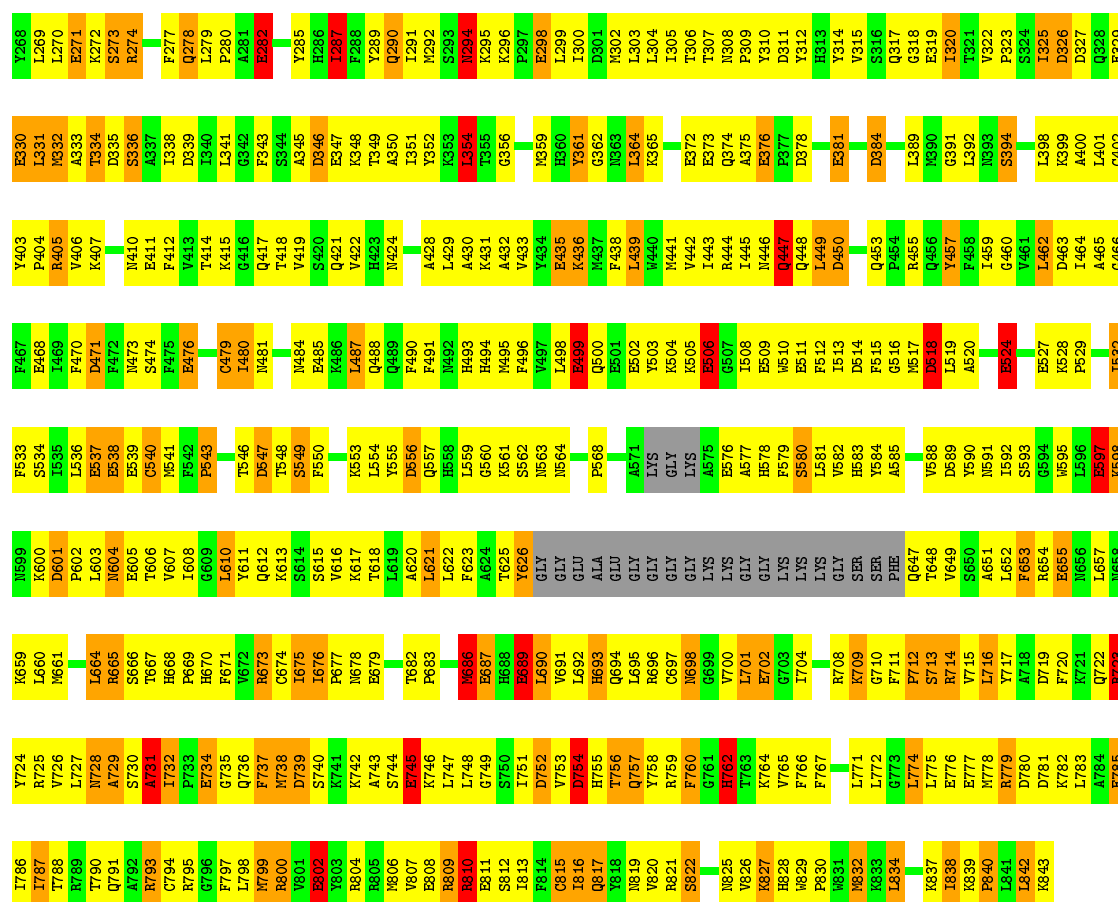
Chain 1-M: 26% 47% 19%



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

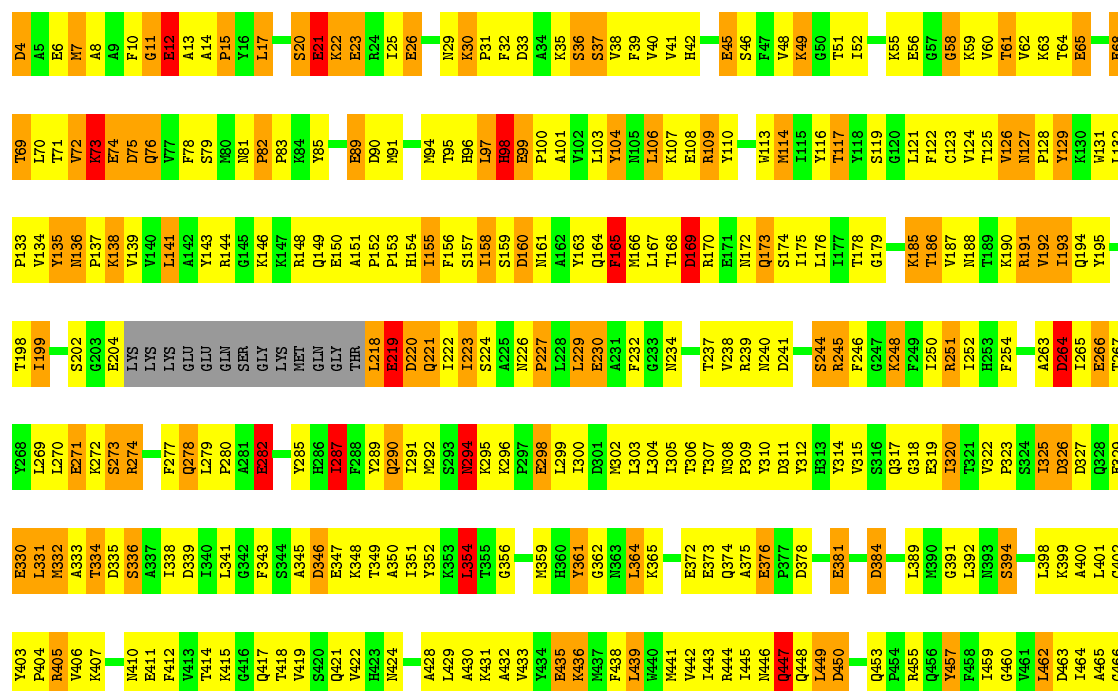
Chain 1-M: 26% 47% 19%

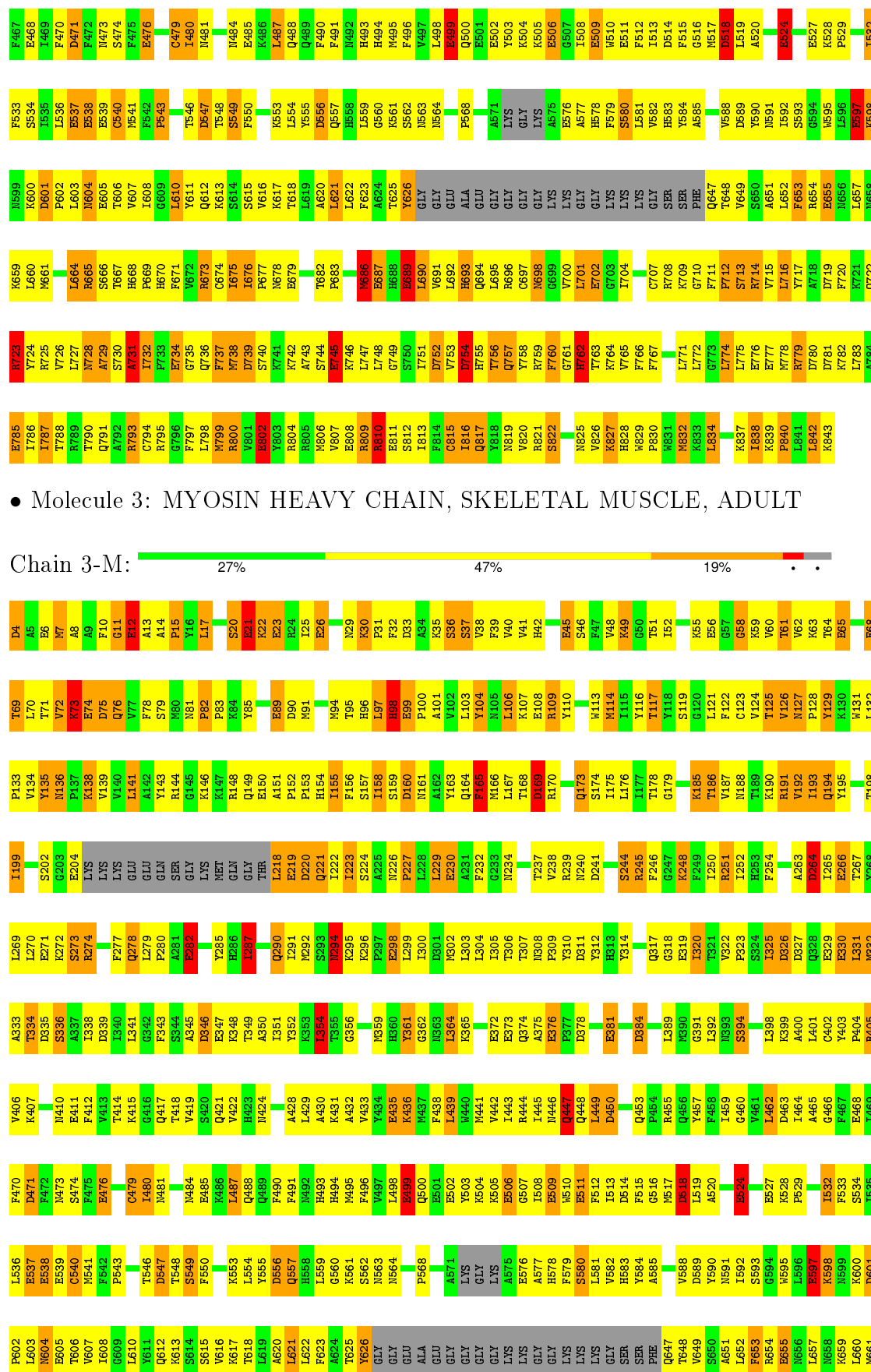




• Molecule 3: MYOSIN HEAVY CHAIN, SKELETAL MUSCLE, ADULT

Chain 2-M: 26% 48% 19%



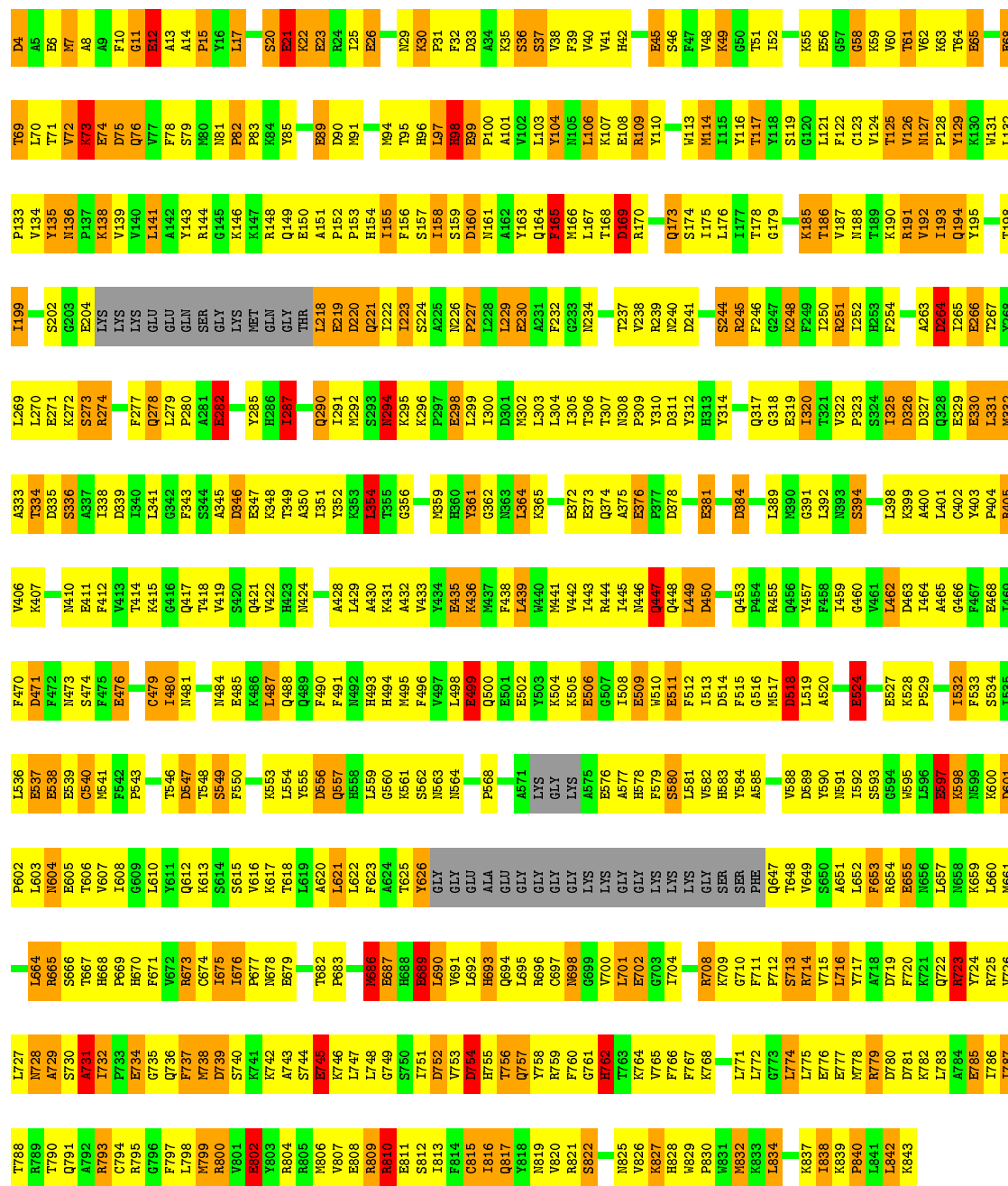




• Molecule 3: MYOSIN HEAVY CHAIN, SKELETAL MUSCLE, ADULT

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

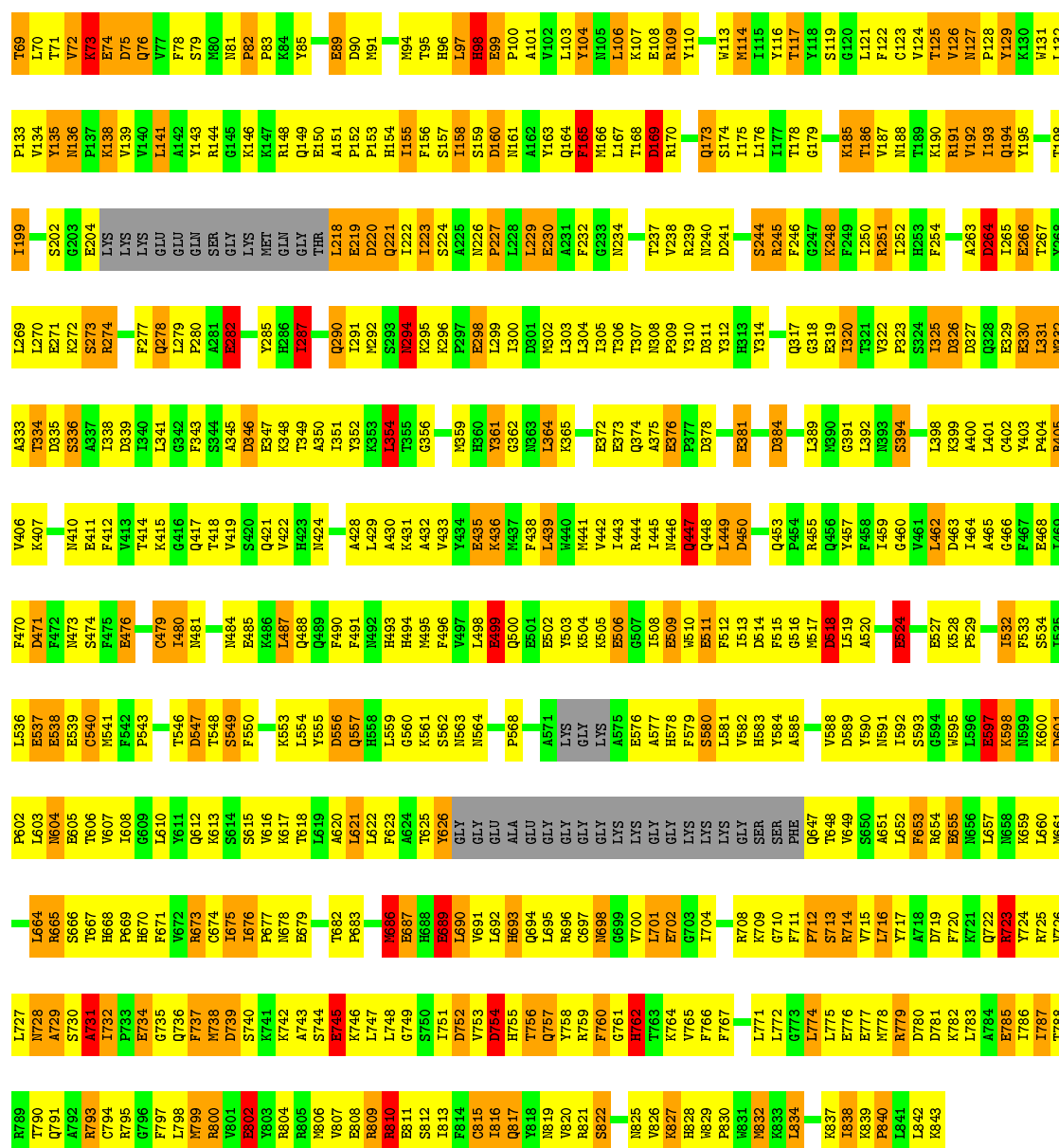
Chain 5-M:  27% 47% 19%



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

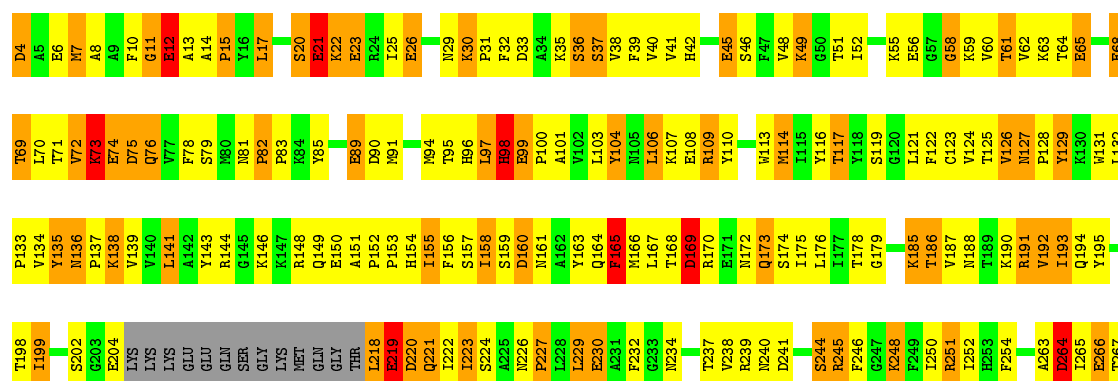
Chain 6-M:  27% 47% 19%





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

Chain 7-M: 26% 48% 19%







[illegible]

Chain 12-M: 



Frequency	Percentage
Daily	28%
Often	46%
Sometimes	19%
Rarely	3%
Never	4%



E271	K272	S273	R274	F277	Q278	L279	P280	A281	E282	Y285	H286	T287	Q290	K291	M292	S293	R294	K295	K296	M299	H360	Y361	G362	N363	K365	E372	E373	Q374	S375	E376	P377	D378	E381	D384	L389	K390	G391	L392	N393	S394	K399	A400	L401	C402	Y403	E329	P404	R405	V406	K407	N410																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
E411	F412	T413	T414	K415	G416	Q417	T418	V419	Q421	V422	H423	N424	A428	L429	K430	K431	A432	V433	Y434	E435	L436	K437	F438	L439	M440	M441	V442	I443	R444	L445	N446	Q447	Q448	F512	I513	D514	F515	G516	M517	R455	Q456	Y457	F458	I459	G460	V461	L462	D463	A465	C466	F467	E468	S469	T469	F470	F471	D472	N473																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
S474	F475	E476	C479	I480	N481	N484	E485	K486	Q487	Q488	Q489	F490	A492	N493	L494	H495	F496	V497	L498	E499	Q500	E501	E502	Y503	K504	K505	V506	G507	E508	E509	M510	E511	F512	I513	D514	F515	G516	M517	R455	Q456	Y457	F458	I459	G460	V461	L462	D463	A465	C466	F467	E468	S469	T469	F470	F471	D472	N473																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
C540	H541	F542	P543	T546	D547	T548	F550	K553	L554	L555	A556	A557	E558	L559	G560	K561	S562	N563	N564	P568	A571	L572	L573	L574	L575	L576	L577	L578	L579	L580	L581	L582	L583	L584	L585	L586	L587	L588	L589	L590	L591	L592	L593	L594	L595	L596	L597	L598	L599	L600	L601	L602	L603	L604	L605																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
T606	V607	L608	L610	L611	Q612	K613	S614	S615	V616	K617	T618	L619	A620	L621	L622	L623	L624	T625	Y626	L627	L628	L629	L630	L631	L632	L633	L634	L635	L636	L637	L638	L639	L640	L641	L642	L643	L644	L645	L646	L647	L648	L649	S650	A651	L652	L653	R654	E655	L656	L657	L658	L659	L660	L661	L662	L663	L664	L665	L666	L667	L668	L669	L670	L671	L672	L673	L674	L675	L676	L677	L678	L679	L680	L681	L682	L683	L684	L685	L686	L687	L688	L689	L690	L691	L692	L693	L694	L695	L696	L697	L698	L699	L700	L701	L702	L703	L704	L705	L706	L707	L708	L709	L710	L711	L712	L713	L714	L715	L716	L717	L718	L719	L720	L721	L722	L723	L724	L725	L726	L727	L728	L729	L730	L731	L732	L733	L734	L735	L736	L737	L738	L739	L740	L741	L742	L743	L744	L745	L746	L747	L748	L749	L750	L751	L752	L753	L754	L755	L756	L757	L758	L759	L760	L761	L762	L763	L764	L765	L766	L767	L768	L769	L770	L771	L772	L773	L774	L775	L776	L777	L778	L779	L780	L781	L782	L783	L784	L785	L786	L787	L788	L789	L790	L791	L792	L793	L794	L795	L796	L797	L798	L799	L800	L801	L802	L803	L804	L805	L806	L807	L808	L809	L810	L811	L812	L813	L814	L815	L816	L817	L818	L819	L820	L821	L822	L823	L824	L825	L826	L827	L828	L829	L830	L831	L832	L833	L834	L835	L836	L837	L838	L839	L840	L841	L842	L843	L844	L845	L846	L847	L848	L849	L850	L851	L852	L853	L854	L855	L856	L857	L858	L859	L860	L861	L862	L863	L864	L865	L866	L867	L868	L869	L870	L871	L872	L873	L874	L875	L876	L877	L878	L879	L880	L881	L882	L883	L884	L885	L886	L887	L888	L889	L890	L891	L892	L893	L894	L895	L896	L897	L898	L899	L900	L901	L902	L903	L904	L905	L906	L907	L908	L909	L910	L911	L912	L913	L914	L915	L916	L917	L918	L919	L920	L921	L922	L923	L924	L925	L926	L927	L928	L929	L930	L931	L932	L933	L934	L935	L936	L937	L938	L939	L940	L941	L942	L943	L944	L945	L946	L947	L948	L949	L950	L951	L952	L953	L954	L955	L956	L957	L958	L959	L960	L961	L962	L963	L964	L965	L966	L967	L968	L969	L970	L971	L972	L973	L974	L975	L976	L977	L978	L979	L980	L981	L982	L983	L984	L985	L986	L987	L988	L989	L990	L991	L992	L993	L994	L995	L996	L997	L998	L999	L1000	L1001	L1002	L1003	L1004	L1005	L1006	L1007	L1008	L1009	L1010	L1011	L1012	L1013	L1014	L1015	L1016	L1017	L1018	L1019	L1020	L1021	L1022	L1023	L1024	L1025	L1026	L1027	L1028	L1029	L1030	L1031	L1032	L1033	L1034	L1035	L1036	L1037	L1038	L1039	L1040	L1041	L1042	L1043	L1044	L1045	L1046	L1047	L1048	L1049	L1050	L1051	L1052	L1053	L1054	L1055	L1056	L1057	L1058	L1059	L1060	L1061	L1062	L1063	L1064	L1065	L1066	L1067	L1068	L1069	L1070	L1071	L1072	L1073	L1074	L1075	L1076	L1077	L1078	L1079	L1080	L1081	L1082	L1083	L1084	L1085	L1086	L1087	L1088	L1089	L1090	L1091	L1092	L1093	L1094	L1095	L1096	L1097	L1098	L1099	L1100	L1101	L1102	L1103	L1104	L1105	L1106	L1107	L1108	L1109	L1110	L1111	L1112	L1113	L1114	L1115	L1116	L1117	L1118	L1119	L1120	L1121	L1122	L1123	L1124	L1125	L1126	L1127	L1128	L1129	L1130	L1131	L1132	L1133	L1134	L1135	L1136	L1137	L1138	L1139	L1140	L1141	L1142	L1143	L1144	L1145	L1146	L1147	L1148	L1149	L1150	L1151	L1152	L1153	L1154	L1155	L1156	L1157	L1158	L1159	L1160	L1161	L1162	L1163	L1164	L1165	L1166	L1167	L1168	L1169	L1170	L1171	L1172	L1173	L1174	L1175	L1176	L1177	L1178	L1179	L1180	L1181	L1182	L1183	L1184	L1185	L1186	L1187	L1188	L1189	L1190	L1191	L1192	L1193	L1194	L1195	L1196	L1197	L1198	L1199	L1200	L1201	L1202	L1203	L1204	L1205	L1206	L1207	L1208	L1209	L1210	L1211	L1212	L1213	L1214	L1215	L1216	L1217	L1218	L1219	L1220	L1221	L1222	L1223	L1224	L1225	L1226	L1227	L1228	L1229	L1230	L1231	L1232	L1233	L1234	L1235	L1236	L1237	L1238	L1239	L1240	L1241	L1242	L1243	L1244	L1245	L1246	L1247	L1248	L1249	L1250	L1251	L1252	L1253	L1254	L1255	L1256	L1257	L1258	L1259	L1260	L1261	L1262	L1263	L1264	L1265	L1266	L1267	L1268	L1269	L1270	L1271	L1272	L1273	L1274	L1275	L1276	L1277	L1278	L1279	L1280	L1281	L1282	L1283	L1284	L1285	L1286	L1287	L1288	L1289	L1290	L1291	L1292	L1293	L1294	L1295	L1296	L1297	L1298	L1299	L1300	L1301	L1302	L1303	L1304	L1305	L1306	L1307	L1308	L1309	L1310	L1311	L1312	L1313	L1314	L1315	L1316	L1317	L1318	L1319	L1320	L1321	L1322	L1323	L1324	L1325	L1326	L1327	L1328	L1329	L1330	L1331	L1332	L1333	L1334	L1335	L1336	L1337	L1338	L1339	L1340	L1341	L1342	L1343	L1344	L1345	L1346	L1347	L1348	L1349	L1350	L1351	L1352	L1353	L1354	L1355	L1356	L1357	L1358	L1359	L1360	L1361	L1362	L1363	L1364	L1365	L1366	L1367	L1368	L1369	L1370	L1371	L1372	L1373	L1374	L1375	L1376	L1377	L1378	L1379	L1380	L1381	L1382	L1383	L1384	L1385	L1386	L1387	L1388	L1389	L1390	L1391	L1392	L1393	L1394	L1395	L1396	L1397	L1398	L1399	L1400	L1401	L1402	L1403	L1404	L1405	L1406	L1407	L1408	L1409	L1410	L1411	L1412	L1413	L1414	L1415	L1416	L1417	L1418	L1419	L1420	L1421	L1422	L1423	L1424	L1425	L1426	L1427	L1428	L1429	L1430	L1431	L1432	L1433	L1434	L1435	L1436	L1437	L1438	L1439	L1440	L1441	L1442	L1443	L1444	L1445	L1446	L1447	L1448	L1449	L1450	L1451	L1452	L1453	L1454	L1455	L1456	L1457	L1458	L1459	L1460	L1461	L1462	L1463	L1464	L1465	L1466	L1467	L1468	L1469	L1470	L1471	L1472	L1473	L1474	L1475	L1476	L1477	L1478	L1479	L1480	L1481	L1482	L1483	L1484	L1485	L1486	L1487	L1488	L1489	L1490	L1491	L1492	L1493	L1494	L1495	L1496	L1497	L1498	L1499	L1500	L1501	L1502	L1503	L1504	L1505	L1506	L1507	L1508	L1509	L1510	L1511	L1512	L1513	L1514	L1515	L1516	L1517	L1518	L1519	L1520	L1521	L1522	L1523	L1524	L1525	L1526	L1527	L1528	L1529	L1530	L1531	L1532	L1533	L1534	L1535	L1536	L1537	L1538	L1539	L1540	L1541	L1542	L1543	L1544	L1545	L1546	L1547	L1548	L1549	L1550	L1551	L1552	L1553	L1554	L1555	L1556	L1557	L1558	L1559	L1560	L1561	L1562	L1563	L1564	L1565	L1566	L1567	L1568	L1569	L1570	L1571	L1572	L1573	L1574	L1575	L1576	L1577	L1578	L1579	L1580	L1581	L1582	L1583	L1584	L1585	L1586	L1587	L1588	L1589	L1590	L1591	L1592	L1593	L1594	L1595	L1596	L1597	L1598	L1599	L1600	L1601	L1602	L1603	L1604	L1605	L1606	L1607	L1608	L1609	L1610	L1611	L1612	L1613	L1614	L1615	L1616	L1617	L1618	L1619	L1620	L1621	L1622	L1623	L1624	L1625	L1626	L1627	L1628	L1629	L1630	L1631	L1632	L1633	L1634	L1635	L1636	L1637	L1638	L1639	L1640	L1641	L1642	L1643	L1644	L1645	L1646	L1647	L1648	L1649	L1650	L1651	L1652	L1653	L1654	L1655	L1656	L1657	L1658	L1659	L1660	L1661	L1662	L1663	L1664	L1665	L1666	L1667	L1668	L1669	L1670	L1671	L1672	L1673	L1674	L1675	L1676	L1677	L1678	L1679	L1680	L1681	L1682	L1683	L1684	L1685	L1686	L1687	L1688	L1689	L1690	L1691	L1692	L1693	L1694	L1695	L1696	L1697	L1698	L1699	L1700	L1701	L1702	L1703	L1704	L1705	L1706	L1707	L1708	L1709	L1710	L1711	L1712	L1713	L1714	L1715	L1716	L1717	L1718	L1719	L1720	L1721	L1722	L1723	L1724	L1725	L1726	L1727	L1728	L1729	L1730	L1731	L1732	L1733	L1734	L1735	L1736	L1737	L1738	L1739	L1740	L1741	L1742	L1743	L1744	L1745	L1746	L1747	L1748	L1749	L1750	L1751	L1752	L1753	L1754	L1755	L1756	L1757	L1758	L1759	L1760	L1761	L1762	L1763	L1764	L1765	L1766	L1767	L1768	L1769	L1770	L1771	L1772	L1773	L1774	L1775	L1776	L1777	L1778	L1779	L1780	L1781	L1782	L1783	L1784	L1785	L1786	L1787	L1788	L1789	L1790	L1791	L1792	L1793	L1794	L1795	L1796	L1797	L1798	L1799	L1800	L1801	L1802	L1803	L1804	L1805	L1806



4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI/PHILIPS CM300FEG/T	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	TIETZ TEM-CAM F224	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 2$	RMSZ	$\# Z > 2$
1	1-B	0.70	0/1199	1.67	18/1617 (1.1%)
1	10-B	0.70	0/1199	1.67	18/1617 (1.1%)
1	11-B	0.70	0/1199	1.67	18/1617 (1.1%)
1	12-B	0.70	0/1199	1.67	18/1617 (1.1%)
1	13-B	0.70	0/1199	1.67	18/1617 (1.1%)
1	14-B	0.70	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%)
2	1-C	0.74	1/1140 (0.1%)	1.58	9/1530 (0.6%)
2	10-C	0.74	1/1140 (0.1%)	1.59	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%)
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%)
3	1-M	1.33	61/6594 (0.9%)	1.54	96/8884 (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%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
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%)
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%)
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	10-B	0	4
1	11-B	0	4
1	12-B	0	4
1	13-B	0	4
1	14-B	0	4
1	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
3	1-M	0	1
3	10-M	0	1
3	11-M	0	1
3	12-M	0	1
3	13-M	0	1
3	14-M	0	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

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	8-M	0	1
3	9-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(°)	Ideal(°)
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 ⓘ

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	19
1	2-B	148/150 (99%)	119 (80%)	17 (12%)	12 (8%)	1	19
1	3-B	148/150 (99%)	119 (80%)	17 (12%)	12 (8%)	1	19
1	4-B	148/150 (99%)	119 (80%)	17 (12%)	12 (8%)	1	19
1	5-B	148/150 (99%)	120 (81%)	16 (11%)	12 (8%)	1	19
1	6-B	148/150 (99%)	119 (80%)	17 (12%)	12 (8%)	1	19
1	7-B	148/150 (99%)	119 (80%)	17 (12%)	12 (8%)	1	19
1	8-B	148/150 (99%)	119 (80%)	17 (12%)	12 (8%)	1	19
1	9-B	148/150 (99%)	120 (81%)	16 (11%)	12 (8%)	1	19
1	10-B	148/150 (99%)	119 (80%)	17 (12%)	12 (8%)	1	19
1	11-B	148/150 (99%)	119 (80%)	17 (12%)	12 (8%)	1	19
1	12-B	148/150 (99%)	119 (80%)	17 (12%)	12 (8%)	1	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	13-B	148/150 (99%)	119 (80%)	17 (12%)	12 (8%)	1	19
1	14-B	148/150 (99%)	119 (80%)	17 (12%)	12 (8%)	1	19
2	1-C	143/145 (99%)	111 (78%)	20 (14%)	12 (8%)	1	18
2	2-C	143/145 (99%)	111 (78%)	20 (14%)	12 (8%)	1	18
2	3-C	143/145 (99%)	111 (78%)	20 (14%)	12 (8%)	1	18
2	4-C	143/145 (99%)	111 (78%)	20 (14%)	12 (8%)	1	18
2	5-C	143/145 (99%)	111 (78%)	20 (14%)	12 (8%)	1	18
2	6-C	143/145 (99%)	111 (78%)	20 (14%)	12 (8%)	1	18
2	7-C	143/145 (99%)	111 (78%)	20 (14%)	12 (8%)	1	18
2	8-C	143/145 (99%)	111 (78%)	20 (14%)	12 (8%)	1	18
2	9-C	143/145 (99%)	111 (78%)	20 (14%)	12 (8%)	1	18
2	10-C	143/145 (99%)	111 (78%)	20 (14%)	12 (8%)	1	18
2	11-C	143/145 (99%)	111 (78%)	20 (14%)	12 (8%)	1	18
2	12-C	143/145 (99%)	111 (78%)	20 (14%)	12 (8%)	1	18
2	13-C	143/145 (99%)	111 (78%)	20 (14%)	12 (8%)	1	18
2	14-C	143/145 (99%)	111 (78%)	20 (14%)	12 (8%)	1	18
3	1-M	788/840 (94%)	651 (83%)	114 (14%)	23 (3%)	6	43
3	2-M	786/840 (94%)	649 (83%)	114 (14%)	23 (3%)	6	43
3	3-M	786/840 (94%)	649 (83%)	115 (15%)	22 (3%)	6	44
3	4-M	786/840 (94%)	649 (83%)	114 (14%)	23 (3%)	6	43
3	5-M	786/840 (94%)	649 (83%)	115 (15%)	22 (3%)	6	44
3	6-M	786/840 (94%)	649 (83%)	115 (15%)	22 (3%)	6	44
3	7-M	788/840 (94%)	651 (83%)	113 (14%)	24 (3%)	5	42
3	8-M	788/840 (94%)	651 (83%)	114 (14%)	23 (3%)	6	43
3	9-M	786/840 (94%)	649 (83%)	115 (15%)	22 (3%)	6	44
3	10-M	786/840 (94%)	649 (83%)	115 (15%)	22 (3%)	6	44
3	11-M	786/840 (94%)	649 (83%)	115 (15%)	22 (3%)	6	44
3	12-M	786/840 (94%)	649 (83%)	115 (15%)	22 (3%)	6	44
3	13-M	786/840 (94%)	649 (83%)	115 (15%)	22 (3%)	6	44
3	14-M	788/840 (94%)	651 (83%)	115 (15%)	22 (3%)	6	44
All	All	15086/15890 (95%)	12316 (82%)	2120 (14%)	650 (4%)	6	34

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 ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1-B	128/130 (98%)	116 (91%)	12 (9%)	11	42
1	2-B	128/130 (98%)	116 (91%)	12 (9%)	11	42
1	3-B	128/130 (98%)	116 (91%)	12 (9%)	11	42
1	4-B	128/130 (98%)	116 (91%)	12 (9%)	11	42
1	5-B	128/130 (98%)	116 (91%)	12 (9%)	11	42
1	6-B	128/130 (98%)	116 (91%)	12 (9%)	11	42
1	7-B	128/130 (98%)	116 (91%)	12 (9%)	11	42
1	8-B	128/130 (98%)	116 (91%)	12 (9%)	11	42
1	9-B	128/130 (98%)	116 (91%)	12 (9%)	11	42
1	10-B	128/130 (98%)	116 (91%)	12 (9%)	11	42
1	11-B	128/130 (98%)	116 (91%)	12 (9%)	11	42
1	12-B	128/130 (98%)	116 (91%)	12 (9%)	11	42
1	13-B	128/130 (98%)	116 (91%)	12 (9%)	11	42
1	14-B	128/130 (98%)	116 (91%)	12 (9%)	11	42
2	1-C	120/122 (98%)	109 (91%)	11 (9%)	11	43
2	2-C	120/122 (98%)	109 (91%)	11 (9%)	11	43
2	3-C	120/122 (98%)	109 (91%)	11 (9%)	11	43
2	4-C	120/122 (98%)	109 (91%)	11 (9%)	11	43
2	5-C	120/122 (98%)	109 (91%)	11 (9%)	11	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	6-C	120/122 (98%)	109 (91%)	11 (9%)	11	43
2	7-C	120/122 (98%)	109 (91%)	11 (9%)	11	43
2	8-C	120/122 (98%)	109 (91%)	11 (9%)	11	43
2	9-C	120/122 (98%)	109 (91%)	11 (9%)	11	43
2	10-C	120/122 (98%)	109 (91%)	11 (9%)	11	43
2	11-C	120/122 (98%)	109 (91%)	11 (9%)	11	43
2	12-C	120/122 (98%)	109 (91%)	11 (9%)	11	43
2	13-C	120/122 (98%)	109 (91%)	11 (9%)	11	43
2	14-C	120/122 (98%)	109 (91%)	11 (9%)	11	43
3	1-M	693/724 (96%)	522 (75%)	171 (25%)	1	6
3	2-M	693/724 (96%)	522 (75%)	171 (25%)	1	6
3	3-M	693/724 (96%)	523 (76%)	170 (24%)	1	6
3	4-M	693/724 (96%)	522 (75%)	171 (25%)	1	6
3	5-M	693/724 (96%)	523 (76%)	170 (24%)	1	6
3	6-M	693/724 (96%)	523 (76%)	170 (24%)	1	6
3	7-M	693/724 (96%)	522 (75%)	171 (25%)	1	6
3	8-M	693/724 (96%)	522 (75%)	171 (25%)	1	6
3	9-M	693/724 (96%)	523 (76%)	170 (24%)	1	6
3	10-M	693/724 (96%)	523 (76%)	170 (24%)	1	6
3	11-M	693/724 (96%)	523 (76%)	170 (24%)	1	6
3	12-M	693/724 (96%)	523 (76%)	170 (24%)	1	6
3	13-M	693/724 (96%)	523 (76%)	170 (24%)	1	6
3	14-M	693/724 (96%)	523 (76%)	170 (24%)	1	6
All	All	13174/13664 (96%)	10467 (80%)	2707 (20%)	4	10

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

Mol	Chain	Res	Type
3	7-M	173	GLN
3	8-M	701	LEU
3	13-M	787	ILE
3	7-M	365	LYS
2	8-C	95	ASP

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

Mol	Chain	Res	Type
3	7-M	194	GLN
3	8-M	698	ASN
3	13-M	757	GLN
3	7-M	417	GLN
2	8-C	40	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.