



## wwPDB EM Validation Summary Report ⓘ

Nov 19, 2022 – 01:11 PM EST

PDB ID : 1O1D  
EMDB ID : EMD-1001  
Title : MOLECULAR MODELS OF AVERAGED RIGOR CROSSBRIDGES FROM TOMOGRAMS OF INSECT FLIGHT MUSCLE  
Authors : Chen, L.F.; Winkler, H.; Reedy, M.K.; Reedy, M.C.; Taylor, K.A.  
Deposited on : 2002-11-18  
Resolution : 70.00 Å (reported)  
Based on initial models : 2MYS, 1ATN

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We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

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<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

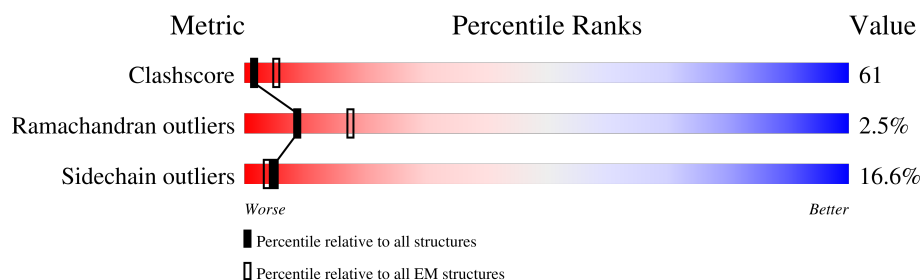
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 70.00 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  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	840	<div> <div>100%</div> <div>24% 51% 21% .</div> </div>
1	D	840	<div> <div>100%</div> <div>25% 51% 19% .</div> </div>
1	G	840	<div> <div>100%</div> <div>25% 51% 20% .</div> </div>
1	J	840	<div> <div>100%</div> <div>26% 50% 21% .</div> </div>
1	M	840	<div> <div>100%</div> <div>24% 51% 21% .</div> </div>
1	P	840	<div> <div>100%</div> <div>25% 50% 20% .</div> </div>
2	B	145	<div> <div>100%</div> <div>65% 26% 6% .</div> </div>
2	E	145	<div> <div>100%</div> <div>64% 27% 6% .</div> </div>

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Mol	Chain	Length	Quality of chain
2	H	145	
2	K	145	
2	N	145	
2	Q	145	
3	C	147	
3	F	147	
3	I	147	
3	L	147	
3	O	147	
3	R	147	
4	0	375	
4	1	375	
4	2	375	
4	3	375	
4	4	375	
4	5	375	
4	7	375	
4	8	375	
4	9	375	
4	V	375	
4	W	375	
4	X	375	
4	Y	375	
4	Z	375	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	MLY	A	505	-	-	X	-
1	MLY	A	553	-	-	X	-
1	MLY	A	764	-	-	X	-
1	MLY	A	768	-	-	X	-
1	MLY	A	782	-	-	X	-
1	MLY	A	839	-	-	X	-
1	MLY	D	553	-	-	X	-
1	MLY	D	764	-	-	X	-
1	MLY	D	768	-	-	X	-
1	MLY	D	782	-	-	X	-
1	MLY	G	553	-	-	X	-
1	MLY	G	764	-	-	X	-
1	MLY	G	768	-	-	X	-
1	MLY	G	84	-	-	X	-
1	MLY	J	505	-	-	X	-
1	MLY	J	553	-	-	X	-
1	MLY	J	839	-	-	X	-
1	MLY	J	84	-	-	X	-
1	MLY	M	35	-	-	X	-
1	MLY	M	505	-	-	X	-
1	MLY	M	553	-	-	X	-
1	MLY	M	782	-	-	X	-
1	MLY	M	839	-	-	X	-
1	MLY	M	84	-	-	X	-
1	MLY	P	764	-	-	X	-
1	MLY	P	839	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 94966 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 SKELETAL MUSCLE MYOSIN II.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	840	Total	C	N	O	S	0	0
			6797	4382	1135	1243	37		
1	D	840	Total	C	N	O	S	0	0
			6797	4382	1135	1243	37		
1	G	840	Total	C	N	O	S	0	0
			6797	4382	1135	1243	37		
1	J	840	Total	C	N	O	S	0	0
			6797	4382	1135	1243	37		
1	M	840	Total	C	N	O	S	0	0
			6797	4382	1135	1243	37		
1	P	840	Total	C	N	O	S	0	0
			6797	4382	1135	1243	37		

- Molecule 2 is a protein called SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	145	Total	C	N	O	S	0	0
			1127	717	177	227	6		
2	E	145	Total	C	N	O	S	0	0
			1127	717	177	227	6		
2	H	145	Total	C	N	O	S	0	0
			1127	717	177	227	6		
2	K	145	Total	C	N	O	S	0	0
			1127	717	177	227	6		
2	N	145	Total	C	N	O	S	0	0
			1127	717	177	227	6		
2	Q	145	Total	C	N	O	S	0	0
			1127	717	177	227	6		

- Molecule 3 is a protein called SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	147	Total	C	N	O	S	0	0
			1123	698	188	230	7		
3	F	147	Total	C	N	O	S	0	0
			1123	698	188	230	7		
3	I	147	Total	C	N	O	S	0	0
			1123	698	188	230	7		
3	L	147	Total	C	N	O	S	0	0
			1123	698	188	230	7		
3	O	147	Total	C	N	O	S	0	0
			1123	698	188	230	7		
3	R	147	Total	C	N	O	S	0	0
			1123	698	188	230	7		

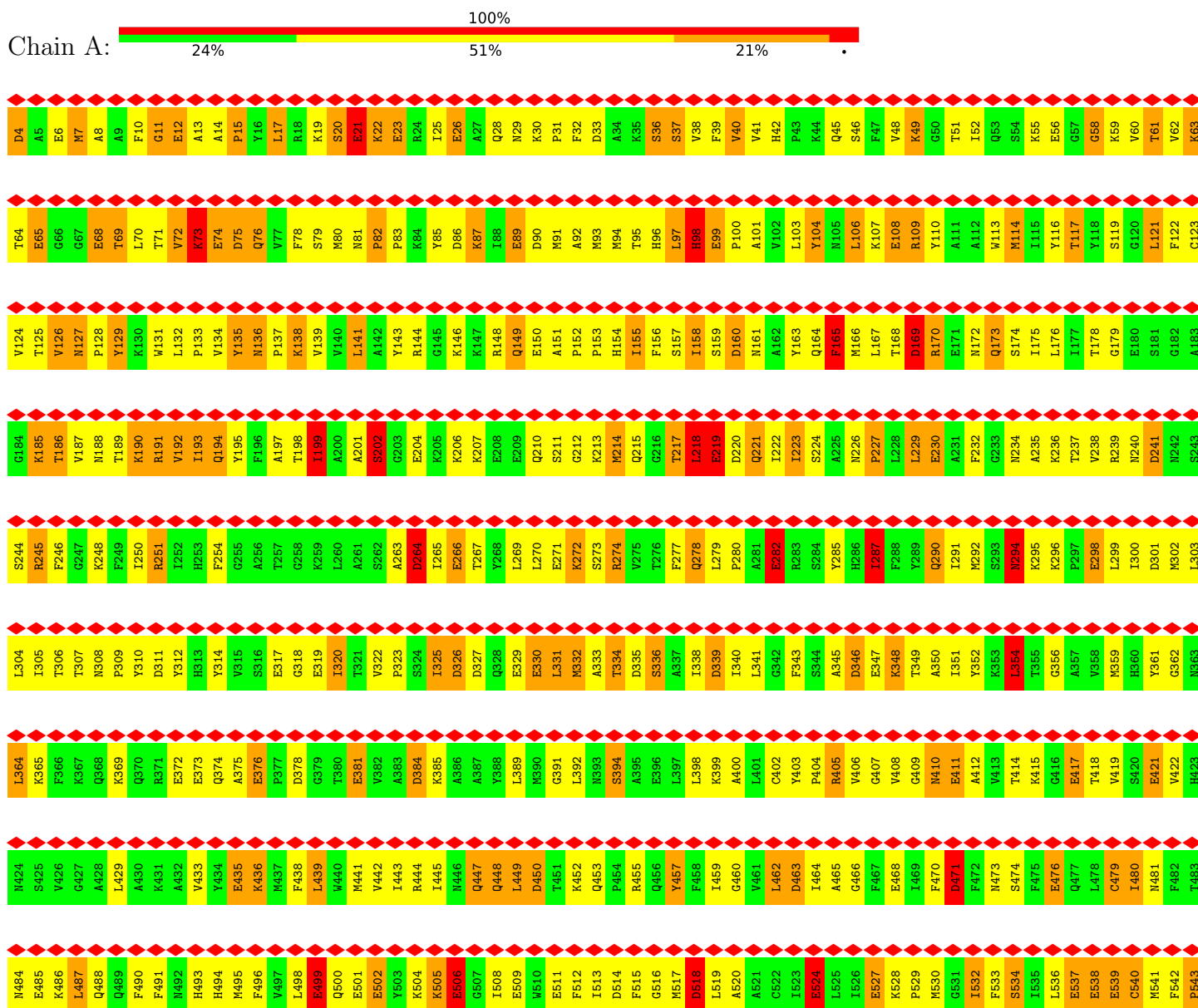
- Molecule 4 is a protein called SKELETAL MUSCLE ACTIN.

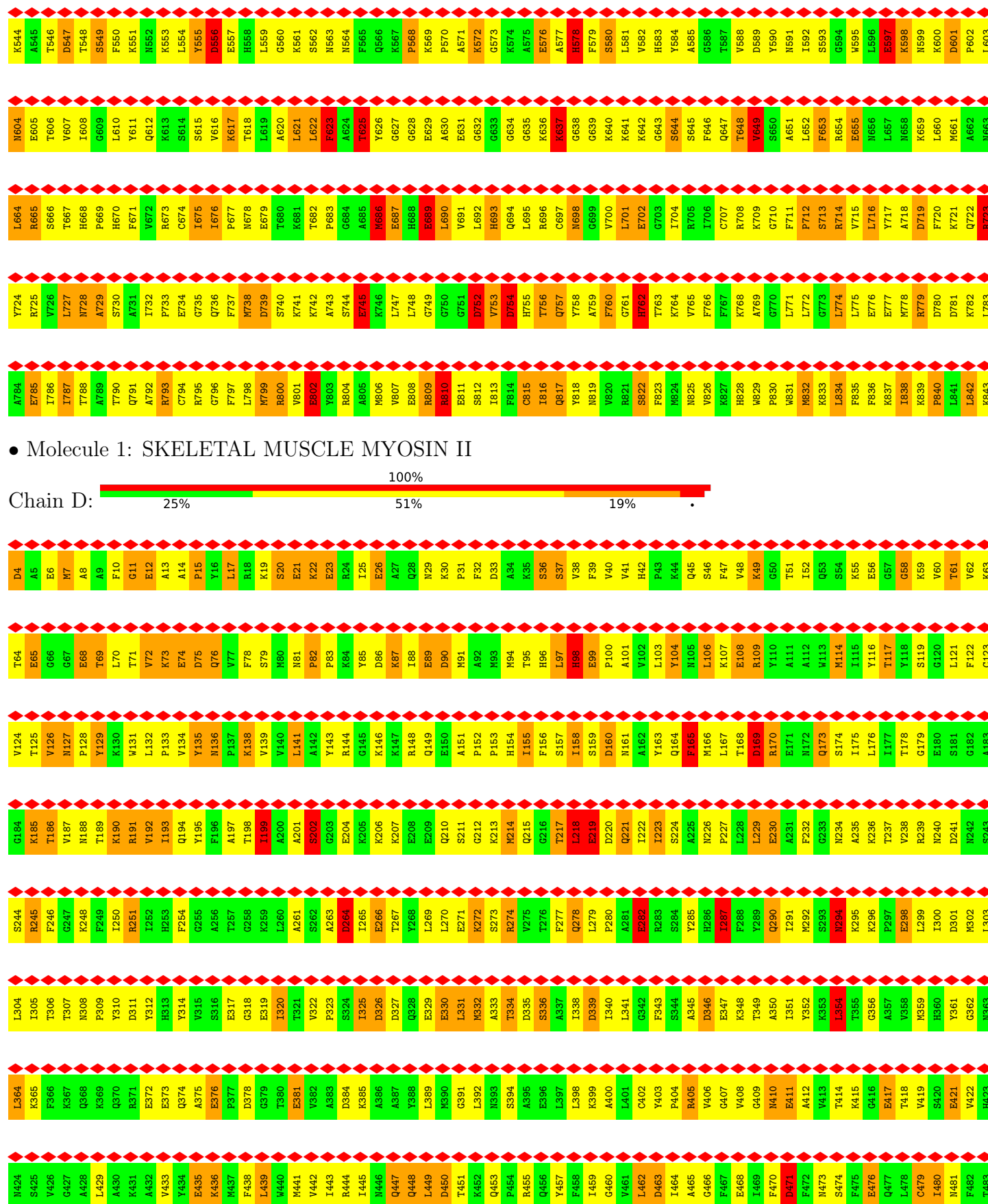
Mol	Chain	Residues	Atoms					AltConf	Trace
4	0	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	1	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	2	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	3	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	4	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	5	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	7	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	8	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	9	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	V	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	W	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	X	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	Y	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	Z	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		

### 3 Residue-property plots

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 and atom inclusion in map density. 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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: SKELETAL MUSCLE MYOSIN II







N484	E485	K486	L487	Q488	Q489	F490	F491	N492	H493	H494	M495	F496	F497	L498	E499	Q500	E501	E502	Y503	K504	K505	E506	G507	I508	E509	W510	E511	F512	I513	D514	F515	G516	M517	D518	L519	A520	A521	C522	I523	E524	L525	I526	E527	K528	P529	M530	G531	I532	F533	S534	I535	L536	E537	E538	E539	C540	M541	F542	P543
K544	E545	T546	D547	T548	S549	F550	K551	N552	K553	L554	Y555	D556	E557	H558	L559	G560	K561	S562	N563	N564	F565	Q566	K567	P568	K569	P570	A571	K572	G573	K574	A575	E576	A577	H578	F579	S580	K581	V582	H583	Y584	A585	G586	T587	V588	D589	Y590	N591	I592	F593	G594	V595	L596	E597	K598	N599	K600	D601	P602	L603
N604	E605	T606	V607	I608	G609	L610	Y611	Q612	K613	S614	S615	I616	K617	T618	L619	A620	L621	L622	F623	A624	T625	Y626	G627	G628	E629	A630	E631	G632	G633	G634	G635	K636	K637	G638	G639	K640	K641	K642	G643	S644	R645	F646	Q647	T648	V649	S650	A651	L652	F653	R654	E655	M656	L657	K658	K659	L660	M661	A662	N663
L664	R665	S666	T667	H668	P669	H670	F671	V672	H673	C674	I675	I676	P677	N678	E679	T680	K681	T682	P683	G684	A685	M686	E687	H688	E689	L690	V691	L692	H693	Q694	L695	R696	C697	M698	G699	V700	L701	E702	G703	I704	R705	I706	C707	R708	K709	G710	F711	L712	S713	R714	V715	L716	T717	A718	D719	F720	T721	Q722	R723
Y724	R725	V726	L727	M728	A729	S730	A731	I732	P733	E734	G735	Q736	F737	M738	D739	S740	K741	K742	A743	S744	E745	K746	L747	L748	G749	G750	G751	D752	V753	D754	H755	T756	Q757	Y758	A759	F760	G761	H762	T763	K764	V765	F766	F767	K768	A769	G770	L771	L772	G773	L774	L775	E776	E777	M778	R779	D780	T781	K782	L783
A784	E785	I786	T787	T788	A789	T790	Q791	R792	A793	C794	R795	G796	F797	L798	M799	R800	V801	E802	Y803	R804	A805	M806	V807	E808	R809	R810	E811	S812	I813	F814	C815	I816	Q817	Y818	N819	V820	R821	S822	F823	M824	N825	V826	K827	H828	H829	P830	M831	M832	K833	L834	F835	F836	T837	T838	K839	P840	L841	L842	K843

## ● Molecule 1: SKELETAL MUSCLE MYOSIN II



L364	L365	F366	K367	Q368	K369	Q370	R371	E372	E373	Q374	A375	E376	P377	D378	G379	T380	E381	V382	A383	D384	K385	A386	A387	Y388	L389	K390	G391	L392	N393	S394	A395	E396	L397	L398	K399	A400	L401	C402	Y403	P404	A405	V406	G407	V408	N409	N410	E411	A412	V413	T414	K415	G416	E417	T418	V419	S420	E421	V422	H423
L304	I305	T306	T307	N308	P309	Y310	D311	Y312	H313	Y314	V315	S316	E317	G318	E319	I320	T321	V322	S323	D324	I325	E326	T327	Q328	E329	E330	L331	M332	A333	T334	D335	S336	V337	I338	D339	T340	L341	G342	F343	S344	A345	D346	E347	K348	T349	A350	I351	Y352	K353	L354	T355	G356	A357	V358	M359	H360	Y361	G362	N363
S244	R245	F246	G247	K248	F249	L250	R251	L252	H253	F254	G255	A256	T257	G258	K259	L260	A261	S262	D263	I265	E266	T267	T268	L269	L270	E271	K272	S273	R274	V275	T276	F277	Q278	L279	P280	A281	E282	R283	S284	Y285	H286	F287	T288	Y289	Q290	I291	M292	S293	R294	K295	K296	E297	E298	L299	I300	D301	M302	L303	
G184	K185	T186	V187	M188	T189	K190	R191	V192	I193	Q194	Y195	F196	A197	T198	I199	A200	A201	S202	G203	E204	K205	K206	K207	E208	E209	Q210	S211	G212	K213	M214	Q215	G216	L217	L218	E219	D220	Q221	I222	I223	S224	A225	N226	P227	L228	L229	E230	A231	F232	G233	N234	A235	K236	T237	V238	R239	E180	D241	N242	S243
V124	T125	V126	N127	P128	Y129	K130	V131	L132	P133	V134	Y135	N136	P137	K138	V139	Y140	L141	A142	Y143	R144	G145	K146	K147	R148	Q149	E150	A151	P152	P153	H154	I155	F156	S157	I158	S159	D160	N161	A162	Q163	Q164	F165	M166	L167	T168	D169	R170	E171	M172	Q173	S174	L175	L176	I177	T178	G179	E180	L181	F182	A183
T64	E65	G66	G67	E68	T69	L70	T71	V72	K73	E74	D75	Y76	V77	F78	S79	M80	N81	P82	P83	K84	Y85	D86	K87	I88	E89	D90	M91	A92	M93	N94	T95	H96	L97	H98	E99	P100	A101	V102	L103	Y104	N105	L106	K107	E108	R109	Y110	A111	A112	W113	M114	I115	Y116	T117	Y118	G119	G120	L121	F122	C123
D4	A5	E6	M7	A8	A9	F10	G11	E12	A13	A14	P15	Y16	L17	R18	K19	S20	E21	K22	E23	R24	I25	E26	A27	Q28	N29	K30	P31	F32	D33	A34	K35	S36	S37	V38	F39	V40	V41	H42	P43	K44	Q45	S46	F47	V48	G49	T51	I52	Q53	S54	K55	E56	G57	G58	K59	V60	T61	V62	K63	

N424	N484	K544	N604	L664	Y724	A784	N424	N484	K544	N604	L664	Y724	A784
S426	E485	A545	E505	R665	R725	E785	S426	E485	A545	E505	R665	R725	E785
V426	K486	T546	T606	S666	V726	I786	V426	K486	T546	T606	S666	V726	I786
G427	L487	D547	V607	T667	L727	T787	G427	L487	D547	V607	T667	L727	T787
N428	Q488	T548	I608	H668	A728	T788	N428	Q488	T548	I608	H668	A728	T788
L429	Q489	S549	G609	P669	A729	A789	L429	Q489	S549	G609	P669	A729	A789
A430	F490	F550	L610	H670	S730	T790	A430	F490	F550	L610	H670	S730	T790
K431	F491	K551	Y611	F671	A731	Q791	K431	F491	K551	Y611	F671	A731	Q791
A432	N492	N552	Q612	V672	I732	A792	A432	N492	N552	Q612	V672	I732	A792
V433	H493	K553	K613	R673	P733	R793	V433	H493	K553	K613	R673	P733	R793
Y434	H494	L554	S614	C674	E734	C794	Y434	H494	L554	S614	C674	E734	C794
E435	M495	Y555	S615	I675	G735	R795	E435	M495	Y555	S615	I675	G735	R795
K436	F496	D556	V616	I676	Q736	G796	K436	F496	D556	V616	I676	Q736	G796
M437	V497	V557	K617	P677	F737	F797	M437	V497	V557	K617	P677	F737	F797
F438	L498	H558	T618	N678	M738	L798	F438	L498	H558	T618	N678	M738	L798
L439	E499	L559	L619	E679	D739	M799	L439	E499	L559	L619	E679	D739	M799
Y440	Q500	G560	A620	T680	S740	R800	Y440	Q500	G560	A620	T680	S740	R800
M441	E501	K561	L621	K681	K741	V601	M441	E501	K561	L621	K681	K741	V601
V442	E502	S562	L622	T682	K742	E502	V442	E502	S562	L622	T682	K742	E502
I443	Y503	N563	F623	P683	A743	R503	I443	Y503	N563	F623	P683	A743	R503
R444	K504	N564	A624	G684	S744	R504	R444	K504	N564	A624	G684	S744	R504
I445	K505	F565	T625	A685	E745	A605	I445	K505	F565	T625	A685	E745	A605
N446	E506	Q566	Y626	M686	K746	M606	N446	E506	Q566	Y626	M686	K746	M606
Q447	G507	K567	G627	H687	L747	V607	Q447	G507	K567	G627	H687	L747	V607
Q448	I508	P568	G628	H688	L748	E508	Q448	I508	P568	G628	H688	L748	E508
L449	E509	K569	E629	E689	G749	R609	L449	E509	K569	E629	E689	G749	R609
D450	W510	P570	A630	L690	G750	R610	D450	W510	P570	A630	L690	G750	R610
T451	E511	A571	E631	V691	G751	E611	T451	E511	A571	E631	V691	G751	E611
K452	F512	K572	G632	L692	D752	S612	K452	F512	K572	G632	L692	D752	S612
Q453	I513	G573	V753	H693	V753	I613	Q453	I513	G573	V753	H693	V753	I613
P454	D514	K574	G634	Q694	D754	F614	P454	D514	K574	G634	Q694	D754	F614
R455	F515	A575	G635	L695	H755	C615	R455	F515	A575	G635	L695	H755	C615
Q456	G516	E576	K636	R696	T756	I616	Q456	G516	E576	K636	R696	T756	I616
Y457	M517	A577	K637	C697	Q757	Q617	Y457	M517	A577	K637	C697	Q757	Q617
F458	D518	H578	G638	N698	Y758	Y618	F458	D518	H578	G638	N698	Y758	Y618
I459	L519	F579	G639	G699	A759	N619	I459	L519	F579	G639	G699	A759	N619
G460	A520	S580	K640	V700	F760	W620	G460	A520	S580	K640	V700	F760	W620
V461	E521	L581	K641	L701	G761	R621	V461	E521	L581	K641	L701	G761	R621
L462	C522	V582	K642	E702	H762	S622	L462	C522	V582	K642	E702	H762	S622
D463	I523	H583	G643	G703	T763	F623	D463	I523	H583	G643	G703	T763	F623
I464	E524	Y584	S644	I704	K764	M624	I464	E524	Y584	S644	I704	K764	M624
A465	L525	A585	S645	R705	V765	N625	A465	L525	A585	S645	R705	V765	N625
G466	I526	G586	F646	I706	F766	V626	G466	I526	G586	F646	I706	F766	V626
F467	E527	T587	Q647	C707	F767	K627	F467	E527	T587	Q647	C707	F767	K627
E468	K528	V588	T648	R708	K768	H628	E468	K528	V588	T648	R708	K768	H628
I469	P529	D589	V649	K709	A769	W629	I469	P529	D589	V649	K709	A769	W629
F470	M530	Y590	S550	G710	G770	P630	F470	M530	Y590	S550	G710	G770	P630
D471	G531	N591	A651	F711	L771	W631	D471	G531	N591	A651	F711	L771	W631
F472	I532	L592	L652	P712	L772	M632	F472	I532	L592	L652	P712	L772	M632
N473	F533	S593	F653	S713	G773	K633	N473	F533	S593	F653	S713	G773	K633
S474	S534	G594	R654	R714	L774	L634	S474	S534	G594	R654	R714	L774	L634
F475	I535	W595	E655	V715	L775	P635	F475	I535	W595	E655	V715	L775	P635
A476	L536	L596	M556	L716	E776	F636	A476	L536	L596	M556	L716	E776	F636
Q477	E537	R597	L657	L717	F777	K637	Q477	E537	R597	L657	L717	F777	K637
L478	E538	K598	M558	A718	M778	T638	L478	E538	K598	M558	A718	M778	T638
C479	E539	N599	K659	D719	R779	K639	C479	E539	N599	K659	D719	R779	K639
I480	C540	K600	L660	F720	D780	P640	I480	C540	K600	L660	F720	D780	P640
N481	M541	D601	M661	K721	D781	L641	N481	M541	D601	M661	K721	D781	L641
F482	F542	P602	A662	Q722	K782	L642	F482	F542	P602	A662	Q722	K782	L642
T483	P543	L603	N663	R723	L783	K643	T483	P543	L603	N663	R723	L783	K643

## ● Molecule 1: SKELETAL MUSCLE MYOSIN II



D4	T64	V124	G184	S244	L304
A5	E65	T125	K185	R245	I305
E6	G66	V126	T186	F246	T306
M7	G67	M127	V187	G247	T307
A8	E68	P128	N188	K248	N308
A9	T69	Y129	T189	F249	P309
F10	L70	K130	K190	L250	Y310
G11	T71	W131	R191	R251	D311
E12	V72	L132	V192	L252	Y312
A13	K73	P133	I193	H253	H313
A14	E74	V134	Q194	F254	Y314
P15	D75	Y135	Y195	G255	V315
Y16	Q76	M136	F196	A256	S316
L17	V77	P137	A197	T257	E317
R18	F78	K138	T198	G258	G318
K19	S79	V139	I199	K259	E319
S20	M80	Y140	A200	L260	I320
E21	N81	L141	A201	A261	T321
K22	P82	A142	S202	S262	V322
R24	K84	Y143	G203	A263	P323
I25	G85	G145	E204	D264	S324
E26	D86	K146	K206	L265	I325
A27	K87	K147	K207	E266	D326
Q28	T88	R148	E208	T267	D327
N29	E89	Q149	E209	V268	Q328
K30	D90	E150	Q210	L269	E329
P31	M91	A151	S211	L270	E330
F32	A92	P152	G212	E271	L331
D33	M93	P153	K213	K272	A332
A34	M94	H154	M214	R274	T334
K35	T95	I155	Q215	V275	D335
S36	H96	F156	G216	G276	S336
S37	L97	S157	T217	T277	A337
V38	H98	I158	L218	Q278	I338
F39	E99	S159	E219	L279	D339
V40	P100	D160	D220	P280	I340
V41	A101	M161	Q221	A281	L341
H42	Y102	A162	I222	E282	G342
P43	L103	Y163	I223	R283	F343
K44	Y104	Q164	S224	S284	S344
Q45	N105	F165	A225	Y285	A345
S46	L106	M166	N226	H286	D346
F47	K107	L167	P227	T287	E347
V48	E108	T168	L228	F288	K348
K49	R109	D169	L229	Y289	T349
G50	Y110	R170	E230	Q290	A350
T51	A111	E171	A231	I291	I351
I52	A112	M172	F232	M292	Y352
Q53	Y113	Q173	G233	S293	K353
S54	M114	S174	N234	L294	L354
K55	I115	T175	A235	K295	T355
E56	Y116	L176	K236	K296	G356
G57	T117	I177	T237	P297	A357
G58	Y118	T178	V238	E298	V358
K59	S119	G179	R239	L299	K359
V60	G120	E180	N240	I300	H360
T61	S121	S181	D241	D301	Y361
V62	F122	G182	N242	M302	G362
K63	C123	A183	S243	L303	N363

A784	L784	Y724	L664	M604	K544	N484	N424	L364
R785	K365	R725	R665	E605	A545	E485	S425	K365
I786	F366	V726	T666	T606	T546	K486	V426	F366
T787	G367	L727	T667	V607	D547	L487	G427	K367
T788	Q368	H728	H668	I608	T548	Q488	A428	Q368
A789	K369	A729	P669	G609	S549	Q489	L429	K369
T790	Q370	S730	H670	L610	F550	F490	A430	Q370
Q791	E371	A731	F671	Y611	K551	F491	K431	E371
A792	R372	I732	V672	Q612	N552	N492	A432	E372
R793	E373	P733	R673	K613	K553	H493	V433	E373
C794	Q374	E734	C674	S614	L554	H494	Y434	Q374
R795	A375	G735	L675	S615	Y555	M495	E435	A375
G796	E376	Q736	L676	V616	D556	F496	K436	E376
F797	P377	F737	P677	K617	E557	V497	M437	P377
M798	D378	M738	N678	H558	H558	L498	F438	D378
M799	G379	D739	E679	L619	L559	E499	L439	G379
V801	T380	S740	T680	A620	G560	Q500	M440	T380
E802	E381	K741	K681	L621	K561	E501	M441	E381
Y803	V382	K742	T682	L622	S562	E502	V442	V382
R804	A383	A743	P683	F623	N563	Y503	I443	A383
A805	D384	S744	G684	A624	N564	K504	R444	D384
M806	K385	E745	A685	T625	F565	K505	I445	K385
V807	A386	K746	M686	V626	Q566	E506	M446	A386
E808	A387	L747	E687	G627	K567	G507	Q447	A387
R809	L388	L748	H688	G628	P568	I508	Q448	L388
R810	L389	G749	E689	E629	K569	E509	L449	L389
E811	M390	G750	L690	A630	P570	W510	D450	M390
S812	G391	G751	V691	E631	A571	E511	T451	G391
L813	L392	D752	L692	G632	K572	F512	K452	L392
F814	N393	V753	H693	G633	G573	I513	Q453	N393
C815	S394	D754	Q694	G634	K574	D514	P454	S394
L816	A395	H755	L695	G635	A575	F515	R455	A395
Q817	E396	T756	R696	K636	E576	G516	Q456	E396
Y818	L397	Q757	G697	K637	A577	M517	Y457	L397
N819	L398	Y758	N698	G638	H578	D518	F458	L398
V820	K399	A759	G699	G639	F579	L519	I459	K399
R821	A400	F760	V700	K640	S580	A520	G460	A400
S822	L401	G761	L701	K641	L581	A521	V461	L401
F823	C402	R762	E702	K642	V582	C522	L462	C402
M824	Y403	T763	G703	G643	H583	I523	D463	Y403
N825	P404	K764	I704	S644	Y584	E524	I464	P404
V826	R405	V765	R705	S645	A585	L525	A465	R405
K827	V406	F766	I706	F646	G586	I526	G466	V406
H828	G407	T767	G707	Q647	T587	E527	F467	G407
V829	V408	K768	R708	T648	V588	K528	E468	V408
M829	G409	A769	K709	V649	D589	P529	I469	G409
M831	N410	G770	G710	S650	Y590	M530	G470	N410
N832	E411	F711	F711	A651	N591	G531	D471	E411
K833	A412	L772	P712	L652	I592	I532	F472	A412
L834	V413	R773	S713	F653	S593	F533	M473	V413
F835	S474	R714	R654	R654	G594	S534	S474	F835
F836	T414	L775	V715	E655	M595	I535	F475	T414
K837	K415	E776	L716	M656	L596	L536	E476	K415
I838	G416	Y717	Y717	L657	E597	E537	Q477	G416
K839	E417	A718	M658	M658	K598	E538	L478	E417
P840	T418	R779	D719	K659	N599	E539	C479	P840
L841	V419	F720	L660	K600	K600	C540	I480	V419
L842	S420	D781	K721	M661	D601	M541	M481	L842
L843	E421	Q722	A662	N662	P602	F452	F482	L843
	H423	L783	R723	N663	L603	P543	T483	H423

• Molecule 1: SKELETAL MUSCLE MYOSIN II



S244	R245	F246	G247	K248	F249	L250	R251	L252	H253	F254	G255	A256	T257	G258	K259	L260	A261	S262	A263	D264	L265	E266	T267	Y268	L269	L270	E271	K272	S273	R274	V275	T276	F277	Q278	L279	P280	A281	E282	R283	S284	Y285	H286	F287	F288	Y289	Q290	T291	N292	M293	S293	N294	K295	K296	P297	E298	L299	I300	D301	M302	L303
G184	K185	T186	V187	N188	T189	K190	R191	V192	I193	Q194	Y195	F196	A197	T198	N199	A200	A201	S202	G203	E204	K205	K206	K207	E208	E209	Q210	S211	G212	K213	M214	Q215	G216	T217	L218	E219	D220	Q221	I222	I223	S224	A225	N226	P227	L228	L229	E230	A231	F232	G233	N234	A235	K236	T237	V238	R239	N240	D241	N242	S243	
V124	T125	V126	N127	P128	Y129	K130	V131	L132	P133	V134	Y135	N136	P137	K138	V139	Y140	L141	A142	Y143	G144	K145	K146	K147	R148	Q149	E150	A151	P152	P153	H154	I155	F156	S157	I158	S159	D160	A161	A162	Y163	Q164	F165	M166	L167	T168	D169	R170	E171	N172	Q173	S174	T175	L176	I177	T178	G179	E180	S181	G182	A183	
T64	E65	G66	G67	E68	T69	L70	T71	V72	K73	E74	D75	Q76	V77	F78	S79	M80	N81	P82	P83	R84	Y85	D86	K87	T88	E89	D90	N91	A92	N93	A94	T95	H96	L97	H98	E99	P100	A101	V102	L103	Y104	N105	L106	K107	E108	R109	Y110	A111	A112	M113	M114	I115	Y116	T117	Y118	S119	G120	L121	F122	C123	
D4	A5	E6	M7	A8	A9	F10	G11	E12	A13	A14	P15	Y16	L17	R18	K19	S20	E21	K22	E23	R24	I25	E26	A27	Q28	N29	K30	P31	F32	D33	A34	K35	S36	S37	V38	F39	V40	V41	H42	P43	K44	Q45	S46	F47	V48	K49	G50	T51	I52	Q53	S54	K55	E56	G57	G58	K59	V60	T61	V62	K63	

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
Y724	R725	V726	L727	N728	A729	S730	A731	I732	P733	E734	G735	Q736	F737	M738	D739	K740	K741	K742	A743	S744	E745	K746	L747	L748	G749	G750	G751	D752	V753	D754	H755	T756	Q757	N758	G759	V760	L761	E762	T763	F764	V765	F766	F767	K768	A769	G770	L771	P772	S773	L774	L775	E776	E777	H778	R779	D780	D781	K782	L783
L664	R665	S666	T667	H668	P669	H670	F671	V672	R673	C674	L675	L676	N677	M678	E679	T680	K681	T682	P683	G684	A685	M686	E687	H688	E689	L690	V691	L692	H693	Q694	L695	R696	G697	N698	G699	V700	L701	E702	G703	K704	R705	I706	C707	T708	K709	G710	F711	P712	S713	L774	L775	E776	E777	H778	R779	D780	D781	K782	L783
M604	E605	T606	V607	T608	G609	L610	Y611	Q612	K613	S614	S615	V616	K617	T618	L619	A620	L621	L622	P623	A624	T625	Y626	G627	G628	E629	A630	E631	G632	G633	G634	G635	K636	K637	G638	G639	K640	K641	K642	G643	S644	P645	Q646	T647	T648	V649	S650	A651	L652	F653	R654	E655	N656	L657	N658	K659	L660	M661	A662	N663
K544	A545	T546	D547	T548	S549	F550	K551	N552	K553	L554	Y555	D556	E557	H558	L559	G560	K561	S562	N563	N564	F565	Q566	K567	P568	K569	P570	A571	K572	G573	K574	A575	E576	A577	H578	F579	S580	L581	V582	H583	Y584	A585	G586	T587	V588	D589	Y590	N591	I592	S593	G594	N595	L596	E597	K598	N599	K600	D601	P602	L603
N484	E485	K486	L487	Q488	Q489	F490	F491	M492	H493	H494	M495	F496	V497	L498	E499	Q500	E501	E502	Y503	K504	K505	E506	G507	I508	E509	W510	E511	F512	I513	D514	F515	G516	N517	D518	L519	A520	A521	C522	I523	E524	L525	I526	E527	K528	P529	M530	G531	I532	F533	S534	I535	L536	E537	E538	E539	C540	M541	F542	P543
N424	S425	V426	G427	A428	L429	A430	K431	A432	V433	Y434	E435	K436	M437	F438	L439	W440	M441	V442	I443	R444	I445	N446	Q447	Q448	L449	D450	T451	K452	Q453	P454	R455	Q456	G457	F458	I459	G460	V461	L462	D463	I464	A465	G466	F467	E468	I469	F470	D471	F472	N473	S474	F475	E476	Q477	L478	C479	I480	N481	F482	T483
L364	K365	F366	K367	Q368	K369	Q370	R371	E372	E373	Q374	A375	S376	P377	D378	G379	T380	E381	V382	A383	D384	K385	A386	A387	Y388	L389	M390	E391	L392	N393	S394	A395	E396	G397	L398	K399	A400	L401	C402	Y403	P404	R405	V406	G407	V408	G409	N410	E411	A412	T413	K414	G415	A416	E417	T418	V419	S420	Y421	V422	H423
L304	I305	T306	T307	N308	P309	Y310	D311	Y312	H313	Y314	V315	S316	E317	G318	E319	I320	T321	V322	P323	S324	I325	D326	Q327	Q328	E329	E330	L331	M332	A333	T334	D335	S336	A337	I338	D339	I340	L341	G342	F343	S344	A345	D346	E347	K348	T349	A350	I351	Y352	K353	L354	T355	G356	A357	V358	M359	H360	Y361	G362	N363

## ● Molecule 1: SKELETAL MUSCLE MYOSIN II



G184	K185	T186	V187	T189	K190	R191	V192	I193	Q194	Y195	F196	A197	I199	A200	A201	S202	G203	E204	K205	K206	K207	E208	E209	Q210	S211	G212	K213	M214	Q215	G216	T217	L218	E219	D220	Q221	I222	I223	S224	A225	N226	P227	L228	L229	E230	A231	F232	G233	N234	A235	K236	T237	V238	R239	N240	D241	N242	S243		
V124	T125	V126	N127	P128	Y129	K130	W131	L132	P133	V134	Y135	N136	P137	K138	V139	V140	L141	A142	Y143	R144	G145	K146	L147	R148	Q149	E150	A151	P152	P153	H154	I155	F156	S157	I158	S159	D160	N161	A162	Y163	Q164	F165	M166	L167	T168	D169	R170	E171	N172	Q173	S174	I175	L176	T177	T178	G179	E180	S181	G182	A183
T64	E65	G66	G67	E68	T69	L70	T71	V72	K73	E74	D75	Q76	V77	F78	S79	M80	N81	P82	P83	K84	Y85	D86	K87	I88	E89	D90	M91	A92	M93	N94	T95	H96	L97	H98	E99	P100	A101	V102	L103	Y104	N105	L106	K107	E108	R109	Y110	A111	A112	W113	M114	I115	Y116	T117	Y118	S119	G120	L121	F122	C123
D4	A5	E6	M7	A8	A9	F10	G11	E12	A13	A14	P15	Y16	L17	R18	K19	S20	E21	K22	E23	K24	I25	E26	Q27	N29	K30	P31	F32	D33	A34	K35	S36	S37	V38	F39	V40	V41	H42	P43	K44	Q45	S46	F47	V48	K49	G50	T51	I52	Q53	S54	K55	E56	G57	G58	K59	V60	T61	V62	K63	

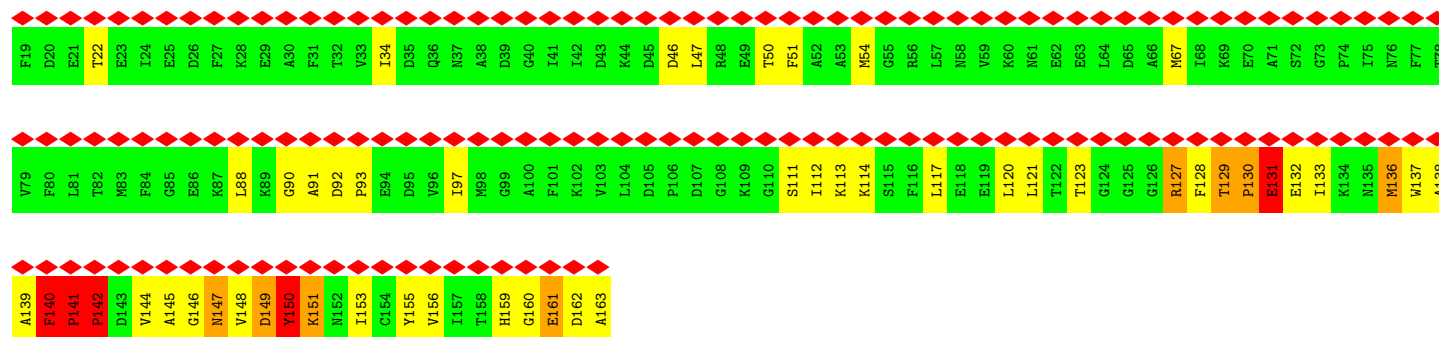
- Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

Device Type	Percentage
Smartphones	100%
Tablets	65%
Feature phones	26%
Other devices	6%

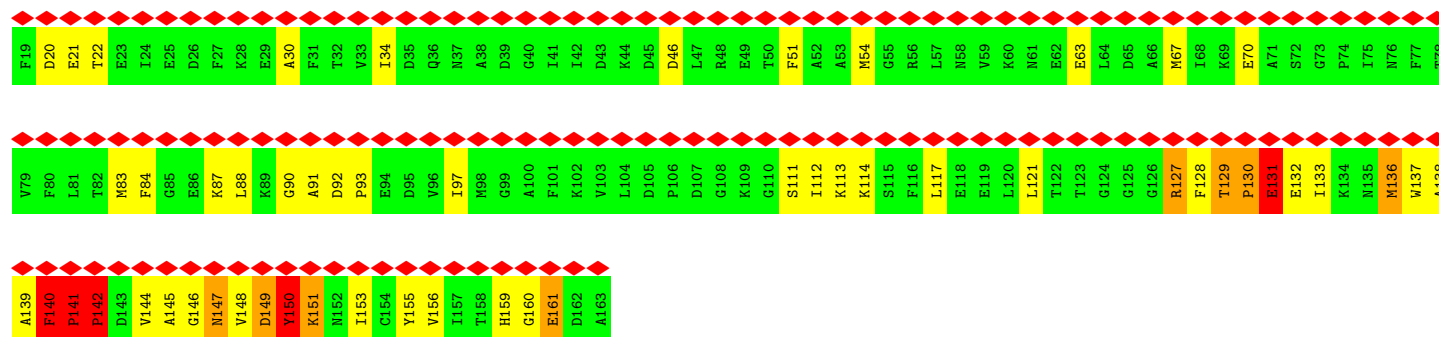


WORLDWIDE  
PDB  
PROTEIN DATA BANK

• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN



• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

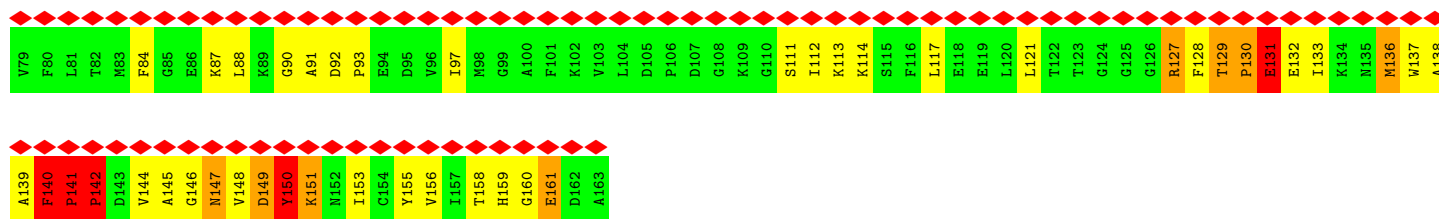


• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

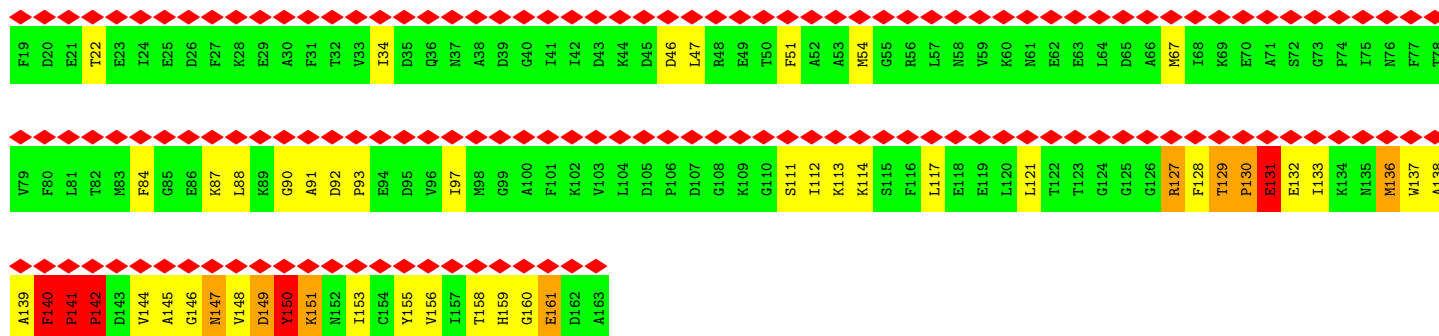


• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

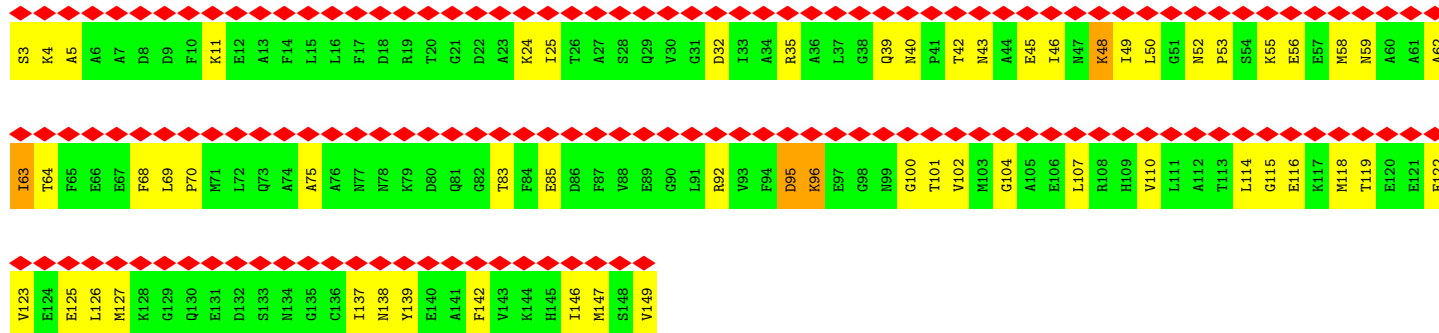




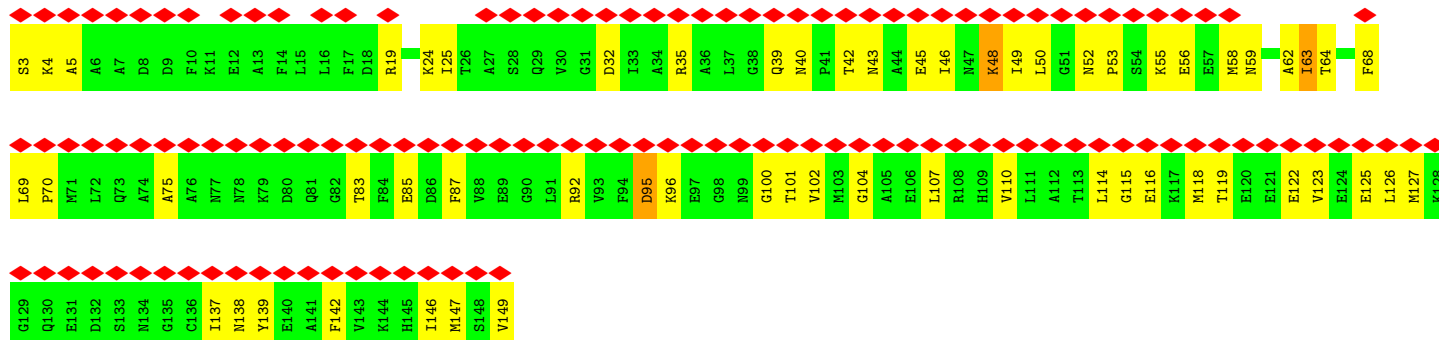
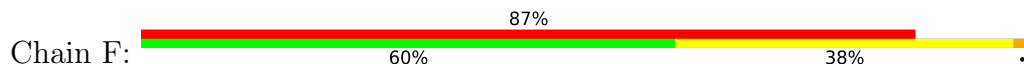
• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN



• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN

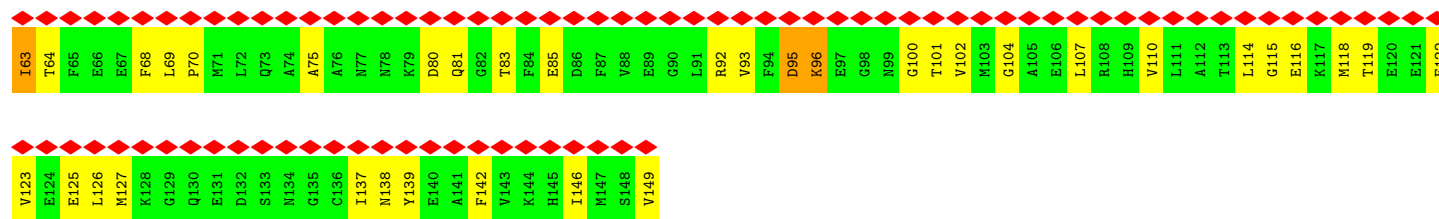


• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN

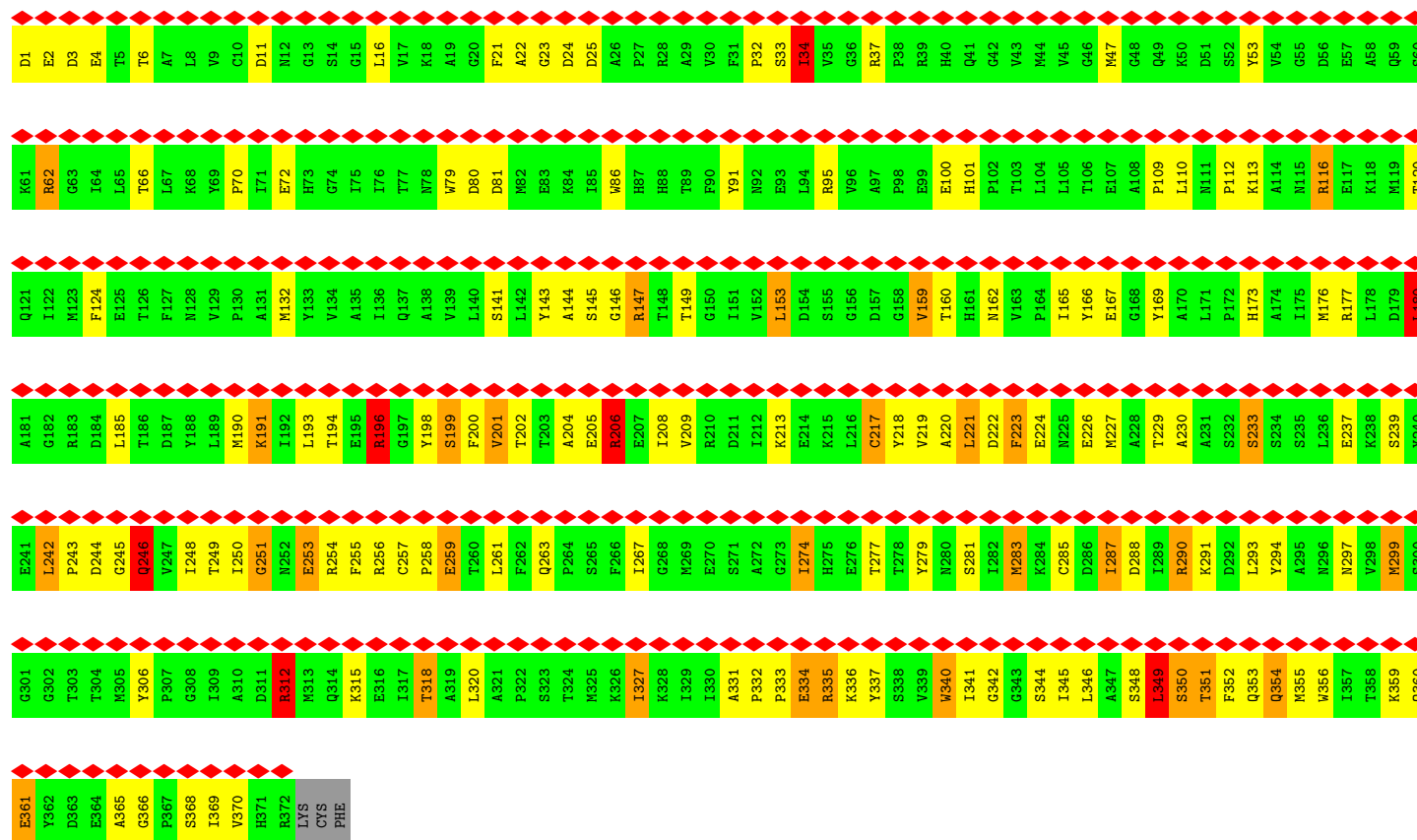




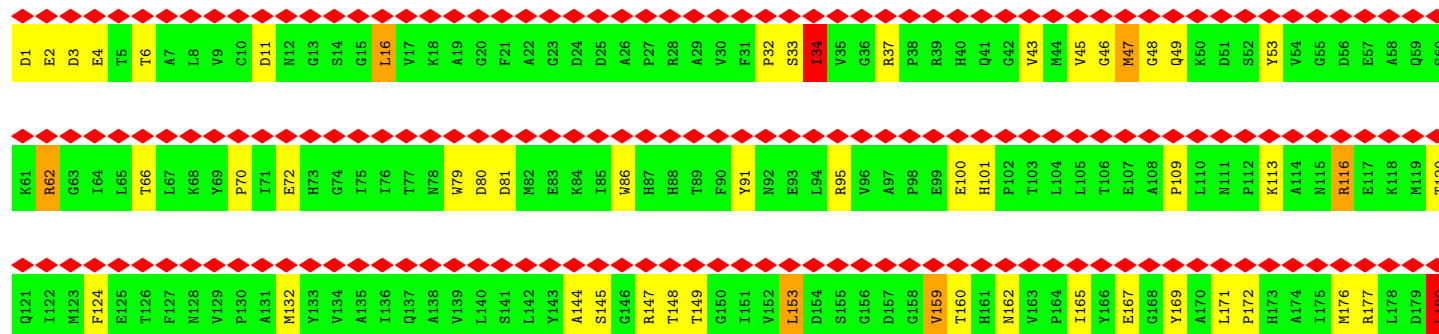




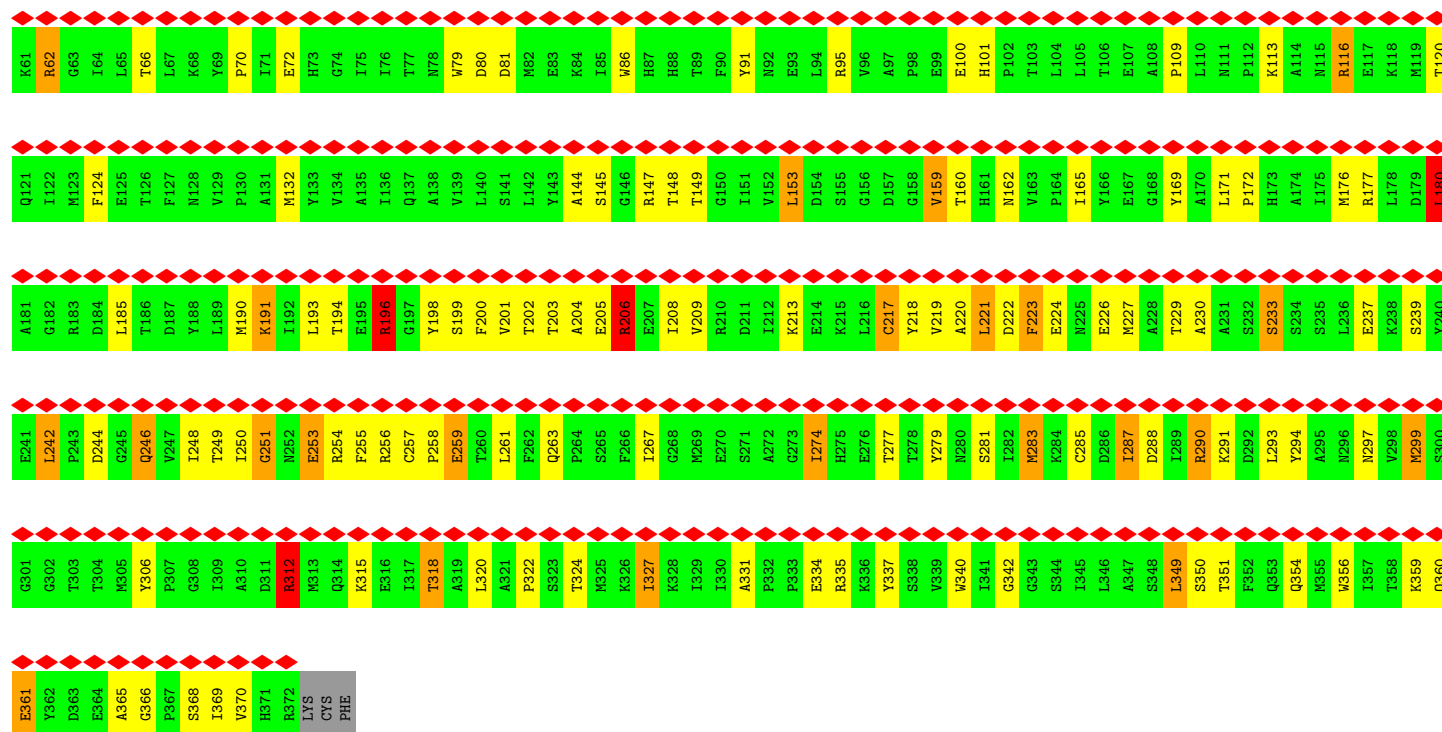
• Molecule 4: SKELETAL MUSCLE ACTIN



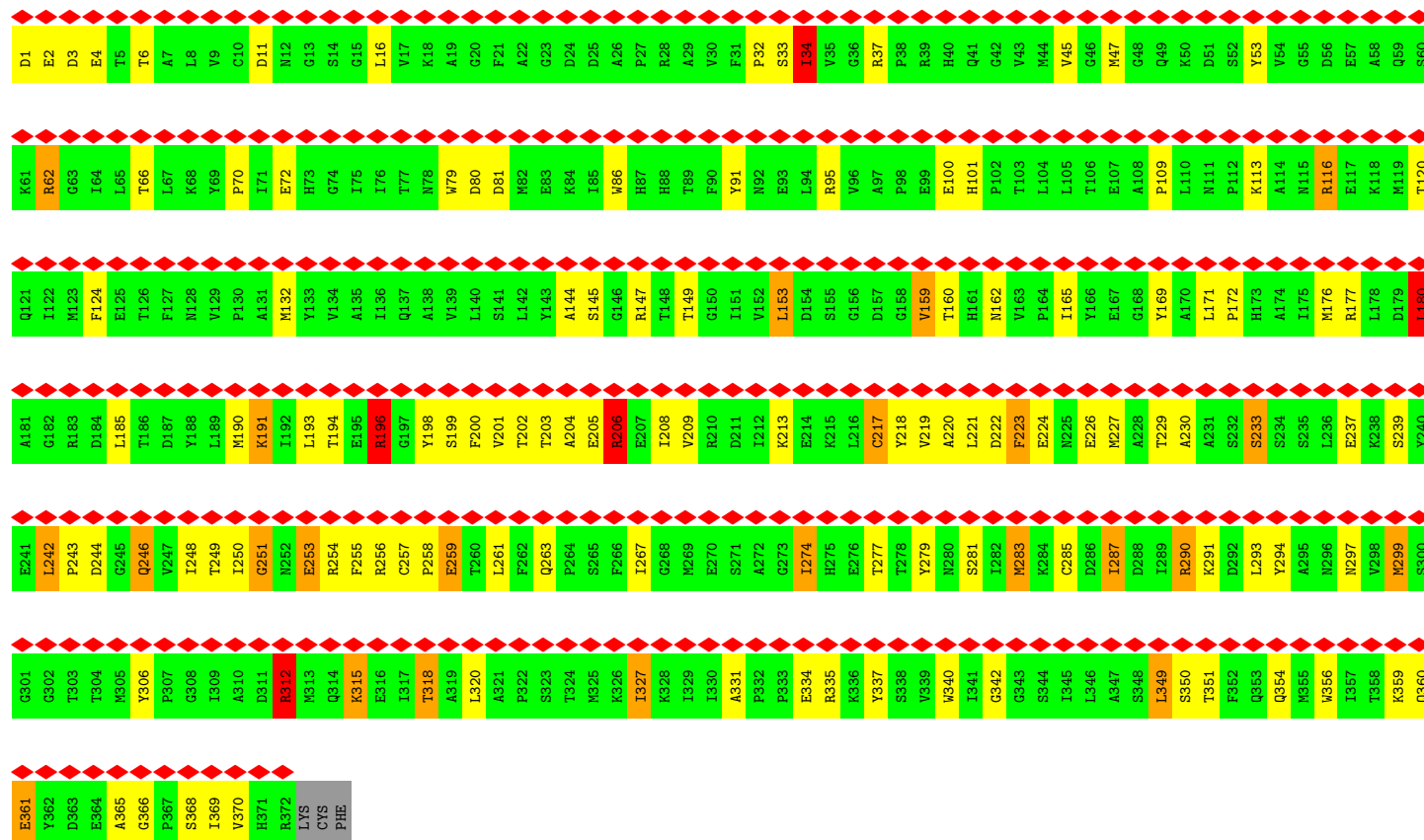
• Molecule 4: SKELETAL MUSCLE ACTIN



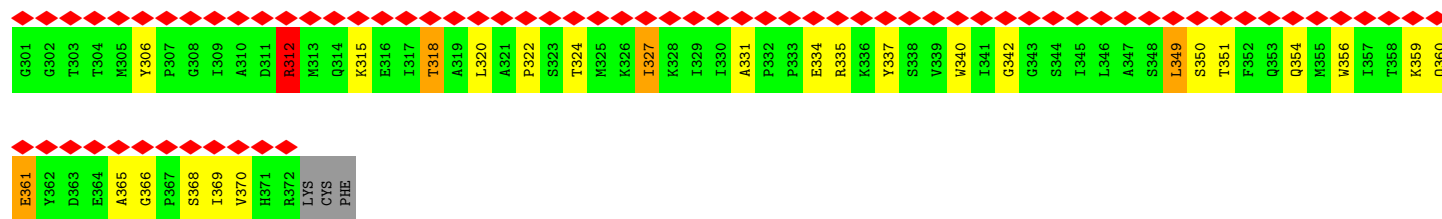




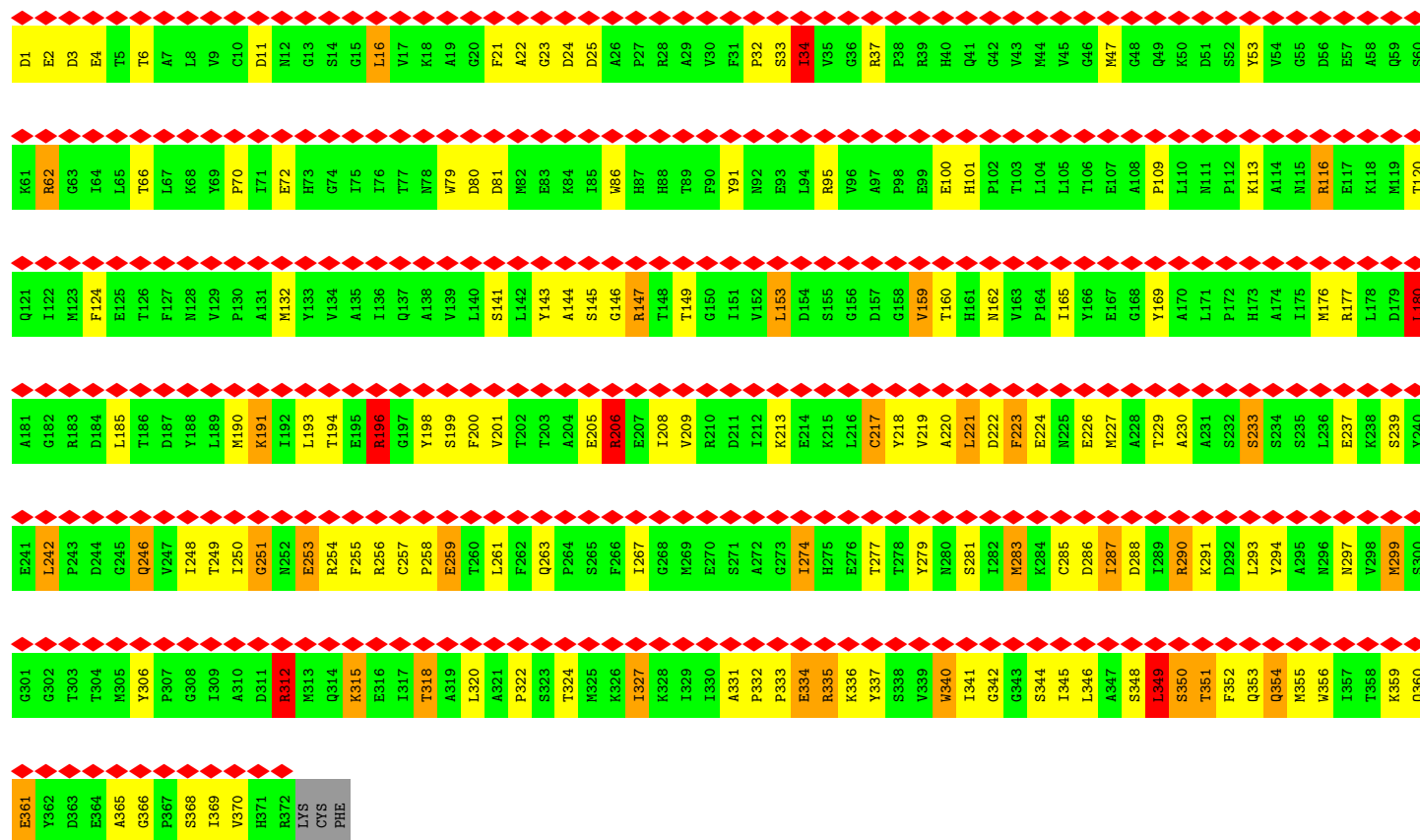
## ● Molecule 4: SKELETAL MUSCLE ACTIN



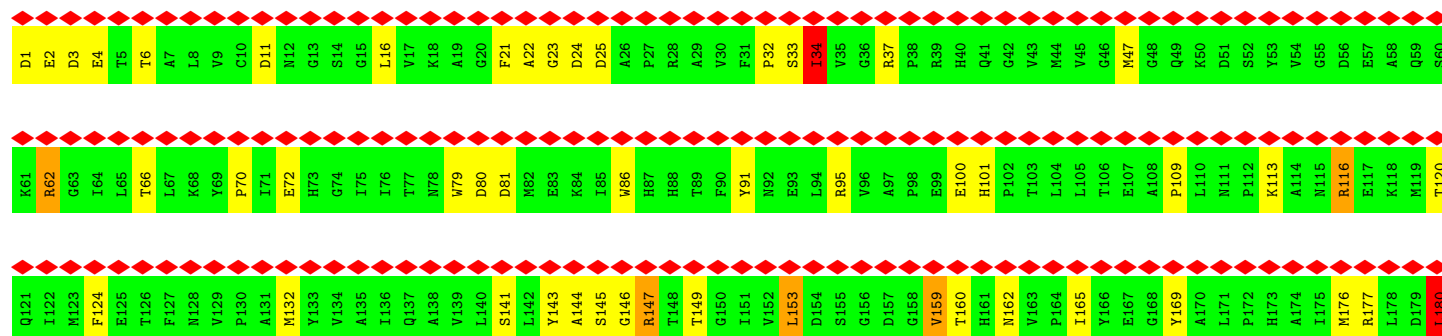




• Molecule 4: SKELETAL MUSCLE ACTIN

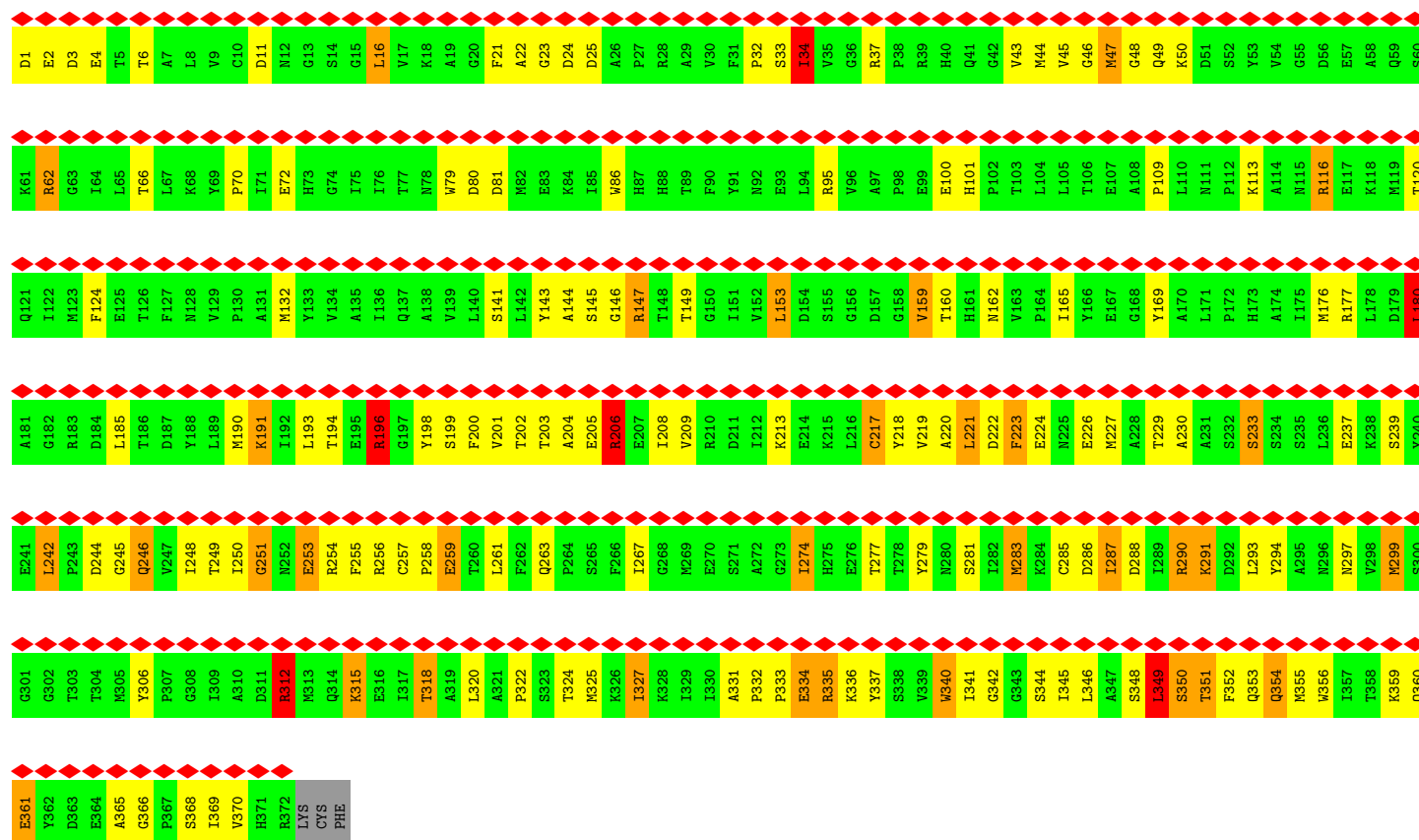


• Molecule 4: SKELETAL MUSCLE ACTIN

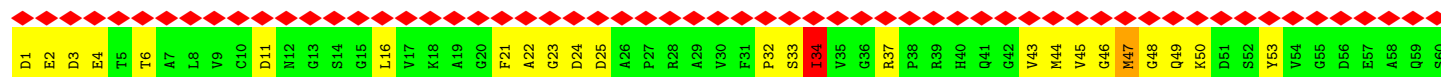


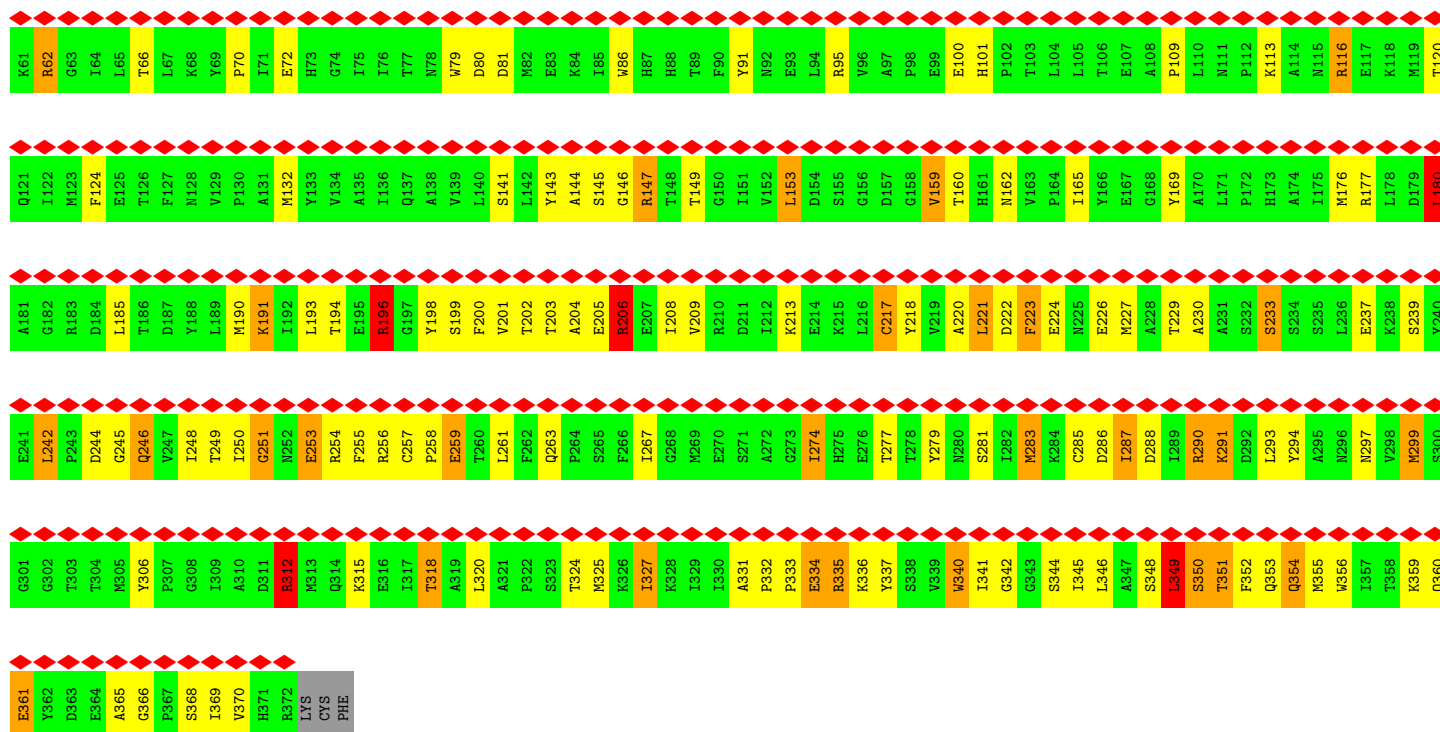


• Molecule 4: SKELETAL MUSCLE ACTIN



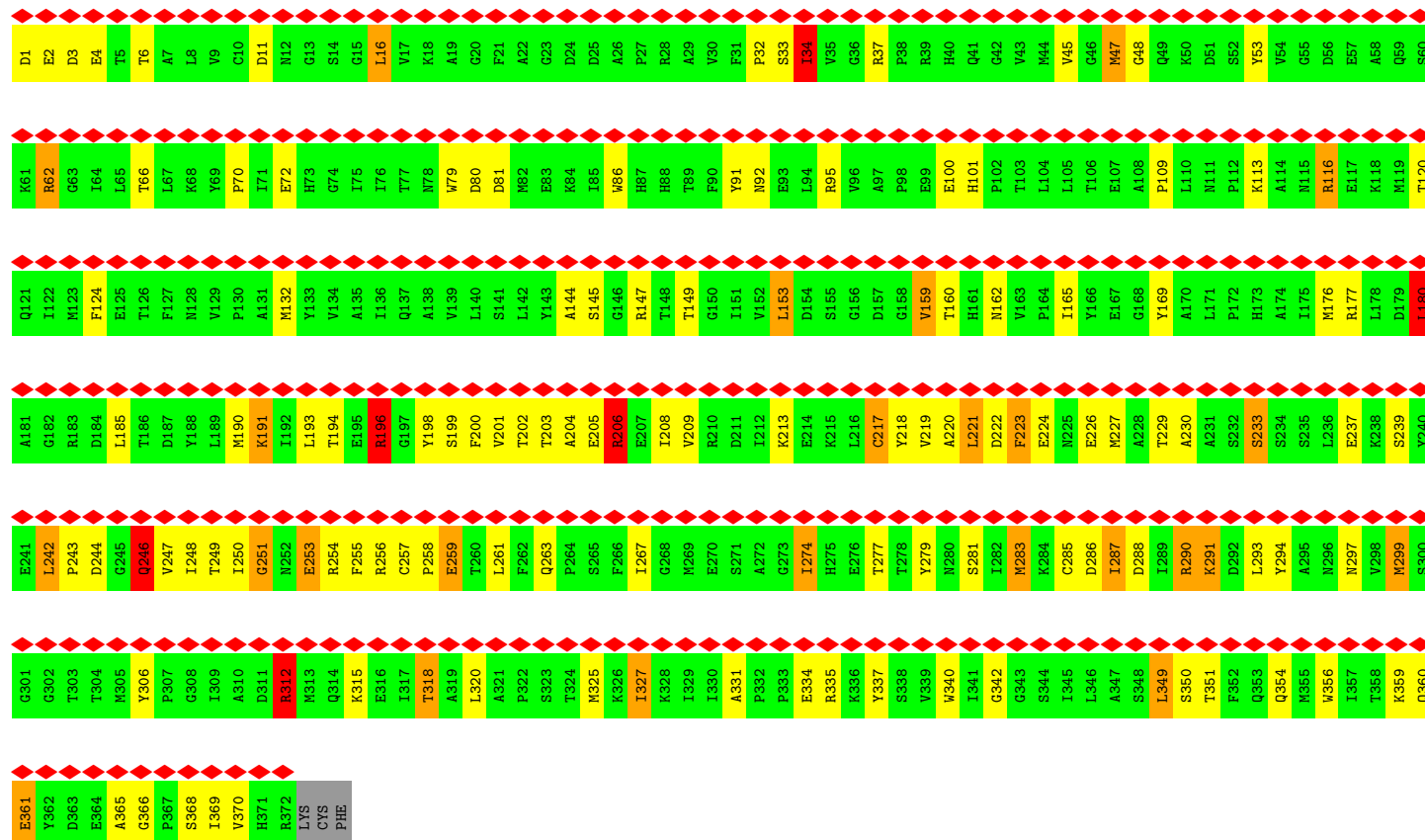
• Molecule 4: SKELETAL MUSCLE ACTIN





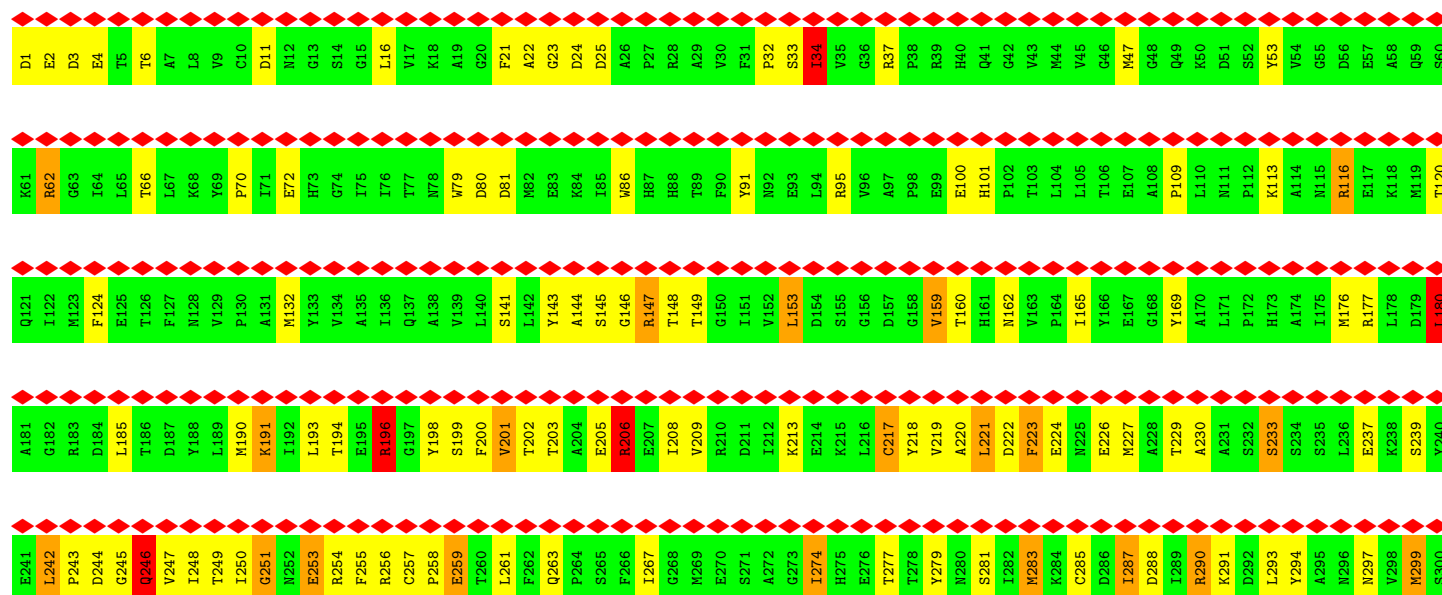
• Molecule 4: SKELETAL MUSCLE ACTIN

Chain Y: 



• Molecule 4: SKELETAL MUSCLE ACTIN

Chain Z: 







## 4 Experimental information

Property	Value	Source
EM reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of tilted images used	Not provided	
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	FEI/PHILIPS EM400	Depositor
Voltage (kV)	100	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	17000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum voxel value	366.680	Depositor
Minimum voxel value	-417.992	Depositor
Average voxel value	1.860	Depositor
Voxel value standard deviation	47.792	Depositor
Recommended contour level	81.2	Depositor
Tomogram size ( $\text{\AA}$ )	9280, 9280, 464	wwPDB
Tomogram dimensions	600, 600, 30	wwPDB
Tomogram angles ( $^\circ$ )	90, 90, 90	wwPDB
Grid spacing ( $\text{\AA}$ )	15.4667, 15.4667, 15.4667	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	A	1.77	67/6448 (1.0%)	1.82	118/8729 (1.4%)
1	D	1.77	63/6448 (1.0%)	1.82	117/8729 (1.3%)
1	G	1.78	67/6449 (1.0%)	1.83	118/8732 (1.4%)
1	J	1.77	68/6449 (1.1%)	1.87	117/8732 (1.3%)
1	M	1.78	66/6446 (1.0%)	1.83	118/8723 (1.4%)
1	P	1.81	67/6448 (1.0%)	1.87	122/8729 (1.4%)
2	B	1.22	10/1148 (0.9%)	1.61	16/1548 (1.0%)
2	E	1.22	10/1148 (0.9%)	1.62	16/1548 (1.0%)
2	H	1.22	10/1148 (0.9%)	1.62	17/1548 (1.1%)
2	K	1.22	10/1148 (0.9%)	1.61	16/1548 (1.0%)
2	N	1.22	10/1148 (0.9%)	1.62	16/1548 (1.0%)
2	Q	1.22	10/1148 (0.9%)	1.61	16/1548 (1.0%)
3	C	0.80	0/1136	0.95	4/1525 (0.3%)
3	F	0.80	0/1136	0.95	4/1525 (0.3%)
3	I	0.80	0/1136	0.94	4/1525 (0.3%)
3	L	0.79	0/1136	0.94	4/1525 (0.3%)
3	O	0.79	0/1136	0.95	4/1525 (0.3%)
3	R	0.79	0/1136	0.94	4/1525 (0.3%)
4	0	0.89	1/2968 (0.0%)	1.64	51/4023 (1.3%)
4	1	0.89	1/2968 (0.0%)	1.64	51/4023 (1.3%)
4	2	0.89	1/2968 (0.0%)	1.64	52/4023 (1.3%)
4	3	0.89	2/2968 (0.1%)	1.64	51/4023 (1.3%)
4	4	0.89	2/2968 (0.1%)	1.64	51/4023 (1.3%)
4	5	0.89	2/2968 (0.1%)	1.64	51/4023 (1.3%)
4	7	0.89	1/2968 (0.0%)	1.64	51/4023 (1.3%)
4	8	0.89	2/2968 (0.1%)	1.64	52/4023 (1.3%)
4	9	0.89	2/2968 (0.1%)	1.64	51/4023 (1.3%)
4	V	0.89	2/2968 (0.1%)	1.64	50/4023 (1.2%)
4	W	0.89	2/2968 (0.1%)	1.64	51/4023 (1.3%)
4	X	0.89	2/2968 (0.1%)	1.64	52/4023 (1.3%)
4	Y	0.89	2/2968 (0.1%)	1.64	51/4023 (1.3%)
4	Z	0.89	2/2968 (0.1%)	1.64	52/4023 (1.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
All	All	1.35	482/93944 (0.5%)	1.69	1548/127134 (1.2%)

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	A	1	4
1	D	1	4
1	G	1	4
1	J	1	6
1	M	1	6
1	P	1	6
2	B	0	3
2	E	0	3
2	H	0	3
2	K	0	3
2	N	0	3
2	Q	0	3
3	C	0	2
3	F	0	2
3	I	0	2
3	L	0	2
3	O	0	2
3	R	0	2
4	0	0	1
4	1	0	1
4	2	0	1
4	3	0	1
4	4	0	1
4	5	0	1
4	7	0	1
4	8	0	1
4	9	0	1
4	V	0	1
4	W	0	1
4	X	0	1
4	Y	0	1
4	Z	0	1
All	All	6	74

The worst 5 of 482 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	649	VAL	CB-CG1	53.30	2.64	1.52
1	G	649	VAL	CB-CG1	53.30	2.64	1.52
1	M	649	VAL	CB-CG1	53.28	2.64	1.52
1	P	649	VAL	CB-CG1	53.28	2.64	1.52
1	D	649	VAL	CB-CG1	53.20	2.64	1.52

The worst 5 of 1548 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	637	LYS	O-C-N	-58.51	23.73	123.20
1	D	637	LYS	O-C-N	-58.48	23.79	123.20
1	M	637	LYS	O-C-N	-58.47	23.80	123.20
1	J	637	LYS	O-C-N	-58.45	23.83	123.20
1	P	637	LYS	O-C-N	-58.45	23.83	123.20

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	648	THR	CB
1	D	648	THR	CB
1	G	648	THR	CB
1	J	648	THR	CB
1	M	648	THR	CB

5 of 74 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	623	PHE	Sidechain
1	A	637	LYS	Mainchain
1	A	649	VAL	Mainchain
1	A	98	HIS	Mainchain
2	B	22	THR	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	A	6797	0	6753	1539	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	6797	0	6758	1519	0
1	G	6797	0	6764	1543	0
1	J	6797	0	6760	1449	0
1	M	6797	0	6765	1504	0
1	P	6797	0	6765	1493	0
2	B	1127	0	1085	226	0
2	E	1127	0	1085	249	0
2	H	1127	0	1087	278	0
2	K	1127	0	1088	282	0
2	N	1127	0	1088	238	0
2	Q	1127	0	1088	253	0
3	C	1123	0	1083	200	0
3	F	1123	0	1084	200	0
3	I	1123	0	1082	211	0
3	L	1123	0	1083	168	0
3	O	1123	0	1084	152	0
3	R	1123	0	1084	238	0
4	0	2906	0	2855	404	0
4	1	2906	0	2858	259	0
4	2	2906	0	2864	173	0
4	3	2906	0	2863	178	0
4	4	2906	0	2865	96	0
4	5	2906	0	2865	97	0
4	7	2906	0	2866	79	0
4	8	2906	0	2857	317	0
4	9	2906	0	2855	341	0
4	V	2906	0	2851	390	0
4	W	2906	0	2851	382	0
4	X	2906	0	2862	208	0
4	Y	2906	0	2863	168	0
4	Z	2906	0	2853	410	0
All	All	94966	0	93614	11439	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 61.

The worst 5 of 11439 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:D:797:PHE:CE2	3:F:126:LEU:HD22	1.31	1.66
1:J:797:PHE:CE1	3:L:146:ILE:HG23	1.26	1.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:797:PHE:CZ	3:I:146:ILE:HD12	1.28	1.66
1:A:505:MLY:HB3	1:A:762:HIS:CD2	1.30	1.65
1:D:508:ILE:HD11	1:D:766:PHE:CE1	1.24	1.65

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	A	789/840 (94%)	651 (82%)	112 (14%)	26 (3%)	4	26
1	D	789/840 (94%)	651 (82%)	112 (14%)	26 (3%)	4	26
1	G	791/840 (94%)	652 (82%)	112 (14%)	27 (3%)	3	26
1	J	791/840 (94%)	652 (82%)	112 (14%)	27 (3%)	3	26
1	M	786/840 (94%)	649 (83%)	111 (14%)	26 (3%)	4	26
1	P	789/840 (94%)	649 (82%)	114 (14%)	26 (3%)	4	26
2	B	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	2	19
2	E	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	2	19
2	H	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	2	19
2	K	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	2	19
2	N	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	2	19
2	Q	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	2	19
3	C	143/147 (97%)	133 (93%)	10 (7%)	0	100	100
3	F	143/147 (97%)	133 (93%)	10 (7%)	0	100	100
3	I	143/147 (97%)	133 (93%)	10 (7%)	0	100	100
3	L	143/147 (97%)	133 (93%)	10 (7%)	0	100	100
3	O	143/147 (97%)	133 (93%)	10 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	R	143/147 (97%)	133 (93%)	10 (7%)	0	100	100
4	0	370/375 (99%)	333 (90%)	31 (8%)	6 (2%)	9	44
4	1	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	9	44
4	2	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	9	44
4	3	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	9	44
4	4	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	9	44
4	5	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	9	44
4	7	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	9	44
4	8	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	9	44
4	9	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	9	44
4	V	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	9	44
4	W	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	9	44
4	X	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	9	44
4	Y	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	9	44
4	Z	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	9	44
All	All	11631/12042 (97%)	10138 (87%)	1203 (10%)	290 (2%)	9	32

5 of 290 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	LYS
1	A	202	SER
1	A	572	LYS
1	A	712	PRO
1	A	729	ALA

### 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	A	672/672 (100%)	510 (76%)	162 (24%)	0	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	672/672 (100%)	514 (76%)	158 (24%)	1	4
1	G	672/672 (100%)	513 (76%)	159 (24%)	1	4
1	J	672/672 (100%)	515 (77%)	157 (23%)	1	4
1	M	672/672 (100%)	514 (76%)	158 (24%)	1	4
1	P	672/672 (100%)	514 (76%)	158 (24%)	1	4
2	B	120/120 (100%)	119 (99%)	1 (1%)	81	89
2	E	120/120 (100%)	119 (99%)	1 (1%)	81	89
2	H	120/120 (100%)	119 (99%)	1 (1%)	81	89
2	K	120/120 (100%)	119 (99%)	1 (1%)	81	89
2	N	120/120 (100%)	119 (99%)	1 (1%)	81	89
2	Q	120/120 (100%)	119 (99%)	1 (1%)	81	89
3	C	117/117 (100%)	112 (96%)	5 (4%)	29	53
3	F	117/117 (100%)	112 (96%)	5 (4%)	29	53
3	I	117/117 (100%)	112 (96%)	5 (4%)	29	53
3	L	117/117 (100%)	112 (96%)	5 (4%)	29	53
3	O	117/117 (100%)	112 (96%)	5 (4%)	29	53
3	R	117/117 (100%)	112 (96%)	5 (4%)	29	53
4	0	315/318 (99%)	269 (85%)	46 (15%)	3	15
4	1	315/318 (99%)	268 (85%)	47 (15%)	3	15
4	2	315/318 (99%)	268 (85%)	47 (15%)	3	15
4	3	315/318 (99%)	269 (85%)	46 (15%)	3	15
4	4	315/318 (99%)	269 (85%)	46 (15%)	3	15
4	5	315/318 (99%)	268 (85%)	47 (15%)	3	15
4	7	315/318 (99%)	269 (85%)	46 (15%)	3	15
4	8	315/318 (99%)	268 (85%)	47 (15%)	3	15
4	9	315/318 (99%)	269 (85%)	46 (15%)	3	15
4	V	315/318 (99%)	268 (85%)	47 (15%)	3	15
4	W	315/318 (99%)	269 (85%)	46 (15%)	3	15
4	X	315/318 (99%)	268 (85%)	47 (15%)	3	15
4	Y	315/318 (99%)	268 (85%)	47 (15%)	3	15
4	Z	315/318 (99%)	269 (85%)	46 (15%)	3	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9864/9906 (100%)	8225 (83%)	1639 (17%)	5 12

5 of 1639 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	543	PRO
4	3	221	LEU
4	Z	100	GLU
1	P	708	ARG
1	P	537	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 237 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	424	ASN
4	X	92	ASN
1	P	481	ASN
4	W	263	GLN
4	Z	263	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

270 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	MLY	P	617	1	9,10,11	0.98	1 (11%)	6,11,13	0.33	0
1	MLY	M	353	1	9,10,11	0.85	0	6,11,13	0.79	0
1	MLY	D	84	1	9,10,11	0.50	0	6,11,13	0.80	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	MLY	D	19	1	9,10,11	1.17	1 (11%)	6,11,13	0.56	0
1	MLY	J	59	1	9,10,11	0.87	0	6,11,13	0.49	0
1	MLY	G	833	1	9,10,11	1.15	2 (22%)	6,11,13	0.32	0
1	MLY	J	659	1	9,10,11	0.81	0	6,11,13	0.58	0
1	MLY	J	84	1	9,10,11	0.49	0	6,11,13	0.80	0
1	MLY	J	600	1	9,10,11	0.53	0	6,11,13	0.36	0
1	MLY	G	505	1	9,10,11	0.90	1 (11%)	6,11,13	0.35	0
1	MLY	D	504	1	9,10,11	0.89	0	6,11,13	0.22	0
1	MLY	D	59	1	9,10,11	0.86	0	6,11,13	0.49	0
1	MLY	A	190	1	9,10,11	1.26	1 (11%)	6,11,13	0.51	0
1	MLY	D	55	1	9,10,11	0.71	0	6,11,13	0.80	0
1	MLY	J	369	1	9,10,11	0.70	0	6,11,13	0.45	0
1	MLY	G	385	1	9,10,11	1.00	1 (11%)	6,11,13	0.43	0
1	MLY	M	35	1	9,10,11	0.72	0	6,11,13	0.39	0
1	MLY	P	367	1	9,10,11	0.63	0	6,11,13	0.36	0
1	MLY	G	782	1	9,10,11	0.77	0	6,11,13	0.35	0
1	MLY	D	839	1	9,10,11	0.70	0	6,11,13	0.79	0
1	MLY	A	553	4,1	9,10,11	0.67	0	6,11,13	0.55	0
1	MLY	M	272	1	9,10,11	1.00	1 (11%)	6,11,13	0.56	0
1	MLY	M	764	1	9,10,11	0.84	0	6,11,13	0.38	0
1	MLY	P	431	1	9,10,11	0.50	0	6,11,13	0.45	0
1	MLY	J	272	1	9,10,11	1.00	1 (11%)	6,11,13	0.56	0
1	MLY	M	782	1	9,10,11	0.78	0	6,11,13	0.38	0
1	MLY	A	348	1	9,10,11	0.87	1 (11%)	6,11,13	0.48	0
1	MLY	J	827	1	9,10,11	0.74	0	6,11,13	0.48	0
1	MLY	A	84	1	9,10,11	0.50	0	6,11,13	0.80	0
1	MLY	P	681	1	9,10,11	0.61	0	6,11,13	0.46	0
1	MLY	P	248	1	9,10,11	0.82	0	6,11,13	0.62	0
1	MLY	J	55	1	9,10,11	0.72	0	6,11,13	0.78	0
1	MLY	J	138	1	9,10,11	1.34	1 (11%)	6,11,13	0.84	0
1	MLY	A	272	1	9,10,11	1.00	1 (11%)	6,11,13	0.55	0
1	MLY	J	130	1	9,10,11	0.76	0	6,11,13	0.75	0
1	MLY	J	35	1	9,10,11	0.72	0	6,11,13	0.39	0
1	MLY	D	63	1	9,10,11	0.90	0	6,11,13	0.45	0
1	MLY	J	598	1	9,10,11	0.88	1 (11%)	6,11,13	0.43	0
1	MLY	P	659	1	9,10,11	0.83	0	6,11,13	0.58	0
1	MLY	M	107	1	9,10,11	0.48	0	6,11,13	0.34	0
1	MLY	P	600	1	9,10,11	0.52	0	6,11,13	0.37	0
1	MLY	J	295	1	9,10,11	0.78	0	6,11,13	0.35	0
1	MLY	J	839	1	9,10,11	0.71	0	6,11,13	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	MLY	P	839	1	9,10,11	0.71	0	6,11,13	0.77	0
1	MLY	A	528	1	9,10,11	0.87	0	6,11,13	0.66	0
1	MLY	D	833	1	9,10,11	1.15	2 (22%)	6,11,13	0.31	0
1	MLY	A	49	1	9,10,11	1.04	1 (11%)	6,11,13	0.74	0
1	MLY	G	19	1	9,10,11	1.15	1 (11%)	6,11,13	0.58	0
1	MLY	G	837	1	9,10,11	0.59	0	6,11,13	0.52	0
1	MLY	P	369	1	9,10,11	0.69	0	6,11,13	0.46	0
1	MLY	M	839	1	9,10,11	0.70	0	6,11,13	0.77	0
1	MLY	J	681	1	9,10,11	0.59	0	6,11,13	0.45	0
1	MLY	M	369	1	9,10,11	0.70	0	6,11,13	0.46	0
1	MLY	A	768	1	9,10,11	0.76	0	6,11,13	0.41	0
1	MLY	P	84	1	9,10,11	0.50	0	6,11,13	0.80	0
1	MLY	G	348	1	9,10,11	0.86	1 (11%)	6,11,13	0.46	0
1	MLY	G	190	1	9,10,11	1.24	1 (11%)	6,11,13	0.52	0
1	MLY	P	19	1	9,10,11	1.18	1 (11%)	6,11,13	0.57	0
1	MLY	M	385	1	9,10,11	1.02	1 (11%)	6,11,13	0.44	0
1	MLY	M	236	1	9,10,11	0.81	1 (11%)	6,11,13	0.47	0
1	MLY	M	431	1	9,10,11	0.52	0	6,11,13	0.44	0
1	MLY	M	84	1	9,10,11	0.50	0	6,11,13	0.81	0
1	MLY	A	551	1	9,10,11	0.51	0	6,11,13	0.19	0
1	MLY	P	55	1	9,10,11	0.72	0	6,11,13	0.78	0
1	MLY	P	138	1	9,10,11	1.34	1 (11%)	6,11,13	0.84	0
1	MLY	P	551	1	9,10,11	0.53	0	6,11,13	0.20	0
1	MLY	P	30	1	9,10,11	0.89	0	6,11,13	0.32	0
1	MLY	G	553	4,1	9,10,11	0.66	0	6,11,13	0.55	0
1	MLY	J	296	1	9,10,11	0.69	0	6,11,13	0.36	0
1	MLY	D	598	1	9,10,11	0.91	1 (11%)	6,11,13	0.43	0
1	MLY	G	504	1	9,10,11	0.88	0	6,11,13	0.22	0
1	MLY	A	505	1	9,10,11	0.90	1 (11%)	6,11,13	0.33	0
1	MLY	A	431	1	9,10,11	0.52	0	6,11,13	0.45	0
1	MLY	G	367	1	9,10,11	0.66	0	6,11,13	0.38	0
1	MLY	J	613	1	9,10,11	0.56	0	6,11,13	0.64	0
1	MLY	G	295	1	9,10,11	0.79	0	6,11,13	0.34	0
1	MLY	M	190	1	9,10,11	1.26	1 (11%)	6,11,13	0.52	0
1	MLY	M	553	4,1	9,10,11	0.67	0	6,11,13	0.54	0
1	MLY	D	553	4,1	9,10,11	0.69	0	6,11,13	0.55	0
1	MLY	G	436	1	9,10,11	1.04	1 (11%)	6,11,13	0.49	0
1	MLY	J	353	1	9,10,11	0.85	0	6,11,13	0.78	0
1	MLY	J	436	1	9,10,11	1.07	1 (11%)	6,11,13	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	MLY	P	436	1	9,10,11	1.08	1 (11%)	6,11,13	0.49	0
1	MLY	M	367	1	9,10,11	0.63	0	6,11,13	0.36	0
1	MLY	G	827	1	9,10,11	0.71	0	6,11,13	0.49	0
1	MLY	M	613	1	9,10,11	0.55	0	6,11,13	0.63	0
1	MLY	G	130	1	9,10,11	0.80	0	6,11,13	0.75	0
1	MLY	D	272	1	9,10,11	0.96	1 (11%)	6,11,13	0.58	0
1	MLY	J	764	1	9,10,11	0.83	0	6,11,13	0.37	0
1	MLY	D	295	1	9,10,11	0.78	0	6,11,13	0.36	0
1	MLY	G	55	1	9,10,11	0.73	0	6,11,13	0.80	0
1	MLY	J	486	1	9,10,11	0.63	0	6,11,13	0.39	0
1	MLY	A	63	1	9,10,11	0.93	1 (11%)	6,11,13	0.44	0
1	MLY	G	59	1	9,10,11	0.83	0	6,11,13	0.50	0
1	MLY	J	528	1	9,10,11	0.88	0	6,11,13	0.66	0
1	MLY	D	827	1	9,10,11	0.68	0	6,11,13	0.47	0
1	MLY	G	49	1	9,10,11	1.07	1 (11%)	6,11,13	0.74	0
1	MLY	D	505	1	9,10,11	0.85	1 (11%)	6,11,13	0.34	0
1	MLY	P	63	1	9,10,11	0.90	0	6,11,13	0.43	0
1	MLY	A	415	1	9,10,11	0.75	0	6,11,13	0.19	0
1	MLY	M	59	1	9,10,11	0.87	0	6,11,13	0.49	0
1	MLY	D	348	1	9,10,11	0.83	0	6,11,13	0.47	0
1	MLY	J	248	1	9,10,11	0.83	0	6,11,13	0.63	0
1	MLY	M	528	1	9,10,11	0.88	0	6,11,13	0.65	0
1	MLY	M	827	1	9,10,11	0.71	0	6,11,13	0.48	0
1	MLY	D	49	1	9,10,11	1.08	1 (11%)	6,11,13	0.74	0
1	MLY	J	107	1	9,10,11	0.48	0	6,11,13	0.33	0
1	MLY	P	553	1	9,10,11	0.67	0	6,11,13	0.54	0
1	MLY	P	833	1	9,10,11	1.17	1 (11%)	6,11,13	0.32	0
1	MLY	J	87	1	9,10,11	1.22	1 (11%)	6,11,13	0.43	0
1	MLY	P	130	1	9,10,11	0.77	0	6,11,13	0.75	0
1	MLY	P	613	1	9,10,11	0.56	0	6,11,13	0.64	0
1	MLY	A	19	1	9,10,11	1.12	1 (11%)	6,11,13	0.56	0
1	MLY	A	236	1	9,10,11	0.79	1 (11%)	6,11,13	0.48	0
1	MLY	A	87	1	9,10,11	1.23	1 (11%)	6,11,13	0.42	0
1	MLY	A	385	1	9,10,11	1.00	1 (11%)	6,11,13	0.43	0
1	MLY	J	30	1	9,10,11	0.88	0	6,11,13	0.31	0
1	MLY	M	19	1	9,10,11	1.17	1 (11%)	6,11,13	0.58	0
1	MLY	G	431	1	9,10,11	0.54	0	6,11,13	0.46	0
1	MLY	G	551	1	9,10,11	0.52	0	6,11,13	0.20	0
1	MLY	P	782	1	9,10,11	0.77	0	6,11,13	0.38	0
1	MLY	D	659	1	9,10,11	0.82	0	6,11,13	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	MLY	A	659	1	9,10,11	0.83	0	6,11,13	0.60	0
1	MLY	D	486	1	9,10,11	0.65	0	6,11,13	0.39	0
1	MLY	G	248	1	9,10,11	0.80	0	6,11,13	0.63	0
1	MLY	G	296	1	9,10,11	0.65	0	6,11,13	0.37	0
1	MLY	P	272	1	9,10,11	1.02	1 (11%)	6,11,13	0.55	0
1	MLY	P	295	1	9,10,11	0.80	0	6,11,13	0.34	0
1	MLY	P	764	1	9,10,11	0.83	0	6,11,13	0.38	0
1	MLY	G	617	1	9,10,11	0.96	1 (11%)	6,11,13	0.34	0
1	MLY	G	138	1	9,10,11	1.36	1 (11%)	6,11,13	0.84	0
1	MLY	P	528	1	9,10,11	0.88	0	6,11,13	0.66	0
1	MLY	A	486	1	9,10,11	0.64	0	6,11,13	0.39	0
1	MLY	P	598	1	9,10,11	0.89	1 (11%)	6,11,13	0.43	0
1	MLY	G	35	1	9,10,11	0.72	0	6,11,13	0.39	0
1	MLY	G	659	1	9,10,11	0.84	0	6,11,13	0.59	0
1	MLY	G	600	1	9,10,11	0.51	0	6,11,13	0.37	0
1	MLY	M	837	1	9,10,11	0.58	0	6,11,13	0.55	0
1	MLY	D	436	1	9,10,11	1.11	1 (11%)	6,11,13	0.49	0
1	MLY	D	248	1	9,10,11	0.84	0	6,11,13	0.62	0
1	MLY	G	839	1	9,10,11	0.73	0	6,11,13	0.80	0
1	MLY	M	598	1	9,10,11	0.87	1 (11%)	6,11,13	0.43	0
1	MLY	J	551	1	9,10,11	0.53	0	6,11,13	0.19	0
1	MLY	J	768	1	9,10,11	0.76	0	6,11,13	0.42	0
1	MLY	P	107	1	9,10,11	0.48	0	6,11,13	0.35	0
1	MLY	P	87	1	9,10,11	1.25	1 (11%)	6,11,13	0.43	0
1	MLY	A	839	1	9,10,11	0.69	0	6,11,13	0.81	0
1	MLY	G	486	1	9,10,11	0.64	0	6,11,13	0.39	0
1	MLY	J	617	1	9,10,11	0.97	1 (11%)	6,11,13	0.33	0
1	MLY	D	138	1	9,10,11	1.38	1 (11%)	6,11,13	0.85	0
1	MLY	D	296	1	9,10,11	0.65	0	6,11,13	0.37	0
1	MLY	A	130	1	9,10,11	0.81	0	6,11,13	0.75	0
1	MLY	G	84	1	9,10,11	0.49	0	6,11,13	0.80	0
1	MLY	D	87	1	9,10,11	1.20	1 (11%)	6,11,13	0.44	0
1	MLY	D	130	1	9,10,11	0.81	0	6,11,13	0.74	0
1	MLY	G	415	1	9,10,11	0.78	0	6,11,13	0.19	0
1	MLY	J	190	1	9,10,11	1.27	1 (11%)	6,11,13	0.52	0
1	MLY	M	63	1	9,10,11	0.92	1 (11%)	6,11,13	0.44	0
1	MLY	M	486	1	9,10,11	0.62	0	6,11,13	0.39	0
1	MLY	M	600	1	9,10,11	0.52	0	6,11,13	0.37	0
1	MLY	P	505	1	9,10,11	0.91	1 (11%)	6,11,13	0.34	0
1	MLY	J	431	1	9,10,11	0.50	0	6,11,13	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	MLY	G	681	1	9,10,11	0.64	0	6,11,13	0.45	0
1	MLY	A	107	1	9,10,11	0.46	0	6,11,13	0.34	0
1	MLY	J	837	1	9,10,11	0.60	0	6,11,13	0.55	0
1	MLY	M	833	1	9,10,11	1.20	1 (11%)	6,11,13	0.32	0
1	MLY	J	385	1	9,10,11	1.02	1 (11%)	6,11,13	0.44	0
1	MLY	G	87	1	9,10,11	1.22	1 (11%)	6,11,13	0.43	0
1	MLY	M	505	1	9,10,11	0.93	1 (11%)	6,11,13	0.34	0
1	MLY	M	436	1	9,10,11	1.08	1 (11%)	6,11,13	0.49	0
1	MLY	A	504	1	9,10,11	0.87	0	6,11,13	0.23	0
1	MLY	D	681	1	9,10,11	0.58	0	6,11,13	0.45	0
1	MLY	A	30	1	9,10,11	0.88	0	6,11,13	0.32	0
1	MLY	D	415	1	9,10,11	0.78	0	6,11,13	0.19	0
1	MLY	G	272	1	9,10,11	0.97	1 (11%)	6,11,13	0.55	0
1	MLY	G	764	1	9,10,11	0.80	0	6,11,13	0.35	0
1	MLY	J	63	1	9,10,11	0.91	1 (11%)	6,11,13	0.44	0
1	MLY	P	768	1	9,10,11	0.78	0	6,11,13	0.41	0
1	MLY	D	35	1	9,10,11	0.72	0	6,11,13	0.38	0
1	MLY	J	505	1	9,10,11	0.92	1 (11%)	6,11,13	0.34	0
1	MLY	M	504	1	9,10,11	0.84	0	6,11,13	0.23	0
1	MLY	A	59	1	9,10,11	0.86	0	6,11,13	0.49	0
1	MLY	M	348	1	9,10,11	0.81	0	6,11,13	0.47	0
1	MLY	J	504	1	9,10,11	0.84	0	6,11,13	0.23	0
1	MLY	J	833	1	9,10,11	1.18	1 (11%)	6,11,13	0.32	0
1	MLY	P	486	1	9,10,11	0.63	0	6,11,13	0.39	0
1	MLY	J	415	1	9,10,11	0.79	0	6,11,13	0.19	0
1	MLY	J	367	1	9,10,11	0.62	0	6,11,13	0.36	0
1	MLY	A	296	1	9,10,11	0.62	0	6,11,13	0.36	0
1	MLY	J	782	1	9,10,11	0.79	0	6,11,13	0.37	0
1	MLY	A	617	1	9,10,11	0.95	1 (11%)	6,11,13	0.34	0
1	MLY	A	613	1	9,10,11	0.57	0	6,11,13	0.63	0
1	MLY	G	63	1	9,10,11	0.90	1 (11%)	6,11,13	0.43	0
1	MLY	M	415	1	9,10,11	0.79	0	6,11,13	0.19	0
1	MLY	J	19	1	9,10,11	1.19	1 (11%)	6,11,13	0.58	0
1	MLY	J	236	1	9,10,11	0.79	1 (11%)	6,11,13	0.48	0
1	MLY	D	353	1	9,10,11	0.85	0	6,11,13	0.79	0
1	MLY	A	353	1	9,10,11	0.88	0	6,11,13	0.79	0
1	MLY	A	367	1	9,10,11	0.64	0	6,11,13	0.36	0
1	MLY	P	236	1	9,10,11	0.80	1 (11%)	6,11,13	0.48	0
1	MLY	D	782	1	9,10,11	0.77	0	6,11,13	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	MLY	P	385	1	9,10,11	1.02	1 (11%)	6,11,13	0.44	0
1	MLY	A	600	1	9,10,11	0.51	0	6,11,13	0.38	0
1	MLY	A	837	1	9,10,11	0.60	0	6,11,13	0.53	0
1	MLY	D	764	1	9,10,11	0.84	0	6,11,13	0.35	0
1	MLY	A	833	1	9,10,11	1.15	1 (11%)	6,11,13	0.32	0
1	MLY	D	431	1	9,10,11	0.54	0	6,11,13	0.46	0
1	MLY	G	613	1	9,10,11	0.59	0	6,11,13	0.63	0
1	MLY	D	551	1	9,10,11	0.53	0	6,11,13	0.20	0
1	MLY	M	248	1	9,10,11	0.82	0	6,11,13	0.62	0
1	MLY	P	59	1	9,10,11	0.88	0	6,11,13	0.49	0
1	MLY	D	768	1	9,10,11	0.73	0	6,11,13	0.41	0
1	MLY	P	348	1	9,10,11	0.83	0	6,11,13	0.47	0
1	MLY	D	528	1	9,10,11	0.90	0	6,11,13	0.65	0
1	MLY	G	353	1	9,10,11	0.85	0	6,11,13	0.80	0
1	MLY	M	49	1	9,10,11	1.09	1 (11%)	6,11,13	0.74	0
1	MLY	P	296	1	9,10,11	0.66	0	6,11,13	0.36	0
1	MLY	M	659	1	9,10,11	0.82	0	6,11,13	0.58	0
1	MLY	M	130	1	9,10,11	0.78	0	6,11,13	0.75	0
1	MLY	M	55	1	9,10,11	0.73	0	6,11,13	0.79	0
1	MLY	M	768	1	9,10,11	0.75	0	6,11,13	0.42	0
1	MLY	A	248	1	9,10,11	0.83	0	6,11,13	0.61	0
1	MLY	P	415	1	9,10,11	0.78	0	6,11,13	0.19	0
1	MLY	G	30	1	9,10,11	0.88	0	6,11,13	0.30	0
1	MLY	P	353	1	9,10,11	0.86	0	6,11,13	0.78	0
1	MLY	D	107	1	9,10,11	0.51	0	6,11,13	0.34	0
1	MLY	A	681	1	9,10,11	0.60	0	6,11,13	0.46	0
1	MLY	A	55	1	9,10,11	0.72	0	6,11,13	0.78	0
1	MLY	M	30	1	9,10,11	0.90	0	6,11,13	0.31	0
1	MLY	D	30	1	9,10,11	0.91	0	6,11,13	0.31	0
1	MLY	P	837	1	9,10,11	0.58	0	6,11,13	0.55	0
1	MLY	A	35	1	9,10,11	0.71	0	6,11,13	0.38	0
1	MLY	G	107	1	9,10,11	0.47	0	6,11,13	0.34	0
1	MLY	P	827	1	9,10,11	0.73	0	6,11,13	0.49	0
1	MLY	A	295	1	9,10,11	0.81	0	6,11,13	0.32	0
1	MLY	M	295	1	9,10,11	0.79	0	6,11,13	0.35	0
1	MLY	J	49	1	9,10,11	1.08	1 (11%)	6,11,13	0.74	0
1	MLY	M	551	1	9,10,11	0.52	0	6,11,13	0.20	0
1	MLY	P	35	1	9,10,11	0.72	0	6,11,13	0.38	0
1	MLY	P	49	1	9,10,11	1.12	1 (11%)	6,11,13	0.75	0
1	MLY	A	436	1	9,10,11	1.07	1 (11%)	6,11,13	0.50	0
1	MLY	A	764	1	9,10,11	0.84	0	6,11,13	0.36	0
1	MLY	A	369	1	9,10,11	0.70	0	6,11,13	0.46	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	MLY	D	190	1	9,10,11	1.22	1 (11%)	6,11,13	0.54	0
1	MLY	A	782	1	9,10,11	0.78	0	6,11,13	0.37	0
1	MLY	A	827	1	9,10,11	0.71	0	6,11,13	0.46	0
1	MLY	D	385	1	9,10,11	0.99	1 (11%)	6,11,13	0.45	0
1	MLY	D	837	1	9,10,11	0.61	0	6,11,13	0.57	0
1	MLY	G	369	1	9,10,11	0.70	0	6,11,13	0.46	0
1	MLY	J	553	1	9,10,11	0.67	0	6,11,13	0.54	0
1	MLY	M	138	1	9,10,11	1.33	1 (11%)	6,11,13	0.83	0
1	MLY	M	681	1	9,10,11	0.58	0	6,11,13	0.45	0
1	MLY	A	138	1	9,10,11	1.33	1 (11%)	6,11,13	0.84	0
1	MLY	P	190	1	9,10,11	1.25	1 (11%)	6,11,13	0.53	0
1	MLY	M	617	1	9,10,11	0.96	1 (11%)	6,11,13	0.33	0
1	MLY	D	613	1	9,10,11	0.57	0	6,11,13	0.63	0
1	MLY	D	617	1	9,10,11	0.99	1 (11%)	6,11,13	0.34	0
1	MLY	M	87	1	9,10,11	1.22	1 (11%)	6,11,13	0.43	0
1	MLY	G	236	1	9,10,11	0.78	1 (11%)	6,11,13	0.47	0
1	MLY	P	504	1	9,10,11	0.83	0	6,11,13	0.22	0
1	MLY	G	528	1	9,10,11	0.89	0	6,11,13	0.66	0
1	MLY	A	598	1	9,10,11	0.90	1 (11%)	6,11,13	0.44	0
1	MLY	G	598	1	9,10,11	0.90	1 (11%)	6,11,13	0.42	0
1	MLY	D	236	1	9,10,11	0.80	1 (11%)	6,11,13	0.47	0
1	MLY	D	600	1	9,10,11	0.51	0	6,11,13	0.38	0
1	MLY	J	348	1	9,10,11	0.80	0	6,11,13	0.47	0
1	MLY	D	369	1	9,10,11	0.69	0	6,11,13	0.45	0
1	MLY	M	296	1	9,10,11	0.69	0	6,11,13	0.36	0
1	MLY	G	768	1	9,10,11	0.72	0	6,11,13	0.42	0
1	MLY	D	367	1	9,10,11	0.60	0	6,11,13	0.40	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	P	617	1	-	1/8/9/11	-
1	MLY	M	353	1	-	4/8/9/11	-
1	MLY	D	84	1	-	4/8/9/11	-
1	MLY	D	19	1	-	4/8/9/11	-
1	MLY	J	59	1	-	3/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	G	833	1	-	6/8/9/11	-
1	MLY	J	659	1	-	3/8/9/11	-
1	MLY	J	84	1	-	4/8/9/11	-
1	MLY	J	600	1	-	3/8/9/11	-
1	MLY	G	505	1	-	5/8/9/11	-
1	MLY	D	504	1	-	4/8/9/11	-
1	MLY	D	59	1	-	3/8/9/11	-
1	MLY	A	190	1	-	5/8/9/11	-
1	MLY	D	55	1	-	6/8/9/11	-
1	MLY	J	369	1	-	2/8/9/11	-
1	MLY	G	385	1	-	2/8/9/11	-
1	MLY	M	35	1	-	3/8/9/11	-
1	MLY	P	367	1	-	2/8/9/11	-
1	MLY	G	782	1	-	6/8/9/11	-
1	MLY	D	839	1	-	3/8/9/11	-
1	MLY	A	553	4,1	-	4/8/9/11	-
1	MLY	M	272	1	-	3/8/9/11	-
1	MLY	M	764	1	-	2/8/9/11	-
1	MLY	P	431	1	-	4/8/9/11	-
1	MLY	J	272	1	-	3/8/9/11	-
1	MLY	M	782	1	-	6/8/9/11	-
1	MLY	A	348	1	-	5/8/9/11	-
1	MLY	J	827	1	-	0/8/9/11	-
1	MLY	A	84	1	-	4/8/9/11	-
1	MLY	P	681	1	-	4/8/9/11	-
1	MLY	P	248	1	-	6/8/9/11	-
1	MLY	J	55	1	-	6/8/9/11	-
1	MLY	J	138	1	-	4/8/9/11	-
1	MLY	A	272	1	-	3/8/9/11	-
1	MLY	J	130	1	-	5/8/9/11	-
1	MLY	J	35	1	-	3/8/9/11	-
1	MLY	D	63	1	-	4/8/9/11	-
1	MLY	J	598	1	-	5/8/9/11	-
1	MLY	P	659	1	-	3/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	M	107	1	-	2/8/9/11	-
1	MLY	P	600	1	-	3/8/9/11	-
1	MLY	J	295	1	-	2/8/9/11	-
1	MLY	J	839	1	-	3/8/9/11	-
1	MLY	P	839	1	-	3/8/9/11	-
1	MLY	A	528	1	-	5/8/9/11	-
1	MLY	D	833	1	-	6/8/9/11	-
1	MLY	A	49	1	-	3/8/9/11	-
1	MLY	G	19	1	-	4/8/9/11	-
1	MLY	G	837	1	-	5/8/9/11	-
1	MLY	P	369	1	-	2/8/9/11	-
1	MLY	M	839	1	-	3/8/9/11	-
1	MLY	J	681	1	-	4/8/9/11	-
1	MLY	M	369	1	-	2/8/9/11	-
1	MLY	A	768	1	-	4/8/9/11	-
1	MLY	P	84	1	-	4/8/9/11	-
1	MLY	G	348	1	-	5/8/9/11	-
1	MLY	G	190	1	-	5/8/9/11	-
1	MLY	P	19	1	-	4/8/9/11	-
1	MLY	M	385	1	-	2/8/9/11	-
1	MLY	M	236	1	-	3/8/9/11	-
1	MLY	M	431	1	-	4/8/9/11	-
1	MLY	M	84	1	-	4/8/9/11	-
1	MLY	A	551	1	-	3/8/9/11	-
1	MLY	P	55	1	-	6/8/9/11	-
1	MLY	P	138	1	-	4/8/9/11	-
1	MLY	P	551	1	-	3/8/9/11	-
1	MLY	P	30	1	-	2/8/9/11	-
1	MLY	G	553	4,1	-	4/8/9/11	-
1	MLY	J	296	1	-	4/8/9/11	-
1	MLY	D	598	1	-	5/8/9/11	-
1	MLY	G	504	1	-	4/8/9/11	-
1	MLY	A	505	1	-	5/8/9/11	-
1	MLY	A	431	1	-	4/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	G	367	1	-	2/8/9/11	-
1	MLY	J	613	1	-	4/8/9/11	-
1	MLY	G	295	1	-	2/8/9/11	-
1	MLY	M	190	1	-	5/8/9/11	-
1	MLY	M	553	4,1	-	4/8/9/11	-
1	MLY	D	553	4,1	-	5/8/9/11	-
1	MLY	G	436	1	-	4/8/9/11	-
1	MLY	J	353	1	-	4/8/9/11	-
1	MLY	J	436	1	-	4/8/9/11	-
1	MLY	P	436	1	-	4/8/9/11	-
1	MLY	M	367	1	-	2/8/9/11	-
1	MLY	G	827	1	-	0/8/9/11	-
1	MLY	M	613	1	-	4/8/9/11	-
1	MLY	G	130	1	-	5/8/9/11	-
1	MLY	D	272	1	-	3/8/9/11	-
1	MLY	J	764	1	-	2/8/9/11	-
1	MLY	D	295	1	-	2/8/9/11	-
1	MLY	G	55	1	-	6/8/9/11	-
1	MLY	J	486	1	-	2/8/9/11	-
1	MLY	A	63	1	-	4/8/9/11	-
1	MLY	G	59	1	-	3/8/9/11	-
1	MLY	J	528	1	-	4/8/9/11	-
1	MLY	D	827	1	-	0/8/9/11	-
1	MLY	G	49	1	-	3/8/9/11	-
1	MLY	D	505	1	-	5/8/9/11	-
1	MLY	P	63	1	-	4/8/9/11	-
1	MLY	A	415	1	-	3/8/9/11	-
1	MLY	M	59	1	-	3/8/9/11	-
1	MLY	D	348	1	-	5/8/9/11	-
1	MLY	J	248	1	-	6/8/9/11	-
1	MLY	M	528	1	-	4/8/9/11	-
1	MLY	M	827	1	-	0/8/9/11	-
1	MLY	D	49	1	-	3/8/9/11	-
1	MLY	J	107	1	-	2/8/9/11	-
1	MLY	P	553	1	-	4/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	P	833	1	-	6/8/9/11	-
1	MLY	J	87	1	-	2/8/9/11	-
1	MLY	P	130	1	-	5/8/9/11	-
1	MLY	P	613	1	-	4/8/9/11	-
1	MLY	A	19	1	-	4/8/9/11	-
1	MLY	A	236	1	-	3/8/9/11	-
1	MLY	A	87	1	-	2/8/9/11	-
1	MLY	A	385	1	-	2/8/9/11	-
1	MLY	J	30	1	-	2/8/9/11	-
1	MLY	M	19	1	-	4/8/9/11	-
1	MLY	G	431	1	-	4/8/9/11	-
1	MLY	G	551	1	-	3/8/9/11	-
1	MLY	P	782	1	-	6/8/9/11	-
1	MLY	D	659	1	-	3/8/9/11	-
1	MLY	A	659	1	-	3/8/9/11	-
1	MLY	D	486	1	-	2/8/9/11	-
1	MLY	G	248	1	-	6/8/9/11	-
1	MLY	G	296	1	-	4/8/9/11	-
1	MLY	P	272	1	-	3/8/9/11	-
1	MLY	P	295	1	-	2/8/9/11	-
1	MLY	P	764	1	-	2/8/9/11	-
1	MLY	G	617	1	-	1/8/9/11	-
1	MLY	G	138	1	-	4/8/9/11	-
1	MLY	P	528	1	-	4/8/9/11	-
1	MLY	A	486	1	-	2/8/9/11	-
1	MLY	P	598	1	-	5/8/9/11	-
1	MLY	G	35	1	-	3/8/9/11	-
1	MLY	G	659	1	-	3/8/9/11	-
1	MLY	G	600	1	-	3/8/9/11	-
1	MLY	M	837	1	-	5/8/9/11	-
1	MLY	D	436	1	-	4/8/9/11	-
1	MLY	D	248	1	-	6/8/9/11	-
1	MLY	G	839	1	-	3/8/9/11	-
1	MLY	M	598	1	-	5/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	J	551	1	-	3/8/9/11	-
1	MLY	J	768	1	-	4/8/9/11	-
1	MLY	P	107	1	-	2/8/9/11	-
1	MLY	P	87	1	-	2/8/9/11	-
1	MLY	A	839	1	-	3/8/9/11	-
1	MLY	G	486	1	-	2/8/9/11	-
1	MLY	J	617	1	-	1/8/9/11	-
1	MLY	D	138	1	-	4/8/9/11	-
1	MLY	D	296	1	-	4/8/9/11	-
1	MLY	A	130	1	-	5/8/9/11	-
1	MLY	G	84	1	-	4/8/9/11	-
1	MLY	D	87	1	-	2/8/9/11	-
1	MLY	D	130	1	-	5/8/9/11	-
1	MLY	G	415	1	-	3/8/9/11	-
1	MLY	J	190	1	-	5/8/9/11	-
1	MLY	M	63	1	-	4/8/9/11	-
1	MLY	M	486	1	-	2/8/9/11	-
1	MLY	M	600	1	-	3/8/9/11	-
1	MLY	P	505	1	-	5/8/9/11	-
1	MLY	J	431	1	-	4/8/9/11	-
1	MLY	G	681	1	-	4/8/9/11	-
1	MLY	A	107	1	-	2/8/9/11	-
1	MLY	J	837	1	-	5/8/9/11	-
1	MLY	M	833	1	-	6/8/9/11	-
1	MLY	J	385	1	-	2/8/9/11	-
1	MLY	G	87	1	-	2/8/9/11	-
1	MLY	M	505	1	-	5/8/9/11	-
1	MLY	M	436	1	-	4/8/9/11	-
1	MLY	A	504	1	-	4/8/9/11	-
1	MLY	D	681	1	-	4/8/9/11	-
1	MLY	A	30	1	-	2/8/9/11	-
1	MLY	D	415	1	-	3/8/9/11	-
1	MLY	G	272	1	-	3/8/9/11	-
1	MLY	G	764	1	-	2/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	J	63	1	-	4/8/9/11	-
1	MLY	P	768	1	-	4/8/9/11	-
1	MLY	D	35	1	-	3/8/9/11	-
1	MLY	J	505	1	-	5/8/9/11	-
1	MLY	M	504	1	-	4/8/9/11	-
1	MLY	A	59	1	-	3/8/9/11	-
1	MLY	M	348	1	-	5/8/9/11	-
1	MLY	J	504	1	-	4/8/9/11	-
1	MLY	J	833	1	-	6/8/9/11	-
1	MLY	P	486	1	-	2/8/9/11	-
1	MLY	J	415	1	-	3/8/9/11	-
1	MLY	J	367	1	-	2/8/9/11	-
1	MLY	A	296	1	-	4/8/9/11	-
1	MLY	J	782	1	-	6/8/9/11	-
1	MLY	A	617	1	-	1/8/9/11	-
1	MLY	A	613	1	-	4/8/9/11	-
1	MLY	G	63	1	-	4/8/9/11	-
1	MLY	M	415	1	-	3/8/9/11	-
1	MLY	J	19	1	-	4/8/9/11	-
1	MLY	J	236	1	-	3/8/9/11	-
1	MLY	D	353	1	-	4/8/9/11	-
1	MLY	A	353	1	-	4/8/9/11	-
1	MLY	A	367	1	-	2/8/9/11	-
1	MLY	P	236	1	-	3/8/9/11	-
1	MLY	D	782	1	-	6/8/9/11	-
1	MLY	P	385	1	-	2/8/9/11	-
1	MLY	A	600	1	-	3/8/9/11	-
1	MLY	A	837	1	-	5/8/9/11	-
1	MLY	D	764	1	-	2/8/9/11	-
1	MLY	A	833	1	-	6/8/9/11	-
1	MLY	D	431	1	-	4/8/9/11	-
1	MLY	G	613	1	-	4/8/9/11	-
1	MLY	D	551	1	-	3/8/9/11	-
1	MLY	M	248	1	-	6/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	P	59	1	-	3/8/9/11	-
1	MLY	D	768	1	-	4/8/9/11	-
1	MLY	P	348	1	-	5/8/9/11	-
1	MLY	D	528	1	-	4/8/9/11	-
1	MLY	G	353	1	-	4/8/9/11	-
1	MLY	M	49	1	-	3/8/9/11	-
1	MLY	P	296	1	-	4/8/9/11	-
1	MLY	M	659	1	-	3/8/9/11	-
1	MLY	M	130	1	-	5/8/9/11	-
1	MLY	M	55	1	-	6/8/9/11	-
1	MLY	M	768	1	-	4/8/9/11	-
1	MLY	A	248	1	-	6/8/9/11	-
1	MLY	P	415	1	-	3/8/9/11	-
1	MLY	G	30	1	-	2/8/9/11	-
1	MLY	P	353	1	-	4/8/9/11	-
1	MLY	D	107	1	-	2/8/9/11	-
1	MLY	A	681	1	-	4/8/9/11	-
1	MLY	A	55	1	-	6/8/9/11	-
1	MLY	M	30	1	-	2/8/9/11	-
1	MLY	D	30	1	-	2/8/9/11	-
1	MLY	P	837	1	-	5/8/9/11	-
1	MLY	A	35	1	-	3/8/9/11	-
1	MLY	G	107	1	-	2/8/9/11	-
1	MLY	P	827	1	-	0/8/9/11	-
1	MLY	A	295	1	-	2/8/9/11	-
1	MLY	M	295	1	-	2/8/9/11	-
1	MLY	J	49	1	-	3/8/9/11	-
1	MLY	M	551	1	-	3/8/9/11	-
1	MLY	P	35	1	-	3/8/9/11	-
1	MLY	P	49	1	-	3/8/9/11	-
1	MLY	A	436	1	-	4/8/9/11	-
1	MLY	A	764	1	-	2/8/9/11	-
1	MLY	A	369	1	-	2/8/9/11	-
1	MLY	D	190	1	-	5/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	A	782	1	-	6/8/9/11	-
1	MLY	A	827	1	-	0/8/9/11	-
1	MLY	D	385	1	-	2/8/9/11	-
1	MLY	D	837	1	-	5/8/9/11	-
1	MLY	G	369	1	-	2/8/9/11	-
1	MLY	J	553	1	-	4/8/9/11	-
1	MLY	M	138	1	-	4/8/9/11	-
1	MLY	M	681	1	-	4/8/9/11	-
1	MLY	A	138	1	-	4/8/9/11	-
1	MLY	P	190	1	-	5/8/9/11	-
1	MLY	M	617	1	-	1/8/9/11	-
1	MLY	D	613	1	-	4/8/9/11	-
1	MLY	D	617	1	-	1/8/9/11	-
1	MLY	M	87	1	-	2/8/9/11	-
1	MLY	G	236	1	-	3/8/9/11	-
1	MLY	P	504	1	-	4/8/9/11	-
1	MLY	G	528	1	-	4/8/9/11	-
1	MLY	A	598	1	-	5/8/9/11	-
1	MLY	G	598	1	-	5/8/9/11	-
1	MLY	D	236	1	-	3/8/9/11	-
1	MLY	D	600	1	-	3/8/9/11	-
1	MLY	J	348	1	-	5/8/9/11	-
1	MLY	D	369	1	-	2/8/9/11	-
1	MLY	M	296	1	-	4/8/9/11	-
1	MLY	G	768	1	-	4/8/9/11	-
1	MLY	D	367	1	-	2/8/9/11	-

The worst 5 of 86 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	138	MLY	CB-CA	-3.79	1.48	1.53
1	G	138	MLY	CB-CA	-3.74	1.48	1.53
1	P	138	MLY	CB-CA	-3.66	1.48	1.53
1	J	138	MLY	CB-CA	-3.64	1.48	1.53
1	M	138	MLY	CB-CA	-3.63	1.48	1.53

There are no bond angle outliers.

There are no chirality outliers.

5 of 956 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	19	MLY	C-CA-CB-CG
1	A	49	MLY	N-CA-CB-CG
1	A	49	MLY	C-CA-CB-CG
1	A	55	MLY	N-CA-CB-CG
1	A	55	MLY	C-CA-CB-CG

There are no ring outliers.

184 monomers are involved in 810 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	P	617	MLY	1	0
1	J	59	MLY	2	0
1	J	659	MLY	2	0
1	J	84	MLY	23	0
1	J	600	MLY	1	0
1	G	505	MLY	1	0
1	D	59	MLY	2	0
1	A	190	MLY	2	0
1	D	55	MLY	1	0
1	M	35	MLY	12	0
1	G	782	MLY	1	0
1	D	839	MLY	4	0
1	A	553	MLY	19	0
1	M	272	MLY	1	0
1	M	764	MLY	6	0
1	J	272	MLY	1	0
1	M	782	MLY	9	0
1	A	348	MLY	5	0
1	P	248	MLY	2	0
1	J	55	MLY	1	0
1	J	138	MLY	1	0
1	A	272	MLY	1	0
1	D	63	MLY	3	0
1	J	598	MLY	1	0
1	P	659	MLY	1	0
1	M	107	MLY	3	0
1	P	600	MLY	1	0
1	J	295	MLY	6	0
1	J	839	MLY	8	0
1	P	839	MLY	12	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	528	MLY	2	0
1	A	49	MLY	3	0
1	G	837	MLY	1	0
1	M	839	MLY	11	0
1	M	369	MLY	1	0
1	A	768	MLY	18	0
1	P	84	MLY	5	0
1	G	348	MLY	4	0
1	G	190	MLY	2	0
1	M	84	MLY	37	0
1	A	551	MLY	2	0
1	P	55	MLY	1	0
1	P	138	MLY	1	0
1	P	30	MLY	1	0
1	G	553	MLY	27	0
1	J	296	MLY	3	0
1	D	598	MLY	1	0
1	A	505	MLY	35	0
1	G	295	MLY	5	0
1	M	190	MLY	2	0
1	M	553	MLY	27	0
1	D	553	MLY	16	0
1	G	436	MLY	2	0
1	J	436	MLY	2	0
1	P	436	MLY	2	0
1	D	272	MLY	1	0
1	J	764	MLY	2	0
1	D	295	MLY	6	0
1	G	55	MLY	1	0
1	J	486	MLY	3	0
1	A	63	MLY	3	0
1	G	59	MLY	3	0
1	J	528	MLY	3	0
1	D	827	MLY	2	0
1	G	49	MLY	2	0
1	P	63	MLY	3	0
1	A	415	MLY	1	0
1	M	59	MLY	2	0
1	D	348	MLY	6	0
1	J	248	MLY	2	0
1	M	528	MLY	3	0
1	D	49	MLY	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	J	107	MLY	3	0
1	P	553	MLY	2	0
1	J	87	MLY	3	0
1	A	87	MLY	3	0
1	J	30	MLY	1	0
1	P	782	MLY	2	0
1	D	659	MLY	2	0
1	A	659	MLY	2	0
1	D	486	MLY	3	0
1	G	248	MLY	2	0
1	G	296	MLY	2	0
1	P	272	MLY	1	0
1	P	295	MLY	6	0
1	P	764	MLY	9	0
1	G	617	MLY	1	0
1	G	138	MLY	1	0
1	P	528	MLY	2	0
1	A	486	MLY	3	0
1	P	598	MLY	1	0
1	G	659	MLY	2	0
1	G	600	MLY	1	0
1	M	837	MLY	1	0
1	D	436	MLY	2	0
1	D	248	MLY	2	0
1	G	839	MLY	4	0
1	M	598	MLY	1	0
1	J	768	MLY	4	0
1	P	107	MLY	3	0
1	P	87	MLY	3	0
1	A	839	MLY	8	0
1	G	486	MLY	3	0
1	J	617	MLY	1	0
1	D	138	MLY	1	0
1	D	296	MLY	3	0
1	G	84	MLY	18	0
1	D	87	MLY	3	0
1	G	415	MLY	1	0
1	J	190	MLY	2	0
1	M	63	MLY	3	0
1	M	486	MLY	3	0
1	M	600	MLY	1	0
1	A	107	MLY	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	J	837	MLY	1	0
1	G	87	MLY	3	0
1	M	505	MLY	12	0
1	M	436	MLY	2	0
1	A	504	MLY	2	0
1	A	30	MLY	1	0
1	D	415	MLY	1	0
1	G	272	MLY	1	0
1	G	764	MLY	22	0
1	J	63	MLY	4	0
1	J	505	MLY	9	0
1	A	59	MLY	2	0
1	M	348	MLY	5	0
1	P	486	MLY	3	0
1	J	415	MLY	1	0
1	A	296	MLY	2	0
1	J	782	MLY	1	0
1	A	617	MLY	1	0
1	G	63	MLY	4	0
1	M	415	MLY	1	0
1	D	782	MLY	87	0
1	A	600	MLY	1	0
1	A	837	MLY	4	0
1	D	764	MLY	9	0
1	D	551	MLY	1	0
1	M	248	MLY	2	0
1	P	59	MLY	2	0
1	D	768	MLY	11	0
1	P	348	MLY	5	0
1	D	528	MLY	3	0
1	M	49	MLY	3	0
1	P	296	MLY	3	0
1	M	659	MLY	2	0
1	M	55	MLY	1	0
1	M	768	MLY	1	0
1	A	248	MLY	2	0
1	P	415	MLY	1	0
1	G	30	MLY	1	0
1	D	107	MLY	2	0
1	A	55	MLY	1	0
1	M	30	MLY	1	0
1	D	30	MLY	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	P	837	MLY	1	0
1	G	107	MLY	2	0
1	A	295	MLY	6	0
1	M	295	MLY	6	0
1	J	49	MLY	2	0
1	M	551	MLY	3	0
1	P	49	MLY	3	0
1	A	436	MLY	2	0
1	A	764	MLY	9	0
1	A	369	MLY	1	0
1	D	190	MLY	2	0
1	A	782	MLY	7	0
1	D	837	MLY	1	0
1	G	369	MLY	1	0
1	J	553	MLY	11	0
1	M	138	MLY	1	0
1	A	138	MLY	1	0
1	P	190	MLY	2	0
1	M	617	MLY	1	0
1	D	617	MLY	1	0
1	M	87	MLY	3	0
1	G	528	MLY	3	0
1	A	598	MLY	1	0
1	G	598	MLY	1	0
1	D	600	MLY	1	0
1	J	348	MLY	5	0
1	M	296	MLY	3	0
1	G	768	MLY	7	0

## 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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	M	7
1	P	6
1	D	4
1	A	4
1	J	3
1	G	3
3	C	1
3	F	1
3	I	1
3	L	1
3	O	1
3	R	1
2	B	1
2	E	1
2	H	1
2	K	1
2	N	1
2	Q	1

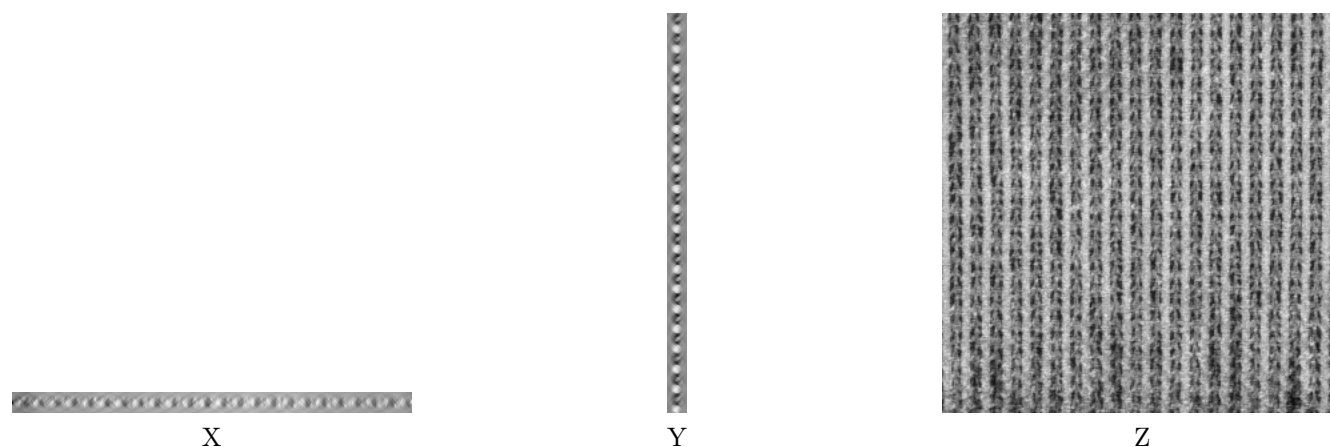
The worst 5 of 39 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	J	769:ALA	C	770:GLY	N	5.54
1	D	769:ALA	C	770:GLY	N	5.18
1	G	769:ALA	C	770:GLY	N	4.67
1	A	709:LYS	C	710:GLY	N	3.39
1	D	709:LYS	C	710:GLY	N	3.25

## 6 Tomogram visualisation [i](#)

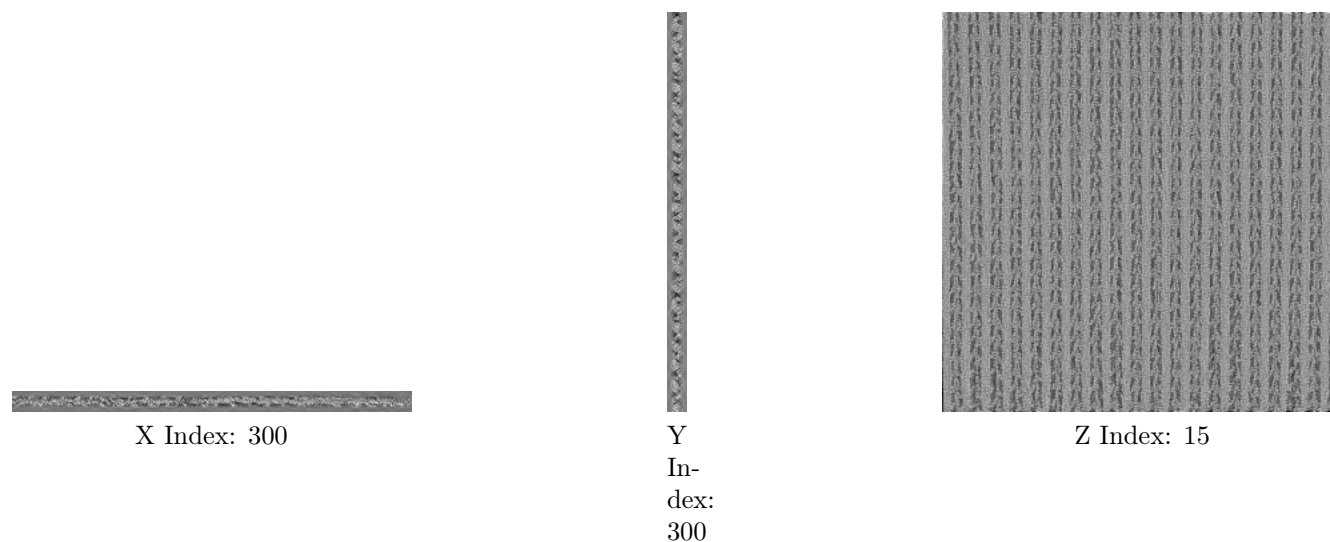
This section contains visualisations of the EMDB entry EMD-1001. These allow visual inspection of the internal detail of the tomogram and identification of artifacts.

### 6.1 Orthogonal projections [i](#)



The images above show the tomogram projected in three orthogonal directions.

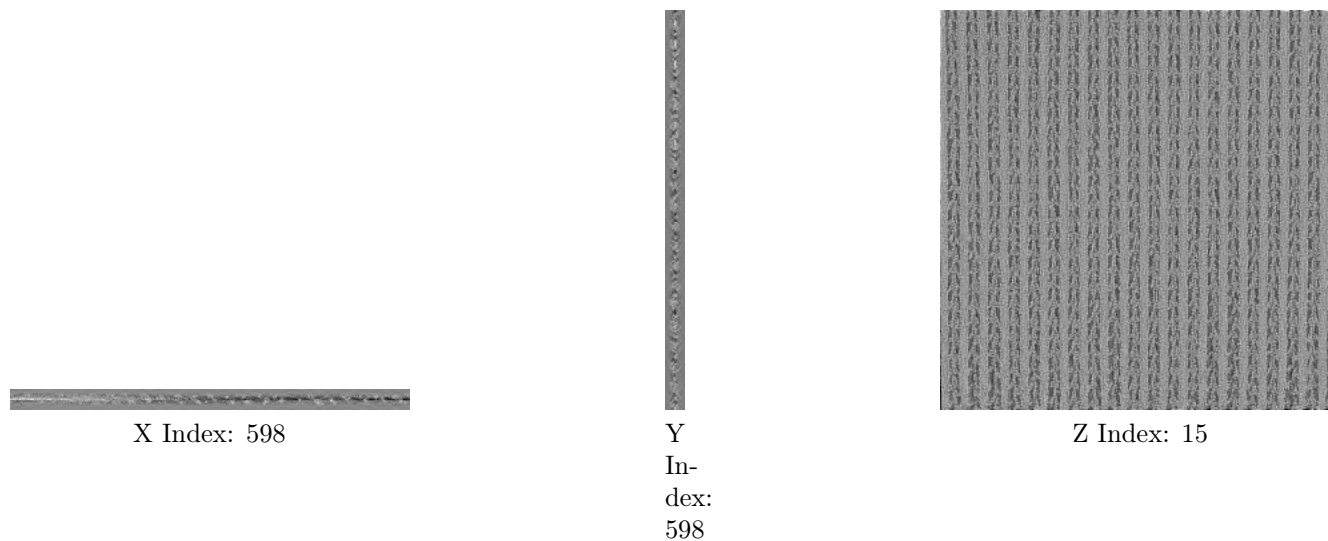
### 6.2 Central slices [i](#)



The images above show central slices of the tomogram in three orthogonal directions.



### 6.3 Largest variance slices [i](#)



The images above show the largest variance slices of the tomogram in three orthogonal directions.

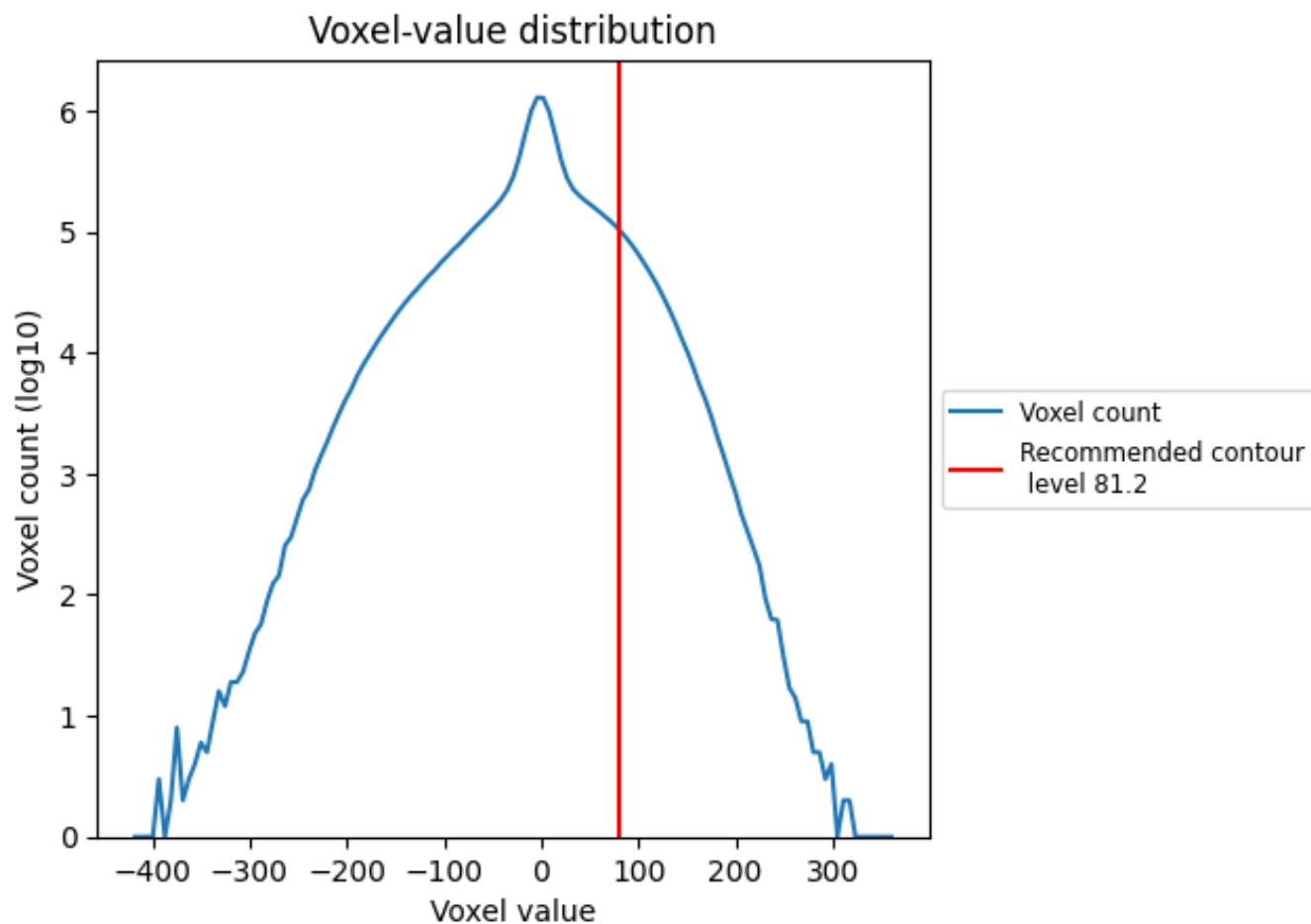
### 6.4 Mask visualisation [i](#)

This section was not generated.

## 7 Tomogram analysis [i](#)

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

### 7.1 Voxel-value distribution [i](#)



The voxel-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic.

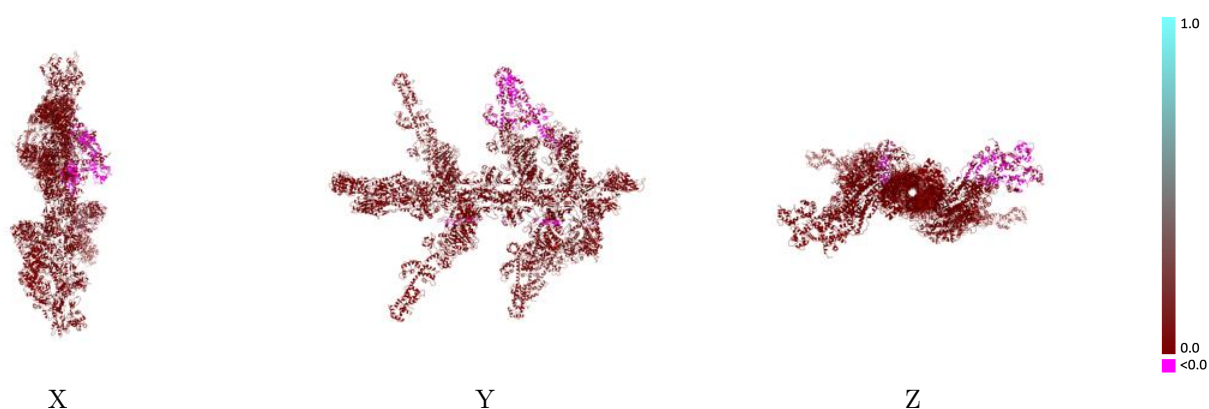
## 8 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-1001 and PDB model 1O1D. Per-residue inclusion information can be found in section 3 on page 7.

### 8.1 Map-model overlay [i](#)

This section was not generated.

### 8.2 Q-score mapped to coordinate model [i](#)

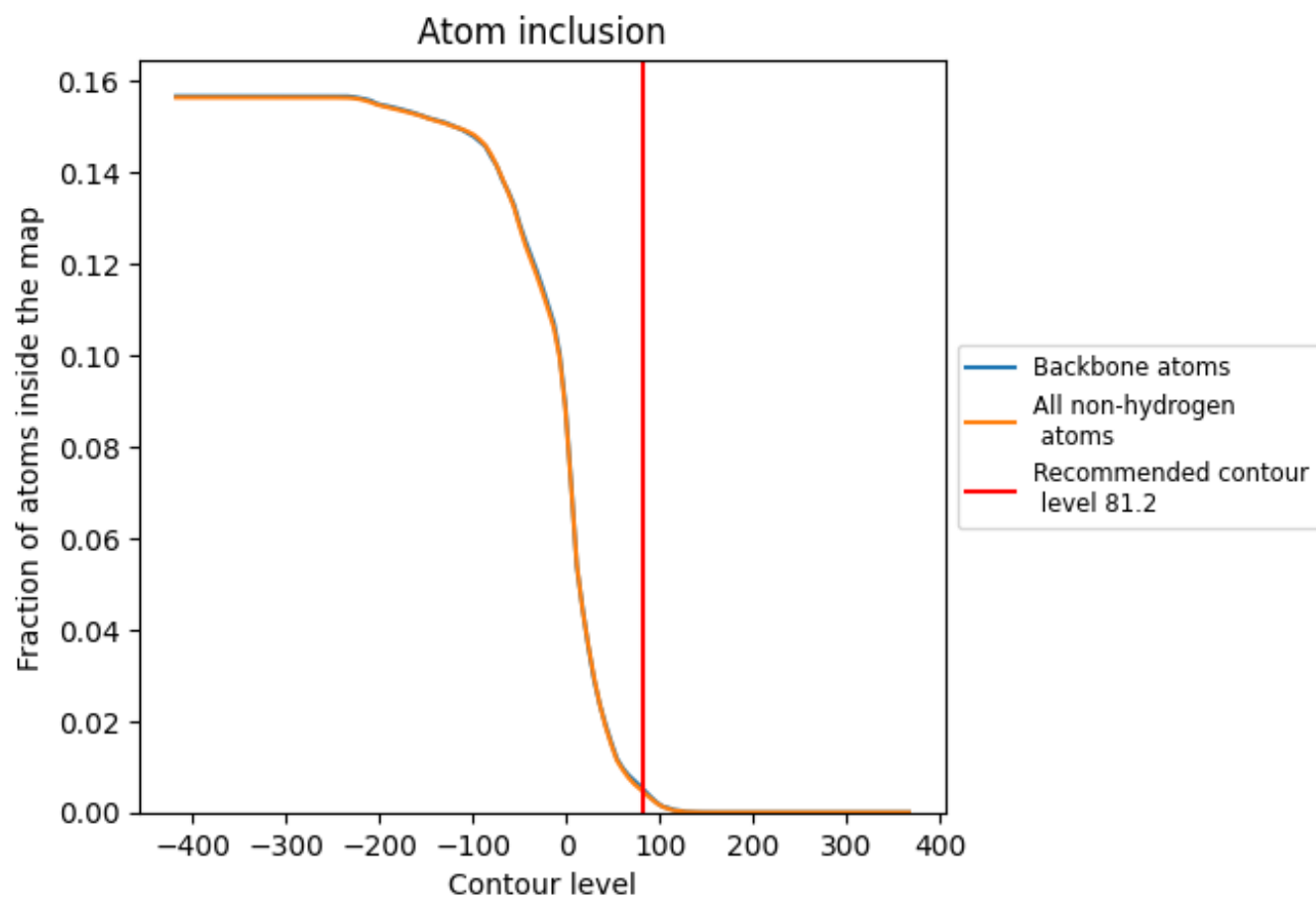


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

### 8.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.



































































## 8.4 Atom inclusion [i](#)



At the recommended contour level, 1% of all backbone atoms, 0% of all non-hydrogen atoms, are inside the map.

## 8.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (81.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.0047	 -0.0000
0	 0.0000	 0.0000
1	 0.0147	 0.0000
2	 0.0000	 0.0000
3	 0.0000	 0.0000
4	 0.0000	 0.0000
5	 0.0000	 0.0000
7	 0.0000	 -0.0000
8	 0.0000	 0.0000
9	 0.0000	 0.0000
A	 0.0000	 -0.0010
B	 0.0000	 0.0000
C	 0.0000	 0.0000
D	 0.0000	 0.0060
E	 0.0000	 -0.0120
F	 0.1158	 0.0020
G	 0.0000	 -0.0040
H	 0.0000	 0.0000
I	 0.0000	 0.0000
J	 0.0000	 -0.0020
K	 0.0152	 0.0000
L	 0.0000	 -0.0070
M	 0.0000	 0.0010
N	 0.0000	 0.0000
O	 0.0000	 0.0000
P	 0.0000	 0.0000
Q	 0.0000	 0.0000
R	 0.0000	 0.0000
V	 0.0000	 -0.0000
W	 0.0000	 0.0000
X	 0.0688	 -0.0010
Y	 0.0000	 0.0000
Z	 0.0189	 0.0030

