



wwPDB EM Validation Summary Report ⓘ

Mar 17, 2026 – 07:09 PM UTC

PDB ID : 1O1C / pdb_00001o1c
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 : 1ATN, 2MYS

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We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

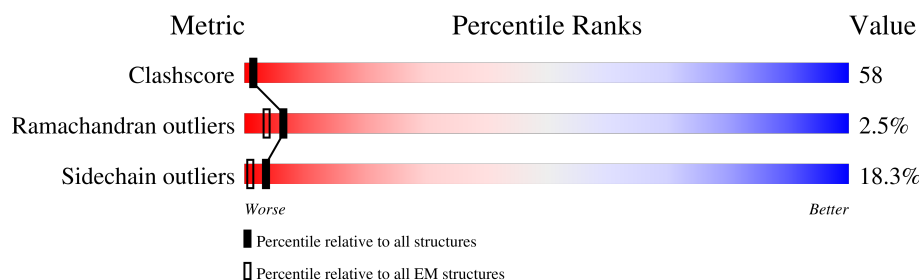
1 Overall quality at a glance

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	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	100% 25% 48% 23% .
1	D	840	100% 25% 49% 22% .
1	G	840	100% 24% 50% 22% .
1	J	840	100% 24% 49% 22% .
1	P	840	100% 24% 49% 22% .
2	B	145	100% 65% 26% 6% .
2	E	145	100% 64% 26% 6% .
2	H	145	100% 61% 30% 5% .

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Mol	Chain	Length	Quality of chain
2	K	145	
2	Q	145	
3	C	147	
3	F	147	
3	I	147	
3	L	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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	MLY	A	505	-	-	X	-
1	MLY	A	553	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	MLY	A	764	-	-	X	-
1	MLY	A	782	-	-	X	-
1	MLY	A	837	-	-	X	-
1	MLY	A	839	-	-	X	-
1	MLY	D	553	-	-	X	-
1	MLY	D	764	-	-	X	-
1	MLY	D	782	-	-	X	-
1	MLY	G	505	-	-	X	-
1	MLY	G	553	-	-	X	-
1	MLY	G	764	-	-	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	P	505	-	-	X	-
1	MLY	P	839	-	-	X	-
1	MLY	P	84	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 85919 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	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	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		

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

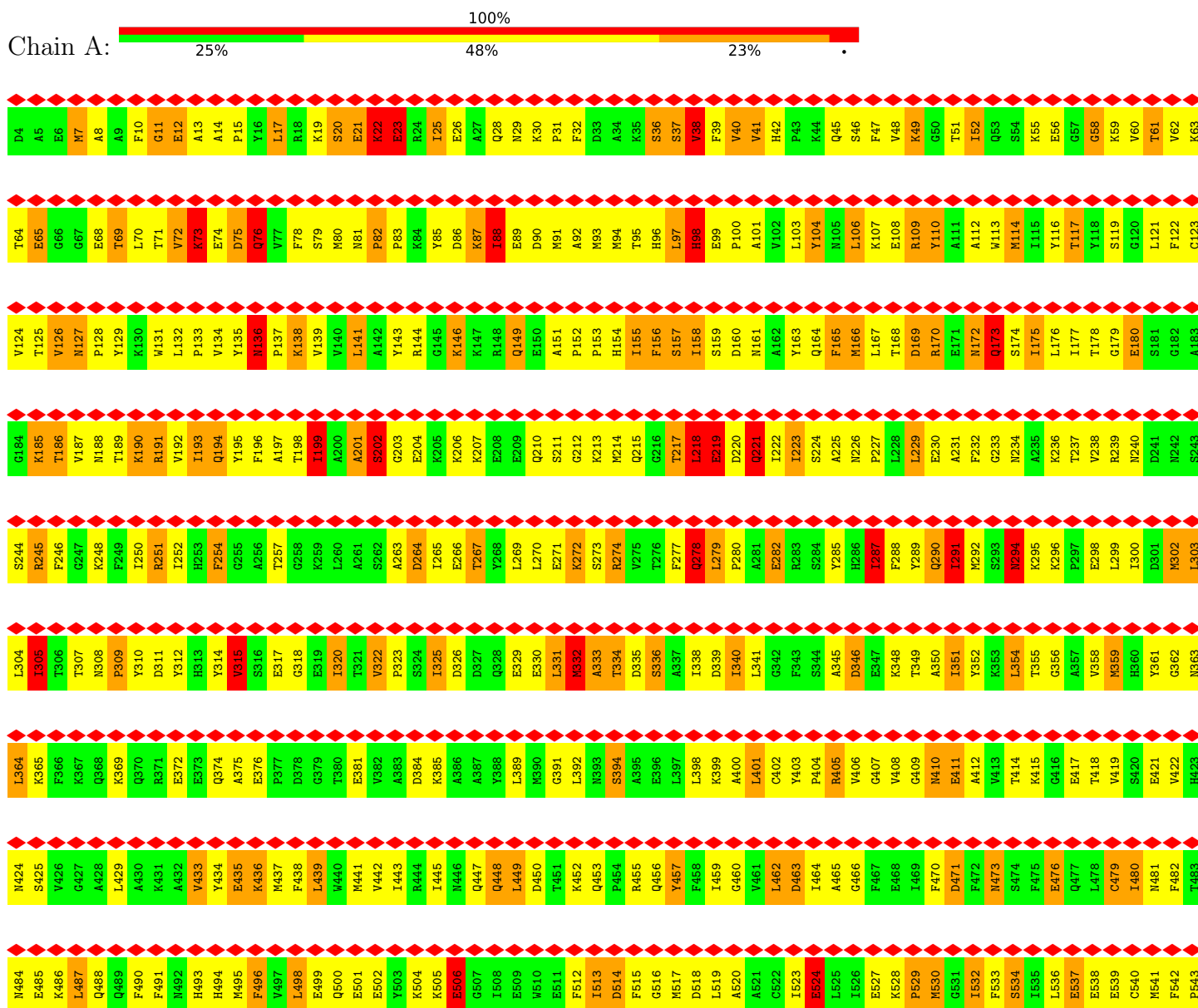
- Molecule 4 is a protein called SKELETAL MUSCLE ACTIN.

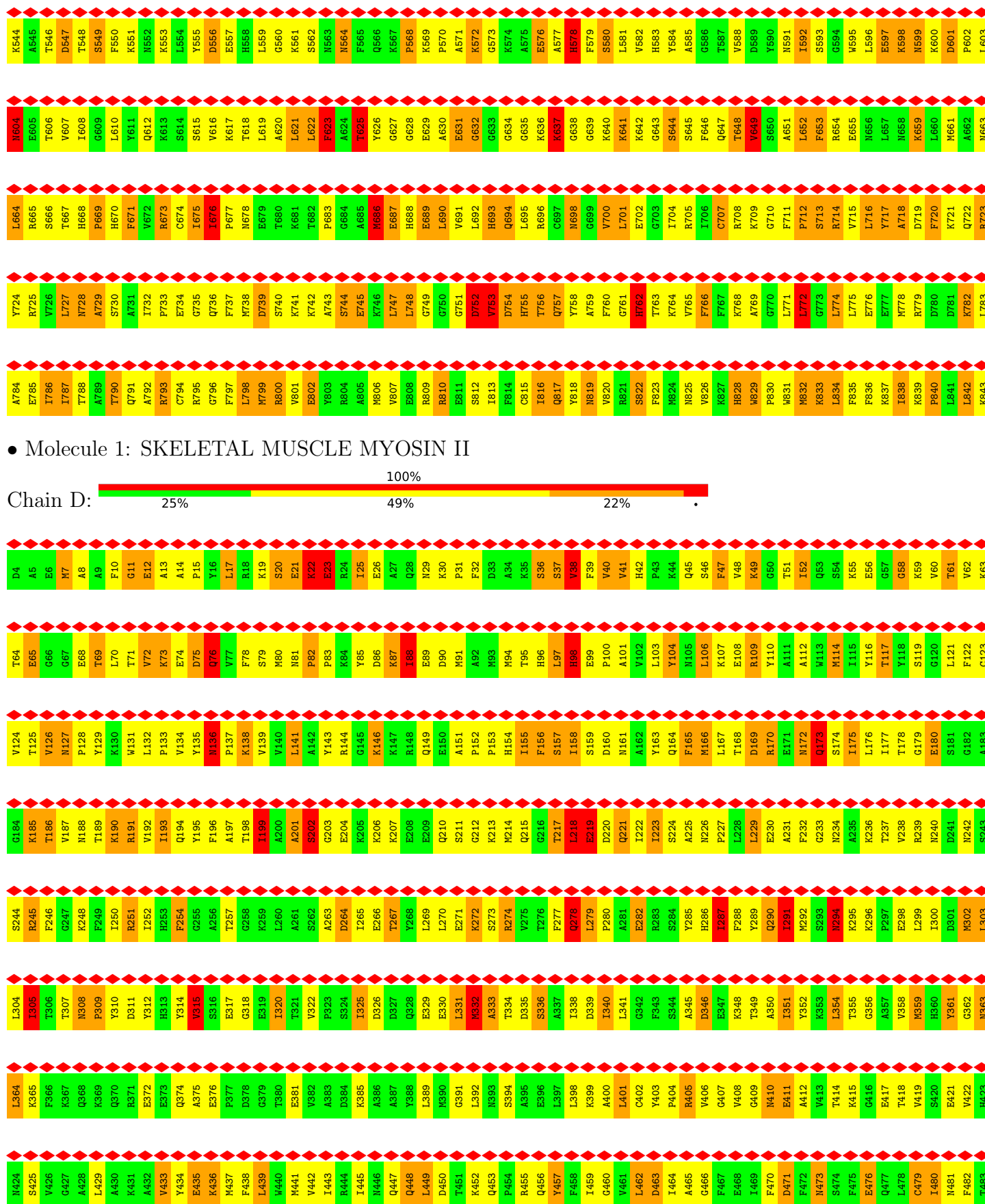
Mol	Chain	Residues	Atoms					AltConf	Trace
4	0	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	1	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	2	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	3	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	4	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
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







N424	N484	K544	L664	Y724	A784	D4	T64	V124	G184	S244	L304
S425	E485	A545	R665	R725	E785	A5	E65	T125	K185	R245	T305
V426	K486	T546	S666	V726	I786	E6	G66	V126	T186	F246	T306
G427	L487	D547	T667	L727	T787	M7	G67	M127	V187	G247	T307
A428	Q488	T548	H668	M728	T788	A8	E68	P128	N188	K248	N308
L429	Q489	S549	P669	A729	A789	A9	E69	Y129	T189	F249	P309
A430	F490	F550	H670	S730	T790	F10	L70	K130	K190	L250	Y310
K431	F491	K551	F671	A731	Q791	G11	T71	V131	R191	R251	D311
A432	N492	N552	V672	I732	A792	E12	V72	L132	V192	L252	D312
V433	H493	K553	R673	P733	R793	A13	K73	P133	T193	H253	Y313
Y434	H494	L554	C674	E734	C794	A14	E74	V134	Q194	F254	Y314
E435	M495	Y555	I675	G735	R795	P15	D75	Y135	Y195	G255	V315
K436	F496	D556	I676	Q736	G796	Y16	Q76	N136	F196	A256	S316
M437	V497	V616	P677	F737	F797	L17	V77	V137	A197	T257	E317
F438	L498	H558	N678	M738	L798	R18	F78	K138	T198	G258	G318
L439	E499	L559	E679	D739	M799	K19	S79	V139	N199	K259	E319
M440	Q500	G560	T680	S740	R800	S20	M80	Y140	A200	L260	I320
M441	E501	K561	K681	K741	V601	E21	E81	L141	A201	A261	T321
V442	E502	S562	T682	K742	E802	K22	P82	A142	S202	S262	V322
I443	Y503	N563	P683	A743	Y803	E23	P83	Y143	G203	A263	P323
R444	K504	N564	G684	S744	R804	R24	K84	G144	E204	D264	S324
I445	K505	F565	A685	E745	A805	I25	Y85	R145	K205	L265	I325
N446	E506	Q566	M686	K746	M806	E26	D86	K146	K206	E266	D326
Q447	G507	K567	E687	L747	V807	A27	K87	K147	K207	T267	D327
Q448	I508	P568	H688	L748	E808	Q28	T88	Q148	E208	T268	Q328
L449	E509	K569	E689	G749	R809	N29	E89	R149	E209	L269	E329
D450	M510	P570	L690	G750	R810	K30	D90	E150	Q210	L270	E330
T451	E511	A571	V691	G751	E811	P31	A91	A151	S211	E271	L331
K452	F512	K572	L692	D752	S812	F32	A92	P152	G212	K272	R332
Q453	I513	G573	H693	V753	I813	D33	M93	P153	K213	S273	A333
P454	D514	K574	Q694	D754	F814	A34	M94	H154	M214	R274	T334
R455	F515	A575	L695	H755	C815	K35	T95	I155	Q215	V275	D335
Q456	G516	E576	R696	T756	I816	S36	H96	F156	G216	T276	S336
Y457	M517	K577	C697	Q757	Q817	S37	L97	S157	T217	F277	A337
F458	D518	H578	N698	Y758	Y818	V38	H98	I158	L218	Q278	I338
I459	L519	F579	G699	A759	N819	F39	E99	S159	E219	L279	D339
G460	A520	S580	V700	F760	V820	V40	P100	D160	D220	P280	I340
V461	E521	L581	L701	G761	R821	V41	A101	A161	Q221	A281	L341
L462	C522	V582	E702	H762	S822	H42	Y102	A162	I222	E282	G342
D463	I523	H583	G703	T763	P823	P43	L103	Y163	I223	R283	F343
I464	E524	Y584	I704	K764	M824	K44	Y104	Q164	S224	S284	S344
A465	L525	A585	R705	V765	N825	Q45	N105	F165	A225	Y285	A345
G466	I526	G586	T706	F766	V826	S46	L106	M166	N226	H286	D346
F467	E527	K587	C707	F767	K827	F47	L107	L167	P227	I287	E347
E468	K528	V588	R708	K768	H828	V48	E108	T168	L228	F288	K348
I469	P529	D589	K709	A769	N829	V49	R109	D169	L229	Y289	T349
F470	M530	Y590	G710	G770	P830	G50	Y110	R170	E230	Q290	A350
D471	G531	N591	F711	L771	M831	T51	A111	E171	A231	I291	I351
F472	I532	L592	P712	L772	M832	I52	A112	M172	F232	M292	Y352
N473	F533	S593	S713	G773	K833	Q53	V113	Q173	G233	S293	K353
S474	S534	G594	R714	L774	L834	S54	M114	S174	N234	N294	L354
F475	I535	V595	V715	L775	P835	K55	I115	I175	A235	K295	T355
E476	L536	L596	L716	E776	P836	E56	Y116	L176	K236	K296	G356
Q477	E537	O597	T717	E777	K837	G57	T117	T177	T237	P297	A357
L478	E538	K598	A718	M778	T838	G58	Y118	T178	V238	E298	V358
C479	E539	N599	D719	R779	K839	S59	S119	G179	R239	L299	K359
I480	C540	K600	F720	D780	P840	V60	G120	E180	N240	T300	H360
N481	M541	D601	K721	L781	L841	T61	G121	S181	D241	I301	Y361
F482	P542	A652	Q722	K782	L842	V62	F122	G182	N242	K302	G362
T483	L603	N663	R723	L783	K843	K63	C123	A183	S243	L303	N363

● Molecule 1: SKELETAL MUSCLE MYOSIN II



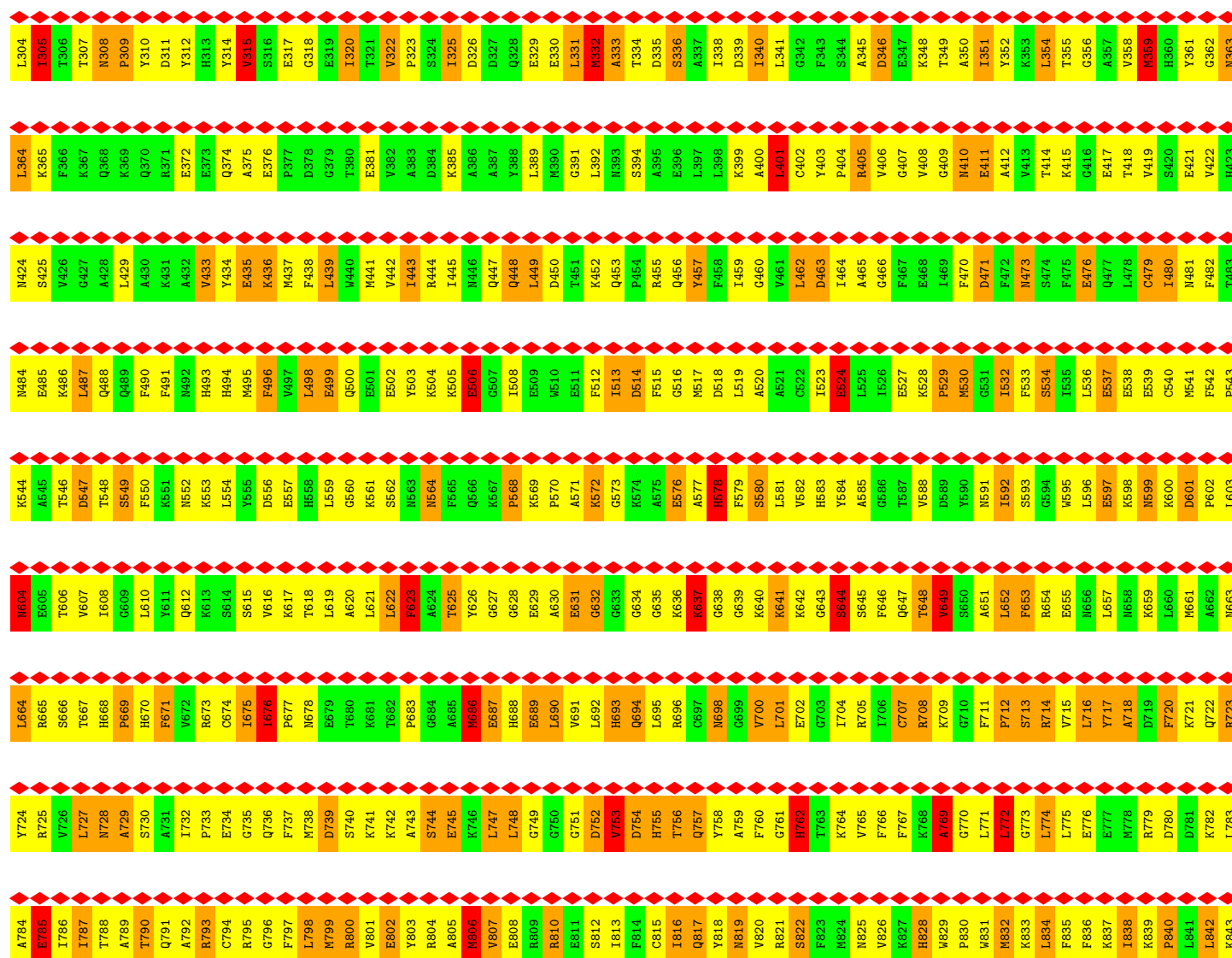
D4	T64	V124	G184	S244	L304
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E6	G66	V126	T186	F246	T306
M7	G67	M127	V187	G247	T307
A8	E68	P128	N188	K248	N308
A9	E69	Y129	T189	F249	P309
F10	L70	K130	K190	L250	Y310
G11	T71	V131	R191	R251	D311
E12	V72	L132	V192	L252	D312
A13	K73	P133	T193	H253	Y313
A14	E74	V134	Q194	F254	Y314
P15	D75	Y135	Y195	G255	V315
Y16	Q76	N136	F196	A256	S316
L17	V77	V137	A197	T257	E317
R18	F78	K138	T198	G258	G318
K19	S79	V139	N199	K259	E319
S20	M80	Y140	A200	L260	I320
E21	E81	L141	A201	A261	T321
K22	P82	A142	S202	S262	V322
E23	P83	Y143	G203	A263	P323
R24	K84	G144	E204	D264	S324
I25	Y85	R145	K205	L265	I325
E26	D86	K146	K206	E266	D326
A27	K87	K147	K207	T267	D327
Q28	T88	Q148	E208	T268	Q328
N29	E89	R149	E209	L269	E329
K30	D90	E150	Q210	L270	E330
P31	A91	A151	S211	E271	L331
F32	A92	P152	G212	K272	R332
D33	M93	P153	K213	S273	A333
A34	M94	H154	M214	R274	T334
K35	T95	I155	Q215	V275	D335
S36	H96	F156	G216	T276	S336
S37	L97	S157	T217	F277	A337
V38	H98	I158	L218	Q278	I338
F39	E99	S159	E219	L279	D339
V40	P100	D160	D220	P280	I340
V41	A101	A161	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	L107	L167	P227	I287	E347
V48	E108	T168	L228	F288	K348
R49	R109	D169	L229	Y289	T349
G50	Y110	R170	E230	Q290	A350
T51	A111	E171	A231	I291	I351
I52	A112	M172	F232	M292	Y352
Q53	V113	Q173	G233	S293	K353
S54	M114	S174	N234	N294	L354
K55	I115	I175	A235	K295	T355
E56	Y116	L176	K236	K296	G356
G57	T117	T177	T237	P297	A357
S58	Y118	T178	V238	E298	V358
K59	S119	G179	R239	L299	K359
V60	G120	E180	N240	T300	H360
T61	G121	S181	D241	I301	Y361
V62	F122	G182	N242	K302	G362
K63	C123	A183	S243	L303	N363

A784	R785	I786	T787	T788	A789	T790	Q791	A792	R793	C794	R795	G796	F797	L798	M799	R800	V801	E802	Y803	R804	A805	M806	V807	E808	R809	R810	E811	S812	L813	F814	C815	L816	Q817	Y818	N819	V820	R821	S822	F823	M824	N825	V826	K827	H828	V829	P830	M831	M832	L833	L834	F835	P836	K837	T838	K839	P840	L841	L842	L843
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	R762	T763	K764	V765	F766	F767	K768	A769	G770	F771	L772	G773	L774	R775	L776	E777	M778	R779	D780	D781	K782	L783
L664	R665	S666	T667	H668	P669	H670	F671	V672	K673	C674	I675	T676	P677	N678	E679	T680	K681	T682	P683	G684	A685	M686	E687	H688	E689	R810	V691	L692	H693	Q694	L695	R696	G697	N698	G699	V700	L701	E702	G703	I704	R705	I706	C707	R708	K709	G710	F711	P712	S713	R714	V715	L716	Y717	A718	D719	F720	K721	Q722	R723
M604	E605	T606	V607	I608	G609	L610	Y611	Q612	K613	S614	S615	V616	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	S645	F646	Q647	T648	V649	S650	A651	L652	F653	R654	E655	M656	L657	M658	K659	L660	M661	A662	
K544	A545	T546	D547	Q548	S549	F550	K551	N552	K553	L554	Y555	D556	E557	H558	L559	G560	K561	S562	N563	N564	F565	Q566	G567	P568	K569	P570	A571	K572	I573	K574	A575	E576	A577	H578	F579	S580	L581	V582	H583	Y584	A585	G586	T587	V588	D589	Y590	N591	I592	S593	S594	W595	L596	E597	K598	N599	K600	D601	P602	L603
N484	E485	K486	L487	Q488	Q489	F490	F491	N492	H493	H494	M495	F496	V497	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
N424	S425	V426	G427	A428	L429	A430	K431	A432	V433	Y434	E435	A436	M437	F438	L439	W440	M441	V442	I443	R444	I445	M446	Q447	Q448	L449	D450	T451	K452	Q453	P454	R455	Q456	Y457	F458	I459	G460	V461	L462	D463	I464	A465	G466	F467	E468	I469	F470	D471	F472	N473	S474	F475	Q476	Q477	L478	C479	I480	M481	F482	T483
L364	K365	F366	K367	Q368	K369	Q370	R371	E372	F373	Q374	A375	F376	P377	D378	G379	T380	E381	V382	A383	D384	K385	A386	A387	Y388	L389	M390	G391	L392	N393	S394	A395	E396	L397	L398	K399	A400	L401	C402	Y403	P404	R405	V406	G407	V408	G409	N410	E411	A412	V413	T414	K415	G416	E417	T418	V419	S420	E421	V422	H423

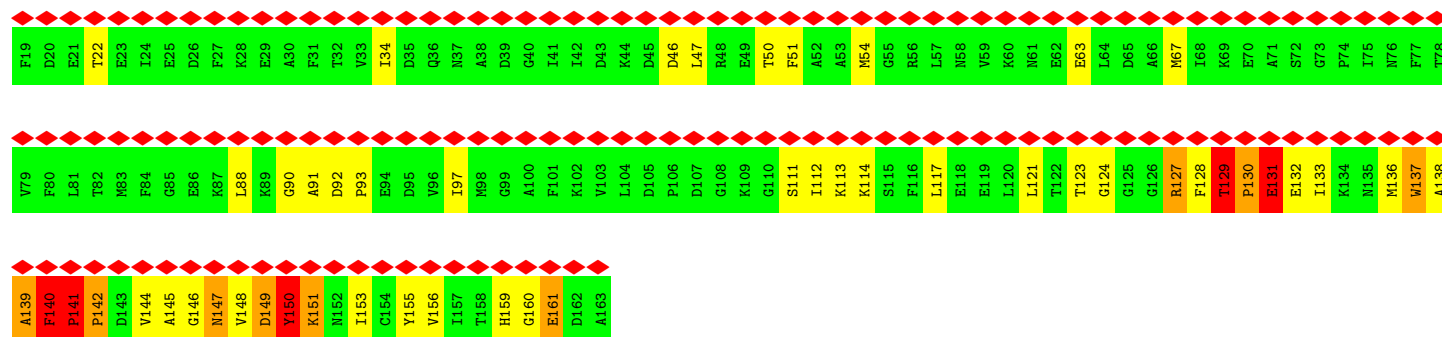
• Molecule 1: SKELETAL MUSCLE MYOSIN II



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	L287	F288	Y289	Q290	I291	M292	K293	N294	K295	K296	P297	E298	L299	L300	D301	M302	L303
G184	K185	T186	V187	N188	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	T217	L218	E219	D220	Q221	I222	I223	S224	A225	N226	P227	L228	L229	E230	A231	F232	G233	N234	A235	K236	V238	R239	L240	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	L148	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	I177	T178	G179	E180	L181	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	L88	E89	D90	N91	A92	M93	M94	T95	H96	L97	H98	E99	P100	A101	V102	L103	Y104	N105	L106	K107	E108	R109	Y110	A111	A112	Q113	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	K28	N29	K30	P31	A32	D33	A34	K35	S36	S37	V38	F39	V40	V41	H42	P43	L44	Y45	S46	F47	V48	K49	G50	T51	I52	Q53	S54	K55	E56	G57	G58	K59	V60	T61	F62	K63

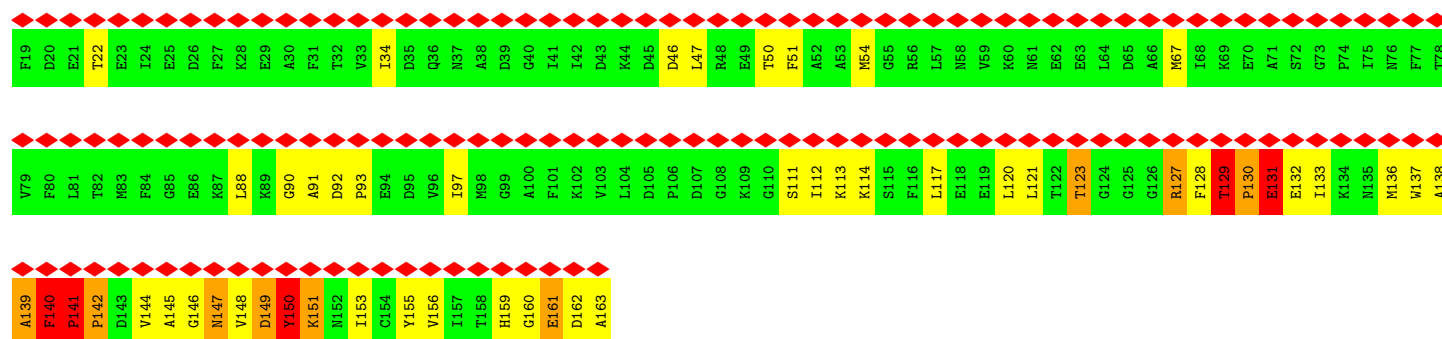


• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

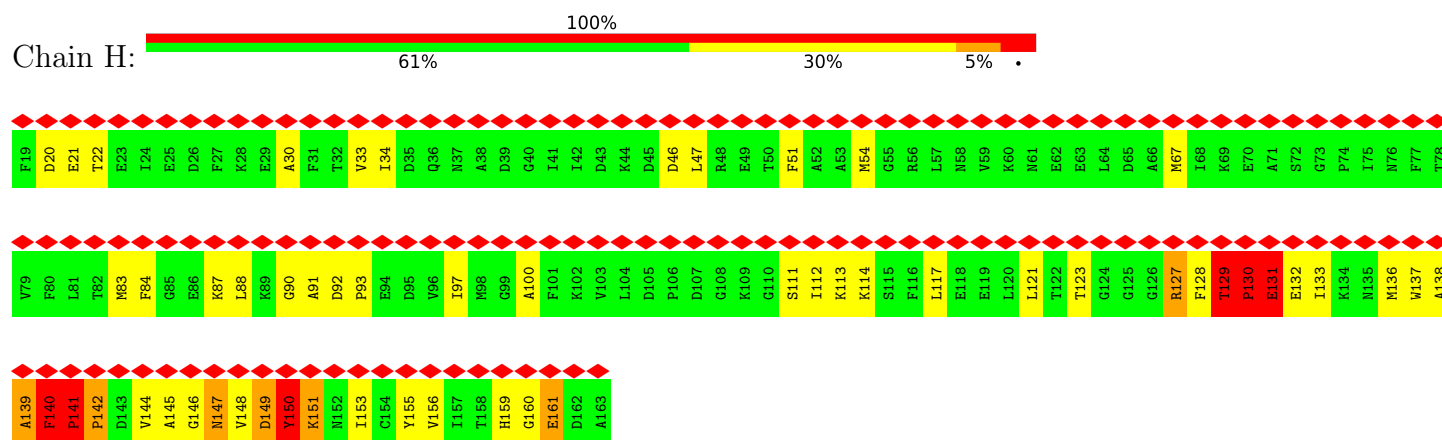


• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

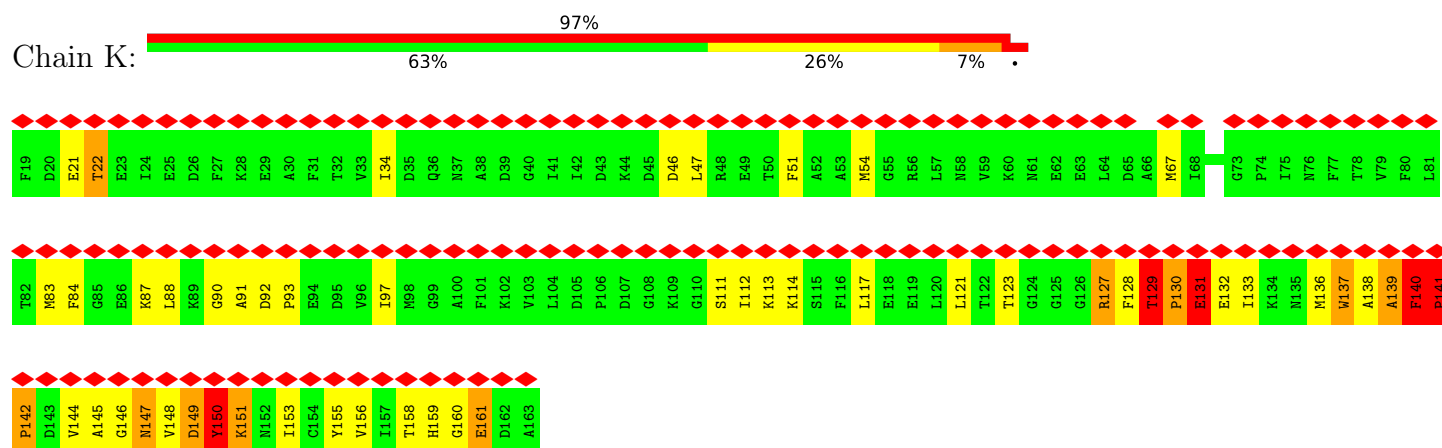




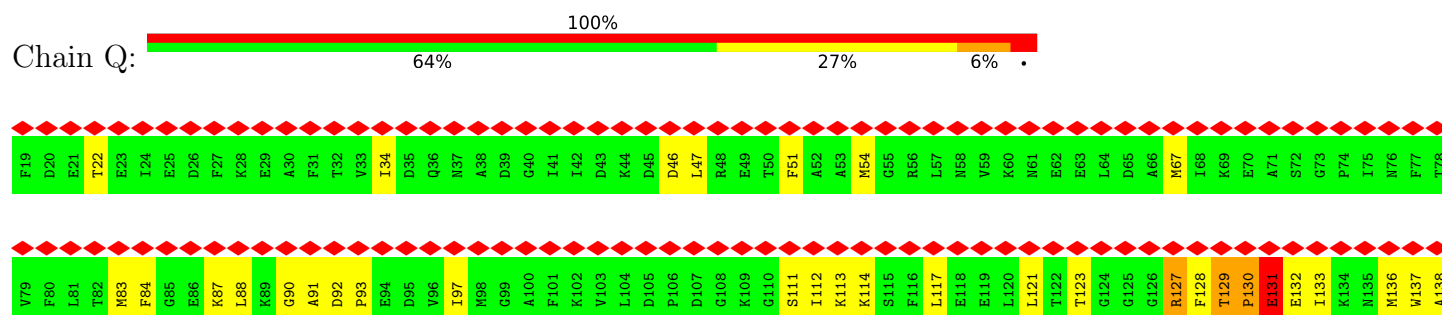
• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN



• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

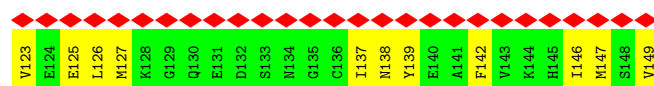


• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

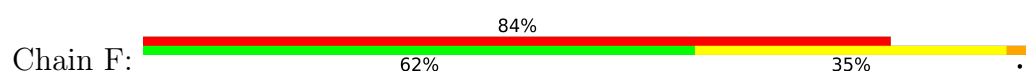




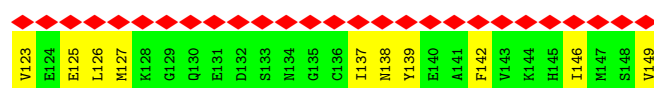
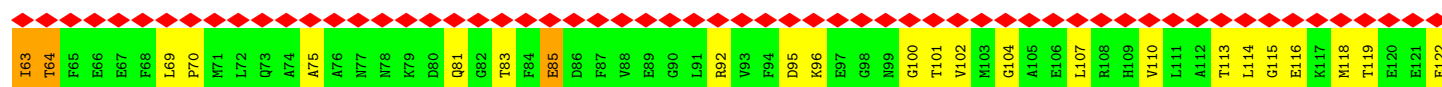
• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN



• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN



• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN

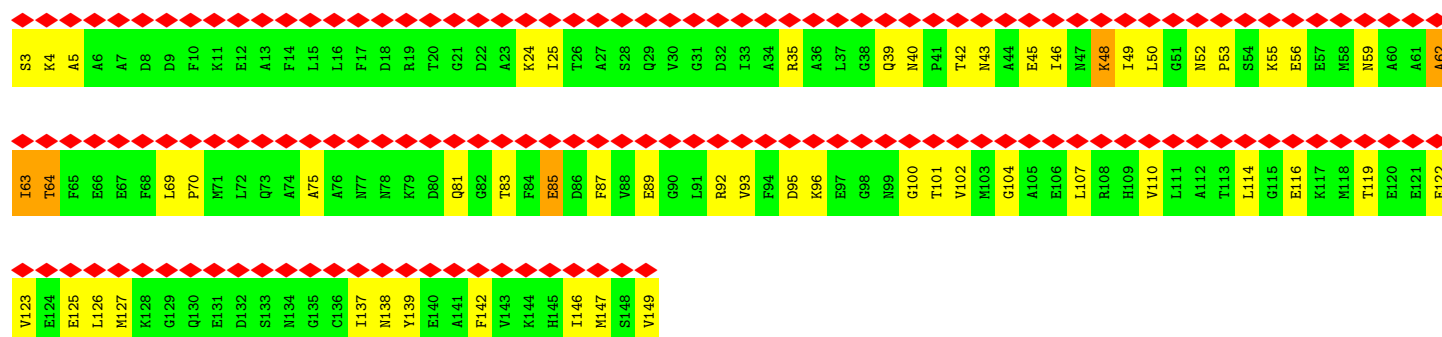


• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN

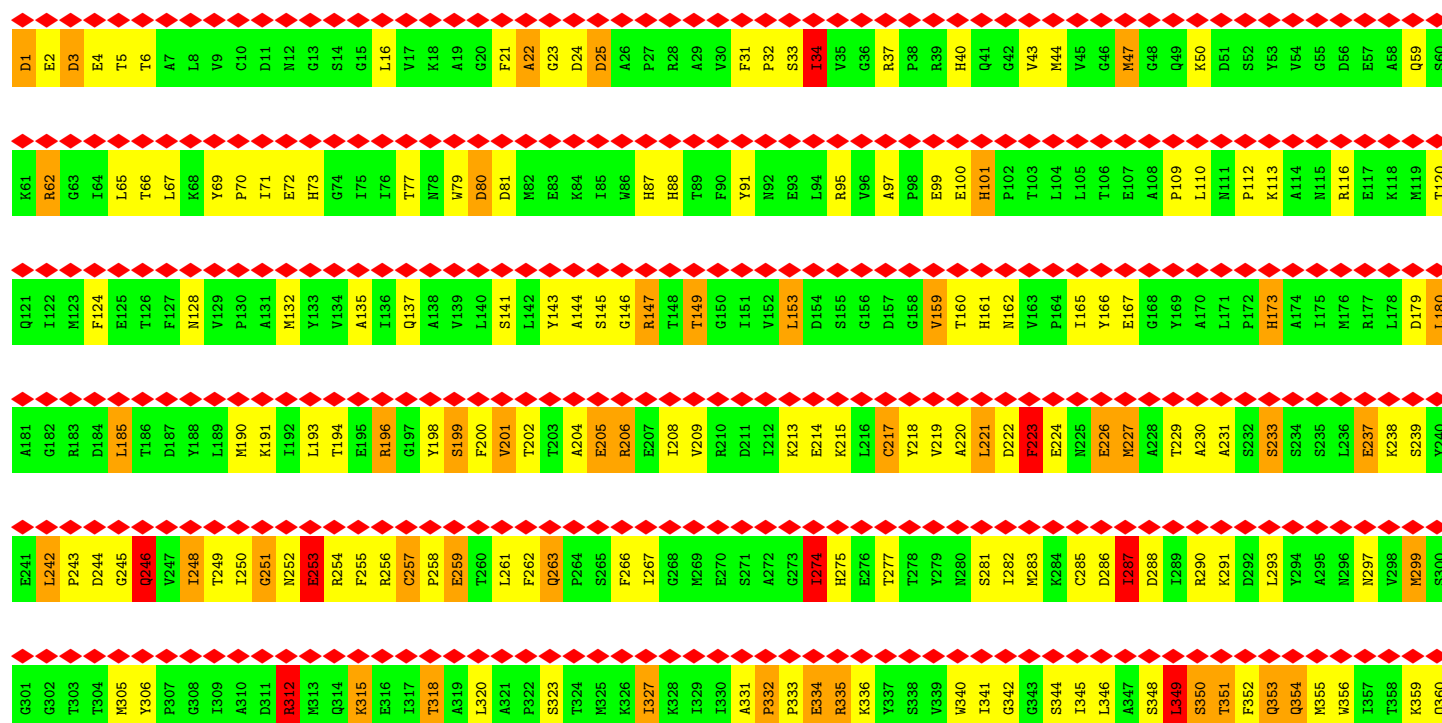


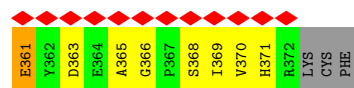


● Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN

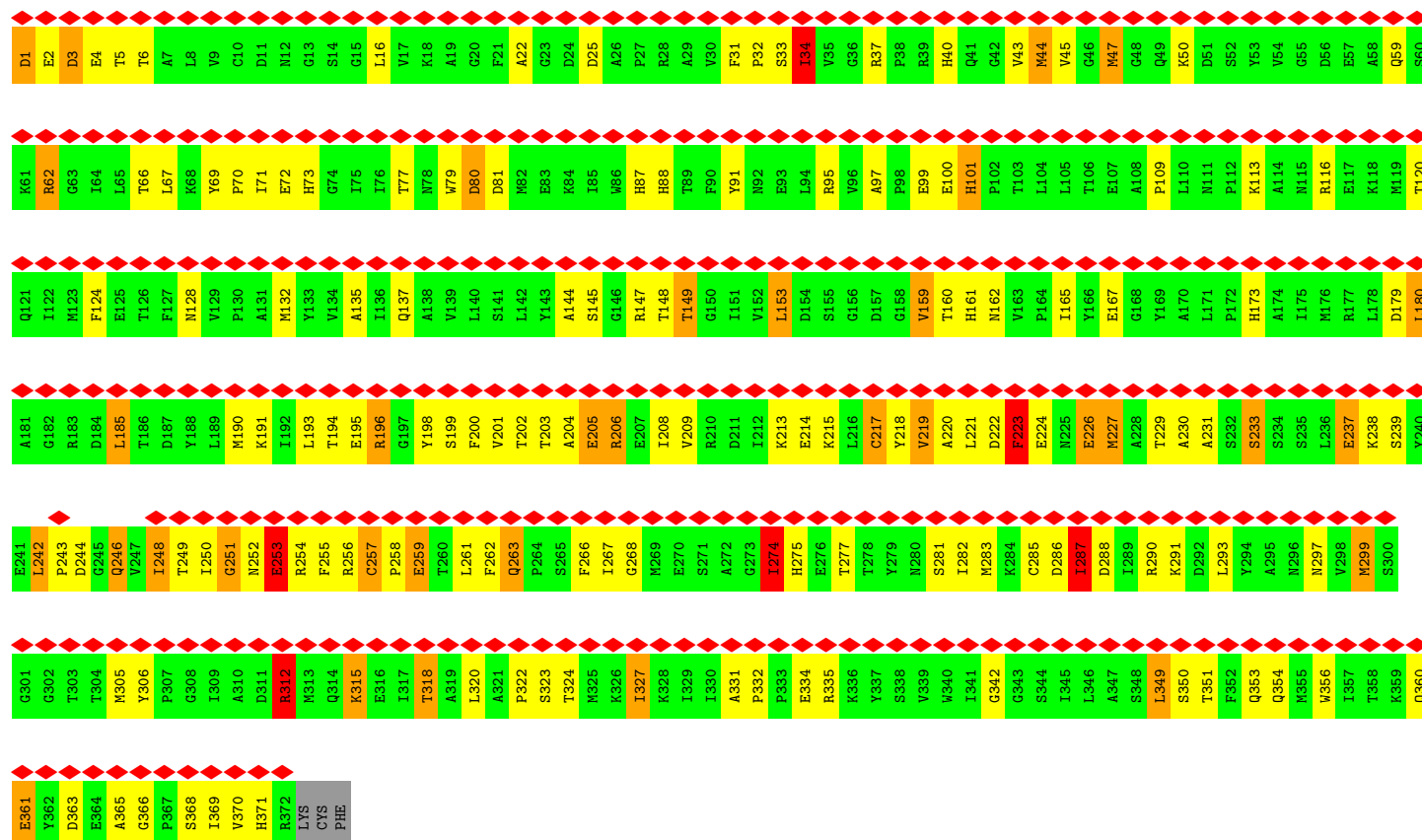


● Molecule 4: SKELETAL MUSCLE ACTIN

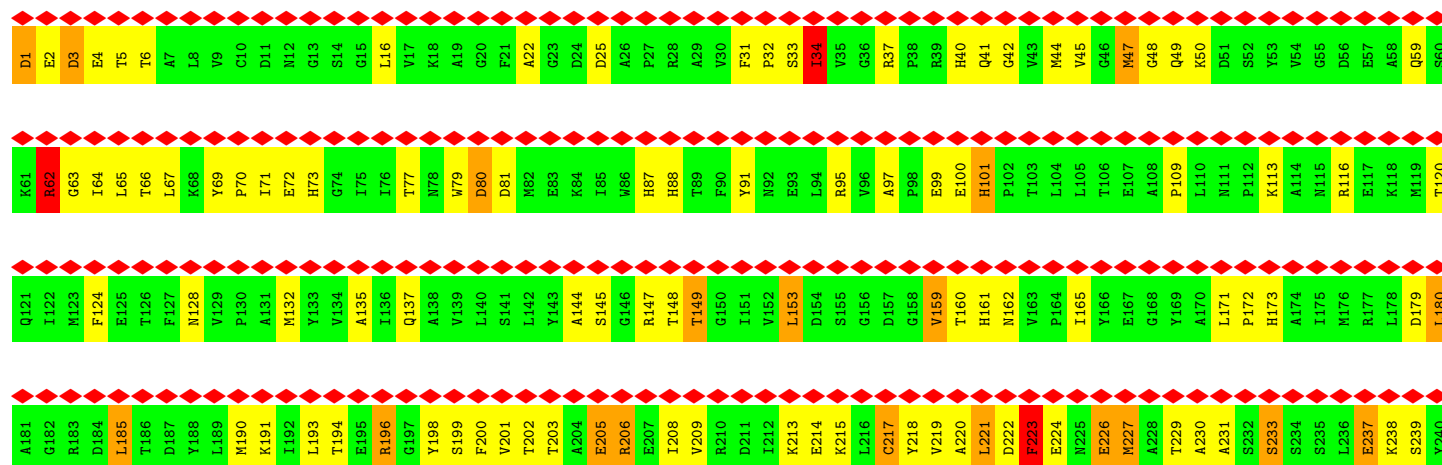




• Molecule 4: SKELETAL MUSCLE ACTIN

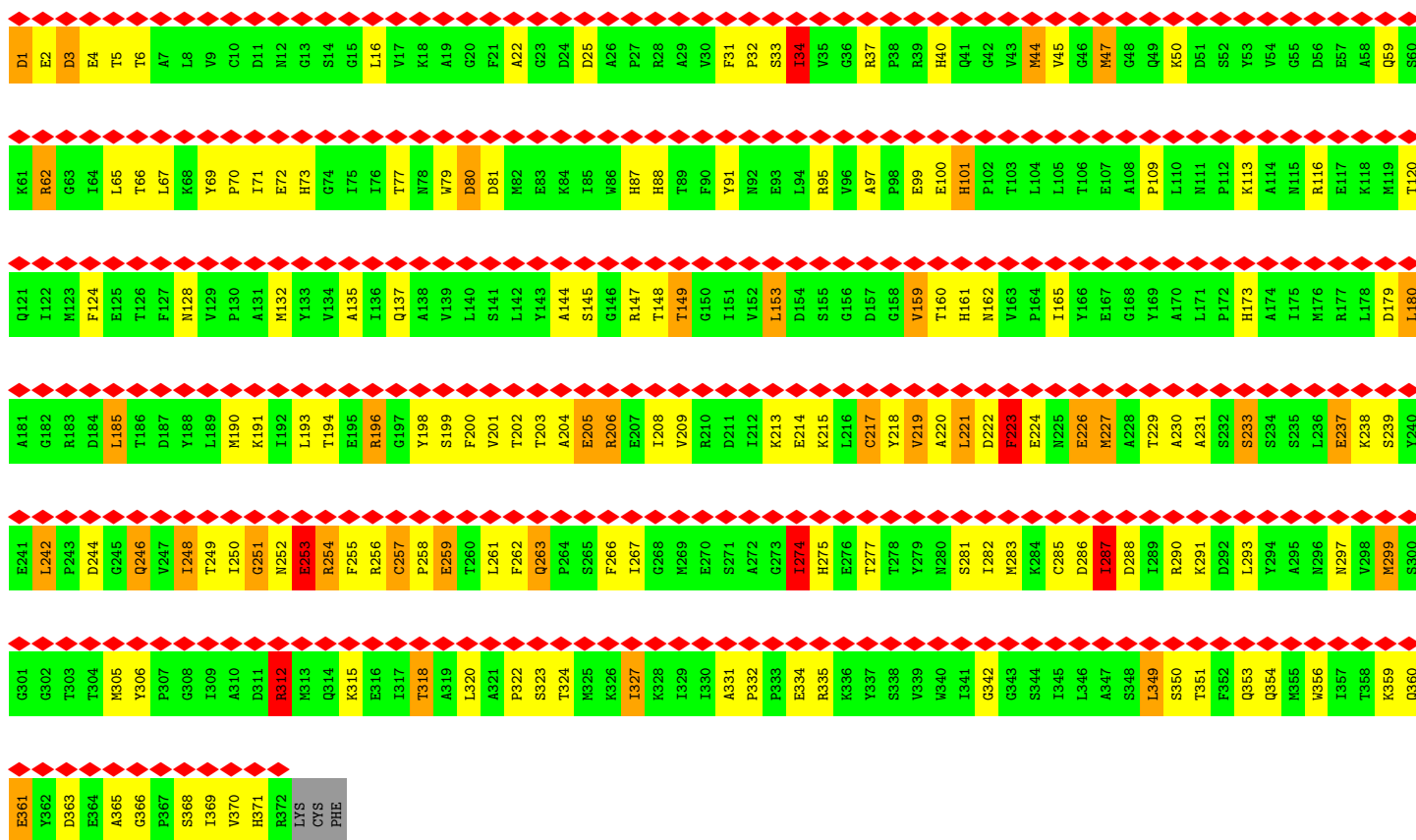


• Molecule 4: SKELETAL MUSCLE ACTIN

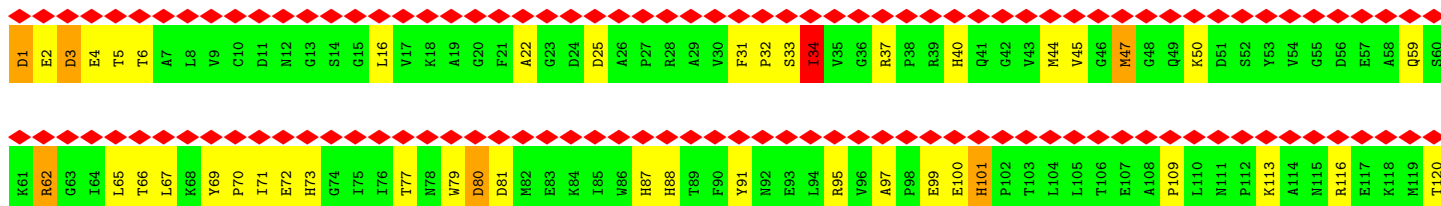


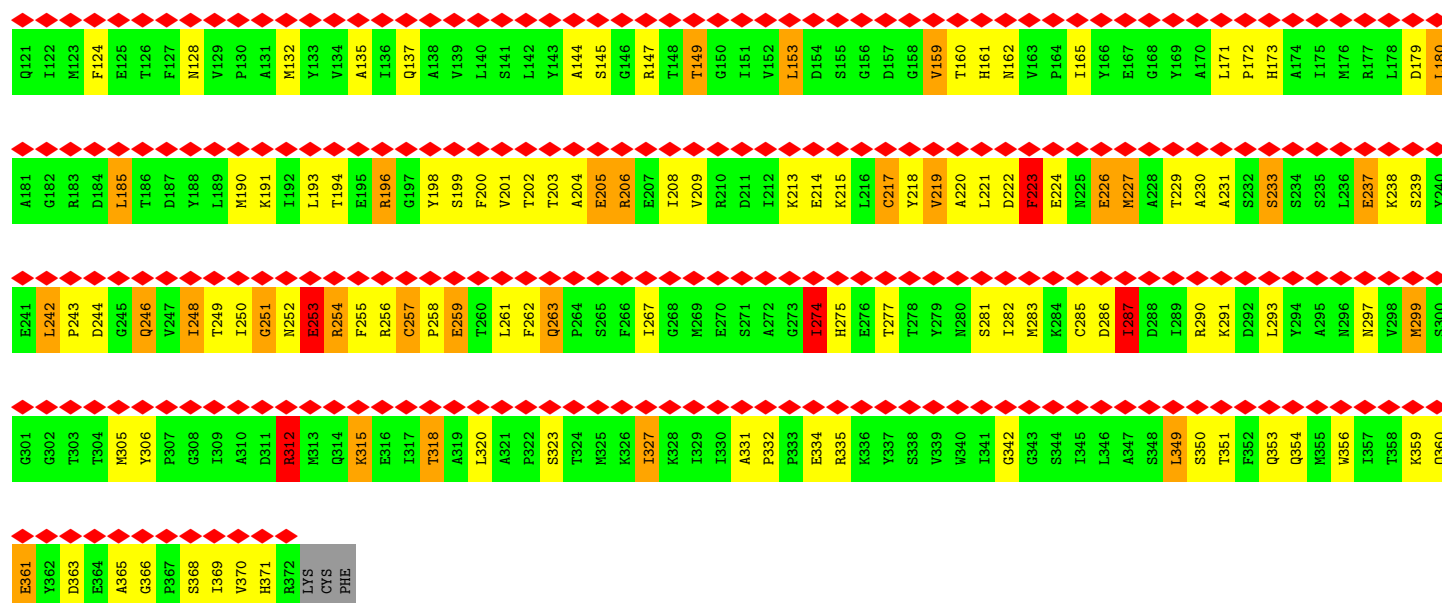


• Molecule 4: SKELETAL MUSCLE ACTIN

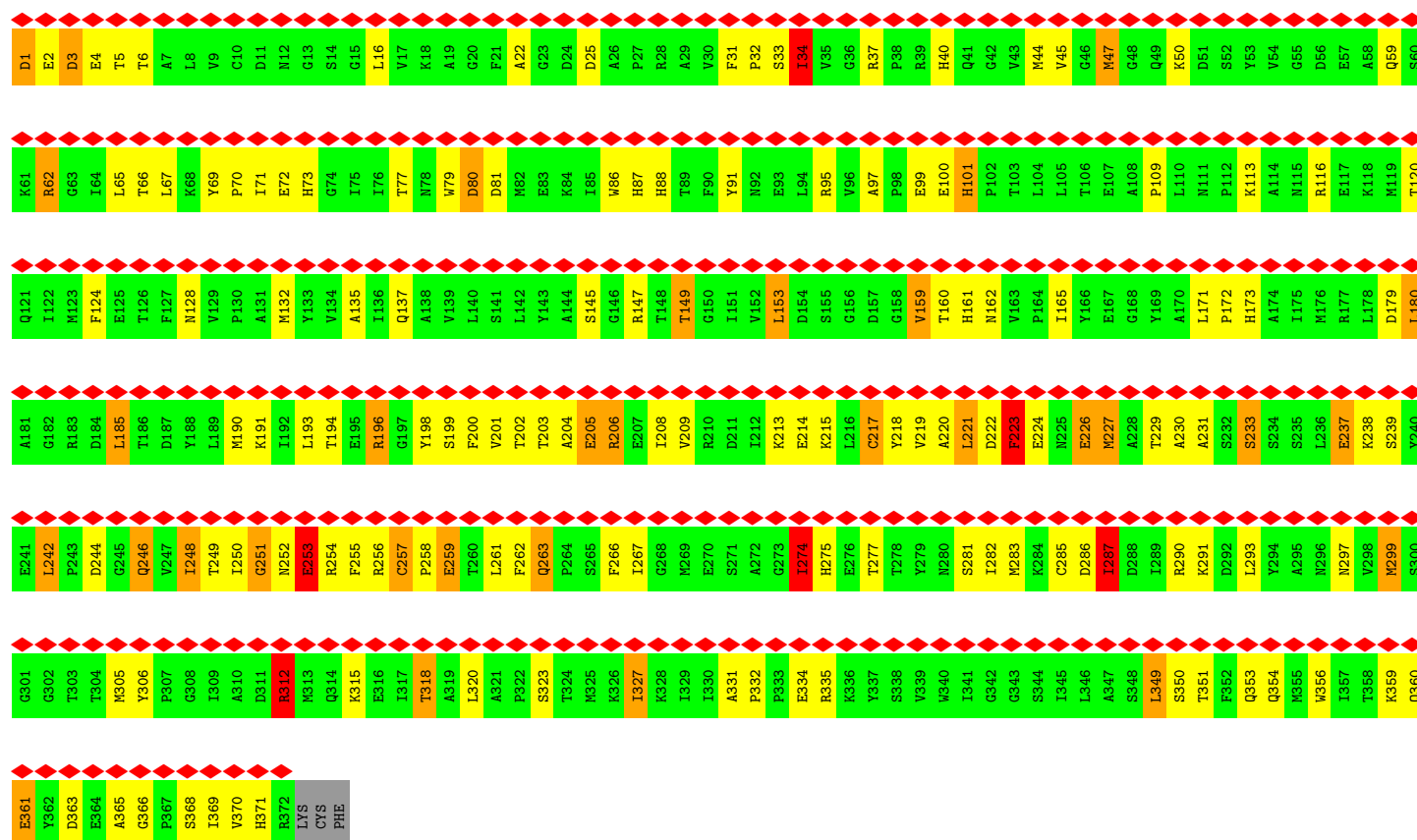


• Molecule 4: SKELETAL MUSCLE ACTIN



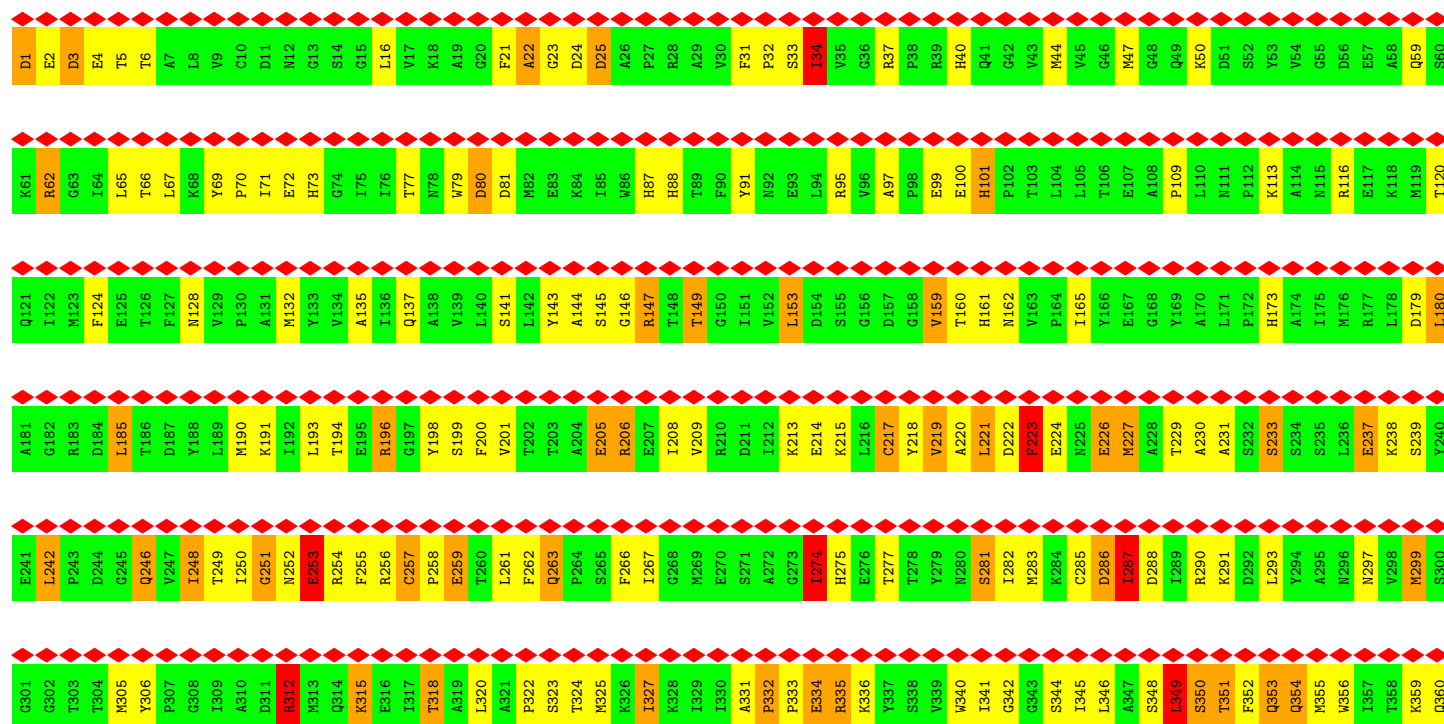


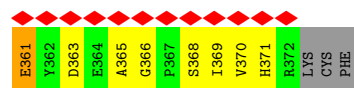
• Molecule 4: SKELETAL MUSCLE ACTIN



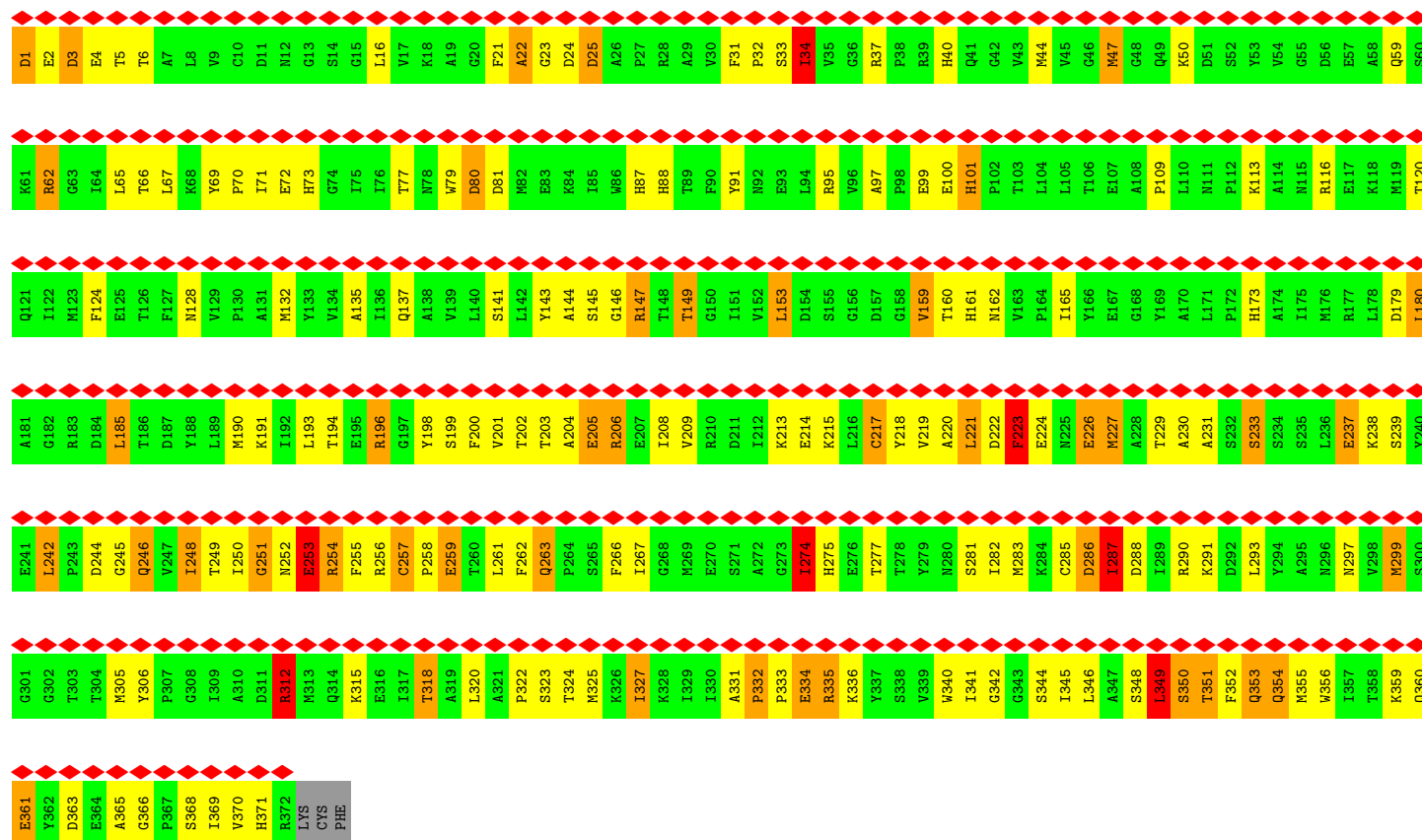
• Molecule 4: SKELETAL MUSCLE ACTIN



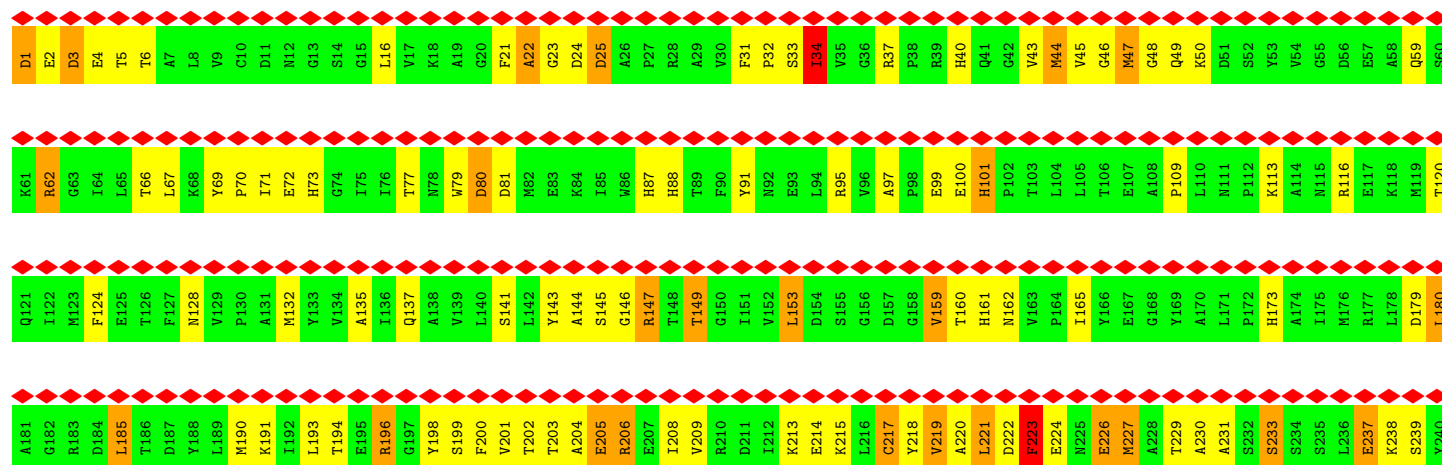


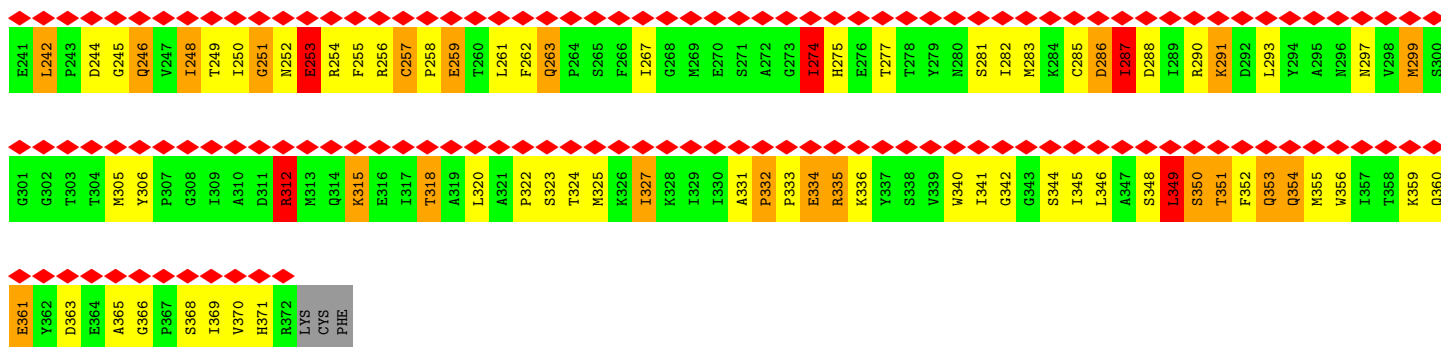


• Molecule 4: SKELETAL MUSCLE ACTIN

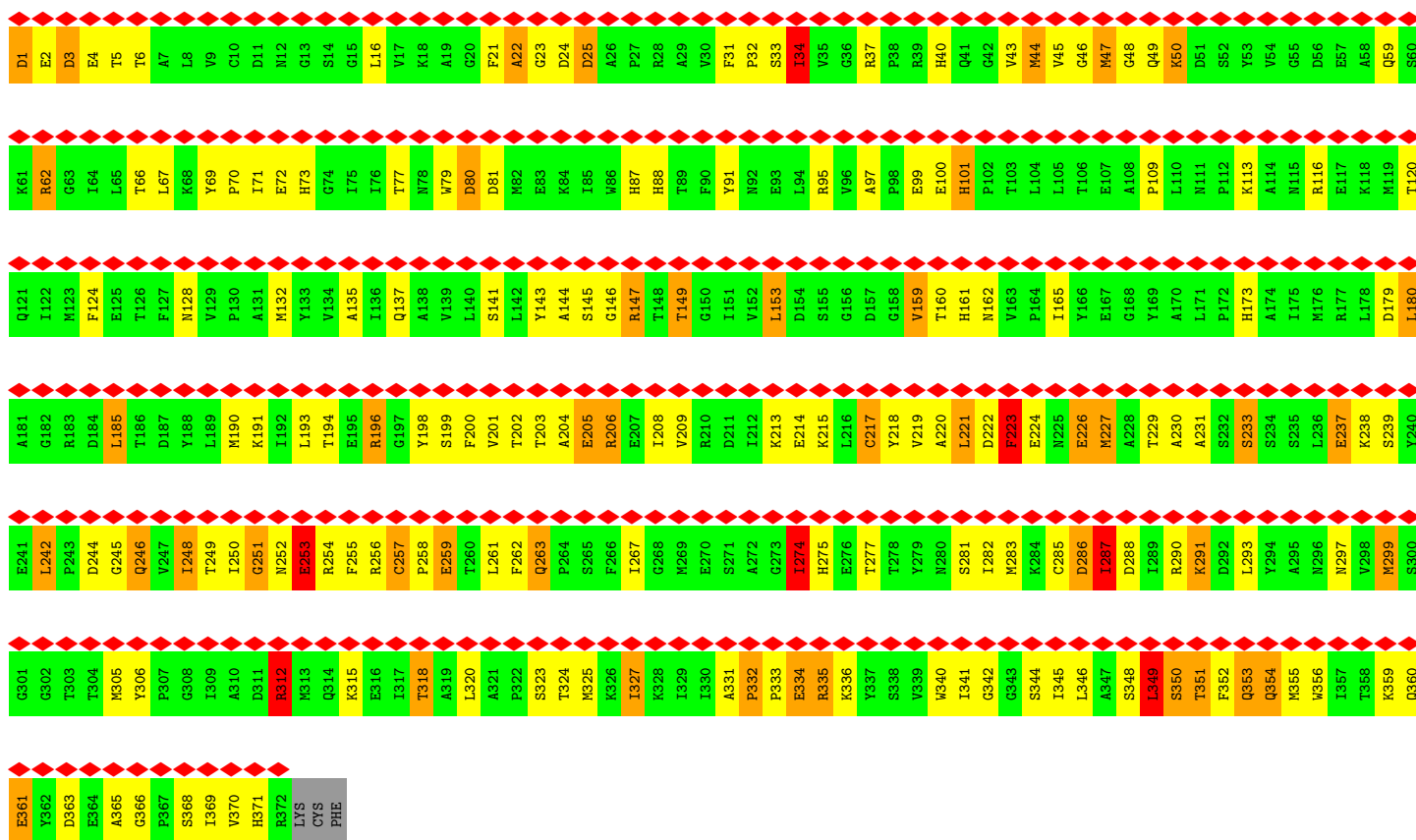


• Molecule 4: SKELETAL MUSCLE ACTIN



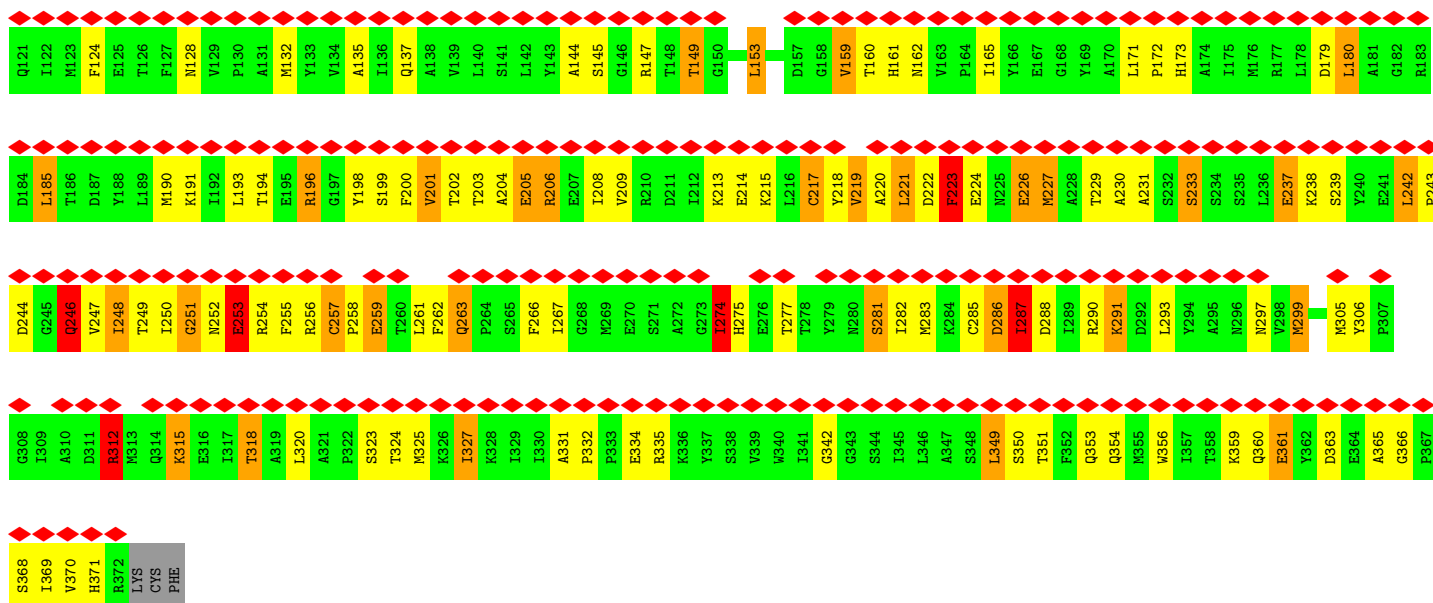


• Molecule 4: SKELETAL MUSCLE ACTIN

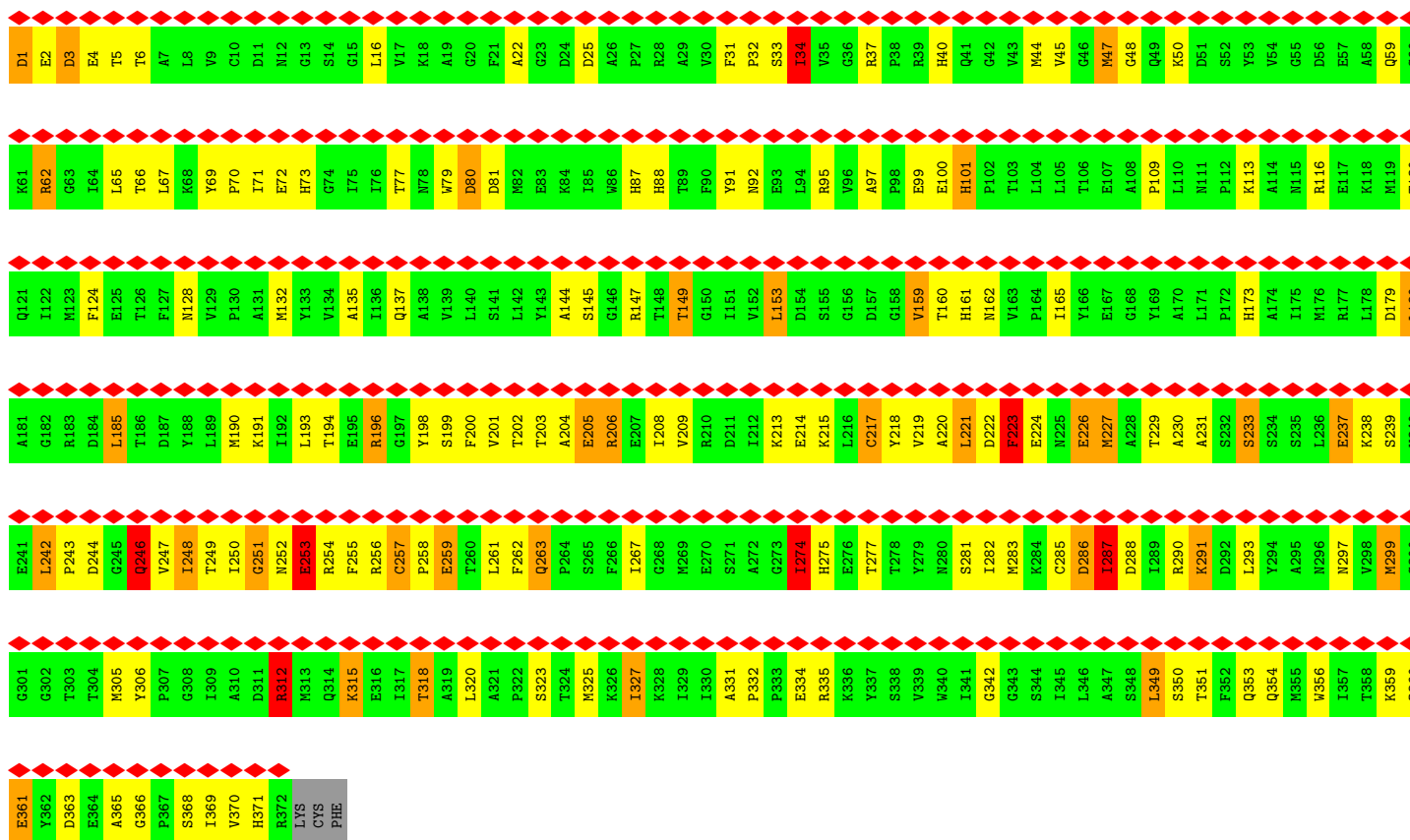


• Molecule 4: SKELETAL MUSCLE ACTIN





• Molecule 4: SKELETAL MUSCLE ACTIN



• Molecule 4: SKELETAL MUSCLE ACTIN



E361	G301	E241	A181	Q121	K61	D1
Y362	G302	L242	G182	I122	R62	E2
D363	T303	R183	P243	M123	G63	D3
E364	T304	D244	D184	F124	T64	E4
A365	M305	G245	L185	E125	L65	T5
G366	Y306	Q246	T186	T126	T66	T6
P367	P307	V247	D187	F127	L67	A7
S368	G308	I248	L188	M128	K68	L8
I369	I309	T249	L189	V129	V69	V9
V370	A310	I250	M190	P130	P70	C10
H371	D311	G251	A191	A131	I71	D11
R372	N252	G252	I192	M132	E72	M12
LYS	M313	E253	L193	Y133	H73	G13
CYS	Q314	R254	T194	V134	G74	S14
PHE	K315	F255	A195	A135	I75	G15
	E316	R256	L196	I136	I76	L16
	I317	C257	G197	Q137	T77	V17
	T318	P258	Y198	A138	N78	K18
	A319	E259	F199	V139	W79	A19
	L320	T260	G200	L140	D80	G20
	A321	L261	V201	S141	D81	F21
	P322	F262	T202	L142	N82	A22
	S323	Q263	T203	Y143	E83	G23
	T324	P264	A204	A144	K84	D24
	M325	S265	E205	S145	I85	D25
	K326	F266	R206	G146	N86	A26
	I327	I267	E207	R147	H87	P27
	K328	G268	T208	T148	H88	R28
	I329	M269	V209	T149	T89	A29
	I330	E270	R210	G150	F90	V30
	A331	S271	D211	I151	Y91	F31
	P332	A272	I212	V152	N92	P32
	P333	G273	K213	L153	E93	S33
	E334	L274	E214	D154	L94	I34
	R335	H275	K215	S155	R95	V35
	K336	E276	L216	G156	N96	G36
	Y337	T277	C217	D157	A97	R37
	S338	T278	Y218	G158	P98	P39
	V339	Y279	V219	V159	E99	R39
	W340	N280	A220	T160	E100	H40
	I341	S281	L221	H161	H101	Q41
	G342	I282	D222	M162	P102	G42
	G343	M283	F223	V163	T103	V43
	S344	K284	E224	P164	L104	M44
	I345	C285	M225	I165	L105	V45
	L346	D286	E226	Y166	T106	G46
	A347	I287	M227	E167	E107	M47
	S348	D288	A228	G168	A108	G49
	L349	I289	T229	V169	P109	Q49
	S350	R290	A230	A170	L110	K50
	T351	K291	A231	L171	N111	D51
	F352	D292	S232	P172	P112	S52
	Q353	L293	S233	H173	K113	V53
	Q354	Y294	S234	A174	A114	V54
	M355	A295	S235	I175	G55	D55
	W356	N296	L236	M176	R116	D56
	I357	N297	E237	R177	E117	E57
	T358	V298	K238	L178	K118	A58
	K359	M299	S239	D179	N119	Q59
	Q360	S300	V240	I180	T120	S60

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	1.85	41/6448 (0.6%)	2.12	154/8729 (1.8%)
1	D	1.85	40/6448 (0.6%)	2.12	149/8729 (1.7%)
1	G	1.85	41/6449 (0.6%)	2.13	160/8732 (1.8%)
1	J	1.86	43/6449 (0.7%)	2.19	148/8732 (1.7%)
1	P	1.92	42/6449 (0.7%)	2.22	159/8732 (1.8%)
2	B	1.36	16/1148 (1.4%)	1.47	21/1548 (1.4%)
2	E	1.37	15/1148 (1.3%)	1.47	21/1548 (1.4%)
2	H	1.37	16/1148 (1.4%)	1.47	21/1548 (1.4%)
2	K	1.37	16/1148 (1.4%)	1.47	21/1548 (1.4%)
2	Q	1.37	15/1148 (1.3%)	1.47	21/1548 (1.4%)
3	C	0.88	4/1136 (0.4%)	1.18	6/1525 (0.4%)
3	F	0.88	4/1136 (0.4%)	1.18	6/1525 (0.4%)
3	I	0.88	4/1136 (0.4%)	1.18	5/1525 (0.3%)
3	L	0.88	4/1136 (0.4%)	1.18	5/1525 (0.3%)
3	R	0.88	4/1136 (0.4%)	1.18	5/1525 (0.3%)
4	0	1.17	13/2968 (0.4%)	2.00	101/4023 (2.5%)
4	1	1.17	12/2968 (0.4%)	2.00	98/4023 (2.4%)
4	2	1.17	13/2968 (0.4%)	2.00	98/4023 (2.4%)
4	3	1.17	13/2968 (0.4%)	2.00	97/4023 (2.4%)
4	4	1.17	13/2968 (0.4%)	2.00	97/4023 (2.4%)
4	5	1.17	13/2968 (0.4%)	2.00	99/4023 (2.5%)
4	7	1.17	13/2968 (0.4%)	2.00	98/4023 (2.4%)
4	8	1.17	13/2968 (0.4%)	2.00	100/4023 (2.5%)
4	9	1.17	13/2968 (0.4%)	2.00	99/4023 (2.5%)
4	V	1.17	12/2968 (0.4%)	2.00	98/4023 (2.4%)
4	W	1.17	13/2968 (0.4%)	2.00	97/4023 (2.4%)
4	X	1.17	13/2968 (0.4%)	2.00	100/4023 (2.5%)
4	Y	1.17	13/2968 (0.4%)	2.00	98/4023 (2.4%)
4	Z	1.17	13/2968 (0.4%)	2.00	97/4023 (2.4%)
All	All	1.47	485/85215 (0.6%)	1.99	2279/115341 (2.0%)

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	A	1	4
1	D	1	4
1	G	2	4
1	J	1	6
1	P	1	9
2	B	0	3
2	E	0	3
2	H	0	3
2	K	0	3
2	Q	0	3
3	C	0	2
3	F	0	2
3	I	0	2
3	L	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	66

The worst 5 of 485 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	648	THR	CB-OG1	42.63	2.12	1.43
1	P	648	THR	CB-OG1	42.62	2.12	1.43
1	J	648	THR	CB-OG1	42.61	2.12	1.43
1	G	648	THR	CB-OG1	42.60	2.12	1.43
1	A	648	THR	CB-OG1	42.59	2.11	1.43

The worst 5 of 2279 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	637	LYS	O-C-N	-74.34	23.71	122.59
1	J	637	LYS	O-C-N	-74.28	23.80	122.59
1	D	637	LYS	O-C-N	-74.27	23.81	122.59
1	P	637	LYS	O-C-N	-74.26	23.82	122.59
1	A	637	LYS	O-C-N	-74.24	23.85	122.59

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	75	ASP	CA
1	G	648	THR	CB
1	J	648	THR	CB

5 of 66 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	6762	1539	0
1	D	6797	0	6763	1442	0
1	G	6797	0	6771	1596	0
1	J	6797	0	6762	1454	0
1	P	6797	0	6773	1556	0
2	B	1127	0	1085	241	0
2	E	1127	0	1086	270	0
2	H	1127	0	1088	297	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	1127	0	1088	272	0
2	Q	1127	0	1088	265	0
3	C	1123	0	1083	196	0
3	F	1123	0	1083	170	0
3	I	1123	0	1083	189	0
3	L	1123	0	1083	164	0
3	R	1123	0	1079	230	0
4	0	2906	0	2855	411	0
4	1	2906	0	2864	217	0
4	2	2906	0	2864	178	0
4	3	2906	0	2863	181	0
4	4	2906	0	2865	100	0
4	5	2906	0	2865	101	0
4	7	2906	0	2866	81	0
4	8	2906	0	2857	323	0
4	9	2906	0	2855	349	0
4	V	2906	0	2851	392	0
4	W	2906	0	2851	390	0
4	X	2906	0	2862	217	0
4	Y	2906	0	2863	173	0
4	Z	2906	0	2862	191	0
All	All	85919	0	84720	9873	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 58.

The worst 5 of 9873 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:J:797:PHE:CE1	3:L:146:ILE:HG23	1.21	1.71
1:G:84:MLY:CH1	1:G:724:TYR:HE2	1.03	1.66
1:P:803:TYR:CD1	1:P:807:VAL:HG11	1.22	1.65
1:G:84:MLY:CG	1:G:723:ARG:HD2	1.17	1.64
1:D:798:LEU:HD11	3:F:126:LEU:CD1	1.26	1.63

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	650 (82%)	113 (14%)	26 (3%)	3	21
1	D	789/840 (94%)	651 (82%)	112 (14%)	26 (3%)	3	21
1	G	791/840 (94%)	651 (82%)	113 (14%)	27 (3%)	3	21
1	J	791/840 (94%)	651 (82%)	113 (14%)	27 (3%)	3	21
1	P	791/840 (94%)	650 (82%)	112 (14%)	29 (4%)	2	20
2	B	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	1	14
2	E	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	1	14
2	H	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	1	14
2	K	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	1	14
2	Q	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	1	14
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	R	143/147 (97%)	133 (93%)	10 (7%)	0	100	100
4	0	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	7	38
4	1	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	7	38
4	2	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	7	38
4	3	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	7	38
4	4	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	7	38
4	5	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	7	38
4	7	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	7	38
4	8	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	7	38
4	9	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	7	38
4	V	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	7	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	W	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	7	38
4	X	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	7	38
4	Y	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	7	38
4	Z	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	7	38
All	All	10561/10910 (97%)	9231 (87%)	1071 (10%)	259 (2%)	6	26

5 of 259 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%)	491 (73%)	181 (27%)	0	3
1	D	672/672 (100%)	490 (73%)	182 (27%)	0	3
1	G	672/672 (100%)	492 (73%)	180 (27%)	0	3
1	J	672/672 (100%)	491 (73%)	181 (27%)	0	3
1	P	672/672 (100%)	490 (73%)	182 (27%)	0	3
2	B	120/120 (100%)	119 (99%)	1 (1%)	73	80
2	E	120/120 (100%)	119 (99%)	1 (1%)	73	80
2	H	120/120 (100%)	119 (99%)	1 (1%)	73	80
2	K	120/120 (100%)	119 (99%)	1 (1%)	73	80
2	Q	120/120 (100%)	120 (100%)	0	100	100
3	C	117/117 (100%)	113 (97%)	4 (3%)	32	54
3	F	117/117 (100%)	113 (97%)	4 (3%)	32	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	I	117/117 (100%)	113 (97%)	4 (3%)	32	54
3	L	117/117 (100%)	113 (97%)	4 (3%)	32	54
3	R	117/117 (100%)	113 (97%)	4 (3%)	32	54
4	0	315/318 (99%)	264 (84%)	51 (16%)	2	11
4	1	315/318 (99%)	265 (84%)	50 (16%)	2	11
4	2	315/318 (99%)	264 (84%)	51 (16%)	2	11
4	3	315/318 (99%)	264 (84%)	51 (16%)	2	11
4	4	315/318 (99%)	264 (84%)	51 (16%)	2	11
4	5	315/318 (99%)	264 (84%)	51 (16%)	2	11
4	7	315/318 (99%)	264 (84%)	51 (16%)	2	11
4	8	315/318 (99%)	264 (84%)	51 (16%)	2	11
4	9	315/318 (99%)	264 (84%)	51 (16%)	2	11
4	V	315/318 (99%)	265 (84%)	50 (16%)	2	11
4	W	315/318 (99%)	265 (84%)	50 (16%)	2	11
4	X	315/318 (99%)	264 (84%)	51 (16%)	2	11
4	Y	315/318 (99%)	264 (84%)	51 (16%)	2	11
4	Z	315/318 (99%)	264 (84%)	51 (16%)	2	11
All	All	8955/8997 (100%)	7314 (82%)	1641 (18%)	3	8

5 of 1641 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	R	48	LYS
4	4	153	LEU
4	Z	99	GLU
4	0	238	LYS
1	P	843	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 254 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	564	ASN
4	V	137	GLN
1	P	481	ASN
4	V	41	GLN

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Mol	Chain	Res	Type
4	X	263	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

225 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	A	553	4,1	9,10,11	0.65	0	6,11,13	0.54	0
1	MLY	A	598	1	9,10,11	0.84	1 (11%)	6,11,13	0.42	0
1	MLY	A	55	1	9,10,11	0.71	0	6,11,13	0.80	0
1	MLY	P	49	1	9,10,11	1.00	1 (11%)	6,11,13	0.75	0
1	MLY	J	415	1	9,10,11	0.76	0	6,11,13	0.19	0
1	MLY	A	600	1	9,10,11	0.53	0	6,11,13	0.39	0
1	MLY	P	138	1	9,10,11	1.21	1 (11%)	6,11,13	0.82	0
1	MLY	D	505	1	9,10,11	0.77	0	6,11,13	0.34	0
1	MLY	P	385	1	9,10,11	0.94	1 (11%)	6,11,13	0.45	0
1	MLY	D	63	1	9,10,11	0.86	0	6,11,13	0.45	0
1	MLY	D	837	1	9,10,11	0.59	0	6,11,13	0.58	0
1	MLY	P	613	1	9,10,11	0.56	0	6,11,13	0.61	0
1	MLY	G	415	1	9,10,11	0.74	0	6,11,13	0.19	0
1	MLY	D	431	1	9,10,11	0.51	0	6,11,13	0.46	0
1	MLY	G	613	1	9,10,11	0.59	0	6,11,13	0.62	0
1	MLY	J	138	1	9,10,11	1.20	1 (11%)	6,11,13	0.82	0
1	MLY	D	681	1	9,10,11	0.53	0	6,11,13	0.46	0
1	MLY	G	296	1	9,10,11	0.62	0	6,11,13	0.36	0
1	MLY	J	84	1	9,10,11	0.51	0	6,11,13	0.80	0
1	MLY	G	553	4,1	9,10,11	0.65	0	6,11,13	0.54	0
1	MLY	G	598	1	9,10,11	0.83	0	6,11,13	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	G	55	1	9,10,11	0.74	0	6,11,13	0.81	0
1	MLY	G	84	1	9,10,11	0.49	0	6,11,13	0.81	0
1	MLY	P	504	1	9,10,11	0.82	0	6,11,13	0.21	0
1	MLY	J	504	1	9,10,11	0.84	0	6,11,13	0.22	0
1	MLY	A	768	1	9,10,11	0.77	0	6,11,13	0.41	0
1	MLY	G	248	1	9,10,11	0.80	0	6,11,13	0.66	0
1	MLY	P	59	1	9,10,11	0.87	0	6,11,13	0.47	0
1	MLY	A	353	1	9,10,11	0.87	0	6,11,13	0.80	0
1	MLY	D	613	1	9,10,11	0.58	0	6,11,13	0.62	0
1	MLY	D	138	1	9,10,11	1.26	1 (11%)	6,11,13	0.83	0
1	MLY	A	30	1	9,10,11	0.91	0	6,11,13	0.32	0
1	MLY	D	782	1	9,10,11	0.81	0	6,11,13	0.35	0
1	MLY	P	837	1	9,10,11	0.58	0	6,11,13	0.57	0
1	MLY	G	431	1	9,10,11	0.52	0	6,11,13	0.46	0
1	MLY	D	827	1	9,10,11	0.65	0	6,11,13	0.48	0
1	MLY	A	248	1	9,10,11	0.81	0	6,11,13	0.64	0
1	MLY	A	528	1	9,10,11	0.89	0	6,11,13	0.67	0
1	MLY	A	659	1	9,10,11	0.84	1 (11%)	6,11,13	0.60	0
1	MLY	A	295	1	9,10,11	0.78	0	6,11,13	0.35	0
1	MLY	A	369	1	9,10,11	0.73	0	6,11,13	0.46	0
1	MLY	G	600	1	9,10,11	0.53	0	6,11,13	0.38	0
1	MLY	G	486	1	9,10,11	0.67	0	6,11,13	0.40	0
1	MLY	D	295	1	9,10,11	0.76	0	6,11,13	0.37	0
1	MLY	G	827	1	9,10,11	0.67	0	6,11,13	0.49	0
1	MLY	P	55	1	9,10,11	0.73	0	6,11,13	0.79	0
1	MLY	A	190	1	9,10,11	1.23	2 (22%)	6,11,13	0.52	0
1	MLY	G	30	1	9,10,11	0.90	0	6,11,13	0.30	0
1	MLY	J	55	1	9,10,11	0.73	0	6,11,13	0.80	0
1	MLY	D	486	1	9,10,11	0.67	0	6,11,13	0.40	0
1	MLY	P	296	1	9,10,11	0.63	0	6,11,13	0.35	0
1	MLY	D	768	1	9,10,11	0.74	0	6,11,13	0.41	0
1	MLY	A	486	1	9,10,11	0.68	0	6,11,13	0.39	0
1	MLY	D	190	1	9,10,11	1.18	2 (22%)	6,11,13	0.54	0
1	MLY	G	659	1	9,10,11	0.84	1 (11%)	6,11,13	0.58	0
1	MLY	G	369	1	9,10,11	0.70	0	6,11,13	0.46	0
1	MLY	J	764	1	9,10,11	0.81	0	6,11,13	0.37	0
1	MLY	D	348	1	9,10,11	0.77	0	6,11,13	0.47	0
1	MLY	J	190	1	9,10,11	1.21	2 (22%)	6,11,13	0.53	0
1	MLY	G	190	1	9,10,11	1.20	2 (22%)	6,11,13	0.53	0
1	MLY	J	553	1	9,10,11	0.65	0	6,11,13	0.53	0
1	MLY	J	295	1	9,10,11	0.76	0	6,11,13	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	D	87	1	9,10,11	1.08	1 (11%)	6,11,13	0.44	0
1	MLY	G	138	1	9,10,11	1.22	1 (11%)	6,11,13	0.83	0
1	MLY	J	486	1	9,10,11	0.65	0	6,11,13	0.40	0
1	MLY	D	528	1	9,10,11	0.92	0	6,11,13	0.64	0
1	MLY	D	30	1	9,10,11	0.92	0	6,11,13	0.31	0
1	MLY	D	617	1	9,10,11	0.90	0	6,11,13	0.35	0
1	MLY	J	107	1	9,10,11	0.49	0	6,11,13	0.33	0
1	MLY	A	764	1	9,10,11	0.82	0	6,11,13	0.35	0
1	MLY	J	768	1	9,10,11	0.77	0	6,11,13	0.42	0
1	MLY	P	35	1	9,10,11	0.73	0	6,11,13	0.38	0
1	MLY	G	107	1	9,10,11	0.48	0	6,11,13	0.33	0
1	MLY	G	59	1	9,10,11	0.84	0	6,11,13	0.48	0
1	MLY	A	236	1	9,10,11	0.84	1 (11%)	6,11,13	0.49	0
1	MLY	P	768	1	9,10,11	0.77	0	6,11,13	0.43	0
1	MLY	G	768	1	9,10,11	0.73	0	6,11,13	0.41	0
1	MLY	P	436	1	9,10,11	0.97	1 (11%)	6,11,13	0.48	0
1	MLY	J	551	1	9,10,11	0.53	0	6,11,13	0.19	0
1	MLY	A	415	1	9,10,11	0.72	0	6,11,13	0.19	0
1	MLY	P	30	1	9,10,11	0.90	0	6,11,13	0.30	0
1	MLY	P	63	1	9,10,11	0.86	0	6,11,13	0.43	0
1	MLY	A	504	1	9,10,11	0.88	0	6,11,13	0.23	0
1	MLY	D	296	1	9,10,11	0.64	0	6,11,13	0.36	0
1	MLY	D	551	1	9,10,11	0.52	0	6,11,13	0.19	0
1	MLY	J	87	1	9,10,11	1.12	1 (11%)	6,11,13	0.43	0
1	MLY	P	87	1	9,10,11	1.15	1 (11%)	6,11,13	0.43	0
1	MLY	P	505	1	9,10,11	0.85	0	6,11,13	0.34	0
1	MLY	G	236	1	9,10,11	0.82	1 (11%)	6,11,13	0.48	0
1	MLY	P	84	1	9,10,11	0.50	0	6,11,13	0.81	0
1	MLY	A	837	1	9,10,11	0.59	0	6,11,13	0.54	0
1	MLY	J	431	1	9,10,11	0.52	0	6,11,13	0.45	0
1	MLY	P	431	1	9,10,11	0.51	0	6,11,13	0.44	0
1	MLY	D	59	1	9,10,11	0.85	0	6,11,13	0.48	0
1	MLY	P	367	1	9,10,11	0.58	0	6,11,13	0.36	0
1	MLY	J	833	1	9,10,11	1.15	2 (22%)	6,11,13	0.31	0
1	MLY	J	49	1	9,10,11	1.00	1 (11%)	6,11,13	0.75	0
1	MLY	G	504	1	9,10,11	0.88	0	6,11,13	0.23	0
1	MLY	D	367	1	9,10,11	0.58	0	6,11,13	0.38	0
1	MLY	P	764	1	9,10,11	0.81	0	6,11,13	0.38	0
1	MLY	A	49	1	9,10,11	0.96	1 (11%)	6,11,13	0.74	0
1	MLY	G	833	1	9,10,11	1.15	1 (11%)	6,11,13	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	J	613	1	9,10,11	0.56	0	6,11,13	0.62	0
1	MLY	A	617	1	9,10,11	0.88	0	6,11,13	0.35	0
1	MLY	A	35	1	9,10,11	0.73	0	6,11,13	0.38	0
1	MLY	A	84	1	9,10,11	0.50	0	6,11,13	0.80	0
1	MLY	G	837	1	9,10,11	0.58	0	6,11,13	0.53	0
1	MLY	P	248	1	9,10,11	0.80	0	6,11,13	0.65	0
1	MLY	D	49	1	9,10,11	0.99	1 (11%)	6,11,13	0.75	0
1	MLY	J	681	1	9,10,11	0.57	0	6,11,13	0.47	0
1	MLY	J	248	1	9,10,11	0.81	0	6,11,13	0.66	0
1	MLY	J	528	1	9,10,11	0.89	0	6,11,13	0.66	0
1	MLY	P	681	1	9,10,11	0.58	0	6,11,13	0.46	0
1	MLY	D	84	1	9,10,11	0.51	0	6,11,13	0.81	0
1	MLY	G	681	1	9,10,11	0.58	0	6,11,13	0.46	0
1	MLY	A	272	1	9,10,11	0.90	1 (11%)	6,11,13	0.56	0
1	MLY	D	272	1	9,10,11	0.89	1 (11%)	6,11,13	0.58	0
1	MLY	G	49	1	9,10,11	1.00	1 (11%)	6,11,13	0.74	0
1	MLY	J	30	1	9,10,11	0.91	0	6,11,13	0.31	0
1	MLY	G	35	1	9,10,11	0.73	0	6,11,13	0.39	0
1	MLY	A	59	1	9,10,11	0.85	0	6,11,13	0.47	0
1	MLY	A	348	1	9,10,11	0.80	0	6,11,13	0.48	0
1	MLY	J	385	1	9,10,11	0.96	1 (11%)	6,11,13	0.45	0
1	MLY	P	353	1	9,10,11	0.86	0	6,11,13	0.80	0
1	MLY	P	236	1	9,10,11	0.84	1 (11%)	6,11,13	0.47	0
1	MLY	G	353	1	9,10,11	0.87	0	6,11,13	0.82	0
1	MLY	G	367	1	9,10,11	0.60	0	6,11,13	0.39	0
1	MLY	G	436	1	9,10,11	0.96	1 (11%)	6,11,13	0.46	0
1	MLY	J	617	1	9,10,11	0.89	0	6,11,13	0.34	0
1	MLY	J	130	1	9,10,11	0.77	0	6,11,13	0.73	0
1	MLY	A	613	1	9,10,11	0.57	0	6,11,13	0.62	0
1	MLY	J	505	1	9,10,11	0.85	1 (11%)	6,11,13	0.33	0
1	MLY	A	107	1	9,10,11	0.47	0	6,11,13	0.34	0
1	MLY	J	19	1	9,10,11	1.08	1 (11%)	6,11,13	0.58	0
1	MLY	J	369	1	9,10,11	0.70	0	6,11,13	0.45	0
1	MLY	G	130	1	9,10,11	0.78	0	6,11,13	0.74	0
1	MLY	J	348	1	9,10,11	0.77	0	6,11,13	0.47	0
1	MLY	J	659	1	9,10,11	0.84	1 (11%)	6,11,13	0.57	0
1	MLY	A	296	1	9,10,11	0.61	0	6,11,13	0.36	0
1	MLY	D	107	1	9,10,11	0.52	0	6,11,13	0.33	0
1	MLY	P	415	1	9,10,11	0.74	0	6,11,13	0.19	0
1	MLY	J	272	1	9,10,11	0.92	1 (11%)	6,11,13	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	D	35	1	9,10,11	0.74	0	6,11,13	0.38	0
1	MLY	D	553	4,1	9,10,11	0.66	0	6,11,13	0.55	0
1	MLY	D	55	1	9,10,11	0.72	0	6,11,13	0.81	0
1	MLY	D	598	1	9,10,11	0.84	1 (11%)	6,11,13	0.42	0
1	MLY	D	130	1	9,10,11	0.80	0	6,11,13	0.72	0
1	MLY	D	600	1	9,10,11	0.52	0	6,11,13	0.38	0
1	MLY	J	827	1	9,10,11	0.72	0	6,11,13	0.47	0
1	MLY	J	436	1	9,10,11	0.94	1 (11%)	6,11,13	0.48	0
1	MLY	P	551	1	9,10,11	0.52	0	6,11,13	0.18	0
1	MLY	G	551	1	9,10,11	0.52	0	6,11,13	0.19	0
1	MLY	D	764	1	9,10,11	0.84	0	6,11,13	0.34	0
1	MLY	A	431	1	9,10,11	0.51	0	6,11,13	0.45	0
1	MLY	A	551	1	9,10,11	0.52	0	6,11,13	0.19	0
1	MLY	J	296	1	9,10,11	0.65	0	6,11,13	0.35	0
1	MLY	J	598	1	9,10,11	0.82	0	6,11,13	0.41	0
1	MLY	J	782	1	9,10,11	0.81	0	6,11,13	0.36	0
1	MLY	A	839	1	9,10,11	0.64	0	6,11,13	0.82	0
1	MLY	A	436	1	9,10,11	0.95	1 (11%)	6,11,13	0.49	0
1	MLY	D	369	1	9,10,11	0.71	0	6,11,13	0.45	0
1	MLY	D	415	1	9,10,11	0.74	0	6,11,13	0.19	0
1	MLY	G	87	1	9,10,11	1.12	1 (11%)	6,11,13	0.42	0
1	MLY	J	236	1	9,10,11	0.84	1 (11%)	6,11,13	0.48	0
1	MLY	J	837	1	9,10,11	0.57	0	6,11,13	0.55	0
1	MLY	A	833	1	9,10,11	1.12	1 (11%)	6,11,13	0.32	0
1	MLY	G	505	1	9,10,11	0.81	0	6,11,13	0.36	0
1	MLY	P	598	1	9,10,11	0.83	0	6,11,13	0.41	0
1	MLY	P	190	1	9,10,11	1.21	2 (22%)	6,11,13	0.53	0
1	MLY	A	87	1	9,10,11	1.12	1 (11%)	6,11,13	0.42	0
1	MLY	J	839	1	9,10,11	0.65	0	6,11,13	0.78	0
1	MLY	A	130	1	9,10,11	0.80	0	6,11,13	0.73	0
1	MLY	D	236	1	9,10,11	0.84	1 (11%)	6,11,13	0.48	0
1	MLY	A	505	1	9,10,11	0.83	0	6,11,13	0.34	0
1	MLY	P	295	1	9,10,11	0.77	0	6,11,13	0.38	0
1	MLY	P	369	1	9,10,11	0.71	0	6,11,13	0.46	0
1	MLY	P	528	1	9,10,11	0.89	0	6,11,13	0.65	0
1	MLY	G	839	1	9,10,11	0.64	0	6,11,13	0.80	0
1	MLY	P	486	1	9,10,11	0.67	0	6,11,13	0.40	0
1	MLY	D	504	1	9,10,11	0.87	0	6,11,13	0.21	0
1	MLY	P	839	1	9,10,11	0.67	0	6,11,13	0.77	0
1	MLY	P	107	1	9,10,11	0.49	0	6,11,13	0.33	0
1	MLY	J	367	1	9,10,11	0.60	0	6,11,13	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	A	681	1	9,10,11	0.56	0	6,11,13	0.45	0
1	MLY	P	348	1	9,10,11	0.77	0	6,11,13	0.47	0
1	MLY	P	782	1	9,10,11	0.80	0	6,11,13	0.39	0
1	MLY	A	367	1	9,10,11	0.59	0	6,11,13	0.36	0
1	MLY	P	600	1	9,10,11	0.54	0	6,11,13	0.38	0
1	MLY	J	600	1	9,10,11	0.53	0	6,11,13	0.38	0
1	MLY	G	764	1	9,10,11	0.81	0	6,11,13	0.36	0
1	MLY	P	827	1	9,10,11	0.68	0	6,11,13	0.47	0
1	MLY	A	19	1	9,10,11	1.02	1 (11%)	6,11,13	0.59	0
1	MLY	D	353	1	9,10,11	0.86	0	6,11,13	0.81	0
1	MLY	D	833	1	9,10,11	1.14	1 (11%)	6,11,13	0.31	0
1	MLY	G	385	1	9,10,11	0.92	1 (11%)	6,11,13	0.45	0
1	MLY	A	782	1	9,10,11	0.83	1 (11%)	6,11,13	0.36	0
1	MLY	P	19	1	9,10,11	1.06	1 (11%)	6,11,13	0.58	0
1	MLY	A	385	1	9,10,11	0.92	1 (11%)	6,11,13	0.44	0
1	MLY	A	827	1	9,10,11	0.70	0	6,11,13	0.44	0
1	MLY	D	19	1	9,10,11	1.07	1 (11%)	6,11,13	0.56	0
1	MLY	P	659	1	9,10,11	0.81	0	6,11,13	0.58	0
1	MLY	G	295	1	9,10,11	0.77	0	6,11,13	0.35	0
1	MLY	P	617	1	9,10,11	0.91	0	6,11,13	0.34	0
1	MLY	D	659	1	9,10,11	0.83	1 (11%)	6,11,13	0.59	0
1	MLY	A	63	1	9,10,11	0.89	0	6,11,13	0.44	0
1	MLY	P	130	1	9,10,11	0.76	0	6,11,13	0.74	0
1	MLY	G	617	1	9,10,11	0.90	0	6,11,13	0.35	0
1	MLY	P	833	1	9,10,11	1.15	2 (22%)	6,11,13	0.30	0
1	MLY	D	248	1	9,10,11	0.80	0	6,11,13	0.65	0
1	MLY	G	19	1	9,10,11	1.05	1 (11%)	6,11,13	0.58	0
1	MLY	J	35	1	9,10,11	0.73	0	6,11,13	0.39	0
1	MLY	G	348	1	9,10,11	0.80	0	6,11,13	0.47	0
1	MLY	A	138	1	9,10,11	1.21	1 (11%)	6,11,13	0.82	0
1	MLY	P	553	1	9,10,11	0.65	0	6,11,13	0.54	0
1	MLY	P	272	1	9,10,11	0.91	1 (11%)	6,11,13	0.55	0
1	MLY	G	782	1	9,10,11	0.80	0	6,11,13	0.36	0
1	MLY	J	353	1	9,10,11	0.86	0	6,11,13	0.80	0
1	MLY	D	839	1	9,10,11	0.64	0	6,11,13	0.79	0
1	MLY	G	272	1	9,10,11	0.88	1 (11%)	6,11,13	0.54	0
1	MLY	D	436	1	9,10,11	0.99	1 (11%)	6,11,13	0.48	0
1	MLY	D	385	1	9,10,11	0.92	1 (11%)	6,11,13	0.45	0
1	MLY	J	59	1	9,10,11	0.85	0	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	J	63	1	9,10,11	0.88	0	6,11,13	0.44	0
1	MLY	G	63	1	9,10,11	0.86	0	6,11,13	0.45	0
1	MLY	G	528	1	9,10,11	0.90	0	6,11,13	0.66	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	A	553	4,1	-	4/8/9/11	-
1	MLY	A	598	1	-	5/8/9/11	-
1	MLY	A	55	1	-	6/8/9/11	-
1	MLY	P	49	1	-	3/8/9/11	-
1	MLY	J	415	1	-	3/8/9/11	-
1	MLY	A	600	1	-	3/8/9/11	-
1	MLY	P	138	1	-	4/8/9/11	-
1	MLY	D	505	1	-	5/8/9/11	-
1	MLY	P	385	1	-	2/8/9/11	-
1	MLY	D	63	1	-	4/8/9/11	-
1	MLY	D	837	1	-	6/8/9/11	-
1	MLY	P	613	1	-	3/8/9/11	-
1	MLY	G	415	1	-	3/8/9/11	-
1	MLY	D	431	1	-	4/8/9/11	-
1	MLY	G	613	1	-	3/8/9/11	-
1	MLY	J	138	1	-	4/8/9/11	-
1	MLY	D	681	1	-	4/8/9/11	-
1	MLY	G	296	1	-	4/8/9/11	-
1	MLY	J	84	1	-	4/8/9/11	-
1	MLY	G	553	4,1	-	4/8/9/11	-
1	MLY	G	598	1	-	5/8/9/11	-
1	MLY	G	55	1	-	6/8/9/11	-
1	MLY	G	84	1	-	4/8/9/11	-
1	MLY	P	504	1	-	4/8/9/11	-
1	MLY	J	504	1	-	4/8/9/11	-
1	MLY	A	768	1	-	4/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	G	248	1	-	6/8/9/11	-
1	MLY	P	59	1	-	3/8/9/11	-
1	MLY	A	353	1	-	4/8/9/11	-
1	MLY	D	613	1	-	3/8/9/11	-
1	MLY	D	138	1	-	4/8/9/11	-
1	MLY	A	30	1	-	3/8/9/11	-
1	MLY	D	782	1	-	6/8/9/11	-
1	MLY	P	837	1	-	6/8/9/11	-
1	MLY	G	431	1	-	4/8/9/11	-
1	MLY	D	827	1	-	1/8/9/11	-
1	MLY	A	248	1	-	6/8/9/11	-
1	MLY	A	528	1	-	4/8/9/11	-
1	MLY	A	659	1	-	3/8/9/11	-
1	MLY	A	295	1	-	2/8/9/11	-
1	MLY	A	369	1	-	2/8/9/11	-
1	MLY	G	600	1	-	3/8/9/11	-
1	MLY	G	486	1	-	2/8/9/11	-
1	MLY	D	295	1	-	2/8/9/11	-
1	MLY	G	827	1	-	1/8/9/11	-
1	MLY	P	55	1	-	6/8/9/11	-
1	MLY	A	190	1	-	4/8/9/11	-
1	MLY	G	30	1	-	3/8/9/11	-
1	MLY	J	55	1	-	6/8/9/11	-
1	MLY	D	486	1	-	2/8/9/11	-
1	MLY	P	296	1	-	4/8/9/11	-
1	MLY	D	768	1	-	4/8/9/11	-
1	MLY	A	486	1	-	2/8/9/11	-
1	MLY	D	190	1	-	4/8/9/11	-
1	MLY	G	659	1	-	3/8/9/11	-
1	MLY	G	369	1	-	2/8/9/11	-
1	MLY	J	764	1	-	2/8/9/11	-
1	MLY	D	348	1	-	5/8/9/11	-
1	MLY	J	190	1	-	4/8/9/11	-
1	MLY	G	190	1	-	4/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	J	553	1	-	4/8/9/11	-
1	MLY	J	295	1	-	2/8/9/11	-
1	MLY	D	87	1	-	2/8/9/11	-
1	MLY	G	138	1	-	4/8/9/11	-
1	MLY	J	486	1	-	2/8/9/11	-
1	MLY	D	528	1	-	4/8/9/11	-
1	MLY	D	30	1	-	3/8/9/11	-
1	MLY	D	617	1	-	2/8/9/11	-
1	MLY	J	107	1	-	2/8/9/11	-
1	MLY	A	764	1	-	2/8/9/11	-
1	MLY	J	768	1	-	4/8/9/11	-
1	MLY	P	35	1	-	3/8/9/11	-
1	MLY	G	107	1	-	2/8/9/11	-
1	MLY	G	59	1	-	3/8/9/11	-
1	MLY	A	236	1	-	3/8/9/11	-
1	MLY	P	768	1	-	4/8/9/11	-
1	MLY	G	768	1	-	4/8/9/11	-
1	MLY	P	436	1	-	4/8/9/11	-
1	MLY	J	551	1	-	3/8/9/11	-
1	MLY	A	415	1	-	3/8/9/11	-
1	MLY	P	30	1	-	3/8/9/11	-
1	MLY	P	63	1	-	4/8/9/11	-
1	MLY	A	504	1	-	4/8/9/11	-
1	MLY	D	296	1	-	4/8/9/11	-
1	MLY	D	551	1	-	3/8/9/11	-
1	MLY	J	87	1	-	2/8/9/11	-
1	MLY	P	87	1	-	2/8/9/11	-
1	MLY	P	505	1	-	5/8/9/11	-
1	MLY	G	236	1	-	3/8/9/11	-
1	MLY	P	84	1	-	4/8/9/11	-
1	MLY	A	837	1	-	6/8/9/11	-
1	MLY	J	431	1	-	4/8/9/11	-
1	MLY	P	431	1	-	4/8/9/11	-
1	MLY	D	59	1	-	3/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	P	367	1	-	2/8/9/11	-
1	MLY	J	833	1	-	6/8/9/11	-
1	MLY	J	49	1	-	3/8/9/11	-
1	MLY	G	504	1	-	4/8/9/11	-
1	MLY	D	367	1	-	2/8/9/11	-
1	MLY	P	764	1	-	2/8/9/11	-
1	MLY	A	49	1	-	3/8/9/11	-
1	MLY	G	833	1	-	6/8/9/11	-
1	MLY	J	613	1	-	3/8/9/11	-
1	MLY	A	617	1	-	2/8/9/11	-
1	MLY	A	35	1	-	3/8/9/11	-
1	MLY	A	84	1	-	4/8/9/11	-
1	MLY	G	837	1	-	6/8/9/11	-
1	MLY	P	248	1	-	6/8/9/11	-
1	MLY	D	49	1	-	3/8/9/11	-
1	MLY	J	681	1	-	4/8/9/11	-
1	MLY	J	248	1	-	6/8/9/11	-
1	MLY	J	528	1	-	4/8/9/11	-
1	MLY	P	681	1	-	4/8/9/11	-
1	MLY	D	84	1	-	4/8/9/11	-
1	MLY	G	681	1	-	4/8/9/11	-
1	MLY	A	272	1	-	3/8/9/11	-
1	MLY	D	272	1	-	3/8/9/11	-
1	MLY	G	49	1	-	3/8/9/11	-
1	MLY	J	30	1	-	3/8/9/11	-
1	MLY	G	35	1	-	3/8/9/11	-
1	MLY	A	59	1	-	3/8/9/11	-
1	MLY	A	348	1	-	5/8/9/11	-
1	MLY	J	385	1	-	2/8/9/11	-
1	MLY	P	353	1	-	4/8/9/11	-
1	MLY	P	236	1	-	3/8/9/11	-
1	MLY	G	353	1	-	4/8/9/11	-
1	MLY	G	367	1	-	2/8/9/11	-
1	MLY	G	436	1	-	4/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	J	617	1	-	2/8/9/11	-
1	MLY	J	130	1	-	5/8/9/11	-
1	MLY	A	613	1	-	3/8/9/11	-
1	MLY	J	505	1	-	5/8/9/11	-
1	MLY	A	107	1	-	2/8/9/11	-
1	MLY	J	19	1	-	4/8/9/11	-
1	MLY	J	369	1	-	2/8/9/11	-
1	MLY	G	130	1	-	5/8/9/11	-
1	MLY	J	348	1	-	5/8/9/11	-
1	MLY	J	659	1	-	3/8/9/11	-
1	MLY	A	296	1	-	4/8/9/11	-
1	MLY	D	107	1	-	2/8/9/11	-
1	MLY	P	415	1	-	3/8/9/11	-
1	MLY	J	272	1	-	3/8/9/11	-
1	MLY	D	35	1	-	3/8/9/11	-
1	MLY	D	553	4,1	-	5/8/9/11	-
1	MLY	D	55	1	-	6/8/9/11	-
1	MLY	D	598	1	-	5/8/9/11	-
1	MLY	D	130	1	-	5/8/9/11	-
1	MLY	D	600	1	-	3/8/9/11	-
1	MLY	J	827	1	-	1/8/9/11	-
1	MLY	J	436	1	-	4/8/9/11	-
1	MLY	P	551	1	-	3/8/9/11	-
1	MLY	G	551	1	-	3/8/9/11	-
1	MLY	D	764	1	-	2/8/9/11	-
1	MLY	A	431	1	-	4/8/9/11	-
1	MLY	A	551	1	-	3/8/9/11	-
1	MLY	J	296	1	-	4/8/9/11	-
1	MLY	J	598	1	-	5/8/9/11	-
1	MLY	J	782	1	-	6/8/9/11	-
1	MLY	A	839	1	-	3/8/9/11	-
1	MLY	A	436	1	-	4/8/9/11	-
1	MLY	D	369	1	-	2/8/9/11	-
1	MLY	D	415	1	-	3/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	G	87	1	-	2/8/9/11	-
1	MLY	J	236	1	-	3/8/9/11	-
1	MLY	J	837	1	-	6/8/9/11	-
1	MLY	A	833	1	-	6/8/9/11	-
1	MLY	G	505	1	-	5/8/9/11	-
1	MLY	P	598	1	-	5/8/9/11	-
1	MLY	P	190	1	-	4/8/9/11	-
1	MLY	A	87	1	-	2/8/9/11	-
1	MLY	J	839	1	-	3/8/9/11	-
1	MLY	A	130	1	-	5/8/9/11	-
1	MLY	D	236	1	-	3/8/9/11	-
1	MLY	A	505	1	-	5/8/9/11	-
1	MLY	P	295	1	-	2/8/9/11	-
1	MLY	P	369	1	-	2/8/9/11	-
1	MLY	P	528	1	-	4/8/9/11	-
1	MLY	G	839	1	-	3/8/9/11	-
1	MLY	P	486	1	-	2/8/9/11	-
1	MLY	D	504	1	-	4/8/9/11	-
1	MLY	P	839	1	-	3/8/9/11	-
1	MLY	P	107	1	-	2/8/9/11	-
1	MLY	J	367	1	-	2/8/9/11	-
1	MLY	A	681	1	-	4/8/9/11	-
1	MLY	P	348	1	-	5/8/9/11	-
1	MLY	P	782	1	-	6/8/9/11	-
1	MLY	A	367	1	-	2/8/9/11	-
1	MLY	P	600	1	-	3/8/9/11	-
1	MLY	J	600	1	-	3/8/9/11	-
1	MLY	G	764	1	-	2/8/9/11	-
1	MLY	P	827	1	-	1/8/9/11	-
1	MLY	A	19	1	-	4/8/9/11	-
1	MLY	D	353	1	-	4/8/9/11	-
1	MLY	D	833	1	-	6/8/9/11	-
1	MLY	G	385	1	-	2/8/9/11	-
1	MLY	A	782	1	-	6/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	P	19	1	-	4/8/9/11	-
1	MLY	A	385	1	-	2/8/9/11	-
1	MLY	A	827	1	-	1/8/9/11	-
1	MLY	D	19	1	-	4/8/9/11	-
1	MLY	P	659	1	-	3/8/9/11	-
1	MLY	G	295	1	-	2/8/9/11	-
1	MLY	P	617	1	-	2/8/9/11	-
1	MLY	D	659	1	-	3/8/9/11	-
1	MLY	A	63	1	-	4/8/9/11	-
1	MLY	P	130	1	-	5/8/9/11	-
1	MLY	G	617	1	-	2/8/9/11	-
1	MLY	P	833	1	-	6/8/9/11	-
1	MLY	D	248	1	-	6/8/9/11	-
1	MLY	G	19	1	-	4/8/9/11	-
1	MLY	J	35	1	-	3/8/9/11	-
1	MLY	G	348	1	-	5/8/9/11	-
1	MLY	A	138	1	-	4/8/9/11	-
1	MLY	P	553	1	-	4/8/9/11	-
1	MLY	P	272	1	-	3/8/9/11	-
1	MLY	G	782	1	-	6/8/9/11	-
1	MLY	J	353	1	-	4/8/9/11	-
1	MLY	D	839	1	-	3/8/9/11	-
1	MLY	G	272	1	-	3/8/9/11	-
1	MLY	D	436	1	-	4/8/9/11	-
1	MLY	D	385	1	-	2/8/9/11	-
1	MLY	J	59	1	-	3/8/9/11	-
1	MLY	J	63	1	-	4/8/9/11	-
1	MLY	G	63	1	-	4/8/9/11	-
1	MLY	G	528	1	-	4/8/9/11	-

The worst 5 of 65 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	138	MLY	CB-CA	-3.35	1.48	1.53
1	G	138	MLY	CB-CA	-3.22	1.48	1.53
1	P	138	MLY	CB-CA	-3.18	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	138	MLY	CB-CA	-3.17	1.48	1.53
1	J	138	MLY	CB-CA	-3.16	1.48	1.53

There are no bond angle outliers.

There are no chirality outliers.

5 of 806 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.

154 monomers are involved in 630 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	553	MLY	18	0
1	A	598	MLY	1	0
1	A	55	MLY	1	0
1	P	49	MLY	4	0
1	J	415	MLY	1	0
1	A	600	MLY	1	0
1	P	138	MLY	2	0
1	D	63	MLY	3	0
1	D	837	MLY	1	0
1	G	415	MLY	1	0
1	J	138	MLY	2	0
1	G	296	MLY	2	0
1	J	84	MLY	18	0
1	G	553	MLY	27	0
1	G	598	MLY	1	0
1	G	55	MLY	1	0
1	G	84	MLY	33	0
1	P	504	MLY	1	0
1	J	504	MLY	1	0
1	A	768	MLY	6	0
1	G	248	MLY	2	0
1	P	59	MLY	2	0
1	D	138	MLY	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	30	MLY	1	0
1	D	782	MLY	43	0
1	P	837	MLY	1	0
1	A	248	MLY	2	0
1	A	528	MLY	2	0
1	A	659	MLY	2	0
1	A	295	MLY	6	0
1	A	369	MLY	1	0
1	G	600	MLY	1	0
1	G	486	MLY	3	0
1	D	295	MLY	6	0
1	P	55	MLY	1	0
1	A	190	MLY	2	0
1	G	30	MLY	1	0
1	J	55	MLY	1	0
1	D	486	MLY	3	0
1	P	296	MLY	3	0
1	A	486	MLY	3	0
1	D	190	MLY	2	0
1	G	659	MLY	2	0
1	G	369	MLY	1	0
1	J	764	MLY	3	0
1	D	348	MLY	6	0
1	J	190	MLY	2	0
1	G	190	MLY	2	0
1	J	553	MLY	11	0
1	J	295	MLY	6	0
1	D	87	MLY	3	0
1	G	138	MLY	2	0
1	J	486	MLY	3	0
1	D	528	MLY	3	0
1	D	30	MLY	1	0
1	D	617	MLY	1	0
1	J	107	MLY	3	0
1	A	764	MLY	11	0
1	J	768	MLY	5	0
1	G	107	MLY	3	0
1	G	59	MLY	3	0
1	G	768	MLY	2	0
1	P	436	MLY	2	0
1	A	415	MLY	1	0
1	P	30	MLY	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	P	63	MLY	4	0
1	A	504	MLY	1	0
1	D	296	MLY	3	0
1	D	551	MLY	1	0
1	J	87	MLY	3	0
1	P	87	MLY	3	0
1	P	505	MLY	8	0
1	P	84	MLY	30	0
1	A	837	MLY	12	0
1	D	59	MLY	2	0
1	J	49	MLY	3	0
1	P	764	MLY	1	0
1	A	49	MLY	3	0
1	A	617	MLY	1	0
1	G	837	MLY	1	0
1	P	248	MLY	2	0
1	D	49	MLY	4	0
1	J	248	MLY	2	0
1	J	528	MLY	3	0
1	A	272	MLY	1	0
1	D	272	MLY	1	0
1	G	49	MLY	3	0
1	J	30	MLY	1	0
1	A	59	MLY	2	0
1	A	348	MLY	5	0
1	G	436	MLY	2	0
1	J	617	MLY	1	0
1	J	505	MLY	10	0
1	A	107	MLY	3	0
1	J	348	MLY	5	0
1	J	659	MLY	2	0
1	A	296	MLY	2	0
1	D	107	MLY	3	0
1	P	415	MLY	1	0
1	J	272	MLY	1	0
1	D	553	MLY	16	0
1	D	55	MLY	1	0
1	D	598	MLY	1	0
1	D	600	MLY	1	0
1	J	436	MLY	2	0
1	D	764	MLY	8	0
1	A	551	MLY	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	J	296	MLY	3	0
1	J	598	MLY	1	0
1	J	782	MLY	1	0
1	A	839	MLY	8	0
1	A	436	MLY	2	0
1	D	415	MLY	1	0
1	G	87	MLY	2	0
1	J	837	MLY	1	0
1	A	833	MLY	1	0
1	G	505	MLY	16	0
1	P	598	MLY	1	0
1	P	190	MLY	2	0
1	A	87	MLY	3	0
1	J	839	MLY	9	0
1	A	505	MLY	25	0
1	P	295	MLY	6	0
1	P	528	MLY	2	0
1	G	839	MLY	4	0
1	P	486	MLY	3	0
1	D	504	MLY	1	0
1	P	839	MLY	8	0
1	P	107	MLY	3	0
1	P	348	MLY	5	0
1	P	782	MLY	1	0
1	P	600	MLY	1	0
1	J	600	MLY	1	0
1	G	764	MLY	20	0
1	A	782	MLY	7	0
1	P	659	MLY	2	0
1	G	295	MLY	6	0
1	P	617	MLY	1	0
1	D	659	MLY	2	0
1	A	63	MLY	4	0
1	G	617	MLY	1	0
1	D	248	MLY	2	0
1	G	348	MLY	4	0
1	A	138	MLY	2	0
1	P	553	MLY	2	0
1	P	272	MLY	1	0
1	G	782	MLY	1	0
1	D	839	MLY	4	0
1	G	272	MLY	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	436	MLY	2	0
1	J	59	MLY	3	0
1	J	63	MLY	3	0
1	G	63	MLY	3	0
1	G	528	MLY	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	P	5
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	R	1
2	B	1
2	E	1
2	H	1
2	K	1
2	Q	1

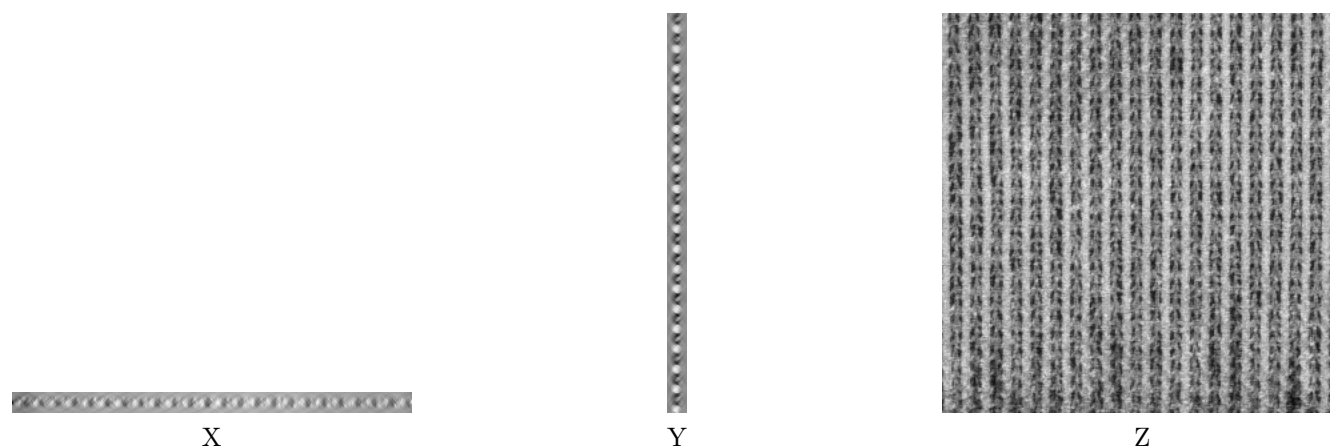
The worst 5 of 29 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	J	769:ALA	C	770:GLY	N	5.57
1	D	769:ALA	C	770:GLY	N	4.97
1	G	769:ALA	C	770:GLY	N	4.52
1	P	786:ILE	C	787:ILE	N	4.06
1	D	709:LYS	C	710:GLY	N	3.41

6 Tomogram visualisation [i](#)

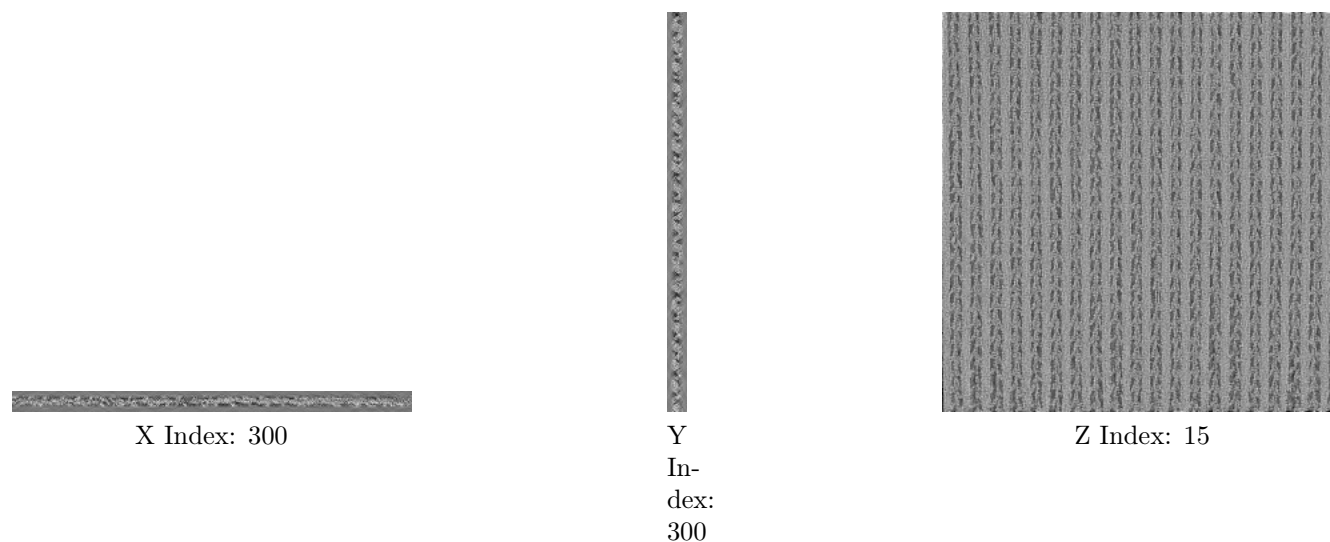
This section contains visualisations of the EMDB entry EMD-1001. These allow visual inspection of the internal detail of the tomogram and identification of artifacts.

6.1 Orthogonal projections [i](#)



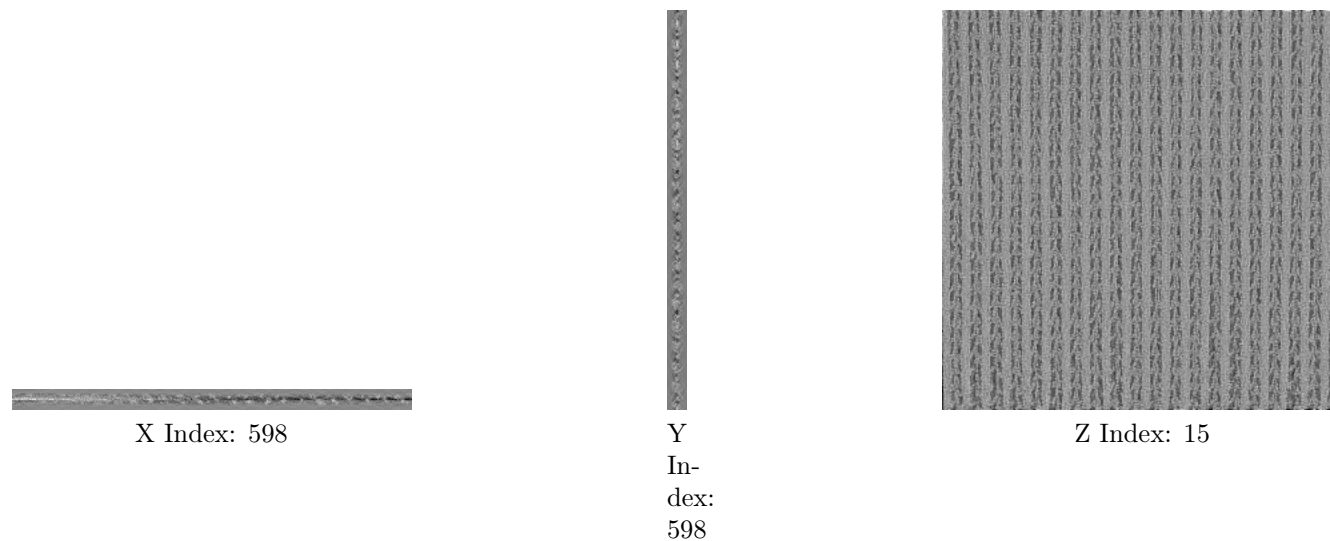
The images above show the tomogram projected in three orthogonal directions.

6.2 Central slices [i](#)



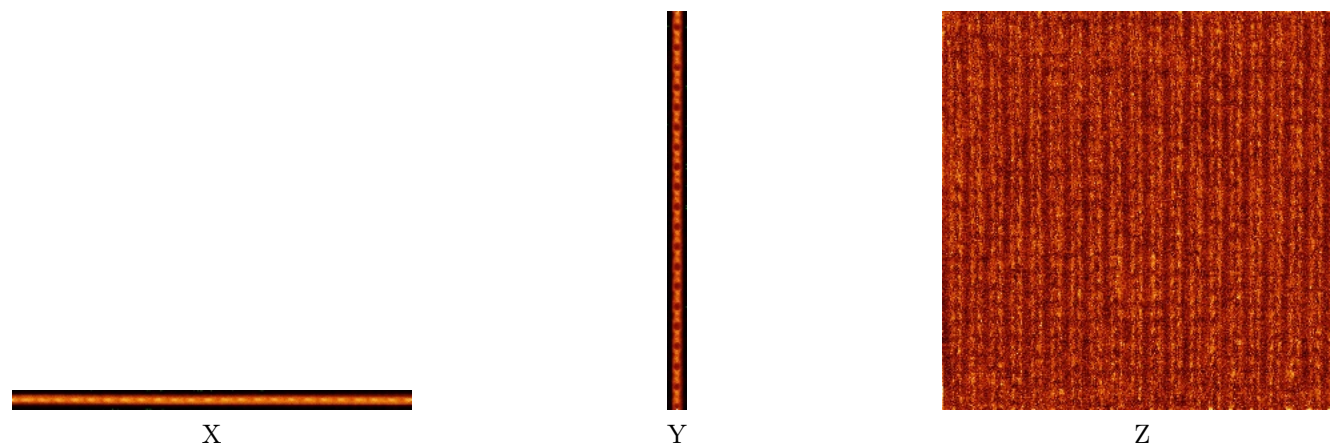
The images above show central slices of the tomogram in three orthogonal directions.

6.3 Largest variance slices [i](#)



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

6.4 Orthogonal standard-deviation projections (False-color) [i](#)



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

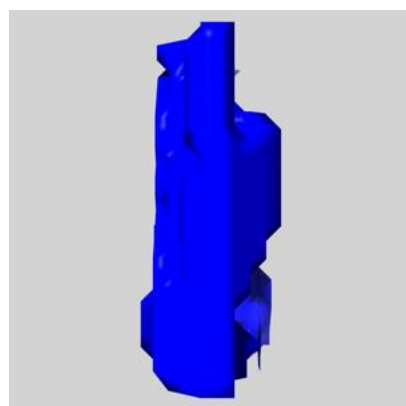
6.5 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

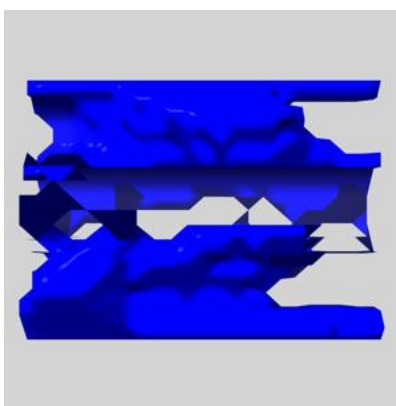
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

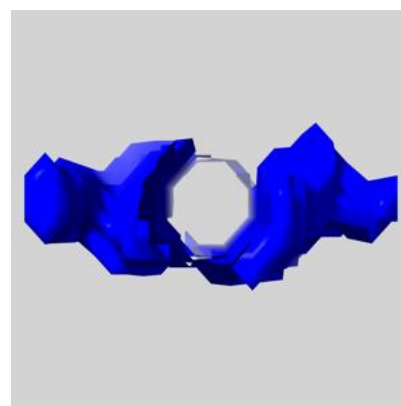
6.5.1 emd_1001_msk_25.map [i](#)



X

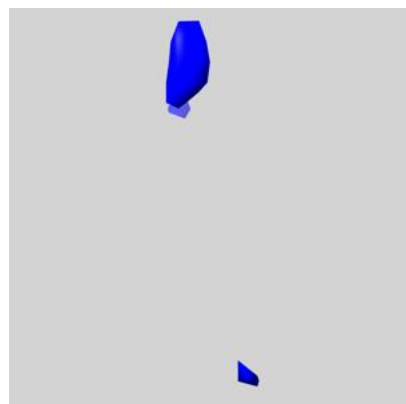


Y

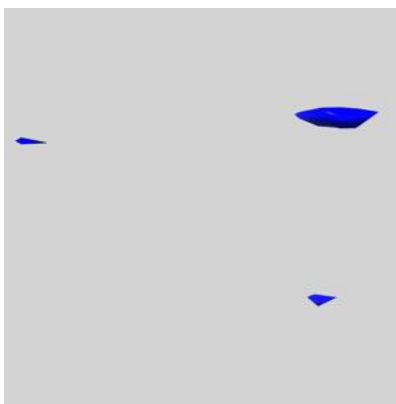


Z

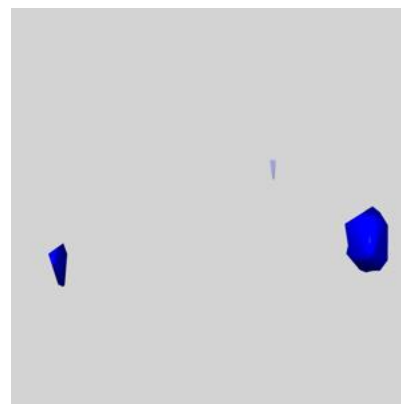
6.5.2 emd_1001_msk_24.map [i](#)



X

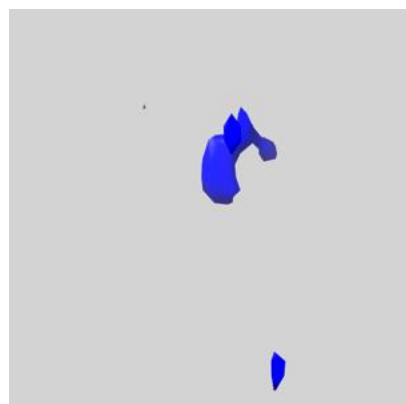


Y

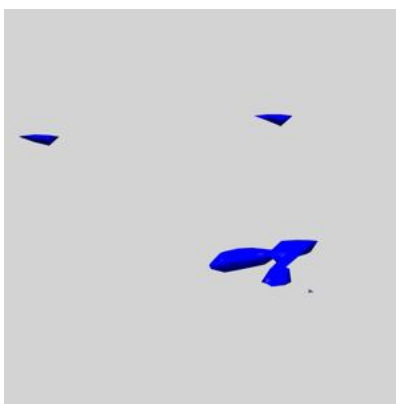


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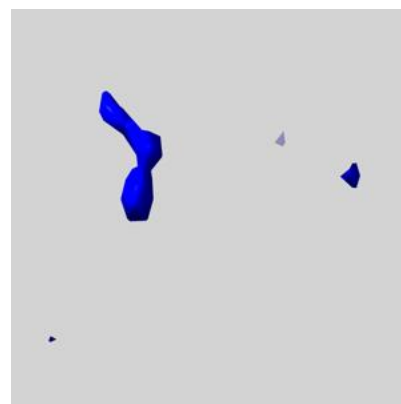
6.5.3 emd_1001_msk_23.map [i](#)



X

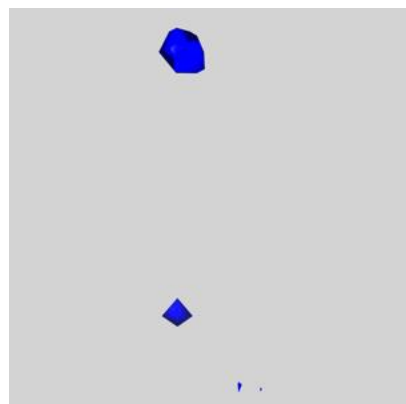


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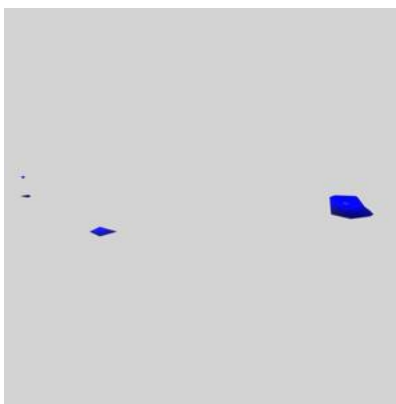


Z

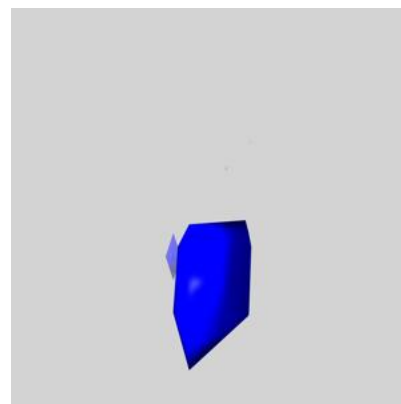
6.5.4 emd_1001_msk_22.map [i](#)



X

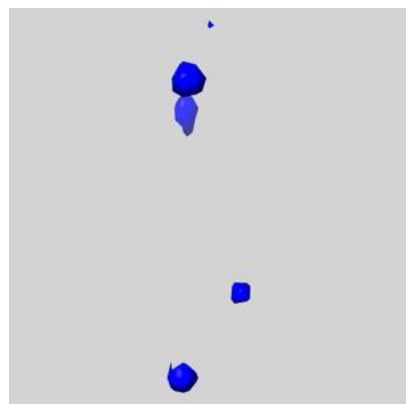


Y

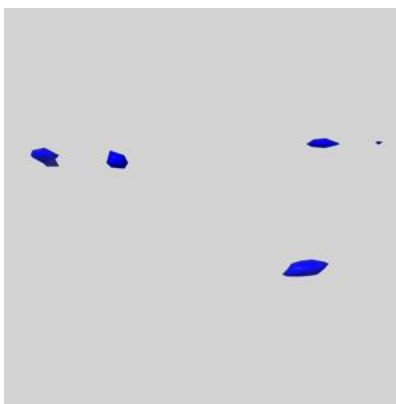


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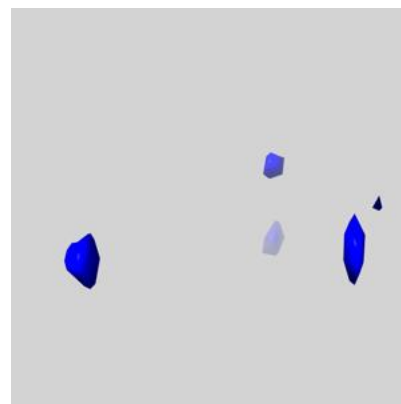
6.5.5 emd_1001_msk_21.map [i](#)



X

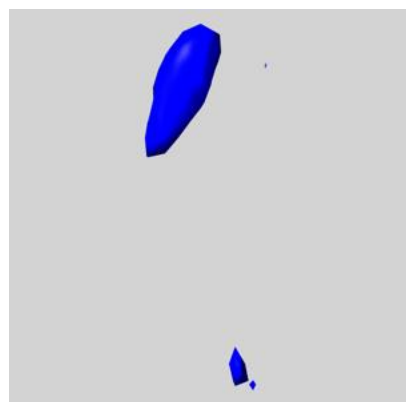


Y

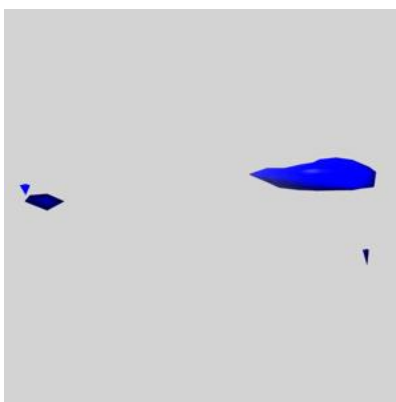


Z

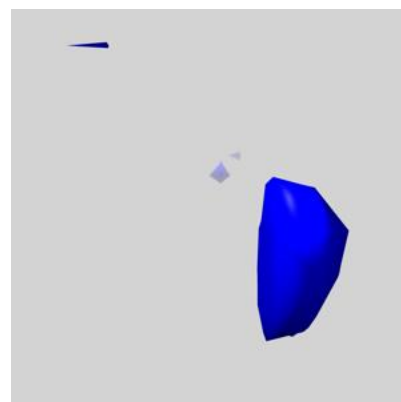
6.5.6 emd_1001_msk_20.map [i](#)



X

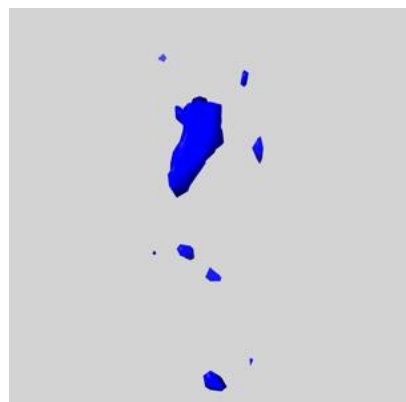


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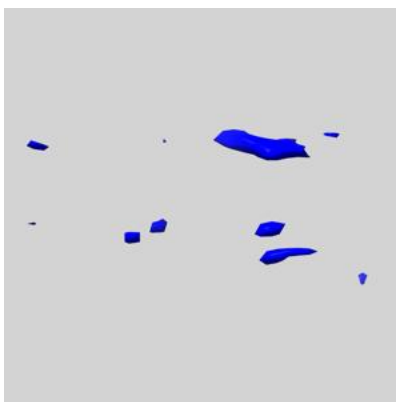


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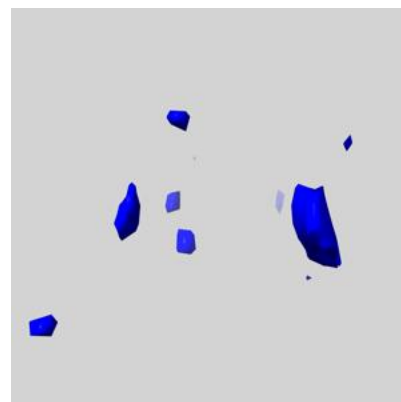
6.5.7 emd_1001_msk_19.map [i](#)



X

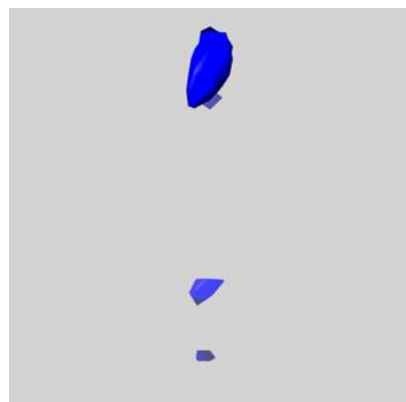


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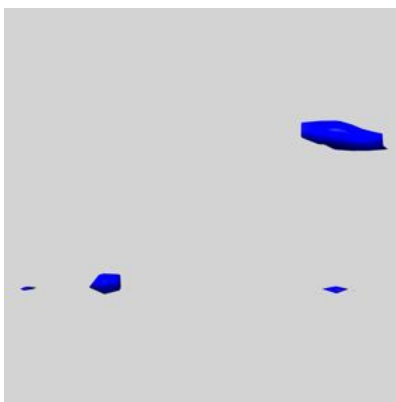


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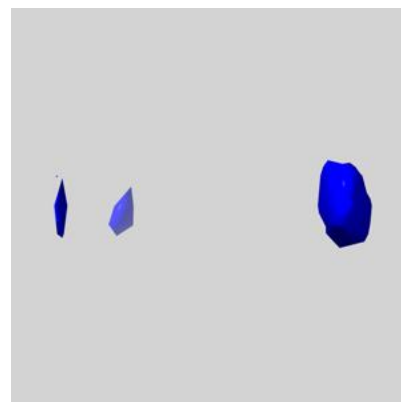
6.5.8 emd_1001_msk_18.map [i](#)



X

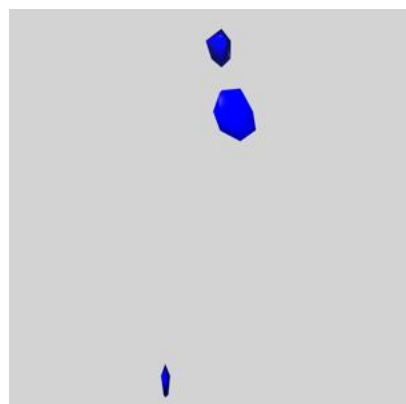


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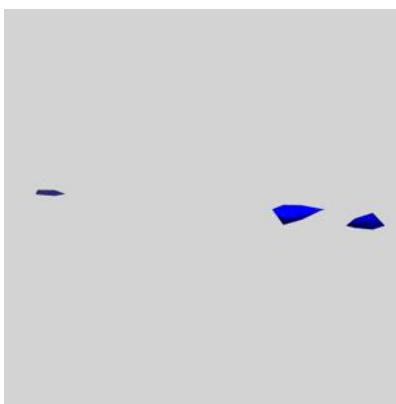


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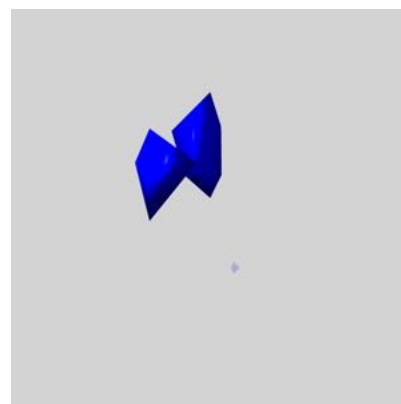
6.5.9 emd_1001_msk_17.map [i](#)



X

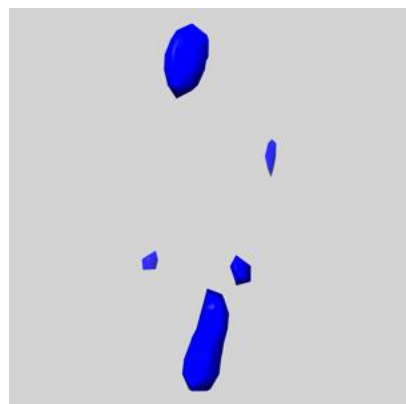


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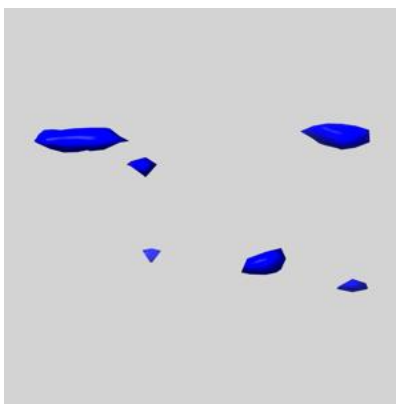


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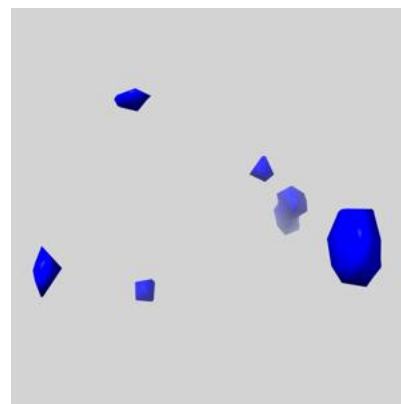
6.5.10 emd_1001_msk_16.map [i](#)



X

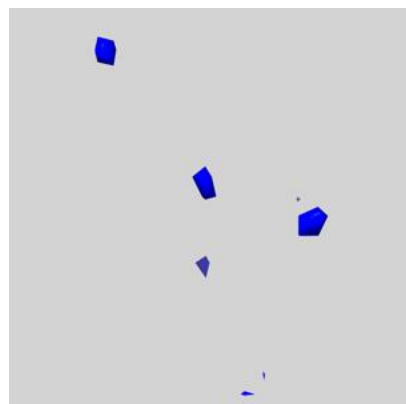


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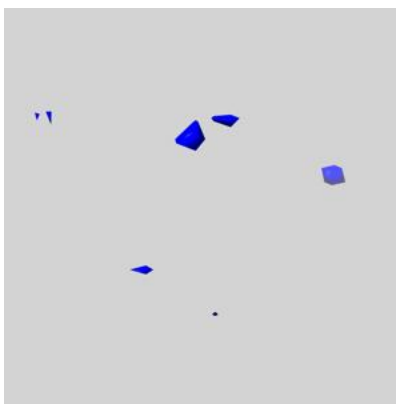


Z

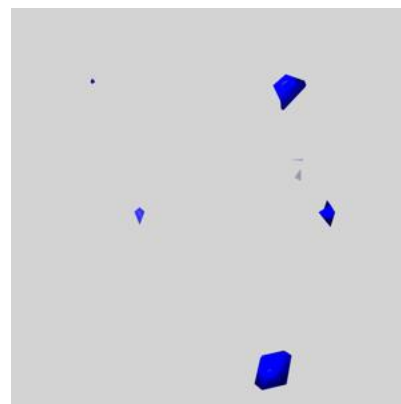
6.5.11 emd_1001_msk_15.map [i](#)



X

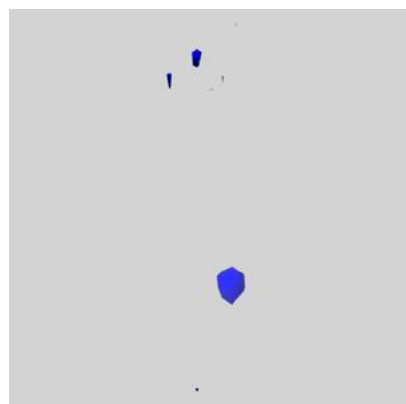


Y

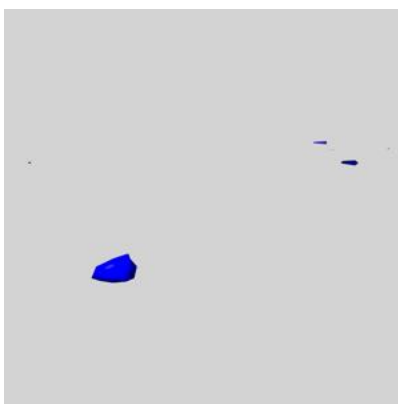


Z

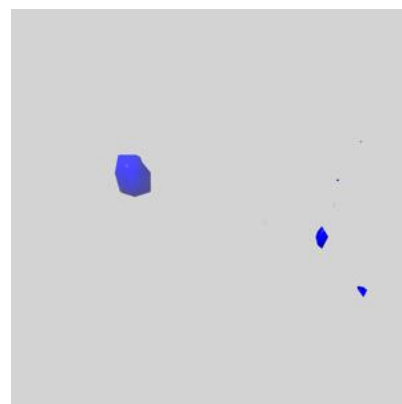
6.5.12 emd_1001_msk_14.map [i](#)



X

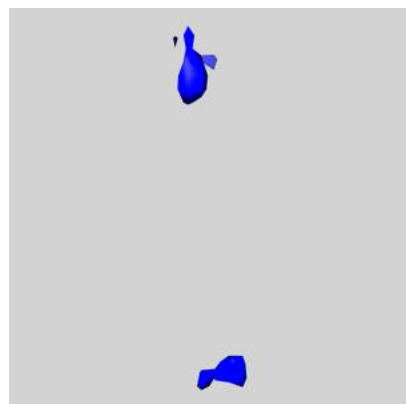


Y

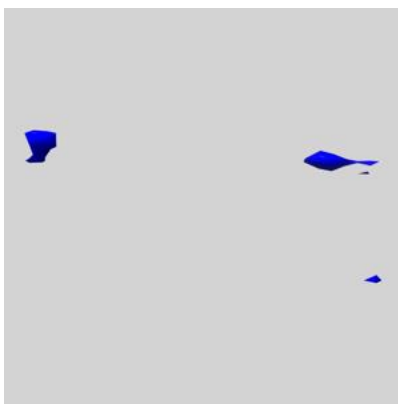


Z

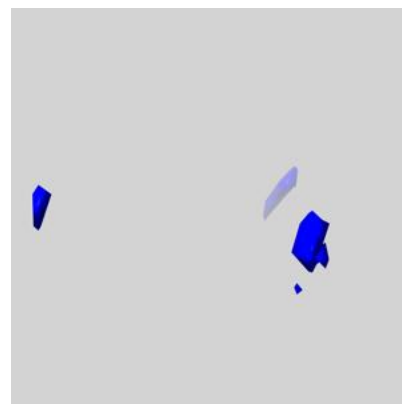
6.5.13 emd_1001_msk_13.map [i](#)



X

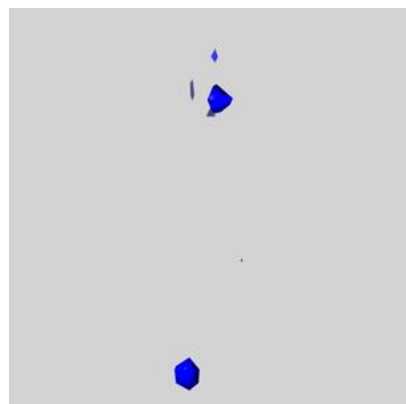


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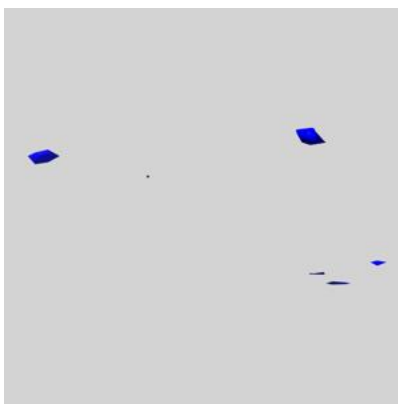


Z

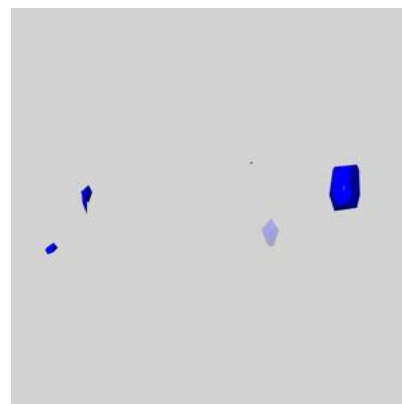
6.5.14 emd_1001_msk_12.map [i](#)



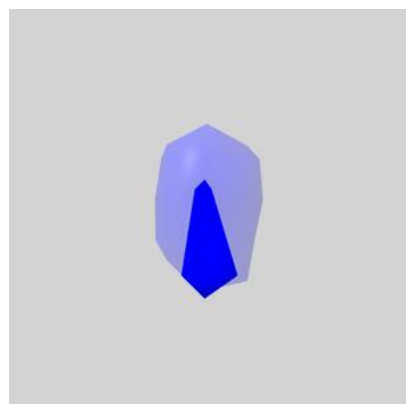
X



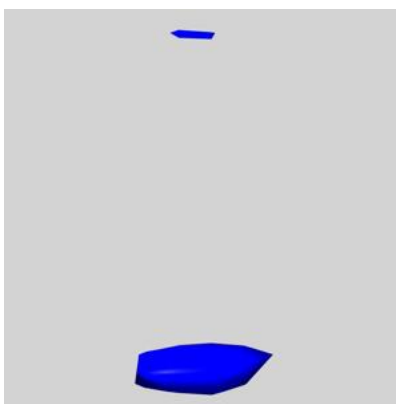
Y



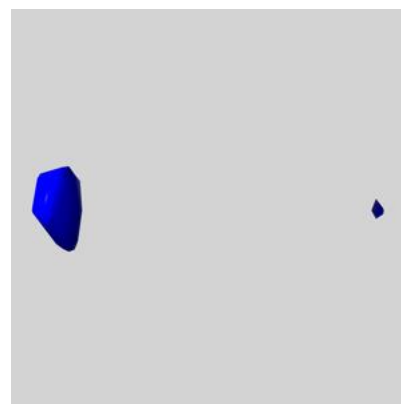
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6.5.15 emd_1001_msk_11.map [i](#)

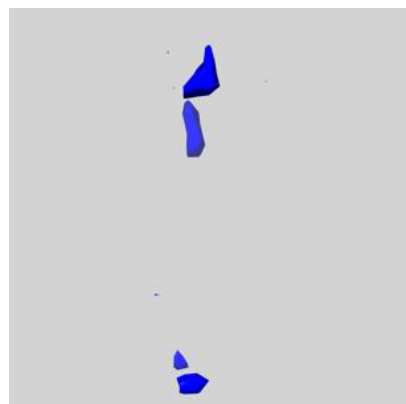
X



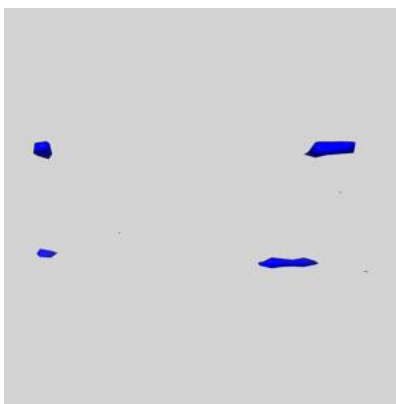
Y



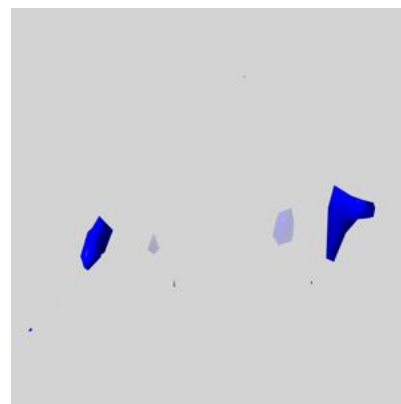
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6.5.16 emd_1001_msk_10.map [i](#)

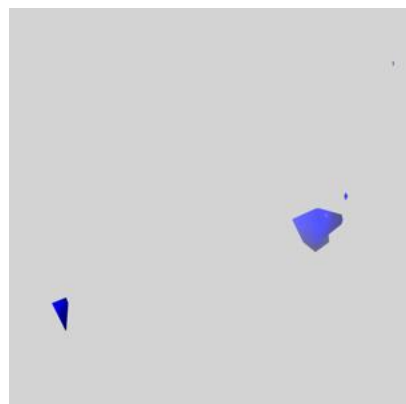
X



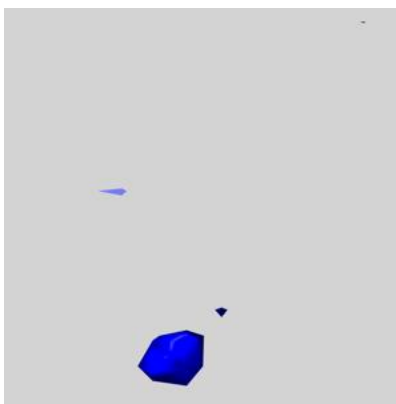
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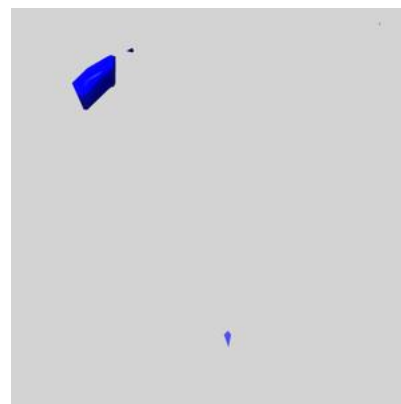
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6.5.17 emd_1001_msk_9.map [i](#)

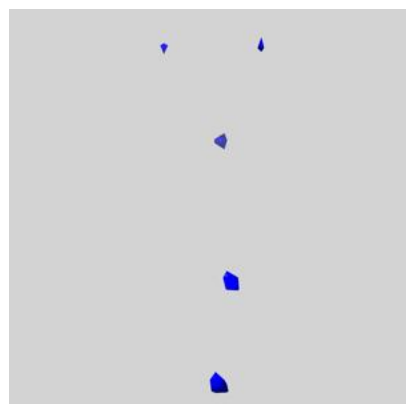
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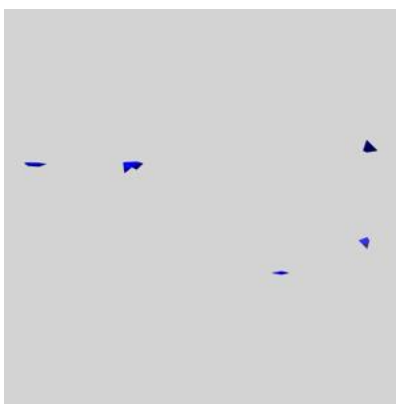
Y



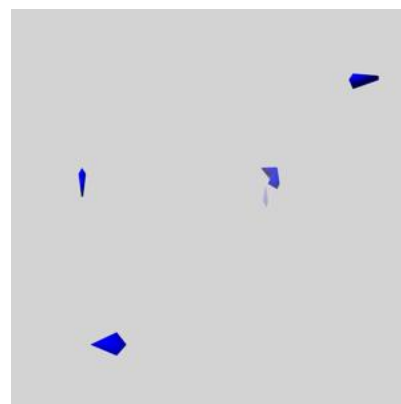
Z

6.5.18 emd_1001_msk_8.map [i](#)

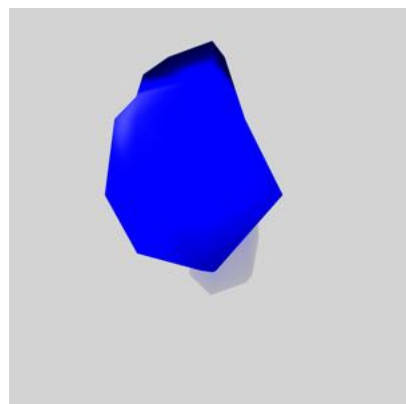
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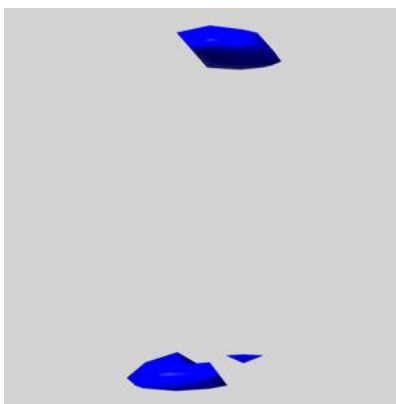
Y



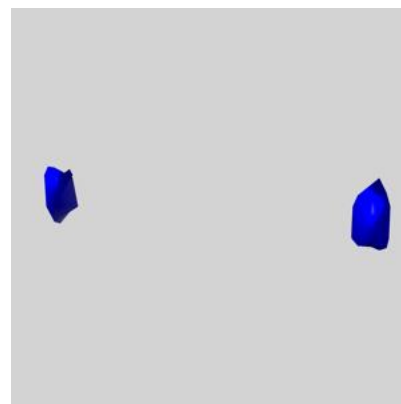
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6.5.19 emd_1001_msk_7.map [i](#)

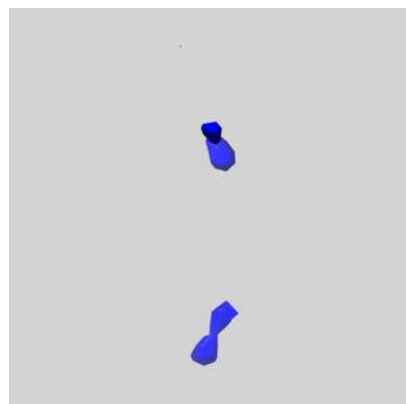
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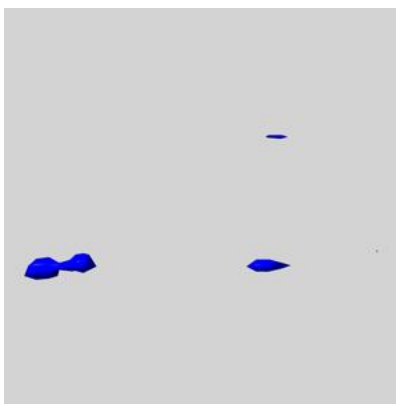
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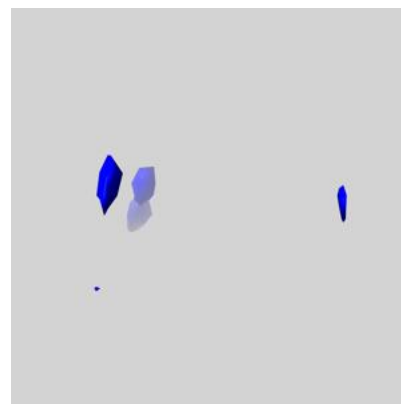
Z

6.5.20 emd_1001_msk_6.map [i](#)

X



Y

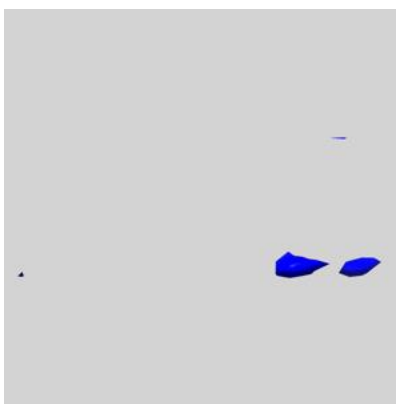


Z

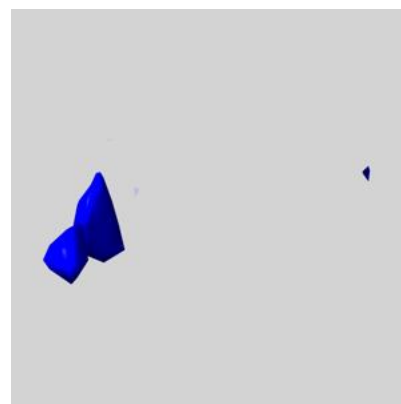
6.5.21 emd_1001_msk_5.map [i](#)



X

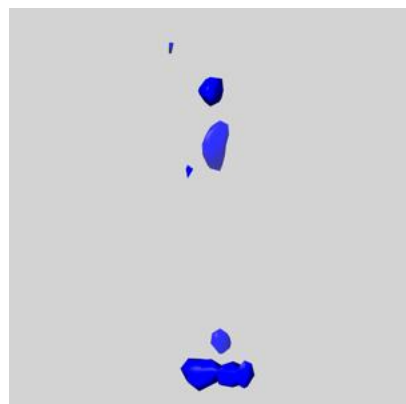


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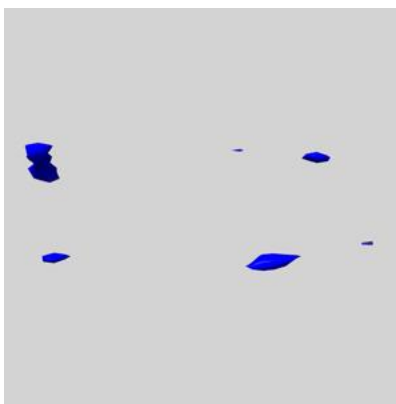


Z

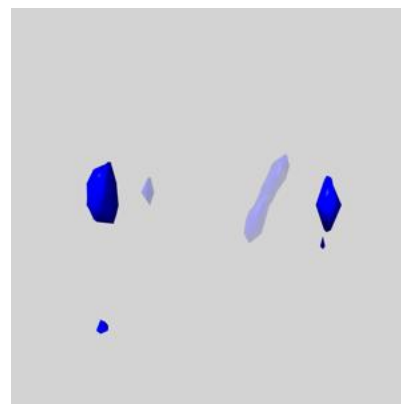
6.5.22 emd_1001_msk_4.map [i](#)



X

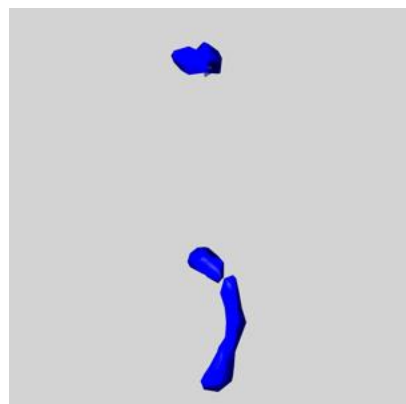


Y

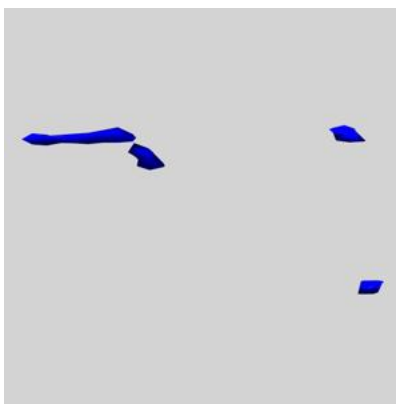


Z

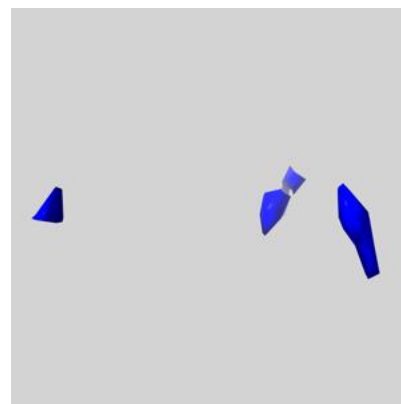
6.5.23 emd_1001_msk_3.map [i](#)



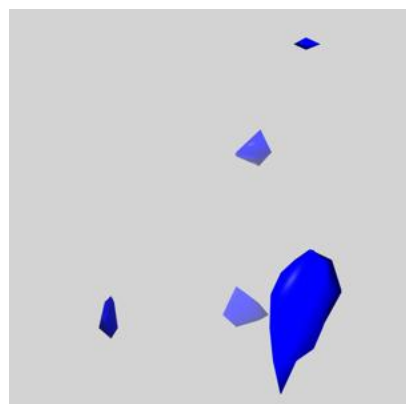
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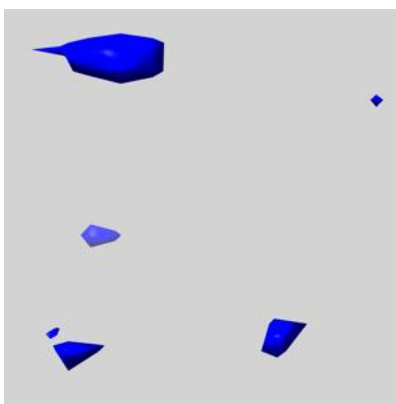
Y



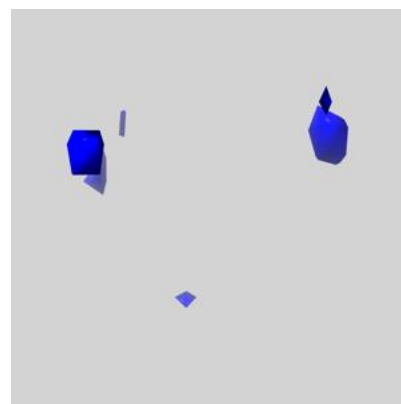
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6.5.24 emd_1001_msk_2.map [i](#)

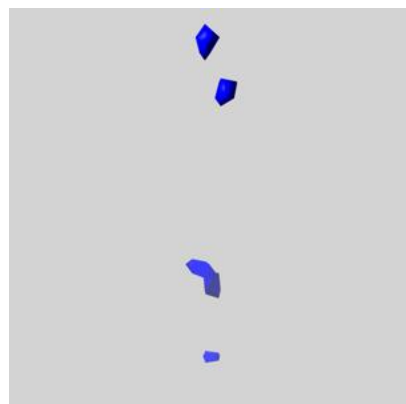
X



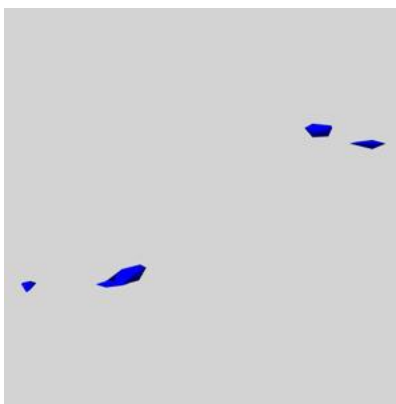
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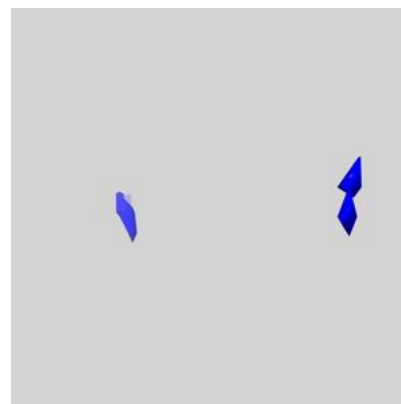
Z

6.5.25 emd_1001_msk_1.map [i](#)

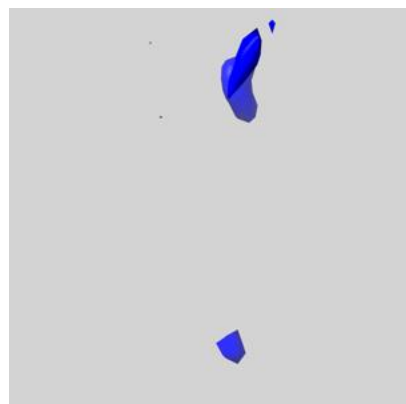
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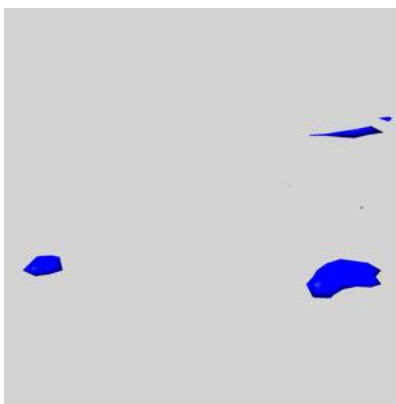
Y



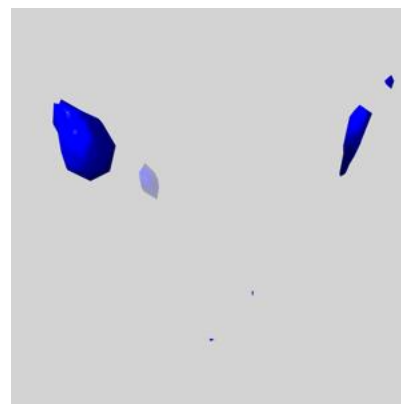
Z

6.5.26 emd_1001_msk_26.map [i](#)

X



Y

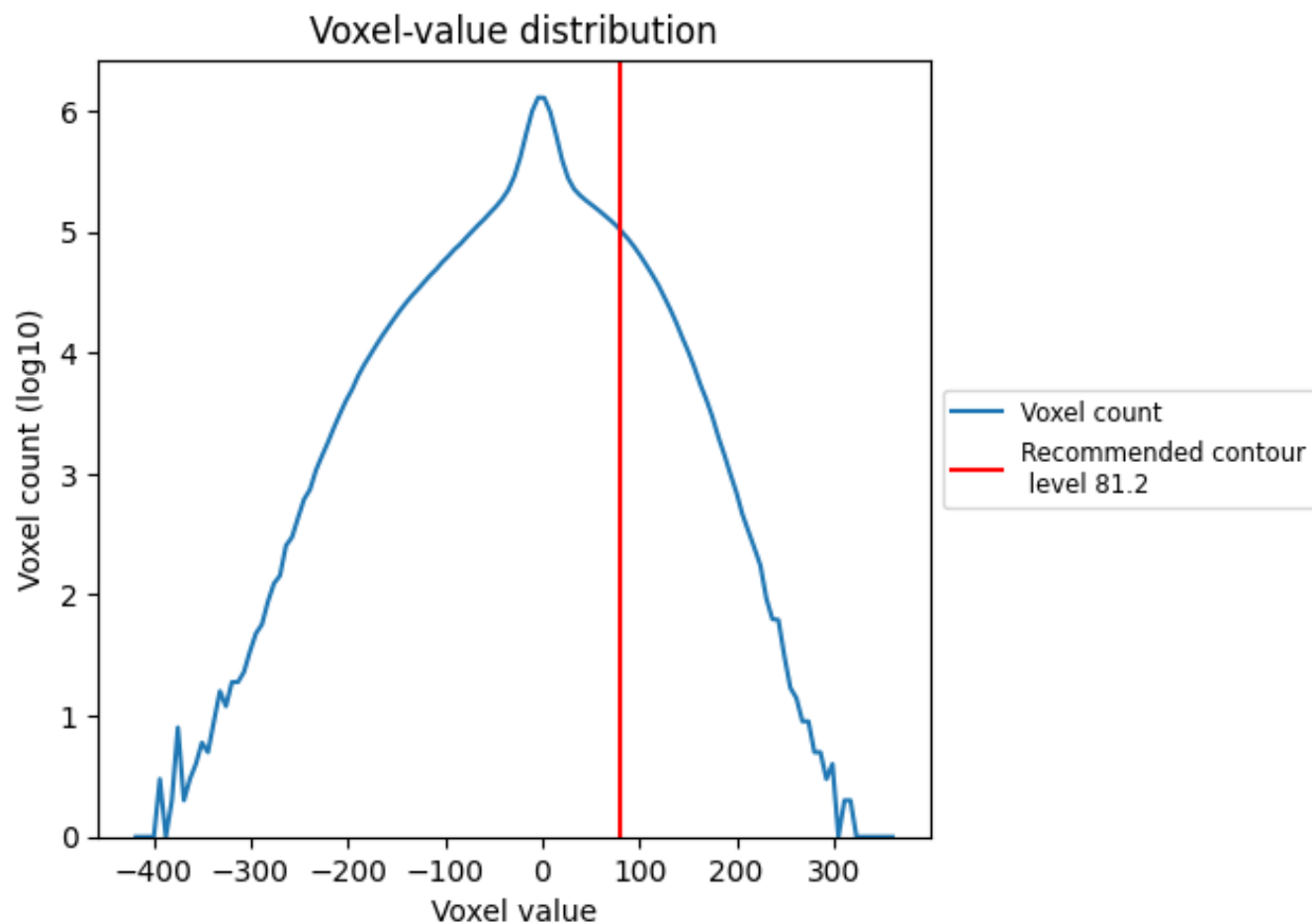


Z

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.

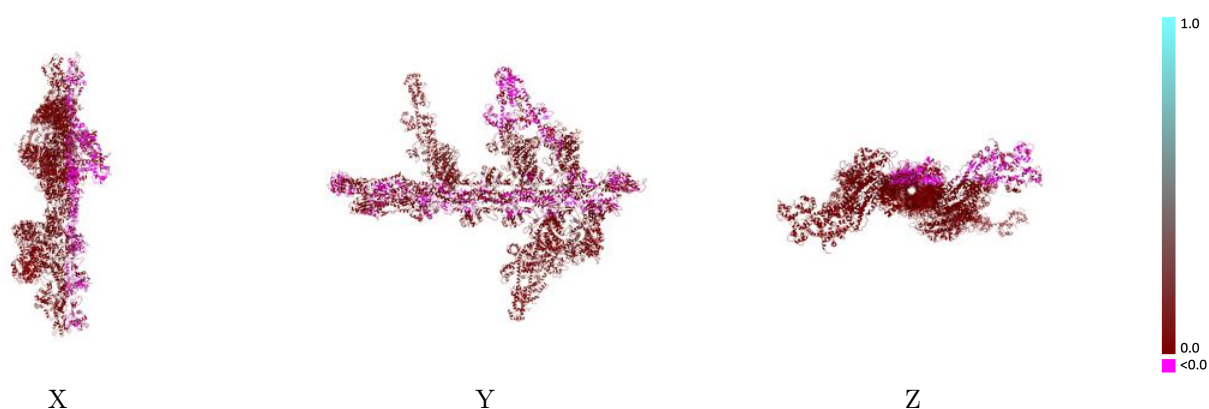
8 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-1001 and PDB model 1O1C. 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](#)

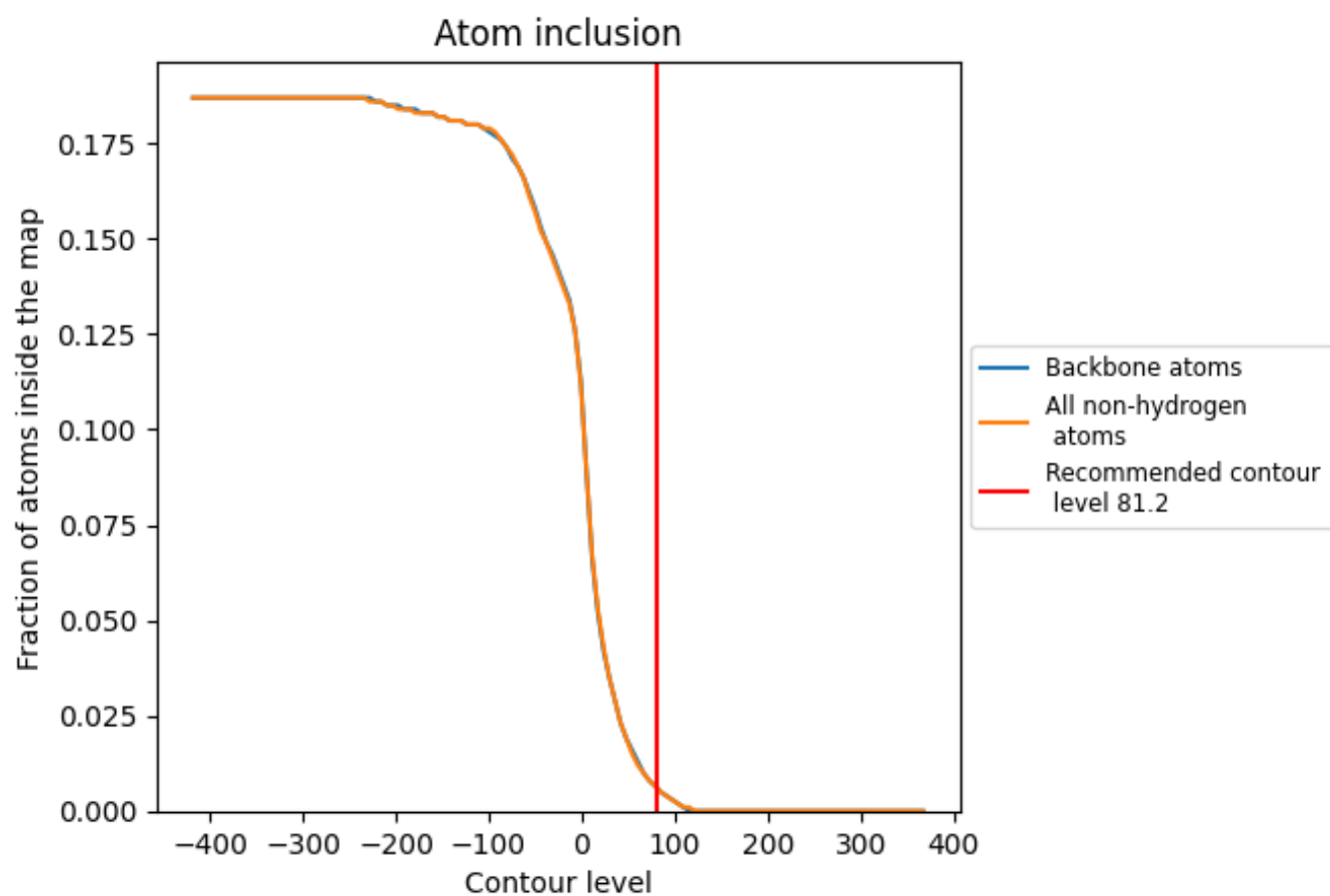


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 1% 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	 0.0060	 -0.0000
0	 0.0000	 0.0000
1	 0.0150	 0.0030
2	 0.0000	 -0.0000
3	 0.0000	 -0.0020
4	 0.0000	 -0.0050
5	 0.0000	 0.0090
7	 0.0000	 -0.0030
8	 0.0000	 -0.0040
9	 0.0000	 -0.0060
A	 0.0000	 0.0000
B	 0.0000	 0.0000
C	 0.0000	 0.0000
D	 0.0000	 0.0080
E	 0.0000	 -0.0160
F	 0.1520	 0.0100
G	 0.0000	 0.0000
H	 0.0000	 0.0000
I	 0.0000	 0.0000
J	 0.0000	 -0.0020
K	 0.0330	 0.0030
L	 0.0000	 -0.0230
P	 0.0000	 0.0000
Q	 0.0000	 0.0000
R	 0.0000	 0.0000
V	 0.0000	 -0.0110
W	 0.0000	 -0.0020
X	 0.0690	 -0.0020
Y	 0.0000	 0.0000
Z	 0.0070	 0.0050

