



wwPDB EM Validation Summary Report ⓘ

Mar 17, 2026 – 08:47 PM UTC

PDB ID : 1O1G / pdb_00001o1g
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 : 2002-11-19
Resolution : 70.00 Å(reported)
Based on initial models : 1ATN, 2MYS

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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:

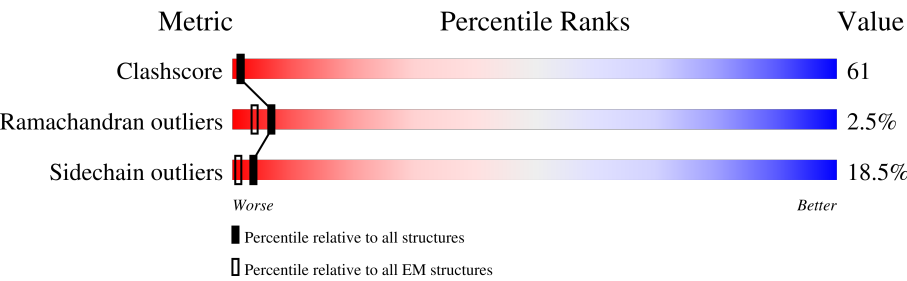
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 i

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%49%23%.
1	D	840	100% 25%49%22%.
1	G	840	99% 24%50%22%.
1	J	840	100% 25%49%22%.
1	M	840	100% 25%49%22%.
1	P	840	100% 25%49%22%.
2	B	145	100% 67%23%7%.
2	E	145	100% 63%26%8%.

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Mol	Chain	Length	Quality of chain
2	H	145	100% 61% 29% 7% .
2	K	145	100% 63% 27% 6% .
2	N	145	100% 63% 28% 6% .
2	Q	145	100% 63% 28% 6% .
3	C	147	100% 61% 35% .
3	F	147	100% 63% 34% .
3	I	147	70% 63% 34% .
3	L	147	100% 63% 34% .
3	O	147	100% 60% 37% ..
3	R	147	100% 61% 35% ..
4	1	375	98% 49% 36% 12% ..
4	2	375	99% 52% 35% 10% ..
4	3	375	99% 54% 34% 9% ..
4	4	375	99% 55% 34% 9% ..
4	5	375	99% 56% 33% 9% ..
4	6	375	99% 55% 33% 9% ..
4	7	375	99% 55% 33% 9% ..
4	8	375	99% 51% 35% 11% ..
4	9	375	99% 50% 35% 12% ..
4	V	375	99% 49% 37% 12% ..
4	W	375	99% 49% 36% 12% ..
4	X	375	99% 54% 34% 9% ..
4	Y	375	97% 54% 35% 9% ..
4	Z	375	99% 51% 36% 11% ..

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	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	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	M	553	-	-	X	-
1	MLY	M	839	-	-	X	-
1	MLY	P	764	-	-	X	-
1	MLY	P	782	-	-	X	-
1	MLY	P	839	-	-	X	-
1	MLY	P	84	-	-	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		

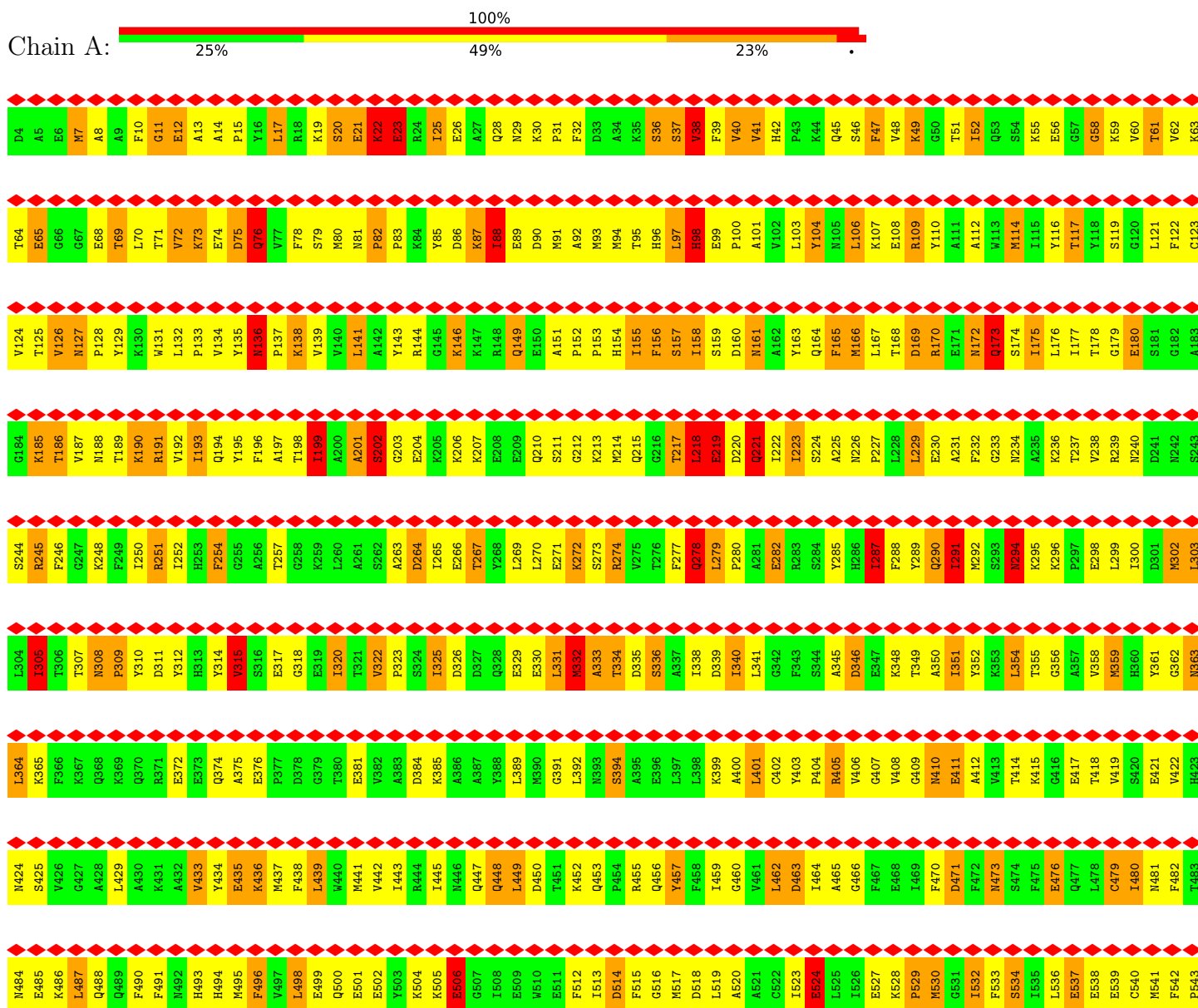
- Molecule 4 is a protein called SKELETAL MUSCLE ACTIN.

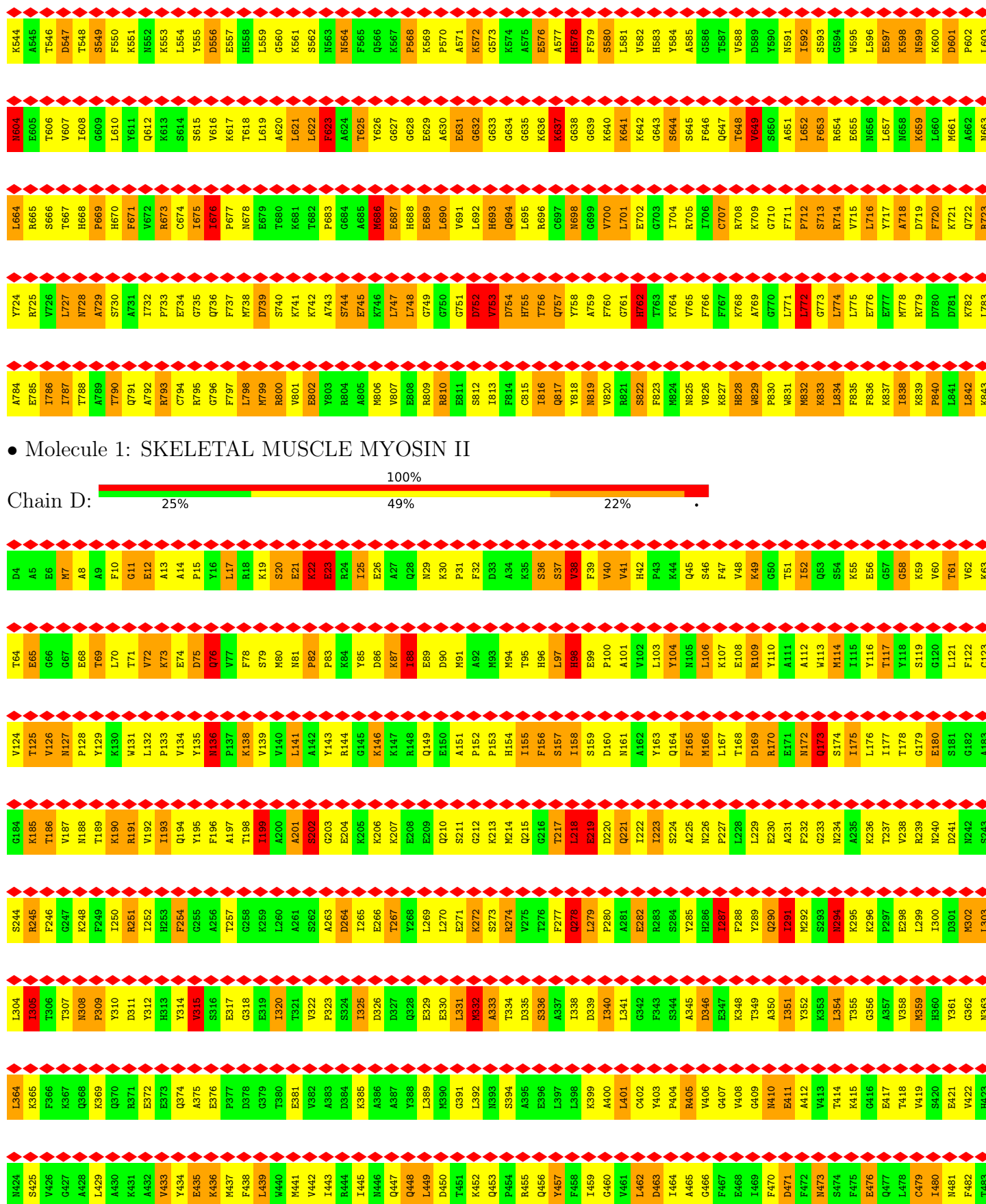
Mol	Chain	Residues	Atoms					AltConf	Trace
4	1	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	2	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	3	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	4	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	5	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	6	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	M128	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	H312
A433	H493	K553	R673	P733	R793	A13	K73	P133	T193	H253	H313
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	M136	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
Y440	Q500	G560	T680	S740	R800	S20	M80	Y140	A200	L260	I320
M441	E501	K561	K681	K741	R801	E21	V81	L141	L41	A261	T321
V442	E502	S562	T682	K742	E802	K22	P82	A142	S202	S262	V322
I443	Y503	N563	P683	A743	R804	E23	P83	Y143	G203	A263	P323
R444	K504	N564	G684	S744	A805	R24	K84	L144	E204	D264	S324
I445	K505	F565	A685	E745	A806	I25	Y85	G145	K205	L265	I325
N446	E506	Q566	M686	K746	V807	E26	D86	K146	K206	E266	D326
Q447	G507	K567	E687	L747	E808	A27	K87	K147	K207	T267	D327
Q448	I508	P568	H688	L748	R809	Q28	T88	R148	E208	T268	Q328
L449	E509	K569	E689	G749	R810	N29	E89	Q149	E209	L269	E329
D450	M510	P570	L690	G750	E811	K30	D90	E150	Q210	L270	E330
T451	E511	A571	V691	G751	S812	P31	A91	A151	S211	E271	L331
K452	F512	K572	L692	D752	T813	F32	A92	P152	G212	K272	R332
Q453	I513	G573	H693	V753	F814	D33	M93	P153	K213	S273	A333
P454	D514	K574	Q694	D754	C815	A34	M94	H154	M214	R274	T334
R455	F515	A575	L695	H755	T816	K35	T95	I155	Q215	V275	D335
Q456	G516	E576	R696	T756	Q817	S36	H96	F156	G216	T276	S336
Y457	M517	A577	C697	Q757	Y818	S37	L97	S157	T217	F277	A337
F458	D518	H578	N698	Y758	R819	V38	H98	I158	L218	Q278	I338
I459	L519	F579	G699	A759	V820	F39	E99	S159	E219	L279	D339
G460	A520	S580	V700	F760	R821	V40	P100	D160	D220	P280	I340
V461	A521	L581	L701	G761	S822	V41	A101	M161	Q221	A281	L341
L462	C522	V582	E702	H762	F823	H42	Y102	A162	I222	E282	G342
D463	I523	H583	G703	T763	M824	P43	L103	L163	I223	R283	F343
I464	E524	Y584	I704	K764	N825	K44	Y104	Q164	S224	S284	S344
A465	L525	A585	R705	V765	V826	Q45	N105	F165	A225	Y285	A345
G466	I526	G586	T706	F766	K827	S46	L106	M166	N226	H286	D346
F467	E527	T587	C707	F767	H828	F47	K107	L167	P227	L287	E347
E468	P528	V588	R708	K768	R829	V48	E108	T168	L228	F288	K348
I469	E529	D589	K709	A769	V830	V49	R109	D169	L229	Y289	T349
F470	M530	Y590	G710	G770	U831	G50	Y110	R170	E230	Q290	A350
D471	G531	N591	F711	L771	M832	T51	A111	E171	A231	L291	I351
F472	I532	L592	P712	L772	K833	I52	A112	M172	F232	M292	Y352
N473	F533	S593	S713	G773	L834	Q53	V113	Q173	G233	K293	K353
S474	S534	G594	R714	L774	F835	S54	M114	S174	N234	N294	L354
F475	I535	V595	V715	L775	P836	K55	I115	I175	A235	K295	T355
A476	L536	L596	L716	E776	K837	E56	Y116	L176	K236	K296	G356
Q477	E537	T597	T717	E777	L838	G57	T117	T177	T237	P297	A357
L478	E538	K598	A718	M778	R839	G58	Y118	T178	V238	E298	V358
C479	E539	N599	D719	R779	K839	S59	S119	G179	R239	L299	K359
I480	C540	K600	F720	D780	L841	V60	G120	E180	N240	T300	H360
N481	M541	D601	K721	L781	L842	T61	L121	S181	D241	D301	Y361
F482	P542	A652	Q722	K782	K843	V62	F122	G182	N242	K302	G362
T483	L603	N663	R723	L783		K63	C123	A183	S243	L303	N363

● Molecule 1: SKELETAL MUSCLE MYOSIN II



D4	T64	V124	G184	S244	L304
A5	E65	T125	K185	R245	T305
E6	G66	V126	T186	F246	T306
M7	G67	M127	V187	G247	T307
A8	E68	M128	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	H312
A13	K73	P133	T193	H253	H313
A14	E74	V134	Q194	F254	Y314
P15	D75	Y135	Y195	G255	V315
Y16	Q76	M136	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	V81	L141	L41	A261	T321
K22	P82	A142	S202	S262	V322
E23	P83	Y143	G203	A263	P323
R24	K84	L144	E204	D264	S324
I25	Y85	G145	K205	L265	I325
E26	D86	K146	K206	E266	D326
A27	K87	K147	K207	T267	D327
Q28	T88	R148	E208	T268	Q328
N29	E89	Q149	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	M161	Q221	A281	L341
H42	Y102	A162	I222	E282	G342
P43	L103	L163	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	L287	E347
V48	E108	T168	L228	F288	K348
R49	R109	D169	L229	Y289	T349
G50	Y110	R170	E230	Q290	A350
T51	A111	E171	A231	L291	I351
I52	A112	M172	F232	M292	Y352
Q53	V113	Q173	G233	K293	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
P59	S119	G179	R239	L299	K359
G120	E180	N240	N240	T300	H360
T61	L121	S181	D241	D301	Y361
V62	F122	G182	N242	K302	G362
K63	C123	A183	S243	L303	N363

A784	L664	Y724	L784	M604	K544	N484	N424	L364	L304
R725	R665	R725	R784	E605	A545	E485	S425	K365	L305
V726	S666	V726	I786	T606	T546	K486	V426	F366	T306
L727	T667	L727	T787	V607	D547	L487	G427	K367	T307
N728	H668	N728	T788	I608	T548	Q488	A428	Q368	N308
A729	P669	A729	T789	G609	S549	Q489	L429	K369	P309
S730	H670	S730	T790	L610	F550	F490	A430	Q370	N308
A731	F671	A731	T791	V611	K551	F491	K431	R371	D311
I732	V672	I732	A792	Q612	N552	N492	A432	E372	Y312
P733	R673	P733	R793	K613	K553	H493	V433	E373	H313
E734	C674	E734	C794	S614	L554	H494	Y434	Q374	Y314
G735	L675	G735	R795	S615	Y555	M495	E435	A375	V315
Q736	L676	Q736	G796	V616	D556	F496	K436	E376	S316
F737	P677	F737	F797	K617	E557	V497	M437	F377	E317
M738	N678	M738	L798	T618	H558	L498	F438	D378	G318
D739	E679	D739	M799	L619	L559	E499	L439	G379	E319
R800	T680	R800	S740	A620	G560	Q500	A440	T380	I320
V801	K681	V801	K741	L621	K561	E501	M441	E381	T321
E802	T682	E802	K742	L622	S562	E502	V442	V382	V322
R803	P683	R803	A743	F623	N563	E603	I443	A383	P323
R804	S744	R804	G804	A624	N564	K504	R444	D384	A324
A805	A685	A805	E745	T625	F565	K505	I445	K385	I325
M806	N686	M806	K746	V626	Q566	E506	N446	A386	D326
V807	E687	V807	L747	G627	K567	G507	Q447	A387	D327
E808	L748	E808	H688	G628	P568	I508	Q448	Y388	Q328
R809	E689	R809	G749	E629	K569	E509	L449	L389	E329
R810	L690	R810	G750	A630	P570	W510	D450	M390	E330
G751	V691	G751	V751	E631	A571	E511	T451	G391	L331
S812	D752	S812	D752	G632	K572	F512	K452	L392	M332
I813	H693	I813	V753	G633	G573	I513	Q453	N393	A333
F814	Q694	F814	D754	G634	K574	D514	P454	S394	T334
C815	L695	C815	H755	G635	A575	F515	R455	A395	D335
L816	R696	L816	T756	G636	E576	G516	Q456	E396	S336
Q817	G697	Q817	Q757	K637	A577	M517	Y457	L397	A337
Y818	N698	Y818	F758	G638	H578	D518	F458	L398	I338
N819	G699	N819	A759	G639	F579	L519	I459	K399	D339
F760	R700	F760	R760	G640	S580	A520	G460	A400	I340
G761	L701	G761	L701	K641	L581	A521	V461	L401	L341
S822	E702	S822	H762	K642	V582	C522	L462	C402	G342
T763	G703	T763	T763	G643	H583	I523	D463	Y403	F343
K764	I704	K764	M824	S644	Y584	E524	I464	P404	S344
R705	R705	R705	N825	S645	A585	L525	A465	R405	A345
F766	T706	F766	R826	F646	G586	I526	G466	V406	D346
F767	C707	F767	K827	Q647	T587	E527	F467	G407	E347
R708	K768	R708	H828	T648	V588	K528	E468	V408	K348
K709	R649	K709	R829	V649	D589	P529	E469	G409	T349
P830	G770	P830	R830	S650	Y590	M530	I469	G409	T349
W831	F711	W831	R831	A651	N591	G531	F470	N410	A350
M832	L772	M832	L772	L651	I591	I532	D471	E411	I351
K833	S713	K833	K773	F653	S593	F533	N473	A412	Y352
L834	R714	L834	L774	R654	G594	S534	S474	V413	K353
R715	V715	R715	L775	E655	N595	I535	F475	L415	T355
L716	L716	L716	E776	N656	L596	L536	E476	G416	G356
E777	Y717	E777	K837	L657	E597	E537	Q477	E417	A357
A718	A718	A718	R838	N658	K598	E538	L478	T418	V358
R779	D719	R779	R839	K659	N599	E539	C479	V419	M359
P840	F720	P840	R840	L660	K600	C540	I480	S420	H360
L841	K721	L841	D781	M661	D601	M541	L480	E421	Y361
L842	Q722	L842	K782	A662	P602	F542	S420	G422	G362
R843	R723	R843	L793	N663	L603	P543	T483	V423	N363

● Molecule 1: SKELETAL MUSCLE MYOSIN II



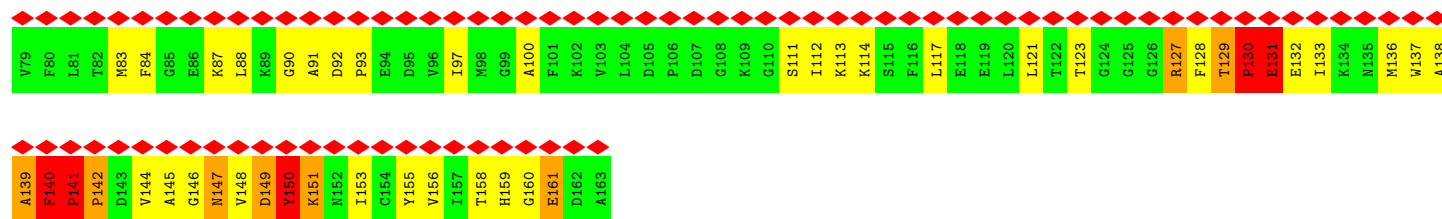
G184	K185	T186	V187	N188	T189	K190	R191	V192	I193	Q194	Y195	F196	A197	T198	I199	A200	A201	S202	G203	E204	K205	K206	K207	E208	E209	Q210	S211	G212	K213	M214	Q215	G216	T217	L218	E219	D220	Q221	I222	I223	S224	A225	N226	P227	L228	L229	E230	A231	F232	G233	N234	A235	K236	T237	V238	R239	N240	D241	N242	S243	
V124	T125	V126	N127	P128	Y129	K130	L131	L132	P133	V134	Y135	N136	P137	K138	V139	V140	L141	A142	Y143	R144	G145	K146	K147	L148	Q149	E150	A151	P152	P153	H154	I155	F156	S157	N158	S159	D160	N161	A162	Y163	Q164	F165	M166	L167	T168	D169	R170	E171	N172	Q173	S174	I175	L176	T177	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	H85	D86	K87	L88	E89	D90	M91	A92	M93	N94	T95	H96	L97	H98	E99	D100	A101	V102	L103	Y104	N105	L106	I107	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	

- Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

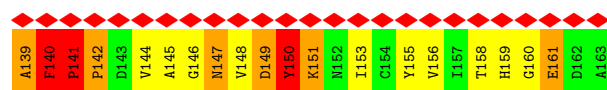
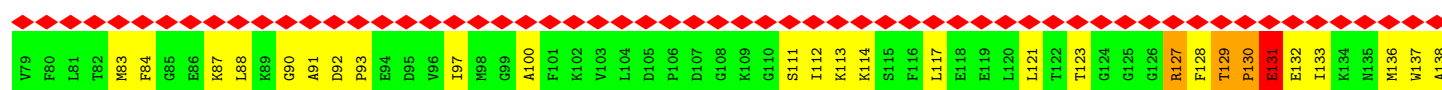
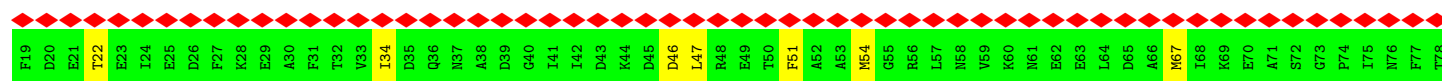
Frequency	Percentage
Daily	67%
Weekly	23%
Monthly	7%







• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN



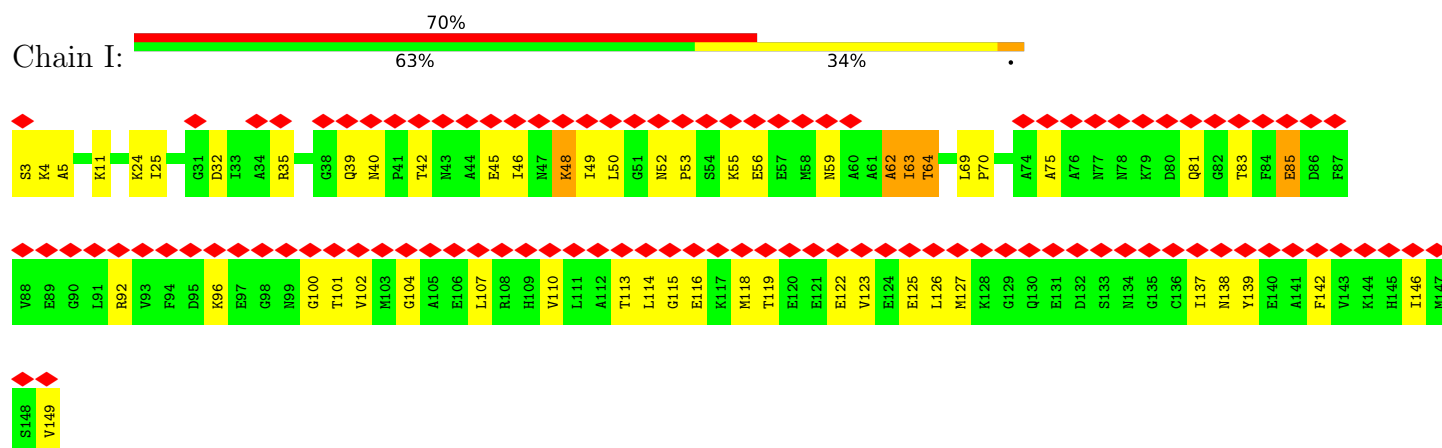
• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN



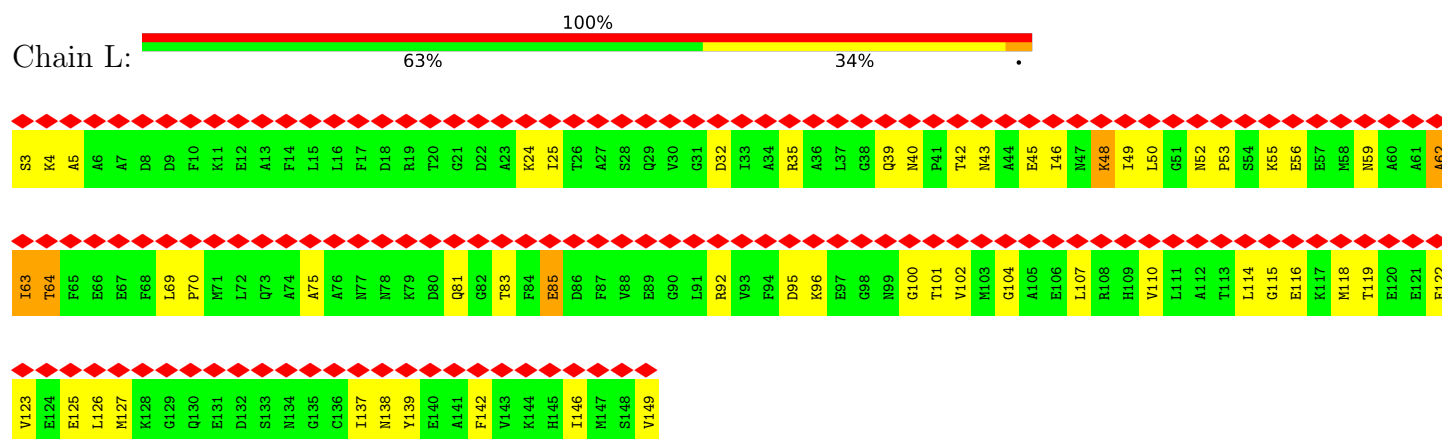
• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN



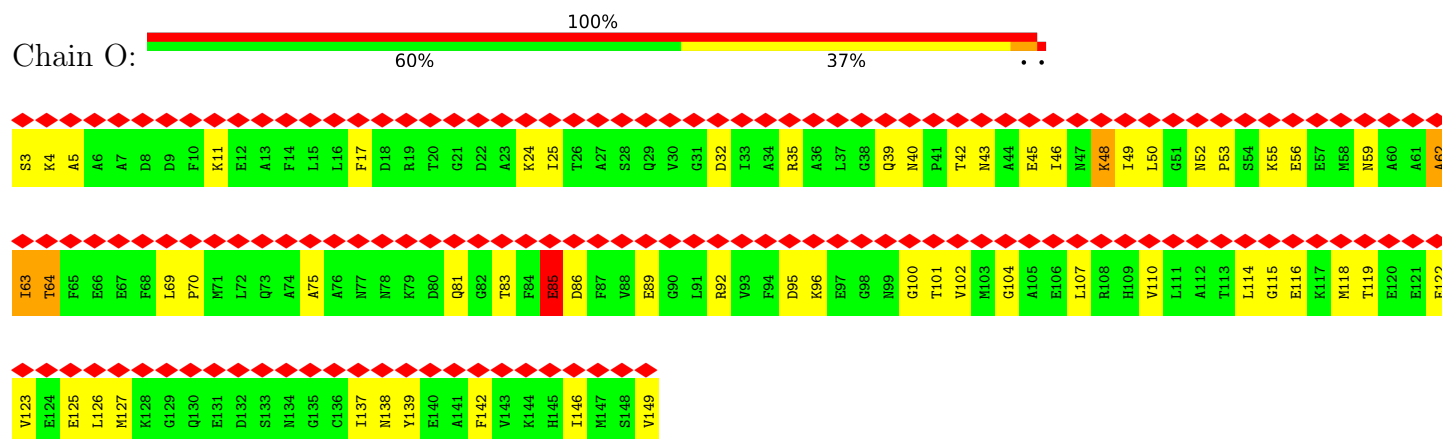
- Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN



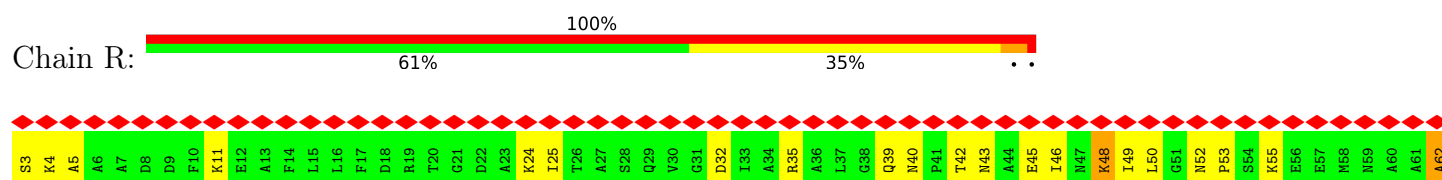
- Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN

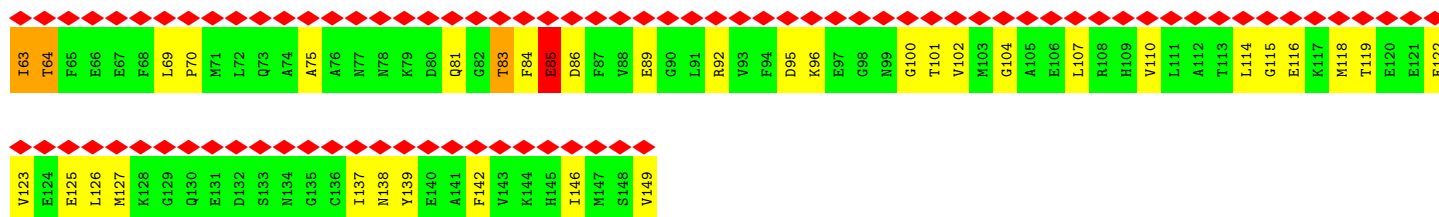


- Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN

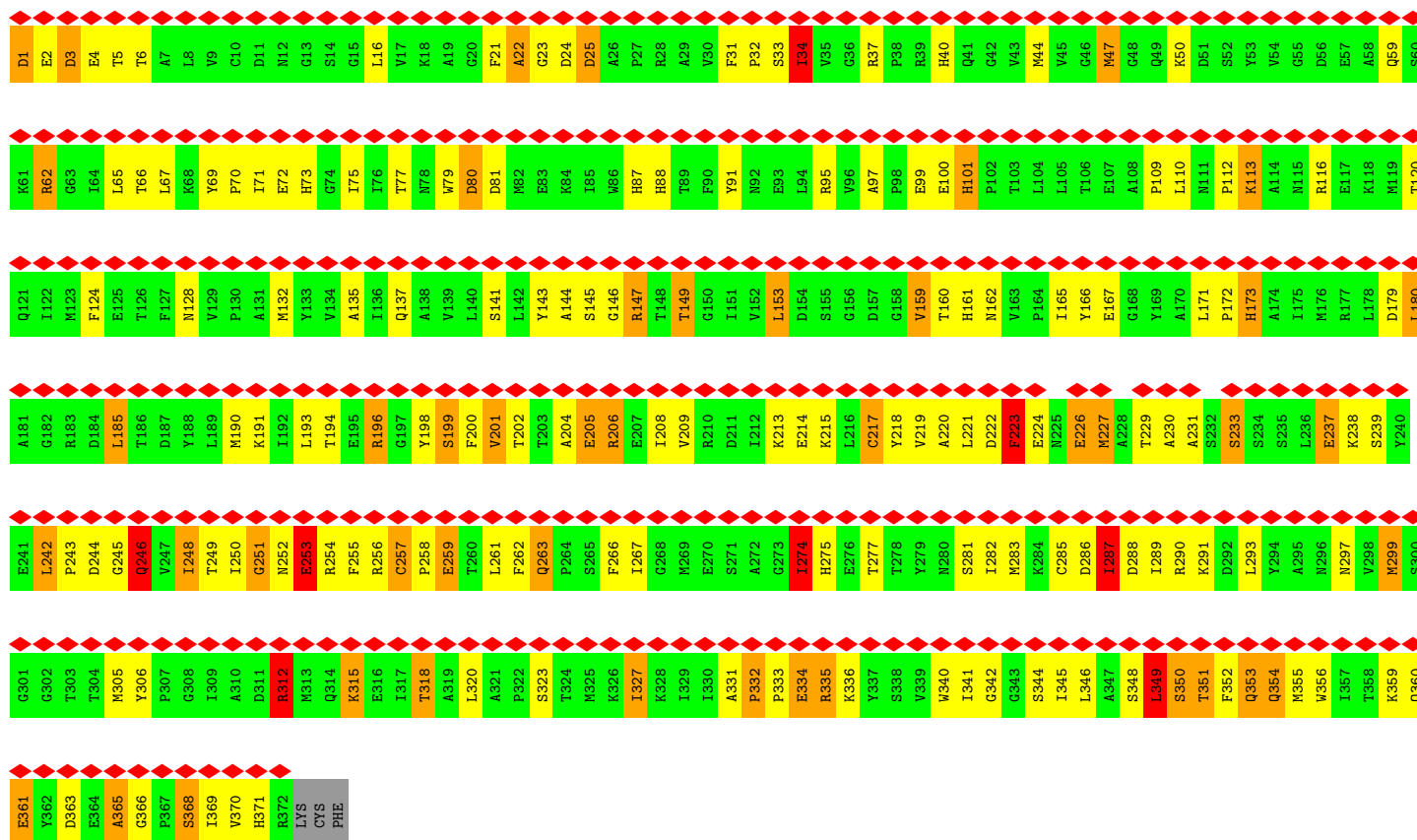


- Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN

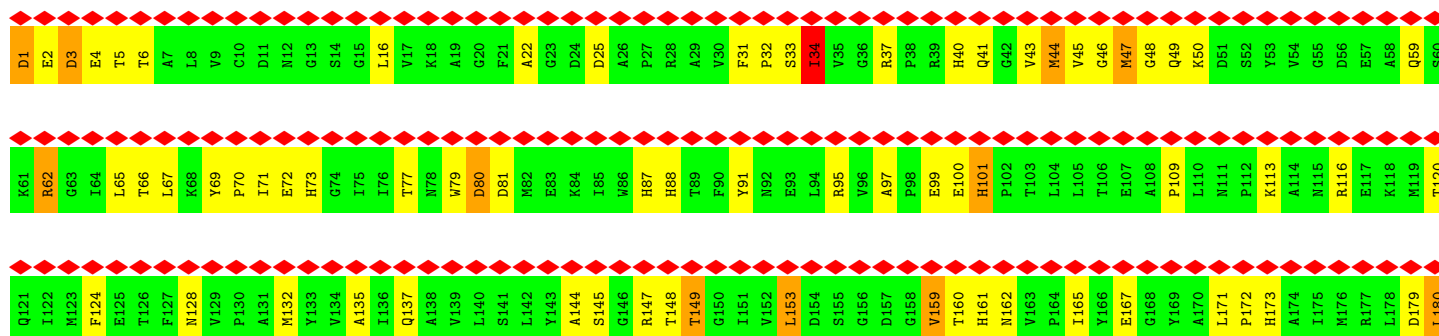


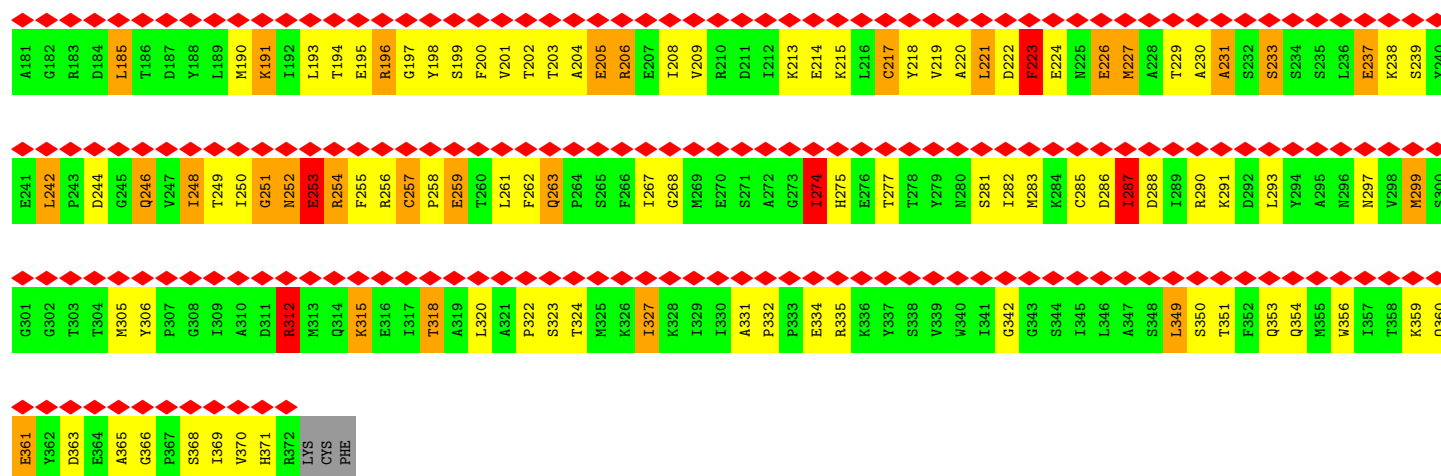


• Molecule 4: SKELETAL MUSCLE ACTIN

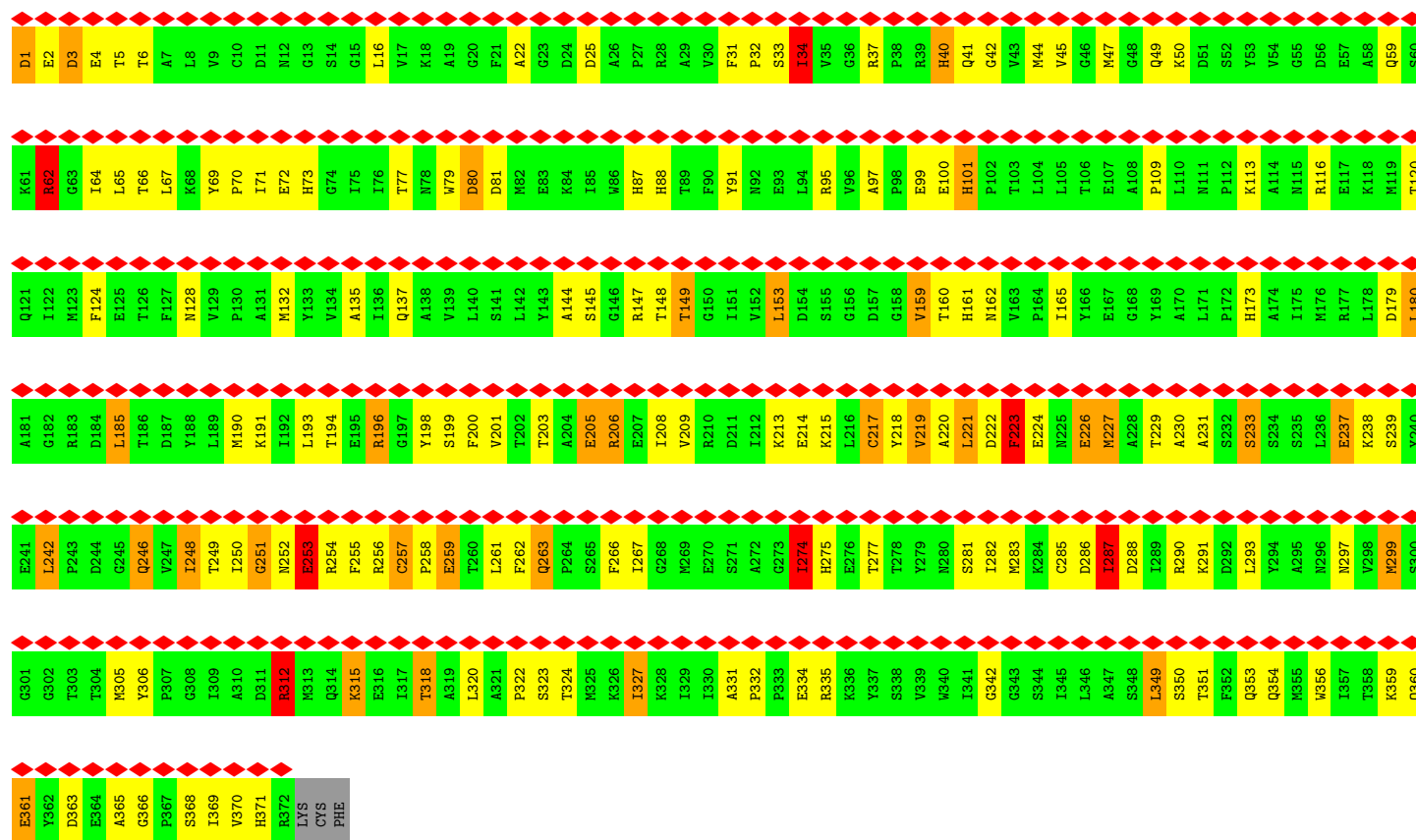


• Molecule 4: SKELETAL MUSCLE ACTIN



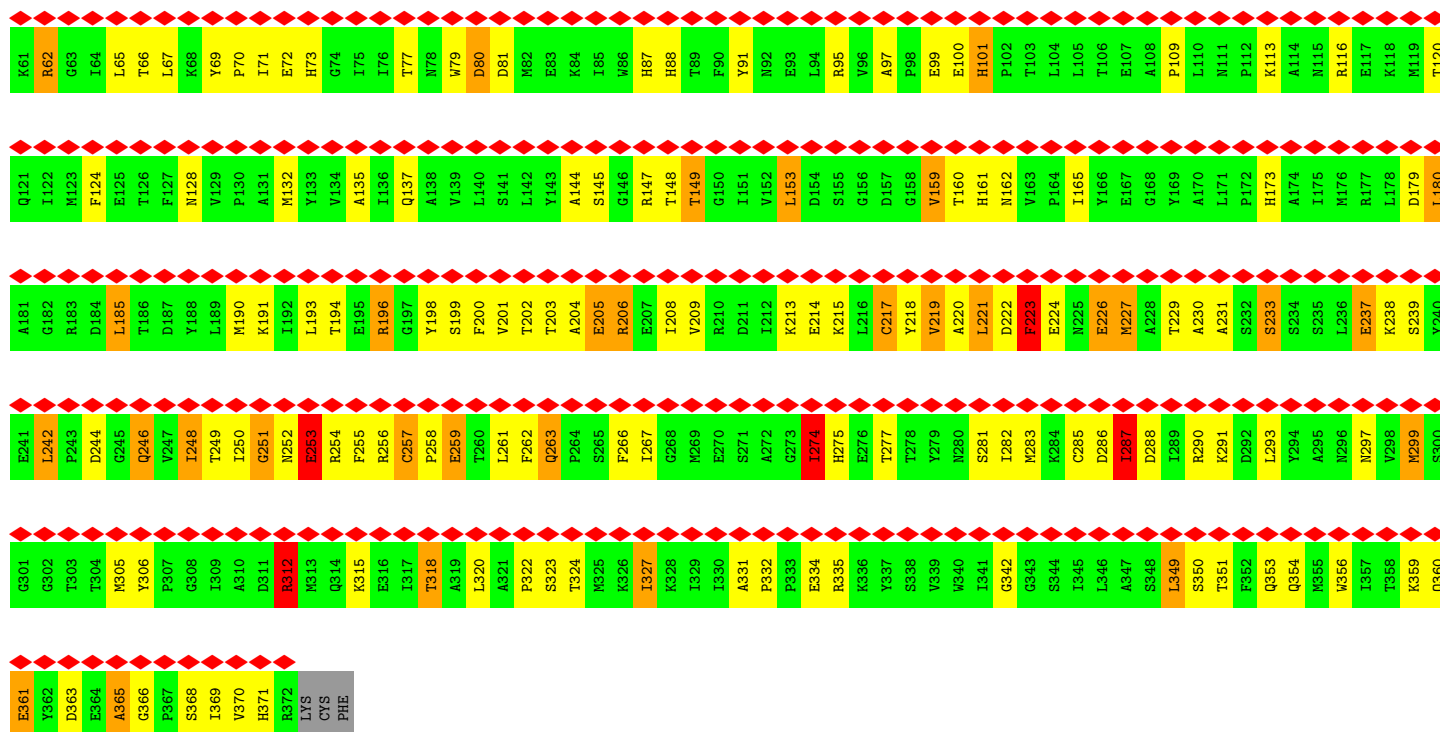


• Molecule 4: SKELETAL MUSCLE ACTIN

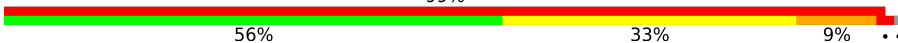


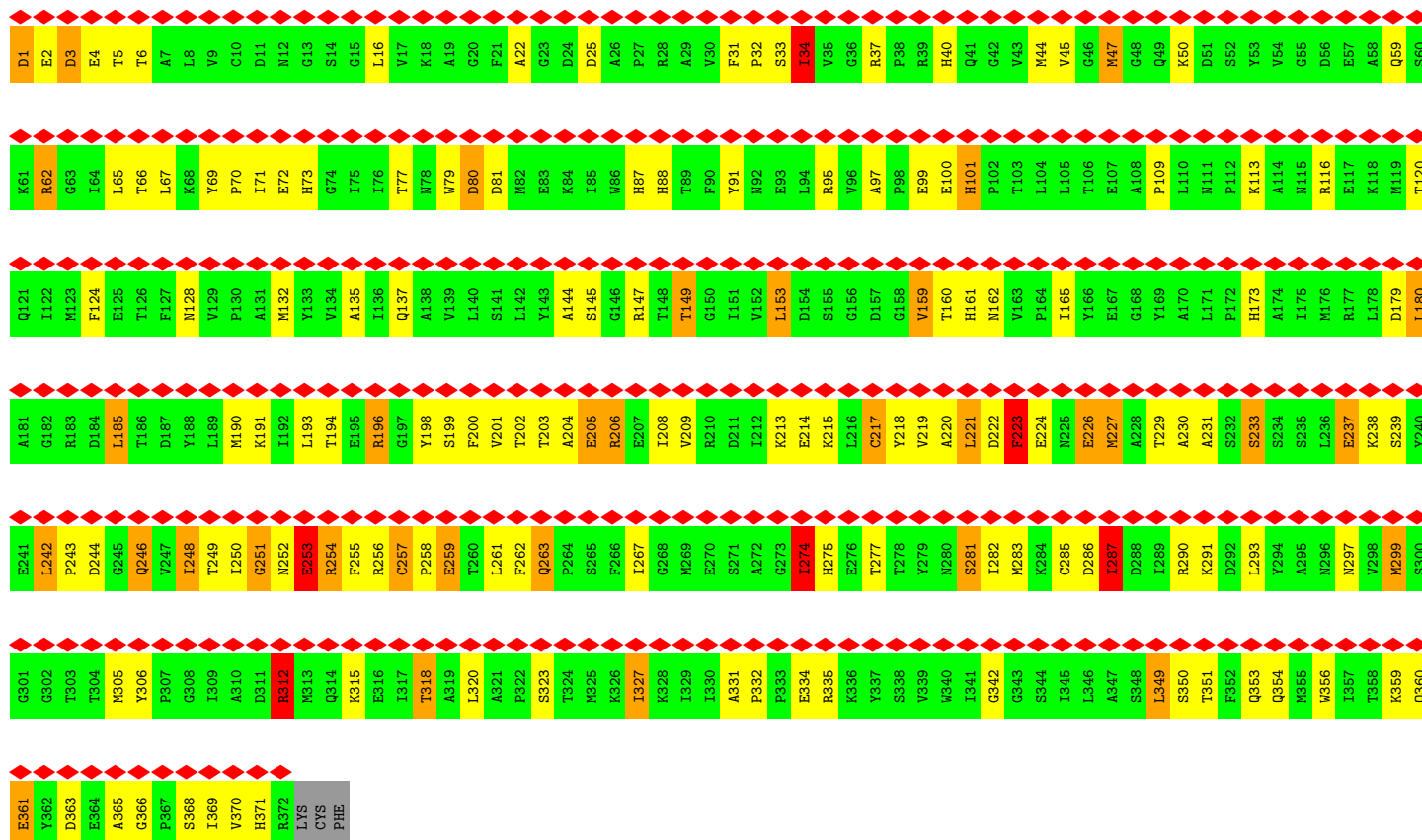
• Molecule 4: SKELETAL MUSCLE ACTIN



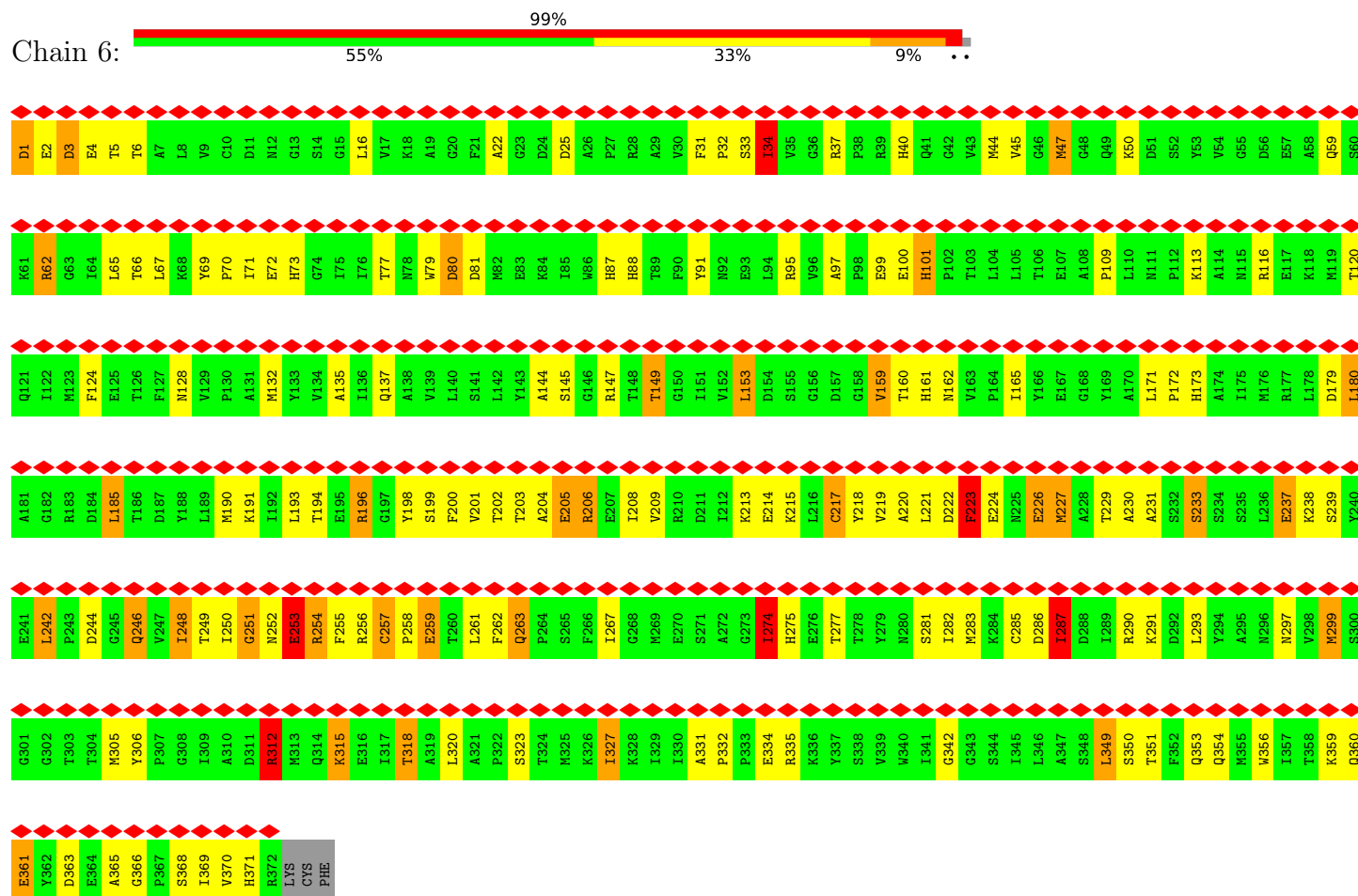


• Molecule 4: SKELETAL MUSCLE ACTIN

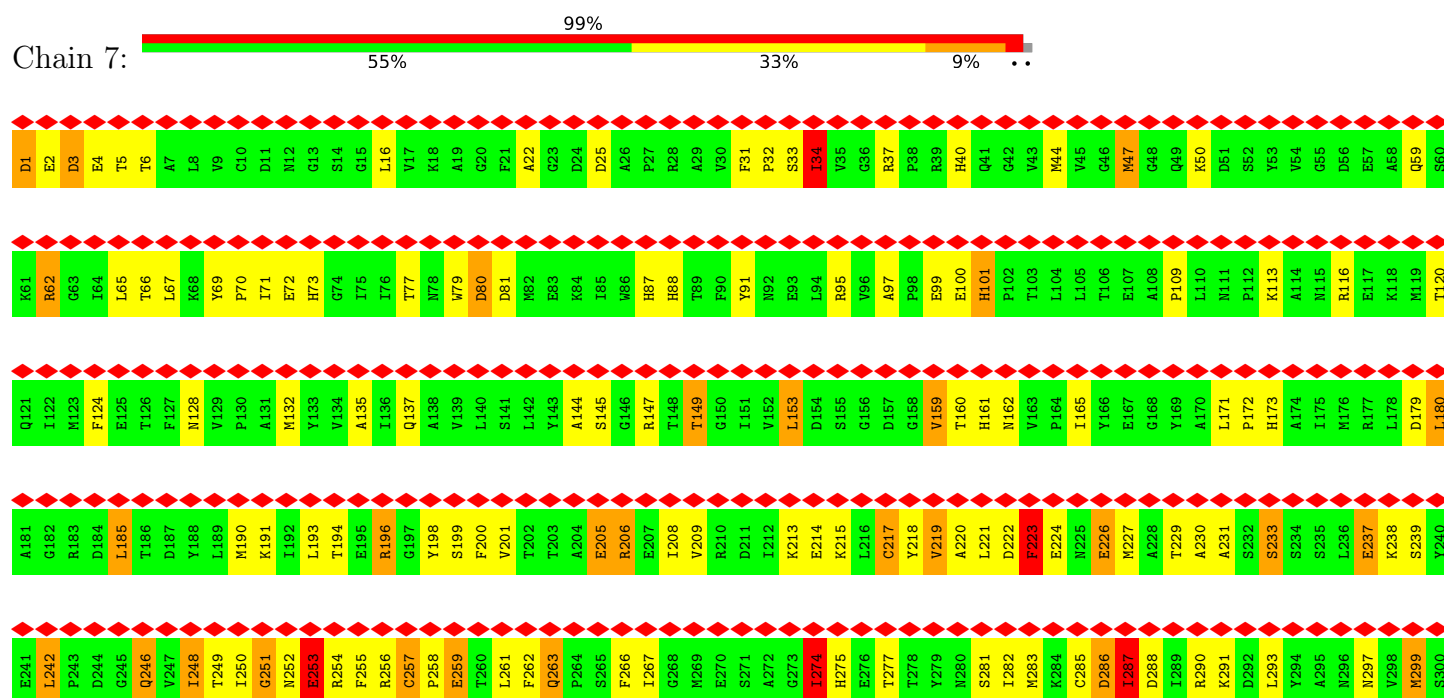
Chain 5: 



• Molecule 4: SKELETAL MUSCLE ACTIN

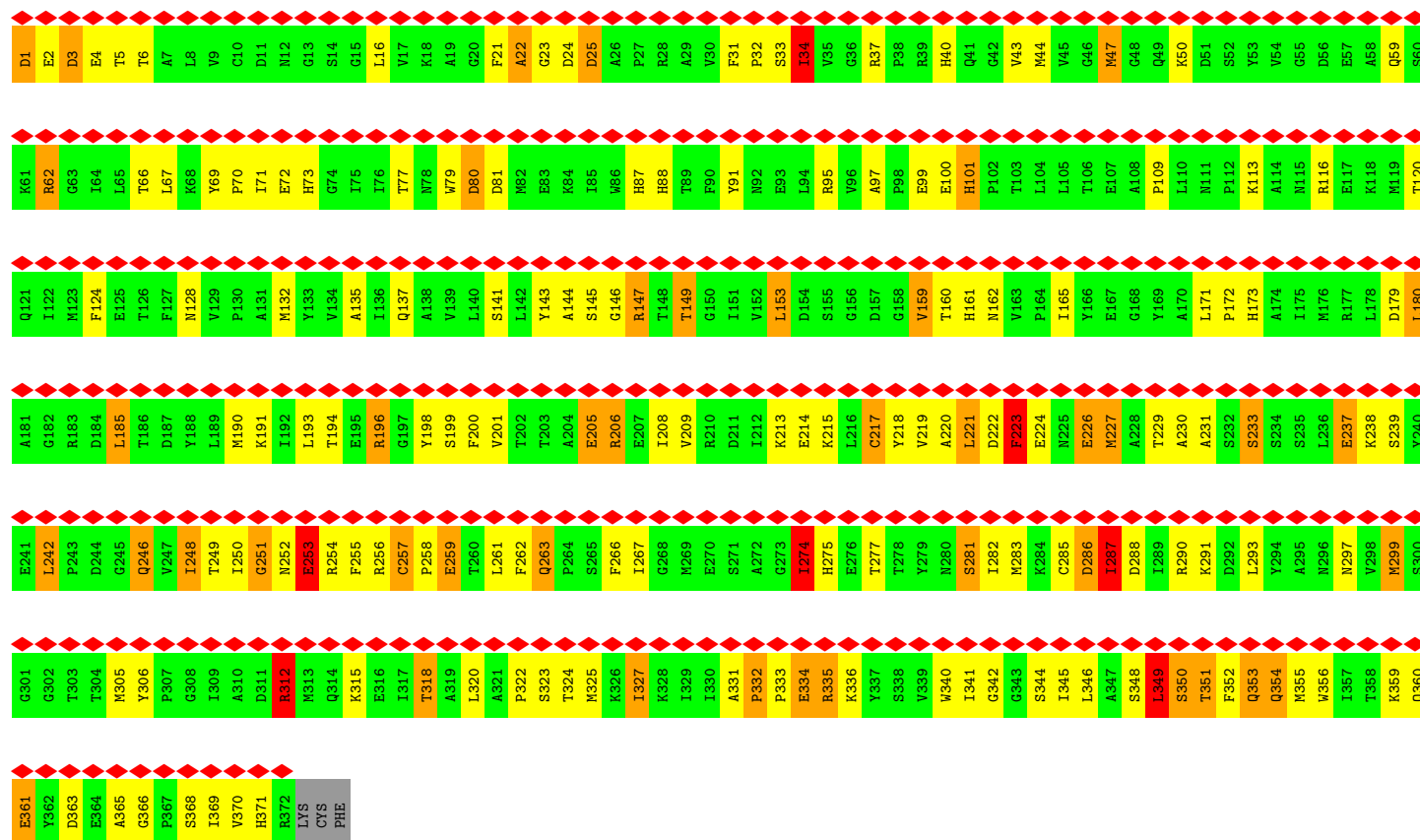


• Molecule 4: SKELETAL MUSCLE ACTIN

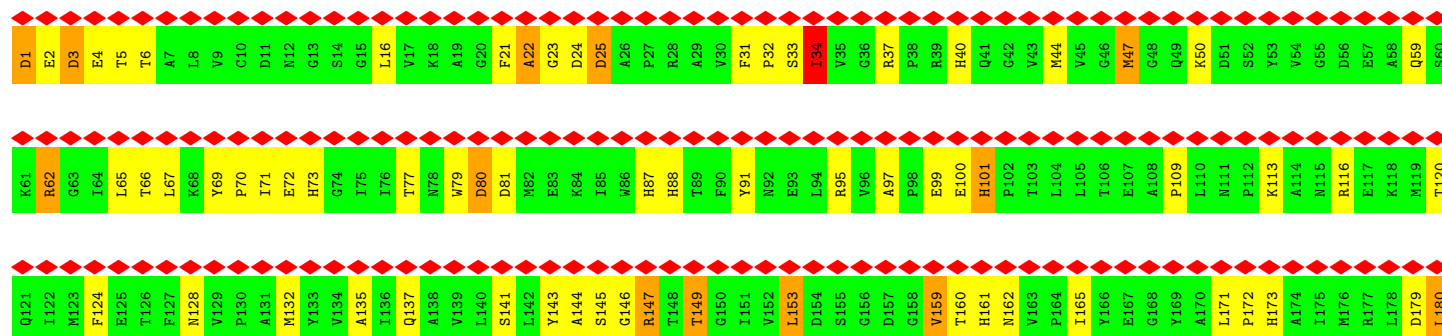


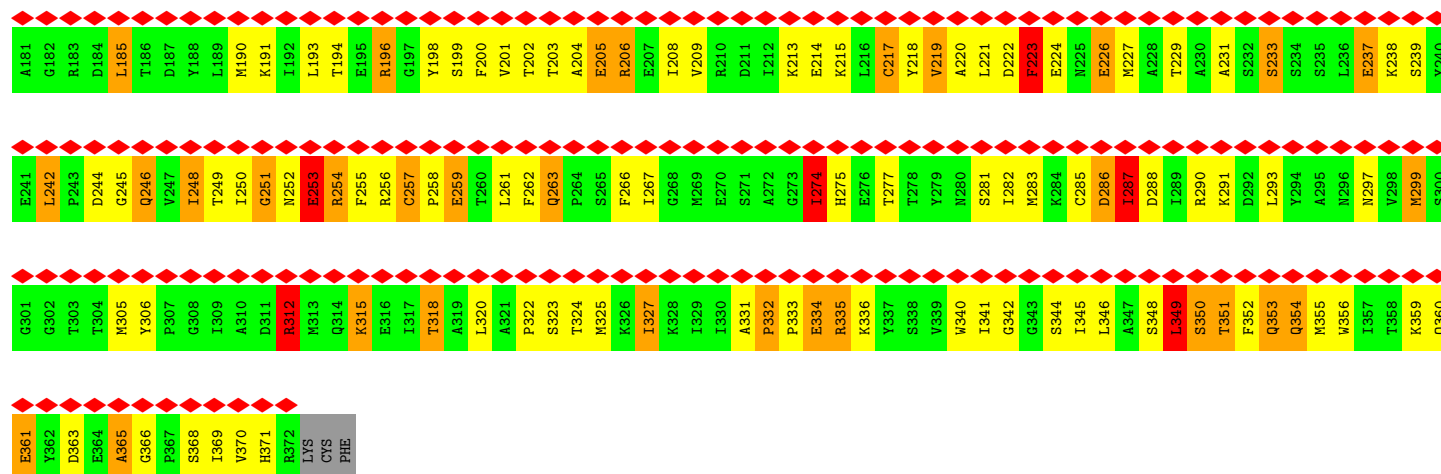


• Molecule 4: SKELETAL MUSCLE ACTIN

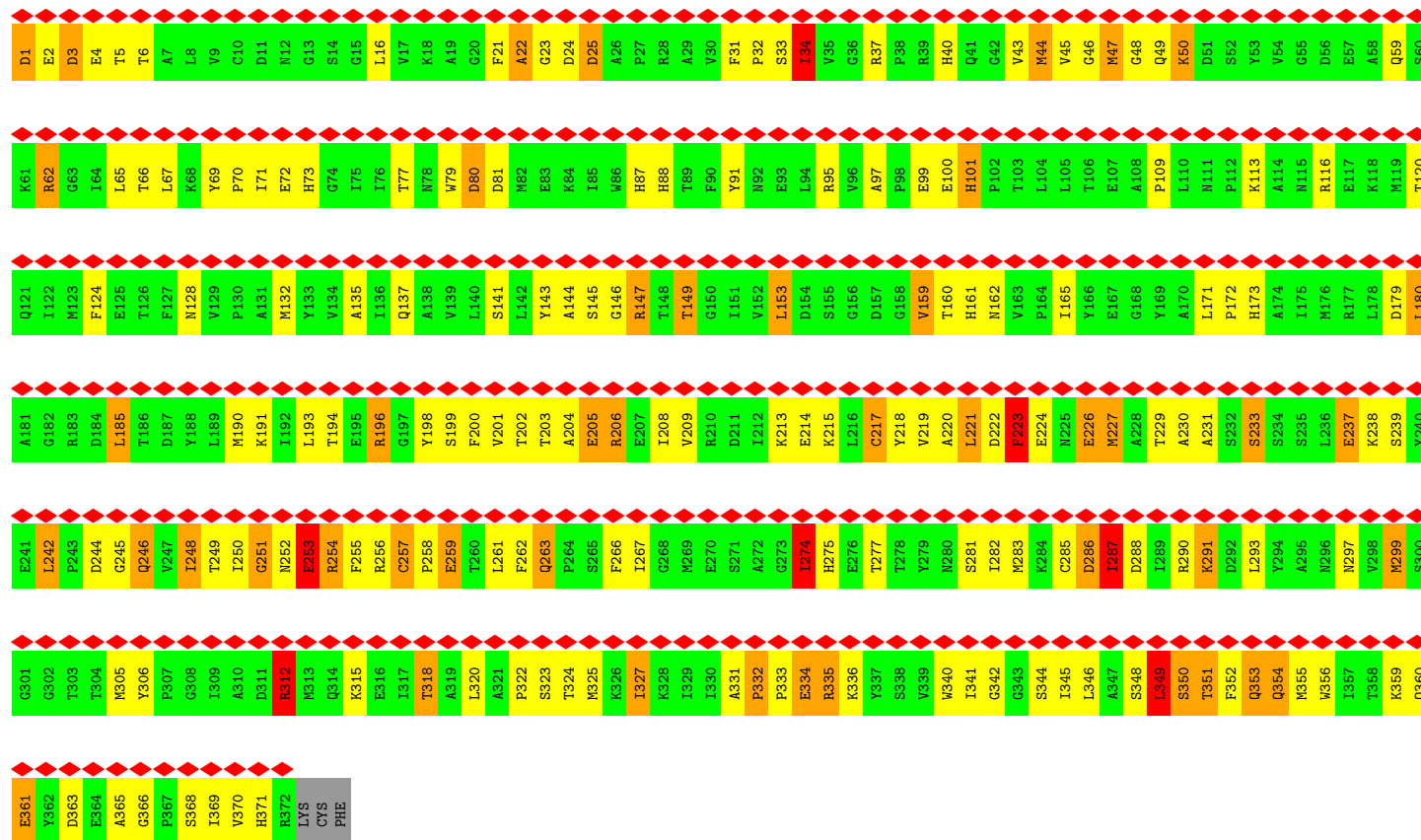


• Molecule 4: SKELETAL MUSCLE ACTIN



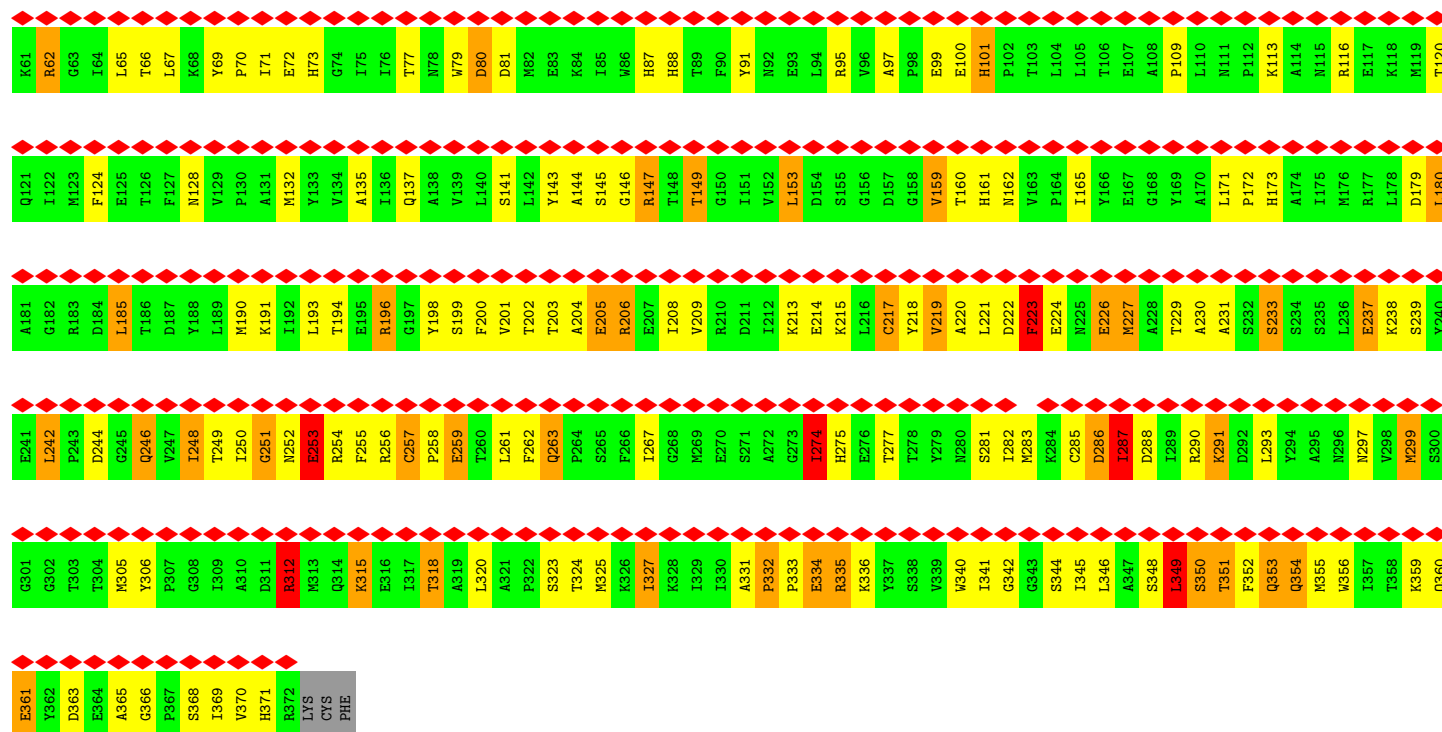


• Molecule 4: SKELETAL MUSCLE ACTIN

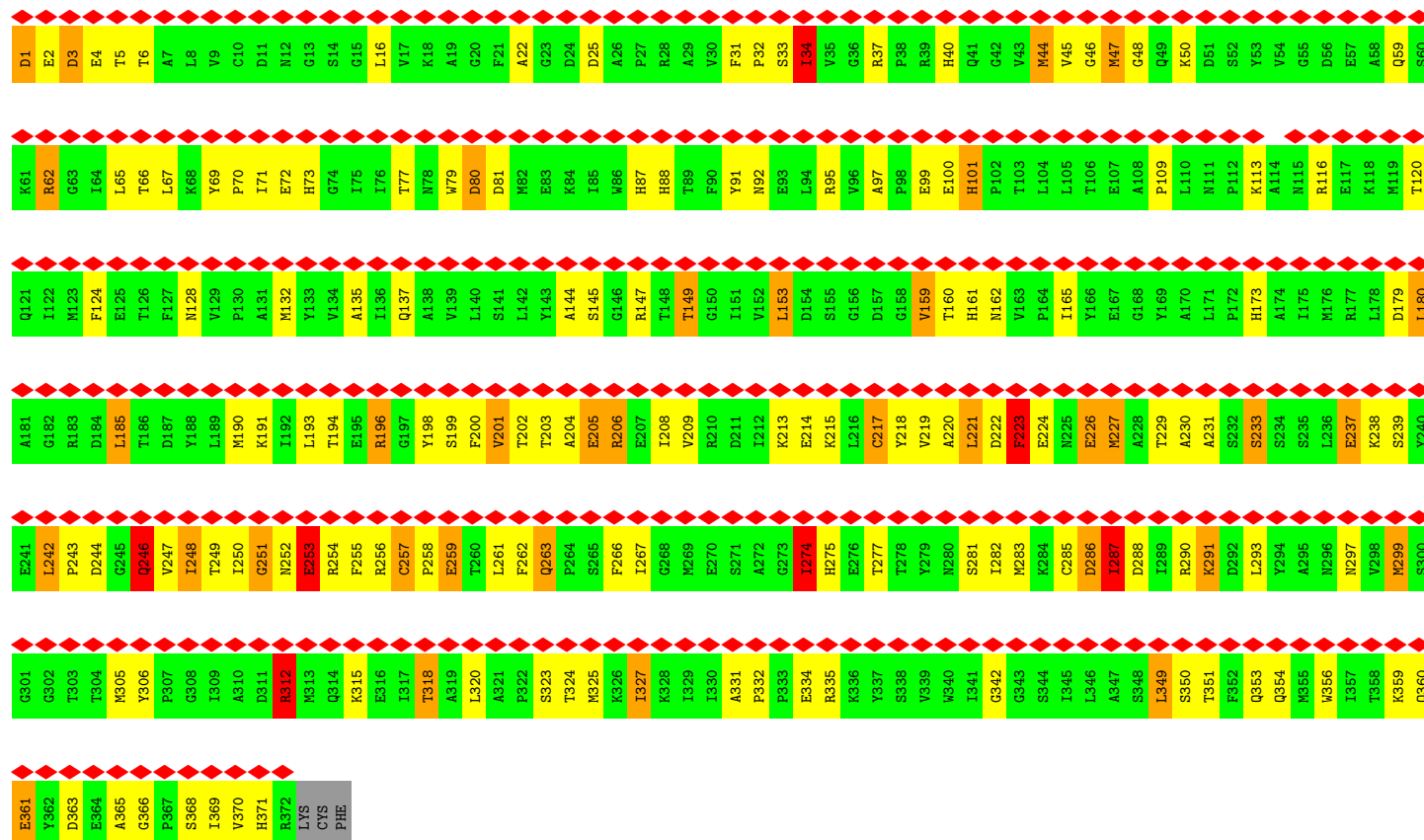


• Molecule 4: SKELETAL MUSCLE ACTIN





• Molecule 4: SKELETAL MUSCLE ACTIN



E361	G301
Y362	G302
D363	T303
E364	T304
A365	M305
G366	Y306
P367	P307
S368	G308
T369	T309
V370	A310
H371	D311
R372	R312
LYS	M313
CYS	Q314
PHE	K315
	E316
	I317
	T318
	A319
	L320
	A321
	P322
	S323
	T324
	M325
	K326
	I327
	K328
	I329
	T330
	A331
	P332
	P333
	E334
	R335
	K336
	Y337
	S338
	V339
	V340
	I341
	G342
	G343
	S344
	I345
	L346
	A347
	S348
	L349
	S350
	T351
	F352
	Q353
	Q354
	M355
	V356
	I357
	T358
	K359
	Q360

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	1.84	39/6448 (0.6%)	2.13	152/8729 (1.7%)
1	D	1.84	39/6448 (0.6%)	2.12	146/8729 (1.7%)
1	G	1.84	41/6449 (0.6%)	2.13	156/8732 (1.8%)
1	J	1.85	43/6449 (0.7%)	2.17	149/8732 (1.7%)
1	M	2.01	43/6449 (0.7%)	2.23	159/8732 (1.8%)
1	P	1.88	40/6448 (0.6%)	2.22	157/8729 (1.8%)
2	B	1.36	15/1148 (1.3%)	1.46	21/1548 (1.4%)
2	E	1.37	16/1148 (1.4%)	1.47	21/1548 (1.4%)
2	H	1.37	16/1148 (1.4%)	1.47	21/1548 (1.4%)
2	K	1.37	14/1148 (1.2%)	1.47	21/1548 (1.4%)
2	N	1.35	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	5/1525 (0.3%)
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	O	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	1	1.17	13/2968 (0.4%)	2.00	99/4023 (2.5%)
4	2	1.17	13/2968 (0.4%)	2.00	98/4023 (2.4%)
4	3	1.17	13/2968 (0.4%)	2.00	98/4023 (2.4%)
4	4	1.17	13/2968 (0.4%)	2.00	99/4023 (2.5%)
4	5	1.17	13/2968 (0.4%)	2.00	98/4023 (2.4%)
4	6	1.17	13/2968 (0.4%)	2.00	97/4023 (2.4%)
4	7	1.17	12/2968 (0.4%)	2.00	97/4023 (2.4%)
4	8	1.17	13/2968 (0.4%)	2.00	102/4023 (2.5%)
4	9	1.17	13/2968 (0.4%)	2.00	98/4023 (2.4%)
4	V	1.17	13/2968 (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	98/4023 (2.4%)
4	Y	1.17	13/2968 (0.4%)	2.00	99/4023 (2.5%)
4	Z	1.17	13/2968 (0.4%)	2.00	98/4023 (2.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	1.50	542/93947 (0.6%)	1.99	2452/127143 (1.9%)

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	M	1	7
1	P	2	7
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	1	0	1
4	2	0	1
4	3	0	1
4	4	0	1
4	5	0	1
4	6	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	8	76

The worst 5 of 542 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	806	MET	C-N	48.52	1.95	1.33
1	A	648	THR	CB-OG1	42.70	2.12	1.43
1	M	648	THR	CB-OG1	42.67	2.12	1.43
1	J	648	THR	CB-OG1	42.66	2.12	1.43
1	G	648	THR	CB-OG1	42.66	2.12	1.43

The worst 5 of 2452 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	-74.30	23.77	122.59
1	D	637	LYS	O-C-N	-74.29	23.78	122.59
1	P	637	LYS	O-C-N	-74.27	23.81	122.59
1	M	637	LYS	O-C-N	-74.26	23.83	122.59

5 of 8 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 76 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	6764	1554	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	6797	0	6764	1411	0
1	G	6797	0	6767	1583	0
1	J	6797	0	6762	1462	0
1	M	6797	0	6777	1457	0
1	P	6797	0	6777	1567	0
2	B	1127	0	1085	246	0
2	E	1127	0	1086	255	0
2	H	1127	0	1088	294	0
2	K	1127	0	1088	275	0
2	N	1127	0	1088	255	0
2	Q	1127	0	1088	261	0
3	C	1123	0	1083	194	0
3	F	1123	0	1083	171	0
3	I	1123	0	1083	192	0
3	L	1123	0	1083	180	0
3	O	1123	0	1084	188	0
3	R	1123	0	1083	268	0
4	1	2906	0	2855	397	0
4	2	2906	0	2862	273	0
4	3	2906	0	2864	142	0
4	4	2906	0	2863	184	0
4	5	2906	0	2865	97	0
4	6	2906	0	2865	105	0
4	7	2906	0	2866	84	0
4	8	2906	0	2857	320	0
4	9	2906	0	2855	351	0
4	V	2906	0	2851	380	0
4	W	2906	0	2851	394	0
4	X	2906	0	2862	198	0
4	Y	2906	0	2863	158	0
4	Z	2906	0	2853	405	0
All	All	94966	0	93665	11460	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 11460 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)
2:E:144:VAL:HG13	2:E:153:ILE:CD1	1.22	1.68
2:N:144:VAL:HG13	2:N:153:ILE:CD1	1.22	1.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:144:VAL:HG13	2:H:153:ILE:CD1	1.22	1.66
1:M:798:LEU:HD11	3:O:126:LEU:CD2	1.21	1.65
1:J:725:ARG:HE	1:J:733:PRO:CB	1.09	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%)	652 (83%)	111 (14%)	26 (3%)	3	21
1	D	789/840 (94%)	651 (82%)	112 (14%)	26 (3%)	3	21
1	G	791/840 (94%)	650 (82%)	114 (14%)	27 (3%)	3	21
1	J	791/840 (94%)	652 (82%)	112 (14%)	27 (3%)	3	21
1	M	791/840 (94%)	655 (83%)	109 (14%)	27 (3%)	3	21
1	P	789/840 (94%)	648 (82%)	114 (14%)	27 (3%)	3	21
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	N	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	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	1	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	7	38
4	2	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	7	38
4	3	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	7	38
4	4	370/375 (99%)	333 (90%)	31 (8%)	6 (2%)	7	38
4	5	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	7	38
4	6	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	7	38
4	7	370/375 (99%)	333 (90%)	31 (8%)	6 (2%)	7	38
4	8	370/375 (99%)	335 (90%)	29 (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
4	W	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	7	38
4	X	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	7	38
4	Y	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	7	38
4	Z	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	7	38
All	All	11636/12042 (97%)	10138 (87%)	1206 (10%)	292 (2%)	6	26

5 of 292 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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	672/672 (100%)	491 (73%)	181 (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	M	672/672 (100%)	491 (73%)	181 (27%)	0	3
1	P	672/672 (100%)	491 (73%)	181 (27%)	0	3
2	B	120/120 (100%)	120 (100%)	0	100	100
2	E	120/120 (100%)	120 (100%)	0	100	100
2	H	120/120 (100%)	120 (100%)	0	100	100
2	K	120/120 (100%)	119 (99%)	1 (1%)	73	80
2	N	120/120 (100%)	120 (100%)	0	100	100
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
3	I	117/117 (100%)	113 (97%)	4 (3%)	32	54
3	L	117/117 (100%)	113 (97%)	4 (3%)	32	54
3	O	117/117 (100%)	113 (97%)	4 (3%)	32	54
3	R	117/117 (100%)	113 (97%)	4 (3%)	32	54
4	1	315/318 (99%)	264 (84%)	51 (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	6	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%)	265 (84%)	50 (16%)	2	11
4	9	315/318 (99%)	264 (84%)	51 (16%)	2	11
4	V	315/318 (99%)	264 (84%)	51 (16%)	2	11
4	W	315/318 (99%)	264 (84%)	51 (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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9864/9906 (100%)	8041 (82%)	1823 (18%)	3 8

5 of 1823 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	12	GLU
4	Z	33	SER
4	1	299	MET
4	Y	291	LYS
4	V	283	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 291 such sidechains are listed below:

Mol	Chain	Res	Type
4	6	40	HIS
4	Z	41	GLN
4	7	40	HIS
4	V	360	GLN
1	J	29	ASN

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	A	764	1	9,10,11	0.81	0	6,11,13	0.36	0
1	MLY	G	35	1	9,10,11	0.75	0	6,11,13	0.38	0
1	MLY	D	130	1	9,10,11	0.79	0	6,11,13	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	M	130	1	9,10,11	0.77	0	6,11,13	0.73	0
1	MLY	J	553	1	9,10,11	0.65	0	6,11,13	0.53	0
1	MLY	D	827	1	9,10,11	0.65	0	6,11,13	0.47	0
1	MLY	P	617	1	9,10,11	0.90	0	6,11,13	0.34	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	0.80	0
1	MLY	A	782	1	9,10,11	0.83	0	6,11,13	0.37	0
1	MLY	D	49	1	9,10,11	1.00	1 (11%)	6,11,13	0.75	0
1	MLY	D	681	1	9,10,11	0.54	0	6,11,13	0.45	0
1	MLY	A	827	1	9,10,11	0.69	0	6,11,13	0.45	0
1	MLY	J	385	1	9,10,11	0.94	1 (11%)	6,11,13	0.43	0
1	MLY	D	87	1	9,10,11	1.06	1 (11%)	6,11,13	0.44	0
1	MLY	M	296	1	9,10,11	0.64	0	6,11,13	0.35	0
1	MLY	D	138	1	9,10,11	1.25	1 (11%)	6,11,13	0.83	0
1	MLY	A	55	1	9,10,11	0.72	0	6,11,13	0.80	0
1	MLY	A	295	1	9,10,11	0.78	0	6,11,13	0.35	0
1	MLY	D	551	1	9,10,11	0.53	0	6,11,13	0.20	0
1	MLY	A	107	1	9,10,11	0.49	0	6,11,13	0.33	0
1	MLY	D	782	1	9,10,11	0.82	0	6,11,13	0.34	0
1	MLY	A	833	1	9,10,11	1.10	1 (11%)	6,11,13	0.32	0
1	MLY	G	59	1	9,10,11	0.83	0	6,11,13	0.48	0
1	MLY	P	236	1	9,10,11	0.84	1 (11%)	6,11,13	0.48	0
1	MLY	P	486	1	9,10,11	0.66	0	6,11,13	0.39	0
1	MLY	D	768	1	9,10,11	0.74	0	6,11,13	0.40	0
1	MLY	P	59	1	9,10,11	0.85	0	6,11,13	0.49	0
1	MLY	A	236	1	9,10,11	0.84	1 (11%)	6,11,13	0.49	0
1	MLY	M	84	1	9,10,11	0.50	0	6,11,13	0.81	0
1	MLY	A	659	1	9,10,11	0.84	1 (11%)	6,11,13	0.60	0
1	MLY	D	190	1	9,10,11	1.18	2 (22%)	6,11,13	0.54	0
1	MLY	A	681	1	9,10,11	0.56	0	6,11,13	0.47	0
1	MLY	D	30	1	9,10,11	0.93	0	6,11,13	0.31	0
1	MLY	G	504	1	9,10,11	0.88	0	6,11,13	0.22	0
1	MLY	P	833	1	9,10,11	1.14	2 (22%)	6,11,13	0.30	0
1	MLY	J	272	1	9,10,11	0.90	1 (11%)	6,11,13	0.56	0
1	MLY	D	369	1	9,10,11	0.70	0	6,11,13	0.44	0
1	MLY	A	551	1	9,10,11	0.54	0	6,11,13	0.20	0
1	MLY	P	385	1	9,10,11	0.95	1 (11%)	6,11,13	0.45	0
1	MLY	D	600	1	9,10,11	0.51	0	6,11,13	0.39	0
1	MLY	M	764	1	9,10,11	0.82	0	6,11,13	0.39	0
1	MLY	J	367	1	9,10,11	0.58	0	6,11,13	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	P	190	1	9,10,11	1.20	2 (22%)	6,11,13	0.53	0
1	MLY	P	295	1	9,10,11	0.75	0	6,11,13	0.38	0
1	MLY	G	415	1	9,10,11	0.74	0	6,11,13	0.19	0
1	MLY	M	19	1	9,10,11	1.05	1 (11%)	6,11,13	0.59	0
1	MLY	M	681	1	9,10,11	0.58	0	6,11,13	0.48	0
1	MLY	J	30	1	9,10,11	0.91	0	6,11,13	0.31	0
1	MLY	M	617	1	9,10,11	0.91	0	6,11,13	0.34	0
1	MLY	J	296	1	9,10,11	0.65	0	6,11,13	0.36	0
1	MLY	G	681	1	9,10,11	0.61	0	6,11,13	0.46	0
1	MLY	M	138	1	9,10,11	1.20	1 (11%)	6,11,13	0.82	0
1	MLY	G	353	1	9,10,11	0.88	0	6,11,13	0.82	0
1	MLY	P	659	1	9,10,11	0.82	0	6,11,13	0.58	0
1	MLY	G	617	1	9,10,11	0.90	0	6,11,13	0.35	0
1	MLY	A	59	1	9,10,11	0.85	0	6,11,13	0.46	0
1	MLY	J	436	1	9,10,11	0.94	1 (11%)	6,11,13	0.48	0
1	MLY	J	782	1	9,10,11	0.80	0	6,11,13	0.35	0
1	MLY	P	55	1	9,10,11	0.72	0	6,11,13	0.79	0
1	MLY	P	505	1	9,10,11	0.87	1 (11%)	6,11,13	0.33	0
1	MLY	D	553	1,4	9,10,11	0.66	0	6,11,13	0.55	0
1	MLY	J	348	1	9,10,11	0.76	0	6,11,13	0.47	0
1	MLY	D	659	1	9,10,11	0.83	1 (11%)	6,11,13	0.59	0
1	MLY	J	839	1	9,10,11	0.67	0	6,11,13	0.77	0
1	MLY	M	659	1	9,10,11	0.83	1 (11%)	6,11,13	0.58	0
1	MLY	G	486	1	9,10,11	0.66	0	6,11,13	0.40	0
1	MLY	D	505	1	9,10,11	0.78	0	6,11,13	0.34	0
1	MLY	J	768	1	9,10,11	0.79	0	6,11,13	0.42	0
1	MLY	M	190	1	9,10,11	1.23	2 (22%)	6,11,13	0.53	0
1	MLY	M	837	1	9,10,11	0.58	0	6,11,13	0.53	0
1	MLY	A	30	1	9,10,11	0.91	0	6,11,13	0.32	0
1	MLY	J	598	1	9,10,11	0.80	0	6,11,13	0.42	0
1	MLY	J	19	1	9,10,11	1.08	1 (11%)	6,11,13	0.57	0
1	MLY	M	295	1	9,10,11	0.75	0	6,11,13	0.36	0
1	MLY	D	55	1	9,10,11	0.72	0	6,11,13	0.80	0
1	MLY	D	436	1	9,10,11	0.96	1 (11%)	6,11,13	0.47	0
1	MLY	J	431	1	9,10,11	0.51	0	6,11,13	0.44	0
1	MLY	J	617	1	9,10,11	0.91	0	6,11,13	0.34	0
1	MLY	P	84	1	9,10,11	0.52	0	6,11,13	0.80	0
1	MLY	G	600	1	9,10,11	0.52	0	6,11,13	0.38	0
1	MLY	J	415	1	9,10,11	0.74	0	6,11,13	0.19	0
1	MLY	J	613	1	9,10,11	0.57	0	6,11,13	0.62	0
1	MLY	A	63	1	9,10,11	0.88	0	6,11,13	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	A	505	1	9,10,11	0.82	0	6,11,13	0.34	0
1	MLY	P	138	1	9,10,11	1.22	1 (11%)	6,11,13	0.82	0
1	MLY	A	296	1	9,10,11	0.60	0	6,11,13	0.34	0
1	MLY	A	598	1	9,10,11	0.86	1 (11%)	6,11,13	0.42	0
1	MLY	P	764	1	9,10,11	0.80	0	6,11,13	0.37	0
1	MLY	D	367	1	9,10,11	0.59	0	6,11,13	0.39	0
1	MLY	P	436	1	9,10,11	0.95	1 (11%)	6,11,13	0.47	0
1	MLY	A	504	1	9,10,11	0.88	0	6,11,13	0.22	0
1	MLY	J	528	1	9,10,11	0.89	0	6,11,13	0.65	0
1	MLY	P	827	1	9,10,11	0.69	0	6,11,13	0.47	0
1	MLY	M	59	1	9,10,11	0.85	0	6,11,13	0.48	0
1	MLY	A	768	1	9,10,11	0.77	0	6,11,13	0.40	0
1	MLY	D	486	1	9,10,11	0.68	0	6,11,13	0.41	0
1	MLY	P	35	1	9,10,11	0.71	0	6,11,13	0.38	0
1	MLY	M	505	1	9,10,11	0.86	1 (11%)	6,11,13	0.34	0
1	MLY	M	30	1	9,10,11	0.90	0	6,11,13	0.31	0
1	MLY	D	504	1	9,10,11	0.87	0	6,11,13	0.21	0
1	MLY	G	63	1	9,10,11	0.87	0	6,11,13	0.44	0
1	MLY	P	415	1	9,10,11	0.72	0	6,11,13	0.19	0
1	MLY	G	837	1	9,10,11	0.59	0	6,11,13	0.54	0
1	MLY	J	504	1	9,10,11	0.84	0	6,11,13	0.24	0
1	MLY	P	504	1	9,10,11	0.85	0	6,11,13	0.24	0
1	MLY	G	367	1	9,10,11	0.60	0	6,11,13	0.38	0
1	MLY	D	348	1	9,10,11	0.77	0	6,11,13	0.47	0
1	MLY	M	551	1	9,10,11	0.53	0	6,11,13	0.18	0
1	MLY	M	415	1	9,10,11	0.77	0	6,11,13	0.19	0
1	MLY	A	528	1	9,10,11	0.89	0	6,11,13	0.67	0
1	MLY	P	369	1	9,10,11	0.71	0	6,11,13	0.45	0
1	MLY	A	600	1	9,10,11	0.52	0	6,11,13	0.39	0
1	MLY	A	348	1	9,10,11	0.79	0	6,11,13	0.48	0
1	MLY	D	63	1	9,10,11	0.86	0	6,11,13	0.45	0
1	MLY	A	353	1	9,10,11	0.88	0	6,11,13	0.81	0
1	MLY	D	598	1	9,10,11	0.83	0	6,11,13	0.42	0
1	MLY	D	19	1	9,10,11	1.06	1 (11%)	6,11,13	0.56	0
1	MLY	G	272	1	9,10,11	0.87	1 (11%)	6,11,13	0.54	0
1	MLY	J	49	1	9,10,11	0.99	1 (11%)	6,11,13	0.75	0
1	MLY	J	505	1	9,10,11	0.86	1 (11%)	6,11,13	0.33	0
1	MLY	J	659	1	9,10,11	0.81	0	6,11,13	0.57	0
1	MLY	G	598	1	9,10,11	0.82	0	6,11,13	0.41	0
1	MLY	M	598	1	9,10,11	0.83	0	6,11,13	0.42	0
1	MLY	P	87	1	9,10,11	1.10	1 (11%)	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	D	617	1	9,10,11	0.91	0	6,11,13	0.35	0
1	MLY	M	768	1	9,10,11	0.78	0	6,11,13	0.42	0
1	MLY	D	613	1	9,10,11	0.59	0	6,11,13	0.61	0
1	MLY	J	353	1	9,10,11	0.86	0	6,11,13	0.80	0
1	MLY	M	553	1	9,10,11	0.66	0	6,11,13	0.53	0
1	MLY	D	385	1	9,10,11	0.92	1 (11%)	6,11,13	0.45	0
1	MLY	M	236	1	9,10,11	0.83	1 (11%)	6,11,13	0.48	0
1	MLY	D	236	1	9,10,11	0.83	1 (11%)	6,11,13	0.47	0
1	MLY	M	486	1	9,10,11	0.65	0	6,11,13	0.40	0
1	MLY	P	528	1	9,10,11	0.89	0	6,11,13	0.66	0
1	MLY	P	598	1	9,10,11	0.82	0	6,11,13	0.42	0
1	MLY	G	19	1	9,10,11	1.03	1 (11%)	6,11,13	0.60	0
1	MLY	M	782	1	9,10,11	0.81	0	6,11,13	0.38	0
1	MLY	G	87	1	9,10,11	1.12	1 (11%)	6,11,13	0.42	0
1	MLY	J	369	1	9,10,11	0.70	0	6,11,13	0.45	0
1	MLY	M	248	1	9,10,11	0.80	0	6,11,13	0.66	0
1	MLY	J	84	1	9,10,11	0.51	0	6,11,13	0.81	0
1	MLY	A	367	1	9,10,11	0.60	0	6,11,13	0.37	0
1	MLY	M	348	1	9,10,11	0.75	0	6,11,13	0.46	0
1	MLY	J	59	1	9,10,11	0.87	0	6,11,13	0.48	0
1	MLY	M	833	1	9,10,11	1.15	2 (22%)	6,11,13	0.29	0
1	MLY	D	833	1	9,10,11	1.12	1 (11%)	6,11,13	0.31	0
1	MLY	P	272	1	9,10,11	0.89	1 (11%)	6,11,13	0.57	0
1	MLY	P	551	1	9,10,11	0.53	0	6,11,13	0.20	0
1	MLY	J	600	1	9,10,11	0.53	0	6,11,13	0.38	0
1	MLY	A	272	1	9,10,11	0.89	1 (11%)	6,11,13	0.56	0
1	MLY	A	190	1	9,10,11	1.22	2 (22%)	6,11,13	0.52	0
1	MLY	P	553	1	9,10,11	0.65	0	6,11,13	0.53	0
1	MLY	P	63	1	9,10,11	0.85	0	6,11,13	0.43	0
1	MLY	D	59	1	9,10,11	0.84	0	6,11,13	0.49	0
1	MLY	G	431	1	9,10,11	0.52	0	6,11,13	0.46	0
1	MLY	J	107	1	9,10,11	0.49	0	6,11,13	0.35	0
1	MLY	M	436	1	9,10,11	0.97	1 (11%)	6,11,13	0.49	0
1	MLY	G	764	1	9,10,11	0.77	0	6,11,13	0.37	0
1	MLY	P	49	1	9,10,11	1.02	1 (11%)	6,11,13	0.75	0
1	MLY	P	681	1	9,10,11	0.55	0	6,11,13	0.47	0
1	MLY	P	296	1	9,10,11	0.64	0	6,11,13	0.35	0
1	MLY	A	837	1	9,10,11	0.61	0	6,11,13	0.55	0
1	MLY	J	236	1	9,10,11	0.84	1 (11%)	6,11,13	0.48	0
1	MLY	M	385	1	9,10,11	0.94	1 (11%)	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	P	782	1	9,10,11	0.81	0	6,11,13	0.36	0
1	MLY	J	681	1	9,10,11	0.57	0	6,11,13	0.46	0
1	MLY	A	49	1	9,10,11	0.95	1 (11%)	6,11,13	0.74	0
1	MLY	G	107	1	9,10,11	0.48	0	6,11,13	0.33	0
1	MLY	G	295	1	9,10,11	0.77	0	6,11,13	0.36	0
1	MLY	J	87	1	9,10,11	1.11	1 (11%)	6,11,13	0.42	0
1	MLY	M	63	1	9,10,11	0.88	0	6,11,13	0.44	0
1	MLY	A	613	1	9,10,11	0.58	0	6,11,13	0.62	0
1	MLY	A	35	1	9,10,11	0.74	0	6,11,13	0.38	0
1	MLY	A	839	1	9,10,11	0.64	0	6,11,13	0.82	0
1	MLY	D	415	1	9,10,11	0.74	0	6,11,13	0.19	0
1	MLY	G	505	1	9,10,11	0.82	0	6,11,13	0.36	0
1	MLY	M	431	1	9,10,11	0.52	0	6,11,13	0.45	0
1	MLY	M	504	1	9,10,11	0.84	0	6,11,13	0.23	0
1	MLY	P	130	1	9,10,11	0.75	0	6,11,13	0.73	0
1	MLY	J	837	1	9,10,11	0.57	0	6,11,13	0.57	0
1	MLY	D	84	1	9,10,11	0.51	0	6,11,13	0.81	0
1	MLY	A	138	1	9,10,11	1.21	1 (11%)	6,11,13	0.83	0
1	MLY	D	272	1	9,10,11	0.86	1 (11%)	6,11,13	0.57	0
1	MLY	A	369	1	9,10,11	0.73	0	6,11,13	0.47	0
1	MLY	G	30	1	9,10,11	0.89	0	6,11,13	0.30	0
1	MLY	J	295	1	9,10,11	0.75	0	6,11,13	0.38	0
1	MLY	A	431	1	9,10,11	0.51	0	6,11,13	0.45	0
1	MLY	D	431	1	9,10,11	0.52	0	6,11,13	0.46	0
1	MLY	A	553	1,4	9,10,11	0.66	0	6,11,13	0.54	0
1	MLY	D	528	1	9,10,11	0.91	0	6,11,13	0.64	0
1	MLY	P	353	1	9,10,11	0.85	0	6,11,13	0.79	0
1	MLY	G	130	1	9,10,11	0.77	0	6,11,13	0.74	0
1	MLY	A	486	1	9,10,11	0.67	0	6,11,13	0.39	0
1	MLY	A	385	1	9,10,11	0.94	1 (11%)	6,11,13	0.45	0
1	MLY	M	49	1	9,10,11	0.98	1 (11%)	6,11,13	0.75	0
1	MLY	P	613	1	9,10,11	0.57	0	6,11,13	0.62	0
1	MLY	P	839	1	9,10,11	0.70	0	6,11,13	0.76	0
1	MLY	D	248	1	9,10,11	0.82	0	6,11,13	0.64	0
1	MLY	M	87	1	9,10,11	1.11	1 (11%)	6,11,13	0.44	0
1	MLY	G	49	1	9,10,11	0.96	1 (11%)	6,11,13	0.74	0
1	MLY	D	837	1	9,10,11	0.60	0	6,11,13	0.59	0
1	MLY	A	248	1	9,10,11	0.80	0	6,11,13	0.64	0
1	MLY	D	295	1	9,10,11	0.76	0	6,11,13	0.38	0
1	MLY	D	296	1	9,10,11	0.63	0	6,11,13	0.38	0
1	MLY	G	190	1	9,10,11	1.19	2 (22%)	6,11,13	0.53	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	0.37	0
1	MLY	M	613	1	9,10,11	0.56	0	6,11,13	0.63	0
1	MLY	M	353	1	9,10,11	0.87	0	6,11,13	0.80	0
1	MLY	D	839	1	9,10,11	0.65	0	6,11,13	0.79	0
1	MLY	G	138	1	9,10,11	1.21	1 (11%)	6,11,13	0.81	0
1	MLY	G	551	1	9,10,11	0.54	0	6,11,13	0.19	0
1	MLY	G	613	1	9,10,11	0.59	0	6,11,13	0.61	0
1	MLY	M	55	1	9,10,11	0.73	0	6,11,13	0.80	0
1	MLY	M	827	1	9,10,11	0.69	0	6,11,13	0.48	0
1	MLY	G	839	1	9,10,11	0.65	0	6,11,13	0.79	0
1	MLY	M	839	1	9,10,11	0.66	0	6,11,13	0.76	0
1	MLY	G	768	1	9,10,11	0.74	0	6,11,13	0.42	0
1	MLY	G	84	1	9,10,11	0.49	0	6,11,13	0.81	0
1	MLY	J	63	1	9,10,11	0.85	0	6,11,13	0.43	0
1	MLY	P	431	1	9,10,11	0.51	0	6,11,13	0.44	0
1	MLY	J	130	1	9,10,11	0.75	0	6,11,13	0.72	0
1	MLY	M	369	1	9,10,11	0.71	0	6,11,13	0.46	0
1	MLY	P	600	1	9,10,11	0.54	0	6,11,13	0.38	0
1	MLY	G	369	1	9,10,11	0.71	0	6,11,13	0.47	0
1	MLY	G	55	1	9,10,11	0.76	0	6,11,13	0.81	0
1	MLY	G	348	1	9,10,11	0.79	0	6,11,13	0.47	0
1	MLY	J	138	1	9,10,11	1.20	1 (11%)	6,11,13	0.82	0
1	MLY	P	248	1	9,10,11	0.81	0	6,11,13	0.64	0
1	MLY	M	528	1	9,10,11	0.90	0	6,11,13	0.65	0
1	MLY	P	107	1	9,10,11	0.48	0	6,11,13	0.34	0
1	MLY	P	768	1	9,10,11	0.77	0	6,11,13	0.42	0
1	MLY	J	35	1	9,10,11	0.73	0	6,11,13	0.38	0
1	MLY	M	600	1	9,10,11	0.53	0	6,11,13	0.38	0
1	MLY	J	486	1	9,10,11	0.66	0	6,11,13	0.40	0
1	MLY	G	296	1	9,10,11	0.61	0	6,11,13	0.35	0
1	MLY	G	528	1	9,10,11	0.90	0	6,11,13	0.66	0
1	MLY	G	827	1	9,10,11	0.70	0	6,11,13	0.47	0
1	MLY	J	764	1	9,10,11	0.81	0	6,11,13	0.36	0
1	MLY	P	367	1	9,10,11	0.60	0	6,11,13	0.36	0
1	MLY	A	130	1	9,10,11	0.79	0	6,11,13	0.74	0
1	MLY	G	782	1	9,10,11	0.80	0	6,11,13	0.36	0
1	MLY	A	436	1	9,10,11	0.95	1 (11%)	6,11,13	0.48	0
1	MLY	D	107	1	9,10,11	0.52	0	6,11,13	0.33	0
1	MLY	G	248	1	9,10,11	0.80	0	6,11,13	0.66	0
1	MLY	J	190	1	9,10,11	1.21	2 (22%)	6,11,13	0.53	0
1	MLY	J	827	1	9,10,11	0.71	0	6,11,13	0.48	0
1	MLY	M	107	1	9,10,11	0.49	0	6,11,13	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	G	833	1	9,10,11	1.15	1 (11%)	6,11,13	0.31	0
1	MLY	J	55	1	9,10,11	0.72	0	6,11,13	0.79	0
1	MLY	J	833	1	9,10,11	1.12	1 (11%)	6,11,13	0.31	0
1	MLY	P	30	1	9,10,11	0.91	0	6,11,13	0.32	0
1	MLY	P	837	1	9,10,11	0.57	0	6,11,13	0.56	0
1	MLY	G	553	1,4	9,10,11	0.64	0	6,11,13	0.55	0
1	MLY	A	87	1	9,10,11	1.09	1 (11%)	6,11,13	0.41	0
1	MLY	A	415	1	9,10,11	0.75	0	6,11,13	0.19	0
1	MLY	G	659	1	9,10,11	0.84	1 (11%)	6,11,13	0.58	0
1	MLY	G	236	1	9,10,11	0.82	1 (11%)	6,11,13	0.48	0
1	MLY	G	385	1	9,10,11	0.92	1 (11%)	6,11,13	0.46	0
1	MLY	P	348	1	9,10,11	0.76	0	6,11,13	0.47	0
1	MLY	M	272	1	9,10,11	0.89	1 (11%)	6,11,13	0.57	0
1	MLY	A	84	1	9,10,11	0.50	0	6,11,13	0.80	0
1	MLY	J	248	1	9,10,11	0.80	0	6,11,13	0.65	0
1	MLY	A	617	1	9,10,11	0.88	0	6,11,13	0.34	0
1	MLY	M	35	1	9,10,11	0.74	0	6,11,13	0.38	0
1	MLY	G	436	1	9,10,11	0.95	1 (11%)	6,11,13	0.46	0
1	MLY	J	551	1	9,10,11	0.52	0	6,11,13	0.20	0
1	MLY	M	367	1	9,10,11	0.57	0	6,11,13	0.37	0
1	MLY	D	764	1	9,10,11	0.82	0	6,11,13	0.34	0
1	MLY	P	19	1	9,10,11	1.08	1 (11%)	6,11,13	0.57	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	764	1	-	2/8/9/11	-
1	MLY	G	35	1	-	3/8/9/11	-
1	MLY	D	130	1	-	5/8/9/11	-
1	MLY	M	130	1	-	5/8/9/11	-
1	MLY	J	553	1	-	4/8/9/11	-
1	MLY	D	827	1	-	1/8/9/11	-
1	MLY	P	617	1	-	2/8/9/11	-
1	MLY	A	19	1	-	4/8/9/11	-
1	MLY	D	353	1	-	4/8/9/11	-
1	MLY	A	782	1	-	6/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	D	49	1	-	3/8/9/11	-
1	MLY	D	681	1	-	4/8/9/11	-
1	MLY	A	827	1	-	1/8/9/11	-
1	MLY	J	385	1	-	2/8/9/11	-
1	MLY	D	87	1	-	2/8/9/11	-
1	MLY	M	296	1	-	4/8/9/11	-
1	MLY	D	138	1	-	4/8/9/11	-
1	MLY	A	55	1	-	6/8/9/11	-
1	MLY	A	295	1	-	2/8/9/11	-
1	MLY	D	551	1	-	3/8/9/11	-
1	MLY	A	107	1	-	2/8/9/11	-
1	MLY	D	782	1	-	6/8/9/11	-
1	MLY	A	833	1	-	6/8/9/11	-
1	MLY	G	59	1	-	3/8/9/11	-
1	MLY	P	236	1	-	3/8/9/11	-
1	MLY	P	486	1	-	2/8/9/11	-
1	MLY	D	768	1	-	4/8/9/11	-
1	MLY	P	59	1	-	3/8/9/11	-
1	MLY	A	236	1	-	3/8/9/11	-
1	MLY	M	84	1	-	4/8/9/11	-
1	MLY	A	659	1	-	3/8/9/11	-
1	MLY	D	190	1	-	4/8/9/11	-
1	MLY	A	681	1	-	4/8/9/11	-
1	MLY	D	30	1	-	3/8/9/11	-
1	MLY	G	504	1	-	4/8/9/11	-
1	MLY	P	833	1	-	6/8/9/11	-
1	MLY	J	272	1	-	3/8/9/11	-
1	MLY	D	369	1	-	2/8/9/11	-
1	MLY	A	551	1	-	3/8/9/11	-
1	MLY	P	385	1	-	2/8/9/11	-
1	MLY	D	600	1	-	3/8/9/11	-
1	MLY	M	764	1	-	2/8/9/11	-
1	MLY	J	367	1	-	2/8/9/11	-
1	MLY	P	190	1	-	4/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	P	295	1	-	2/8/9/11	-
1	MLY	G	415	1	-	3/8/9/11	-
1	MLY	M	19	1	-	4/8/9/11	-
1	MLY	M	681	1	-	4/8/9/11	-
1	MLY	J	30	1	-	3/8/9/11	-
1	MLY	M	617	1	-	2/8/9/11	-
1	MLY	J	296	1	-	4/8/9/11	-
1	MLY	G	681	1	-	4/8/9/11	-
1	MLY	M	138	1	-	4/8/9/11	-
1	MLY	G	353	1	-	4/8/9/11	-
1	MLY	P	659	1	-	3/8/9/11	-
1	MLY	G	617	1	-	2/8/9/11	-
1	MLY	A	59	1	-	3/8/9/11	-
1	MLY	J	436	1	-	4/8/9/11	-
1	MLY	J	782	1	-	6/8/9/11	-
1	MLY	P	55	1	-	6/8/9/11	-
1	MLY	P	505	1	-	5/8/9/11	-
1	MLY	D	553	1,4	-	5/8/9/11	-
1	MLY	J	348	1	-	5/8/9/11	-
1	MLY	D	659	1	-	3/8/9/11	-
1	MLY	J	839	1	-	3/8/9/11	-
1	MLY	M	659	1	-	3/8/9/11	-
1	MLY	G	486	1	-	2/8/9/11	-
1	MLY	D	505	1	-	5/8/9/11	-
1	MLY	J	768	1	-	4/8/9/11	-
1	MLY	M	190	1	-	4/8/9/11	-
1	MLY	M	837	1	-	6/8/9/11	-
1	MLY	A	30	1	-	3/8/9/11	-
1	MLY	J	598	1	-	5/8/9/11	-
1	MLY	J	19	1	-	4/8/9/11	-
1	MLY	M	295	1	-	2/8/9/11	-
1	MLY	D	55	1	-	6/8/9/11	-
1	MLY	D	436	1	-	4/8/9/11	-
1	MLY	J	431	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	P	84	1	-	4/8/9/11	-
1	MLY	G	600	1	-	3/8/9/11	-
1	MLY	J	415	1	-	3/8/9/11	-
1	MLY	J	613	1	-	3/8/9/11	-
1	MLY	A	63	1	-	4/8/9/11	-
1	MLY	A	505	1	-	5/8/9/11	-
1	MLY	P	138	1	-	4/8/9/11	-
1	MLY	A	296	1	-	4/8/9/11	-
1	MLY	A	598	1	-	5/8/9/11	-
1	MLY	P	764	1	-	2/8/9/11	-
1	MLY	D	367	1	-	2/8/9/11	-
1	MLY	P	436	1	-	4/8/9/11	-
1	MLY	A	504	1	-	4/8/9/11	-
1	MLY	J	528	1	-	4/8/9/11	-
1	MLY	P	827	1	-	1/8/9/11	-
1	MLY	M	59	1	-	3/8/9/11	-
1	MLY	A	768	1	-	4/8/9/11	-
1	MLY	D	486	1	-	2/8/9/11	-
1	MLY	P	35	1	-	3/8/9/11	-
1	MLY	M	505	1	-	5/8/9/11	-
1	MLY	M	30	1	-	3/8/9/11	-
1	MLY	D	504	1	-	4/8/9/11	-
1	MLY	G	63	1	-	4/8/9/11	-
1	MLY	P	415	1	-	3/8/9/11	-
1	MLY	G	837	1	-	6/8/9/11	-
1	MLY	J	504	1	-	4/8/9/11	-
1	MLY	P	504	1	-	4/8/9/11	-
1	MLY	G	367	1	-	2/8/9/11	-
1	MLY	D	348	1	-	5/8/9/11	-
1	MLY	M	551	1	-	3/8/9/11	-
1	MLY	M	415	1	-	3/8/9/11	-
1	MLY	A	528	1	-	4/8/9/11	-
1	MLY	P	369	1	-	2/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	A	600	1	-	3/8/9/11	-
1	MLY	A	348	1	-	5/8/9/11	-
1	MLY	D	63	1	-	4/8/9/11	-
1	MLY	A	353	1	-	4/8/9/11	-
1	MLY	D	598	1	-	5/8/9/11	-
1	MLY	D	19	1	-	4/8/9/11	-
1	MLY	G	272	1	-	3/8/9/11	-
1	MLY	J	49	1	-	3/8/9/11	-
1	MLY	J	505	1	-	5/8/9/11	-
1	MLY	J	659	1	-	3/8/9/11	-
1	MLY	G	598	1	-	5/8/9/11	-
1	MLY	M	598	1	-	5/8/9/11	-
1	MLY	P	87	1	-	2/8/9/11	-
1	MLY	D	617	1	-	2/8/9/11	-
1	MLY	M	768	1	-	4/8/9/11	-
1	MLY	D	613	1	-	3/8/9/11	-
1	MLY	J	353	1	-	4/8/9/11	-
1	MLY	M	553	1	-	4/8/9/11	-
1	MLY	D	385	1	-	2/8/9/11	-
1	MLY	M	236	1	-	3/8/9/11	-
1	MLY	D	236	1	-	3/8/9/11	-
1	MLY	M	486	1	-	2/8/9/11	-
1	MLY	P	528	1	-	4/8/9/11	-
1	MLY	P	598	1	-	5/8/9/11	-
1	MLY	G	19	1	-	4/8/9/11	-
1	MLY	M	782	1	-	6/8/9/11	-
1	MLY	G	87	1	-	2/8/9/11	-
1	MLY	J	369	1	-	2/8/9/11	-
1	MLY	M	248	1	-	6/8/9/11	-
1	MLY	J	84	1	-	4/8/9/11	-
1	MLY	A	367	1	-	2/8/9/11	-
1	MLY	M	348	1	-	5/8/9/11	-
1	MLY	J	59	1	-	3/8/9/11	-
1	MLY	M	833	1	-	6/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	D	833	1	-	6/8/9/11	-
1	MLY	P	272	1	-	3/8/9/11	-
1	MLY	P	551	1	-	3/8/9/11	-
1	MLY	J	600	1	-	3/8/9/11	-
1	MLY	A	272	1	-	3/8/9/11	-
1	MLY	A	190	1	-	4/8/9/11	-
1	MLY	P	553	1	-	4/8/9/11	-
1	MLY	P	63	1	-	4/8/9/11	-
1	MLY	D	59	1	-	3/8/9/11	-
1	MLY	G	431	1	-	4/8/9/11	-
1	MLY	J	107	1	-	2/8/9/11	-
1	MLY	M	436	1	-	4/8/9/11	-
1	MLY	G	764	1	-	2/8/9/11	-
1	MLY	P	49	1	-	3/8/9/11	-
1	MLY	P	681	1	-	4/8/9/11	-
1	MLY	P	296	1	-	4/8/9/11	-
1	MLY	A	837	1	-	6/8/9/11	-
1	MLY	J	236	1	-	3/8/9/11	-
1	MLY	M	385	1	-	2/8/9/11	-
1	MLY	P	782	1	-	6/8/9/11	-
1	MLY	J	681	1	-	4/8/9/11	-
1	MLY	A	49	1	-	3/8/9/11	-
1	MLY	G	107	1	-	2/8/9/11	-
1	MLY	G	295	1	-	2/8/9/11	-
1	MLY	J	87	1	-	2/8/9/11	-
1	MLY	M	63	1	-	4/8/9/11	-
1	MLY	A	613	1	-	3/8/9/11	-
1	MLY	A	35	1	-	3/8/9/11	-
1	MLY	A	839	1	-	3/8/9/11	-
1	MLY	D	415	1	-	3/8/9/11	-
1	MLY	G	505	1	-	5/8/9/11	-
1	MLY	M	431	1	-	4/8/9/11	-
1	MLY	M	504	1	-	4/8/9/11	-
1	MLY	P	130	1	-	5/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	J	837	1	-	6/8/9/11	-
1	MLY	D	84	1	-	4/8/9/11	-
1	MLY	A	138	1	-	4/8/9/11	-
1	MLY	D	272	1	-	3/8/9/11	-
1	MLY	A	369	1	-	2/8/9/11	-
1	MLY	G	30	1	-	3/8/9/11	-
1	MLY	J	295	1	-	2/8/9/11	-
1	MLY	A	431	1	-	4/8/9/11	-
1	MLY	D	431	1	-	4/8/9/11	-
1	MLY	A	553	1,4	-	4/8/9/11	-
1	MLY	D	528	1	-	4/8/9/11	-
1	MLY	P	353	1	-	4/8/9/11	-
1	MLY	G	130	1	-	5/8/9/11	-
1	MLY	A	486	1	-	2/8/9/11	-
1	MLY	A	385	1	-	2/8/9/11	-
1	MLY	M	49	1	-	3/8/9/11	-
1	MLY	P	613	1	-	3/8/9/11	-
1	MLY	P	839	1	-	3/8/9/11	-
1	MLY	D	248	1	-	6/8/9/11	-
1	MLY	M	87	1	-	2/8/9/11	-
1	MLY	G	49	1	-	3/8/9/11	-
1	MLY	D	837	1	-	6/8/9/11	-
1	MLY	A	248	1	-	6/8/9/11	-
1	MLY	D	295	1	-	2/8/9/11	-
1	MLY	D	296	1	-	4/8/9/11	-
1	MLY	G	190	1	-	4/8/9/11	-
1	MLY	D	35	1	-	3/8/9/11	-
1	MLY	M	613	1	-	3/8/9/11	-
1	MLY	M	353	1	-	4/8/9/11	-
1	MLY	D	839	1	-	3/8/9/11	-
1	MLY	G	138	1	-	4/8/9/11	-
1	MLY	G	551	1	-	3/8/9/11	-
1	MLY	G	613	1	-	3/8/9/11	-
1	MLY	M	55	1	-	6/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	M	827	1	-	1/8/9/11	-
1	MLY	G	839	1	-	3/8/9/11	-
1	MLY	M	839	1	-	3/8/9/11	-
1	MLY	G	768	1	-	4/8/9/11	-
1	MLY	G	84	1	-	4/8/9/11	-
1	MLY	J	63	1	-	4/8/9/11	-
1	MLY	P	431	1	-	4/8/9/11	-
1	MLY	J	130	1	-	5/8/9/11	-
1	MLY	M	369	1	-	2/8/9/11	-
1	MLY	P	600	1	-	3/8/9/11	-
1	MLY	G	369	1	-	2/8/9/11	-
1	MLY	G	55	1	-	6/8/9/11	-
1	MLY	G	348	1	-	5/8/9/11	-
1	MLY	J	138	1	-	4/8/9/11	-
1	MLY	P	248	1	-	6/8/9/11	-
1	MLY	M	528	1	-	4/8/9/11	-
1	MLY	P	107	1	-	2/8/9/11	-
1	MLY	P	768	1	-	4/8/9/11	-
1	MLY	J	35	1	-	3/8/9/11	-
1	MLY	M	600	1	-	3/8/9/11	-
1	MLY	J	486	1	-	2/8/9/11	-
1	MLY	G	296	1	-	4/8/9/11	-
1	MLY	G	528	1	-	4/8/9/11	-
1	MLY	G	827	1	-	1/8/9/11	-
1	MLY	J	764	1	-	2/8/9/11	-
1	MLY	P	367	1	-	2/8/9/11	-
1	MLY	A	130	1	-	5/8/9/11	-
1	MLY	G	782	1	-	6/8/9/11	-
1	MLY	A	436	1	-	4/8/9/11	-
1	MLY	D	107	1	-	2/8/9/11	-
1	MLY	G	248	1	-	6/8/9/11	-
1	MLY	J	190	1	-	4/8/9/11	-
1	MLY	J	827	1	-	1/8/9/11	-
1	MLY	M	107	1	-	2/8/9/11	-
1	MLY	G	833	1	-	6/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	J	55	1	-	6/8/9/11	-
1	MLY	J	833	1	-	6/8/9/11	-
1	MLY	P	30	1	-	3/8/9/11	-
1	MLY	P	837	1	-	6/8/9/11	-
1	MLY	G	553	1,4	-	4/8/9/11	-
1	MLY	A	87	1	-	2/8/9/11	-
1	MLY	A	415	1	-	3/8/9/11	-
1	MLY	G	659	1	-	3/8/9/11	-
1	MLY	G	236	1	-	3/8/9/11	-
1	MLY	G	385	1	-	2/8/9/11	-
1	MLY	P	348	1	-	5/8/9/11	-
1	MLY	M	272	1	-	3/8/9/11	-
1	MLY	A	84	1	-	4/8/9/11	-
1	MLY	J	248	1	-	6/8/9/11	-
1	MLY	A	617	1	-	2/8/9/11	-
1	MLY	M	35	1	-	3/8/9/11	-
1	MLY	G	436	1	-	4/8/9/11	-
1	MLY	J	551	1	-	3/8/9/11	-
1	MLY	M	367	1	-	2/8/9/11	-
1	MLY	D	764	1	-	2/8/9/11	-
1	MLY	P	19	1	-	4/8/9/11	-

The worst 5 of 76 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	138	MLY	CB-CA	-3.32	1.48	1.53
1	P	138	MLY	CB-CA	-3.22	1.48	1.53
1	G	138	MLY	CB-CA	-3.19	1.48	1.53
1	A	138	MLY	CB-CA	-3.19	1.48	1.53
1	M	138	MLY	CB-CA	-3.17	1.48	1.53

There are no bond angle outliers.

There are no chirality outliers.

5 of 967 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.

185 monomers are involved in 687 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	764	MLY	9	0
1	J	553	MLY	11	0
1	P	617	MLY	1	0
1	A	782	MLY	7	0
1	D	49	MLY	3	0
1	A	827	MLY	1	0
1	D	87	MLY	3	0
1	M	296	MLY	3	0
1	D	138	MLY	2	0
1	A	55	MLY	1	0
1	A	295	MLY	6	0
1	D	551	MLY	2	0
1	A	107	MLY	3	0
1	D	782	MLY	58	0
1	A	833	MLY	1	0
1	G	59	MLY	3	0
1	P	486	MLY	3	0
1	P	59	MLY	2	0
1	A	659	MLY	2	0
1	D	190	MLY	2	0
1	D	30	MLY	1	0
1	G	504	MLY	1	0
1	J	272	MLY	1	0
1	D	369	MLY	1	0
1	A	551	MLY	2	0
1	D	600	MLY	1	0
1	M	764	MLY	2	0
1	P	190	MLY	2	0
1	P	295	MLY	6	0
1	G	415	MLY	1	0
1	J	30	MLY	1	0
1	M	617	MLY	1	0
1	J	296	MLY	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	M	138	MLY	2	0
1	P	659	MLY	2	0
1	G	617	MLY	1	0
1	A	59	MLY	2	0
1	J	436	MLY	2	0
1	J	782	MLY	1	0
1	P	55	MLY	1	0
1	P	505	MLY	1	0
1	D	553	MLY	17	0
1	J	348	MLY	4	0
1	D	659	MLY	2	0
1	J	839	MLY	9	0
1	M	659	MLY	2	0
1	G	486	MLY	3	0
1	J	768	MLY	1	0
1	M	190	MLY	2	0
1	M	837	MLY	1	0
1	A	30	MLY	1	0
1	J	598	MLY	1	0
1	M	295	MLY	6	0
1	D	55	MLY	1	0
1	D	436	MLY	2	0
1	J	617	MLY	1	0
1	P	84	MLY	9	0
1	G	600	MLY	1	0
1	J	415	MLY	1	0
1	A	63	MLY	3	0
1	A	505	MLY	19	0
1	P	138	MLY	2	0
1	A	296	MLY	2	0
1	A	598	MLY	1	0
1	P	764	MLY	7	0
1	P	436	MLY	2	0
1	A	504	MLY	1	0
1	J	528	MLY	3	0
1	M	59	MLY	3	0
1	A	768	MLY	8	0
1	D	486	MLY	3	0
1	M	30	MLY	1	0
1	D	504	MLY	1	0
1	G	63	MLY	3	0
1	P	415	MLY	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	G	837	MLY	1	0
1	J	504	MLY	1	0
1	D	348	MLY	4	0
1	M	415	MLY	1	0
1	A	528	MLY	3	0
1	P	369	MLY	1	0
1	A	600	MLY	1	0
1	A	348	MLY	5	0
1	D	63	MLY	4	0
1	D	598	MLY	1	0
1	G	272	MLY	1	0
1	J	49	MLY	3	0
1	J	505	MLY	10	0
1	J	659	MLY	2	0
1	G	598	MLY	1	0
1	M	598	MLY	1	0
1	P	87	MLY	3	0
1	D	617	MLY	1	0
1	M	553	MLY	9	0
1	M	486	MLY	3	0
1	P	528	MLY	3	0
1	P	598	MLY	1	0
1	M	782	MLY	3	0
1	G	87	MLY	3	0
1	J	369	MLY	1	0
1	M	248	MLY	2	0
1	J	84	MLY	19	0
1	M	348	MLY	5	0
1	J	59	MLY	2	0
1	P	272	MLY	1	0
1	J	600	MLY	1	0
1	A	272	MLY	1	0
1	A	190	MLY	2	0
1	P	553	MLY	2	0
1	P	63	MLY	4	0
1	D	59	MLY	3	0
1	J	107	MLY	3	0
1	M	436	MLY	2	0
1	G	764	MLY	11	0
1	P	49	MLY	3	0
1	P	296	MLY	2	0
1	A	837	MLY	11	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	P	782	MLY	21	0
1	A	49	MLY	4	0
1	G	107	MLY	3	0
1	G	295	MLY	6	0
1	J	87	MLY	3	0
1	M	63	MLY	4	0
1	A	839	MLY	7	0
1	D	415	MLY	1	0
1	G	505	MLY	5	0
1	M	504	MLY	1	0
1	J	837	MLY	1	0
1	A	138	MLY	2	0
1	D	272	MLY	1	0
1	G	30	MLY	1	0
1	J	295	MLY	6	0
1	A	553	MLY	16	0
1	D	528	MLY	3	0
1	A	486	MLY	3	0
1	M	49	MLY	4	0
1	P	839	MLY	8	0
1	D	248	MLY	2	0
1	M	87	MLY	2	0
1	G	49	MLY	4	0
1	D	837	MLY	1	0
1	A	248	MLY	2	0
1	D	295	MLY	6	0
1	D	296	MLY	2	0
1	G	190	MLY	2	0
1	D	839	MLY	4	0
1	G	138	MLY	1	0
1	M	55	MLY	1	0
1	G	839	MLY	4	0
1	M	839	MLY	8	0
1	G	768	MLY	2	0
1	G	84	MLY	30	0
1	J	63	MLY	4	0
1	P	600	MLY	1	0
1	G	55	MLY	1	0
1	G	348	MLY	4	0
1	J	138	MLY	2	0
1	P	248	MLY	2	0
1	M	528	MLY	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	P	107	MLY	3	0
1	P	768	MLY	4	0
1	M	600	MLY	1	0
1	J	486	MLY	3	0
1	G	296	MLY	2	0
1	G	528	MLY	2	0
1	J	764	MLY	2	0
1	G	782	MLY	1	0
1	A	436	MLY	3	0
1	D	107	MLY	3	0
1	G	248	MLY	2	0
1	J	190	MLY	2	0
1	M	107	MLY	3	0
1	J	55	MLY	1	0
1	P	30	MLY	1	0
1	P	837	MLY	1	0
1	G	553	MLY	26	0
1	A	87	MLY	3	0
1	A	415	MLY	1	0
1	G	659	MLY	2	0
1	P	348	MLY	5	0
1	M	272	MLY	1	0
1	J	248	MLY	2	0
1	A	617	MLY	1	0
1	G	436	MLY	2	0
1	D	764	MLY	8	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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	M	5
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	O	1
3	R	1
2	B	1
2	E	1
2	H	1
2	K	1
2	N	1
2	Q	1

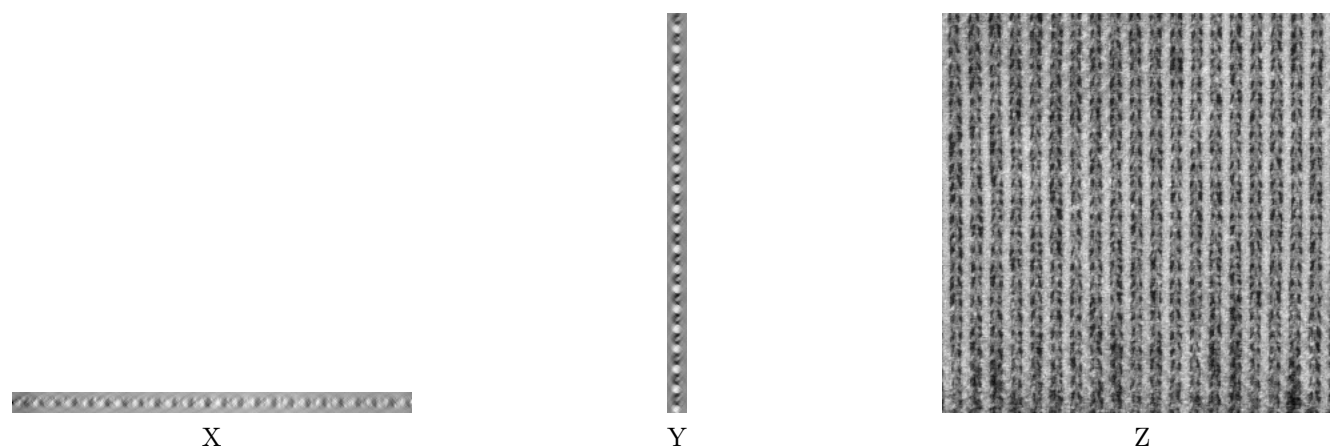
The worst 5 of 36 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	J	769:ALA	C	770:GLY	N	5.56
1	D	769:ALA	C	770:GLY	N	4.62
1	G	769:ALA	C	770:GLY	N	4.48
1	D	709:LYS	C	710:GLY	N	3.36
1	A	709:LYS	C	710:GLY	N	2.70

6 Tomogram visualisation [i](#)

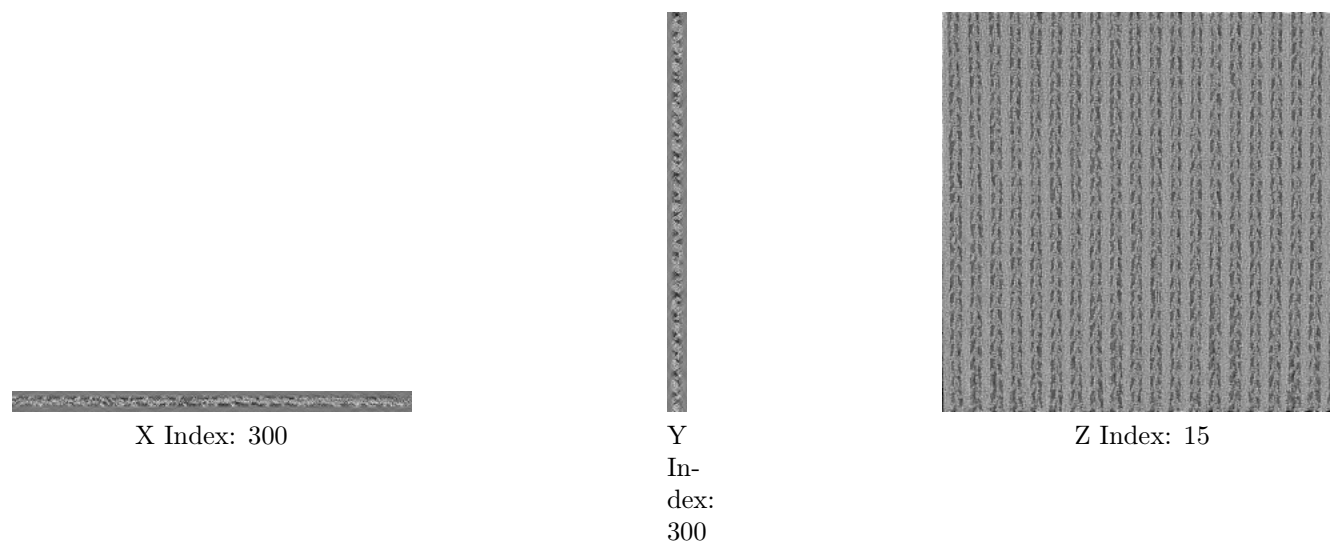
This section contains visualisations of the EMDB entry EMD-1001. These allow visual inspection of the internal detail of the tomogram and identification of artifacts.

6.1 Orthogonal projections [i](#)



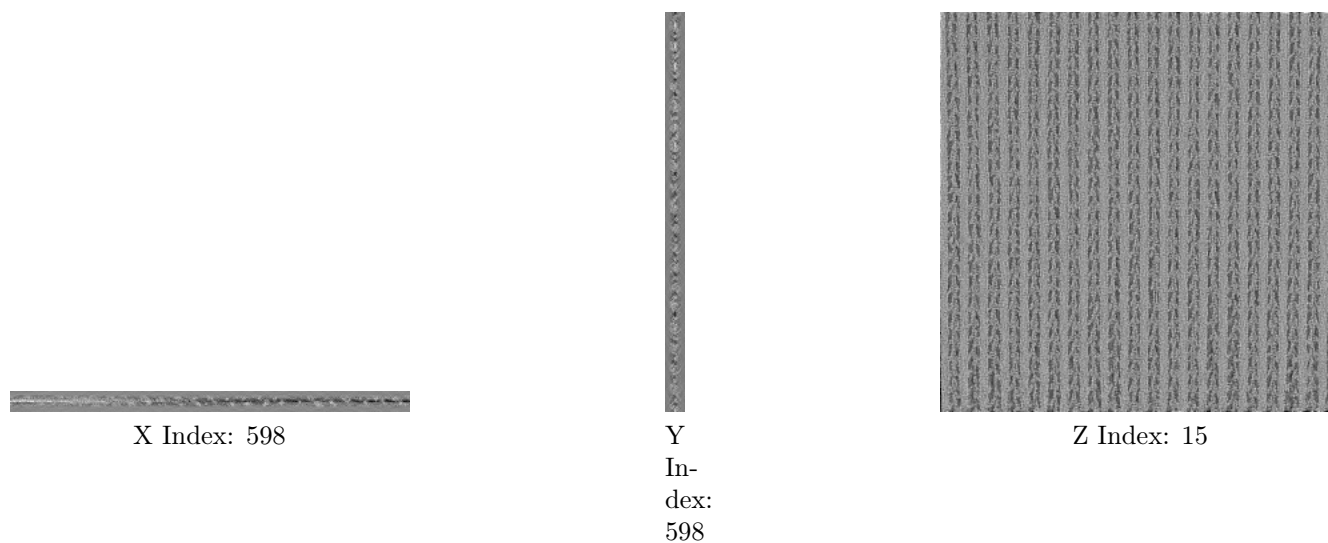
The images above show the tomogram projected in three orthogonal directions.

6.2 Central slices [i](#)



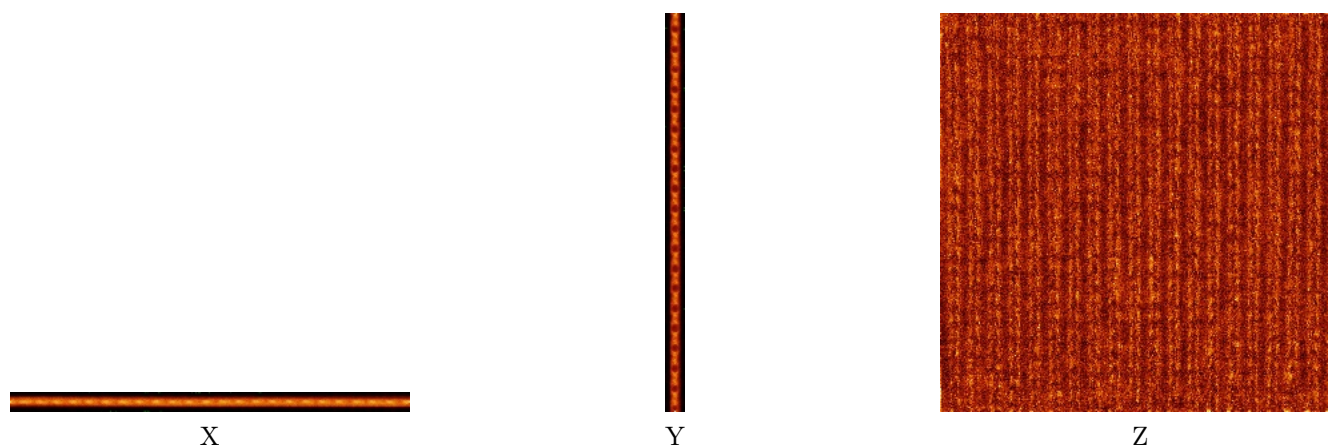
The images above show central slices of the tomogram in three orthogonal directions.

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.

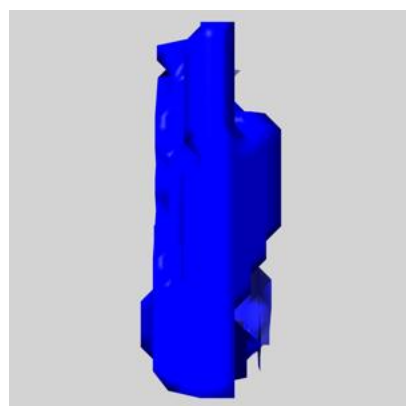
6.5 Mask visualisation [i](#)

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

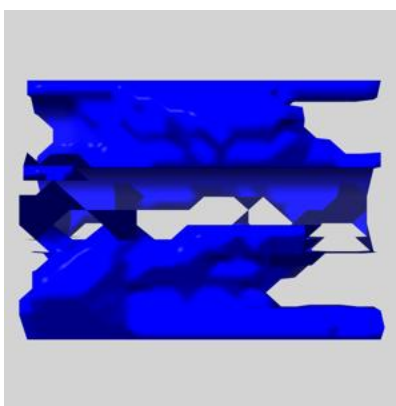
A mask typically either:

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

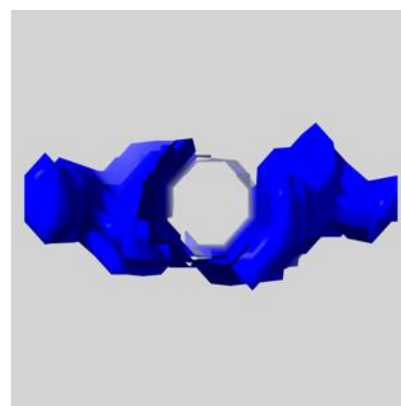
6.5.1 emd_1001_msk_25.map [i](#)



X

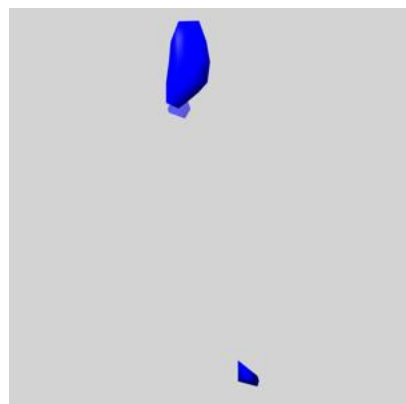


Y

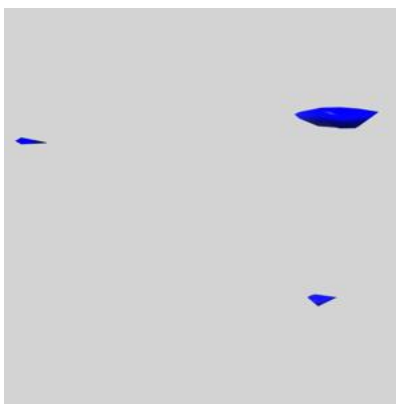


Z

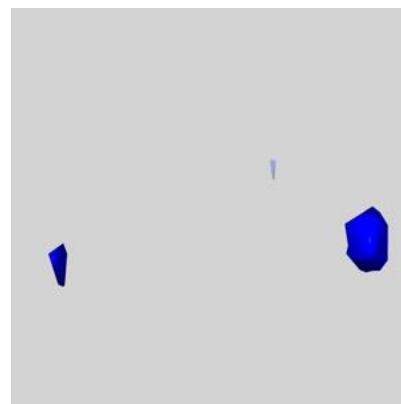
6.5.2 emd_1001_msk_24.map [i](#)



X

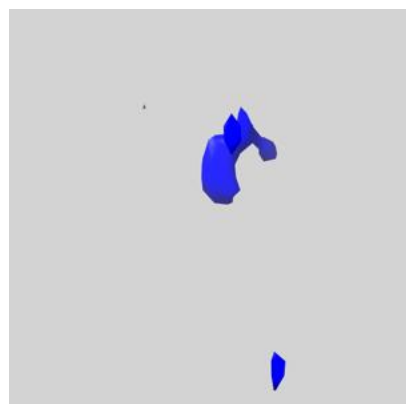


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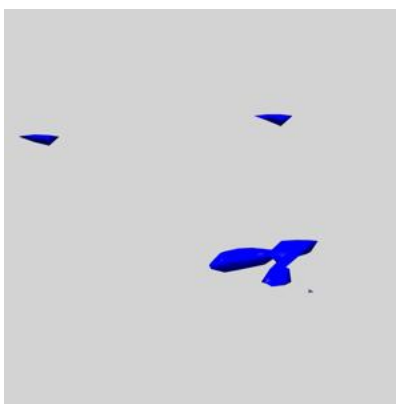


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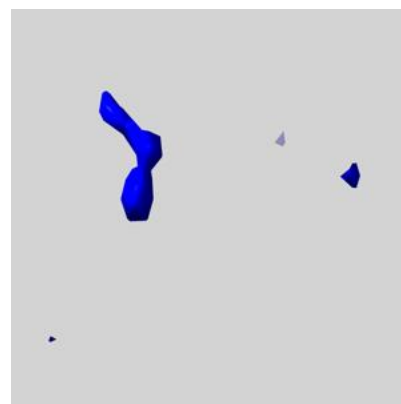
6.5.3 emd_1001_msk_23.map [i](#)



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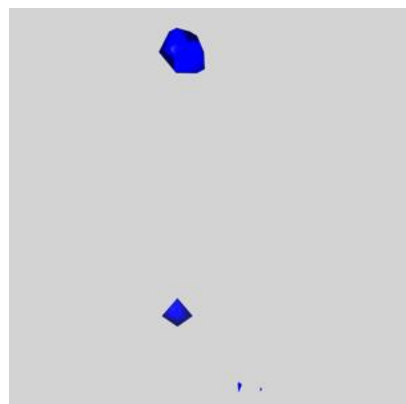


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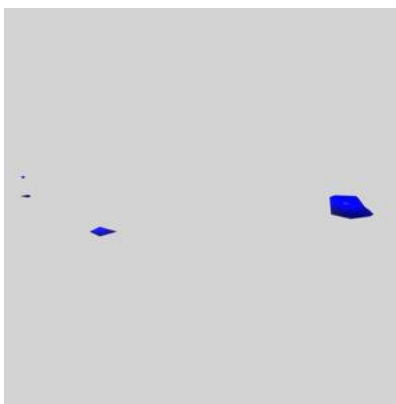


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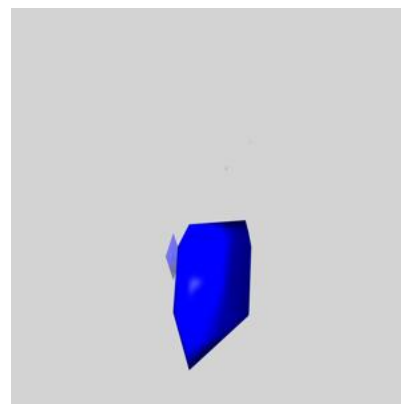
6.5.4 emd_1001_msk_22.map [i](#)



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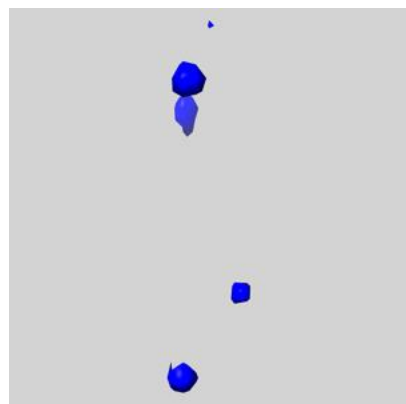


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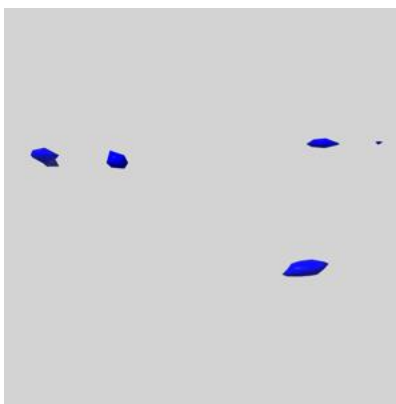


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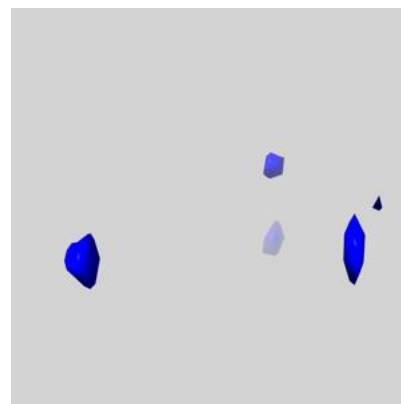
6.5.5 emd_1001_msk_21.map [i](#)



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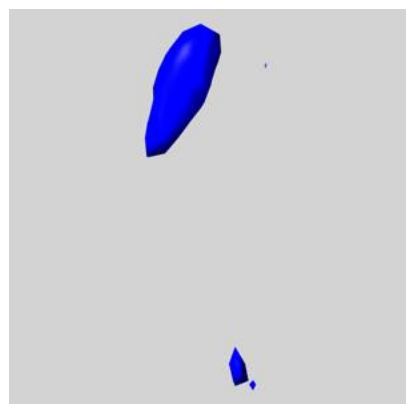


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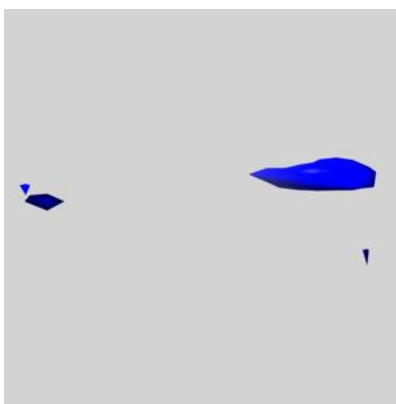


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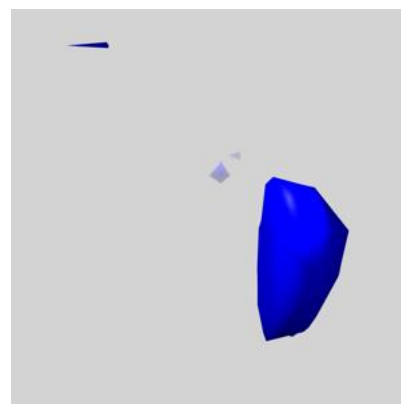
6.5.6 emd_1001_msk_20.map [i](#)



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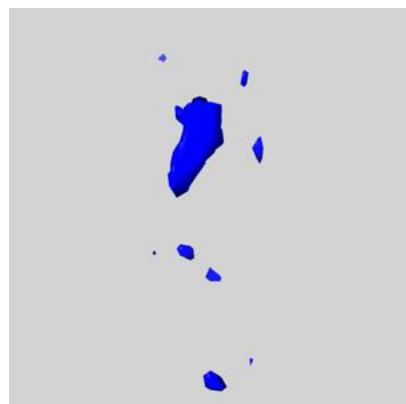


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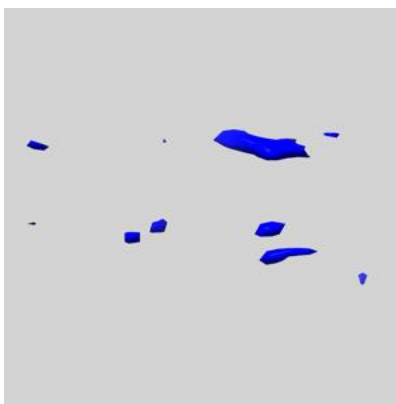


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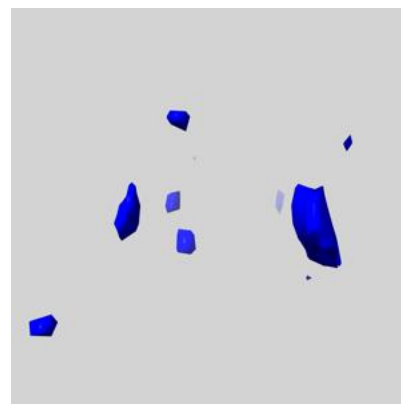
6.5.7 emd_1001_msk_19.map [i](#)



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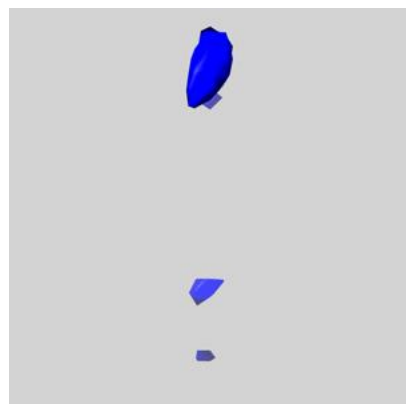


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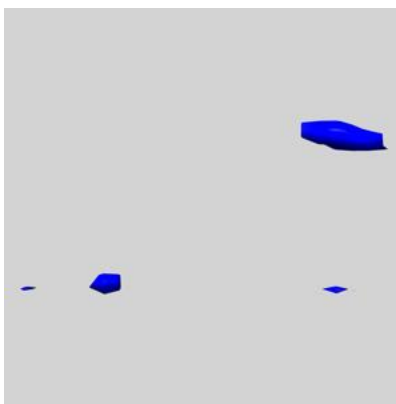


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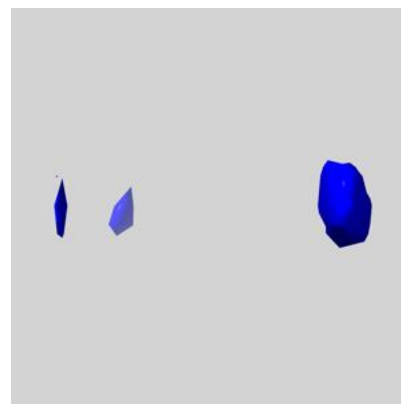
6.5.8 emd_1001_msk_18.map [i](#)



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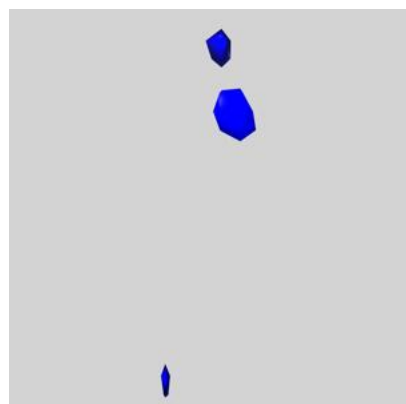


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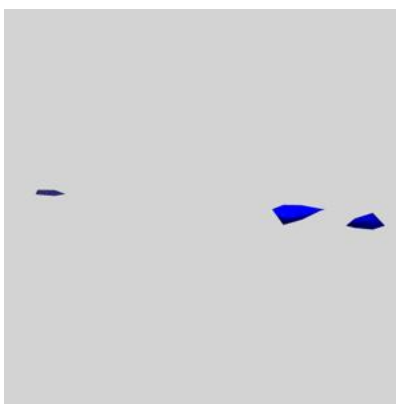


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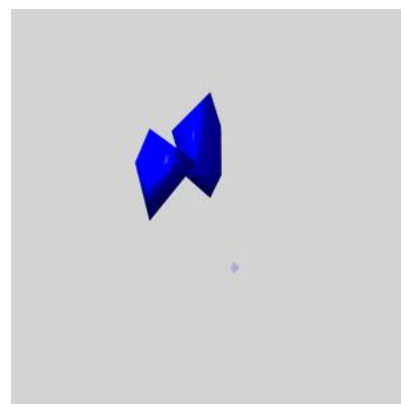
6.5.9 emd_1001_msk_17.map [i](#)



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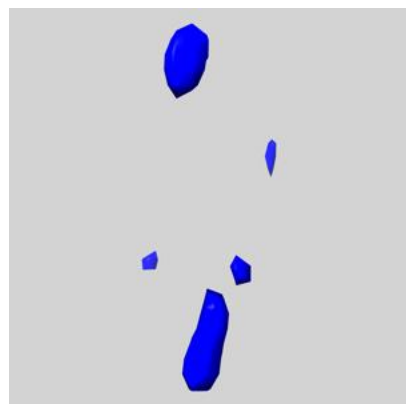


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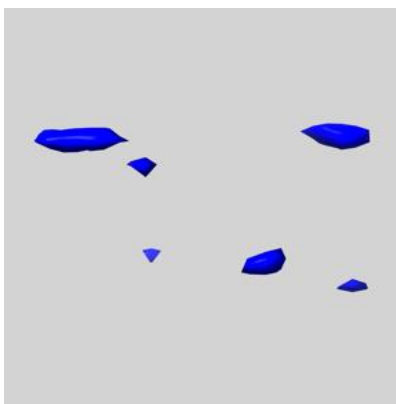


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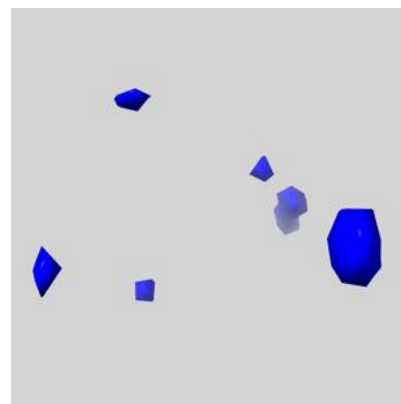
6.5.10 emd_1001_msk_16.map [i](#)



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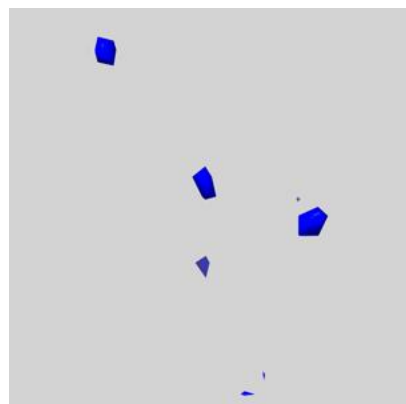


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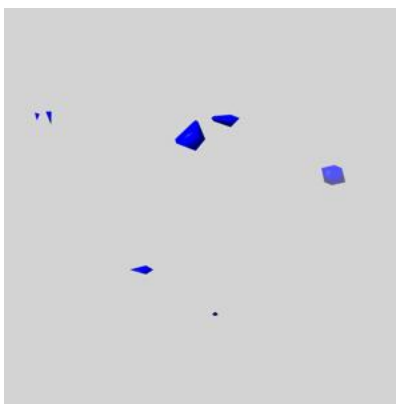


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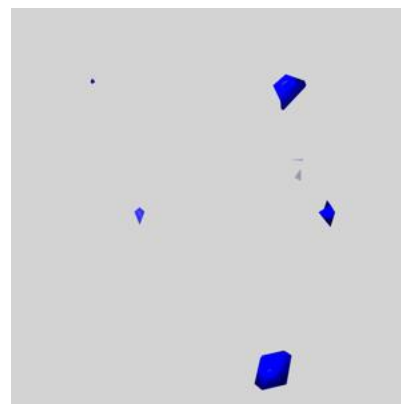
6.5.11 emd_1001_msk_15.map [i](#)



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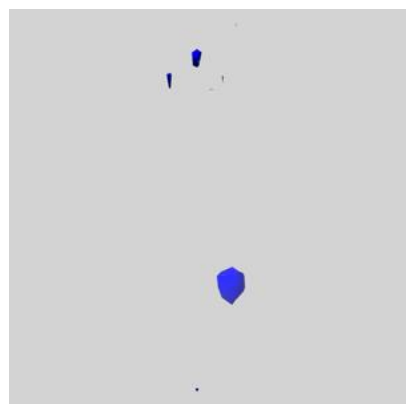


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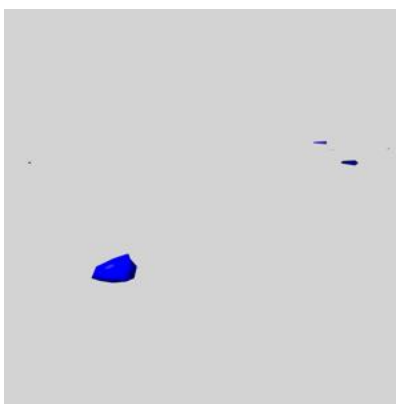


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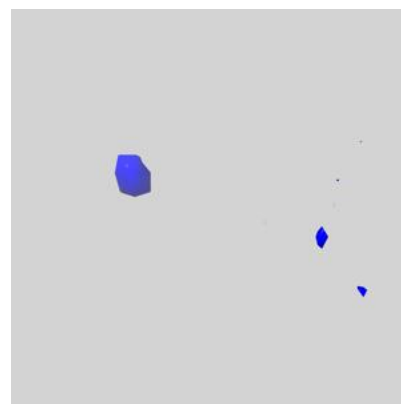
6.5.12 emd_1001_msk_14.map [i](#)



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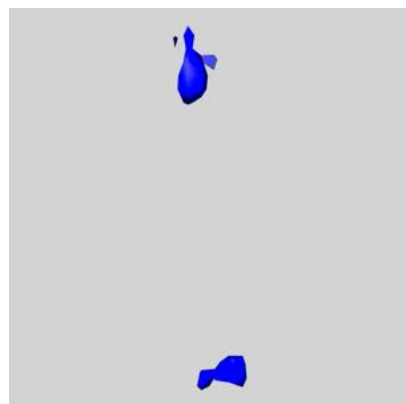


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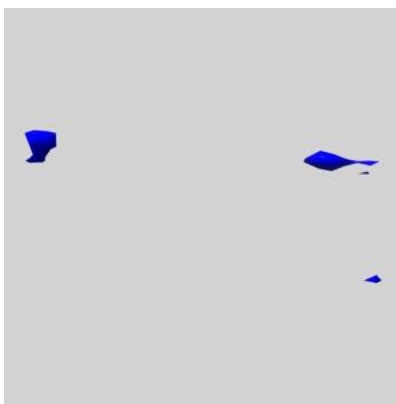


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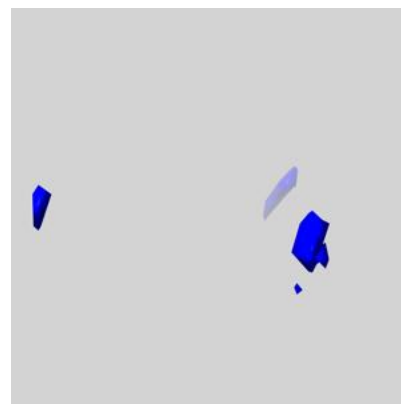
6.5.13 emd_1001_msk_13.map [i](#)



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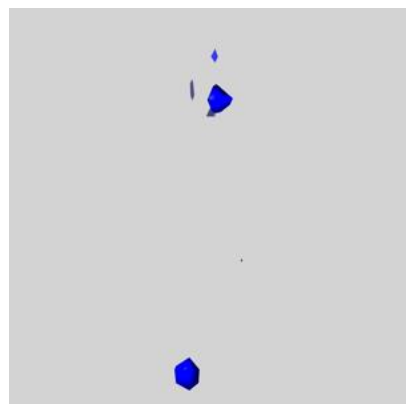


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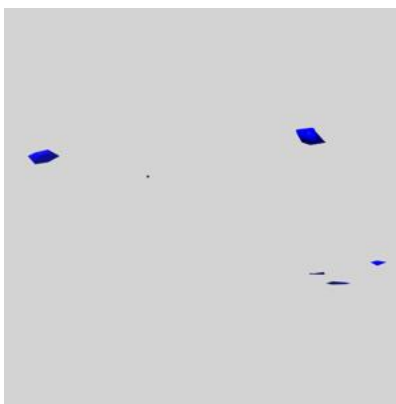


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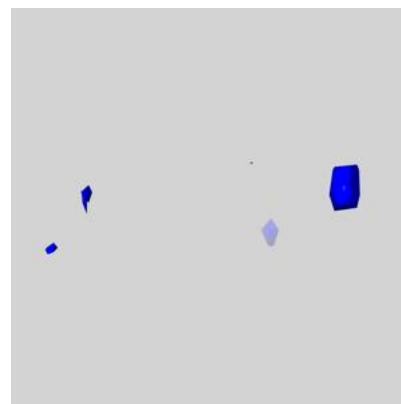
6.5.14 emd_1001_msk_12.map [i](#)



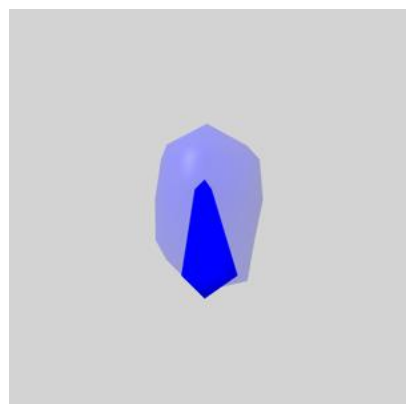
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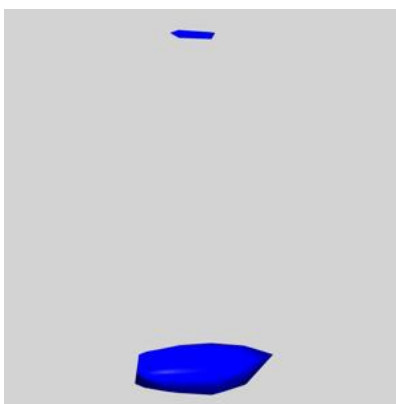
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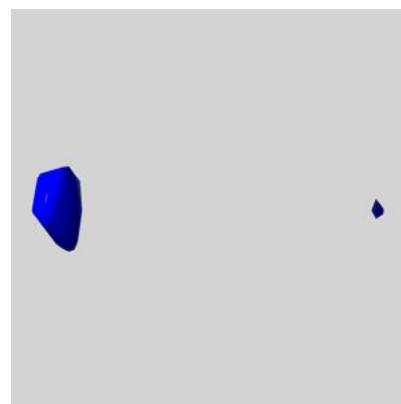
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6.5.15 emd_1001_msk_11.map [i](#)

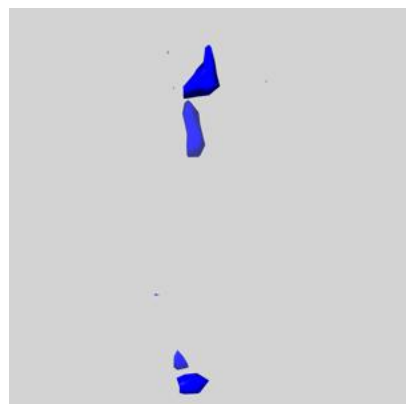
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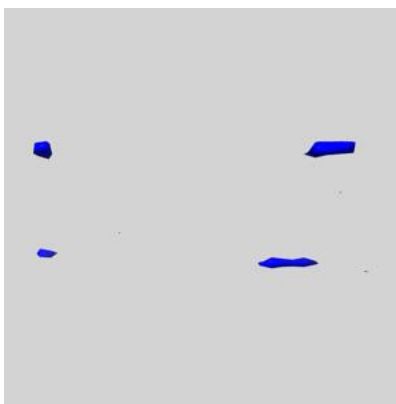
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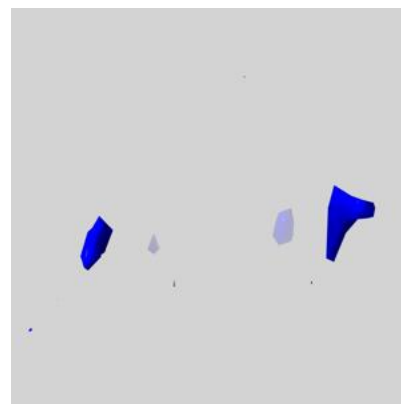
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6.5.16 emd_1001_msk_10.map [i](#)

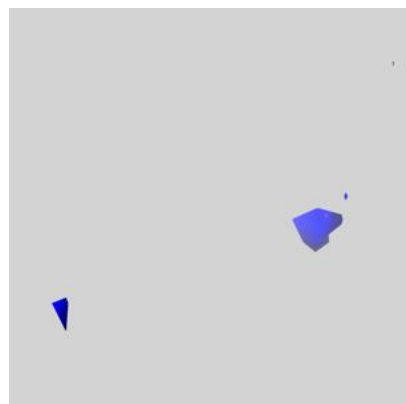
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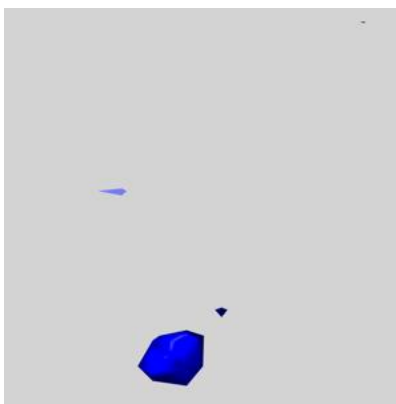
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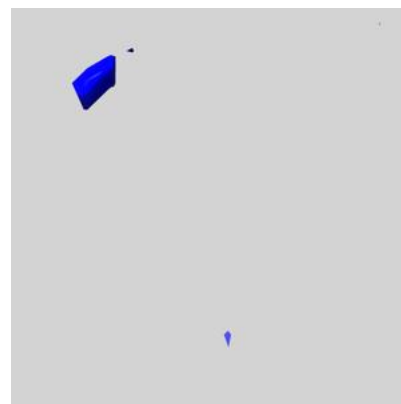
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6.5.17 emd_1001_msk_9.map [i](#)

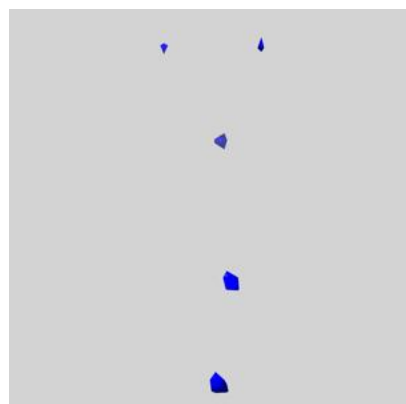
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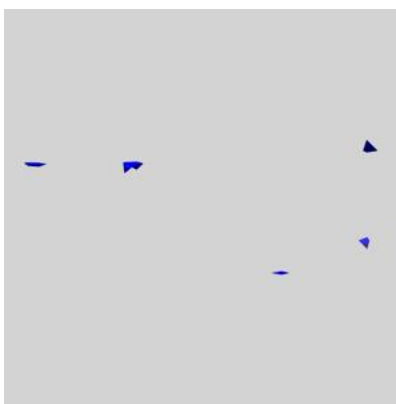
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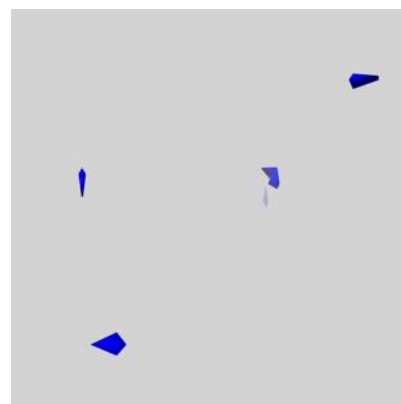
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6.5.18 emd_1001_msk_8.map [i](#)

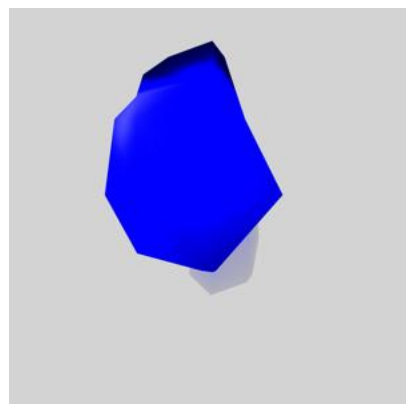
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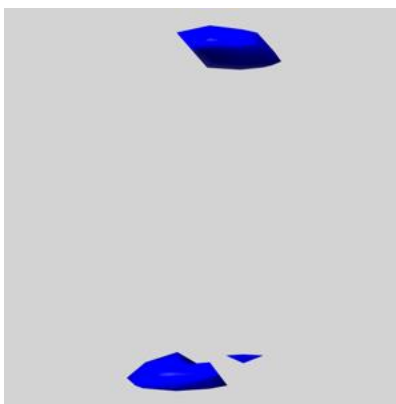
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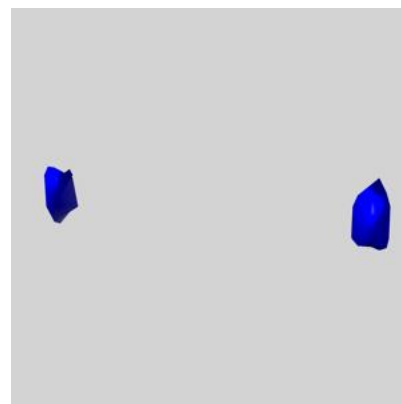
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6.5.19 emd_1001_msk_7.map [i](#)

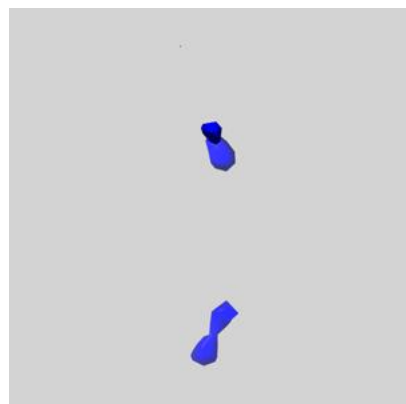
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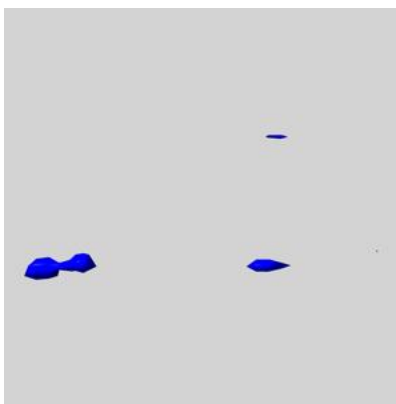
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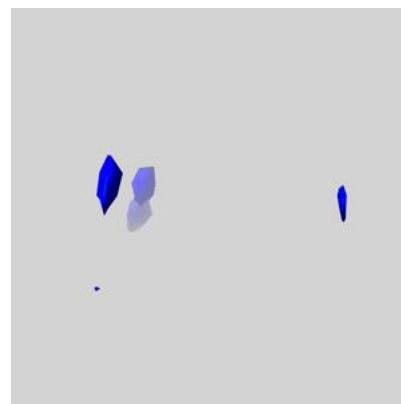
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6.5.20 emd_1001_msk_6.map [i](#)

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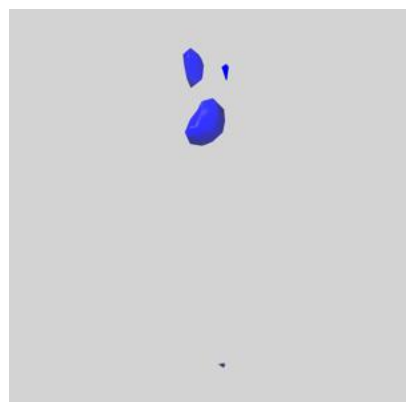


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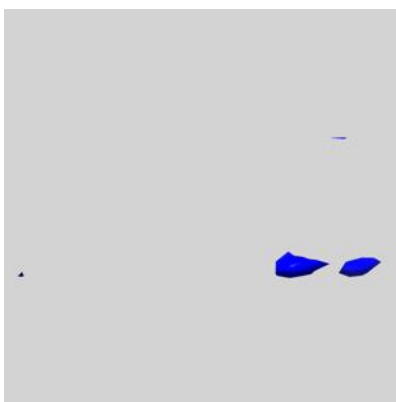


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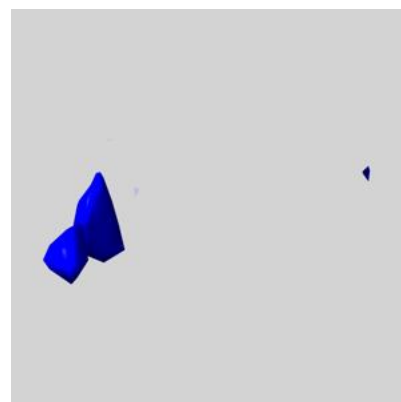
6.5.21 emd_1001_msk_5.map [i](#)



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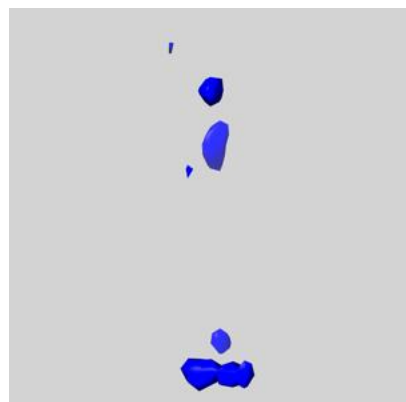


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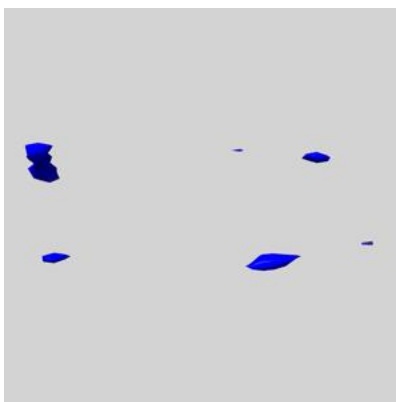


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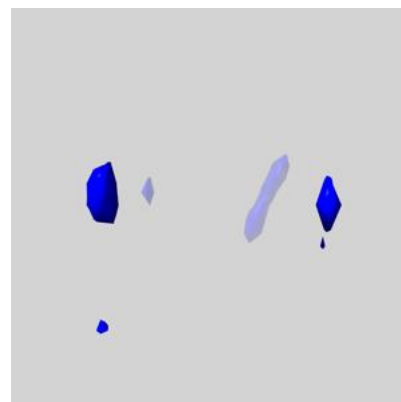
6.5.22 emd_1001_msk_4.map [i](#)



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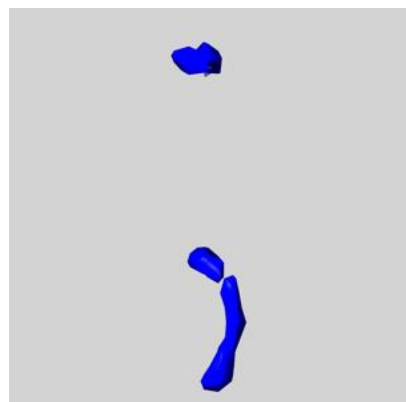


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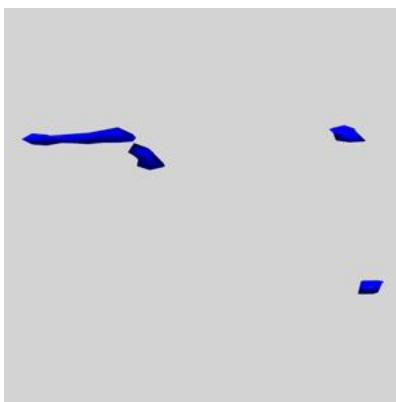


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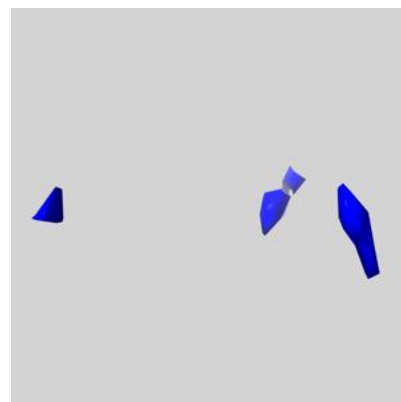
6.5.23 emd_1001_msk_3.map [i](#)



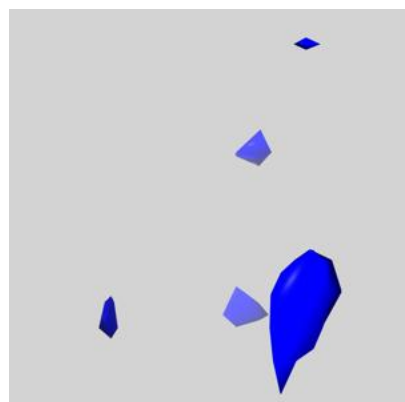
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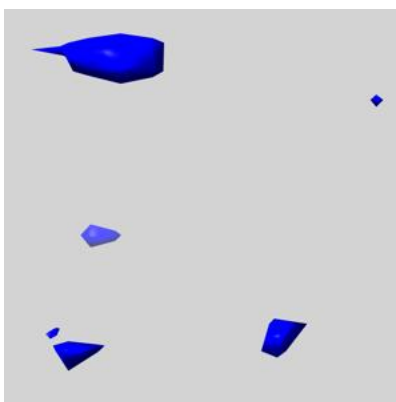
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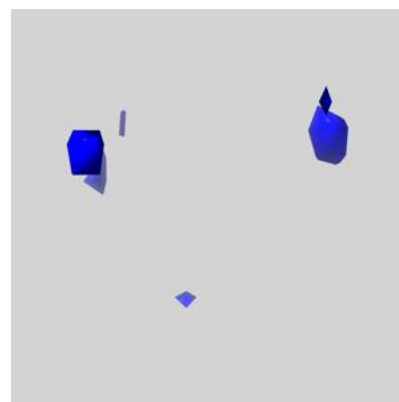
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6.5.24 emd_1001_msk_2.map [i](#)

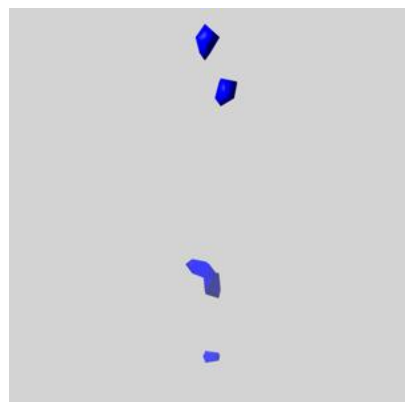
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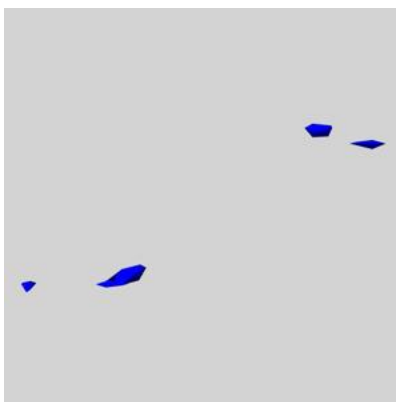
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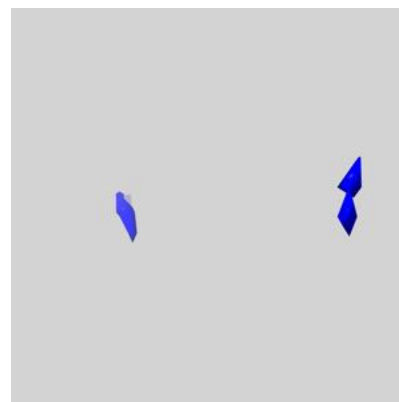
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6.5.25 emd_1001_msk_1.map [i](#)

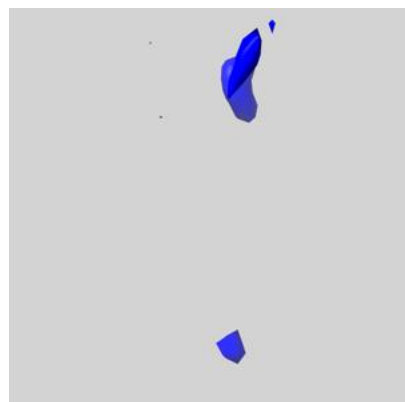
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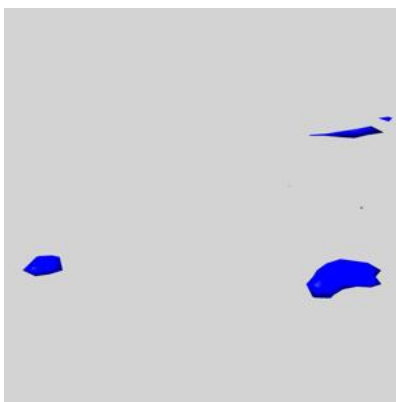
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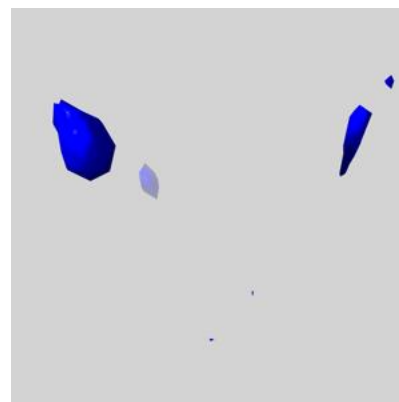
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6.5.26 emd_1001_msk_26.map [i](#)

X



Y

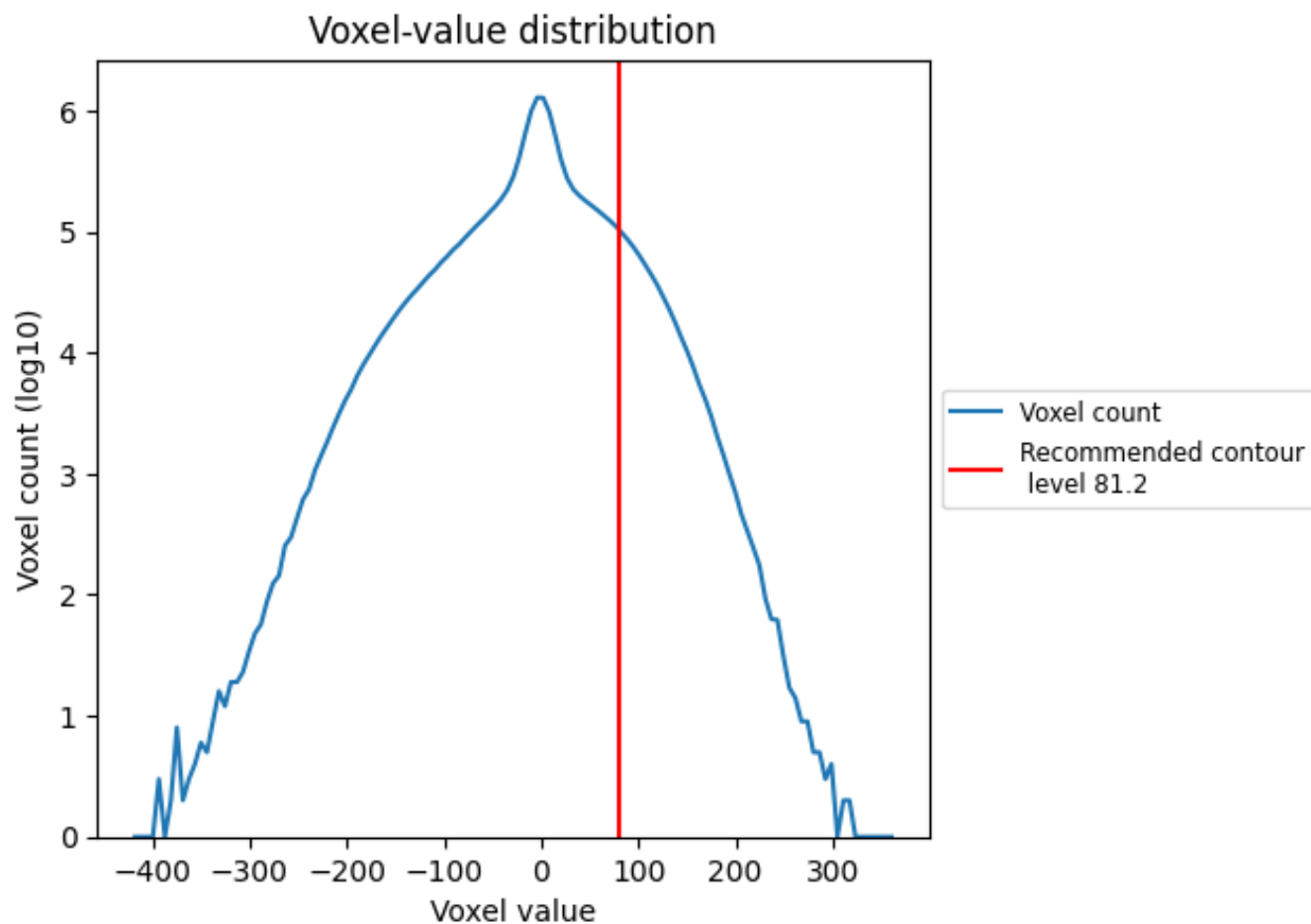


Z

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.

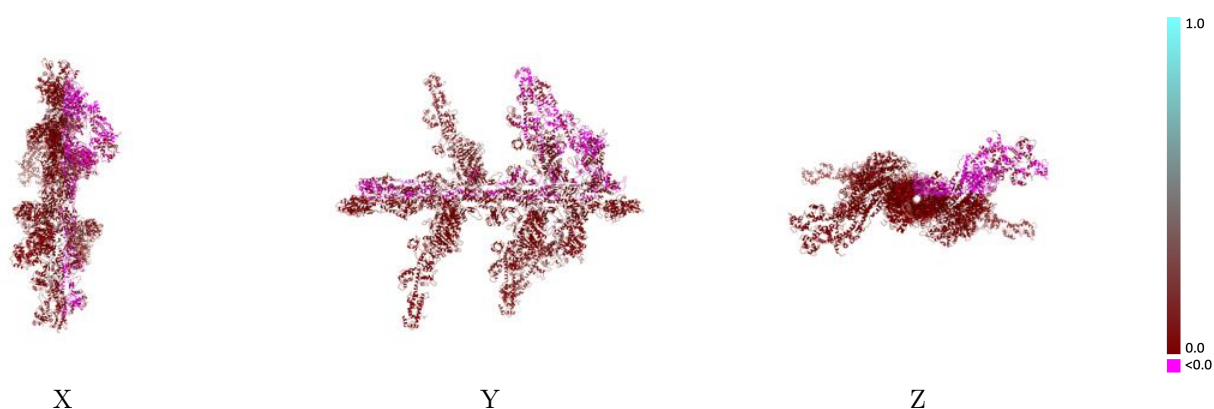
8 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-1001 and PDB model 1O1G. 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](#)

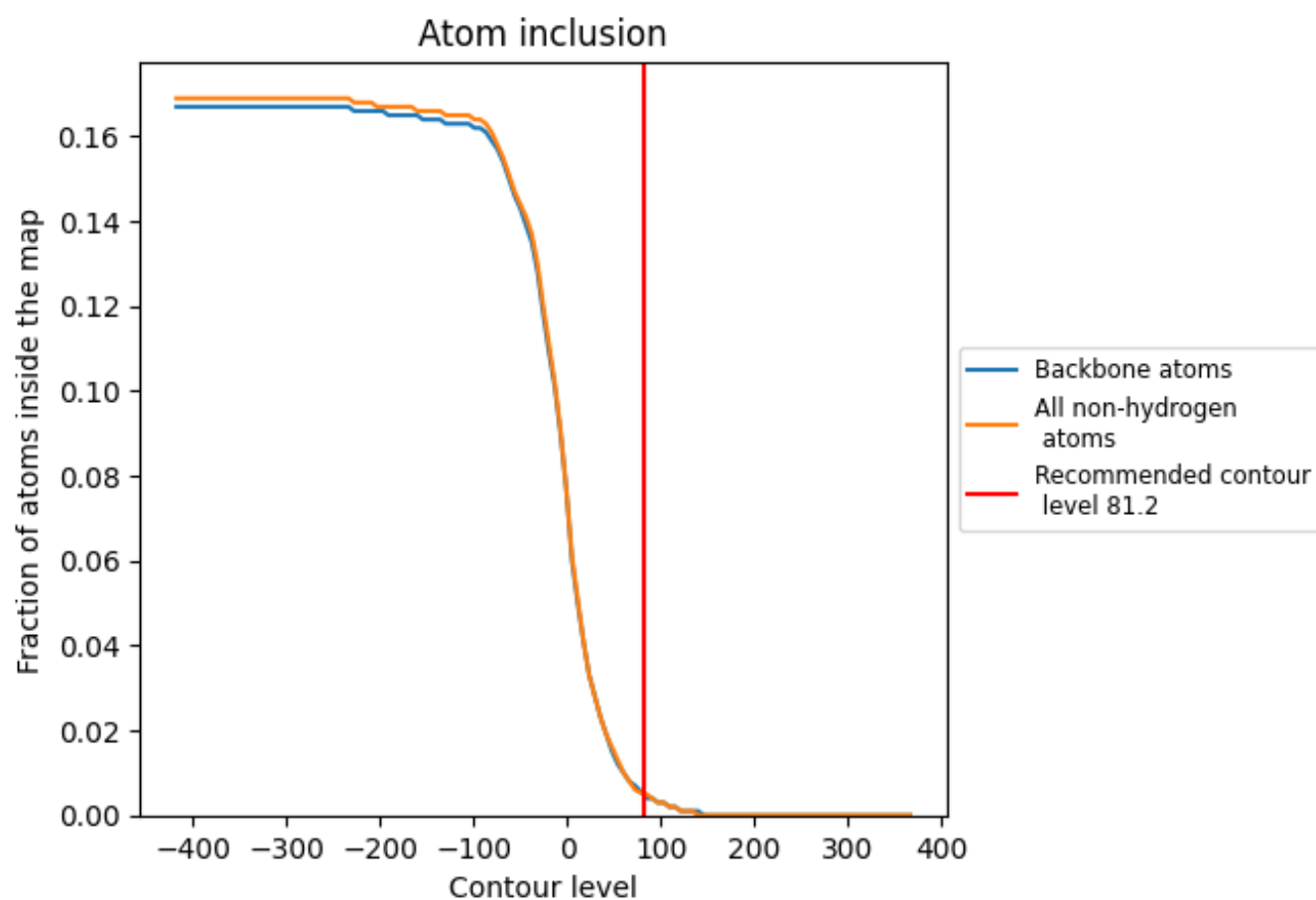


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 0% 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	 0.0050	 -0.0020
1	 0.0070	 0.0040
2	 0.0000	 0.0000
3	 0.0000	 -0.0030
4	 0.0000	 -0.0000
5	 0.0000	 -0.0160
6	 0.0000	 -0.0000
7	 0.0000	 0.0010
8	 0.0000	 -0.0030
9	 0.0000	 -0.0020
A	 0.0000	 -0.0160
B	 0.0000	 0.0050
C	 0.0000	 -0.0090
D	 0.0000	 0.0000
E	 0.0000	 0.0000
F	 0.0000	 0.0000
G	 0.0060	 -0.0020
H	 0.0000	 0.0100
I	 0.2890	 0.0220
J	 0.0000	 0.0000
K	 0.0000	 0.0000
L	 0.0000	 0.0000
M	 0.0000	 0.0000
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	 0.0020
W	 0.0010	 -0.0010
X	 0.0020	 -0.0060
Y	 0.0280	 0.0020
Z	 0.0000	 0.0010

