



wwPDB EM Validation Summary Report ⓘ

Mar 17, 2026 – 05:34 PM UTC

PDB ID : 1O18 / pdb_00001o18
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 : 2002-11-04
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

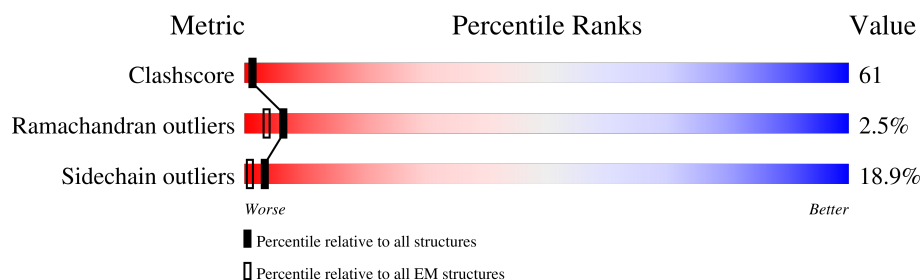
1 Overall quality at a glance

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% 26% 48% 22% .
1	D	840	100% 25% 49% 22% .
1	G	840	100% 24% 49% 22% 5%
1	J	840	100% 24% 50% 22% .
1	M	840	100% 25% 49% 22% .
1	P	840	100% 25% 50% 22% .
2	E	145	100% 65% 25% 7% .
2	H	145	100% 62% 29% 6% .

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Mol	Chain	Length	Quality of chain
2	K	145	100% 63% 26% 7% .
2	N	145	100% 63% 28% 6% .
2	Q	145	100% 61% 30% 6% .
3	F	147	100% 62% 35% .
3	I	147	84% 62% 35% .
3	L	147	100% 62% 35% .
3	O	147	100% 61% 35% ..
3	R	147	100% 61% 35% ..
4	1	375	98% 50% 35% 12% ..
4	2	375	99% 52% 36% 9% ..
4	3	375	99% 54% 35% 9% ..
4	4	375	99% 54% 34% 9% ..
4	5	375	99% 55% 33% 9% ..
4	6	375	99% 56% 33% 9% ..
4	7	375	99% 56% 33% 9% ..
4	8	375	99% 52% 34% 11% ..
4	9	375	99% 50% 35% 12% ..
4	V	375	99% 50% 35% 12% ..
4	W	375	97% 49% 35% 13% ..
4	X	375	99% 54% 34% 10% ..
4	Y	375	99% 54% 34% 9% ..
4	Z	375	99% 50% 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 criteria:

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	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	839	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 92716 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	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	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	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		

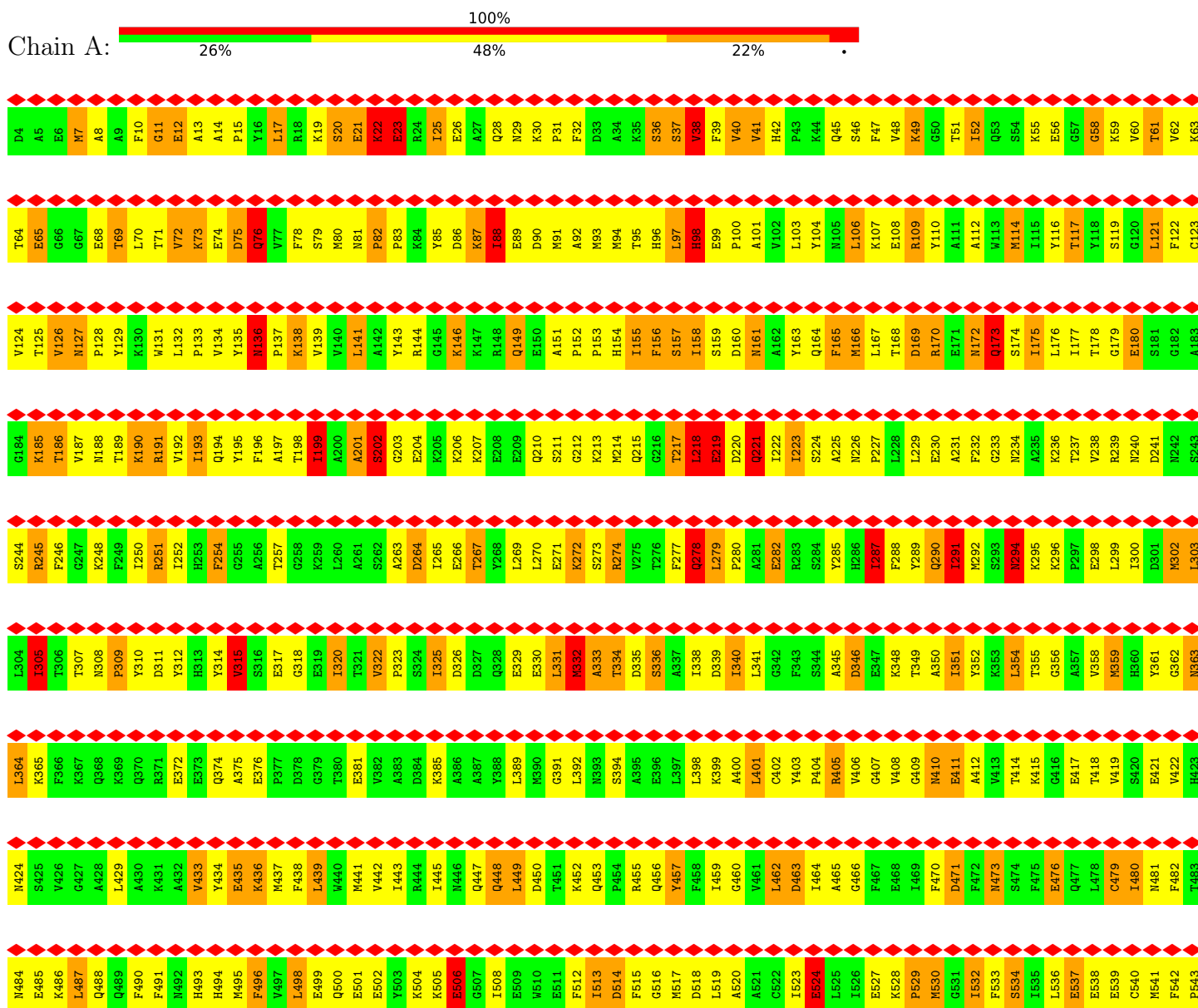
- Molecule 4 is a protein called SKELETAL MUSCLE ACTIN.

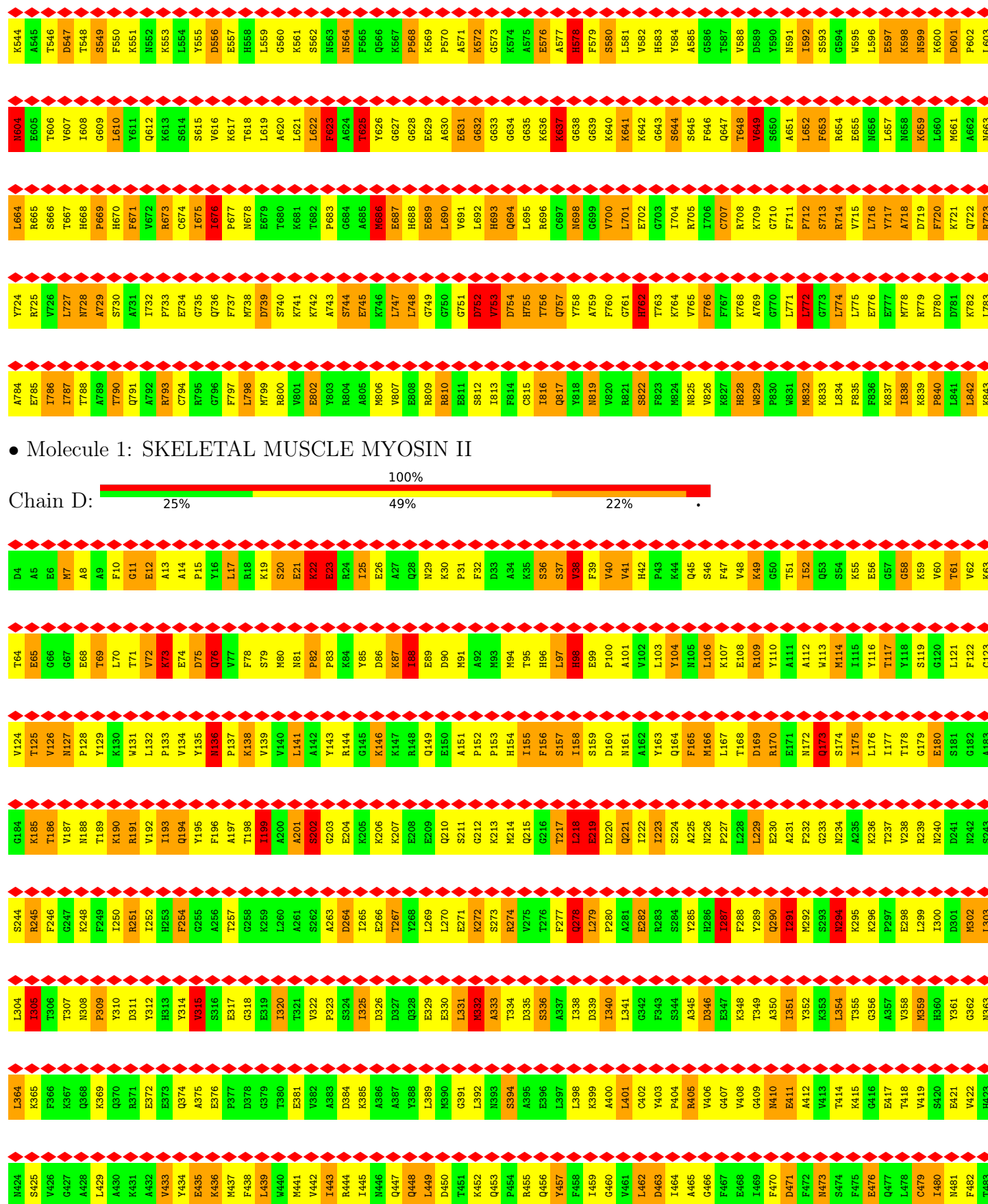
Mol	Chain	Residues	Atoms					AltConf	Trace
4	1	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	2	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	3	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	4	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	5	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
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		

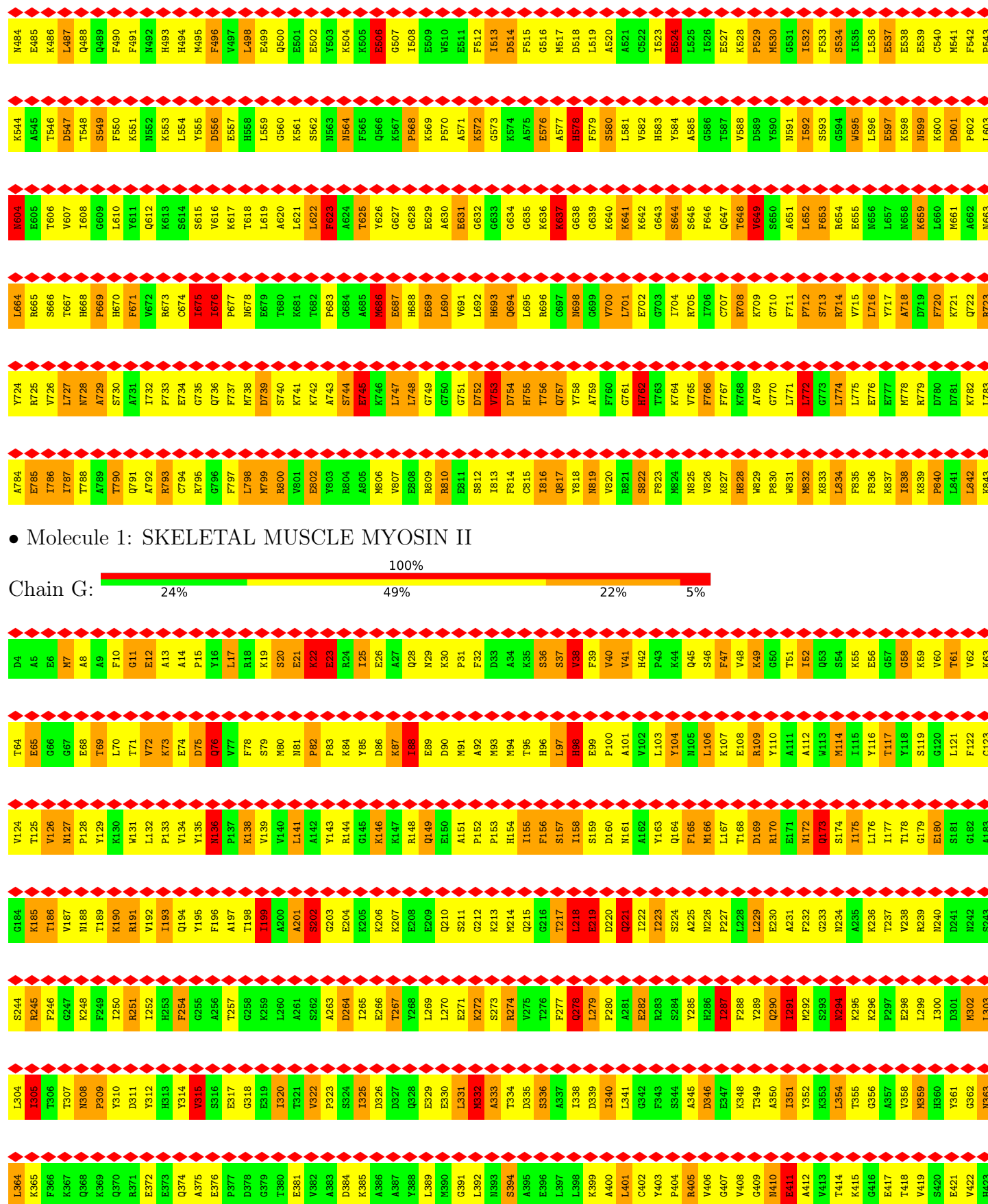
3 Residue-property plots

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	N127	V187	G247	T307
A428	Q488	T548	H668	M728	T788	A8	E68	P128	N188	K248	N308
L429	Q489	S549	P669	A729	A789	A9	T69	Y129	T189	F249	N309
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	T72	L132	V192	L252	Y312
A433	H493	K553	R673	P733	R793	A13	K73	P133	I193	H253	Y313
Y434	H494	L554	C674	E734	C794	A14	E74	V134	Q194	F254	Y314
E435	M495	Y555	I675	G735	R795	P15	E75	Y135	Y195	G255	V315
K436	F496	D556	I676	Q736	G796	Y16	Q76	N136	F196	A256	S316
M437	V497	V616	T677	F737	F797	L17	V77	P137	A197	T257	E317
F438	L498	H558	N678	M738	L798	R18	F78	K138	T198	G258	G318
L439	E499	L559	E679	D739	M799	K19	S79	V139	I199	K259	E319
Y440	Q500	G560	T680	S740	R800	S20	M80	Y140	A200	L260	I320
M441	E501	K561	K681	K741	V801	E21	N81	L141	A201	A261	T321
V442	E502	S562	T682	K742	E802	K22	P82	A142	S202	S262	V322
I443	Y503	N563	P683	A743	A805	E23	P83	Y143	G203	A263	P323
R444	K504	N564	G684	S744	M806	I24	K84	R144	E204	D264	S324
I445	K505	F565	A685	E745	M807	R25	Y85	G145	K205	L265	I325
N446	E506	Q566	M686	K746	E808	E26	D86	K146	K206	E266	D326
Q447	G507	Q567	E687	L747	E809	A27	I88	K147	K207	T267	D327
Q448	I508	P568	H688	L748	R809	Q28	E89	R148	E208	T268	Q328
L449	E509	K569	E689	G749	R810	N29	D90	Q149	E209	L269	E329
D450	W510	P570	L690	G750	E811	K30	D91	E150	Q210	L270	E330
T451	E511	A571	V691	G751	S812	P31	M91	A151	S211	E271	L331
K452	F512	K572	L692	D752	I813	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	I816	K35	T95	I155	Q215	V275	D335
Q456	G516	E576	R696	T756	Q817	S36	H96	F156	G216	T276	S336
Y457	M517	K577	C697	Q757	Y818	S37	L97	S157	T217	F277	A337
F458	D518	H578	N698	Y758	N819	V38	E98	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	E521	L581	L701	G761	S822	V41	A101	N161	Q221	A281	L341
L462	C522	V582	E702	H762	F823	H42	Y102	A162	I222	E282	G342
D463	I523	H583	G703	T763	N824	P43	L103	Q163	I223	R283	F343
I464	E524	Y584	I704	K764	N825	K44	Y104	Q164	S224	S284	S344
A465	E525	A585	R705	V765	V826	Q45	N105	F165	A225	Y285	A345
G466	I526	G586	I706	F766	K327	S46	L106	M166	N226	H286	D346
F467	E527	T587	C707	F767	H828	F47	K107	L167	P227	L287	E347
E468	K528	V588	R708	T768	W829	V48	E108	T168	T228	F288	K348
I469	P529	D589	K709	A769	P830	V49	K49	D169	L229	Y289	T349
F470	M530	Y590	G710	G770	W831	G50	K89	R170	E230	Q290	A350
D471	G531	N591	F711	L771	N832	T51	N832	E171	A231	I291	I351
F472	I532	L592	P712	L772	K833	I52	A112	M172	F232	M292	Y352
N473	F533	S593	S713	G773	L834	Q53	L834	Q173	Q233	S293	K353
S474	S534	G594	R714	L774	P835	S54	F835	M114	N234	N294	L354
F475	I535	W595	V715	L775	F836	K55	F836	I115	A235	K295	T355
E476	L536	L596	T716	E776	K837	E56	K837	Y116	L176	K296	G356
Q477	E537	T597	L717	E777	T838	G57	T838	T117	L177	P297	A357
L478	E538	K598	A718	M778	K839	G58	K839	Y118	T178	E298	V358
C479	E539	N599	D719	R779	P840	V60	P840	S119	G179	L299	K359
I480	C540	K600	F720	D780	L841	V61	G120	E180	E180	T300	H360
N481	M541	D601	K721	D781	L842	V62	G121	S181	L121	D301	Y361
F482	P542	A662	Q722	K782	K843		F122	G182	F122	K302	G362
T483	L603	N663	R723	L783			G123	A183		L303	N363

• Molecule 1: SKELETAL MUSCLE MYOSIN II



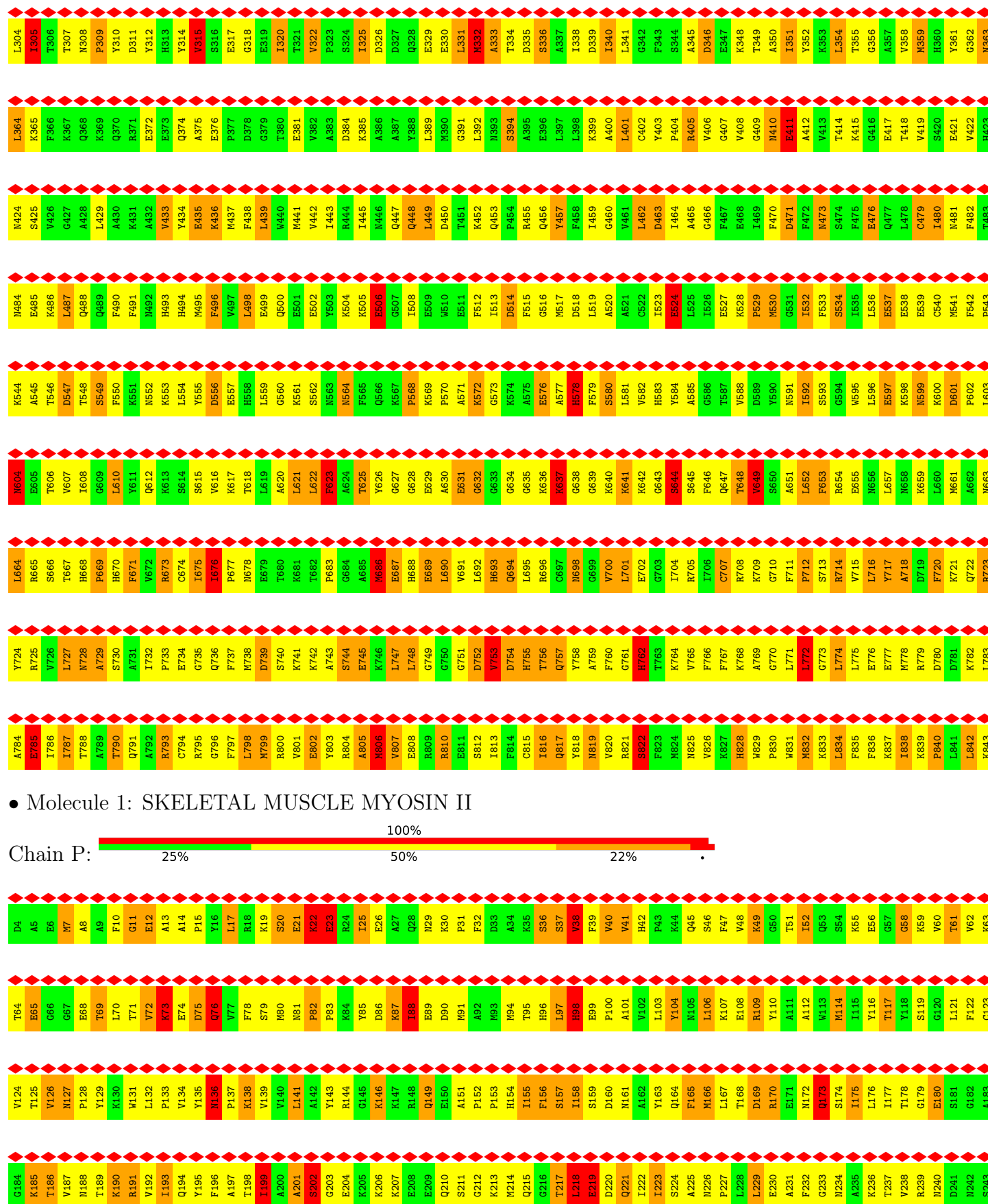
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A5	E65	T125	K185	R245	T305
E6	G66	V126	T186	F246	T306
M7	G67	N127	V187	G247	T307
A8	E68	P128	N188	K248	N308
A9	T69	Y129	T189	F249	N309
F10	L70	K130	K190	L250	Y310
G11	T71	V131	R191	R251	D311
E12	T72	L132	V192	L252	Y312
A13	K73	P133	I193	H253	Y313
A14	E74	V134	Q194	F254	Y314
P15	E75	Y135	Y195	G255	V315
Y16	Q76	N136	F196	A256	S316
L17	V77	P137	A197	T257	E317
R18	F78	K138	T198	G258	G318
K19	S79	V139	I199	K259	E319
S20	M80	Y140	A200	L260	I320
E21	N81	L141	A201	A261	T321
K22	P82	A142	S202	S262	V322
E23	P83	Y143	G203	A263	P323
I24	K84	R144	E204	D264	S324
R25	Y85	G145	K205	L265	I325
E26	D86	K146	K206	E266	D326
A27	I88	K147	K207	T267	D327
Q28	E89	R148	E208	T268	Q328
N29	D90	Q149	E209	L269	E329
K30	D91	E150	Q210	L270	E330
P31	M91	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	E98	I158	L218	Q278	I338
F39	E99	S159	E219	L279	D339
V40	P100	D160	D220	P280	I340
V41	A101	N161	Q221	A281	L341
H42	Y102	A162	I222	E282	G342
P43	L103	Q163	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	T228	F288	K348
K49	D169	L229	L229	Y289	T349
G50	R170	E230	E230	Q290	A350
T51	E171	A231	A231	I291	I351
I52	M172	F232	F232	M292	Y352
Q53	Q173	Q233	Q233	S293	K353
S54	M114	N234	N234	N294	L354
K55	I115	A235	A235	K295	T355
E56	L176	K236	K236	K296	G356
G57	T117	T237	T237	P297	A357
G58	Y118	V238	V238	E298	V358
N59	S119	R239	R239	L299	K359
V60	G120	E180	N240	T300	H360
T61	S181	L121	D241	D301	Y361
V62	F122	G182	N242	K302	G362
K63		A183		L303	N363

L364	K365	F366	K367	K368	K369	Q370	R371	E372	E373	Q374	A375	E376	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
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	E476	Q477	L478	C479	I480	M481	F482	T483
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
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	G573	K574	A575	E576	A577	H578	F579	S580	L581	V582	H583	Y584	A585	G586	T587	V588	D589	Y590	N591	I592	F593	S594	W595	L596	E597	K598	N599	K600	D601	P602	L603
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	N663
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	L690	V691	L692	H693	Q694	L695	R696	G697	N698	G699	V700	L701	E702	G703	I704	R705	I706	F707	R708	K709	G710	F711	P712	S713	R714	V715	L716	A717	D718	F719	F720	Q721	R722	R723
Y724	R725	V726	L727	M728	A729	S730	A731	I732	P733	E734	G735	Q736	F737	M738	D739	S740	K741	T682	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	L771	L772	G773	L774	L775	E776	M777	R778	D779	D780	L781	K782	L783
A784	E785	I786	T787	T788	A789	T790	Q791	A792	R793	C794	R795	G796	F797	L798	M799	R800	V801	E802	Y803	R804	A805	M806	E807	E808	R809	R810	E811	S812	I813	F814	C815	L816	Q817	Y818	N819	V820	R821	S822	F823	M824	N825	V826	K827	H828	V829	P830	M831	N832	K833	L834	F835	P836	K837	T838	K839	P840	L841	L842	K843

• Molecule 1: SKELETAL MUSCLE MYOSIN II



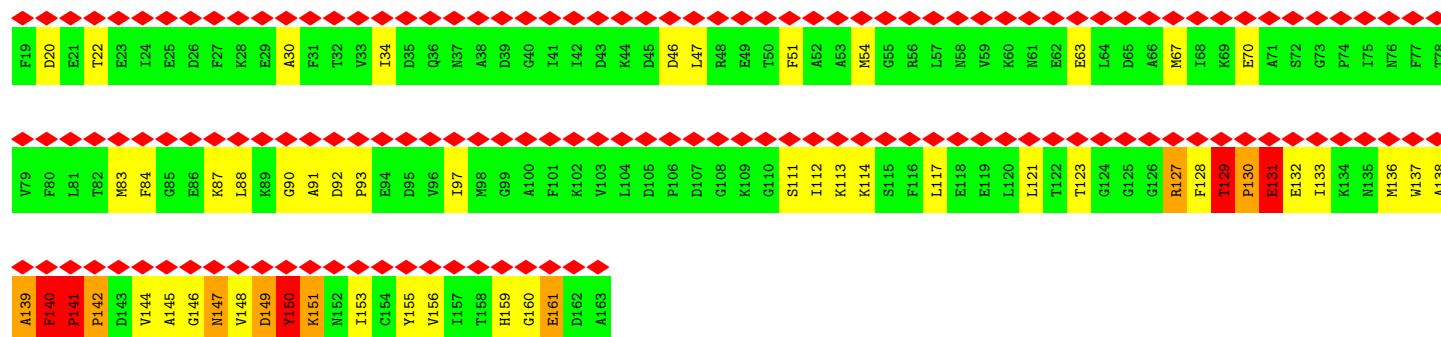
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G184	K185	T186	V187	N188	T189	K190	R191	V192	I193	Q194	Y195	F196	A197	T198	N199	A200	A201	S202	G203	E204	K205	K206	K207	E208	E209	Q210	S211	G212	K213	M214	Q215	G216	T217	L218	E219	D220	Q221	I222	I223	S224	A225	N226	P227	L228	L229	E230	A231	F232	G233	N234	A235	K236	T237	V238	R239	N240	D241	K242	L243
V124	T125	V126	N127	N128	Y129	K130	V131	L132	P133	V134	Y135	N136	P137	K138	V139	Y140	L141	A142	Y143	R144	G145	K146	L147	R148	Q149	E150	A151	P152	P153	H154	I155	F156	S157	I158	S159	D160	N161	A162	Y163	Q164	F165	M166	L167	T168	D169	R170	E171	N172	Q173	S174	I175	L176	T177	T178	G179	E180	L181	G182	A183
T64	E65	G66	G67	E68	T69	L70	T71	V72	K73	E74	D75	Q76	V77	F78	S79	M80	N81	P82	P83	G84	H85	D86	K87	E88	E89	D90	N91	A92	H93	M94	T95	H96	L97	H98	E99	P100	A101	V102	L103	Y104	N105	L106	K107	E108	R109	Y110	A111	A112	Y113	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	R23	R24	I25	E26	Q27	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	K58	K59	V60	T61	V62	K63



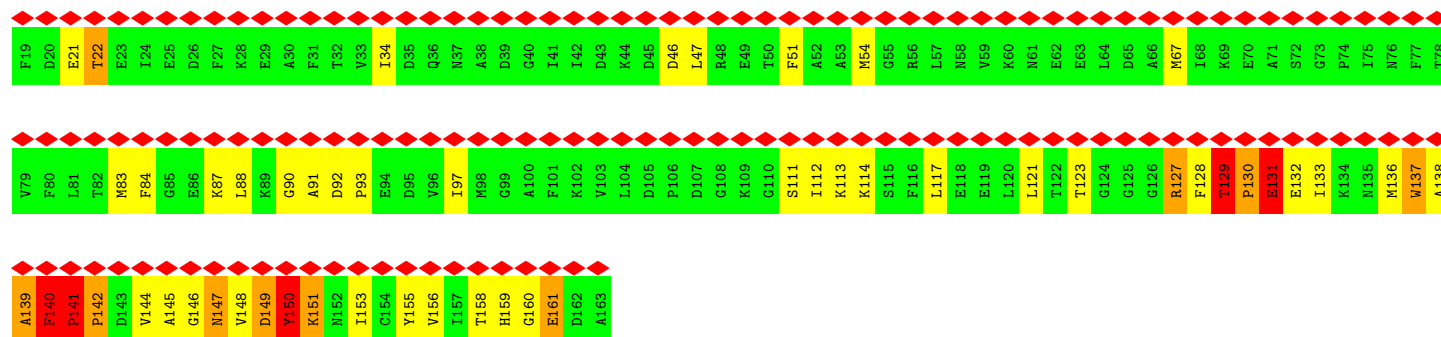
- Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

A139	F19	V79	
F140	D20	F80	
P141	E21	L81	
P142	T22	T82	
D143	E23	M83	
V144	T24	F84	
A145	E25	G85	
G146	D26	E86	
N147	F27	K87	
V148	X28	L88	
D149	E29	K89	
Y150	A30	G90	
K151	F31	A91	
H152	T32	D92	
I153	V33	P93	
C154	T34	E94	
	D35	D95	
	Q36	V96	
	N37	I97	
T158	A38	M98	
H159	D39	G99	
G160	G40	A100	
E161	I41	F101	
D162	I42	K102	
A163	D43	V103	
	X44	L104	
	D45	D105	
	D46	P106	
	L47	D107	
	A48	G108	
	E49	K109	
	T50	G110	
	F51	S111	
	A52	I112	
	A53	K113	
	M54	K114	
	G55	S115	
	R56	F116	
	L57	L117	
	M58	E118	
	V59	E119	
	X60	L120	
	M61	L121	
	E62	T122	
	E63	T123	
	L64	G124	
	D65	G125	
	A66	G126	
	M67	R127	
	T68	F128	
	K69	T129	
	E70	P130	
	A71	E131	
	S72	E132	
	G73	I133	
	P74	K134	
	I75	M135	
	M76	M136	
	F77	W137	
	T78	A138	

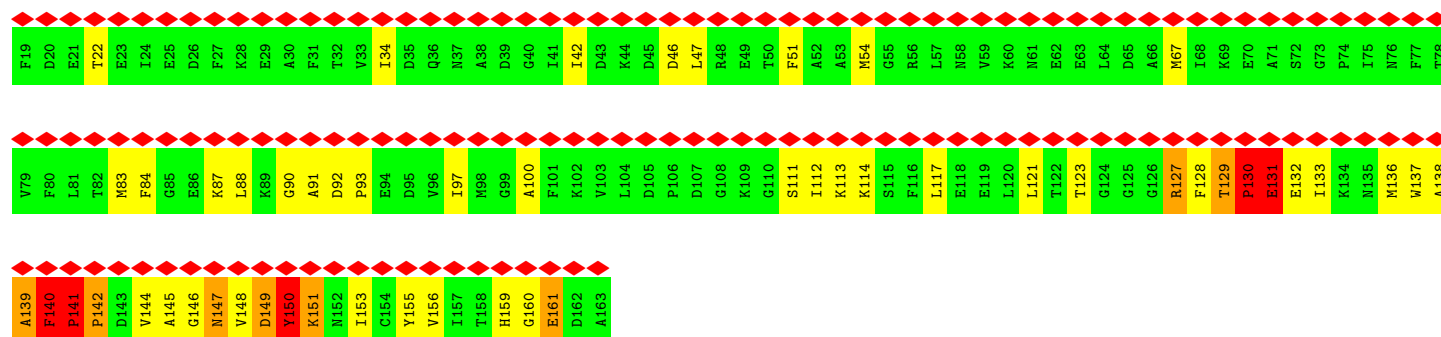
• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN



• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

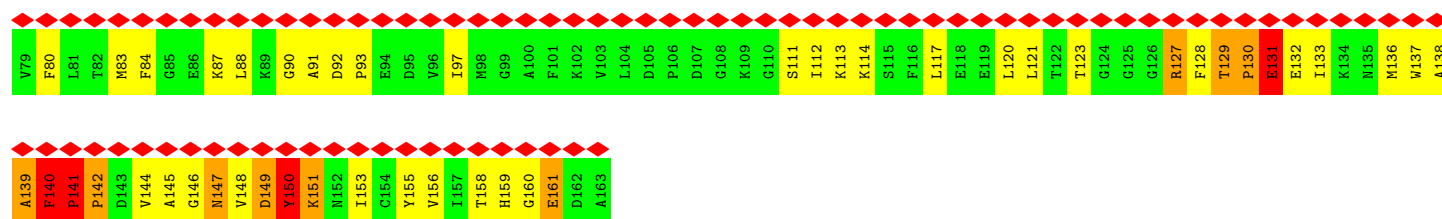


• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

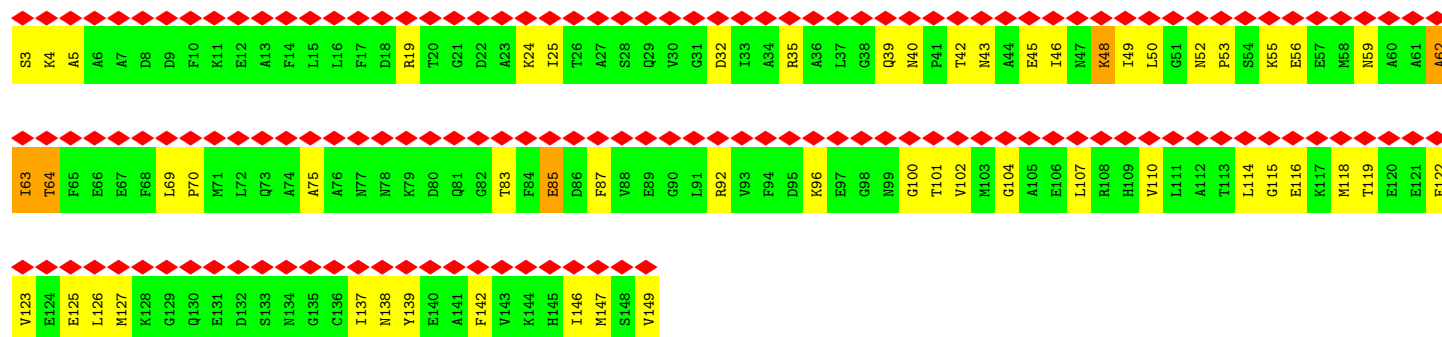


• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

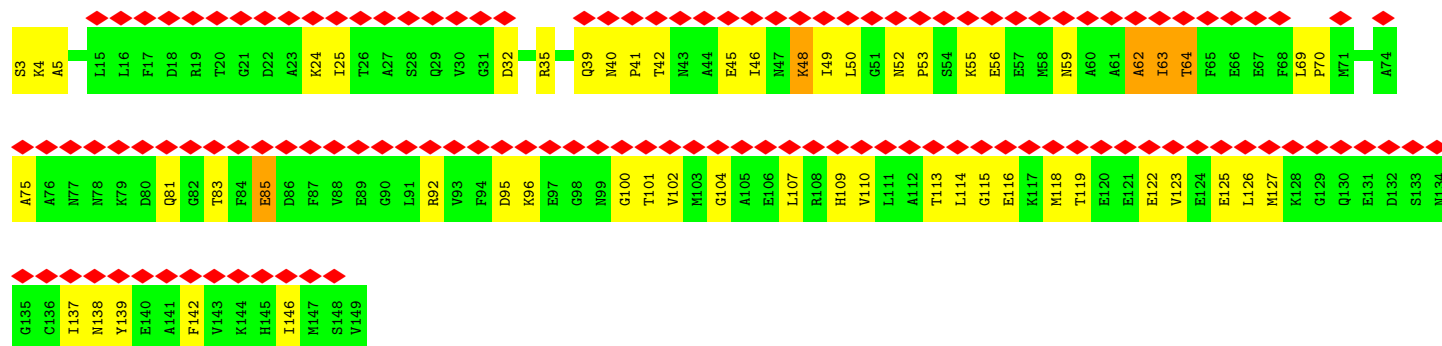
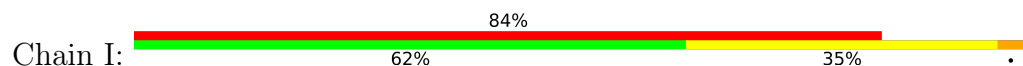




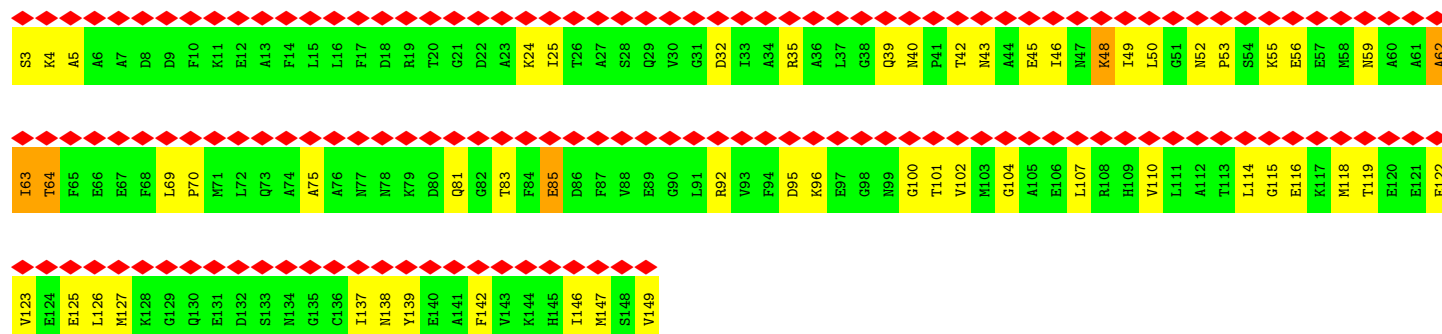
• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN



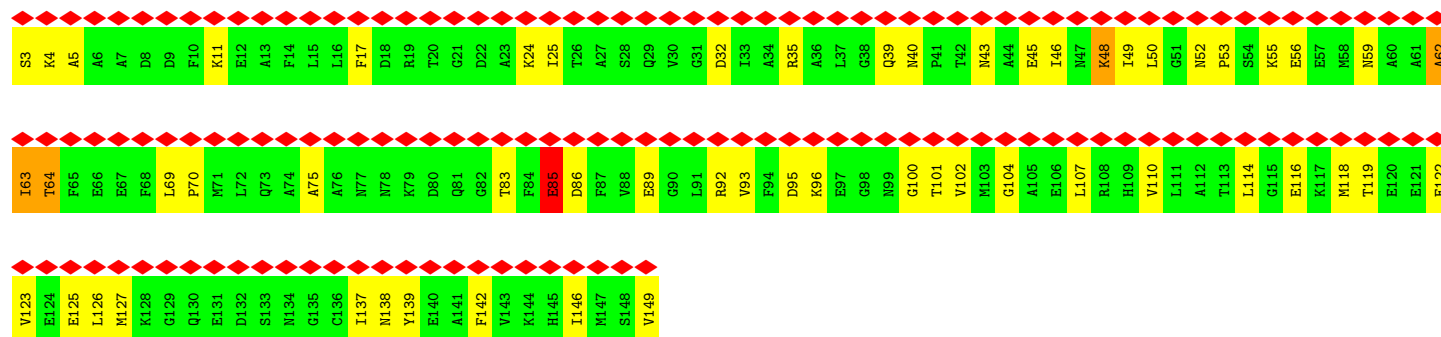
• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN



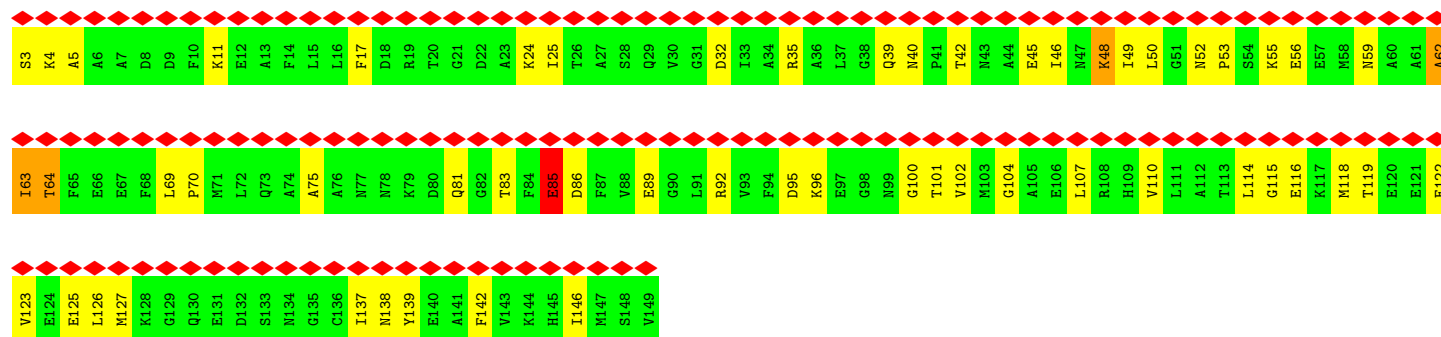
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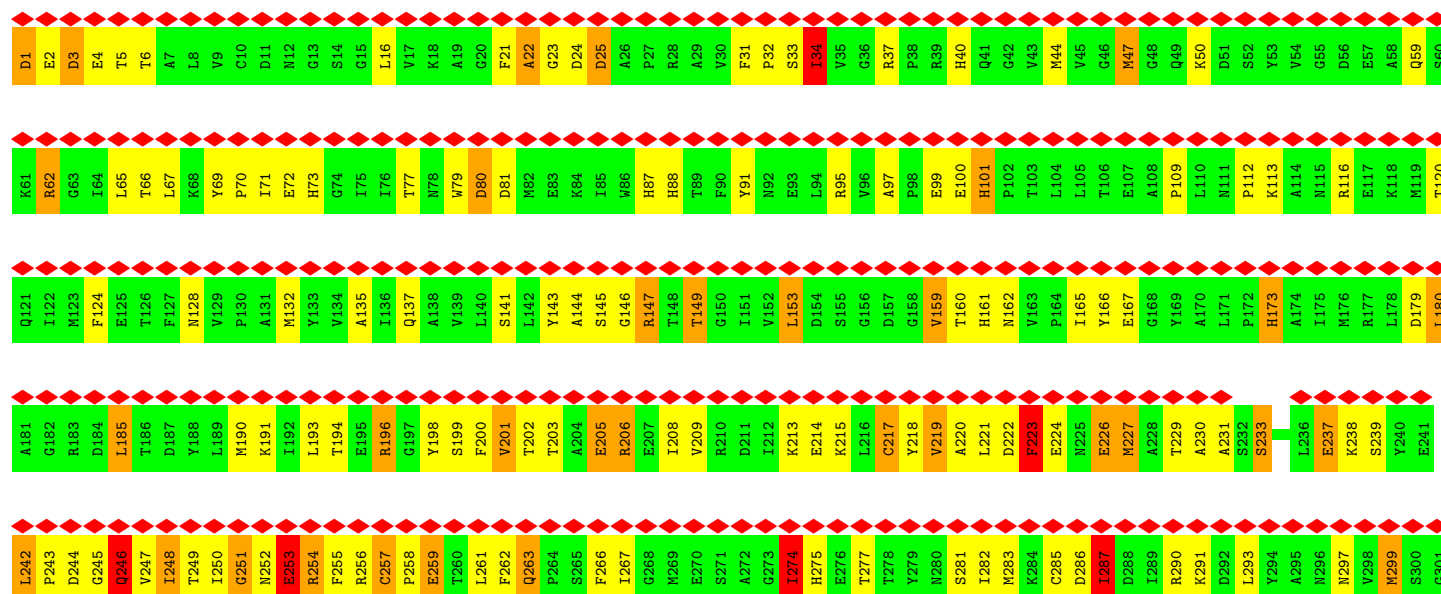
● Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN



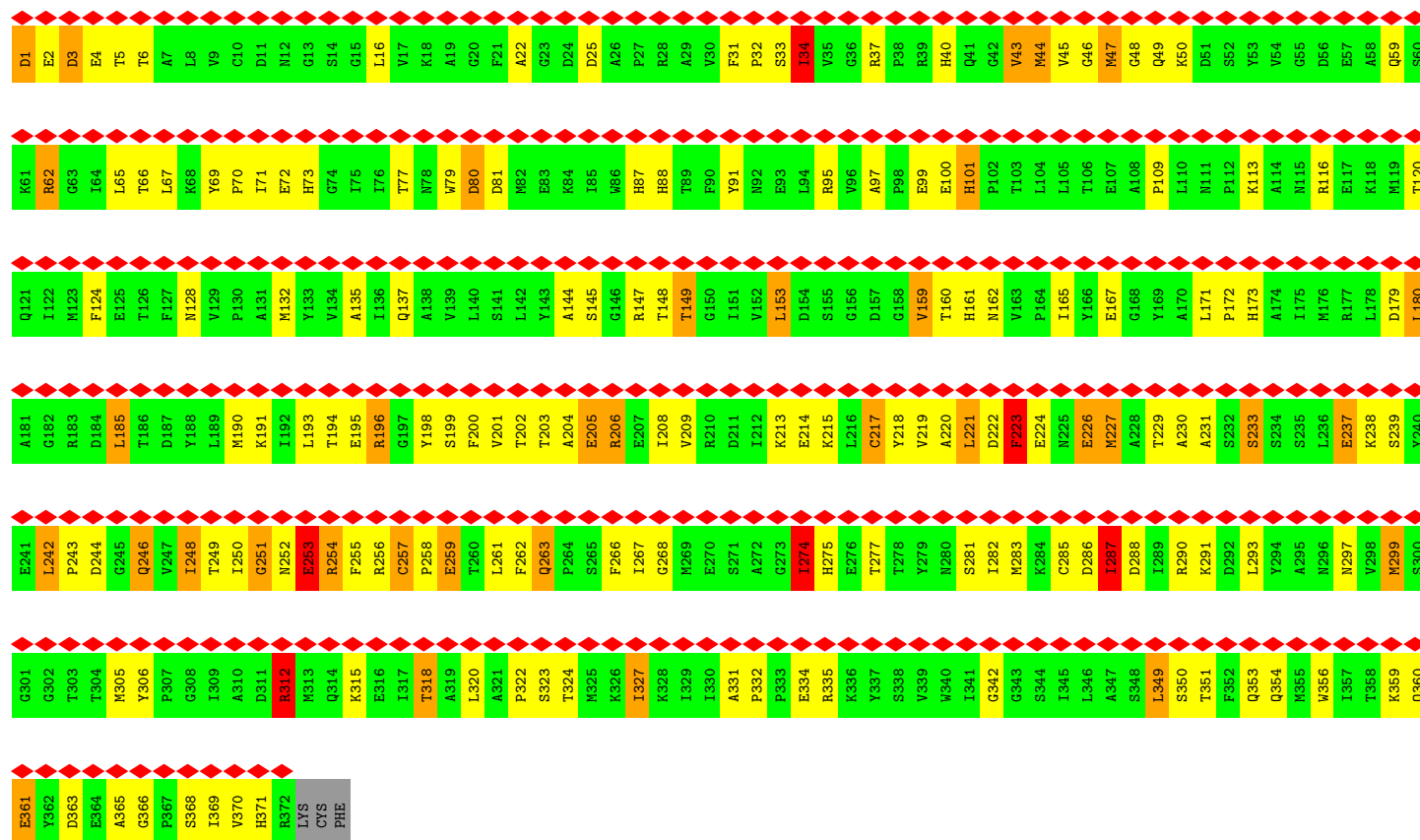
● Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN



● Molecule 4: SKELETAL MUSCLE ACTIN

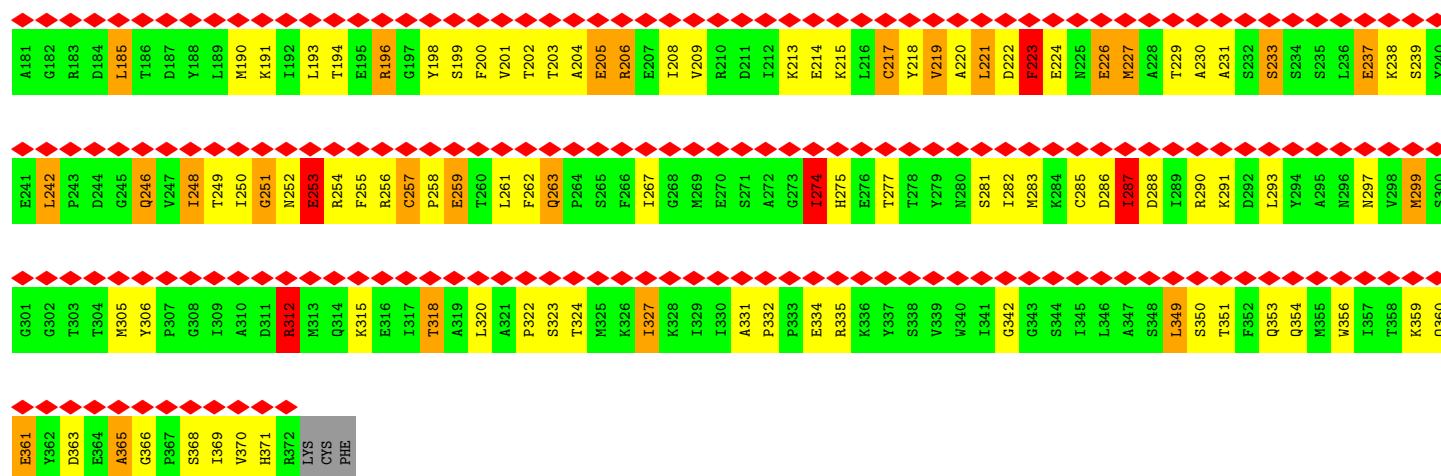


- Molecule 4: SKELETAL MUSCLE ACTIN

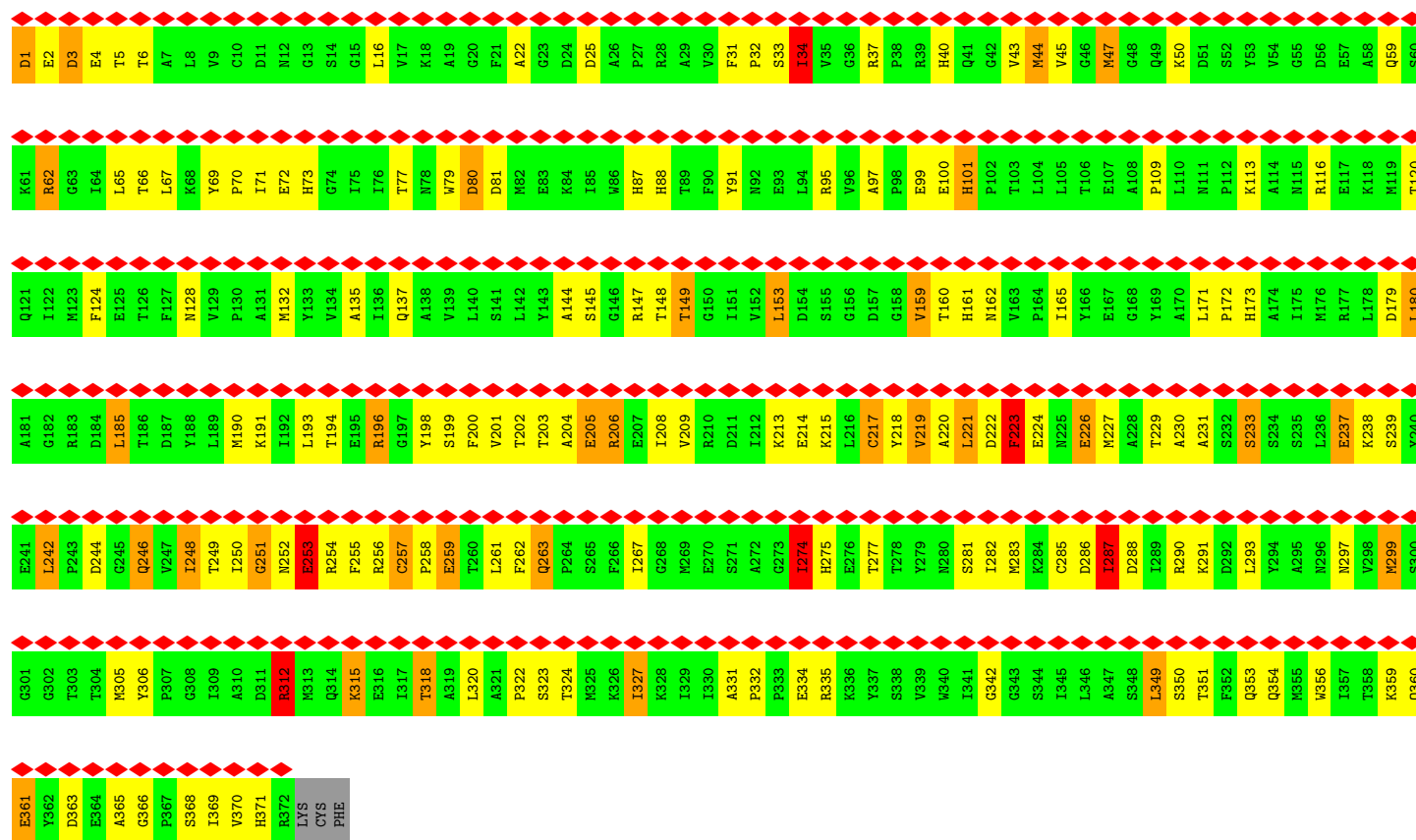


- Molecule 4: SKELETAL MUSCLE ACTIN



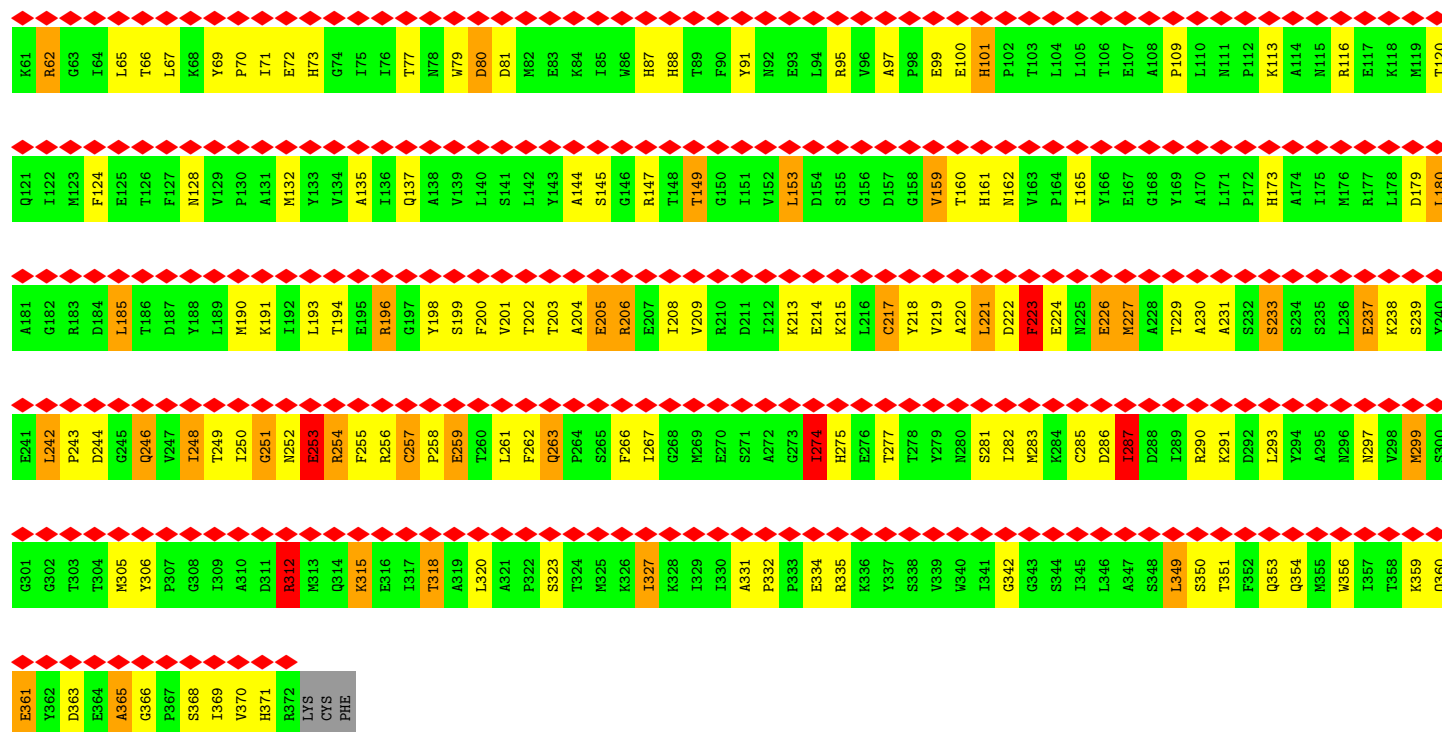


• Molecule 4: SKELETAL MUSCLE ACTIN

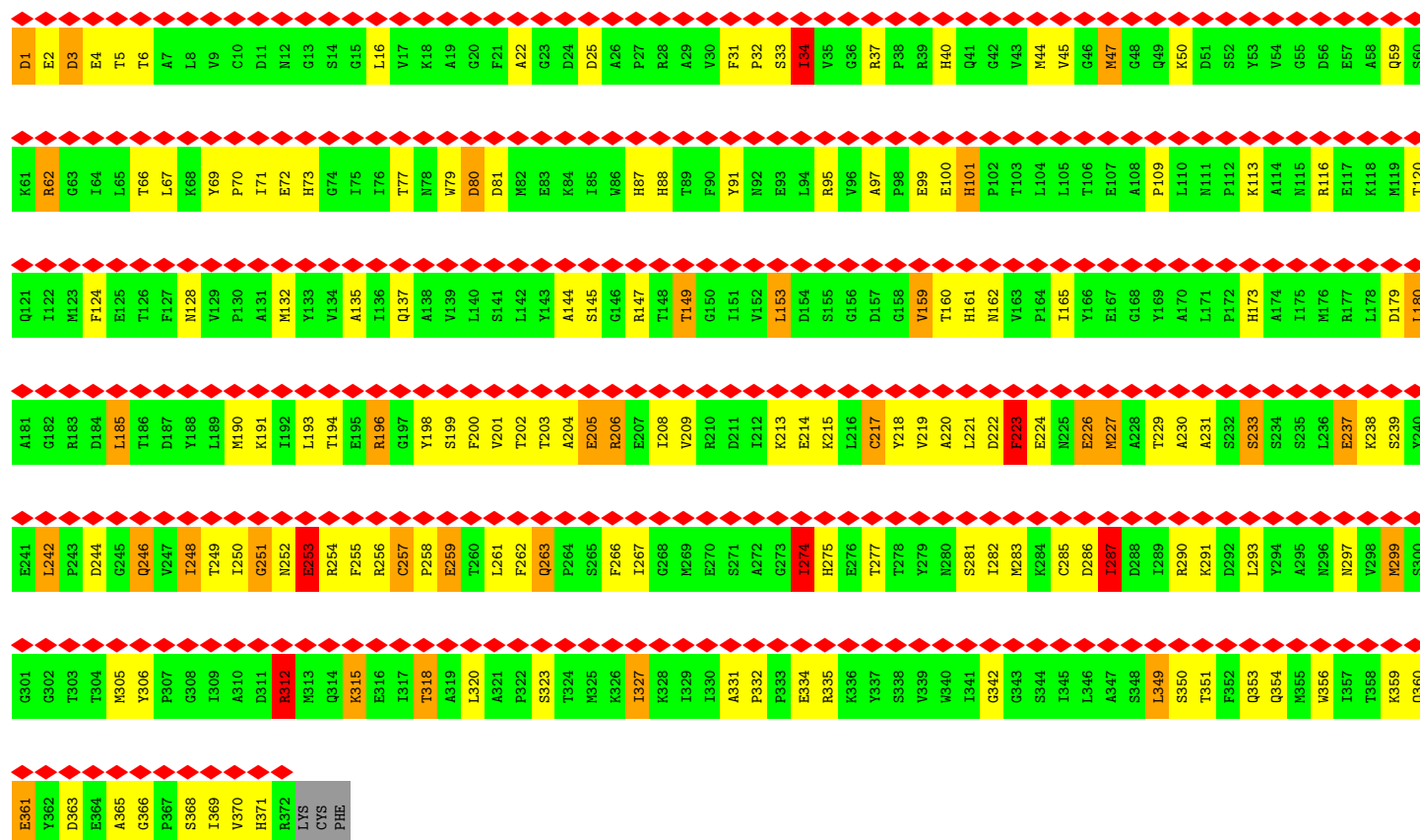


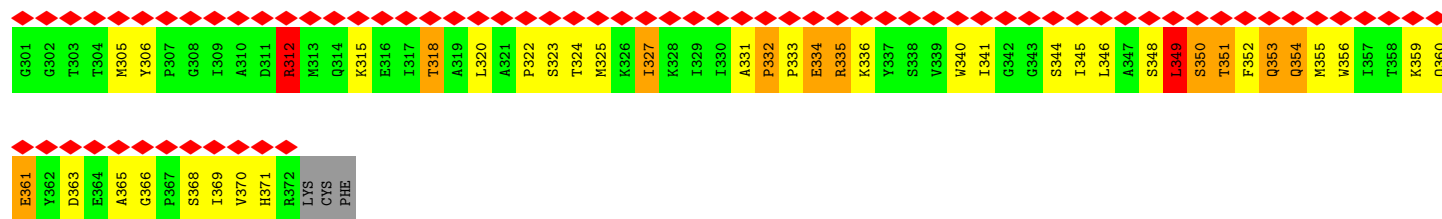
• Molecule 4: SKELETAL MUSCLE ACTIN



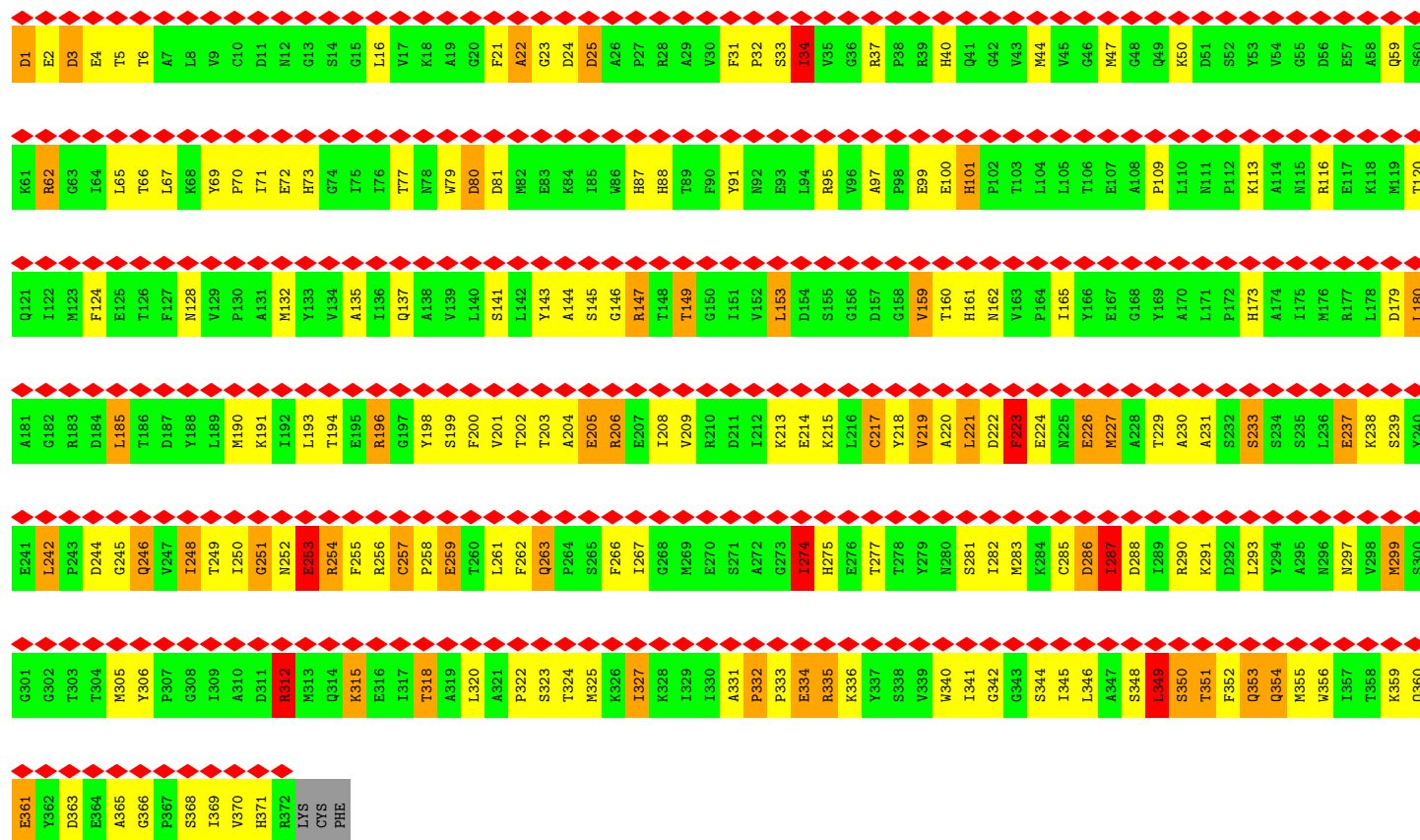


• Molecule 4: SKELETAL MUSCLE ACTIN

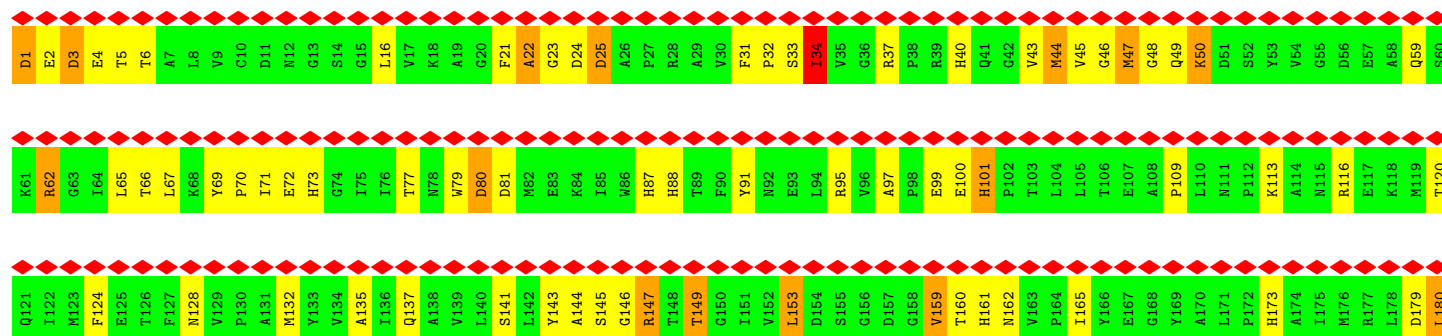


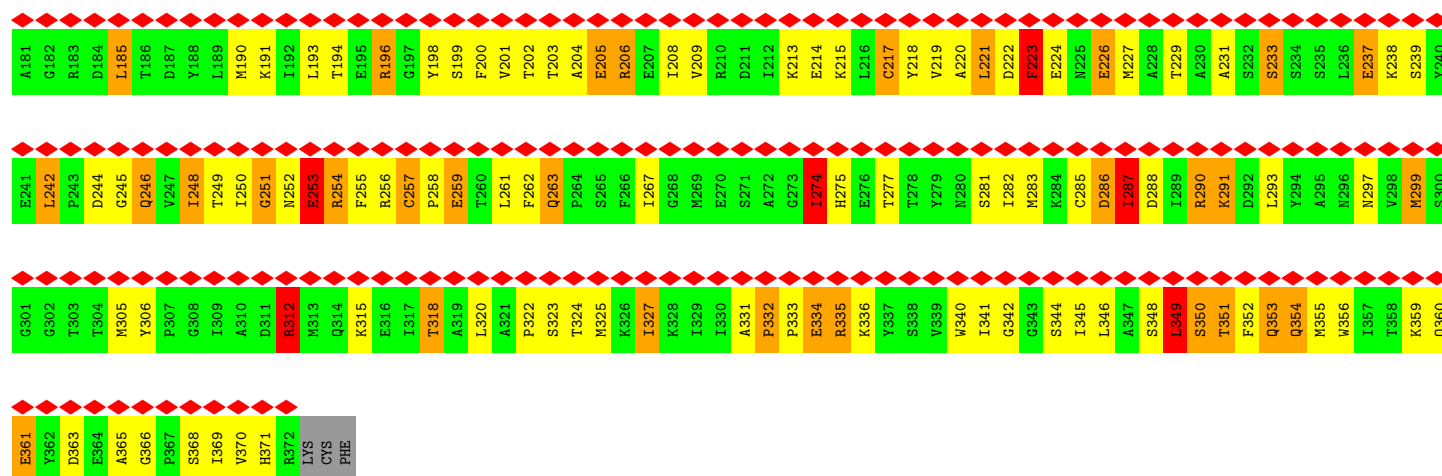


• Molecule 4: SKELETAL MUSCLE ACTIN

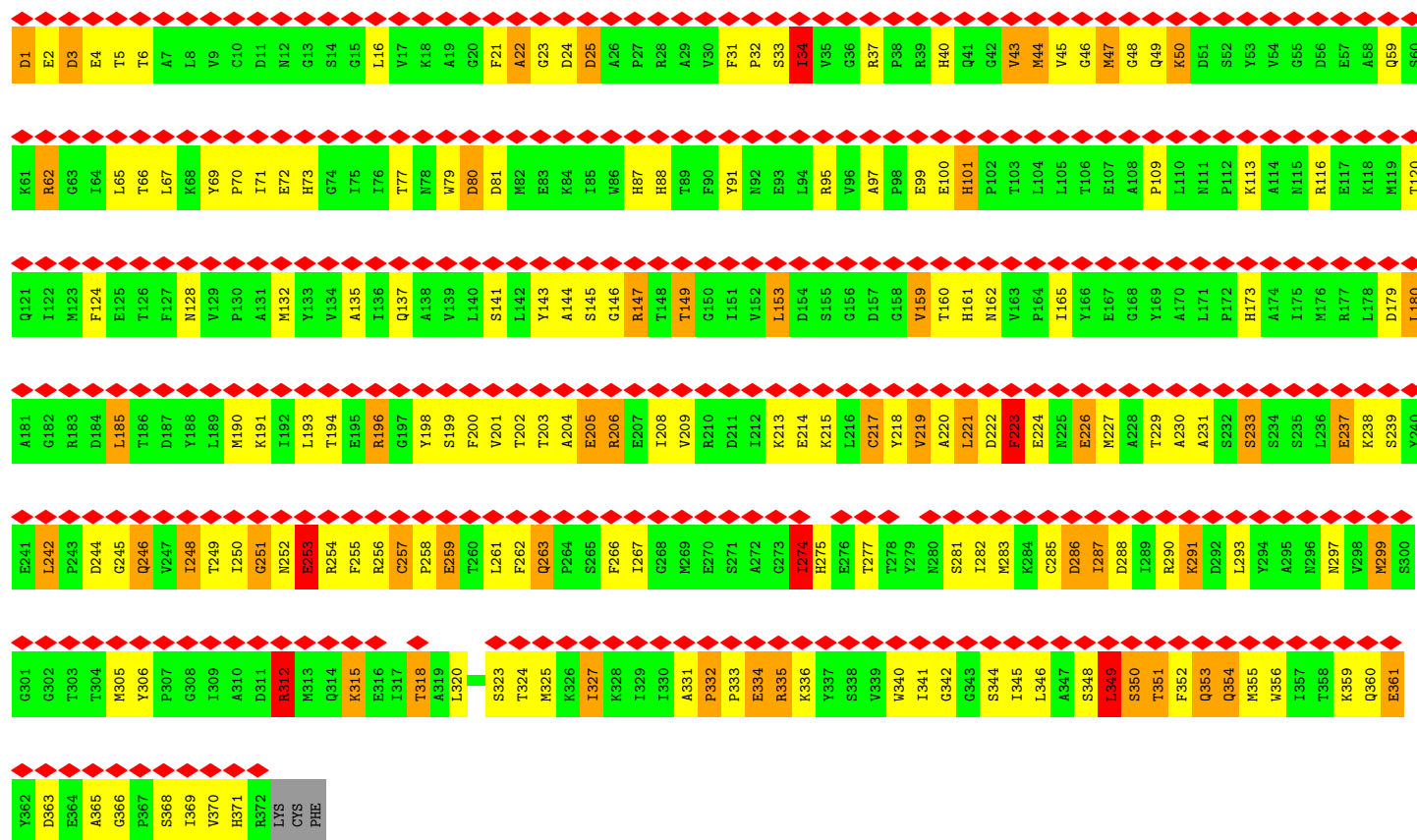


• Molecule 4: SKELETAL MUSCLE ACTIN

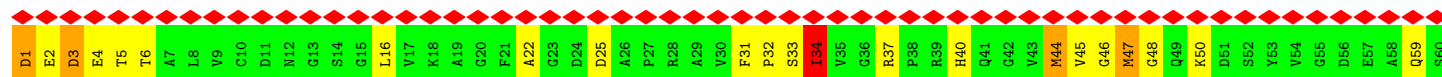


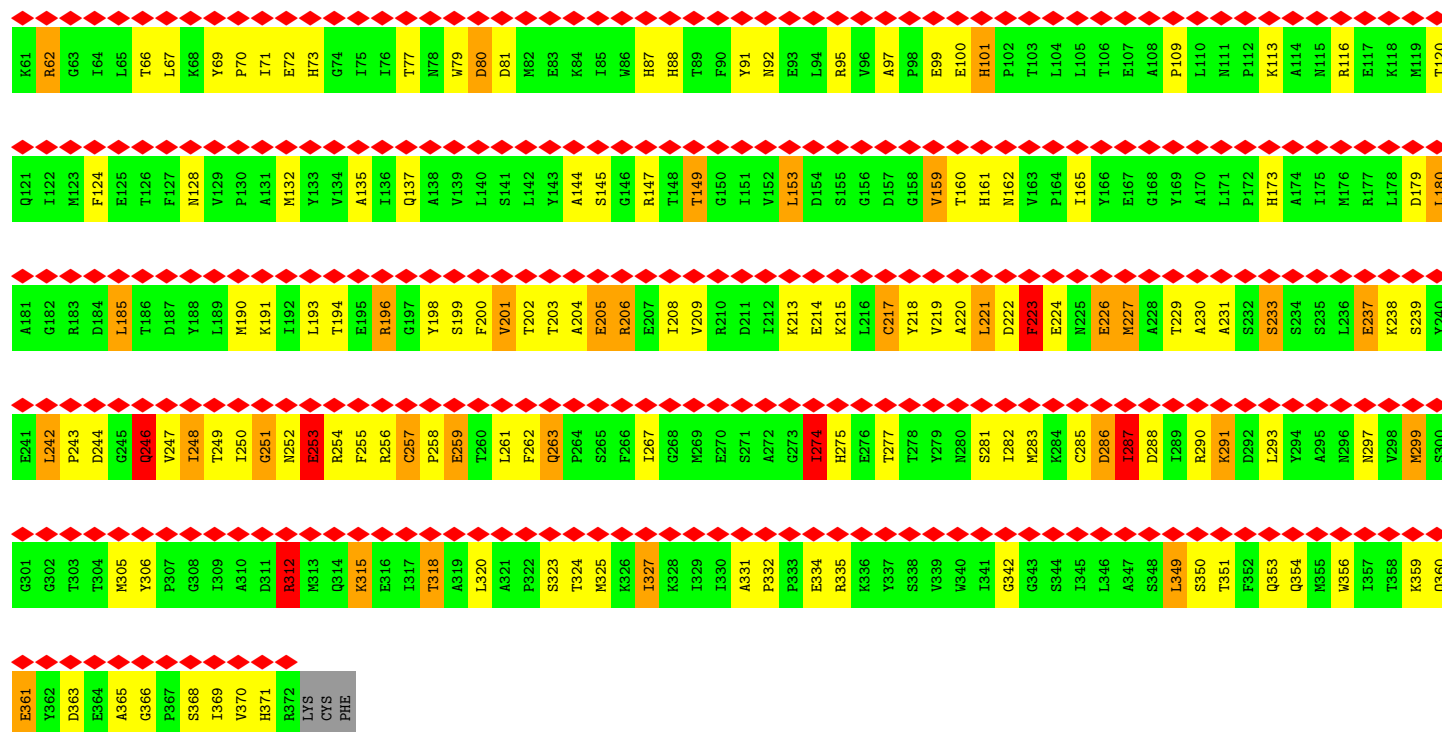


• Molecule 4: SKELETAL MUSCLE ACTIN

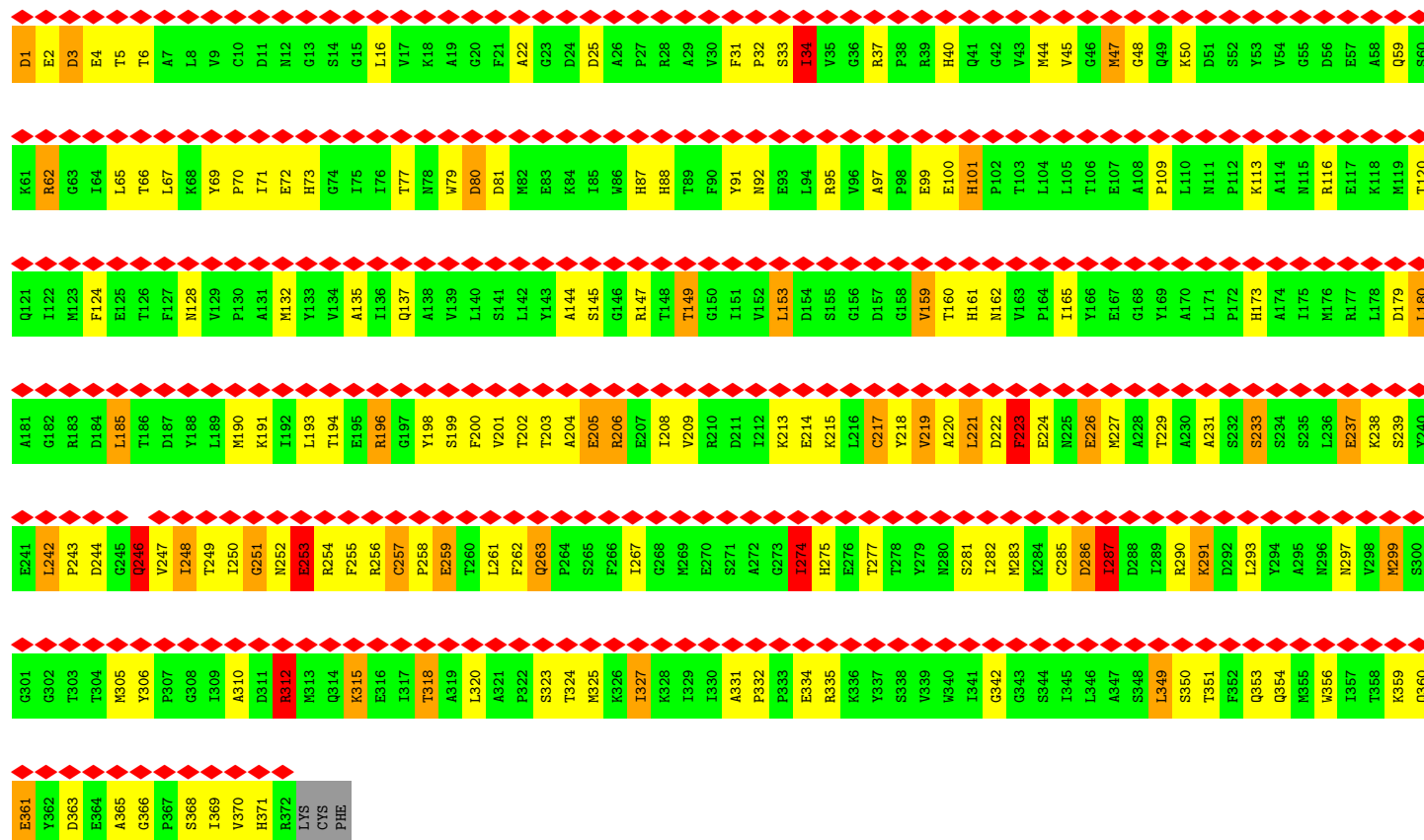


• Molecule 4: SKELETAL MUSCLE ACTIN

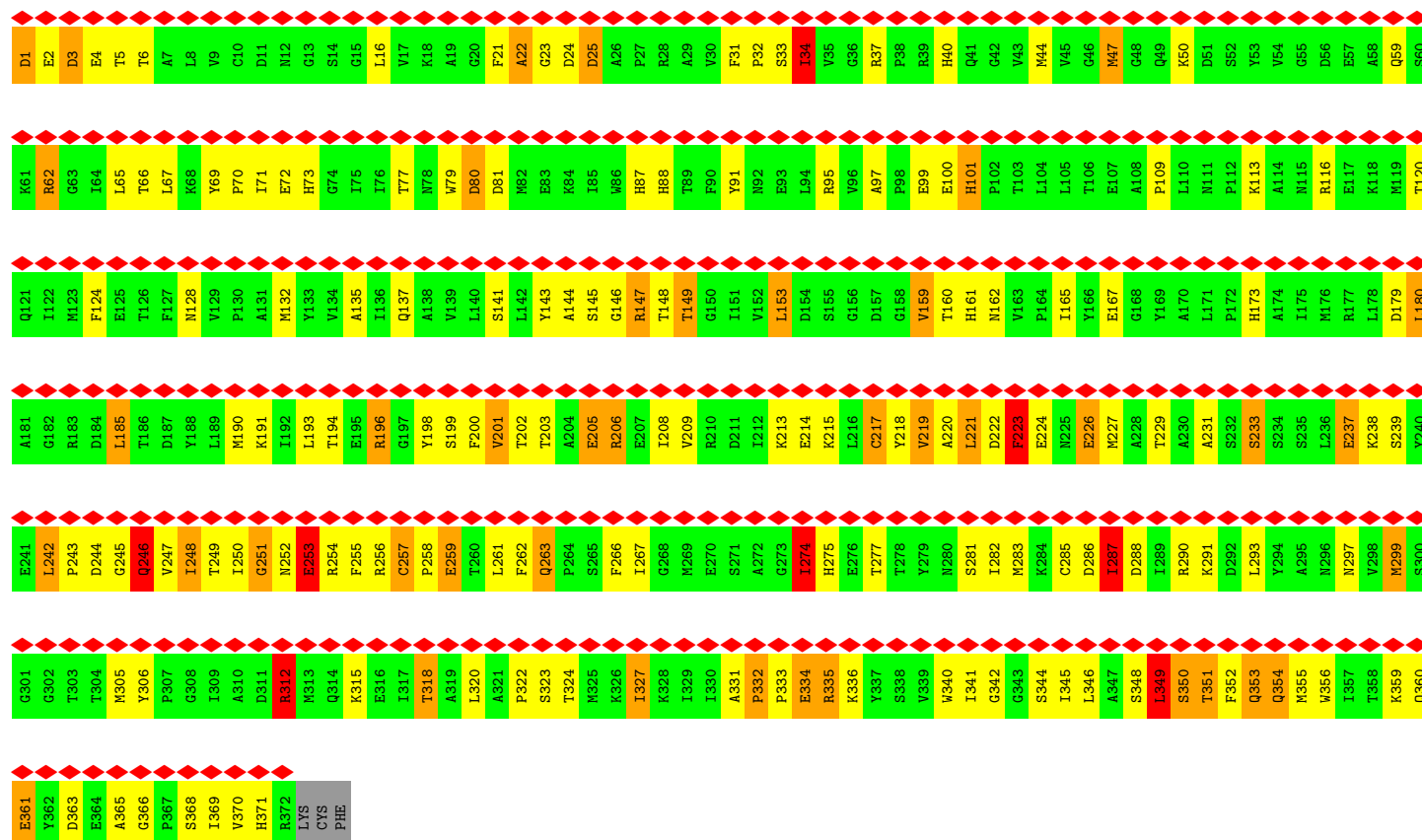




• Molecule 4: SKELETAL MUSCLE ACTIN



Chain Z: 99% 50% 36% 11%



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 (Å)	9280, 9280, 464	wwPDB
Tomogram dimensions	600, 600, 30	wwPDB
Tomogram angles (°)	90, 90, 90	wwPDB
Grid spacing (Å)	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%)	2.12	150/8729 (1.7%)
1	D	1.84	40/6448 (0.6%)	2.12	149/8729 (1.7%)
1	G	1.85	44/6449 (0.7%)	2.13	154/8732 (1.8%)
1	J	1.86	42/6449 (0.7%)	2.22	151/8732 (1.7%)
1	M	1.90	42/6447 (0.7%)	2.25	154/8726 (1.8%)
1	P	1.87	42/6448 (0.7%)	2.27	157/8729 (1.8%)
2	E	1.35	16/1148 (1.4%)	1.47	21/1548 (1.4%)
2	H	1.37	15/1148 (1.3%)	1.47	21/1548 (1.4%)
2	K	1.37	16/1148 (1.4%)	1.47	21/1548 (1.4%)
2	N	1.37	16/1148 (1.4%)	1.47	21/1548 (1.4%)
2	Q	1.37	14/1148 (1.2%)	1.47	21/1548 (1.4%)
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	6/1525 (0.4%)
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	99/4023 (2.5%)
4	3	1.17	13/2968 (0.4%)	2.00	98/4023 (2.4%)
4	4	1.16	13/2968 (0.4%)	2.00	96/4023 (2.4%)
4	5	1.17	13/2968 (0.4%)	2.00	98/4023 (2.4%)
4	6	1.17	13/2968 (0.4%)	2.00	100/4023 (2.5%)
4	7	1.17	13/2968 (0.4%)	2.00	101/4023 (2.5%)
4	8	1.17	13/2968 (0.4%)	2.01	100/4023 (2.5%)
4	9	1.17	13/2968 (0.4%)	2.00	99/4023 (2.5%)
4	V	1.17	13/2968 (0.4%)	2.00	99/4023 (2.5%)
4	W	1.17	13/2968 (0.4%)	2.00	98/4023 (2.4%)
4	X	1.17	13/2968 (0.4%)	2.00	97/4023 (2.4%)
4	Y	1.16	13/2968 (0.4%)	2.00	98/4023 (2.4%)
4	Z	1.17	13/2968 (0.4%)	2.00	99/4023 (2.5%)
All	All	1.50	528/91661 (0.6%)	2.02	2428/124064 (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	M	1	7
1	P	1	8
2	E	0	3
2	H	0	3
2	K	0	3
2	N	0	3
2	Q	0	3
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	7	72

The worst 5 of 528 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	648	THR	CB-OG1	42.69	2.12	1.43
1	G	648	THR	CB-OG1	42.68	2.12	1.43
1	J	648	THR	CB-OG1	42.67	2.12	1.43
1	A	648	THR	CB-OG1	42.66	2.12	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	648	THR	CB-OG1	42.66	2.12	1.43

The worst 5 of 2428 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	637	LYS	O-C-N	-74.35	23.70	122.59
1	M	637	LYS	O-C-N	-74.31	23.75	122.59
1	D	637	LYS	O-C-N	-74.28	23.79	122.59
1	A	637	LYS	O-C-N	-74.28	23.79	122.59
1	J	637	LYS	O-C-N	-74.27	23.81	122.59

5 of 7 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 72 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
1	D	98	HIS	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	6768	1331	0
1	D	6797	0	6766	1489	0
1	G	6797	0	6772	1578	0
1	J	6797	0	6770	1478	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	M	6797	0	6775	1484	0
1	P	6797	0	6774	1535	0
2	E	1127	0	1086	261	0
2	H	1127	0	1088	272	0
2	K	1127	0	1088	288	0
2	N	1127	0	1089	279	0
2	Q	1127	0	1089	281	0
3	F	1123	0	1084	186	0
3	I	1123	0	1082	211	0
3	L	1123	0	1082	167	0
3	O	1123	0	1084	192	0
3	R	1123	0	1083	208	0
4	1	2906	0	2856	428	0
4	2	2906	0	2861	257	0
4	3	2906	0	2863	175	0
4	4	2906	0	2863	184	0
4	5	2906	0	2865	97	0
4	6	2906	0	2865	99	0
4	7	2906	0	2866	83	0
4	8	2906	0	2857	317	0
4	9	2906	0	2855	355	0
4	V	2906	0	2851	384	0
4	W	2906	0	2851	400	0
4	X	2906	0	2862	214	0
4	Y	2906	0	2863	192	0
4	Z	2906	0	2853	432	0
All	All	92716	0	91511	11198	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 11198 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:A:757:GLN:HB3	1:A:771:LEU:CD1	1.23	1.67
4:2:287:ILE:CG2	4:4:202:THR:HB	1.23	1.66
1:A:505:MLY:HB3	1:A:762:HIS:CD2	1.28	1.64
2:E:144:VAL:HG13	2:E:153:ILE:CG1	1.17	1.64
1:G:797:PHE:CE2	3:I:126:LEU:HD22	1.23	1.64

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%)	650 (82%)	113 (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	M	787/840 (94%)	648 (82%)	110 (14%)	29 (4%)	2	20
1	P	789/840 (94%)	650 (82%)	112 (14%)	27 (3%)	3	21
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	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
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%)	333 (90%)	31 (8%)	6 (2%)	7	38
4	4	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	7	38
4	5	370/375 (99%)	333 (90%)	31 (8%)	6 (2%)	7	38
4	6	370/375 (99%)	334 (90%)	30 (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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	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%)	334 (90%)	30 (8%)	6 (2%)	7	38
All	All	11346/11750 (97%)	9872 (87%)	1188 (10%)	286 (2%)	6	26

5 of 286 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%)	491 (73%)	181 (27%)	0	3
1	G	672/672 (100%)	492 (73%)	180 (27%)	0	3
1	J	672/672 (100%)	490 (73%)	182 (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	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	N	120/120 (100%)	120 (100%)	0	100	100
2	Q	120/120 (100%)	120 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	265 (84%)	50 (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%)	265 (84%)	50 (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%)	264 (84%)	51 (16%)	2	11
4	W	315/318 (99%)	264 (84%)	51 (16%)	2	11
4	X	315/318 (99%)	265 (84%)	50 (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	9627/9669 (100%)	7807 (81%)	1820 (19%)	3	8

5 of 1820 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	17	LEU
4	Z	65	LEU
4	1	305	MET
4	Y	299	MET
4	V	291	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 293 such sidechains are listed below:

Mol	Chain	Res	Type
4	6	41	GLN

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Mol	Chain	Res	Type
4	Y	263	GLN
4	7	40	HIS
4	V	78	ASN
1	J	164	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	MLY	A	353	1	9,10,11	0.89	0	6,11,13	0.81	0
1	MLY	P	236	1	9,10,11	0.84	1 (11%)	6,11,13	0.48	0
1	MLY	D	415	1	9,10,11	0.75	0	6,11,13	0.19	0
1	MLY	G	63	1	9,10,11	0.84	0	6,11,13	0.44	0
1	MLY	M	348	1	9,10,11	0.75	0	6,11,13	0.46	0
1	MLY	M	84	1	9,10,11	0.51	0	6,11,13	0.81	0
1	MLY	P	827	1	9,10,11	0.68	0	6,11,13	0.48	0
1	MLY	P	385	1	9,10,11	0.93	1 (11%)	6,11,13	0.44	0
1	MLY	D	827	1	9,10,11	0.66	0	6,11,13	0.47	0
1	MLY	A	431	1	9,10,11	0.50	0	6,11,13	0.44	0
1	MLY	G	613	1	9,10,11	0.62	0	6,11,13	0.62	0
1	MLY	P	839	1	9,10,11	0.68	0	6,11,13	0.79	0
1	MLY	A	764	1	9,10,11	0.81	0	6,11,13	0.36	0
1	MLY	J	107	1	9,10,11	0.49	0	6,11,13	0.34	0
1	MLY	J	553	1	9,10,11	0.64	0	6,11,13	0.54	0
1	MLY	G	764	1	9,10,11	0.80	0	6,11,13	0.36	0
1	MLY	D	295	1	9,10,11	0.73	0	6,11,13	0.37	0
1	MLY	D	107	1	9,10,11	0.52	0	6,11,13	0.32	0
1	MLY	D	236	1	9,10,11	0.82	1 (11%)	6,11,13	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	M	600	1	9,10,11	0.53	0	6,11,13	0.38	0
1	MLY	M	30	1	9,10,11	0.91	0	6,11,13	0.32	0
1	MLY	G	296	1	9,10,11	0.60	0	6,11,13	0.37	0
1	MLY	J	598	1	9,10,11	0.82	0	6,11,13	0.41	0
1	MLY	M	59	1	9,10,11	0.86	0	6,11,13	0.47	0
1	MLY	G	385	1	9,10,11	0.94	1 (11%)	6,11,13	0.45	0
1	MLY	J	295	1	9,10,11	0.74	0	6,11,13	0.37	0
1	MLY	G	837	1	9,10,11	0.59	0	6,11,13	0.54	0
1	MLY	J	613	1	9,10,11	0.58	0	6,11,13	0.62	0
1	MLY	D	600	1	9,10,11	0.51	0	6,11,13	0.39	0
1	MLY	G	272	1	9,10,11	0.86	1 (11%)	6,11,13	0.54	0
1	MLY	P	138	1	9,10,11	1.21	1 (11%)	6,11,13	0.80	0
1	MLY	D	30	1	9,10,11	0.93	0	6,11,13	0.31	0
1	MLY	G	617	1	9,10,11	0.88	0	6,11,13	0.35	0
1	MLY	P	837	1	9,10,11	0.57	0	6,11,13	0.56	0
1	MLY	G	87	1	9,10,11	1.11	1 (11%)	6,11,13	0.42	0
1	MLY	M	385	1	9,10,11	0.94	1 (11%)	6,11,13	0.45	0
1	MLY	M	486	1	9,10,11	0.66	0	6,11,13	0.39	0
1	MLY	P	272	1	9,10,11	0.89	1 (11%)	6,11,13	0.56	0
1	MLY	D	528	1	9,10,11	0.91	0	6,11,13	0.64	0
1	MLY	J	504	1	9,10,11	0.84	0	6,11,13	0.23	0
1	MLY	M	617	1	9,10,11	0.91	0	6,11,13	0.33	0
1	MLY	D	598	1	9,10,11	0.84	0	6,11,13	0.41	0
1	MLY	M	782	1	9,10,11	0.82	0	6,11,13	0.38	0
1	MLY	A	553	4,1	9,10,11	0.66	0	6,11,13	0.55	0
1	MLY	J	190	1	9,10,11	1.20	2 (22%)	6,11,13	0.53	0
1	MLY	P	84	1	9,10,11	0.50	0	6,11,13	0.81	0
1	MLY	M	528	1	9,10,11	0.90	0	6,11,13	0.65	0
1	MLY	G	681	1	9,10,11	0.62	0	6,11,13	0.45	0
1	MLY	D	63	1	9,10,11	0.87	0	6,11,13	0.45	0
1	MLY	A	504	1	9,10,11	0.88	0	6,11,13	0.24	0
1	MLY	A	833	1	9,10,11	1.11	1 (11%)	6,11,13	0.32	0
1	MLY	G	30	1	9,10,11	0.90	0	6,11,13	0.30	0
1	MLY	J	353	1	9,10,11	0.87	0	6,11,13	0.79	0
1	MLY	A	659	1	9,10,11	0.84	1 (11%)	6,11,13	0.60	0
1	MLY	G	55	1	9,10,11	0.74	0	6,11,13	0.80	0
1	MLY	A	55	1	9,10,11	0.72	0	6,11,13	0.80	0
1	MLY	D	833	1	9,10,11	1.11	1 (11%)	6,11,13	0.31	0
1	MLY	M	827	1	9,10,11	0.67	0	6,11,13	0.47	0
1	MLY	J	63	1	9,10,11	0.85	0	6,11,13	0.44	0
1	MLY	P	764	1	9,10,11	0.82	0	6,11,13	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	G	130	1	9,10,11	0.79	0	6,11,13	0.73	0
1	MLY	G	138	1	9,10,11	1.20	1 (11%)	6,11,13	0.82	0
1	MLY	P	35	1	9,10,11	0.73	0	6,11,13	0.38	0
1	MLY	P	415	1	9,10,11	0.74	0	6,11,13	0.19	0
1	MLY	M	35	1	9,10,11	0.73	0	6,11,13	0.38	0
1	MLY	D	35	1	9,10,11	0.74	0	6,11,13	0.37	0
1	MLY	A	63	1	9,10,11	0.87	0	6,11,13	0.44	0
1	MLY	P	367	1	9,10,11	0.59	0	6,11,13	0.36	0
1	MLY	D	764	1	9,10,11	0.81	0	6,11,13	0.35	0
1	MLY	A	505	1	9,10,11	0.82	0	6,11,13	0.33	0
1	MLY	A	49	1	9,10,11	0.96	1 (11%)	6,11,13	0.74	0
1	MLY	D	617	1	9,10,11	0.90	0	6,11,13	0.36	0
1	MLY	G	190	1	9,10,11	1.20	2 (22%)	6,11,13	0.53	0
1	MLY	M	248	1	9,10,11	0.79	0	6,11,13	0.65	0
1	MLY	J	837	1	9,10,11	0.58	0	6,11,13	0.56	0
1	MLY	G	19	1	9,10,11	1.04	1 (11%)	6,11,13	0.58	0
1	MLY	M	236	1	9,10,11	0.84	1 (11%)	6,11,13	0.48	0
1	MLY	D	130	1	9,10,11	0.77	0	6,11,13	0.72	0
1	MLY	J	839	1	9,10,11	0.67	0	6,11,13	0.77	0
1	MLY	D	659	1	9,10,11	0.85	1 (11%)	6,11,13	0.58	0
1	MLY	G	782	1	9,10,11	0.79	0	6,11,13	0.36	0
1	MLY	P	248	1	9,10,11	0.81	0	6,11,13	0.65	0
1	MLY	P	551	1	9,10,11	0.52	0	6,11,13	0.19	0
1	MLY	P	600	1	9,10,11	0.54	0	6,11,13	0.39	0
1	MLY	G	49	1	9,10,11	0.98	1 (11%)	6,11,13	0.74	0
1	MLY	P	782	1	9,10,11	0.83	0	6,11,13	0.35	0
1	MLY	P	30	1	9,10,11	0.91	0	6,11,13	0.32	0
1	MLY	D	768	1	9,10,11	0.75	0	6,11,13	0.41	0
1	MLY	A	87	1	9,10,11	1.11	1 (11%)	6,11,13	0.41	0
1	MLY	J	505	1	9,10,11	0.85	0	6,11,13	0.33	0
1	MLY	D	436	1	9,10,11	1.00	1 (11%)	6,11,13	0.47	0
1	MLY	D	19	1	9,10,11	1.07	1 (11%)	6,11,13	0.57	0
1	MLY	A	130	1	9,10,11	0.79	0	6,11,13	0.74	0
1	MLY	M	87	1	9,10,11	1.12	1 (11%)	6,11,13	0.44	0
1	MLY	D	553	4,1	9,10,11	0.65	0	6,11,13	0.55	0
1	MLY	M	681	1	9,10,11	0.58	0	6,11,13	0.47	0
1	MLY	G	248	1	9,10,11	0.78	0	6,11,13	0.66	0
1	MLY	P	59	1	9,10,11	0.84	0	6,11,13	0.47	0
1	MLY	M	768	1	9,10,11	0.76	0	6,11,13	0.43	0
1	MLY	J	272	1	9,10,11	0.90	1 (11%)	6,11,13	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	J	55	1	9,10,11	0.74	0	6,11,13	0.79	0
1	MLY	M	107	1	9,10,11	0.49	0	6,11,13	0.33	0
1	MLY	P	768	1	9,10,11	0.77	0	6,11,13	0.43	0
1	MLY	P	295	1	9,10,11	0.76	0	6,11,13	0.37	0
1	MLY	G	486	1	9,10,11	0.67	0	6,11,13	0.40	0
1	MLY	P	528	1	9,10,11	0.90	0	6,11,13	0.65	0
1	MLY	G	353	1	9,10,11	0.88	0	6,11,13	0.81	0
1	MLY	G	415	1	9,10,11	0.74	0	6,11,13	0.19	0
1	MLY	P	486	1	9,10,11	0.65	0	6,11,13	0.41	0
1	MLY	A	19	1	9,10,11	1.01	1 (11%)	6,11,13	0.58	0
1	MLY	J	348	1	9,10,11	0.77	0	6,11,13	0.47	0
1	MLY	M	295	1	9,10,11	0.75	0	6,11,13	0.37	0
1	MLY	M	598	1	9,10,11	0.82	0	6,11,13	0.41	0
1	MLY	M	613	1	9,10,11	0.58	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	G	431	1	9,10,11	0.51	0	6,11,13	0.46	0
1	MLY	A	272	1	9,10,11	0.88	1 (11%)	6,11,13	0.57	0
1	MLY	J	369	1	9,10,11	0.70	0	6,11,13	0.45	0
1	MLY	P	598	1	9,10,11	0.82	0	6,11,13	0.41	0
1	MLY	G	59	1	9,10,11	0.83	0	6,11,13	0.48	0
1	MLY	G	768	1	9,10,11	0.75	0	6,11,13	0.41	0
1	MLY	J	782	1	9,10,11	0.81	0	6,11,13	0.37	0
1	MLY	J	296	1	9,10,11	0.65	0	6,11,13	0.35	0
1	MLY	J	659	1	9,10,11	0.83	1 (11%)	6,11,13	0.58	0
1	MLY	J	681	1	9,10,11	0.57	0	6,11,13	0.45	0
1	MLY	G	367	1	9,10,11	0.60	0	6,11,13	0.39	0
1	MLY	G	504	1	9,10,11	0.88	0	6,11,13	0.23	0
1	MLY	J	59	1	9,10,11	0.84	0	6,11,13	0.47	0
1	MLY	D	837	1	9,10,11	0.60	0	6,11,13	0.58	0
1	MLY	J	138	1	9,10,11	1.19	1 (11%)	6,11,13	0.81	0
1	MLY	J	415	1	9,10,11	0.76	0	6,11,13	0.19	0
1	MLY	A	59	1	9,10,11	0.84	0	6,11,13	0.48	0
1	MLY	G	84	1	9,10,11	0.50	0	6,11,13	0.81	0
1	MLY	D	87	1	9,10,11	1.07	1 (11%)	6,11,13	0.43	0
1	MLY	A	436	1	9,10,11	0.95	1 (11%)	6,11,13	0.47	0
1	MLY	G	348	1	9,10,11	0.78	0	6,11,13	0.47	0
1	MLY	G	598	1	9,10,11	0.81	0	6,11,13	0.41	0
1	MLY	J	248	1	9,10,11	0.80	0	6,11,13	0.65	0
1	MLY	A	295	1	9,10,11	0.77	0	6,11,13	0.36	0
1	MLY	D	248	1	9,10,11	0.81	0	6,11,13	0.66	0
1	MLY	A	138	1	9,10,11	1.21	1 (11%)	6,11,13	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	A	600	1	9,10,11	0.51	0	6,11,13	0.39	0
1	MLY	A	415	1	9,10,11	0.73	0	6,11,13	0.19	0
1	MLY	P	130	1	9,10,11	0.76	0	6,11,13	0.72	0
1	MLY	P	613	1	9,10,11	0.56	0	6,11,13	0.61	0
1	MLY	A	369	1	9,10,11	0.72	0	6,11,13	0.47	0
1	MLY	G	505	1	9,10,11	0.81	0	6,11,13	0.36	0
1	MLY	A	837	1	9,10,11	0.61	0	6,11,13	0.55	0
1	MLY	P	617	1	9,10,11	0.90	0	6,11,13	0.33	0
1	MLY	D	839	1	9,10,11	0.64	0	6,11,13	0.80	0
1	MLY	G	833	1	9,10,11	1.13	1 (11%)	6,11,13	0.31	0
1	MLY	G	659	1	9,10,11	0.85	1 (11%)	6,11,13	0.59	0
1	MLY	A	348	1	9,10,11	0.80	0	6,11,13	0.47	0
1	MLY	P	87	1	9,10,11	1.13	1 (11%)	6,11,13	0.42	0
1	MLY	M	504	1	9,10,11	0.85	0	6,11,13	0.23	0
1	MLY	P	681	1	9,10,11	0.58	0	6,11,13	0.48	0
1	MLY	M	367	1	9,10,11	0.59	0	6,11,13	0.37	0
1	MLY	J	30	1	9,10,11	0.91	0	6,11,13	0.32	0
1	MLY	A	486	1	9,10,11	0.66	0	6,11,13	0.40	0
1	MLY	D	59	1	9,10,11	0.86	0	6,11,13	0.48	0
1	MLY	J	764	1	9,10,11	0.81	0	6,11,13	0.37	0
1	MLY	M	659	1	9,10,11	0.83	0	6,11,13	0.58	0
1	MLY	P	659	1	9,10,11	0.84	1 (11%)	6,11,13	0.57	0
1	MLY	J	431	1	9,10,11	0.51	0	6,11,13	0.44	0
1	MLY	A	248	1	9,10,11	0.80	0	6,11,13	0.64	0
1	MLY	G	827	1	9,10,11	0.69	0	6,11,13	0.48	0
1	MLY	D	367	1	9,10,11	0.58	0	6,11,13	0.38	0
1	MLY	J	768	1	9,10,11	0.78	0	6,11,13	0.43	0
1	MLY	D	504	1	9,10,11	0.88	0	6,11,13	0.21	0
1	MLY	P	107	1	9,10,11	0.49	0	6,11,13	0.34	0
1	MLY	D	431	1	9,10,11	0.52	0	6,11,13	0.45	0
1	MLY	D	138	1	9,10,11	1.23	1 (11%)	6,11,13	0.84	0
1	MLY	A	30	1	9,10,11	0.91	0	6,11,13	0.32	0
1	MLY	G	436	1	9,10,11	0.96	1 (11%)	6,11,13	0.46	0
1	MLY	G	528	1	9,10,11	0.91	0	6,11,13	0.66	0
1	MLY	G	236	1	9,10,11	0.83	1 (11%)	6,11,13	0.47	0
1	MLY	G	553	4,1	9,10,11	0.65	0	6,11,13	0.55	0
1	MLY	D	84	1	9,10,11	0.50	0	6,11,13	0.80	0
1	MLY	D	190	1	9,10,11	1.17	2 (22%)	6,11,13	0.54	0
1	MLY	J	551	1	9,10,11	0.53	0	6,11,13	0.20	0
1	MLY	D	55	1	9,10,11	0.74	0	6,11,13	0.80	0
1	MLY	M	63	1	9,10,11	0.87	0	6,11,13	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	P	436	1	9,10,11	0.95	1 (11%)	6,11,13	0.48	0
1	MLY	P	19	1	9,10,11	1.08	1 (11%)	6,11,13	0.58	0
1	MLY	M	505	1	9,10,11	0.83	0	6,11,13	0.34	0
1	MLY	M	49	1	9,10,11	0.98	1 (11%)	6,11,13	0.74	0
1	MLY	D	551	1	9,10,11	0.54	0	6,11,13	0.19	0
1	MLY	G	369	1	9,10,11	0.71	0	6,11,13	0.47	0
1	MLY	J	84	1	9,10,11	0.50	0	6,11,13	0.81	0
1	MLY	J	528	1	9,10,11	0.89	0	6,11,13	0.65	0
1	MLY	P	296	1	9,10,11	0.63	0	6,11,13	0.35	0
1	MLY	D	782	1	9,10,11	0.82	0	6,11,13	0.36	0
1	MLY	A	367	1	9,10,11	0.59	0	6,11,13	0.36	0
1	MLY	M	55	1	9,10,11	0.73	0	6,11,13	0.79	0
1	MLY	A	782	1	9,10,11	0.83	0	6,11,13	0.36	0
1	MLY	A	768	1	9,10,11	0.77	0	6,11,13	0.40	0
1	MLY	D	49	1	9,10,11	0.98	1 (11%)	6,11,13	0.75	0
1	MLY	P	190	1	9,10,11	1.21	2 (22%)	6,11,13	0.54	0
1	MLY	A	84	1	9,10,11	0.51	0	6,11,13	0.80	0
1	MLY	J	600	1	9,10,11	0.53	0	6,11,13	0.38	0
1	MLY	A	528	1	9,10,11	0.89	0	6,11,13	0.67	0
1	MLY	J	827	1	9,10,11	0.70	0	6,11,13	0.47	0
1	MLY	D	613	1	9,10,11	0.59	0	6,11,13	0.62	0
1	MLY	M	296	1	9,10,11	0.66	0	6,11,13	0.35	0
1	MLY	A	551	1	9,10,11	0.53	0	6,11,13	0.19	0
1	MLY	A	296	1	9,10,11	0.59	0	6,11,13	0.35	0
1	MLY	M	272	1	9,10,11	0.91	1 (11%)	6,11,13	0.57	0
1	MLY	J	833	1	9,10,11	1.14	1 (11%)	6,11,13	0.29	0
1	MLY	A	827	1	9,10,11	0.69	0	6,11,13	0.44	0
1	MLY	D	296	1	9,10,11	0.63	0	6,11,13	0.36	0
1	MLY	J	385	1	9,10,11	0.94	1 (11%)	6,11,13	0.44	0
1	MLY	D	385	1	9,10,11	0.90	1 (11%)	6,11,13	0.46	0
1	MLY	A	598	1	9,10,11	0.84	1 (11%)	6,11,13	0.43	0
1	MLY	J	486	1	9,10,11	0.64	0	6,11,13	0.40	0
1	MLY	M	431	1	9,10,11	0.51	0	6,11,13	0.45	0
1	MLY	M	369	1	9,10,11	0.71	0	6,11,13	0.46	0
1	MLY	M	839	1	9,10,11	0.70	0	6,11,13	0.77	0
1	MLY	D	272	1	9,10,11	0.85	1 (11%)	6,11,13	0.57	0
1	MLY	A	35	1	9,10,11	0.73	0	6,11,13	0.37	0
1	MLY	J	436	1	9,10,11	0.94	1 (11%)	6,11,13	0.48	0
1	MLY	D	486	1	9,10,11	0.67	0	6,11,13	0.41	0
1	MLY	J	236	1	9,10,11	0.84	1 (11%)	6,11,13	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	P	353	1	9,10,11	0.86	0	6,11,13	0.80	0
1	MLY	P	553	1	9,10,11	0.66	0	6,11,13	0.54	0
1	MLY	D	353	1	9,10,11	0.85	0	6,11,13	0.81	0
1	MLY	P	369	1	9,10,11	0.71	0	6,11,13	0.45	0
1	MLY	G	35	1	9,10,11	0.72	0	6,11,13	0.38	0
1	MLY	D	369	1	9,10,11	0.70	0	6,11,13	0.44	0
1	MLY	J	19	1	9,10,11	1.06	1 (11%)	6,11,13	0.58	0
1	MLY	P	504	1	9,10,11	0.84	0	6,11,13	0.23	0
1	MLY	M	553	1	9,10,11	0.65	0	6,11,13	0.54	0
1	MLY	A	190	1	9,10,11	1.21	2 (22%)	6,11,13	0.51	0
1	MLY	A	236	1	9,10,11	0.84	1 (11%)	6,11,13	0.49	0
1	MLY	P	833	1	9,10,11	1.14	2 (22%)	6,11,13	0.30	0
1	MLY	M	837	1	9,10,11	0.58	0	6,11,13	0.55	0
1	MLY	G	107	1	9,10,11	0.49	0	6,11,13	0.33	0
1	MLY	M	190	1	9,10,11	1.20	2 (22%)	6,11,13	0.53	0
1	MLY	J	367	1	9,10,11	0.59	0	6,11,13	0.37	0
1	MLY	P	348	1	9,10,11	0.76	0	6,11,13	0.47	0
1	MLY	G	839	1	9,10,11	0.65	0	6,11,13	0.79	0
1	MLY	A	385	1	9,10,11	0.92	1 (11%)	6,11,13	0.45	0
1	MLY	G	551	1	9,10,11	0.53	0	6,11,13	0.19	0
1	MLY	M	833	1	9,10,11	1.13	1 (11%)	6,11,13	0.30	0
1	MLY	M	138	1	9,10,11	1.22	1 (11%)	6,11,13	0.81	0
1	MLY	A	839	1	9,10,11	0.64	0	6,11,13	0.81	0
1	MLY	P	63	1	9,10,11	0.84	0	6,11,13	0.43	0
1	MLY	P	431	1	9,10,11	0.53	0	6,11,13	0.44	0
1	MLY	G	295	1	9,10,11	0.76	0	6,11,13	0.36	0
1	MLY	A	613	1	9,10,11	0.59	0	6,11,13	0.62	0
1	MLY	A	681	1	9,10,11	0.58	0	6,11,13	0.45	0
1	MLY	P	505	1	9,10,11	0.84	0	6,11,13	0.33	0
1	MLY	P	49	1	9,10,11	1.00	1 (11%)	6,11,13	0.76	0
1	MLY	D	348	1	9,10,11	0.75	0	6,11,13	0.47	0
1	MLY	M	764	1	9,10,11	0.81	0	6,11,13	0.38	0
1	MLY	J	49	1	9,10,11	0.99	1 (11%)	6,11,13	0.75	0
1	MLY	M	436	1	9,10,11	0.95	1 (11%)	6,11,13	0.48	0
1	MLY	G	600	1	9,10,11	0.52	0	6,11,13	0.37	0
1	MLY	A	107	1	9,10,11	0.48	0	6,11,13	0.33	0
1	MLY	J	87	1	9,10,11	1.11	1 (11%)	6,11,13	0.43	0
1	MLY	M	19	1	9,10,11	1.07	1 (11%)	6,11,13	0.59	0
1	MLY	J	130	1	9,10,11	0.74	0	6,11,13	0.73	0
1	MLY	J	35	1	9,10,11	0.74	0	6,11,13	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	D	505	1	9,10,11	0.78	0	6,11,13	0.35	0
1	MLY	M	353	1	9,10,11	0.87	0	6,11,13	0.81	0
1	MLY	M	415	1	9,10,11	0.77	0	6,11,13	0.19	0
1	MLY	D	681	1	9,10,11	0.55	0	6,11,13	0.46	0
1	MLY	M	130	1	9,10,11	0.75	0	6,11,13	0.73	0
1	MLY	P	55	1	9,10,11	0.74	0	6,11,13	0.80	0
1	MLY	J	617	1	9,10,11	0.90	0	6,11,13	0.34	0
1	MLY	M	551	1	9,10,11	0.54	0	6,11,13	0.19	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	353	1	-	4/8/9/11	-
1	MLY	P	236	1	-	3/8/9/11	-
1	MLY	D	415	1	-	3/8/9/11	-
1	MLY	G	63	1	-	4/8/9/11	-
1	MLY	M	348	1	-	5/8/9/11	-
1	MLY	M	84	1	-	4/8/9/11	-
1	MLY	P	827	1	-	1/8/9/11	-
1	MLY	P	385	1	-	2/8/9/11	-
1	MLY	D	827	1	-	1/8/9/11	-
1	MLY	A	431	1	-	4/8/9/11	-
1	MLY	G	613	1	-	3/8/9/11	-
1	MLY	P	839	1	-	3/8/9/11	-
1	MLY	A	764	1	-	2/8/9/11	-
1	MLY	J	107	1	-	2/8/9/11	-
1	MLY	J	553	1	-	4/8/9/11	-
1	MLY	G	764	1	-	2/8/9/11	-
1	MLY	D	295	1	-	2/8/9/11	-
1	MLY	D	107	1	-	2/8/9/11	-
1	MLY	D	236	1	-	3/8/9/11	-
1	MLY	M	600	1	-	3/8/9/11	-
1	MLY	M	30	1	-	3/8/9/11	-
1	MLY	G	296	1	-	4/8/9/11	-
1	MLY	J	598	1	-	5/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	M	59	1	-	3/8/9/11	-
1	MLY	G	385	1	-	2/8/9/11	-
1	MLY	J	295	1	-	2/8/9/11	-
1	MLY	G	837	1	-	6/8/9/11	-
1	MLY	J	613	1	-	3/8/9/11	-
1	MLY	D	600	1	-	3/8/9/11	-
1	MLY	G	272	1	-	3/8/9/11	-
1	MLY	P	138	1	-	4/8/9/11	-
1	MLY	D	30	1	-	3/8/9/11	-
1	MLY	G	617	1	-	2/8/9/11	-
1	MLY	P	837	1	-	6/8/9/11	-
1	MLY	G	87	1	-	2/8/9/11	-
1	MLY	M	385	1	-	2/8/9/11	-
1	MLY	M	486	1	-	2/8/9/11	-
1	MLY	P	272	1	-	3/8/9/11	-
1	MLY	D	528	1	-	4/8/9/11	-
1	MLY	J	504	1	-	4/8/9/11	-
1	MLY	M	617	1	-	2/8/9/11	-
1	MLY	D	598	1	-	5/8/9/11	-
1	MLY	M	782	1	-	6/8/9/11	-
1	MLY	A	553	4,1	-	4/8/9/11	-
1	MLY	J	190	1	-	4/8/9/11	-
1	MLY	P	84	1	-	4/8/9/11	-
1	MLY	M	528	1	-	4/8/9/11	-
1	MLY	G	681	1	-	4/8/9/11	-
1	MLY	D	63	1	-	4/8/9/11	-
1	MLY	A	504	1	-	4/8/9/11	-
1	MLY	A	833	1	-	6/8/9/11	-
1	MLY	G	30	1	-	3/8/9/11	-
1	MLY	J	353	1	-	4/8/9/11	-
1	MLY	A	659	1	-	3/8/9/11	-
1	MLY	G	55	1	-	6/8/9/11	-
1	MLY	A	55	1	-	6/8/9/11	-
1	MLY	D	833	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	J	63	1	-	4/8/9/11	-
1	MLY	P	764	1	-	2/8/9/11	-
1	MLY	G	130	1	-	5/8/9/11	-
1	MLY	G	138	1	-	4/8/9/11	-
1	MLY	P	35	1	-	3/8/9/11	-
1	MLY	P	415	1	-	3/8/9/11	-
1	MLY	M	35	1	-	3/8/9/11	-
1	MLY	D	35	1	-	3/8/9/11	-
1	MLY	A	63	1	-	4/8/9/11	-
1	MLY	P	367	1	-	2/8/9/11	-
1	MLY	D	764	1	-	2/8/9/11	-
1	MLY	A	505	1	-	5/8/9/11	-
1	MLY	A	49	1	-	3/8/9/11	-
1	MLY	D	617	1	-	2/8/9/11	-
1	MLY	G	190	1	-	4/8/9/11	-
1	MLY	M	248	1	-	6/8/9/11	-
1	MLY	J	837	1	-	6/8/9/11	-
1	MLY	G	19	1	-	4/8/9/11	-
1	MLY	M	236	1	-	3/8/9/11	-
1	MLY	D	130	1	-	5/8/9/11	-
1	MLY	J	839	1	-	3/8/9/11	-
1	MLY	D	659	1	-	3/8/9/11	-
1	MLY	G	782	1	-	6/8/9/11	-
1	MLY	P	248	1	-	6/8/9/11	-
1	MLY	P	551	1	-	3/8/9/11	-
1	MLY	P	600	1	-	3/8/9/11	-
1	MLY	G	49	1	-	3/8/9/11	-
1	MLY	P	782	1	-	6/8/9/11	-
1	MLY	P	30	1	-	3/8/9/11	-
1	MLY	D	768	1	-	4/8/9/11	-
1	MLY	A	87	1	-	2/8/9/11	-
1	MLY	J	505	1	-	5/8/9/11	-
1	MLY	D	436	1	-	4/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	D	19	1	-	4/8/9/11	-
1	MLY	A	130	1	-	5/8/9/11	-
1	MLY	M	87	1	-	2/8/9/11	-
1	MLY	D	553	4,1	-	4/8/9/11	-
1	MLY	M	681	1	-	4/8/9/11	-
1	MLY	G	248	1	-	6/8/9/11	-
1	MLY	P	59	1	-	3/8/9/11	-
1	MLY	M	768	1	-	4/8/9/11	-
1	MLY	J	272	1	-	3/8/9/11	-
1	MLY	J	55	1	-	6/8/9/11	-
1	MLY	M	107	1	-	2/8/9/11	-
1	MLY	P	768	1	-	4/8/9/11	-
1	MLY	P	295	1	-	2/8/9/11	-
1	MLY	G	486	1	-	2/8/9/11	-
1	MLY	P	528	1	-	4/8/9/11	-
1	MLY	G	353	1	-	4/8/9/11	-
1	MLY	G	415	1	-	3/8/9/11	-
1	MLY	P	486	1	-	2/8/9/11	-
1	MLY	A	19	1	-	4/8/9/11	-
1	MLY	J	348	1	-	5/8/9/11	-
1	MLY	M	295	1	-	2/8/9/11	-
1	MLY	M	598	1	-	5/8/9/11	-
1	MLY	M	613	1	-	3/8/9/11	-
1	MLY	A	617	1	-	2/8/9/11	-
1	MLY	G	431	1	-	4/8/9/11	-
1	MLY	A	272	1	-	3/8/9/11	-
1	MLY	J	369	1	-	2/8/9/11	-
1	MLY	P	598	1	-	5/8/9/11	-
1	MLY	G	59	1	-	3/8/9/11	-
1	MLY	G	768	1	-	4/8/9/11	-
1	MLY	J	782	1	-	6/8/9/11	-
1	MLY	J	296	1	-	4/8/9/11	-
1	MLY	J	659	1	-	3/8/9/11	-
1	MLY	J	681	1	-	4/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	G	367	1	-	2/8/9/11	-
1	MLY	G	504	1	-	4/8/9/11	-
1	MLY	J	59	1	-	3/8/9/11	-
1	MLY	D	837	1	-	6/8/9/11	-
1	MLY	J	138	1	-	4/8/9/11	-
1	MLY	J	415	1	-	3/8/9/11	-
1	MLY	A	59	1	-	3/8/9/11	-
1	MLY	G	84	1	-	4/8/9/11	-
1	MLY	D	87	1	-	2/8/9/11	-
1	MLY	A	436	1	-	4/8/9/11	-
1	MLY	G	348	1	-	5/8/9/11	-
1	MLY	G	598	1	-	5/8/9/11	-
1	MLY	J	248	1	-	6/8/9/11	-
1	MLY	A	295	1	-	2/8/9/11	-
1	MLY	D	248	1	-	6/8/9/11	-
1	MLY	A	138	1	-	4/8/9/11	-
1	MLY	A	600	1	-	3/8/9/11	-
1	MLY	A	415	1	-	3/8/9/11	-
1	MLY	P	130	1	-	5/8/9/11	-
1	MLY	P	613	1	-	3/8/9/11	-
1	MLY	A	369	1	-	2/8/9/11	-
1	MLY	G	505	1	-	5/8/9/11	-
1	MLY	A	837	1	-	6/8/9/11	-
1	MLY	P	617	1	-	2/8/9/11	-
1	MLY	D	839	1	-	3/8/9/11	-
1	MLY	G	833	1	-	6/8/9/11	-
1	MLY	G	659	1	-	3/8/9/11	-
1	MLY	A	348	1	-	5/8/9/11	-
1	MLY	P	87	1	-	2/8/9/11	-
1	MLY	M	504	1	-	4/8/9/11	-
1	MLY	P	681	1	-	4/8/9/11	-
1	MLY	M	367	1	-	2/8/9/11	-
1	MLY	J	30	1	-	3/8/9/11	-
1	MLY	A	486	1	-	2/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	D	59	1	-	3/8/9/11	-
1	MLY	J	764	1	-	2/8/9/11	-
1	MLY	M	659	1	-	3/8/9/11	-
1	MLY	P	659	1	-	3/8/9/11	-
1	MLY	J	431	1	-	4/8/9/11	-
1	MLY	A	248	1	-	6/8/9/11	-
1	MLY	G	827	1	-	1/8/9/11	-
1	MLY	D	367	1	-	2/8/9/11	-
1	MLY	J	768	1	-	4/8/9/11	-
1	MLY	D	504	1	-	4/8/9/11	-
1	MLY	P	107	1	-	2/8/9/11	-
1	MLY	D	431	1	-	4/8/9/11	-
1	MLY	D	138	1	-	4/8/9/11	-
1	MLY	A	30	1	-	3/8/9/11	-
1	MLY	G	436	1	-	4/8/9/11	-
1	MLY	G	528	1	-	4/8/9/11	-
1	MLY	G	236	1	-	3/8/9/11	-
1	MLY	G	553	4,1	-	4/8/9/11	-
1	MLY	D	84	1	-	4/8/9/11	-
1	MLY	D	190	1	-	4/8/9/11	-
1	MLY	J	551	1	-	3/8/9/11	-
1	MLY	D	55	1	-	6/8/9/11	-
1	MLY	M	63	1	-	4/8/9/11	-
1	MLY	P	436	1	-	4/8/9/11	-
1	MLY	P	19	1	-	4/8/9/11	-
1	MLY	M	505	1	-	5/8/9/11	-
1	MLY	M	49	1	-	3/8/9/11	-
1	MLY	D	551	1	-	3/8/9/11	-
1	MLY	G	369	1	-	2/8/9/11	-
1	MLY	J	84	1	-	4/8/9/11	-
1	MLY	J	528	1	-	4/8/9/11	-
1	MLY	P	296	1	-	4/8/9/11	-
1	MLY	D	782	1	-	6/8/9/11	-
1	MLY	A	367	1	-	2/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	M	55	1	-	6/8/9/11	-
1	MLY	A	782	1	-	6/8/9/11	-
1	MLY	A	768	1	-	4/8/9/11	-
1	MLY	D	49	1	-	3/8/9/11	-
1	MLY	P	190	1	-	4/8/9/11	-
1	MLY	A	84	1	-	4/8/9/11	-
1	MLY	J	600	1	-	3/8/9/11	-
1	MLY	A	528	1	-	4/8/9/11	-
1	MLY	J	827	1	-	1/8/9/11	-
1	MLY	D	613	1	-	3/8/9/11	-
1	MLY	M	296	1	-	4/8/9/11	-
1	MLY	A	551	1	-	3/8/9/11	-
1	MLY	A	296	1	-	4/8/9/11	-
1	MLY	M	272	1	-	3/8/9/11	-
1	MLY	J	833	1	-	6/8/9/11	-
1	MLY	A	827	1	-	1/8/9/11	-
1	MLY	D	296	1	-	4/8/9/11	-
1	MLY	J	385	1	-	2/8/9/11	-
1	MLY	D	385	1	-	2/8/9/11	-
1	MLY	A	598	1	-	5/8/9/11	-
1	MLY	J	486	1	-	2/8/9/11	-
1	MLY	M	431	1	-	4/8/9/11	-
1	MLY	M	369	1	-	2/8/9/11	-
1	MLY	M	839	1	-	3/8/9/11	-
1	MLY	D	272	1	-	3/8/9/11	-
1	MLY	A	35	1	-	3/8/9/11	-
1	MLY	J	436	1	-	4/8/9/11	-
1	MLY	D	486	1	-	2/8/9/11	-
1	MLY	J	236	1	-	3/8/9/11	-
1	MLY	P	353	1	-	4/8/9/11	-
1	MLY	P	553	1	-	4/8/9/11	-
1	MLY	D	353	1	-	4/8/9/11	-
1	MLY	P	369	1	-	2/8/9/11	-
1	MLY	G	35	1	-	3/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	D	369	1	-	2/8/9/11	-
1	MLY	J	19	1	-	4/8/9/11	-
1	MLY	P	504	1	-	4/8/9/11	-
1	MLY	M	553	1	-	4/8/9/11	-
1	MLY	A	190	1	-	4/8/9/11	-
1	MLY	A	236	1	-	3/8/9/11	-
1	MLY	P	833	1	-	6/8/9/11	-
1	MLY	M	837	1	-	6/8/9/11	-
1	MLY	G	107	1	-	2/8/9/11	-
1	MLY	M	190	1	-	4/8/9/11	-
1	MLY	J	367	1	-	2/8/9/11	-
1	MLY	P	348	1	-	5/8/9/11	-
1	MLY	G	839	1	-	3/8/9/11	-
1	MLY	A	385	1	-	2/8/9/11	-
1	MLY	G	551	1	-	3/8/9/11	-
1	MLY	M	833	1	-	6/8/9/11	-
1	MLY	M	138	1	-	4/8/9/11	-
1	MLY	A	839	1	-	3/8/9/11	-
1	MLY	P	63	1	-	4/8/9/11	-
1	MLY	P	431	1	-	4/8/9/11	-
1	MLY	G	295	1	-	2/8/9/11	-
1	MLY	A	613	1	-	3/8/9/11	-
1	MLY	A	681	1	-	4/8/9/11	-
1	MLY	P	505	1	-	5/8/9/11	-
1	MLY	P	49	1	-	3/8/9/11	-
1	MLY	D	348	1	-	5/8/9/11	-
1	MLY	M	764	1	-	2/8/9/11	-
1	MLY	J	49	1	-	3/8/9/11	-
1	MLY	M	436	1	-	4/8/9/11	-
1	MLY	G	600	1	-	3/8/9/11	-
1	MLY	A	107	1	-	2/8/9/11	-
1	MLY	J	87	1	-	2/8/9/11	-
1	MLY	M	19	1	-	4/8/9/11	-
1	MLY	J	130	1	-	5/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	J	35	1	-	3/8/9/11	-
1	MLY	D	505	1	-	5/8/9/11	-
1	MLY	M	353	1	-	4/8/9/11	-
1	MLY	M	415	1	-	3/8/9/11	-
1	MLY	D	681	1	-	4/8/9/11	-
1	MLY	M	130	1	-	5/8/9/11	-
1	MLY	P	55	1	-	6/8/9/11	-
1	MLY	J	617	1	-	2/8/9/11	-
1	MLY	M	551	1	-	3/8/9/11	-

The worst 5 of 73 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	138	MLY	CB-CA	-3.26	1.48	1.53
1	M	138	MLY	CB-CA	-3.22	1.48	1.53
1	A	138	MLY	CB-CA	-3.21	1.48	1.53
1	P	138	MLY	CB-CA	-3.20	1.48	1.53
1	G	138	MLY	CB-CA	-3.17	1.48	1.53

There are no bond angle outliers.

There are no chirality outliers.

5 of 966 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 731 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	415	MLY	1	0
1	G	63	MLY	3	0
1	M	348	MLY	5	0
1	D	827	MLY	2	0
1	P	839	MLY	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	764	MLY	9	0
1	J	107	MLY	3	0
1	J	553	MLY	12	0
1	G	764	MLY	19	0
1	D	295	MLY	6	0
1	D	107	MLY	3	0
1	M	600	MLY	1	0
1	M	30	MLY	1	0
1	G	296	MLY	3	0
1	J	598	MLY	1	0
1	M	59	MLY	2	0
1	J	295	MLY	6	0
1	G	837	MLY	1	0
1	D	600	MLY	1	0
1	G	272	MLY	1	0
1	P	138	MLY	2	0
1	D	30	MLY	1	0
1	G	617	MLY	1	0
1	P	837	MLY	1	0
1	G	87	MLY	3	0
1	M	486	MLY	3	0
1	P	272	MLY	1	0
1	D	528	MLY	3	0
1	J	504	MLY	1	0
1	M	617	MLY	1	0
1	D	598	MLY	1	0
1	M	782	MLY	3	0
1	A	553	MLY	17	0
1	J	190	MLY	2	0
1	M	528	MLY	2	0
1	D	63	MLY	3	0
1	A	504	MLY	4	0
1	G	30	MLY	1	0
1	A	659	MLY	2	0
1	G	55	MLY	1	0
1	A	55	MLY	1	0
1	J	63	MLY	3	0
1	P	764	MLY	9	0
1	G	138	MLY	2	0
1	P	415	MLY	1	0
1	A	63	MLY	3	0
1	D	764	MLY	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	505	MLY	35	0
1	A	49	MLY	3	0
1	D	617	MLY	1	0
1	G	190	MLY	2	0
1	M	248	MLY	2	0
1	J	837	MLY	1	0
1	J	839	MLY	8	0
1	D	659	MLY	2	0
1	G	782	MLY	1	0
1	P	248	MLY	2	0
1	P	600	MLY	1	0
1	G	49	MLY	4	0
1	P	782	MLY	1	0
1	P	30	MLY	1	0
1	A	87	MLY	3	0
1	J	505	MLY	9	0
1	D	436	MLY	2	0
1	M	87	MLY	3	0
1	D	553	MLY	18	0
1	G	248	MLY	2	0
1	P	59	MLY	3	0
1	M	768	MLY	3	0
1	J	272	MLY	1	0
1	J	55	MLY	1	0
1	M	107	MLY	3	0
1	P	768	MLY	2	0
1	P	295	MLY	6	0
1	G	486	MLY	3	0
1	P	528	MLY	3	0
1	G	415	MLY	1	0
1	P	486	MLY	3	0
1	J	348	MLY	5	0
1	M	295	MLY	6	0
1	M	598	MLY	1	0
1	A	617	MLY	1	0
1	A	272	MLY	1	0
1	J	369	MLY	1	0
1	P	598	MLY	1	0
1	G	59	MLY	2	0
1	G	768	MLY	5	0
1	J	782	MLY	1	0
1	J	296	MLY	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	J	659	MLY	2	0
1	G	504	MLY	1	0
1	J	59	MLY	3	0
1	D	837	MLY	1	0
1	J	138	MLY	2	0
1	J	415	MLY	1	0
1	A	59	MLY	3	0
1	G	84	MLY	22	0
1	D	87	MLY	3	0
1	A	436	MLY	2	0
1	G	348	MLY	5	0
1	G	598	MLY	1	0
1	J	248	MLY	2	0
1	A	295	MLY	6	0
1	D	248	MLY	2	0
1	A	138	MLY	2	0
1	A	600	MLY	1	0
1	A	415	MLY	1	0
1	G	505	MLY	1	0
1	A	837	MLY	3	0
1	P	617	MLY	1	0
1	D	839	MLY	4	0
1	G	659	MLY	2	0
1	A	348	MLY	6	0
1	P	87	MLY	2	0
1	M	504	MLY	1	0
1	J	30	MLY	1	0
1	A	486	MLY	3	0
1	D	59	MLY	3	0
1	J	764	MLY	4	0
1	M	659	MLY	1	0
1	P	659	MLY	2	0
1	A	248	MLY	2	0
1	J	768	MLY	6	0
1	D	504	MLY	1	0
1	P	107	MLY	3	0
1	D	138	MLY	2	0
1	A	30	MLY	1	0
1	G	436	MLY	2	0
1	G	528	MLY	2	0
1	G	553	MLY	27	0
1	D	190	MLY	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	55	MLY	1	0
1	M	63	MLY	4	0
1	P	436	MLY	2	0
1	M	505	MLY	1	0
1	M	49	MLY	3	0
1	D	551	MLY	2	0
1	J	84	MLY	27	0
1	J	528	MLY	3	0
1	P	296	MLY	2	0
1	D	782	MLY	88	0
1	M	55	MLY	1	0
1	A	782	MLY	7	0
1	A	768	MLY	18	0
1	D	49	MLY	3	0
1	P	190	MLY	2	0
1	J	600	MLY	1	0
1	A	528	MLY	3	0
1	M	296	MLY	3	0
1	A	551	MLY	2	0
1	A	296	MLY	3	0
1	M	272	MLY	1	0
1	D	296	MLY	2	0
1	A	598	MLY	1	0
1	J	486	MLY	3	0
1	M	839	MLY	8	0
1	D	272	MLY	1	0
1	J	436	MLY	2	0
1	D	486	MLY	3	0
1	P	553	MLY	3	0
1	P	369	MLY	1	0
1	D	369	MLY	1	0
1	P	504	MLY	1	0
1	M	553	MLY	12	0
1	A	190	MLY	2	0
1	M	837	MLY	1	0
1	G	107	MLY	3	0
1	M	190	MLY	2	0
1	P	348	MLY	4	0
1	G	839	MLY	4	0
1	M	138	MLY	2	0
1	A	839	MLY	4	0
1	P	63	MLY	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	G	295	MLY	6	0
1	P	49	MLY	3	0
1	D	348	MLY	5	0
1	M	764	MLY	1	0
1	J	49	MLY	3	0
1	M	436	MLY	2	0
1	G	600	MLY	1	0
1	A	107	MLY	3	0
1	J	87	MLY	3	0
1	M	415	MLY	1	0
1	P	55	MLY	1	0
1	J	617	MLY	1	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	M	6
1	P	6
1	D	4
1	A	4
1	J	3
1	G	3
3	F	1
3	I	1
3	L	1

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

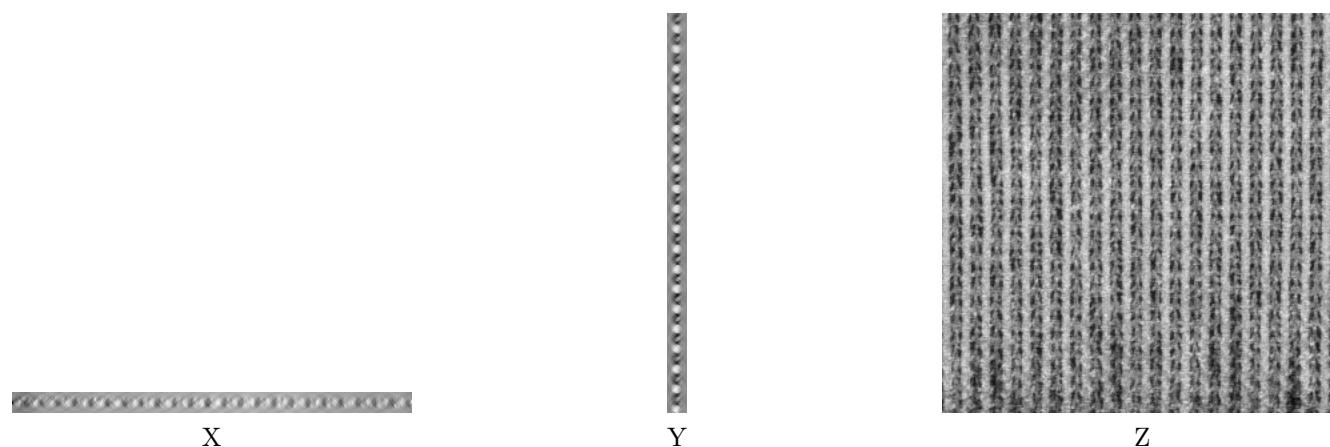
The worst 5 of 36 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	J	769:ALA	C	770:GLY	N	5.52
1	D	769:ALA	C	770:GLY	N	5.23
1	G	769:ALA	C	770:GLY	N	4.70
1	A	709:LYS	C	710:GLY	N	3.41
1	D	709:LYS	C	710:GLY	N	3.08

6 Tomogram visualisation [i](#)

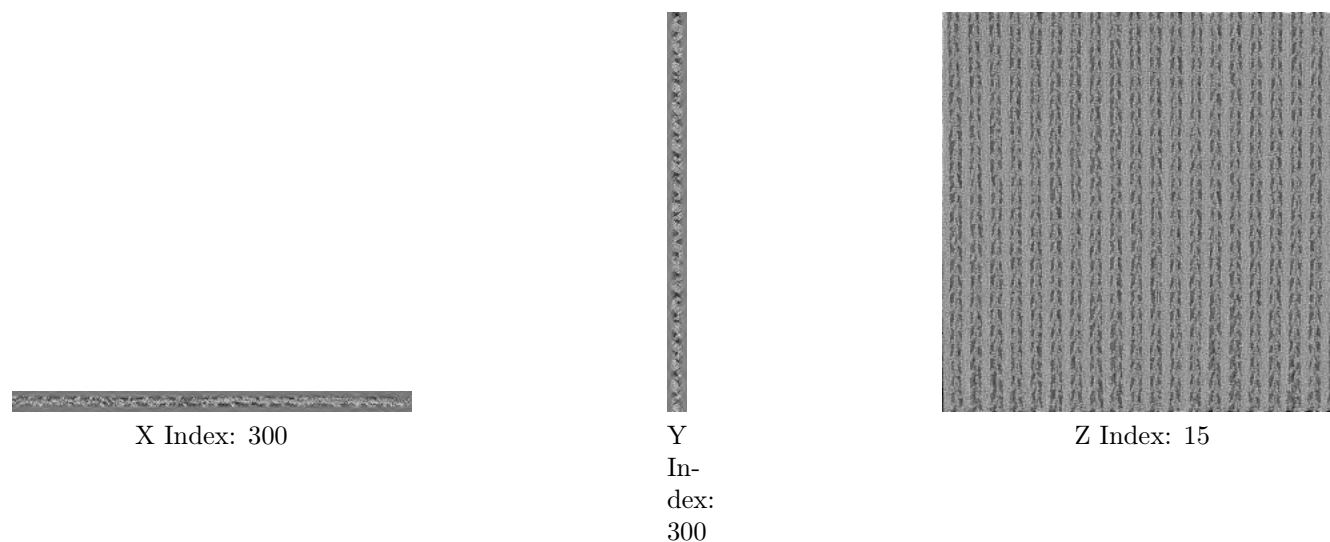
This section contains visualisations of the EMDB entry EMD-1001. These allow visual inspection of the internal detail of the tomogram and identification of artifacts.

6.1 Orthogonal projections [i](#)



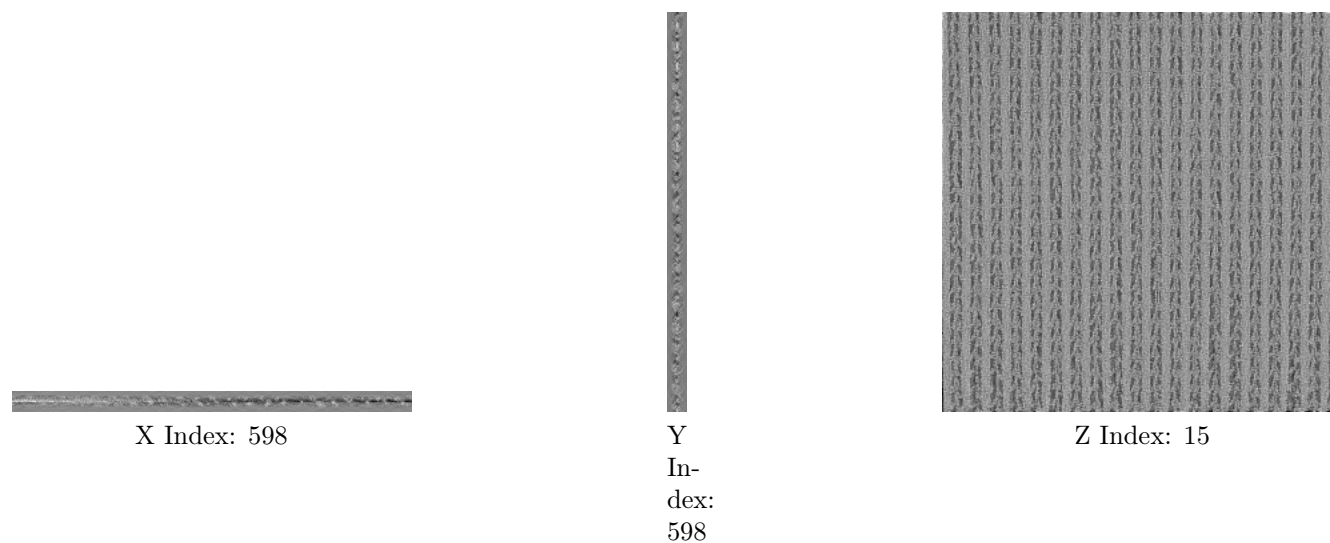
The images above show the tomogram projected in three orthogonal directions.

6.2 Central slices [i](#)



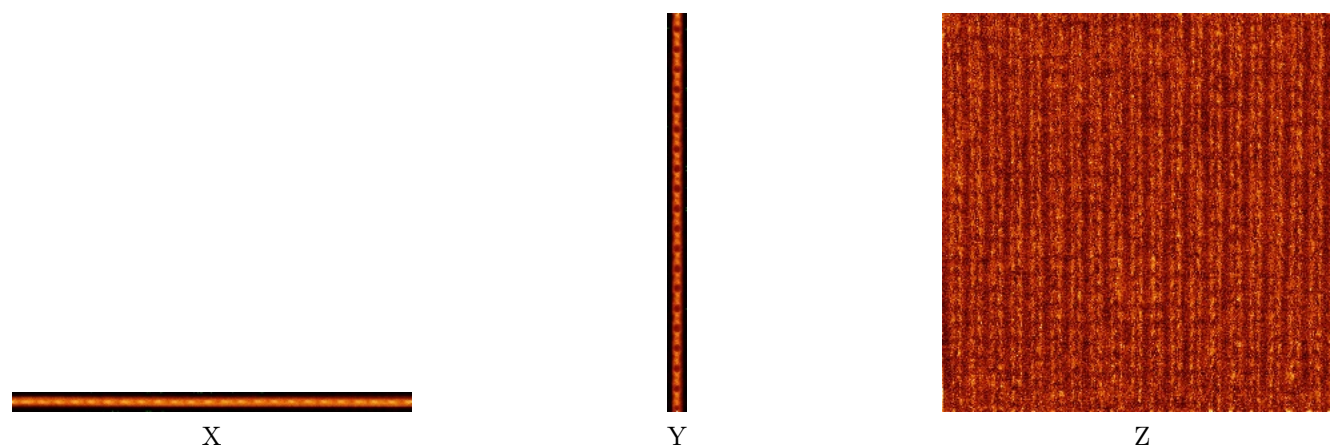
The images above show central slices of the tomogram in three orthogonal directions.

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.

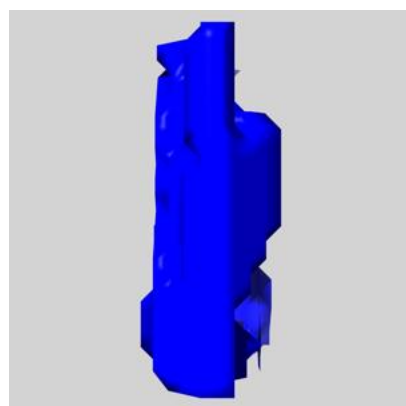
6.5 Mask visualisation [i](#)

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

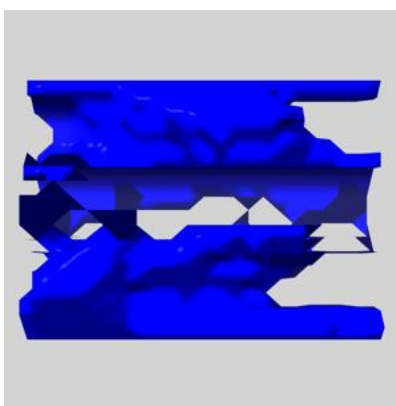
A mask typically either:

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

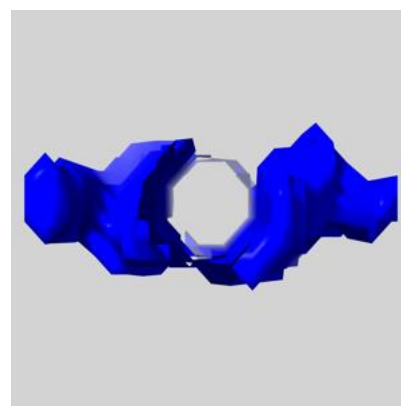
6.5.1 emd_1001_msk_25.map [i](#)



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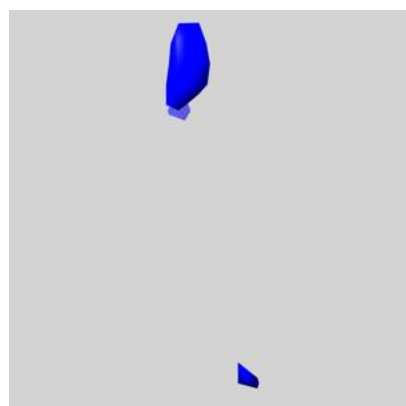


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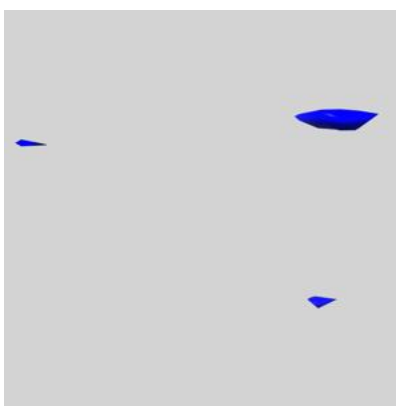


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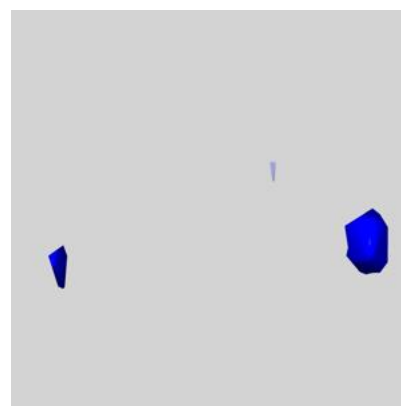
6.5.2 emd_1001_msk_24.map [i](#)



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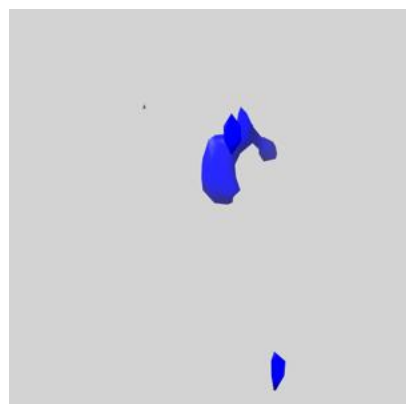


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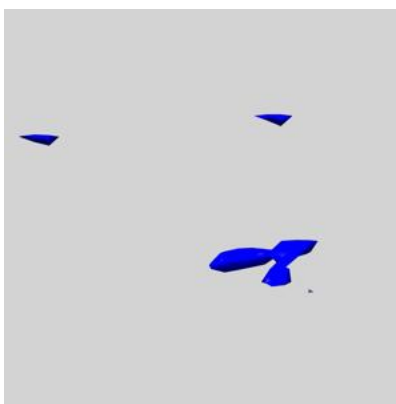


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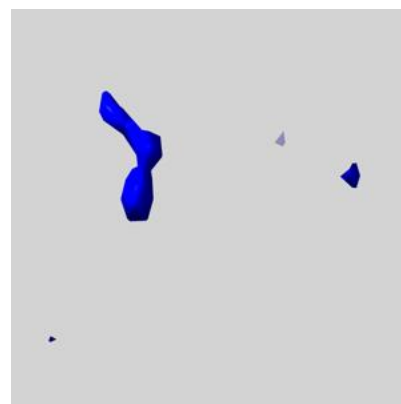
6.5.3 emd_1001_msk_23.map [i](#)



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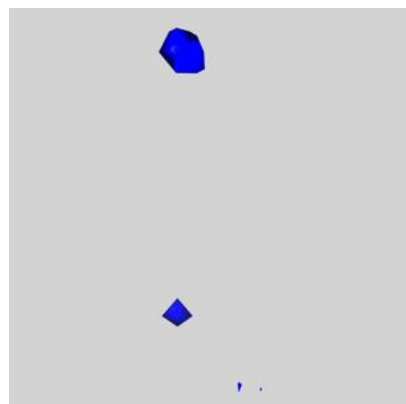


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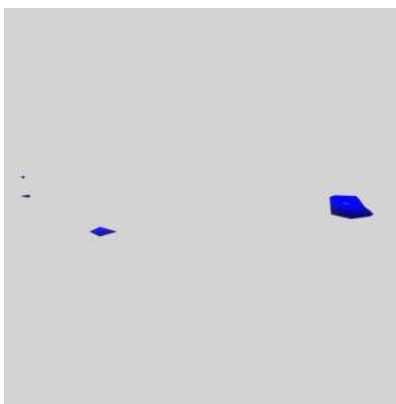


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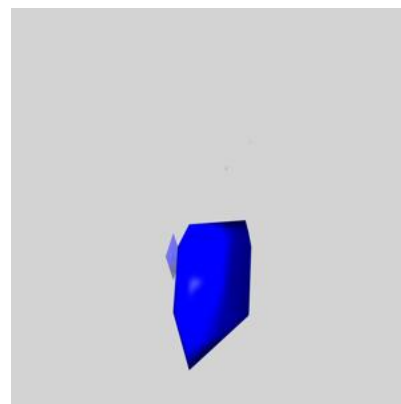
6.5.4 emd_1001_msk_22.map [i](#)



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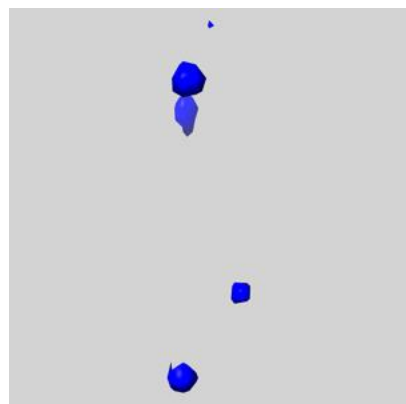


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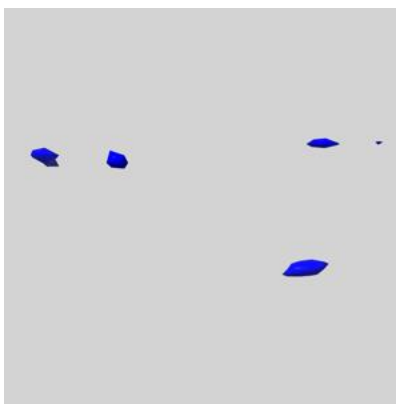


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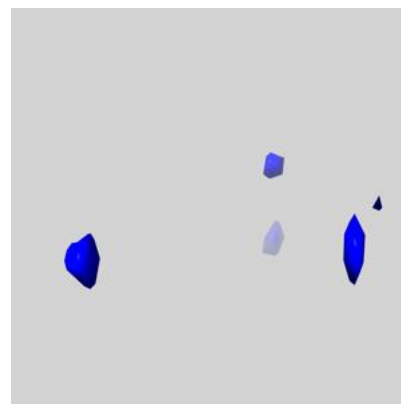
6.5.5 emd_1001_msk_21.map [i](#)



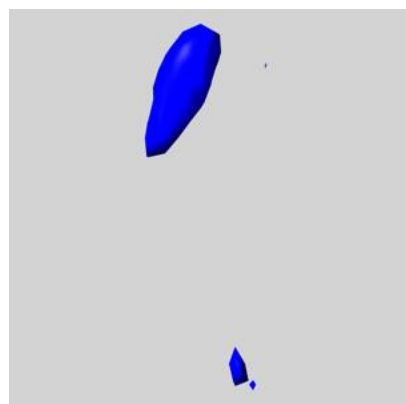
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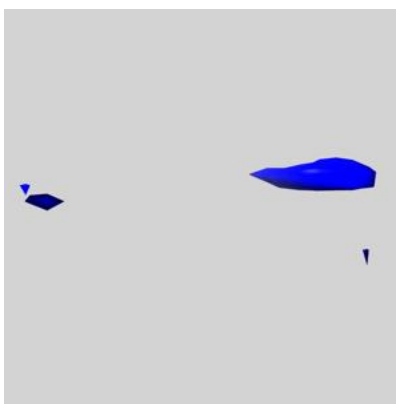
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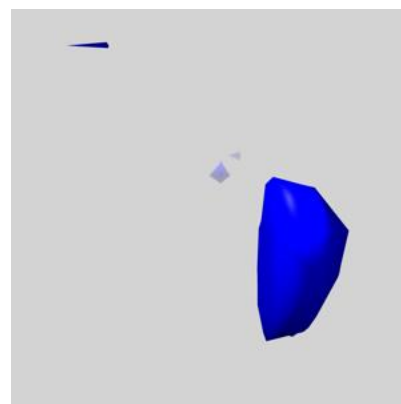
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6.5.6 emd_1001_msk_20.map [i](#)

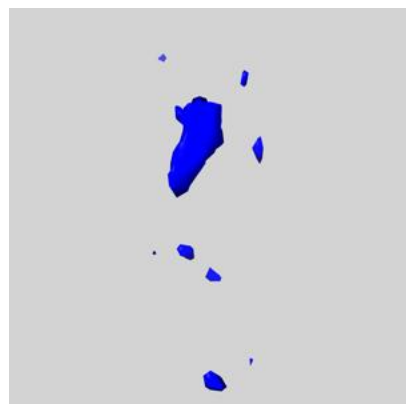
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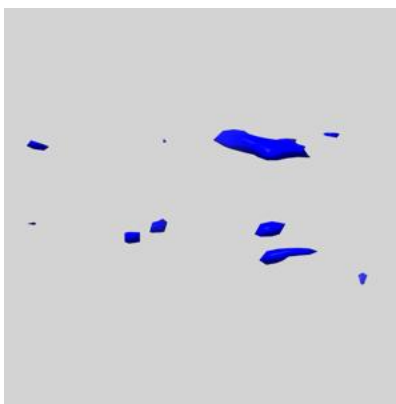
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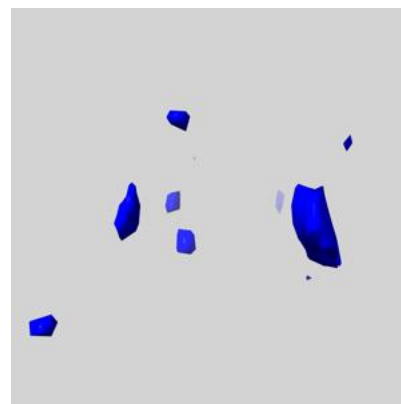
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6.5.7 emd_1001_msk_19.map [i](#)

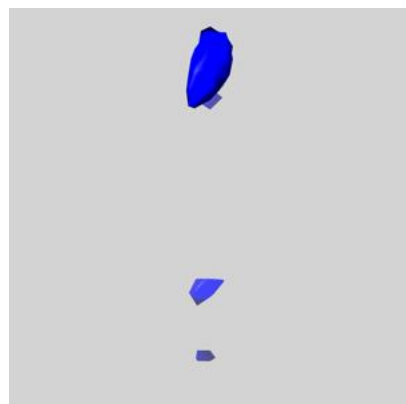
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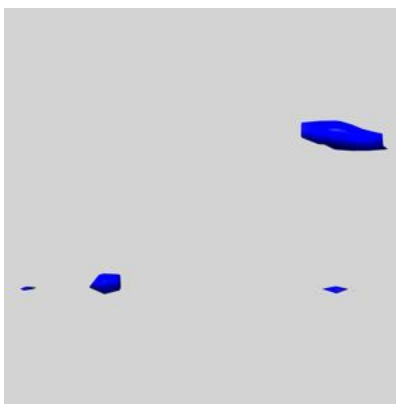
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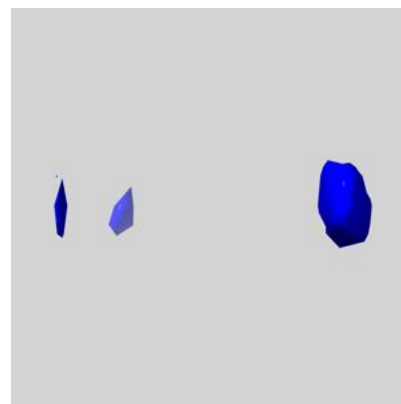
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6.5.8 emd_1001_msk_18.map [i](#)

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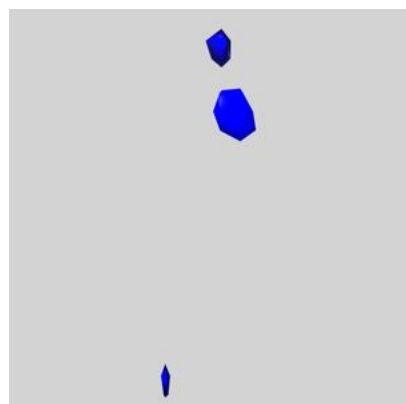


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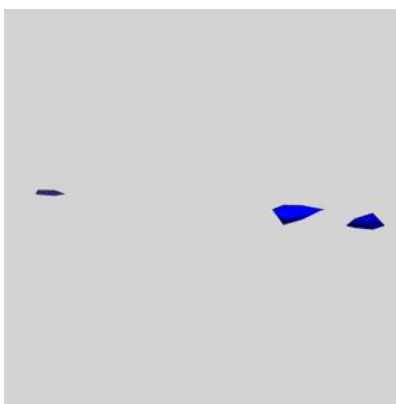


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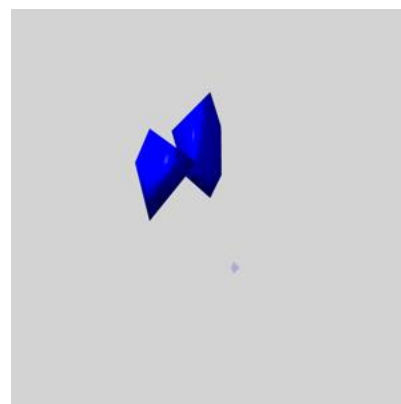
6.5.9 emd_1001_msk_17.map [i](#)



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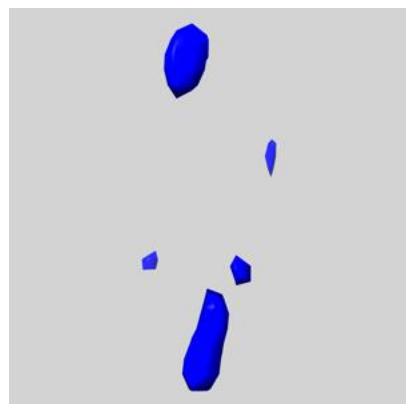


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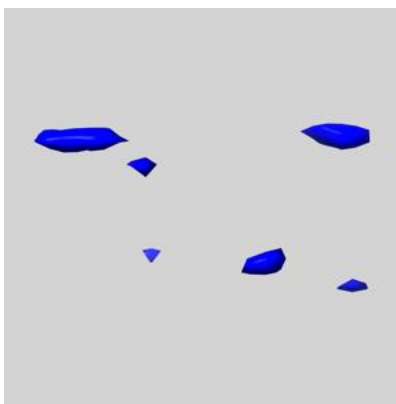


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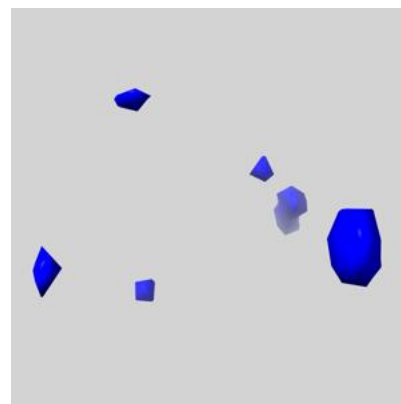
6.5.10 emd_1001_msk_16.map [i](#)



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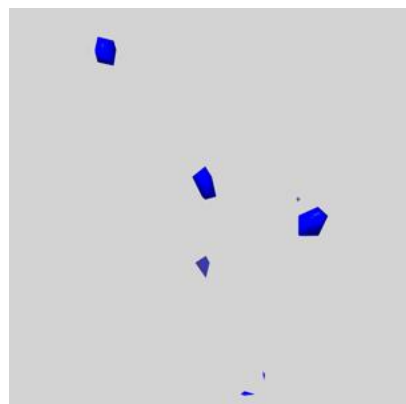


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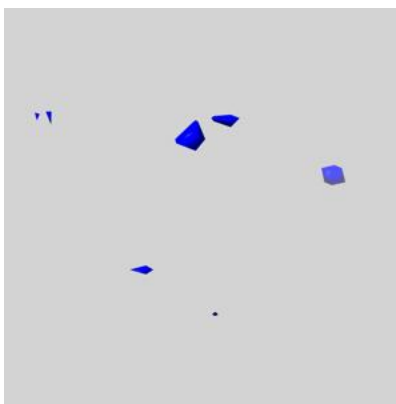


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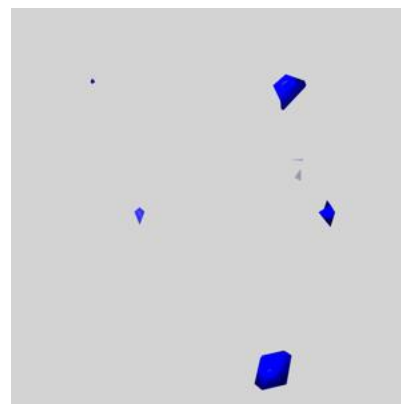
6.5.11 emd_1001_msk_15.map [i](#)



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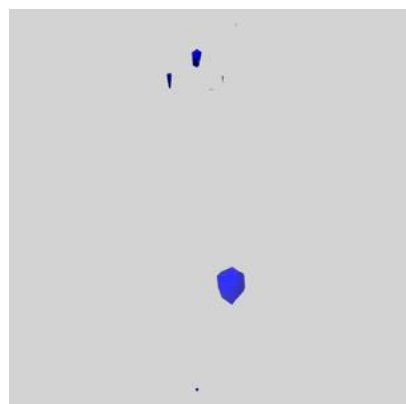


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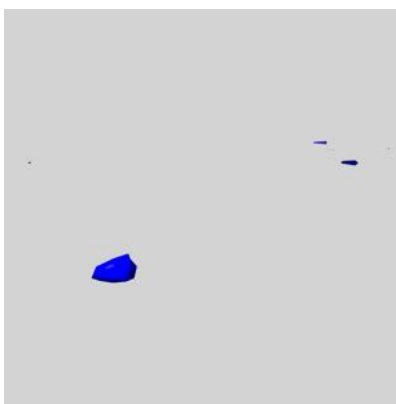


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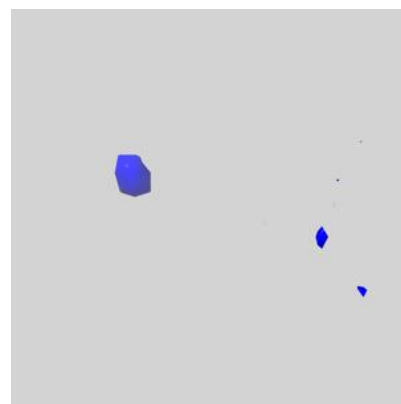
6.5.12 emd_1001_msk_14.map [i](#)



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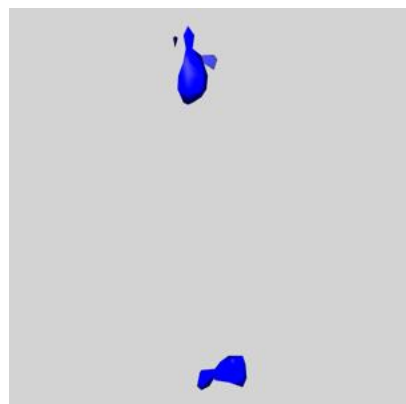


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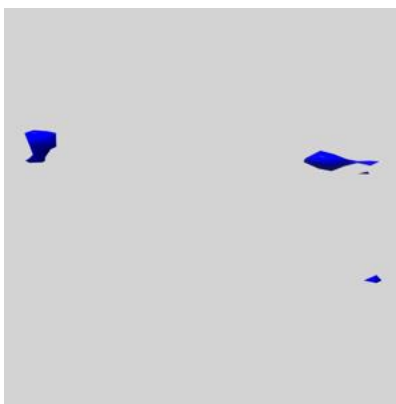


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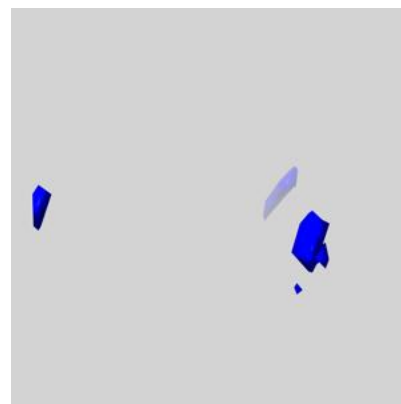
6.5.13 emd_1001_msk_13.map [i](#)



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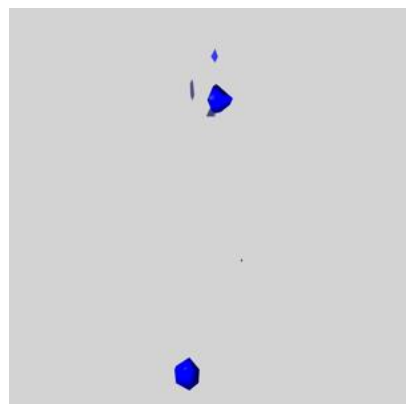


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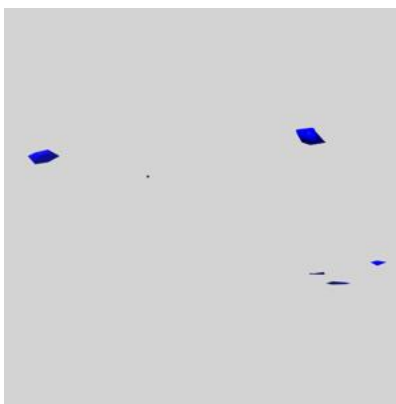


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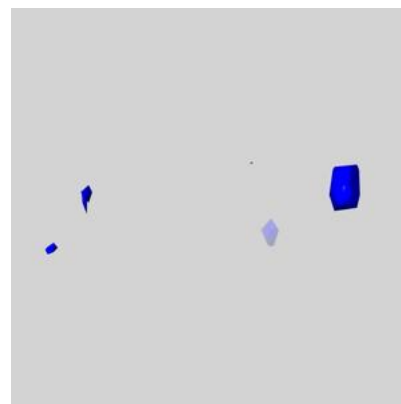
6.5.14 emd_1001_msk_12.map [i](#)



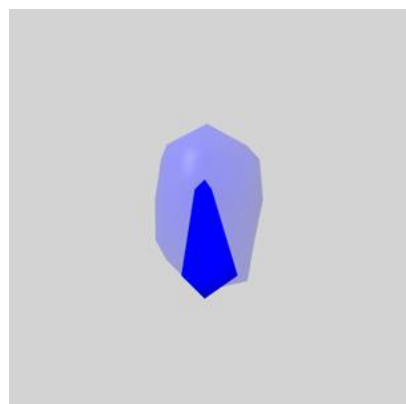
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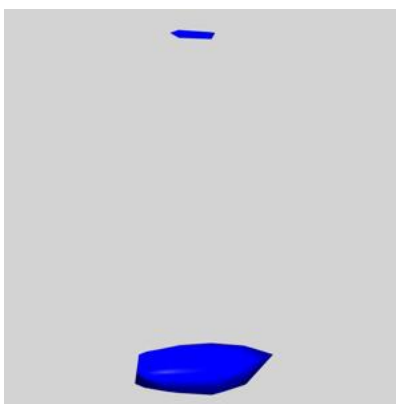
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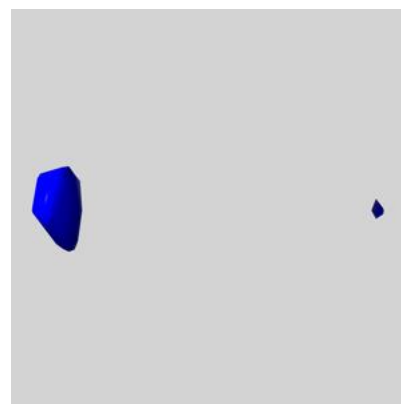
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6.5.15 emd_1001_msk_11.map [i](#)

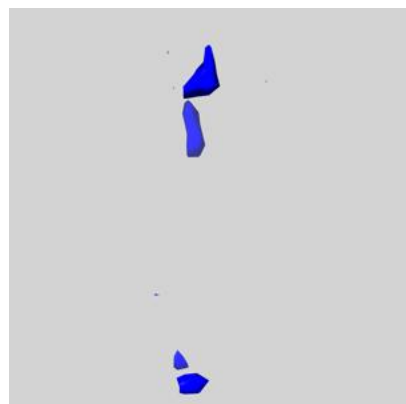
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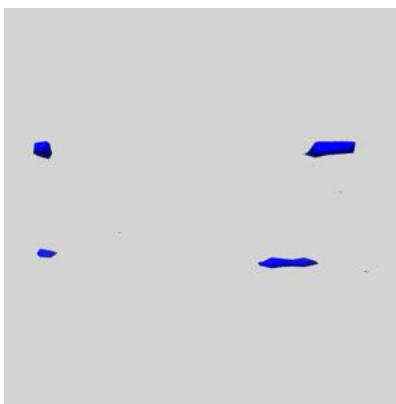
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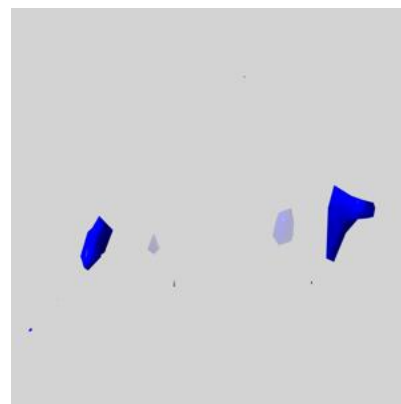
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6.5.16 emd_1001_msk_10.map [i](#)

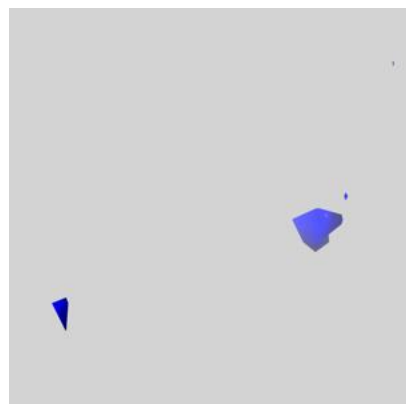
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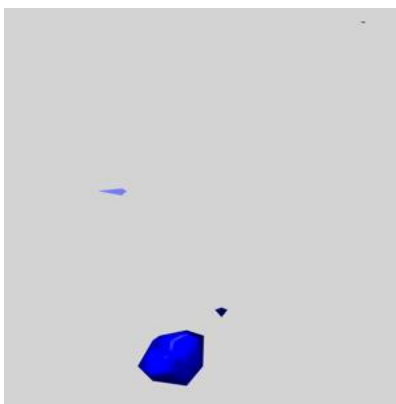
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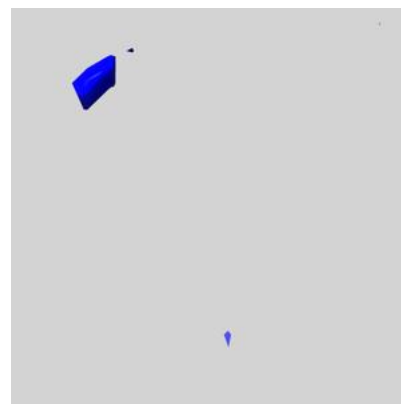
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6.5.17 emd_1001_msk_9.map [i](#)

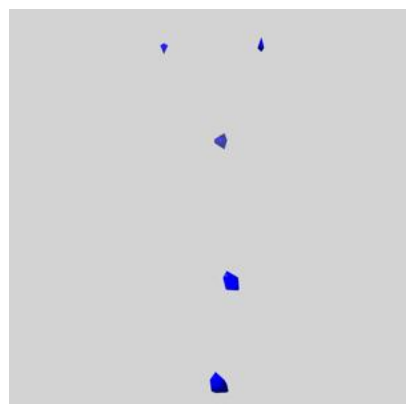
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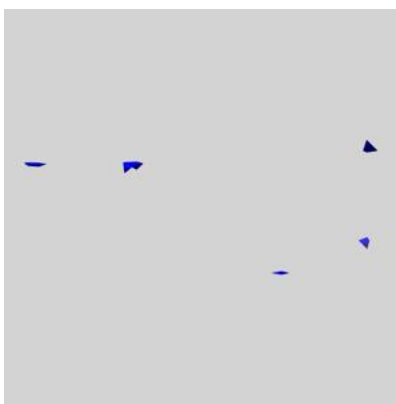
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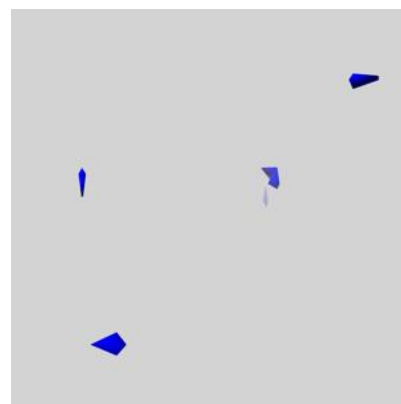
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6.5.18 emd_1001_msk_8.map [i](#)

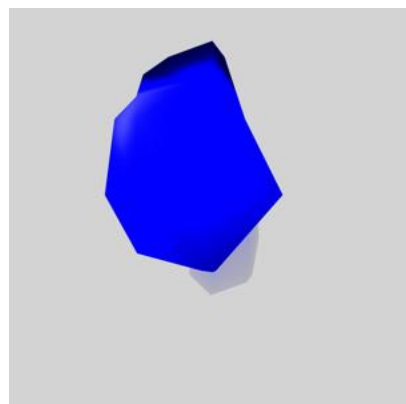
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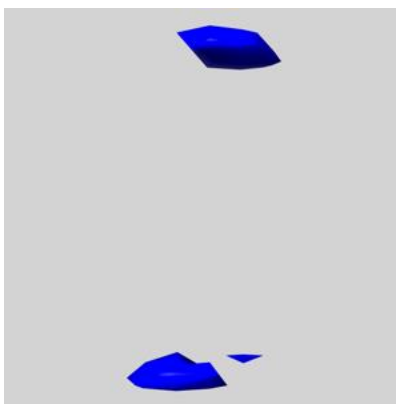
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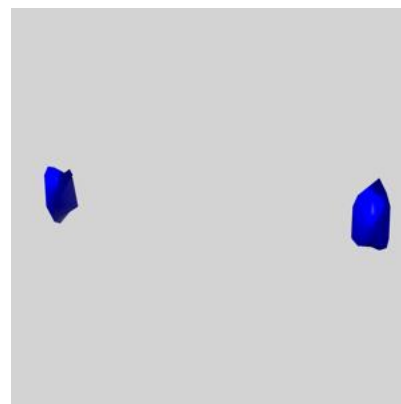
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6.5.19 emd_1001_msk_7.map [i](#)

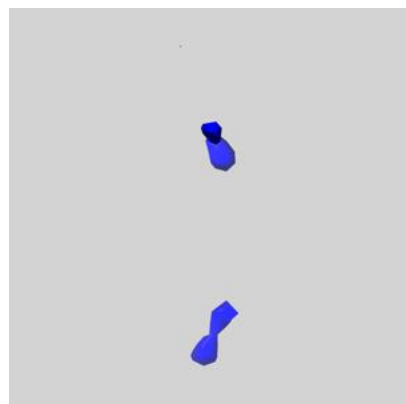
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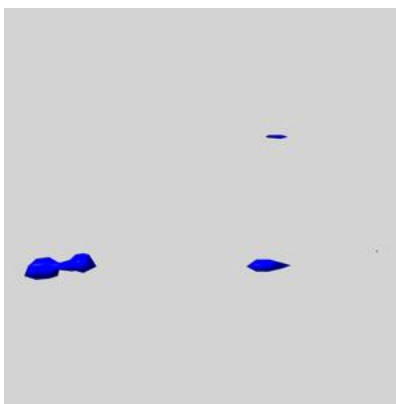
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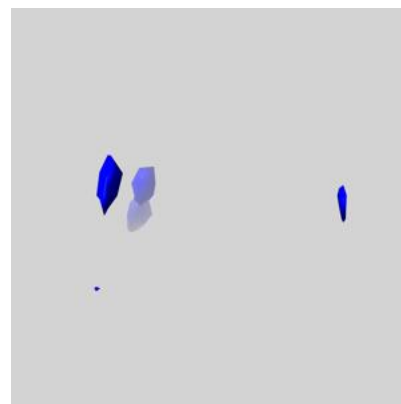
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6.5.20 emd_1001_msk_6.map [i](#)

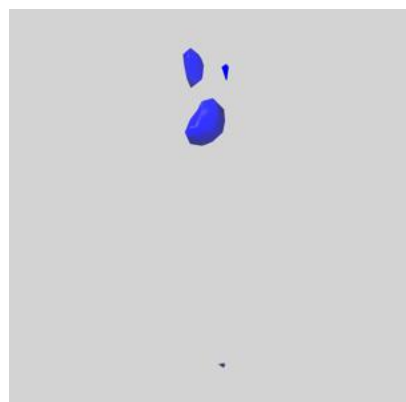
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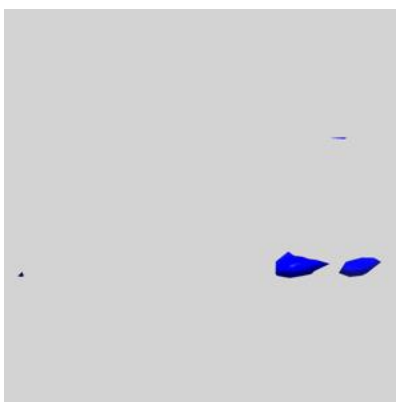
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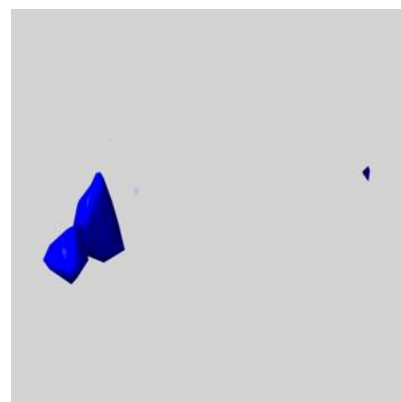
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6.5.21 emd_1001_msk_5.map [i](#)

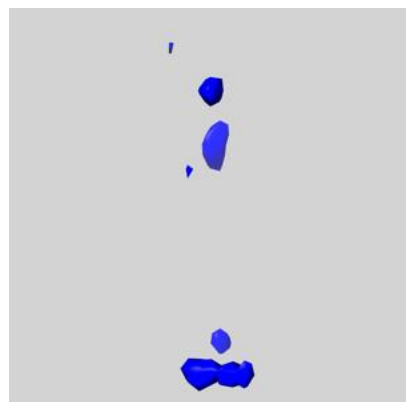
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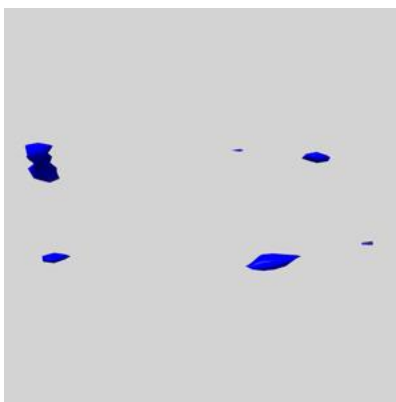
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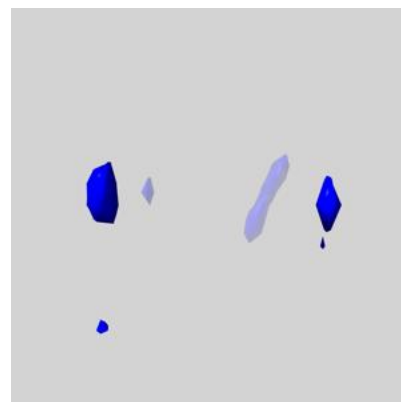
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6.5.22 emd_1001_msk_4.map [i](#)

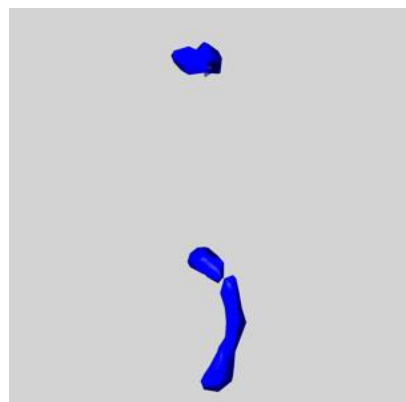
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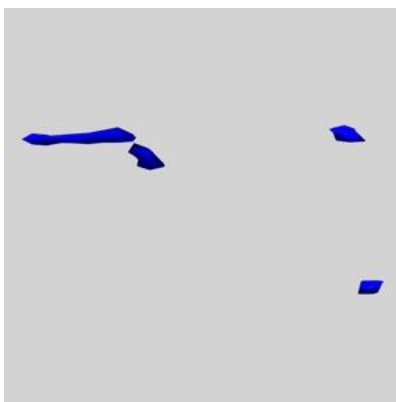
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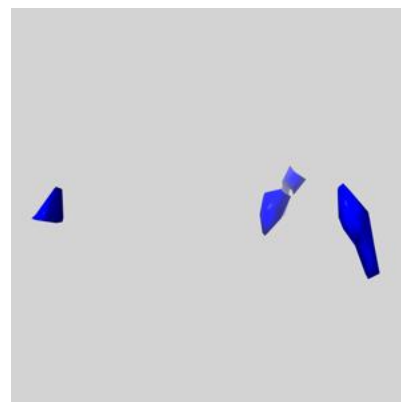
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6.5.23 emd_1001_msk_3.map [i](#)

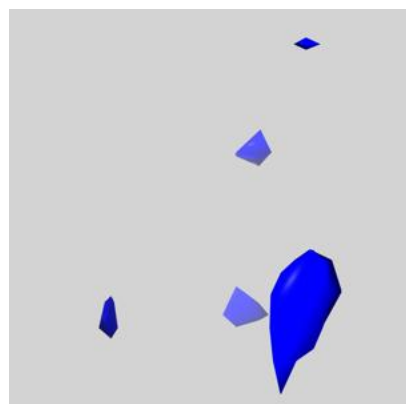
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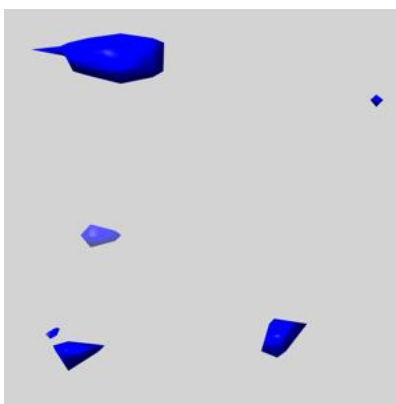
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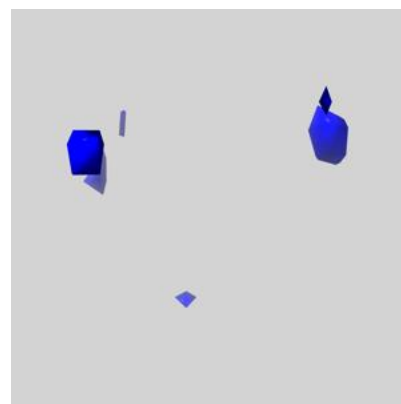
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6.5.24 emd_1001_msk_2.map [i](#)

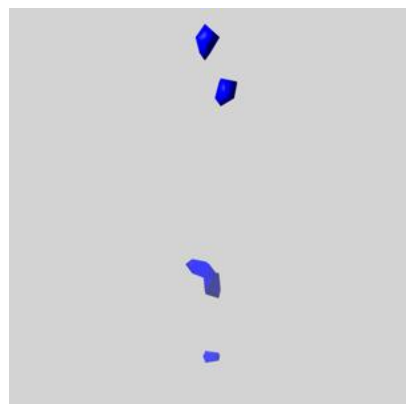
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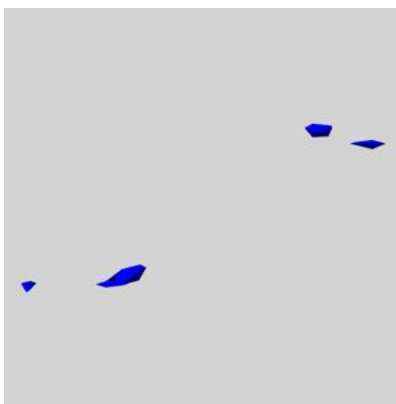
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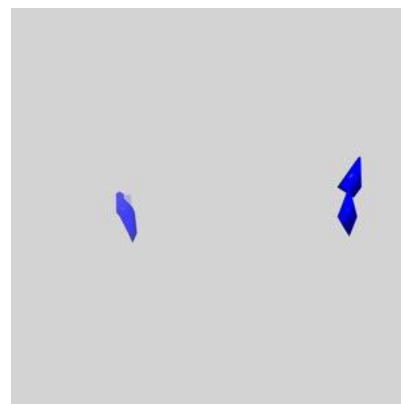
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6.5.25 emd_1001_msk_1.map [i](#)

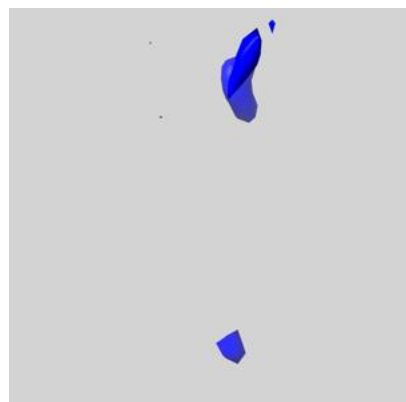
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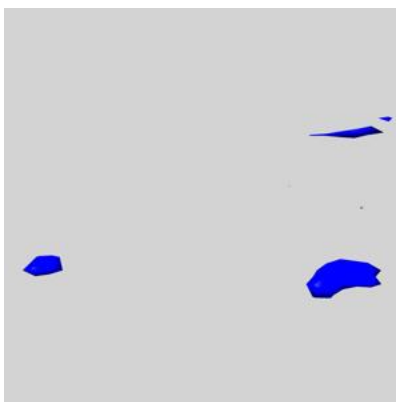
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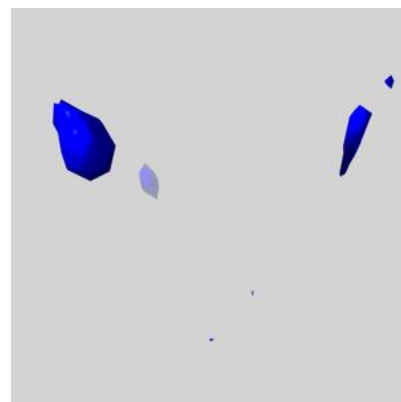
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6.5.26 emd_1001_msk_26.map [i](#)

X



Y

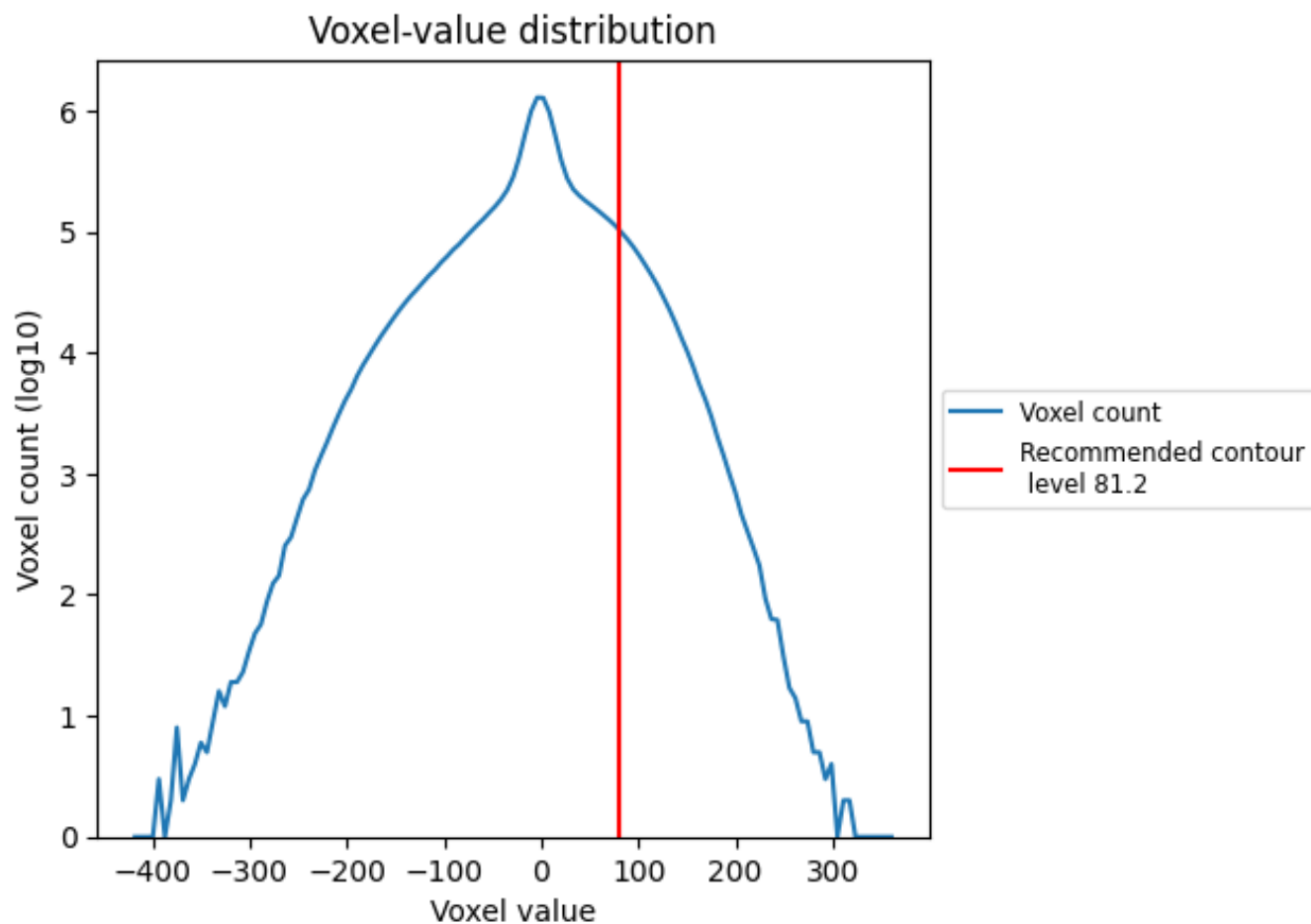


Z

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.

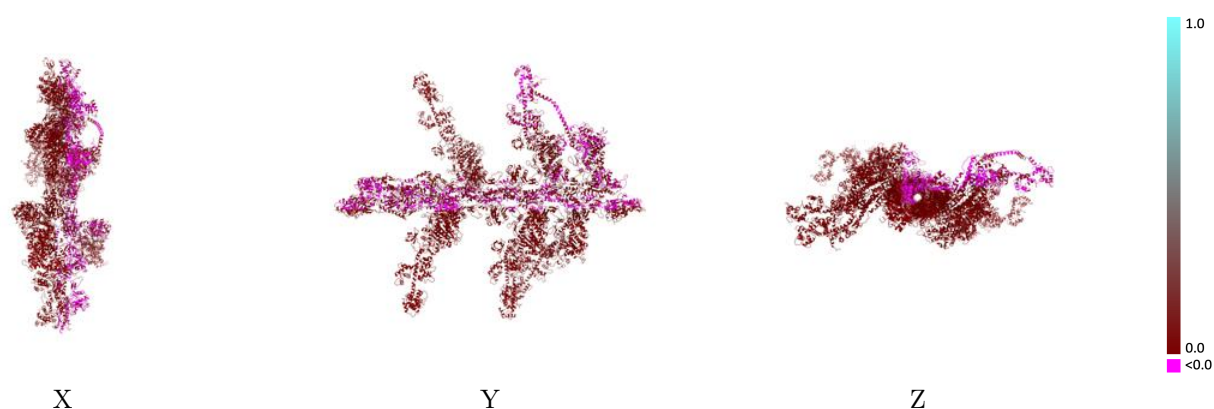
8 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-1001 and PDB model 1O18. Per-residue inclusion information can be found in section 3 on page 7.

8.1 Map-model overlay [i](#)

This section was not generated.

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

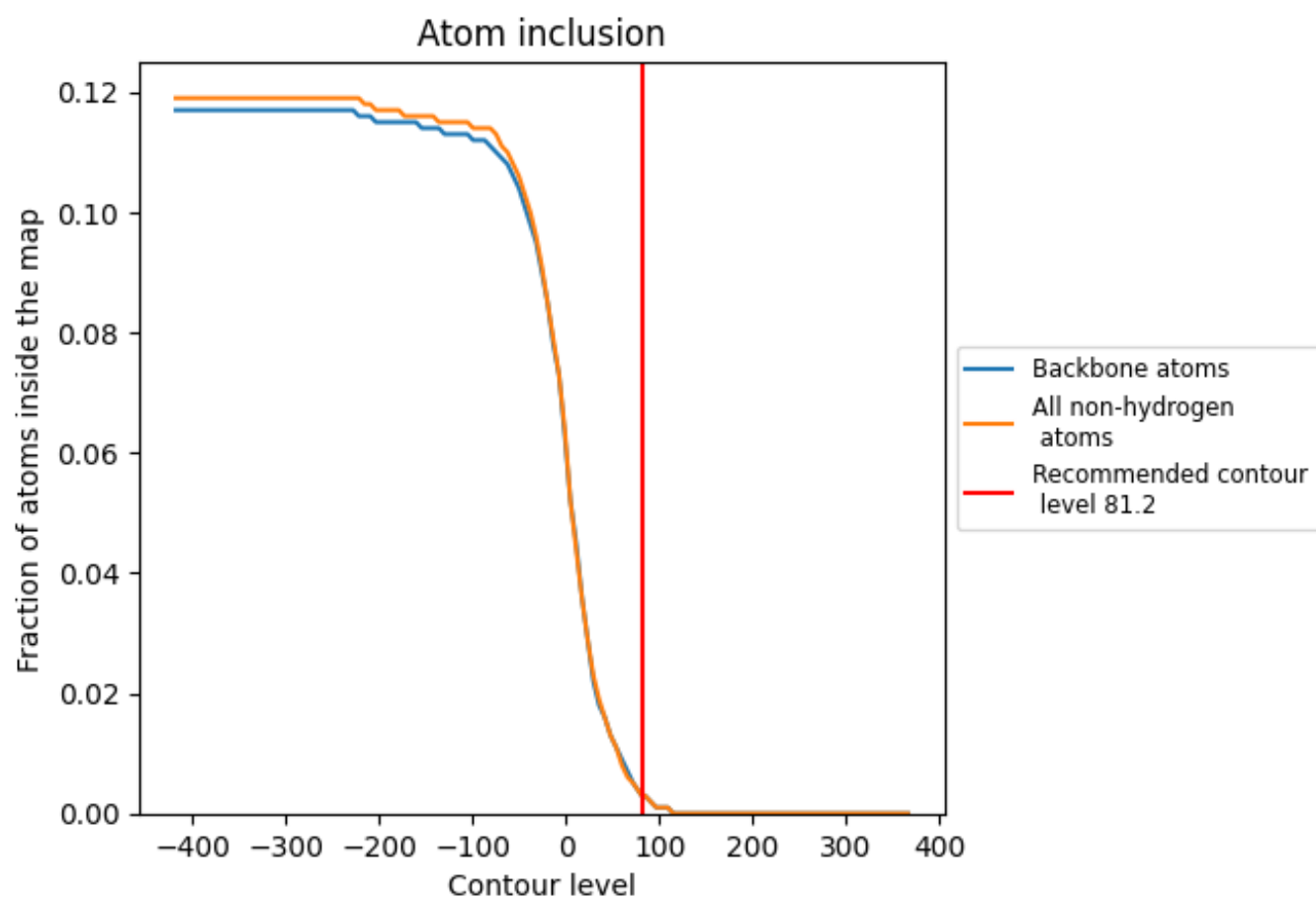


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

8.4 Atom inclusion [i](#)



At the recommended contour level, 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	 0.0030	 -0.0020
1	 0.0080	 0.0020
2	 0.0000	 -0.0050
3	 0.0000	 -0.0170
4	 0.0000	 -0.0030
5	 0.0000	 -0.0110
6	 0.0000	 -0.0060
7	 0.0000	 0.0020
8	 0.0000	 -0.0030
9	 0.0000	 -0.0040
A	 0.0010	 0.0010
D	 0.0000	 0.0000
E	 0.0000	 0.0000
F	 0.0000	 0.0000
G	 0.0030	 0.0020
H	 0.0000	 -0.0180
I	 0.1530	 0.0240
J	 0.0000	 -0.0010
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	 -0.0060
Q	 0.0000	 0.0000
R	 0.0000	 0.0000
V	 0.0000	 -0.0030
W	 0.0180	 -0.0060
X	 0.0000	 -0.0010
Y	 0.0020	 0.0070
Z	 0.0000	 0.0010

