



wwPDB EM Validation Summary Report ⓘ

Mar 17, 2026 – 07:34 PM UTC

PDB ID : 1O1D / pdb_00001o1d
EMDB ID : EMD-1001
Title : MOLECULAR MODELS OF AVERAGED RIGOR CROSSBRIDGES FROM
TOMOGRAMS OF INSECT FLIGHT MUSCLE
Authors : Chen, L.F.; Winkler, H.; Reedy, M.K.; Reedy, M.C.; Taylor, K.A.
Deposited on : 2002-11-18
Resolution : 70.00 Å(reported)
Based on initial models : 2MYS, 1ATN

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:

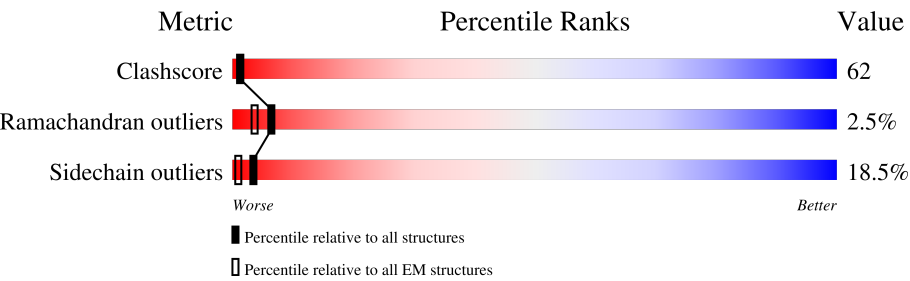
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)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

1 Overall quality at a glance 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% 24%49%22%. .
1	D	840	100% 25%49%22%. .
1	G	840	100% 24%49%22%. .
1	J	840	100% 25%49%23%. .
1	M	840	100% 23%50%23%. .
1	P	840	100% 24%49%22%. .
2	B	145	100% 64%26%7%. .
2	E	145	100% 64%26%8%. .

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Mol	Chain	Length	Quality of chain		
2	H	145	100%	62%	29% 5% .
2	K	145	99%	63%	27% 7% .
2	N	145	100%	64%	26% 7% .
2	Q	145	100%	64%	27% 6% .
3	C	147	100%	61%	35% .
3	F	147	87%	61%	35% .
3	I	147	100%	61%	35% .
3	L	147	100%	61%	35% .
3	O	147	100%	61%	35% .
3	R	147	100%	61%	35% .
4	0	375	99%	50%	35% 12% ..
4	1	375	97%	53%	36% 9% ..
4	2	375	99%	53%	36% 8% ..
4	3	375	99%	54%	34% 9% ..
4	4	375	99%	55%	34% 9% ..
4	5	375	99%	55%	34% 9% ..
4	7	375	99%	56%	33% 9% ..
4	8	375	99%	51%	35% 11% ..
4	9	375	99%	50%	35% 12% ..
4	V	375	99%	49%	36% 13% ..
4	W	375	99%	49%	36% 12% ..
4	X	375	92%	54%	34% 10% ..
4	Y	375	99%	54%	34% 9% ..
4	Z	375	97%	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 crite-

ria:

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

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 94966 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called SKELETAL MUSCLE MYOSIN II.

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

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

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

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

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

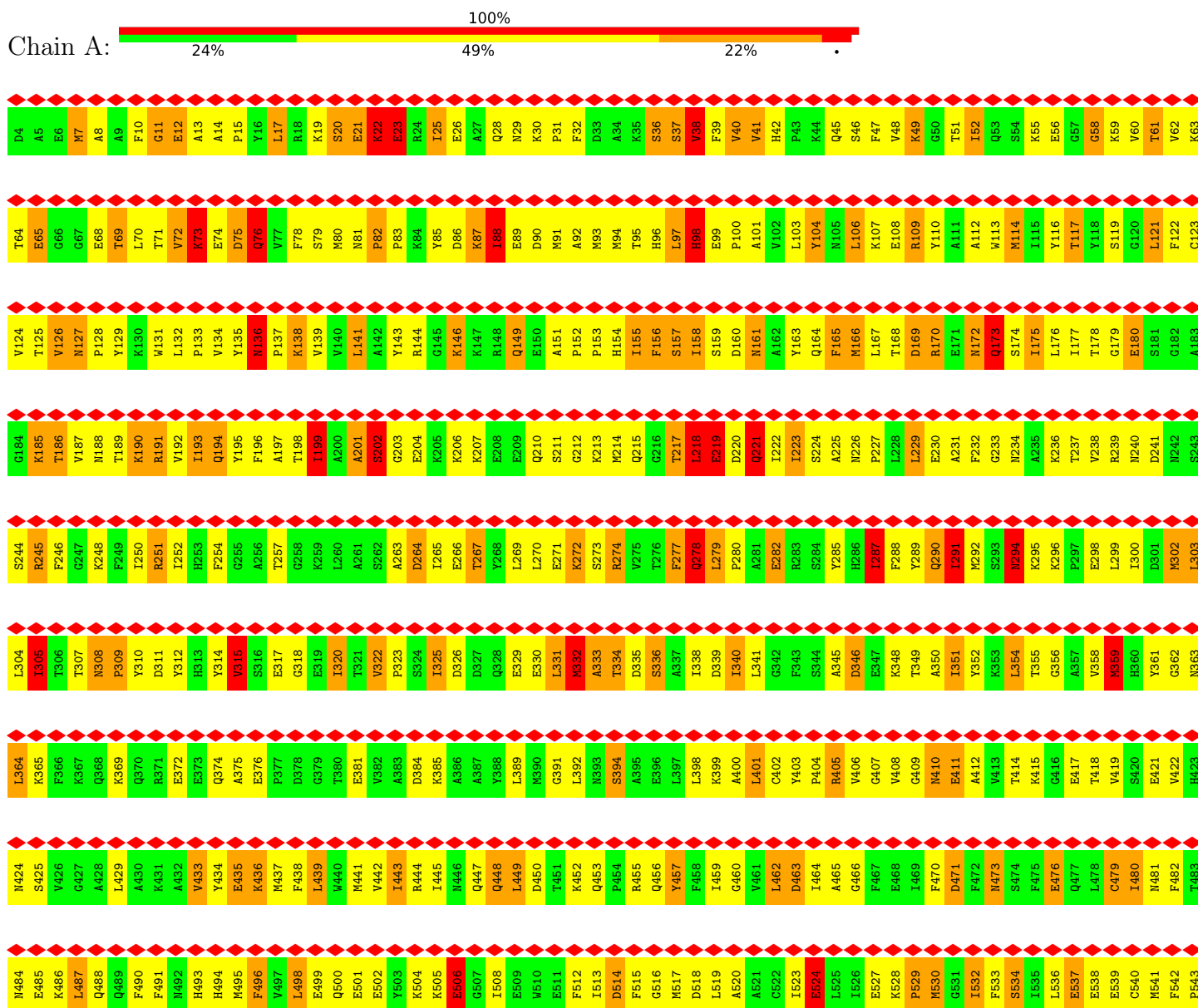
- Molecule 4 is a protein called SKELETAL MUSCLE ACTIN.

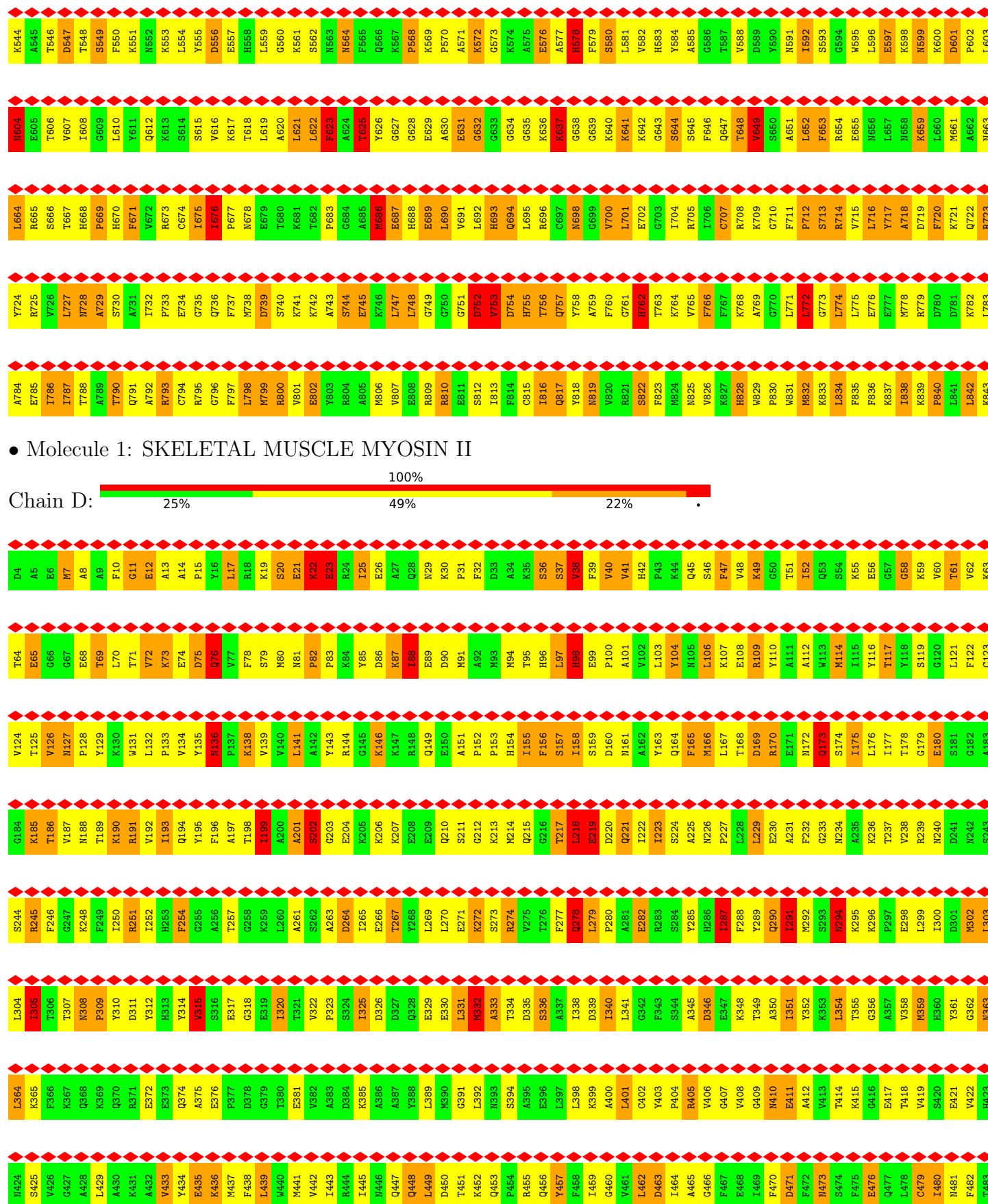
Mol	Chain	Residues	Atoms					AltConf	Trace
4	0	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	1	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	2	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	3	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	4	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20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

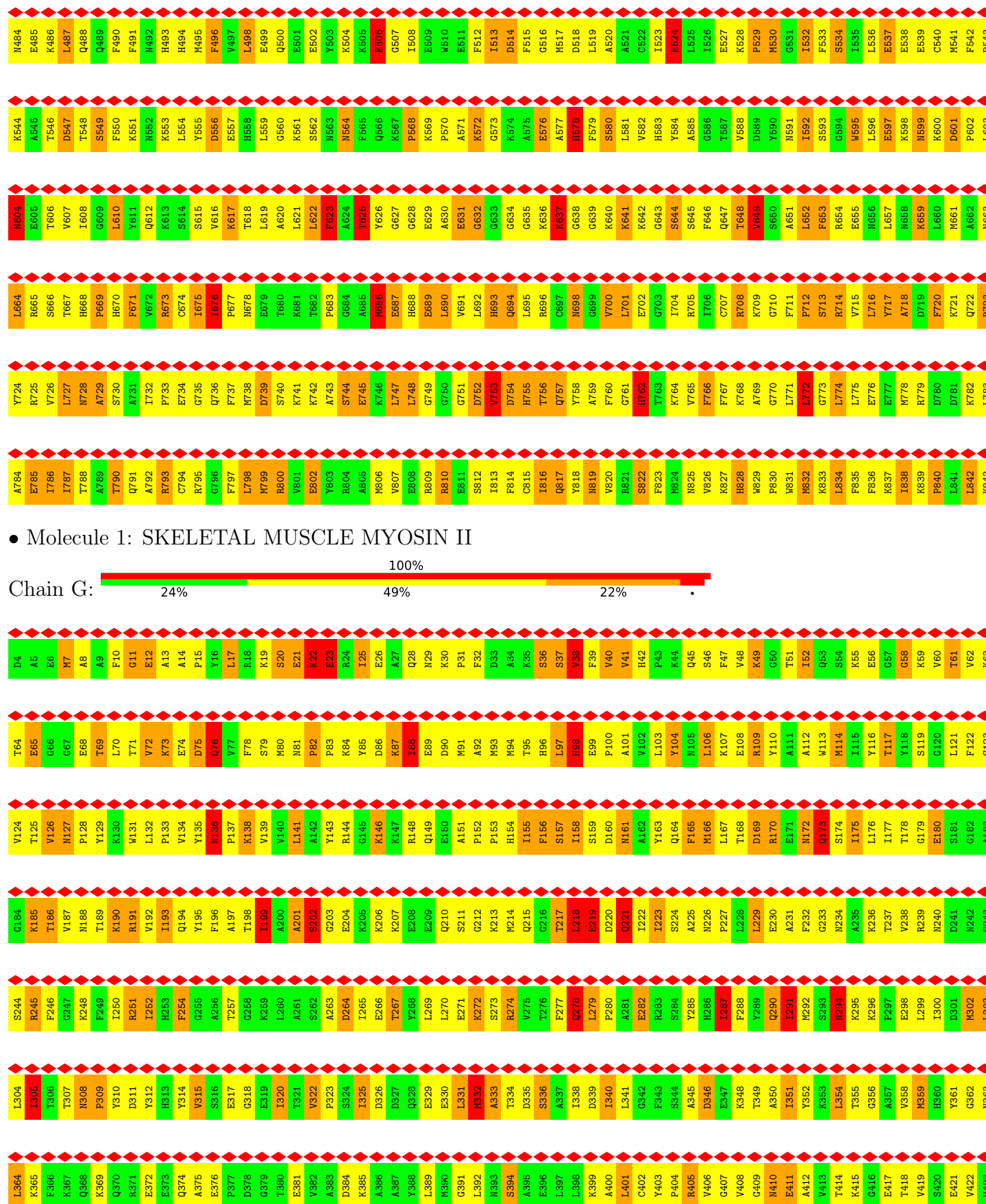
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: SKELETAL MUSCLE MYOSIN II







N424	N484	K544	L664	Y724	A784	N425	E485	K545	R665	R725	A785	V426	E486	T546	S666	L726	T786	E688	T690	F791	A792	V427	L487	D547	T667	H687	A789	T790	G791	A793	V428	Q488	S549	F669	H689	A791	F671	A794	E734	C794	R795	G796	F797	L429	Q489	F550	K551	Q612	N552	V430	F490	F491	N492	V431	H493	H494	E495	F496	V497	M498	F438	L498	E499	L439	Q500	Q501	E502	V440	M441	R444	I443	K504	K505	E506	Q447	G507	I508	Q448	E509	K569	P570	W510	E511	F512	K452	Q453	D514	F454	R455	F515	G516	Q456	M517	F457	D518	I459	G460	A520	V461	C522	I523	E524	I464	L465	L526	F467	E527	K528	P529	M530	D471	G531	I532	N473	F533	S534	S474	F475	I535	L536	Q477	E537	E538	C479	C540	M541	F542	P543	T483
K544	L664	Y724	A784	T64	V124	G184	K185	T125	V126	M127	N128	A129	K130	W131	L132	P133	V134	Y135	M136	K138	V139	W140	L141	A142	G143	R144	G145	K146	E147	T148	Q149	E150	A151	P152	G153	A154	T155	F156	S157	I158	S159	D160	A161	V162	G163	H164	I165	L166	K167	E168	D169	R170	A171	E172	M173	Q173	M174	I175	L176	T177	T178	G179	E180	L181	F182	N183	S244	R245	F246	G247	K248	F249	L250	R251	L252	H253	F254	G255	A256	T257	G258	K259	L260	A261	S262	A263	L265	E266	T267	G268	Q269	L270	E271	K272	S273	R274	V275	T276	F277	Q278	L279	P280	A281	E282	R283	S284	Y285	H286	E287	F288	Y289	Q290	L291	M292	K293	L354	T355	G356	A357	V358	K359	H360	Y361	G362	N363				

● Molecule 1: SKELETAL MUSCLE MYOSIN II



L304	L305	T306	T307	N308	P309	D310	D311	D312	H313	H314	G315	S316	E317	G318	E319	I320	T321	V322	P323	S324	I325	D326	D327	G328	E329	E330	L331	M332	A333	T334	D335	S336	A337	I338	L339	I340	L341	G342	F343	S344	A345	D346	E347	K348	T349	I350	F352	K353	T355	G356	A357	V358	K359	H360	Y361	G362	N363		
S244	R245	F246	G247	K248	F249	I250	R251	L252	H253	F254	G255	A256	T257	G258	K259	L260	A261	S262	A263	L265	E266	T267	G268	Q269	L269	L270	E271	K272	S273	R274	V275	T276	F277	Q278	L279	P280	A281	E282	R283	S284	Y285	H286	E287	F288	Y289	Q290	L291	M292	S293	N294	K295	K296	P297	E298	L299	I300	D301	M302	L303
G184	K185	T186	V187	N188	T189	K190	R191	V192	I193	Q194	Y195	F196	A197	I198	E199	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	G232	G233	N234	A235	K236	T237	V238	R239	T240	D241	N242	S243
V124	T125	V126	N127	P128	Y129	K130	W131	L132	P133	V134	Y135	N136	P137	K138	V139	V140	L141	A142	Y143	R144	G145	K146	K147	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	I177	T178	G179	E180	S181	G182	A183
T64	E65	G66	G67	E68	T69	L70	T71	V72	K73	E74	D75	Q76	V77	F78	S79	M80	N81	P82	P83	K84	Y85	D86	K87	T88	E89	D90	M91	A92	M93	A94	T95	H96	L97	H98	E99	P100	A101	V102	L103	Y104	N105	L106	K107	E108	R109	Y110	A111	A112	W113	M114	I115	Y116	T117	Y118	S119	G120	F121	L122	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

A784	R785	I786	T787	T788	A789	S790	Q791	A792	R793	C794	R795	G796	F797	L798	M799	R800	V801	E802	Y803	R804	A805	M806	E807	E808	R809	R810	E811	S812	L813	F814	C815	L816	Q817	Y818	N819	V820	R821	S822	F823	M824	N825	V826	K827	H828	V829	P830	M831	N832	L833	L834	F835	P836	K837	T838	K839	P840	L841	L842	R843	
Y724	R725	V726	L727	M728	A729	S730	A731	T732	P733	E734	G735	Q736	F737	M738	D739	S740	K741	T742	A743	S744	E745	K746	L747	L748	G749	G750	G751	D752	V753	D754	H755	T756	Q757	Y758	A759	F760	G761	R762	T763	K764	V765	F766	F767	K768	A769	G770	F771	L772	G773	L774	R775	E776	E777	M778	R779	D780	D781	L842	L843	
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	K640	K641	K642	G643	S644	S645	F646	Q647	T648	V649	S650	A651	L652	F653	R654	E655	M656	L657	M658	K659	L660	M661	A662	N663
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	
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	G572	I573	K574	A575	E576	A577	H578	F579	S580	L581	V582	H583	Y584	A585	G586	T587	V588	D589	Y590	N591	I592	F593	S593	G594	W595	L596	E597	K598	N599	K600	D601	P602	L603
N484	E485	K486	L487	Q488	Q489	F490	F491	N492	H493	H494	M495	F496	V497	L498	E499	Q500	E501	E502	Y503	K504	K505	E506	G507	I508	E509	W510	E511	F512	I513	D514	F515	G516	M517	D518	L519	A520	A521	C522	I523	E524	L525	I526	E527	K528	P529	M530	G531	I532	F533	S534	I535	L536	E537	E538	E539	C540	M541	F542	P543	
N424	S425	V426	G427	A428	L429	A430	K431	A432	V433	Y434	E435	A436	M437	F438	L439	W440	M441	V442	I443	I444	I445	M446	Q447	Q448	L449	D450	T451	K452	Q453	P454	A455	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	
L364	K365	F366	K367	Q368	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	

● Molecule 1: SKELETAL MUSCLE MYOSIN II



S244	R245	F246	G247	F249	L250	R251	L252	H253	F254	G255	A256	T257	G258	K259	L260	A261	S262	A263	D264	L265	E266	T267	Y268	L269	L270	E271	K272	S273	R274	V275	T276	F277	Q278	L279	P280	A281	E282	R283	S284	Y285	H286	L287	F288	Y289	Q290	I291	M292	G293	N294	K295	K296	P297	E298	L299	I300	D301	M302	L303	
G184	K185	T186	V187	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	L222	T223	S224	A225	N226	P227	L228	L229	E230	A231	F232	G233	N234	A235	K236	T237	V238	R239	N240	D241	N242	S243	
V124	T125	V126	N127	N128	Y129	K130	V131	L132	P133	V134	Y135	N136	P137	K138	V139	Y140	L141	A142	Y143	G145	K146	K147	R148	Q149	E150	A151	P152	P153	H154	I155	F156	S157	I158	S159	D160	N161	A162	V163	Q164	F165	M166	L167	T168	D169	R170	N172	E171	Q173	S174	I175	L176	T177	T178	G179	E180	S181	G182	A183	
T64	E65	G66	G67	E68	T69	L70	T71	V72	K73	E74	D75	Q76	V77	F78	S79	M80	N81	P82	P83	K84	Y85	D86	K87	H88	E89	D90	N91	A92	M93	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	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

L304	L305	L306	L307	N308	P309	Y310	D311	Y312	H313	Y314	V315	S316	E317	G318	E319	I320	T321	V322	P323	S324	I325	D326	Q327	Q328	E329	E330	L331	M332	A333	T334	D335	S336	A337	I338	D339	I340	L341	G342	F343	S344	A345	D346	E347	K348	T349	A350	I351	Y352	K353	L354	T355	G356	A357	V358	M359	H360	Y361	G362	N363
L364	K365	F366	K367	Q368	K369	Q370	R371	E372	E373	Q374	A375	E376	P377	D378	G379	E380	E381	V382	A383	D384	K385	A386	A387	Y388	L389	M390	G391	L392	N393	S394	A395	E396	G397	L398	D399	K400	L401	C402	Y403	D404	A405	V406	G407	V408	G409	N410	E411	A412	T414	K415	G416	E417	T418	V419	S420	E421	V422	H423	
N424	S425	V426	G427	A428	L429	A430	K431	A432	A433	Y434	E435	A436	M437	F438	E439	W440	M441	V442	I443	R444	I445	N446	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	S474	F475	E476	Q477	L478	C479	I480	N481	F482	T483	
M484	E485	K486	L487	Q488	Q489	F490	F491	M492	H493	H494	M495	F496	V497	L498	E499	Q500	E501	E502	Y503	K504	K505	E506	G507	I508	E509	W510	E511	F512	I513	D514	F515	G516	M517	D518	L519	A520	A521	C522	I523	E524	L525	I526	E527	K528	P529	M530	G531	I532	K533	S534	I535	L536	E537	E538	E539	C540	M541	F542	P543
K544	A545	T546	D547	T548	S549	F550	K551	N552	K553	L554	Y555	D556	E557	H558	L559	G560	K561	S562	N563	N564	F565	Q566	K567	P568	K569	P570	A571	K572	G573	K574	A575	E576	A577	H578	F579	S580	L581	V582	H583	Y584	A585	G586	V587	V588	D589	Y590	N591	I592	S593	G594	N595	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	F646	Q647	T648	V649	S650	A651	L652	F653	R654	E655	N656	L657	N658	K659	L660	M661	A662	N663	
L664	R665	S666	T667	H668	P669	H670	F671	V672	R673	C674	L675	L676	P677	N678	E679	T680	K681	T682	P683	G684	A685	N686	E687	H688	E689	L690	V691	L692	H693	Q694	L695	R696	G697	N698	G699	V700	L701	E702	G703	I704	R705	I706	C707	R708	K709	G710	F711	P712	S713	R714	V715	L716	Y717	A718	D719	F720	K721	Q722	R723
Y724	R725	V726	L727	N728	A729	S730	A731	I732	P733	E734	G735	Q736	F737	N738	D739	S740	K741	K742	A743	S744	E745	K746	L747	L748	G749	G750	G751	D752	F753	D754	H755	T756	Q757	Y758	A759	F760	G761	H762	T763	K764	V765	F766	K767	T768	A769	G770	L771	L772	G773	L774	L775	E776	N777	N778	R779	D780	L781	K782	L783
A784	E785	I786	I787	T788	A789	T790	Q791	A792	R793	C794	R795	G796	F797	L798	M799	R800	V801	E802	R803	R804	A805	M806	V807	E808	R809	R810	E811	S812	R813	F814	C815	L816	Q817	Y818	N819	V820	R821	S822	F823	H824	N825	V826	H828	V829	P830	W831	H832	K833	L834	F835	F836	L838	K839	P840	L841	L842	K843		
D4	A5	E6	M7	A8	A9	F10	G11	E12	A13	A14	P15	Y16	L17	R18	K19	S20	K22	E23	R24	I25	E26	A27	Q28	N29	K30	P31	F32	D33	A34	K35	S36	S37	Y38	F39	V40	V41	H42	P43	K44	Q45	S46	F47	V48	G50	T51	I52	Q53	S54	K55	E56	G58	K59	V60	L61	F62	K63			
T64	E65	G66	G67	E68	T69	L70	T71	V72	K73	E74	D75	Q76	V77	F78	S79	M80	N81	P82	P83	K84	Y85	D86	L88	E89	D90	N91	A92	N93	M94	T95	H96	L97	N98	E99	D100	A101	V102	L103	Y104	N105	L106	I107	R108	R109	Y110	A111	A112	W113	M114	I115	Y116	T117	Y118	S119	G120	L121	F122	C123	
V124	T125	V126	N127	P128	Y129	K130	W131	L132	P133	V134	Y135	N136	P137	K138	V139	V140	A142	Y143	R144	G145	K146	K147	R148	Q149	E150	A151	P152	P153	H154	T155	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	
G184	K185	T186	N187	N188	T189	K190	R191	V192	I193	Q194	Y195	F196	A197	T198	I199	A200	S202	G203	E204	E205	K206	K207	E208	E209	Q210	S211	G212	K213	M214	Q215	G216	T217	L218	E219	D220	Q221	I222	I223	S224	N226	P227	L228	L229	E230	A231	F232	G233	N234	A235	K236	T237	V238	R239	N240	D241	N242	S243		

● Molecule 1: SKELETAL MUSCLE MYOSIN II

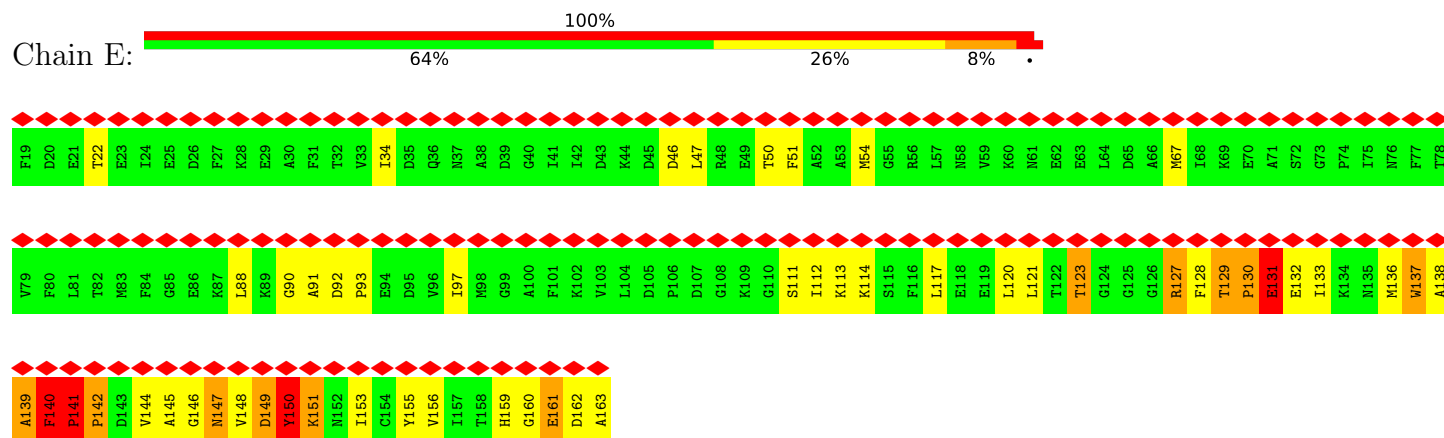




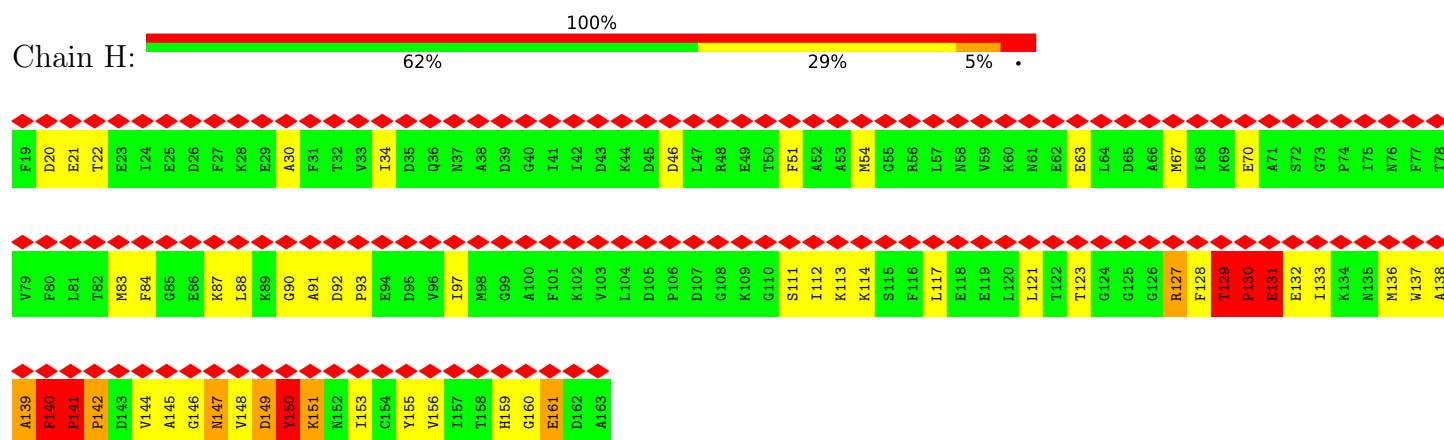
Service	Percentage
Service 1	100%
Service 2	64%
Service 3	26%
Service 4	7%



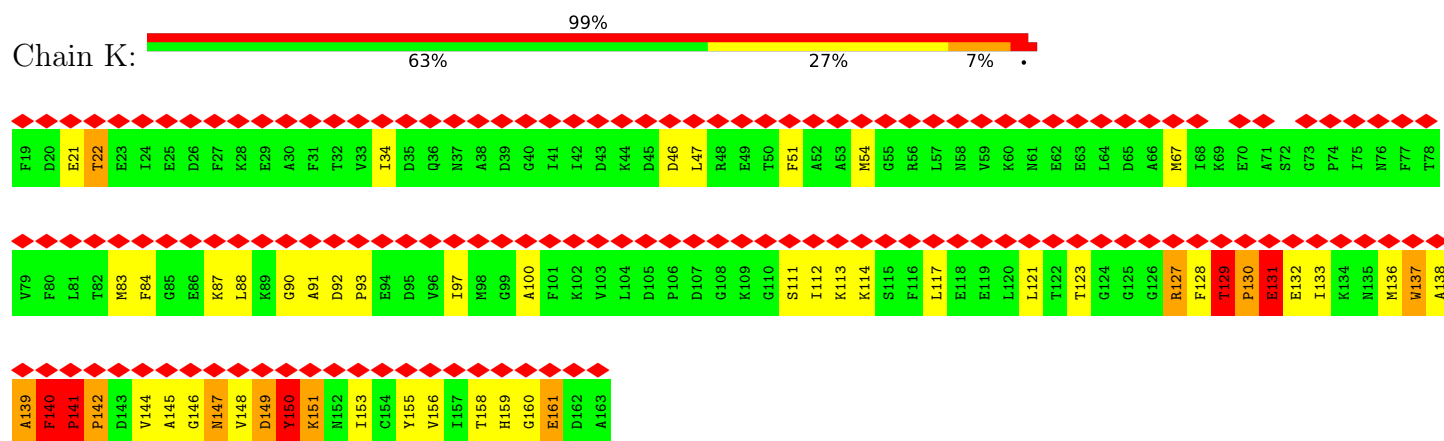
• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN



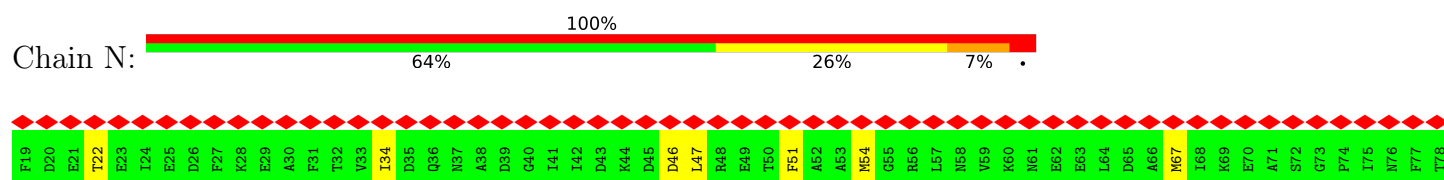
• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

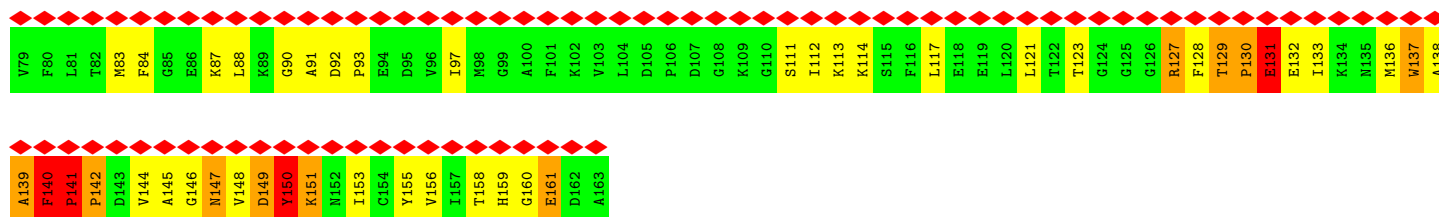


• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

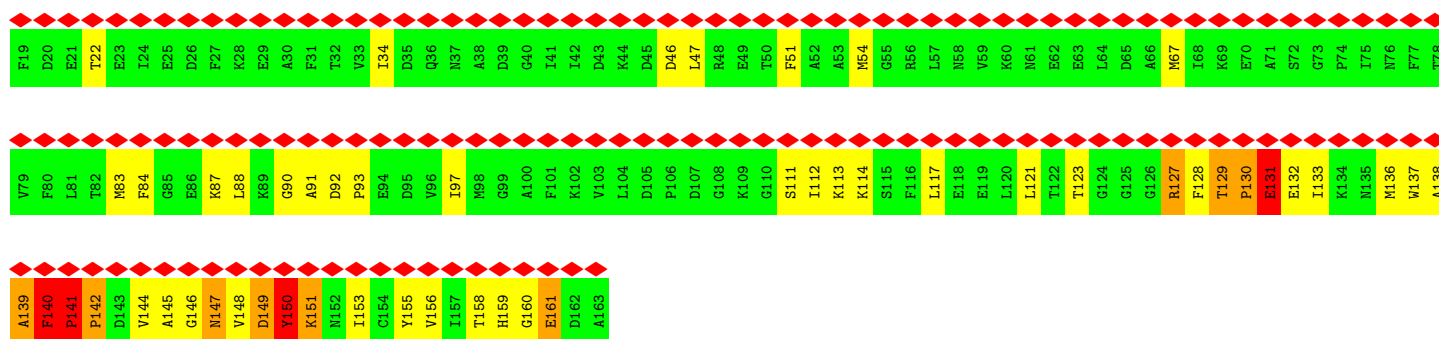


• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

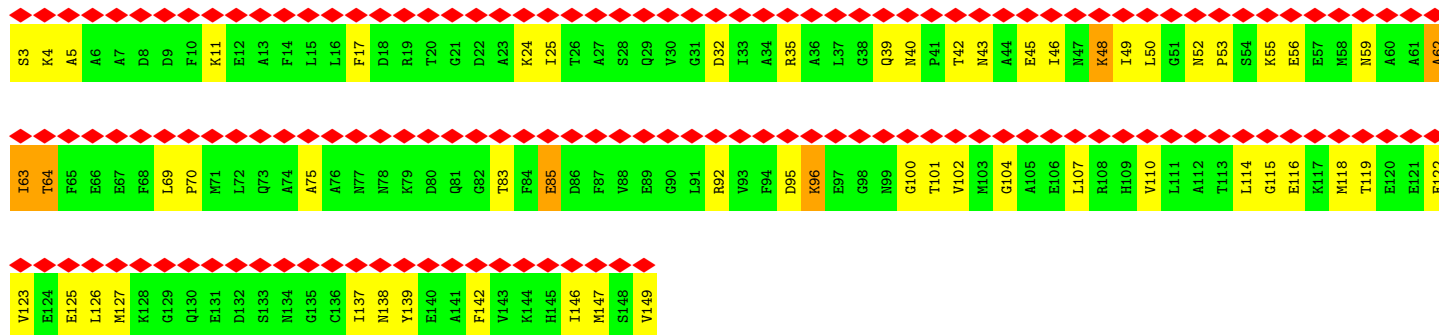




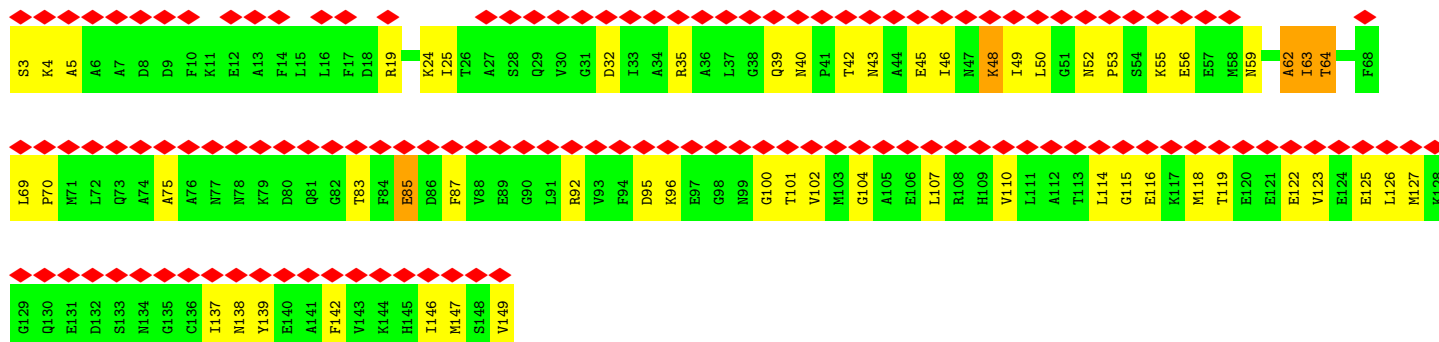
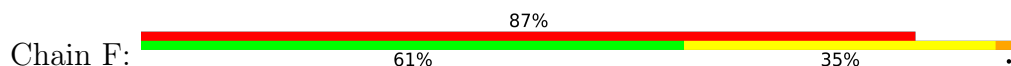
• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN



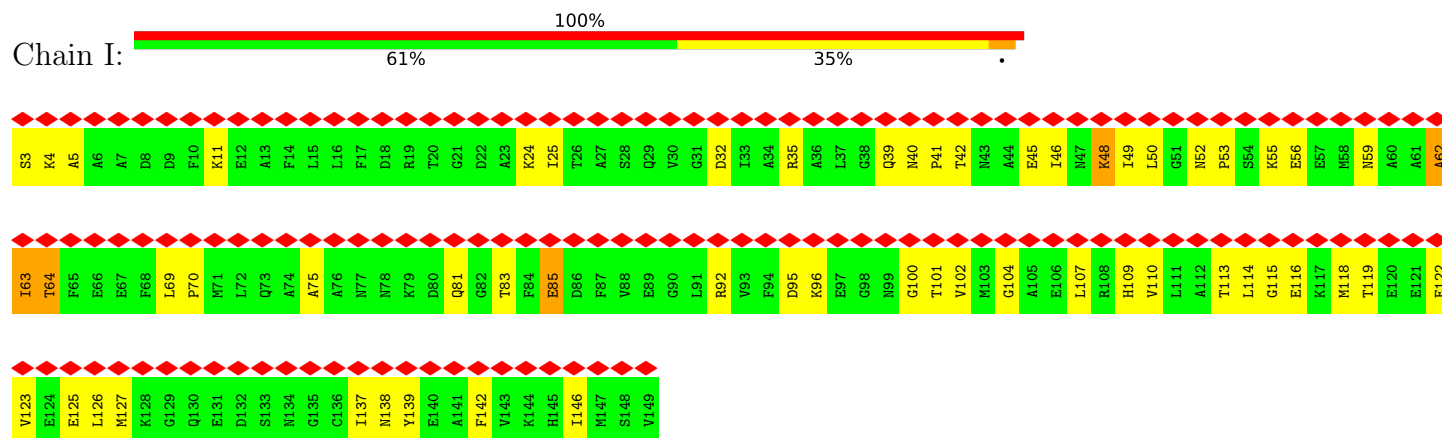
• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN



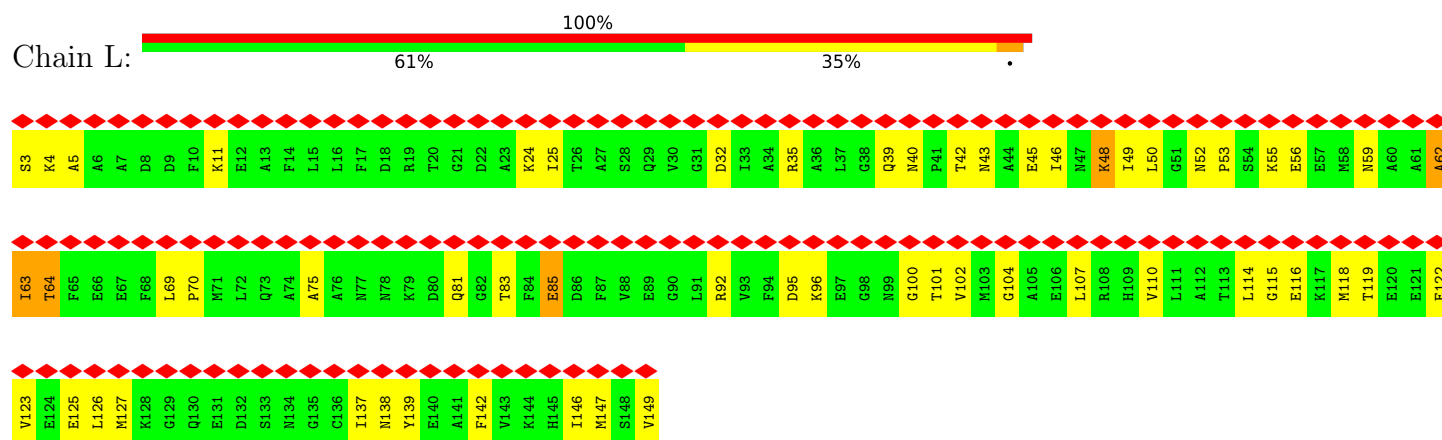
• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN



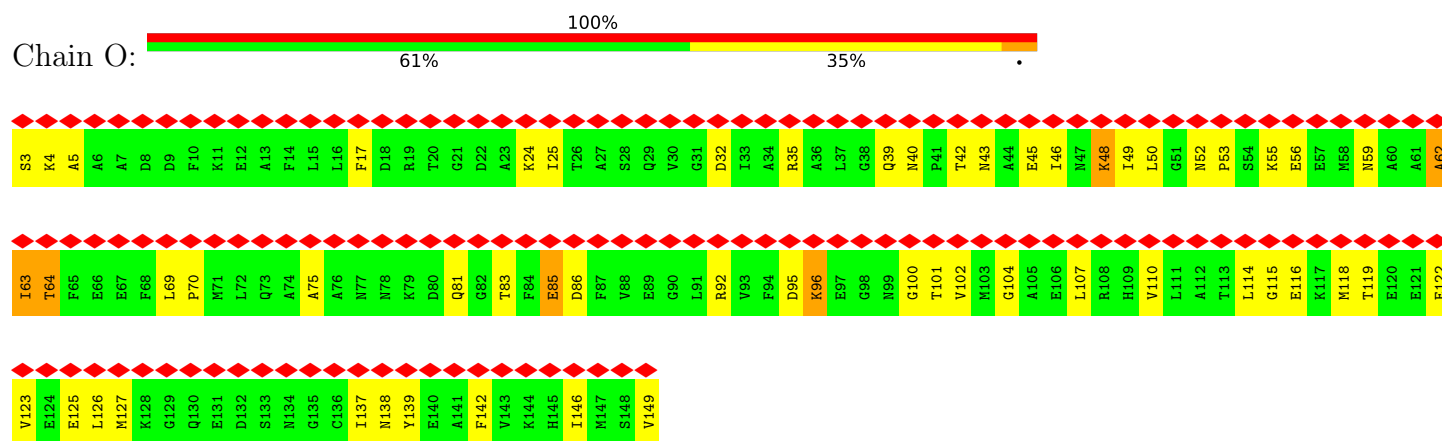
● Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN



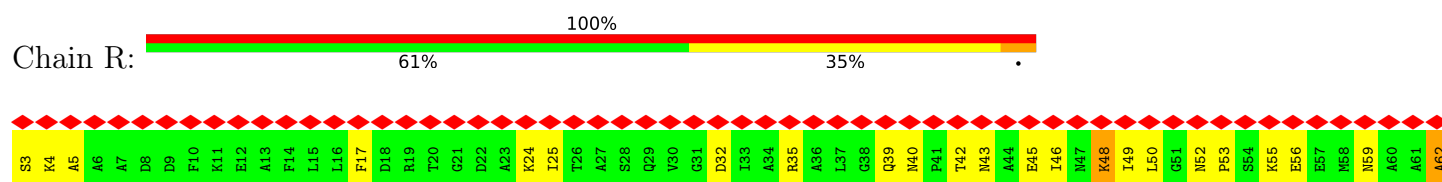
● Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN

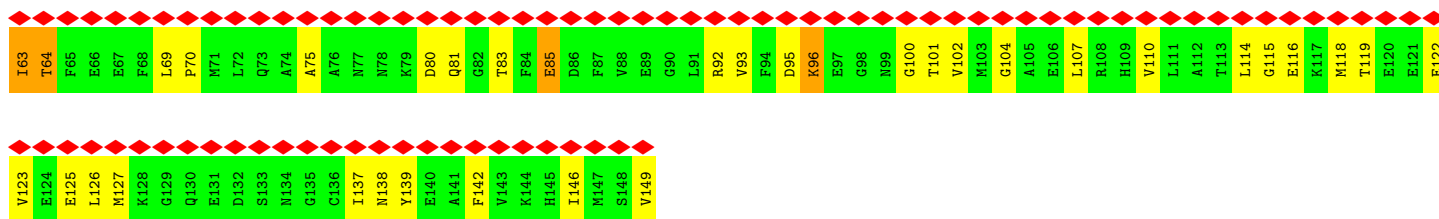


● Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN

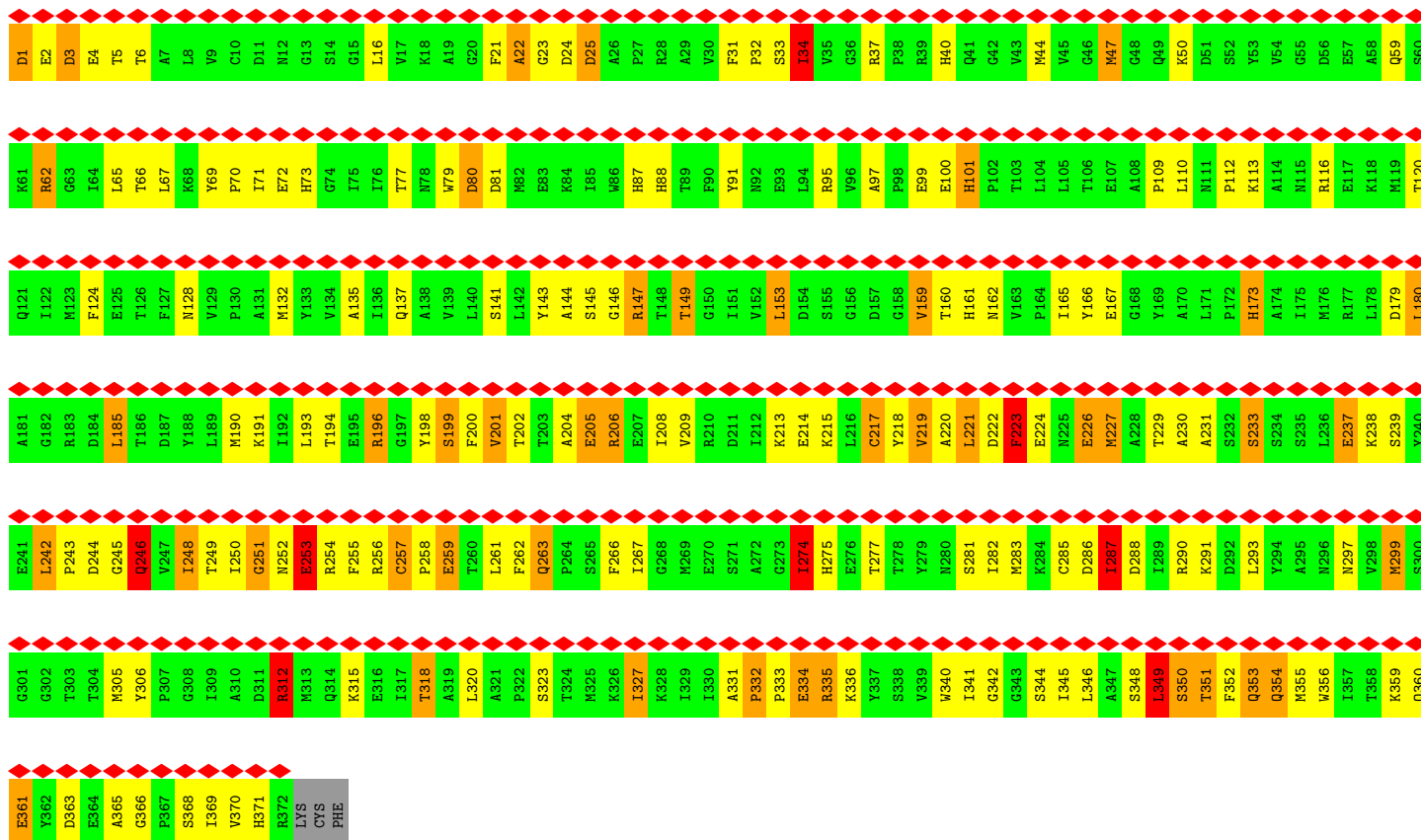


● Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN

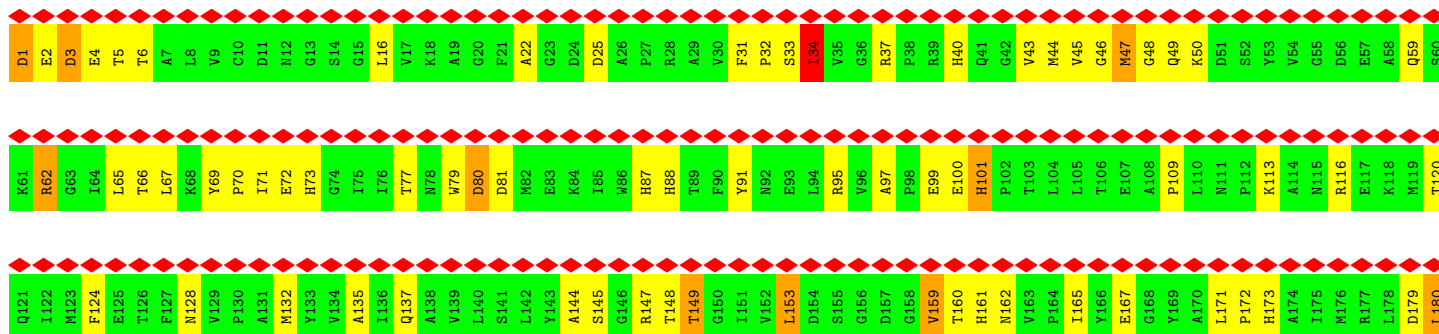


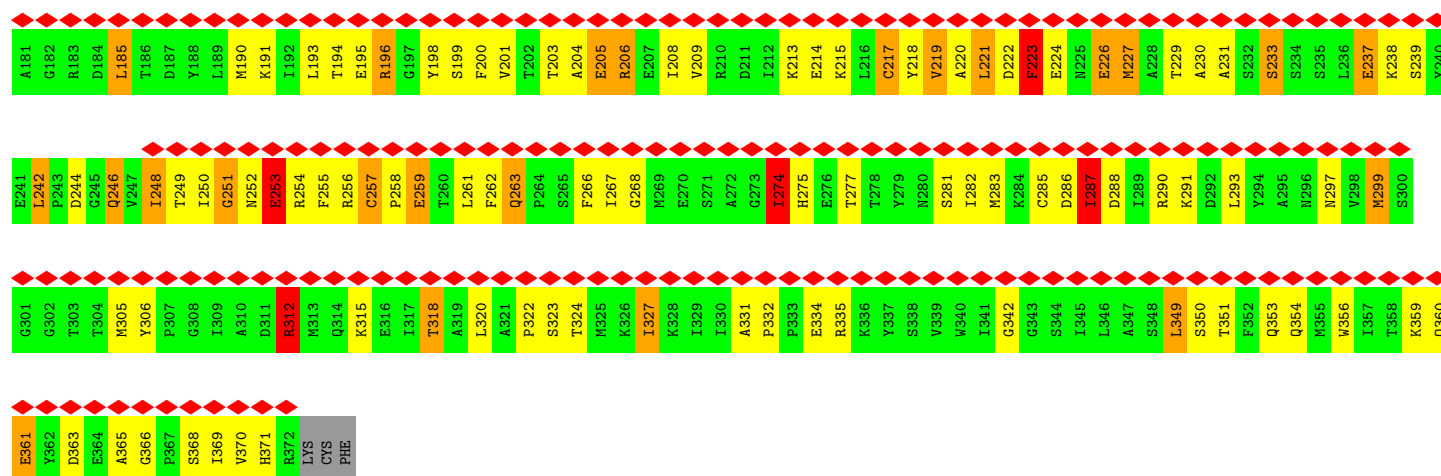


• Molecule 4: SKELETAL MUSCLE ACTIN

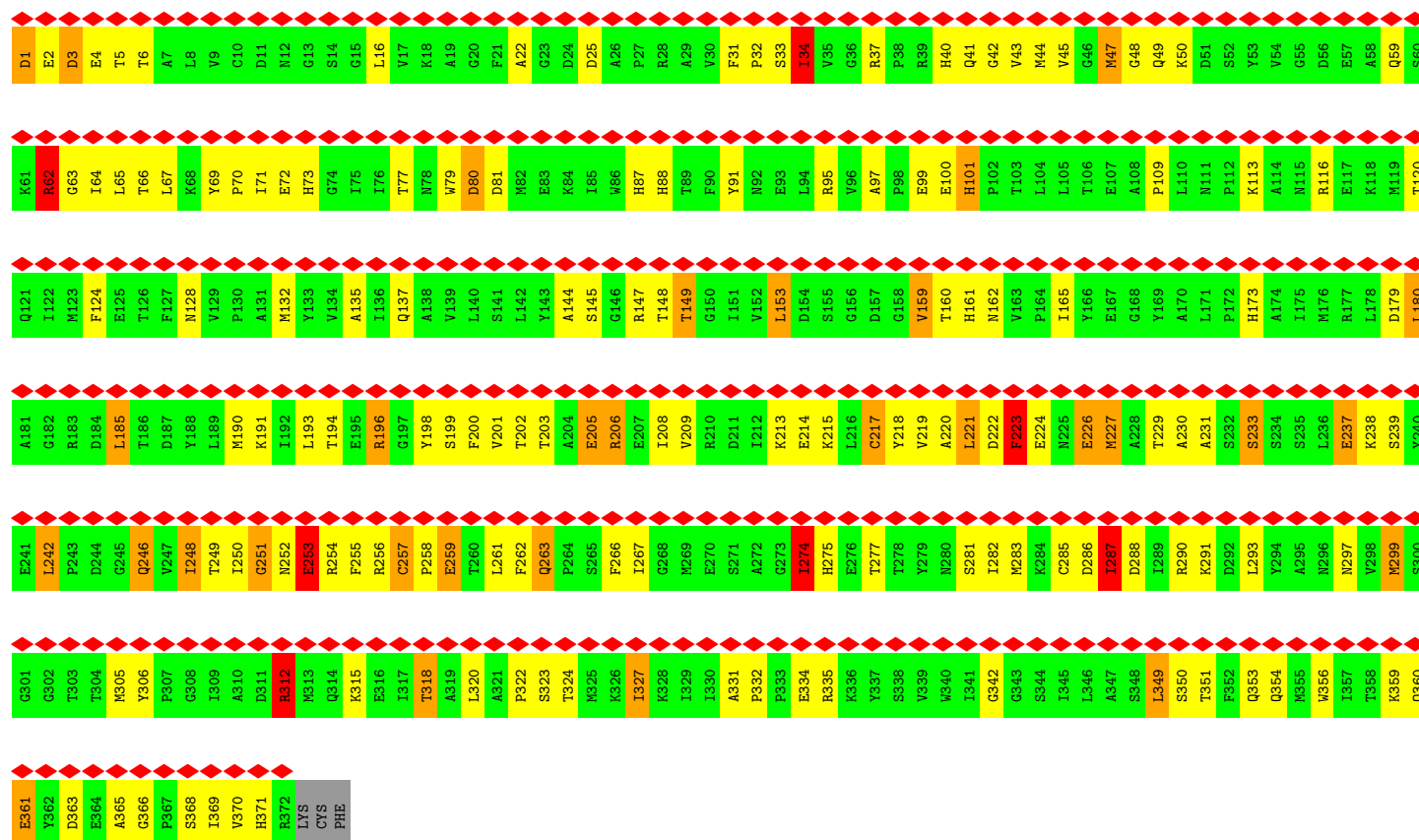


• Molecule 4: SKELETAL MUSCLE ACTIN



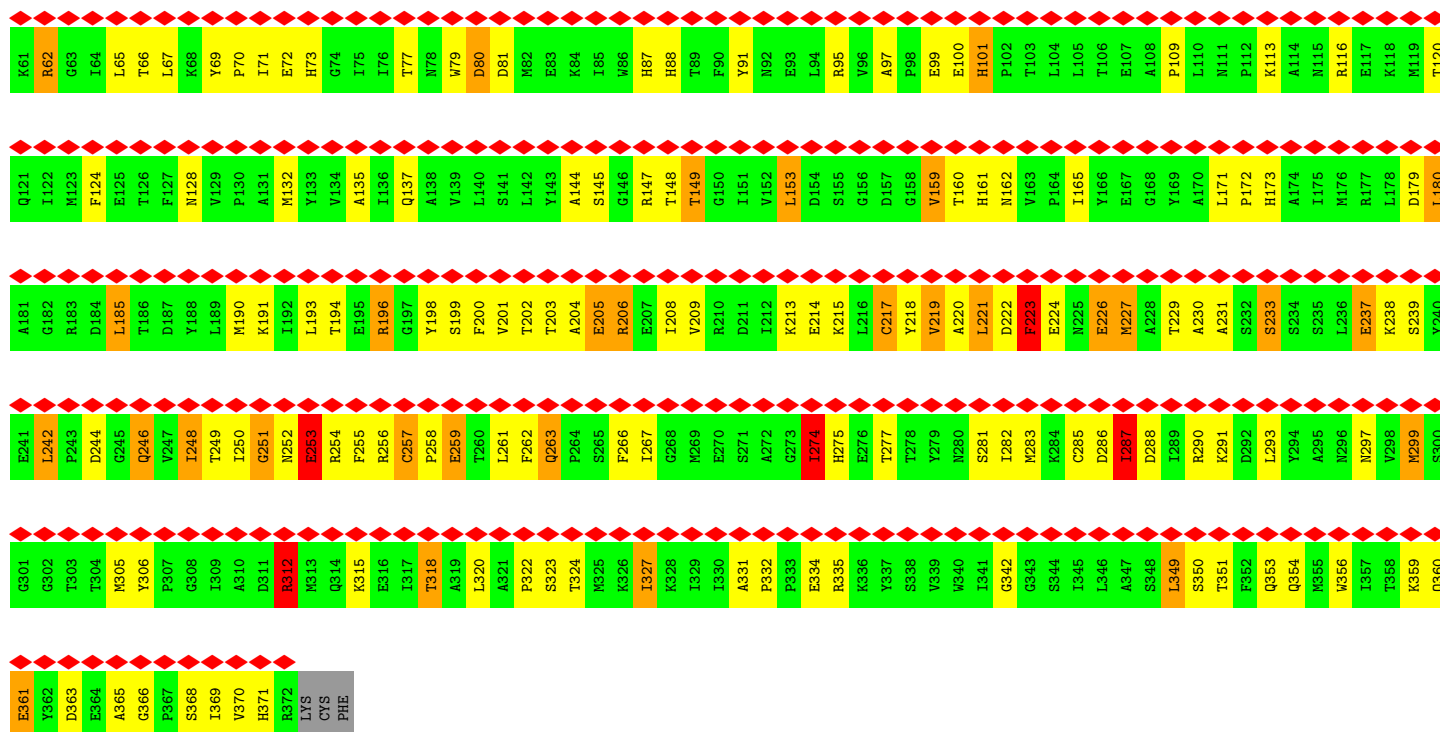


• Molecule 4: SKELETAL MUSCLE ACTIN

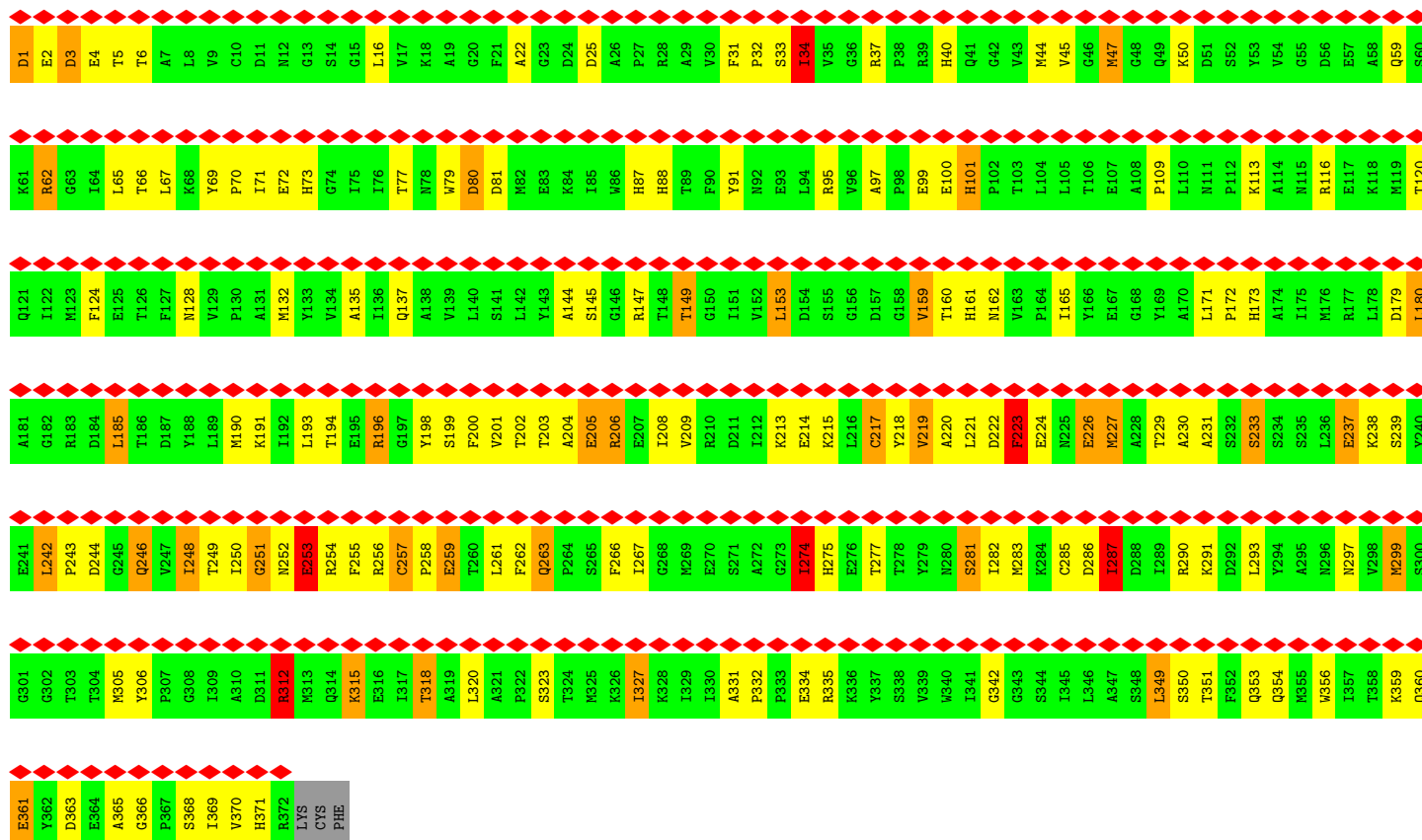


• Molecule 4: SKELETAL MUSCLE ACTIN

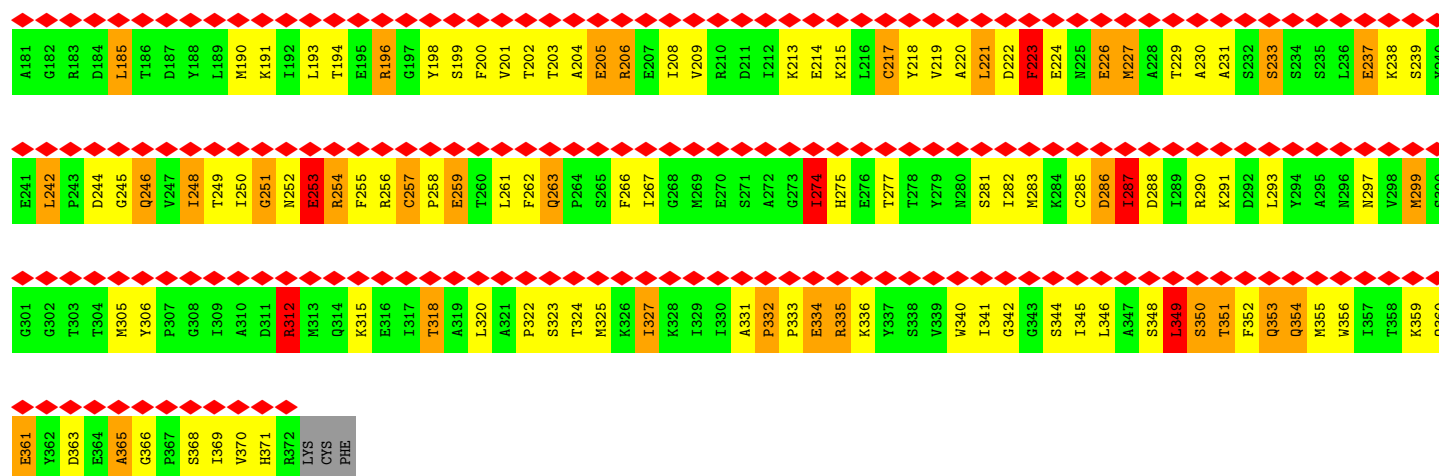




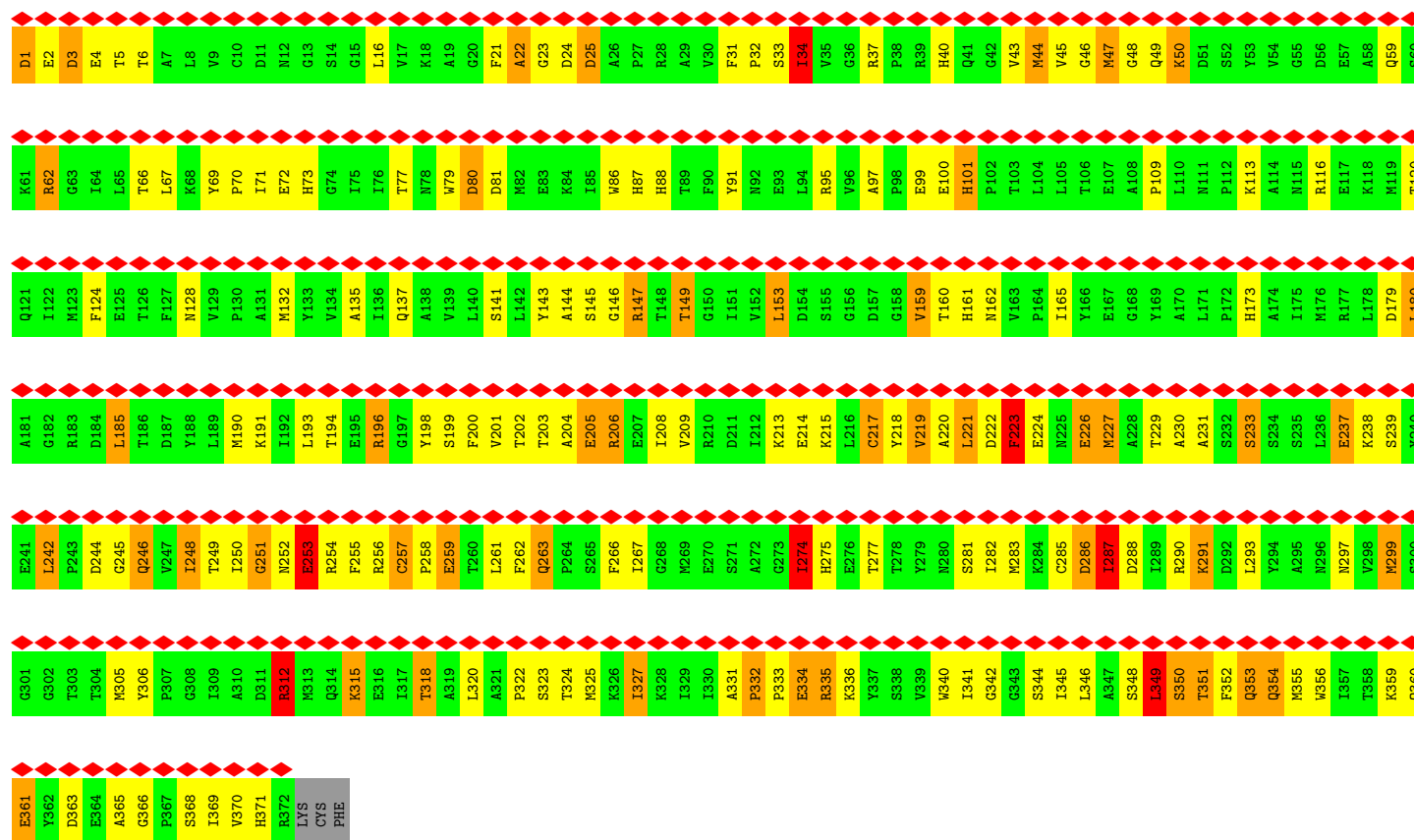
● Molecule 4: SKELETAL MUSCLE ACTIN





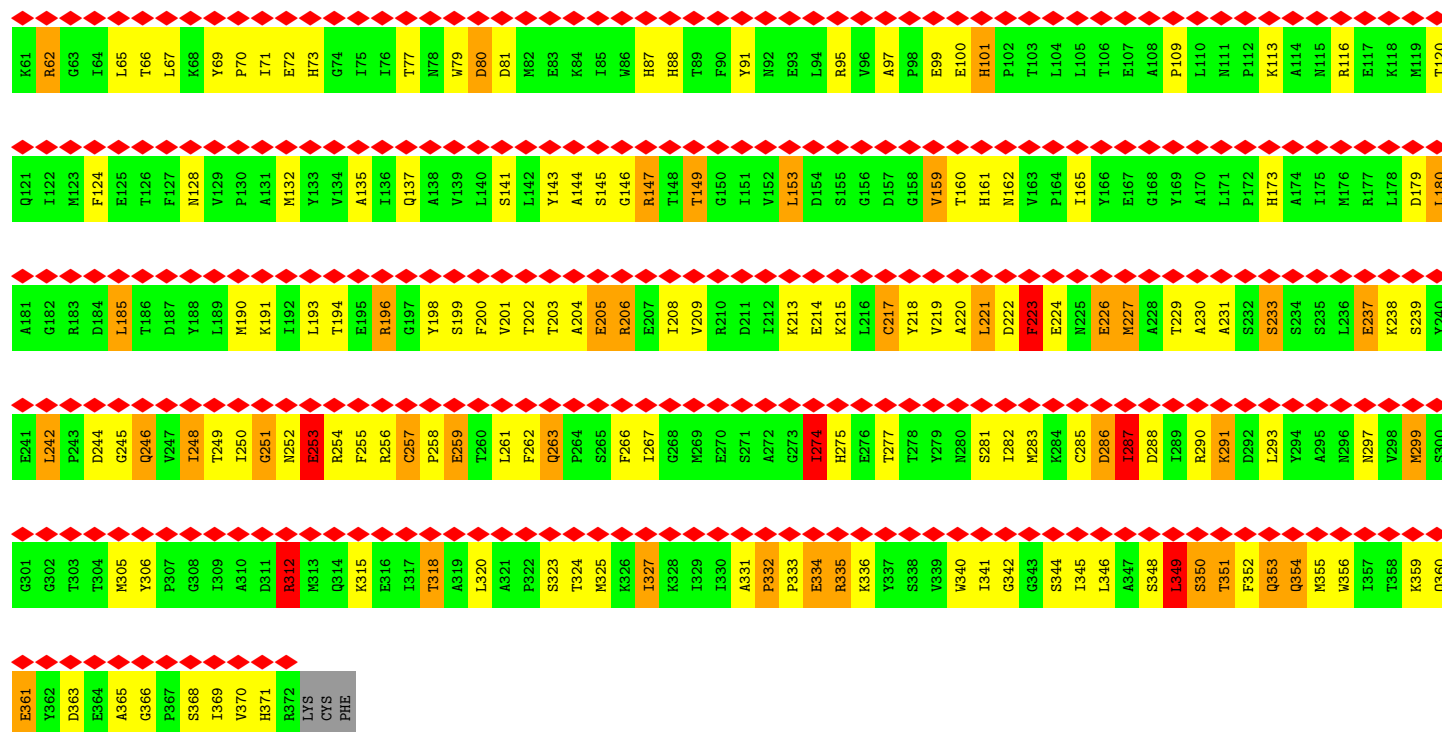


• Molecule 4: SKELETAL MUSCLE ACTIN

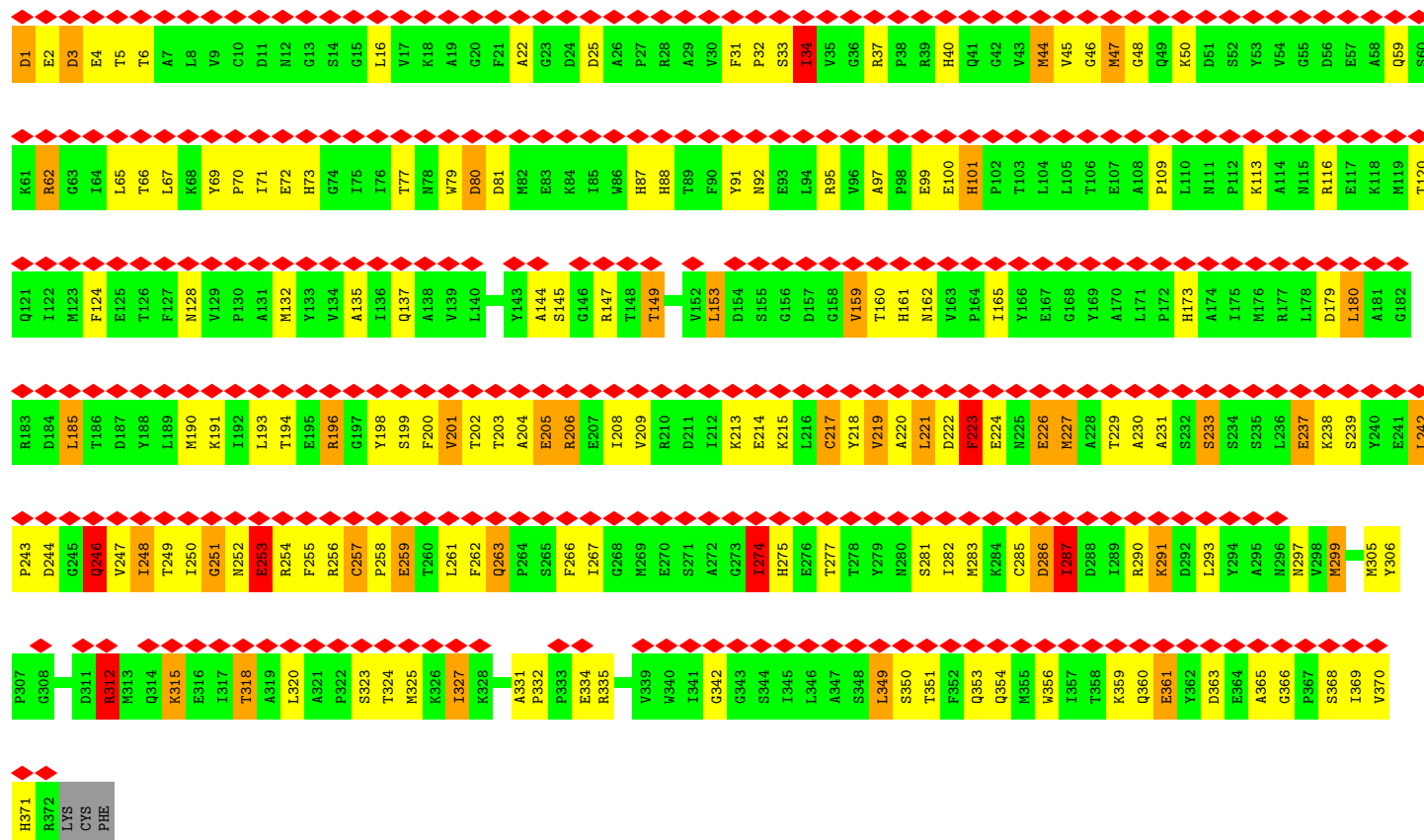
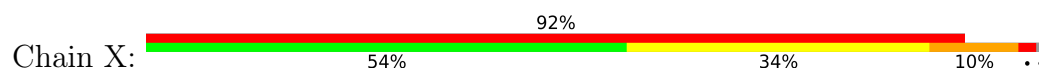


• Molecule 4: SKELETAL MUSCLE ACTIN





● Molecule 4: SKELETAL MUSCLE ACTIN





4 Experimental information

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.85	42/6448 (0.7%)	2.12	150/8729 (1.7%)
1	D	1.85	39/6448 (0.6%)	2.13	150/8729 (1.7%)
1	G	1.86	42/6449 (0.7%)	2.13	160/8732 (1.8%)
1	J	1.86	43/6449 (0.7%)	2.23	149/8732 (1.7%)
1	M	1.86	44/6446 (0.7%)	2.14	151/8723 (1.7%)
1	P	2.00	45/6448 (0.7%)	2.20	156/8729 (1.8%)
2	B	1.36	16/1148 (1.4%)	1.47	21/1548 (1.4%)
2	E	1.37	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	15/1148 (1.3%)	1.47	21/1548 (1.4%)
3	C	0.88	4/1136 (0.4%)	1.18	6/1525 (0.4%)
3	F	0.88	4/1136 (0.4%)	1.18	5/1525 (0.3%)
3	I	0.88	4/1136 (0.4%)	1.18	5/1525 (0.3%)
3	L	0.87	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	0	1.17	13/2968 (0.4%)	2.00	100/4023 (2.5%)
4	1	1.17	13/2968 (0.4%)	2.00	99/4023 (2.5%)
4	2	1.17	13/2968 (0.4%)	2.00	100/4023 (2.5%)
4	3	1.17	13/2968 (0.4%)	2.00	98/4023 (2.4%)
4	4	1.17	13/2968 (0.4%)	2.00	100/4023 (2.5%)
4	5	1.17	13/2968 (0.4%)	2.00	100/4023 (2.5%)
4	7	1.17	13/2968 (0.4%)	2.00	98/4023 (2.4%)
4	8	1.17	13/2968 (0.4%)	2.00	100/4023 (2.5%)
4	9	1.17	12/2968 (0.4%)	2.00	100/4023 (2.5%)
4	V	1.17	12/2968 (0.4%)	2.00	99/4023 (2.5%)
4	W	1.17	13/2968 (0.4%)	2.00	99/4023 (2.5%)
4	X	1.17	13/2968 (0.4%)	2.00	96/4023 (2.4%)
4	Y	1.17	13/2968 (0.4%)	2.00	100/4023 (2.5%)
4	Z	1.17	12/2968 (0.4%)	2.00	101/4023 (2.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	1.50	552/93944 (0.6%)	1.99	2464/127134 (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	1	4
1	J	1	6
1	M	1	6
1	P	1	6
2	B	0	3
2	E	0	3
2	H	0	3
2	K	0	3
2	N	0	3
2	Q	0	3
3	C	0	2
3	F	0	2
3	I	0	2
3	L	0	2
3	O	0	2
3	R	0	2
4	0	0	1
4	1	0	1
4	2	0	1
4	3	0	1
4	4	0	1
4	5	0	1
4	7	0	1
4	8	0	1
4	9	0	1
4	V	0	1
4	W	0	1
4	X	0	1
4	Y	0	1
4	Z	0	1
All	All	6	74

The worst 5 of 552 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	786	ILE	C-N	46.74	1.89	1.33
1	A	648	THR	CB-OG1	42.69	2.12	1.43
1	D	648	THR	CB-OG1	42.67	2.12	1.43
1	G	648	THR	CB-OG1	42.63	2.12	1.43
1	P	648	THR	CB-OG1	42.63	2.12	1.43

The worst 5 of 2464 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	637	LYS	O-C-N	-74.33	23.73	122.59
1	D	637	LYS	O-C-N	-74.28	23.79	122.59
1	M	637	LYS	O-C-N	-74.28	23.80	122.59
1	J	637	LYS	O-C-N	-74.26	23.83	122.59
1	P	637	LYS	O-C-N	-74.25	23.83	122.59

5 of 6 chirality outliers are listed below:

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

5 of 74 planarity outliers are listed below:

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

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6797	0	6761	1573	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	6797	0	6766	1539	0
1	G	6797	0	6772	1573	0
1	J	6797	0	6768	1479	0
1	M	6797	0	6774	1543	0
1	P	6797	0	6774	1525	0
2	B	1127	0	1085	231	0
2	E	1127	0	1085	252	0
2	H	1127	0	1087	277	0
2	K	1127	0	1088	283	0
2	N	1127	0	1088	246	0
2	Q	1127	0	1088	263	0
3	C	1123	0	1083	201	0
3	F	1123	0	1084	196	0
3	I	1123	0	1082	211	0
3	L	1123	0	1083	171	0
3	O	1123	0	1084	155	0
3	R	1123	0	1084	238	0
4	0	2906	0	2855	409	0
4	1	2906	0	2858	259	0
4	2	2906	0	2864	177	0
4	3	2906	0	2863	180	0
4	4	2906	0	2865	98	0
4	5	2906	0	2865	99	0
4	7	2906	0	2866	85	0
4	8	2906	0	2857	322	0
4	9	2906	0	2855	349	0
4	V	2906	0	2851	398	0
4	W	2906	0	2851	388	0
4	X	2906	0	2862	212	0
4	Y	2906	0	2863	173	0
4	Z	2906	0	2853	412	0
All	All	94966	0	93664	11693	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 62.

The worst 5 of 11693 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:797:PHE:CE2	3:F:126:LEU:HD22	1.31	1.66
1:J:797:PHE:CE1	3:L:146:ILE:HG23	1.26	1.66

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

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	789/840 (94%)	651 (82%)	112 (14%)	26 (3%)	3	21
1	D	789/840 (94%)	651 (82%)	112 (14%)	26 (3%)	3	21
1	G	791/840 (94%)	652 (82%)	112 (14%)	27 (3%)	3	21
1	J	791/840 (94%)	652 (82%)	112 (14%)	27 (3%)	3	21
1	M	786/840 (94%)	649 (83%)	111 (14%)	26 (3%)	3	21
1	P	789/840 (94%)	649 (82%)	114 (14%)	26 (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	0	370/375 (99%)	333 (90%)	31 (8%)	6 (2%)	7	38
4	1	370/375 (99%)	335 (90%)	29 (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%)	334 (90%)	30 (8%)	6 (2%)	7	38
4	5	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	7	38
4	7	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	7	38
4	8	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	7	38
4	9	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	7	38
4	V	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	7	38
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%)	334 (90%)	30 (8%)	6 (2%)	7	38
4	Z	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	7	38
All	All	11631/12042 (97%)	10138 (87%)	1203 (10%)	290 (2%)	6	26

5 of 290 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	672/672 (100%)	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%)	490 (73%)	182 (27%)	0	3
1	P	672/672 (100%)	490 (73%)	182 (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%)	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
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	0	315/318 (99%)	264 (84%)	51 (16%)	2	11
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	7	315/318 (99%)	265 (84%)	50 (16%)	2	11
4	8	315/318 (99%)	264 (84%)	51 (16%)	2	11
4	9	315/318 (99%)	264 (84%)	51 (16%)	2	11
4	V	315/318 (99%)	265 (84%)	50 (16%)	2	11
4	W	315/318 (99%)	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%)	8039 (82%)	1825 (18%)	3 8

5 of 1825 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	O	96	LYS
4	Y	368	SER
4	O	291	LYS
4	Y	283	MET
4	V	274	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 282 such sidechains are listed below:

Mol	Chain	Res	Type
4	7	41	GLN
4	8	78	ASN
4	W	263	GLN
3	I	81	GLN
1	G	791	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	M	348	1	9,10,11	0.76	0	6,11,13	0.47	0
1	MLY	G	504	1	9,10,11	0.88	0	6,11,13	0.22	0
1	MLY	G	59	1	9,10,11	0.82	0	6,11,13	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	G	768	1	9,10,11	0.73	0	6,11,13	0.42	0
1	MLY	A	49	1	9,10,11	0.96	1 (11%)	6,11,13	0.74	0
1	MLY	M	107	1	9,10,11	0.49	0	6,11,13	0.33	0
1	MLY	P	598	1	9,10,11	0.82	0	6,11,13	0.42	0
1	MLY	G	130	1	9,10,11	0.78	0	6,11,13	0.74	0
1	MLY	P	833	1	9,10,11	1.13	1 (11%)	6,11,13	0.31	0
1	MLY	D	613	1	9,10,11	0.57	0	6,11,13	0.61	0
1	MLY	D	353	1	9,10,11	0.85	0	6,11,13	0.81	0
1	MLY	P	49	1	9,10,11	1.02	1 (11%)	6,11,13	0.75	0
1	MLY	M	431	1	9,10,11	0.52	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	385	1	9,10,11	0.91	1 (11%)	6,11,13	0.46	0
1	MLY	A	436	1	9,10,11	0.96	1 (11%)	6,11,13	0.48	0
1	MLY	G	659	1	9,10,11	0.85	1 (11%)	6,11,13	0.59	0
1	MLY	A	431	1	9,10,11	0.52	0	6,11,13	0.45	0
1	MLY	G	353	1	9,10,11	0.86	0	6,11,13	0.81	0
1	MLY	M	84	1	9,10,11	0.51	0	6,11,13	0.81	0
1	MLY	M	138	1	9,10,11	1.21	1 (11%)	6,11,13	0.81	0
1	MLY	M	827	1	9,10,11	0.69	0	6,11,13	0.48	0
1	MLY	G	782	1	9,10,11	0.80	0	6,11,13	0.36	0
1	MLY	P	613	1	9,10,11	0.57	0	6,11,13	0.62	0
1	MLY	M	385	1	9,10,11	0.94	1 (11%)	6,11,13	0.45	0
1	MLY	D	551	1	9,10,11	0.53	0	6,11,13	0.20	0
1	MLY	M	613	1	9,10,11	0.56	0	6,11,13	0.61	0
1	MLY	J	598	1	9,10,11	0.81	0	6,11,13	0.41	0
1	MLY	P	296	1	9,10,11	0.64	0	6,11,13	0.35	0
1	MLY	J	130	1	9,10,11	0.75	0	6,11,13	0.73	0
1	MLY	G	553	1,4	9,10,11	0.64	0	6,11,13	0.55	0
1	MLY	D	659	1	9,10,11	0.83	1 (11%)	6,11,13	0.60	0
1	MLY	G	63	1	9,10,11	0.86	0	6,11,13	0.43	0
1	MLY	P	617	1	9,10,11	0.92	0	6,11,13	0.34	0
1	MLY	M	87	1	9,10,11	1.13	1 (11%)	6,11,13	0.43	0
1	MLY	D	782	1	9,10,11	0.80	0	6,11,13	0.35	0
1	MLY	D	30	1	9,10,11	0.93	0	6,11,13	0.31	0
1	MLY	A	385	1	9,10,11	0.92	1 (11%)	6,11,13	0.44	0
1	MLY	G	367	1	9,10,11	0.62	0	6,11,13	0.38	0
1	MLY	M	296	1	9,10,11	0.66	0	6,11,13	0.35	0
1	MLY	M	833	1	9,10,11	1.16	2 (22%)	6,11,13	0.31	0
1	MLY	M	528	1	9,10,11	0.89	0	6,11,13	0.65	0
1	MLY	P	385	1	9,10,11	0.94	1 (11%)	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	D	837	1	9,10,11	0.60	0	6,11,13	0.58	0
1	MLY	G	30	1	9,10,11	0.90	0	6,11,13	0.30	0
1	MLY	J	295	1	9,10,11	0.76	0	6,11,13	0.37	0
1	MLY	P	35	1	9,10,11	0.73	0	6,11,13	0.38	0
1	MLY	P	505	1	9,10,11	0.84	0	6,11,13	0.34	0
1	MLY	G	600	1	9,10,11	0.52	0	6,11,13	0.38	0
1	MLY	M	681	1	9,10,11	0.55	0	6,11,13	0.45	0
1	MLY	P	248	1	9,10,11	0.80	0	6,11,13	0.65	0
1	MLY	M	598	1	9,10,11	0.80	0	6,11,13	0.41	0
1	MLY	A	486	1	9,10,11	0.67	0	6,11,13	0.40	0
1	MLY	P	837	1	9,10,11	0.57	0	6,11,13	0.56	0
1	MLY	M	839	1	9,10,11	0.66	0	6,11,13	0.78	0
1	MLY	J	839	1	9,10,11	0.67	0	6,11,13	0.77	0
1	MLY	P	87	1	9,10,11	1.15	1 (11%)	6,11,13	0.43	0
1	MLY	P	551	1	9,10,11	0.53	0	6,11,13	0.20	0
1	MLY	M	63	1	9,10,11	0.88	0	6,11,13	0.45	0
1	MLY	P	827	1	9,10,11	0.70	0	6,11,13	0.48	0
1	MLY	G	272	1	9,10,11	0.87	1 (11%)	6,11,13	0.55	0
1	MLY	J	504	1	9,10,11	0.84	0	6,11,13	0.22	0
1	MLY	G	436	1	9,10,11	0.93	1 (11%)	6,11,13	0.47	0
1	MLY	J	837	1	9,10,11	0.59	0	6,11,13	0.56	0
1	MLY	M	553	1,4	9,10,11	0.65	0	6,11,13	0.54	0
1	MLY	A	551	1	9,10,11	0.51	0	6,11,13	0.18	0
1	MLY	G	431	1	9,10,11	0.52	0	6,11,13	0.46	0
1	MLY	P	764	1	9,10,11	0.80	0	6,11,13	0.38	0
1	MLY	A	84	1	9,10,11	0.51	0	6,11,13	0.80	0
1	MLY	A	369	1	9,10,11	0.72	0	6,11,13	0.46	0
1	MLY	D	827	1	9,10,11	0.66	0	6,11,13	0.47	0
1	MLY	M	295	1	9,10,11	0.77	0	6,11,13	0.37	0
1	MLY	A	768	1	9,10,11	0.77	0	6,11,13	0.41	0
1	MLY	M	49	1	9,10,11	1.00	1 (11%)	6,11,13	0.74	0
1	MLY	A	130	1	9,10,11	0.79	0	6,11,13	0.73	0
1	MLY	G	827	1	9,10,11	0.68	0	6,11,13	0.48	0
1	MLY	A	296	1	9,10,11	0.60	0	6,11,13	0.36	0
1	MLY	D	505	1	9,10,11	0.79	0	6,11,13	0.34	0
1	MLY	J	19	1	9,10,11	1.07	1 (11%)	6,11,13	0.58	0
1	MLY	J	827	1	9,10,11	0.72	0	6,11,13	0.47	0
1	MLY	D	130	1	9,10,11	0.80	0	6,11,13	0.72	0
1	MLY	A	600	1	9,10,11	0.52	0	6,11,13	0.39	0
1	MLY	D	107	1	9,10,11	0.52	0	6,11,13	0.33	0
1	MLY	M	764	1	9,10,11	0.81	0	6,11,13	0.37	0
1	MLY	M	837	1	9,10,11	0.58	0	6,11,13	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	A	295	1	9,10,11	0.77	0	6,11,13	0.34	0
1	MLY	P	553	1	9,10,11	0.65	0	6,11,13	0.54	0
1	MLY	A	782	1	9,10,11	0.81	0	6,11,13	0.37	0
1	MLY	J	764	1	9,10,11	0.81	0	6,11,13	0.37	0
1	MLY	J	768	1	9,10,11	0.77	0	6,11,13	0.42	0
1	MLY	M	505	1	9,10,11	0.85	1 (11%)	6,11,13	0.34	0
1	MLY	G	348	1	9,10,11	0.80	0	6,11,13	0.46	0
1	MLY	D	504	1	9,10,11	0.88	0	6,11,13	0.21	0
1	MLY	J	617	1	9,10,11	0.91	0	6,11,13	0.33	0
1	MLY	M	248	1	9,10,11	0.80	0	6,11,13	0.66	0
1	MLY	D	600	1	9,10,11	0.52	0	6,11,13	0.39	0
1	MLY	A	553	1,4	9,10,11	0.64	0	6,11,13	0.55	0
1	MLY	J	436	1	9,10,11	0.96	1 (11%)	6,11,13	0.47	0
1	MLY	J	505	1	9,10,11	0.85	1 (11%)	6,11,13	0.34	0
1	MLY	G	486	1	9,10,11	0.66	0	6,11,13	0.40	0
1	MLY	G	598	1	9,10,11	0.83	0	6,11,13	0.41	0
1	MLY	A	504	1	9,10,11	0.86	0	6,11,13	0.23	0
1	MLY	A	59	1	9,10,11	0.84	0	6,11,13	0.47	0
1	MLY	A	837	1	9,10,11	0.59	0	6,11,13	0.54	0
1	MLY	D	19	1	9,10,11	1.06	1 (11%)	6,11,13	0.57	0
1	MLY	D	764	1	9,10,11	0.82	0	6,11,13	0.35	0
1	MLY	J	296	1	9,10,11	0.65	0	6,11,13	0.36	0
1	MLY	P	839	1	9,10,11	0.67	0	6,11,13	0.78	0
1	MLY	A	272	1	9,10,11	0.90	1 (11%)	6,11,13	0.56	0
1	MLY	A	87	1	9,10,11	1.13	1 (11%)	6,11,13	0.41	0
1	MLY	J	353	1	9,10,11	0.86	0	6,11,13	0.79	0
1	MLY	D	617	1	9,10,11	0.93	1 (11%)	6,11,13	0.35	0
1	MLY	D	87	1	9,10,11	1.10	1 (11%)	6,11,13	0.44	0
1	MLY	P	19	1	9,10,11	1.06	1 (11%)	6,11,13	0.58	0
1	MLY	G	236	1	9,10,11	0.82	1 (11%)	6,11,13	0.47	0
1	MLY	P	107	1	9,10,11	0.49	0	6,11,13	0.34	0
1	MLY	G	84	1	9,10,11	0.49	0	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	M	617	1	9,10,11	0.90	0	6,11,13	0.34	0
1	MLY	P	369	1	9,10,11	0.71	0	6,11,13	0.46	0
1	MLY	D	486	1	9,10,11	0.67	0	6,11,13	0.40	0
1	MLY	P	295	1	9,10,11	0.77	0	6,11,13	0.36	0
1	MLY	J	272	1	9,10,11	0.90	1 (11%)	6,11,13	0.56	0
1	MLY	J	348	1	9,10,11	0.75	0	6,11,13	0.47	0
1	MLY	G	49	1	9,10,11	0.98	1 (11%)	6,11,13	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	G	613	1	9,10,11	0.59	0	6,11,13	0.61	0
1	MLY	M	551	1	9,10,11	0.52	0	6,11,13	0.19	0
1	MLY	D	59	1	9,10,11	0.84	0	6,11,13	0.47	0
1	MLY	J	59	1	9,10,11	0.85	0	6,11,13	0.47	0
1	MLY	P	600	1	9,10,11	0.53	0	6,11,13	0.38	0
1	MLY	A	348	1	9,10,11	0.81	0	6,11,13	0.48	0
1	MLY	D	431	1	9,10,11	0.53	0	6,11,13	0.46	0
1	MLY	G	296	1	9,10,11	0.61	0	6,11,13	0.36	0
1	MLY	J	553	1	9,10,11	0.65	0	6,11,13	0.54	0
1	MLY	J	551	1	9,10,11	0.53	0	6,11,13	0.19	0
1	MLY	M	272	1	9,10,11	0.90	1 (11%)	6,11,13	0.56	0
1	MLY	P	138	1	9,10,11	1.21	1 (11%)	6,11,13	0.82	0
1	MLY	D	236	1	9,10,11	0.83	1 (11%)	6,11,13	0.47	0
1	MLY	D	138	1	9,10,11	1.25	1 (11%)	6,11,13	0.84	0
1	MLY	D	833	1	9,10,11	1.12	1 (11%)	6,11,13	0.30	0
1	MLY	P	190	1	9,10,11	1.21	2 (22%)	6,11,13	0.53	0
1	MLY	J	659	1	9,10,11	0.82	1 (11%)	6,11,13	0.58	0
1	MLY	M	59	1	9,10,11	0.85	0	6,11,13	0.47	0
1	MLY	A	528	1	9,10,11	0.88	0	6,11,13	0.66	0
1	MLY	G	55	1	9,10,11	0.74	0	6,11,13	0.81	0
1	MLY	G	833	1	9,10,11	1.13	1 (11%)	6,11,13	0.32	0
1	MLY	G	190	1	9,10,11	1.20	2 (22%)	6,11,13	0.52	0
1	MLY	G	528	1	9,10,11	0.90	0	6,11,13	0.66	0
1	MLY	P	782	1	9,10,11	0.80	0	6,11,13	0.38	0
1	MLY	D	839	1	9,10,11	0.65	0	6,11,13	0.80	0
1	MLY	G	505	1	9,10,11	0.83	0	6,11,13	0.35	0
1	MLY	M	367	1	9,10,11	0.59	0	6,11,13	0.36	0
1	MLY	G	35	1	9,10,11	0.74	0	6,11,13	0.39	0
1	MLY	M	19	1	9,10,11	1.05	1 (11%)	6,11,13	0.59	0
1	MLY	D	768	1	9,10,11	0.74	0	6,11,13	0.41	0
1	MLY	G	248	1	9,10,11	0.78	0	6,11,13	0.66	0
1	MLY	P	681	1	9,10,11	0.58	0	6,11,13	0.46	0
1	MLY	A	598	1	9,10,11	0.83	0	6,11,13	0.43	0
1	MLY	A	353	1	9,10,11	0.88	0	6,11,13	0.80	0
1	MLY	P	59	1	9,10,11	0.85	0	6,11,13	0.47	0
1	MLY	D	272	1	9,10,11	0.87	1 (11%)	6,11,13	0.58	0
1	MLY	D	348	1	9,10,11	0.78	0	6,11,13	0.47	0
1	MLY	P	504	1	9,10,11	0.83	0	6,11,13	0.22	0
1	MLY	J	248	1	9,10,11	0.80	0	6,11,13	0.66	0
1	MLY	D	369	1	9,10,11	0.70	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	839	1	9,10,11	0.65	0	6,11,13	0.82	0
1	MLY	J	369	1	9,10,11	0.71	0	6,11,13	0.45	0
1	MLY	M	35	1	9,10,11	0.73	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	M	504	1	9,10,11	0.84	0	6,11,13	0.22	0
1	MLY	M	768	1	9,10,11	0.76	0	6,11,13	0.42	0
1	MLY	P	431	1	9,10,11	0.50	0	6,11,13	0.45	0
1	MLY	A	367	1	9,10,11	0.60	0	6,11,13	0.36	0
1	MLY	D	35	1	9,10,11	0.73	0	6,11,13	0.37	0
1	MLY	M	436	1	9,10,11	0.97	1 (11%)	6,11,13	0.47	0
1	MLY	A	19	1	9,10,11	1.01	1 (11%)	6,11,13	0.57	0
1	MLY	A	764	1	9,10,11	0.81	0	6,11,13	0.36	0
1	MLY	P	236	1	9,10,11	0.84	1 (11%)	6,11,13	0.48	0
1	MLY	D	367	1	9,10,11	0.57	0	6,11,13	0.39	0
1	MLY	A	107	1	9,10,11	0.47	0	6,11,13	0.33	0
1	MLY	J	190	1	9,10,11	1.22	2 (22%)	6,11,13	0.53	0
1	MLY	M	369	1	9,10,11	0.71	0	6,11,13	0.46	0
1	MLY	P	659	1	9,10,11	0.83	0	6,11,13	0.58	0
1	MLY	P	436	1	9,10,11	0.97	1 (11%)	6,11,13	0.48	0
1	MLY	P	353	1	9,10,11	0.86	0	6,11,13	0.79	0
1	MLY	P	84	1	9,10,11	0.51	0	6,11,13	0.80	0
1	MLY	A	827	1	9,10,11	0.68	0	6,11,13	0.45	0
1	MLY	P	768	1	9,10,11	0.78	0	6,11,13	0.41	0
1	MLY	G	385	1	9,10,11	0.93	1 (11%)	6,11,13	0.45	0
1	MLY	M	353	1	9,10,11	0.86	0	6,11,13	0.80	0
1	MLY	J	30	1	9,10,11	0.90	0	6,11,13	0.31	0
1	MLY	P	415	1	9,10,11	0.75	0	6,11,13	0.19	0
1	MLY	J	600	1	9,10,11	0.54	0	6,11,13	0.38	0
1	MLY	J	782	1	9,10,11	0.81	0	6,11,13	0.37	0
1	MLY	P	272	1	9,10,11	0.91	1 (11%)	6,11,13	0.55	0
1	MLY	J	49	1	9,10,11	0.99	1 (11%)	6,11,13	0.74	0
1	MLY	M	415	1	9,10,11	0.76	0	6,11,13	0.19	0
1	MLY	D	436	1	9,10,11	1.00	1 (11%)	6,11,13	0.48	0
1	MLY	G	551	1	9,10,11	0.52	0	6,11,13	0.19	0
1	MLY	A	55	1	9,10,11	0.72	0	6,11,13	0.80	0
1	MLY	D	296	1	9,10,11	0.62	0	6,11,13	0.36	0
1	MLY	J	107	1	9,10,11	0.49	0	6,11,13	0.32	0
1	MLY	P	63	1	9,10,11	0.86	0	6,11,13	0.44	0
1	MLY	A	505	1	9,10,11	0.83	0	6,11,13	0.33	0
1	MLY	G	87	1	9,10,11	1.12	1 (11%)	6,11,13	0.43	0
1	MLY	J	486	1	9,10,11	0.66	0	6,11,13	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	M	782	1	9,10,11	0.81	0	6,11,13	0.38	0
1	MLY	A	35	1	9,10,11	0.73	0	6,11,13	0.38	0
1	MLY	M	130	1	9,10,11	0.77	0	6,11,13	0.73	0
1	MLY	D	598	1	9,10,11	0.84	0	6,11,13	0.42	0
1	MLY	D	55	1	9,10,11	0.72	0	6,11,13	0.81	0
1	MLY	A	248	1	9,10,11	0.81	0	6,11,13	0.65	0
1	MLY	J	833	1	9,10,11	1.14	1 (11%)	6,11,13	0.31	0
1	MLY	J	431	1	9,10,11	0.50	0	6,11,13	0.45	0
1	MLY	D	190	1	9,10,11	1.18	2 (22%)	6,11,13	0.54	0
1	MLY	M	236	1	9,10,11	0.85	1 (11%)	6,11,13	0.47	0
1	MLY	M	30	1	9,10,11	0.92	0	6,11,13	0.31	0
1	MLY	M	659	1	9,10,11	0.83	1 (11%)	6,11,13	0.58	0
1	MLY	M	486	1	9,10,11	0.65	0	6,11,13	0.40	0
1	MLY	P	348	1	9,10,11	0.78	0	6,11,13	0.47	0
1	MLY	D	553	1,4	9,10,11	0.66	0	6,11,13	0.55	0
1	MLY	G	839	1	9,10,11	0.68	0	6,11,13	0.80	0
1	MLY	J	138	1	9,10,11	1.21	1 (11%)	6,11,13	0.82	0
1	MLY	G	415	1	9,10,11	0.75	0	6,11,13	0.19	0
1	MLY	J	84	1	9,10,11	0.50	0	6,11,13	0.81	0
1	MLY	J	236	1	9,10,11	0.83	1 (11%)	6,11,13	0.48	0
1	MLY	M	55	1	9,10,11	0.74	0	6,11,13	0.80	0
1	MLY	J	385	1	9,10,11	0.94	1 (11%)	6,11,13	0.45	0
1	MLY	G	19	1	9,10,11	1.04	1 (11%)	6,11,13	0.59	0
1	MLY	G	764	1	9,10,11	0.78	0	6,11,13	0.35	0
1	MLY	D	295	1	9,10,11	0.74	0	6,11,13	0.38	0
1	MLY	D	528	1	9,10,11	0.91	0	6,11,13	0.65	0
1	MLY	G	107	1	9,10,11	0.48	0	6,11,13	0.33	0
1	MLY	D	415	1	9,10,11	0.75	0	6,11,13	0.19	0
1	MLY	G	617	1	9,10,11	0.90	0	6,11,13	0.35	0
1	MLY	D	49	1	9,10,11	0.99	1 (11%)	6,11,13	0.75	0
1	MLY	A	617	1	9,10,11	0.89	0	6,11,13	0.34	0
1	MLY	J	55	1	9,10,11	0.72	0	6,11,13	0.80	0
1	MLY	J	367	1	9,10,11	0.59	0	6,11,13	0.36	0
1	MLY	J	613	1	9,10,11	0.57	0	6,11,13	0.62	0
1	MLY	P	130	1	9,10,11	0.76	0	6,11,13	0.73	0
1	MLY	A	30	1	9,10,11	0.90	0	6,11,13	0.32	0
1	MLY	A	659	1	9,10,11	0.83	1 (11%)	6,11,13	0.60	0
1	MLY	G	369	1	9,10,11	0.71	0	6,11,13	0.46	0
1	MLY	D	681	1	9,10,11	0.55	0	6,11,13	0.46	0
1	MLY	J	681	1	9,10,11	0.56	0	6,11,13	0.46	0
1	MLY	A	613	1	9,10,11	0.58	0	6,11,13	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	J	87	1	9,10,11	1.13	1 (11%)	6,11,13	0.43	0
1	MLY	D	63	1	9,10,11	0.87	0	6,11,13	0.46	0
1	MLY	P	55	1	9,10,11	0.73	0	6,11,13	0.80	0
1	MLY	G	681	1	9,10,11	0.60	0	6,11,13	0.45	0
1	MLY	J	528	1	9,10,11	0.89	0	6,11,13	0.66	0
1	MLY	A	681	1	9,10,11	0.57	0	6,11,13	0.46	0
1	MLY	G	138	1	9,10,11	1.23	1 (11%)	6,11,13	0.82	0
1	MLY	M	190	1	9,10,11	1.21	2 (22%)	6,11,13	0.53	0
1	MLY	G	295	1	9,10,11	0.76	0	6,11,13	0.36	0
1	MLY	G	837	1	9,10,11	0.59	0	6,11,13	0.52	0
1	MLY	P	30	1	9,10,11	0.91	0	6,11,13	0.31	0
1	MLY	A	190	1	9,10,11	1.22	2 (22%)	6,11,13	0.52	0
1	MLY	A	833	1	9,10,11	1.12	1 (11%)	6,11,13	0.31	0
1	MLY	A	63	1	9,10,11	0.88	0	6,11,13	0.45	0
1	MLY	D	84	1	9,10,11	0.51	0	6,11,13	0.81	0
1	MLY	D	248	1	9,10,11	0.81	0	6,11,13	0.66	0
1	MLY	P	486	1	9,10,11	0.66	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	J	63	1	9,10,11	0.87	0	6,11,13	0.44	0
1	MLY	M	600	1	9,10,11	0.53	0	6,11,13	0.38	0
1	MLY	J	35	1	9,10,11	0.73	0	6,11,13	0.39	0
1	MLY	A	138	1	9,10,11	1.20	1 (11%)	6,11,13	0.82	0
1	MLY	A	236	1	9,10,11	0.83	1 (11%)	6,11,13	0.48	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	M	348	1	-	5/8/9/11	-
1	MLY	G	504	1	-	4/8/9/11	-
1	MLY	G	59	1	-	3/8/9/11	-
1	MLY	G	768	1	-	4/8/9/11	-
1	MLY	A	49	1	-	3/8/9/11	-
1	MLY	M	107	1	-	2/8/9/11	-
1	MLY	P	598	1	-	5/8/9/11	-
1	MLY	G	130	1	-	5/8/9/11	-
1	MLY	P	833	1	-	6/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	D	613	1	-	3/8/9/11	-
1	MLY	D	353	1	-	4/8/9/11	-
1	MLY	P	49	1	-	3/8/9/11	-
1	MLY	M	431	1	-	4/8/9/11	-
1	MLY	P	367	1	-	2/8/9/11	-
1	MLY	D	385	1	-	2/8/9/11	-
1	MLY	A	436	1	-	4/8/9/11	-
1	MLY	G	659	1	-	3/8/9/11	-
1	MLY	A	431	1	-	4/8/9/11	-
1	MLY	G	353	1	-	4/8/9/11	-
1	MLY	M	84	1	-	4/8/9/11	-
1	MLY	M	138	1	-	4/8/9/11	-
1	MLY	M	827	1	-	1/8/9/11	-
1	MLY	G	782	1	-	6/8/9/11	-
1	MLY	P	613	1	-	3/8/9/11	-
1	MLY	M	385	1	-	2/8/9/11	-
1	MLY	D	551	1	-	3/8/9/11	-
1	MLY	M	613	1	-	3/8/9/11	-
1	MLY	J	598	1	-	5/8/9/11	-
1	MLY	P	296	1	-	4/8/9/11	-
1	MLY	J	130	1	-	5/8/9/11	-
1	MLY	G	553	1,4	-	4/8/9/11	-
1	MLY	D	659	1	-	3/8/9/11	-
1	MLY	G	63	1	-	4/8/9/11	-
1	MLY	P	617	1	-	2/8/9/11	-
1	MLY	M	87	1	-	2/8/9/11	-
1	MLY	D	782	1	-	6/8/9/11	-
1	MLY	D	30	1	-	3/8/9/11	-
1	MLY	A	385	1	-	2/8/9/11	-
1	MLY	G	367	1	-	2/8/9/11	-
1	MLY	M	296	1	-	4/8/9/11	-
1	MLY	M	833	1	-	6/8/9/11	-
1	MLY	M	528	1	-	4/8/9/11	-
1	MLY	P	385	1	-	2/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	D	837	1	-	6/8/9/11	-
1	MLY	G	30	1	-	3/8/9/11	-
1	MLY	J	295	1	-	2/8/9/11	-
1	MLY	P	35	1	-	3/8/9/11	-
1	MLY	P	505	1	-	5/8/9/11	-
1	MLY	G	600	1	-	3/8/9/11	-
1	MLY	M	681	1	-	4/8/9/11	-
1	MLY	P	248	1	-	6/8/9/11	-
1	MLY	M	598	1	-	5/8/9/11	-
1	MLY	A	486	1	-	2/8/9/11	-
1	MLY	P	837	1	-	6/8/9/11	-
1	MLY	M	839	1	-	3/8/9/11	-
1	MLY	J	839	1	-	3/8/9/11	-
1	MLY	P	87	1	-	2/8/9/11	-
1	MLY	P	551	1	-	3/8/9/11	-
1	MLY	M	63	1	-	4/8/9/11	-
1	MLY	P	827	1	-	1/8/9/11	-
1	MLY	G	272	1	-	3/8/9/11	-
1	MLY	J	504	1	-	4/8/9/11	-
1	MLY	G	436	1	-	4/8/9/11	-
1	MLY	J	837	1	-	6/8/9/11	-
1	MLY	M	553	1,4	-	4/8/9/11	-
1	MLY	A	551	1	-	3/8/9/11	-
1	MLY	G	431	1	-	4/8/9/11	-
1	MLY	P	764	1	-	2/8/9/11	-
1	MLY	A	84	1	-	4/8/9/11	-
1	MLY	A	369	1	-	2/8/9/11	-
1	MLY	D	827	1	-	1/8/9/11	-
1	MLY	M	295	1	-	2/8/9/11	-
1	MLY	A	768	1	-	4/8/9/11	-
1	MLY	M	49	1	-	3/8/9/11	-
1	MLY	A	130	1	-	5/8/9/11	-
1	MLY	G	827	1	-	1/8/9/11	-
1	MLY	A	296	1	-	4/8/9/11	-
1	MLY	D	505	1	-	5/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	J	19	1	-	4/8/9/11	-
1	MLY	J	827	1	-	1/8/9/11	-
1	MLY	D	130	1	-	5/8/9/11	-
1	MLY	A	600	1	-	3/8/9/11	-
1	MLY	D	107	1	-	2/8/9/11	-
1	MLY	M	764	1	-	2/8/9/11	-
1	MLY	M	837	1	-	6/8/9/11	-
1	MLY	A	295	1	-	2/8/9/11	-
1	MLY	P	553	1	-	4/8/9/11	-
1	MLY	A	782	1	-	6/8/9/11	-
1	MLY	J	764	1	-	2/8/9/11	-
1	MLY	J	768	1	-	4/8/9/11	-
1	MLY	M	505	1	-	5/8/9/11	-
1	MLY	G	348	1	-	5/8/9/11	-
1	MLY	D	504	1	-	4/8/9/11	-
1	MLY	J	617	1	-	2/8/9/11	-
1	MLY	M	248	1	-	6/8/9/11	-
1	MLY	D	600	1	-	3/8/9/11	-
1	MLY	A	553	1,4	-	4/8/9/11	-
1	MLY	J	436	1	-	4/8/9/11	-
1	MLY	J	505	1	-	5/8/9/11	-
1	MLY	G	486	1	-	2/8/9/11	-
1	MLY	G	598	1	-	5/8/9/11	-
1	MLY	A	504	1	-	4/8/9/11	-
1	MLY	A	59	1	-	3/8/9/11	-
1	MLY	A	837	1	-	6/8/9/11	-
1	MLY	D	19	1	-	4/8/9/11	-
1	MLY	D	764	1	-	2/8/9/11	-
1	MLY	J	296	1	-	4/8/9/11	-
1	MLY	P	839	1	-	3/8/9/11	-
1	MLY	A	272	1	-	3/8/9/11	-
1	MLY	A	87	1	-	2/8/9/11	-
1	MLY	J	353	1	-	4/8/9/11	-
1	MLY	D	617	1	-	2/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	D	87	1	-	2/8/9/11	-
1	MLY	P	19	1	-	4/8/9/11	-
1	MLY	G	236	1	-	3/8/9/11	-
1	MLY	P	107	1	-	2/8/9/11	-
1	MLY	G	84	1	-	4/8/9/11	-
1	MLY	J	415	1	-	3/8/9/11	-
1	MLY	M	617	1	-	2/8/9/11	-
1	MLY	P	369	1	-	2/8/9/11	-
1	MLY	D	486	1	-	2/8/9/11	-
1	MLY	P	295	1	-	2/8/9/11	-
1	MLY	J	272	1	-	3/8/9/11	-
1	MLY	J	348	1	-	5/8/9/11	-
1	MLY	G	49	1	-	3/8/9/11	-
1	MLY	G	613	1	-	3/8/9/11	-
1	MLY	M	551	1	-	3/8/9/11	-
1	MLY	D	59	1	-	3/8/9/11	-
1	MLY	J	59	1	-	3/8/9/11	-
1	MLY	P	600	1	-	3/8/9/11	-
1	MLY	A	348	1	-	5/8/9/11	-
1	MLY	D	431	1	-	4/8/9/11	-
1	MLY	G	296	1	-	4/8/9/11	-
1	MLY	J	553	1	-	4/8/9/11	-
1	MLY	J	551	1	-	3/8/9/11	-
1	MLY	M	272	1	-	3/8/9/11	-
1	MLY	P	138	1	-	4/8/9/11	-
1	MLY	D	236	1	-	3/8/9/11	-
1	MLY	D	138	1	-	4/8/9/11	-
1	MLY	D	833	1	-	6/8/9/11	-
1	MLY	P	190	1	-	4/8/9/11	-
1	MLY	J	659	1	-	3/8/9/11	-
1	MLY	M	59	1	-	3/8/9/11	-
1	MLY	A	528	1	-	4/8/9/11	-
1	MLY	G	55	1	-	6/8/9/11	-
1	MLY	G	833	1	-	6/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	G	190	1	-	4/8/9/11	-
1	MLY	G	528	1	-	4/8/9/11	-
1	MLY	P	782	1	-	6/8/9/11	-
1	MLY	D	839	1	-	3/8/9/11	-
1	MLY	G	505	1	-	5/8/9/11	-
1	MLY	M	367	1	-	2/8/9/11	-
1	MLY	G	35	1	-	3/8/9/11	-
1	MLY	M	19	1	-	4/8/9/11	-
1	MLY	D	768	1	-	4/8/9/11	-
1	MLY	G	248	1	-	6/8/9/11	-
1	MLY	P	681	1	-	4/8/9/11	-
1	MLY	A	598	1	-	5/8/9/11	-
1	MLY	A	353	1	-	4/8/9/11	-
1	MLY	P	59	1	-	3/8/9/11	-
1	MLY	D	272	1	-	3/8/9/11	-
1	MLY	D	348	1	-	5/8/9/11	-
1	MLY	P	504	1	-	4/8/9/11	-
1	MLY	J	248	1	-	6/8/9/11	-
1	MLY	D	369	1	-	2/8/9/11	-
1	MLY	A	839	1	-	3/8/9/11	-
1	MLY	J	369	1	-	2/8/9/11	-
1	MLY	M	35	1	-	3/8/9/11	-
1	MLY	A	415	1	-	3/8/9/11	-
1	MLY	M	504	1	-	4/8/9/11	-
1	MLY	M	768	1	-	4/8/9/11	-
1	MLY	P	431	1	-	4/8/9/11	-
1	MLY	A	367	1	-	2/8/9/11	-
1	MLY	D	35	1	-	3/8/9/11	-
1	MLY	M	436	1	-	4/8/9/11	-
1	MLY	A	19	1	-	4/8/9/11	-
1	MLY	A	764	1	-	2/8/9/11	-
1	MLY	P	236	1	-	3/8/9/11	-
1	MLY	D	367	1	-	2/8/9/11	-
1	MLY	A	107	1	-	2/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	J	190	1	-	4/8/9/11	-
1	MLY	M	369	1	-	2/8/9/11	-
1	MLY	P	659	1	-	3/8/9/11	-
1	MLY	P	436	1	-	4/8/9/11	-
1	MLY	P	353	1	-	4/8/9/11	-
1	MLY	P	84	1	-	4/8/9/11	-
1	MLY	A	827	1	-	1/8/9/11	-
1	MLY	P	768	1	-	4/8/9/11	-
1	MLY	G	385	1	-	2/8/9/11	-
1	MLY	M	353	1	-	4/8/9/11	-
1	MLY	J	30	1	-	3/8/9/11	-
1	MLY	P	415	1	-	3/8/9/11	-
1	MLY	J	600	1	-	3/8/9/11	-
1	MLY	J	782	1	-	6/8/9/11	-
1	MLY	P	272	1	-	3/8/9/11	-
1	MLY	J	49	1	-	3/8/9/11	-
1	MLY	M	415	1	-	3/8/9/11	-
1	MLY	D	436	1	-	4/8/9/11	-
1	MLY	G	551	1	-	3/8/9/11	-
1	MLY	A	55	1	-	6/8/9/11	-
1	MLY	D	296	1	-	4/8/9/11	-
1	MLY	J	107	1	-	2/8/9/11	-
1	MLY	P	63	1	-	4/8/9/11	-
1	MLY	A	505	1	-	5/8/9/11	-
1	MLY	G	87	1	-	2/8/9/11	-
1	MLY	J	486	1	-	2/8/9/11	-
1	MLY	M	782	1	-	6/8/9/11	-
1	MLY	A	35	1	-	3/8/9/11	-
1	MLY	M	130	1	-	5/8/9/11	-
1	MLY	D	598	1	-	5/8/9/11	-
1	MLY	D	55	1	-	6/8/9/11	-
1	MLY	A	248	1	-	6/8/9/11	-
1	MLY	J	833	1	-	6/8/9/11	-
1	MLY	J	431	1	-	4/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	D	190	1	-	4/8/9/11	-
1	MLY	M	236	1	-	3/8/9/11	-
1	MLY	M	30	1	-	3/8/9/11	-
1	MLY	M	659	1	-	3/8/9/11	-
1	MLY	M	486	1	-	2/8/9/11	-
1	MLY	P	348	1	-	5/8/9/11	-
1	MLY	D	553	1,4	-	5/8/9/11	-
1	MLY	G	839	1	-	3/8/9/11	-
1	MLY	J	138	1	-	4/8/9/11	-
1	MLY	G	415	1	-	3/8/9/11	-
1	MLY	J	84	1	-	4/8/9/11	-
1	MLY	J	236	1	-	3/8/9/11	-
1	MLY	M	55	1	-	6/8/9/11	-
1	MLY	J	385	1	-	2/8/9/11	-
1	MLY	G	19	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	528	1	-	4/8/9/11	-
1	MLY	G	107	1	-	2/8/9/11	-
1	MLY	D	415	1	-	3/8/9/11	-
1	MLY	G	617	1	-	2/8/9/11	-
1	MLY	D	49	1	-	3/8/9/11	-
1	MLY	A	617	1	-	2/8/9/11	-
1	MLY	J	55	1	-	6/8/9/11	-
1	MLY	J	367	1	-	2/8/9/11	-
1	MLY	J	613	1	-	3/8/9/11	-
1	MLY	P	130	1	-	5/8/9/11	-
1	MLY	A	30	1	-	3/8/9/11	-
1	MLY	A	659	1	-	3/8/9/11	-
1	MLY	G	369	1	-	2/8/9/11	-
1	MLY	D	681	1	-	4/8/9/11	-
1	MLY	J	681	1	-	4/8/9/11	-
1	MLY	A	613	1	-	3/8/9/11	-
1	MLY	J	87	1	-	2/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	D	63	1	-	4/8/9/11	-
1	MLY	P	55	1	-	6/8/9/11	-
1	MLY	G	681	1	-	4/8/9/11	-
1	MLY	J	528	1	-	4/8/9/11	-
1	MLY	A	681	1	-	4/8/9/11	-
1	MLY	G	138	1	-	4/8/9/11	-
1	MLY	M	190	1	-	4/8/9/11	-
1	MLY	G	295	1	-	2/8/9/11	-
1	MLY	G	837	1	-	6/8/9/11	-
1	MLY	P	30	1	-	3/8/9/11	-
1	MLY	A	190	1	-	4/8/9/11	-
1	MLY	A	833	1	-	6/8/9/11	-
1	MLY	A	63	1	-	4/8/9/11	-
1	MLY	D	84	1	-	4/8/9/11	-
1	MLY	D	248	1	-	6/8/9/11	-
1	MLY	P	486	1	-	2/8/9/11	-
1	MLY	P	528	1	-	4/8/9/11	-
1	MLY	J	63	1	-	4/8/9/11	-
1	MLY	M	600	1	-	3/8/9/11	-
1	MLY	J	35	1	-	3/8/9/11	-
1	MLY	A	138	1	-	4/8/9/11	-
1	MLY	A	236	1	-	3/8/9/11	-

The worst 5 of 75 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	G	138	MLY	CB-CA	-3.28	1.48	1.53
1	P	138	MLY	CB-CA	-3.21	1.48	1.53
1	J	138	MLY	CB-CA	-3.19	1.48	1.53
1	M	138	MLY	CB-CA	-3.19	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.

189 monomers are involved in 833 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	M	348	MLY	5	0
1	G	504	MLY	1	0
1	G	59	MLY	3	0
1	G	768	MLY	7	0
1	A	49	MLY	3	0
1	M	107	MLY	3	0
1	P	598	MLY	1	0
1	P	49	MLY	4	0
1	A	436	MLY	2	0
1	G	659	MLY	2	0
1	M	84	MLY	37	0
1	M	138	MLY	2	0
1	G	782	MLY	1	0
1	D	551	MLY	1	0
1	J	598	MLY	1	0
1	P	296	MLY	3	0
1	G	553	MLY	27	0
1	D	659	MLY	2	0
1	G	63	MLY	4	0
1	P	617	MLY	1	0
1	M	87	MLY	3	0
1	D	782	MLY	87	0
1	D	30	MLY	1	0
1	M	296	MLY	3	0
1	M	528	MLY	3	0
1	D	837	MLY	1	0
1	G	30	MLY	1	0
1	J	295	MLY	6	0
1	G	600	MLY	1	0
1	P	248	MLY	2	0
1	M	598	MLY	1	0
1	A	486	MLY	3	0
1	P	837	MLY	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	M	839	MLY	11	0
1	J	839	MLY	8	0
1	P	87	MLY	3	0
1	M	63	MLY	3	0
1	G	272	MLY	1	0
1	J	504	MLY	1	0
1	G	436	MLY	2	0
1	J	837	MLY	1	0
1	M	553	MLY	27	0
1	A	551	MLY	2	0
1	P	764	MLY	9	0
1	A	369	MLY	1	0
1	D	827	MLY	2	0
1	M	295	MLY	6	0
1	A	768	MLY	18	0
1	M	49	MLY	3	0
1	A	296	MLY	2	0
1	A	600	MLY	1	0
1	D	107	MLY	3	0
1	M	764	MLY	7	0
1	M	837	MLY	1	0
1	A	295	MLY	6	0
1	P	553	MLY	2	0
1	A	782	MLY	7	0
1	J	764	MLY	3	0
1	J	768	MLY	4	0
1	M	505	MLY	12	0
1	G	348	MLY	4	0
1	D	504	MLY	1	0
1	J	617	MLY	1	0
1	M	248	MLY	2	0
1	D	600	MLY	1	0
1	A	553	MLY	19	0
1	J	436	MLY	2	0
1	J	505	MLY	9	0
1	G	486	MLY	3	0
1	G	598	MLY	1	0
1	A	504	MLY	3	0
1	A	59	MLY	2	0
1	A	837	MLY	4	0
1	D	764	MLY	9	0
1	J	296	MLY	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	P	839	MLY	12	0
1	A	272	MLY	1	0
1	A	87	MLY	3	0
1	D	617	MLY	1	0
1	D	87	MLY	3	0
1	P	107	MLY	3	0
1	G	84	MLY	19	0
1	J	415	MLY	1	0
1	M	617	MLY	1	0
1	D	486	MLY	3	0
1	P	295	MLY	6	0
1	J	272	MLY	1	0
1	J	348	MLY	5	0
1	G	49	MLY	3	0
1	M	551	MLY	3	0
1	D	59	MLY	2	0
1	J	59	MLY	2	0
1	P	600	MLY	1	0
1	A	348	MLY	5	0
1	G	296	MLY	2	0
1	J	553	MLY	11	0
1	M	272	MLY	1	0
1	P	138	MLY	2	0
1	D	138	MLY	2	0
1	P	190	MLY	2	0
1	J	659	MLY	2	0
1	M	59	MLY	2	0
1	A	528	MLY	2	0
1	G	55	MLY	1	0
1	G	190	MLY	2	0
1	G	528	MLY	3	0
1	P	782	MLY	2	0
1	D	839	MLY	4	0
1	G	505	MLY	1	0
1	D	768	MLY	11	0
1	G	248	MLY	2	0
1	A	598	MLY	1	0
1	P	59	MLY	2	0
1	D	272	MLY	1	0
1	D	348	MLY	6	0
1	P	504	MLY	1	0
1	J	248	MLY	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	839	MLY	8	0
1	M	35	MLY	12	0
1	A	415	MLY	1	0
1	M	504	MLY	1	0
1	M	768	MLY	1	0
1	M	436	MLY	2	0
1	A	764	MLY	10	0
1	A	107	MLY	3	0
1	J	190	MLY	2	0
1	M	369	MLY	1	0
1	P	659	MLY	1	0
1	P	436	MLY	2	0
1	P	84	MLY	5	0
1	J	30	MLY	1	0
1	P	415	MLY	1	0
1	J	600	MLY	1	0
1	J	782	MLY	1	0
1	P	272	MLY	1	0
1	J	49	MLY	3	0
1	M	415	MLY	1	0
1	D	436	MLY	2	0
1	A	55	MLY	1	0
1	D	296	MLY	3	0
1	J	107	MLY	3	0
1	P	63	MLY	3	0
1	A	505	MLY	35	0
1	G	87	MLY	3	0
1	J	486	MLY	3	0
1	M	782	MLY	9	0
1	D	598	MLY	1	0
1	D	55	MLY	1	0
1	A	248	MLY	2	0
1	D	190	MLY	2	0
1	M	30	MLY	1	0
1	M	659	MLY	2	0
1	M	486	MLY	3	0
1	P	348	MLY	5	0
1	D	553	MLY	16	0
1	G	839	MLY	4	0
1	J	138	MLY	2	0
1	G	415	MLY	1	0
1	J	84	MLY	23	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	M	55	MLY	1	0
1	G	764	MLY	21	0
1	D	295	MLY	6	0
1	D	528	MLY	3	0
1	G	107	MLY	3	0
1	D	415	MLY	1	0
1	G	617	MLY	1	0
1	D	49	MLY	4	0
1	A	617	MLY	1	0
1	J	55	MLY	1	0
1	A	30	MLY	1	0
1	A	659	MLY	2	0
1	G	369	MLY	1	0
1	J	87	MLY	3	0
1	D	63	MLY	3	0
1	P	55	MLY	1	0
1	J	528	MLY	3	0
1	G	138	MLY	2	0
1	M	190	MLY	2	0
1	G	295	MLY	6	0
1	G	837	MLY	1	0
1	P	30	MLY	1	0
1	A	190	MLY	2	0
1	A	63	MLY	3	0
1	D	248	MLY	2	0
1	P	486	MLY	3	0
1	P	528	MLY	2	0
1	J	63	MLY	4	0
1	M	600	MLY	1	0
1	A	138	MLY	2	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	7
1	P	6
1	D	4
1	A	4
1	J	3
1	G	3
3	C	1
3	F	1
3	I	1
3	L	1
3	O	1
3	R	1
2	B	1
2	E	1
2	H	1
2	K	1
2	N	1
2	Q	1

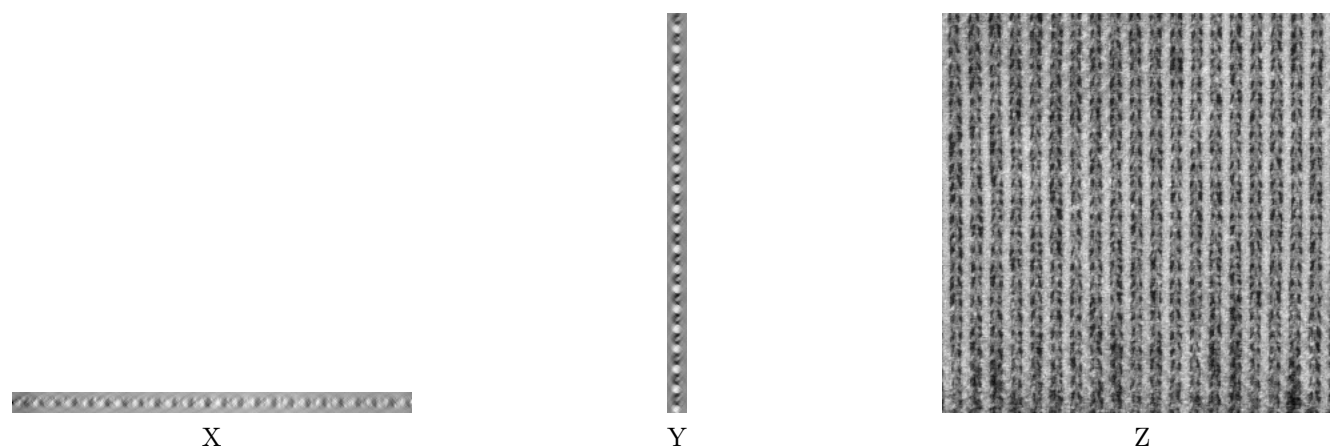
The worst 5 of 39 chain breaks are listed below:

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

6 Tomogram visualisation [i](#)

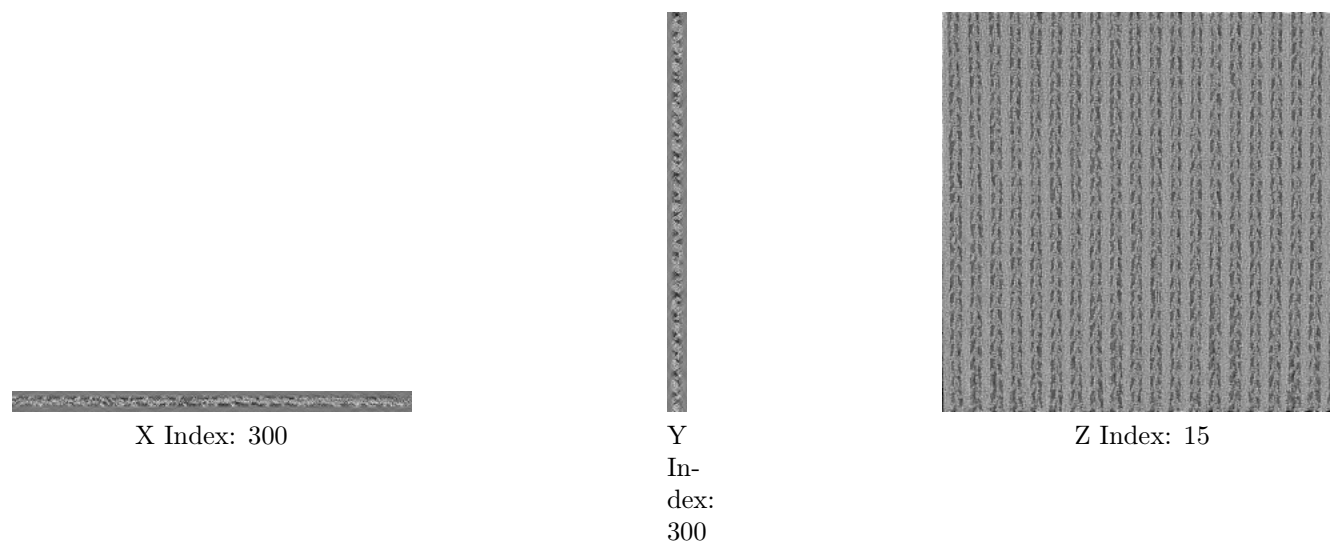
This section contains visualisations of the EMDB entry EMD-1001. These allow visual inspection of the internal detail of the tomogram and identification of artifacts.

6.1 Orthogonal projections [i](#)



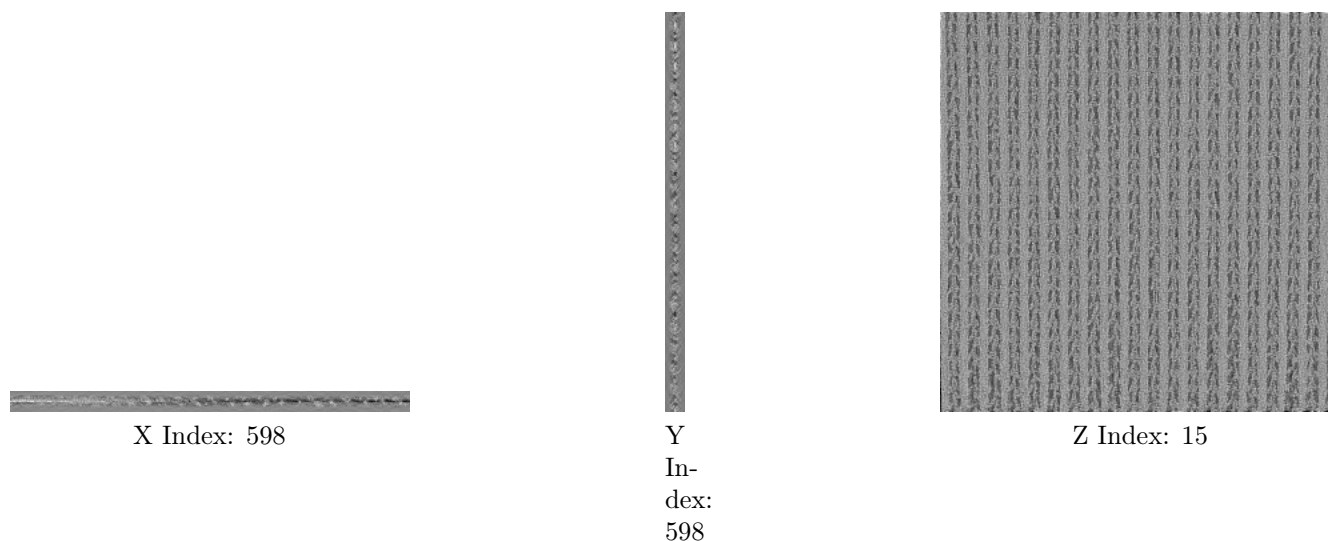
The images above show the tomogram projected in three orthogonal directions.

6.2 Central slices [i](#)



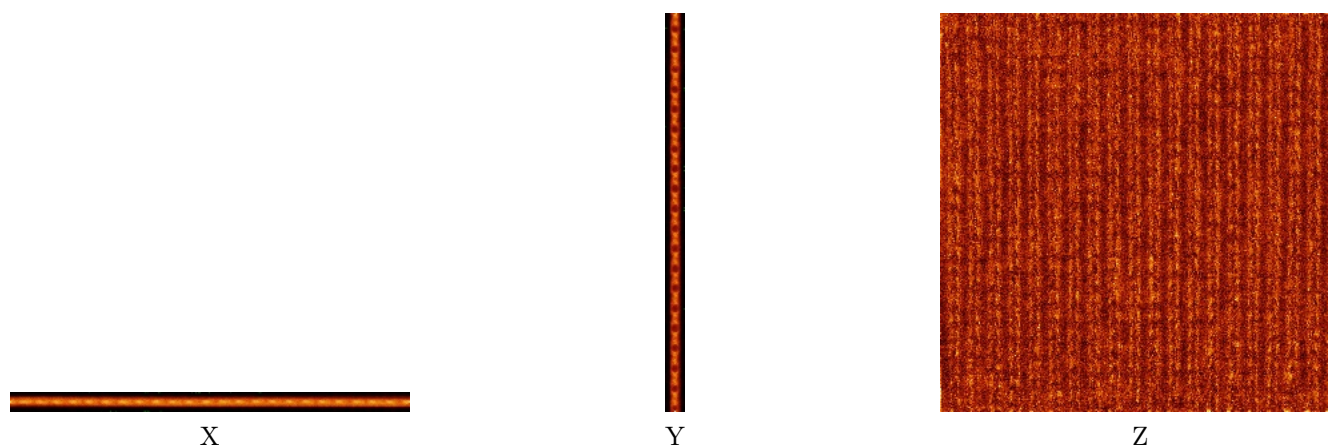
The images above show central slices of the tomogram in three orthogonal directions.

6.3 Largest variance slices [i](#)



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

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



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

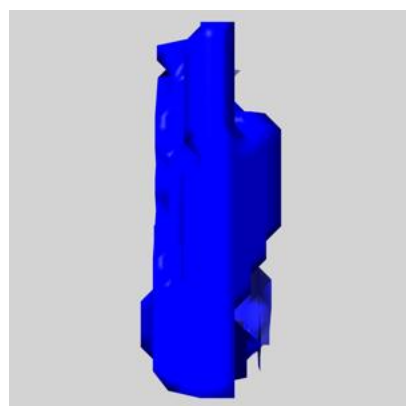
6.5 Mask visualisation [i](#)

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

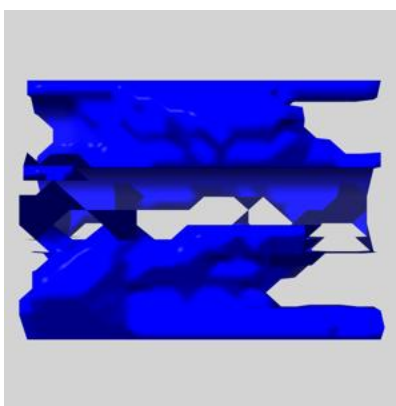
A mask typically either:

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

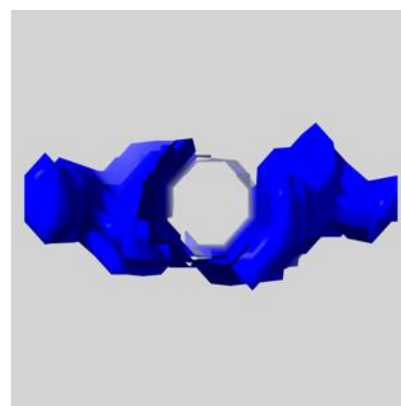
6.5.1 emd_1001_msk_25.map [i](#)



X

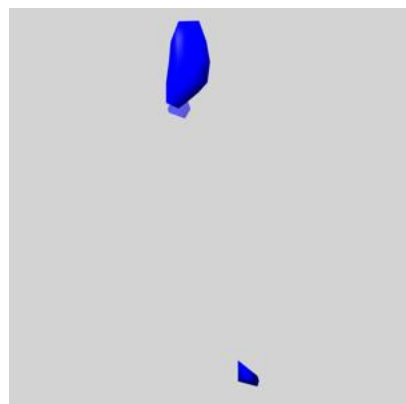


Y

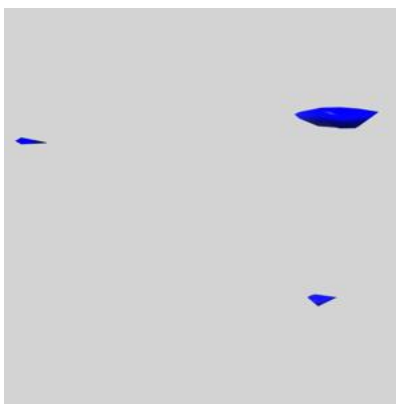


Z

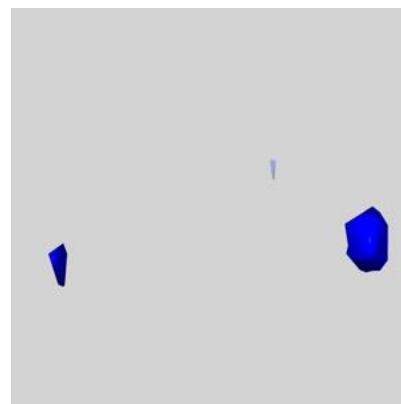
6.5.2 emd_1001_msk_24.map [i](#)



X

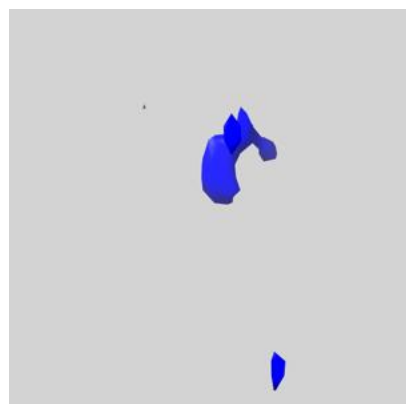


Y

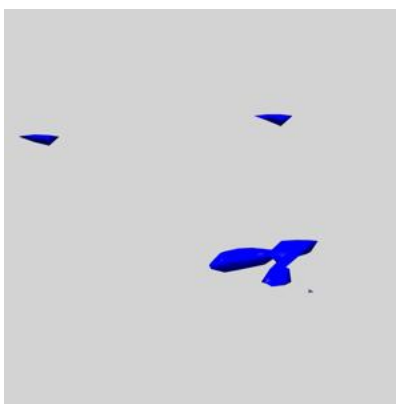


Z

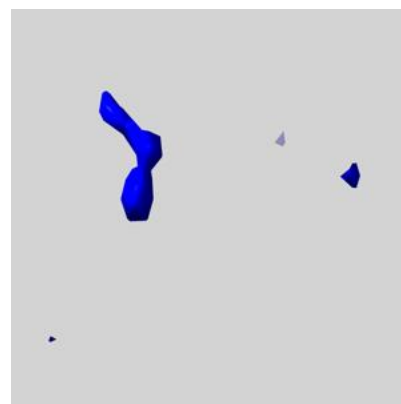
6.5.3 emd_1001_msk_23.map [i](#)



X

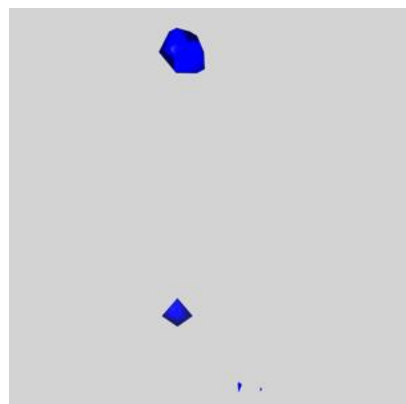


Y

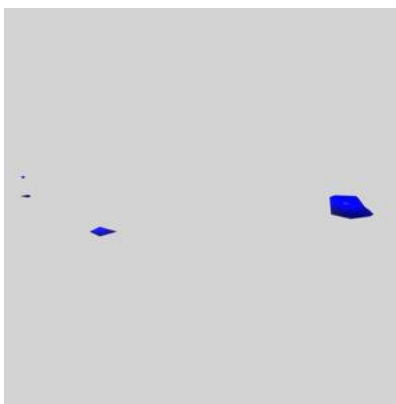


Z

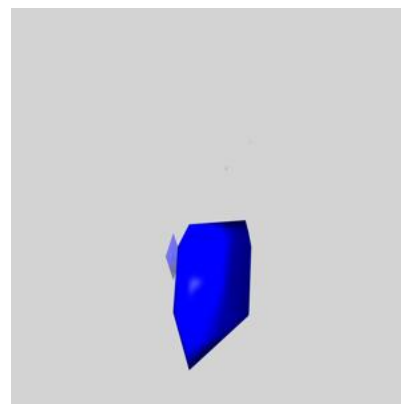
6.5.4 emd_1001_msk_22.map [i](#)



X

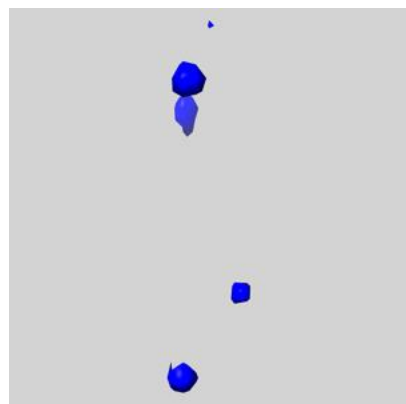


Y

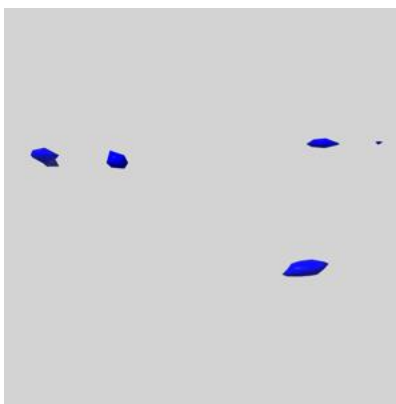


Z

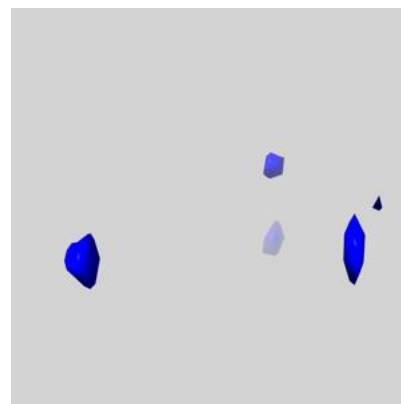
6.5.5 emd_1001_msk_21.map [i](#)



X

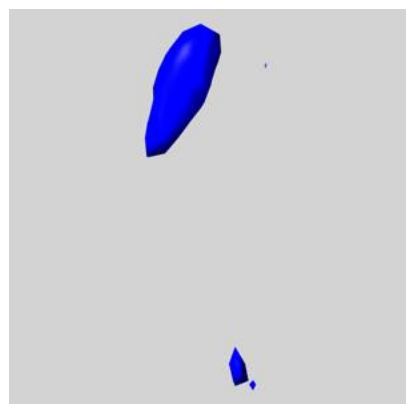


Y

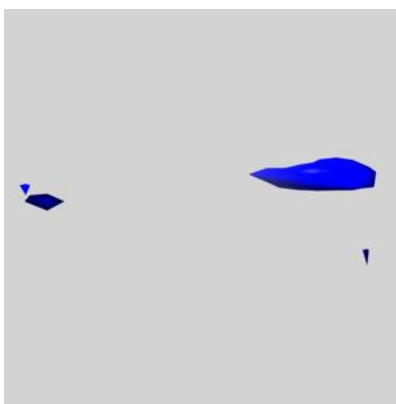


Z

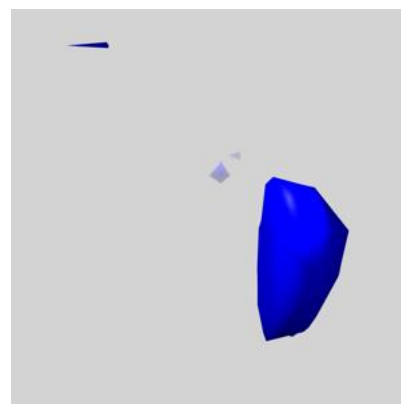
6.5.6 emd_1001_msk_20.map [i](#)



X

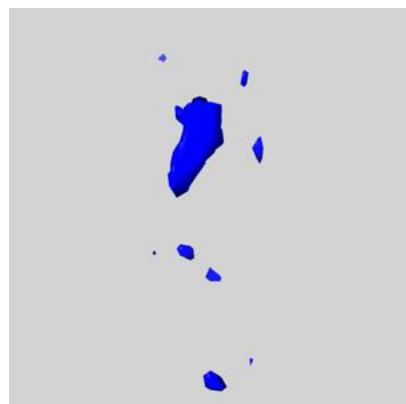


Y

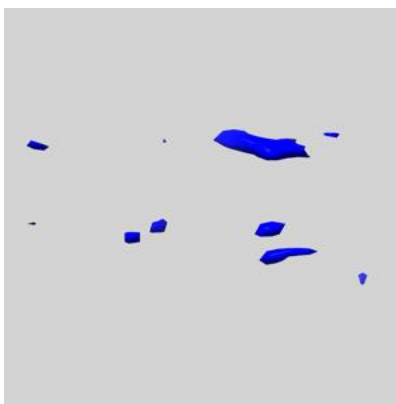


Z

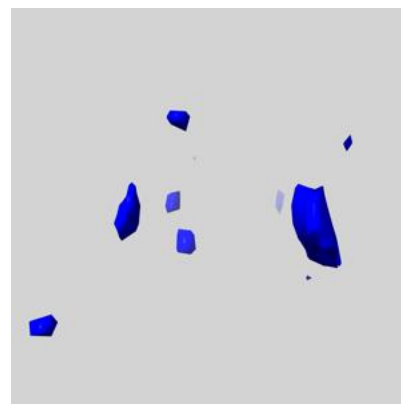
6.5.7 emd_1001_msk_19.map [i](#)



X

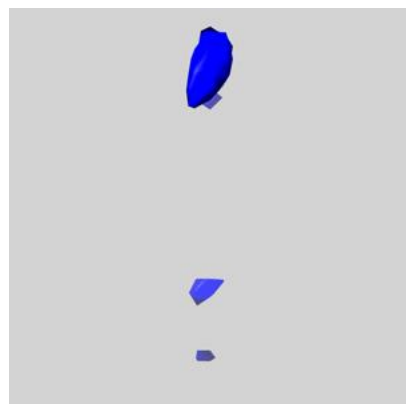


Y

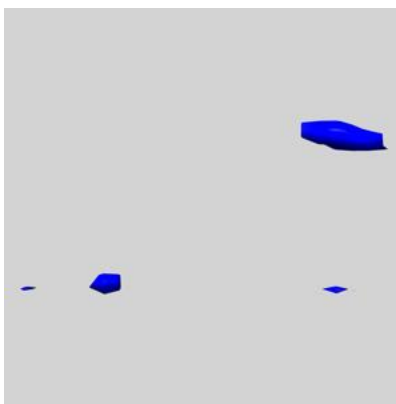


Z

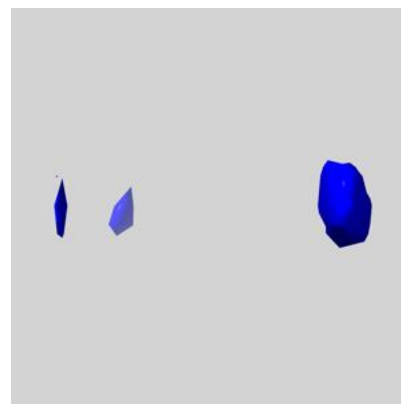
6.5.8 emd_1001_msk_18.map [i](#)



X

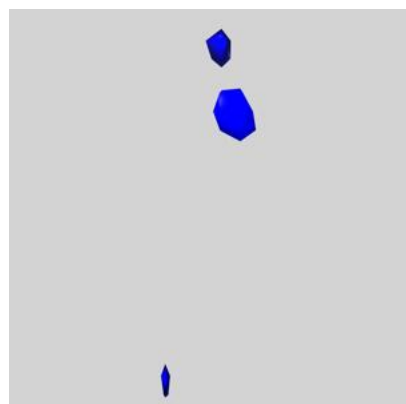


Y

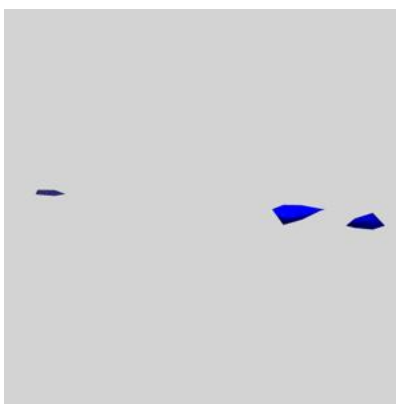


Z

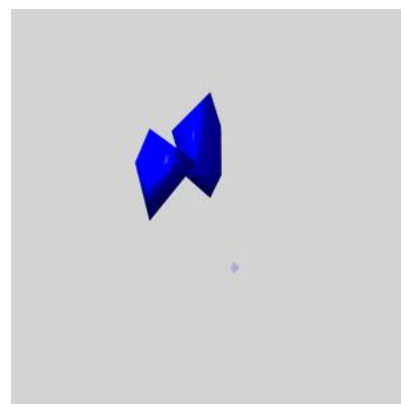
6.5.9 emd_1001_msk_17.map [i](#)



X

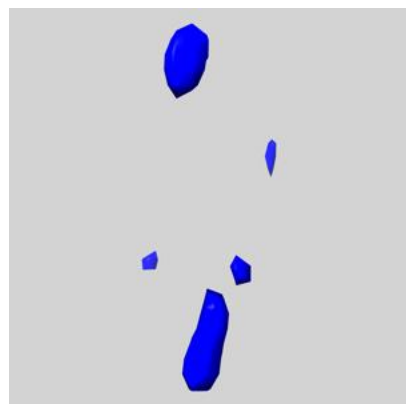


Y

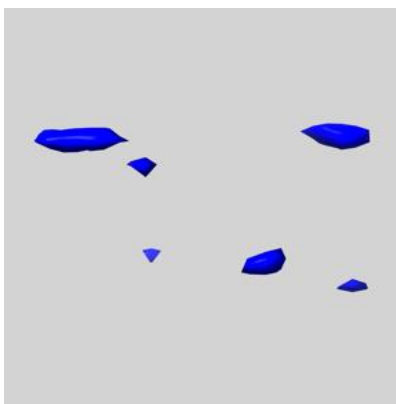


Z

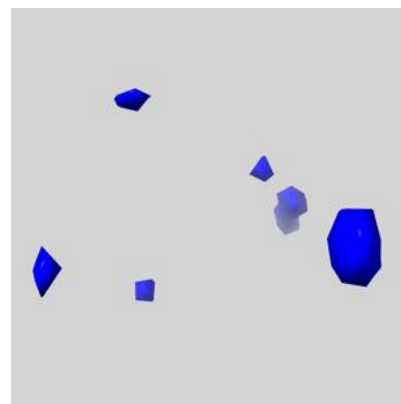
6.5.10 emd_1001_msk_16.map [i](#)



X

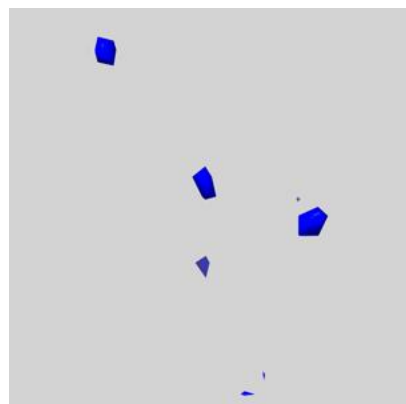


Y

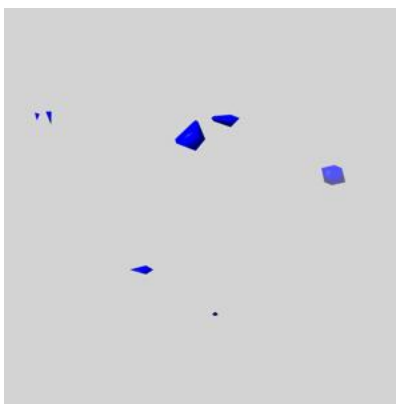


Z

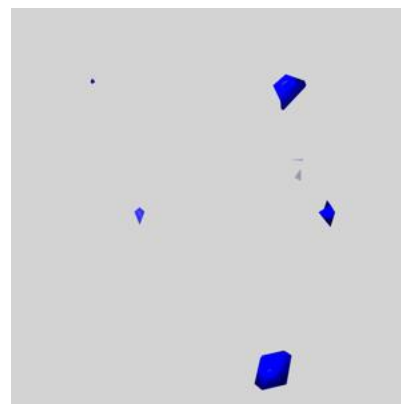
6.5.11 emd_1001_msk_15.map [i](#)



X

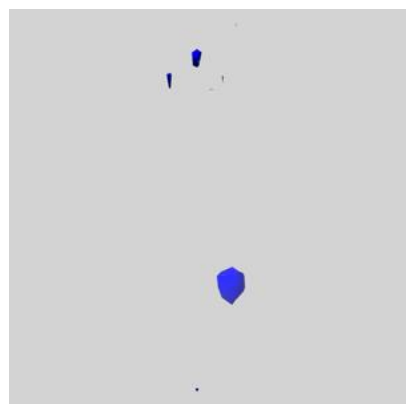


Y

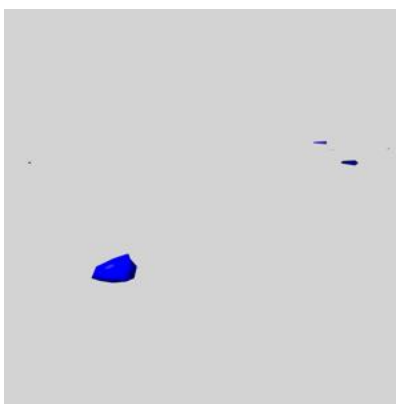


Z

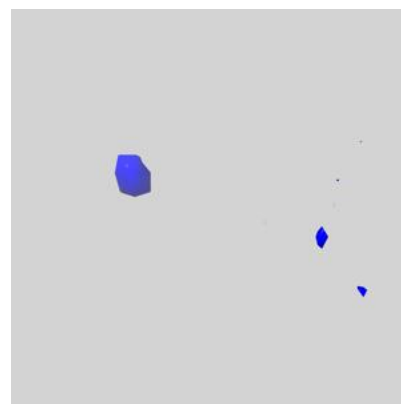
6.5.12 emd_1001_msk_14.map [i](#)



X

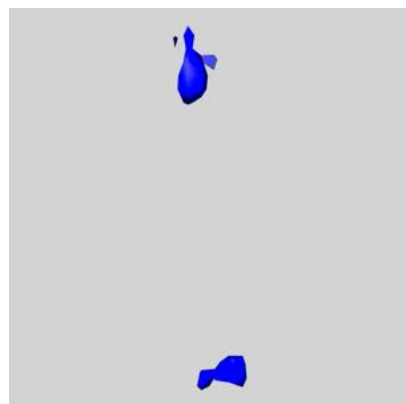


Y

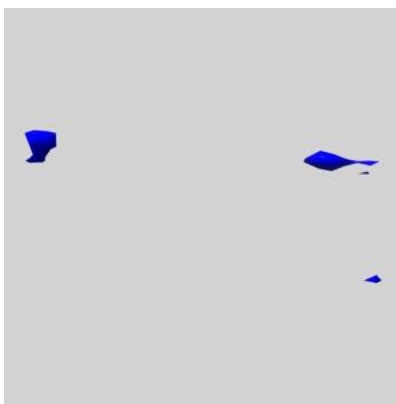


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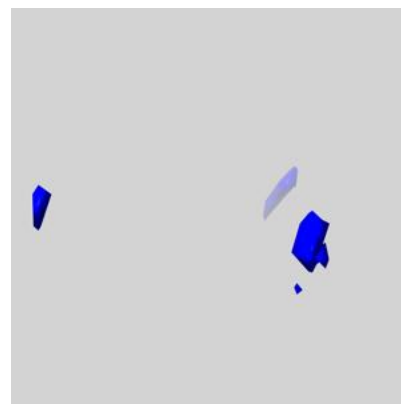
6.5.13 emd_1001_msk_13.map [i](#)



X

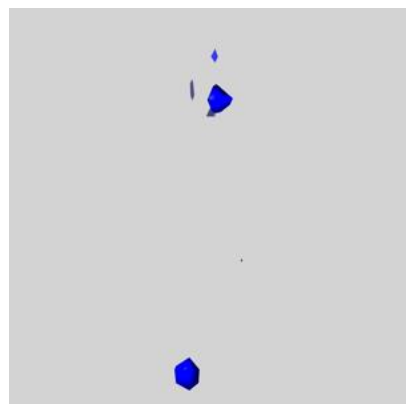


Y

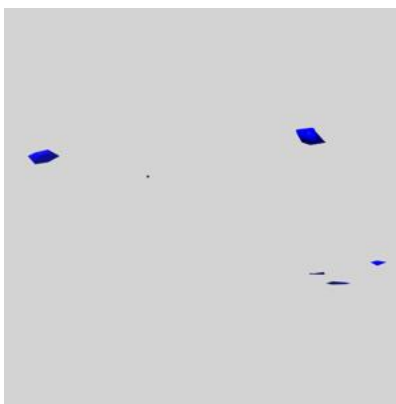


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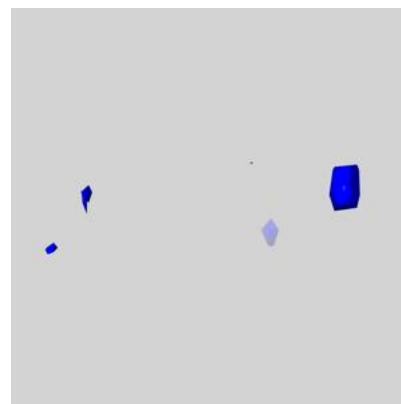
6.5.14 emd_1001_msk_12.map [i](#)



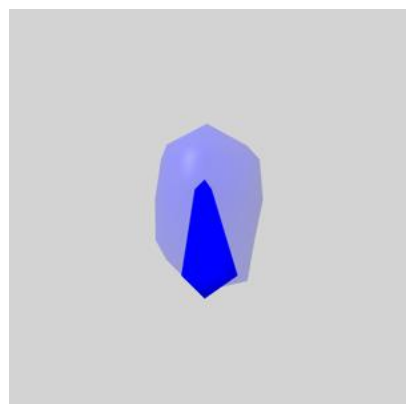
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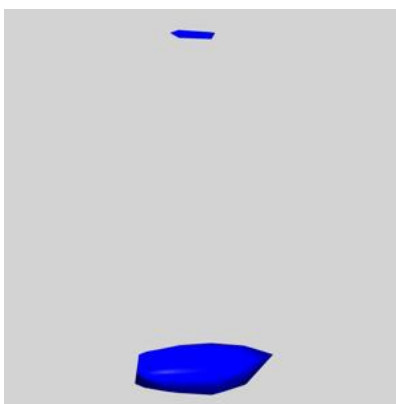
Y



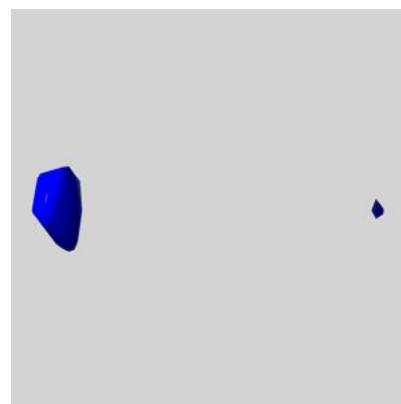
Z

6.5.15 emd_1001_msk_11.map [i](#)

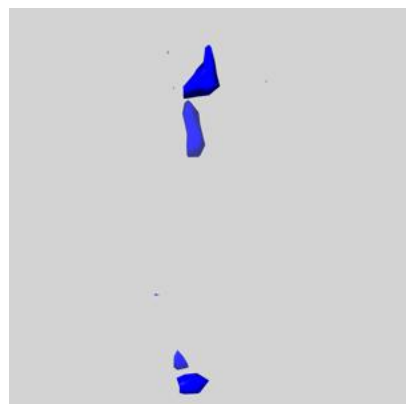
X



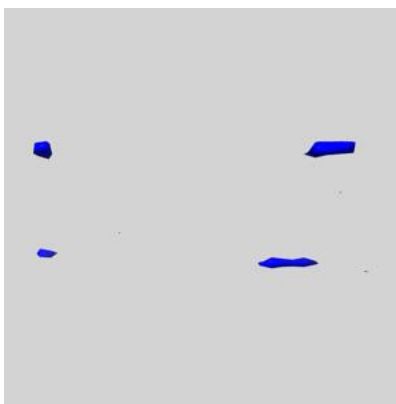
Y



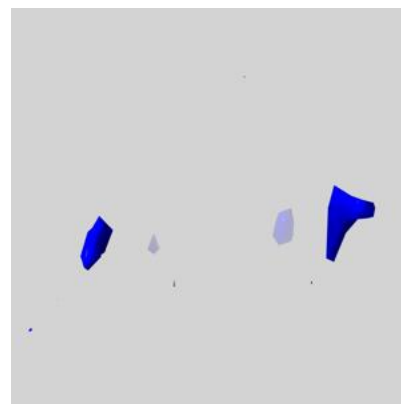
Z

6.5.16 emd_1001_msk_10.map [i](#)

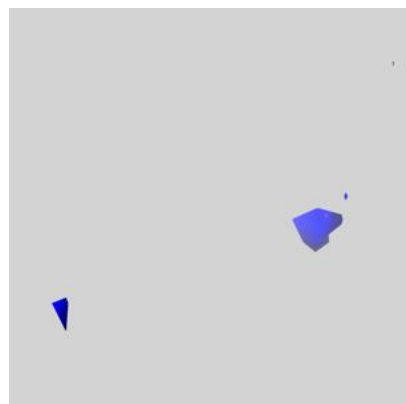
X



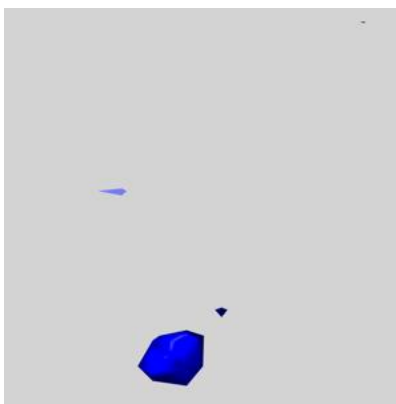
Y



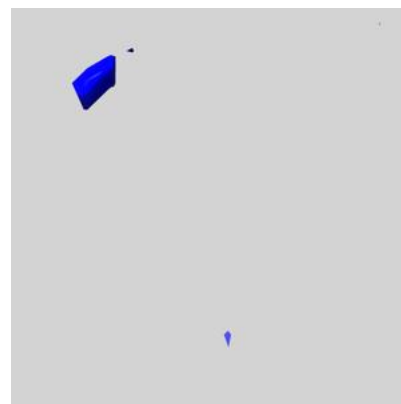
Z

6.5.17 emd_1001_msk_9.map [i](#)

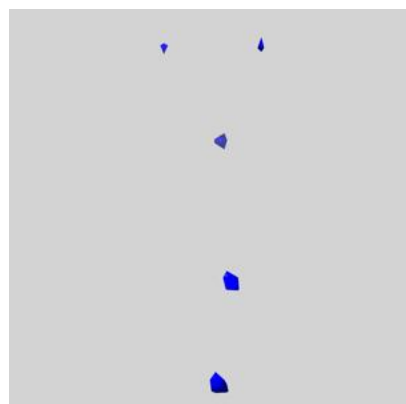
X



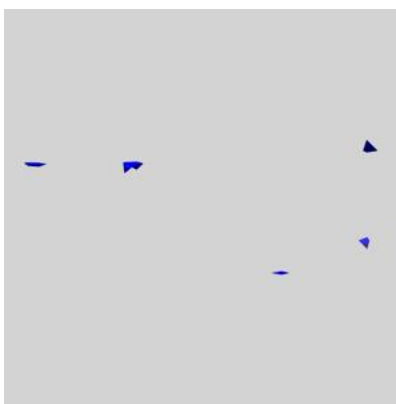
Y



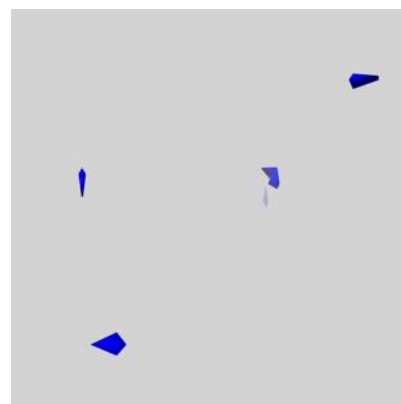
Z

6.5.18 emd_1001_msk_8.map [i](#)

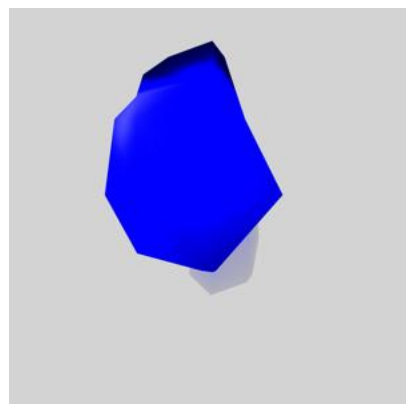
X



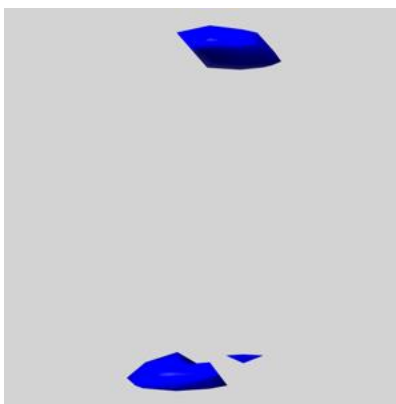
Y



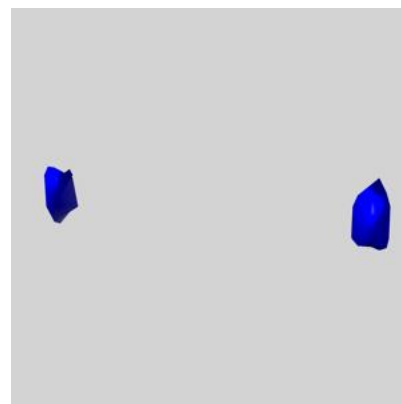
Z

6.5.19 emd_1001_msk_7.map [i](#)

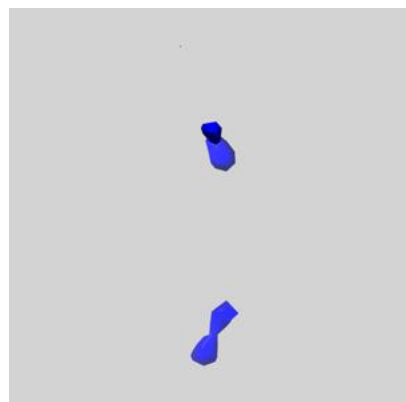
X



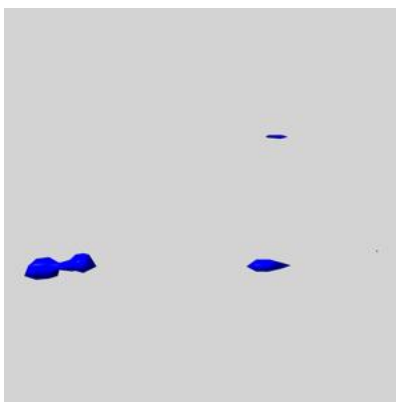
Y



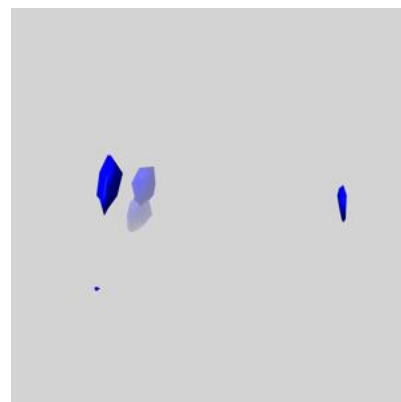
Z

6.5.20 emd_1001_msk_6.map [i](#)

X



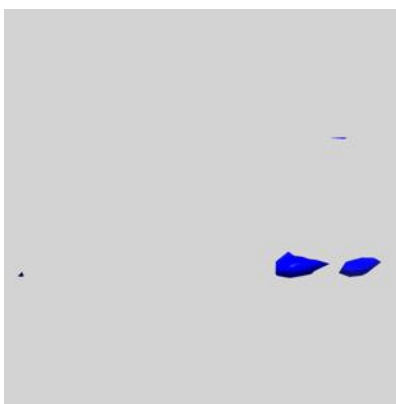
Y



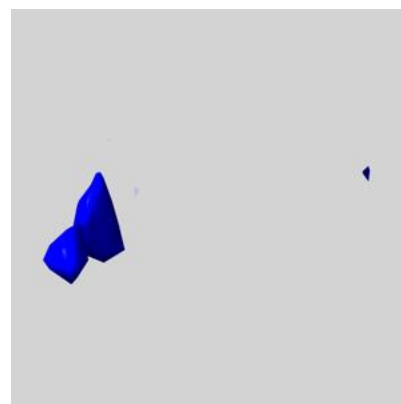
Z

6.5.21 emd_1001_msk_5.map [i](#)

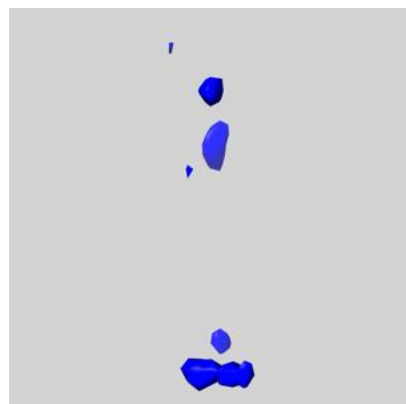
X



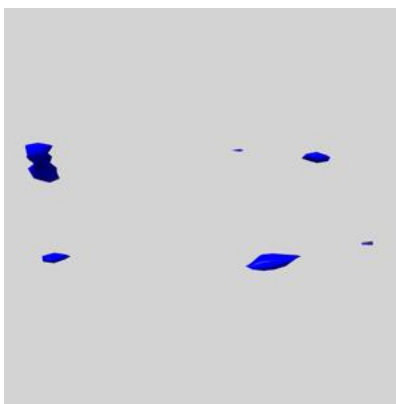
Y



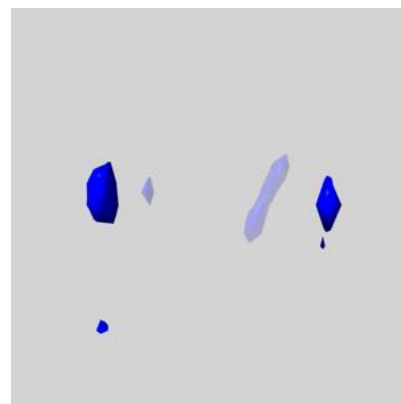
Z

6.5.22 emd_1001_msk_4.map [i](#)

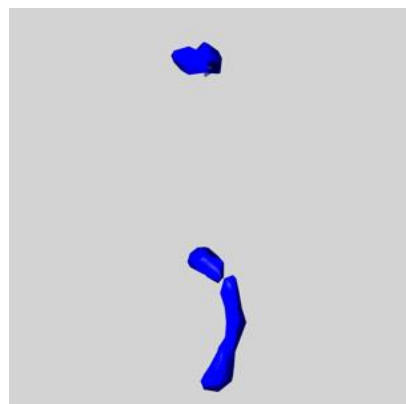
X



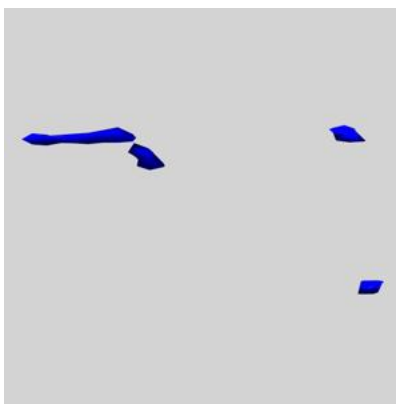
Y



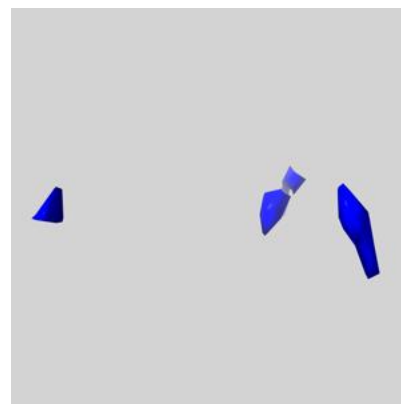
Z

6.5.23 emd_1001_msk_3.map [i](#)

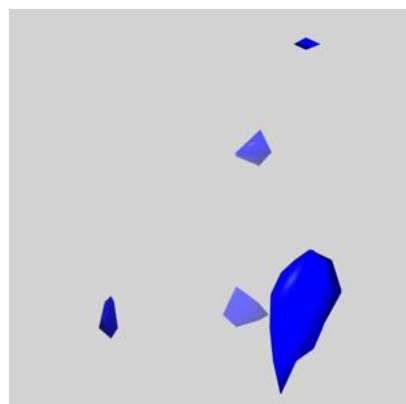
X



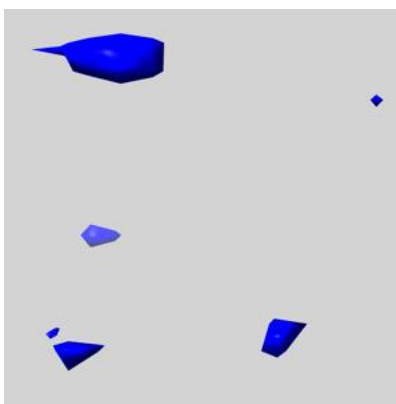
Y



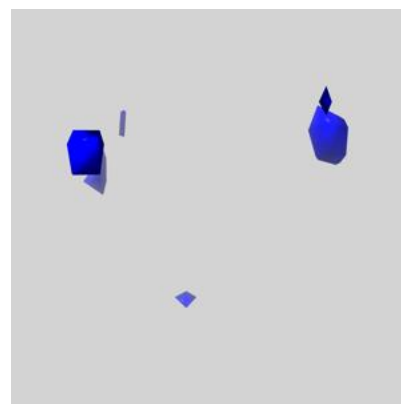
Z

6.5.24 emd_1001_msk_2.map [i](#)

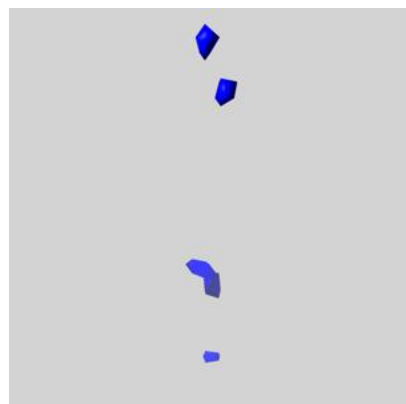
X



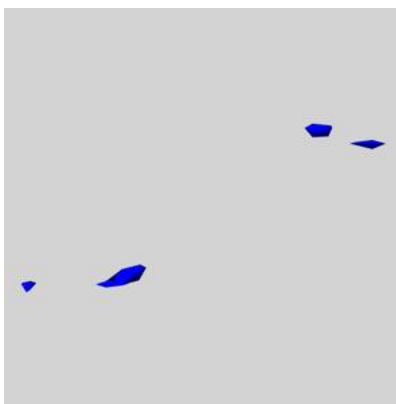
Y



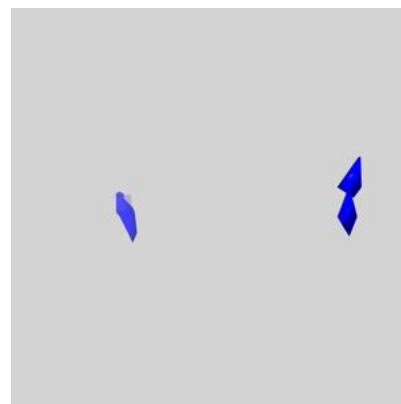
Z

6.5.25 emd_1001_msk_1.map [i](#)

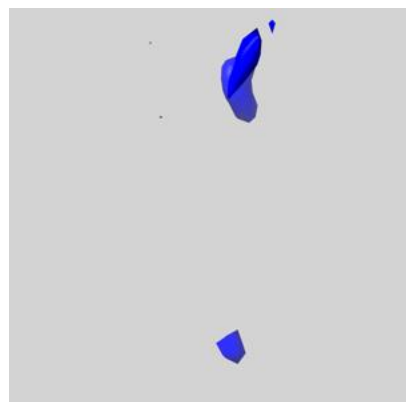
X



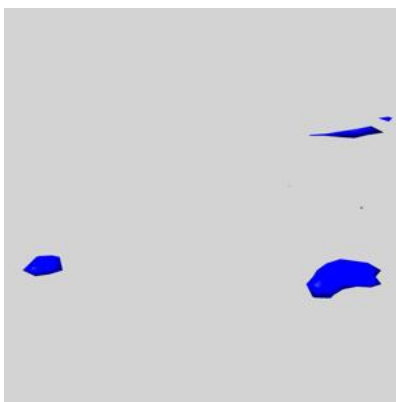
Y



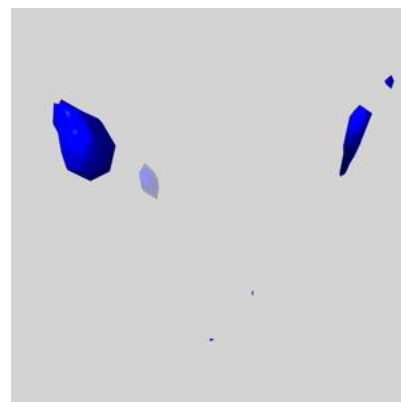
Z

6.5.26 emd_1001_msk_26.map [i](#)

X



Y

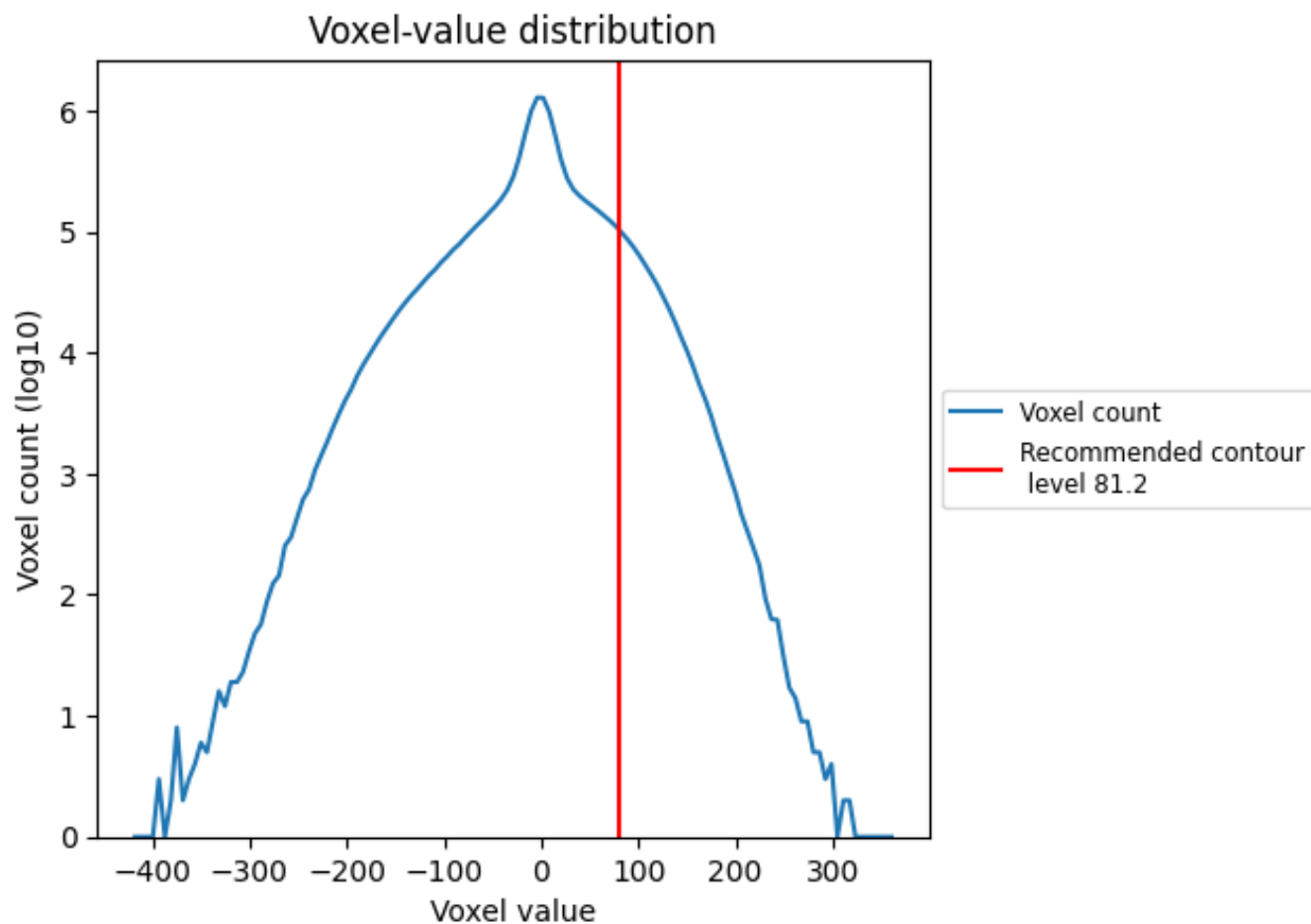


Z

7 Tomogram analysis [i](#)

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

7.1 Voxel-value distribution [i](#)



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

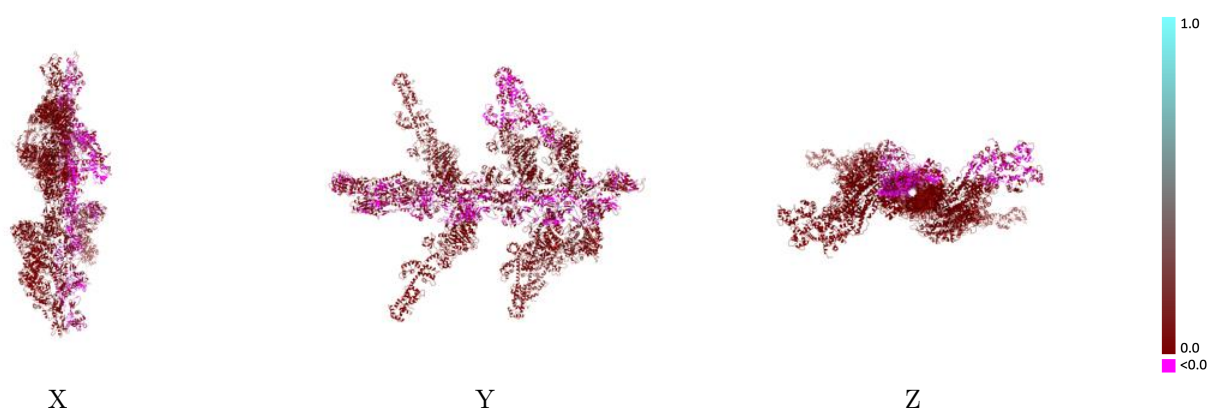
8 Map-model fit [i](#)

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

8.1 Map-model overlay [i](#)

This section was not generated.

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

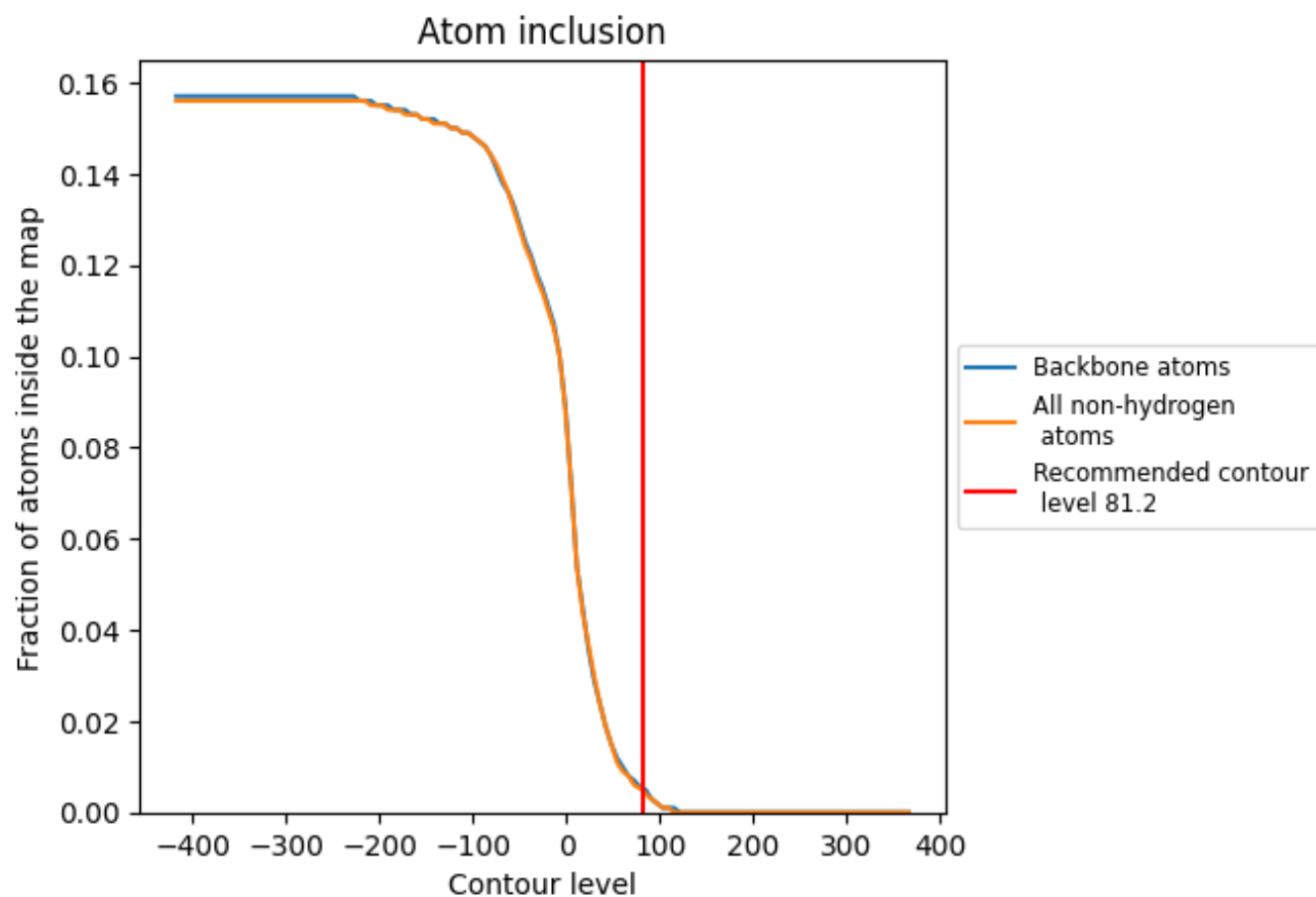


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

8.4 Atom inclusion [i](#)



At the recommended contour level, 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	 -0.0000
0	 0.0000	 0.0000
1	 0.0150	 0.0180
2	 0.0000	 -0.0100
3	 0.0000	 0.0040
4	 0.0000	 -0.0020
5	 0.0000	 0.0090
7	 0.0000	 0.0000
8	 0.0000	 -0.0080
9	 0.0000	 -0.0040
A	 0.0000	 -0.0020
B	 0.0000	 0.0000
C	 0.0000	 0.0000
D	 0.0000	 0.0080
E	 0.0000	 -0.0140
F	 0.1160	 0.0080
G	 0.0000	 -0.0030
H	 0.0000	 0.0000
I	 0.0000	 0.0000
J	 0.0000	 -0.0010
K	 0.0150	 0.0060
L	 0.0000	 -0.0230
M	 0.0000	 0.0030
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	 -0.0170
W	 0.0000	 0.0020
X	 0.0690	 0.0040
Y	 0.0000	 0.0010
Z	 0.0190	 -0.0040

