



wwPDB EM Validation Summary Report ⓘ

Mar 17, 2026 – 06:46 PM UTC

PDB ID : 1O1B / pdb_00001o1b
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 : 2002-11-15
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 : 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

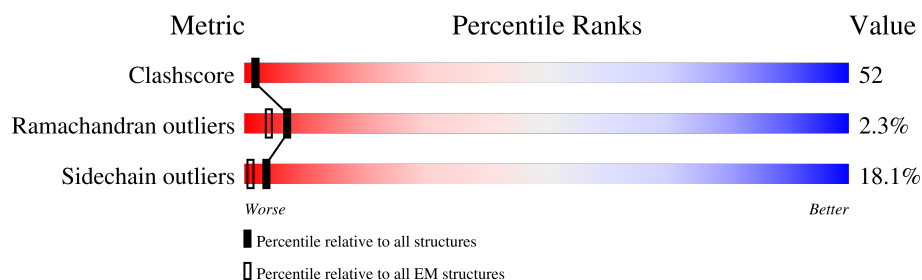
1 Overall quality at a glance

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% 25% 49% 22% .
1	D	840	100% 25% 49% 23% .
1	G	840	100% 24% 49% 22% .
1	J	840	99% 24% 49% 23% .
2	B	145	100% 66% 25% 7% .
2	E	145	100% 63% 28% 6% .
2	H	145	100% 62% 29% 6% .
2	K	145	92% 64% 26% 7% .

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Mol	Chain	Length	Quality of chain
3	C	147	
3	F	147	
3	I	147	
3	L	147	
4	0	375	
4	1	375	
4	2	375	
4	3	375	
4	4	375	
4	5	375	
4	7	375	
4	8	375	
4	9	375	
4	V	375	
4	W	375	
4	X	375	
4	Y	375	
4	Z	375	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	MLY	A	505	-	-	X	-
1	MLY	A	553	-	-	X	-
1	MLY	A	764	-	-	X	-
1	MLY	A	768	-	-	X	-
1	MLY	A	839	-	-	X	-
1	MLY	D	553	-	-	X	-
1	MLY	D	768	-	-	X	-

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

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 76872 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		

- 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		

- 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		

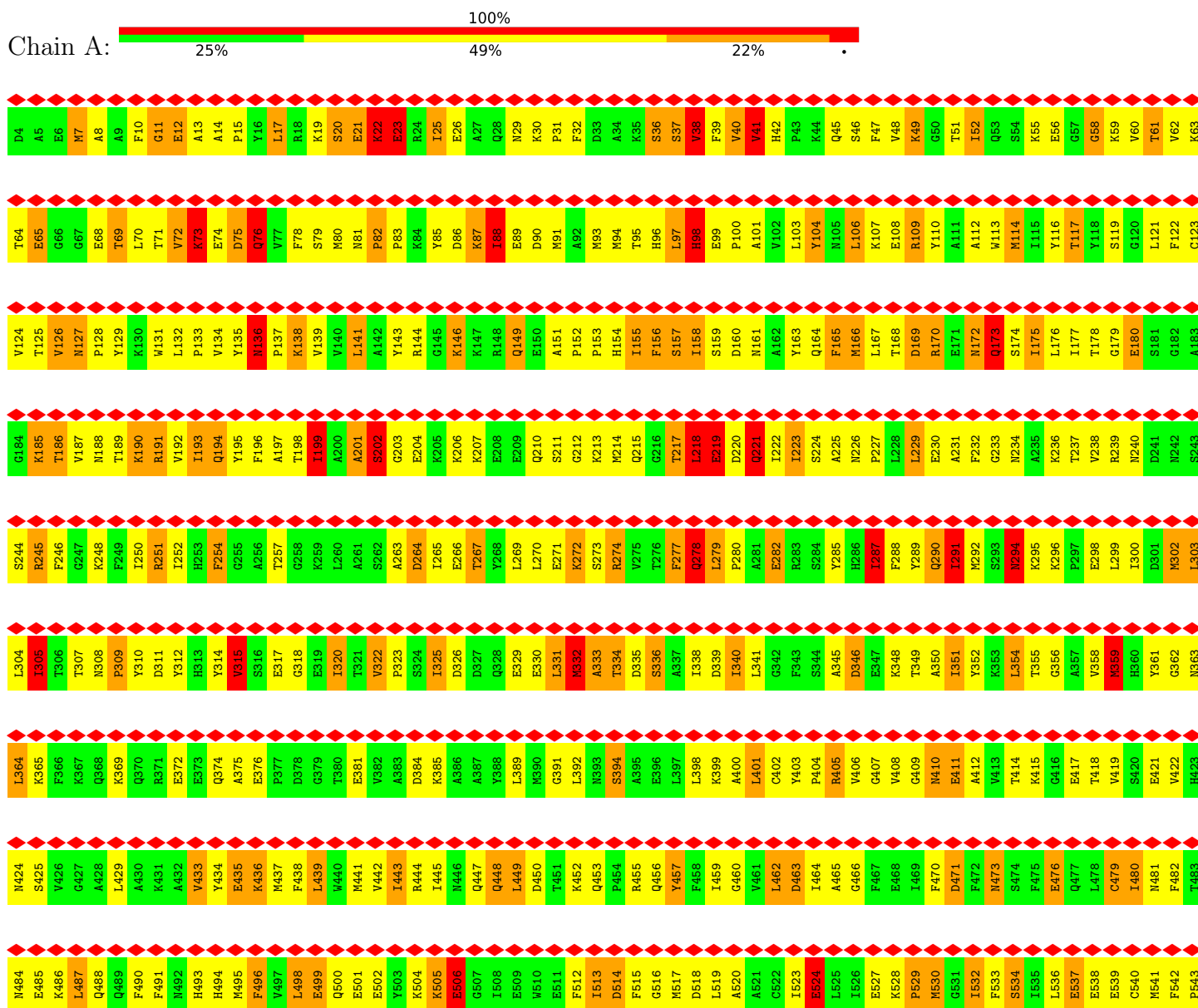
- Molecule 4 is a protein called SKELETAL MUSCLE ACTIN.

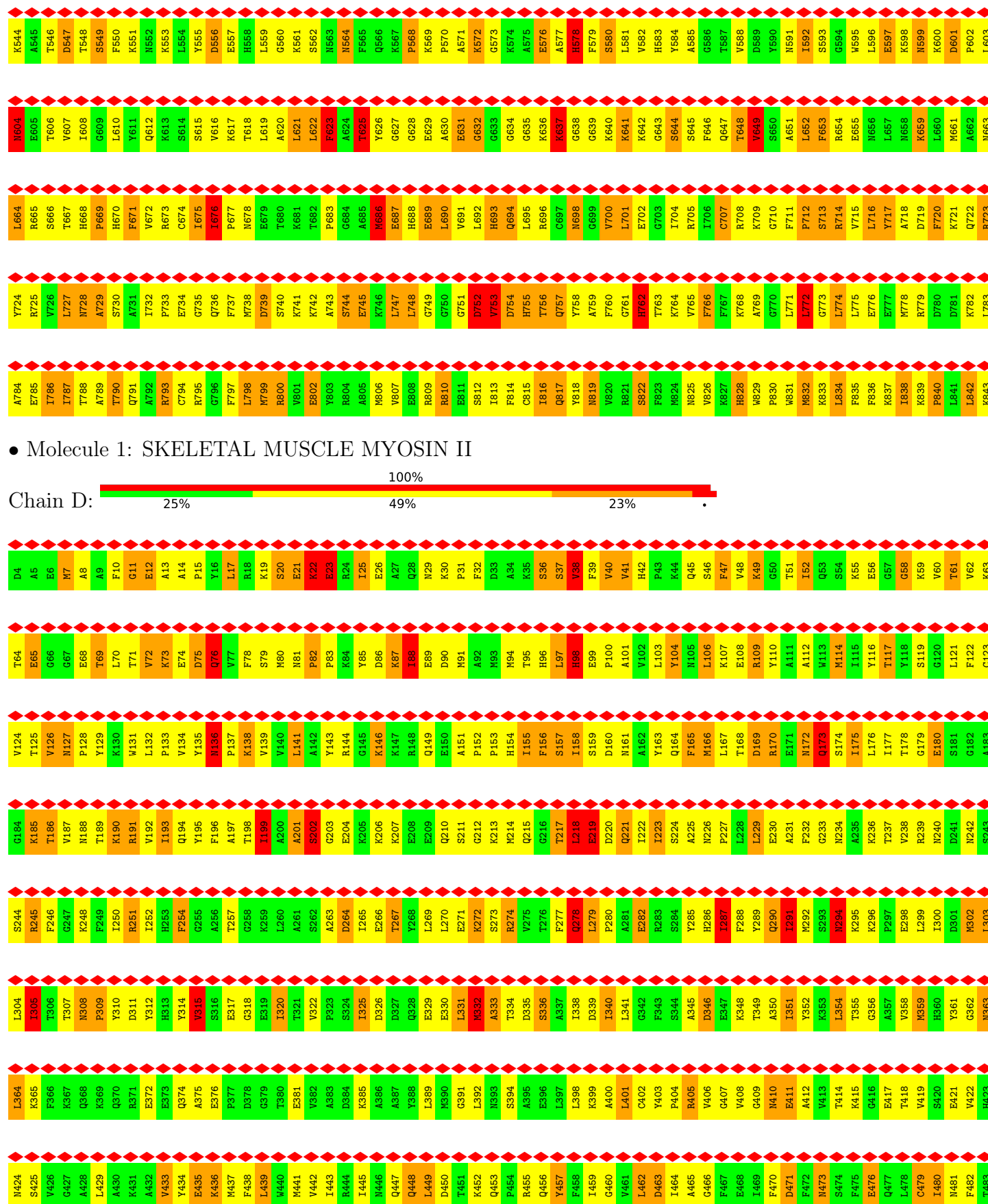
Mol	Chain	Residues	Atoms					AltConf	Trace
4	0	372	Total 2906	C 1836	N 489	O 561	S 20	0	0
4	1	372	Total 2906	C 1836	N 489	O 561	S 20	0	0
4	2	372	Total 2906	C 1836	N 489	O 561	S 20	0	0
4	3	372	Total 2906	C 1836	N 489	O 561	S 20	0	0
4	4	372	Total 2906	C 1836	N 489	O 561	S 20	0	0
4	5	372	Total 2906	C 1836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

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

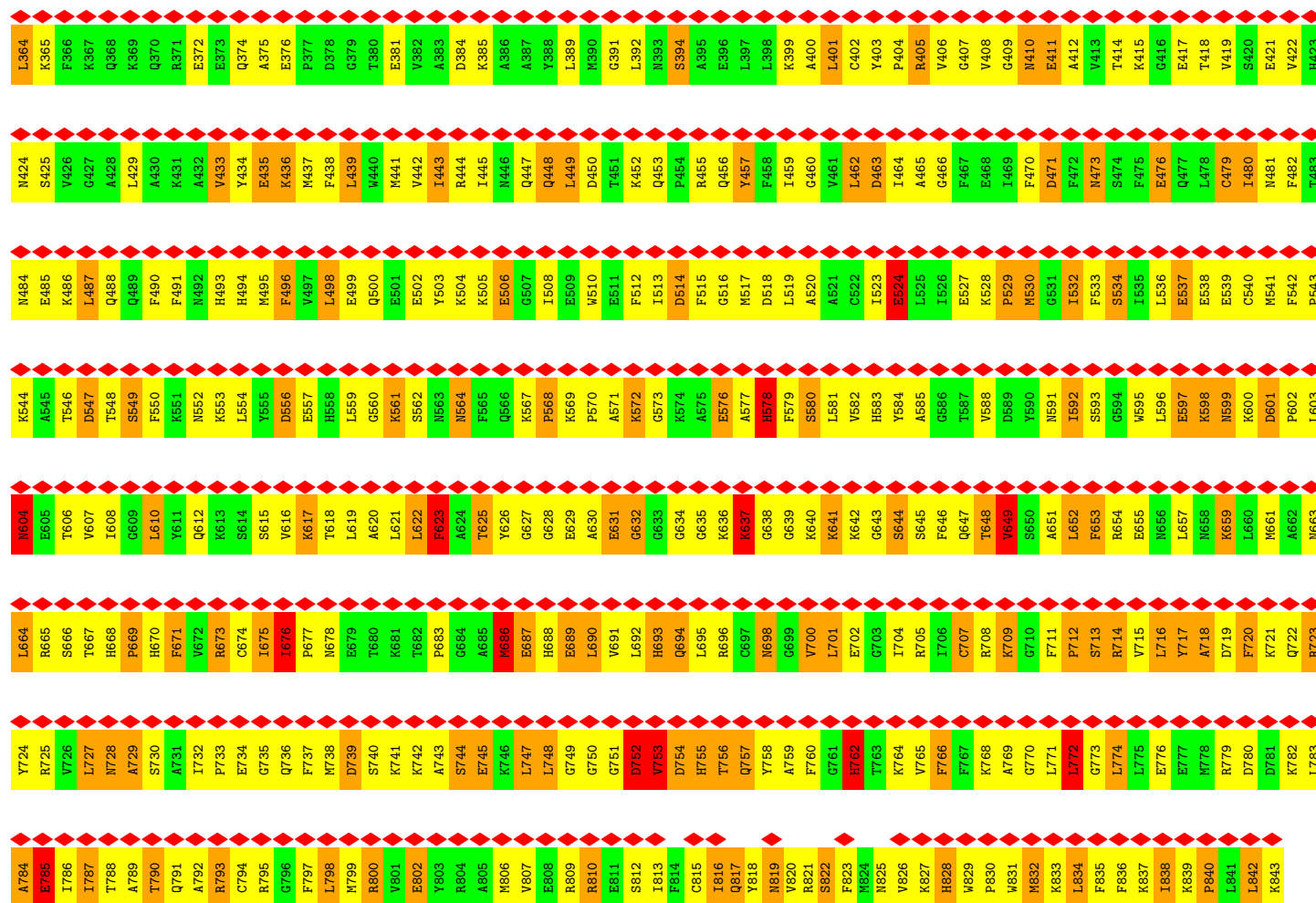




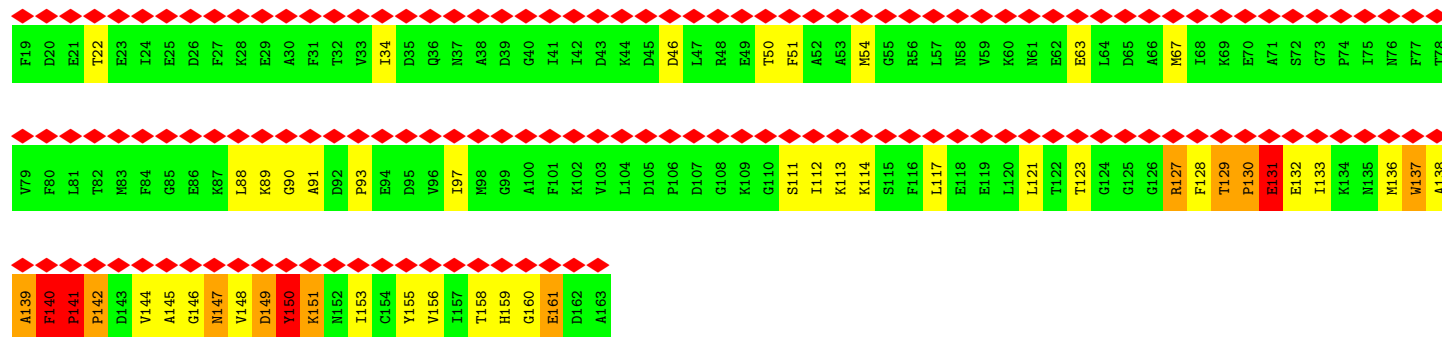
N424	N484	K544	L664	Y724	A784	D4	T64	V124	G184	S244	L304
S425	E485	K545	R665	R725	E785	A5	E65	T125	K185	R245	T305
V426	K486	T546	S666	V726	I786	E6	G66	V126	T186	F246	T306
G427	L487	D547	T667	L727	T787	M7	G67	M127	V187	G247	T307
A428	Q488	T548	H668	M728	T788	A8	E68	P128	N188	K248	N308
L429	Q489	S549	P669	A729	A789	A9	E69	Y129	T189	F249	P309
A430	F490	F550	H670	S730	T790	F10	L70	K130	K190	L250	Y310
K431	F491	K551	F671	A731	Q791	G11	T71	V131	R191	R251	D311
A432	N492	N552	V672	I732	A792	E12	V72	L132	V192	L252	Y312
V433	H493	K553	G673	P733	T793	A13	K73	P133	T193	H253	H313
Y434	H494	L554	C674	E734	C794	A14	E74	V134	Q194	F254	Y314
E435	M495	Y555	I675	G735	R795	P15	D75	Y135	Y195	G255	Y315
K436	F496	D556	T676	Q736	G796	Y16	V76	N136	F196	A256	S316
M437	V497	V557	F677	F737	F797	L17	V77	K137	A197	T257	E317
F438	L498	H558	N678	M738	L798	R18	F78	K138	T198	G258	G318
L439	E499	L559	E679	D739	M799	K19	S79	V139	N199	K259	E319
M440	Q500	G560	T680	S740	R800	S20	M80	Y140	A200	L260	I320
M441	E501	K561	K681	K741	V801	E21	E81	L141	A201	A261	T321
V442	E502	S562	T682	K742	E802	K22	P82	A142	S202	S262	V322
I443	Y503	N563	P683	A743	Y803	E23	P83	Y143	G203	A263	P323
R444	K504	N564	G684	S744	R804	R24	K84	G144	E204	D264	S324
I445	K505	F565	A685	E745	A805	I25	Y85	R145	K205	L265	I325
V446	E506	Q566	M686	K746	M806	E26	D86	K146	K206	E266	D326
Q447	G507	Q567	E687	L747	V807	A27	T87	K147	K207	T267	D327
Q448	I508	P568	H688	L748	E808	Q28	T88	Q148	E208	G268	Q328
L449	E509	K569	E689	G749	R809	N29	E89	R149	E209	L269	E329
D450	M510	P570	L690	G750	R810	K30	D90	E150	Q210	L270	E330
T451	E511	A571	V691	G751	E811	P31	N91	A151	S211	E271	L331
K452	F512	K572	L692	D752	S812	F32	A92	P152	G212	K272	R332
Q453	I513	G573	H693	V753	I813	D33	N93	P153	K213	S273	A333
V454	D514	K574	Q694	D754	F814	A34	M94	H154	M214	R274	T334
R455	F515	A575	L695	H755	C815	K35	T95	I155	Q215	V275	D335
Q456	G516	E576	R696	T756	I816	S36	H96	F156	G216	T276	S336
Y457	M517	Q577	C697	Q757	Q817	S37	L97	S157	T217	F277	A337
F458	D518	H578	N698	Y758	Y818	V38	H98	I158	L218	Q278	I338
I459	L519	F579	G699	A759	N819	F39	E99	S159	E219	L279	D339
G460	A520	S580	V700	F760	V820	V40	P100	D160	D220	P280	I340
V461	E521	L581	L701	G761	R821	V41	A101	A161	Q221	A281	L341
L462	C522	V582	E702	H762	S822	H42	Y102	A162	I222	E282	G342
D463	I523	H583	G703	T763	P823	P43	L103	Y163	I223	R283	F343
I464	E524	Y584	I704	K764	M824	K44	Y104	Q164	S224	S284	S344
A465	L525	A585	R705	V765	N825	Q45	N105	F165	A225	Y285	A345
G466	I526	G586	T706	F766	V826	S46	L106	M166	N226	H286	D346
F467	E527	T587	C707	F767	V827	F47	E107	L167	P227	L287	E347
E468	P528	V588	R708	K768	H828	V48	E108	T168	L228	F288	K348
I469	E529	D589	K709	A769	N829	K49	R109	D169	L229	Y289	T349
F470	M530	Y590	G710	G770	P830	G50	Y110	R170	E230	Q290	A350
D471	G531	N591	F711	L771	M831	T51	A111	E171	A231	I291	I351
F472	I532	L592	P712	L772	M832	I52	A112	M172	F232	M292	Y352
N473	F533	S593	S713	G773	K833	Q53	V113	Q173	G233	S293	K353
S474	S534	G594	R714	L774	L834	S54	M114	S174	N234	N294	L354
F475	I535	V595	V715	L775	P835	K55	I115	I175	A235	K295	T355
A476	L536	L596	T716	E776	P836	E56	Y116	Y176	K236	K296	G356
Q477	E537	T597	K837	F777	K837	G57	T117	T177	T237	P297	A357
L478	E538	K598	A718	M778	T838	G58	Y118	T178	V238	E298	V358
C479	E539	N599	D719	R779	K839	K59	S119	G179	R239	L299	K359
I480	C540	K600	F720	D780	P840	V60	G120	E180	N240	T300	H360
N481	M541	D601	K721	L781	L841	T61	G121	S181	D241	I361	Y361
F482	P542	A662	Q722	K782	L842	V62	F122	G182	N242	K362	G362
T483	L603	N663	R723	L783	K843	K63	C123	A183	S243	L303	N363

• Molecule 1: SKELETAL MUSCLE MYOSIN II

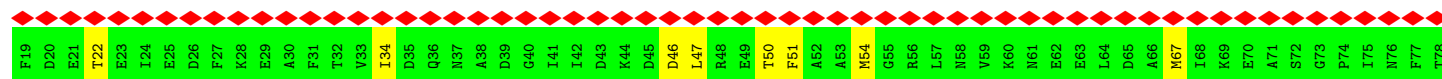


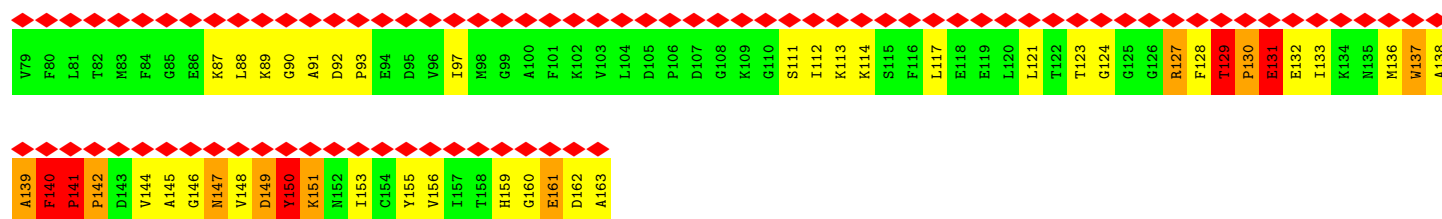


• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

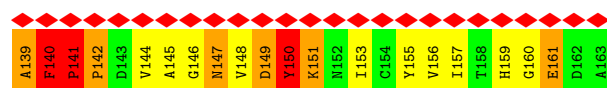
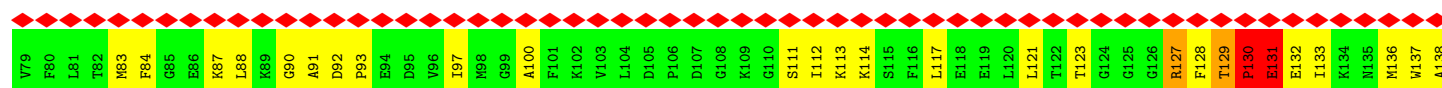
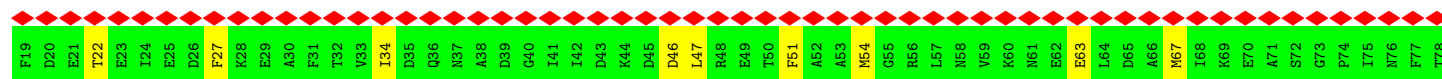


• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

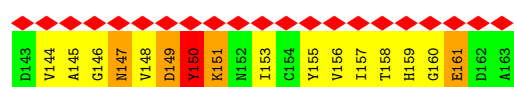
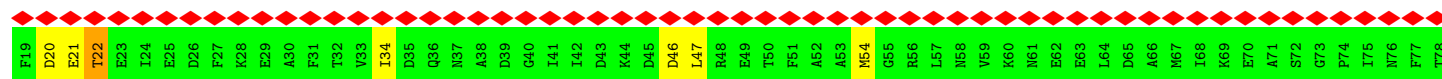




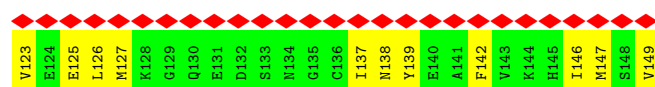
• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN



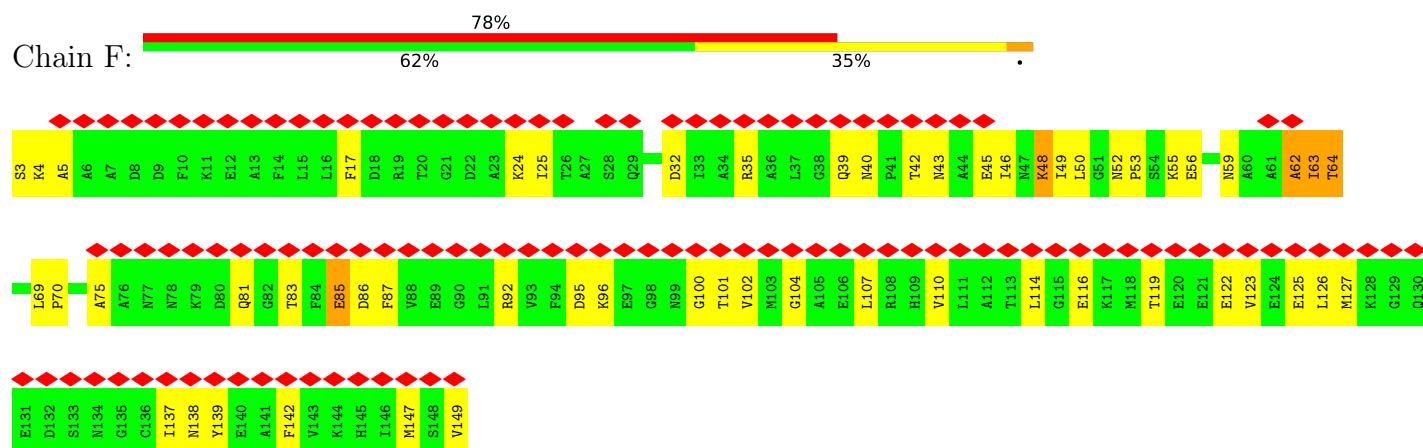
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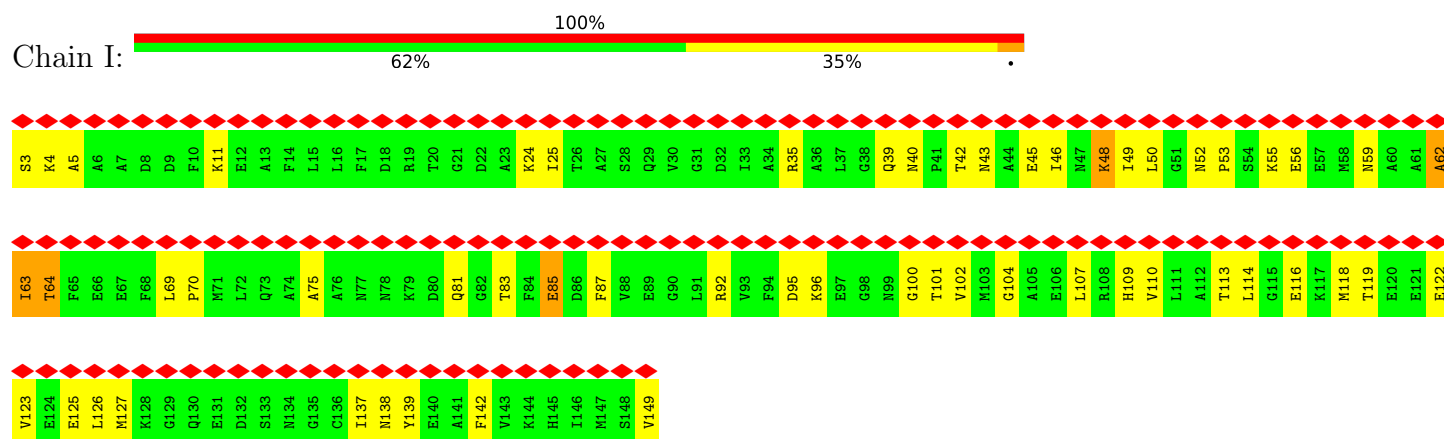
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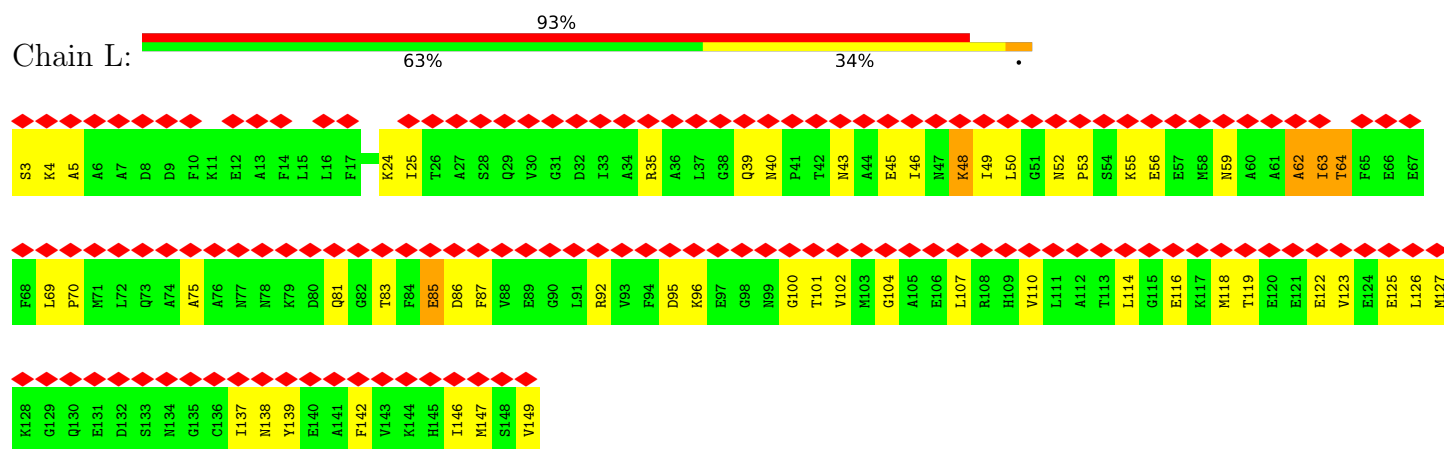
- Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN



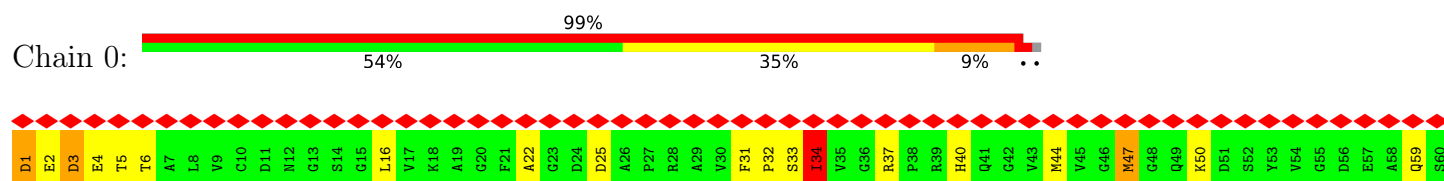
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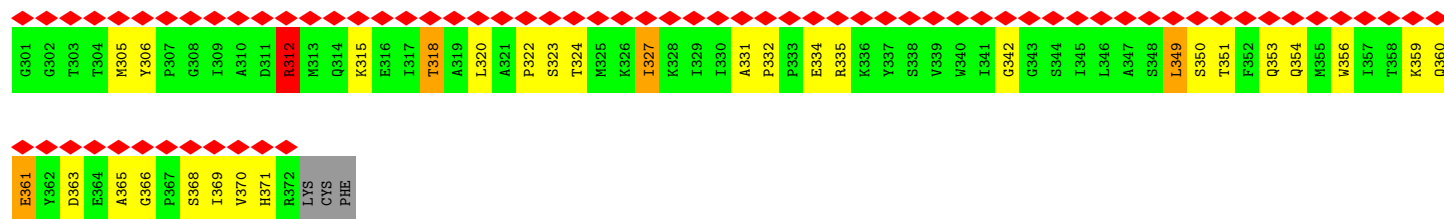


- Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN

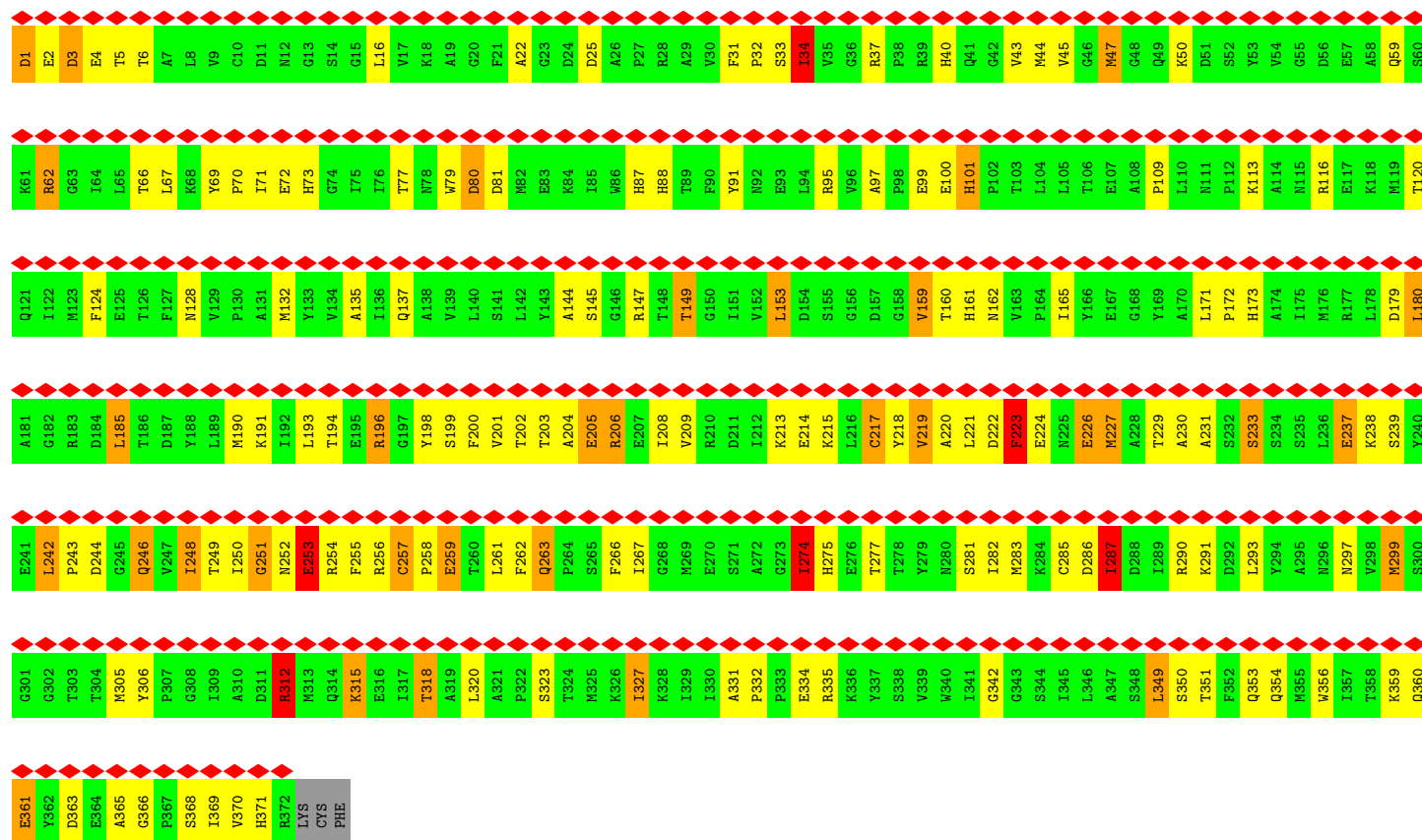


- Molecule 4: SKELETAL MUSCLE ACTIN

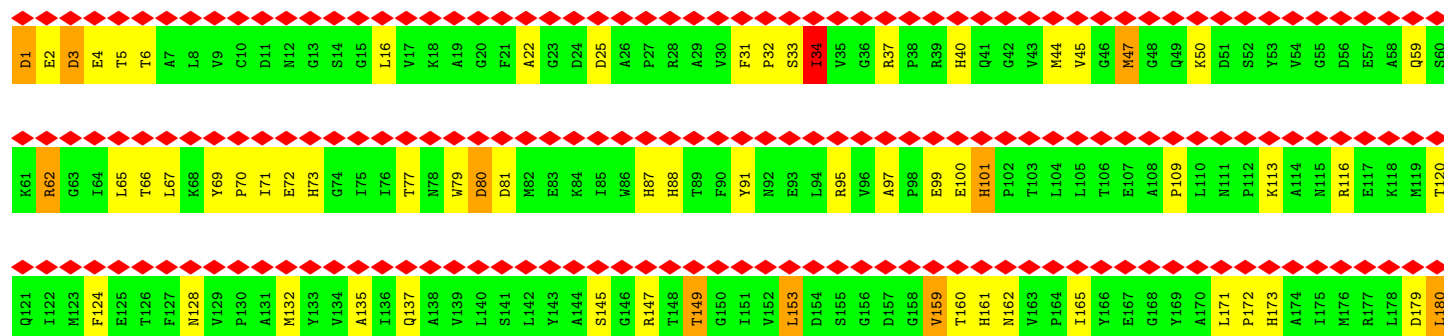


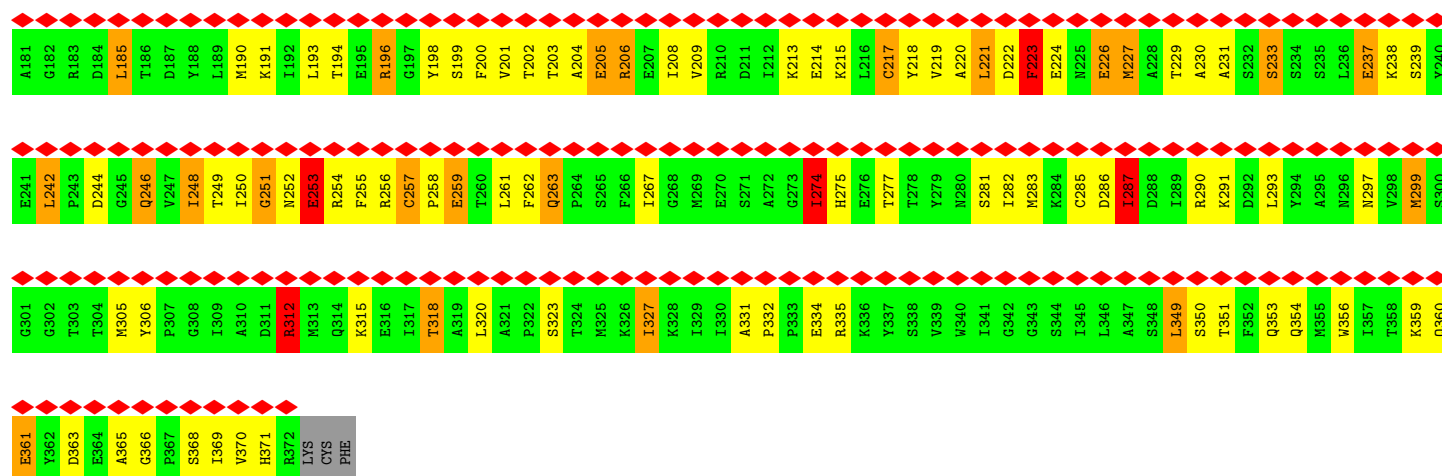


• Molecule 4: SKELETAL MUSCLE ACTIN

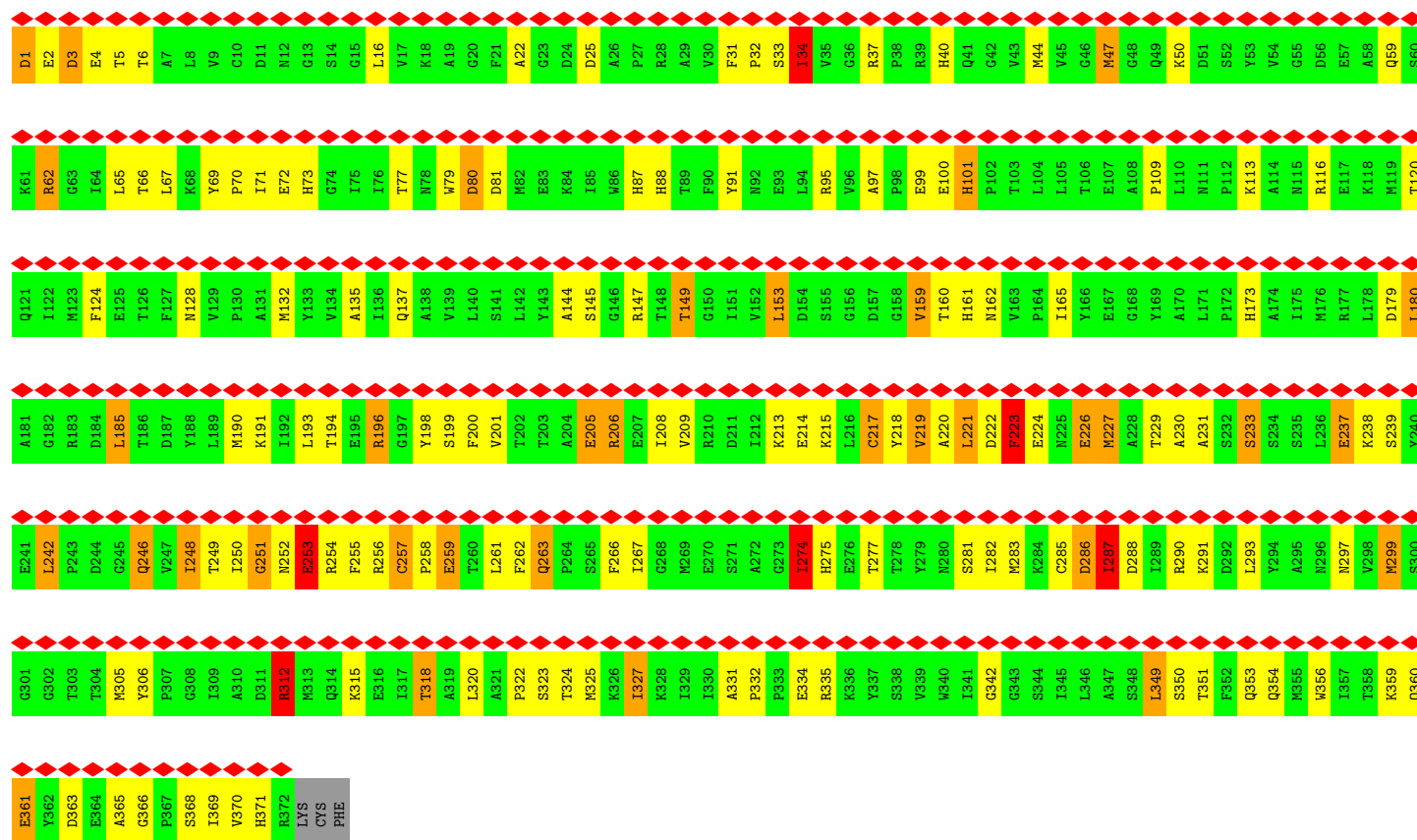


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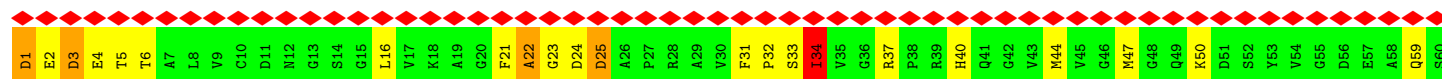




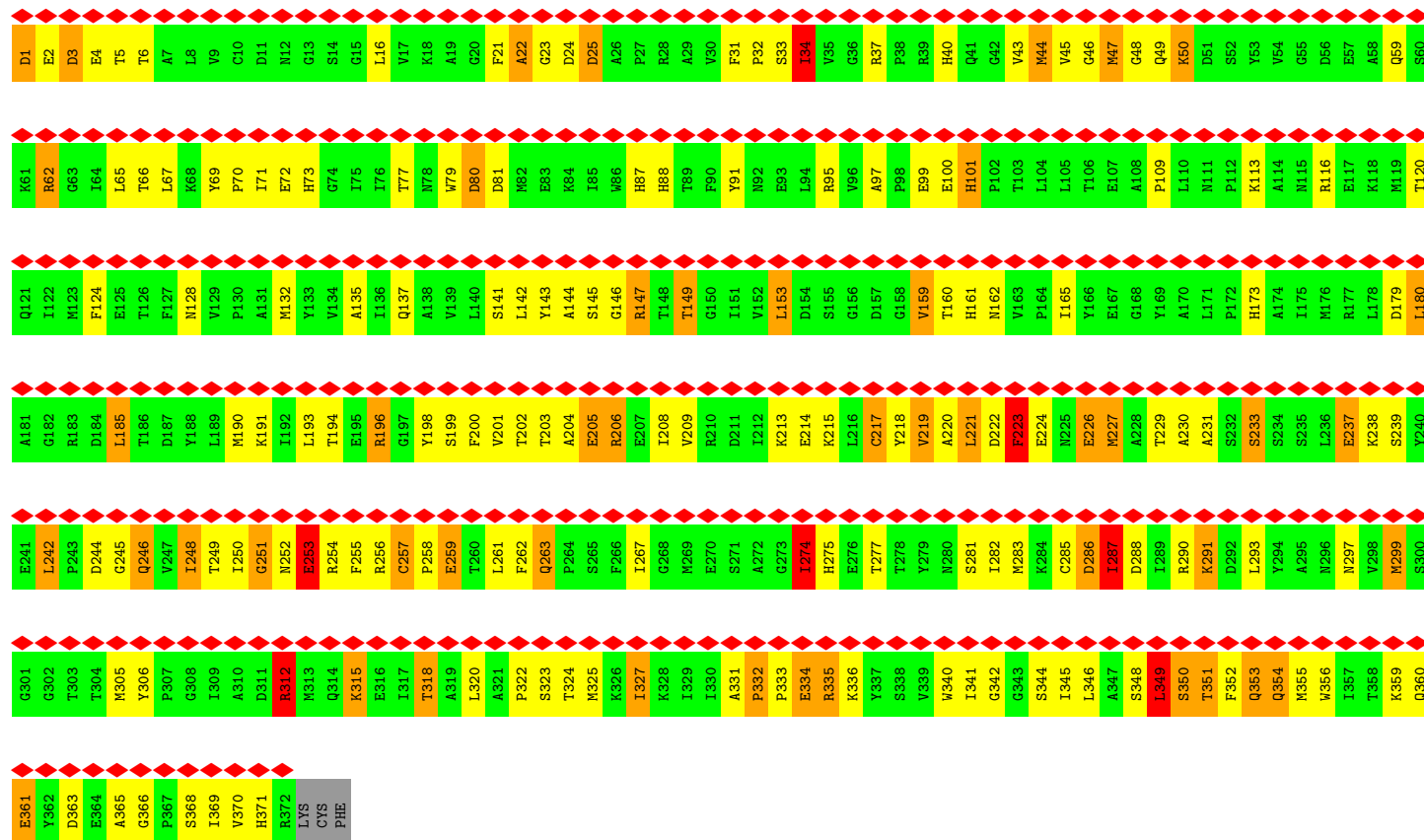
• Molecule 4: SKELETAL MUSCLE ACTIN



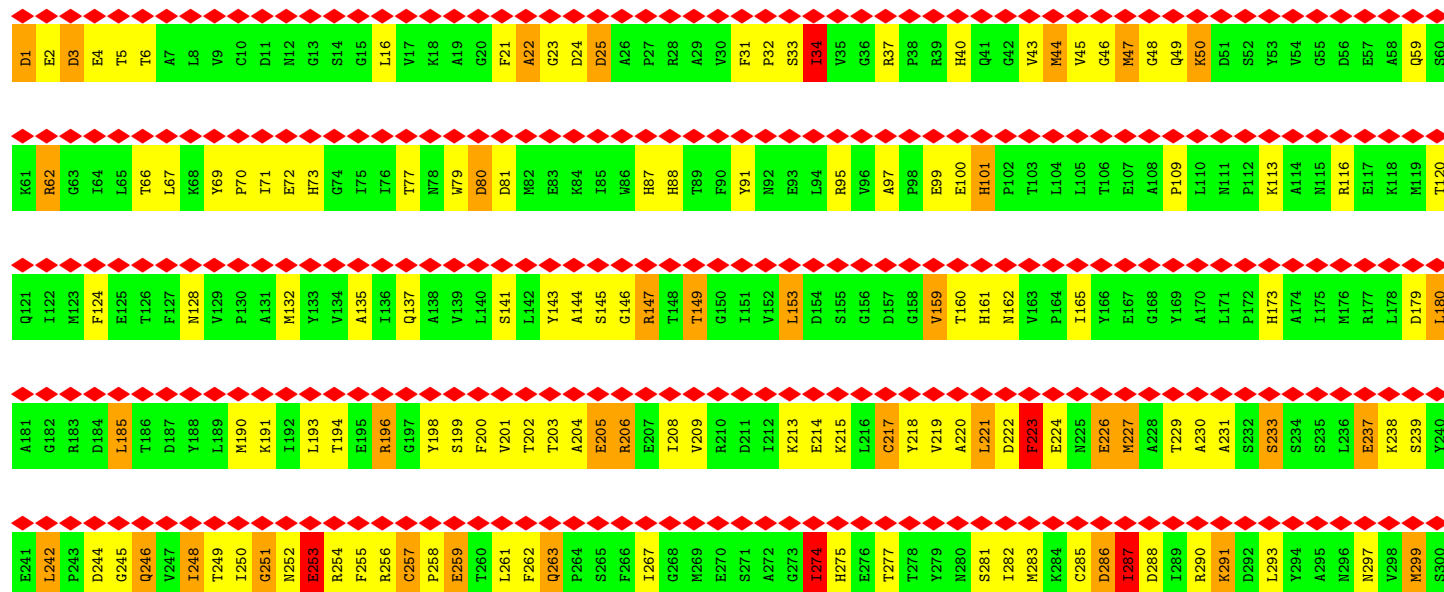
• Molecule 4: SKELETAL MUSCLE ACTIN

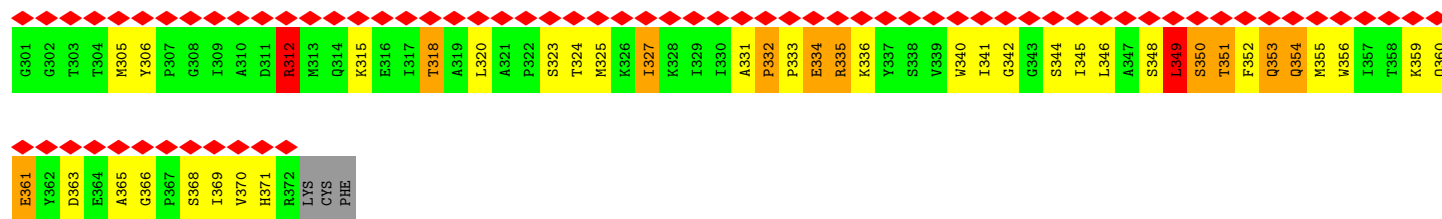


Chain V:

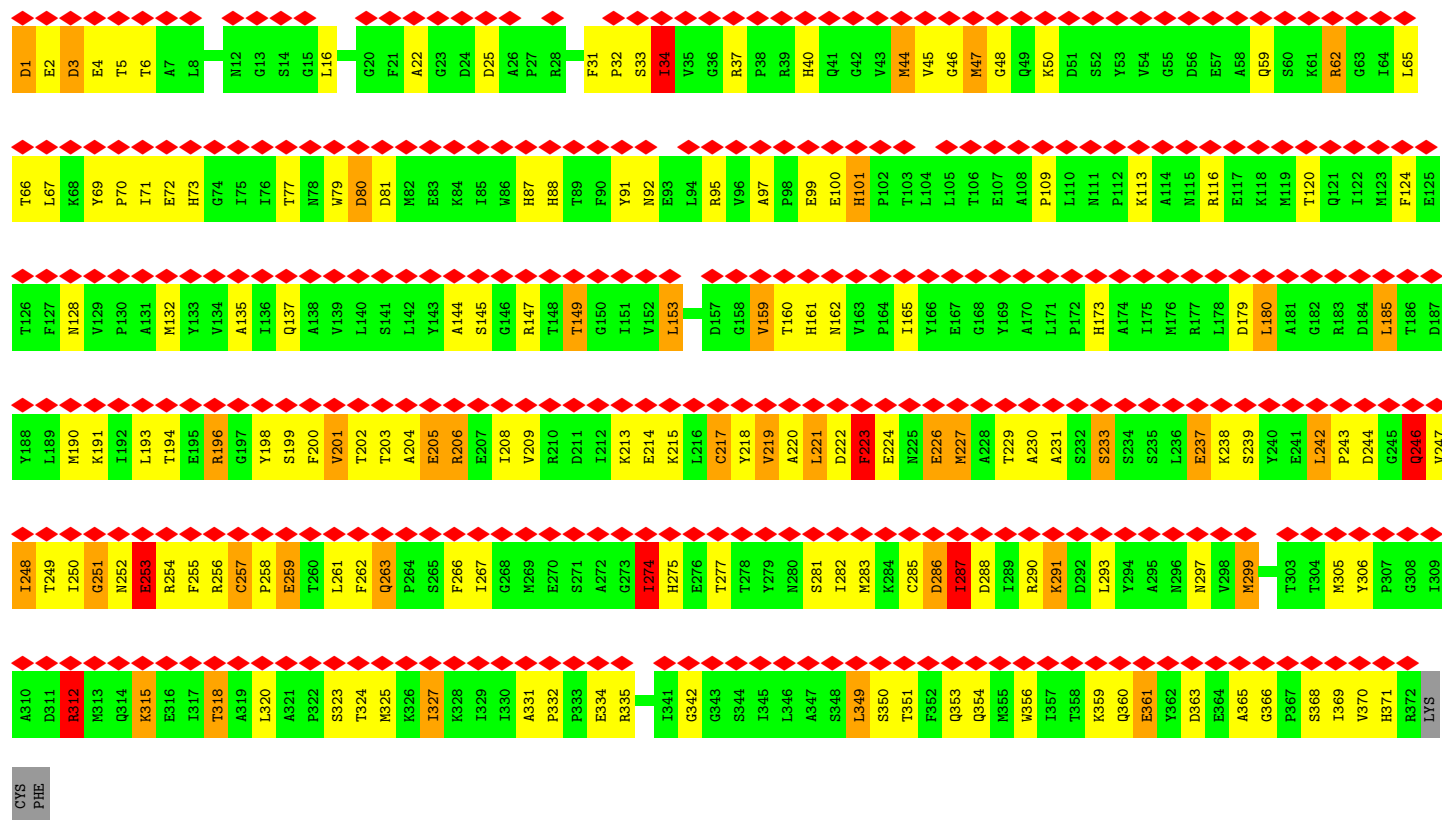


Chain W:

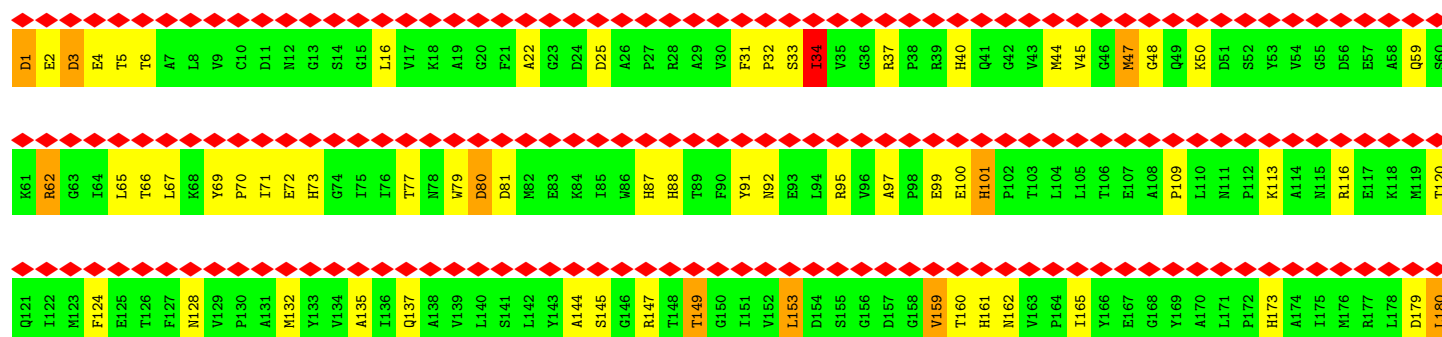


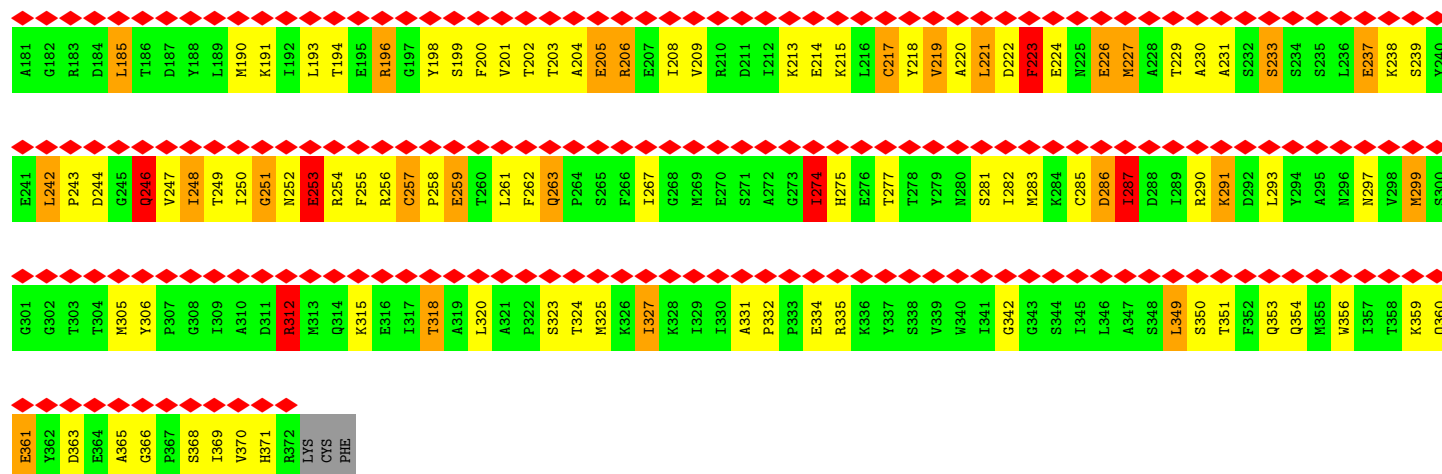


• Molecule 4: SKELETAL MUSCLE ACTIN

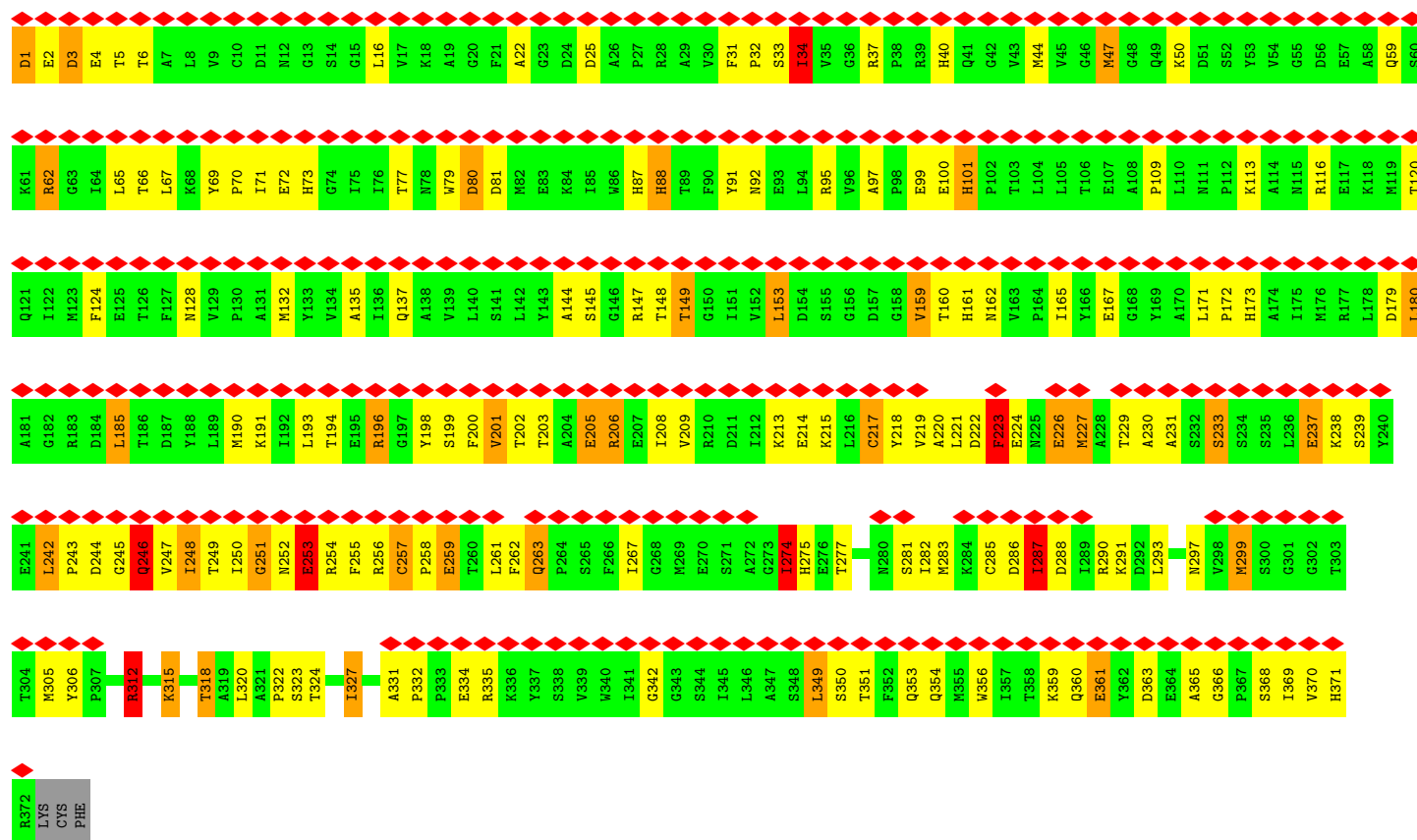
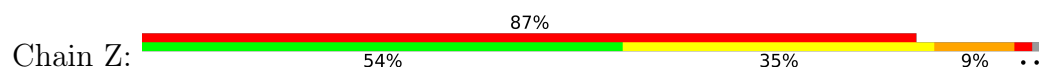


• Molecule 4: SKELETAL MUSCLE ACTIN





• 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	44/6448 (0.7%)	2.12	152/8729 (1.7%)
1	D	1.85	39/6448 (0.6%)	2.13	151/8729 (1.7%)
1	G	1.86	41/6448 (0.6%)	2.13	156/8729 (1.8%)
1	J	2.05	44/6449 (0.7%)	2.16	149/8732 (1.7%)
2	B	1.38	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	16/1148 (1.4%)	1.47	21/1548 (1.4%)
2	K	1.37	15/1148 (1.3%)	1.47	21/1548 (1.4%)
3	C	0.88	4/1136 (0.4%)	1.18	6/1525 (0.4%)
3	F	0.88	4/1136 (0.4%)	1.18	6/1525 (0.4%)
3	I	0.88	4/1136 (0.4%)	1.18	5/1525 (0.3%)
3	L	0.87	4/1136 (0.4%)	1.18	5/1525 (0.3%)
4	0	1.17	12/2968 (0.4%)	2.00	96/4023 (2.4%)
4	1	1.17	13/2968 (0.4%)	2.00	101/4023 (2.5%)
4	2	1.17	13/2968 (0.4%)	2.00	98/4023 (2.4%)
4	3	1.17	13/2968 (0.4%)	2.00	98/4023 (2.4%)
4	4	1.17	13/2968 (0.4%)	2.00	100/4023 (2.5%)
4	5	1.17	13/2968 (0.4%)	2.00	98/4023 (2.4%)
4	7	1.17	13/2968 (0.4%)	2.00	99/4023 (2.5%)
4	8	1.17	12/2968 (0.4%)	2.00	97/4023 (2.4%)
4	9	1.17	12/2968 (0.4%)	2.00	98/4023 (2.4%)
4	V	1.17	12/2968 (0.4%)	2.00	98/4023 (2.4%)
4	W	1.17	13/2968 (0.4%)	2.00	98/4023 (2.4%)
4	X	1.17	13/2968 (0.4%)	2.00	98/4023 (2.4%)
4	Y	1.17	13/2968 (0.4%)	2.00	99/4023 (2.5%)
4	Z	1.17	13/2968 (0.4%)	2.00	99/4023 (2.5%)
All	All	1.46	425/76481 (0.6%)	1.98	2091/103533 (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	1	4
1	J	1	6
2	B	0	3
2	E	0	3
2	H	0	3
2	K	0	3
3	C	0	2
3	F	0	2
3	I	0	2
3	L	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	4	52

The worst 5 of 425 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	709	LYS	C-N	-68.49	0.33	1.33
1	A	648	THR	CB-OG1	42.59	2.11	1.43
1	G	648	THR	CB-OG1	42.57	2.11	1.43
1	J	648	THR	CB-OG1	42.55	2.11	1.43
1	D	648	THR	CB-OG1	42.53	2.11	1.43

The worst 5 of 2091 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	637	LYS	O-C-N	-74.34	23.72	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	637	LYS	O-C-N	-74.28	23.80	122.59
1	J	637	LYS	O-C-N	-74.27	23.81	122.59
1	A	637	LYS	O-C-N	-74.23	23.87	122.59
1	J	648	THR	CA-CB-OG1	-44.78	42.43	109.60

All (4) 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

5 of 52 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

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	6760	1441	0
1	D	6797	0	6769	1466	0
1	G	6797	0	6768	1432	0
1	J	6797	0	6775	1448	0
2	B	1127	0	1086	253	0
2	E	1127	0	1087	325	0
2	H	1127	0	1087	231	0
2	K	1127	0	1087	232	0
3	C	1123	0	1084	180	0
3	F	1123	0	1082	143	0
3	I	1123	0	1084	169	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	1123	0	1084	167	0
4	0	2906	0	2865	182	0
4	1	2906	0	2865	207	0
4	2	2906	0	2865	139	0
4	3	2906	0	2863	182	0
4	4	2906	0	2865	98	0
4	5	2906	0	2865	100	0
4	7	2906	0	2866	84	0
4	8	2906	0	2857	324	0
4	9	2906	0	2855	348	0
4	V	2906	0	2851	392	0
4	W	2906	0	2851	389	0
4	X	2906	0	2862	217	0
4	Y	2906	0	2863	191	0
4	Z	2906	0	2862	194	0
All	All	76872	0	75808	7895	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 52.

The worst 5 of 7895 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:G:797:PHE:CD1	3:I:149:VAL:HG11	1.21	1.69
2:E:144:VAL:HG13	2:E:153:ILE:CD1	1.22	1.66
1:A:725:ARG:HE	1:A:733:PRO:CB	1.09	1.64
1:D:725:ARG:HE	1:D:733:PRO:CB	1.09	1.64
1:G:798:LEU:CD1	3:I:126:LEU:HD21	1.22	1.64

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%)	650 (82%)	113 (14%)	26 (3%)	3	21
1	D	789/840 (94%)	650 (82%)	113 (14%)	26 (3%)	3	21
1	G	789/840 (94%)	650 (82%)	112 (14%)	27 (3%)	3	21
1	J	791/840 (94%)	652 (82%)	112 (14%)	27 (3%)	3	21
2	B	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	1	14
2	E	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	1	14
2	H	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	1	14
2	K	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	1	14
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
4	0	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	7	38
4	1	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	7	38
4	2	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	7	38
4	3	370/375 (99%)	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%)	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%)	333 (90%)	31 (8%)	6 (2%)	7	38
4	V	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	7	38
4	W	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	7	38
4	X	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	7	38
4	Y	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	7	38
4	Z	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	7	38
All	All	9482/9778 (97%)	8316 (88%)	944 (10%)	222 (2%)	7	28

5 of 222 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	LYS
1	A	202	SER
1	A	572	LYS

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Mol	Chain	Res	Type
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%)	490 (73%)	182 (27%)	0	3
1	D	672/672 (100%)	490 (73%)	182 (27%)	0	3
1	G	672/672 (100%)	492 (73%)	180 (27%)	0	3
1	J	672/672 (100%)	491 (73%)	181 (27%)	0	3
2	B	120/120 (100%)	120 (100%)	0	100	100
2	E	120/120 (100%)	119 (99%)	1 (1%)	73	80
2	H	120/120 (100%)	120 (100%)	0	100	100
2	K	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
4	0	315/318 (99%)	264 (84%)	51 (16%)	2	11
4	1	315/318 (99%)	265 (84%)	50 (16%)	2	11
4	2	315/318 (99%)	264 (84%)	51 (16%)	2	11
4	3	315/318 (99%)	264 (84%)	51 (16%)	2	11
4	4	315/318 (99%)	265 (84%)	50 (16%)	2	11
4	5	315/318 (99%)	264 (84%)	51 (16%)	2	11
4	7	315/318 (99%)	264 (84%)	51 (16%)	2	11
4	8	315/318 (99%)	264 (84%)	51 (16%)	2	11
4	9	315/318 (99%)	264 (84%)	51 (16%)	2	11
4	V	315/318 (99%)	264 (84%)	51 (16%)	2	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	W	315/318 (99%)	265 (84%)	50 (16%)	2	11
4	X	315/318 (99%)	264 (84%)	51 (16%)	2	11
4	Y	315/318 (99%)	264 (84%)	51 (16%)	2	11
4	Z	315/318 (99%)	264 (84%)	51 (16%)	2	11
All	All	8046/8088 (100%)	6593 (82%)	1453 (18%)	3	9

5 of 1453 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	3	287	ILE
4	8	361	GLU
4	4	99	GLU
4	3	283	MET
4	5	350	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 233 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	424	ASN
4	Y	137	GLN
4	1	40	HIS
4	Y	78	ASN
4	V	78	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

180 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	D	19	1	9,10,11	1.09	1 (11%)	6,11,13	0.58	0
1	MLY	D	59	1	9,10,11	0.85	0	6,11,13	0.47	0
1	MLY	D	296	1	9,10,11	0.63	0	6,11,13	0.35	0
1	MLY	J	839	1	9,10,11	0.65	0	6,11,13	0.77	0
1	MLY	D	84	1	9,10,11	0.52	0	6,11,13	0.81	0
1	MLY	G	248	1	9,10,11	0.80	0	6,11,13	0.66	0
1	MLY	G	19	1	9,10,11	1.04	1 (11%)	6,11,13	0.58	0
1	MLY	G	272	1	9,10,11	0.87	1 (11%)	6,11,13	0.53	0
1	MLY	A	659	1	9,10,11	0.85	1 (11%)	6,11,13	0.60	0
1	MLY	D	190	1	9,10,11	1.17	2 (22%)	6,11,13	0.54	0
1	MLY	J	35	1	9,10,11	0.73	0	6,11,13	0.38	0
1	MLY	J	84	1	9,10,11	0.52	0	6,11,13	0.81	0
1	MLY	G	436	1	9,10,11	0.95	1 (11%)	6,11,13	0.47	0
1	MLY	D	764	1	9,10,11	0.83	0	6,11,13	0.35	0
1	MLY	A	295	1	9,10,11	0.80	0	6,11,13	0.34	0
1	MLY	A	55	1	9,10,11	0.72	0	6,11,13	0.80	0
1	MLY	G	827	1	9,10,11	0.68	0	6,11,13	0.49	0
1	MLY	J	827	1	9,10,11	0.71	0	6,11,13	0.48	0
1	MLY	D	130	1	9,10,11	0.80	0	6,11,13	0.72	0
1	MLY	A	87	1	9,10,11	1.11	1 (11%)	6,11,13	0.41	0
1	MLY	A	768	1	9,10,11	0.76	0	6,11,13	0.41	0
1	MLY	J	528	1	9,10,11	0.88	0	6,11,13	0.66	0
1	MLY	A	504	1	9,10,11	0.88	0	6,11,13	0.24	0
1	MLY	J	782	1	9,10,11	0.81	0	6,11,13	0.36	0
1	MLY	A	833	1	9,10,11	1.13	1 (11%)	6,11,13	0.32	0
1	MLY	A	598	1	9,10,11	0.83	0	6,11,13	0.42	0
1	MLY	J	369	1	9,10,11	0.71	0	6,11,13	0.45	0
1	MLY	D	681	1	9,10,11	0.56	0	6,11,13	0.46	0
1	MLY	J	415	1	9,10,11	0.75	0	6,11,13	0.19	0
1	MLY	G	659	1	9,10,11	0.84	1 (11%)	6,11,13	0.59	0
1	MLY	G	681	1	9,10,11	0.58	0	6,11,13	0.45	0
1	MLY	D	385	1	9,10,11	0.91	1 (11%)	6,11,13	0.44	0
1	MLY	G	613	1	9,10,11	0.59	0	6,11,13	0.62	0
1	MLY	D	486	1	9,10,11	0.67	0	6,11,13	0.41	0
1	MLY	J	486	1	9,10,11	0.66	0	6,11,13	0.39	0
1	MLY	D	504	1	9,10,11	0.87	0	6,11,13	0.20	0
1	MLY	G	87	1	9,10,11	1.16	1 (11%)	6,11,13	0.43	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	0.42	0
1	MLY	J	837	1	9,10,11	0.59	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	837	1	9,10,11	0.59	0	6,11,13	0.54	0
1	MLY	D	553	1,4	9,10,11	0.64	0	6,11,13	0.55	0
1	MLY	A	551	1	9,10,11	0.51	0	6,11,13	0.18	0
1	MLY	A	782	1	9,10,11	0.81	0	6,11,13	0.37	0
1	MLY	D	436	1	9,10,11	1.00	1 (11%)	6,11,13	0.48	0
1	MLY	J	138	1	9,10,11	1.22	1 (11%)	6,11,13	0.82	0
1	MLY	G	348	1	9,10,11	0.80	0	6,11,13	0.47	0
1	MLY	G	367	1	9,10,11	0.60	0	6,11,13	0.39	0
1	MLY	D	63	1	9,10,11	0.87	0	6,11,13	0.46	0
1	MLY	A	49	1	9,10,11	0.94	1 (11%)	6,11,13	0.74	0
1	MLY	G	55	1	9,10,11	0.74	0	6,11,13	0.81	0
1	MLY	G	600	1	9,10,11	0.52	0	6,11,13	0.38	0
1	MLY	G	617	1	9,10,11	0.92	0	6,11,13	0.35	0
1	MLY	D	107	1	9,10,11	0.52	0	6,11,13	0.32	0
1	MLY	D	837	1	9,10,11	0.59	0	6,11,13	0.58	0
1	MLY	A	30	1	9,10,11	0.90	0	6,11,13	0.31	0
1	MLY	J	19	1	9,10,11	1.07	1 (11%)	6,11,13	0.58	0
1	MLY	D	551	1	9,10,11	0.52	0	6,11,13	0.19	0
1	MLY	A	486	1	9,10,11	0.68	0	6,11,13	0.39	0
1	MLY	G	833	1	9,10,11	1.16	2 (22%)	6,11,13	0.31	0
1	MLY	J	505	1	9,10,11	0.85	1 (11%)	6,11,13	0.34	0
1	MLY	G	296	1	9,10,11	0.62	0	6,11,13	0.37	0
1	MLY	D	236	1	9,10,11	0.84	1 (11%)	6,11,13	0.48	0
1	MLY	J	598	1	9,10,11	0.83	1 (11%)	6,11,13	0.42	0
1	MLY	G	764	1	9,10,11	0.80	0	6,11,13	0.36	0
1	MLY	G	598	1	9,10,11	0.83	1 (11%)	6,11,13	0.41	0
1	MLY	D	55	1	9,10,11	0.72	0	6,11,13	0.81	0
1	MLY	D	353	1	9,10,11	0.85	0	6,11,13	0.81	0
1	MLY	D	87	1	9,10,11	1.10	1 (11%)	6,11,13	0.44	0
1	MLY	D	49	1	9,10,11	1.00	1 (11%)	6,11,13	0.74	0
1	MLY	D	833	1	9,10,11	1.11	1 (11%)	6,11,13	0.31	0
1	MLY	A	617	1	9,10,11	0.88	0	6,11,13	0.35	0
1	MLY	G	505	1	9,10,11	0.83	1 (11%)	6,11,13	0.34	0
1	MLY	J	59	1	9,10,11	0.84	0	6,11,13	0.48	0
1	MLY	G	35	1	9,10,11	0.73	0	6,11,13	0.39	0
1	MLY	A	436	1	9,10,11	0.96	1 (11%)	6,11,13	0.48	0
1	MLY	A	505	1	9,10,11	0.84	1 (11%)	6,11,13	0.32	0
1	MLY	J	613	1	9,10,11	0.55	0	6,11,13	0.62	0
1	MLY	G	353	1	9,10,11	0.85	0	6,11,13	0.81	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	D	348	1	9,10,11	0.77	0	6,11,13	0.47	0
1	MLY	J	348	1	9,10,11	0.78	0	6,11,13	0.47	0
1	MLY	D	367	1	9,10,11	0.59	0	6,11,13	0.38	0
1	MLY	D	35	1	9,10,11	0.73	0	6,11,13	0.37	0
1	MLY	J	768	1	9,10,11	0.75	0	6,11,13	0.42	0
1	MLY	A	138	1	9,10,11	1.23	1 (11%)	6,11,13	0.82	0
1	MLY	J	764	1	9,10,11	0.81	0	6,11,13	0.37	0
1	MLY	G	553	1,4	9,10,11	0.64	0	6,11,13	0.55	0
1	MLY	D	617	1	9,10,11	0.91	0	6,11,13	0.35	0
1	MLY	D	248	1	9,10,11	0.81	0	6,11,13	0.65	0
1	MLY	J	248	1	9,10,11	0.81	0	6,11,13	0.65	0
1	MLY	A	528	1	9,10,11	0.89	0	6,11,13	0.67	0
1	MLY	G	295	1	9,10,11	0.77	0	6,11,13	0.36	0
1	MLY	J	272	1	9,10,11	0.92	1 (11%)	6,11,13	0.56	0
1	MLY	D	782	1	9,10,11	0.80	0	6,11,13	0.35	0
1	MLY	A	839	1,2	9,10,11	0.66	0	6,11,13	0.82	0
1	MLY	G	236	1	9,10,11	0.82	1 (11%)	6,11,13	0.48	0
1	MLY	J	236	1	9,10,11	0.83	1 (11%)	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	J	681	1	9,10,11	0.57	0	6,11,13	0.46	0
1	MLY	J	130	1	9,10,11	0.76	0	6,11,13	0.74	0
1	MLY	G	190	1	9,10,11	1.21	2 (22%)	6,11,13	0.52	0
1	MLY	G	837	1	9,10,11	0.60	0	6,11,13	0.53	0
1	MLY	G	385	1	9,10,11	0.92	1 (11%)	6,11,13	0.45	0
1	MLY	A	348	1	9,10,11	0.79	0	6,11,13	0.48	0
1	MLY	J	190	1	9,10,11	1.22	2 (22%)	6,11,13	0.52	0
1	MLY	A	63	1	9,10,11	0.88	0	6,11,13	0.43	0
1	MLY	D	30	1	9,10,11	0.92	0	6,11,13	0.31	0
1	MLY	J	49	1	9,10,11	0.99	1 (11%)	6,11,13	0.75	0
1	MLY	D	839	1	9,10,11	0.66	0	6,11,13	0.79	0
1	MLY	J	504	1	9,10,11	0.83	0	6,11,13	0.22	0
1	MLY	G	839	1	9,10,11	0.66	0	6,11,13	0.79	0
1	MLY	J	385	1	9,10,11	0.95	1 (11%)	6,11,13	0.45	0
1	MLY	J	659	1	9,10,11	0.82	1 (11%)	6,11,13	0.58	0
1	MLY	A	272	1	9,10,11	0.92	1 (11%)	6,11,13	0.56	0
1	MLY	D	431	1	9,10,11	0.52	0	6,11,13	0.46	0
1	MLY	D	505	1	9,10,11	0.80	0	6,11,13	0.35	0
1	MLY	D	528	1	9,10,11	0.92	0	6,11,13	0.65	0
1	MLY	G	30	1	9,10,11	0.90	0	6,11,13	0.30	0
1	MLY	A	613	1	9,10,11	0.56	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	A	415	1	9,10,11	0.74	0	6,11,13	0.20	0
1	MLY	J	295	1	9,10,11	0.76	0	6,11,13	0.37	0
1	MLY	A	130	1	9,10,11	0.79	0	6,11,13	0.73	0
1	MLY	A	431	1	9,10,11	0.52	0	6,11,13	0.44	0
1	MLY	A	107	1	9,10,11	0.47	0	6,11,13	0.32	0
1	MLY	G	504	1	9,10,11	0.88	0	6,11,13	0.22	0
1	MLY	G	551	1	9,10,11	0.51	0	6,11,13	0.19	0
1	MLY	J	833	1	9,10,11	1.15	2 (22%)	6,11,13	0.30	0
1	MLY	D	369	1	9,10,11	0.71	0	6,11,13	0.45	0
1	MLY	J	353	1	9,10,11	0.87	0	6,11,13	0.79	0
1	MLY	D	613	1	9,10,11	0.57	0	6,11,13	0.62	0
1	MLY	D	415	1	9,10,11	0.76	0	6,11,13	0.20	0
1	MLY	G	49	1	9,10,11	1.01	1 (11%)	6,11,13	0.74	0
1	MLY	J	553	1	9,10,11	0.64	0	6,11,13	0.53	0
1	MLY	J	107	1	9,10,11	0.48	0	6,11,13	0.33	0
1	MLY	A	190	1	9,10,11	1.25	2 (22%)	6,11,13	0.52	0
1	MLY	J	600	1	9,10,11	0.54	0	6,11,13	0.38	0
1	MLY	A	553	1,4	9,10,11	0.65	0	6,11,13	0.55	0
1	MLY	A	827	1	9,10,11	0.70	0	6,11,13	0.44	0
1	MLY	G	138	1	9,10,11	1.21	1 (11%)	6,11,13	0.82	0
1	MLY	A	35	1	9,10,11	0.74	0	6,11,13	0.38	0
1	MLY	D	138	1	9,10,11	1.26	1 (11%)	6,11,13	0.84	0
1	MLY	G	431	1	9,10,11	0.52	0	6,11,13	0.47	0
1	MLY	J	30	1	9,10,11	0.91	0	6,11,13	0.31	0
1	MLY	J	367	1	9,10,11	0.58	0	6,11,13	0.37	0
1	MLY	D	598	1	9,10,11	0.86	1 (11%)	6,11,13	0.42	0
1	MLY	G	415	1	9,10,11	0.74	0	6,11,13	0.19	0
1	MLY	J	296	1	9,10,11	0.67	0	6,11,13	0.35	0
1	MLY	G	107	1	9,10,11	0.49	0	6,11,13	0.32	0
1	MLY	A	248	1	9,10,11	0.81	0	6,11,13	0.64	0
1	MLY	J	551	1	9,10,11	0.51	0	6,11,13	0.18	0
1	MLY	D	272	1	9,10,11	0.89	1 (11%)	6,11,13	0.58	0
1	MLY	A	385	1	9,10,11	0.93	1 (11%)	6,11,13	0.44	0
1	MLY	G	782	1	9,10,11	0.82	1 (11%)	6,11,13	0.35	0
1	MLY	G	528	1	9,10,11	0.91	0	6,11,13	0.66	0
1	MLY	A	353	1	9,10,11	0.87	0	6,11,13	0.79	0
1	MLY	D	295	1	9,10,11	0.76	0	6,11,13	0.37	0
1	MLY	A	600	1	9,10,11	0.53	0	6,11,13	0.39	0
1	MLY	G	130	1	9,10,11	0.78	0	6,11,13	0.74	0
1	MLY	D	827	1	9,10,11	0.66	0	6,11,13	0.48	0
1	MLY	J	55	1	9,10,11	0.73	0	6,11,13	0.80	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	G	63	1	9,10,11	0.86	0	6,11,13	0.44	0
1	MLY	G	369	1	9,10,11	0.71	0	6,11,13	0.47	0
1	MLY	J	63	1	9,10,11	0.88	0	6,11,13	0.44	0
1	MLY	A	367	1	9,10,11	0.59	0	6,11,13	0.37	0
1	MLY	J	436	1	9,10,11	0.98	1 (11%)	6,11,13	0.48	0
1	MLY	A	369	1	9,10,11	0.72	0	6,11,13	0.46	0
1	MLY	A	236	1	9,10,11	0.83	1 (11%)	6,11,13	0.48	0
1	MLY	A	19	1	9,10,11	1.03	1 (11%)	6,11,13	0.57	0
1	MLY	A	59	1	9,10,11	0.85	0	6,11,13	0.48	0
1	MLY	A	296	1	9,10,11	0.60	0	6,11,13	0.34	0
1	MLY	J	431	1	9,10,11	0.52	0	6,11,13	0.45	0
1	MLY	D	768	1	9,10,11	0.73	0	6,11,13	0.41	0
1	MLY	A	84	1	9,10,11	0.50	0	6,11,13	0.80	0
1	MLY	D	659	1	9,10,11	0.85	1 (11%)	6,11,13	0.59	0
1	MLY	D	600	1	9,10,11	0.52	0	6,11,13	0.39	0
1	MLY	A	681	1	9,10,11	0.57	0	6,11,13	0.46	0
1	MLY	J	617	1	9,10,11	0.91	1 (11%)	6,11,13	0.34	0
1	MLY	G	486	1	9,10,11	0.67	0	6,11,13	0.40	0
1	MLY	J	87	1	9,10,11	1.12	1 (11%)	6,11,13	0.43	0
1	MLY	A	764	1	9,10,11	0.82	0	6,11,13	0.36	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	D	19	1	-	4/8/9/11	-
1	MLY	D	59	1	-	3/8/9/11	-
1	MLY	D	296	1	-	4/8/9/11	-
1	MLY	J	839	1	-	3/8/9/11	-
1	MLY	D	84	1	-	4/8/9/11	-
1	MLY	G	248	1	-	6/8/9/11	-
1	MLY	G	19	1	-	4/8/9/11	-
1	MLY	G	272	1	-	3/8/9/11	-
1	MLY	A	659	1	-	3/8/9/11	-
1	MLY	D	190	1	-	4/8/9/11	-
1	MLY	J	35	1	-	3/8/9/11	-
1	MLY	J	84	1	-	4/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	G	436	1	-	4/8/9/11	-
1	MLY	D	764	1	-	2/8/9/11	-
1	MLY	A	295	1	-	2/8/9/11	-
1	MLY	A	55	1	-	6/8/9/11	-
1	MLY	G	827	1	-	1/8/9/11	-
1	MLY	J	827	1	-	1/8/9/11	-
1	MLY	D	130	1	-	5/8/9/11	-
1	MLY	A	87	1	-	2/8/9/11	-
1	MLY	A	768	1	-	4/8/9/11	-
1	MLY	J	528	1	-	4/8/9/11	-
1	MLY	A	504	1	-	4/8/9/11	-
1	MLY	J	782	1	-	6/8/9/11	-
1	MLY	A	833	1	-	6/8/9/11	-
1	MLY	A	598	1	-	5/8/9/11	-
1	MLY	J	369	1	-	2/8/9/11	-
1	MLY	D	681	1	-	4/8/9/11	-
1	MLY	J	415	1	-	3/8/9/11	-
1	MLY	G	659	1	-	3/8/9/11	-
1	MLY	G	681	1	-	4/8/9/11	-
1	MLY	D	385	1	-	2/8/9/11	-
1	MLY	G	613	1	-	3/8/9/11	-
1	MLY	D	486	1	-	2/8/9/11	-
1	MLY	J	486	1	-	2/8/9/11	-
1	MLY	D	504	1	-	4/8/9/11	-
1	MLY	G	87	1	-	2/8/9/11	-
1	MLY	G	59	1	-	3/8/9/11	-
1	MLY	G	768	1	-	4/8/9/11	-
1	MLY	J	837	1	-	6/8/9/11	-
1	MLY	A	837	1	-	6/8/9/11	-
1	MLY	D	553	1,4	-	5/8/9/11	-
1	MLY	A	551	1	-	3/8/9/11	-
1	MLY	A	782	1	-	6/8/9/11	-
1	MLY	D	436	1	-	4/8/9/11	-
1	MLY	J	138	1	-	4/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	G	348	1	-	5/8/9/11	-
1	MLY	G	367	1	-	2/8/9/11	-
1	MLY	D	63	1	-	4/8/9/11	-
1	MLY	A	49	1	-	3/8/9/11	-
1	MLY	G	55	1	-	6/8/9/11	-
1	MLY	G	600	1	-	3/8/9/11	-
1	MLY	G	617	1	-	2/8/9/11	-
1	MLY	D	107	1	-	2/8/9/11	-
1	MLY	D	837	1	-	6/8/9/11	-
1	MLY	A	30	1	-	3/8/9/11	-
1	MLY	J	19	1	-	4/8/9/11	-
1	MLY	D	551	1	-	3/8/9/11	-
1	MLY	A	486	1	-	2/8/9/11	-
1	MLY	G	833	1	-	6/8/9/11	-
1	MLY	J	505	1	-	5/8/9/11	-
1	MLY	G	296	1	-	4/8/9/11	-
1	MLY	D	236	1	-	3/8/9/11	-
1	MLY	J	598	1	-	5/8/9/11	-
1	MLY	G	764	1	-	2/8/9/11	-
1	MLY	G	598	1	-	5/8/9/11	-
1	MLY	D	55	1	-	6/8/9/11	-
1	MLY	D	353	1	-	4/8/9/11	-
1	MLY	D	87	1	-	2/8/9/11	-
1	MLY	D	49	1	-	3/8/9/11	-
1	MLY	D	833	1	-	6/8/9/11	-
1	MLY	A	617	1	-	2/8/9/11	-
1	MLY	G	505	1	-	5/8/9/11	-
1	MLY	J	59	1	-	3/8/9/11	-
1	MLY	G	35	1	-	3/8/9/11	-
1	MLY	A	436	1	-	4/8/9/11	-
1	MLY	A	505	1	-	5/8/9/11	-
1	MLY	J	613	1	-	3/8/9/11	-
1	MLY	G	353	1	-	4/8/9/11	-
1	MLY	D	348	1	-	5/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	J	348	1	-	5/8/9/11	-
1	MLY	D	367	1	-	2/8/9/11	-
1	MLY	D	35	1	-	3/8/9/11	-
1	MLY	J	768	1	-	4/8/9/11	-
1	MLY	A	138	1	-	4/8/9/11	-
1	MLY	J	764	1	-	2/8/9/11	-
1	MLY	G	553	1,4	-	4/8/9/11	-
1	MLY	D	617	1	-	2/8/9/11	-
1	MLY	D	248	1	-	6/8/9/11	-
1	MLY	J	248	1	-	6/8/9/11	-
1	MLY	A	528	1	-	4/8/9/11	-
1	MLY	G	295	1	-	2/8/9/11	-
1	MLY	J	272	1	-	3/8/9/11	-
1	MLY	D	782	1	-	6/8/9/11	-
1	MLY	A	839	1,2	-	3/8/9/11	-
1	MLY	G	236	1	-	3/8/9/11	-
1	MLY	J	236	1	-	3/8/9/11	-
1	MLY	G	84	1	-	4/8/9/11	-
1	MLY	J	681	1	-	4/8/9/11	-
1	MLY	J	130	1	-	5/8/9/11	-
1	MLY	G	190	1	-	4/8/9/11	-
1	MLY	G	837	1	-	6/8/9/11	-
1	MLY	G	385	1	-	2/8/9/11	-
1	MLY	A	348	1	-	5/8/9/11	-
1	MLY	J	190	1	-	4/8/9/11	-
1	MLY	A	63	1	-	4/8/9/11	-
1	MLY	D	30	1	-	3/8/9/11	-
1	MLY	J	49	1	-	3/8/9/11	-
1	MLY	D	839	1	-	3/8/9/11	-
1	MLY	J	504	1	-	4/8/9/11	-
1	MLY	G	839	1	-	3/8/9/11	-
1	MLY	J	385	1	-	2/8/9/11	-
1	MLY	J	659	1	-	3/8/9/11	-
1	MLY	A	272	1	-	3/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	D	431	1	-	4/8/9/11	-
1	MLY	D	505	1	-	5/8/9/11	-
1	MLY	D	528	1	-	4/8/9/11	-
1	MLY	G	30	1	-	3/8/9/11	-
1	MLY	A	613	1	-	3/8/9/11	-
1	MLY	A	415	1	-	3/8/9/11	-
1	MLY	J	295	1	-	2/8/9/11	-
1	MLY	A	130	1	-	5/8/9/11	-
1	MLY	A	431	1	-	4/8/9/11	-
1	MLY	A	107	1	-	2/8/9/11	-
1	MLY	G	504	1	-	4/8/9/11	-
1	MLY	G	551	1	-	3/8/9/11	-
1	MLY	J	833	1	-	6/8/9/11	-
1	MLY	D	369	1	-	2/8/9/11	-
1	MLY	J	353	1	-	4/8/9/11	-
1	MLY	D	613	1	-	3/8/9/11	-
1	MLY	D	415	1	-	3/8/9/11	-
1	MLY	G	49	1	-	3/8/9/11	-
1	MLY	J	553	1	-	4/8/9/11	-
1	MLY	J	107	1	-	2/8/9/11	-
1	MLY	A	190	1	-	4/8/9/11	-
1	MLY	J	600	1	-	3/8/9/11	-
1	MLY	A	553	1,4	-	4/8/9/11	-
1	MLY	A	827	1	-	1/8/9/11	-
1	MLY	G	138	1	-	4/8/9/11	-
1	MLY	A	35	1	-	3/8/9/11	-
1	MLY	D	138	1	-	4/8/9/11	-
1	MLY	G	431	1	-	4/8/9/11	-
1	MLY	J	30	1	-	3/8/9/11	-
1	MLY	J	367	1	-	2/8/9/11	-
1	MLY	D	598	1	-	5/8/9/11	-
1	MLY	G	415	1	-	3/8/9/11	-
1	MLY	J	296	1	-	4/8/9/11	-
1	MLY	G	107	1	-	2/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	A	248	1	-	6/8/9/11	-
1	MLY	J	551	1	-	3/8/9/11	-
1	MLY	D	272	1	-	3/8/9/11	-
1	MLY	A	385	1	-	2/8/9/11	-
1	MLY	G	782	1	-	6/8/9/11	-
1	MLY	G	528	1	-	4/8/9/11	-
1	MLY	A	353	1	-	4/8/9/11	-
1	MLY	D	295	1	-	2/8/9/11	-
1	MLY	A	600	1	-	3/8/9/11	-
1	MLY	G	130	1	-	5/8/9/11	-
1	MLY	D	827	1	-	1/8/9/11	-
1	MLY	J	55	1	-	6/8/9/11	-
1	MLY	G	63	1	-	4/8/9/11	-
1	MLY	G	369	1	-	2/8/9/11	-
1	MLY	J	63	1	-	4/8/9/11	-
1	MLY	A	367	1	-	2/8/9/11	-
1	MLY	J	436	1	-	4/8/9/11	-
1	MLY	A	369	1	-	2/8/9/11	-
1	MLY	A	236	1	-	3/8/9/11	-
1	MLY	A	19	1	-	4/8/9/11	-
1	MLY	A	59	1	-	3/8/9/11	-
1	MLY	A	296	1	-	4/8/9/11	-
1	MLY	J	431	1	-	4/8/9/11	-
1	MLY	D	768	1	-	4/8/9/11	-
1	MLY	A	84	1	-	4/8/9/11	-
1	MLY	D	659	1	-	3/8/9/11	-
1	MLY	D	600	1	-	3/8/9/11	-
1	MLY	A	681	1	-	4/8/9/11	-
1	MLY	J	617	1	-	2/8/9/11	-
1	MLY	G	486	1	-	2/8/9/11	-
1	MLY	J	87	1	-	2/8/9/11	-
1	MLY	A	764	1	-	2/8/9/11	-

The worst 5 of 58 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	138	MLY	CB-CA	-3.37	1.48	1.53
1	A	138	MLY	CB-CA	-3.23	1.48	1.53
1	J	138	MLY	CB-CA	-3.21	1.48	1.53
1	G	138	MLY	CB-CA	-3.20	1.48	1.53
1	G	87	MLY	CB-CA	-2.92	1.49	1.53

There are no bond angle outliers.

There are no chirality outliers.

5 of 645 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.

125 monomers are involved in 534 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	59	MLY	2	0
1	D	296	MLY	3	0
1	J	839	MLY	5	0
1	G	248	MLY	2	0
1	G	272	MLY	1	0
1	A	659	MLY	2	0
1	D	190	MLY	2	0
1	J	84	MLY	25	0
1	G	436	MLY	2	0
1	D	764	MLY	2	0
1	A	295	MLY	6	0
1	A	55	MLY	1	0
1	G	827	MLY	1	0
1	J	827	MLY	1	0
1	A	87	MLY	3	0
1	A	768	MLY	14	0
1	J	528	MLY	3	0
1	A	504	MLY	5	0
1	J	782	MLY	1	0
1	A	598	MLY	1	0
1	J	415	MLY	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	G	659	MLY	2	0
1	D	486	MLY	3	0
1	J	486	MLY	3	0
1	D	504	MLY	1	0
1	G	87	MLY	2	0
1	G	59	MLY	3	0
1	G	768	MLY	13	0
1	J	837	MLY	1	0
1	A	837	MLY	1	0
1	D	553	MLY	16	0
1	A	551	MLY	2	0
1	A	782	MLY	1	0
1	D	436	MLY	2	0
1	J	138	MLY	2	0
1	G	348	MLY	4	0
1	D	63	MLY	3	0
1	A	49	MLY	3	0
1	G	55	MLY	1	0
1	G	600	MLY	1	0
1	G	617	MLY	1	0
1	D	107	MLY	3	0
1	D	837	MLY	1	0
1	A	30	MLY	1	0
1	D	551	MLY	1	0
1	A	486	MLY	3	0
1	G	296	MLY	2	0
1	J	598	MLY	1	0
1	G	764	MLY	13	0
1	G	598	MLY	1	0
1	D	55	MLY	1	0
1	D	87	MLY	3	0
1	D	49	MLY	4	0
1	A	617	MLY	1	0
1	J	59	MLY	3	0
1	A	436	MLY	2	0
1	A	505	MLY	11	0
1	D	348	MLY	6	0
1	J	348	MLY	5	0
1	J	768	MLY	40	0
1	A	138	MLY	2	0
1	J	764	MLY	22	0
1	G	553	MLY	27	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	617	MLY	1	0
1	D	248	MLY	2	0
1	J	248	MLY	2	0
1	A	528	MLY	2	0
1	G	295	MLY	6	0
1	J	272	MLY	1	0
1	D	782	MLY	31	0
1	A	839	MLY	15	0
1	G	84	MLY	18	0
1	G	190	MLY	2	0
1	G	837	MLY	1	0
1	A	348	MLY	5	0
1	J	190	MLY	2	0
1	A	63	MLY	3	0
1	D	30	MLY	1	0
1	J	49	MLY	3	0
1	D	839	MLY	16	0
1	J	504	MLY	1	0
1	G	839	MLY	4	0
1	J	659	MLY	2	0
1	A	272	MLY	1	0
1	D	528	MLY	3	0
1	G	30	MLY	1	0
1	A	415	MLY	1	0
1	J	295	MLY	6	0
1	A	107	MLY	3	0
1	G	504	MLY	1	0
1	D	415	MLY	1	0
1	G	49	MLY	3	0
1	J	553	MLY	11	0
1	J	107	MLY	3	0
1	A	190	MLY	2	0
1	J	600	MLY	1	0
1	A	553	MLY	17	0
1	G	138	MLY	2	0
1	D	138	MLY	2	0
1	J	30	MLY	1	0
1	D	598	MLY	1	0
1	G	415	MLY	1	0
1	J	296	MLY	3	0
1	G	107	MLY	3	0
1	A	248	MLY	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	272	MLY	1	0
1	G	782	MLY	1	0
1	G	528	MLY	3	0
1	D	295	MLY	6	0
1	A	600	MLY	1	0
1	J	55	MLY	1	0
1	G	63	MLY	3	0
1	G	369	MLY	1	0
1	J	63	MLY	4	0
1	J	436	MLY	2	0
1	A	369	MLY	1	0
1	A	59	MLY	2	0
1	A	296	MLY	2	0
1	D	768	MLY	7	0
1	D	659	MLY	2	0
1	D	600	MLY	1	0
1	J	617	MLY	1	0
1	G	486	MLY	3	0
1	J	87	MLY	3	0
1	A	764	MLY	7	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	G	4

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Mol	Chain	Number of breaks
1	J	4
1	D	4
1	A	4
3	C	1
3	F	1
3	I	1
3	L	1
2	B	1
2	E	1
2	H	1
2	K	1

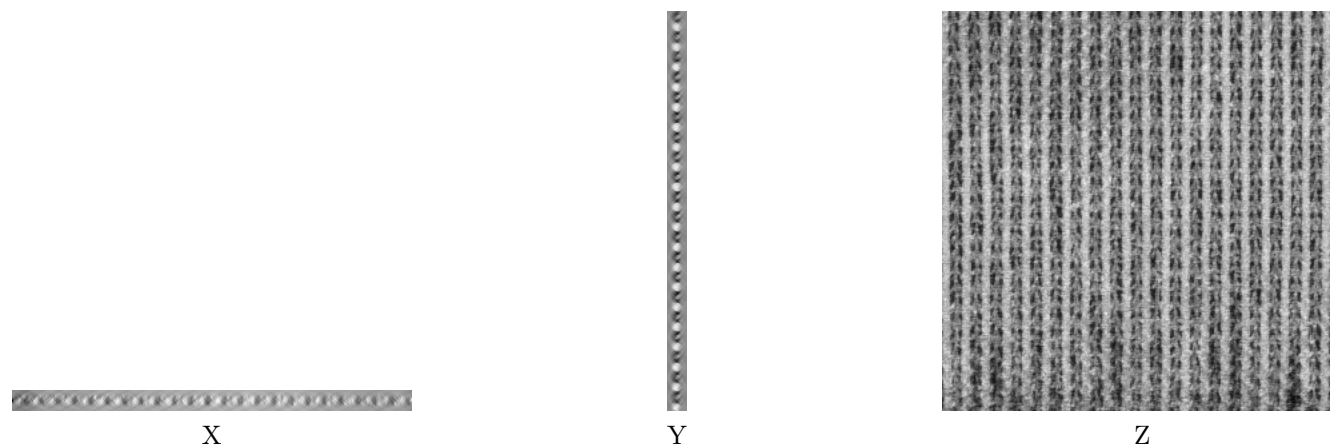
The worst 5 of 24 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	769:ALA	C	770:GLY	N	4.88
1	J	769:ALA	C	770:GLY	N	4.64
1	D	769:ALA	C	770:GLY	N	4.52
1	D	709:LYS	C	710:GLY	N	3.32
1	A	709:LYS	C	710:GLY	N	3.27

6 Tomogram visualisation [i](#)

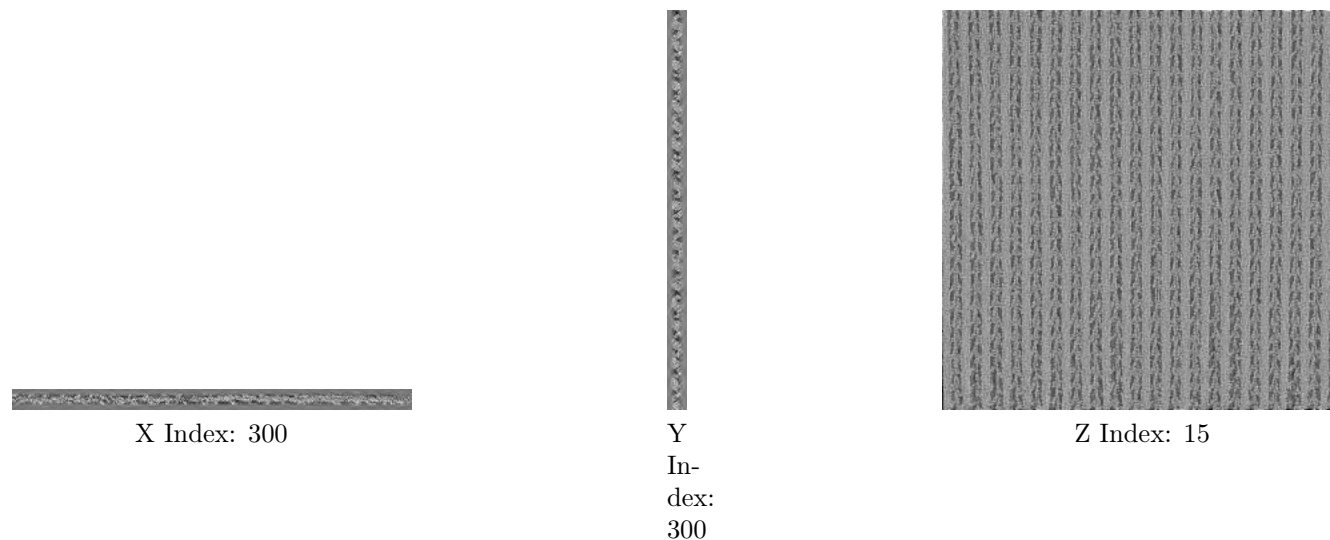
This section contains visualisations of the EMDB entry EMD-1001. These allow visual inspection of the internal detail of the tomogram and identification of artifacts.

6.1 Orthogonal projections [i](#)



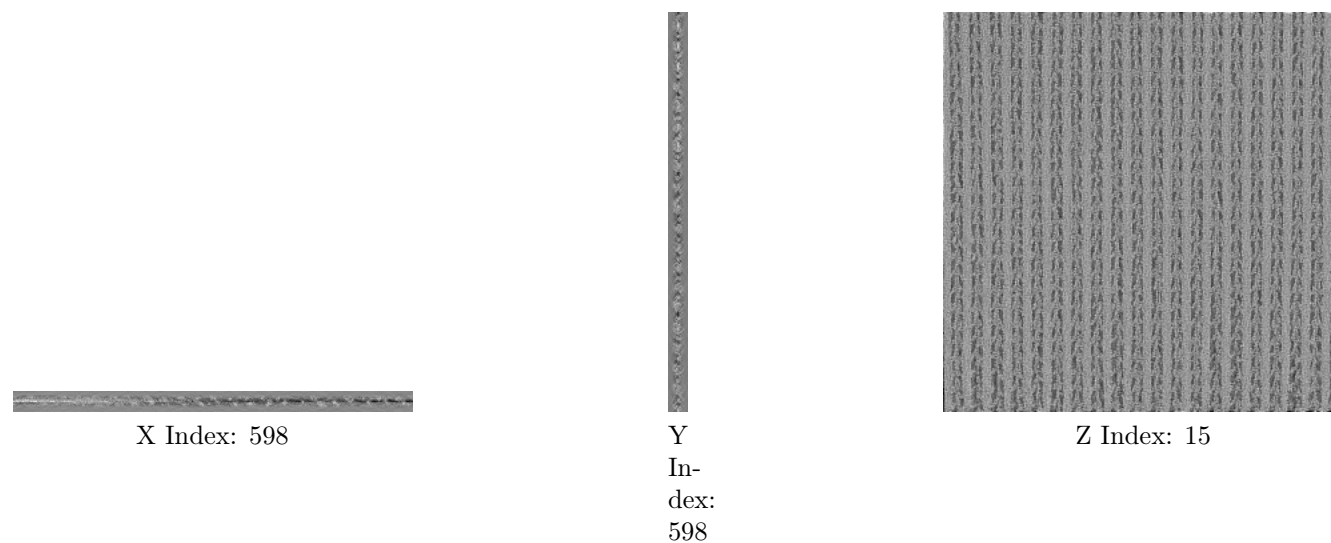
The images above show the tomogram projected in three orthogonal directions.

6.2 Central slices [i](#)



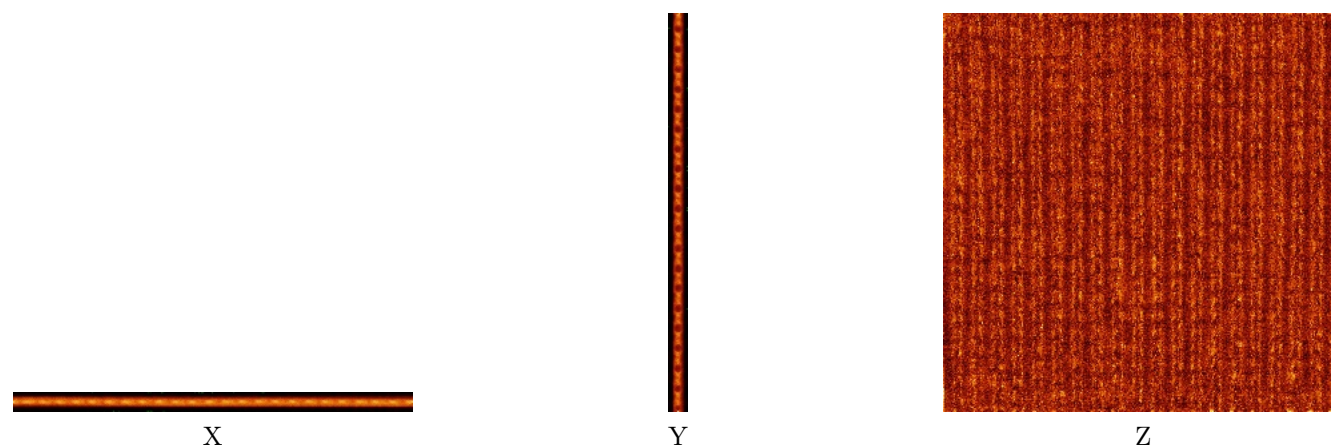
The images above show central slices of the tomogram in three orthogonal directions.

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.

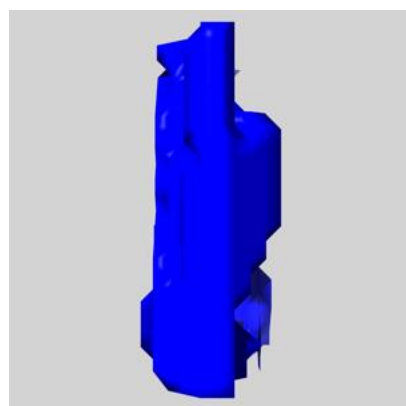
6.5 Mask visualisation [i](#)

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

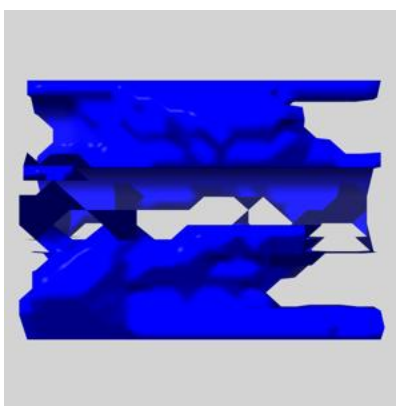
A mask typically either:

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

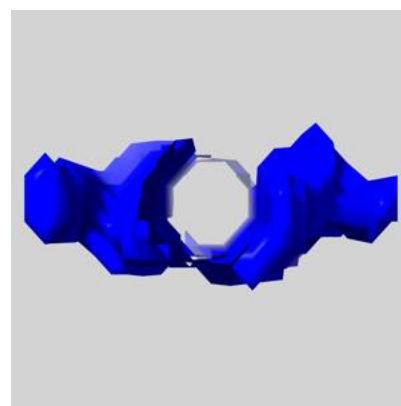
6.5.1 emd_1001_msk_25.map [i](#)



X

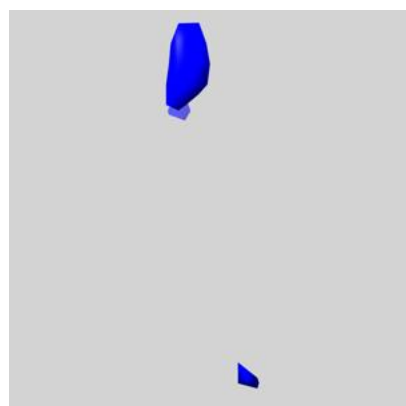


Y

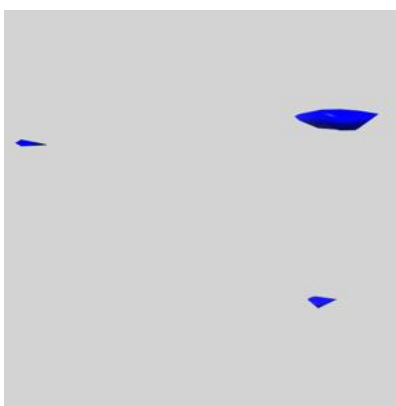


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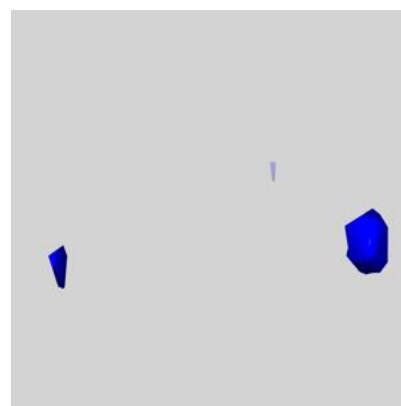
6.5.2 emd_1001_msk_24.map [i](#)



X

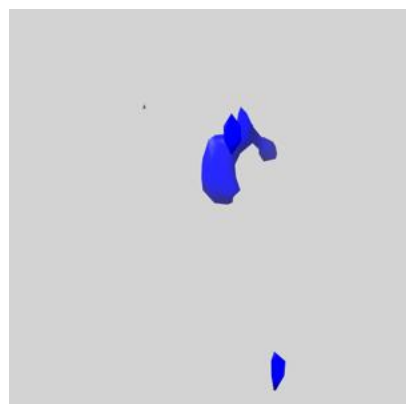


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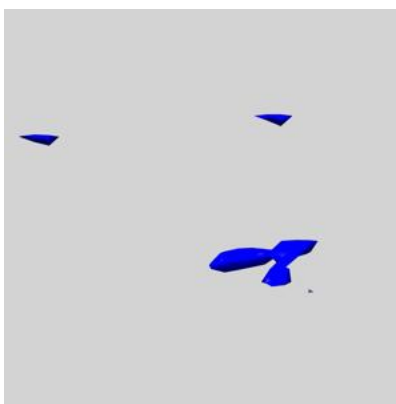


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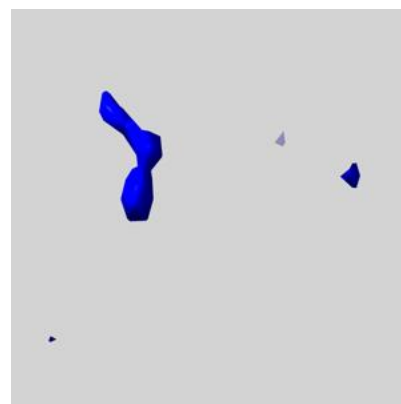
6.5.3 emd_1001_msk_23.map [i](#)



X

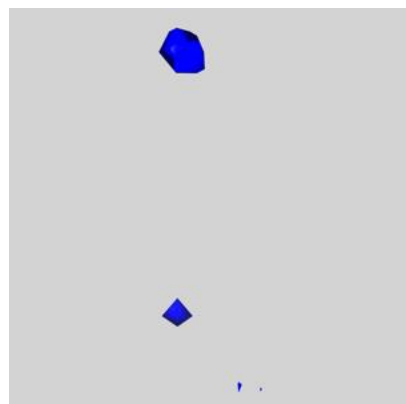


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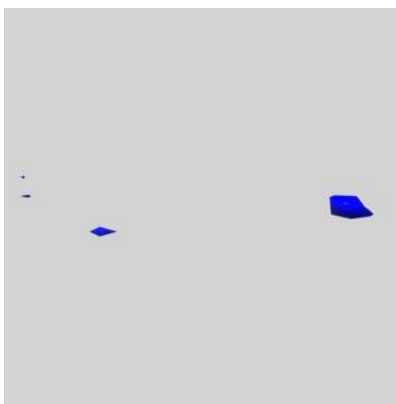


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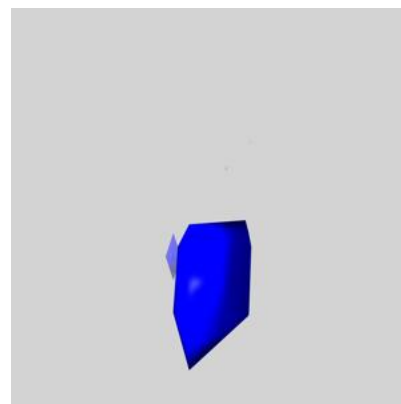
6.5.4 emd_1001_msk_22.map [i](#)



X

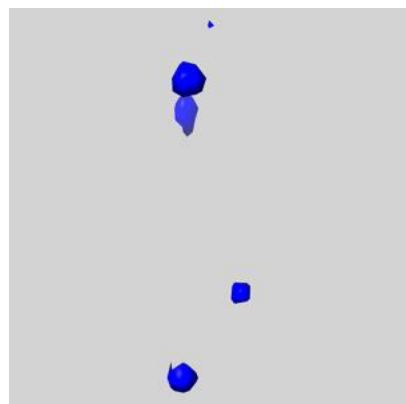


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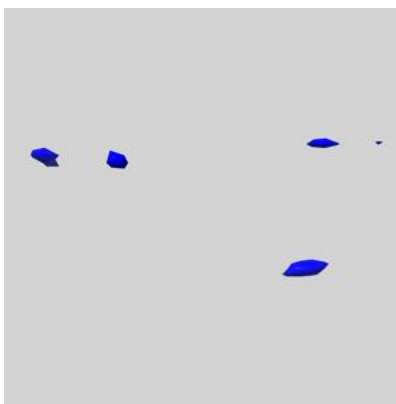


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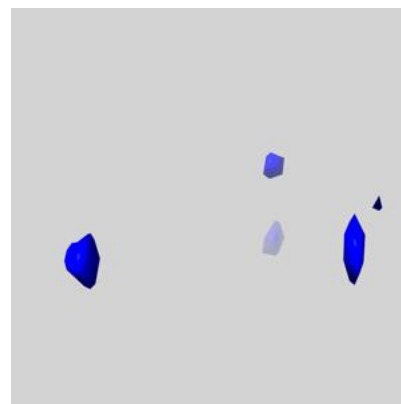
6.5.5 emd_1001_msk_21.map [i](#)



X

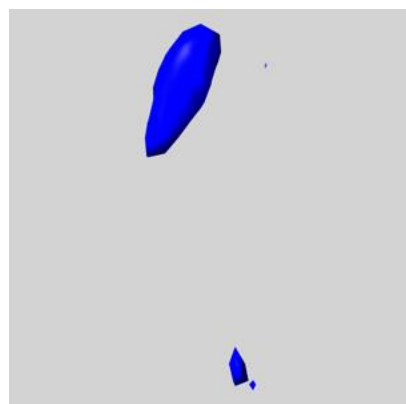


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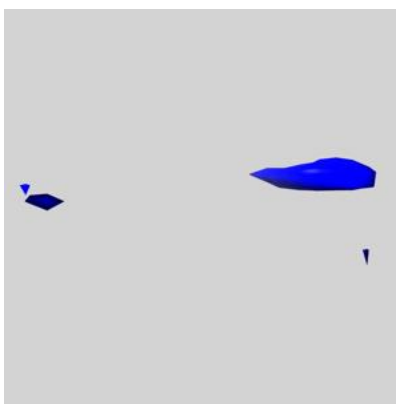


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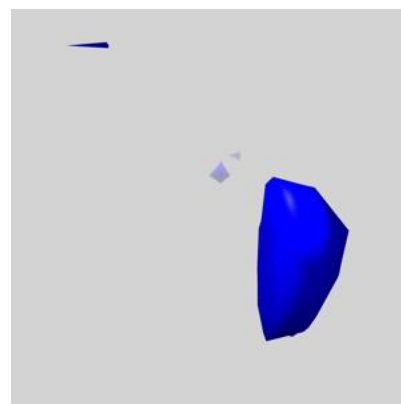
6.5.6 emd_1001_msk_20.map [i](#)



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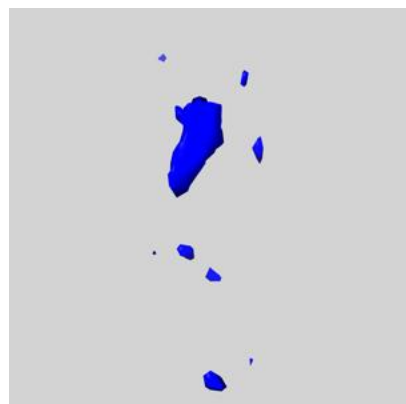


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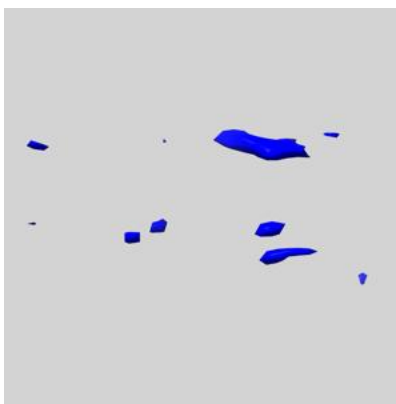


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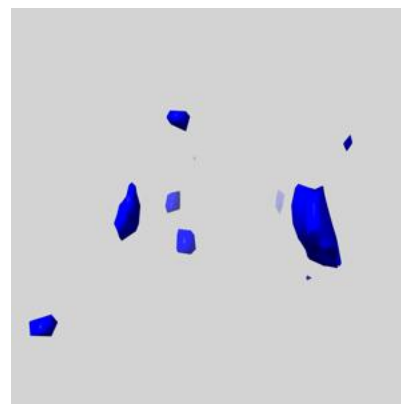
6.5.7 emd_1001_msk_19.map [i](#)



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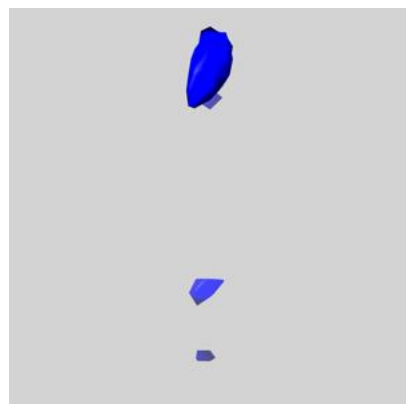


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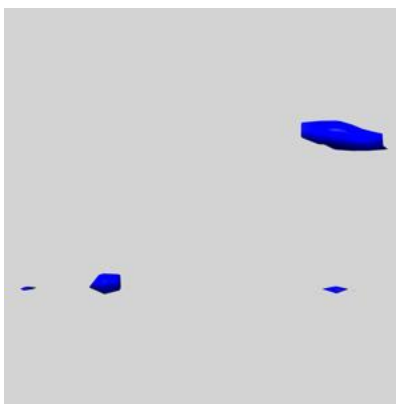


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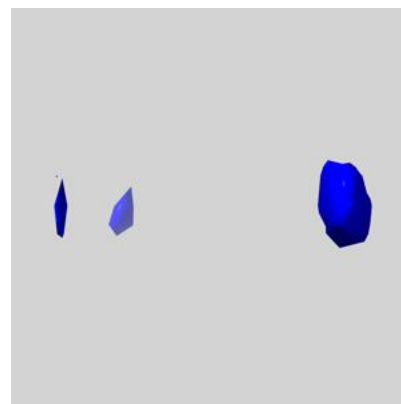
6.5.8 emd_1001_msk_18.map [i](#)



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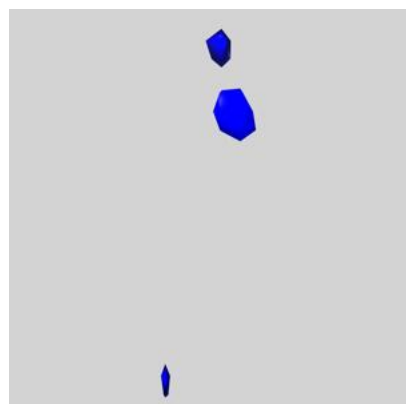


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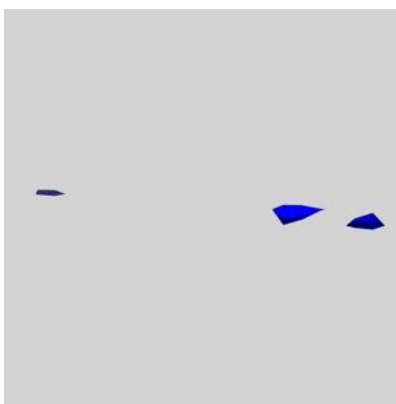


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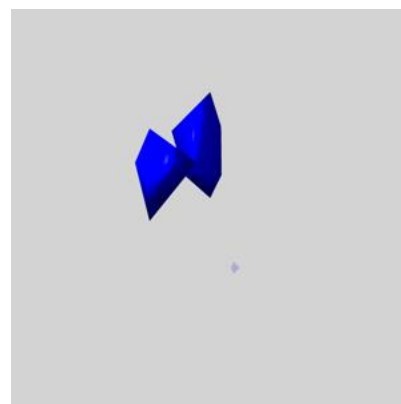
6.5.9 emd_1001_msk_17.map [i](#)



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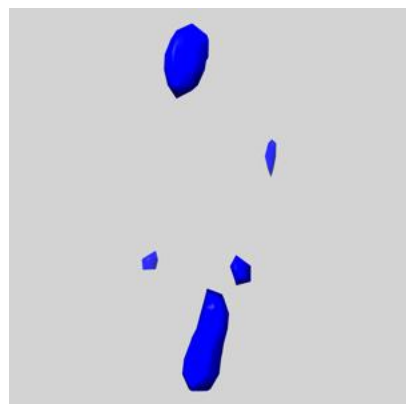


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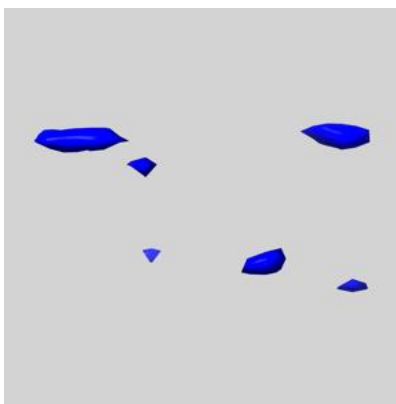


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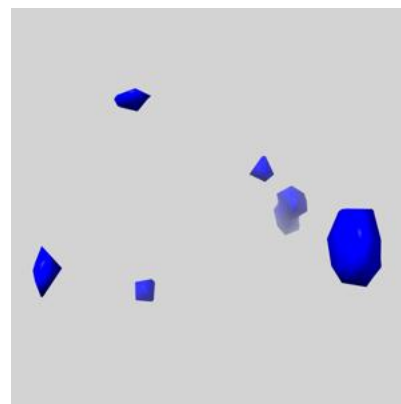
6.5.10 emd_1001_msk_16.map [i](#)



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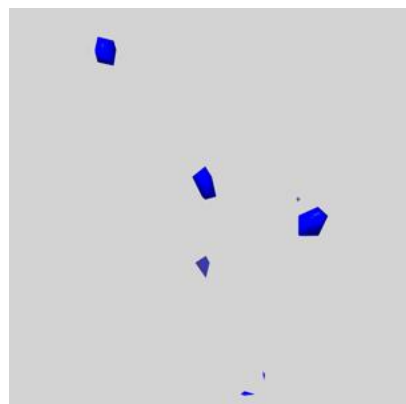


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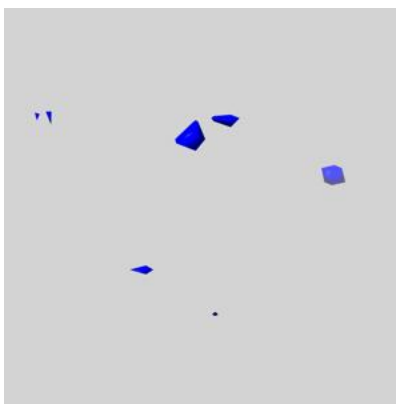


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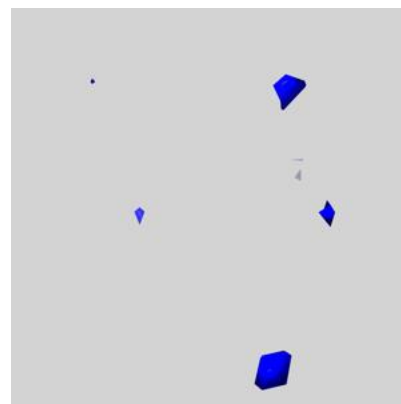
6.5.11 emd_1001_msk_15.map [i](#)



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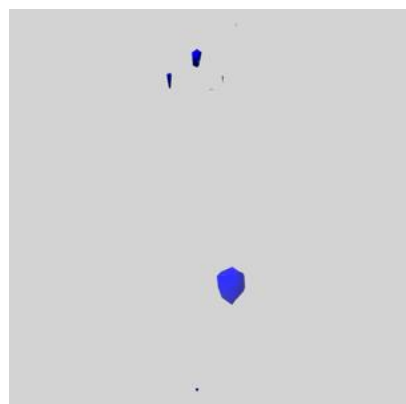


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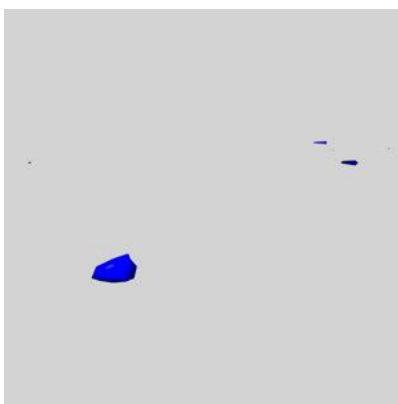


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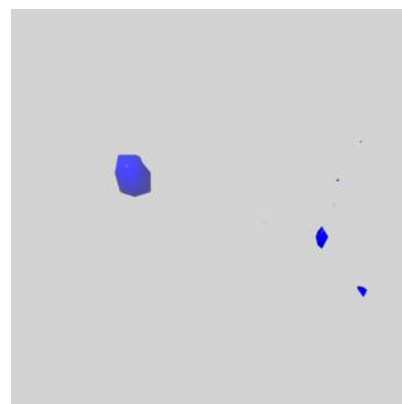
6.5.12 emd_1001_msk_14.map [i](#)



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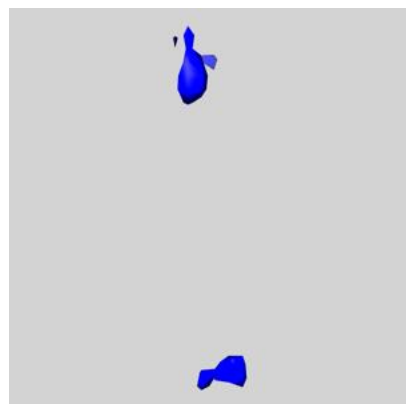


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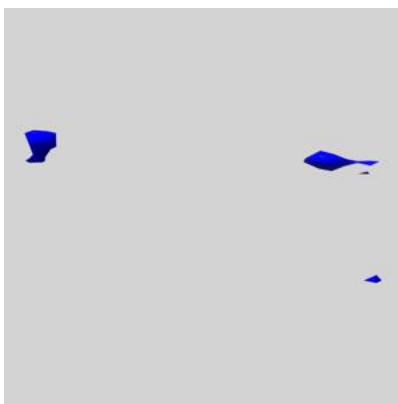


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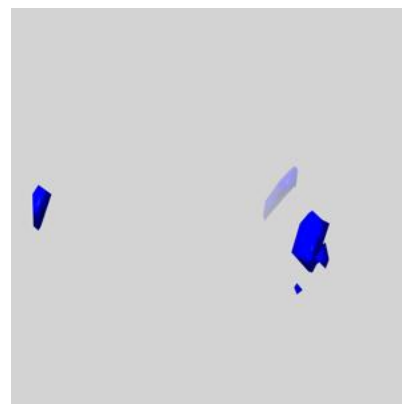
6.5.13 emd_1001_msk_13.map [i](#)



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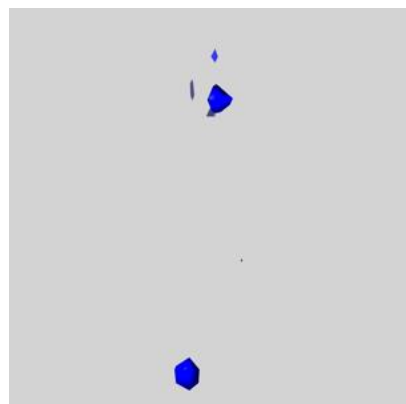


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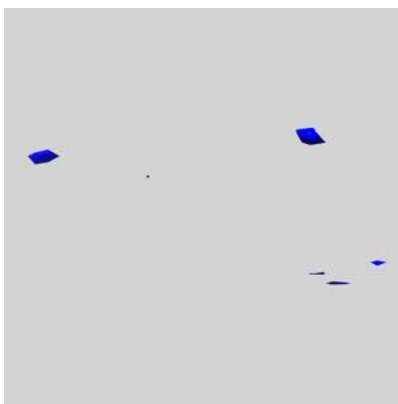


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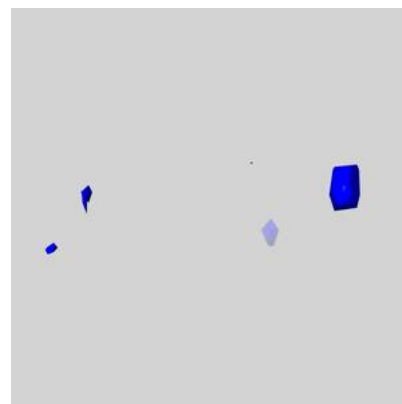
6.5.14 emd_1001_msk_12.map [i](#)



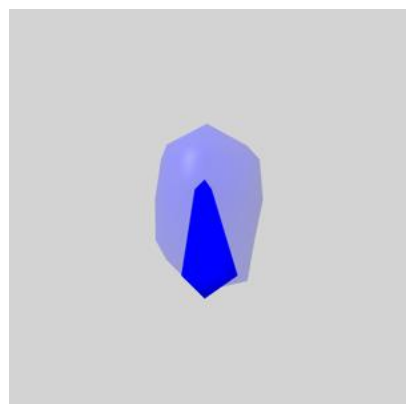
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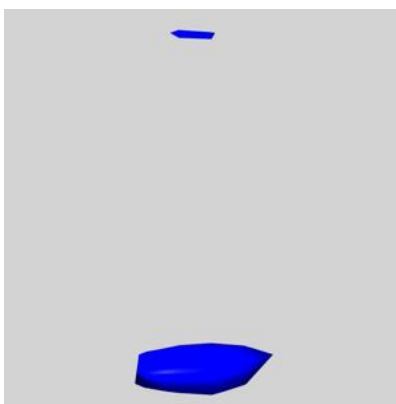
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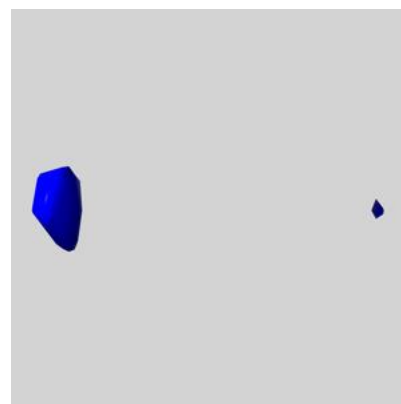
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6.5.15 emd_1001_msk_11.map [i](#)

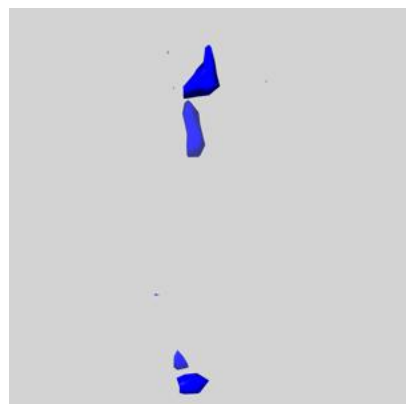
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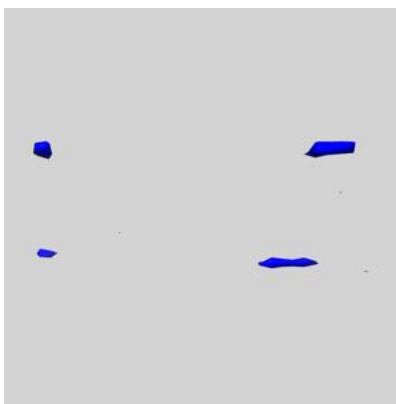
Y



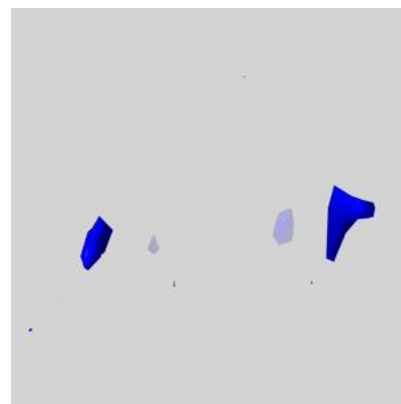
Z

6.5.16 emd_1001_msk_10.map [i](#)

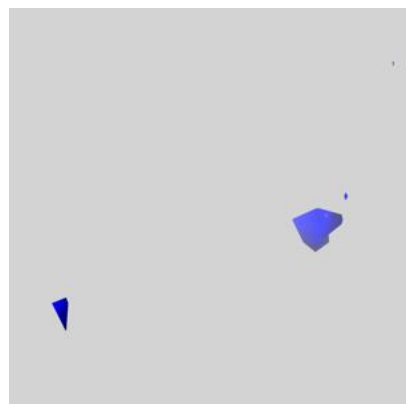
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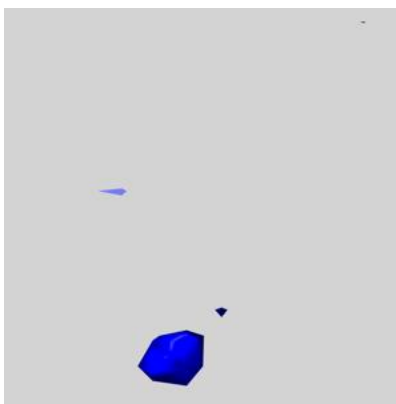
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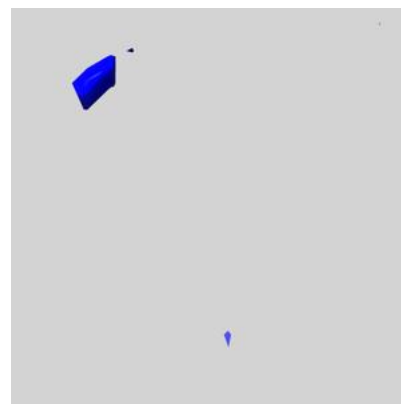
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6.5.17 emd_1001_msk_9.map [i](#)

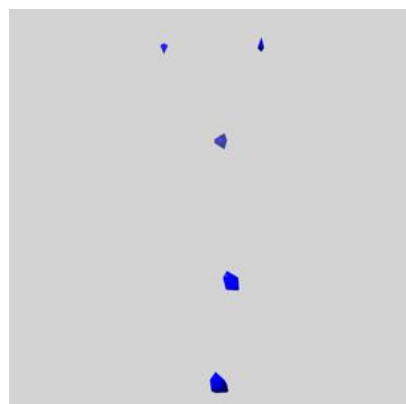
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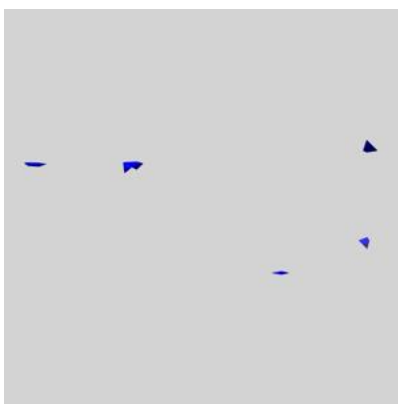
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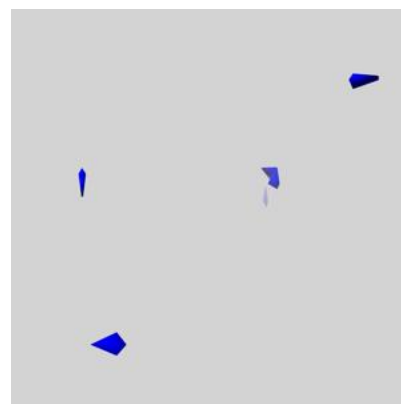
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6.5.18 emd_1001_msk_8.map [i](#)

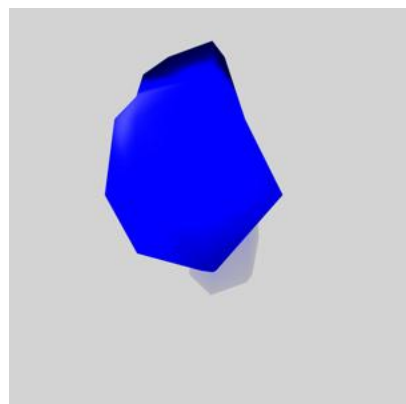
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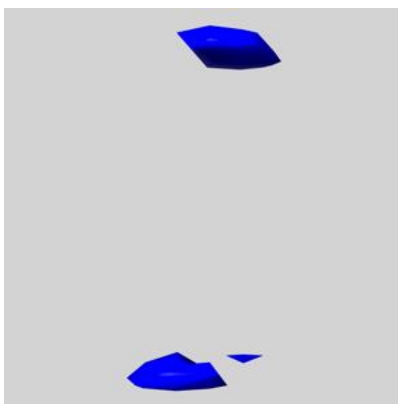
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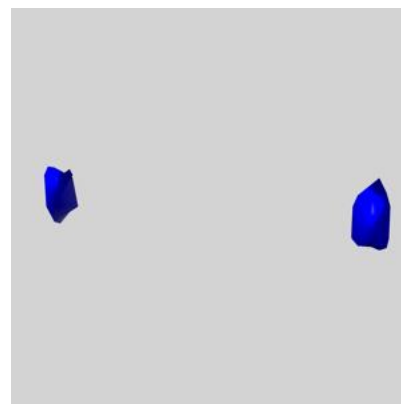
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6.5.19 emd_1001_msk_7.map [i](#)

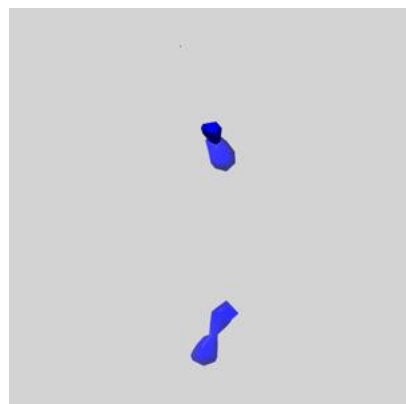
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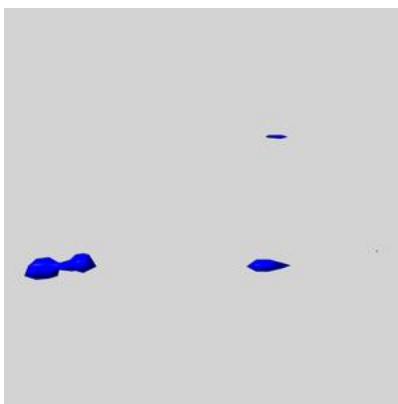
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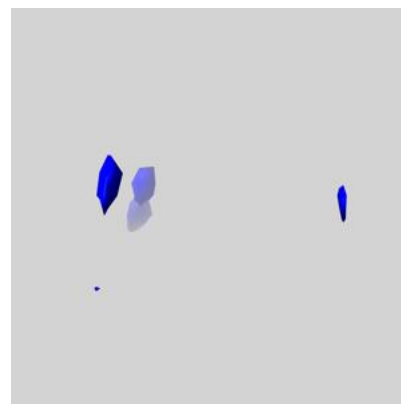
Z

6.5.20 emd_1001_msk_6.map [i](#)

X



Y

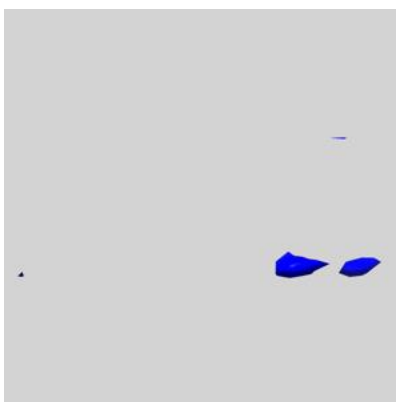


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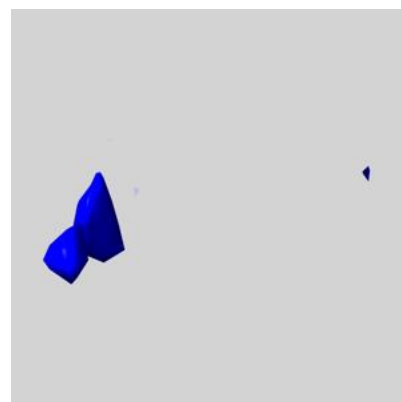
6.5.21 emd_1001_msk_5.map [i](#)



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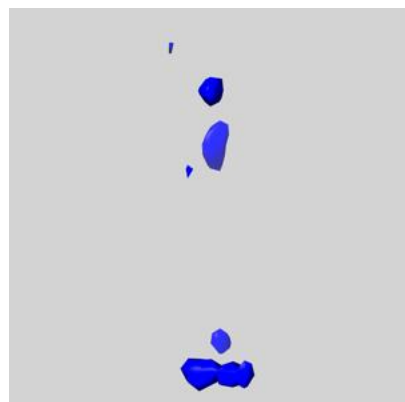


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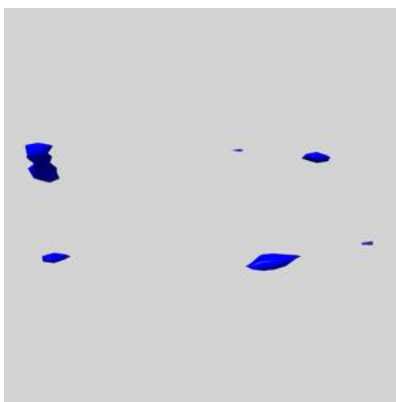


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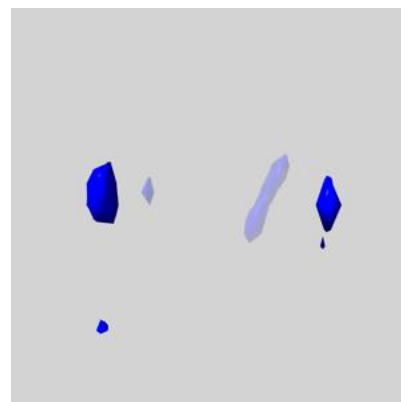
6.5.22 emd_1001_msk_4.map [i](#)



X

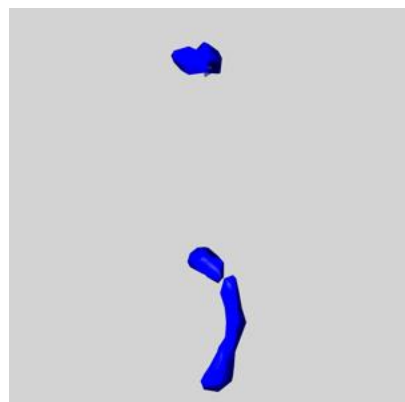


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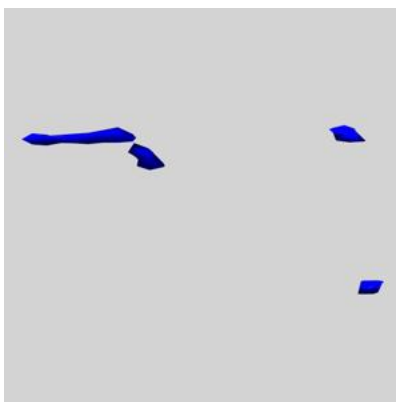


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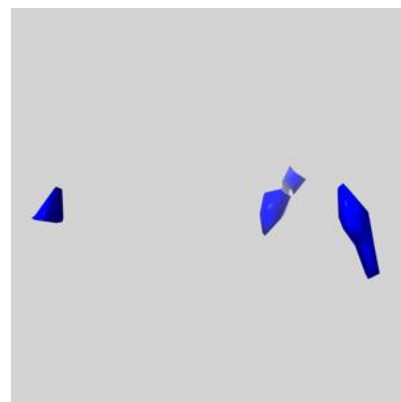
6.5.23 emd_1001_msk_3.map [i](#)



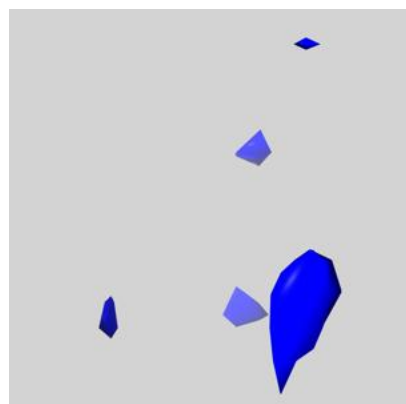
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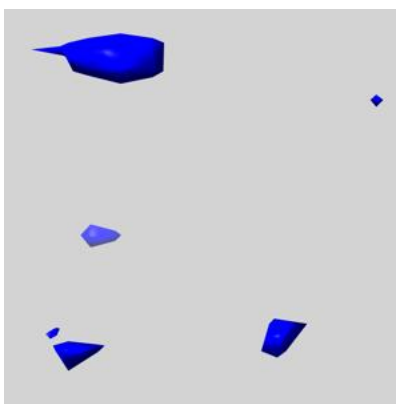
Y



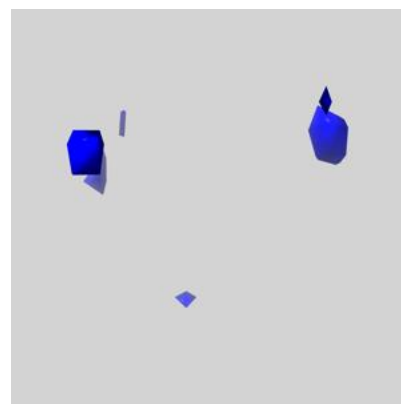
Z

6.5.24 emd_1001_msk_2.map [i](#)

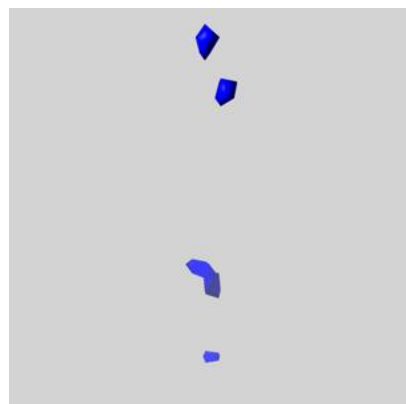
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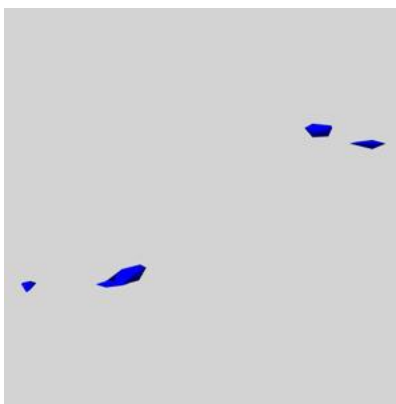
Y



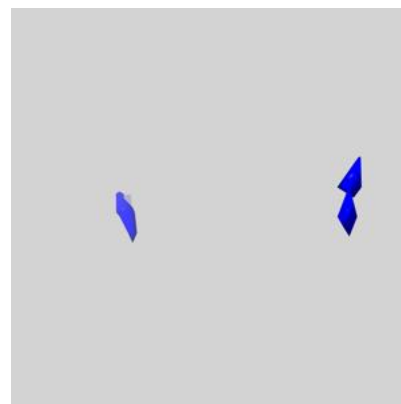
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6.5.25 emd_1001_msk_1.map [i](#)

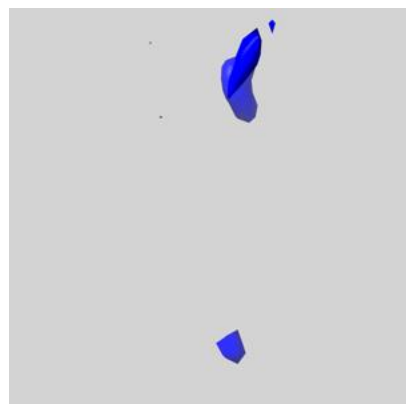
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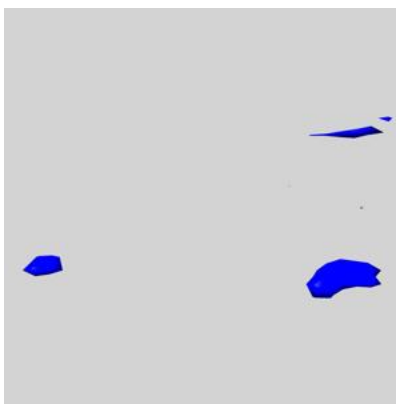
Y



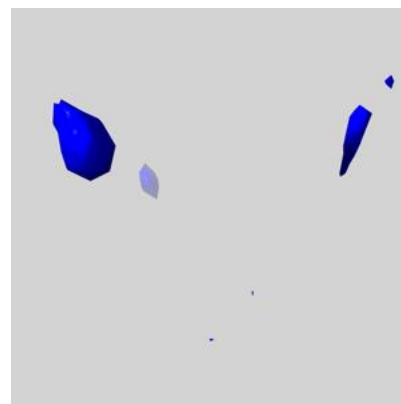
Z

6.5.26 emd_1001_msk_26.map [i](#)

X



Y

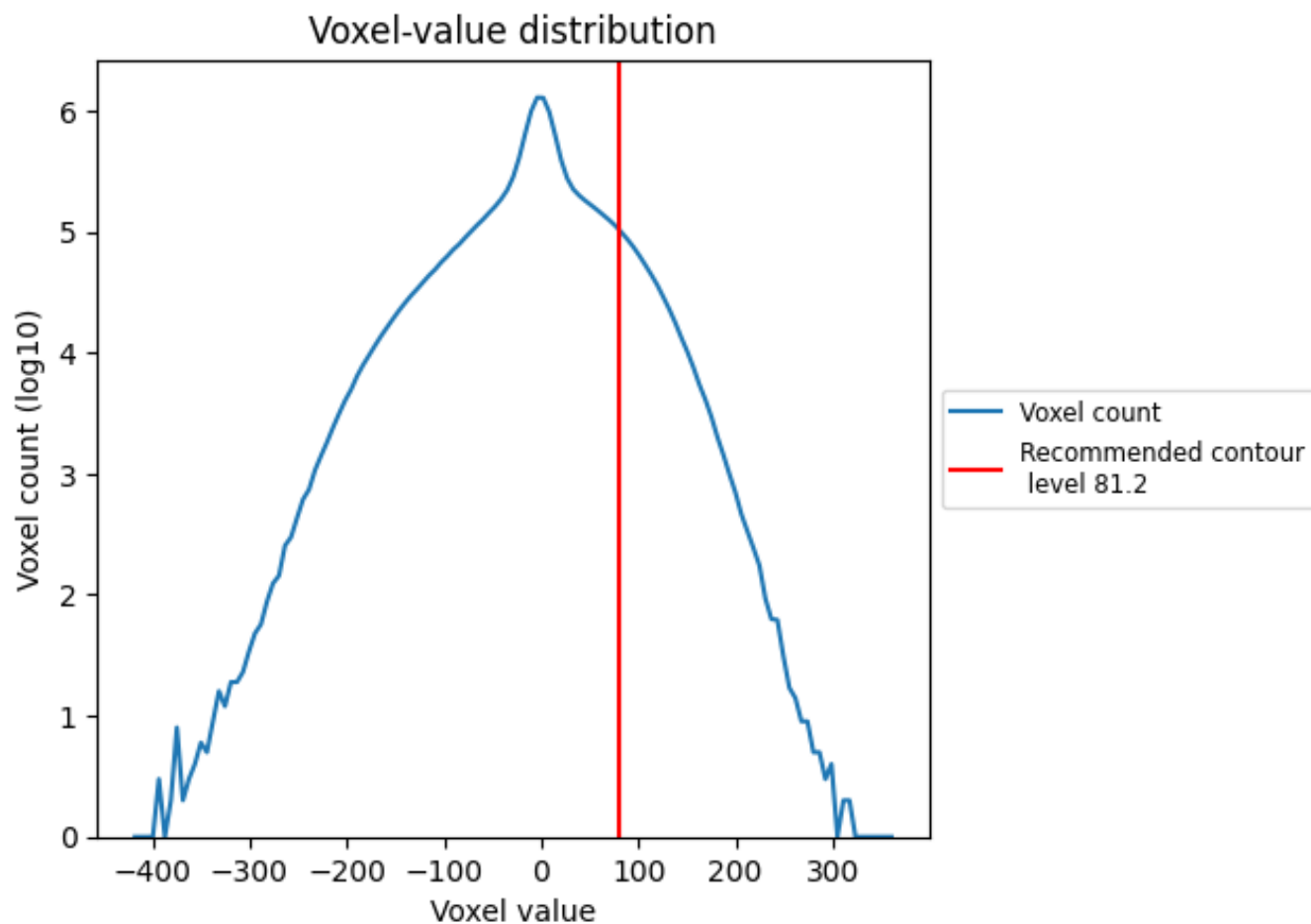


Z

7 Tomogram analysis [i](#)

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

7.1 Voxel-value distribution [i](#)



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

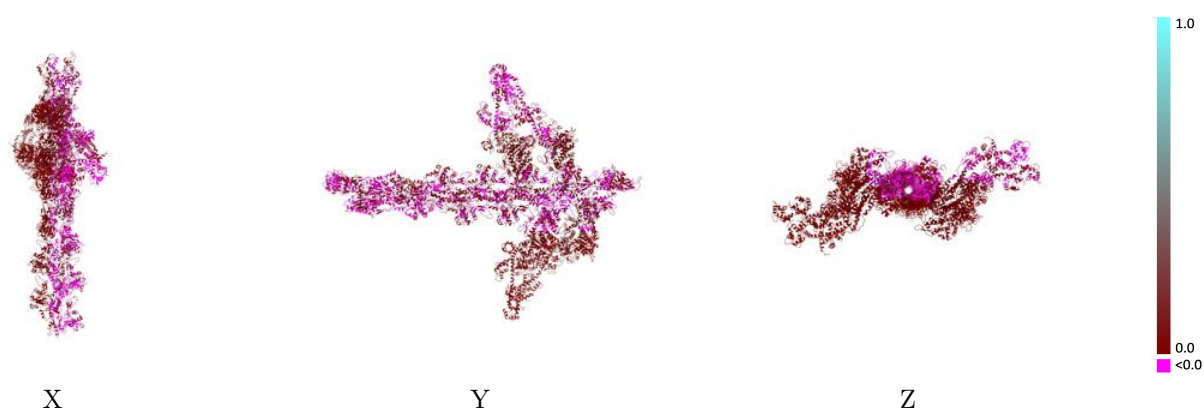
8 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-1001 and PDB model 1O1B. Per-residue inclusion information can be found in section 3 on page 7.

8.1 Map-model overlay [i](#)

This section was not generated.

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

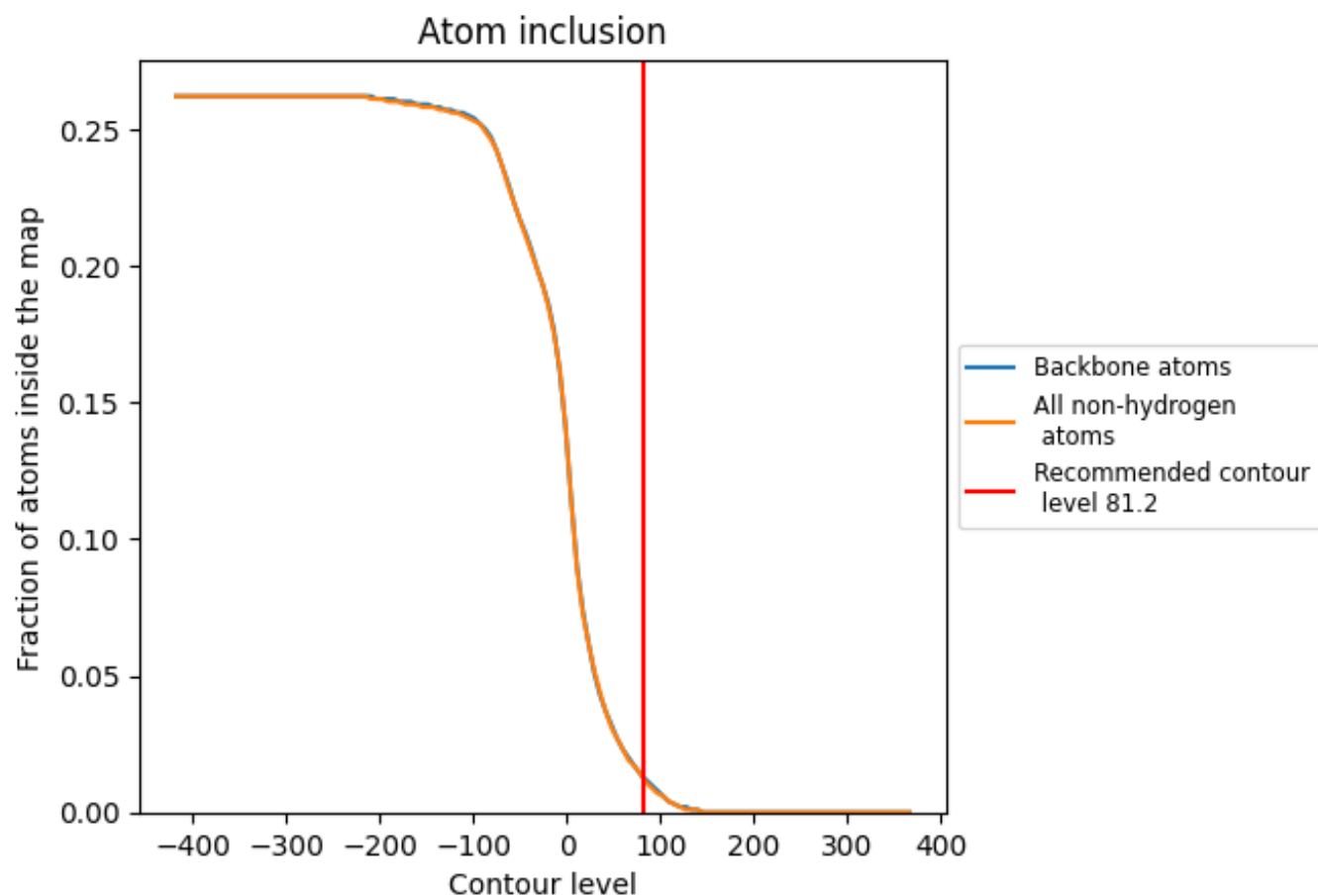


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

8.4 Atom inclusion [i](#)



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

8.5 Map-model fit summary

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

Chain	Atom inclusion	Q-score
All	 0.0130	 -0.0010
0	 0.0000	 -0.0040
1	 0.0000	 -0.0070
2	 0.0000	 -0.0100
3	 0.0000	 -0.0110
4	 0.0000	 -0.0080
5	 0.0000	 0.0020
7	 0.0000	 0.0040
8	 0.0000	 0.0080
9	 0.0000	 0.0100
A	 0.0000	 -0.0020
B	 0.0000	 0.0000
C	 0.0000	 0.0000
D	 0.0000	 0.0070
E	 0.0000	 -0.0440
F	 0.2030	 0.0400
G	 0.0000	 -0.0050
H	 0.0000	 0.0000
I	 0.0000	 0.0000
J	 0.0090	 -0.0010
K	 0.0620	 0.0150
L	 0.0780	 -0.0100
V	 0.0000	 -0.0260
W	 0.0000	 0.0030
X	 0.0610	 0.0140
Y	 0.0000	 0.0000
Z	 0.1200	 0.0110

