



wwPDB EM Validation Summary Report ⓘ

Mar 17, 2026 – 06:00 PM UTC

PDB ID : 1O19 / pdb_00001o19
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

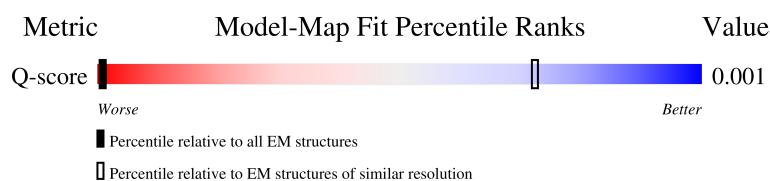
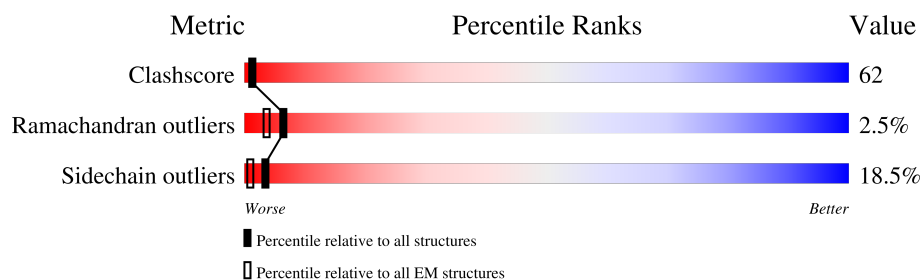
1 Overall quality at a glance

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	18 (40.00 - 40.00)

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% 22% .
1	G	840	100% 24% 50% 22% .
1	J	840	99% 25% 49% 22% .

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Mol	Chain	Length	Quality of chain		
1	M	840	100%	24%	22%
1	S	840	100%	24%	21%
2	B	145	100%	65%	26%
2	E	145	90%	64%	26%
2	H	145	100%	63%	28%
2	K	145	100%	63%	26%
2	N	145	100%	63%	28%
2	T	145	100%	63%	27%
3	C	147	100%	61%	35%
3	F	147	96%	61%	35%
3	I	147	100%	62%	35%
3	L	147	82%	62%	35%
3	O	147	100%	62%	35%
3	U	147	100%	59%	37%
4	1	375	99%	54%	34%
4	2	375	96%	49%	36%
4	3	375	99%	54%	35%
4	4	375	99%	54%	35%
4	5	375	99%	55%	33%
4	6	375	99%	56%	34%
4	7	375	99%	56%	33%
4	8	375	99%	51%	35%
4	9	375	99%	50%	36%
4	V	375	99%	48%	37%
4	W	375	99%	49%	36%

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Mol	Chain	Length	Quality of chain
4	X	375	93% 54% 33% 10% ..
4	Y	375	99% 53% 34% 10% ..
4	Z	375	99% 50% 35% 12% ..

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	MLY	A	505	-	-	X	-
1	MLY	A	553	-	-	X	-
1	MLY	A	764	-	-	X	-
1	MLY	A	768	-	-	X	-
1	MLY	A	782	-	-	X	-
1	MLY	A	839	-	-	X	-
1	MLY	D	553	-	-	X	-
1	MLY	D	782	-	-	X	-
1	MLY	D	839	-	-	X	-
1	MLY	G	295	-	-	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	768	-	-	X	-
1	MLY	J	839	-	-	X	-
1	MLY	J	84	-	-	X	-
1	MLY	M	35	-	-	X	-
1	MLY	M	553	-	-	X	-
1	MLY	M	839	-	-	X	-
1	MLY	M	84	-	-	X	-
1	MLY	S	505	-	-	X	-
1	MLY	S	764	-	-	X	-
1	MLY	S	839	-	-	X	-
1	MLY	S	84	-	-	X	-

2 Entry composition

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	840	Total	C	N	O	S	0	0
			6797	4382	1135	1243	37		
1	D	840	Total	C	N	O	S	0	0
			6797	4382	1135	1243	37		
1	G	840	Total	C	N	O	S	0	0
			6797	4382	1135	1243	37		
1	J	840	Total	C	N	O	S	0	0
			6797	4382	1135	1243	37		
1	M	840	Total	C	N	O	S	0	0
			6797	4382	1135	1243	37		
1	S	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	T	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	U	147	Total	C	N	O	S	0	0
			1123	698	188	230	7		

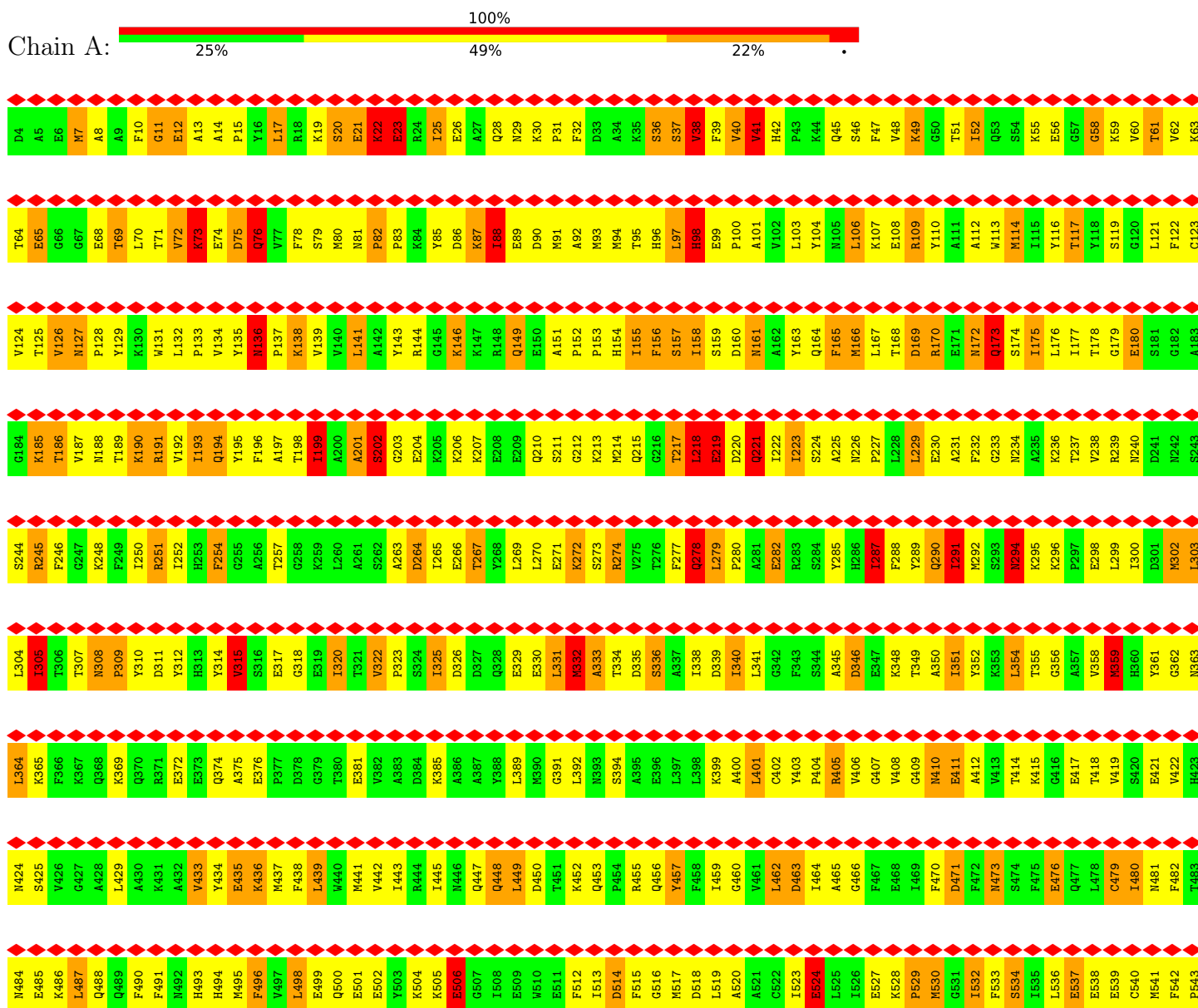
- Molecule 4 is a protein called SKELETAL MUSCLE ACTIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	1	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	2	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	3	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	4	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	5	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	6	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	7	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	8	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	9	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	V	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	W	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	X	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	Y	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	Z	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		

3 Residue-property plots

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

• Molecule 1: SKELETAL MUSCLE MYOSIN II





N424	N484	K544	L664	Y724	A784	N424	N484	K544	L664	Y724	A784
S425	E485	A545	R665	R725	E785	S425	E485	A545	R665	R725	E785
V426	K486	T546	S666	V726	I786	V426	K486	T546	S666	V726	I786
G427	L487	D547	T667	L727	T787	G427	L487	D547	T667	L727	T787
A428	Q488	T548	H668	M728	T788	A428	Q488	T548	H668	M728	T788
L429	Q489	S549	P669	A729	A789	L429	Q489	S549	P669	A729	A789
A430	F490	F550	H670	S730	T790	A430	F490	F550	H670	S730	T790
K431	F491	K551	F671	A731	Q791	K431	F491	K551	F671	A731	Q791
A432	N492	N552	V672	I732	A792	A432	N492	N552	V672	I732	A792
V433	H493	K553	R673	T733	R793	V433	H493	K553	R673	T733	R793
Y434	H494	L554	C674	E734	C794	Y434	H494	L554	C674	E734	C794
E435	M495	Y555	I675	G735	R795	E435	M495	Y555	I675	G735	R795
K436	F496	D556	I676	Q736	G796	K436	F496	D556	I676	Q736	G796
M437	V497	V616	P677	F737	F797	M437	V497	V616	P677	F737	F797
F438	L498	H558	N678	M738	L798	F438	L498	H558	N678	M738	L798
L439	E499	L559	E679	D739	M799	L439	E499	L559	E679	D739	M799
A440	Q500	G560	T680	S740	R800	A440	Q500	G560	T680	S740	R800
M441	E501	G561	K681	K741	V601	M441	E501	G561	K681	K741	V601
V442	E502	S562	T682	K742	E602	V442	E502	S562	T682	K742	E602
I443	Y503	N563	P683	A743	R603	I443	Y503	N563	P683	A743	R603
R444	K504	N564	G684	S744	R604	R444	K504	N564	G684	S744	R604
I445	K505	F565	A685	E745	A605	I445	K505	F565	A685	E745	A605
N446	E506	Q566	M686	K746	M606	N446	E506	Q566	M686	K746	M606
Q447	G507	K567	E687	L747	V607	Q447	G507	K567	E687	L747	V607
Q448	I508	P568	H688	L748	E608	Q448	I508	P568	H688	L748	E608
L449	E509	K569	E689	G749	R609	L449	E509	K569	E689	G749	R609
D450	W510	P570	L690	G750	R610	D450	W510	P570	L690	G750	R610
T451	E511	A571	V691	G751	E611	T451	E511	A571	V691	G751	E611
K452	F512	K572	L692	D752	S612	K452	F512	K572	L692	D752	S612
Q453	I513	G573	H693	V753	I613	Q453	I513	G573	H693	V753	I613
P454	D514	K574	Q694	D754	F614	P454	D514	K574	Q694	D754	F614
R455	F515	A575	L695	H755	C615	R455	F515	A575	L695	H755	C615
Q456	G516	E576	R696	T756	I616	Q456	G516	E576	R696	T756	I616
Y457	M517	K577	C697	Q757	Q617	Y457	M517	K577	C697	Q757	Q617
F458	D518	H578	N698	Y758	Y618	F458	D518	H578	N698	Y758	Y618
I459	L519	F579	G699	A759	N619	I459	L519	F579	G699	A759	N619
G460	A520	S580	V700	F760	W620	G460	A520	S580	V700	F760	W620
V461	E521	L581	L701	G761	R621	V461	E521	L581	L701	G761	R621
L462	C522	V582	E702	H762	S622	L462	C522	V582	E702	H762	S622
D463	I523	H583	G703	T763	F623	D463	I523	H583	G703	T763	F623
I464	E524	Y584	I704	K764	M624	I464	E524	Y584	I704	K764	M624
A465	L525	A585	R705	V765	N625	A465	L525	A585	R705	V765	N625
G466	I526	G586	I706	F766	V626	G466	I526	G586	I706	F766	V626
F467	E527	T587	R708	F767	K627	F467	E527	T587	R708	F767	K627
E468	P528	V588	K708	K768	H628	E468	P528	V588	K708	K768	H628
I469	E529	D589	V649	A769	N629	I469	E529	D589	V649	A769	N629
F470	M530	Y590	G710	G770	P630	F470	M530	Y590	G710	G770	P630
D471	G531	N591	F711	L771	W631	D471	G531	N591	F711	L771	W631
F472	I532	L592	F712	L772	M632	F472	I532	L592	F712	L772	M632
N473	F533	S593	S713	G773	K633	N473	F533	S593	S713	G773	K633
S474	S534	G594	R714	L774	L634	S474	S534	G594	R714	L774	L634
F475	I535	W595	V715	L775	P635	F475	I535	W595	V715	L775	P635
Q476	L536	L596	L716	E776	F636	Q476	L536	L596	L716	E776	F636
E477	E537	O597	Y717	E777	K637	E477	E537	O597	Y717	E777	K637
L478	E538	K598	A718	M778	T638	L478	E538	K598	A718	M778	T638
C479	E539	N599	D719	R779	K639	C479	E539	N599	D719	R779	K639
I480	C540	K600	F720	D780	P640	I480	C540	K600	F720	D780	P640
N481	M541	D601	K721	L781	L641	N481	M541	D601	K721	L781	L641
F482	P542	A602	Q722	K782	L642	F482	P542	A602	Q722	K782	L642
T483	P543	N603	R723	L783	K643	T483	P543	N603	R723	L783	K643

• Molecule 1: SKELETAL MUSCLE MYOSIN II



D4	T64	V124	G184	S244	L304
A5	E65	T125	K185	R245	T305
E6	G66	V126	T186	F246	T306
M7	G67	M127	V187	G247	T307
A8	E68	M128	N188	K248	N308
A9	T69	Y129	T189	F249	P309
F10	L70	K130	K190	L250	Y310
G11	T71	W131	R191	R251	D311
E12	V72	L132	V192	L252	Y312
A13	K73	P133	T193	H253	H313
A14	E74	V134	Q194	F254	Y314
P15	D75	Y135	Y195	G255	V315
Y16	Q76	M136	F196	A256	S316
L17	V77	L137	A197	T257	E317
R18	F78	K138	T198	G258	G318
K19	S79	V139	N199	K259	E319
S20	M80	Y140	A200	L260	I320
E21	N81	L141	A201	A261	T321
K22	P82	A142	S202	S262	V322
E23	K83	Y143	G203	A263	P323
R24	K84	L144	E204	D264	S324
I25	Y85	G145	K205	L265	I325
E26	D86	K146	K206	E266	D326
A27	K87	K147	K207	T267	D327
Q28	T88	L148	E208	T268	Q328
N29	E89	Q149	E209	L269	E329
K30	D90	E150	Q210	L270	E330
P31	N91	A151	S211	E271	L331
F32	A92	P152	G212	K272	R332
D33	M93	P153	K213	S273	A333
A34	M94	H154	M214	R274	T334
K35	T95	I155	Q215	V275	D335
S36	H96	F156	G216	T276	S336
S37	L97	S157	T217	F277	A337
V38	H98	I158	L218	Q278	I338
F39	E99	S159	E219	L279	D339
V40	P100	D160	D220	P280	I340
V41	A101	M161	Q221	A281	L341
H42	Y102	A162	I222	E282	G342
P43	L103	Y163	I223	R283	F343
K44	Y104	Q164	S224	S284	S344
Q45	N105	F165	A225	Y285	A345
S46	L106	M166	N226	H286	D346
F47	K107	L167	P227	L287	E347
V48	E108	T168	L228	F288	K348
K49	R109	D169	L229	Y289	T349
Y110	Y110	R170	E230	Q290	A350
T51	A111	E171	A231	L291	I351
I52	M112	M172	F232	M292	Y352
Q53	W113	Q173	G233	S293	K353
S54	M114	S174	N234	N294	L354
K55	I115	T175	A235	K295	T355
E56	Y116	L176	K236	K296	G356
G57	T117	T177	T237	P297	A357
G58	Y118	T178	V238	E298	V358
K59	S119	G179	R239	L299	K359
V60	G120	E180	N240	T300	H360
T61	L121	S181	D241	Y361	G362
V62	F122	G182	N242	K363	N363

A784	L784	Y724	L664	M604	K544	N484	N424	L364
E785	R785	R725	R665	E605	A545	E485	S425	K365
I786	V726	V726	S666	T606	T546	K486	V426	F366
T787	L727	L727	T667	V607	D547	L487	G427	K367
T788	M728	M728	H668	I608	T548	Q488	A428	Q368
A789	A729	A729	P669	G609	S549	Q489	L429	K369
T790	S730	S730	H670	L610	F550	F490	A430	Q370
Q791	A731	A731	F671	Y611	K551	F491	K431	R371
A792	V672	V672	V672	Q612	N552	N492	A432	E372
R793	R733	R733	R673	K613	K553	H493	V433	E373
C794	E734	E734	S614	S614	L554	H494	Y434	Q374
R795	G735	G735	I675	S615	Y555	M495	E435	A375
G796	Q736	Q736	I676	V616	D556	F496	K436	E376
F797	L737	L737	P677	K617	E557	V497	M437	P377
L798	M738	M738	N678	T618	H558	L498	F438	D378
R800	D739	D739	E679	L619	L559	E499	L439	G379
V801	S740	S740	T680	A620	G560	Q500	W440	T380
E802	K741	K741	K681	L621	K561	E501	M441	E381
Y803	K742	K742	T682	L622	S562	E502	V442	V382
R804	A743	A743	P683	F623	N563	Y603	I443	A383
A805	S744	S744	G684	A624	N564	K504	R444	D384
M806	E745	E745	A685	T625	F565	K505	I445	K385
V807	K746	K746	M686	Y626	Q566	E506	M446	A386
E808	L747	L747	E687	G627	K567	G507	Q447	A387
R809	L748	L748	H688	G628	P568	I508	Q448	Y388
R810	G749	G749	E689	E629	K569	E509	L449	L389
E811	G750	G750	L690	A630	P570	W510	D450	M390
S812	G751	G751	V691	E631	A571	E511	T451	G391
L813	D752	D752	L692	G632	K572	F512	K452	L392
F814	V753	V753	H693	G633	G573	T513	Q453	N393
C815	D754	D754	Q694	G634	K574	D514	S394	S394
L816	H755	H755	L695	G635	A575	F515	R455	A395
Q817	T756	T756	R696	K636	E576	G516	Q456	E396
N819	Q757	Q757	G697	K637	A577	M517	Y457	L397
V820	Y758	Y758	N698	G638	H578	D518	F458	L398
R821	A759	A759	G699	G639	F579	L519	I459	K399
S822	F760	F760	V700	K640	S580	A520	G460	A400
F823	G761	G761	L701	K641	L581	A521	V461	L401
M824	E762	E762	E702	K642	V582	C522	L462	C402
N825	G703	G703	G643	G643	H583	I523	D463	Y403
V826	K764	K764	I704	S644	Y584	E524	I464	P404
K827	V765	V765	R705	S645	A585	L525	A465	R405
H828	F766	F766	I706	F646	G586	I526	G466	V406
W829	F767	F767	C707	Q647	T587	E527	F467	G407
P830	K768	K768	R708	T648	V588	K528	E468	V408
W831	A769	A769	K709	V649	D589	P529	I469	G409
M832	G770	G770	G710	S650	Y590	M530	G469	N410
K833	L771	L771	F711	A651	N591	G531	D471	E411
L834	L772	L772	P712	L652	I592	I532	F472	A412
F835	G773	G773	S713	F653	S593	F533	M473	V413
F836	L774	L774	R714	R654	G594	S534	T414	T414
K837	L775	L775	V715	E655	N595	I535	F475	K415
I838	E776	E776	L716	M656	L596	L536	E476	G416
K839	E777	E777	Y717	L657	E597	E537	Q477	E417
P840	M778	M778	A718	M658	K598	E538	L478	T418
L841	R779	R779	D719	K659	N599	E539	C479	V419
L842	D780	D780	F720	L660	K600	C540	I480	S420
L843	D781	D781	K721	M661	D601	M541	N481	E421
			Q722	A662	P602	F542	F482	V422
			R723	N663	L603	P543	T483	H423

• Molecule 1: SKELETAL MUSCLE MYOSIN II



S244	R245	F246	G247	F249	I250	R251	I252	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	S293	N294	K295	K296	P297	E298	L299	I300	D301	K302	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	I222	I223	S224	A225	N226	P227	L228	L229	E230	A231	F232	G233	N234	A235	K236	T237	V238	R239	N240	D241	N242	S243
V124	T125	V126	N127	N128	Y129	K130	V131	L132	P133	V134	Y135	N136	P137	K138	V139	Y140	L141	A142	Y143	R144	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	H85	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	V113	M114	I115	Y116	T117	Y118	S119	G120	F122	C123
D4	A5	E6	M7	A8	A9	F10	G11	E12	A13	A14	P15	Y16	L17	R18	K19	S20	E21	K22	E23	R24	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

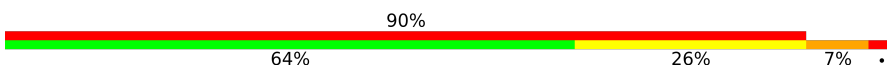
A784	L784	Y724	L664	M604	K544	N484	N424	L364	L304
R725	R665	R726	R666	E605	A545	E485	S425	K365	T306
I786	T666	V726	T667	T606	T546	K486	V426	F366	T307
T787	T667	L727	T668	V607	D547	L487	G427	K367	N308
T788	H668	N728	H668	T608	T548	Q488	A428	Q368	P309
A789	P669	A729	P669	G609	S549	Q489	L429	K369	P309
T790	H670	S730	H670	L610	F550	F490	A430	Q370	Y310
Q791	F671	A731	F671	V611	K551	F491	K431	R371	D311
A792	V672	I732	V672	D612	N552	N492	A432	E372	Y312
R793	R673	P733	R673	K613	K553	H493	V433	E373	H313
C794	C674	E734	C674	S614	L554	H494	Y434	Q374	Y314
R795	L675	G735	L675	S615	Y555	M495	E435	A375	V315
G796	L676	Q736	L676	V616	D556	F496	K436	E376	S316
F797	P677	F737	P677	K617	E557	V497	M437	F377	E317
L798	N678	M738	N678	T618	H558	L498	F438	D378	G318
M799	E679	D739	E679	L619	L559	E499	L439	G379	E319
R800	T680	S740	T680	A620	G560	Q500	A440	T380	I320
V801	K681	K741	K681	L621	K561	E501	M441	E381	T321
E802	T682	K742	T682	L622	S562	E502	V442	V382	V322
R803	P683	A743	P683	F623	N563	E603	I443	A383	P323
R804	S744	S744	G684	A624	N564	K504	R444	D384	S324
A805	A685	E745	A685	T625	F565	K505	I445	K385	I325
M806	K746	K746	N686	Y626	Q566	E506	N446	A386	D326
V807	E687	L747	E687	G627	K567	G507	Q447	A387	D327
E808	L748	H688	L748	G628	P568	I508	Q448	V388	Q328
R809	E689	G749	E689	E629	K569	E509	L449	L389	E329
R810	G750	G750	L690	A630	P570	W510	D450	M390	E330
E811	G751	Q751	V691	E631	A571	E511	T451	G391	L331
S812	D752	D752	L692	G632	K572	F512	K452	L392	M332
I813	H693	V753	H693	G633	G573	I513	Q453	N393	A333
F814	Q694	D754	Q694	G634	K574	D514	P454	S394	T334
C815	L695	H755	L695	G635	A575	F515	R455	A395	D335
L816	R696	T756	R696	G636	E576	G516	Q456	E396	S336
Q817	G697	Q757	G697	K637	A577	M517	Y457	L397	A337
Y818	N698	Y758	N698	G638	H578	D518	F458	L398	I338
N819	G699	A759	G699	G639	F579	L519	I459	K399	D339
V820	F760	F760	V700	K640	S580	A520	G460	A400	I340
R821	L701	G761	L701	K641	L581	A521	V461	L401	L341
S822	E702	R762	E702	K642	V582	C522	L462	C402	G342
T763	G703	T763	G703	G643	H583	I523	D463	Y403	F343
M824	K704	I704	K764	S644	Y584	E524	I464	P404	S344
N825	R705	V765	R705	S645	A585	L525	A465	R405	A345
R826	F766	F766	F706	F646	G586	I526	G466	V406	D346
K827	C707	F767	C707	Q647	T587	E527	F467	G407	E347
H828	R708	K768	R708	T648	V588	K528	E468	V408	K348
W829	K709	A769	K709	V649	D589	P529	I469	G409	T349
P830	G710	G770	G710	S650	Y590	M530	F470	A350	A350
W831	F711	L771	F711	A651	N591	G531	D471	E411	I351
M832	L772	L772	L772	P651	I592	I532	F472	A412	Y352
K833	G773	K773	G773	F653	S593	F533	N473	V413	K353
L834	L774	R714	L774	R654	G594	S534	S474	L354	L354
F835	L775	V715	L775	E655	N595	I535	F475	K415	T355
R836	L716	L716	L716	N656	L596	L536	E476	G416	G356
K837	E777	Y717	E777	L657	E597	E537	Q477	E417	A357
I838	A718	A718	A718	N658	K598	E538	L478	T418	V358
K839	D719	R779	D719	K659	N599	E539	C479	V419	M359
P840	F720	D780	F720	L660	K600	C540	I480	S420	H360
L841	K721	D781	K721	M661	D601	M541	N481	E421	Y361
L842	Q722	K782	Q722	A662	P602	F542	F482	V422	G362
R843	R773	L793	R773	N663	L603	P543	T483	H423	N363

● Molecule 1: SKELETAL MUSCLE MYOSIN II



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	Q29	K30	P31	F32	D33	A34	K35	S36	S37	V38	F39	V40	V41	H42	P43	K44	Q45	S46	F47	V48	R49	G50	T51	I52	Q53	S54	K55	E56	G57	G58	K59	V60	V62	K63	
T64	E65	G66	G67	E68	T69	L70	T71	V72	K73	E74	D75	Q76	V77	F78	S79	M80	N81	P82	P83	K84	H85	D86	L87	L88	E89	D90	N91	A92	N93	M94	T95	H96	L97	H98	E99	D100	A101	V102	L103	Y104	L106	L107	E108	R109	Y110	A111	A112	Q113	M114	T115	Y116	L117	Y118	S119	G120	L121	F122	C123	
V124	T125	V126	N127	P128	Y129	K130	Y131	L132	P133	V134	Y135	N136	P137	K138	V139	Y140	A141	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	T175	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	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	T228	L229	E230	A231	F232	G233	N234	A235	K236	T237	V238	R239	N240	D241	N242	S243

• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

Chain E: 



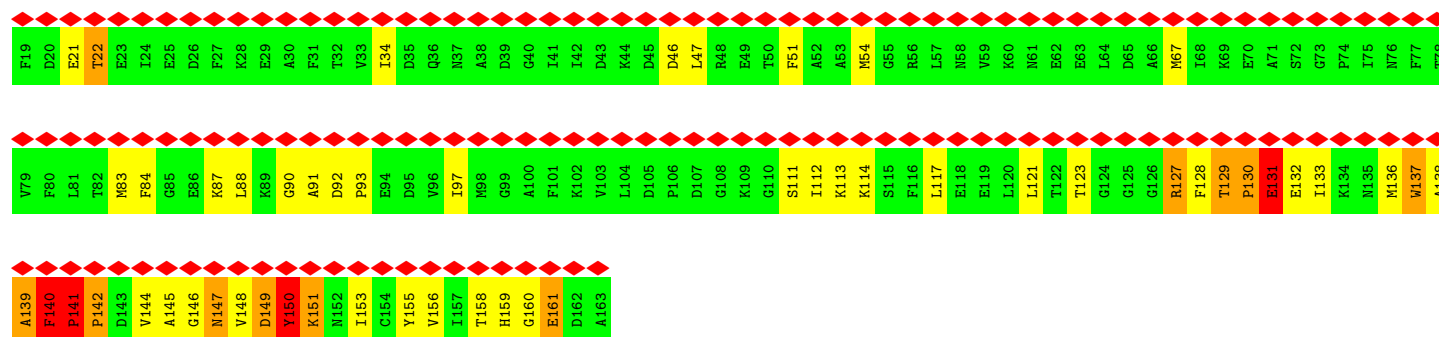
• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

Chain H: 



• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

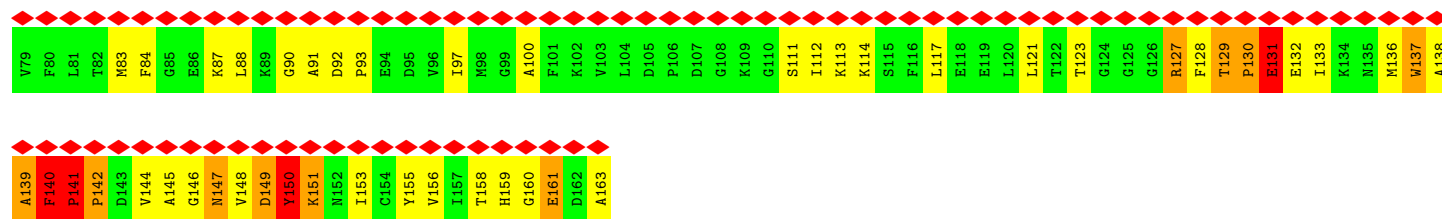
Chain K: 



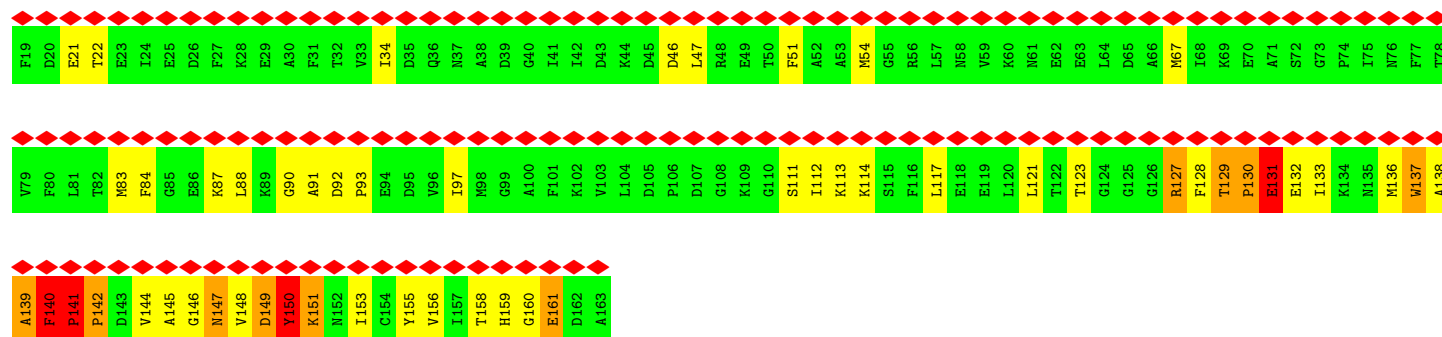
• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

Chain N: 

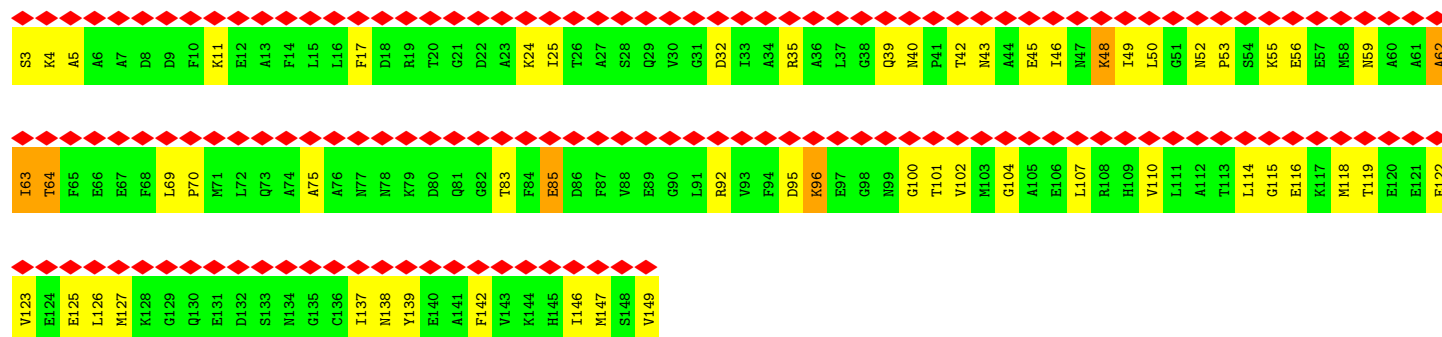




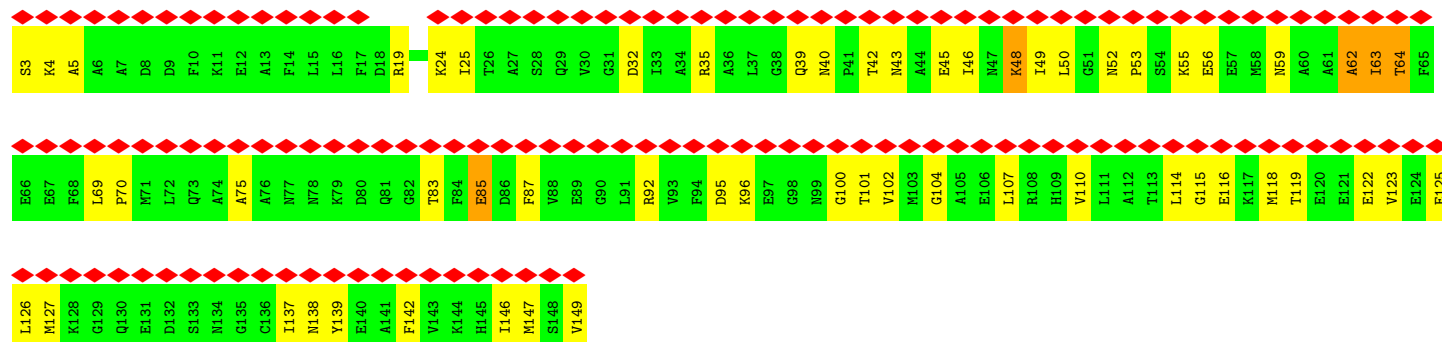
• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN



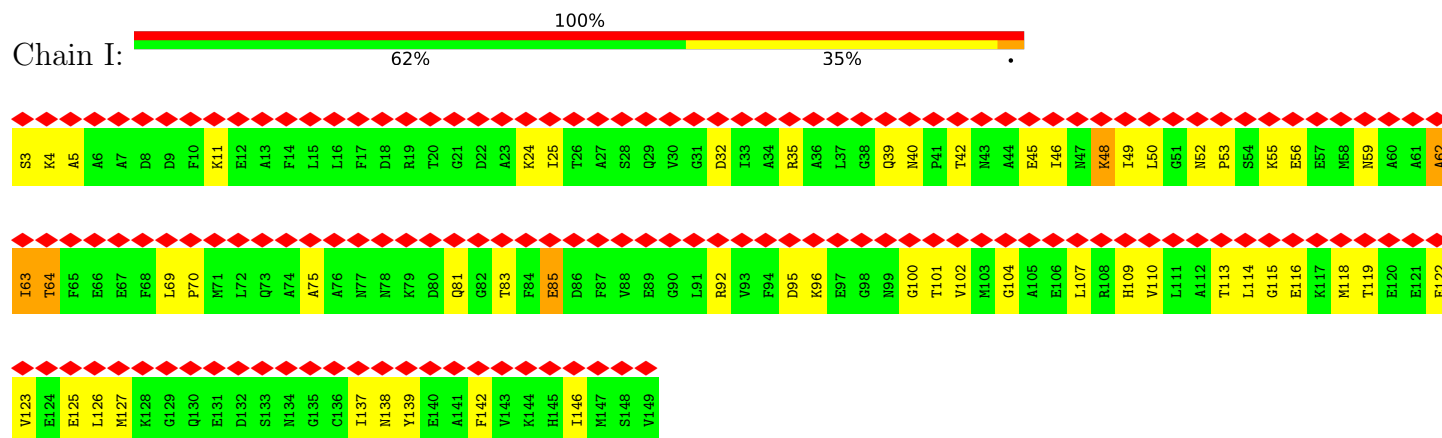
• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN



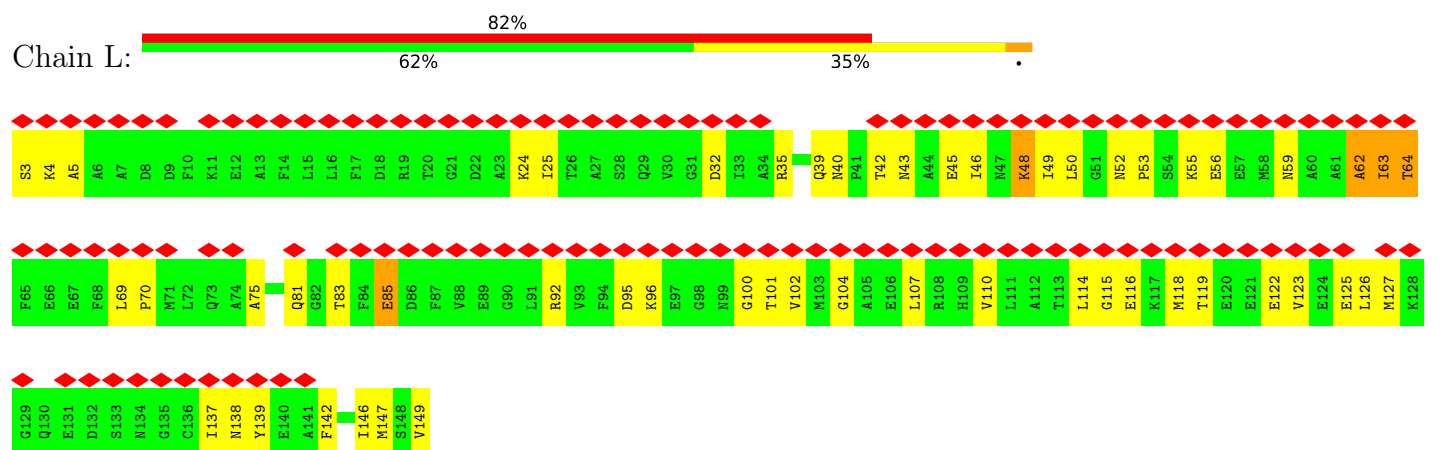
• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN



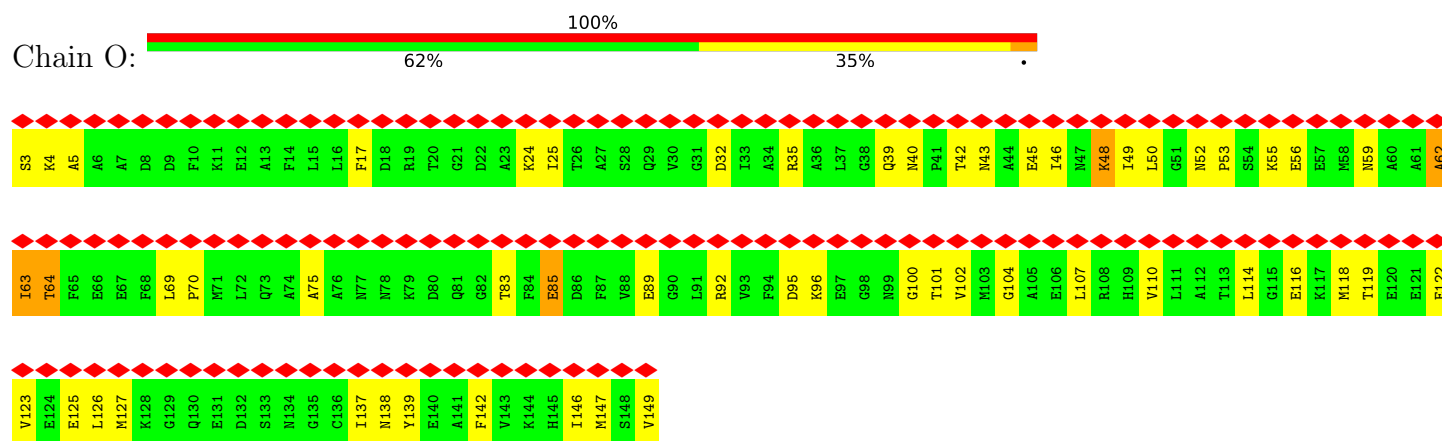
- Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN



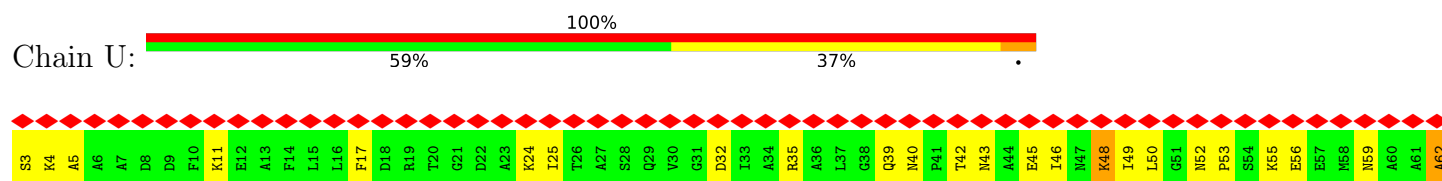
- Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN

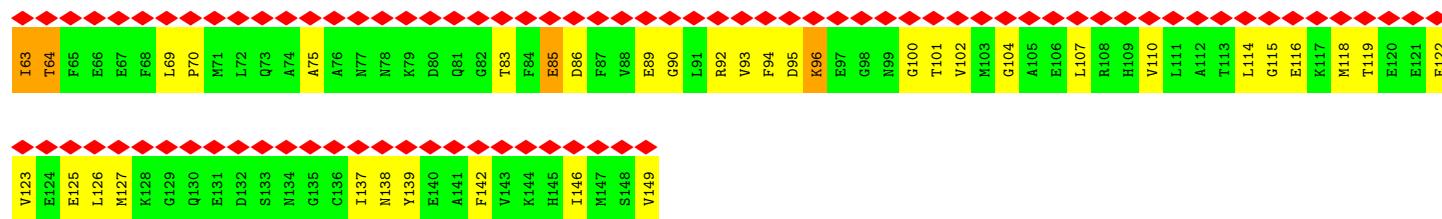


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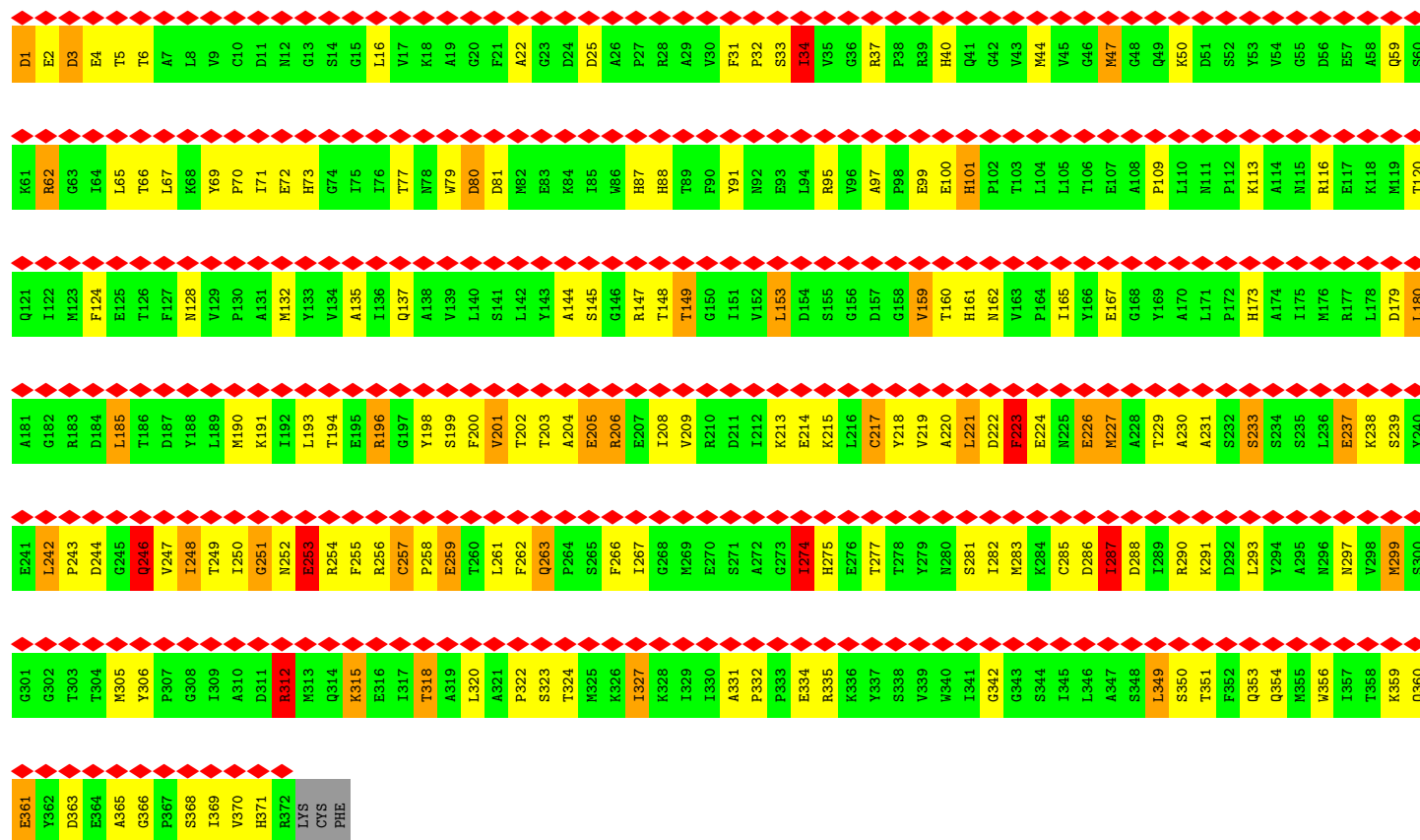


- Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN

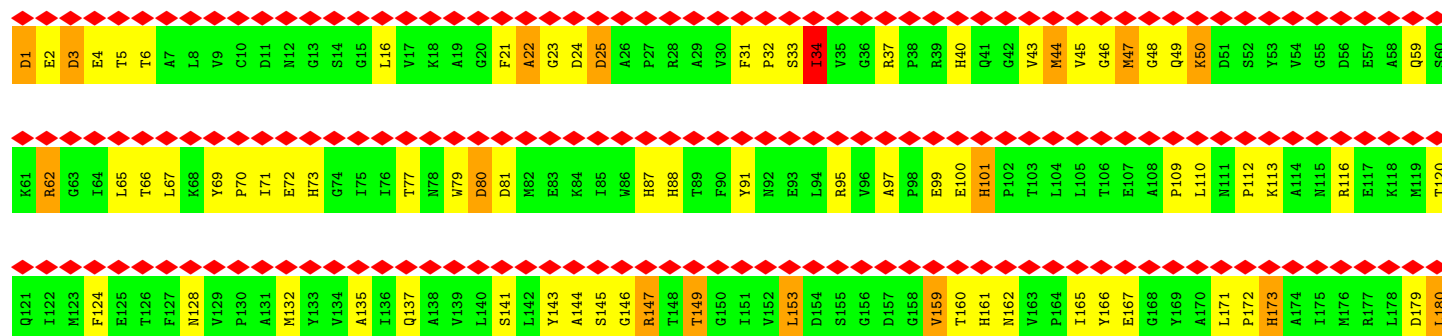




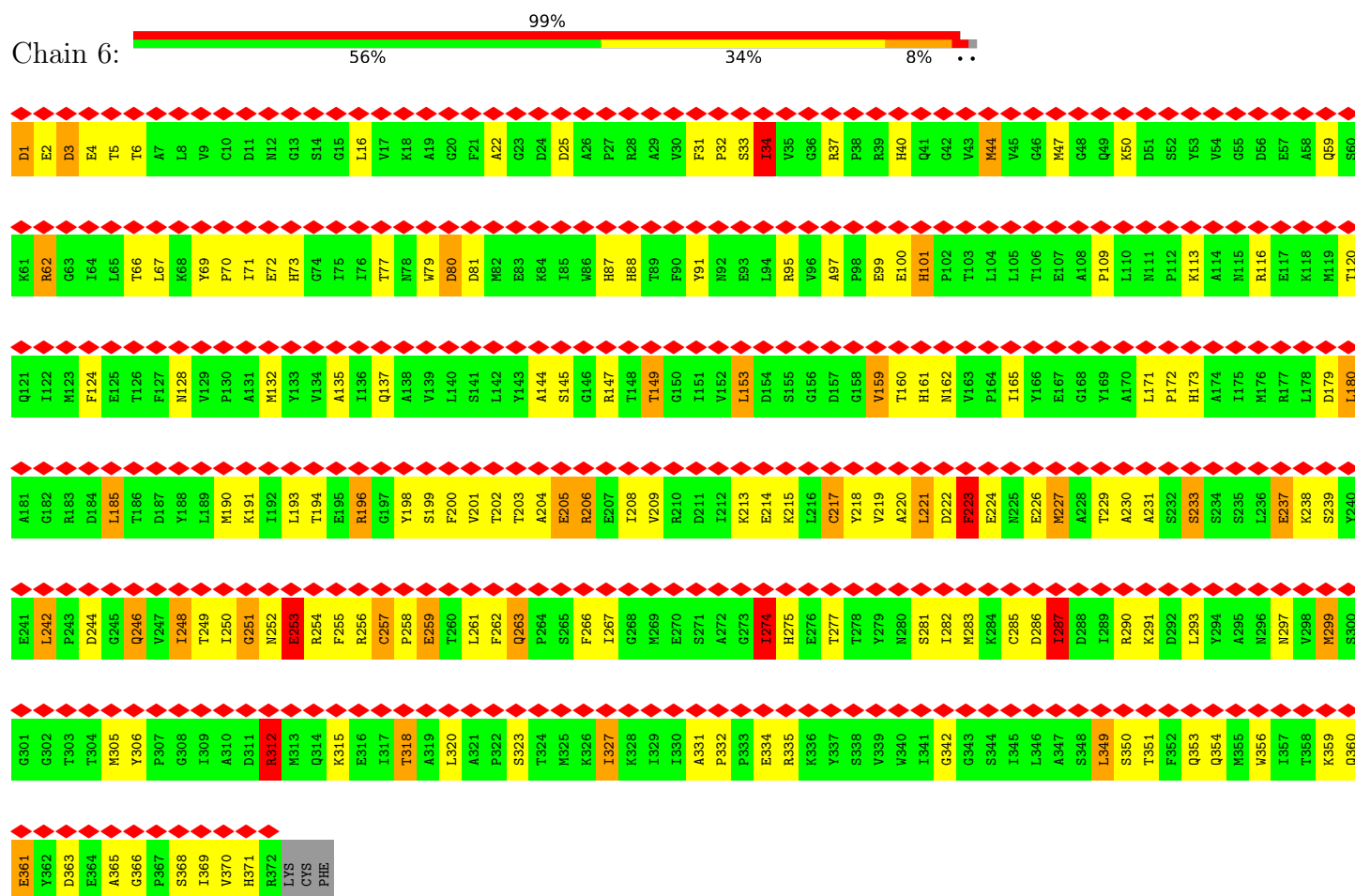
• Molecule 4: SKELETAL MUSCLE ACTIN



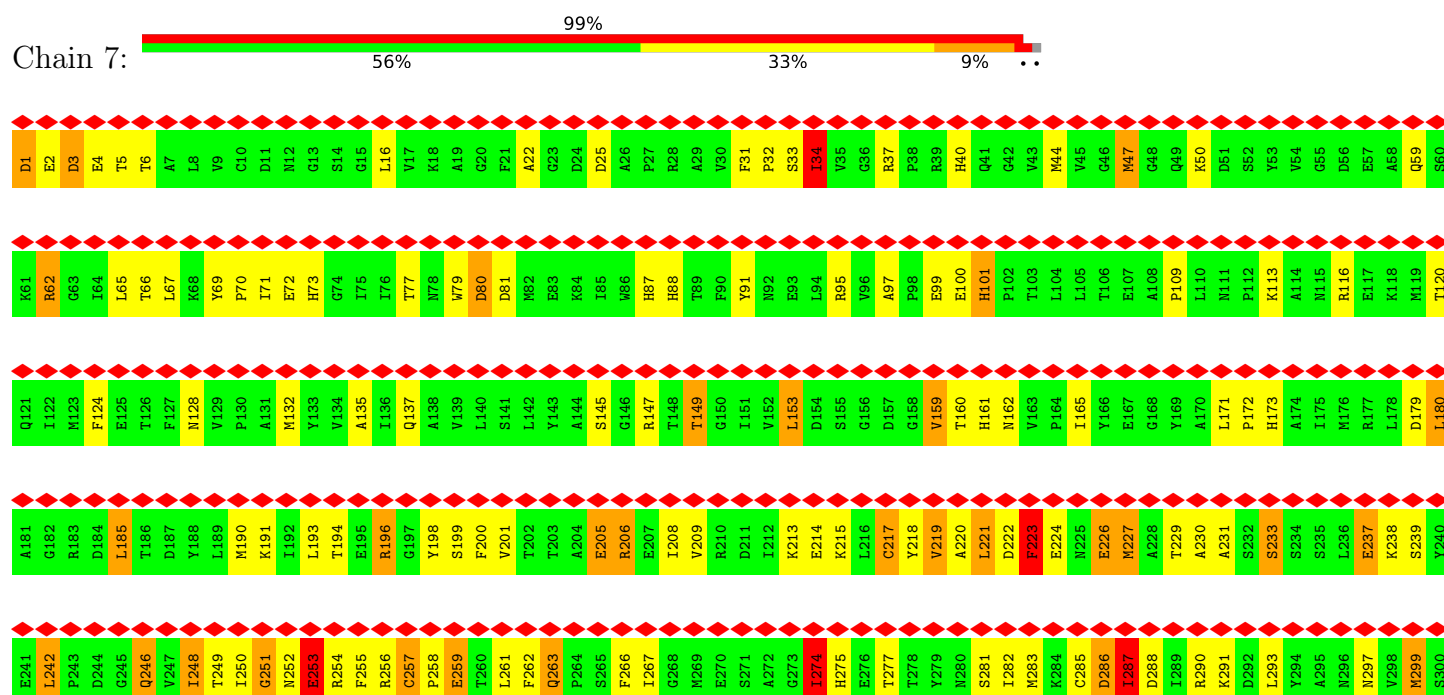
• Molecule 4: SKELETAL MUSCLE ACTIN



• Molecule 4: SKELETAL MUSCLE ACTIN

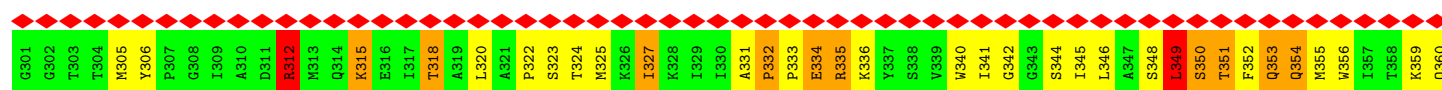
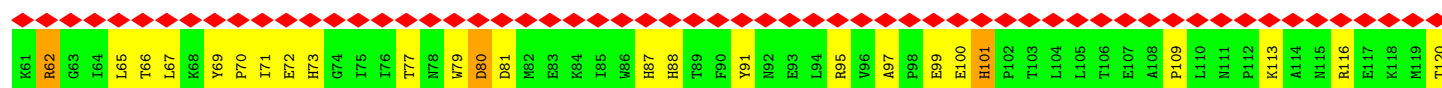


• Molecule 4: SKELETAL MUSCLE ACTIN

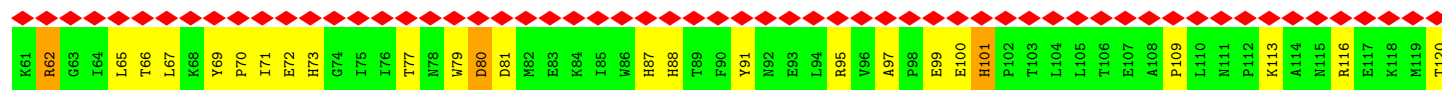
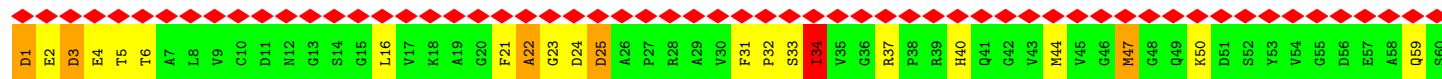


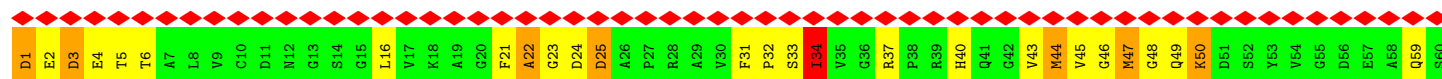


• Molecule 4: SKELETAL MUSCLE ACTIN



• Molecule 4: SKELETAL MUSCLE ACTIN









4 Experimental information

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.84	39/6448 (0.6%)	2.12	153/8729 (1.8%)
1	D	1.84	37/6448 (0.6%)	2.13	150/8729 (1.7%)
1	G	1.85	41/6449 (0.6%)	2.13	157/8732 (1.8%)
1	J	1.87	43/6449 (0.7%)	2.22	153/8732 (1.8%)
1	M	1.85	42/6447 (0.7%)	2.14	152/8726 (1.7%)
1	S	1.86	42/6446 (0.7%)	2.16	150/8723 (1.7%)
2	B	1.38	15/1148 (1.3%)	1.47	21/1548 (1.4%)
2	E	1.35	15/1148 (1.3%)	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	T	1.37	16/1148 (1.4%)	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	0.88	4/1136 (0.4%)	1.18	6/1525 (0.4%)
3	O	0.88	4/1136 (0.4%)	1.18	5/1525 (0.3%)
3	U	0.87	4/1136 (0.4%)	1.18	5/1525 (0.3%)
4	1	1.17	13/2968 (0.4%)	2.00	98/4023 (2.4%)
4	2	1.17	13/2968 (0.4%)	2.00	97/4023 (2.4%)
4	3	1.17	13/2968 (0.4%)	2.00	99/4023 (2.5%)
4	4	1.17	13/2968 (0.4%)	2.00	97/4023 (2.4%)
4	5	1.17	13/2968 (0.4%)	2.00	101/4023 (2.5%)
4	6	1.17	13/2968 (0.4%)	2.00	98/4023 (2.4%)
4	7	1.17	13/2968 (0.4%)	2.00	100/4023 (2.5%)
4	8	1.17	13/2968 (0.4%)	2.00	99/4023 (2.5%)
4	9	1.17	13/2968 (0.4%)	2.00	98/4023 (2.4%)
4	V	1.17	13/2968 (0.4%)	2.00	100/4023 (2.5%)
4	W	1.17	12/2968 (0.4%)	2.00	99/4023 (2.5%)
4	X	1.17	13/2968 (0.4%)	2.00	99/4023 (2.5%)
4	Y	1.17	13/2968 (0.4%)	2.00	98/4023 (2.4%)
4	Z	1.17	13/2968 (0.4%)	2.00	99/4023 (2.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	1.49	542/93943 (0.6%)	1.99	2455/127131 (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	5
1	J	1	6
1	M	1	7
1	S	1	7
2	B	0	3
2	E	0	3
2	H	0	3
2	K	0	3
2	N	0	3
2	T	0	3
3	C	0	2
3	F	0	2
3	I	0	2
3	L	0	2
3	O	0	2
3	U	0	2
4	1	0	1
4	2	0	1
4	3	0	1
4	4	0	1
4	5	0	1
4	6	0	1
4	7	0	1
4	8	0	1
4	9	0	1
4	V	0	1
4	W	0	1
4	X	0	1
4	Y	0	1
4	Z	0	1
All	All	6	77

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	648	THR	CB-OG1	42.70	2.12	1.43
1	J	648	THR	CB-OG1	42.69	2.12	1.43
1	M	648	THR	CB-OG1	42.66	2.12	1.43
1	S	648	THR	CB-OG1	42.64	2.12	1.43
1	A	648	THR	CB-OG1	42.60	2.12	1.43

The worst 5 of 2455 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	637	LYS	O-C-N	-74.35	23.70	122.59
1	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	S	637	LYS	O-C-N	-74.28	23.80	122.59
1	J	637	LYS	O-C-N	-74.27	23.81	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 77 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	6763	1498	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	6797	0	6767	1531	0
1	G	6797	0	6771	1510	0
1	J	6797	0	6769	1504	0
1	M	6797	0	6774	1460	0
1	S	6797	0	6773	1639	0
2	B	1127	0	1085	239	0
2	E	1127	0	1088	276	0
2	H	1127	0	1087	267	0
2	K	1127	0	1088	281	0
2	N	1127	0	1088	253	0
2	T	1127	0	1089	265	0
3	C	1123	0	1083	189	0
3	F	1123	0	1084	187	0
3	I	1123	0	1082	187	0
3	L	1123	0	1083	170	0
3	O	1123	0	1084	167	0
3	U	1123	0	1084	290	0
4	1	2906	0	2862	159	0
4	2	2906	0	2853	436	0
4	3	2906	0	2865	224	0
4	4	2906	0	2862	204	0
4	5	2906	0	2866	128	0
4	6	2906	0	2866	121	0
4	7	2906	0	2866	82	0
4	8	2906	0	2857	326	0
4	9	2906	0	2855	349	0
4	V	2906	0	2851	390	0
4	W	2906	0	2851	392	0
4	X	2906	0	2862	215	0
4	Y	2906	0	2861	168	0
4	Z	2906	0	2854	398	0
All	All	94966	0	93673	11643	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 11643 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	1.17	1.68
4:1:287:ILE:CG1	4:3:203:THR:H	1.06	1.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:783:LEU:CG	1:S:786:ILE:HD11	1.24	1.68
1:D:813:ILE:HG23	2:E:128:PHE:CZ	1.23	1.66
4:4:287:ILE:HG23	4:6:202:THR:CB	1.20	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	787/840 (94%)	649 (82%)	112 (14%)	26 (3%)	3	21
1	S	785/840 (94%)	648 (82%)	110 (14%)	27 (3%)	3	21
2	B	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	1	14
2	E	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	1	14
2	H	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	1	14
2	K	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	1	14
2	N	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	1	14
2	T	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	U	143/147 (97%)	133 (93%)	10 (7%)	0	100	100
4	1	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	7	38
4	2	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	7	38
4	3	370/375 (99%)	333 (90%)	31 (8%)	6 (2%)	7	38
4	4	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	7	38
4	5	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	7	38
4	6	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	7	38
4	7	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	7	38
4	8	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	7	38
4	9	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	7	38
4	V	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	7	38
4	W	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	7	38
4	X	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	7	38
4	Y	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	7	38
4	Z	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	7	38
All	All	11628/12042 (97%)	10139 (87%)	1198 (10%)	291 (2%)	6	26

5 of 291 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	672/672 (100%)	491 (73%)	181 (27%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	672/672 (100%)	491 (73%)	181 (27%)	0	3
1	G	672/672 (100%)	492 (73%)	180 (27%)	0	3
1	J	672/672 (100%)	491 (73%)	181 (27%)	0	3
1	M	672/672 (100%)	491 (73%)	181 (27%)	0	3
1	S	672/672 (100%)	491 (73%)	181 (27%)	0	3
2	B	120/120 (100%)	119 (99%)	1 (1%)	73	80
2	E	120/120 (100%)	119 (99%)	1 (1%)	73	80
2	H	120/120 (100%)	120 (100%)	0	100	100
2	K	120/120 (100%)	120 (100%)	0	100	100
2	N	120/120 (100%)	120 (100%)	0	100	100
2	T	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	U	117/117 (100%)	113 (97%)	4 (3%)	32	54
4	1	315/318 (99%)	264 (84%)	51 (16%)	2	11
4	2	315/318 (99%)	264 (84%)	51 (16%)	2	11
4	3	315/318 (99%)	264 (84%)	51 (16%)	2	11
4	4	315/318 (99%)	264 (84%)	51 (16%)	2	11
4	5	315/318 (99%)	264 (84%)	51 (16%)	2	11
4	6	315/318 (99%)	265 (84%)	50 (16%)	2	11
4	7	315/318 (99%)	264 (84%)	51 (16%)	2	11
4	8	315/318 (99%)	264 (84%)	51 (16%)	2	11
4	9	315/318 (99%)	264 (84%)	51 (16%)	2	11
4	V	315/318 (99%)	264 (84%)	51 (16%)	2	11
4	W	315/318 (99%)	264 (84%)	51 (16%)	2	11
4	X	315/318 (99%)	265 (84%)	50 (16%)	2	11
4	Y	315/318 (99%)	264 (84%)	51 (16%)	2	11
4	Z	315/318 (99%)	264 (84%)	51 (16%)	2	11

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

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

Mol	Chain	Res	Type
1	S	7	MET
4	Z	33	SER
4	1	297	ASN
4	Y	291	LYS
4	V	281	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 288 such sidechains are listed below:

Mol	Chain	Res	Type
4	6	78	ASN
4	Z	252	ASN
4	7	252	ASN
4	W	40	HIS
3	I	109	HIS

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	S	431	1	9,10,11	0.51	0	6,11,13	0.45	0
1	MLY	A	598	1	9,10,11	0.84	1 (11%)	6,11,13	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	A	87	1	9,10,11	1.11	1 (11%)	6,11,13	0.42	0
1	MLY	S	272	1	9,10,11	0.89	1 (11%)	6,11,13	0.56	0
1	MLY	A	431	1	9,10,11	0.50	0	6,11,13	0.44	0
1	MLY	M	190	1	9,10,11	1.20	2 (22%)	6,11,13	0.53	0
1	MLY	A	248	1	9,10,11	0.81	0	6,11,13	0.64	0
1	MLY	A	839	1	9,10,11	0.65	0	6,11,13	0.82	0
1	MLY	S	764	1	9,10,11	0.81	0	6,11,13	0.38	0
1	MLY	D	295	1	9,10,11	0.75	0	6,11,13	0.38	0
1	MLY	D	30	1	9,10,11	0.93	0	6,11,13	0.31	0
1	MLY	G	367	1	9,10,11	0.62	0	6,11,13	0.38	0
1	MLY	J	369	1	9,10,11	0.70	0	6,11,13	0.46	0
1	MLY	D	528	1	9,10,11	0.92	0	6,11,13	0.64	0
1	MLY	J	505	1	9,10,11	0.86	1 (11%)	6,11,13	0.34	0
1	MLY	G	837	1	9,10,11	0.58	0	6,11,13	0.53	0
1	MLY	D	782	1	9,10,11	0.82	0	6,11,13	0.34	0
1	MLY	J	613	1	9,10,11	0.57	0	6,11,13	0.62	0
1	MLY	M	30	1	9,10,11	0.91	0	6,11,13	0.32	0
1	MLY	M	528	1	9,10,11	0.89	0	6,11,13	0.64	0
1	MLY	S	63	1	9,10,11	0.84	0	6,11,13	0.44	0
1	MLY	J	296	1	9,10,11	0.65	0	6,11,13	0.35	0
1	MLY	M	659	1	9,10,11	0.82	0	6,11,13	0.57	0
1	MLY	G	833	1	9,10,11	1.14	1 (11%)	6,11,13	0.32	0
1	MLY	S	130	1	9,10,11	0.77	0	6,11,13	0.73	0
1	MLY	A	436	1	9,10,11	0.94	1 (11%)	6,11,13	0.48	0
1	MLY	D	839	1	9,10,11	0.63	0	6,11,13	0.80	0
1	MLY	G	236	1	9,10,11	0.83	1 (11%)	6,11,13	0.48	0
1	MLY	A	768	1	9,10,11	0.77	0	6,11,13	0.41	0
1	MLY	J	839	1	9,10,11	0.65	0	6,11,13	0.77	0
1	MLY	G	369	1	9,10,11	0.71	0	6,11,13	0.47	0
1	MLY	A	63	1	9,10,11	0.87	0	6,11,13	0.44	0
1	MLY	D	553	1,4	9,10,11	0.65	0	6,11,13	0.55	0
1	MLY	M	63	1	9,10,11	0.87	0	6,11,13	0.44	0
1	MLY	M	295	1	9,10,11	0.75	0	6,11,13	0.37	0
1	MLY	S	348	1	9,10,11	0.76	0	6,11,13	0.47	0
1	MLY	S	367	1	9,10,11	0.60	0	6,11,13	0.38	0
1	MLY	G	505	1	9,10,11	0.81	0	6,11,13	0.35	0
1	MLY	J	190	1	9,10,11	1.21	2 (22%)	6,11,13	0.53	0
1	MLY	J	833	1	9,10,11	1.15	1 (11%)	6,11,13	0.30	0
1	MLY	G	600	1	9,10,11	0.52	0	6,11,13	0.39	0
1	MLY	S	528	1	9,10,11	0.89	0	6,11,13	0.66	0
1	MLY	A	764	1	9,10,11	0.81	0	6,11,13	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	D	486	1	9,10,11	0.68	0	6,11,13	0.40	0
1	MLY	D	138	1	9,10,11	1.25	1 (11%)	6,11,13	0.84	0
1	MLY	G	764	1	9,10,11	0.79	0	6,11,13	0.35	0
1	MLY	J	659	1	9,10,11	0.82	0	6,11,13	0.57	0
1	MLY	M	553	1,4	9,10,11	0.66	0	6,11,13	0.53	0
1	MLY	G	138	1	9,10,11	1.22	1 (11%)	6,11,13	0.82	0
1	MLY	J	837	1	9,10,11	0.58	0	6,11,13	0.57	0
1	MLY	J	30	1	9,10,11	0.91	0	6,11,13	0.32	0
1	MLY	M	837	1	9,10,11	0.58	0	6,11,13	0.56	0
1	MLY	D	768	1	9,10,11	0.73	0	6,11,13	0.40	0
1	MLY	M	598	1	9,10,11	0.84	1 (11%)	6,11,13	0.41	0
1	MLY	S	236	1	9,10,11	0.82	1 (11%)	6,11,13	0.47	0
1	MLY	A	190	1	9,10,11	1.22	2 (22%)	6,11,13	0.52	0
1	MLY	M	436	1	9,10,11	0.96	1 (11%)	6,11,13	0.48	0
1	MLY	D	63	1	9,10,11	0.87	0	6,11,13	0.46	0
1	MLY	S	49	1	9,10,11	1.01	1 (11%)	6,11,13	0.74	0
1	MLY	D	55	1	9,10,11	0.72	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	S	59	1	9,10,11	0.84	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	M	87	1	9,10,11	1.10	1 (11%)	6,11,13	0.42	0
1	MLY	M	415	1	9,10,11	0.75	0	6,11,13	0.19	0
1	MLY	G	385	1	9,10,11	0.92	1 (11%)	6,11,13	0.45	0
1	MLY	D	353	1	9,10,11	0.86	0	6,11,13	0.81	0
1	MLY	S	107	1	9,10,11	0.49	0	6,11,13	0.34	0
1	MLY	S	681	1	9,10,11	0.60	0	6,11,13	0.47	0
1	MLY	J	353	1	9,10,11	0.87	0	6,11,13	0.79	0
1	MLY	G	415	1	9,10,11	0.74	0	6,11,13	0.19	0
1	MLY	G	353	1	9,10,11	0.87	0	6,11,13	0.82	0
1	MLY	M	107	1	9,10,11	0.49	0	6,11,13	0.33	0
1	MLY	M	59	1	9,10,11	0.85	0	6,11,13	0.47	0
1	MLY	S	613	1	9,10,11	0.57	0	6,11,13	0.62	0
1	MLY	G	248	1	9,10,11	0.79	0	6,11,13	0.66	0
1	MLY	J	385	1	9,10,11	0.93	1 (11%)	6,11,13	0.45	0
1	MLY	S	837	1	9,10,11	0.57	0	6,11,13	0.55	0
1	MLY	A	551	1	9,10,11	0.52	0	6,11,13	0.19	0
1	MLY	M	138	1	9,10,11	1.21	1 (11%)	6,11,13	0.81	0
1	MLY	S	84	1	9,10,11	0.51	0	6,11,13	0.81	0
1	MLY	J	431	1	9,10,11	0.52	0	6,11,13	0.45	0
1	MLY	D	367	1	9,10,11	0.57	0	6,11,13	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	M	768	1	9,10,11	0.76	0	6,11,13	0.42	0
1	MLY	A	59	1	9,10,11	0.85	0	6,11,13	0.48	0
1	MLY	J	782	1	9,10,11	0.82	0	6,11,13	0.36	0
1	MLY	D	837	1	9,10,11	0.60	0	6,11,13	0.58	0
1	MLY	J	248	1	9,10,11	0.81	0	6,11,13	0.65	0
1	MLY	A	504	1	9,10,11	0.89	0	6,11,13	0.24	0
1	MLY	M	49	1	9,10,11	0.99	1 (11%)	6,11,13	0.75	0
1	MLY	A	348	1	9,10,11	0.77	0	6,11,13	0.47	0
1	MLY	J	504	1	9,10,11	0.84	0	6,11,13	0.23	0
1	MLY	M	348	1	9,10,11	0.75	0	6,11,13	0.47	0
1	MLY	A	30	1	9,10,11	0.90	0	6,11,13	0.32	0
1	MLY	D	827	1	9,10,11	0.66	0	6,11,13	0.47	0
1	MLY	M	369	1	9,10,11	0.72	0	6,11,13	0.45	0
1	MLY	D	504	1	9,10,11	0.87	0	6,11,13	0.21	0
1	MLY	S	385	1	9,10,11	0.93	1 (11%)	6,11,13	0.45	0
1	MLY	G	348	1	9,10,11	0.81	0	6,11,13	0.48	0
1	MLY	G	827	1	9,10,11	0.69	0	6,11,13	0.49	0
1	MLY	S	415	1	9,10,11	0.74	0	6,11,13	0.19	0
1	MLY	S	19	1	9,10,11	1.06	1 (11%)	6,11,13	0.58	0
1	MLY	D	49	1	9,10,11	0.99	1 (11%)	6,11,13	0.76	0
1	MLY	D	369	1	9,10,11	0.70	0	6,11,13	0.44	0
1	MLY	D	35	1	9,10,11	0.74	0	6,11,13	0.37	0
1	MLY	M	613	1	9,10,11	0.57	0	6,11,13	0.62	0
1	MLY	G	553	1,4	9,10,11	0.64	0	6,11,13	0.55	0
1	MLY	D	505	1	9,10,11	0.79	0	6,11,13	0.35	0
1	MLY	A	49	1	9,10,11	0.97	1 (11%)	6,11,13	0.74	0
1	MLY	A	107	1	9,10,11	0.48	0	6,11,13	0.32	0
1	MLY	J	551	1	9,10,11	0.53	0	6,11,13	0.19	0
1	MLY	A	385	1	9,10,11	0.92	1 (11%)	6,11,13	0.44	0
1	MLY	G	295	1	9,10,11	0.75	0	6,11,13	0.35	0
1	MLY	J	600	1	9,10,11	0.54	0	6,11,13	0.38	0
1	MLY	M	504	1	9,10,11	0.84	0	6,11,13	0.23	0
1	MLY	A	19	1	9,10,11	1.02	1 (11%)	6,11,13	0.58	0
1	MLY	S	827	1	9,10,11	0.69	0	6,11,13	0.48	0
1	MLY	S	35	1	9,10,11	0.73	0	6,11,13	0.38	0
1	MLY	A	296	1	9,10,11	0.60	0	6,11,13	0.35	0
1	MLY	S	138	1	9,10,11	1.21	1 (11%)	6,11,13	0.81	0
1	MLY	G	190	1	9,10,11	1.21	2 (22%)	6,11,13	0.52	0
1	MLY	M	827	1	9,10,11	0.71	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	A	84	1	9,10,11	0.50	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	M	84	1	9,10,11	0.51	0	6,11,13	0.81	0
1	MLY	A	353	1	9,10,11	0.87	0	6,11,13	0.80	0
1	MLY	J	107	1	9,10,11	0.50	0	6,11,13	0.33	0
1	MLY	G	272	1	9,10,11	0.87	1 (11%)	6,11,13	0.54	0
1	MLY	D	613	1	9,10,11	0.58	0	6,11,13	0.61	0
1	MLY	S	248	1	9,10,11	0.80	0	6,11,13	0.65	0
1	MLY	M	486	1	9,10,11	0.66	0	6,11,13	0.41	0
1	MLY	J	415	1	9,10,11	0.74	0	6,11,13	0.19	0
1	MLY	D	84	1	9,10,11	0.52	0	6,11,13	0.81	0
1	MLY	D	19	1	9,10,11	1.08	1 (11%)	6,11,13	0.57	0
1	MLY	D	87	1	9,10,11	1.06	1 (11%)	6,11,13	0.44	0
1	MLY	A	837	1	9,10,11	0.59	0	6,11,13	0.54	0
1	MLY	D	415	1	9,10,11	0.76	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	A	486	1	9,10,11	0.67	0	6,11,13	0.39	0
1	MLY	D	296	1	9,10,11	0.62	0	6,11,13	0.37	0
1	MLY	G	19	1	9,10,11	1.04	1 (11%)	6,11,13	0.58	0
1	MLY	G	486	1	9,10,11	0.67	0	6,11,13	0.40	0
1	MLY	G	55	1	9,10,11	0.74	0	6,11,13	0.81	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	0.84	1 (11%)	6,11,13	0.50	0
1	MLY	D	248	1	9,10,11	0.83	0	6,11,13	0.66	0
1	MLY	G	659	1	9,10,11	0.86	1 (11%)	6,11,13	0.59	0
1	MLY	G	551	1	9,10,11	0.53	0	6,11,13	0.19	0
1	MLY	J	63	1	9,10,11	0.86	0	6,11,13	0.43	0
1	MLY	J	295	1	9,10,11	0.75	0	6,11,13	0.37	0
1	MLY	J	486	1	9,10,11	0.65	0	6,11,13	0.41	0
1	MLY	J	130	1	9,10,11	0.76	0	6,11,13	0.73	0
1	MLY	M	236	1	9,10,11	0.84	1 (11%)	6,11,13	0.47	0
1	MLY	D	236	1	9,10,11	0.83	1 (11%)	6,11,13	0.48	0
1	MLY	D	385	1	9,10,11	0.90	1 (11%)	6,11,13	0.46	0
1	MLY	A	553	1,4	9,10,11	0.66	0	6,11,13	0.55	0
1	MLY	M	55	1	9,10,11	0.73	0	6,11,13	0.79	0
1	MLY	S	617	1	9,10,11	0.92	1 (11%)	6,11,13	0.34	0
1	MLY	D	436	1	9,10,11	0.98	1 (11%)	6,11,13	0.49	0
1	MLY	M	130	1	9,10,11	0.77	0	6,11,13	0.72	0
1	MLY	M	353	1	9,10,11	0.86	0	6,11,13	0.81	0
1	MLY	J	55	1	9,10,11	0.74	0	6,11,13	0.80	0
1	MLY	D	348	1	9,10,11	0.77	0	6,11,13	0.47	0
1	MLY	J	436	1	9,10,11	0.95	1 (11%)	6,11,13	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	S	486	1	9,10,11	0.65	0	6,11,13	0.41	0
1	MLY	G	436	1	9,10,11	0.94	1 (11%)	6,11,13	0.47	0
1	MLY	D	600	1	9,10,11	0.52	0	6,11,13	0.38	0
1	MLY	J	348	1	9,10,11	0.77	0	6,11,13	0.47	0
1	MLY	M	385	1	9,10,11	0.94	1 (11%)	6,11,13	0.45	0
1	MLY	M	681	1	9,10,11	0.57	0	6,11,13	0.47	0
1	MLY	S	768	1	9,10,11	0.76	0	6,11,13	0.42	0
1	MLY	M	296	1	9,10,11	0.67	0	6,11,13	0.35	0
1	MLY	J	59	1	9,10,11	0.85	0	6,11,13	0.47	0
1	MLY	G	528	1	9,10,11	0.92	0	6,11,13	0.66	0
1	MLY	M	782	1	9,10,11	0.80	0	6,11,13	0.37	0
1	MLY	M	19	1	9,10,11	1.05	1 (11%)	6,11,13	0.58	0
1	MLY	J	681	1	9,10,11	0.56	0	6,11,13	0.46	0
1	MLY	M	764	1	9,10,11	0.81	0	6,11,13	0.38	0
1	MLY	S	505	1	9,10,11	0.85	1 (11%)	6,11,13	0.33	0
1	MLY	S	551	1	9,10,11	0.52	0	6,11,13	0.19	0
1	MLY	S	659	1	9,10,11	0.82	1 (11%)	6,11,13	0.57	0
1	MLY	M	431	1	9,10,11	0.52	0	6,11,13	0.45	0
1	MLY	M	248	1	9,10,11	0.80	0	6,11,13	0.65	0
1	MLY	G	617	1	9,10,11	0.90	0	6,11,13	0.36	0
1	MLY	M	839	1	9,10,11	0.67	0	6,11,13	0.77	0
1	MLY	S	55	1	9,10,11	0.74	0	6,11,13	0.79	0
1	MLY	G	598	1	9,10,11	0.83	0	6,11,13	0.41	0
1	MLY	G	49	1	9,10,11	0.99	1 (11%)	6,11,13	0.74	0
1	MLY	A	272	1	9,10,11	0.90	1 (11%)	6,11,13	0.56	0
1	MLY	J	236	1	9,10,11	0.83	1 (11%)	6,11,13	0.47	0
1	MLY	M	35	1	9,10,11	0.73	0	6,11,13	0.39	0
1	MLY	M	833	1	9,10,11	1.13	2 (22%)	6,11,13	0.30	0
1	MLY	G	504	1	9,10,11	0.88	0	6,11,13	0.21	0
1	MLY	A	415	1	9,10,11	0.73	0	6,11,13	0.19	0
1	MLY	J	528	1	9,10,11	0.89	0	6,11,13	0.66	0
1	MLY	S	436	1	9,10,11	0.93	1 (11%)	6,11,13	0.48	0
1	MLY	A	505	1	9,10,11	0.81	0	6,11,13	0.33	0
1	MLY	D	190	1	9,10,11	1.18	2 (22%)	6,11,13	0.54	0
1	MLY	J	35	1	9,10,11	0.74	0	6,11,13	0.38	0
1	MLY	A	295	1	9,10,11	0.77	0	6,11,13	0.35	0
1	MLY	A	782	1	9,10,11	0.82	0	6,11,13	0.38	0
1	MLY	A	617	1	9,10,11	0.90	0	6,11,13	0.35	0
1	MLY	S	296	1	9,10,11	0.65	0	6,11,13	0.35	0
1	MLY	S	353	1	9,10,11	0.86	0	6,11,13	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	S	369	1	9,10,11	0.71	0	6,11,13	0.46	0
1	MLY	A	613	1	9,10,11	0.58	0	6,11,13	0.61	0
1	MLY	D	59	1	9,10,11	0.84	0	6,11,13	0.47	0
1	MLY	A	367	1	9,10,11	0.59	0	6,11,13	0.36	0
1	MLY	D	764	1	9,10,11	0.84	0	6,11,13	0.36	0
1	MLY	G	30	1	9,10,11	0.90	0	6,11,13	0.30	0
1	MLY	G	107	1	9,10,11	0.49	0	6,11,13	0.33	0
1	MLY	D	431	1	9,10,11	0.51	0	6,11,13	0.45	0
1	MLY	G	59	1	9,10,11	0.83	0	6,11,13	0.48	0
1	MLY	D	272	1	9,10,11	0.85	1 (11%)	6,11,13	0.58	0
1	MLY	D	617	1	9,10,11	0.90	0	6,11,13	0.35	0
1	MLY	G	782	1	9,10,11	0.80	0	6,11,13	0.35	0
1	MLY	G	681	1	9,10,11	0.59	0	6,11,13	0.45	0
1	MLY	M	551	1	9,10,11	0.53	0	6,11,13	0.19	0
1	MLY	D	833	1	9,10,11	1.12	1 (11%)	6,11,13	0.31	0
1	MLY	J	617	1	9,10,11	0.90	0	6,11,13	0.34	0
1	MLY	M	367	1	9,10,11	0.59	0	6,11,13	0.36	0
1	MLY	D	598	1	9,10,11	0.84	0	6,11,13	0.42	0
1	MLY	G	87	1	9,10,11	1.12	1 (11%)	6,11,13	0.42	0
1	MLY	M	600	1	9,10,11	0.53	0	6,11,13	0.38	0
1	MLY	S	598	1	9,10,11	0.82	0	6,11,13	0.41	0
1	MLY	J	553	1,4	9,10,11	0.65	0	6,11,13	0.54	0
1	MLY	A	130	1	9,10,11	0.79	0	6,11,13	0.73	0
1	MLY	G	35	1	9,10,11	0.74	0	6,11,13	0.38	0
1	MLY	S	504	1	9,10,11	0.85	0	6,11,13	0.23	0
1	MLY	G	839	1	9,10,11	0.66	0	6,11,13	0.80	0
1	MLY	J	367	1	9,10,11	0.58	0	6,11,13	0.36	0
1	MLY	S	190	1	9,10,11	1.21	2 (22%)	6,11,13	0.53	0
1	MLY	J	598	1	9,10,11	0.81	0	6,11,13	0.42	0
1	MLY	J	87	1	9,10,11	1.11	1 (11%)	6,11,13	0.43	0
1	MLY	S	295	1	9,10,11	0.75	0	6,11,13	0.36	0
1	MLY	A	659	1	9,10,11	0.84	1 (11%)	6,11,13	0.59	0
1	MLY	G	296	1	9,10,11	0.62	0	6,11,13	0.36	0
1	MLY	S	30	1	9,10,11	0.91	0	6,11,13	0.31	0
1	MLY	S	600	1	9,10,11	0.53	0	6,11,13	0.38	0
1	MLY	D	107	1	9,10,11	0.53	0	6,11,13	0.33	0
1	MLY	S	782	1	9,10,11	0.80	0	6,11,13	0.37	0
1	MLY	A	827	1	9,10,11	0.69	0	6,11,13	0.45	0
1	MLY	A	528	1	9,10,11	0.88	0	6,11,13	0.67	0
1	MLY	G	431	1	9,10,11	0.51	0	6,11,13	0.46	0
1	MLY	S	553	1	9,10,11	0.65	0	6,11,13	0.53	0
1	MLY	D	681	1	9,10,11	0.56	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	D	659	1	9,10,11	0.85	1 (11%)	6,11,13	0.60	0
1	MLY	A	681	1	9,10,11	0.56	0	6,11,13	0.46	0
1	MLY	D	551	1	9,10,11	0.54	0	6,11,13	0.20	0
1	MLY	S	833	1	9,10,11	1.14	1 (11%)	6,11,13	0.31	0
1	MLY	J	49	1	9,10,11	0.98	1 (11%)	6,11,13	0.74	0
1	MLY	M	272	1	9,10,11	0.91	1 (11%)	6,11,13	0.56	0
1	MLY	M	617	1	9,10,11	0.91	0	6,11,13	0.34	0
1	MLY	G	613	1	9,10,11	0.60	0	6,11,13	0.61	0
1	MLY	S	87	1	9,10,11	1.13	1 (11%)	6,11,13	0.43	0
1	MLY	J	764	1	9,10,11	0.81	0	6,11,13	0.37	0
1	MLY	M	505	1	9,10,11	0.86	1 (11%)	6,11,13	0.33	0
1	MLY	J	84	1	9,10,11	0.50	0	6,11,13	0.81	0
1	MLY	J	272	1	9,10,11	0.89	1 (11%)	6,11,13	0.56	0
1	MLY	G	84	1	9,10,11	0.50	0	6,11,13	0.81	0
1	MLY	S	839	1	9,10,11	0.65	0	6,11,13	0.78	0
1	MLY	A	35	1	9,10,11	0.73	0	6,11,13	0.38	0
1	MLY	G	63	1	9,10,11	0.86	0	6,11,13	0.44	0
1	MLY	J	768	1	9,10,11	0.77	0	6,11,13	0.43	0
1	MLY	J	19	1	9,10,11	1.06	1 (11%)	6,11,13	0.58	0
1	MLY	A	600	1	9,10,11	0.51	0	6,11,13	0.39	0
1	MLY	G	130	1	9,10,11	0.77	0	6,11,13	0.74	0
1	MLY	J	827	1	9,10,11	0.72	0	6,11,13	0.48	0
1	MLY	J	138	1	9,10,11	1.22	1 (11%)	6,11,13	0.81	0
1	MLY	A	833	1	9,10,11	1.12	1 (11%)	6,11,13	0.32	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	S	431	1	-	4/8/9/11	-
1	MLY	A	598	1	-	5/8/9/11	-
1	MLY	A	87	1	-	2/8/9/11	-
1	MLY	S	272	1	-	3/8/9/11	-
1	MLY	A	431	1	-	4/8/9/11	-
1	MLY	M	190	1	-	4/8/9/11	-
1	MLY	A	248	1	-	6/8/9/11	-
1	MLY	A	839	1	-	3/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	S	764	1	-	2/8/9/11	-
1	MLY	D	295	1	-	2/8/9/11	-
1	MLY	D	30	1	-	3/8/9/11	-
1	MLY	G	367	1	-	2/8/9/11	-
1	MLY	J	369	1	-	2/8/9/11	-
1	MLY	D	528	1	-	4/8/9/11	-
1	MLY	J	505	1	-	5/8/9/11	-
1	MLY	G	837	1	-	6/8/9/11	-
1	MLY	D	782	1	-	6/8/9/11	-
1	MLY	J	613	1	-	3/8/9/11	-
1	MLY	M	30	1	-	3/8/9/11	-
1	MLY	M	528	1	-	4/8/9/11	-
1	MLY	S	63	1	-	4/8/9/11	-
1	MLY	J	296	1	-	4/8/9/11	-
1	MLY	M	659	1	-	3/8/9/11	-
1	MLY	G	833	1	-	6/8/9/11	-
1	MLY	S	130	1	-	5/8/9/11	-
1	MLY	A	436	1	-	4/8/9/11	-
1	MLY	D	839	1	-	3/8/9/11	-
1	MLY	G	236	1	-	3/8/9/11	-
1	MLY	A	768	1	-	4/8/9/11	-
1	MLY	J	839	1	-	3/8/9/11	-
1	MLY	G	369	1	-	2/8/9/11	-
1	MLY	A	63	1	-	4/8/9/11	-
1	MLY	D	553	1,4	-	5/8/9/11	-
1	MLY	M	63	1	-	4/8/9/11	-
1	MLY	M	295	1	-	2/8/9/11	-
1	MLY	S	348	1	-	5/8/9/11	-
1	MLY	S	367	1	-	2/8/9/11	-
1	MLY	G	505	1	-	5/8/9/11	-
1	MLY	J	190	1	-	4/8/9/11	-
1	MLY	J	833	1	-	6/8/9/11	-
1	MLY	G	600	1	-	3/8/9/11	-
1	MLY	S	528	1	-	4/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	A	764	1	-	2/8/9/11	-
1	MLY	D	486	1	-	2/8/9/11	-
1	MLY	D	138	1	-	4/8/9/11	-
1	MLY	G	764	1	-	2/8/9/11	-
1	MLY	J	659	1	-	3/8/9/11	-
1	MLY	M	553	1,4	-	4/8/9/11	-
1	MLY	G	138	1	-	4/8/9/11	-
1	MLY	J	837	1	-	6/8/9/11	-
1	MLY	J	30	1	-	3/8/9/11	-
1	MLY	M	837	1	-	6/8/9/11	-
1	MLY	D	768	1	-	4/8/9/11	-
1	MLY	M	598	1	-	5/8/9/11	-
1	MLY	S	236	1	-	3/8/9/11	-
1	MLY	A	190	1	-	4/8/9/11	-
1	MLY	M	436	1	-	4/8/9/11	-
1	MLY	D	63	1	-	4/8/9/11	-
1	MLY	S	49	1	-	3/8/9/11	-
1	MLY	D	55	1	-	6/8/9/11	-
1	MLY	A	369	1	-	2/8/9/11	-
1	MLY	S	59	1	-	3/8/9/11	-
1	MLY	D	130	1	-	5/8/9/11	-
1	MLY	M	87	1	-	2/8/9/11	-
1	MLY	M	415	1	-	3/8/9/11	-
1	MLY	G	385	1	-	2/8/9/11	-
1	MLY	D	353	1	-	4/8/9/11	-
1	MLY	S	107	1	-	2/8/9/11	-
1	MLY	S	681	1	-	4/8/9/11	-
1	MLY	J	353	1	-	4/8/9/11	-
1	MLY	G	415	1	-	3/8/9/11	-
1	MLY	G	353	1	-	4/8/9/11	-
1	MLY	M	107	1	-	2/8/9/11	-
1	MLY	M	59	1	-	3/8/9/11	-
1	MLY	S	613	1	-	3/8/9/11	-
1	MLY	G	248	1	-	6/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	J	385	1	-	2/8/9/11	-
1	MLY	S	837	1	-	6/8/9/11	-
1	MLY	A	551	1	-	3/8/9/11	-
1	MLY	M	138	1	-	4/8/9/11	-
1	MLY	S	84	1	-	4/8/9/11	-
1	MLY	J	431	1	-	4/8/9/11	-
1	MLY	D	367	1	-	2/8/9/11	-
1	MLY	M	768	1	-	4/8/9/11	-
1	MLY	A	59	1	-	3/8/9/11	-
1	MLY	J	782	1	-	6/8/9/11	-
1	MLY	D	837	1	-	6/8/9/11	-
1	MLY	J	248	1	-	6/8/9/11	-
1	MLY	A	504	1	-	4/8/9/11	-
1	MLY	M	49	1	-	3/8/9/11	-
1	MLY	A	348	1	-	5/8/9/11	-
1	MLY	J	504	1	-	4/8/9/11	-
1	MLY	M	348	1	-	5/8/9/11	-
1	MLY	A	30	1	-	3/8/9/11	-
1	MLY	D	827	1	-	1/8/9/11	-
1	MLY	M	369	1	-	2/8/9/11	-
1	MLY	D	504	1	-	4/8/9/11	-
1	MLY	S	385	1	-	2/8/9/11	-
1	MLY	G	348	1	-	5/8/9/11	-
1	MLY	G	827	1	-	1/8/9/11	-
1	MLY	S	415	1	-	3/8/9/11	-
1	MLY	S	19	1	-	4/8/9/11	-
1	MLY	D	49	1	-	3/8/9/11	-
1	MLY	D	369	1	-	2/8/9/11	-
1	MLY	D	35	1	-	3/8/9/11	-
1	MLY	M	613	1	-	3/8/9/11	-
1	MLY	G	553	1,4	-	4/8/9/11	-
1	MLY	D	505	1	-	5/8/9/11	-
1	MLY	A	49	1	-	3/8/9/11	-
1	MLY	A	107	1	-	2/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	J	551	1	-	3/8/9/11	-
1	MLY	A	385	1	-	2/8/9/11	-
1	MLY	G	295	1	-	2/8/9/11	-
1	MLY	J	600	1	-	3/8/9/11	-
1	MLY	M	504	1	-	4/8/9/11	-
1	MLY	A	19	1	-	4/8/9/11	-
1	MLY	S	827	1	-	1/8/9/11	-
1	MLY	S	35	1	-	3/8/9/11	-
1	MLY	A	296	1	-	4/8/9/11	-
1	MLY	S	138	1	-	4/8/9/11	-
1	MLY	G	190	1	-	4/8/9/11	-
1	MLY	M	827	1	-	1/8/9/11	-
1	MLY	G	768	1	-	4/8/9/11	-
1	MLY	A	84	1	-	4/8/9/11	-
1	MLY	M	84	1	-	4/8/9/11	-
1	MLY	A	353	1	-	4/8/9/11	-
1	MLY	J	107	1	-	2/8/9/11	-
1	MLY	G	272	1	-	3/8/9/11	-
1	MLY	D	613	1	-	3/8/9/11	-
1	MLY	S	248	1	-	6/8/9/11	-
1	MLY	M	486	1	-	2/8/9/11	-
1	MLY	J	415	1	-	3/8/9/11	-
1	MLY	D	84	1	-	4/8/9/11	-
1	MLY	D	19	1	-	4/8/9/11	-
1	MLY	D	87	1	-	2/8/9/11	-
1	MLY	A	837	1	-	6/8/9/11	-
1	MLY	D	415	1	-	3/8/9/11	-
1	MLY	A	55	1	-	6/8/9/11	-
1	MLY	A	486	1	-	2/8/9/11	-
1	MLY	D	296	1	-	4/8/9/11	-
1	MLY	G	19	1	-	4/8/9/11	-
1	MLY	G	486	1	-	2/8/9/11	-
1	MLY	G	55	1	-	6/8/9/11	-
1	MLY	A	138	1	-	4/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	A	236	1	-	3/8/9/11	-
1	MLY	D	248	1	-	6/8/9/11	-
1	MLY	G	659	1	-	3/8/9/11	-
1	MLY	G	551	1	-	3/8/9/11	-
1	MLY	J	63	1	-	4/8/9/11	-
1	MLY	J	295	1	-	2/8/9/11	-
1	MLY	J	486	1	-	2/8/9/11	-
1	MLY	J	130	1	-	5/8/9/11	-
1	MLY	M	236	1	-	3/8/9/11	-
1	MLY	D	236	1	-	3/8/9/11	-
1	MLY	D	385	1	-	2/8/9/11	-
1	MLY	A	553	1,4	-	4/8/9/11	-
1	MLY	M	55	1	-	6/8/9/11	-
1	MLY	S	617	1	-	2/8/9/11	-
1	MLY	D	436	1	-	4/8/9/11	-
1	MLY	M	130	1	-	5/8/9/11	-
1	MLY	M	353	1	-	4/8/9/11	-
1	MLY	J	55	1	-	6/8/9/11	-
1	MLY	D	348	1	-	5/8/9/11	-
1	MLY	J	436	1	-	4/8/9/11	-
1	MLY	S	486	1	-	2/8/9/11	-
1	MLY	G	436	1	-	4/8/9/11	-
1	MLY	D	600	1	-	3/8/9/11	-
1	MLY	J	348	1	-	5/8/9/11	-
1	MLY	M	385	1	-	2/8/9/11	-
1	MLY	M	681	1	-	4/8/9/11	-
1	MLY	S	768	1	-	4/8/9/11	-
1	MLY	M	296	1	-	4/8/9/11	-
1	MLY	J	59	1	-	3/8/9/11	-
1	MLY	G	528	1	-	4/8/9/11	-
1	MLY	M	782	1	-	6/8/9/11	-
1	MLY	M	19	1	-	4/8/9/11	-
1	MLY	J	681	1	-	4/8/9/11	-
1	MLY	M	764	1	-	2/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	S	505	1	-	5/8/9/11	-
1	MLY	S	551	1	-	3/8/9/11	-
1	MLY	S	659	1	-	3/8/9/11	-
1	MLY	M	431	1	-	4/8/9/11	-
1	MLY	M	248	1	-	6/8/9/11	-
1	MLY	G	617	1	-	2/8/9/11	-
1	MLY	M	839	1	-	3/8/9/11	-
1	MLY	S	55	1	-	6/8/9/11	-
1	MLY	G	598	1	-	5/8/9/11	-
1	MLY	G	49	1	-	3/8/9/11	-
1	MLY	A	272	1	-	3/8/9/11	-
1	MLY	J	236	1	-	3/8/9/11	-
1	MLY	M	35	1	-	3/8/9/11	-
1	MLY	M	833	1	-	6/8/9/11	-
1	MLY	G	504	1	-	4/8/9/11	-
1	MLY	A	415	1	-	3/8/9/11	-
1	MLY	J	528	1	-	4/8/9/11	-
1	MLY	S	436	1	-	4/8/9/11	-
1	MLY	A	505	1	-	5/8/9/11	-
1	MLY	D	190	1	-	4/8/9/11	-
1	MLY	J	35	1	-	3/8/9/11	-
1	MLY	A	295	1	-	2/8/9/11	-
1	MLY	A	782	1	-	6/8/9/11	-
1	MLY	A	617	1	-	2/8/9/11	-
1	MLY	S	296	1	-	4/8/9/11	-
1	MLY	S	353	1	-	4/8/9/11	-
1	MLY	S	369	1	-	2/8/9/11	-
1	MLY	A	613	1	-	3/8/9/11	-
1	MLY	D	59	1	-	3/8/9/11	-
1	MLY	A	367	1	-	2/8/9/11	-
1	MLY	D	764	1	-	2/8/9/11	-
1	MLY	G	30	1	-	3/8/9/11	-
1	MLY	G	107	1	-	2/8/9/11	-
1	MLY	D	431	1	-	4/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	G	59	1	-	3/8/9/11	-
1	MLY	D	272	1	-	3/8/9/11	-
1	MLY	D	617	1	-	2/8/9/11	-
1	MLY	G	782	1	-	6/8/9/11	-
1	MLY	G	681	1	-	4/8/9/11	-
1	MLY	M	551	1	-	3/8/9/11	-
1	MLY	D	833	1	-	6/8/9/11	-
1	MLY	J	617	1	-	2/8/9/11	-
1	MLY	M	367	1	-	2/8/9/11	-
1	MLY	D	598	1	-	5/8/9/11	-
1	MLY	G	87	1	-	2/8/9/11	-
1	MLY	M	600	1	-	3/8/9/11	-
1	MLY	S	598	1	-	5/8/9/11	-
1	MLY	J	553	1,4	-	4/8/9/11	-
1	MLY	A	130	1	-	5/8/9/11	-
1	MLY	G	35	1	-	3/8/9/11	-
1	MLY	S	504	1	-	4/8/9/11	-
1	MLY	G	839	1	-	3/8/9/11	-
1	MLY	J	367	1	-	2/8/9/11	-
1	MLY	S	190	1	-	4/8/9/11	-
1	MLY	J	598	1	-	5/8/9/11	-
1	MLY	J	87	1	-	2/8/9/11	-
1	MLY	S	295	1	-	2/8/9/11	-
1	MLY	A	659	1	-	3/8/9/11	-
1	MLY	G	296	1	-	4/8/9/11	-
1	MLY	S	30	1	-	3/8/9/11	-
1	MLY	S	600	1	-	3/8/9/11	-
1	MLY	D	107	1	-	2/8/9/11	-
1	MLY	S	782	1	-	6/8/9/11	-
1	MLY	A	827	1	-	1/8/9/11	-
1	MLY	A	528	1	-	4/8/9/11	-
1	MLY	G	431	1	-	4/8/9/11	-
1	MLY	S	553	1	-	4/8/9/11	-
1	MLY	D	681	1	-	4/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	D	659	1	-	3/8/9/11	-
1	MLY	A	681	1	-	4/8/9/11	-
1	MLY	D	551	1	-	3/8/9/11	-
1	MLY	S	833	1	-	6/8/9/11	-
1	MLY	J	49	1	-	3/8/9/11	-
1	MLY	M	272	1	-	3/8/9/11	-
1	MLY	M	617	1	-	2/8/9/11	-
1	MLY	G	613	1	-	3/8/9/11	-
1	MLY	S	87	1	-	2/8/9/11	-
1	MLY	J	764	1	-	2/8/9/11	-
1	MLY	M	505	1	-	5/8/9/11	-
1	MLY	J	84	1	-	4/8/9/11	-
1	MLY	J	272	1	-	3/8/9/11	-
1	MLY	G	84	1	-	4/8/9/11	-
1	MLY	S	839	1	-	3/8/9/11	-
1	MLY	A	35	1	-	3/8/9/11	-
1	MLY	G	63	1	-	4/8/9/11	-
1	MLY	J	768	1	-	4/8/9/11	-
1	MLY	J	19	1	-	4/8/9/11	-
1	MLY	A	600	1	-	3/8/9/11	-
1	MLY	G	130	1	-	5/8/9/11	-
1	MLY	J	827	1	-	1/8/9/11	-
1	MLY	J	138	1	-	4/8/9/11	-
1	MLY	A	833	1	-	6/8/9/11	-

The worst 5 of 77 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	138	MLY	CB-CA	-3.34	1.48	1.53
1	G	138	MLY	CB-CA	-3.25	1.48	1.53
1	J	138	MLY	CB-CA	-3.22	1.48	1.53
1	M	138	MLY	CB-CA	-3.21	1.48	1.53
1	S	138	MLY	CB-CA	-3.18	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.

190 monomers are involved in 828 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	598	MLY	1	0
1	A	87	MLY	3	0
1	S	272	MLY	1	0
1	M	190	MLY	2	0
1	A	248	MLY	2	0
1	A	839	MLY	9	0
1	S	764	MLY	29	0
1	D	295	MLY	6	0
1	D	30	MLY	1	0
1	D	528	MLY	3	0
1	J	505	MLY	9	0
1	G	837	MLY	1	0
1	D	782	MLY	71	0
1	M	30	MLY	1	0
1	M	528	MLY	3	0
1	S	63	MLY	3	0
1	J	296	MLY	3	0
1	M	659	MLY	2	0
1	A	436	MLY	3	0
1	D	839	MLY	7	0
1	A	768	MLY	12	0
1	J	839	MLY	15	0
1	G	369	MLY	1	0
1	A	63	MLY	3	0
1	D	553	MLY	16	0
1	M	63	MLY	4	0
1	M	295	MLY	6	0
1	S	348	MLY	6	0
1	J	190	MLY	2	0
1	G	600	MLY	1	0
1	S	528	MLY	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	764	MLY	11	0
1	D	486	MLY	3	0
1	D	138	MLY	2	0
1	G	764	MLY	8	0
1	J	659	MLY	2	0
1	M	553	MLY	17	0
1	G	138	MLY	2	0
1	J	837	MLY	1	0
1	J	30	MLY	1	0
1	M	837	MLY	1	0
1	D	768	MLY	1	0
1	M	598	MLY	1	0
1	A	190	MLY	2	0
1	M	436	MLY	2	0
1	D	63	MLY	4	0
1	S	49	MLY	3	0
1	D	55	MLY	1	0
1	A	369	MLY	1	0
1	S	59	MLY	2	0
1	M	87	MLY	3	0
1	M	415	MLY	1	0
1	S	107	MLY	3	0
1	G	415	MLY	1	0
1	M	107	MLY	3	0
1	M	59	MLY	2	0
1	G	248	MLY	2	0
1	S	837	MLY	1	0
1	A	551	MLY	2	0
1	M	138	MLY	2	0
1	S	84	MLY	14	0
1	M	768	MLY	1	0
1	A	59	MLY	2	0
1	J	782	MLY	1	0
1	D	837	MLY	1	0
1	J	248	MLY	2	0
1	A	504	MLY	4	0
1	M	49	MLY	3	0
1	A	348	MLY	5	0
1	J	504	MLY	1	0
1	M	348	MLY	6	0
1	A	30	MLY	1	0
1	D	827	MLY	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	M	369	MLY	1	0
1	G	348	MLY	4	0
1	G	827	MLY	1	0
1	S	415	MLY	1	0
1	D	49	MLY	3	0
1	G	553	MLY	26	0
1	A	49	MLY	3	0
1	A	107	MLY	3	0
1	G	295	MLY	7	0
1	J	600	MLY	1	0
1	M	504	MLY	1	0
1	A	296	MLY	3	0
1	S	138	MLY	2	0
1	G	190	MLY	2	0
1	G	768	MLY	9	0
1	M	84	MLY	23	0
1	J	107	MLY	3	0
1	G	272	MLY	1	0
1	S	248	MLY	2	0
1	M	486	MLY	3	0
1	J	415	MLY	1	0
1	D	87	MLY	3	0
1	A	837	MLY	1	0
1	D	415	MLY	1	0
1	A	55	MLY	1	0
1	A	486	MLY	3	0
1	D	296	MLY	3	0
1	G	486	MLY	3	0
1	G	55	MLY	1	0
1	A	138	MLY	2	0
1	D	248	MLY	2	0
1	G	659	MLY	2	0
1	J	63	MLY	4	0
1	J	295	MLY	6	0
1	J	486	MLY	3	0
1	A	553	MLY	17	0
1	M	55	MLY	1	0
1	S	617	MLY	1	0
1	D	436	MLY	3	0
1	J	55	MLY	1	0
1	D	348	MLY	6	0
1	J	436	MLY	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	S	486	MLY	3	0
1	G	436	MLY	2	0
1	D	600	MLY	1	0
1	J	348	MLY	5	0
1	M	296	MLY	3	0
1	J	59	MLY	2	0
1	G	528	MLY	3	0
1	M	782	MLY	3	0
1	M	764	MLY	4	0
1	S	505	MLY	8	0
1	S	659	MLY	2	0
1	M	248	MLY	2	0
1	G	617	MLY	1	0
1	M	839	MLY	7	0
1	S	55	MLY	1	0
1	G	598	MLY	1	0
1	G	49	MLY	3	0
1	A	272	MLY	1	0
1	M	35	MLY	13	0
1	G	504	MLY	1	0
1	A	415	MLY	1	0
1	J	528	MLY	3	0
1	S	436	MLY	2	0
1	A	505	MLY	24	0
1	D	190	MLY	2	0
1	A	295	MLY	6	0
1	A	782	MLY	8	0
1	A	617	MLY	1	0
1	S	296	MLY	3	0
1	S	369	MLY	1	0
1	D	59	MLY	2	0
1	D	764	MLY	6	0
1	G	30	MLY	1	0
1	G	107	MLY	3	0
1	G	59	MLY	2	0
1	D	272	MLY	1	0
1	D	617	MLY	1	0
1	G	782	MLY	1	0
1	M	551	MLY	1	0
1	J	617	MLY	1	0
1	D	598	MLY	1	0
1	G	87	MLY	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	M	600	MLY	1	0
1	S	598	MLY	1	0
1	J	553	MLY	27	0
1	S	504	MLY	1	0
1	G	839	MLY	4	0
1	S	190	MLY	2	0
1	J	598	MLY	1	0
1	J	87	MLY	3	0
1	S	295	MLY	6	0
1	A	659	MLY	2	0
1	G	296	MLY	2	0
1	S	30	MLY	1	0
1	S	600	MLY	1	0
1	D	107	MLY	3	0
1	S	782	MLY	1	0
1	A	528	MLY	3	0
1	S	553	MLY	3	0
1	D	659	MLY	2	0
1	D	551	MLY	2	0
1	J	49	MLY	4	0
1	M	272	MLY	1	0
1	M	617	MLY	1	0
1	S	87	MLY	3	0
1	J	764	MLY	6	0
1	M	505	MLY	2	0
1	J	84	MLY	44	0
1	J	272	MLY	1	0
1	G	84	MLY	16	0
1	S	839	MLY	15	0
1	G	63	MLY	4	0
1	J	768	MLY	9	0
1	A	600	MLY	1	0
1	J	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	S	8
1	M	5
1	J	4
1	D	4
1	A	4
1	G	3
3	C	1
3	F	1
3	I	1
3	L	1
3	O	1
3	U	1
2	H	1
2	B	1
2	E	1
2	K	1
2	N	1
2	T	1

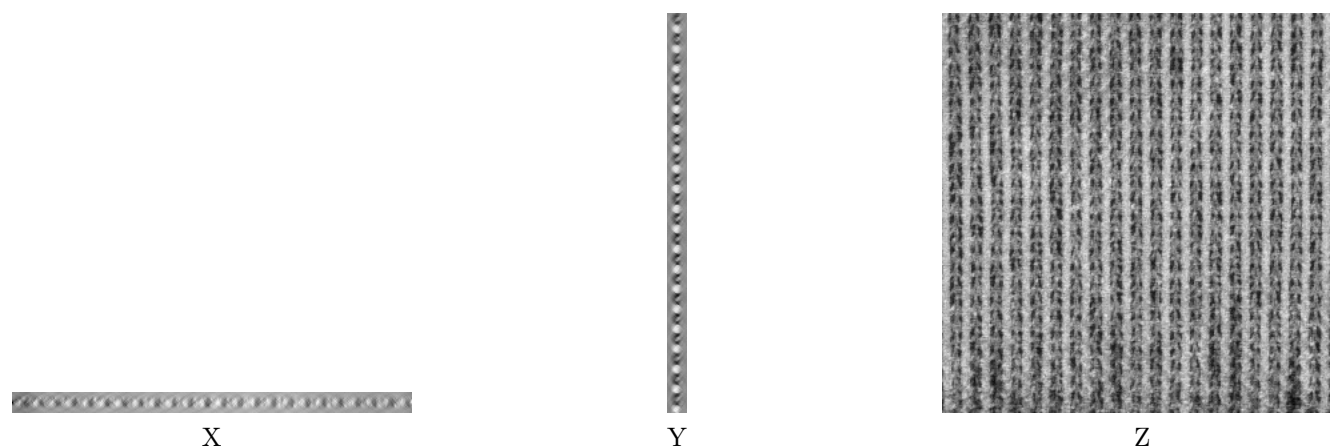
The worst 5 of 40 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	J	769:ALA	C	770:GLY	N	5.58
1	D	769:ALA	C	770:GLY	N	5.32
1	G	769:ALA	C	770:GLY	N	4.88
1	M	769:ALA	C	770:GLY	N	3.92
1	A	709:LYS	C	710:GLY	N	3.14

6 Tomogram visualisation [i](#)

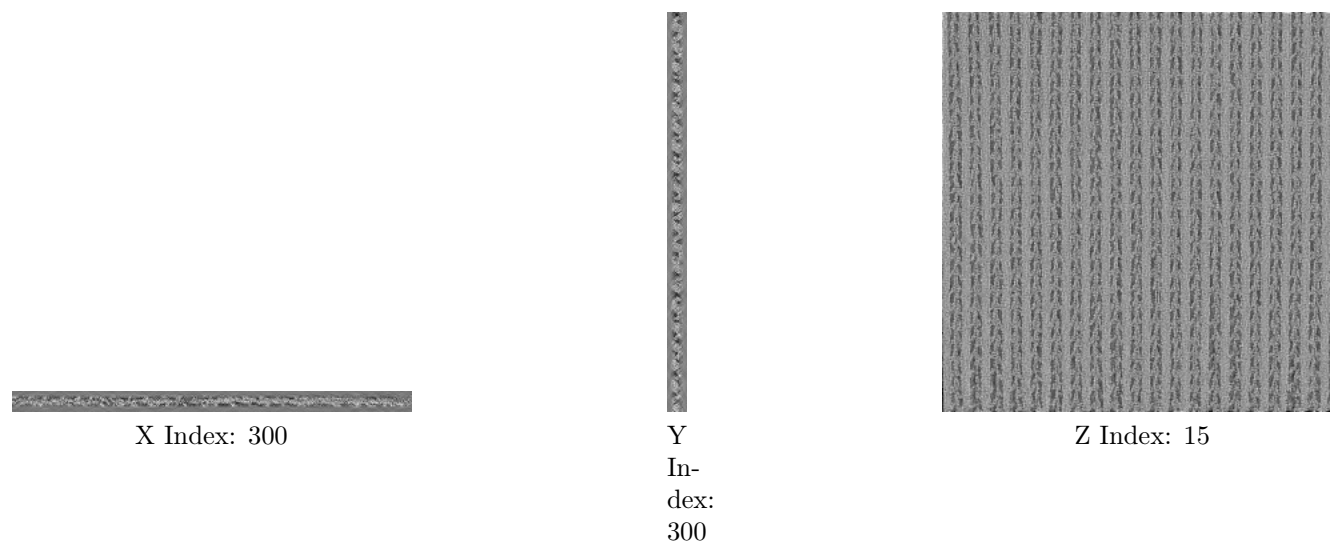
This section contains visualisations of the EMDB entry EMD-1001. These allow visual inspection of the internal detail of the tomogram and identification of artifacts.

6.1 Orthogonal projections [i](#)



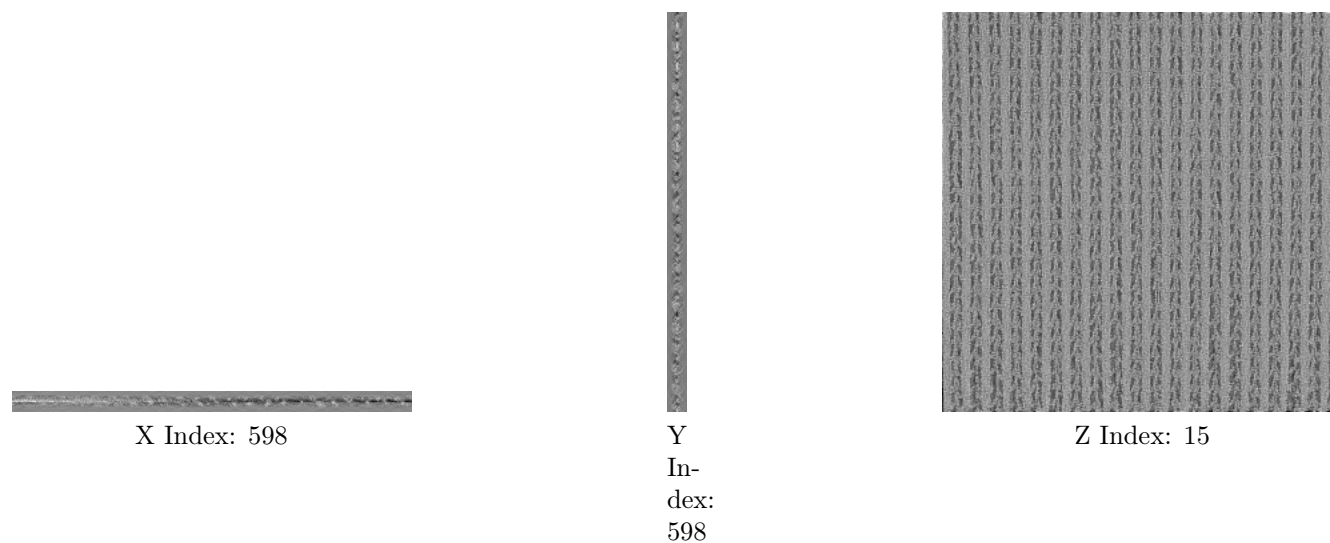
The images above show the tomogram projected in three orthogonal directions.

6.2 Central slices [i](#)



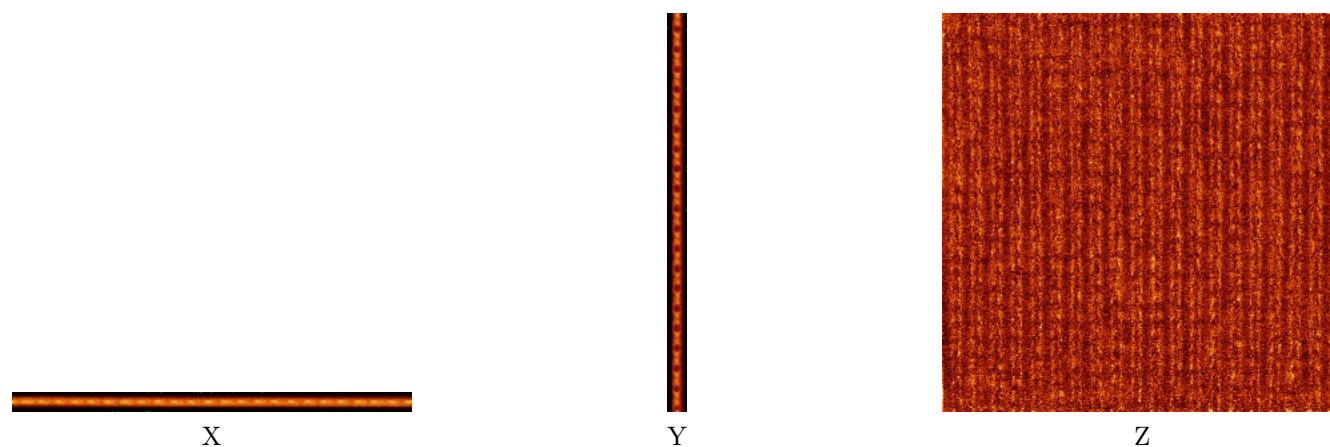
The images above show central slices of the tomogram in three orthogonal directions.

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.

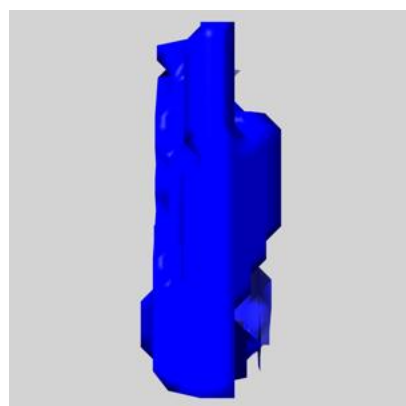
6.5 Mask visualisation [i](#)

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

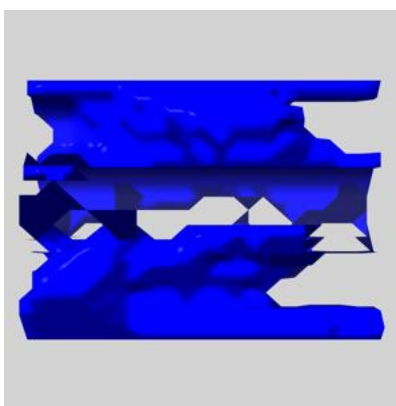
A mask typically either:

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

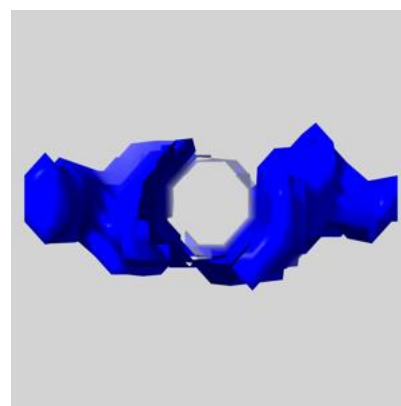
6.5.1 emd_1001_msk_25.map [i](#)



X

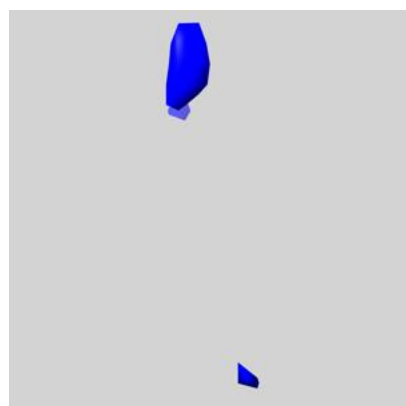


Y

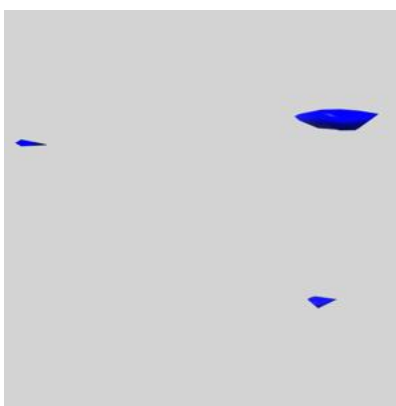


Z

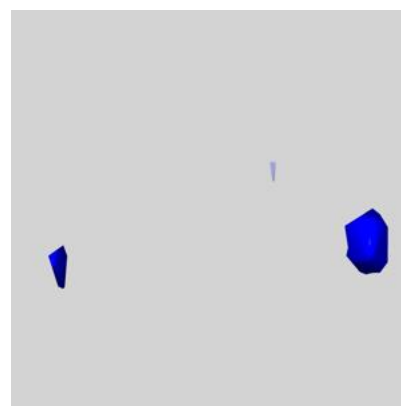
6.5.2 emd_1001_msk_24.map [i](#)



X

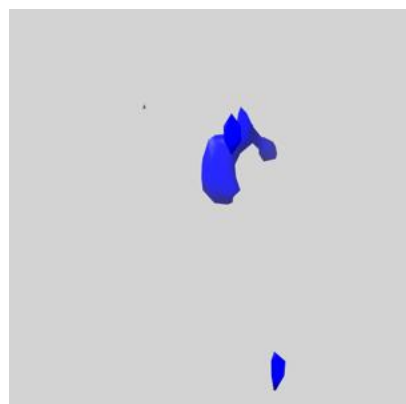


Y

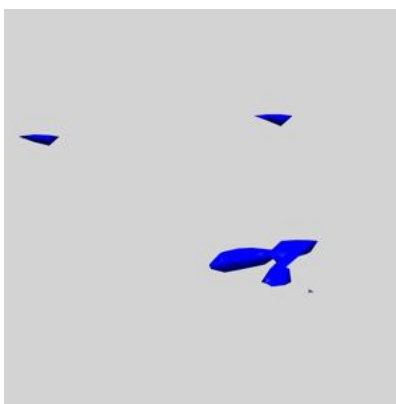


Z

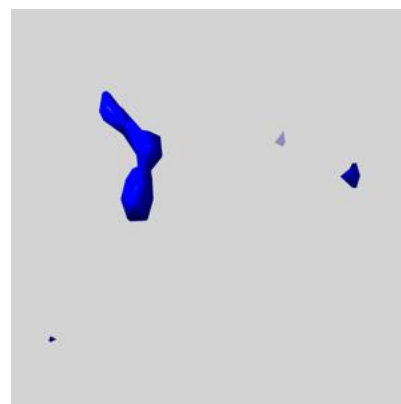
6.5.3 emd_1001_msk_23.map [i](#)



X

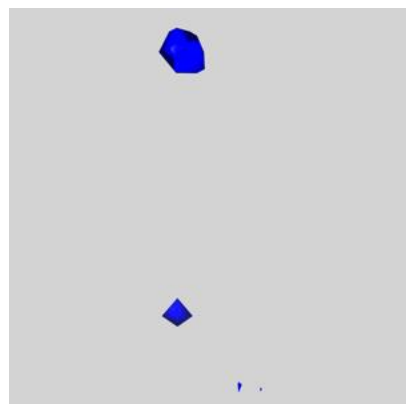


Y

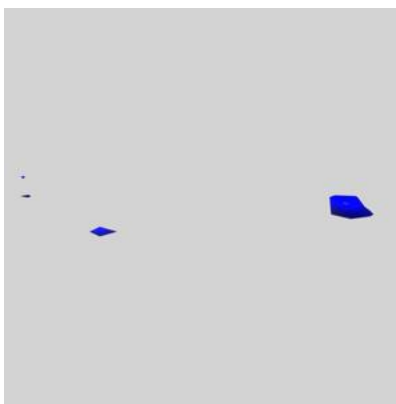


Z

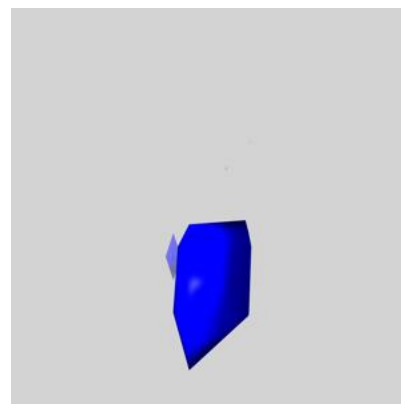
6.5.4 emd_1001_msk_22.map [i](#)



X

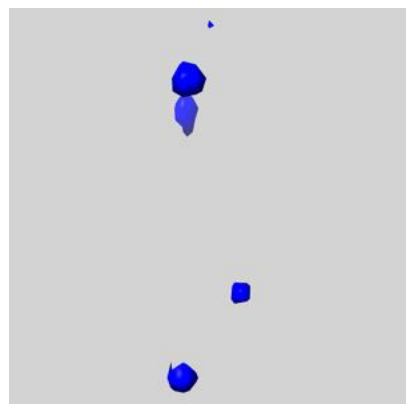


Y

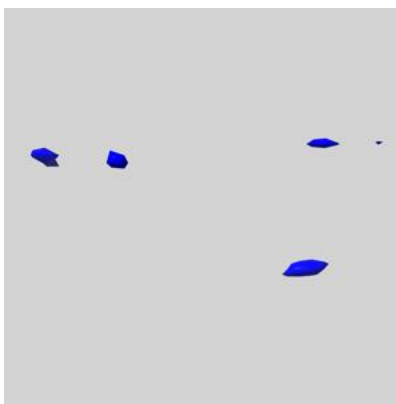


Z

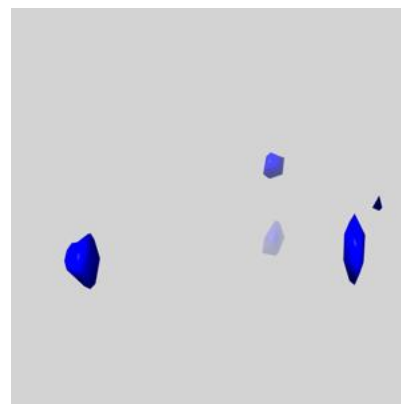
6.5.5 emd_1001_msk_21.map [i](#)



X

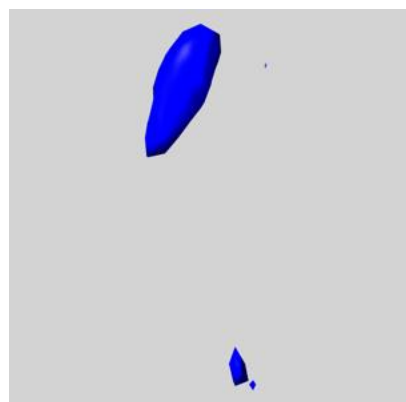


Y

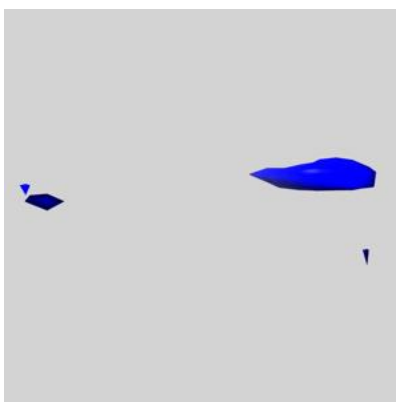


Z

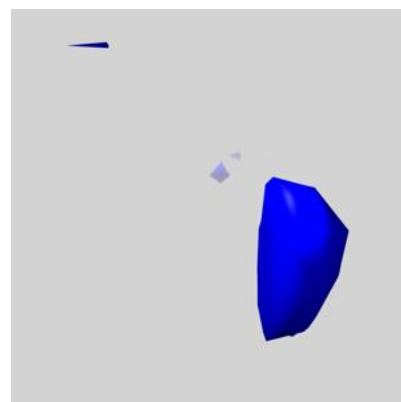
6.5.6 emd_1001_msk_20.map [i](#)



X

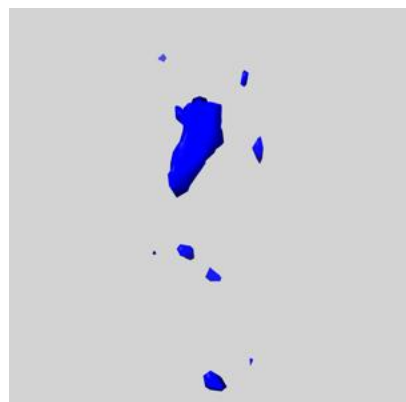


Y

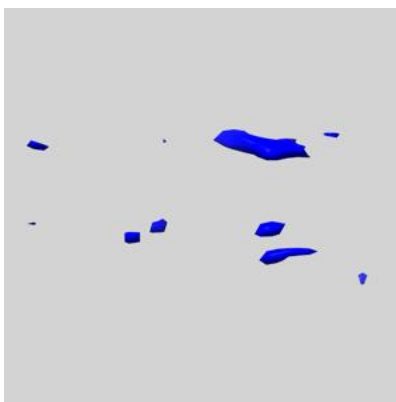


Z

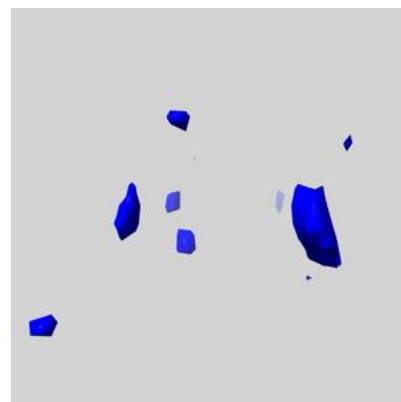
6.5.7 emd_1001_msk_19.map [i](#)



X

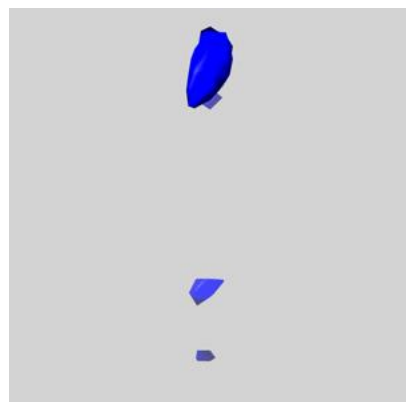


Y

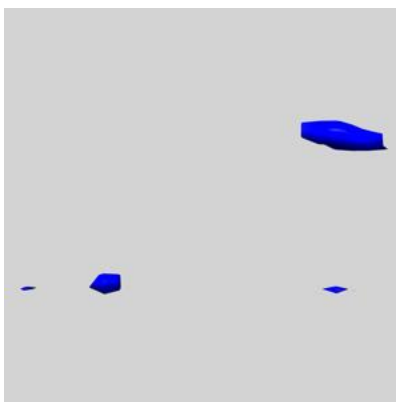


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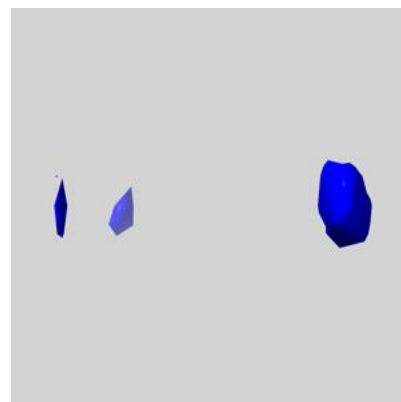
6.5.8 emd_1001_msk_18.map [i](#)



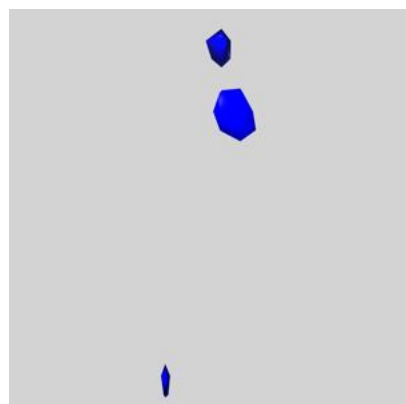
X



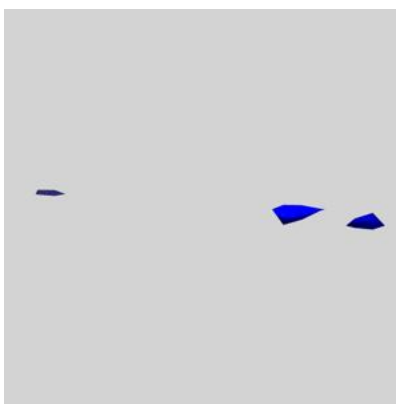
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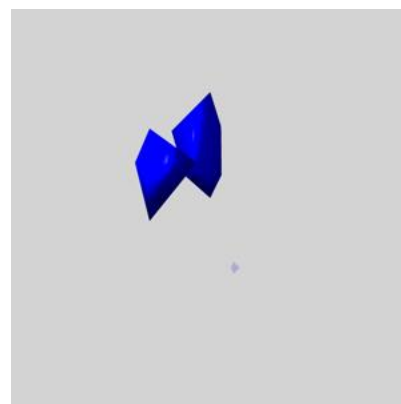
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6.5.9 emd_1001_msk_17.map [i](#)

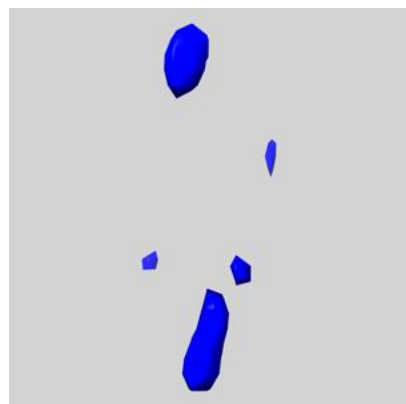
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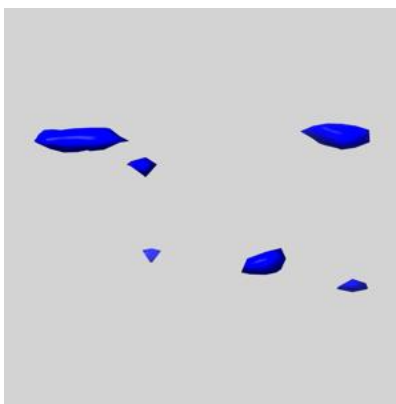
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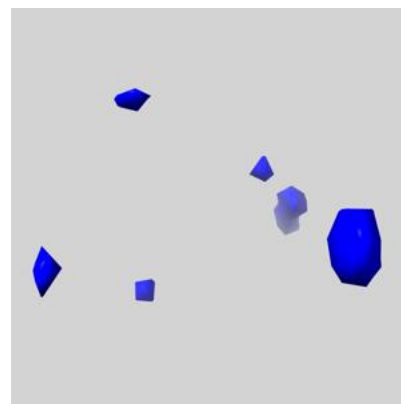
Z

6.5.10 emd_1001_msk_16.map [i](#)

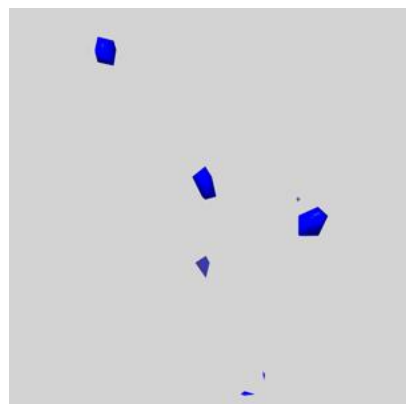
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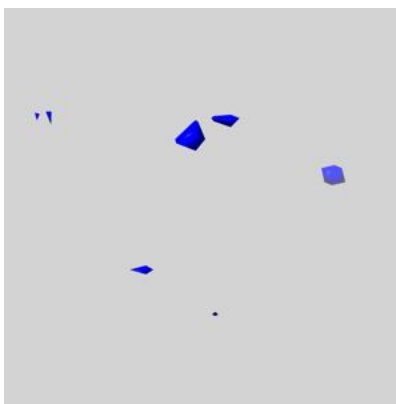
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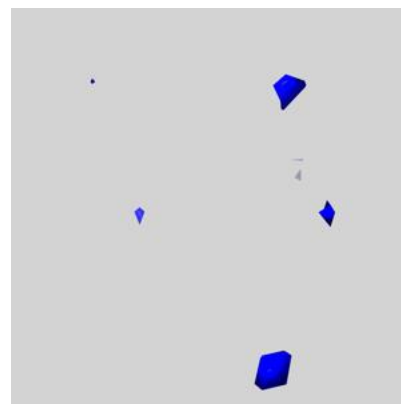
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6.5.11 emd_1001_msk_15.map [i](#)

X

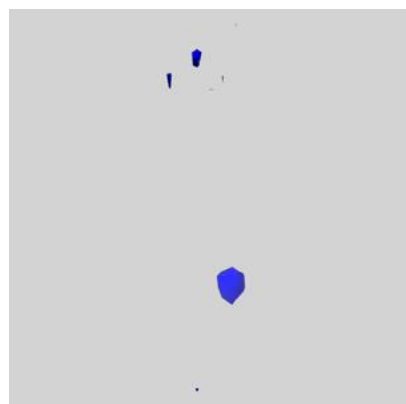


Y

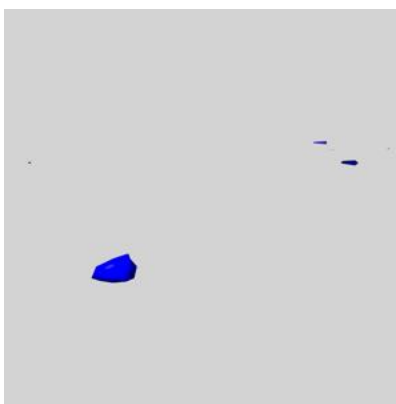


Z

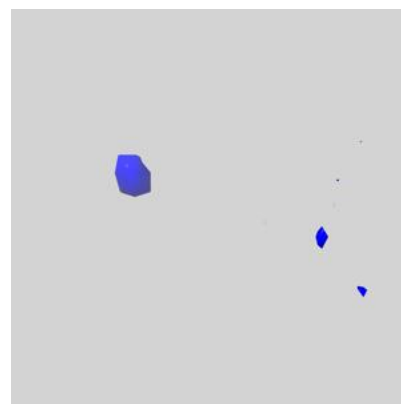
6.5.12 emd_1001_msk_14.map [i](#)



X

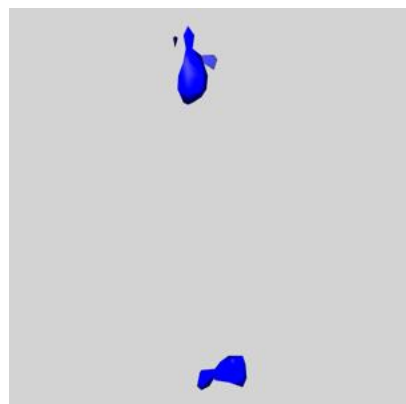


Y

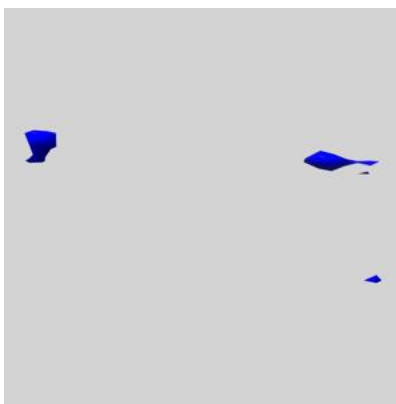


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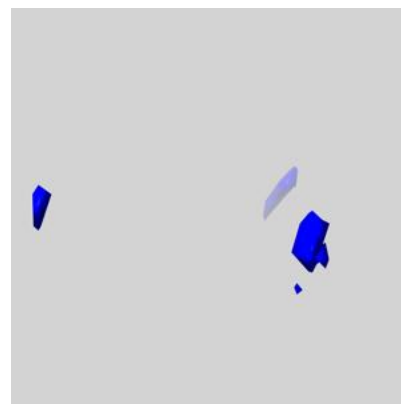
6.5.13 emd_1001_msk_13.map [i](#)



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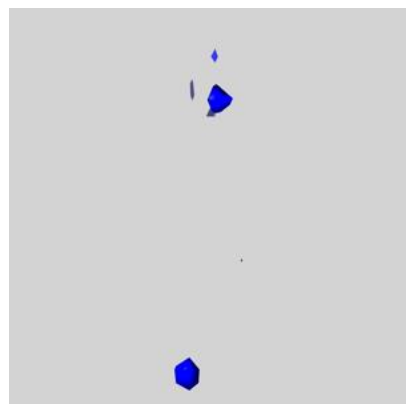


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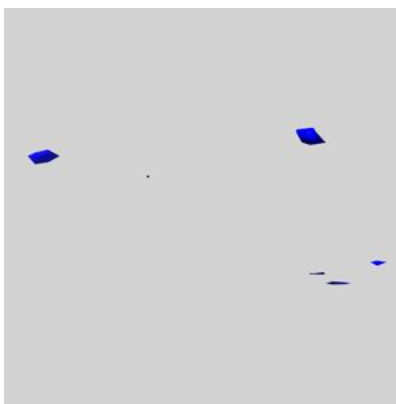


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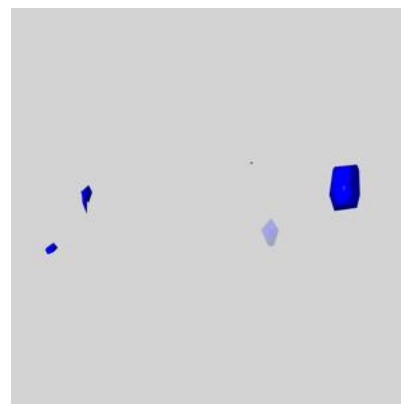
6.5.14 emd_1001_msk_12.map [i](#)



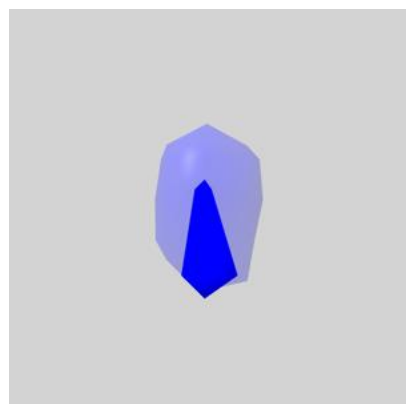
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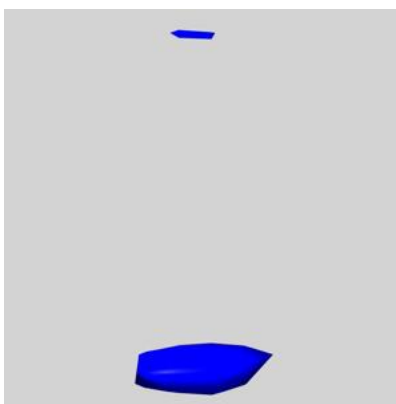
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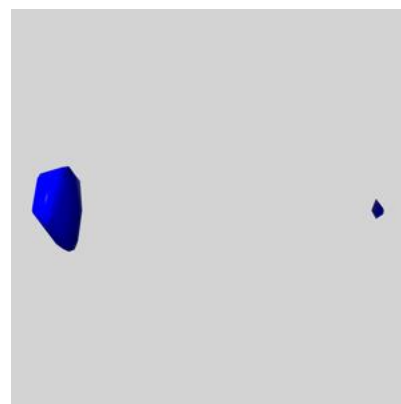
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6.5.15 emd_1001_msk_11.map [i](#)

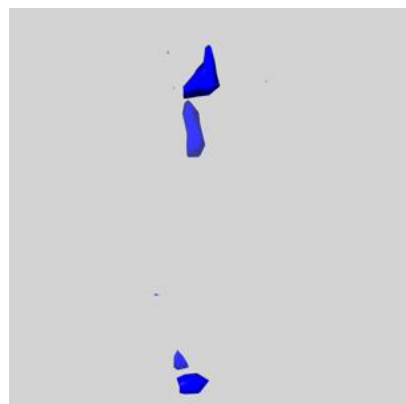
X



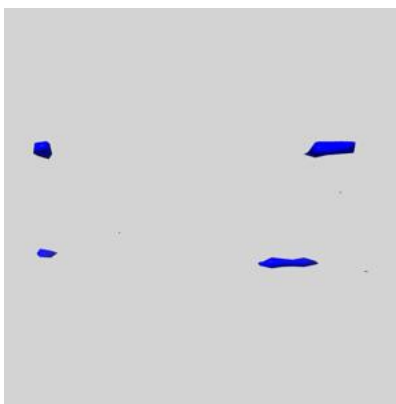
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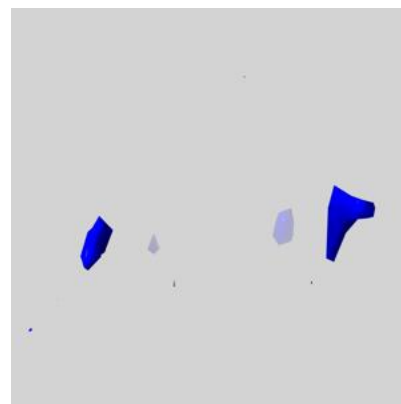
Z

6.5.16 emd_1001_msk_10.map [i](#)

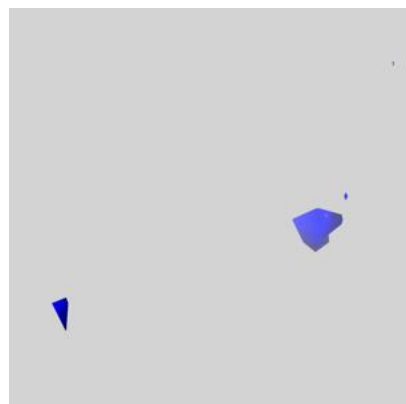
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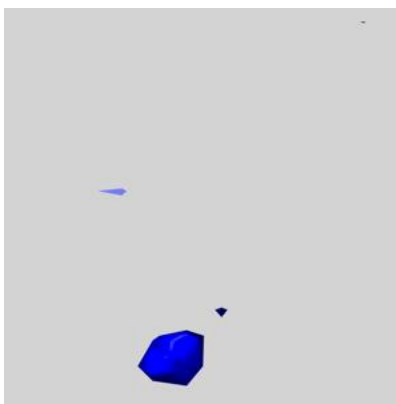
Y



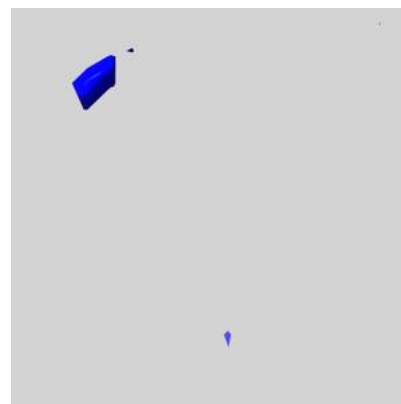
Z

6.5.17 emd_1001_msk_9.map [i](#)

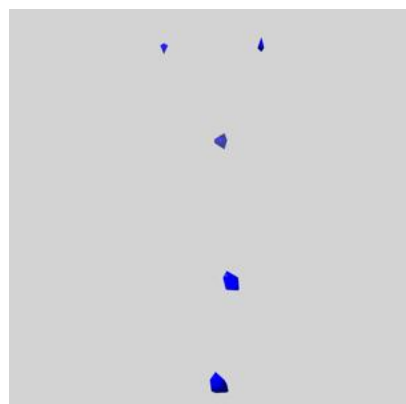
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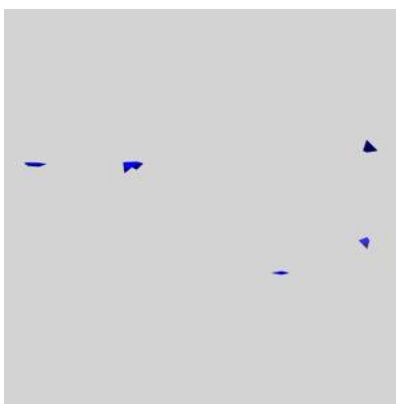
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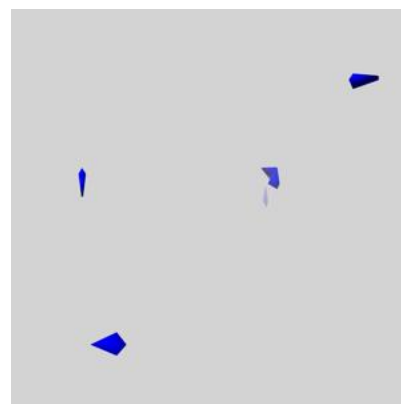
Z

6.5.18 emd_1001_msk_8.map [i](#)

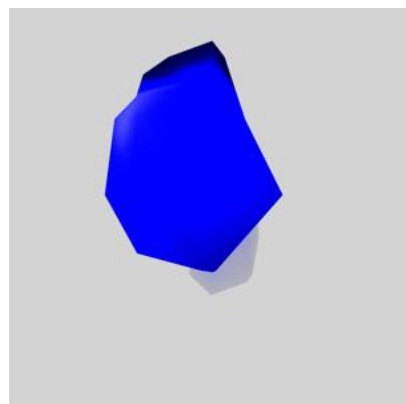
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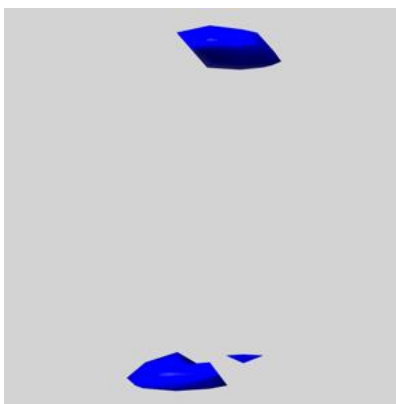
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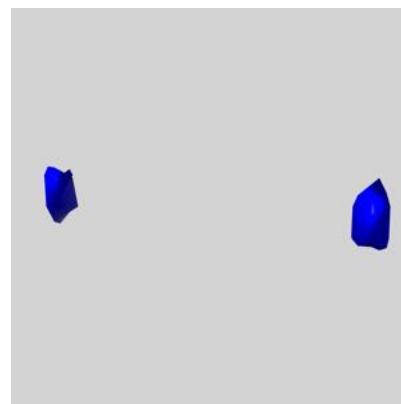
Z

6.5.19 emd_1001_msk_7.map [i](#)

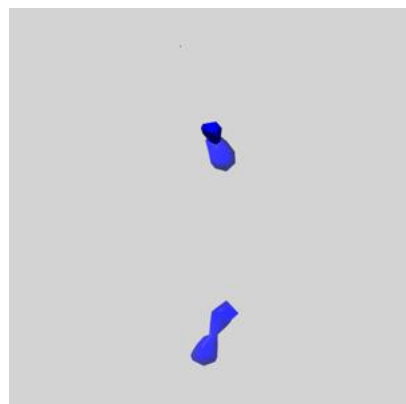
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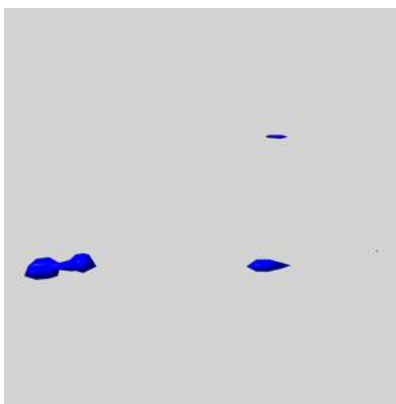
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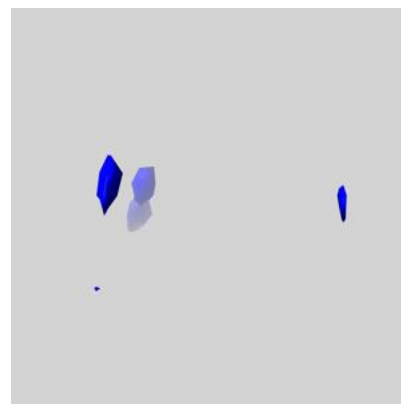
Z

6.5.20 emd_1001_msk_6.map [i](#)

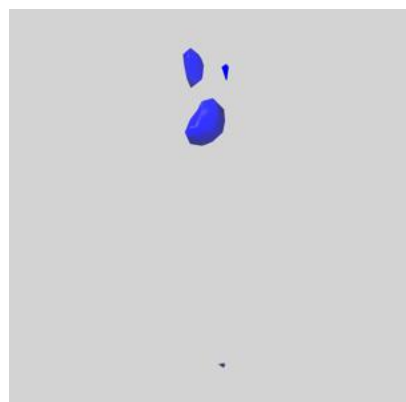
X



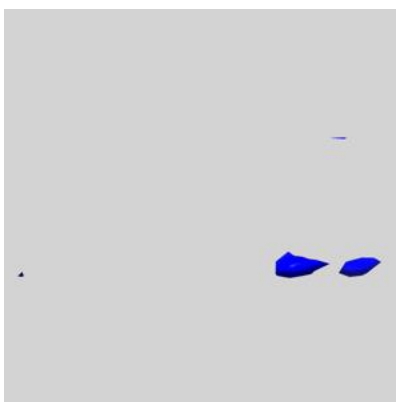
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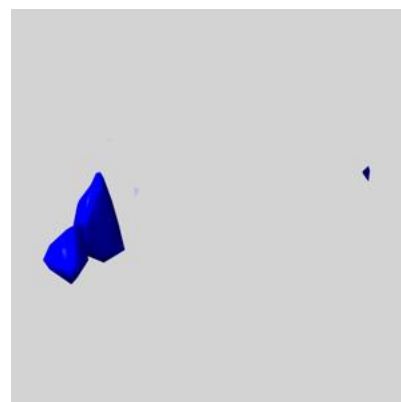
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6.5.21 emd_1001_msk_5.map [i](#)

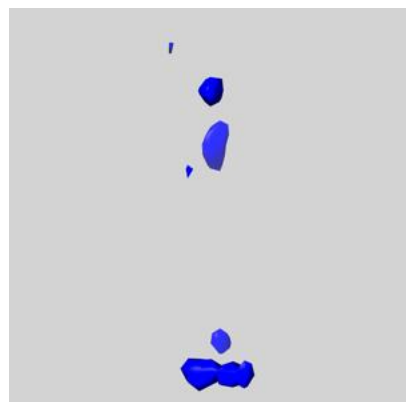
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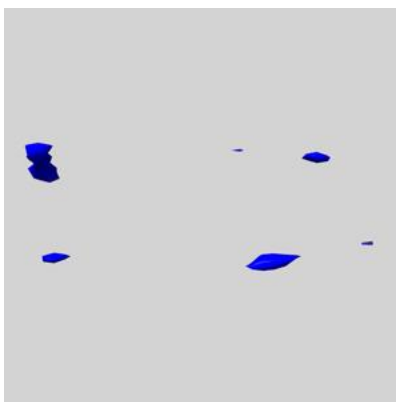
Y



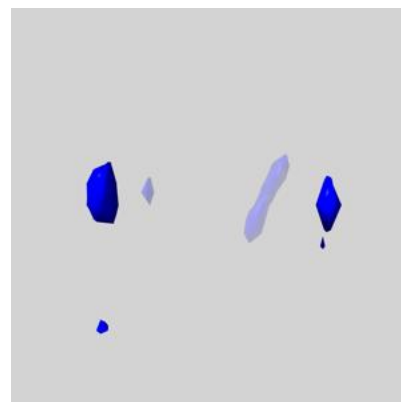
Z

6.5.22 emd_1001_msk_4.map [i](#)

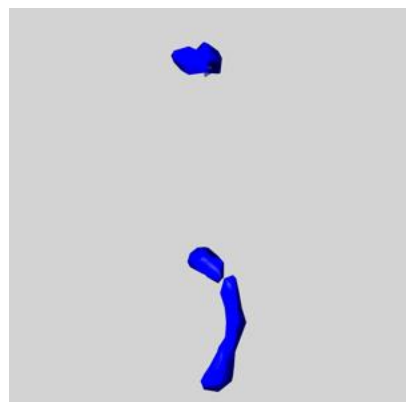
X



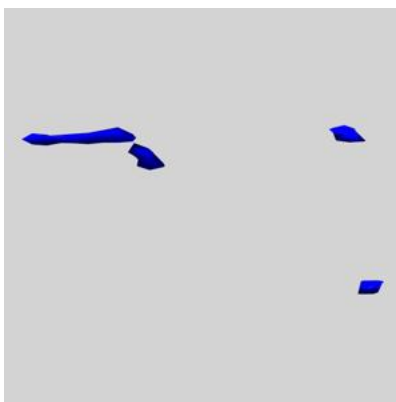
Y



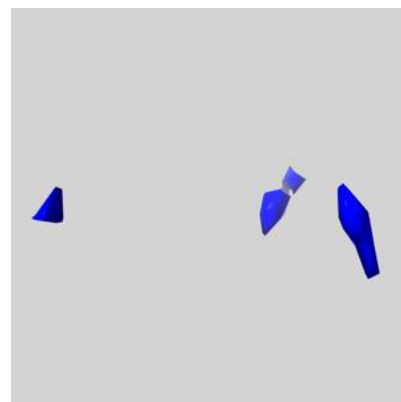
Z

6.5.23 emd_1001_msk_3.map [i](#)

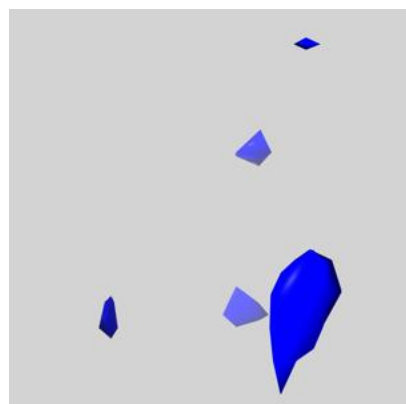
X



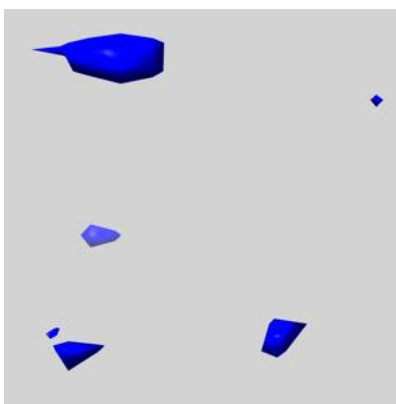
Y



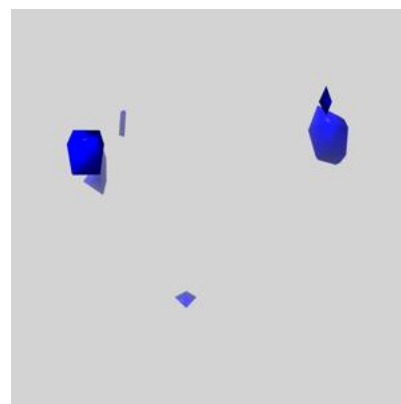
Z

6.5.24 emd_1001_msk_2.map [i](#)

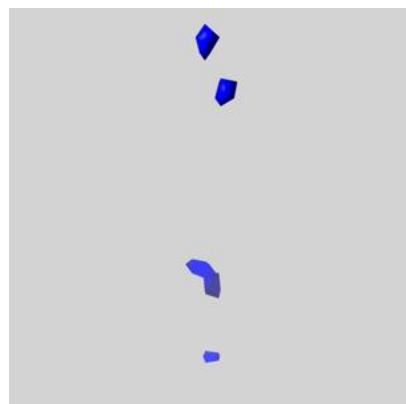
X



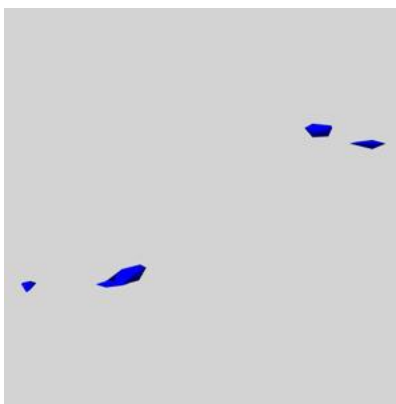
Y



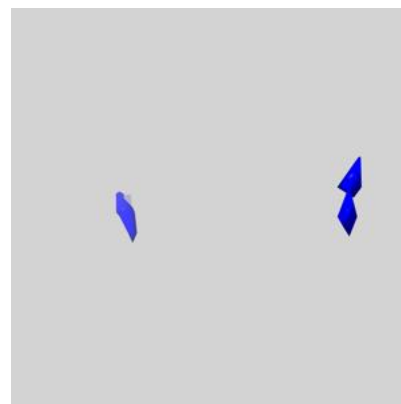
Z

6.5.25 emd_1001_msk_1.map [i](#)

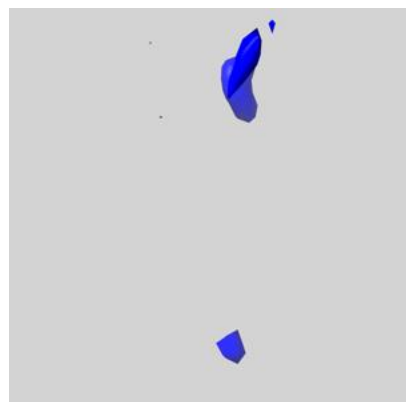
X



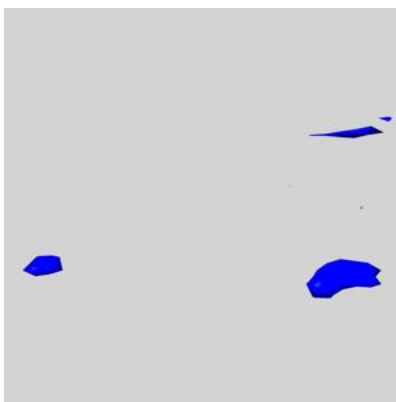
Y



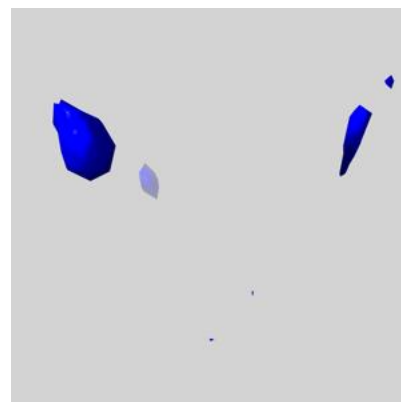
Z

6.5.26 emd_1001_msk_26.map [i](#)

X



Y

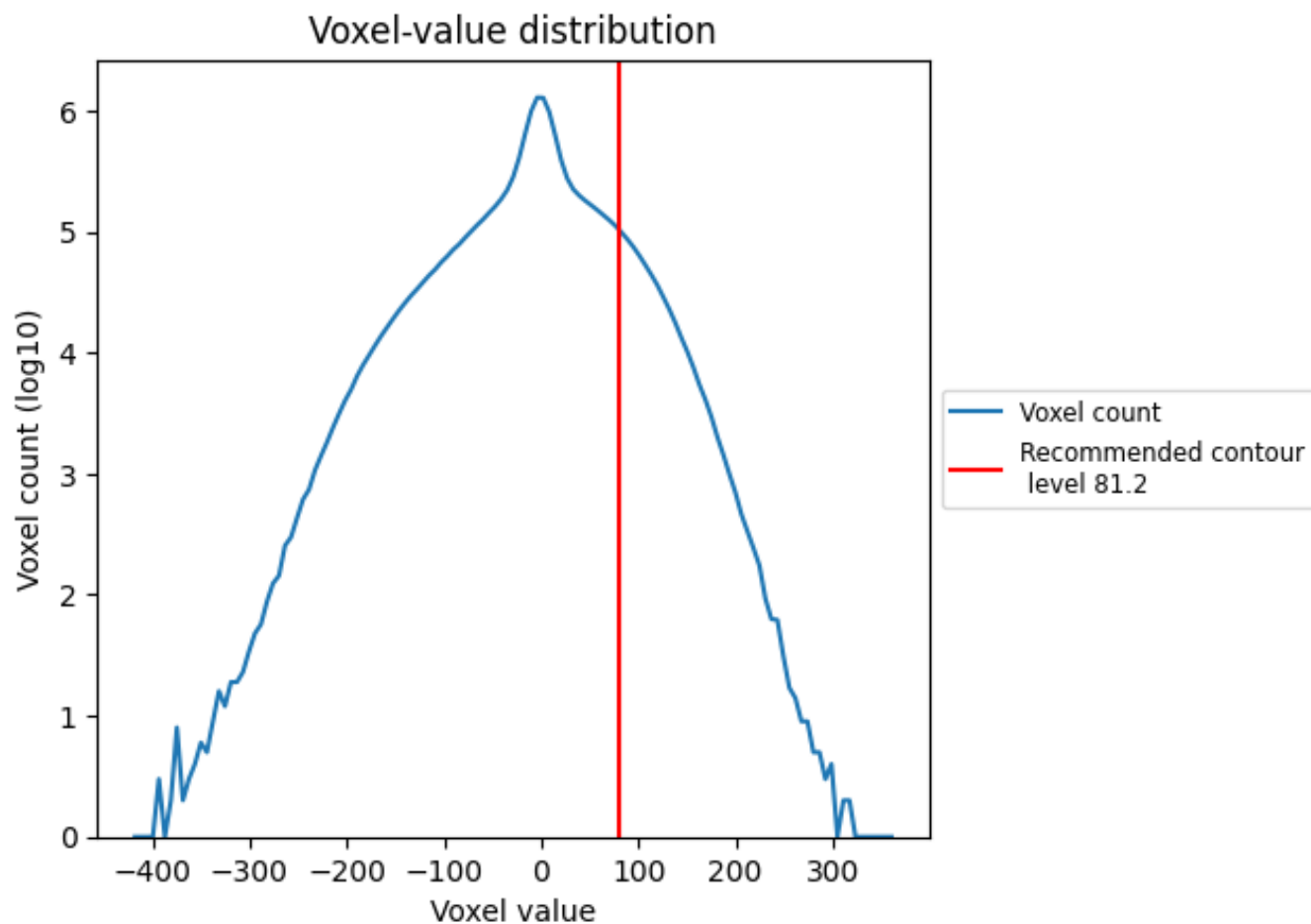


Z

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.

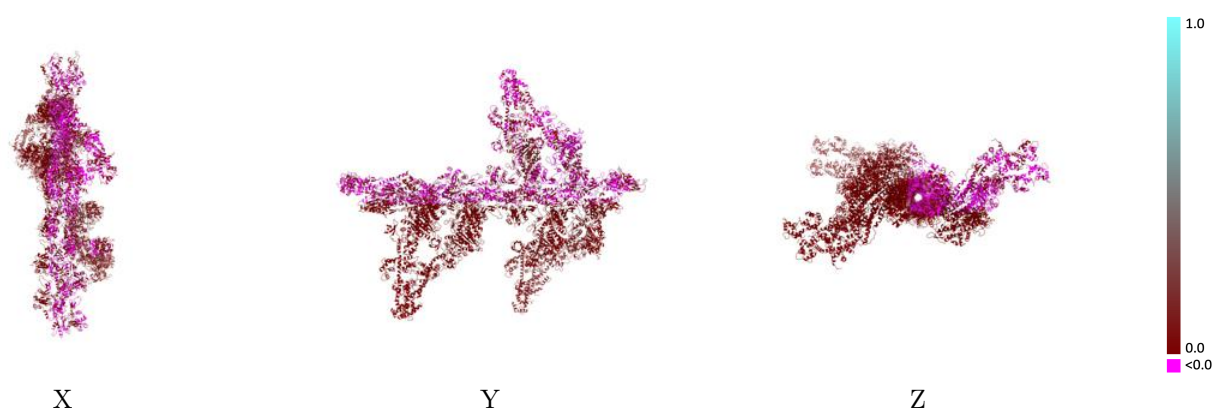
8 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-1001 and PDB model 1O19. 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](#)

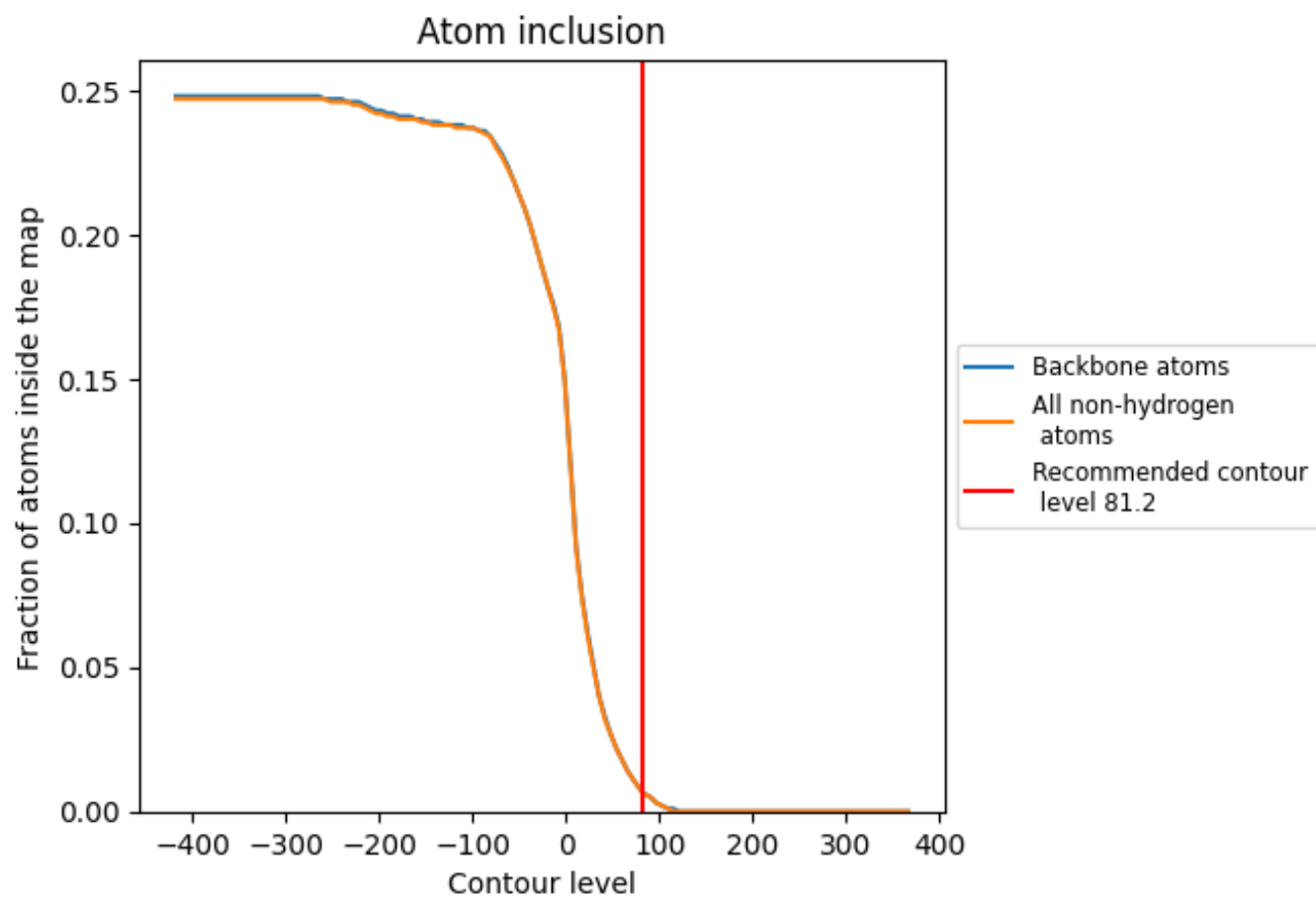


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 ⓘ



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	 0.0070	 0.0010
1	 0.0000	 0.0010
2	 0.0280	 0.0010
3	 0.0000	 -0.0060
4	 0.0000	 0.0120
5	 0.0000	 -0.0020
6	 0.0000	 0.0010
7	 0.0000	 0.0010
8	 0.0000	 0.0030
9	 0.0000	 0.0070
A	 0.0000	 0.0000
B	 0.0000	 0.0000
C	 0.0000	 0.0000
D	 0.0020	 -0.0030
E	 0.1030	 0.0240
F	 0.0400	 -0.0110
G	 0.0000	 0.0000
H	 0.0000	 0.0000
I	 0.0000	 0.0000
J	 0.0110	 0.0070
K	 0.0000	 -0.0200
L	 0.1700	 0.0250
M	 0.0000	 0.0000
N	 0.0000	 0.0000
O	 0.0000	 0.0000
S	 0.0000	 0.0010
T	 0.0000	 0.0000
U	 0.0000	 0.0000
V	 0.0000	 -0.0010
W	 0.0000	 -0.0080
X	 0.0540	 0.0100
Y	 0.0000	 0.0040
Z	 0.0000	 -0.0200

