



wwPDB EM Validation Summary Report ⓘ

Dec 18, 2023 – 11:50 PM EST

PDB ID : 1O19
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 : 1ATN, 2MYS

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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.dev70
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

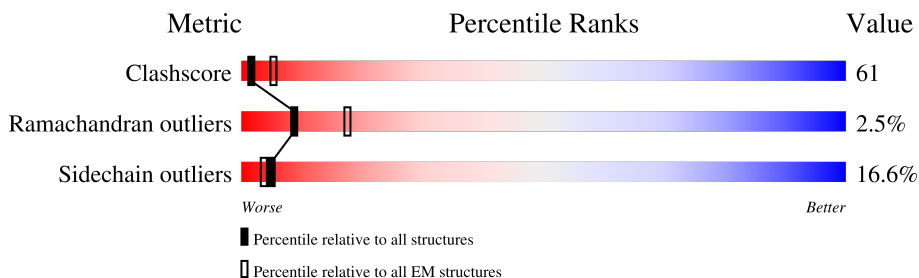
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 70.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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% 51% 20% .
1	D	840	100% 25% 50% 20% .
1	G	840	100% 24% 51% 20% .
1	J	840	99% 26% 50% 20% .
1	M	840	100% 26% 50% 21% .
1	S	840	100% 25% 51% 20% .
2	B	145	100% 66% 26% 6% .
2	E	145	90% 64% 27% 6% .

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Mol	Chain	Length	Quality of chain				
2	H	145	100%	64%	27%	6%	.
2	K	145	100%	64%	26%	6%	.
2	N	145	100%	64%	27%	6%	.
2	T	145	100%	65%	26%	6%	.
3	C	147	100%	60%	37%		.
3	F	147	96%	60%	38%		.
3	I	147	100%	61%	37%		.
3	L	147	82%	61%	37%		.
3	O	147	100%	61%	37%		.
3	U	147	100%	57%	40%		.
4	1	375	99%	62%	29%	6%	..
4	2	375	96%	55%	34%	9%	..
4	3	375	99%	62%	30%	6%	..
4	4	375	99%	62%	30%	6%	..
4	5	375	99%	63%	29%	6%	..
4	6	375	99%	64%	28%	6%	..
4	7	375	99%	64%	27%	6%	..
4	8	375	99%	58%	31%	8%	..
4	9	375	99%	58%	32%	8%	..
4	V	375	99%	55%	34%	8%	..
4	W	375	99%	55%	33%	9%	..
4	X	375	93%	61%	30%	7%	..
4	Y	375	99%	61%	30%	7%	..
4	Z	375	99%	57%	32%	8%	..

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	MLY	A	505	-	-	X	-
1	MLY	A	553	-	-	X	-
1	MLY	A	764	-	-	X	-
1	MLY	A	768	-	-	X	-
1	MLY	A	782	-	-	X	-
1	MLY	A	839	-	-	X	-
1	MLY	D	553	-	-	X	-
1	MLY	D	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	295	-	-	X	-
1	MLY	J	505	-	-	X	-
1	MLY	J	553	-	-	X	-
1	MLY	J	764	-	-	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 [i](#)

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
			Total	C	N	O	S		
1	A	840	6797	4382	1135	1243	37	0	0
1	D	840	6797	4382	1135	1243	37	0	0
1	G	840	6797	4382	1135	1243	37	0	0
1	J	840	6797	4382	1135	1243	37	0	0
1	M	840	6797	4382	1135	1243	37	0	0
1	S	840	6797	4382	1135	1243	37	0	0

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

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

- 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		

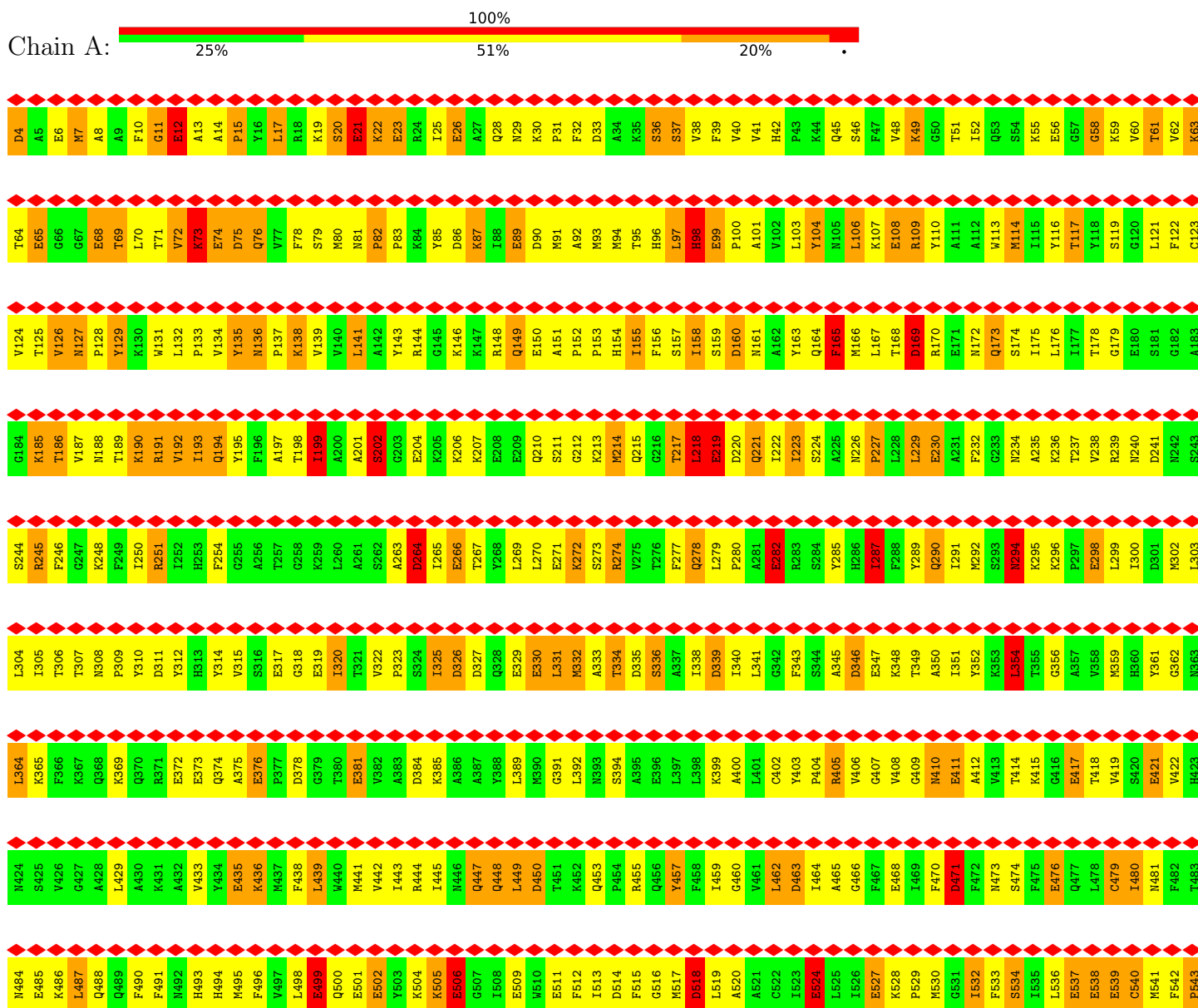
- Molecule 4 is a protein called SKELETAL MUSCLE ACTIN.

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 [i](#)

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



K544	E605	L664	Y724	E784
E604	E604	R665	R725	E785
T546	T606	S666	V726	I786
D647	V607	T667	L727	I787
T548	V608	H668	M728	T788
S649	G609	P669	A729	A789
F550	L610	H670	S730	T790
K651	Y611	F671	A731	Q791
N552	Q612	V672	I732	R792
K553	K613	K673	P733	A793
L554	S614	C674	E734	C794
Y555	S615	I675	G735	R795
D556	V616	I676	Q736	G796
E557	K617	F677	F737	F797
H558	T618	M678	M738	L798
L659	L619	E679	D739	M799
G660	A620	T680	S740	R800
K661	L621	K681	K741	V801
S662	L622	T682	K742	E802
N663	F623	P683	A743	Y803
N664	A624	G684	S744	R804
F665	T625	A685	E745	A805
Q666	Y626	M686	K746	M806
K667	G627	E687	L747	V807
P668	G628	H688	L748	E808
K669	E629	E689	G749	R809
P570	A630	L690	G750	R810
A571	E631	V691	G751	E811
K572	G632	L692	D752	S812
G573	G633	G693	V753	I813
K574	G634	Q694	D754	F814
A575	G635	L695	H755	C815
E576	K636	R696	T756	I816
A577	K637	C697	Q757	Q817
H578	G638	M698	Y758	Y818
F579	G639	G699	A759	N819
S680	K640	V700	F760	V820
L681	K641	L701	G61	R821
V682	K642	E702	H62	S822
H683	G643	G703	T763	F823
Y684	S644	I704	K764	M824
G686	S645	R705	V765	N825
T687	F646	I706	F766	V826
V688	Q647	C707	F767	K827
D689	T648	R708	K768	H828
Y690	V649	K709	A769	N829
N691	S650	G710	G770	P830
L692	A651	F711	L771	M831
S693	L652	P712	L772	M832
G694	F653	S713	G773	K833
V695	R654	R714	L774	L834
L696	E655	V715	L775	F835
E697	M656	L716	E776	F836
K698	L657	Y717	K777	K837
N699	M658	A718	M778	I838
K600	K659	D719	R779	K839
D601	L660	F720	D780	P840
P602	M661	K721	D781	L841
L603	A662	Q722	K782	L842
	N663	R723	L783	K843

● Molecule 1: SKELETAL MUSCLE MYOSIN II



D4	A5	G184	V124	S244	L304	L364	N424
A5	G66	K185	T125	R245	L305	K365	S425
E6	G66	T186	V126	F246	T306	F366	V426
M7	G67	V187	N127	G247	T307	K367	G427
A8	E68	N188	P128	K248	N308	Q368	A428
A9	A8	T189	Y129	F249	P309	K369	L429
F10	L70	K190	K130	I250	Y310	Q370	A430
G11	E11	R191	V131	R251	D311	R371	K431
E12	E12	R192	L132	I252	Y312	E372	A432
A13	K73	I193	P133	H253	H313	E373	V433
A14	E74	Q194	V134	F254	Y314	Q374	Y434
P15	D75	Y195	Y135	G255	V315	A375	E435
Y16	V76	F196	N136	A256	S316	E376	K436
L17	V77	A197	P137	T257	E317	P377	K437
R18	F78	T198	K138	G258	G318	D378	F438
K19	S79	I199	V139	K259	E319	G379	L439
S20	M80	A200	Y140	L260	I320	T380	W440
E21	N81	A201	L141	A261	T321	E381	M441
K22	P82	S202	A142	S262	V322	V382	V442
E23	P83	G203	Y143	A263	P323	A383	L443
A24	K84	E204	R144	D264	S224	D384	R444
I25	Y85	K205	G145	E265	I325	K385	I445
E26	D86	K206	K146	E266	D326	A386	N446
Q27	K87	K207	K147	T267	D327	A387	Q447
A28	I88	E208	L148	Y268	Q328	Y388	L448
N29	R89	E209	Q149	L269	E329	L389	L449
K30	D90	Q210	E150	L270	E330	N390	D450
P31	M91	S211	A151	E271	L331	G391	T451
F32	A92	G212	P152	K272	M332	L392	K452
D33	M93	K213	P153	S273	A333	N393	R453
A34	M94	M214	H154	R274	T334	S394	F454
K35	T95	Q215	I155	V275	D335	A395	R455
S36	H96	G216	F156	T276	S336	E396	Q456
S37	L97	G217	S157	F277	A337	L397	Y457
V38	H88	L218	I158	Q278	I338	L398	F458
F39	E99	E219	S159	L279	D339	K399	L459
V40	P100	D220	D160	P280	I340	A400	G460
A41	A101	Q221	N161	A281	L341	L401	V461
H42	V102	I222	A162	E282	G342	C402	L462
K43	L103	I223	Y163	R283	F343	Y403	D463
K44	Y104	S224	Q164	S284	S344	P404	I464
Q45	N105	A225	F165	Y285	A345	A405	A465
S46	L106	M226	M166	H286	D346	V406	G466
F47	K107	P227	L167	I287	E347	Q407	F467
V48	E108	L228	T168	F288	K348	V408	E468
K49	R109	L229	D169	Y289	T349	Q409	L469
G50	Y110	E230	R170	Q290	A350	N410	F470
T51	A111	A231	E171	I291	I351	E411	D471
I52	M112	F232	M172	M292	Y352	A412	F472
Q53	M113	G233	Q173	S293	K353	V413	N473
S54	M114	M234	S174	M294	L354	T414	S474
K55	I115	A235	I175	K295	T355	K415	F475
E56	Y116	K236	L176	K296	G356	G416	E476
G57	T117	T237	I177	P297	E357	E417	Q477
G58	Y118	V238	T178	E298	V358	T418	L478
K59	S119	R239	G179	L299	N359	V419	C479
V60	G120	M240	E180	I300	H360	S420	I480
T61	L121	D241	L181	D301	Y361	E421	N481
V62	F122	M242	G182	K302	G362	V422	F482
K63	C123	S243	A183	L303	N363	H423	T483

M484	M485	E486	K486	L487	Q488	Q489	F490	F491	M492	H493	H494	M495	F496	V497	L498	E499	Q500	E501	Y503	K504	K505	E506	G507	I508	E509	M510	E511	F512	I513	D514	F515	G516	M517	M518	D518	L519	A520	A521	C522	I523	E524	L525	L526	E527	K528	P529	K530	G531	L532	F533	F534	L535	L536	E537	E538	E539	C540	M541	F542	P543
K544	A545	T546	D547	T548	S549	F550	K551	M552	K553	L554	Y555	D556	H557	H558	L559	G560	K561	S562	M563	N564	F565	Q566	K567	P568	K569	P570	A571	K572	G573	K574	A575	E576	A577	H578	F579	S580	K581	V582	H583	Y584	G585	G586	T587	V588	D589	Y590	N591	L592	F593	F594	G595	L596	L597	K598	N599	K600	D601	P602	L603	
N604	E605	T606	V607	I608	G609	L610	Y611	Q612	K613	S614	S615	L616	K617	T618	L619	A620	L621	L622	F623	N624	T625	Y626	G627	G628	E629	A630	E631	G632	G633	G634	G635	K636	K637	G638	G639	K640	L641	K642	G643	S644	S645	F646	Q647	T648	V649	S650	A651	L652	F653	F654	R655	E656	L657	M658	K659	L660	M661	A662	N663	
L664	R665	S666	T667	H668	P669	H670	F671	H672	K673	C674	I675	I676	P677	M678	E679	T680	K681	L682	P683	G684	A685	M686	E687	H688	E689	L689	V691	L692	H693	Q694	L695	R696	C697	M698	G699	V700	K640	E702	G703	I704	S705	I706	C707	R708	K709	G710	F711	L652	S713	R714	V715	L716	L717	A718	D719	F720	K721	Q722	R723	
Y724	R725	V726	L727	M728	A729	S730	A731	I732	P733	E734	G735	F736	M737	M738	D739	S740	K741	K742	A743	G844	E745	K746	L747	L748	G749	G750	G751	D752	V753	D754	H755	T756	Q757	Y758	A759	F760	G761	H762	T763	K764	V765	F766	F767	K768	A769	G770	L771	L772	G773	L774	L775	E776	E777	M778	R779	D780	L781	K782	L783	
A784	E785	I786	I787	A788	T789	Q791	A792	R793	C794	R795	G796	L797	L798	M799	V800	E801	E802	Y803	R804	A805	M806	V807	E808	R809	R810	E811	S812	I813	F814	C815	I816	Q817	Y818	N819	V820	R821	S822	F823	M824	N825	V826	K827	H828	M829	P830	M831	M832	K833	L834	F835	F836	K837	L838	K839	P840	L841	L842	K843		

• 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	N29	K30	P31	F32	I33	A34	K35	S36	S37	V38	F39	V40	V41	H42	P43	K44	Q45	S46	F47	K48	V49	G50	T51	I52	Q53	S54	K55	E56	G57	G58	K59	V60	T61	V62	K63
T64	E65	G66	G67	E68	T69	L70	T71	H72	K73	E74	D75	V76	V77	F78	S79	M80	N81	P82	P83	K84	Y85	D86	K87	I88	E89	M91	A92	M93	M94	T95	H96	L97	H98	E99	P100	A101	Y102	L103	Y104	N105	L106	K107	E108	R109	Y110	A111	A112	M113	M114	I115	Y116	T117	Y118	S119	G120	F121	F122	C123	
V124	T125	V126	M127	A128	P129	K130	V131	L132	P133	V134	Y135	M136	P137	K138	V139	Y140	A141	Y143	R144	G145	K146	K147	R148	Q149	E150	A151	P152	P153	H154	I155	F156	S157	I158	S159	D160	M161	A162	Y163	Q164	F165	M166	L167	L168	D169	R170	E171	M172	Q173	S174	I175	L176	L177	T178	G179	E180	L181	G182	A183	
G184	K185	T186	V187	M188	T189	K190	R191	L192	I193	Q194	Y195	F196	A197	T198	I199	A200	E201	S202	G203	E204	K205	K206	K207	E208	E209	Q210	S211	G212	K213	M214	Q215	G216	L218	E219	D220	Q221	I222	I223	S224	A225	M226	P227	L228	L229	E230	A231	F232	G233	M234	A235	K236	T237	V238	R239	M240	D241	M242	S243	
S244	R245	F246	G247	K248	F249	I250	R251	L252	H253	F254	G255	A256	T257	G258	K259	L260	A261	S262	A263	D264	I265	E266	T267	Y268	L269	L270	E271	K272	S273	K274	V275	T276	F277	Q278	L279	P280	E282	R283	S284	H286	F288	Y289	Q290	I291	M292	S293	K294	K295	K296	P297	E298	L299	I300	D301	M302	L303			
L304	T305	T306	T307	N308	P309	Y310	D311	Y312	H313	Y314	V315	S316	E317	G318	E319	I320	T321	V322	P323	S324	I325	D326	D327	Q328	E329	E330	L331	M332	A333	S334	D335	S336	L338	D339	L340	L341	G342	F343	S344	D346	E347	K348	A350	I351	Y352	M353	L354	T355	G356	V358	K359	H360	G362	N363					
L364	K365	F366	K367	Q368	K369	Q370	R371	E372	E373	Q374	A375	E376	P377	D378	Q379	T380	E381	Y382	A383	D384	K385	A386	A387	Y388	L389	M390	G391	L392	N393	S394	A395	E396	L397	L398	K399	A400	C402	Y403	P404	R405	V406	G407	V408	N410	E411	A412	V413	L414	T415	G416	E417	T418	V419	S420	E421	V422	H423		

N424	N484	K544	N604	L664	Y724	A784	D4	T64	V124	G184	S244	L304
S425	E485	A545	E605	R665	R725	E785	A5	E65	T125	K185	R245	I305
V426	K486	T546	T606	S666	V726	I786	E6	G66	V126	T186	F246	T306
G427	L487	D547	V607	T667	L727	I787	M7	G67	M127	V187	G247	T307
A428	Q488	T548	I608	H668	A728	T788	A8	E68	P128	M188	K248	T308
L429	Q489	S549	G609	P669	A729	A789	A9	T69	Y129	T189	F249	P309
A430	F490	F550	L610	H670	S730	T790	F10	L70	K130	K190	I250	Y310
K431	F491	K551	Y611	F671	A731	Q791	G11	T71	M131	R191	R251	D311
A432	N492	N552	Q612	V672	I732	A792	E12	V72	L132	V192	I252	H312
V433	H493	K553	K613	H673	P733	R793	A13	W73	P133	L193	H253	H313
Y434	H494	L554	S614	C674	E734	C794	A14	E74	V134	Q194	F254	Y314
E435	M495	Y555	S615	I675	G735	R795	P15	D75	Y135	Y195	G255	V315
K436	F496	D556	V616	I676	Q736	G796	Y16	V76	M136	F196	A256	S316
M437	V497	E557	K617	P677	F737	F797	L17	V77	P137	A197	T257	E317
F438	L498	H558	T618	N678	M738	L798	R18	F78	K138	T198	Q258	G318
L439	E499	L559	L619	E679	D739	M799	K19	S79	V139	I199	K259	E319
V440	Q500	G560	A620	T680	S740	R800	S20	M80	Y140	A200	L260	I320
M441	E501	K561	L621	K681	K741	V801	E21	N81	L141	A201	A261	T321
V442	E502	S562	L622	T682	K742	E802	K22	P82	A142	S202	S262	V322
I443	Y503	N563	F623	P683	A743	Y803	E23	P83	Y143	G203	A263	P323
R444	K504	N564	A624	G684	S744	R804	I25	K84	G144	E204	D264	S324
I445	K505	F565	G625	H685	E745	A805	E26	D86	K146	K206	I266	I325
N446	E506	Q566	Y626	M686	K746	M806	E27	K87	K147	K207	T267	D326
Q447	G507	P568	G627	H688	L747	V807	Q28	I88	R148	E208	T268	Q327
Q448	I508	P568	G628	H688	L748	E808	N29	S89	Q149	Q209	L269	E328
L449	E509	K569	E629	E689	G749	R809	K30	D90	E150	Q210	L270	E329
D450	W510	P570	A630	L690	G750	R810	P31	M91	A151	S211	L271	E330
A451	E511	A571	E631	V691	G751	E811	F32	A92	P152	G212	E272	L331
K452	F512	K572	G632	H692	D752	S812	D33	A93	P153	K213	K273	M332
Q453	I513	G573	K633	H693	V753	I813	A34	H94	H154	M214	R274	A333
P454	D514	K574	G634	Q694	D754	F814	K35	T95	I155	Q215	V275	T334
R455	F515	A575	G635	L695	H755	C815	S36	H96	F156	G216	V276	D335
Q456	G516	E576	K636	R696	T756	I816	S37	S97	S157	G217	T277	S336
Y457	M517	A577	K637	C697	Q757	Q817	S38	L98	Q157	T217	F277	A337
F458	D518	H578	G638	M698	Y758	Y818	V38	H98	I158	L218	Q278	I338
I459	L519	F579	G639	G699	A759	N819	F39	E99	S159	E219	L279	D339
G460	A520	S580	K640	V700	F760	W820	V40	P100	D160	Q220	P280	I340
V461	L521	L581	K641	L701	G761	R821	V41	A101	M161	D221	A281	L341
L462	C522	V582	K642	E702	H762	S822	H42	Y102	A162	I222	E282	G342
D463	I523	H583	G643	G703	T763	F823	P43	L103	Y163	I223	R283	F343
I464	E524	Y584	S644	I704	K764	M824	K44	Y104	Q164	A224	S284	S344
A465	L525	A585	S645	R705	V765	N825	Q45	N105	F165	A225	Y285	A345
G466	I526	G586	F646	I706	F766	V826	S46	L106	M166	N226	H286	D346
F467	E527	T587	F647	C707	F767	K827	F47	E108	L167	P227	I287	E347
E468	K528	V588	T648	R708	K768	H828	V48	E109	T168	T228	F288	K348
I469	P529	D589	V649	K709	A769	M829	K49	R109	D169	L229	Y289	T349
F470	M530	Y590	S550	G710	G770	P830	G50	Y110	R170	E230	Q290	A350
D471	G531	N591	A651	F711	L771	M831	T51	A111	E171	A231	I291	I351
F472	I532	I592	L652	F712	L772	M832	S52	A112	M172	F232	M292	Y352
M473	F533	S593	F653	S713	G773	K833	Q53	W113	Q173	G233	S293	Y353
S474	S534	G594	R654	R714	L774	L834	S54	M114	S174	M234	N294	L354
F475	I535	W595	E655	V715	L775	P835	K55	I115	I175	A235	K295	T355
A476	L536	L596	M556	L716	E776	F836	E56	Y116	L176	K236	K296	G356
Q477	E537	E597	M557	L717	E777	K837	G57	T117	I177	T237	P297	A357
L478	E538	K598	M558	A718	M778	L838	G58	Y118	T178	V238	E298	V358
C479	E539	N599	K659	D719	R779	K839	R59	S119	G179	R239	L299	K359
M480	C540	K600	L660	F720	D780	P840	V60	G120	E180	N240	I300	H360
I481	M541	D601	M661	K721	D781	L841	T61	L121	S181	D241	Y301	I361
F482	F542	P602	A662	Q722	K782	L842	L62	F122	G182	M242	M302	G362
T483	L603	N663	R723	R723	L783	K843	K63	C123	A183	S243	L303	N363

• Molecule 1: SKELETAL MUSCLE MYOSIN II



D4	T64	V124	G184	S244	L304
A5	E65	T125	K185	R245	I305
E6	G66	V126	T186	F246	T306
M7	G67	M127	V187	G247	T307
A8	E68	P128	M188	K248	T308
A9	T69	Y129	T189	F249	P309
F10	L70	K130	K190	I250	Y310
G11	T71	M131	R191	R251	D311
E12	V72	L132	V192	I252	H312
A13	K73	P133	L193	H253	H313
A14	E74	V134	Q194	F254	Y314
P15	D75	Y135	Y195	G255	V315
Y16	V76	M136	F196	A256	S316
L17	V77	P137	A197	T257	E317
R18	F78	K138	T198	Q258	G318
K19	S79	V139	I199	K259	E319
S20	M80	Y140	A200	L260	I320
E21	N81	L141	A201	A261	T321
K22	P82	A142	S202	S262	V322
E23	P83	Y143	G203	A263	P323
K24	K84	G144	E204	D264	S324
I25	Y85	R146	K206	I266	I325
E26	D86	K146	K206	E266	D326
A27	K87	K147	K207	T267	D327
Q28	I88	R148	E208	T268	Q327
N29	S89	Q149	Q209	L269	E328
K30	D90	E150	Q210	L270	E329
P31	M91	A151	S211	L271	E330
F32	A92	P152	G212	E272	L331
D33	A93	P153	K213	K273	M332
A34	H94	H154	M214	R274	A333
K35	T95	I155	Q215	V275	T334
S36	H96	F156	G216	V276	D335
S37	L97	S157	G217	T277	S336
V38	H98	I158	L218	Q278	A337
F39	E99	S159	E219	L279	I338
V40	P100	D160	Q220	P280	D339
V41	A101	M161	D221	A281	I340
H42	Y102	A162	I222	E282	L341
P43	L103	Y163	I223	R283	G342
K44	Y104	Q164	A224	S284	F343
Q45	N105	F165	A225	Y285	S344
S46	L106	M166	N226	H286	A345
F47	E108	L167	P227	I287	D346
V48	E109	T168	T228	F288	E347
R49	D169	D169	L229	Y289	K348
G50	Y110	R170	E230	Q290	A350
T51	A111	E171	A231	I291	I351
S52	A112	M172	F232	M292	Y352
Q53	W113	Q173	G233	S293	Y353
S54	M114	S174	M234	N294	L354
K55	I115	I175	A235	K295	T355
E56	Y116	L176	K236	K296	G356
G57	T117	I177	T237	P297	A357
G58	Y118	T178	V238	E298	V358
R59	S119	G179	R239	L299	K359
V60	G120	E180	N240	I300	H360
T61	L121	S181	D241	Y301	I361
L62	F122	G182	M242	M302	G362
K63	C123	A183	S243	L303	N363

L364	K365	F366	K367	Q368	K369	Q370	R371	E372	E373	Q374	A375	E376	P377	D378	G379	T380	E381	V382	A383	D384	K385	A386	A387	Y388	L389	M390	G391	L392	S394	A395	E396	L397	L398	K399	A400	C402	Y403	P404	R405	V406	G407	V408	G409	N410	E411	A412	A413	T414	K415	G416	T418	V419	S420	A422	H423			
M424	S425	V426	G427	A428	L429	A430	K431	A432	V433	Y434	E435	A436	M437	F438	L439	W440	M441	V442	I443	R444	I445	M446	Q447	Q448	L449	D450	T451	K452	P454	R455	Q456	Y457	F458	I459	G460	V461	L462	D463	I464	A465	G466	F467	E468	I469	F470	D471	M472	F473	S474	F475	E476	Q477	L478	C479	I480	M481	F482	T483
M484	E485	K486	L487	Q488	Q489	F490	F491	M492	H493	H494	M495	F496	L497	L498	E499	Q500	E501	Y503	K504	K505	E506	G507	I508	E509	W510	E511	F512	I513	D514	F515	G516	M517	D518	L519	A520	A521	C522	I523	E524	L525	I526	E527	K528	P529	M530	G531	I532	F533	S534	I535	L536	E537	E538	E539	C540	M541	F542	P543
K544	A545	T546	D547	S549	F550	K551	N552	K553	L554	Y555	D556	F557	H558	L559	G560	K561	S562	N563	R564	F565	Q566	G567	P568	K569	P570	E571	K572	G573	K574	A575	E576	A577	H578	F579	S580	L581	C582	H583	Y584	G585	G586	T587	V588	D589	Y590	N591	I592	F593	G594	M595	L596	E597	K598	N599	K600	D601	P602	L603
N604	E605	T606	V607	I608	L610	Y611	K612	K613	S614	S615	V616	K617	T618	L619	A620	L621	L622	F623	A624	Y626	G627	G628	E629	A630	E631	G632	G633	G634	G635	K636	K637	G638	G639	K640	K641	K642	G643	S644	F646	Q647	T648	D649	S650	A651	L652	F653	R654	E655	M656	M658	K659	L660	M661	A662	N663			
L664	R665	S666	T667	H668	P669	H670	F671	V672	R673	C674	I675	I676	P677	N678	E679	T680	K681	P683	G684	A685	M686	E687	H688	E689	L690	V691	L692	H693	Q694	L695	R696	M698	G699	V700	L701	E702	G703	I704	R705	I706	G707	R708	K709	G710	F711	L712	S713	R714	V715	L716	A718	D719	F720	M721	Q722	R723		
Y724	R725	V726	L727	M728	A729	S730	A731	I732	P733	E734	G735	Q736	M738	D739	S740	K741	K742	A743	E744	K746	L747	L748	G749	G750	G751	D752	V753	Q754	H755	T756	Q757	Y758	A759	F760	G761	R762	T763	K764	V765	I766	F767	K768	A769	G770	L771	L772	G773	L774	L775	E776	M778	R779	D780	K782	L783			
A784	E785	I786	T787	T788	A789	T790	Q791	A792	R793	C794	R795	G796	F797	L798	M799	R800	E802	R803	A805	M806	V807	E808	R809	R810	E811	S812	L813	F814	C815	L816	Q817	Y818	N819	V820	R821	S822	F823	M824	N825	V826	K827	H828	M829	P830	M831	M832	K833	L834	F835	F836	K837	L838	K839	P840	L841	L842	K843	

• Molecule 1: SKELETAL MUSCLE MYOSIN II



D4	A5	E6	M7	A8	A9	F10	G11	E12	A13	E14	P15	Y16	L17	R18	K19	S20	E21	K22	E23	R24	L25	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	L53	Q53	S54	K55	E56	G57	G58	K59	V60	T61	V62	K63
T64	E65	G66	G67	E68	T69	L70	T71	V72	K73	E74	D75	Q76	F77	F78	S79	M80	N81	P82	K83	K84	Y85	D86	K87	I88	E89	Q90	A91	A92	N93	M94	T95	H96	L97	H98	E99	P100	A101	V102	L103	Y104	N105	L106	E107	E108	R109	Y110	A111	A112	I113	M114	I115	Y116	E117	Y118	S119	G120	F122	C123		
V124	T125	V126	N127	P128	Y129	K130	M131	L132	P133	V134	Y135	M136	K137	K138	V139	L140	A141	A142	Y143	R144	G145	K146	K147	R148	Q149	E150	A151	P152	P153	H154	I155	F156	S157	I158	S159	D160	N161	A162	L163	Q164	F165	M166	L167	T168	D169	R170	E171	M172	Q173	Q174	S175	L176	L177	I178	G179	E180	L181	G182	A183	
G184	K185	T186	V187	M188	T189	K190	R191	V192	L193	Q194	Y195	F196	L197	T198	L199	A200	A201	S202	G203	E204	K205	K206	K207	E208	E209	Q210	S211	G212	K213	M214	Q215	G216	L218	E219	D220	Q221	I222	I223	S224	A225	M226	P227	L228	L229	E230	A231	F232	G233	Q234	M235	K236	T237	V238	R239	M240	D241	M242	S243		
S244	R245	F246	G247	K248	F249	L250	R251	L252	H253	F254	G255	A256	G258	K259	L260	A261	S262	D264	L265	E266	T267	Y268	L269	L270	E271	K272	S273	R274	V275	T276	F277	Q278	L279	P280	A281	E282	R283	S284	Y285	H286	F288	Y289	Q290	L291	M292	S293	M294	K295	K296	T297	E298	L299	I300	D301	K302	L303				

L304	I305	T306	T307	N308	P309	Y310	D311	H312	Y314	V315	S316	E317	G318	E319	I320	T321	V322	P323	S324	I325	D326	D327	Q328	E329	E330	L331	M332	A333	T334	D335	S336	A337	I338	D339	I340	L341	G342	F343	S344	A345	D346	E347	K348	T349	A350	I351	Y352	K353	L354	T355	G356	A357	V358	M359	H360	G362	N363		
L364	K365	F366	K367	K368	K369	Q370	R371	E372	H373	Q374	A375	E376	P377	D378	G379	T380	E381	V382	A383	D384	K385	A386	A387	Y388	L389	M390	G391	L392	N393	S394	A395	E396	S397	L398	D399	A400	L401	C402	Y403	R404	P405	V406	G407	V408	G409	N410	E411	A412	V413	T414	K415	G416	A417	T418	V419	S420	H423		
N424	S425	G426	A427	A428	L429	A430	K431	A432	V433	Y434	E435	K436	M437	F438	L439	W440	V442	I443	R444	I445	M446	Q447	Q448	L449	D450	I451	K452	Q453	P454	R455	Q456	L457	F458	I459	G460	L462	D463	I464	A465	G466	F467	E468	I469	F470	D471	N472	M473	S474	F475	E476	Q477	L478	C479	I480	M481	F482	T483		
M484	E485	K486	L487	Q488	Q489	F490	F491	M492	H493	H494	M495	F496	V497	L498	E499	Q500	E502	Y503	K504	K505	E506	G507	I508	E509	M510	E511	F512	I513	D514	F515	G516	M517	D518	L519	A520	A521	C522	I523	E524	I526	E527	K528	P529	M530	G531	I532	M533	S534	I535	L536	E537	E538	E539	C540	M541	F542	P543		
K544	A545	T546	D547	T548	S549	F550	K551	N552	K553	L554	Y555	D556	H557	H558	L559	G560	K561	S562	N563	N564	F565	Q566	K567	P568	K569	P570	A571	K572	G573	K574	A575	E576	H577	H578	F579	S580	L581	V582	H583	Y584	E585	G586	T587	V588	D589	Y590	N591	I592	S593	S594	N595	L596	E597	K598	N599	K600	D601	P602	L603
M604	E605	T606	V607	I608	G609	L610	Y611	Q612	K613	S614	S615	V616	K617	T618	L619	A620	L621	L622	F623	A624	T625	Y626	G627	G628	E629	A630	E631	G632	G633	G634	G635	K636	K637	G638	G639	K640	L641	K642	G643	S644	F646	Q647	T648	V649	S650	A651	L652	F653	R654	E655	M656	L657	M658	K659	L660	M661	A662	N663	
L664	R665	S666	T667	H668	P669	H670	F671	V672	R673	C674	L675	L676	P677	N678	E679	T680	K681	T682	P683	G684	A685	M686	E687	H688	E689	L690	V691	L692	Q694	L695	R696	K697	N698	G699	V700	L701	E702	G703	I704	R705	I706	C707	R708	K709	G710	F711	P712	S713	R714	V715	L716	A717	D718	F719	L720	M721	Q722	R723	
Y724	R725	V726	L727	N728	A729	S730	A731	I732	P733	E734	G735	Q736	F737	M738	D739	S740	K741	A743	S744	E745	K746	L747	L748	G749	G750	G751	D752	V753	D754	H755	T756	Q757	Y758	A759	F760	L761	R762	T763	K764	F766	F767	K768	A769	G770	L771	L772	G773	L774	L775	E776	E777	M778	R779	D780	D781	K782	L783		
A784	E785	I786	I787	T788	A789	T790	Q791	A792	C794	R795	G796	F797	L798	M799	R800	E802	Y803	R804	A805	M806	H807	E808	R809	R810	E811	S812	F814	C815	L816	Q817	Y818	N819	V820	V821	S822	F823	M824	N825	V826	K827	H828	H829	P830	M831	H832	K833	L834	F835	F836	K837	L838	K839	P840	L841	L842	K843			

• 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	K24	I25	E26	A27	Q28	Q29	K30	P31	F32	D33	A34	K35	S36	S37	V38	F39	V40	V41	H42	P43	K44	Q45	S46	F47	V48	K49	G50	T51	I52	M53	Q54	I55	Y56	E57	G58	K59	V60	L61	F62	C63
T64	E65	G66	G67	E68	T69	L70	T71	V72	K73	E74	D75	Q76	V77	F78	S79	M80	N81	P82	P83	K84	Y85	D86	K87	I88	E89	D90	N91	A92	N93	M94	T95	H96	L97	H98	E99	P100	V101	V102	L103	Y104	N105	L106	K107	E108	R109	Y110	A111	M112	M113	M114	I115	Y116	E117	Y118	S119	G120	L121	F122	C123
V124	T125	V126	N127	P128	Y129	K130	W131	L132	P133	V134	Y135	M136	P137	K138	V139	Y140	A142	Y143	R144	G145	K146	K147	R148	Q149	E150	A151	P152	P153	H154	I155	F156	S157	I158	S159	D160	N161	A162	Y163	Q164	F165	M166	L167	T168	E169	R170	E171	M172	Q173	S174	I175	L176	I177	T178	G179	E180	L181	G182	A183	
G184	K185	T186	V187	M188	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	M226	P227	L228	E230	A231	F232	G233	M234	A235	K236	T237	V238	R239	M240	D241	N242	S243		

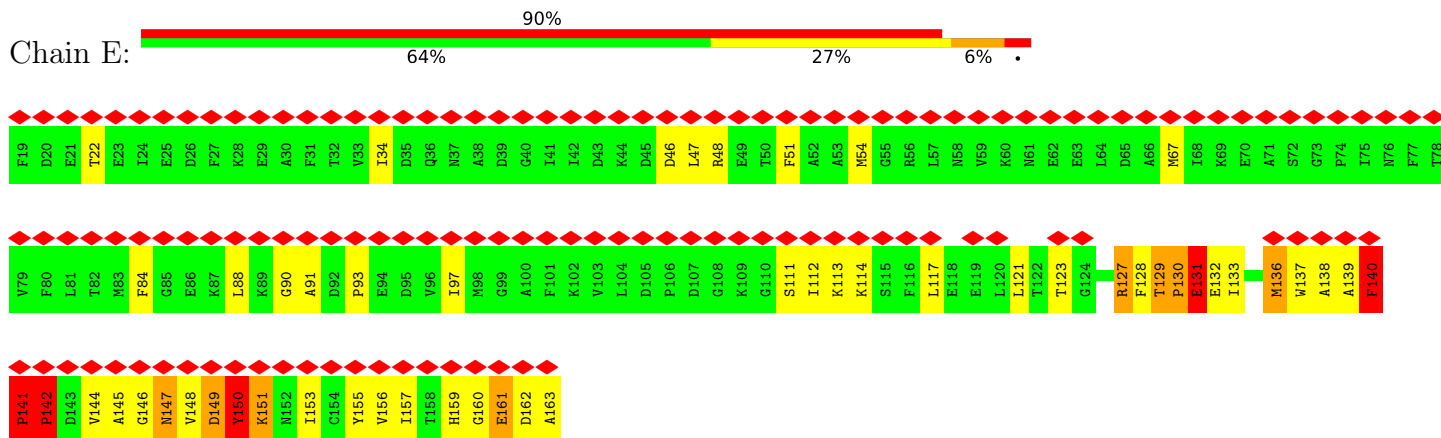
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L304	I305	T306	T307	N308	P309	Y310	D311	Y312	H313	Y314	V315	S316	E317	G318	E319	I320	T321	V322	P323	A324	I325	D326	D327	Q328	E329	E330	L331	M332	A333	T334	D335	S336	I338	D339	I340	L341	G342	F343	S344	A345	D346	E347	K348	T349	A350	I351	Y352	K353	L354	K355	G356	P357	V358	M359	H360	G362	N363	
L364	K365	F366	K367	Q368	K369	Q370	R371	E372	E373	Q374	A375	E376	P377	D378	G379	T380	V382	A383	D384	K385	A386	A387	Y388	E389	M390	G391	L392	L393	S394	A395	E396	L397	L398	K399	A400	C402	Y403	P404	A405	V406	G407	V408	G409	M410	A411	A412	A413	T414	K415	G416	E417	T418	V419	S420	A421	V422	H423	
M424	S425	V426	G427	A428	L429	A430	K431	A432	A433	Y434	E435	K436	M437	F438	L439	M440	V442	I443	R444	I445	M446	Q447	Q448	L449	D450	K451	F452	Q453	P454	R455	Q456	F457	F458	I459	G460	L462	D463	I464	A465	G466	F467	E468	I469	F470	D471	F472	M473	S474	F475	E476	Q477	L478	C479	I480	M481	F482	T483	
M484	E485	K486	L487	Q488	Q489	F490	F491	M492	M493	H494	M495	F496	V497	L498	E499	Q500	E502	Y503	K504	K505	E506	G507	I508	E509	M510	E511	F512	I513	D514	R455	Q456	M517	D518	L519	A520	A521	C522	I523	E524	L525	I526	E527	K528	P529	M530	G531	I532	F533	S534	I535	L536	E537	E538	E539	C540	M541	F542	P543
K544	A545	T546	D547	T548	S549	F550	K551	N552	K553	L554	Y555	D556	E557	H558	L559	G560	S562	N563	N564	F565	Q566	P568	K569	P570	A571	K572	G573	G574	A575	E576	A577	H578	F579	S580	L581	V582	H583	Y584	A585	G586	T587	V588	D589	Y590	N591	I592	S593	G594	N595	L596	E597	K598	N599	K600	D601	P602	L603	
N604	E605	T606	V607	I608	G609	L610	Y611	Q612	K613	S614	S615	V616	T618	L619	A620	K621	L622	F623	A624	T625	Y626	G627	G628	E629	A630	E631	G632	G633	G634	G635	K636	G638	G639	K640	K642	G643	S644	S645	F646	G647	T648	V649	S650	A651	L652	F653	R654	E655	N656	L657	N658	K659	L660	M661	A662	N663		
L664	R665	S666	T667	H668	P669	H670	F671	V672	R673	C674	L675	L676	N678	E679	T680	K681	T682	P683	G684	A685	R686	E687	H688	E689	L690	V691	L692	H693	Q694	L695	R696	G697	N698	V700	L701	E702	G703	I704	R705	I706	C707	R708	K709	G710	F711	P712	S713	R714	V715	L716	L717	A718	D719	F720	L721	Q722	R723	
Y724	R725	V726	L727	M728	A729	S730	A731	I732	P733	E734	G735	Q736	M738	D739	S740	K741	K742	A743	S744	E745	K746	L747	L748	G749	G750	G751	D752	V753	D754	H755	T756	Q757	Y758	A759	F760	G761	H762	T763	K764	V765	F766	F767	K768	R769	G770	L771	L772	G773	L774	L775	E776	E777	M778	R779	D780	D781	K782	L783
A784	E785	I786	I787	T788	A789	T790	Q791	A792	R793	C794	R795	G796	L798	M799	R800	E802	Y803	R804	A805	M806	E808	R809	R810	E811	S812	L813	F814	C815	L816	L817	Y818	N819	V820	R821	S822	F823	H824	N825	V826	K827	H828	H829	P830	M831	H832	L834	F835	F836	K837	L838	K839	P840	L841	L842	K843			

● Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

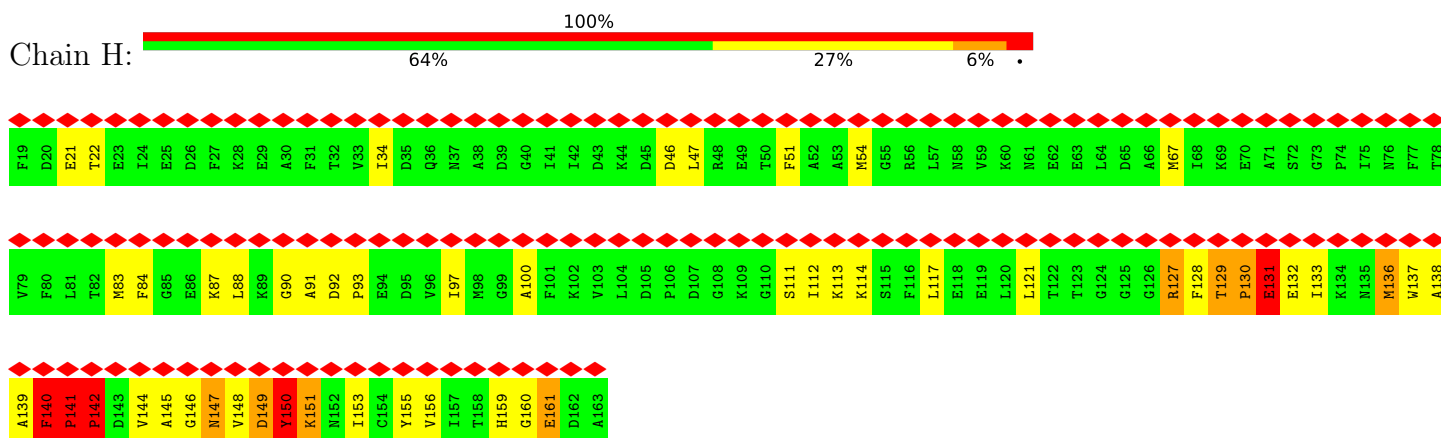


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Y79	F80	L81	T82	M83	F84	C85	E86	K87	L88	H89	G90	A91	D92	P93	E94	D95	V96	I97	N98	G99	A100	F101	K102	L103	L104	D105	P106	D107	G108	K109	G110	L111	L112	K113	K114	S115	F116	L117	E118	E119	L120	L121	T122	L123	G124	G125	G126	R127	T129	P130	E131	L132	I133	K134	M135	I136	W137	A138	
A139	F140	P141	P142	D143	V144	A145	G146	M147	V148	D149	Y150	K151	H152	I153	C154	Y155	V156	I157	T158	H159	G160	E161	D162	A163																																			

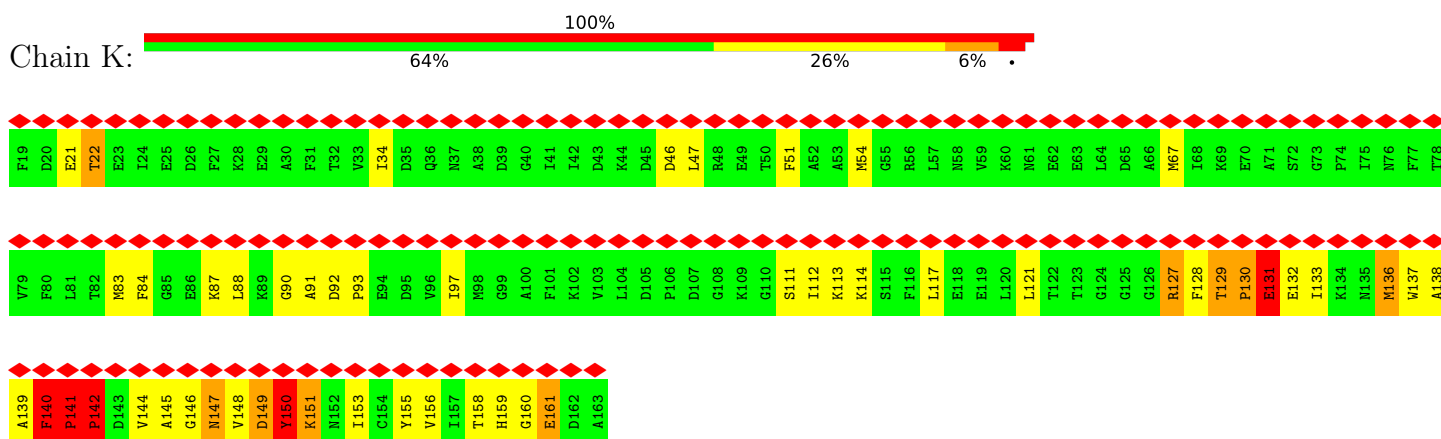
• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN



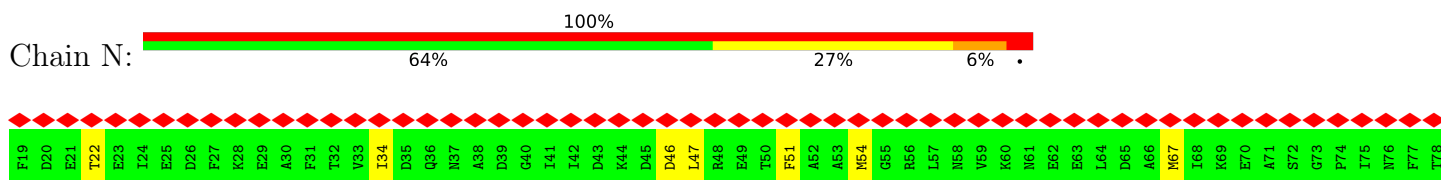
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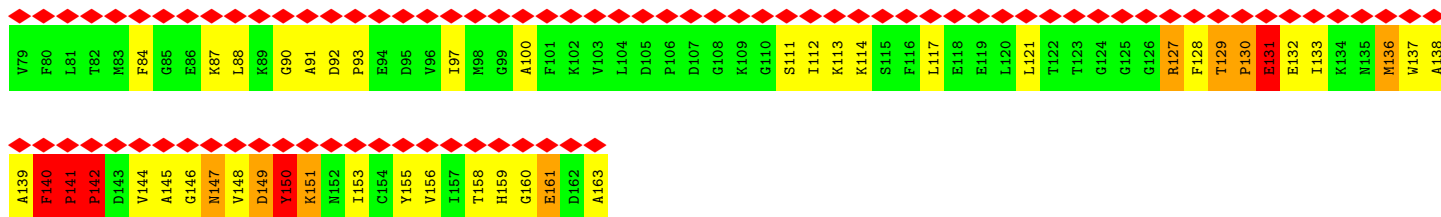


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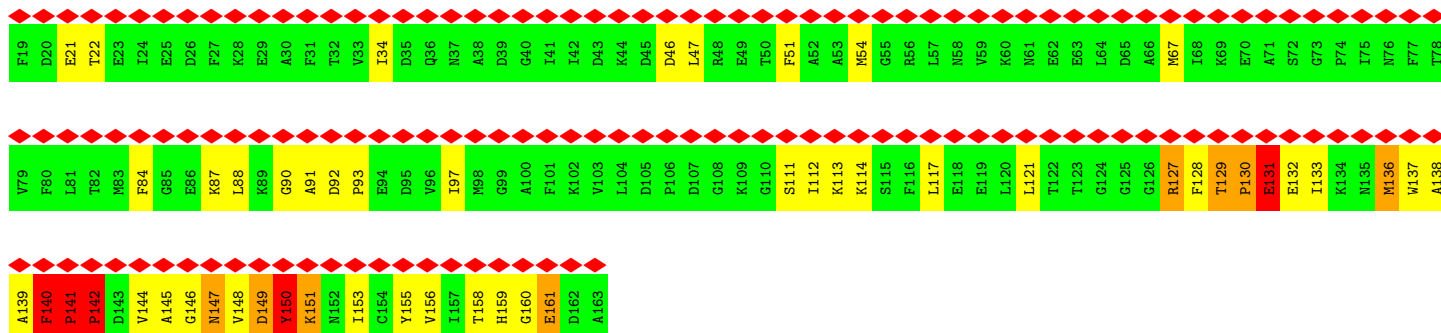


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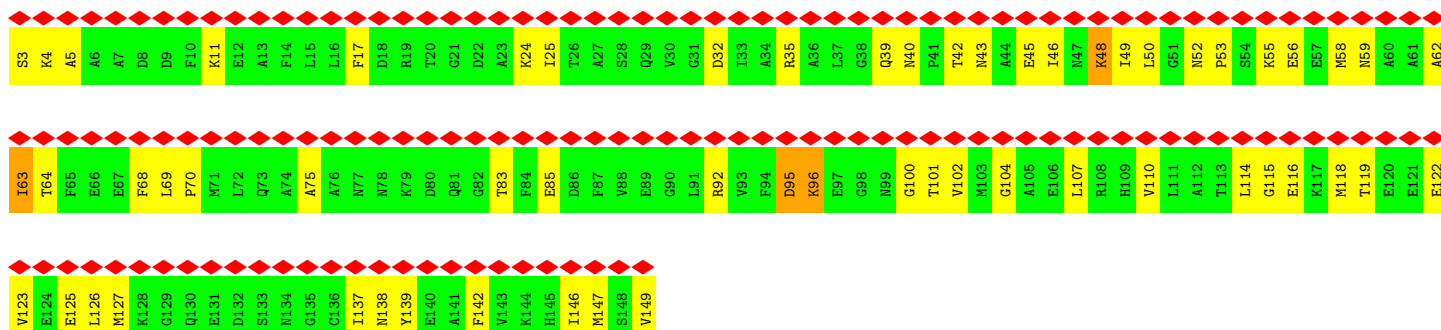




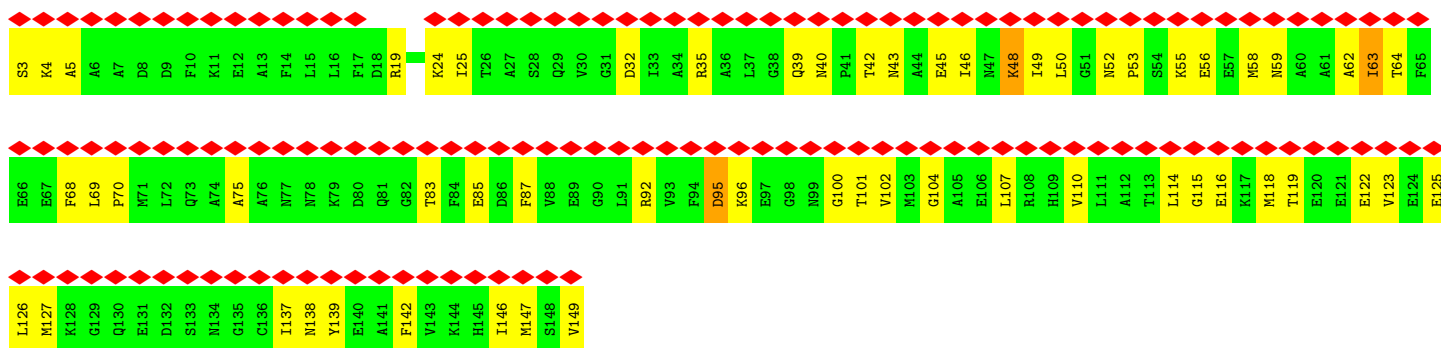
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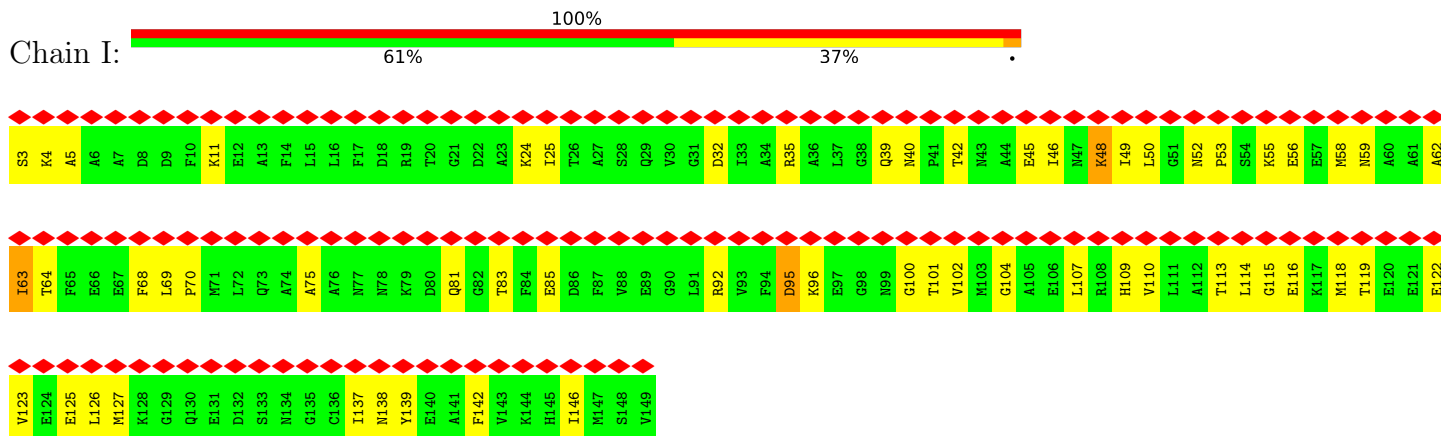
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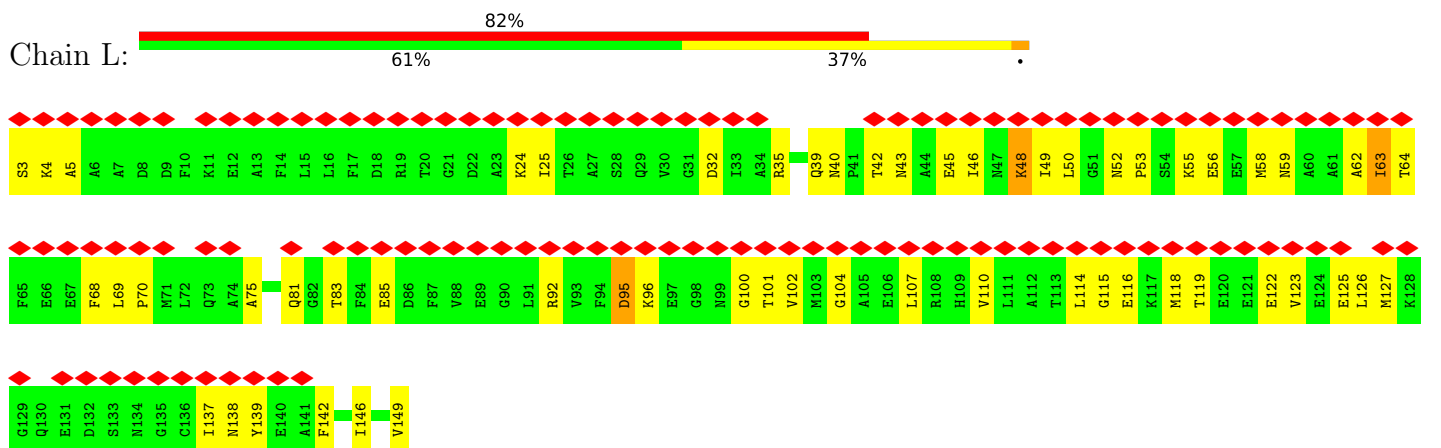
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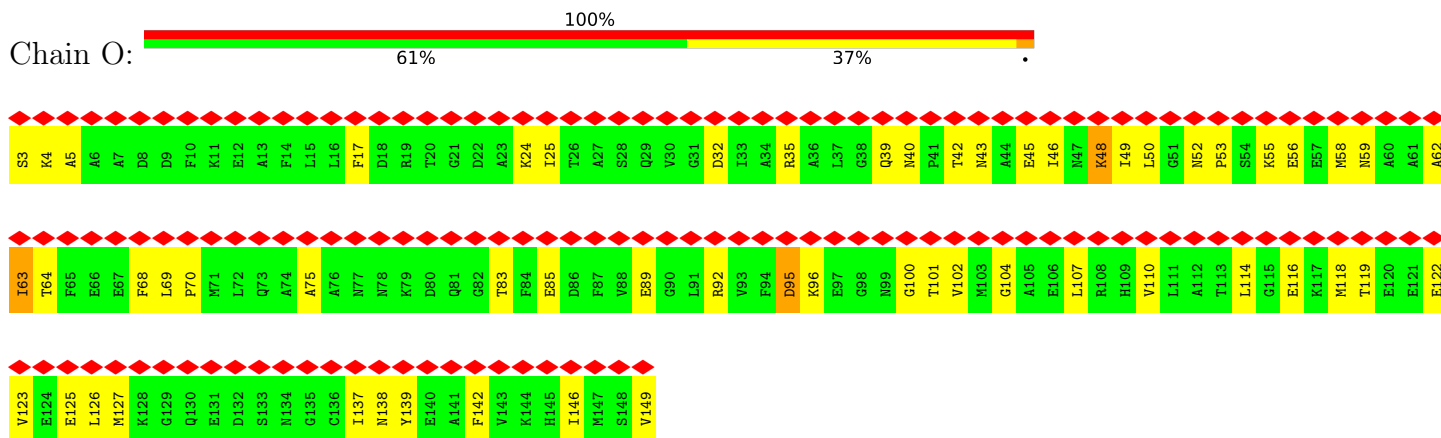
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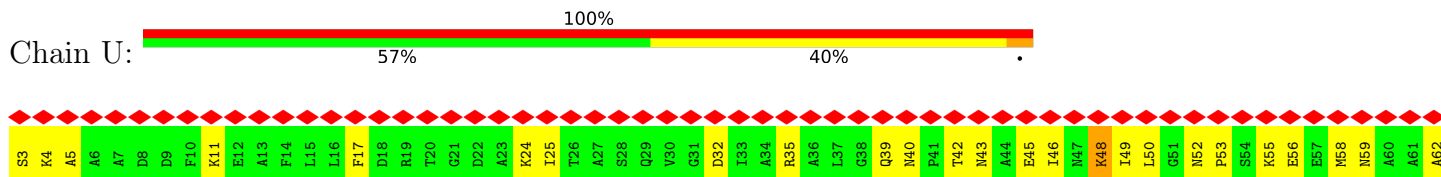
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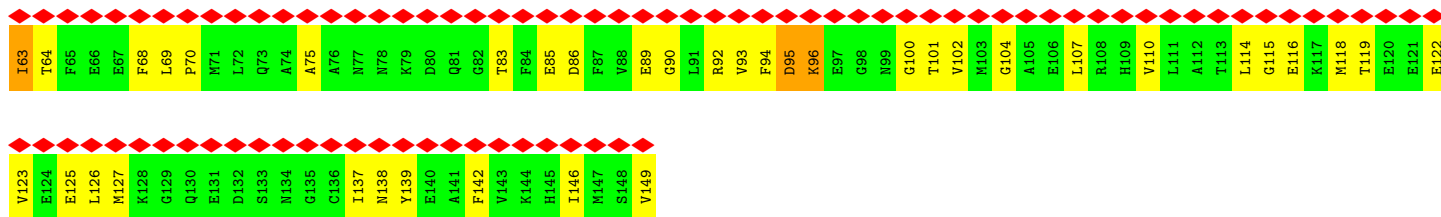


• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN

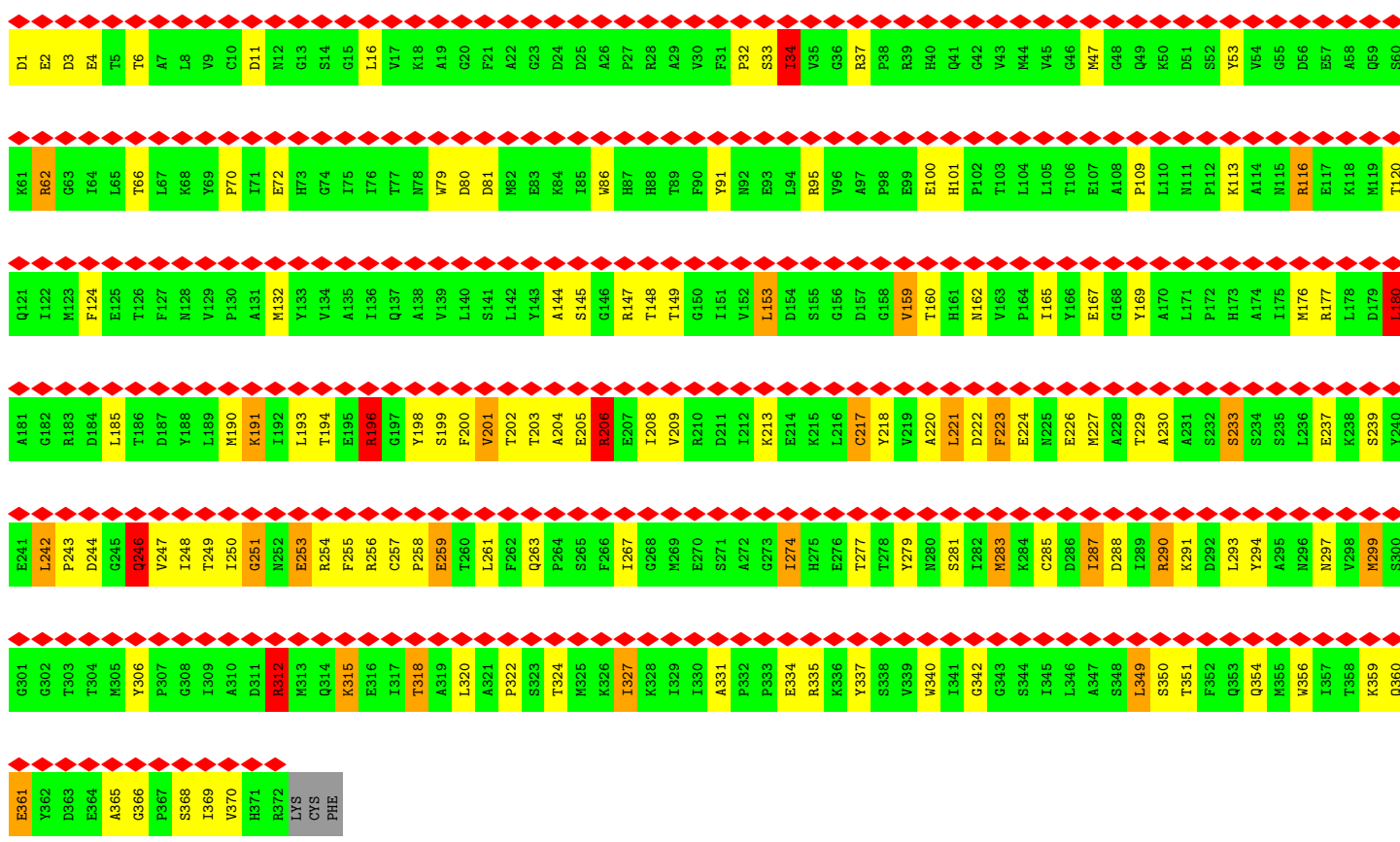


• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN

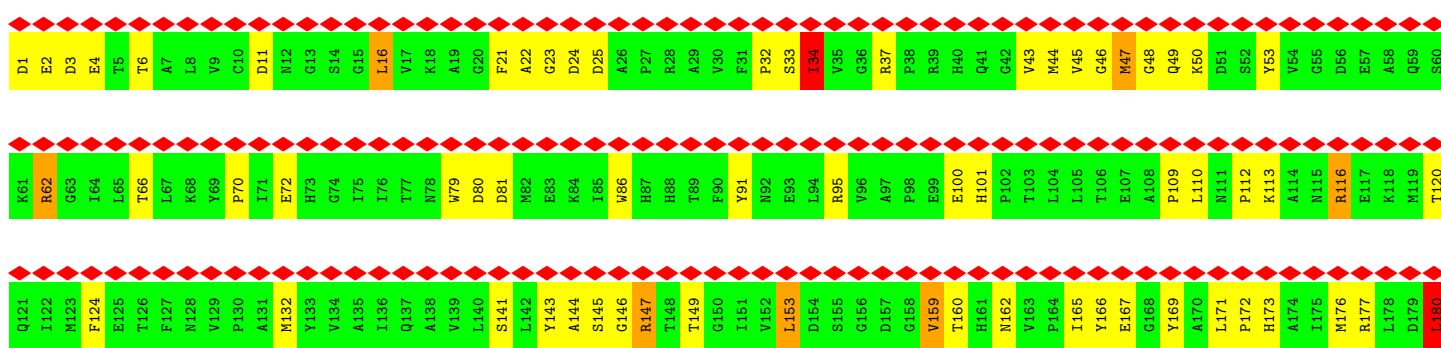


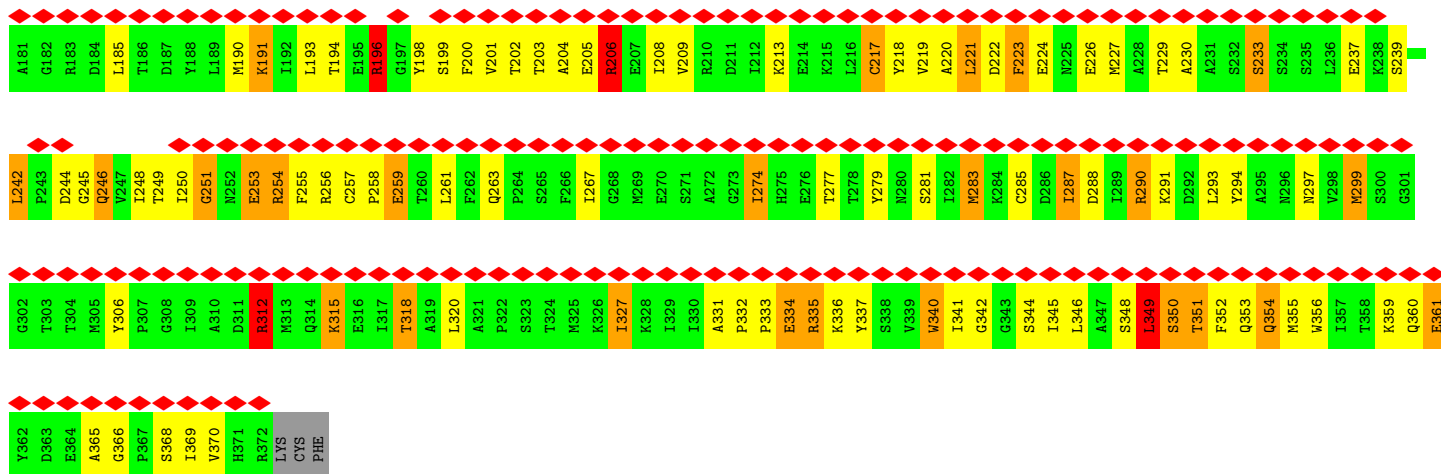


• Molecule 4: SKELETAL MUSCLE ACTIN

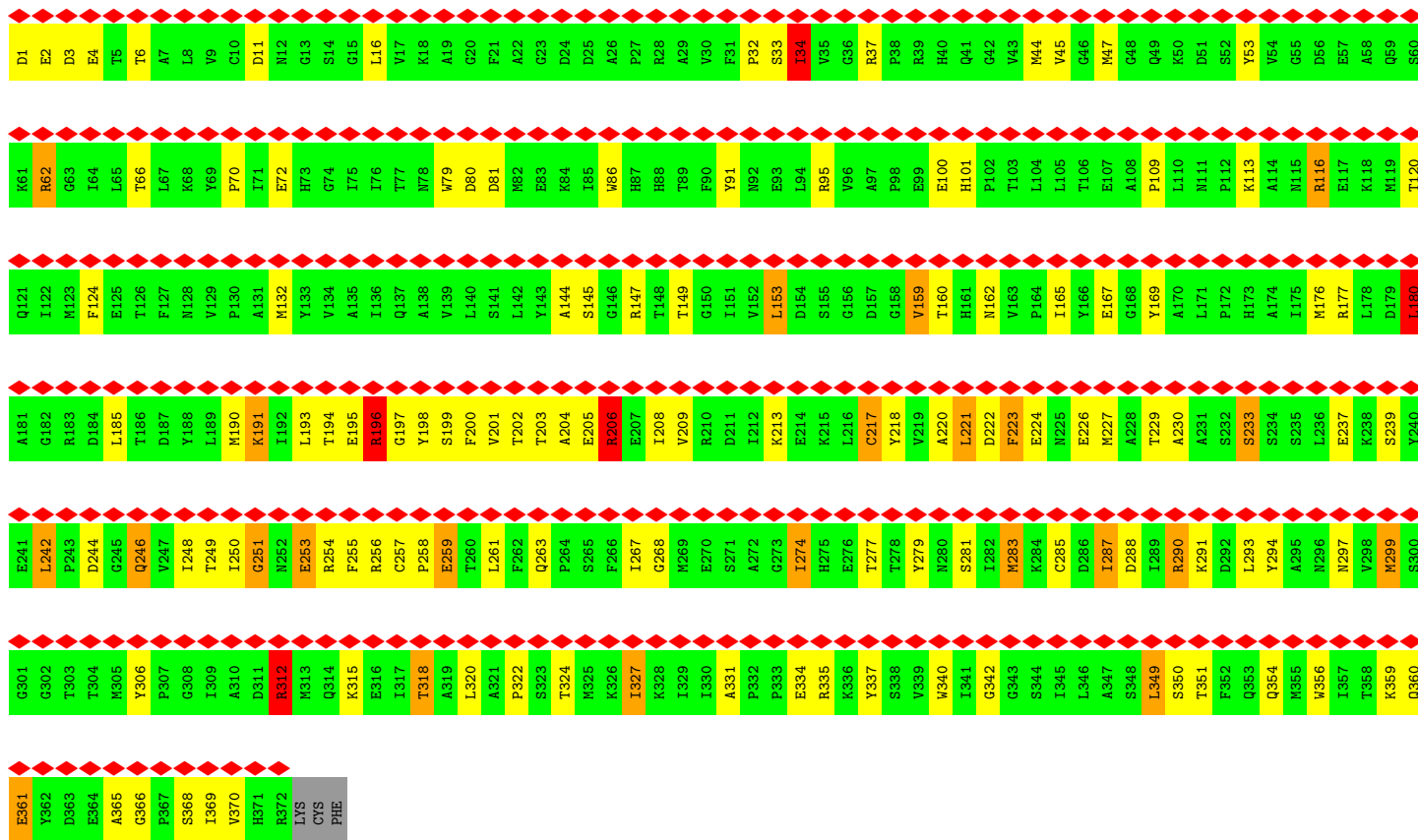


• Molecule 4: SKELETAL MUSCLE ACTIN

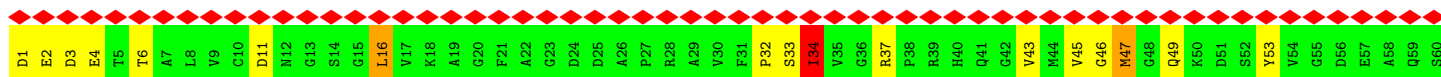


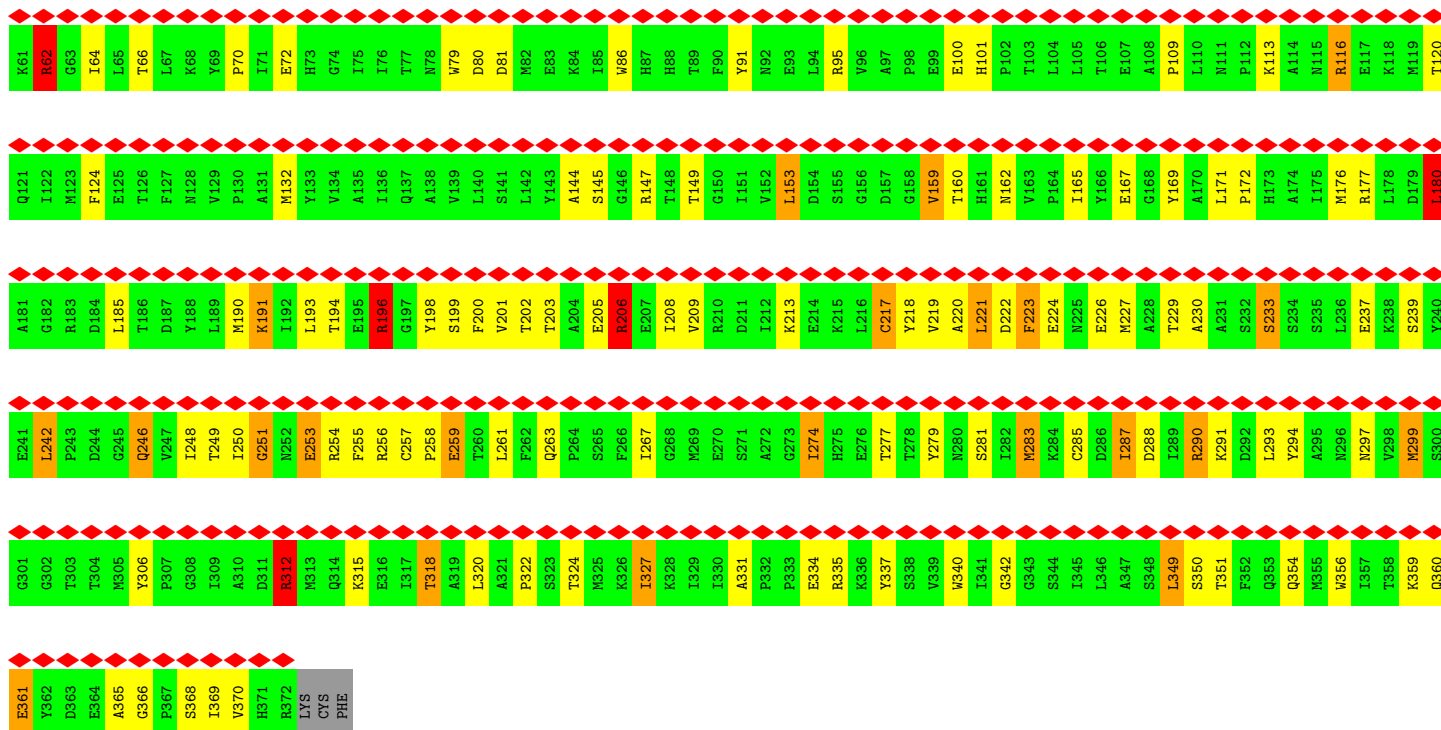


• Molecule 4: SKELETAL MUSCLE ACTIN

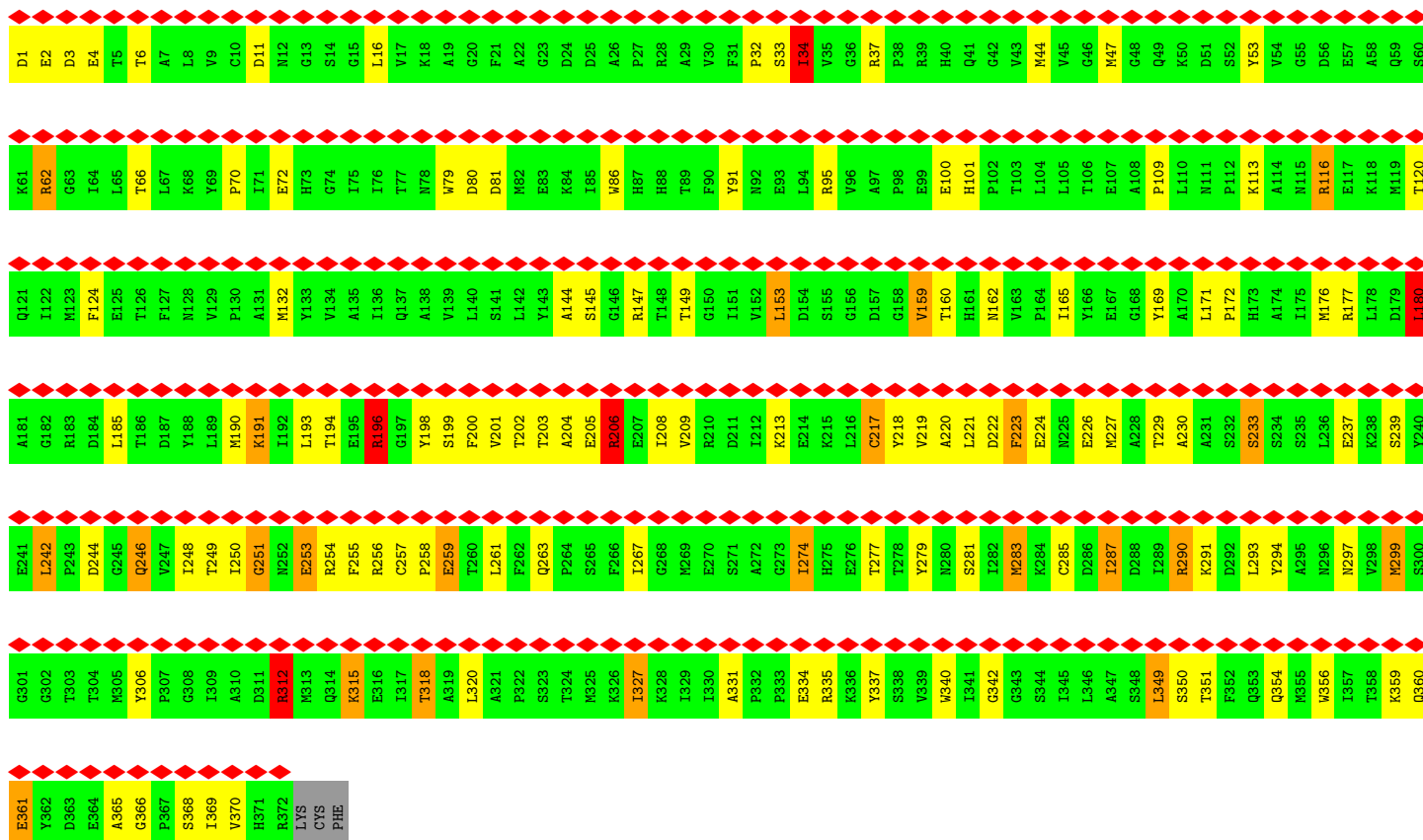


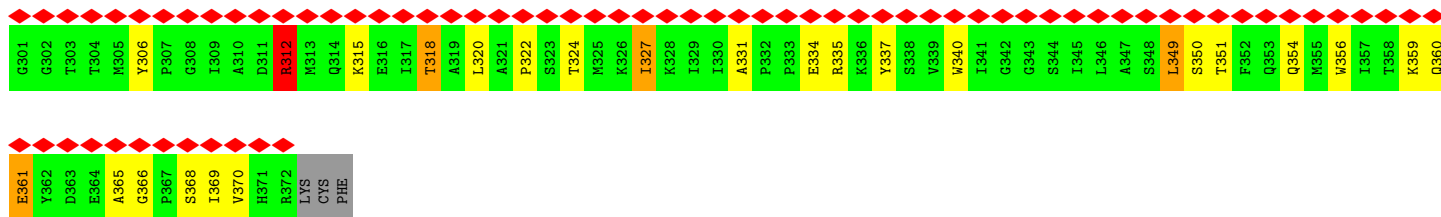
• Molecule 4: SKELETAL MUSCLE ACTIN



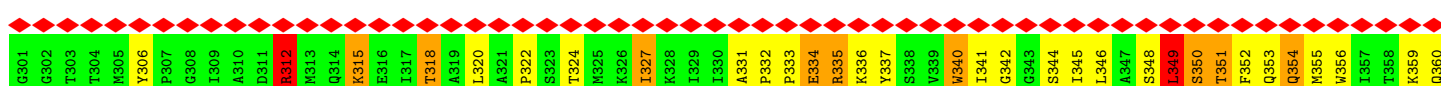
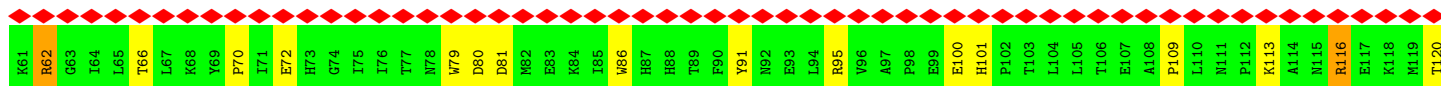
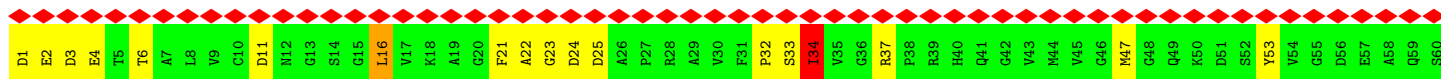


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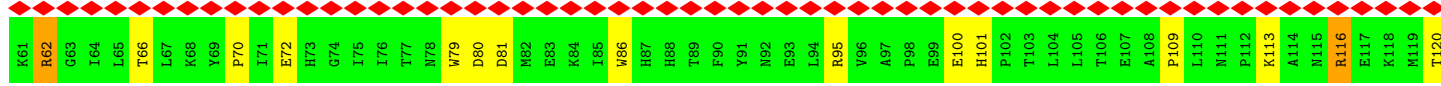
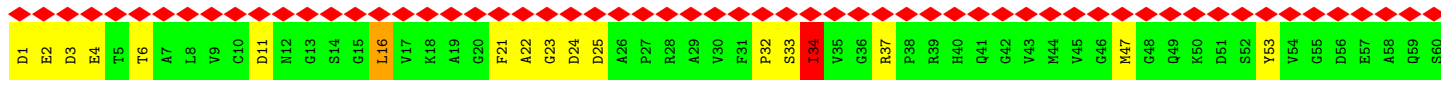




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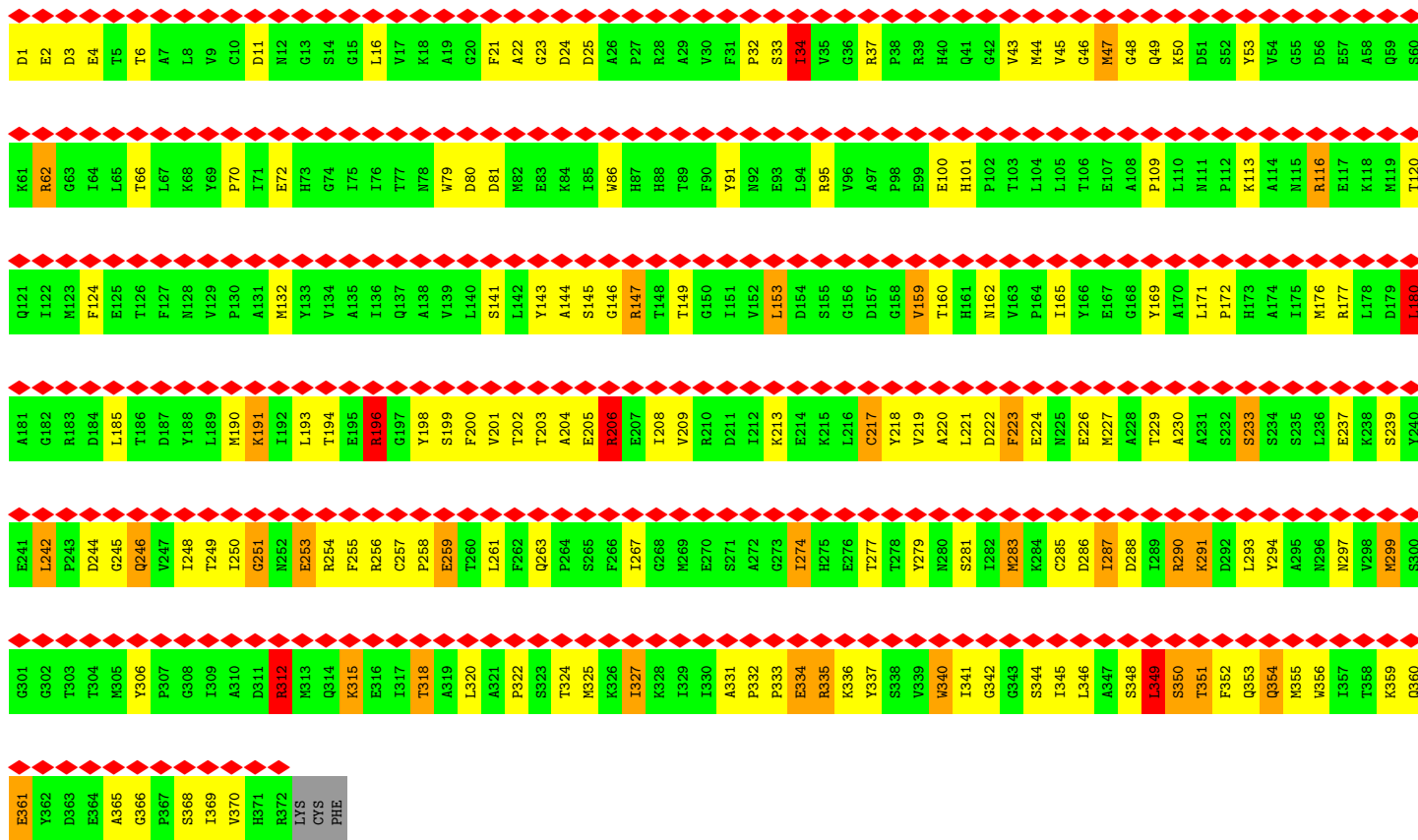


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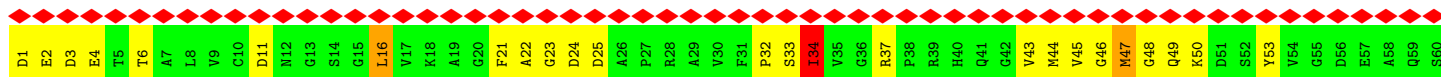


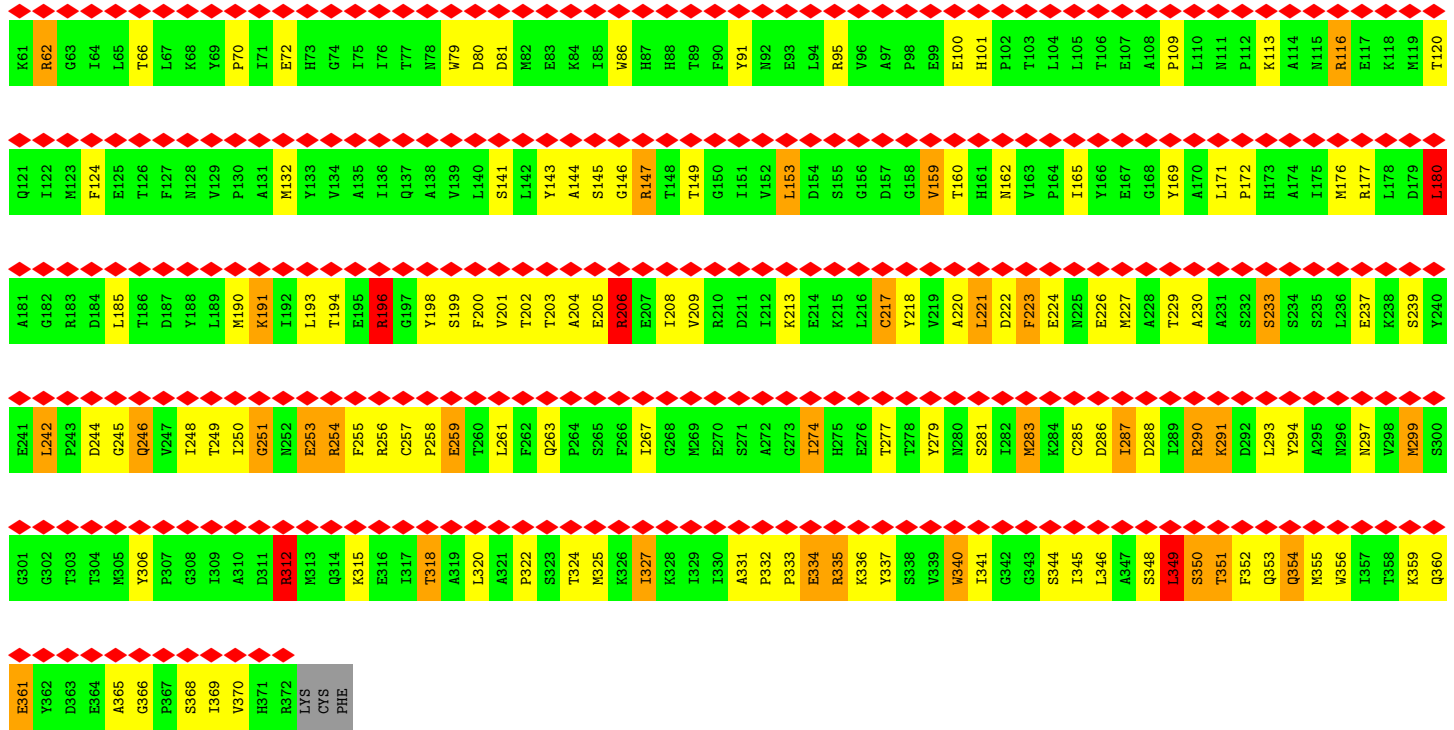


• Molecule 4: SKELETAL MUSCLE ACTIN

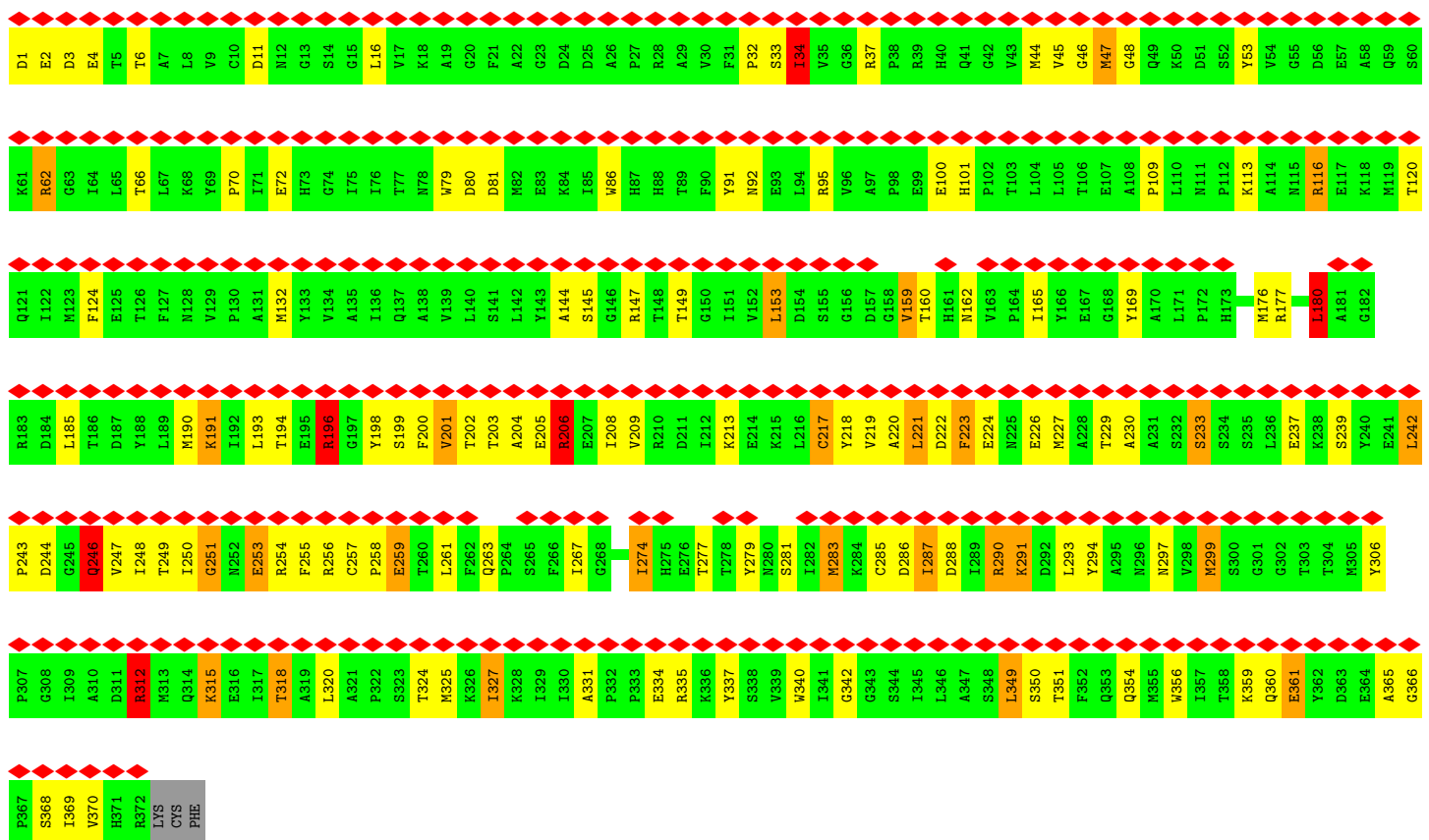
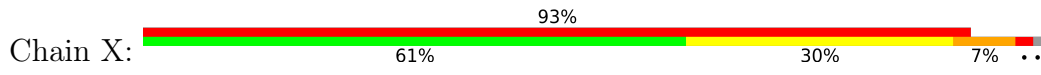


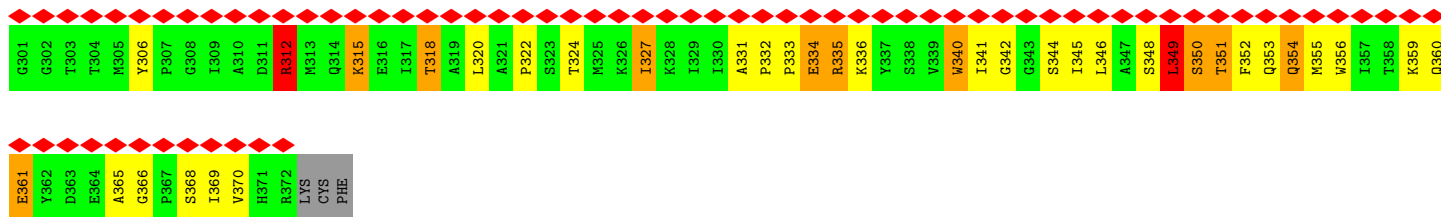
• Molecule 4: SKELETAL MUSCLE ACTIN





● 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 (\AA)	9280, 9280, 464	wwPDB
Tomogram dimensions	600, 600, 30	wwPDB
Tomogram angles ($^\circ$)	90, 90, 90	wwPDB
Grid spacing (\AA)	15.4667, 15.4667, 15.4667	Depositor

5 Model quality i

5.1 Standard geometry i

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	1.77	68/6448 (1.1%)	1.82	116/8729 (1.3%)
1	D	1.77	66/6448 (1.0%)	1.82	115/8729 (1.3%)
1	G	1.77	67/6449 (1.0%)	1.82	118/8732 (1.4%)
1	J	1.79	68/6449 (1.1%)	1.87	118/8732 (1.4%)
1	M	1.77	66/6447 (1.0%)	1.83	119/8726 (1.4%)
1	S	1.78	69/6446 (1.1%)	1.85	119/8723 (1.4%)
2	B	1.22	10/1148 (0.9%)	1.61	16/1548 (1.0%)
2	E	1.21	10/1148 (0.9%)	1.62	16/1548 (1.0%)
2	H	1.22	10/1148 (0.9%)	1.62	16/1548 (1.0%)
2	K	1.22	10/1148 (0.9%)	1.61	16/1548 (1.0%)
2	N	1.22	10/1148 (0.9%)	1.61	16/1548 (1.0%)
2	T	1.22	10/1148 (0.9%)	1.61	16/1548 (1.0%)
3	C	0.80	0/1136	0.95	4/1525 (0.3%)
3	F	0.80	0/1136	0.95	4/1525 (0.3%)
3	I	0.80	0/1136	0.95	4/1525 (0.3%)
3	L	0.79	0/1136	0.95	4/1525 (0.3%)
3	O	0.79	0/1136	0.95	4/1525 (0.3%)
3	U	0.80	0/1136	0.95	4/1525 (0.3%)
4	1	0.89	2/2968 (0.1%)	1.64	51/4023 (1.3%)
4	2	0.89	2/2968 (0.1%)	1.64	52/4023 (1.3%)
4	3	0.89	2/2968 (0.1%)	1.64	52/4023 (1.3%)
4	4	0.89	2/2968 (0.1%)	1.64	50/4023 (1.2%)
4	5	0.89	2/2968 (0.1%)	1.64	51/4023 (1.3%)
4	6	0.89	1/2968 (0.0%)	1.64	52/4023 (1.3%)
4	7	0.89	2/2968 (0.1%)	1.64	51/4023 (1.3%)
4	8	0.89	2/2968 (0.1%)	1.64	52/4023 (1.3%)
4	9	0.89	2/2968 (0.1%)	1.64	50/4023 (1.2%)
4	V	0.89	2/2968 (0.1%)	1.64	51/4023 (1.3%)
4	W	0.89	2/2968 (0.1%)	1.64	51/4023 (1.3%)
4	X	0.89	1/2968 (0.0%)	1.64	52/4023 (1.3%)
4	Y	0.89	2/2968 (0.1%)	1.64	52/4023 (1.3%)
4	Z	0.89	2/2968 (0.1%)	1.64	50/4023 (1.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	1.34	490/93943 (0.5%)	1.68	1542/127131 (1.2%)

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 490 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	649	VAL	CB-CG1	53.33	2.64	1.52
1	S	649	VAL	CB-CG1	53.30	2.64	1.52
1	M	649	VAL	CB-CG1	53.28	2.64	1.52
1	G	649	VAL	CB-CG1	53.26	2.64	1.52
1	D	649	VAL	CB-CG1	53.22	2.64	1.52

The worst 5 of 1542 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	637	LYS	O-C-N	-58.53	23.70	123.20
1	D	637	LYS	O-C-N	-58.47	23.79	123.20
1	M	637	LYS	O-C-N	-58.47	23.80	123.20
1	S	637	LYS	O-C-N	-58.47	23.80	123.20
1	J	637	LYS	O-C-N	-58.47	23.81	123.20

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	6755	1473	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	6797	0	6759	1500	0
1	G	6797	0	6762	1471	0
1	J	6797	0	6761	1483	0
1	M	6797	0	6766	1434	0
1	S	6797	0	6764	1607	0
2	B	1127	0	1085	237	0
2	E	1127	0	1088	272	0
2	H	1127	0	1087	258	0
2	K	1127	0	1088	282	0
2	N	1127	0	1088	252	0
2	T	1127	0	1089	262	0
3	C	1123	0	1083	191	0
3	F	1123	0	1084	187	0
3	I	1123	0	1082	184	0
3	L	1123	0	1083	163	0
3	O	1123	0	1084	164	0
3	U	1123	0	1084	292	0
4	1	2906	0	2862	156	0
4	2	2906	0	2853	428	0
4	3	2906	0	2865	219	0
4	4	2906	0	2862	199	0
4	5	2906	0	2866	124	0
4	6	2906	0	2866	117	0
4	7	2906	0	2866	77	0
4	8	2906	0	2857	321	0
4	9	2906	0	2855	339	0
4	V	2906	0	2851	383	0
4	W	2906	0	2851	388	0
4	X	2906	0	2862	210	0
4	Y	2906	0	2861	167	0
4	Z	2906	0	2854	390	0
All	All	94966	0	93623	11394	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 61.

The worst 5 of 11394 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%)	4	26
1	D	789/840 (94%)	651 (82%)	112 (14%)	26 (3%)	4	26
1	G	791/840 (94%)	652 (82%)	112 (14%)	27 (3%)	3	26
1	J	791/840 (94%)	652 (82%)	112 (14%)	27 (3%)	3	26
1	M	787/840 (94%)	649 (82%)	112 (14%)	26 (3%)	4	26
1	S	785/840 (94%)	648 (82%)	110 (14%)	27 (3%)	3	26
2	B	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	2	19
2	E	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	2	19
2	H	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	2	19
2	K	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	2	19
2	N	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	2	19
2	T	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	2	19
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%)	9	44
4	2	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	9	44
4	3	370/375 (99%)	333 (90%)	31 (8%)	6 (2%)	9	44
4	4	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	9	44
4	5	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	9	44
4	6	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	9	44
4	7	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	9	44
4	8	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	9	44
4	9	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	9	44
4	V	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	9	44
4	W	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	9	44
4	X	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	9	44
4	Y	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	9	44
4	Z	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	9	44
All	All	11628/12042 (97%)	10139 (87%)	1198 (10%)	291 (2%)	9	32

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 [i](#)

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%)	512 (76%)	160 (24%)	0	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	672/672 (100%)	513 (76%)	159 (24%)	1	4
1	G	672/672 (100%)	513 (76%)	159 (24%)	1	4
1	J	672/672 (100%)	515 (77%)	157 (23%)	1	4
1	M	672/672 (100%)	514 (76%)	158 (24%)	1	4
1	S	672/672 (100%)	515 (77%)	157 (23%)	1	4
2	B	120/120 (100%)	119 (99%)	1 (1%)	81	89
2	E	120/120 (100%)	119 (99%)	1 (1%)	81	89
2	H	120/120 (100%)	119 (99%)	1 (1%)	81	89
2	K	120/120 (100%)	119 (99%)	1 (1%)	81	89
2	N	120/120 (100%)	119 (99%)	1 (1%)	81	89
2	T	120/120 (100%)	119 (99%)	1 (1%)	81	89
3	C	117/117 (100%)	112 (96%)	5 (4%)	29	53
3	F	117/117 (100%)	112 (96%)	5 (4%)	29	53
3	I	117/117 (100%)	112 (96%)	5 (4%)	29	53
3	L	117/117 (100%)	112 (96%)	5 (4%)	29	53
3	O	117/117 (100%)	112 (96%)	5 (4%)	29	53
3	U	117/117 (100%)	112 (96%)	5 (4%)	29	53
4	1	315/318 (99%)	269 (85%)	46 (15%)	3	15
4	2	315/318 (99%)	268 (85%)	47 (15%)	3	15
4	3	315/318 (99%)	269 (85%)	46 (15%)	3	15
4	4	315/318 (99%)	268 (85%)	47 (15%)	3	15
4	5	315/318 (99%)	269 (85%)	46 (15%)	3	15
4	6	315/318 (99%)	269 (85%)	46 (15%)	3	15
4	7	315/318 (99%)	268 (85%)	47 (15%)	3	15
4	8	315/318 (99%)	268 (85%)	47 (15%)	3	15
4	9	315/318 (99%)	268 (85%)	47 (15%)	3	15
4	V	315/318 (99%)	269 (85%)	46 (15%)	3	15
4	W	315/318 (99%)	268 (85%)	47 (15%)	3	15
4	X	315/318 (99%)	269 (85%)	46 (15%)	3	15
4	Y	315/318 (99%)	269 (85%)	46 (15%)	3	15
4	Z	315/318 (99%)	268 (85%)	47 (15%)	3	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9864/9906 (100%)	8227 (83%)	1637 (17%)	5 12

5 of 1637 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	S	561	LYS
4	4	229	THR
4	Z	116	ARG
1	S	714	ARG
1	S	549	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 236 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	221	GLN
4	X	137	GLN
1	S	424	ASN
4	X	41	GLN
4	8	41	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	MLY	A	107	1	9,10,11	0.47	0	6,11,13	0.33	0
1	MLY	S	272	1	9,10,11	0.99	1 (11%)	6,11,13	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	A	617	1	9,10,11	0.96	1 (11%)	6,11,13	0.34	0
1	MLY	A	486	1	9,10,11	0.65	0	6,11,13	0.38	0
1	MLY	M	827	1	9,10,11	0.73	0	6,11,13	0.48	0
1	MLY	A	659	1	9,10,11	0.84	0	6,11,13	0.59	0
1	MLY	G	436	1	9,10,11	1.04	1 (11%)	6,11,13	0.48	0
1	MLY	D	505	1	9,10,11	0.86	1 (11%)	6,11,13	0.35	0
1	MLY	M	19	1	9,10,11	1.16	1 (11%)	6,11,13	0.57	0
1	MLY	S	833	1	9,10,11	1.18	1 (11%)	6,11,13	0.31	0
1	MLY	A	553	1,4	9,10,11	0.68	0	6,11,13	0.55	0
1	MLY	D	431	1	9,10,11	0.53	0	6,11,13	0.45	0
1	MLY	D	598	1	9,10,11	0.91	1 (11%)	6,11,13	0.43	0
1	MLY	J	369	1	9,10,11	0.69	0	6,11,13	0.46	0
1	MLY	G	236	1	9,10,11	0.79	1 (11%)	6,11,13	0.48	0
1	MLY	M	768	1	9,10,11	0.76	0	6,11,13	0.42	0
1	MLY	S	839	1	9,10,11	0.69	0	6,11,13	0.77	0
1	MLY	S	369	1	9,10,11	0.70	0	6,11,13	0.46	0
1	MLY	A	837	1	9,10,11	0.60	0	6,11,13	0.54	0
1	MLY	D	63	1	9,10,11	0.91	0	6,11,13	0.46	0
1	MLY	D	837	1	9,10,11	0.61	0	6,11,13	0.57	0
1	MLY	G	30	1	9,10,11	0.88	0	6,11,13	0.30	0
1	MLY	G	190	1	9,10,11	1.26	1 (11%)	6,11,13	0.51	0
1	MLY	M	55	1	9,10,11	0.73	0	6,11,13	0.78	0
1	MLY	S	19	1	9,10,11	1.17	1 (11%)	6,11,13	0.57	0
1	MLY	J	833	1	9,10,11	1.19	1 (11%)	6,11,13	0.31	0
1	MLY	A	19	1	9,10,11	1.12	1 (11%)	6,11,13	0.58	0
1	MLY	J	49	1	9,10,11	1.08	1 (11%)	6,11,13	0.74	0
1	MLY	M	190	1	9,10,11	1.24	1 (11%)	6,11,13	0.53	0
1	MLY	S	431	1	9,10,11	0.51	0	6,11,13	0.44	0
1	MLY	M	236	1	9,10,11	0.80	1 (11%)	6,11,13	0.47	0
1	MLY	M	30	1	9,10,11	0.89	0	6,11,13	0.32	0
1	MLY	A	248	1	9,10,11	0.83	0	6,11,13	0.61	0
1	MLY	G	839	1	9,10,11	0.71	0	6,11,13	0.80	0
1	MLY	J	617	1	9,10,11	0.96	1 (11%)	6,11,13	0.33	0
1	MLY	J	107	1	9,10,11	0.49	0	6,11,13	0.34	0
1	MLY	D	87	1	9,10,11	1.15	1 (11%)	6,11,13	0.45	0
1	MLY	D	528	1	9,10,11	0.91	0	6,11,13	0.64	0
1	MLY	D	138	1	9,10,11	1.39	1 (11%)	6,11,13	0.86	0
1	MLY	G	681	1	9,10,11	0.62	0	6,11,13	0.45	0
1	MLY	J	659	1	9,10,11	0.82	0	6,11,13	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	M	782	1	9,10,11	0.78	0	6,11,13	0.36	0
1	MLY	A	764	1	9,10,11	0.84	0	6,11,13	0.36	0
1	MLY	S	107	1	9,10,11	0.48	0	6,11,13	0.35	0
1	MLY	S	436	1	9,10,11	1.04	1 (11%)	6,11,13	0.49	0
1	MLY	D	272	1	9,10,11	0.95	1 (11%)	6,11,13	0.58	0
1	MLY	S	768	1	9,10,11	0.75	0	6,11,13	0.42	0
1	MLY	J	598	1	9,10,11	0.88	1 (11%)	6,11,13	0.43	0
1	MLY	G	369	1	9,10,11	0.70	0	6,11,13	0.46	0
1	MLY	G	84	1	9,10,11	0.49	0	6,11,13	0.80	0
1	MLY	G	504	1	9,10,11	0.88	0	6,11,13	0.22	0
1	MLY	D	613	1	9,10,11	0.58	0	6,11,13	0.63	0
1	MLY	J	84	1	9,10,11	0.49	0	6,11,13	0.80	0
1	MLY	J	63	1	9,10,11	0.89	0	6,11,13	0.43	0
1	MLY	M	505	1	9,10,11	0.93	1 (11%)	6,11,13	0.33	0
1	MLY	G	55	1	9,10,11	0.73	0	6,11,13	0.79	0
1	MLY	S	190	1	9,10,11	1.25	1 (11%)	6,11,13	0.52	0
1	MLY	D	59	1	9,10,11	0.86	0	6,11,13	0.49	0
1	MLY	M	613	1	9,10,11	0.56	0	6,11,13	0.64	0
1	MLY	S	63	1	9,10,11	0.88	0	6,11,13	0.43	0
1	MLY	G	833	1	9,10,11	1.17	2 (22%)	6,11,13	0.33	0
1	MLY	M	84	1	9,10,11	0.50	0	6,11,13	0.80	0
1	MLY	M	600	1	9,10,11	0.53	0	6,11,13	0.37	0
1	MLY	J	295	1	9,10,11	0.78	0	6,11,13	0.35	0
1	MLY	S	367	1	9,10,11	0.63	0	6,11,13	0.38	0
1	MLY	A	190	1	9,10,11	1.26	1 (11%)	6,11,13	0.51	0
1	MLY	J	248	1	9,10,11	0.84	0	6,11,13	0.62	0
1	MLY	M	431	1	9,10,11	0.53	0	6,11,13	0.44	0
1	MLY	G	138	1	9,10,11	1.35	1 (11%)	6,11,13	0.84	0
1	MLY	S	528	1	9,10,11	0.89	0	6,11,13	0.66	0
1	MLY	S	681	1	9,10,11	0.63	0	6,11,13	0.46	0
1	MLY	G	87	1	9,10,11	1.22	1 (11%)	6,11,13	0.43	0
1	MLY	S	55	1	9,10,11	0.73	0	6,11,13	0.77	0
1	MLY	J	505	1	9,10,11	0.93	1 (11%)	6,11,13	0.34	0
1	MLY	M	107	1	9,10,11	0.48	0	6,11,13	0.34	0
1	MLY	J	35	1	9,10,11	0.72	0	6,11,13	0.38	0
1	MLY	M	617	1	9,10,11	0.97	1 (11%)	6,11,13	0.33	0
1	MLY	A	296	1	9,10,11	0.62	0	6,11,13	0.36	0
1	MLY	A	385	1	9,10,11	0.99	1 (11%)	6,11,13	0.43	0
1	MLY	D	35	1	9,10,11	0.73	0	6,11,13	0.37	0
1	MLY	D	107	1	9,10,11	0.51	0	6,11,13	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	M	486	1	9,10,11	0.64	0	6,11,13	0.40	0
1	MLY	D	617	1	9,10,11	0.96	1 (11%)	6,11,13	0.34	0
1	MLY	J	59	1	9,10,11	0.87	0	6,11,13	0.49	0
1	MLY	G	837	1	9,10,11	0.59	0	6,11,13	0.53	0
1	MLY	M	553	1,4	9,10,11	0.68	0	6,11,13	0.53	0
1	MLY	M	436	1	9,10,11	1.07	1 (11%)	6,11,13	0.50	0
1	MLY	D	553	1,4	9,10,11	0.68	0	6,11,13	0.55	0
1	MLY	S	49	1	9,10,11	1.11	1 (11%)	6,11,13	0.74	0
1	MLY	A	87	1	9,10,11	1.20	1 (11%)	6,11,13	0.42	0
1	MLY	A	504	1	9,10,11	0.90	0	6,11,13	0.24	0
1	MLY	D	504	1	9,10,11	0.88	0	6,11,13	0.21	0
1	MLY	M	369	1	9,10,11	0.70	0	6,11,13	0.45	0
1	MLY	D	839	1	9,10,11	0.67	0	6,11,13	0.79	0
1	MLY	D	369	1	9,10,11	0.69	0	6,11,13	0.44	0
1	MLY	G	295	1	9,10,11	0.78	0	6,11,13	0.33	0
1	MLY	A	600	1	9,10,11	0.50	0	6,11,13	0.37	0
1	MLY	G	248	1	9,10,11	0.81	0	6,11,13	0.63	0
1	MLY	A	138	1	9,10,11	1.33	1 (11%)	6,11,13	0.84	0
1	MLY	S	617	1	9,10,11	0.98	1 (11%)	6,11,13	0.34	0
1	MLY	A	367	1	9,10,11	0.63	0	6,11,13	0.36	0
1	MLY	M	272	1	9,10,11	1.02	1 (11%)	6,11,13	0.56	0
1	MLY	J	431	1	9,10,11	0.53	0	6,11,13	0.45	0
1	MLY	A	436	1	9,10,11	1.04	1 (11%)	6,11,13	0.49	0
1	MLY	G	49	1	9,10,11	1.08	1 (11%)	6,11,13	0.74	0
1	MLY	M	295	1	9,10,11	0.78	0	6,11,13	0.34	0
1	MLY	M	248	1	9,10,11	0.82	0	6,11,13	0.62	0
1	MLY	G	35	1	9,10,11	0.72	0	6,11,13	0.39	0
1	MLY	G	272	1	9,10,11	0.97	1 (11%)	6,11,13	0.54	0
1	MLY	S	764	1	9,10,11	0.83	0	6,11,13	0.38	0
1	MLY	M	87	1	9,10,11	1.20	1 (11%)	6,11,13	0.43	0
1	MLY	A	236	1	9,10,11	0.80	1 (11%)	6,11,13	0.50	0
1	MLY	A	30	1	9,10,11	0.88	0	6,11,13	0.32	0
1	MLY	G	59	1	9,10,11	0.84	0	6,11,13	0.50	0
1	MLY	J	768	1	9,10,11	0.77	0	6,11,13	0.42	0
1	MLY	M	35	1	9,10,11	0.71	0	6,11,13	0.39	0
1	MLY	D	768	1	9,10,11	0.73	0	6,11,13	0.40	0
1	MLY	A	295	1	9,10,11	0.80	0	6,11,13	0.33	0
1	MLY	J	504	1	9,10,11	0.85	0	6,11,13	0.24	0
1	MLY	S	295	1	9,10,11	0.77	0	6,11,13	0.34	0
1	MLY	J	87	1	9,10,11	1.20	1 (11%)	6,11,13	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	S	348	1	9,10,11	0.80	0	6,11,13	0.47	0
1	MLY	S	782	1	9,10,11	0.77	0	6,11,13	0.37	0
1	MLY	S	248	1	9,10,11	0.82	0	6,11,13	0.62	0
1	MLY	A	827	1	9,10,11	0.72	0	6,11,13	0.46	0
1	MLY	A	839	1	9,10,11	0.68	0	6,11,13	0.81	0
1	MLY	M	59	1	9,10,11	0.88	0	6,11,13	0.49	0
1	MLY	D	600	1	9,10,11	0.51	0	6,11,13	0.37	0
1	MLY	S	827	1	9,10,11	0.72	0	6,11,13	0.49	0
1	MLY	A	782	1	9,10,11	0.79	0	6,11,13	0.37	0
1	MLY	D	367	1	9,10,11	0.61	0	6,11,13	0.38	0
1	MLY	G	431	1	9,10,11	0.52	0	6,11,13	0.46	0
1	MLY	M	504	1	9,10,11	0.85	0	6,11,13	0.23	0
1	MLY	J	353	1	9,10,11	0.86	0	6,11,13	0.78	0
1	MLY	G	130	1	9,10,11	0.78	0	6,11,13	0.75	0
1	MLY	S	505	1	9,10,11	0.92	1 (11%)	6,11,13	0.33	0
1	MLY	G	505	1	9,10,11	0.88	1 (11%)	6,11,13	0.35	0
1	MLY	G	782	1	9,10,11	0.77	0	6,11,13	0.35	0
1	MLY	D	353	1	9,10,11	0.85	0	6,11,13	0.79	0
1	MLY	D	295	1	9,10,11	0.78	0	6,11,13	0.36	0
1	MLY	A	369	1	9,10,11	0.71	0	6,11,13	0.46	0
1	MLY	D	248	1	9,10,11	0.86	0	6,11,13	0.62	0
1	MLY	J	415	1	9,10,11	0.77	0	6,11,13	0.18	0
1	MLY	D	681	1	9,10,11	0.59	0	6,11,13	0.45	0
1	MLY	A	59	1	9,10,11	0.87	0	6,11,13	0.49	0
1	MLY	G	617	1	9,10,11	0.95	1 (11%)	6,11,13	0.35	0
1	MLY	D	415	1	9,10,11	0.79	0	6,11,13	0.19	0
1	MLY	S	84	1	9,10,11	0.50	0	6,11,13	0.80	0
1	MLY	S	296	1	9,10,11	0.68	0	6,11,13	0.36	0
1	MLY	A	63	1	9,10,11	0.92	1 (11%)	6,11,13	0.44	0
1	MLY	A	598	1	9,10,11	0.91	1 (11%)	6,11,13	0.44	0
1	MLY	J	486	1	9,10,11	0.63	0	6,11,13	0.40	0
1	MLY	A	551	1	9,10,11	0.52	0	6,11,13	0.19	0
1	MLY	G	659	1	9,10,11	0.85	0	6,11,13	0.59	0
1	MLY	G	553	1,4	9,10,11	0.67	0	6,11,13	0.55	0
1	MLY	M	764	1	9,10,11	0.83	0	6,11,13	0.38	0
1	MLY	S	385	1	9,10,11	1.01	1 (11%)	6,11,13	0.44	0
1	MLY	D	486	1	9,10,11	0.66	0	6,11,13	0.38	0
1	MLY	S	353	1	9,10,11	0.86	0	6,11,13	0.78	0
1	MLY	M	659	1	9,10,11	0.81	0	6,11,13	0.57	0
1	MLY	G	613	1	9,10,11	0.59	0	6,11,13	0.63	0
1	MLY	G	600	1	9,10,11	0.52	0	6,11,13	0.37	0
1	MLY	J	55	1	9,10,11	0.73	0	6,11,13	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	S	504	1	9,10,11	0.85	0	6,11,13	0.23	0
1	MLY	S	600	1	9,10,11	0.53	0	6,11,13	0.37	0
1	MLY	S	837	1	9,10,11	0.58	0	6,11,13	0.54	0
1	MLY	J	837	1	9,10,11	0.59	0	6,11,13	0.56	0
1	MLY	M	367	1	9,10,11	0.62	0	6,11,13	0.36	0
1	MLY	S	486	1	9,10,11	0.63	0	6,11,13	0.40	0
1	MLY	A	348	1	9,10,11	0.82	0	6,11,13	0.48	0
1	MLY	A	681	1	9,10,11	0.59	0	6,11,13	0.46	0
1	MLY	G	353	1	9,10,11	0.86	0	6,11,13	0.80	0
1	MLY	J	528	1	9,10,11	0.88	0	6,11,13	0.65	0
1	MLY	A	833	1	9,10,11	1.15	1 (11%)	6,11,13	0.32	0
1	MLY	J	130	1	9,10,11	0.77	0	6,11,13	0.75	0
1	MLY	D	130	1	9,10,11	0.80	0	6,11,13	0.74	0
1	MLY	G	598	1	9,10,11	0.90	1 (11%)	6,11,13	0.42	0
1	MLY	A	84	1	9,10,11	0.49	0	6,11,13	0.79	0
1	MLY	G	528	1	9,10,11	0.91	0	6,11,13	0.66	0
1	MLY	J	190	1	9,10,11	1.25	1 (11%)	6,11,13	0.53	0
1	MLY	D	436	1	9,10,11	1.09	1 (11%)	6,11,13	0.50	0
1	MLY	J	551	1	9,10,11	0.54	0	6,11,13	0.19	0
1	MLY	G	486	1	9,10,11	0.65	0	6,11,13	0.39	0
1	MLY	J	764	1	9,10,11	0.83	0	6,11,13	0.37	0
1	MLY	S	30	1	9,10,11	0.89	0	6,11,13	0.32	0
1	MLY	A	55	1	9,10,11	0.71	0	6,11,13	0.79	0
1	MLY	D	551	1	9,10,11	0.54	0	6,11,13	0.20	0
1	MLY	S	59	1	9,10,11	0.86	0	6,11,13	0.50	0
1	MLY	S	551	1	9,10,11	0.53	0	6,11,13	0.19	0
1	MLY	M	415	1	9,10,11	0.78	0	6,11,13	0.19	0
1	MLY	D	385	1	9,10,11	0.97	1 (11%)	6,11,13	0.44	0
1	MLY	D	236	1	9,10,11	0.79	1 (11%)	6,11,13	0.48	0
1	MLY	D	659	1	9,10,11	0.84	0	6,11,13	0.60	0
1	MLY	J	839	1	9,10,11	0.68	0	6,11,13	0.77	0
1	MLY	J	348	1	9,10,11	0.82	0	6,11,13	0.47	0
1	MLY	D	190	1	9,10,11	1.21	1 (11%)	6,11,13	0.54	0
1	MLY	J	681	1	9,10,11	0.59	0	6,11,13	0.46	0
1	MLY	J	782	1	9,10,11	0.79	0	6,11,13	0.36	0
1	MLY	A	528	1	9,10,11	0.88	0	6,11,13	0.67	0
1	MLY	A	49	1	9,10,11	1.06	1 (11%)	6,11,13	0.74	0
1	MLY	D	348	1	9,10,11	0.82	0	6,11,13	0.47	0
1	MLY	G	107	1	9,10,11	0.48	0	6,11,13	0.34	0
1	MLY	G	19	1	9,10,11	1.15	1 (11%)	6,11,13	0.58	0
1	MLY	M	839	1	9,10,11	0.71	0	6,11,13	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	D	827	1	9,10,11	0.67	0	6,11,13	0.48	0
1	MLY	A	272	1	9,10,11	1.00	1 (11%)	6,11,13	0.56	0
1	MLY	G	385	1	9,10,11	0.99	1 (11%)	6,11,13	0.44	0
1	MLY	S	415	1	9,10,11	0.77	0	6,11,13	0.18	0
1	MLY	S	598	1	9,10,11	0.89	1 (11%)	6,11,13	0.43	0
1	MLY	D	84	1	9,10,11	0.51	0	6,11,13	0.80	0
1	MLY	G	551	1	9,10,11	0.53	0	6,11,13	0.19	0
1	MLY	S	553	1	9,10,11	0.67	0	6,11,13	0.53	0
1	MLY	G	764	1	9,10,11	0.81	0	6,11,13	0.35	0
1	MLY	M	130	1	9,10,11	0.78	0	6,11,13	0.74	0
1	MLY	D	55	1	9,10,11	0.72	0	6,11,13	0.79	0
1	MLY	G	63	1	9,10,11	0.90	0	6,11,13	0.43	0
1	MLY	M	49	1	9,10,11	1.08	1 (11%)	6,11,13	0.75	0
1	MLY	M	528	1	9,10,11	0.89	0	6,11,13	0.64	0
1	MLY	J	385	1	9,10,11	1.01	1 (11%)	6,11,13	0.44	0
1	MLY	M	598	1	9,10,11	0.91	1 (11%)	6,11,13	0.43	0
1	MLY	J	296	1	9,10,11	0.69	0	6,11,13	0.36	0
1	MLY	D	296	1	9,10,11	0.64	0	6,11,13	0.38	0
1	MLY	M	551	1	9,10,11	0.53	0	6,11,13	0.19	0
1	MLY	J	553	1,4	9,10,11	0.67	0	6,11,13	0.54	0
1	MLY	A	431	1	9,10,11	0.51	0	6,11,13	0.44	0
1	MLY	G	768	1	9,10,11	0.74	0	6,11,13	0.42	0
1	MLY	M	385	1	9,10,11	1.02	1 (11%)	6,11,13	0.44	0
1	MLY	G	348	1	9,10,11	0.87	1 (11%)	6,11,13	0.48	0
1	MLY	D	49	1	9,10,11	1.08	1 (11%)	6,11,13	0.75	0
1	MLY	J	367	1	9,10,11	0.61	0	6,11,13	0.37	0
1	MLY	S	87	1	9,10,11	1.23	1 (11%)	6,11,13	0.43	0
1	MLY	J	827	1	9,10,11	0.75	0	6,11,13	0.48	0
1	MLY	S	138	1	9,10,11	1.33	1 (11%)	6,11,13	0.83	0
1	MLY	G	367	1	9,10,11	0.66	0	6,11,13	0.38	0
1	MLY	J	138	1	9,10,11	1.34	1 (11%)	6,11,13	0.83	0
1	MLY	M	348	1	9,10,11	0.79	0	6,11,13	0.47	0
1	MLY	J	613	1	9,10,11	0.57	0	6,11,13	0.64	0
1	MLY	A	35	1	9,10,11	0.71	0	6,11,13	0.38	0
1	MLY	D	764	1	9,10,11	0.86	0	6,11,13	0.36	0
1	MLY	S	35	1	9,10,11	0.72	0	6,11,13	0.38	0
1	MLY	S	659	1	9,10,11	0.81	0	6,11,13	0.57	0
1	MLY	M	681	1	9,10,11	0.60	0	6,11,13	0.46	0
1	MLY	S	613	1	9,10,11	0.56	0	6,11,13	0.63	0
1	MLY	A	768	1	9,10,11	0.76	0	6,11,13	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	J	436	1	9,10,11	1.05	1 (11%)	6,11,13	0.50	0
1	MLY	S	130	1	9,10,11	0.78	0	6,11,13	0.75	0
1	MLY	D	833	1	9,10,11	1.15	2 (22%)	6,11,13	0.32	0
1	MLY	A	613	1	9,10,11	0.57	0	6,11,13	0.63	0
1	MLY	M	353	1	9,10,11	0.85	0	6,11,13	0.79	0
1	MLY	G	296	1	9,10,11	0.65	0	6,11,13	0.37	0
1	MLY	G	415	1	9,10,11	0.77	0	6,11,13	0.19	0
1	MLY	J	236	1	9,10,11	0.79	1 (11%)	6,11,13	0.47	0
1	MLY	M	837	1	9,10,11	0.59	0	6,11,13	0.56	0
1	MLY	M	63	1	9,10,11	0.91	0	6,11,13	0.43	0
1	MLY	J	30	1	9,10,11	0.89	0	6,11,13	0.32	0
1	MLY	J	19	1	9,10,11	1.18	1 (11%)	6,11,13	0.57	0
1	MLY	S	236	1	9,10,11	0.78	1 (11%)	6,11,13	0.47	0
1	MLY	D	30	1	9,10,11	0.92	0	6,11,13	0.32	0
1	MLY	D	19	1	9,10,11	1.19	1 (11%)	6,11,13	0.56	0
1	MLY	M	833	1	9,10,11	1.17	1 (11%)	6,11,13	0.31	0
1	MLY	A	353	1	9,10,11	0.86	0	6,11,13	0.79	0
1	MLY	J	600	1	9,10,11	0.53	0	6,11,13	0.37	0
1	MLY	M	296	1	9,10,11	0.71	0	6,11,13	0.36	0
1	MLY	A	130	1	9,10,11	0.80	0	6,11,13	0.74	0
1	MLY	D	782	1	9,10,11	0.79	0	6,11,13	0.34	0
1	MLY	G	827	1	9,10,11	0.71	0	6,11,13	0.49	0
1	MLY	A	505	1	9,10,11	0.88	1 (11%)	6,11,13	0.33	0
1	MLY	J	272	1	9,10,11	0.99	1 (11%)	6,11,13	0.56	0
1	MLY	A	415	1	9,10,11	0.76	0	6,11,13	0.19	0
1	MLY	M	138	1	9,10,11	1.34	1 (11%)	6,11,13	0.83	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	A	107	1	-	2/8/9/11	-
1	MLY	S	272	1	-	3/8/9/11	-
1	MLY	A	617	1	-	1/8/9/11	-
1	MLY	A	486	1	-	2/8/9/11	-
1	MLY	M	827	1	-	0/8/9/11	-
1	MLY	A	659	1	-	3/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	G	436	1	-	4/8/9/11	-
1	MLY	D	505	1	-	5/8/9/11	-
1	MLY	M	19	1	-	4/8/9/11	-
1	MLY	S	833	1	-	6/8/9/11	-
1	MLY	A	553	1,4	-	4/8/9/11	-
1	MLY	D	431	1	-	4/8/9/11	-
1	MLY	D	598	1	-	5/8/9/11	-
1	MLY	J	369	1	-	2/8/9/11	-
1	MLY	G	236	1	-	3/8/9/11	-
1	MLY	M	768	1	-	4/8/9/11	-
1	MLY	S	839	1	-	3/8/9/11	-
1	MLY	S	369	1	-	2/8/9/11	-
1	MLY	A	837	1	-	5/8/9/11	-
1	MLY	D	63	1	-	4/8/9/11	-
1	MLY	D	837	1	-	5/8/9/11	-
1	MLY	G	30	1	-	2/8/9/11	-
1	MLY	G	190	1	-	5/8/9/11	-
1	MLY	M	55	1	-	6/8/9/11	-
1	MLY	S	19	1	-	4/8/9/11	-
1	MLY	J	833	1	-	6/8/9/11	-
1	MLY	A	19	1	-	4/8/9/11	-
1	MLY	J	49	1	-	3/8/9/11	-
1	MLY	M	190	1	-	5/8/9/11	-
1	MLY	S	431	1	-	4/8/9/11	-
1	MLY	M	236	1	-	3/8/9/11	-
1	MLY	M	30	1	-	2/8/9/11	-
1	MLY	A	248	1	-	6/8/9/11	-
1	MLY	G	839	1	-	3/8/9/11	-
1	MLY	J	617	1	-	1/8/9/11	-
1	MLY	J	107	1	-	2/8/9/11	-
1	MLY	D	87	1	-	2/8/9/11	-
1	MLY	D	528	1	-	4/8/9/11	-
1	MLY	D	138	1	-	4/8/9/11	-
1	MLY	G	681	1	-	4/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	J	659	1	-	3/8/9/11	-
1	MLY	M	782	1	-	6/8/9/11	-
1	MLY	A	764	1	-	2/8/9/11	-
1	MLY	S	107	1	-	2/8/9/11	-
1	MLY	S	436	1	-	4/8/9/11	-
1	MLY	D	272	1	-	3/8/9/11	-
1	MLY	S	768	1	-	4/8/9/11	-
1	MLY	J	598	1	-	5/8/9/11	-
1	MLY	G	369	1	-	2/8/9/11	-
1	MLY	G	84	1	-	4/8/9/11	-
1	MLY	G	504	1	-	4/8/9/11	-
1	MLY	D	613	1	-	4/8/9/11	-
1	MLY	J	84	1	-	4/8/9/11	-
1	MLY	J	63	1	-	4/8/9/11	-
1	MLY	M	505	1	-	5/8/9/11	-
1	MLY	G	55	1	-	6/8/9/11	-
1	MLY	S	190	1	-	5/8/9/11	-
1	MLY	D	59	1	-	3/8/9/11	-
1	MLY	M	613	1	-	4/8/9/11	-
1	MLY	S	63	1	-	4/8/9/11	-
1	MLY	G	833	1	-	6/8/9/11	-
1	MLY	M	84	1	-	4/8/9/11	-
1	MLY	M	600	1	-	3/8/9/11	-
1	MLY	J	295	1	-	2/8/9/11	-
1	MLY	S	367	1	-	2/8/9/11	-
1	MLY	A	190	1	-	5/8/9/11	-
1	MLY	J	248	1	-	6/8/9/11	-
1	MLY	M	431	1	-	4/8/9/11	-
1	MLY	G	138	1	-	4/8/9/11	-
1	MLY	S	528	1	-	4/8/9/11	-
1	MLY	S	681	1	-	4/8/9/11	-
1	MLY	G	87	1	-	2/8/9/11	-
1	MLY	S	55	1	-	6/8/9/11	-
1	MLY	J	505	1	-	5/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	M	107	1	-	2/8/9/11	-
1	MLY	J	35	1	-	3/8/9/11	-
1	MLY	M	617	1	-	1/8/9/11	-
1	MLY	A	296	1	-	4/8/9/11	-
1	MLY	A	385	1	-	2/8/9/11	-
1	MLY	D	35	1	-	3/8/9/11	-
1	MLY	D	107	1	-	2/8/9/11	-
1	MLY	M	486	1	-	2/8/9/11	-
1	MLY	D	617	1	-	1/8/9/11	-
1	MLY	J	59	1	-	3/8/9/11	-
1	MLY	G	837	1	-	5/8/9/11	-
1	MLY	M	553	1,4	-	4/8/9/11	-
1	MLY	M	436	1	-	4/8/9/11	-
1	MLY	D	553	1,4	-	5/8/9/11	-
1	MLY	S	49	1	-	3/8/9/11	-
1	MLY	A	87	1	-	2/8/9/11	-
1	MLY	A	504	1	-	4/8/9/11	-
1	MLY	D	504	1	-	4/8/9/11	-
1	MLY	M	369	1	-	2/8/9/11	-
1	MLY	D	839	1	-	3/8/9/11	-
1	MLY	D	369	1	-	2/8/9/11	-
1	MLY	G	295	1	-	2/8/9/11	-
1	MLY	A	600	1	-	3/8/9/11	-
1	MLY	G	248	1	-	6/8/9/11	-
1	MLY	A	138	1	-	4/8/9/11	-
1	MLY	S	617	1	-	1/8/9/11	-
1	MLY	A	367	1	-	2/8/9/11	-
1	MLY	M	272	1	-	3/8/9/11	-
1	MLY	J	431	1	-	4/8/9/11	-
1	MLY	A	436	1	-	4/8/9/11	-
1	MLY	G	49	1	-	3/8/9/11	-
1	MLY	M	295	1	-	2/8/9/11	-
1	MLY	M	248	1	-	6/8/9/11	-
1	MLY	G	35	1	-	3/8/9/11	-
1	MLY	G	272	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	M	87	1	-	2/8/9/11	-
1	MLY	A	236	1	-	3/8/9/11	-
1	MLY	A	30	1	-	2/8/9/11	-
1	MLY	G	59	1	-	3/8/9/11	-
1	MLY	J	768	1	-	4/8/9/11	-
1	MLY	M	35	1	-	3/8/9/11	-
1	MLY	D	768	1	-	4/8/9/11	-
1	MLY	A	295	1	-	2/8/9/11	-
1	MLY	J	504	1	-	4/8/9/11	-
1	MLY	S	295	1	-	2/8/9/11	-
1	MLY	J	87	1	-	2/8/9/11	-
1	MLY	S	348	1	-	5/8/9/11	-
1	MLY	S	782	1	-	6/8/9/11	-
1	MLY	S	248	1	-	6/8/9/11	-
1	MLY	A	827	1	-	0/8/9/11	-
1	MLY	A	839	1	-	3/8/9/11	-
1	MLY	M	59	1	-	3/8/9/11	-
1	MLY	D	600	1	-	3/8/9/11	-
1	MLY	S	827	1	-	0/8/9/11	-
1	MLY	A	782	1	-	6/8/9/11	-
1	MLY	D	367	1	-	2/8/9/11	-
1	MLY	G	431	1	-	4/8/9/11	-
1	MLY	M	504	1	-	4/8/9/11	-
1	MLY	J	353	1	-	4/8/9/11	-
1	MLY	G	130	1	-	5/8/9/11	-
1	MLY	S	505	1	-	5/8/9/11	-
1	MLY	G	505	1	-	5/8/9/11	-
1	MLY	G	782	1	-	6/8/9/11	-
1	MLY	D	353	1	-	4/8/9/11	-
1	MLY	D	295	1	-	2/8/9/11	-
1	MLY	A	369	1	-	2/8/9/11	-
1	MLY	D	248	1	-	6/8/9/11	-
1	MLY	J	415	1	-	3/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	D	681	1	-	4/8/9/11	-
1	MLY	A	59	1	-	3/8/9/11	-
1	MLY	G	617	1	-	1/8/9/11	-
1	MLY	D	415	1	-	3/8/9/11	-
1	MLY	S	84	1	-	4/8/9/11	-
1	MLY	S	296	1	-	4/8/9/11	-
1	MLY	A	63	1	-	4/8/9/11	-
1	MLY	A	598	1	-	5/8/9/11	-
1	MLY	J	486	1	-	2/8/9/11	-
1	MLY	A	551	1	-	3/8/9/11	-
1	MLY	G	659	1	-	3/8/9/11	-
1	MLY	G	553	1,4	-	4/8/9/11	-
1	MLY	M	764	1	-	2/8/9/11	-
1	MLY	S	385	1	-	2/8/9/11	-
1	MLY	D	486	1	-	2/8/9/11	-
1	MLY	S	353	1	-	4/8/9/11	-
1	MLY	M	659	1	-	3/8/9/11	-
1	MLY	G	613	1	-	4/8/9/11	-
1	MLY	G	600	1	-	3/8/9/11	-
1	MLY	J	55	1	-	6/8/9/11	-
1	MLY	S	504	1	-	4/8/9/11	-
1	MLY	S	600	1	-	3/8/9/11	-
1	MLY	S	837	1	-	5/8/9/11	-
1	MLY	J	837	1	-	5/8/9/11	-
1	MLY	M	367	1	-	2/8/9/11	-
1	MLY	S	486	1	-	2/8/9/11	-
1	MLY	A	348	1	-	5/8/9/11	-
1	MLY	A	681	1	-	4/8/9/11	-
1	MLY	G	353	1	-	4/8/9/11	-
1	MLY	J	528	1	-	5/8/9/11	-
1	MLY	A	833	1	-	6/8/9/11	-
1	MLY	J	130	1	-	5/8/9/11	-
1	MLY	D	130	1	-	5/8/9/11	-
1	MLY	G	598	1	-	5/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	A	84	1	-	4/8/9/11	-
1	MLY	G	528	1	-	4/8/9/11	-
1	MLY	J	190	1	-	5/8/9/11	-
1	MLY	D	436	1	-	4/8/9/11	-
1	MLY	J	551	1	-	3/8/9/11	-
1	MLY	G	486	1	-	2/8/9/11	-
1	MLY	J	764	1	-	2/8/9/11	-
1	MLY	S	30	1	-	2/8/9/11	-
1	MLY	A	55	1	-	6/8/9/11	-
1	MLY	D	551	1	-	3/8/9/11	-
1	MLY	S	59	1	-	3/8/9/11	-
1	MLY	S	551	1	-	3/8/9/11	-
1	MLY	M	415	1	-	3/8/9/11	-
1	MLY	D	385	1	-	2/8/9/11	-
1	MLY	D	236	1	-	3/8/9/11	-
1	MLY	D	659	1	-	3/8/9/11	-
1	MLY	J	839	1	-	3/8/9/11	-
1	MLY	J	348	1	-	5/8/9/11	-
1	MLY	D	190	1	-	5/8/9/11	-
1	MLY	J	681	1	-	4/8/9/11	-
1	MLY	J	782	1	-	6/8/9/11	-
1	MLY	A	528	1	-	5/8/9/11	-
1	MLY	A	49	1	-	3/8/9/11	-
1	MLY	D	348	1	-	5/8/9/11	-
1	MLY	G	107	1	-	2/8/9/11	-
1	MLY	G	19	1	-	4/8/9/11	-
1	MLY	M	839	1	-	3/8/9/11	-
1	MLY	D	827	1	-	0/8/9/11	-
1	MLY	A	272	1	-	3/8/9/11	-
1	MLY	G	385	1	-	2/8/9/11	-
1	MLY	S	415	1	-	3/8/9/11	-
1	MLY	S	598	1	-	5/8/9/11	-
1	MLY	D	84	1	-	4/8/9/11	-
1	MLY	G	551	1	-	3/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	S	553	1	-	4/8/9/11	-
1	MLY	G	764	1	-	2/8/9/11	-
1	MLY	M	130	1	-	5/8/9/11	-
1	MLY	D	55	1	-	6/8/9/11	-
1	MLY	G	63	1	-	4/8/9/11	-
1	MLY	M	49	1	-	3/8/9/11	-
1	MLY	M	528	1	-	5/8/9/11	-
1	MLY	J	385	1	-	2/8/9/11	-
1	MLY	M	598	1	-	5/8/9/11	-
1	MLY	J	296	1	-	4/8/9/11	-
1	MLY	D	296	1	-	4/8/9/11	-
1	MLY	M	551	1	-	3/8/9/11	-
1	MLY	J	553	1,4	-	4/8/9/11	-
1	MLY	A	431	1	-	4/8/9/11	-
1	MLY	G	768	1	-	4/8/9/11	-
1	MLY	M	385	1	-	2/8/9/11	-
1	MLY	G	348	1	-	5/8/9/11	-
1	MLY	D	49	1	-	3/8/9/11	-
1	MLY	J	367	1	-	2/8/9/11	-
1	MLY	S	87	1	-	2/8/9/11	-
1	MLY	J	827	1	-	0/8/9/11	-
1	MLY	S	138	1	-	4/8/9/11	-
1	MLY	G	367	1	-	2/8/9/11	-
1	MLY	J	138	1	-	4/8/9/11	-
1	MLY	M	348	1	-	5/8/9/11	-
1	MLY	J	613	1	-	4/8/9/11	-
1	MLY	A	35	1	-	3/8/9/11	-
1	MLY	D	764	1	-	2/8/9/11	-
1	MLY	S	35	1	-	3/8/9/11	-
1	MLY	S	659	1	-	3/8/9/11	-
1	MLY	M	681	1	-	4/8/9/11	-
1	MLY	S	613	1	-	4/8/9/11	-
1	MLY	A	768	1	-	4/8/9/11	-
1	MLY	J	436	1	-	4/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	S	130	1	-	5/8/9/11	-
1	MLY	D	833	1	-	6/8/9/11	-
1	MLY	A	613	1	-	4/8/9/11	-
1	MLY	M	353	1	-	4/8/9/11	-
1	MLY	G	296	1	-	4/8/9/11	-
1	MLY	G	415	1	-	3/8/9/11	-
1	MLY	J	236	1	-	3/8/9/11	-
1	MLY	M	837	1	-	5/8/9/11	-
1	MLY	M	63	1	-	4/8/9/11	-
1	MLY	J	30	1	-	2/8/9/11	-
1	MLY	J	19	1	-	4/8/9/11	-
1	MLY	S	236	1	-	3/8/9/11	-
1	MLY	D	30	1	-	2/8/9/11	-
1	MLY	D	19	1	-	4/8/9/11	-
1	MLY	M	833	1	-	6/8/9/11	-
1	MLY	A	353	1	-	4/8/9/11	-
1	MLY	J	600	1	-	3/8/9/11	-
1	MLY	M	296	1	-	4/8/9/11	-
1	MLY	A	130	1	-	5/8/9/11	-
1	MLY	D	782	1	-	6/8/9/11	-
1	MLY	G	827	1	-	0/8/9/11	-
1	MLY	A	505	1	-	5/8/9/11	-
1	MLY	J	272	1	-	3/8/9/11	-
1	MLY	A	415	1	-	3/8/9/11	-
1	MLY	M	138	1	-	4/8/9/11	-

The worst 5 of 82 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	138	MLY	CB-CA	-3.81	1.48	1.53
1	G	138	MLY	CB-CA	-3.70	1.48	1.53
1	J	138	MLY	CB-CA	-3.67	1.48	1.53
1	M	138	MLY	CB-CA	-3.66	1.48	1.53
1	S	138	MLY	CB-CA	-3.62	1.48	1.53

There are no bond angle outliers.

There are no chirality outliers.

5 of 958 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.

186 monomers are involved in 820 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	107	MLY	2	0
1	S	272	MLY	1	0
1	A	617	MLY	1	0
1	A	486	MLY	3	0
1	A	659	MLY	2	0
1	G	436	MLY	2	0
1	A	553	MLY	17	0
1	D	598	MLY	1	0
1	M	768	MLY	1	0
1	S	839	MLY	15	0
1	S	369	MLY	1	0
1	A	837	MLY	1	0
1	D	63	MLY	4	0
1	D	837	MLY	1	0
1	G	30	MLY	1	0
1	G	190	MLY	2	0
1	M	55	MLY	1	0
1	J	49	MLY	4	0
1	M	190	MLY	2	0
1	M	30	MLY	1	0
1	A	248	MLY	2	0
1	G	839	MLY	4	0
1	J	617	MLY	1	0
1	J	107	MLY	3	0
1	D	87	MLY	3	0
1	D	528	MLY	3	0
1	D	138	MLY	1	0
1	J	659	MLY	2	0
1	M	782	MLY	3	0
1	A	764	MLY	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	S	107	MLY	3	0
1	S	436	MLY	2	0
1	D	272	MLY	1	0
1	J	598	MLY	1	0
1	G	369	MLY	1	0
1	G	84	MLY	16	0
1	J	84	MLY	43	0
1	J	63	MLY	4	0
1	M	505	MLY	2	0
1	G	55	MLY	1	0
1	S	190	MLY	2	0
1	D	59	MLY	2	0
1	S	63	MLY	3	0
1	M	84	MLY	23	0
1	M	600	MLY	1	0
1	J	295	MLY	7	0
1	A	190	MLY	2	0
1	J	248	MLY	2	0
1	G	138	MLY	1	0
1	S	528	MLY	3	0
1	G	87	MLY	3	0
1	S	55	MLY	1	0
1	J	505	MLY	9	0
1	M	107	MLY	4	0
1	M	617	MLY	1	0
1	A	296	MLY	3	0
1	D	107	MLY	3	0
1	M	486	MLY	3	0
1	D	617	MLY	1	0
1	J	59	MLY	2	0
1	G	837	MLY	1	0
1	M	553	MLY	17	0
1	M	436	MLY	2	0
1	D	553	MLY	16	0
1	S	49	MLY	3	0
1	A	87	MLY	3	0
1	A	504	MLY	4	0
1	M	369	MLY	1	0
1	D	839	MLY	7	0
1	G	295	MLY	7	0
1	A	600	MLY	1	0
1	G	248	MLY	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	138	MLY	1	0
1	S	617	MLY	1	0
1	M	272	MLY	1	0
1	A	436	MLY	3	0
1	G	49	MLY	3	0
1	M	295	MLY	6	0
1	M	248	MLY	2	0
1	G	272	MLY	1	0
1	S	764	MLY	31	0
1	M	87	MLY	3	0
1	A	30	MLY	1	0
1	G	59	MLY	2	0
1	J	768	MLY	9	0
1	M	35	MLY	13	0
1	D	768	MLY	1	0
1	A	295	MLY	6	0
1	S	295	MLY	6	0
1	J	87	MLY	3	0
1	S	348	MLY	6	0
1	S	782	MLY	1	0
1	S	248	MLY	2	0
1	A	839	MLY	9	0
1	M	59	MLY	2	0
1	D	600	MLY	1	0
1	A	782	MLY	8	0
1	S	505	MLY	8	0
1	G	782	MLY	1	0
1	D	295	MLY	6	0
1	A	369	MLY	1	0
1	D	248	MLY	2	0
1	J	415	MLY	1	0
1	A	59	MLY	2	0
1	G	617	MLY	1	0
1	D	415	MLY	1	0
1	S	84	MLY	14	0
1	S	296	MLY	3	0
1	A	63	MLY	3	0
1	A	598	MLY	1	0
1	J	486	MLY	3	0
1	A	551	MLY	2	0
1	G	659	MLY	2	0
1	G	553	MLY	26	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	M	764	MLY	5	0
1	D	486	MLY	3	0
1	M	659	MLY	2	0
1	G	600	MLY	1	0
1	J	55	MLY	1	0
1	S	600	MLY	1	0
1	S	837	MLY	1	0
1	J	837	MLY	1	0
1	S	486	MLY	3	0
1	A	348	MLY	5	0
1	J	528	MLY	3	0
1	G	598	MLY	1	0
1	G	528	MLY	3	0
1	J	190	MLY	2	0
1	D	436	MLY	3	0
1	G	486	MLY	3	0
1	J	764	MLY	7	0
1	S	30	MLY	1	0
1	A	55	MLY	1	0
1	D	551	MLY	2	0
1	S	59	MLY	2	0
1	M	415	MLY	1	0
1	D	659	MLY	2	0
1	J	839	MLY	15	0
1	J	348	MLY	5	0
1	D	190	MLY	2	0
1	J	782	MLY	1	0
1	A	528	MLY	3	0
1	A	49	MLY	3	0
1	D	348	MLY	6	0
1	G	107	MLY	2	0
1	M	839	MLY	7	0
1	D	827	MLY	3	0
1	A	272	MLY	1	0
1	S	415	MLY	1	0
1	S	598	MLY	1	0
1	S	553	MLY	3	0
1	G	764	MLY	8	0
1	D	55	MLY	1	0
1	G	63	MLY	4	0
1	M	49	MLY	3	0
1	M	528	MLY	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	M	598	MLY	1	0
1	J	296	MLY	3	0
1	D	296	MLY	3	0
1	M	551	MLY	1	0
1	J	553	MLY	27	0
1	G	768	MLY	9	0
1	G	348	MLY	4	0
1	D	49	MLY	3	0
1	S	87	MLY	3	0
1	S	138	MLY	1	0
1	J	138	MLY	1	0
1	M	348	MLY	6	0
1	D	764	MLY	6	0
1	S	659	MLY	2	0
1	A	768	MLY	12	0
1	J	436	MLY	2	0
1	G	296	MLY	2	0
1	G	415	MLY	1	0
1	M	837	MLY	1	0
1	M	63	MLY	4	0
1	J	30	MLY	1	0
1	D	30	MLY	1	0
1	J	600	MLY	1	0
1	M	296	MLY	3	0
1	D	782	MLY	71	0
1	G	827	MLY	1	0
1	A	505	MLY	24	0
1	J	272	MLY	1	0
1	A	415	MLY	1	0
1	M	138	MLY	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides 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

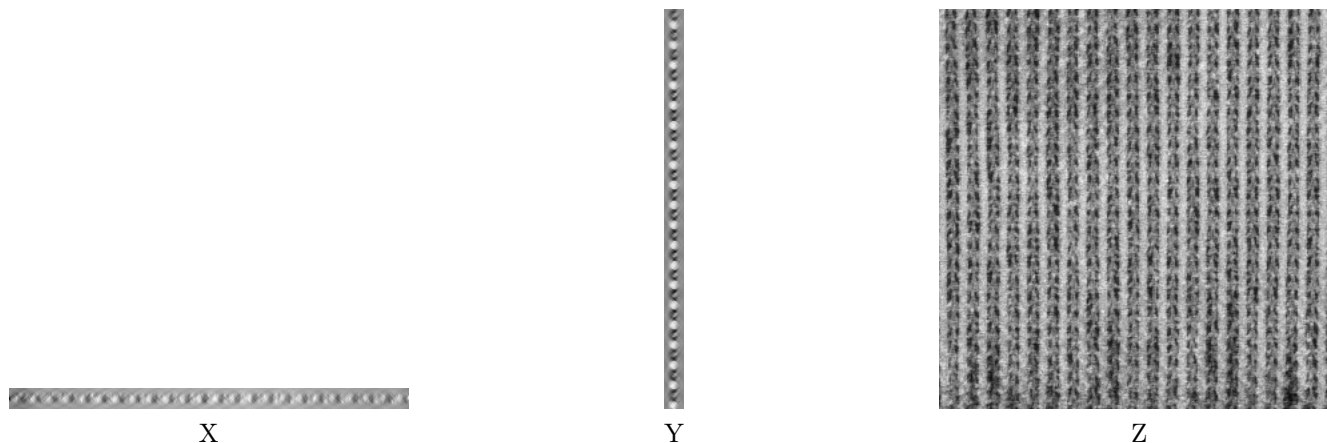
The worst 5 of 40 chain breaks are listed below:

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](#)

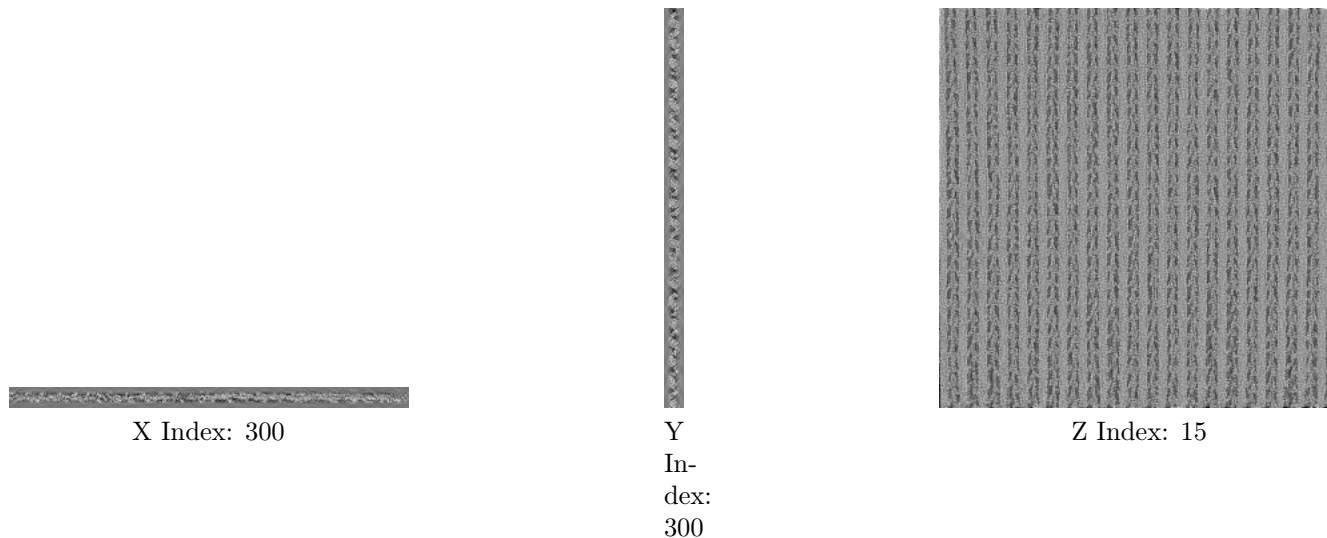
This section contains visualisations of the EMDB entry EMD-1001. These allow visual inspection of the internal detail of the tomogram and identification of artifacts.

6.1 Orthogonal projections [i](#)



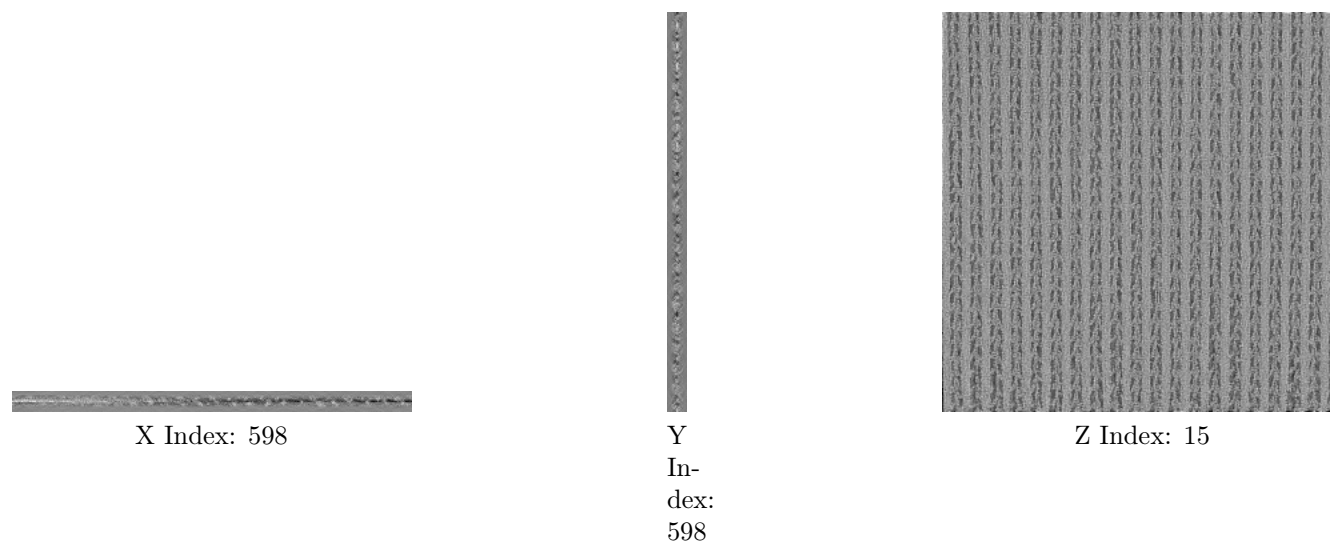
The images above show the tomogram projected in three orthogonal directions.

6.2 Central slices [i](#)



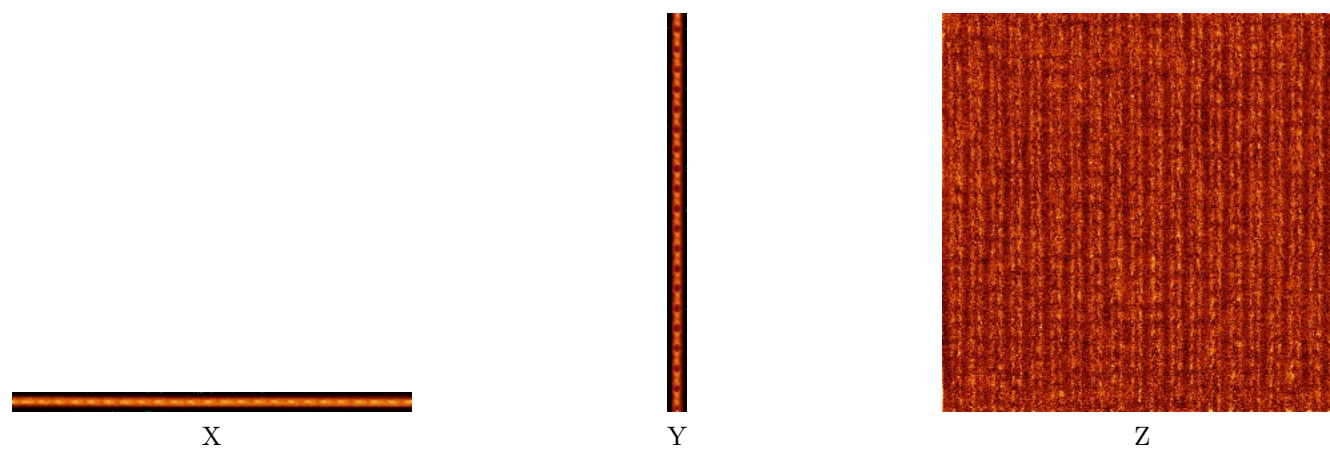
The images above show central slices of the tomogram in three orthogonal directions.

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.

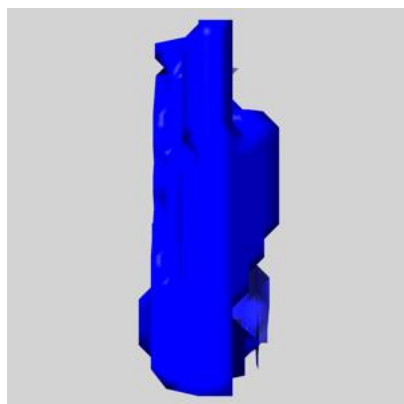
6.5 Mask visualisation [i](#)

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

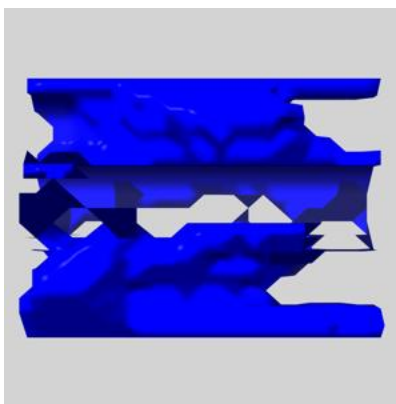
A mask typically either:

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

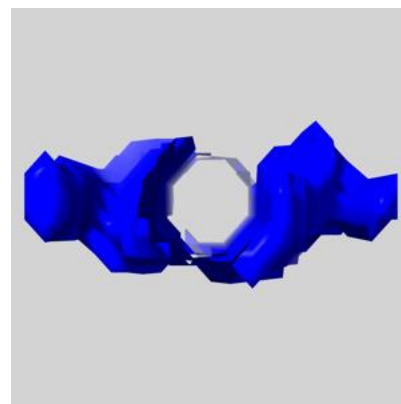
6.5.1 emd_1001_msk_25.map [i](#)



X

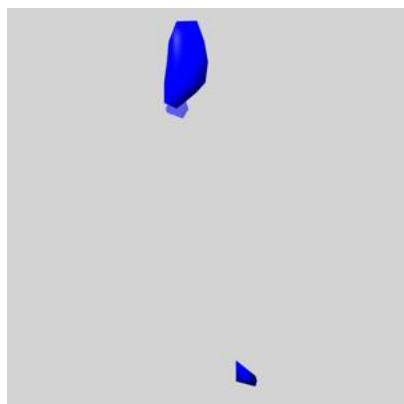


Y

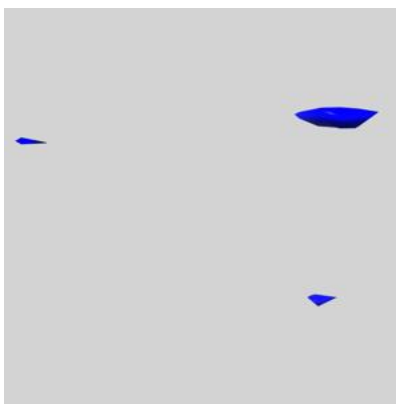


Z

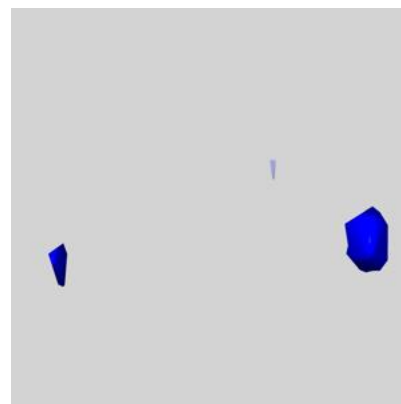
6.5.2 emd_1001_msk_24.map [i](#)



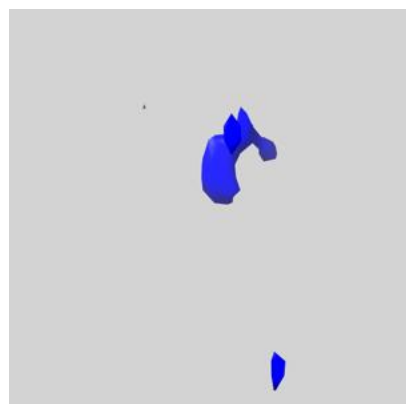
X



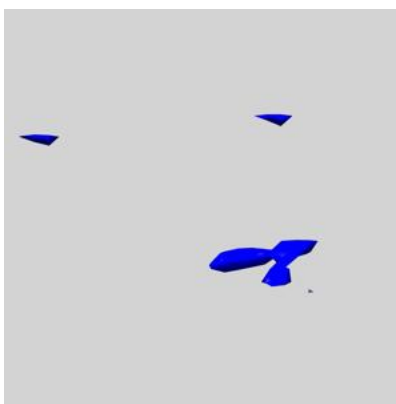
Y



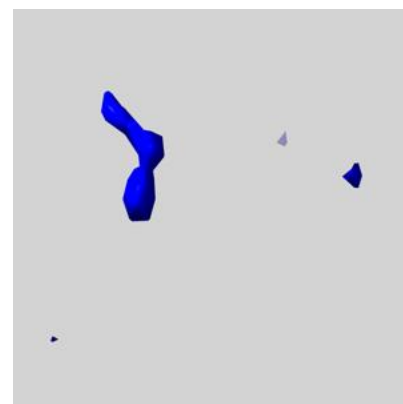
Z

6.5.3 emd_1001_msk_23.map [i](#)

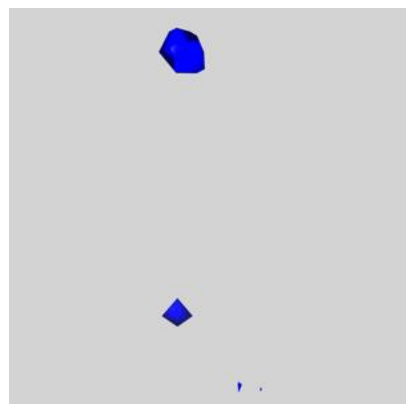
X



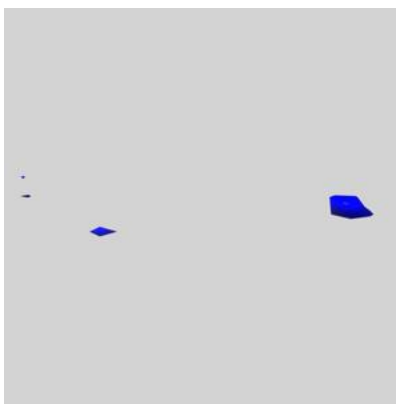
Y



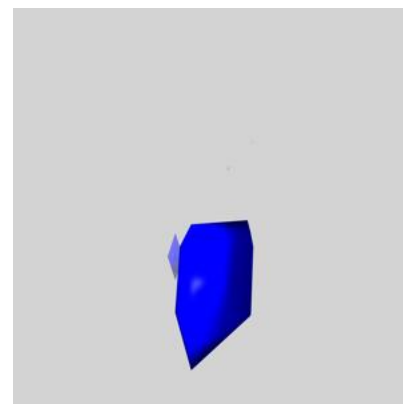
Z

6.5.4 emd_1001_msk_22.map [i](#)

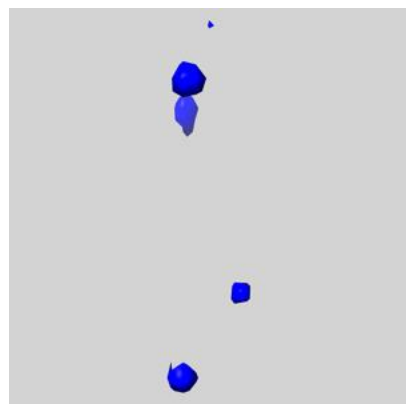
X



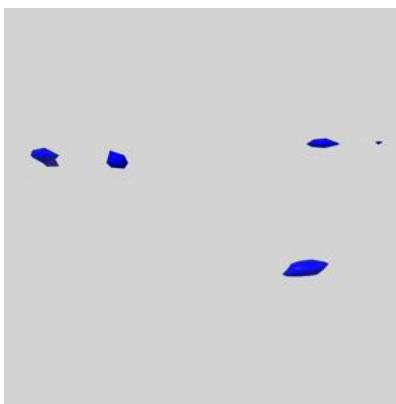
Y



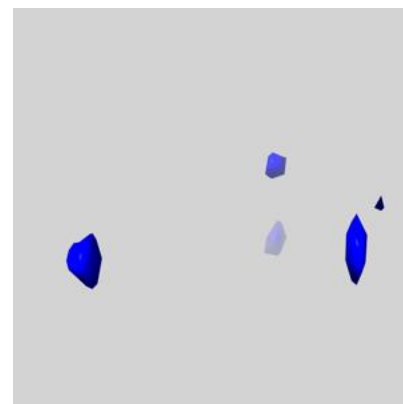
Z

6.5.5 emd_1001_msk_21.map [i](#)

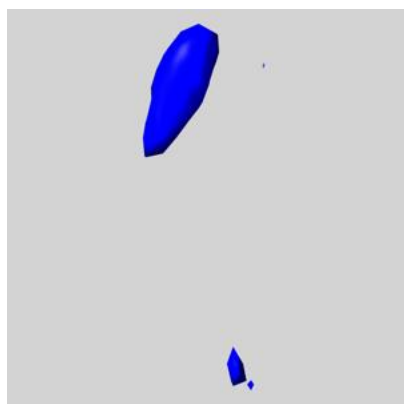
X



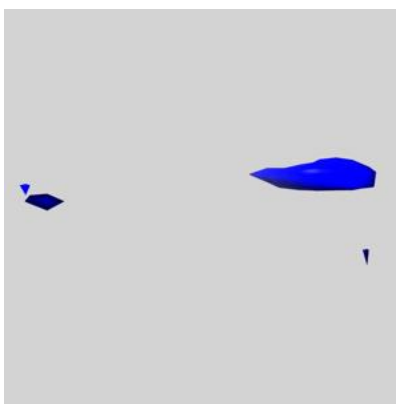
Y



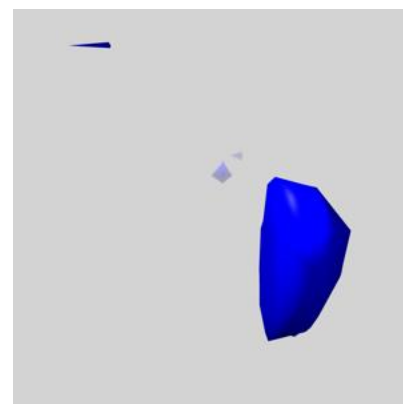
Z

6.5.6 `emd_1001_msk_20.map` [i](#)

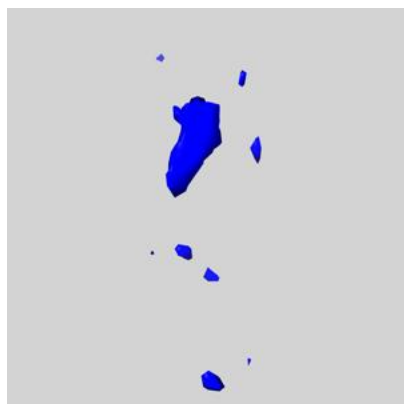
X



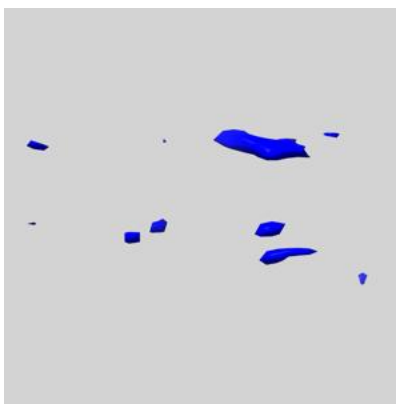
Y



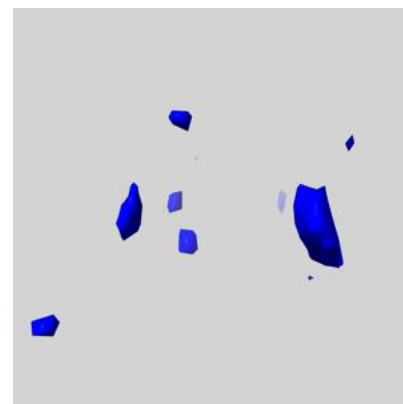
Z

6.5.7 `emd_1001_msk_19.map` [i](#)

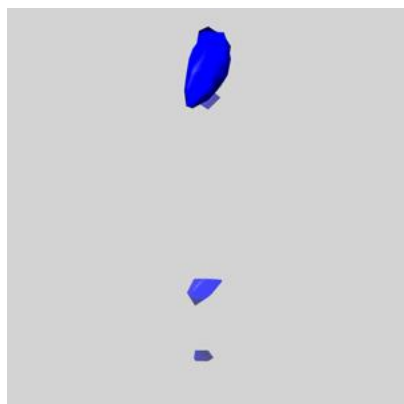
X



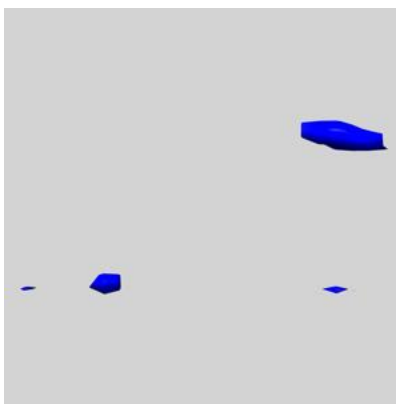
Y



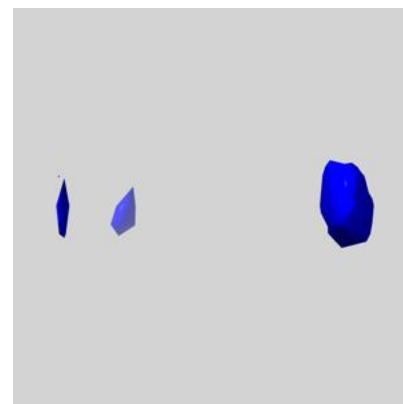
Z

6.5.8 `emd_1001_msk_18.map` [i](#)

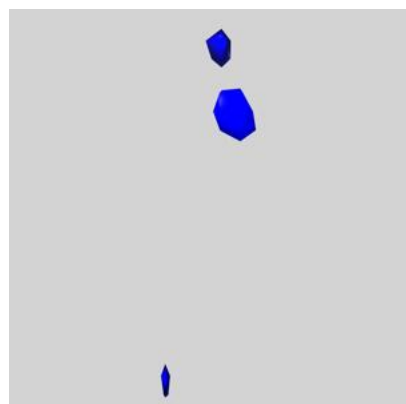
X



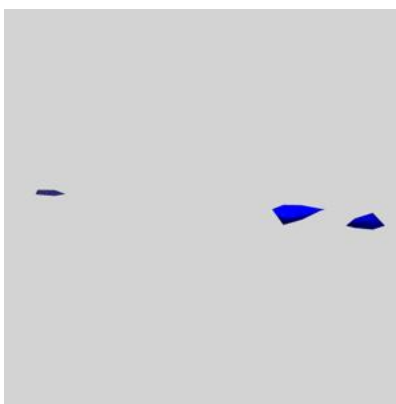
Y



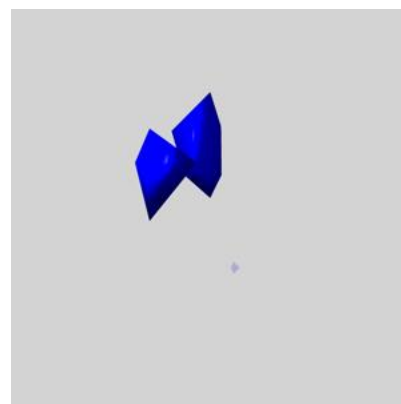
Z

6.5.9 emd_1001_msk_17.map [i](#)

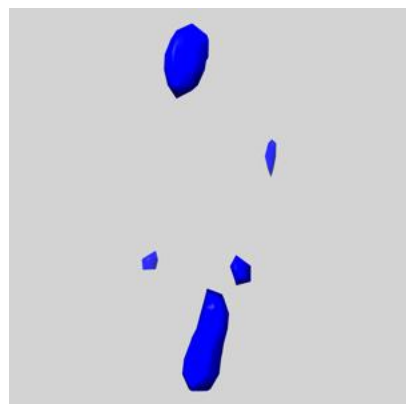
X



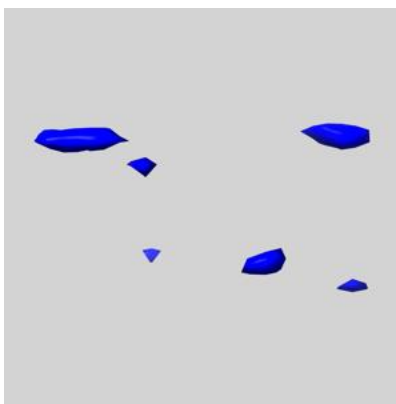
Y



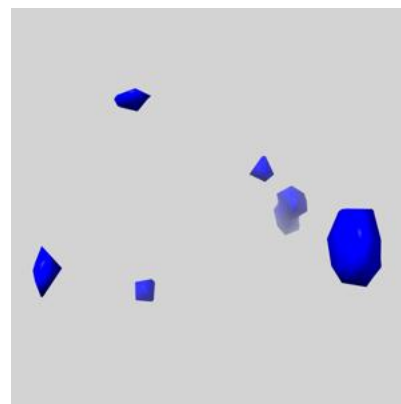
Z

6.5.10 emd_1001_msk_16.map [i](#)

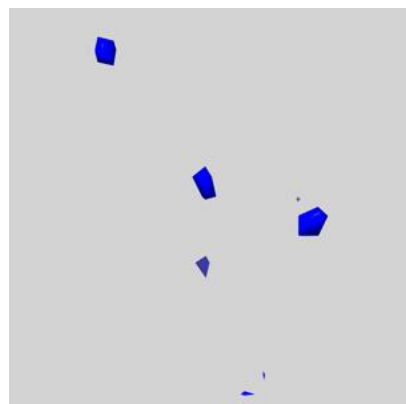
X



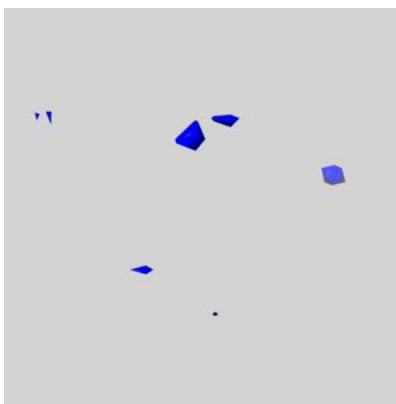
Y



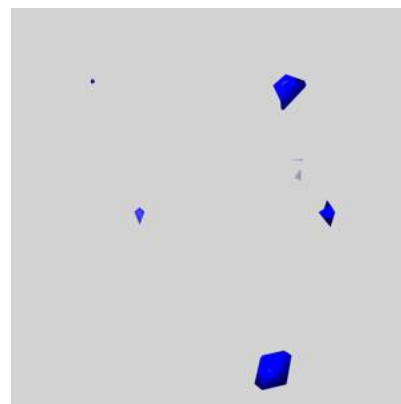
Z

6.5.11 emd_1001_msk_15.map [i](#)

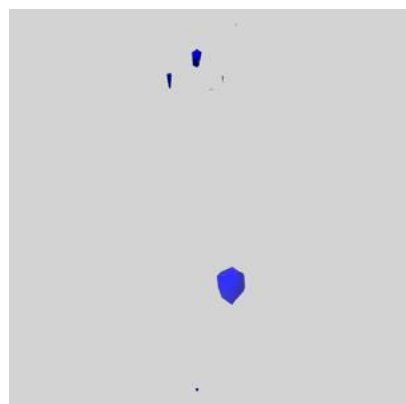
X



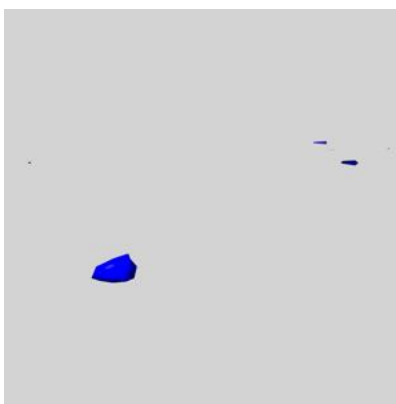
Y



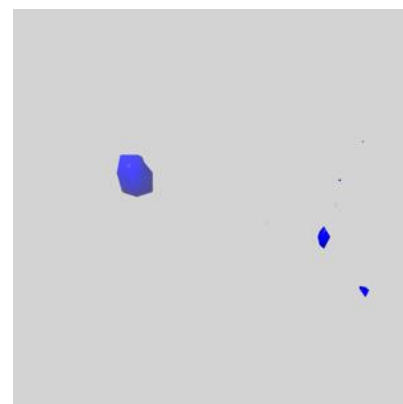
Z

6.5.12 emd_1001_msk_14.map [i](#)

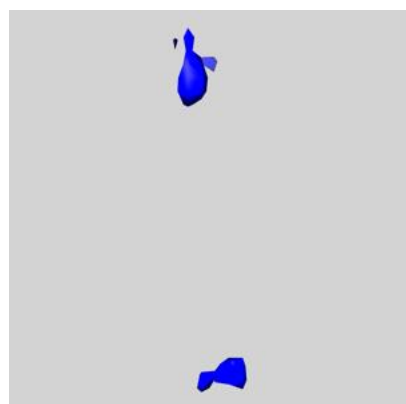
X



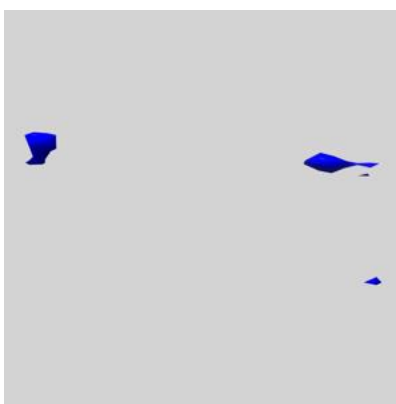
Y



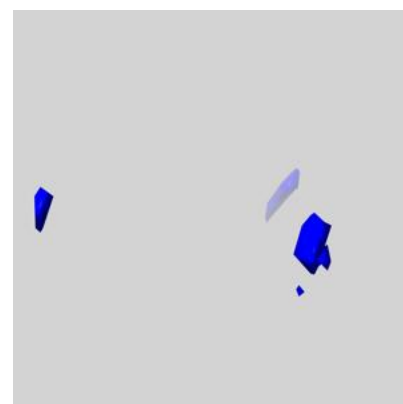
Z

6.5.13 emd_1001_msk_13.map [i](#)

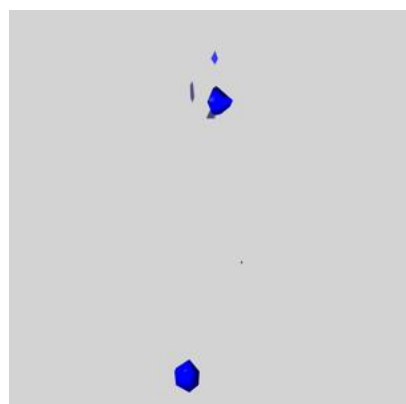
X



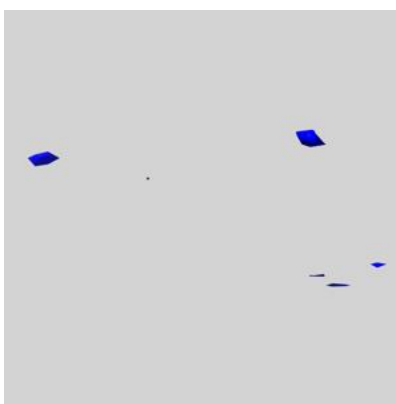
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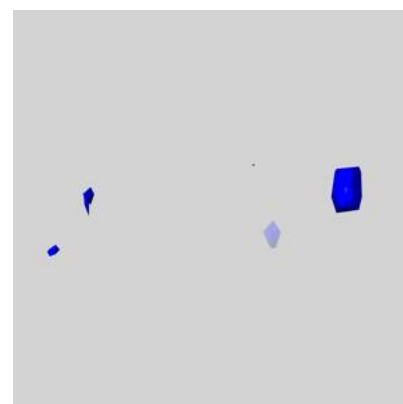
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6.5.14 emd_1001_msk_12.map [i](#)

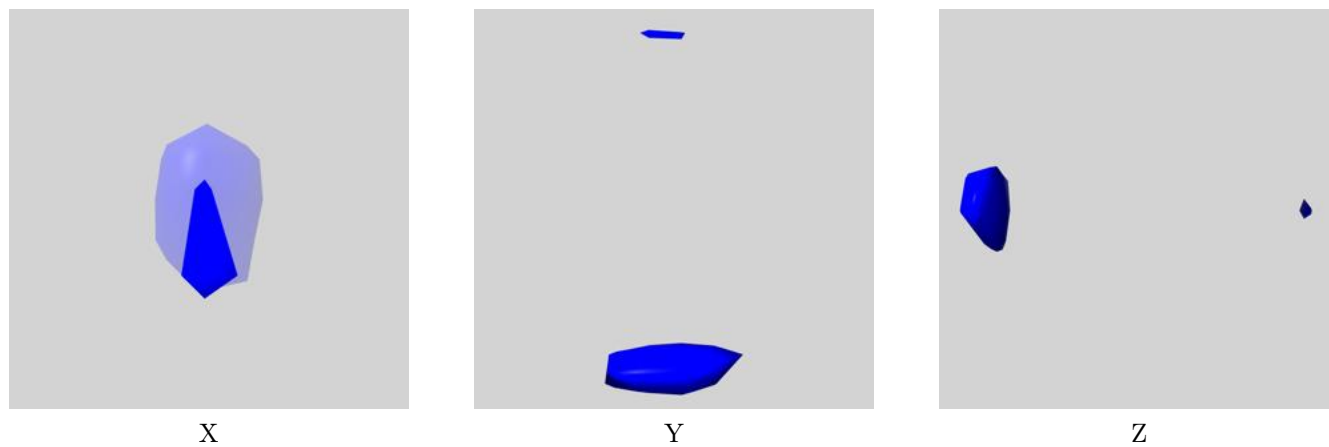
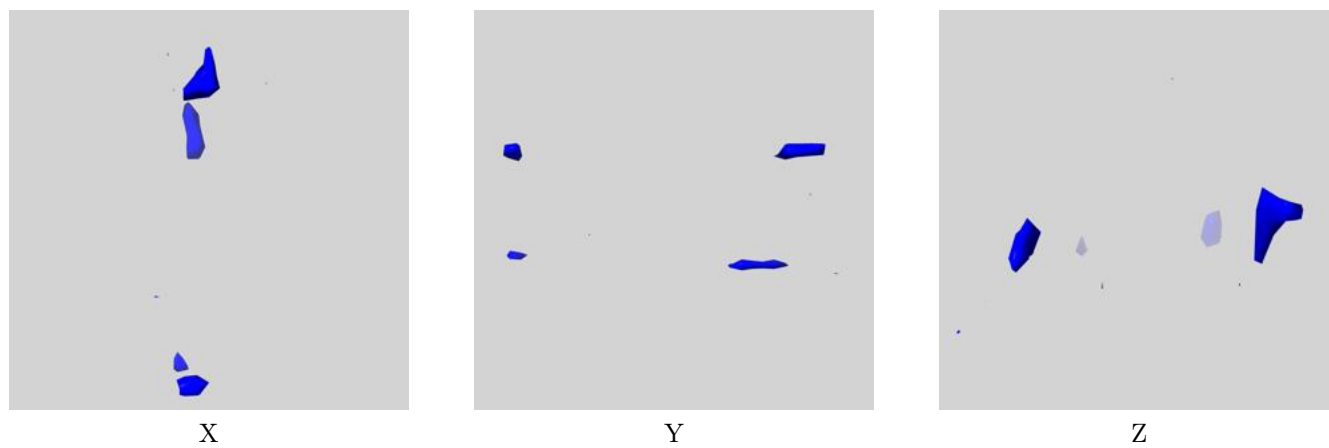
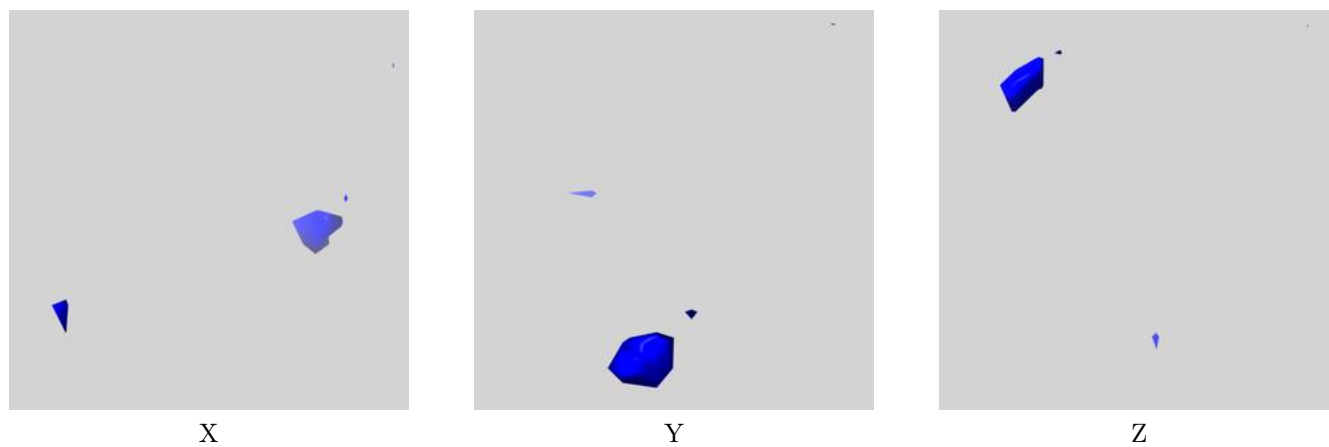
X

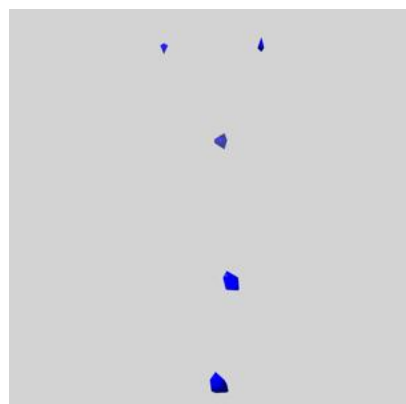


Y

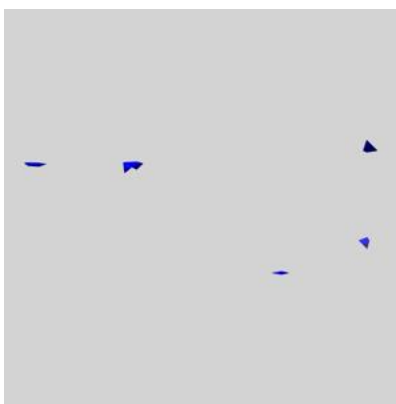


Z

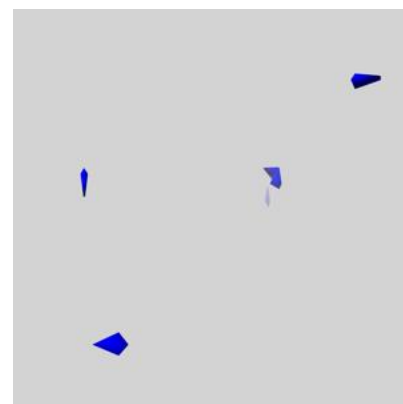
6.5.15 emd_1001_msk_11.map [i](#)6.5.16 emd_1001_msk_10.map [i](#)6.5.17 emd_1001_msk_9.map [i](#)

6.5.18 emd_1001_msk_8.map [i](#)

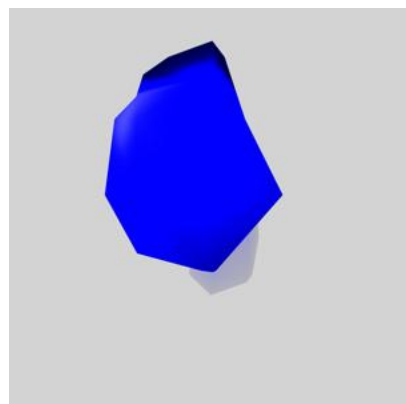
X



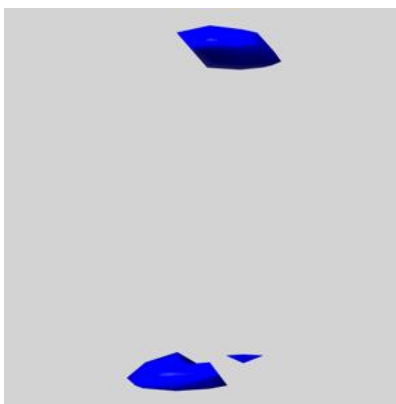
Y



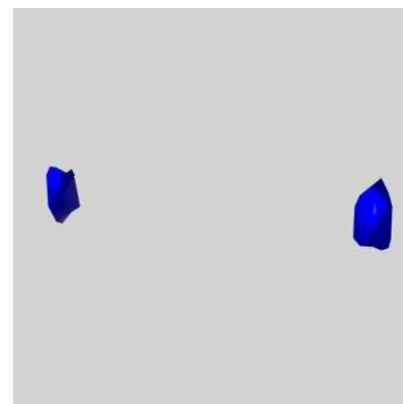
Z

6.5.19 emd_1001_msk_7.map [i](#)

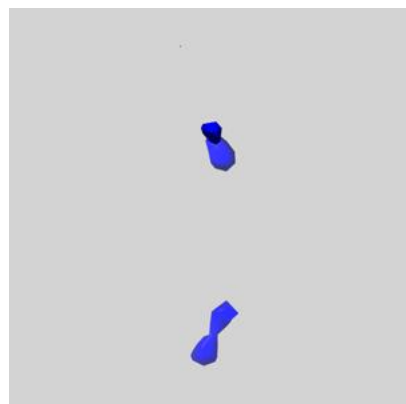
X



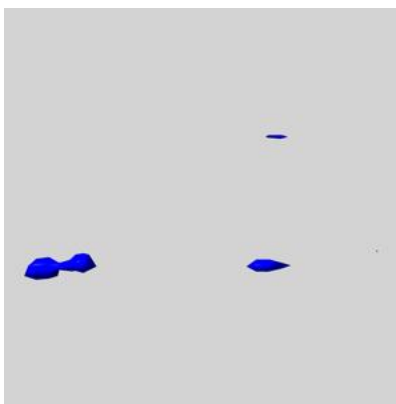
Y



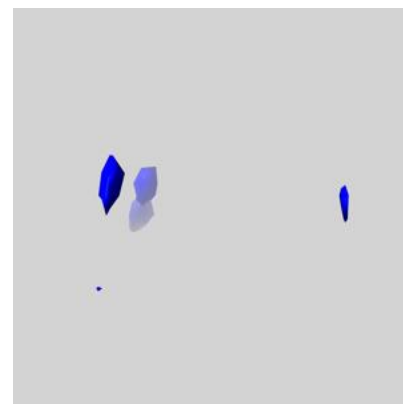
Z

6.5.20 emd_1001_msk_6.map [i](#)

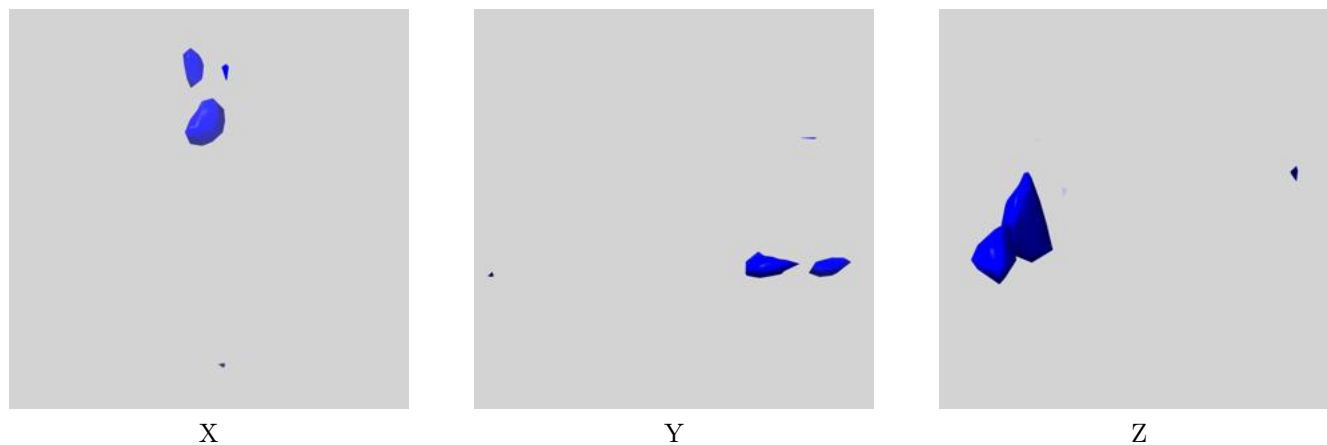
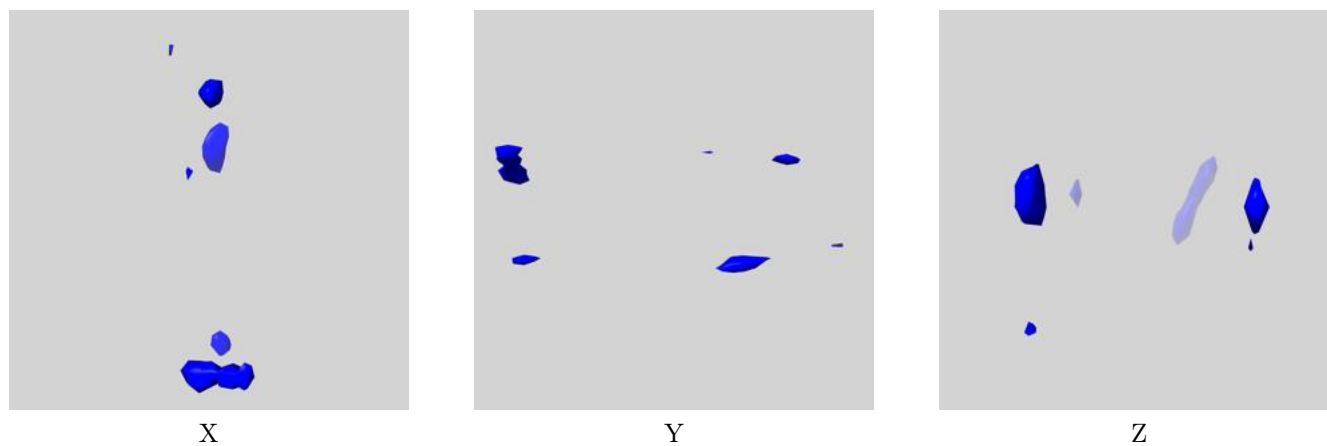
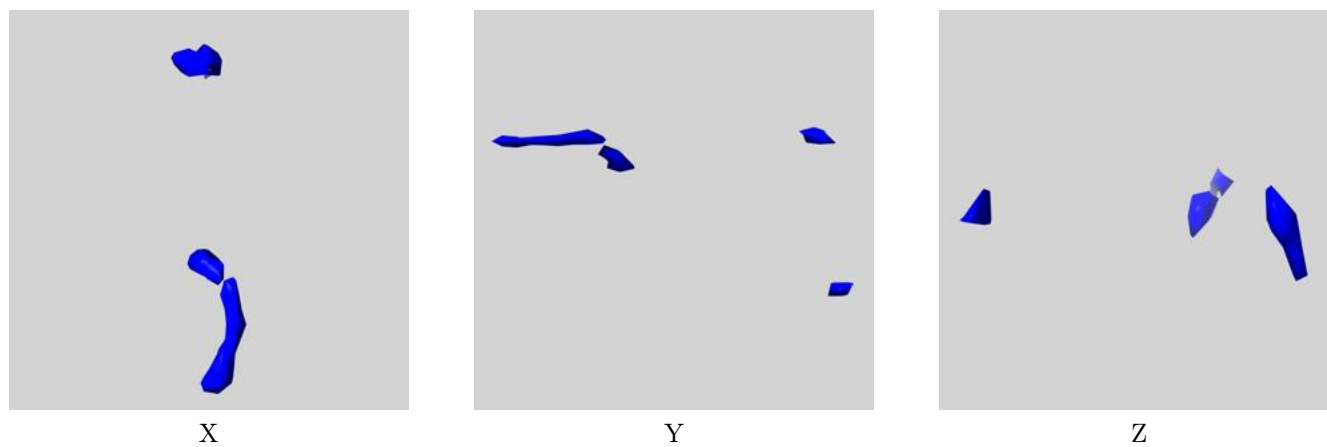
X

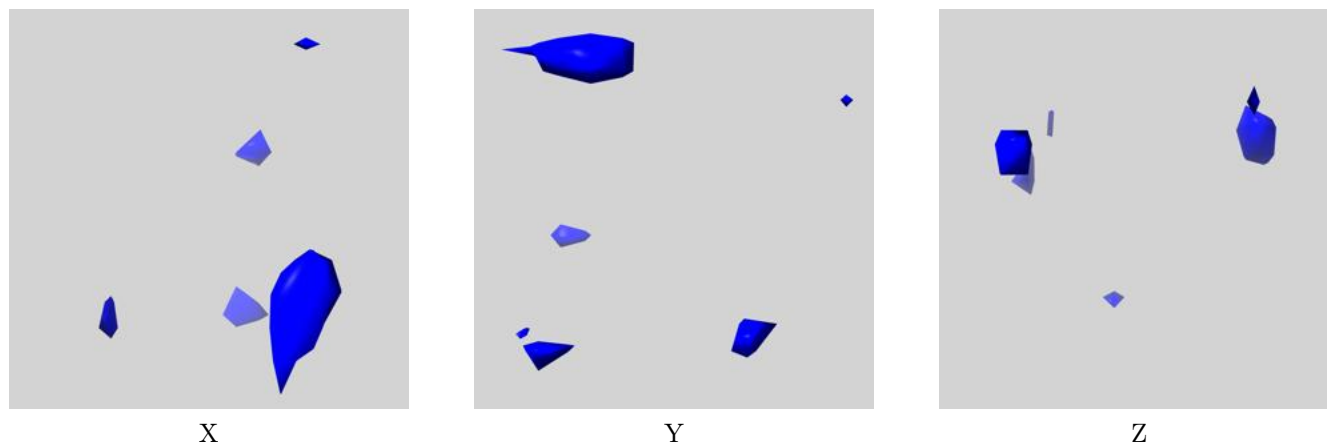
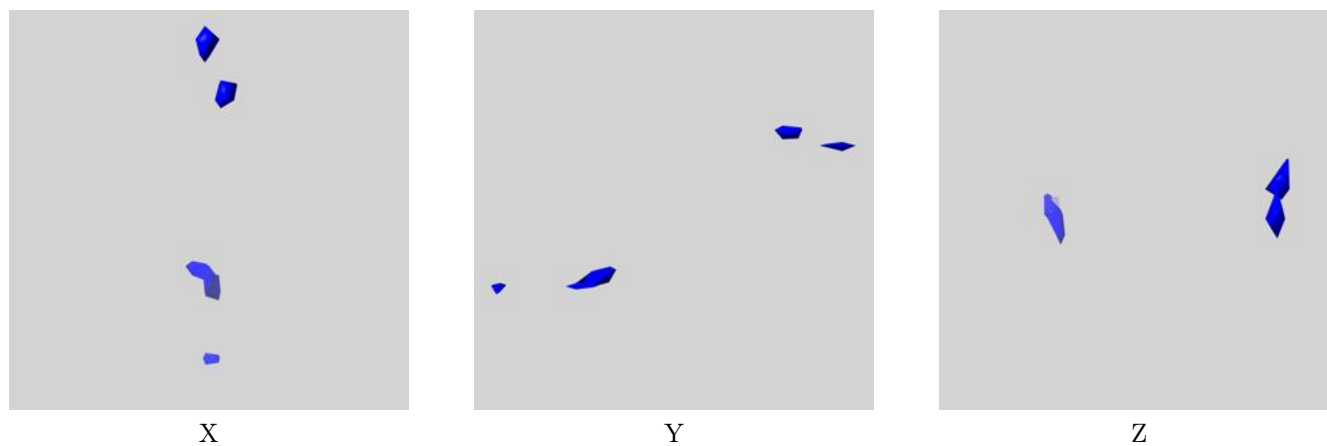
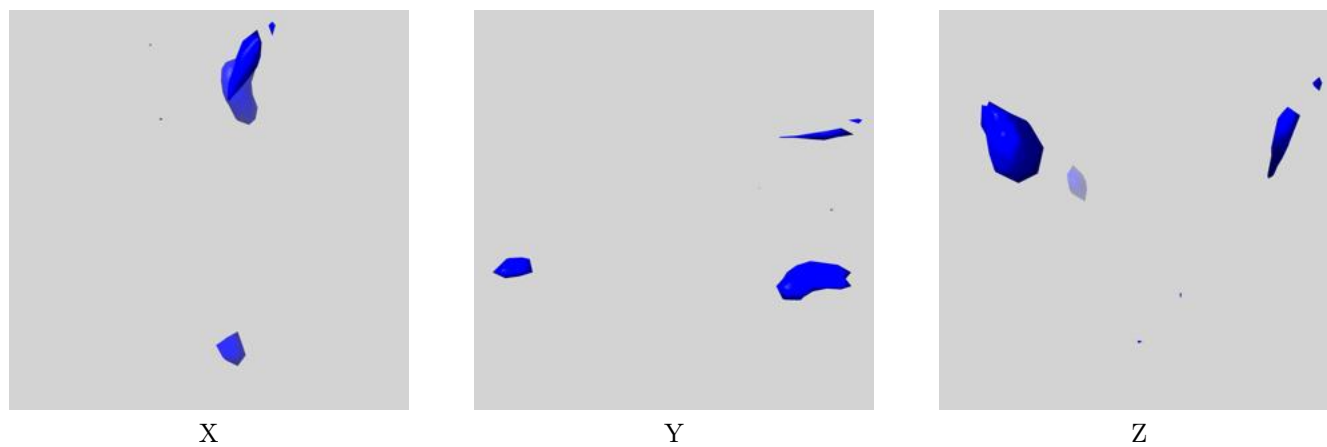


Y



Z

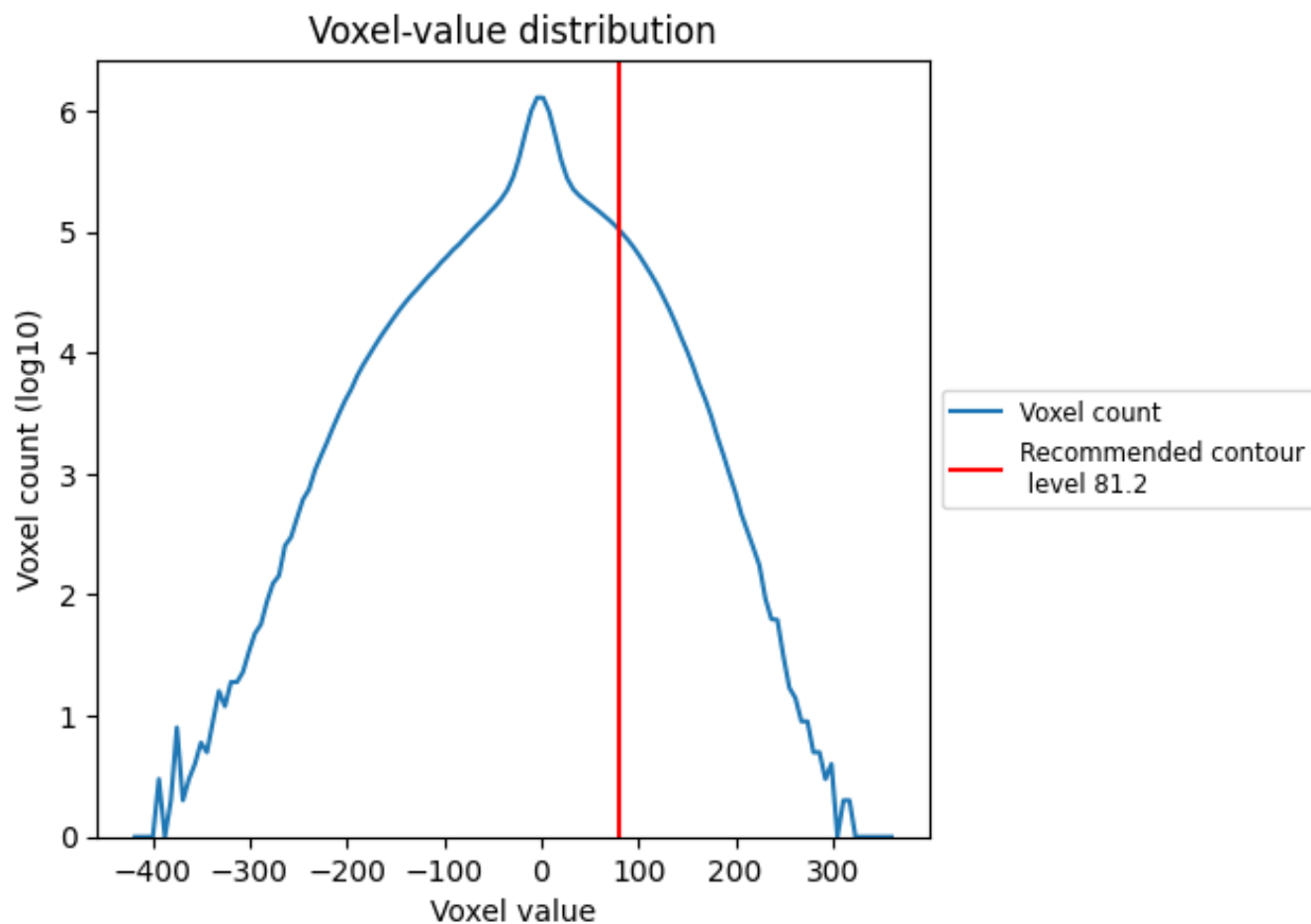
6.5.21 emd_1001_msk_5.map [i](#)6.5.22 emd_1001_msk_4.map [i](#)6.5.23 emd_1001_msk_3.map [i](#)

6.5.24 emd_1001_msk_2.map [i](#)6.5.25 emd_1001_msk_1.map [i](#)6.5.26 emd_1001_msk_26.map [i](#)

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.

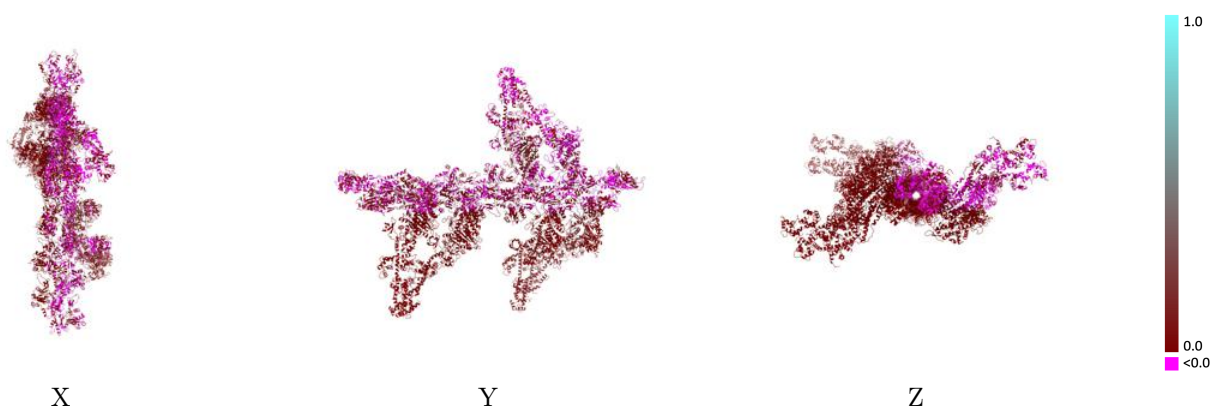
8 Map-model fit [i](#)

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](#)

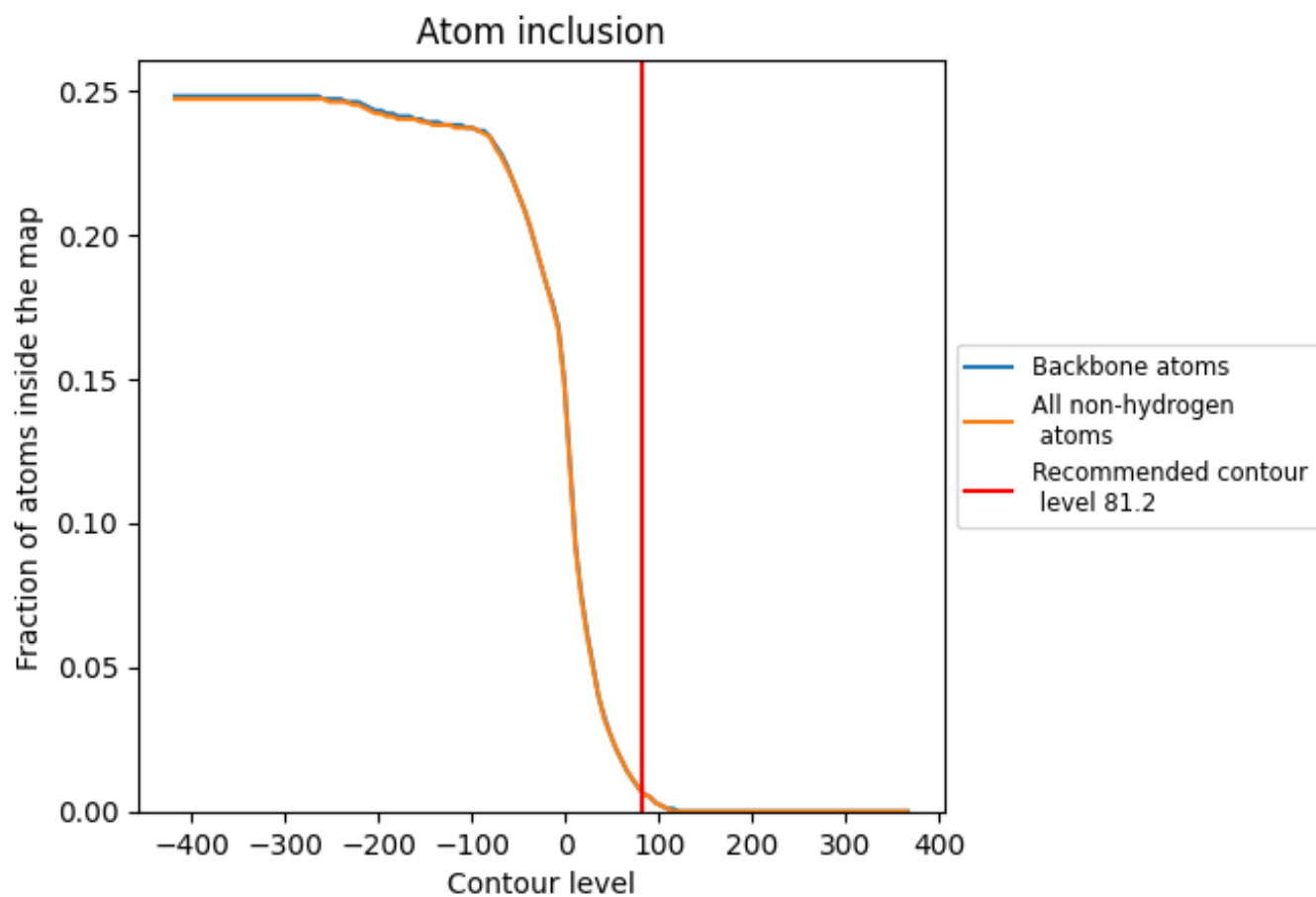


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 [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	 0.0070	 0.0020
1	 0.0000	 0.0050
2	 0.0280	 0.0120
3	 0.0000	 -0.0070
4	 0.0000	 0.0150
5	 0.0000	 -0.0040
6	 0.0000	 0.0040
7	 0.0000	 -0.0010
8	 0.0000	 0.0020
9	 0.0000	 -0.0020
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	 0.0020
T	 0.0000	 0.0000
U	 0.0000	 0.0000
V	 0.0000	 0.0070
W	 0.0000	 -0.0040
X	 0.0540	 0.0060
Y	 0.0000	 0.0050
Z	 0.0000	 -0.0080

