



wwPDB EM Validation Summary Report ⓘ

Nov 19, 2022 – 09:12 AM 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 : 2MYS, 1ATN

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev43
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) : 2.31.3

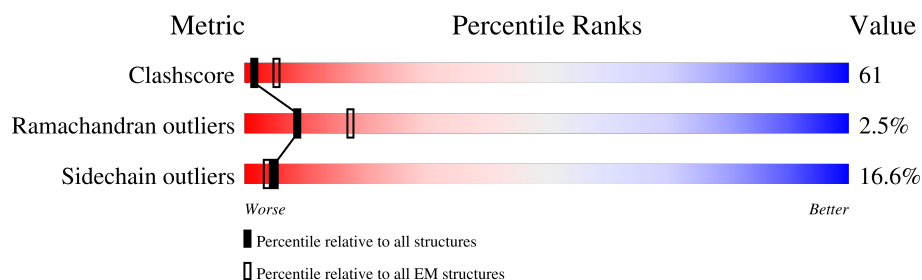
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 70.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	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	<div> <div>100%</div> <div>25% 51% 20% .</div> </div>
1	D	840	<div> <div>100%</div> <div>25% 50% 20% .</div> </div>
1	G	840	<div> <div>100%</div> <div>24% 51% 20% .</div> </div>
1	J	840	<div> <div>99%</div> <div>26% 50% 20% .</div> </div>
1	M	840	<div> <div>100%</div> <div>26% 50% 21% .</div> </div>
1	S	840	<div> <div>100%</div> <div>25% 51% 20% .</div> </div>
2	B	145	<div> <div>100%</div> <div>66% 26% 6% .</div> </div>
2	E	145	<div> <div>90%</div> <div>64% 27% 6% .</div> </div>

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

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

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

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

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

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

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

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

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

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

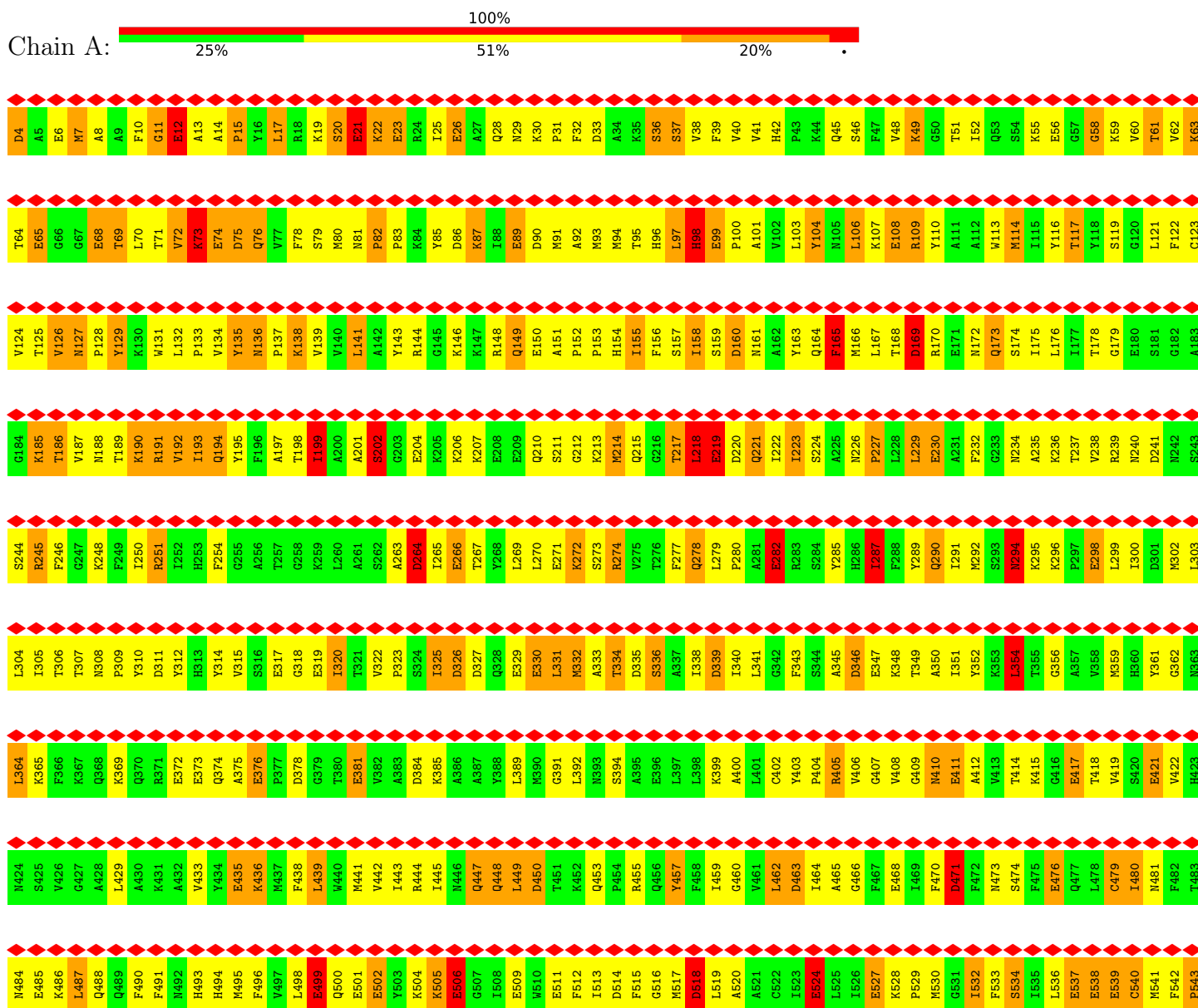
- Molecule 4 is a protein called SKELETAL MUSCLE ACTIN.

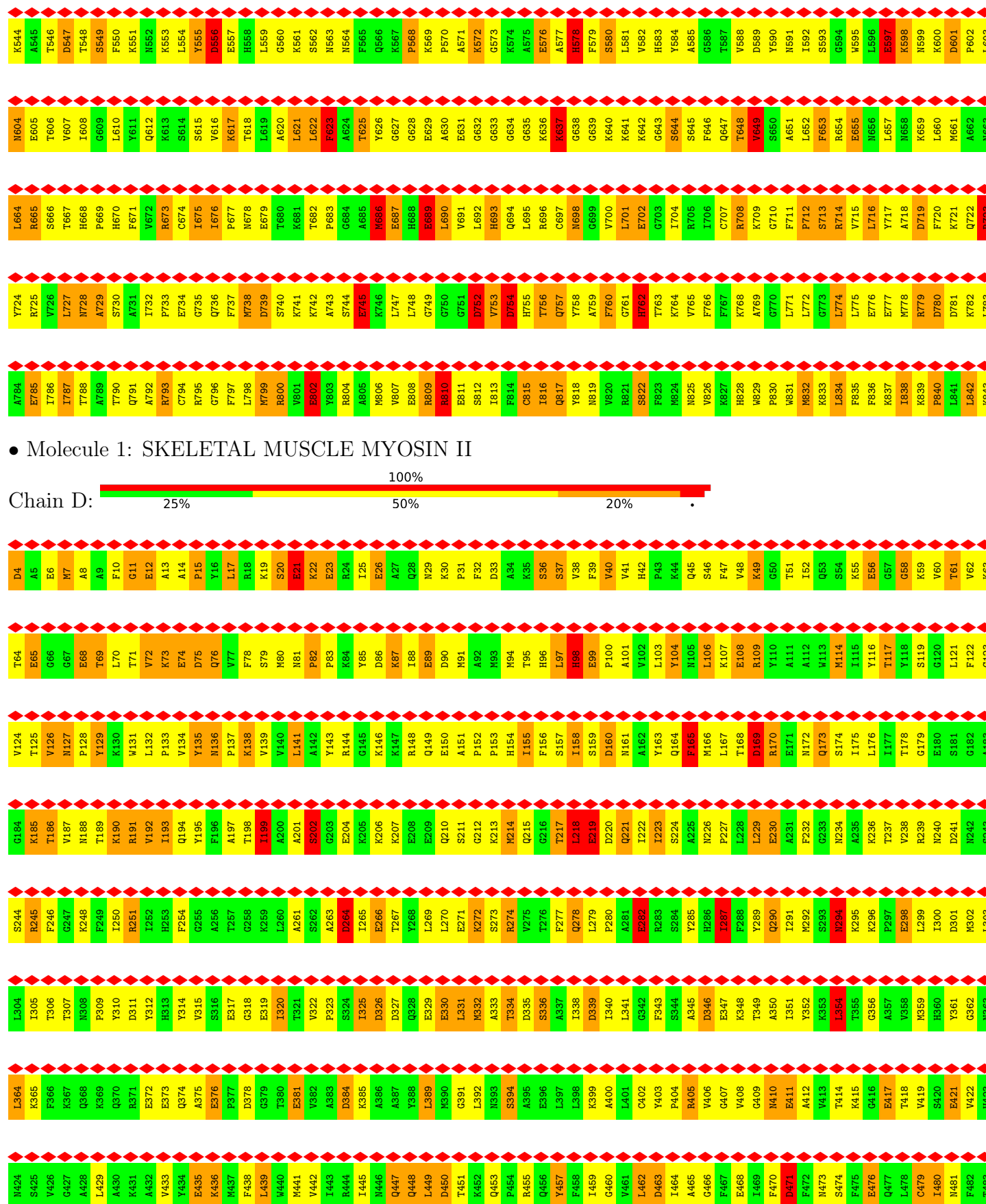
Mol	Chain	Residues	Atoms					AltConf	Trace
4	1	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	2	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	3	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	4	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	5	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20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

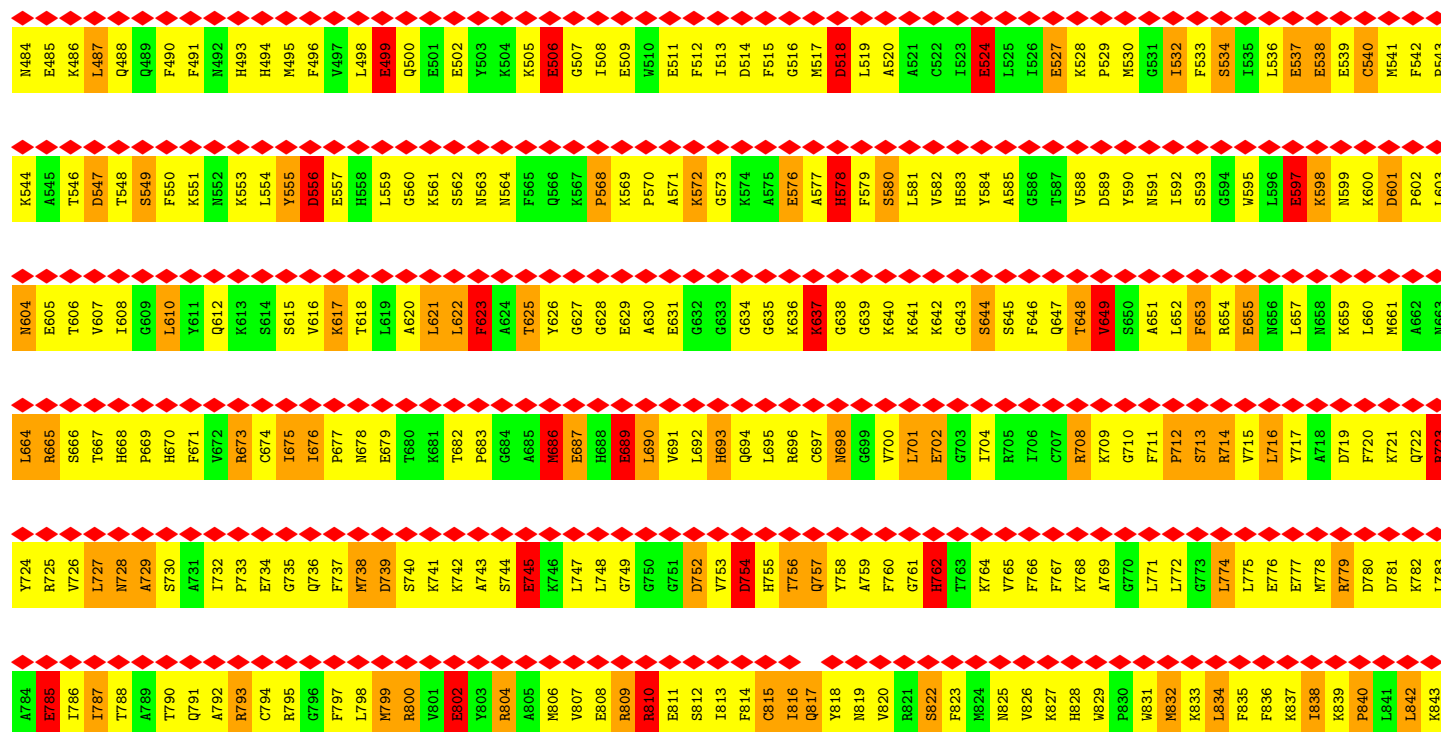
3 Residue-property plots

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

• Molecule 1: SKELETAL MUSCLE MYOSIN II







N424	N484	K544	N604	L664	Y724	A784	N424	N484	K544	N604	L664	Y724	A784
S425	E485	A545	E505	R665	R725	E785	S425	E485	A545	E505	R665	R725	E785
V426	K486	T546	T606	S666	V726	I786	V426	K486	T546	T606	S666	V726	I786
G427	L487	D547	V607	T667	L727	T787	G427	L487	D547	V607	T667	L727	T787
N428	Q488	T548	G608	H668	A728	T788	N428	Q488	T548	G608	H668	A728	T788
L429	Q489	S549	G609	P669	A729	A789	L429	Q489	S549	G609	P669	A729	A789
A430	F490	F550	L610	H670	S730	T790	A430	F490	F550	L610	H670	S730	T790
K431	F491	K551	Y611	F671	A731	Q791	K431	F491	K551	Y611	F671	A731	Q791
A432	N492	N552	Q612	F672	I732	A792	A432	N492	N552	Q612	F672	I732	A792
V433	H493	K553	K613	R673	P733	R793	V433	H493	K553	K613	R673	P733	R793
Y434	H494	L554	S614	C674	E734	C794	Y434	H494	L554	S614	C674	E734	C794
E435	M495	Y555	S615	I675	G735	R795	E435	M495	Y555	S615	I675	G735	R795
K436	F496	D556	V616	I676	Q736	G796	K436	F496	D556	V616	I676	Q736	G796
M437	V497	V557	K617	P677	F737	F797	M437	V497	V557	K617	P677	F737	F797
F438	L498	H558	T618	N678	M738	L798	F438	L498	H558	T618	N678	M738	L798
L439	E499	L559	L619	E679	D739	M799	L439	E499	L559	L619	E679	D739	M799
V440	Q500	G560	A620	T680	S740	R800	V440	Q500	G560	A620	T680	S740	R800
M441	E501	K561	L621	K681	K741	V601	M441	E501	K561	L621	K681	K741	V601
V442	E502	S562	L622	T682	K742	E502	V442	E502	S562	L622	T682	K742	E502
I443	Y503	N563	F623	P683	A743	E503	I443	Y503	N563	F623	P683	A743	E503
R444	K504	N564	A624	G684	S744	R804	R444	K504	N564	A624	G684	S744	R804
I445	K505	F565	T625	A685	E745	A805	I445	K505	F565	T625	A685	E745	A805
N446	E506	Q566	Y626	M686	K746	M806	N446	E506	Q566	Y626	M686	K746	M806
Q447	G507	K567	G627	H687	L747	V607	Q447	G507	K567	G627	H687	L747	V607
Q448	I508	P568	G628	H688	L748	E508	Q448	I508	P568	G628	H688	L748	E508
L449	E509	K569	E629	E689	G749	R809	L449	E509	K569	E629	E689	G749	R809
D450	W510	P570	A630	L690	G750	R810	D450	W510	P570	A630	L690	G750	R810
T451	E511	A571	E631	V691	G751	E811	T451	E511	A571	E631	V691	G751	E811
K452	F512	K572	G632	L692	D752	S812	K452	F512	K572	G632	L692	D752	S812
Q453	I513	G573	V753	H693	E753	I813	Q453	I513	G573	V753	H693	E753	I813
P454	D514	K574	Q634	Q694	D754	F814	P454	D514	K574	Q634	Q694	D754	F814
R455	F515	A575	G635	L695	H755	C815	R455	F515	A575	G635	L695	H755	C815
Q456	G516	E576	K636	R696	T756	I816	Q456	G516	E576	K636	R696	T756	I816
Y457	M517	A577	P637	C697	Q757	Q817	Y457	M517	A577	P637	C697	Q757	Q817
F458	D518	H578	G638	N698	Y758	Y818	F458	D518	H578	G638	N698	Y758	Y818
I459	L519	F579	K639	G699	A759	N819	I459	L519	F579	K639	G699	A759	N819
G460	A520	S580	V640	V700	F760	V820	G460	A520	S580	V640	V700	F760	V820
V461	E521	L581	K641	L701	G761	R821	V461	E521	L581	K641	L701	G761	R821
L462	C522	V582	K642	E702	H762	S822	L462	C522	V582	K642	E702	H762	S822
D463	I523	H583	G643	G703	T763	F823	D463	I523	H583	G643	G703	T763	F823
I464	E524	Y584	S644	I704	K764	M824	I464	E524	Y584	S644	I704	K764	M824
A465	L525	A585	S645	R705	V765	N825	A465	L525	A585	S645	R705	V765	N825
G466	I526	G586	F646	I706	F766	V826	G466	I526	G586	F646	I706	F766	V826
F467	E527	T587	Q647	C707	F767	K827	F467	E527	T587	Q647	C707	F767	K827
E468	K528	V588	T648	R708	K768	H828	E468	K528	V588	T648	R708	K768	H828
I469	P529	D589	V649	K709	A769	N829	I469	P529	D589	V649	K709	A769	N829
F470	M530	Y590	S550	G710	G770	P830	F470	M530	Y590	S550	G710	G770	P830
D471	G531	N591	A651	F711	L771	M831	D471	G531	N591	A651	F711	L771	M831
F472	I532	L592	L652	P712	L772	M832	F472	I532	L592	L652	P712	L772	M832
N473	F533	S593	F653	S713	G773	K833	N473	F533	S593	F653	S713	G773	K833
S474	S534	G594	R654	R714	L774	L834	S474	S534	G594	R654	R714	L774	L834
F475	I535	W595	E655	V715	L775	P835	F475	I535	W595	E655	V715	L775	P835
A476	L536	L596	M556	L716	E776	F836	A476	L536	L596	M556	L716	E776	F836
Q477	E537	R597	L657	Y717	E777	K837	Q477	E537	R597	L657	Y717	E777	K837
L478	E538	K598	M558	A718	M778	T838	L478	E538	K598	M558	A718	M778	T838
C479	E539	N599	K659	D719	R779	K839	C479	E539	N599	K659	D719	R779	K839
I480	C540	K600	L660	F720	D780	P840	I480	C540	K600	L660	F720	D780	P840
N481	M541	D601	M661	K721	D781	L841	N481	M541	D601	M661	K721	D781	L841
F482	F542	P602	A662	Q722	K782	L842	F482	F542	P602	A662	Q722	K782	L842
T483	P543	L603	N663	R723	L783	K843	T483	P543	L603	N663	R723	L783	K843

● 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	N188	K248	N308
A9	T69	Y129	T189	F249	P309
F10	L70	K130	K190	L250	Y310
G11	T71	W131	R191	R251	D311
E12	V72	L132	V192	L252	Y312
A13	K73	P133	T193	H253	H313
A14	E74	V134	Q194	F254	Y314
P15	D75	Y135	Y195	G255	V315
Y16	Q76	M136	F196	A256	S316
L17	V77	P137	A197	T257	E317
R18	F78	K138	T198	G258	G318
K19	S79	V139	I199	K259	E319
S20	M80	Y140	A200	L260	I320
E21	N81	L141	A201	A261	T321
K22	P82	A142	S202	S262	V322
R23	K83	Y143	G203	A263	P323
I25	D86	G145	E204	D264	S324
E26	K87	K146	K206	T265	T325
A27	T88	E147	K207	E266	D326
Q28	I89	R148	E208	T267	D327
N29	E90	Q149	E209	T268	Q328
K30	D90	E150	Q210	L269	E329
P31	N91	A151	S211	L270	E330
F32	A92	P152	G212	E271	L331
D33	M93	P153	K213	K272	A332
A34	M94	H154	M214	R273	T334
K35	T95	I155	Q215	V275	D335
S36	H96	F156	G216	T276	S336
S37	L97	S157	T217	F277	A337
V38	H98	I158	L218	Q278	I338
F39	E99	S159	E219	L279	D339
V40	P100	D160	D220	P280	I340
V41	A101	M161	Q221	A281	L341
H42	Y102	A162	I222	E282	G342
P43	L103	Y163	I223	R283	F343
K44	Y104	Q164	S224	S284	S344
Q45	N105	F165	A225	Y285	A345
S46	L106	M166	N226	H286	D346
F47	K107	L167	P227	T287	E347
V48	E108	T168	L228	F288	K348
K49	R109	D169	L229	Y289	T349
G50	Y110	R170	E230	Q290	A350
T51	A111	E171	A231	T291	L351
I52	A112	M172	F232	M292	Y352
Q53	V113	Q173	G233	K293	K353
S54	M114	S174	N234	L294	L354
K55	I115	T175	A235	K295	T355
E56	Y116	L176	K236	K296	G356
G57	T117	I177	T237	P297	A357
G58	Y118	T178	V238	E298	V358
K59	S119	G179	R239	L299	K359
V60	G120	E180	N240	T300	H360
T61	S121	S181	D241	D301	Y361
V62	F122	G182	N242	K302	G362
K63	C123	A183	S243	L303	N363

A784	E785	I786	I787	T788	A789	T790	Q791	A792	R793	C794	R795	G796	F797	L798	M799	R800	E801	E802	Y803	R804	A805	M806	V807	E808	R809	R810	E811	L812	F813	C815	L816	Q817	Y818	L819	V820	R821	S822	F823	M824	N825	V826	K827	H828	M829	P830	K831	M832	K833	L834	F835	F836	K837	L838	K839	P840	L841	L842	K843		
Y724	R725	V726	L727	H728	A729	S730	A731	I732	P733	E734	G735	Q736	F737	M738	D739	S740	K741	K742	A743	S744	E745	K746	L747	L748	G749	G750	G751	D752	F753	D754	H755	T756	Q757	Y758	A759	F760	G761	R762	T763	K764	V765	F766	F767	K768	A769	G770	L771	L772	G773	L774	L775	E776	E777	M778	R779	D780	D781	K782	L783	
L664	R665	S666	T667	H668	P669	H670	F671	V672	K673	C674	G675	I676	P677	N678	E679	T680	K681	T682	P683	G684	A685	M686	L687	H688	E689	L690	V691	L692	H693	Q694	L695	R696	G697	N698	G699	V700	L701	E702	G703	K704	R705	I706	G707	K708	K709	G710	F711	P712	S713	R714	V715	L716	Y717	A718	D719	F720	D721	Q722	R723	
N604	E605	T606	V607	I608	G609	L610	Y611	Q612	K613	S614	S615	V616	K617	T618	L619	A620	L621	L622	F623	A624	Y625	Y626	G627	G628	E629	A630	E631	G632	G633	G634	G635	K636	K637	G638	G639	K640	K641	K642	G643	S644	S645	F646	Q647	T648	V649	S650	A651	L652	F653	R654	E655	M656	L657	M658	K659	L660	M661	A662	N663	
K544	A545	T546	D547	L548	S549	F550	K551	N552	K553	L554	E555	D556	E557	H558	L559	G560	S561	S562	N563	N564	F565	Q566	K567	P568	K569	P570	A571	K572	G573	K574	A575	E576	A577	H578	F579	S580	L581	V582	H583	Y584	A585	G586	T587	V588	D589	Y590	N591	I592	S593	S594	L595	L596	E597	K598	N599	K600	D601	P602	L603	
N484	E485	K486	L487	Q488	Q489	F490	F491	N492	H493	H494	M495	F496	M497	L498	E499	Q500	M501	E502	Y503	K504	K505	E506	G507	I508	L509	E509	M510	E511	F512	I513	D514	F515	G516	M517	D518	L519	A520	A521	C522	I523	E524	L525	I526	E527	K528	P529	M530	G531	I532	F533	S534	I535	L536	E537	E538	E539	C540	M541	F542	P543
N424	S425	V426	G427	A428	L429	A430	K431	A432	V433	Y434	E435	A436	M437	F438	L439	Q440	Q441	V442	I443	R444	I445	M446	Q447	Q448	L449	D450	T451	K452	Q453	P454	R455	Q456	Y457	F458	I459	G460	V461	L462	D463	I464	A465	G466	F467	E468	I469	F470	D471	F472	N473	S474	F475	E476	Q477	L478	C479	I480	M481	F482	T483	
L364	K365	F366	K367	Q368	K369	Q370	R371	E372	E373	Q374	A375	E376	P377	D378	G379	T380	E381	V382	A383	D384	K385	A386	A387	Y388	L389	M390	G391	L392	N393	S394	A395	E396	L397	L398	K399	A400	L401	C402	Y403	P404	R405	V406	G407	V408	G409	N410	E411	A412	V413	T414	K415	G416	E417	T418	V419	S420	E421	V422	H423	

• Molecule 1: SKELETAL MUSCLE MYOSIN II



S244	R245	F246	G247	K248	F249	L250	R251	H253	F254	G255	A256	T257	G258	K259	L260	A261	S262	D263	D264	L265	E266	T267	Y268	L269	L270	E271	K272	S273	R274	V275	T276	F277	Q278	L279	P280	A281	E282	R283	S284	Y285	H286	F287	F288	Y289	Q290	I291	M292	S293	N294	K295	K296	P297	E298	L299	I300	D301	M302	K303	
G184	K185	T186	V187	N188	T189	K190	R191	V192	I193	Q194	Y195	F196	A197	T198	L199	A200	A201	S202	G203	E204	K205	K206	K207	E208	E209	Q210	S211	G212	K213	M214	Q215	G216	T217	L218	E219	S220	Q221	I222	I223	S224	A225	N226	P227	L228	L229	E230	A231	F232	G233	N234	A235	K236	T237	V238	R239	N240	D241	N242	S243
V124	T125	V126	N127	P128	Y129	K130	V131	L132	P133	V134	Y135	N136	P137	K138	V139	Y140	L141	A142	Y143	R144	G145	K146	L147	R148	Q149	E150	A151	P152	P153	H154	I155	F156	S157	I158	S159	D160	N161	A162	V163	Q164	F165	M166	L167	T168	D169	R170	E171	N172	Q173	S174	I175	L176	I177	T178	G179	E180	S181	G182	A183
D4	A5	E6	M7	A8	A9	F10	G11	E12	A13	A14	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	Q53	S54	K55	E56	G57	G58	K59	V60	T61	V62	K63

L304	L364	N424	N484	K544	N604	L664	Y724	A784	L844	L904	L964	L1024	L1084	L1144	L1204	L1264	L1324	L1384	L1444	L1504	L1564	L1624	L1684	L1744	L1804	L1864	L1924	L1984	L2044	L2104	L2164	L2224	L2284	L2344	L2404	L2464	L2524	L2584	L2644	L2704	L2764	L2824	L2884	L2944	L3004	L3064	L3124	L3184	L3244	L3304	L3364	L3424	L3484	L3544	L3604	L3664	L3724	L3784	L3844	L3904	L3964	L4024	L4084	L4144	L4204	L4264	L4324	L4384	L4444	L4504	L4564	L4624	L4684	L4744	L4804	L4864	L4924	L4984	L5044	L5104	L5164	L5224	L5284	L5344	L5404	L5464	L5524	L5584	L5644	L5704	L5764	L5824	L5884	L5944	L6004	L6064	L6124	L6184	L6244	L6304	L6364	L6424	L6484	L6544	L6604	L6664	L6724	L6784	L6844	L6904	L6964	L7024	L7084	L7144	L7204	L7264	L7324	L7384	L7444	L7504	L7564	L7624	L7684	L7744	L7804	L7864	L7924	L7984	L8044	L8104	L8164	L8224	L8284	L8344	L8404	L8464	L8524	L8584	L8644	L8704	L8764	L8824	L8884	L8944	L9004	L9064	L9124	L9184	L9244	L9304	L9364	L9424	L9484	L9544	L9604	L9664	L9724	L9784	L9844	L9904	L9964	L10024	L10084	L10144	L10204	L10264	L10324	L10384	L10444	L10504	L10564	L10624	L10684	L10744	L10804	L10864	L10924	L10984	L11044	L11104	L11164	L11224	L11284	L11344	L11404	L11464	L11524	L11584	L11644	L11704	L11764	L11824	L11884	L11944	L12004	L12064	L12124	L12184	L12244	L12304	L12364	L12424	L12484	L12544	L12604	L12664	L12724	L12784	L12844	L12904	L12964	L13024	L13084	L13144	L13204	L13264	L13324	L13384	L13444	L13504	L13564	L13624	L13684	L13744	L13804	L13864	L13924	L13984	L14044	L14104	L14164	L14224	L14284	L14344	L14404	L14464	L14524	L14584	L14644	L14704	L14764	L14824	L14884	L14944	L15004	L15064	L15124	L15184	L15244	L15304	L15364	L15424	L15484	L15544	L15604	L15664	L15724	L15784	L15844	L15904	L15964	L16024	L16084	L16144	L16204	L16264	L16324	L16384	L16444	L16504	L16564	L16624	L16684	L16744	L16804	L16864	L16924	L16984	L17044	L17104	L17164	L17224	L17284	L17344	L17404	L17464	L17524	L17584	L17644	L17704	L17764	L17824	L17884	L17944	L18004	L18064	L18124	L18184	L18244	L18304	L18364	L18424	L18484	L18544	L18604	L18664	L18724	L18784	L18844	L18904	L18964	L19024	L19084	L19144	L19204	L19264	L19324	L19384	L19444	L19504	L19564	L19624	L19684	L19744	L19804	L19864	L19924	L19984	L20044	L20104	L20164	L20224	L20284	L20344	L20404	L20464	L20524	L20584	L20644	L20704	L20764	L20824	L20884	L20944	L21004	L21064	L21124	L21184	L21244	L21304	L21364	L21424	L21484	L21544	L21604	L21664	L21724	L21784	L21844	L21904	L21964	L22024	L22084	L22144	L22204	L22264	L22324	L22384	L22444	L22504	L22564	L22624	L22684	L22744	L22804	L22864	L22924	L22984	L23044	L23104	L23164	L23224	L23284	L23344	L23404	L23464	L23524	L23584	L23644	L23704	L23764	L23824	L23884	L23944	L24004	L24064	L24124	L24184	L24244	L24304	L24364	L24424	L24484	L24544	L24604	L24664	L24724	L24784	L24844	L24904	L24964	L25024	L25084	L25144	L25204	L25264	L25324	L25384	L25444	L25504	L25564	L25624	L25684	L25744	L25804	L25864	L25924	L25984	L26044	L26104	L26164	L26224	L26284	L26344	L26404	L26464	L26524	L26584	L26644	L26704	L26764	L26824	L26884	L26944	L27004	L27064	L27124	L27184	L27244	L27304	L27364	L27424	L27484	L27544	L27604	L27664	L27724	L27784	L27844	L27904	L27964	L28024	L28084	L28144	L28204	L28264	L28324	L28384	L28444	L28504	L28564	L28624	L28684	L28744	L28804	L28864	L28924	L28984	L29044	L29104	L29164	L29224	L29284	L29344	L29404	L29464	L29524	L29584	L29644	L29704	L29764	L29824	L29884	L29944	L30004	L30064	L30124	L30184	L30244	L30304	L30364	L30424	L30484	L30544	L30604	L30664	L30724	L30784	L30844	L30904	L30964	L31024	L31084	L31144	L31204	L31264	L31324	L31384	L31444	L31504	L31564	L31624	L31684	L31744	L31804	L31864	L31924	L31984	L32044	L32104	L32164	L32224	L32284	L32344	L32404	L32464	L32524	L32584	L32644	L32704	L32764	L32824	L32884	L32944	L33004	L33064	L33124	L33184	L33244	L33304	L33364	L33424	L33484	L33544	L33604	L33664	L33724	L33784	L33844	L33904	L33964	L34024	L34084	L34144	L34204	L34264	L34324	L34384	L34444	L34504	L34564	L34624	L34684	L34744	L34804	L34864	L34924	L34984	L35044	L35104	L35164	L35224	L35284	L35344	L35404	L35464	L35524	L35584	L35644	L35704	L35764	L35824	L35884	L35944	L36004	L36064	L36124	L36184	L36244	L36304	L36364	L36424	L36484	L36544	L36604	L36664	L36724	L36784	L36844	L36904	L36964	L37024	L37084	L37144	L37204	L37264	L37324	L37384	L37444	L37504	L37564	L37624	L37684	L37744	L37804	L37864	L37924	L37984	L38044	L38104	L38164	L38224	L38284	L38344	L38404	L38464	L38524	L38584	L38644	L38704	L38764	L38824	L38884	L38944	L39004	L39064	L39124	L39184	L39244	L39304	L39364	L39424	L39484	L39544	L39604	L39664	L39724	L39784	L39844	L39904	L39964	L40024	L40084	L40144	L40204	L40264	L40324	L40384	L40444	L40504	L40564	L40624	L40684	L40744	L40804	L40864	L40924	L40984	L41044	L41104	L41164	L41224	L41284	L41344	L41404	L41464	L41524	L41584	L41644	L41704	L41764	L41824	L41884	L41944	L42004	L42064	L42124	L42184	L42244	L42304	L42364	L42424	L42484	L42544	L42604	L42664	L42724	L42784	L42844	L42904	L42964	L43024	L43084	L43144	L43204	L43264	L43324	L43384	L43444	L43504	L43564	L43624	L43684	L43744	L43804	L43864	L43924	L43984	L44044	L44104	L44164	L44224	L44284	L44344	L44404	L44464	L44524	L44584	L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• Molecule 1: SKELETAL MUSCLE MYOSIN II



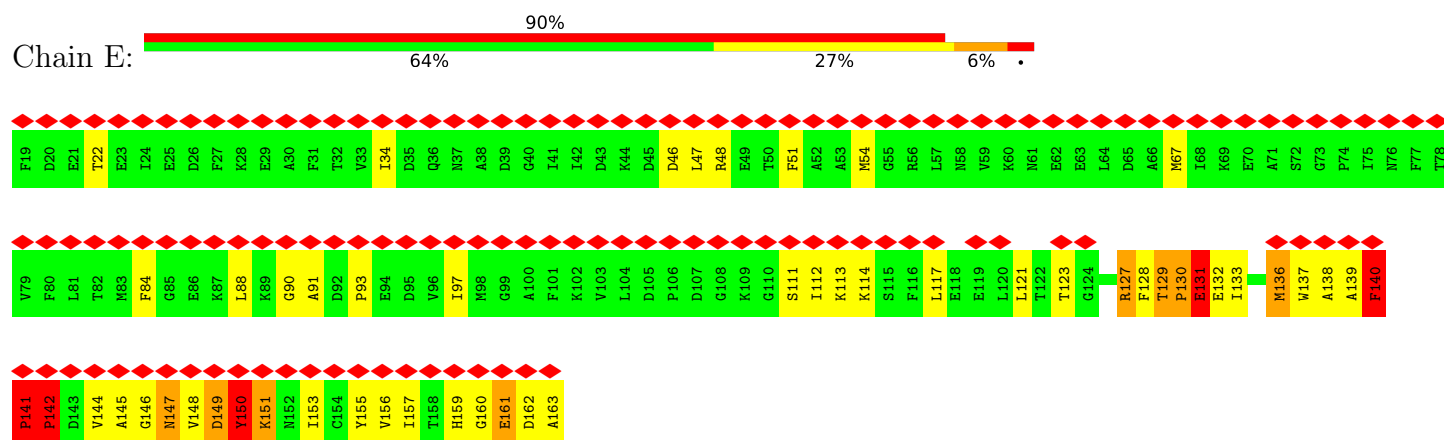
G184	K185	T186	V187	N188	T189	K190	R191	V192	I193	Q194	Y195	F196	A197	T198	I199	A201	S202	G203	E204	K205	K206	K207	E208	E209	Q210	S211	G212	K213	M214	Q215	G216	T217	L218	E219	D220	Q221	I222	I223	S224	A225	N226	P227	L228	L229	E230	A231	F232	G233	N234	A235	K236	T237	V238	R239	N240	D241	N242	S243	
V124	T125	N126	P127	N128	Y129	K130	W131	L132	P133	V134	Y135	N136	P137	K138	V139	V140	L141	A142	Y143	R144	G145	K146	L147	R148	Q149	E150	A151	P152	P153	H154	I155	F156	S157	I158	S159	D160	N161	A162	Y163	Q164	F165	M166	L167	T168	D169	R170	E171	N172	Q173	S174	I175	L176	T177	T178	G179	E180	S181	G182	A183
T64	E65	G66	G67	E68	T69	L70	T71	V72	K73	E74	D75	Q76	V77	F78	S79	M80	N81	P82	P83	K84	Y85	D86	K87	I88	E89	D90	M91	A92	M93	M94	T95	H96	L97	H98	E99	P100	A101	V102	L103	Y104	N105	L106	K107	E108	R109	Y110	A111	A112	Q113	M114	I115	Y116	T117	Y118	S119	G120	L121	F122	C123
D4	A5	E6	M7	A8	A9	F10	G11	E12	A13	A14	P15	Y16	L17	R18	K19	S20	E21	K22	E23	R24	I25	E26	A27	Q28	N29	K30	P31	F32	D33	A34	K35	S36	S37	V38	F39	V40	V41	H42	P43	K44	Q45	S46	F47	V48	K49	G50	T51	I52	Q53	S54	K55	E56	G57	G58	K59	V60	T61	V62	K63



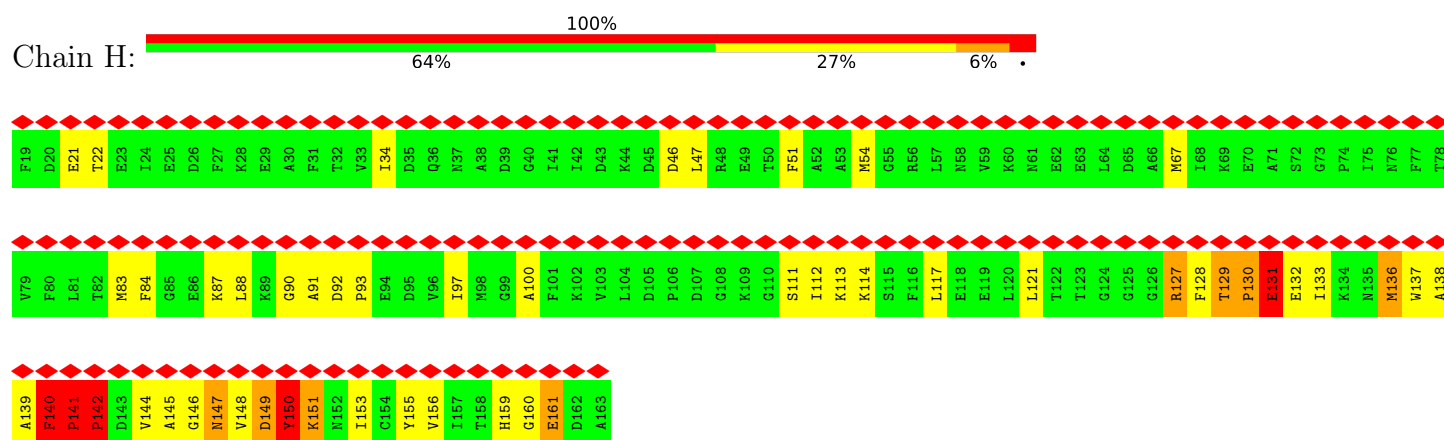
Frequency	Percentage
100%	100%
66%	66%
26%	26%
6%	6%



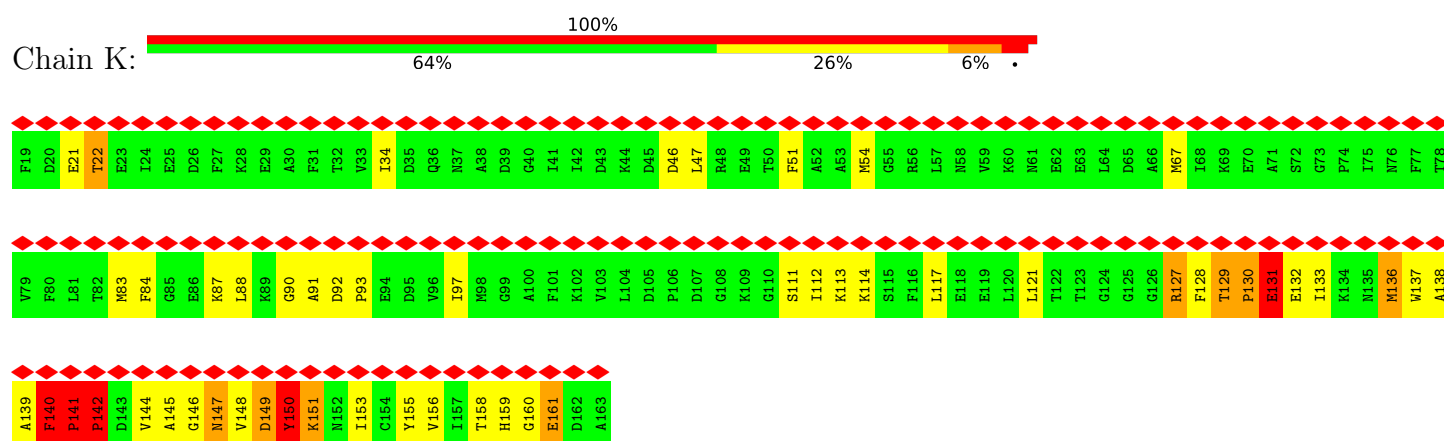
• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN



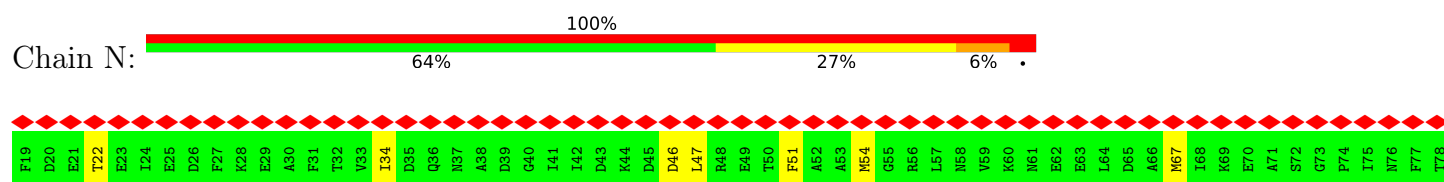
• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

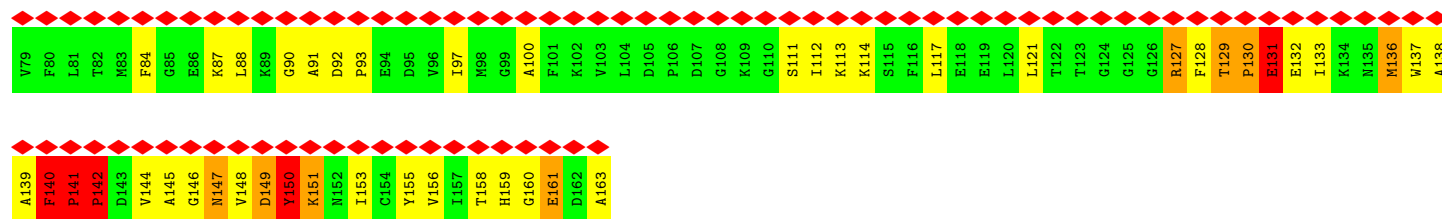


• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

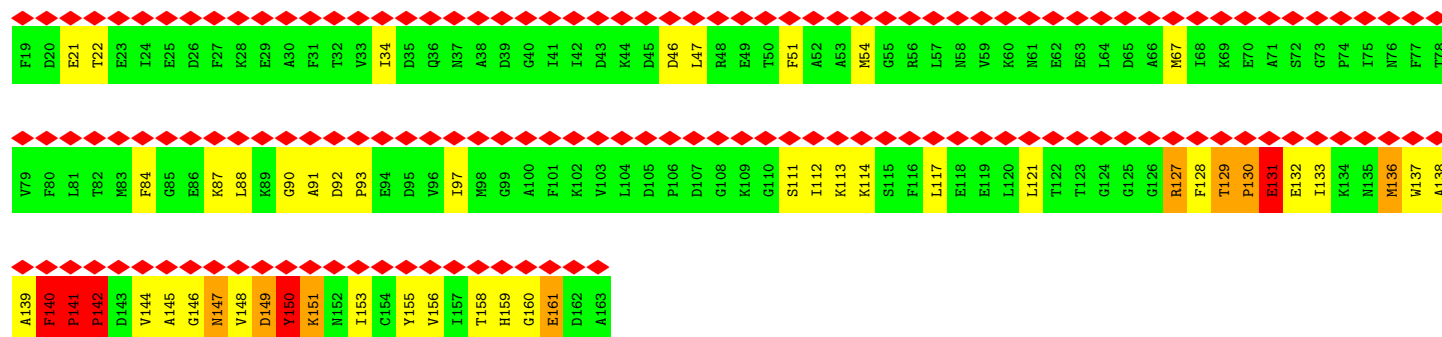


• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

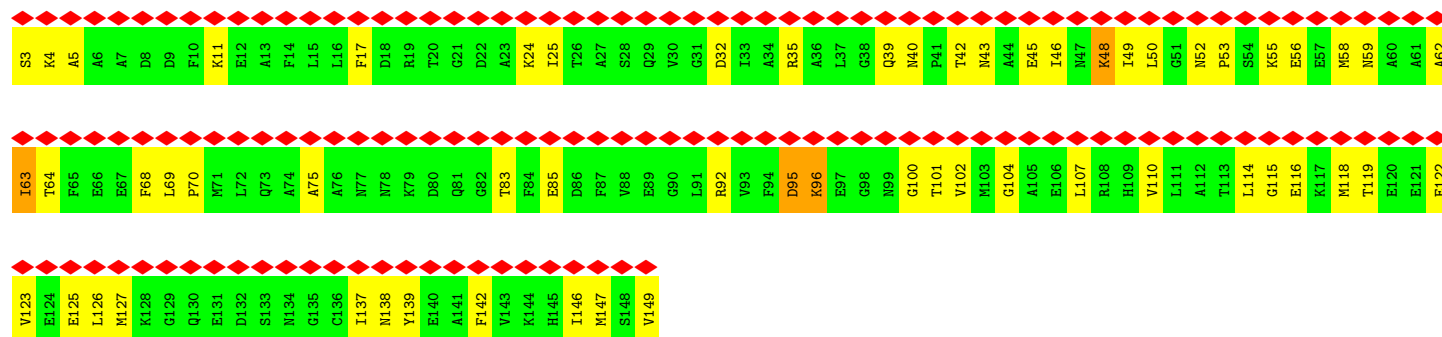




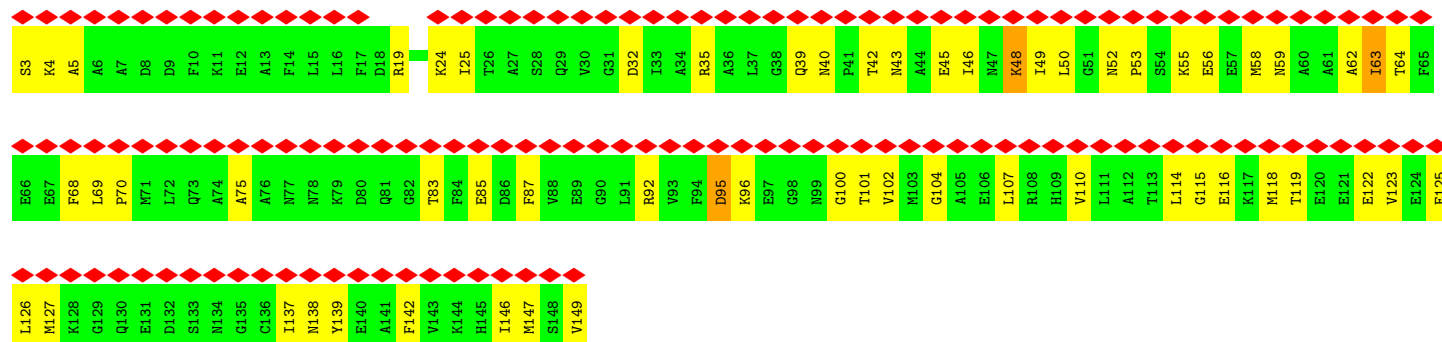
• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN



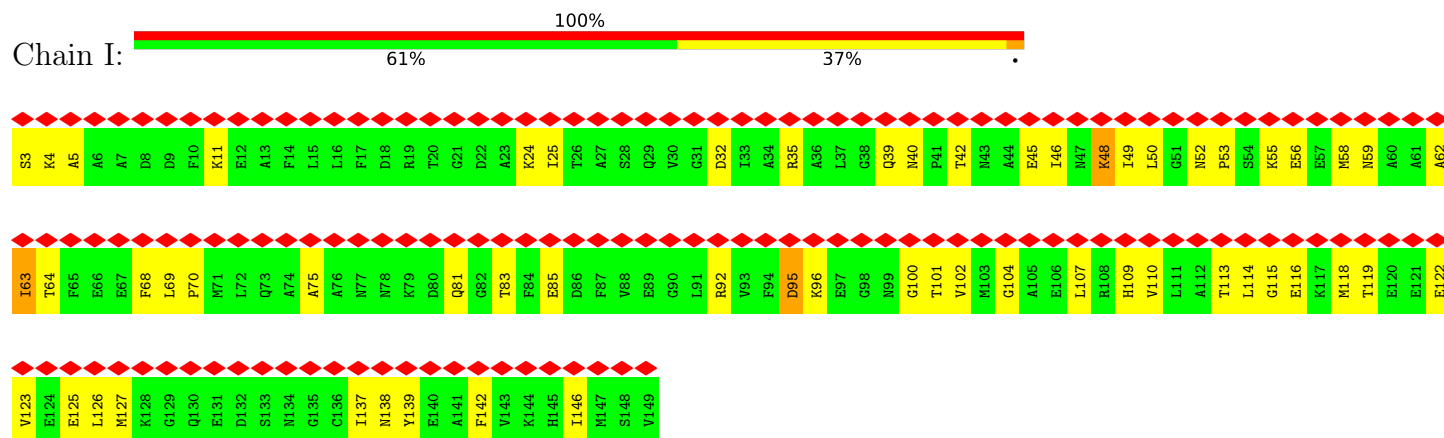
• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN



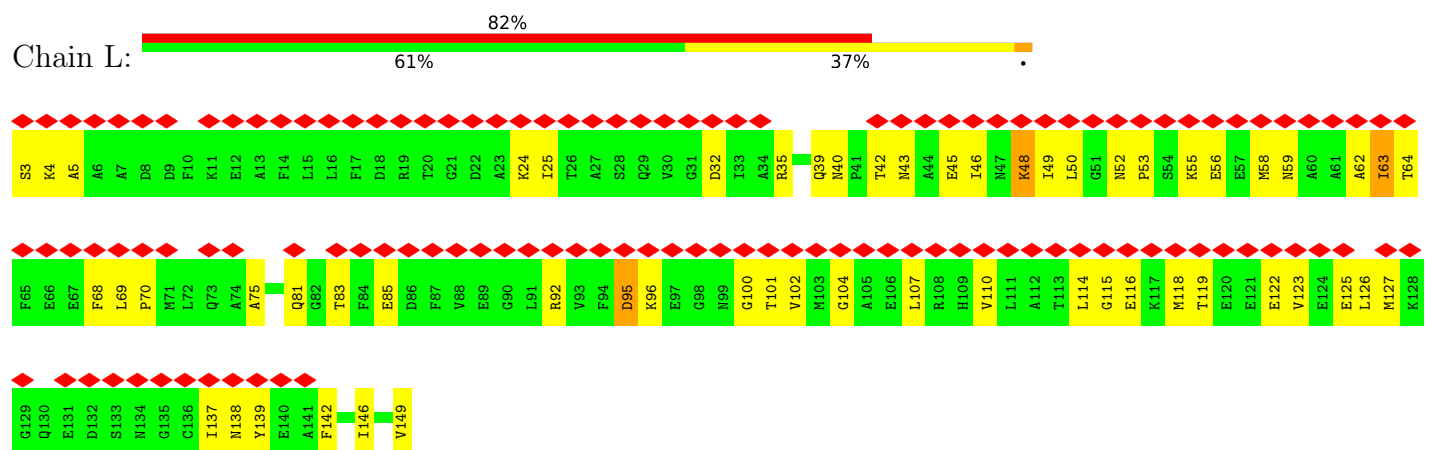
• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN



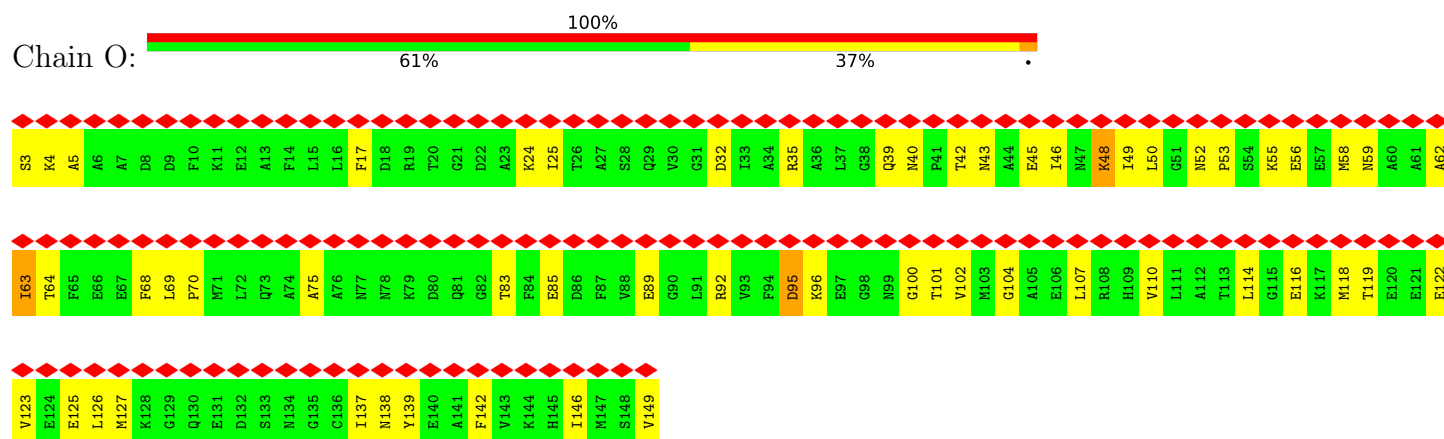
- Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN



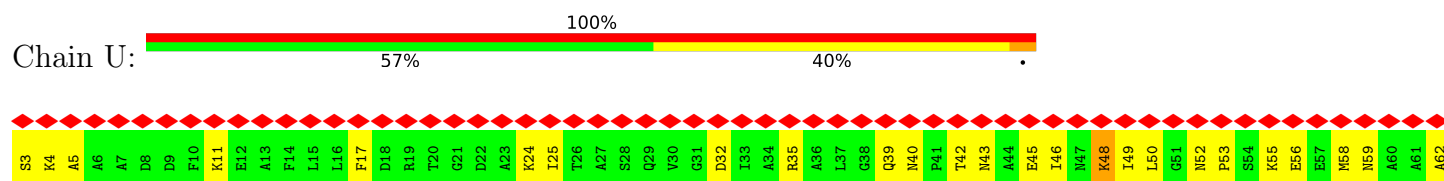
- Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN

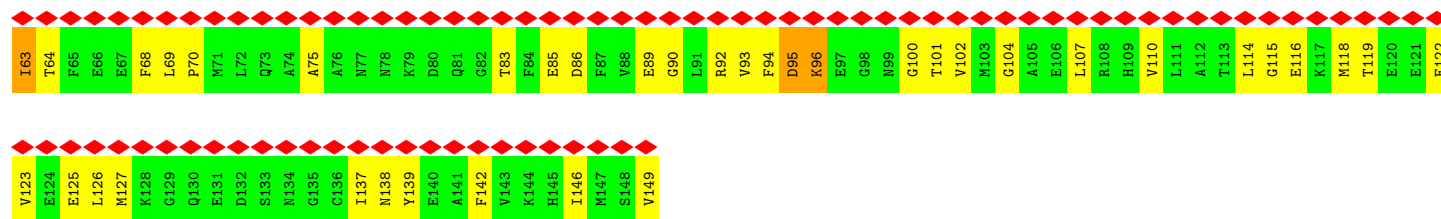


- Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN

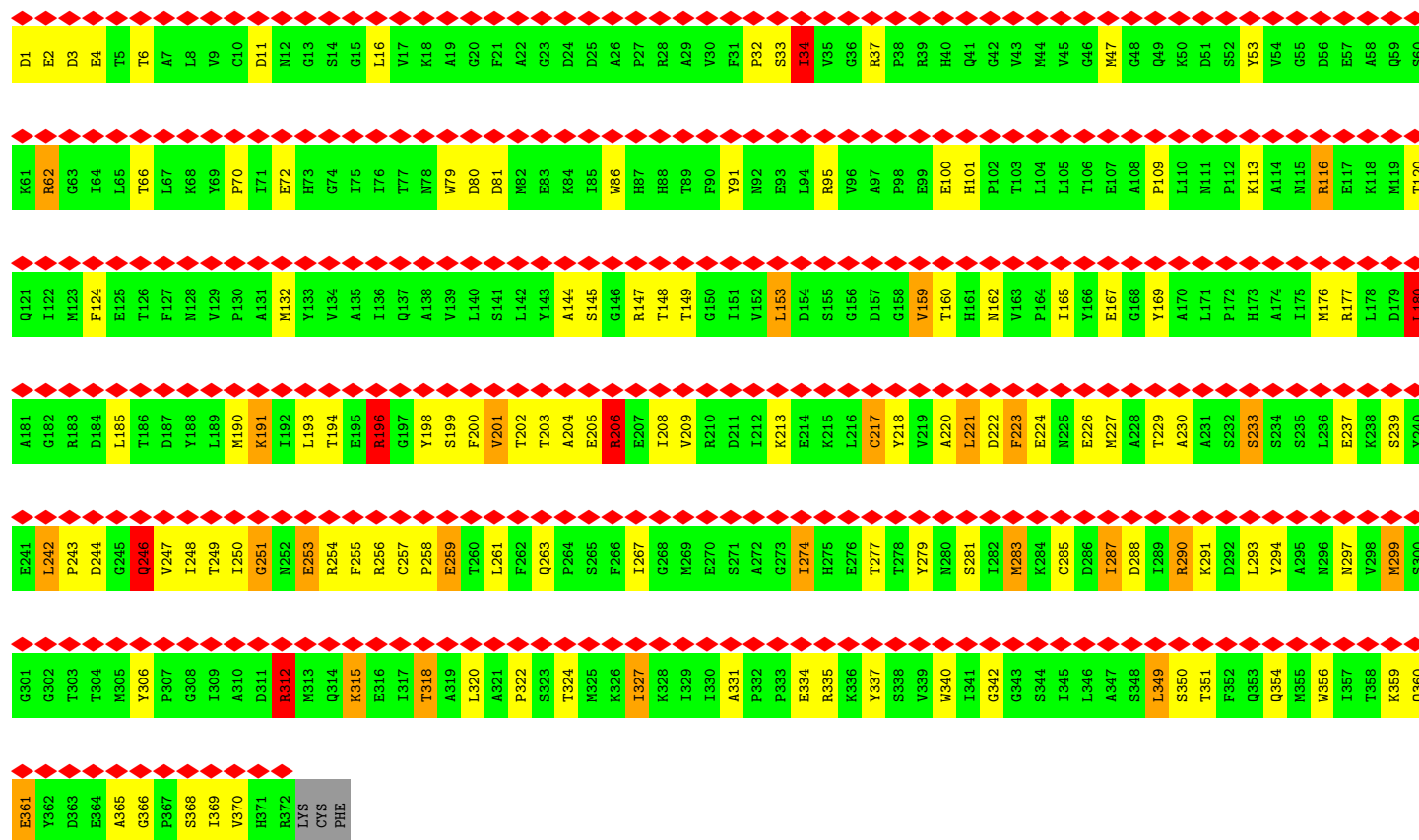


- Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN

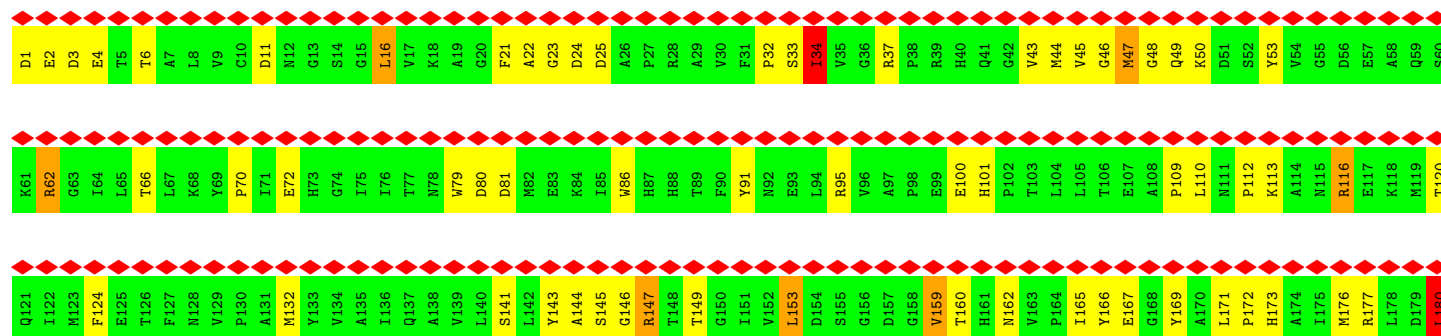


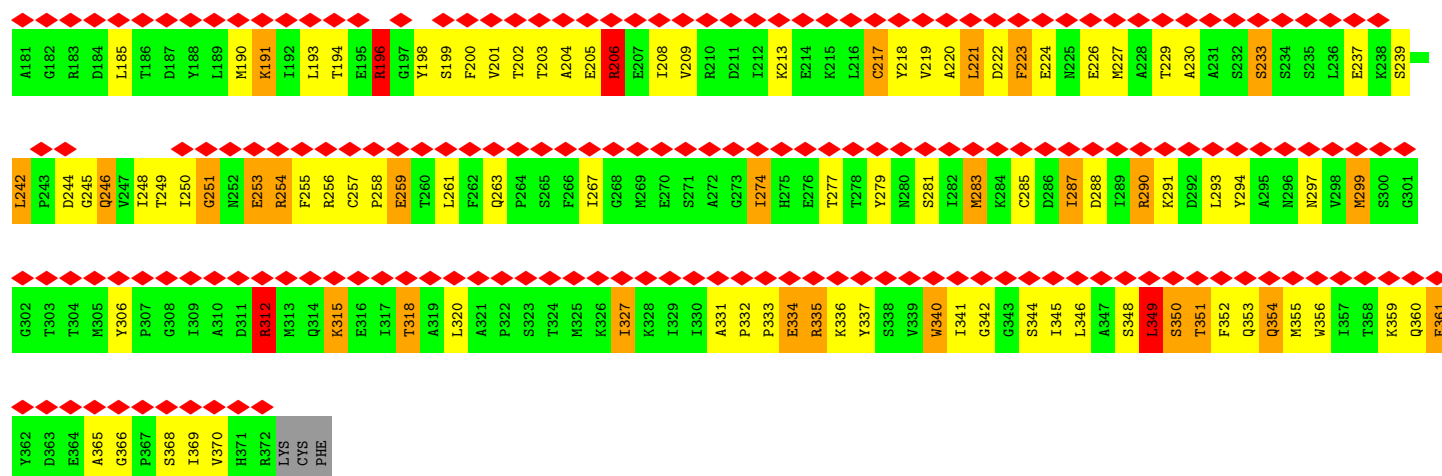


• Molecule 4: SKELETAL MUSCLE ACTIN

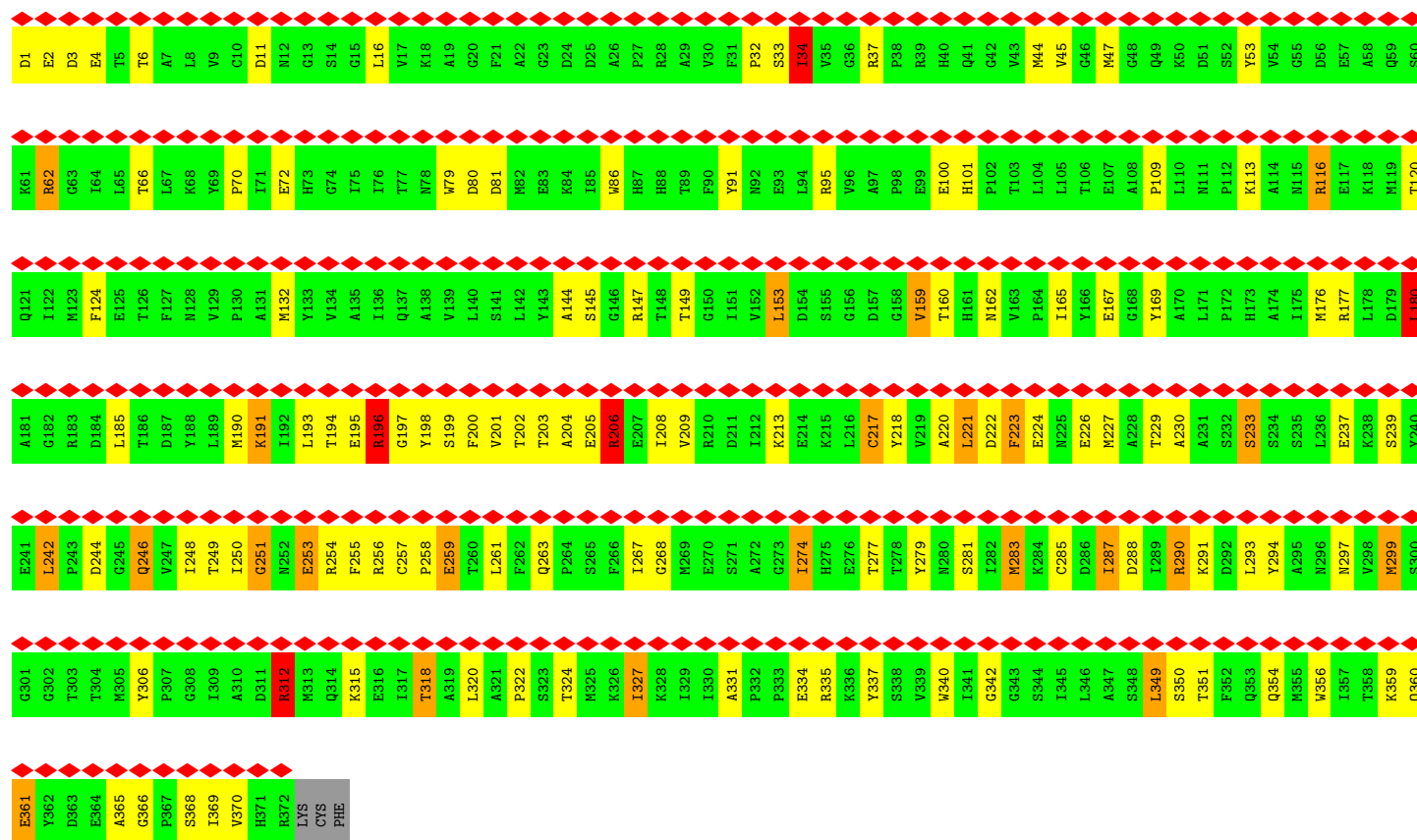


• Molecule 4: SKELETAL MUSCLE ACTIN

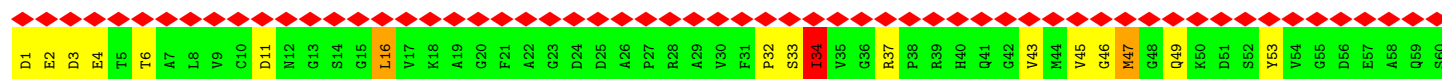




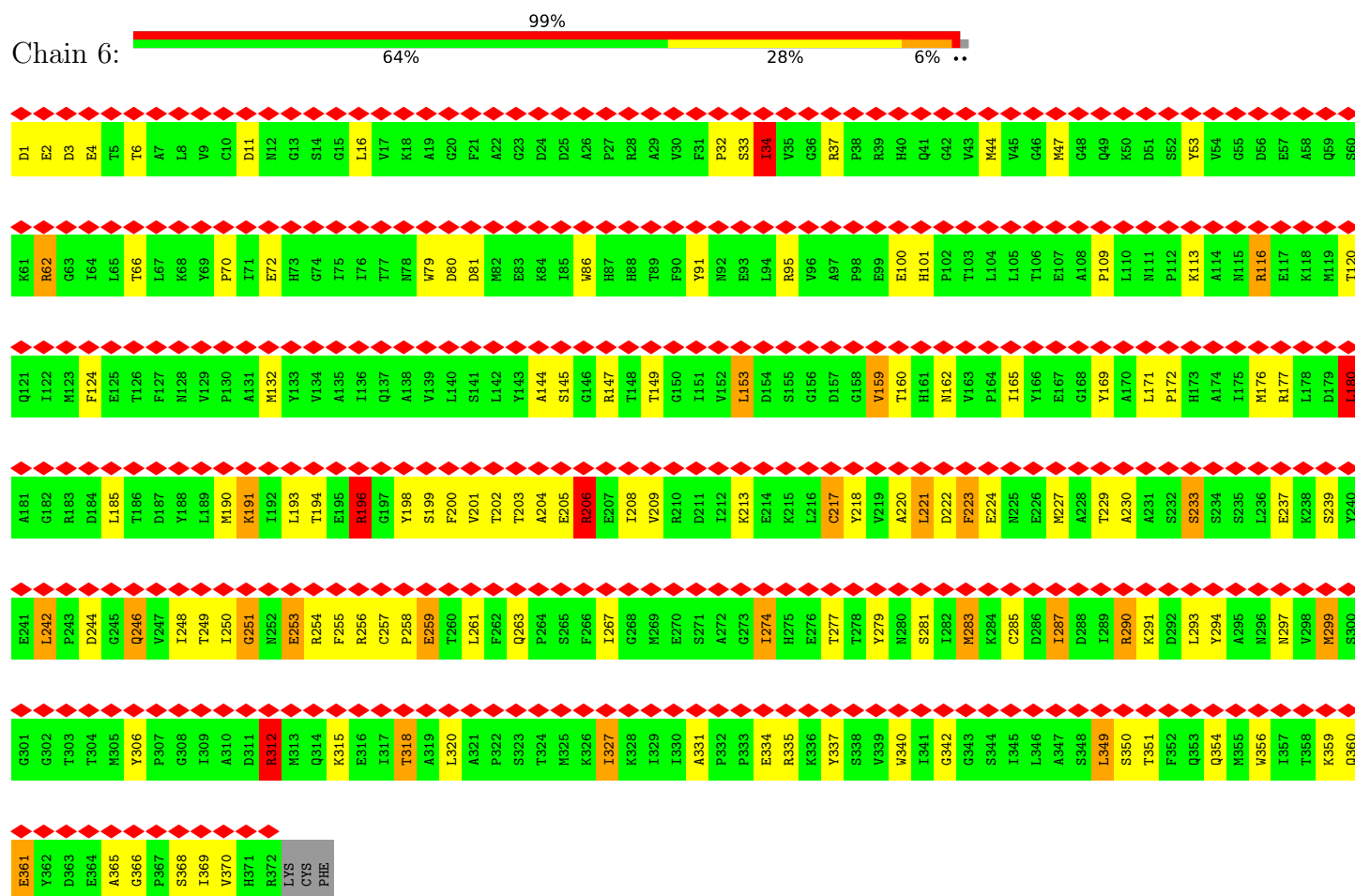
• Molecule 4: SKELETAL MUSCLE ACTIN



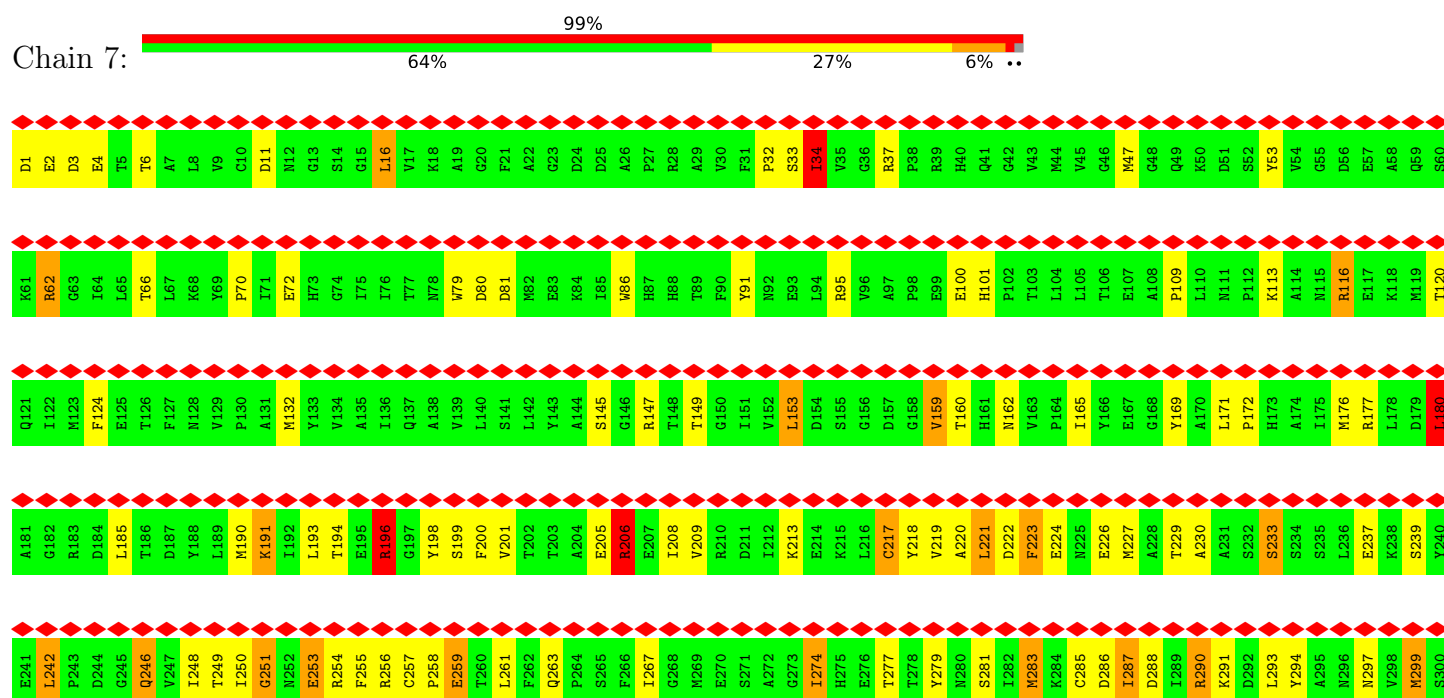
• Molecule 4: SKELETAL MUSCLE ACTIN



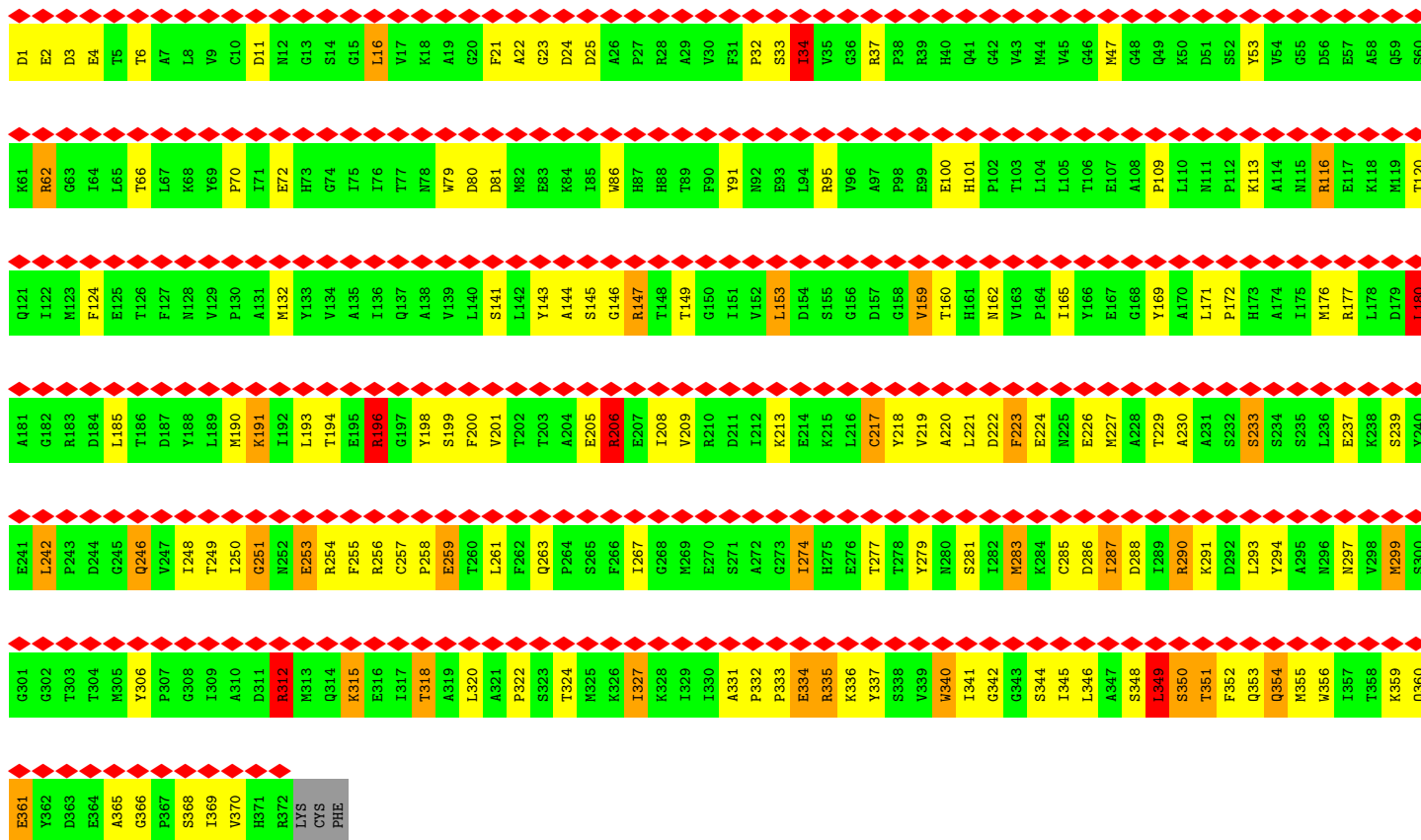
● Molecule 4: SKELETAL MUSCLE ACTIN



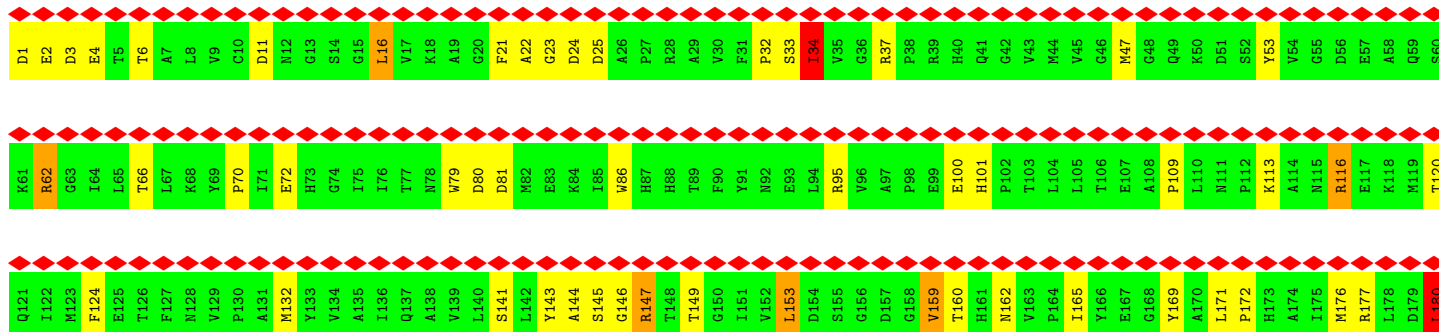
● Molecule 4: SKELETAL MUSCLE ACTIN

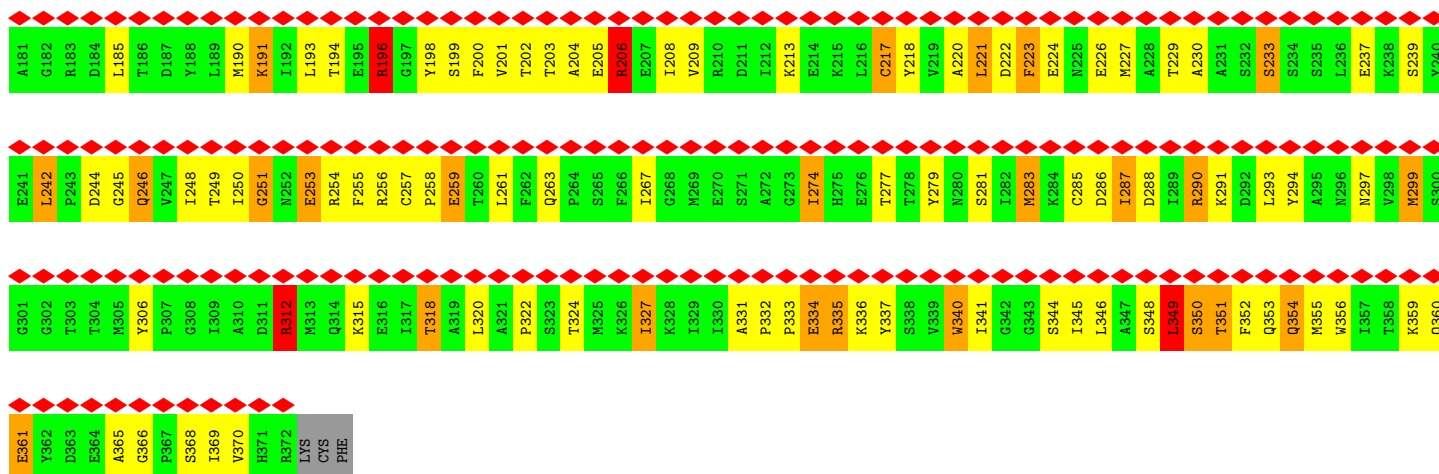


- Molecule 4: SKELETAL MUSCLE ACTIN

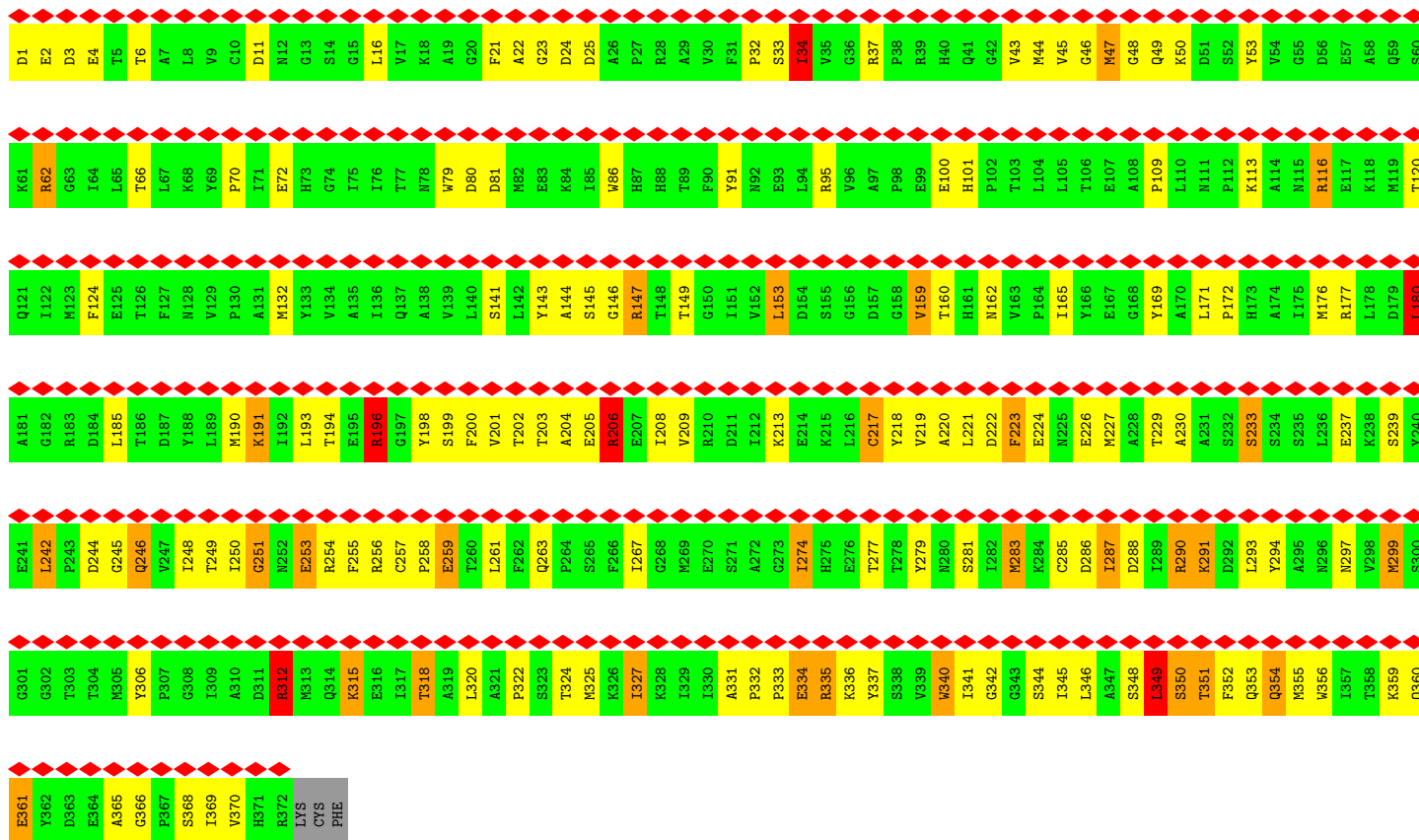


- Molecule 4: SKELETAL MUSCLE ACTIN

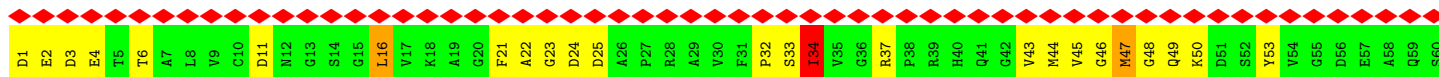


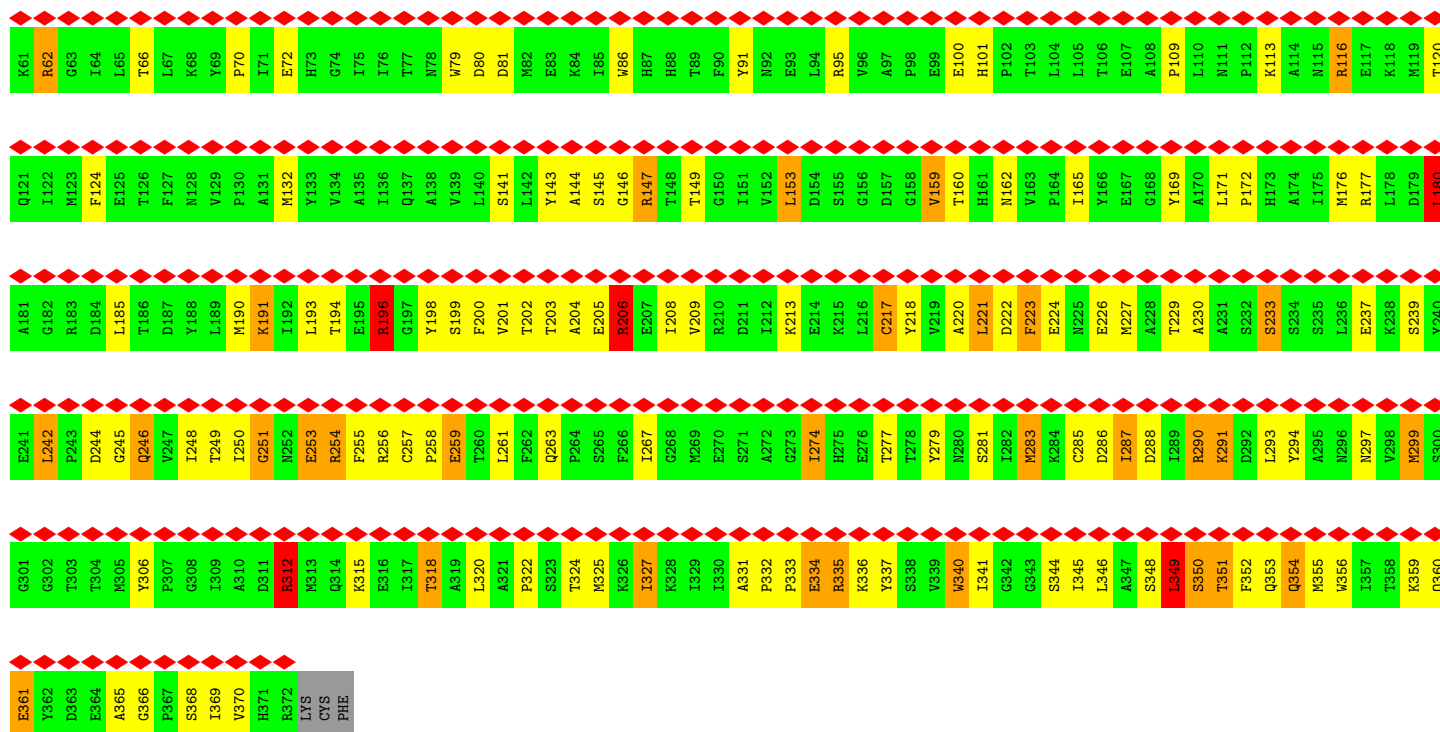


• Molecule 4: SKELETAL MUSCLE ACTIN

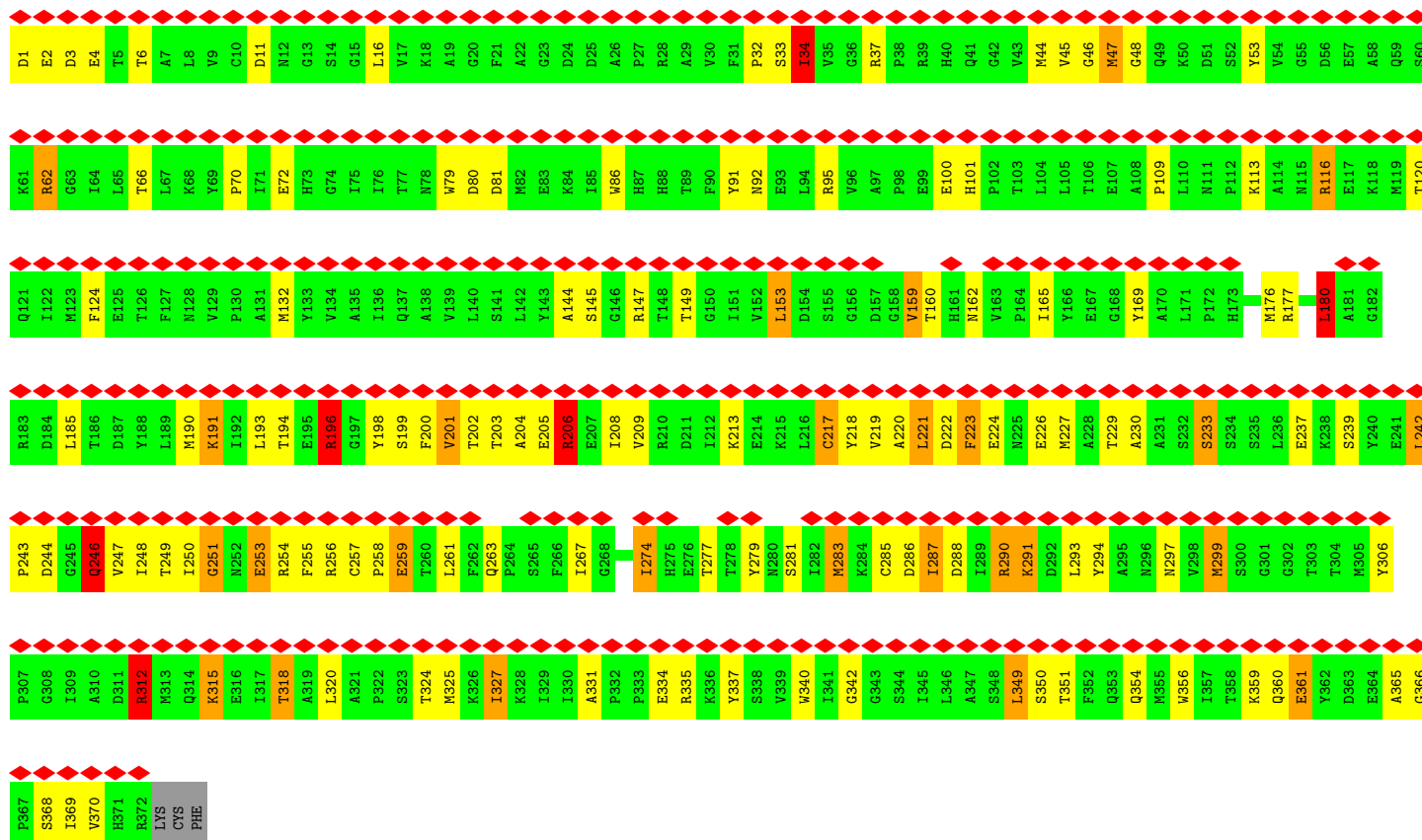
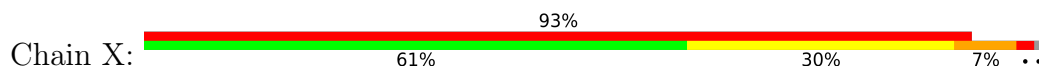


• Molecule 4: SKELETAL MUSCLE ACTIN





Molecule 4: SKELETAL MUSCLE ACTIN



E361	G301
Y362	G302
D363	T303
E364	T304
A365	M305
G366	Y306
P367	P307
S368	G308
T369	T309
V370	A310
H371	D311
R372	R312
LYS	M313
CYS	Q314
PHE	K315
	E316
	I317
	T318
	A319
	L320
	A321
	P322
	S323
	T324
	M325
	K326
	I327
	K328
	I329
	T330
	A331
	P332
	P333
	E334
	R335
	K336
	Y337
	S338
	V339
	W340
	I341
	G342
	G343
	S344
	I345
	L346
	A347
	S348
	L349
	S350
	T351
	F352
	Q353
	Q354
	M355
	W356
	I357
	T358
	K359
	Q360

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 ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.77	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 ⓘ

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 ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	MLY	G	551	1	9,10,11	0.53	0	6,11,13	0.19	0
1	MLY	S	353	1	9,10,11	0.86	0	6,11,13	0.78	0
1	MLY	D	385	1	9,10,11	0.97	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	M	504	1	9,10,11	0.85	0	6,11,13	0.23	0
1	MLY	M	107	1	9,10,11	0.48	0	6,11,13	0.34	0
1	MLY	S	833	1	9,10,11	1.18	1 (11%)	6,11,13	0.31	0
1	MLY	J	528	1	9,10,11	0.88	0	6,11,13	0.65	0
1	MLY	S	827	1	9,10,11	0.72	0	6,11,13	0.49	0
1	MLY	G	369	1	9,10,11	0.70	0	6,11,13	0.46	0
1	MLY	A	782	1	9,10,11	0.79	0	6,11,13	0.37	0
1	MLY	D	839	1	9,10,11	0.67	0	6,11,13	0.79	0
1	MLY	J	49	1	9,10,11	1.08	1 (11%)	6,11,13	0.74	0
1	MLY	J	295	1	9,10,11	0.78	0	6,11,13	0.35	0
1	MLY	A	659	1	9,10,11	0.84	0	6,11,13	0.59	0
1	MLY	A	296	1	9,10,11	0.62	0	6,11,13	0.36	0
1	MLY	G	63	1	9,10,11	0.90	0	6,11,13	0.43	0
1	MLY	J	63	1	9,10,11	0.89	0	6,11,13	0.43	0
1	MLY	A	353	1	9,10,11	0.86	0	6,11,13	0.79	0
1	MLY	J	681	1	9,10,11	0.59	0	6,11,13	0.46	0
1	MLY	S	84	1	9,10,11	0.50	0	6,11,13	0.80	0
1	MLY	D	598	1	9,10,11	0.91	1 (11%)	6,11,13	0.43	0
1	MLY	S	528	1	9,10,11	0.89	0	6,11,13	0.66	0
1	MLY	G	272	1	9,10,11	0.97	1 (11%)	6,11,13	0.54	0
1	MLY	J	272	1	9,10,11	0.99	1 (11%)	6,11,13	0.56	0
1	MLY	M	353	1	9,10,11	0.85	0	6,11,13	0.79	0
1	MLY	M	385	1	9,10,11	1.02	1 (11%)	6,11,13	0.44	0
1	MLY	A	553	1,4	9,10,11	0.68	0	6,11,13	0.55	0
1	MLY	S	295	1	9,10,11	0.77	0	6,11,13	0.34	0
1	MLY	D	504	1	9,10,11	0.88	0	6,11,13	0.21	0
1	MLY	S	681	1	9,10,11	0.63	0	6,11,13	0.46	0
1	MLY	S	837	1	9,10,11	0.58	0	6,11,13	0.54	0
1	MLY	A	613	1	9,10,11	0.57	0	6,11,13	0.63	0
1	MLY	D	272	1	9,10,11	0.95	1 (11%)	6,11,13	0.58	0
1	MLY	G	385	1	9,10,11	0.99	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	J	415	1	9,10,11	0.77	0	6,11,13	0.18	0
1	MLY	S	30	1	9,10,11	0.89	0	6,11,13	0.32	0
1	MLY	G	431	1	9,10,11	0.52	0	6,11,13	0.46	0
1	MLY	D	130	1	9,10,11	0.80	0	6,11,13	0.74	0
1	MLY	D	528	1	9,10,11	0.91	0	6,11,13	0.64	0
1	MLY	G	367	1	9,10,11	0.66	0	6,11,13	0.38	0
1	MLY	G	553	1,4	9,10,11	0.67	0	6,11,13	0.55	0
1	MLY	J	768	1	9,10,11	0.77	0	6,11,13	0.42	0
1	MLY	G	138	1	9,10,11	1.35	1 (11%)	6,11,13	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	A	19	1	9,10,11	1.12	1 (11%)	6,11,13	0.58	0
1	MLY	M	505	1	9,10,11	0.93	1 (11%)	6,11,13	0.33	0
1	MLY	S	415	1	9,10,11	0.77	0	6,11,13	0.18	0
1	MLY	G	87	1	9,10,11	1.22	1 (11%)	6,11,13	0.43	0
1	MLY	G	436	1	9,10,11	1.04	1 (11%)	6,11,13	0.48	0
1	MLY	D	353	1	9,10,11	0.85	0	6,11,13	0.79	0
1	MLY	A	138	1	9,10,11	1.33	1 (11%)	6,11,13	0.84	0
1	MLY	J	385	1	9,10,11	1.01	1 (11%)	6,11,13	0.44	0
1	MLY	S	551	1	9,10,11	0.53	0	6,11,13	0.19	0
1	MLY	S	768	1	9,10,11	0.75	0	6,11,13	0.42	0
1	MLY	J	833	1	9,10,11	1.19	1 (11%)	6,11,13	0.31	0
1	MLY	A	369	1	9,10,11	0.71	0	6,11,13	0.46	0
1	MLY	D	505	1	9,10,11	0.86	1 (11%)	6,11,13	0.35	0
1	MLY	J	600	1	9,10,11	0.53	0	6,11,13	0.37	0
1	MLY	J	84	1	9,10,11	0.49	0	6,11,13	0.80	0
1	MLY	A	55	1	9,10,11	0.71	0	6,11,13	0.79	0
1	MLY	A	415	1	9,10,11	0.76	0	6,11,13	0.19	0
1	MLY	G	353	1	9,10,11	0.86	0	6,11,13	0.80	0
1	MLY	A	431	1	9,10,11	0.51	0	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	D	827	1	9,10,11	0.67	0	6,11,13	0.48	0
1	MLY	M	551	1	9,10,11	0.53	0	6,11,13	0.19	0
1	MLY	D	782	1	9,10,11	0.79	0	6,11,13	0.34	0
1	MLY	A	551	1	9,10,11	0.52	0	6,11,13	0.19	0
1	MLY	D	84	1	9,10,11	0.51	0	6,11,13	0.80	0
1	MLY	J	598	1	9,10,11	0.88	1 (11%)	6,11,13	0.43	0
1	MLY	D	659	1	9,10,11	0.84	0	6,11,13	0.60	0
1	MLY	G	130	1	9,10,11	0.78	0	6,11,13	0.75	0
1	MLY	M	84	1	9,10,11	0.50	0	6,11,13	0.80	0
1	MLY	M	348	1	9,10,11	0.79	0	6,11,13	0.47	0
1	MLY	J	505	1	9,10,11	0.93	1 (11%)	6,11,13	0.34	0
1	MLY	M	598	1	9,10,11	0.91	1 (11%)	6,11,13	0.43	0
1	MLY	S	486	1	9,10,11	0.63	0	6,11,13	0.40	0
1	MLY	M	190	1	9,10,11	1.24	1 (11%)	6,11,13	0.53	0
1	MLY	M	59	1	9,10,11	0.88	0	6,11,13	0.49	0
1	MLY	A	617	1	9,10,11	0.96	1 (11%)	6,11,13	0.34	0
1	MLY	D	248	1	9,10,11	0.86	0	6,11,13	0.62	0
1	MLY	S	35	1	9,10,11	0.72	0	6,11,13	0.38	0
1	MLY	A	30	1	9,10,11	0.88	0	6,11,13	0.32	0
1	MLY	S	764	1	9,10,11	0.83	0	6,11,13	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	J	107	1	9,10,11	0.49	0	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	A	827	1	9,10,11	0.72	0	6,11,13	0.46	0
1	MLY	D	49	1	9,10,11	1.08	1 (11%)	6,11,13	0.75	0
1	MLY	G	35	1	9,10,11	0.72	0	6,11,13	0.39	0
1	MLY	G	837	1	9,10,11	0.59	0	6,11,13	0.53	0
1	MLY	D	30	1	9,10,11	0.92	0	6,11,13	0.32	0
1	MLY	J	87	1	9,10,11	1.20	1 (11%)	6,11,13	0.44	0
1	MLY	J	436	1	9,10,11	1.05	1 (11%)	6,11,13	0.50	0
1	MLY	J	837	1	9,10,11	0.59	0	6,11,13	0.56	0
1	MLY	M	30	1	9,10,11	0.89	0	6,11,13	0.32	0
1	MLY	S	272	1	9,10,11	0.99	1 (11%)	6,11,13	0.56	0
1	MLY	G	49	1	9,10,11	1.08	1 (11%)	6,11,13	0.74	0
1	MLY	S	431	1	9,10,11	0.51	0	6,11,13	0.44	0
1	MLY	S	617	1	9,10,11	0.98	1 (11%)	6,11,13	0.34	0
1	MLY	D	348	1	9,10,11	0.82	0	6,11,13	0.47	0
1	MLY	G	236	1	9,10,11	0.79	1 (11%)	6,11,13	0.48	0
1	MLY	G	296	1	9,10,11	0.65	0	6,11,13	0.37	0
1	MLY	J	236	1	9,10,11	0.79	1 (11%)	6,11,13	0.47	0
1	MLY	J	353	1	9,10,11	0.86	0	6,11,13	0.78	0
1	MLY	S	385	1	9,10,11	1.01	1 (11%)	6,11,13	0.44	0
1	MLY	D	431	1	9,10,11	0.53	0	6,11,13	0.45	0
1	MLY	G	505	1	9,10,11	0.88	1 (11%)	6,11,13	0.35	0
1	MLY	S	63	1	9,10,11	0.88	0	6,11,13	0.43	0
1	MLY	A	764	1	9,10,11	0.84	0	6,11,13	0.36	0
1	MLY	D	138	1	9,10,11	1.39	1 (11%)	6,11,13	0.86	0
1	MLY	M	138	1	9,10,11	1.34	1 (11%)	6,11,13	0.83	0
1	MLY	G	528	1	9,10,11	0.91	0	6,11,13	0.66	0
1	MLY	D	681	1	9,10,11	0.59	0	6,11,13	0.45	0
1	MLY	S	367	1	9,10,11	0.63	0	6,11,13	0.38	0
1	MLY	S	600	1	9,10,11	0.53	0	6,11,13	0.37	0
1	MLY	M	827	1	9,10,11	0.73	0	6,11,13	0.48	0
1	MLY	S	87	1	9,10,11	1.23	1 (11%)	6,11,13	0.43	0
1	MLY	M	764	1	9,10,11	0.83	0	6,11,13	0.38	0
1	MLY	M	782	1	9,10,11	0.78	0	6,11,13	0.36	0
1	MLY	S	49	1	9,10,11	1.11	1 (11%)	6,11,13	0.74	0
1	MLY	S	436	1	9,10,11	1.04	1 (11%)	6,11,13	0.49	0
1	MLY	M	617	1	9,10,11	0.97	1 (11%)	6,11,13	0.33	0
1	MLY	G	839	1	9,10,11	0.71	0	6,11,13	0.80	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	G	681	1	9,10,11	0.62	0	6,11,13	0.45	0
1	MLY	G	613	1	9,10,11	0.59	0	6,11,13	0.63	0
1	MLY	J	613	1	9,10,11	0.57	0	6,11,13	0.64	0
1	MLY	M	613	1	9,10,11	0.56	0	6,11,13	0.64	0
1	MLY	G	768	1	9,10,11	0.74	0	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	A	505	1	9,10,11	0.88	1 (11%)	6,11,13	0.33	0
1	MLY	J	659	1	9,10,11	0.82	0	6,11,13	0.57	0
1	MLY	M	600	1	9,10,11	0.53	0	6,11,13	0.37	0
1	MLY	D	600	1	9,10,11	0.51	0	6,11,13	0.37	0
1	MLY	A	768	1	9,10,11	0.76	0	6,11,13	0.41	0
1	MLY	A	528	1	9,10,11	0.88	0	6,11,13	0.67	0
1	MLY	D	87	1	9,10,11	1.15	1 (11%)	6,11,13	0.45	0
1	MLY	M	19	1	9,10,11	1.16	1 (11%)	6,11,13	0.57	0
1	MLY	J	551	1	9,10,11	0.54	0	6,11,13	0.19	0
1	MLY	J	30	1	9,10,11	0.89	0	6,11,13	0.32	0
1	MLY	J	138	1	9,10,11	1.34	1 (11%)	6,11,13	0.83	0
1	MLY	D	764	1	9,10,11	0.86	0	6,11,13	0.36	0
1	MLY	G	600	1	9,10,11	0.52	0	6,11,13	0.37	0
1	MLY	J	296	1	9,10,11	0.69	0	6,11,13	0.36	0
1	MLY	J	348	1	9,10,11	0.82	0	6,11,13	0.47	0
1	MLY	A	295	1	9,10,11	0.80	0	6,11,13	0.33	0
1	MLY	G	248	1	9,10,11	0.81	0	6,11,13	0.63	0
1	MLY	G	504	1	9,10,11	0.88	0	6,11,13	0.22	0
1	MLY	J	55	1	9,10,11	0.73	0	6,11,13	0.78	0
1	MLY	A	681	1	9,10,11	0.59	0	6,11,13	0.46	0
1	MLY	J	504	1	9,10,11	0.85	0	6,11,13	0.24	0
1	MLY	G	59	1	9,10,11	0.84	0	6,11,13	0.50	0
1	MLY	M	431	1	9,10,11	0.53	0	6,11,13	0.44	0
1	MLY	A	837	1	9,10,11	0.60	0	6,11,13	0.54	0
1	MLY	J	59	1	9,10,11	0.87	0	6,11,13	0.49	0
1	MLY	M	528	1	9,10,11	0.89	0	6,11,13	0.64	0
1	MLY	M	295	1	9,10,11	0.78	0	6,11,13	0.34	0
1	MLY	D	295	1	9,10,11	0.78	0	6,11,13	0.36	0
1	MLY	S	19	1	9,10,11	1.17	1 (11%)	6,11,13	0.57	0
1	MLY	M	768	1	9,10,11	0.76	0	6,11,13	0.42	0
1	MLY	M	681	1	9,10,11	0.60	0	6,11,13	0.46	0
1	MLY	J	839	1	9,10,11	0.68	0	6,11,13	0.77	0
1	MLY	G	30	1	9,10,11	0.88	0	6,11,13	0.30	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	659	1	9,10,11	0.85	0	6,11,13	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	M	63	1	9,10,11	0.91	0	6,11,13	0.43	0
1	MLY	M	833	1	9,10,11	1.17	1 (11%)	6,11,13	0.31	0
1	MLY	M	837	1	9,10,11	0.59	0	6,11,13	0.56	0
1	MLY	S	55	1	9,10,11	0.73	0	6,11,13	0.77	0
1	MLY	S	505	1	9,10,11	0.92	1 (11%)	6,11,13	0.33	0
1	MLY	S	504	1	9,10,11	0.85	0	6,11,13	0.23	0
1	MLY	S	59	1	9,10,11	0.86	0	6,11,13	0.50	0
1	MLY	G	84	1	9,10,11	0.49	0	6,11,13	0.80	0
1	MLY	G	827	1	9,10,11	0.71	0	6,11,13	0.49	0
1	MLY	M	369	1	9,10,11	0.70	0	6,11,13	0.45	0
1	MLY	G	782	1	9,10,11	0.77	0	6,11,13	0.35	0
1	MLY	J	782	1	9,10,11	0.79	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	M	415	1	9,10,11	0.78	0	6,11,13	0.19	0
1	MLY	G	190	1	9,10,11	1.26	1 (11%)	6,11,13	0.51	0
1	MLY	A	59	1	9,10,11	0.87	0	6,11,13	0.49	0
1	MLY	S	598	1	9,10,11	0.89	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	M	55	1	9,10,11	0.73	0	6,11,13	0.78	0
1	MLY	G	107	1	9,10,11	0.48	0	6,11,13	0.34	0
1	MLY	D	551	1	9,10,11	0.54	0	6,11,13	0.20	0
1	MLY	A	367	1	9,10,11	0.63	0	6,11,13	0.36	0
1	MLY	D	59	1	9,10,11	0.86	0	6,11,13	0.49	0
1	MLY	D	768	1	9,10,11	0.73	0	6,11,13	0.40	0
1	MLY	J	130	1	9,10,11	0.77	0	6,11,13	0.75	0
1	MLY	M	367	1	9,10,11	0.62	0	6,11,13	0.36	0
1	MLY	S	839	1	9,10,11	0.69	0	6,11,13	0.77	0
1	MLY	A	87	1	9,10,11	1.20	1 (11%)	6,11,13	0.42	0
1	MLY	D	190	1	9,10,11	1.21	1 (11%)	6,11,13	0.54	0
1	MLY	A	436	1	9,10,11	1.04	1 (11%)	6,11,13	0.49	0
1	MLY	A	833	1	9,10,11	1.15	1 (11%)	6,11,13	0.32	0
1	MLY	D	369	1	9,10,11	0.69	0	6,11,13	0.44	0
1	MLY	S	659	1	9,10,11	0.81	0	6,11,13	0.57	0
1	MLY	D	613	1	9,10,11	0.58	0	6,11,13	0.63	0
1	MLY	G	19	1	9,10,11	1.15	1 (11%)	6,11,13	0.58	0
1	MLY	J	19	1	9,10,11	1.18	1 (11%)	6,11,13	0.57	0
1	MLY	M	35	1	9,10,11	0.71	0	6,11,13	0.39	0
1	MLY	S	107	1	9,10,11	0.48	0	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	D	833	1	9,10,11	1.15	2 (22%)	6,11,13	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	S	130	1	9,10,11	0.78	0	6,11,13	0.75	0
1	MLY	J	248	1	9,10,11	0.84	0	6,11,13	0.62	0
1	MLY	S	553	1	9,10,11	0.67	0	6,11,13	0.53	0
1	MLY	D	19	1	9,10,11	1.19	1 (11%)	6,11,13	0.56	0
1	MLY	A	504	1	9,10,11	0.90	0	6,11,13	0.24	0
1	MLY	S	782	1	9,10,11	0.77	0	6,11,13	0.37	0
1	MLY	A	107	1	9,10,11	0.47	0	6,11,13	0.33	0
1	MLY	G	415	1	9,10,11	0.77	0	6,11,13	0.19	0
1	MLY	A	130	1	9,10,11	0.80	0	6,11,13	0.74	0
1	MLY	J	431	1	9,10,11	0.53	0	6,11,13	0.45	0
1	MLY	A	63	1	9,10,11	0.92	1 (11%)	6,11,13	0.44	0
1	MLY	D	55	1	9,10,11	0.72	0	6,11,13	0.79	0
1	MLY	S	248	1	9,10,11	0.82	0	6,11,13	0.62	0
1	MLY	J	190	1	9,10,11	1.25	1 (11%)	6,11,13	0.53	0
1	MLY	M	130	1	9,10,11	0.78	0	6,11,13	0.74	0
1	MLY	A	49	1	9,10,11	1.06	1 (11%)	6,11,13	0.74	0
1	MLY	D	486	1	9,10,11	0.66	0	6,11,13	0.38	0
1	MLY	G	295	1	9,10,11	0.78	0	6,11,13	0.33	0
1	MLY	M	49	1	9,10,11	1.08	1 (11%)	6,11,13	0.75	0
1	MLY	S	236	1	9,10,11	0.78	1 (11%)	6,11,13	0.47	0
1	MLY	A	35	1	9,10,11	0.71	0	6,11,13	0.38	0
1	MLY	S	296	1	9,10,11	0.68	0	6,11,13	0.36	0
1	MLY	M	839	1	9,10,11	0.71	0	6,11,13	0.77	0
1	MLY	G	833	1	9,10,11	1.17	2 (22%)	6,11,13	0.33	0
1	MLY	M	436	1	9,10,11	1.07	1 (11%)	6,11,13	0.50	0
1	MLY	D	436	1	9,10,11	1.09	1 (11%)	6,11,13	0.50	0
1	MLY	S	190	1	9,10,11	1.25	1 (11%)	6,11,13	0.52	0
1	MLY	A	600	1	9,10,11	0.50	0	6,11,13	0.37	0
1	MLY	M	248	1	9,10,11	0.82	0	6,11,13	0.62	0
1	MLY	J	369	1	9,10,11	0.69	0	6,11,13	0.46	0
1	MLY	G	764	1	9,10,11	0.81	0	6,11,13	0.35	0
1	MLY	A	248	1	9,10,11	0.83	0	6,11,13	0.61	0
1	MLY	G	598	1	9,10,11	0.90	1 (11%)	6,11,13	0.42	0
1	MLY	A	190	1	9,10,11	1.26	1 (11%)	6,11,13	0.51	0
1	MLY	J	553	1,4	9,10,11	0.67	0	6,11,13	0.54	0
1	MLY	D	107	1	9,10,11	0.51	0	6,11,13	0.34	0
1	MLY	M	272	1	9,10,11	1.02	1 (11%)	6,11,13	0.56	0
1	MLY	J	367	1	9,10,11	0.61	0	6,11,13	0.37	0
1	MLY	J	827	1	9,10,11	0.75	0	6,11,13	0.48	0
1	MLY	S	369	1	9,10,11	0.70	0	6,11,13	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	S	613	1	9,10,11	0.56	0	6,11,13	0.63	0
1	MLY	M	553	1,4	9,10,11	0.68	0	6,11,13	0.53	0
1	MLY	D	553	1,4	9,10,11	0.68	0	6,11,13	0.55	0
1	MLY	J	35	1	9,10,11	0.72	0	6,11,13	0.38	0
1	MLY	S	348	1	9,10,11	0.80	0	6,11,13	0.47	0
1	MLY	D	367	1	9,10,11	0.61	0	6,11,13	0.38	0
1	MLY	A	839	1	9,10,11	0.68	0	6,11,13	0.81	0
1	MLY	G	617	1	9,10,11	0.95	1 (11%)	6,11,13	0.35	0
1	MLY	J	764	1	9,10,11	0.83	0	6,11,13	0.37	0
1	MLY	J	617	1	9,10,11	0.96	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	138	1	9,10,11	1.33	1 (11%)	6,11,13	0.83	0
1	MLY	A	272	1	9,10,11	1.00	1 (11%)	6,11,13	0.56	0
1	MLY	G	486	1	9,10,11	0.65	0	6,11,13	0.39	0
1	MLY	J	486	1	9,10,11	0.63	0	6,11,13	0.40	0
1	MLY	M	486	1	9,10,11	0.64	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	M	659	1	9,10,11	0.81	0	6,11,13	0.57	0
1	MLY	D	617	1	9,10,11	0.96	1 (11%)	6,11,13	0.34	0
1	MLY	M	87	1	9,10,11	1.20	1 (11%)	6,11,13	0.43	0
1	MLY	M	236	1	9,10,11	0.80	1 (11%)	6,11,13	0.47	0
1	MLY	D	236	1	9,10,11	0.79	1 (11%)	6,11,13	0.48	0
1	MLY	D	35	1	9,10,11	0.73	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	D	296	1	9,10,11	0.64	0	6,11,13	0.38	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	G	551	1	-	3/8/9/11	-
1	MLY	S	353	1	-	4/8/9/11	-
1	MLY	D	385	1	-	2/8/9/11	-
1	MLY	M	504	1	-	4/8/9/11	-
1	MLY	M	107	1	-	2/8/9/11	-
1	MLY	S	833	1	-	6/8/9/11	-
1	MLY	J	528	1	-	5/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	S	827	1	-	0/8/9/11	-
1	MLY	G	369	1	-	2/8/9/11	-
1	MLY	A	782	1	-	6/8/9/11	-
1	MLY	D	839	1	-	3/8/9/11	-
1	MLY	J	49	1	-	3/8/9/11	-
1	MLY	J	295	1	-	2/8/9/11	-
1	MLY	A	659	1	-	3/8/9/11	-
1	MLY	A	296	1	-	4/8/9/11	-
1	MLY	G	63	1	-	4/8/9/11	-
1	MLY	J	63	1	-	4/8/9/11	-
1	MLY	A	353	1	-	4/8/9/11	-
1	MLY	J	681	1	-	4/8/9/11	-
1	MLY	S	84	1	-	4/8/9/11	-
1	MLY	D	598	1	-	5/8/9/11	-
1	MLY	S	528	1	-	4/8/9/11	-
1	MLY	G	272	1	-	3/8/9/11	-
1	MLY	J	272	1	-	3/8/9/11	-
1	MLY	M	353	1	-	4/8/9/11	-
1	MLY	M	385	1	-	2/8/9/11	-
1	MLY	A	553	1,4	-	4/8/9/11	-
1	MLY	S	295	1	-	2/8/9/11	-
1	MLY	D	504	1	-	4/8/9/11	-
1	MLY	S	681	1	-	4/8/9/11	-
1	MLY	S	837	1	-	5/8/9/11	-
1	MLY	A	613	1	-	4/8/9/11	-
1	MLY	D	272	1	-	3/8/9/11	-
1	MLY	G	385	1	-	2/8/9/11	-
1	MLY	G	348	1	-	5/8/9/11	-
1	MLY	J	415	1	-	3/8/9/11	-
1	MLY	S	30	1	-	2/8/9/11	-
1	MLY	G	431	1	-	4/8/9/11	-
1	MLY	D	130	1	-	5/8/9/11	-
1	MLY	D	528	1	-	4/8/9/11	-
1	MLY	G	367	1	-	2/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	G	553	1,4	-	4/8/9/11	-
1	MLY	J	768	1	-	4/8/9/11	-
1	MLY	G	138	1	-	4/8/9/11	-
1	MLY	A	19	1	-	4/8/9/11	-
1	MLY	M	505	1	-	5/8/9/11	-
1	MLY	S	415	1	-	3/8/9/11	-
1	MLY	G	87	1	-	2/8/9/11	-
1	MLY	G	436	1	-	4/8/9/11	-
1	MLY	D	353	1	-	4/8/9/11	-
1	MLY	A	138	1	-	4/8/9/11	-
1	MLY	J	385	1	-	2/8/9/11	-
1	MLY	S	551	1	-	3/8/9/11	-
1	MLY	S	768	1	-	4/8/9/11	-
1	MLY	J	833	1	-	6/8/9/11	-
1	MLY	A	369	1	-	2/8/9/11	-
1	MLY	D	505	1	-	5/8/9/11	-
1	MLY	J	600	1	-	3/8/9/11	-
1	MLY	J	84	1	-	4/8/9/11	-
1	MLY	A	55	1	-	6/8/9/11	-
1	MLY	A	415	1	-	3/8/9/11	-
1	MLY	G	353	1	-	4/8/9/11	-
1	MLY	A	431	1	-	4/8/9/11	-
1	MLY	A	598	1	-	5/8/9/11	-
1	MLY	D	827	1	-	0/8/9/11	-
1	MLY	M	551	1	-	3/8/9/11	-
1	MLY	D	782	1	-	6/8/9/11	-
1	MLY	A	551	1	-	3/8/9/11	-
1	MLY	D	84	1	-	4/8/9/11	-
1	MLY	J	598	1	-	5/8/9/11	-
1	MLY	D	659	1	-	3/8/9/11	-
1	MLY	G	130	1	-	5/8/9/11	-
1	MLY	M	84	1	-	4/8/9/11	-
1	MLY	M	348	1	-	5/8/9/11	-
1	MLY	J	505	1	-	5/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	M	598	1	-	5/8/9/11	-
1	MLY	S	486	1	-	2/8/9/11	-
1	MLY	M	190	1	-	5/8/9/11	-
1	MLY	M	59	1	-	3/8/9/11	-
1	MLY	A	617	1	-	1/8/9/11	-
1	MLY	D	248	1	-	6/8/9/11	-
1	MLY	S	35	1	-	3/8/9/11	-
1	MLY	A	30	1	-	2/8/9/11	-
1	MLY	S	764	1	-	2/8/9/11	-
1	MLY	J	107	1	-	2/8/9/11	-
1	MLY	A	486	1	-	2/8/9/11	-
1	MLY	A	827	1	-	0/8/9/11	-
1	MLY	D	49	1	-	3/8/9/11	-
1	MLY	G	35	1	-	3/8/9/11	-
1	MLY	G	837	1	-	5/8/9/11	-
1	MLY	D	30	1	-	2/8/9/11	-
1	MLY	J	87	1	-	2/8/9/11	-
1	MLY	J	436	1	-	4/8/9/11	-
1	MLY	J	837	1	-	5/8/9/11	-
1	MLY	M	30	1	-	2/8/9/11	-
1	MLY	S	272	1	-	3/8/9/11	-
1	MLY	G	49	1	-	3/8/9/11	-
1	MLY	S	431	1	-	4/8/9/11	-
1	MLY	S	617	1	-	1/8/9/11	-
1	MLY	D	348	1	-	5/8/9/11	-
1	MLY	G	236	1	-	3/8/9/11	-
1	MLY	G	296	1	-	4/8/9/11	-
1	MLY	J	236	1	-	3/8/9/11	-
1	MLY	J	353	1	-	4/8/9/11	-
1	MLY	S	385	1	-	2/8/9/11	-
1	MLY	D	431	1	-	4/8/9/11	-
1	MLY	G	505	1	-	5/8/9/11	-
1	MLY	S	63	1	-	4/8/9/11	-
1	MLY	A	764	1	-	2/8/9/11	-
1	MLY	D	138	1	-	4/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	M	138	1	-	4/8/9/11	-
1	MLY	G	528	1	-	4/8/9/11	-
1	MLY	D	681	1	-	4/8/9/11	-
1	MLY	S	367	1	-	2/8/9/11	-
1	MLY	S	600	1	-	3/8/9/11	-
1	MLY	M	827	1	-	0/8/9/11	-
1	MLY	S	87	1	-	2/8/9/11	-
1	MLY	M	764	1	-	2/8/9/11	-
1	MLY	M	782	1	-	6/8/9/11	-
1	MLY	S	49	1	-	3/8/9/11	-
1	MLY	S	436	1	-	4/8/9/11	-
1	MLY	M	617	1	-	1/8/9/11	-
1	MLY	G	839	1	-	3/8/9/11	-
1	MLY	G	681	1	-	4/8/9/11	-
1	MLY	G	613	1	-	4/8/9/11	-
1	MLY	J	613	1	-	4/8/9/11	-
1	MLY	M	613	1	-	4/8/9/11	-
1	MLY	G	768	1	-	4/8/9/11	-
1	MLY	A	84	1	-	4/8/9/11	-
1	MLY	A	505	1	-	5/8/9/11	-
1	MLY	J	659	1	-	3/8/9/11	-
1	MLY	M	600	1	-	3/8/9/11	-
1	MLY	D	600	1	-	3/8/9/11	-
1	MLY	A	768	1	-	4/8/9/11	-
1	MLY	A	528	1	-	5/8/9/11	-
1	MLY	D	87	1	-	2/8/9/11	-
1	MLY	M	19	1	-	4/8/9/11	-
1	MLY	J	551	1	-	3/8/9/11	-
1	MLY	J	30	1	-	2/8/9/11	-
1	MLY	J	138	1	-	4/8/9/11	-
1	MLY	D	764	1	-	2/8/9/11	-
1	MLY	G	600	1	-	3/8/9/11	-
1	MLY	J	296	1	-	4/8/9/11	-
1	MLY	J	348	1	-	5/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	A	295	1	-	2/8/9/11	-
1	MLY	G	248	1	-	6/8/9/11	-
1	MLY	G	504	1	-	4/8/9/11	-
1	MLY	J	55	1	-	6/8/9/11	-
1	MLY	A	681	1	-	4/8/9/11	-
1	MLY	J	504	1	-	4/8/9/11	-
1	MLY	G	59	1	-	3/8/9/11	-
1	MLY	M	431	1	-	4/8/9/11	-
1	MLY	A	837	1	-	5/8/9/11	-
1	MLY	J	59	1	-	3/8/9/11	-
1	MLY	M	528	1	-	5/8/9/11	-
1	MLY	M	295	1	-	2/8/9/11	-
1	MLY	D	295	1	-	2/8/9/11	-
1	MLY	S	19	1	-	4/8/9/11	-
1	MLY	M	768	1	-	4/8/9/11	-
1	MLY	M	681	1	-	4/8/9/11	-
1	MLY	J	839	1	-	3/8/9/11	-
1	MLY	G	30	1	-	2/8/9/11	-
1	MLY	D	63	1	-	4/8/9/11	-
1	MLY	D	837	1	-	5/8/9/11	-
1	MLY	G	659	1	-	3/8/9/11	-
1	MLY	M	63	1	-	4/8/9/11	-
1	MLY	M	833	1	-	6/8/9/11	-
1	MLY	M	837	1	-	5/8/9/11	-
1	MLY	S	55	1	-	6/8/9/11	-
1	MLY	S	505	1	-	5/8/9/11	-
1	MLY	S	504	1	-	4/8/9/11	-
1	MLY	S	59	1	-	3/8/9/11	-
1	MLY	G	84	1	-	4/8/9/11	-
1	MLY	G	827	1	-	0/8/9/11	-
1	MLY	M	369	1	-	2/8/9/11	-
1	MLY	G	782	1	-	6/8/9/11	-
1	MLY	J	782	1	-	6/8/9/11	-
1	MLY	A	385	1	-	2/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	M	415	1	-	3/8/9/11	-
1	MLY	G	190	1	-	5/8/9/11	-
1	MLY	A	59	1	-	3/8/9/11	-
1	MLY	S	598	1	-	5/8/9/11	-
1	MLY	A	236	1	-	3/8/9/11	-
1	MLY	M	55	1	-	6/8/9/11	-
1	MLY	G	107	1	-	2/8/9/11	-
1	MLY	D	551	1	-	3/8/9/11	-
1	MLY	A	367	1	-	2/8/9/11	-
1	MLY	D	59	1	-	3/8/9/11	-
1	MLY	D	768	1	-	4/8/9/11	-
1	MLY	J	130	1	-	5/8/9/11	-
1	MLY	M	367	1	-	2/8/9/11	-
1	MLY	S	839	1	-	3/8/9/11	-
1	MLY	A	87	1	-	2/8/9/11	-
1	MLY	D	190	1	-	5/8/9/11	-
1	MLY	A	436	1	-	4/8/9/11	-
1	MLY	A	833	1	-	6/8/9/11	-
1	MLY	D	369	1	-	2/8/9/11	-
1	MLY	S	659	1	-	3/8/9/11	-
1	MLY	D	613	1	-	4/8/9/11	-
1	MLY	G	19	1	-	4/8/9/11	-
1	MLY	J	19	1	-	4/8/9/11	-
1	MLY	M	35	1	-	3/8/9/11	-
1	MLY	S	107	1	-	2/8/9/11	-
1	MLY	D	415	1	-	3/8/9/11	-
1	MLY	D	833	1	-	6/8/9/11	-
1	MLY	S	130	1	-	5/8/9/11	-
1	MLY	J	248	1	-	6/8/9/11	-
1	MLY	S	553	1	-	4/8/9/11	-
1	MLY	D	19	1	-	4/8/9/11	-
1	MLY	A	504	1	-	4/8/9/11	-
1	MLY	S	782	1	-	6/8/9/11	-
1	MLY	A	107	1	-	2/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	G	415	1	-	3/8/9/11	-
1	MLY	A	130	1	-	5/8/9/11	-
1	MLY	J	431	1	-	4/8/9/11	-
1	MLY	A	63	1	-	4/8/9/11	-
1	MLY	D	55	1	-	6/8/9/11	-
1	MLY	S	248	1	-	6/8/9/11	-
1	MLY	J	190	1	-	5/8/9/11	-
1	MLY	M	130	1	-	5/8/9/11	-
1	MLY	A	49	1	-	3/8/9/11	-
1	MLY	D	486	1	-	2/8/9/11	-
1	MLY	G	295	1	-	2/8/9/11	-
1	MLY	M	49	1	-	3/8/9/11	-
1	MLY	S	236	1	-	3/8/9/11	-
1	MLY	A	35	1	-	3/8/9/11	-
1	MLY	S	296	1	-	4/8/9/11	-
1	MLY	M	839	1	-	3/8/9/11	-
1	MLY	G	833	1	-	6/8/9/11	-
1	MLY	M	436	1	-	4/8/9/11	-
1	MLY	D	436	1	-	4/8/9/11	-
1	MLY	S	190	1	-	5/8/9/11	-
1	MLY	A	600	1	-	3/8/9/11	-
1	MLY	M	248	1	-	6/8/9/11	-
1	MLY	J	369	1	-	2/8/9/11	-
1	MLY	G	764	1	-	2/8/9/11	-
1	MLY	A	248	1	-	6/8/9/11	-
1	MLY	G	598	1	-	5/8/9/11	-
1	MLY	A	190	1	-	5/8/9/11	-
1	MLY	J	553	1,4	-	4/8/9/11	-
1	MLY	D	107	1	-	2/8/9/11	-
1	MLY	M	272	1	-	3/8/9/11	-
1	MLY	J	367	1	-	2/8/9/11	-
1	MLY	J	827	1	-	0/8/9/11	-
1	MLY	S	369	1	-	2/8/9/11	-
1	MLY	S	613	1	-	4/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	M	553	1,4	-	4/8/9/11	-
1	MLY	D	553	1,4	-	5/8/9/11	-
1	MLY	J	35	1	-	3/8/9/11	-
1	MLY	S	348	1	-	5/8/9/11	-
1	MLY	D	367	1	-	2/8/9/11	-
1	MLY	A	839	1	-	3/8/9/11	-
1	MLY	G	617	1	-	1/8/9/11	-
1	MLY	J	764	1	-	2/8/9/11	-
1	MLY	J	617	1	-	1/8/9/11	-
1	MLY	G	55	1	-	6/8/9/11	-
1	MLY	S	138	1	-	4/8/9/11	-
1	MLY	A	272	1	-	3/8/9/11	-
1	MLY	G	486	1	-	2/8/9/11	-
1	MLY	J	486	1	-	2/8/9/11	-
1	MLY	M	486	1	-	2/8/9/11	-
1	MLY	A	348	1	-	5/8/9/11	-
1	MLY	M	659	1	-	3/8/9/11	-
1	MLY	D	617	1	-	1/8/9/11	-
1	MLY	M	87	1	-	2/8/9/11	-
1	MLY	M	236	1	-	3/8/9/11	-
1	MLY	D	236	1	-	3/8/9/11	-
1	MLY	D	35	1	-	3/8/9/11	-
1	MLY	M	296	1	-	4/8/9/11	-
1	MLY	D	296	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	M	107	MLY	4	0
1	J	528	MLY	3	0
1	G	369	MLY	1	0
1	A	782	MLY	8	0
1	D	839	MLY	7	0
1	J	49	MLY	4	0
1	J	295	MLY	7	0
1	A	659	MLY	2	0
1	A	296	MLY	3	0
1	G	63	MLY	4	0
1	J	63	MLY	4	0
1	S	84	MLY	14	0
1	D	598	MLY	1	0
1	S	528	MLY	3	0
1	G	272	MLY	1	0
1	J	272	MLY	1	0
1	A	553	MLY	17	0
1	S	295	MLY	6	0
1	S	837	MLY	1	0
1	D	272	MLY	1	0
1	G	348	MLY	4	0
1	J	415	MLY	1	0
1	S	30	MLY	1	0
1	D	528	MLY	3	0
1	G	553	MLY	26	0
1	J	768	MLY	9	0
1	G	138	MLY	1	0
1	M	505	MLY	2	0
1	S	415	MLY	1	0
1	G	87	MLY	3	0
1	G	436	MLY	2	0
1	A	138	MLY	1	0
1	A	369	MLY	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	J	600	MLY	1	0
1	J	84	MLY	43	0
1	A	55	MLY	1	0
1	A	415	MLY	1	0
1	A	598	MLY	1	0
1	D	827	MLY	3	0
1	M	551	MLY	1	0
1	D	782	MLY	71	0
1	A	551	MLY	2	0
1	J	598	MLY	1	0
1	D	659	MLY	2	0
1	M	84	MLY	23	0
1	M	348	MLY	6	0
1	J	505	MLY	9	0
1	M	598	MLY	1	0
1	S	486	MLY	3	0
1	M	190	MLY	2	0
1	M	59	MLY	2	0
1	A	617	MLY	1	0
1	D	248	MLY	2	0
1	A	30	MLY	1	0
1	S	764	MLY	31	0
1	J	107	MLY	3	0
1	A	486	MLY	3	0
1	D	49	MLY	3	0
1	G	837	MLY	1	0
1	D	30	MLY	1	0
1	J	87	MLY	3	0
1	J	436	MLY	2	0
1	J	837	MLY	1	0
1	M	30	MLY	1	0
1	S	272	MLY	1	0
1	G	49	MLY	3	0
1	S	617	MLY	1	0
1	D	348	MLY	6	0
1	G	296	MLY	2	0
1	S	63	MLY	3	0
1	A	764	MLY	10	0
1	D	138	MLY	1	0
1	M	138	MLY	1	0
1	G	528	MLY	3	0
1	S	600	MLY	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	S	87	MLY	3	0
1	M	764	MLY	5	0
1	M	782	MLY	3	0
1	S	49	MLY	3	0
1	S	436	MLY	2	0
1	M	617	MLY	1	0
1	G	839	MLY	4	0
1	G	768	MLY	9	0
1	A	505	MLY	24	0
1	J	659	MLY	2	0
1	M	600	MLY	1	0
1	D	600	MLY	1	0
1	A	768	MLY	12	0
1	A	528	MLY	3	0
1	D	87	MLY	3	0
1	J	30	MLY	1	0
1	J	138	MLY	1	0
1	D	764	MLY	6	0
1	G	600	MLY	1	0
1	J	296	MLY	3	0
1	J	348	MLY	5	0
1	A	295	MLY	6	0
1	G	248	MLY	2	0
1	J	55	MLY	1	0
1	G	59	MLY	2	0
1	A	837	MLY	1	0
1	J	59	MLY	2	0
1	M	528	MLY	3	0
1	M	295	MLY	6	0
1	D	295	MLY	6	0
1	M	768	MLY	1	0
1	J	839	MLY	15	0
1	G	30	MLY	1	0
1	D	63	MLY	4	0
1	D	837	MLY	1	0
1	G	659	MLY	2	0
1	M	63	MLY	4	0
1	M	837	MLY	1	0
1	S	55	MLY	1	0
1	S	505	MLY	8	0
1	S	59	MLY	2	0
1	G	84	MLY	16	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	G	827	MLY	1	0
1	M	369	MLY	1	0
1	G	782	MLY	1	0
1	J	782	MLY	1	0
1	M	415	MLY	1	0
1	G	190	MLY	2	0
1	A	59	MLY	2	0
1	S	598	MLY	1	0
1	M	55	MLY	1	0
1	G	107	MLY	2	0
1	D	551	MLY	2	0
1	D	59	MLY	2	0
1	D	768	MLY	1	0
1	S	839	MLY	15	0
1	A	87	MLY	3	0
1	D	190	MLY	2	0
1	A	436	MLY	3	0
1	S	659	MLY	2	0
1	M	35	MLY	13	0
1	S	107	MLY	3	0
1	D	415	MLY	1	0
1	J	248	MLY	2	0
1	S	553	MLY	3	0
1	A	504	MLY	4	0
1	S	782	MLY	1	0
1	A	107	MLY	2	0
1	G	415	MLY	1	0
1	A	63	MLY	3	0
1	D	55	MLY	1	0
1	S	248	MLY	2	0
1	J	190	MLY	2	0
1	A	49	MLY	3	0
1	D	486	MLY	3	0
1	G	295	MLY	7	0
1	M	49	MLY	3	0
1	S	296	MLY	3	0
1	M	839	MLY	7	0
1	M	436	MLY	2	0
1	D	436	MLY	3	0
1	S	190	MLY	2	0
1	A	600	MLY	1	0
1	M	248	MLY	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	G	764	MLY	8	0
1	A	248	MLY	2	0
1	G	598	MLY	1	0
1	A	190	MLY	2	0
1	J	553	MLY	27	0
1	D	107	MLY	3	0
1	M	272	MLY	1	0
1	S	369	MLY	1	0
1	M	553	MLY	17	0
1	D	553	MLY	16	0
1	S	348	MLY	6	0
1	A	839	MLY	9	0
1	G	617	MLY	1	0
1	J	764	MLY	7	0
1	J	617	MLY	1	0
1	G	55	MLY	1	0
1	S	138	MLY	1	0
1	A	272	MLY	1	0
1	G	486	MLY	3	0
1	J	486	MLY	3	0
1	M	486	MLY	3	0
1	A	348	MLY	5	0
1	M	659	MLY	2	0
1	D	617	MLY	1	0
1	M	87	MLY	3	0
1	M	296	MLY	3	0
1	D	296	MLY	3	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

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

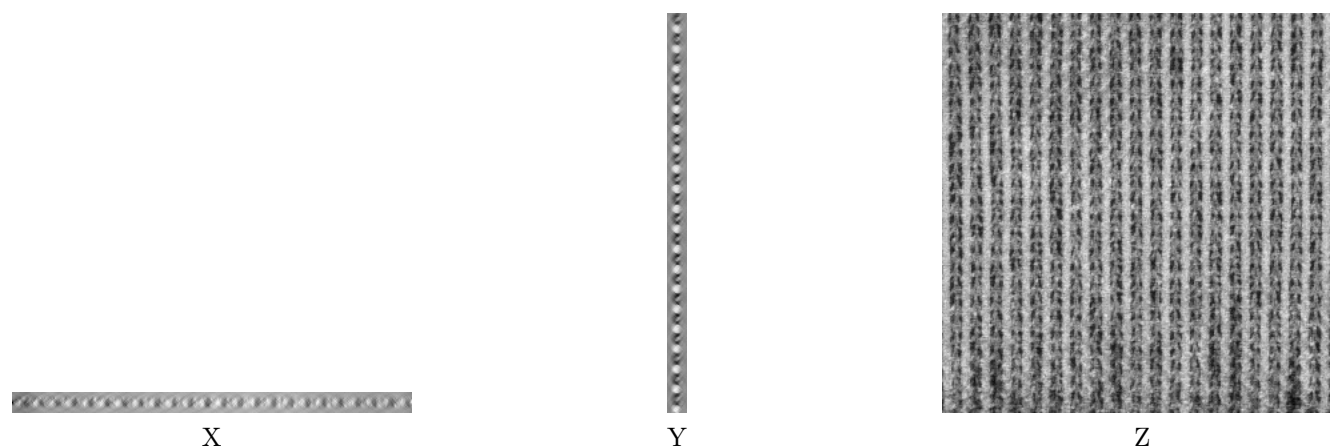
The worst 5 of 40 chain breaks are listed below:

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](#)

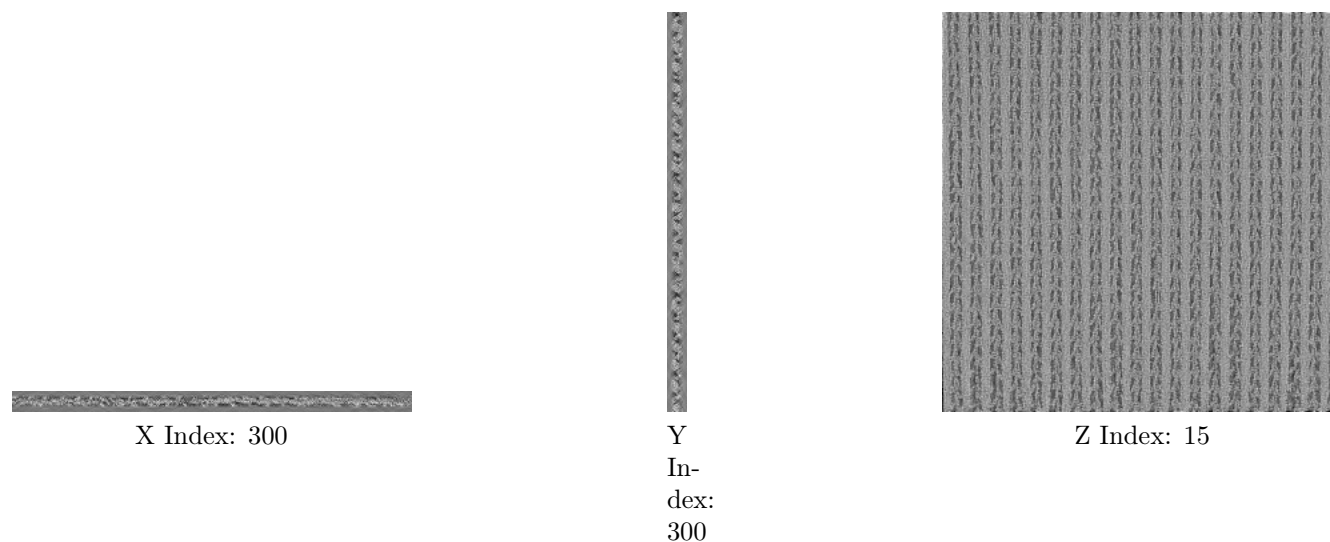
This section contains visualisations of the EMDB entry EMD-1001. These allow visual inspection of the internal detail of the tomogram and identification of artifacts.

6.1 Orthogonal projections [i](#)



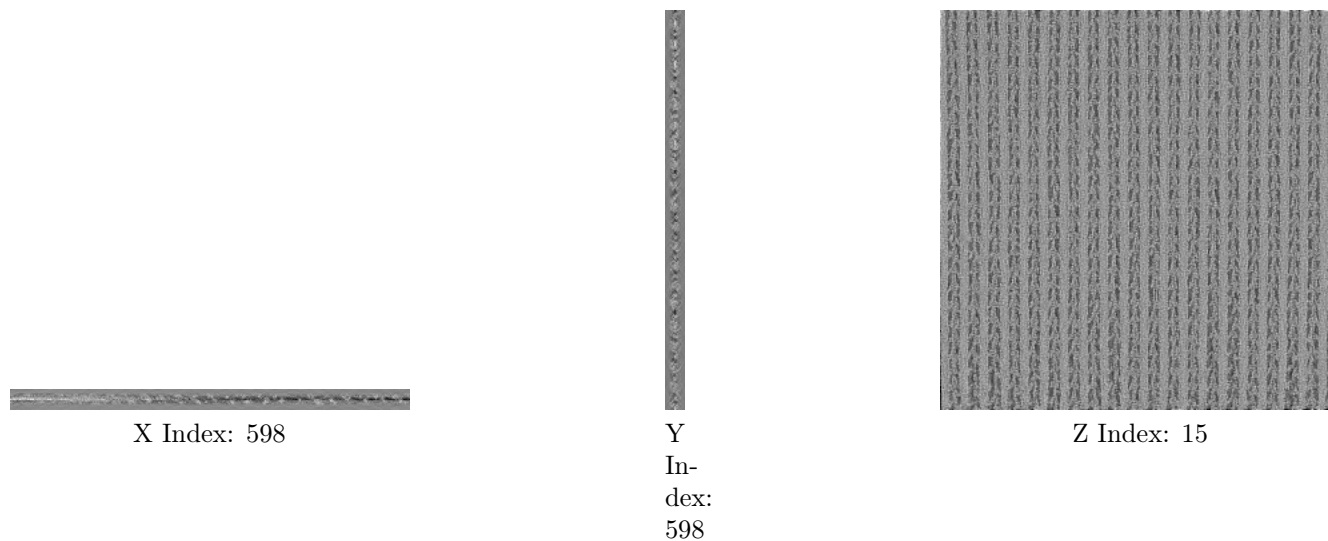
The images above show the tomogram projected in three orthogonal directions.

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.

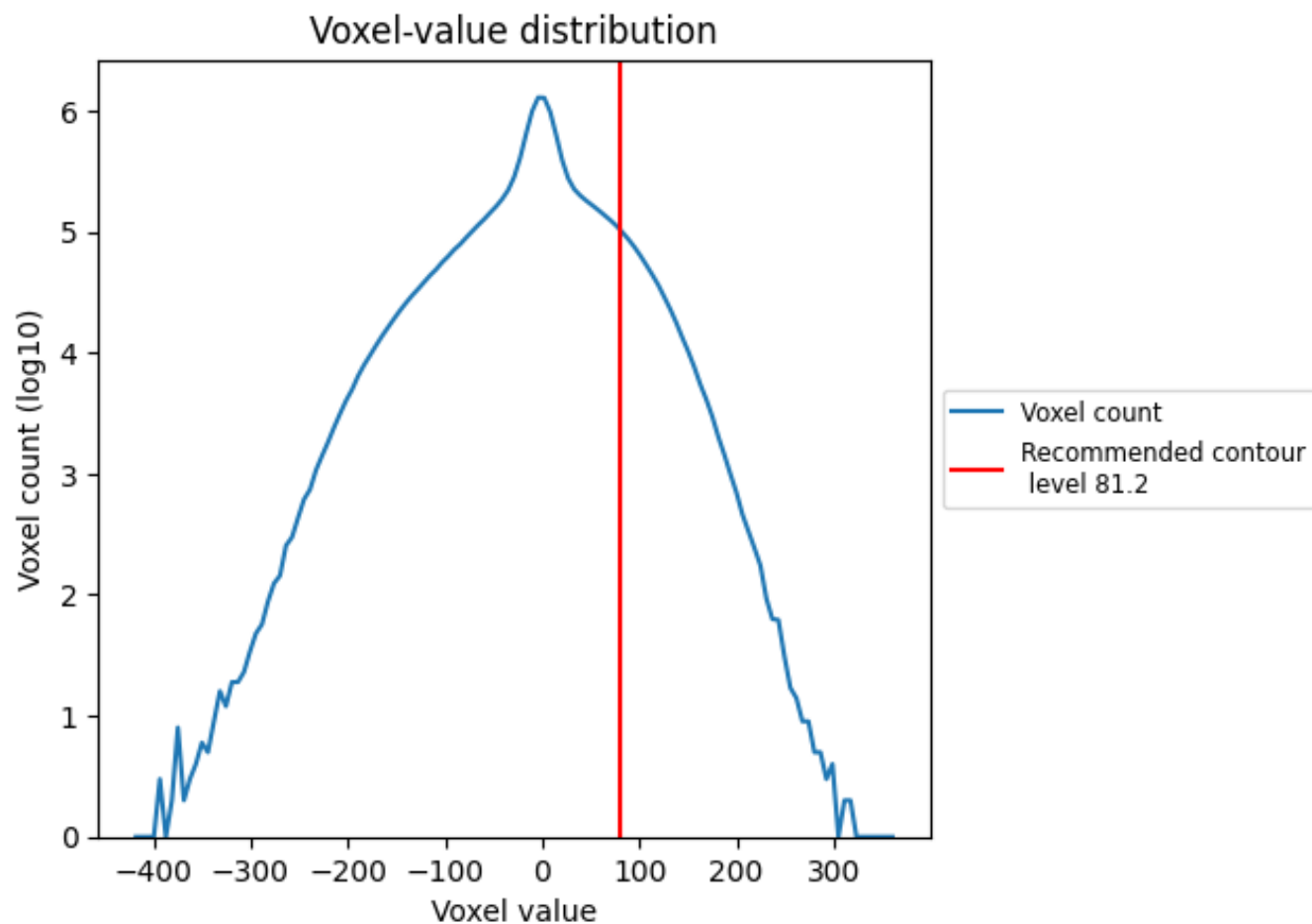
6.4 Mask visualisation [i](#)

This section was not generated.

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.

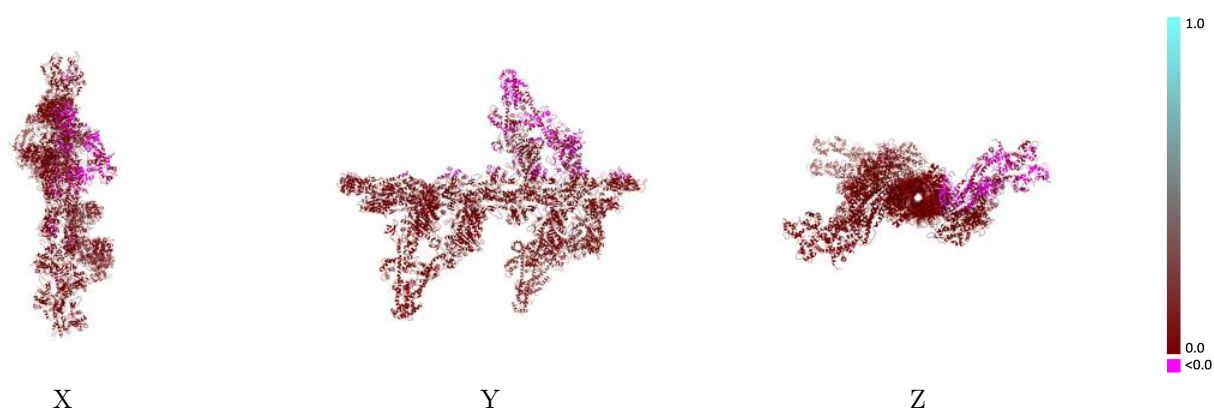
8 Map-model fit [i](#)

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](#)

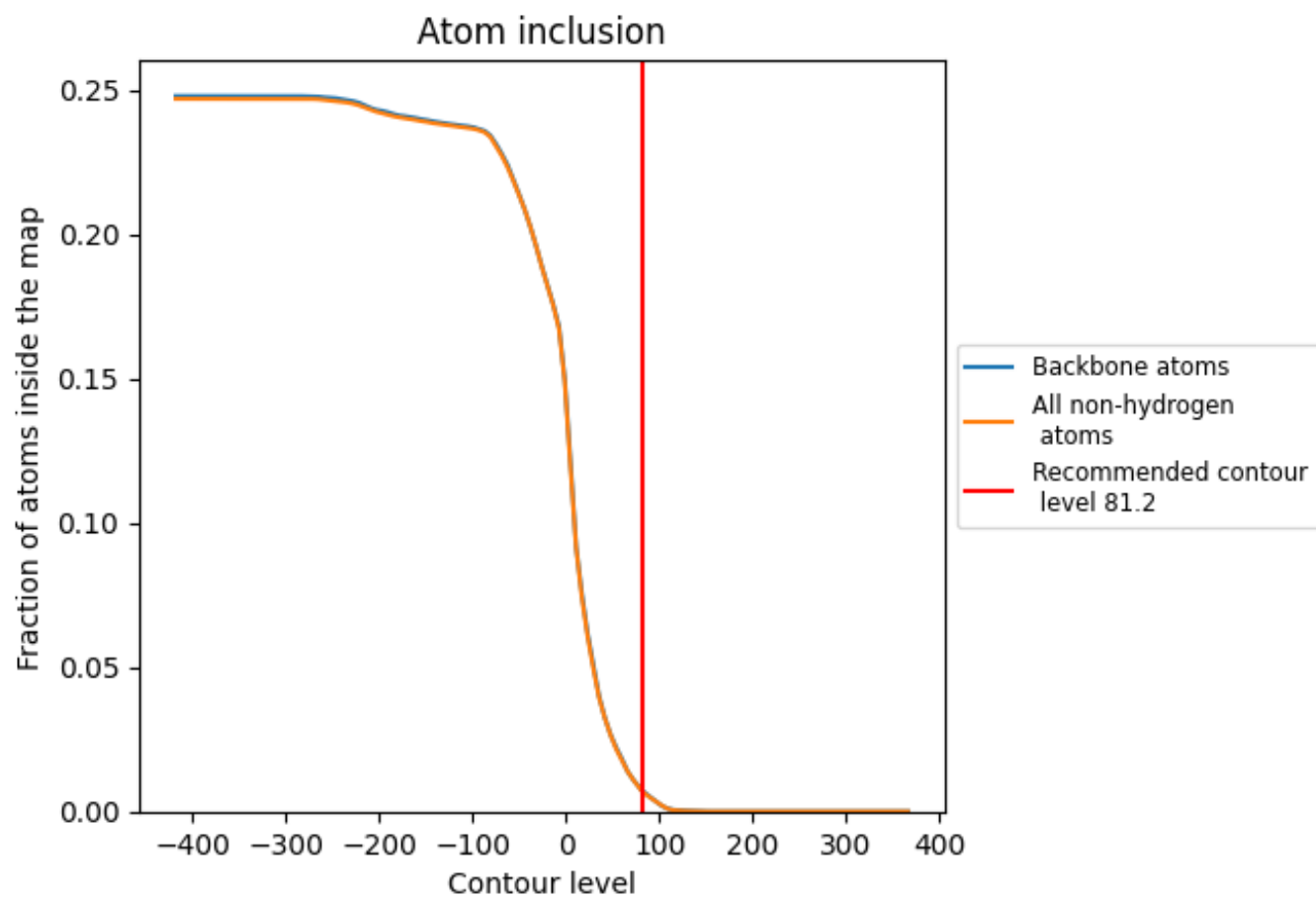


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	 0.0072	 0.0010
1	 0.0000	 -0.0020
2	 0.0284	 -0.0000
3	 0.0000	 0.0000
4	 0.0000	 0.0030
5	 0.0000	 0.0000
6	 0.0000	 0.0020
7	 0.0000	 0.0020
8	 0.0000	 0.0000
9	 0.0000	 0.0020
A	 0.0000	 0.0000
B	 0.0000	 0.0000
C	 0.0000	 0.0000
D	 0.0018	 0.0000
E	 0.1029	 0.0190
F	 0.0395	 -0.0110
G	 0.0000	 0.0000
H	 0.0000	 0.0000
I	 0.0000	 0.0000
J	 0.0111	 0.0050
K	 0.0000	 -0.0200
L	 0.1697	 0.0230
M	 0.0000	 0.0000
N	 0.0000	 0.0000
O	 0.0000	 0.0000
S	 0.0000	 0.0000
T	 0.0000	 0.0000
U	 0.0000	 0.0000
V	 0.0000	 0.0000
W	 0.0000	 0.0020
X	 0.0537	 0.0000
Y	 0.0000	 0.0020
Z	 0.0000	 0.0000

