



## wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 11:30 am GMT

PDB ID : 1O1A  
EMDB ID: : EMD-1001  
Title : MOLECULAR MODELS OF AVERAGED RIGOR CROSSBRIDGES FROM  
TOMOGRAMS OF INSECT FLIGHT MUSCLE  
Authors : Chen, L.F.; Winkler, H.; Reedy, M.K.; Reedy, M.C.; Taylor, K.A.  
Deposited on : 2002-11-18  
Resolution : 70.00 Å(reported)

This is a wwPDB/EMDatabank EM Map/Model Validation Summary Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc29047

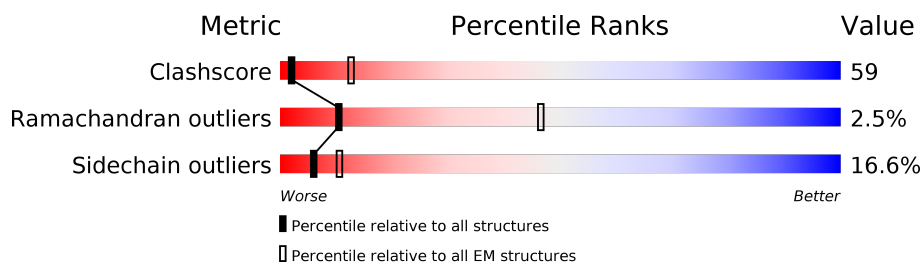
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

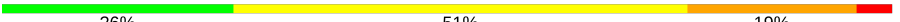








The reported resolution of this entry is 70.00 Å.

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.















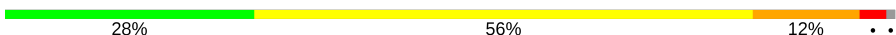



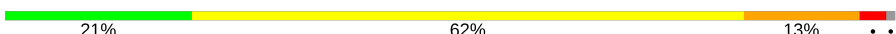
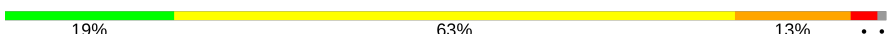





Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	840	 26% 51% 19% .
1	D	840	 27% 51% 18% .
1	G	840	 25% 51% 19% .
1	J	840	 25% 51% 19% .
1	M	840	 27% 50% 19% .
1	P	840	 26% 50% 20% .
2	B	145	 68% 23% 6% .
2	E	145	 64% 27% 6% .
2	H	145	 61% 30% 6% .

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Mol	Chain	Length	Quality of chain
2	K	145	
2	N	145	
2	Q	145	
3	C	147	
3	F	147	
3	I	147	
3	L	147	
3	O	147	
3	R	147	
4	1	375	
4	2	375	
4	3	375	
4	4	375	
4	5	375	
4	6	375	
4	7	375	
4	8	375	
4	9	375	
4	V	375	
4	W	375	
4	X	375	
4	Y	375	
4	Z	375	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	MLY	A	505	-	-	X	-
1	MLY	A	553	-	-	X	-
1	MLY	A	764	-	-	X	-
1	MLY	A	837	-	-	X	-
1	MLY	A	839	-	-	X	-
1	MLY	D	553	-	-	X	-
1	MLY	D	764	-	-	X	-
1	MLY	D	782	-	-	X	-
1	MLY	G	505	-	-	X	-
1	MLY	G	553	-	-	X	-
1	MLY	G	764	-	-	X	-
1	MLY	G	84	-	-	X	-
1	MLY	J	505	-	-	X	-
1	MLY	J	553	-	-	X	-
1	MLY	J	839	-	-	X	-
1	MLY	J	84	-	-	X	-
1	MLY	M	839	-	-	X	-
1	MLY	P	839	-	-	X	-

## 2 Entry composition

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

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

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

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

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

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

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

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

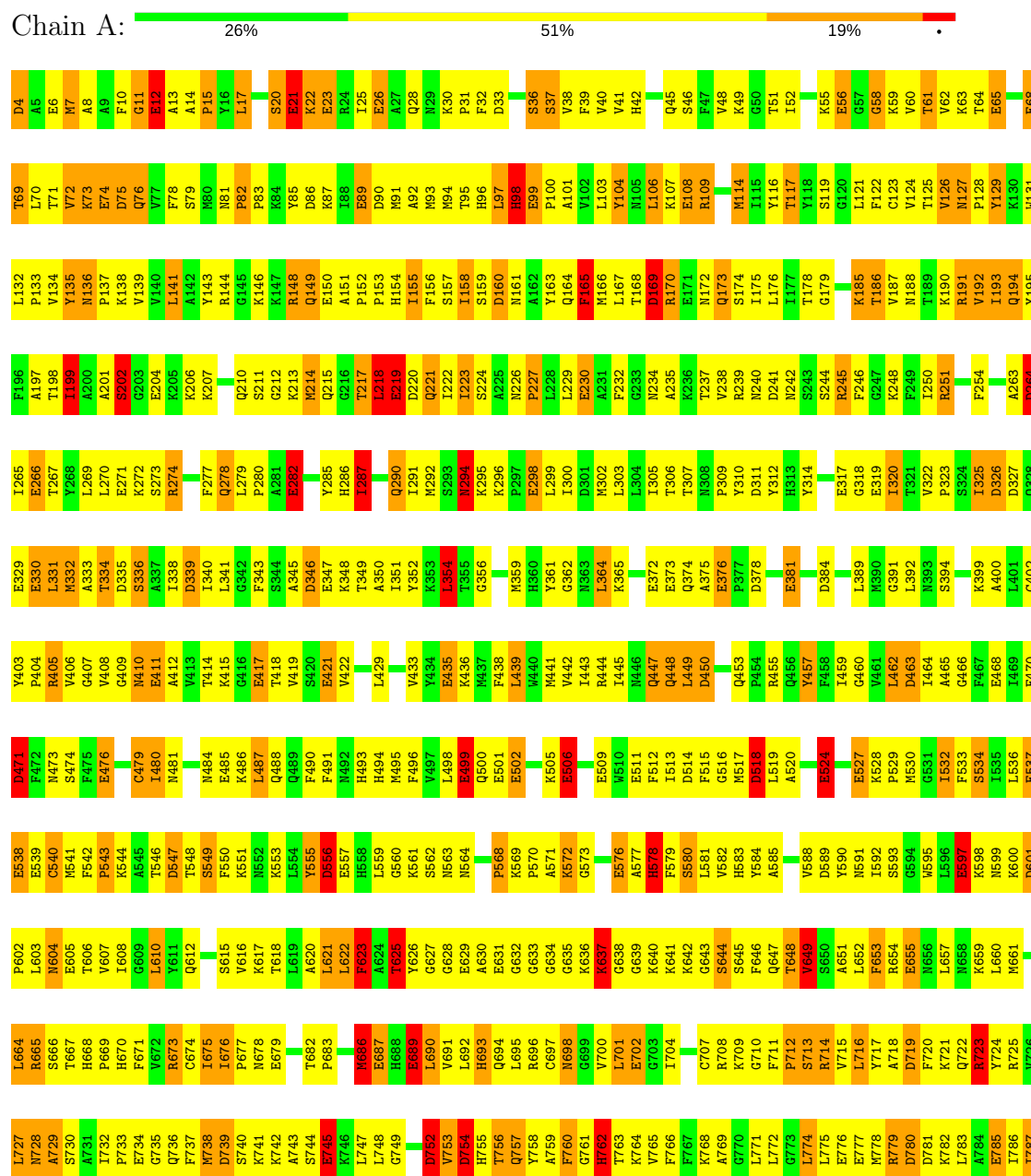
- Molecule 4 is a protein called SKELETAL MUSCLE ACTIN.

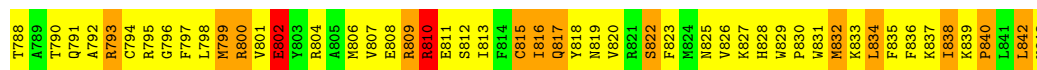
Mol	Chain	Residues	Atoms					AltConf	Trace
4	1	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	2	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	3	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	4	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	5	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
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 and DNA 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. 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. 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.

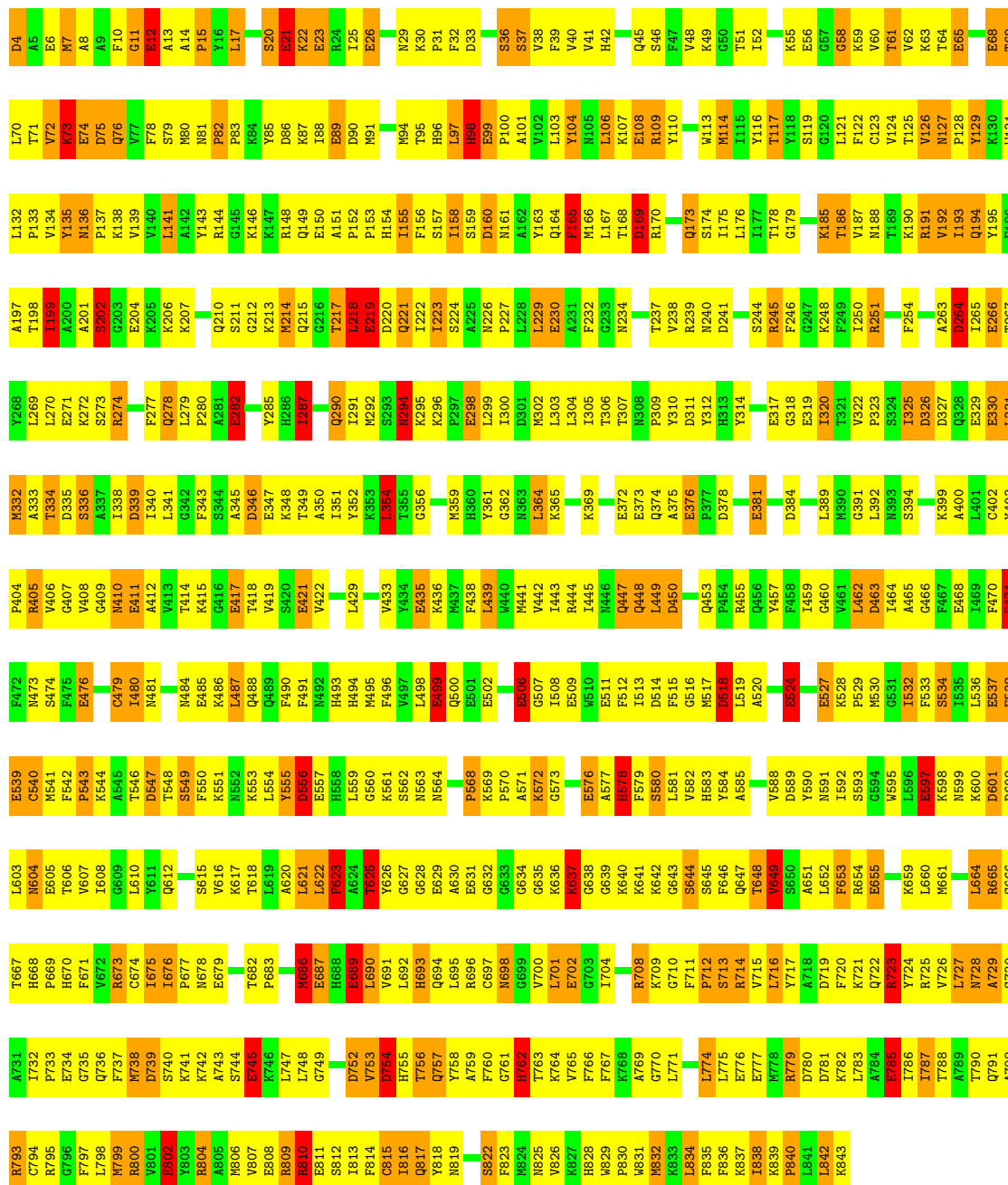
#### • Molecule 1: SKELETAL MUSCLE MYOSIN II





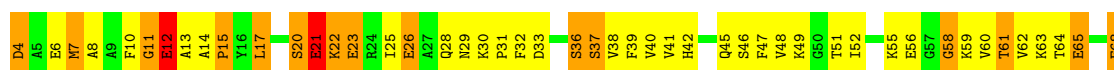
### • Molecule 1: SKELETAL MUSCLE MYOSIN II

Chain D: 27% 51% 18%



### • Molecule 1: SKELETAL MUSCLE MYOSIN II

Chain G: 25% 51% 19%



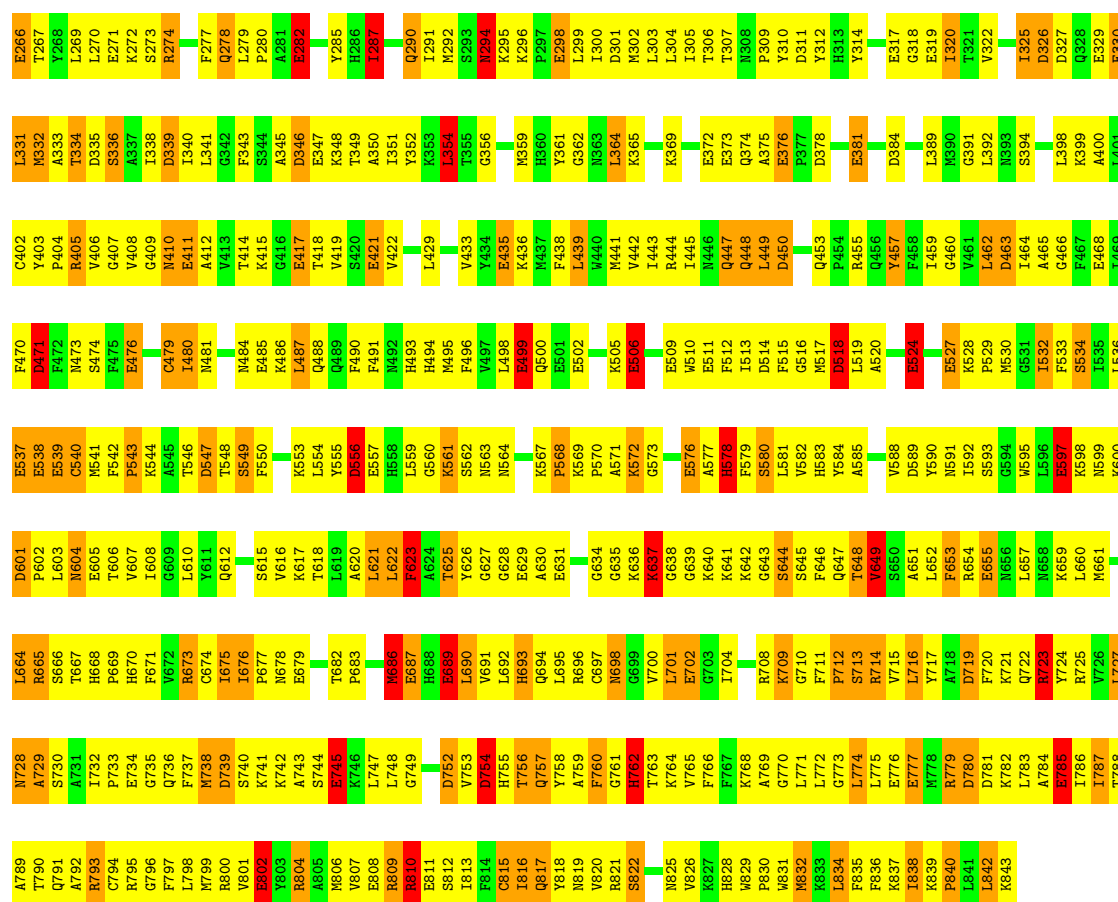


F196	A197	F198	E266	G326	C402	F470	F535	K598	M661	L727	T788
A197	A197	T198	T267	E329	Y403	D471	L536	N599	M661	M728	A789
T198	T198	T199	Y268	E330	P404	F472	E537	N600	L664	M729	A790
K73	L200	A201	L269	E331	R405	M473	E538	D601	R665	S730	T790
E74	A201	S202	L270	E332	V406	S474	E539	P602	S666	A731	Q791
D75	S202	S203	E271	A333	Q407	F475	E540	L603	T667	T732	A792
Q76	S203	E204	K272	A334	Q408	E476	M541	N604	H668	P733	C794
V77	E204	K205	R273	D336	Q409		F542	E605	P669	E734	R795
F78	K205	K206	S274	E337	N410	C479	P543	T606	H670	G735	G796
S79	K206	K207	F277	A338	A411	M481	E544	L608	F671	Q736	L797
M80	K207		Q278	E339	A412	M484	E545	G609	R673	M738	M799
N81			L279	E340	A413	M484	T546	G610	C674	D739	R800
P82	G145		P280	E341	K415	E485	T547	T611	I675	S740	V801
K83	K146		E281	G342	G416	E486	T548	Q612	I676	K741	E802
E84	K147		E282	F343	E417	L487	F549		P677	K742	R803
Y85	R148		Y285	S344	T418	Q488	F550	S615	M678	A743	R804
D86	Q149		H286	A345	V419	F490	K552	V616	E679	S744	A805
K87	E150		L287	D346	E421	F491	K553	T617	T682	E745	M806
E88	A151		P288	E347	V422	M492	L554	T618	P683	K746	V807
E89	P152		Y289	E348			F555	L619		L747	E808
D90	P153		Q290	A350	L429	H494	E557	A620	M686	L748	R809
N91	H154		I291	E352	V433	M495	E558	L621	E687	G749	R810
A92	I155		M292	K353	Y434	F496	L559	L622	H688		E811
M93	F156		Q221	R353	E435	E497	G560	F623	E689	D752	S812
N94	S157		I222	L354	E436	M498	E562	T625	E690	V753	I813
T95	I158		I223	R355	E437	E499	S562	Y626	L690	H754	C815
H96	S159		K296	G356	M437	Q500	N564	G627	V691	T756	R816
L97	D160		N297		F438	E501		G628	H693	Q757	Q817
N98	N161		P297		L439	E502	K567	E629	Q694	Y758	Y818
E99	A162		L298		V440	Y503	P568	A630	L695	A759	N819
P100	Q163		I300		M441	R504	E569	G632	R696	F760	N820
A101	Q164		D301		V442	K505	P570	G633	C697	G761	R821
V102	M166		M302		I443	E506	E571	G634	M698	H762	S822
L103	L167		L303		R444	G507	K572	G635	G699	T763	R823
Y104	T168		L304		I445	I508	E573	G636	V700	K764	M824
N105	D169		I305		V446	E509	G573	K637	L701	V765	N825
L106	R170		T306		Q447	M510	E576	G638	E702	F766	V826
K107	E171		T307		Q448	E511	E577	G639	C707	F767	K827
R109	Q173		R239		L449	F512	A577	K640	R708	K768	H828
	M166		Y310		D450	I513	H578	K641	K709	A769	W829
M114	S174		D241			D514	F579	K642	L711	G770	P830
T115	L175		Y312		Q453	F515	S580	G643	F712	L771	N831
Y116	L176		S242		P454	G516	L581	G644	P713	L772	M832
T117	G179		S243		R455	M517	V582	S645	R714	G773	K833
Y118	T178		R245		Q456	E518	H583	P646	S713	L774	L834
S119	G179		V315		Y457	F519	Y584	Q647	R715	L775	F835
G120			F246		F458	A520	A585	T648	V716	E777	R836
L121	K185		G247		I459	E524	V588	V649	L717	K778	K837
F122	T186		K248		Q460	E527	D589	S650	A718	H779	I838
C123	V187		F249		V461	E527	E590	A651	D719	D780	K839
V124	N188		T250		L462	E527	F591	L652	F720	T781	P840
T125	T189		R251		D463	P529	N591	L653	K721	L841	T841
N126	K190		K191		K393	M530	I592	F654	K722	K782	L842
N127	R191		P323		S394	E531	S593	G655	Q722	L783	K843
P128	V192		S294		G466	G531	G594	E655	R723	A784	
I129	I193		I325		P467	L532	W595	K659	T724	E785	
K130	D264		D327		E468	F533	L596	L725	R726	E786	
Y195	I195		I265		I469	S534	E597	L660	V726	L787	

● Molecule 1: SKELETAL MUSCLE MYOSIN II

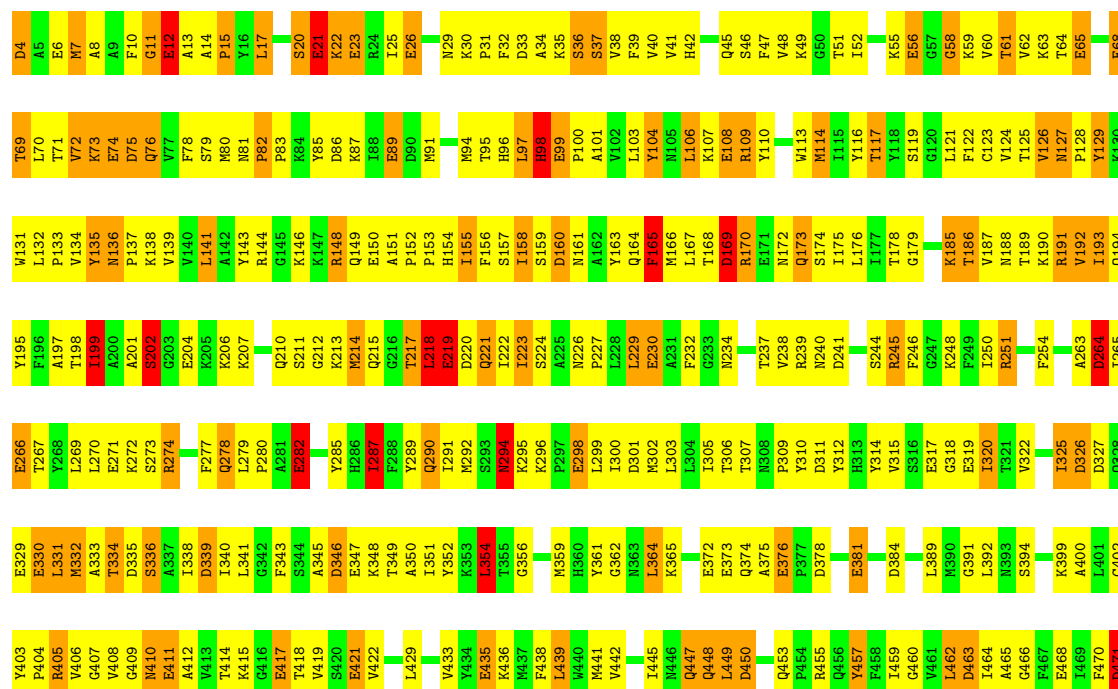
Chain J:  25% 51% 19%

D4	A5	A6	T69	L132	F196
E6	A7	A8	L70	P133	A197
M7	A9	A10	T71	V134	T198
A8	F10	F11	W72	Y135	T199
C794	G11	E12	K73	N136	A200
R795	E12	E13	E74	P137	A201
L796	A13	A14	D75	K138	S202
L798	F78	F79	Q76	V139	E203
M799	A14	A15	V77	V140	G204
R800	F79	F80	S78	A141	K205
V801	A15	A16	M80	A142	K206
E802	P15	P16	N81	R144	K207
R803	L17	L18	P82	G145	
R804	S20	S21	K83	K146	Q210
A805	E21	E22	Y85	K147	S211
M806	K22	K23	D86	R148	K213
V807	E23	E24	K87	Q149	M214
E808	E24	E25	I88	E150	Q215
R809	L25	L26	E89	A151	G216
R810	A27	A28	N91	P152	T217
E811	Q28	Q29	M92	P153	L218
S812	N29	N30	A92	H154	E219
I813	K30	K31	M93	I155	M155
C815	P31	P32	N94	S157	Q221
T816	F32	F33	T95	I158	I222
Q817	L97	L98	H96	S159	I223
Y818	D97	D98	L97	D160	A225
N819	S96	S97	N98	N161	N226
V820	E37	E38	E99	A162	P227
R821	V38	V39	P100	Y163	L228
S822	F39	F40	A101	Q164	L229
R823	M103	M104	V102	F165	E230
M824	V41	V42	L103	M166	A231
N825	H42	H43	Y104	F232	F232
V826	Q45	Q46	N105	L167	G233
K827	S46	S47	L106	T168	N234
H828	F47	F48	K107	D169	A235
W829	V48	V49	E108	R170	K236
P830	K49	K50	R109	E171	T237
N831	G50	G51	M114	Q173	V238
M832	T51	T52	T115	S174	R239
K833	L52	L53	Y116	I175	N240
L834	K55	K56	T117	L176	D241
F835	E56	E57	S119	G179	
R836	G57	G58	G120	K185	S244
K837	G58	G59	L121	T186	R245
I838	K59	K60	F122	V187	G247
R839	T60	T61	C123	T188	K248
L841	T61	T62	V124	N188	F249
L842	V62	V63	T125	T189	T250
K843	K63	K64	N126	K190	R251
	T64	T65	N127	R191	F254
	E65	E66	P128	V192	
	L786	L787	I129	I193	A263
	V726	V727	K130	D264	D264
			Y195	I195	I265

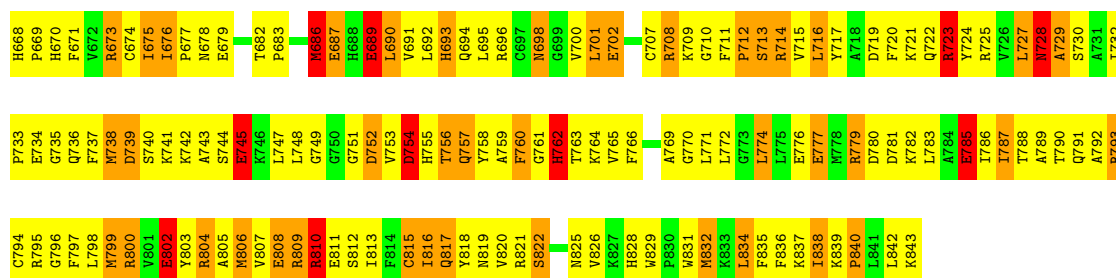


## • Molecule 1: SKELETAL MUSCLE MYOSIN II

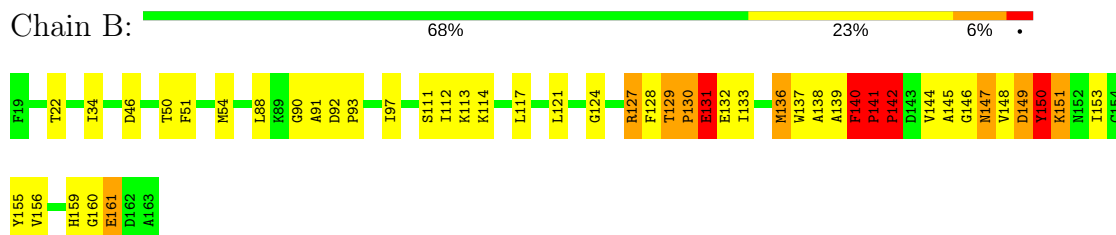
Chain M: 27% 50% 19%



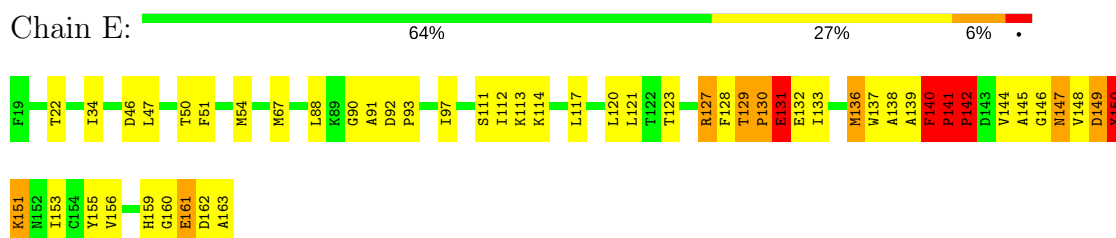




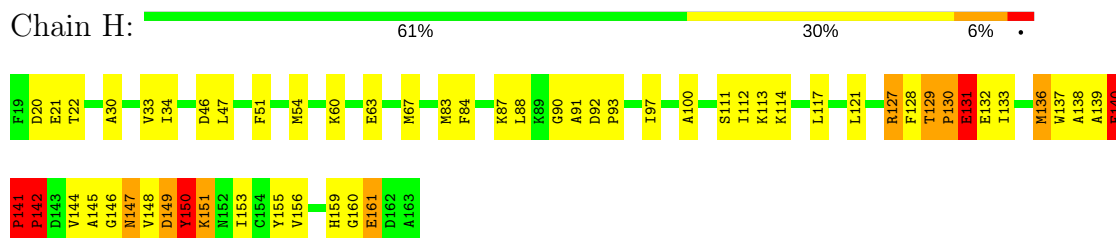
• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN



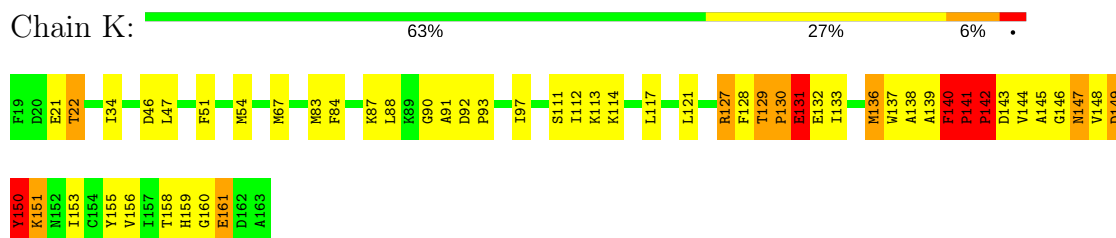
• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN



• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

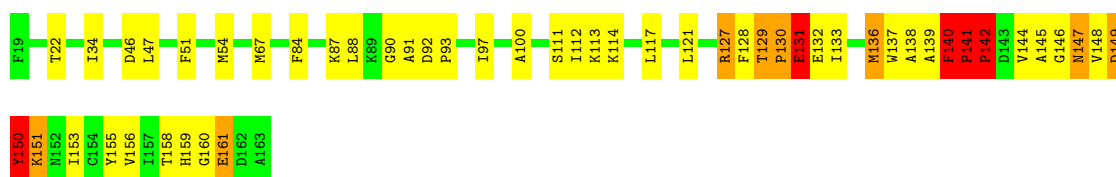


• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN



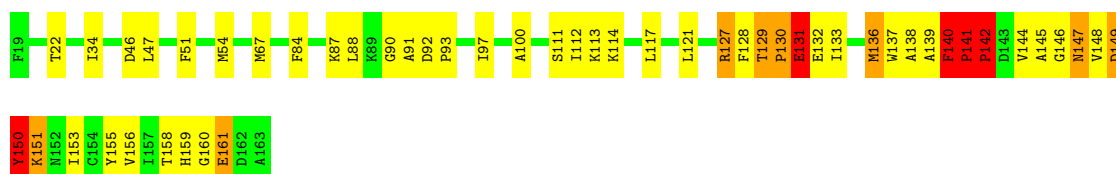
• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN





• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

Chain Q: 65% 26% 6%



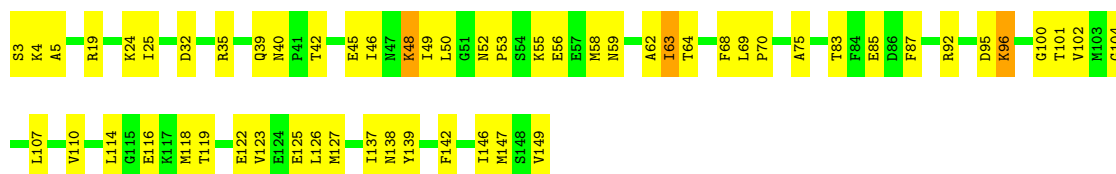
• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN

Chain C: 60% 38%



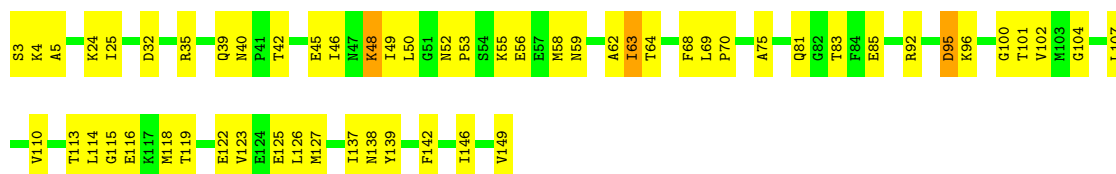
• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN

Chain F: 61% 37%



• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN

Chain I: 61% 37%



• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN

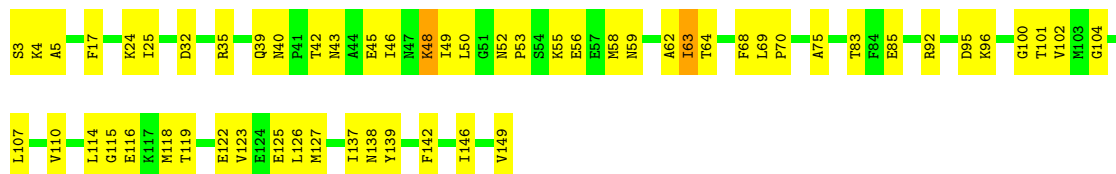
Chain L: 62% 36%





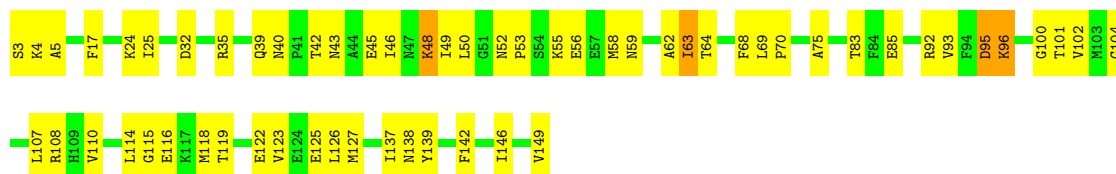
• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN

Chain O: 61% 37%



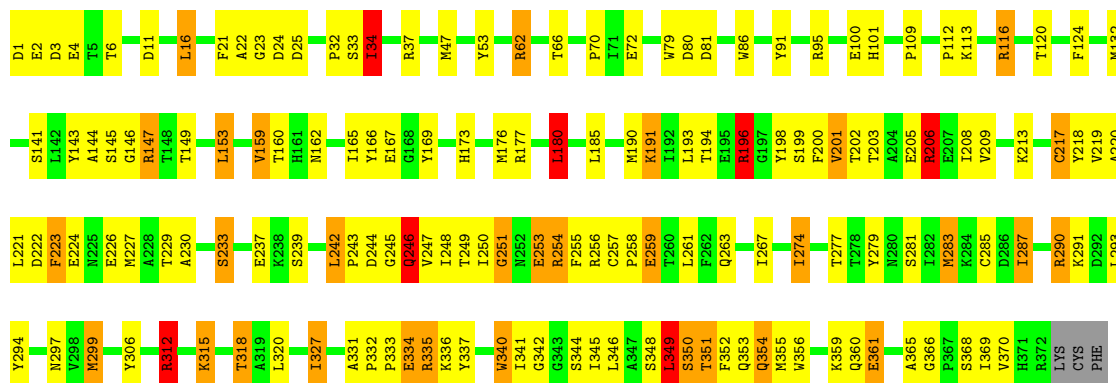
• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN

Chain R: 60% 37%



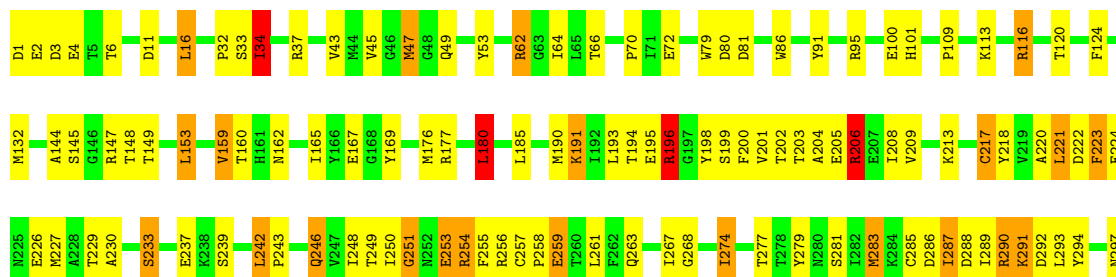
• Molecule 4: SKELETAL MUSCLE ACTIN

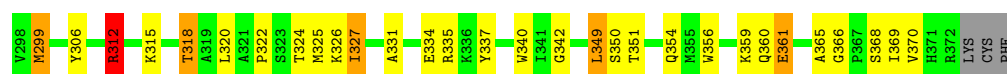
Chain 1: 57% 32% 8%



• Molecule 4: SKELETAL MUSCLE ACTIN

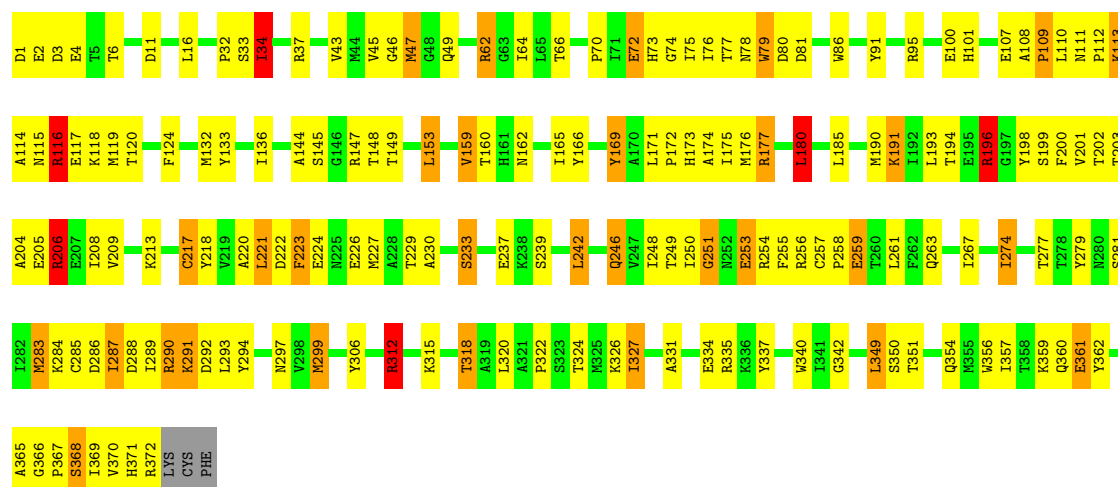
Chain 2: 60% 31% 7%





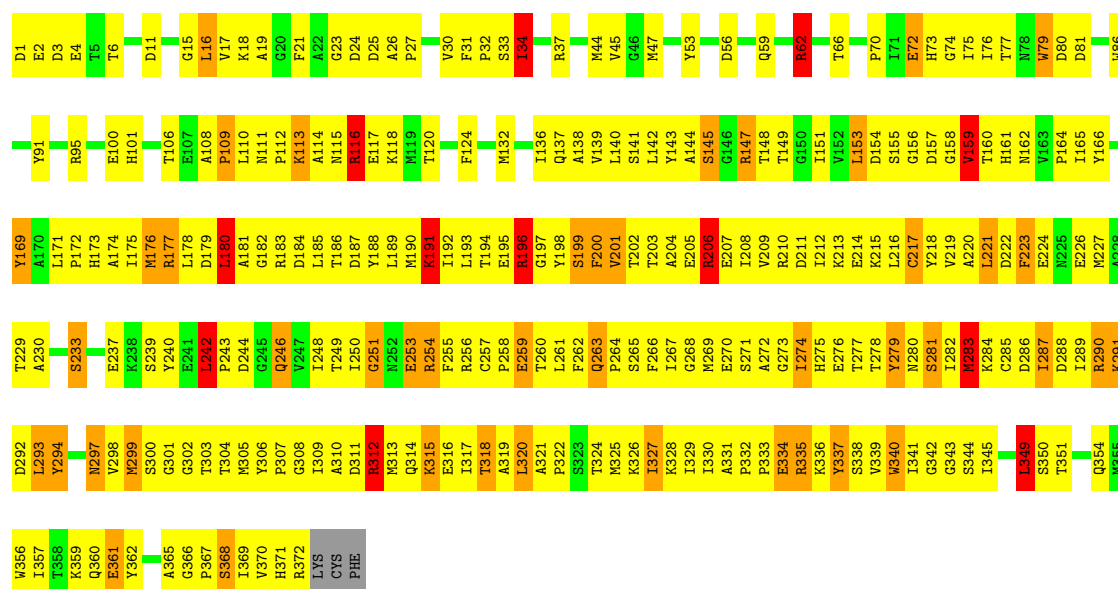
### • Molecule 4: SKELETAL MUSCLE ACTIN

Chain 3: 53% 36% 8% ..



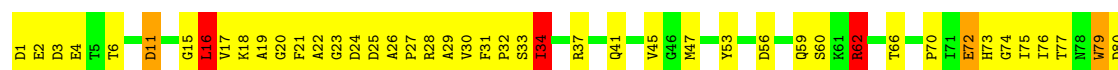
### • Molecule 4: SKELETAL MUSCLE ACTIN

Chain 4: 28% 56% 12% ..



### • Molecule 4: SKELETAL MUSCLE ACTIN

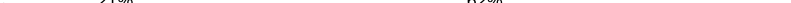
Chain 5: 26% 58% 12% ..

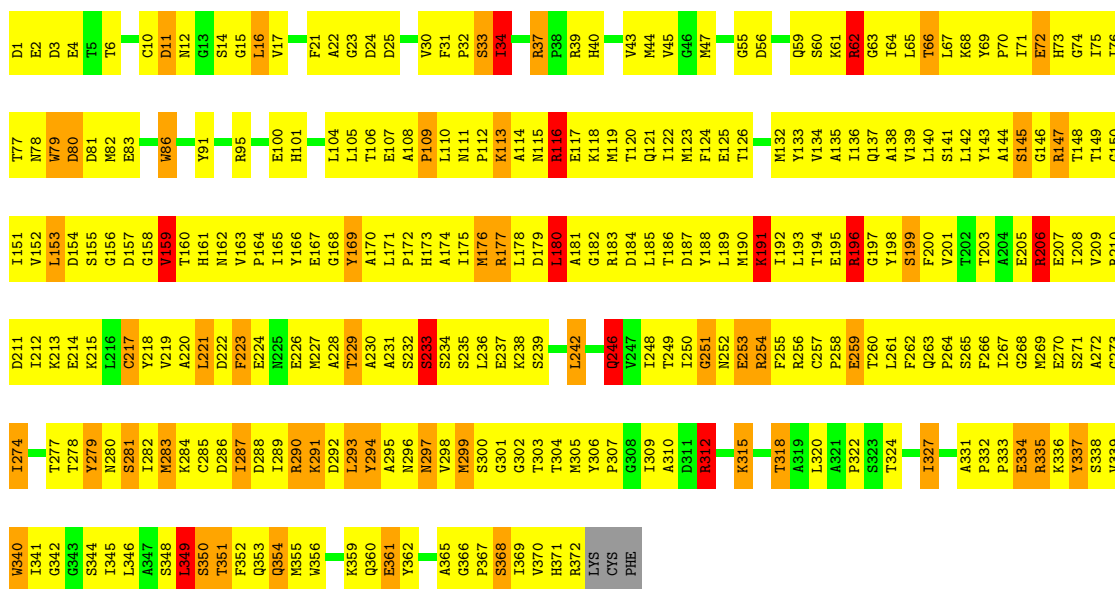






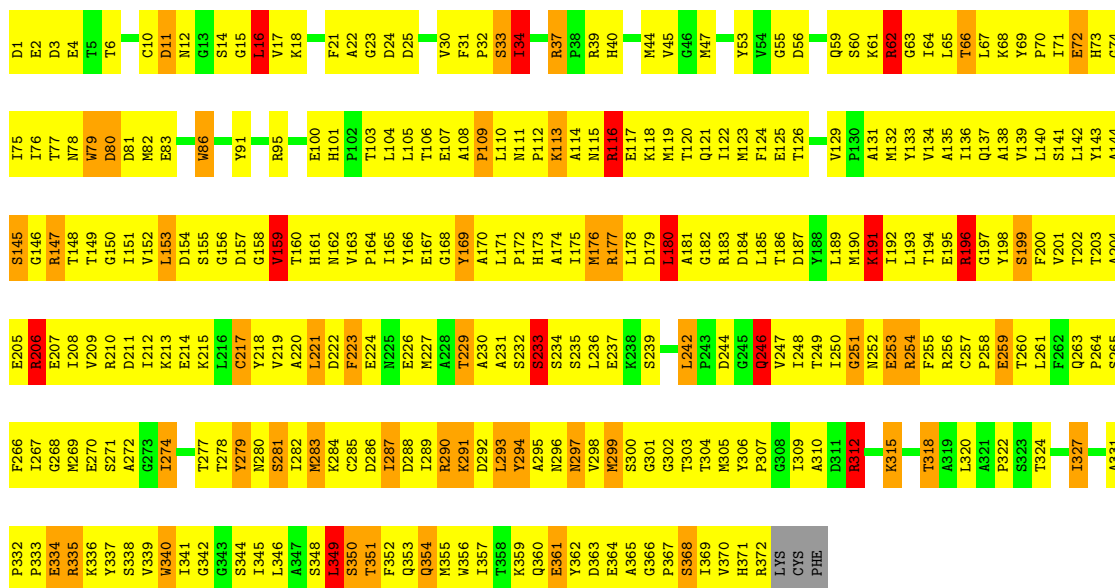
● Molecule 4: SKELETAL MUSCLE ACTIN

Chain 8:  21% 62% 13% . .

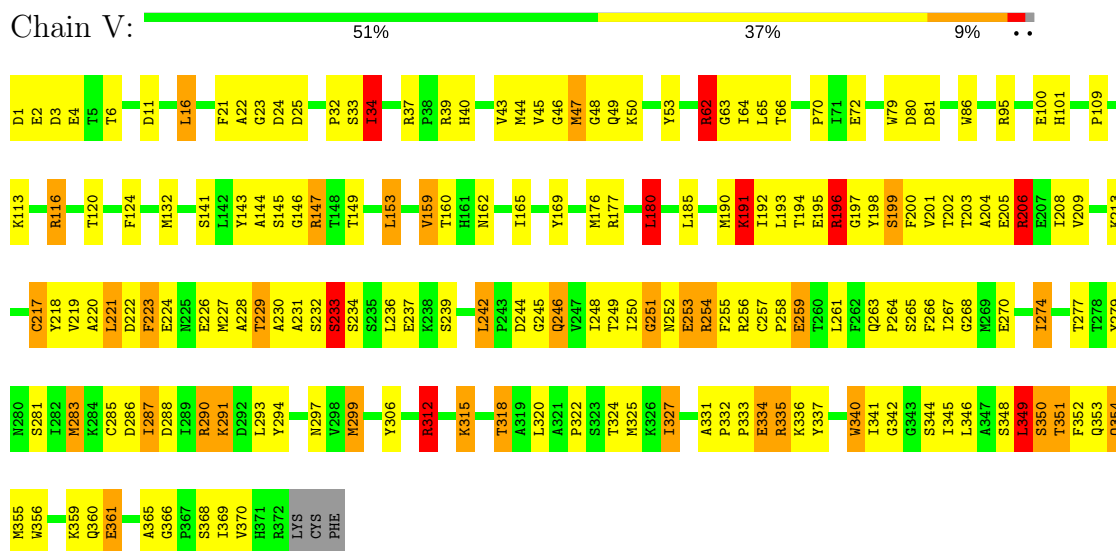


• Molecule 4: SKELETAL MUSCLE ACTIN

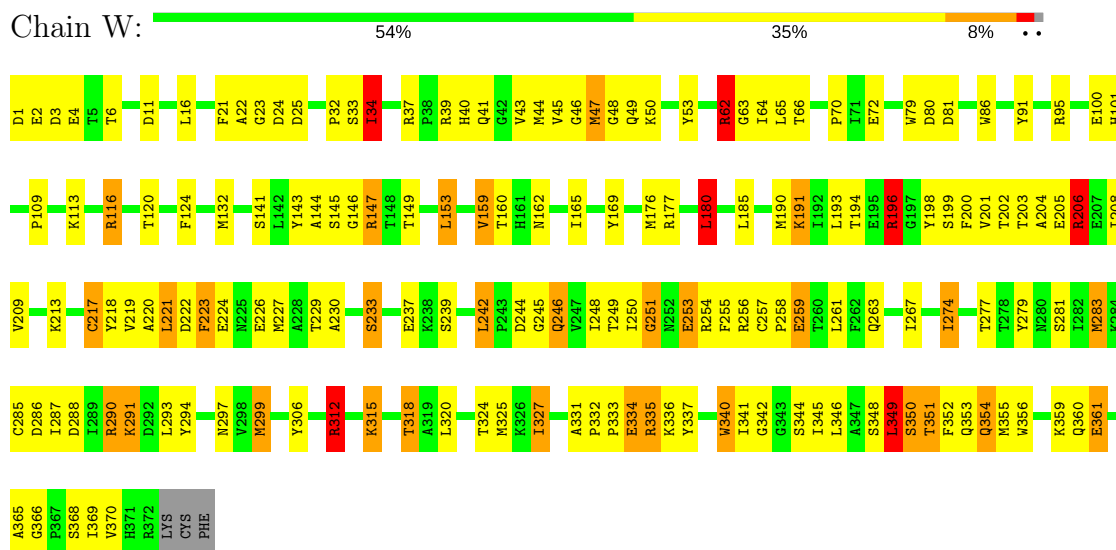
Chain 9:  19% 63% 13% ..



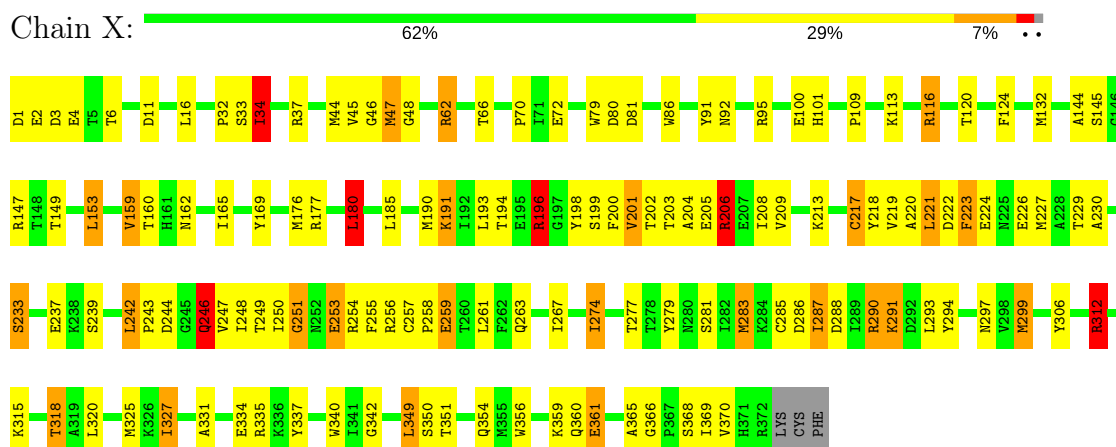
- Molecule 4: SKELETAL MUSCLE ACTIN



• Molecule 4: SKELETAL MUSCLE ACTIN

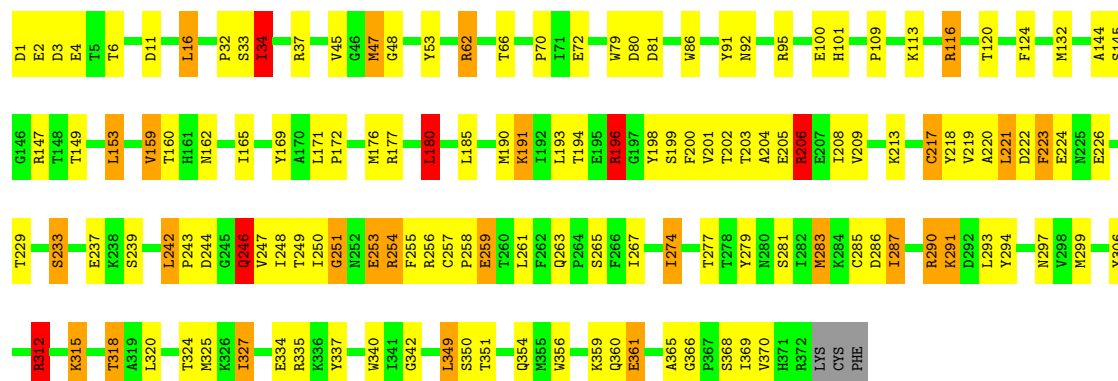


• Molecule 4: SKELETAL MUSCLE ACTIN



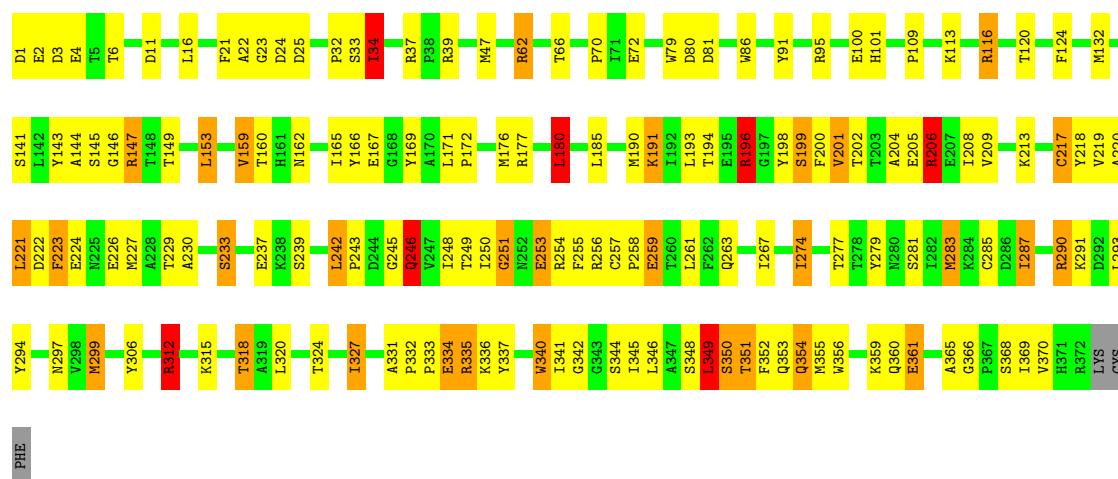
● Molecule 4: SKELETAL MUSCLE ACTIN

Chain Y:  62% 29% 7% ..



● Molecule 4: SKELETAL MUSCLE ACTIN

Chain Z:  58% 32% 8% ..



PHE

## 4 Experimental information

Property	Value	Source
Reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of tilted images used	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	Not provided	Depositor
Voltage (kV)	Not provided	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	KODAK S0163 FILM	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  >2	RMSZ	# Z  >2
1	A	1.77	68/6448 (1.1%)	1.82	116/8729 (1.3%)
1	D	1.77	67/6448 (1.0%)	1.82	115/8729 (1.3%)
1	G	1.77	69/6449 (1.1%)	1.83	118/8732 (1.4%)
1	J	1.77	69/6449 (1.1%)	1.86	119/8732 (1.4%)
1	M	1.86	70/6447 (1.1%)	1.85	120/8726 (1.4%)
1	P	1.78	68/6447 (1.1%)	1.87	123/8726 (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	17/1548 (1.1%)
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	Q	1.22	10/1148 (0.9%)	1.62	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	0.94	4/1525 (0.3%)
3	L	0.80	0/1136	0.95	4/1525 (0.3%)
3	O	0.79	0/1136	0.95	4/1525 (0.3%)
3	R	0.80	0/1136	0.95	4/1525 (0.3%)
4	1	0.89	2/2968 (0.1%)	1.64	52/4023 (1.3%)
4	2	0.89	2/2968 (0.1%)	1.64	51/4023 (1.3%)
4	3	0.89	2/2968 (0.1%)	1.64	51/4023 (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	52/4023 (1.3%)
4	6	0.89	2/2968 (0.1%)	1.64	51/4023 (1.3%)
4	7	0.89	2/2968 (0.1%)	1.64	50/4023 (1.2%)
4	8	0.89	1/2968 (0.0%)	1.64	50/4023 (1.2%)
4	9	0.89	2/2968 (0.1%)	1.64	51/4023 (1.3%)
4	V	0.89	2/2968 (0.1%)	1.64	51/4023 (1.3%)
4	W	0.89	2/2968 (0.1%)	1.64	52/4023 (1.3%)
4	X	0.89	2/2968 (0.1%)	1.64	50/4023 (1.2%)
4	Y	0.89	2/2968 (0.1%)	1.64	51/4023 (1.3%)
4	Z	0.89	2/2968 (0.1%)	1.64	51/4023 (1.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
All	All	1.35	498/93944 (0.5%)	1.69	1545/127134 (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	4
1	J	1	6
1	M	1	4
1	P	1	6
2	B	0	3
2	E	0	3
2	H	0	3
2	K	0	3
2	N	0	3
2	Q	0	3
3	C	0	2
3	F	0	2
3	I	0	2
3	L	0	2
3	O	0	2
3	R	0	2
4	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	72

The worst 5 of 498 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	649	VAL	CB-CG1	53.37	2.65	1.52
1	M	649	VAL	CB-CG1	53.35	2.64	1.52
1	J	649	VAL	CB-CG1	53.27	2.64	1.52
1	P	649	VAL	CB-CG1	53.24	2.64	1.52
1	A	649	VAL	CB-CG1	53.21	2.64	1.52

The worst 5 of 1545 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	637	LYS	O-C-N	-58.52	23.72	123.20
1	M	637	LYS	O-C-N	-58.47	23.80	123.20
1	D	637	LYS	O-C-N	-58.47	23.81	123.20
1	P	637	LYS	O-C-N	-58.47	23.81	123.20
1	A	637	LYS	O-C-N	-58.46	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 72 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	6756	1513	18

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	6797	0	6756	1419	28
1	G	6797	0	6764	1560	0
1	J	6797	0	6755	1414	0
1	M	6797	0	6769	1360	0
1	P	6797	0	6766	1424	0
2	B	1127	0	1085	248	0
2	E	1127	0	1086	266	0
2	H	1127	0	1088	300	5
2	K	1127	0	1088	271	5
2	N	1127	0	1088	248	0
2	Q	1127	0	1088	250	0
3	C	1123	0	1083	194	0
3	F	1123	0	1083	173	0
3	I	1123	0	1083	185	0
3	L	1123	0	1083	158	0
3	O	1123	0	1084	183	0
3	R	1123	0	1084	189	0
4	1	2906	0	2856	418	0
4	2	2906	0	2860	207	86
4	3	2906	0	2863	169	610
4	4	2906	0	2863	179	3050
4	5	2906	0	2865	94	3249
4	6	2906	0	2865	99	3357
4	7	2906	0	2866	74	3176
4	8	2906	0	2857	315	3192
4	9	2906	0	2855	344	3429
4	V	2906	0	2851	379	419
4	W	2906	0	2851	395	90
4	X	2906	0	2863	179	0
4	Y	2906	0	2863	193	0
4	Z	2906	0	2855	380	0
All	All	94966	0	93622	11072	10357

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 59.

The worst 5 of 11072 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)
2:N:144:VAL:HG13	2:N:153:ILE:CD1	1.22	1.68
1:J:797:PHE:CE1	3:L:146:ILE:HG23	1.24	1.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:831:TRP:CZ3	2:B:50:THR:HG21	1.27	1.67
1:A:753:VAL:HG12	1:A:775:LEU:CG	1.22	1.66
4:2:287:ILE:CG2	4:4:202:THR:HB	1.23	1.66

The worst 5 of 10357 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:300:SER:CB	4:7:107:GLU:OE1[1_554]	0.08	2.12
4:6:28:ARG:CB	4:9:126:THR:CG2[1_554]	0.12	2.08
4:5:341:ILE:CB	4:8:120:THR:OG1[1_554]	0.15	2.05
4:6:173:HIS:CE1	4:V:265:SER:C[1_554]	0.15	2.05
4:5:154:ASP:N	4:8:109:PRO:C[1_554]	0.17	2.03

## 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%)	652 (83%)	111 (14%)	26 (3%)	4	35
1	D	789/840 (94%)	651 (82%)	112 (14%)	26 (3%)	4	35
1	G	791/840 (94%)	650 (82%)	114 (14%)	27 (3%)	4	35
1	J	791/840 (94%)	652 (82%)	112 (14%)	27 (3%)	4	35
1	M	788/840 (94%)	651 (83%)	110 (14%)	27 (3%)	4	35
1	P	787/840 (94%)	651 (83%)	109 (14%)	27 (3%)	4	35
2	B	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	2	25
2	E	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	2	25
2	H	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	2	25
2	K	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	2	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	N	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	2	25
2	Q	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	2	25
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
3	R	143/147 (97%)	133 (93%)	10 (7%)	0	100	100
4	1	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	11	51
4	2	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	11	51
4	3	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	11	51
4	4	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	11	51
4	5	370/375 (99%)	333 (90%)	31 (8%)	6 (2%)	11	51
4	6	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	11	51
4	7	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	11	51
4	8	370/375 (99%)	333 (90%)	31 (8%)	6 (2%)	11	51
4	9	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	11	51
4	V	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	11	51
4	W	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	11	51
4	X	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	11	51
4	Y	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	11	51
4	Z	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	11	51
All	All	11631/12042 (97%)	10138 (87%)	1201 (10%)	292 (2%)	10	41

5 of 292 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%)	1	5
1	D	672/672 (100%)	514 (76%)	158 (24%)	1	5
1	G	672/672 (100%)	514 (76%)	158 (24%)	1	5
1	J	672/672 (100%)	513 (76%)	159 (24%)	1	5
1	M	672/672 (100%)	513 (76%)	159 (24%)	1	5
1	P	672/672 (100%)	515 (77%)	157 (23%)	1	5
2	B	120/120 (100%)	119 (99%)	1 (1%)	85	92
2	E	120/120 (100%)	119 (99%)	1 (1%)	85	92
2	H	120/120 (100%)	119 (99%)	1 (1%)	85	92
2	K	120/120 (100%)	119 (99%)	1 (1%)	85	92
2	N	120/120 (100%)	119 (99%)	1 (1%)	85	92
2	Q	120/120 (100%)	119 (99%)	1 (1%)	85	92
3	C	117/117 (100%)	112 (96%)	5 (4%)	33	64
3	F	117/117 (100%)	112 (96%)	5 (4%)	33	64
3	I	117/117 (100%)	112 (96%)	5 (4%)	33	64
3	L	117/117 (100%)	112 (96%)	5 (4%)	33	64
3	O	117/117 (100%)	112 (96%)	5 (4%)	33	64
3	R	117/117 (100%)	112 (96%)	5 (4%)	33	64
4	1	315/318 (99%)	268 (85%)	47 (15%)	3	20
4	2	315/318 (99%)	268 (85%)	47 (15%)	3	20
4	3	315/318 (99%)	269 (85%)	46 (15%)	3	21
4	4	315/318 (99%)	269 (85%)	46 (15%)	3	21
4	5	315/318 (99%)	268 (85%)	47 (15%)	3	20
4	6	315/318 (99%)	268 (85%)	47 (15%)	3	20
4	7	315/318 (99%)	269 (85%)	46 (15%)	3	21
4	8	315/318 (99%)	269 (85%)	46 (15%)	3	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	9	315/318 (99%)	268 (85%)	47 (15%)	3	20
4	V	315/318 (99%)	268 (85%)	47 (15%)	3	20
4	W	315/318 (99%)	269 (85%)	46 (15%)	3	21
4	X	315/318 (99%)	269 (85%)	46 (15%)	3	21
4	Y	315/318 (99%)	268 (85%)	47 (15%)	3	20
4	Z	315/318 (99%)	269 (85%)	46 (15%)	3	21
All	All	9864/9906 (100%)	8226 (83%)	1638 (17%)	6	16

5 of 1638 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	410	ASN
1	P	495	MET
4	X	196	ARG
1	M	543	PRO
1	P	36	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 231 such sidechains are listed below:

Mol	Chain	Res	Type
3	L	52	ASN
3	O	52	ASN
4	W	263	GLN
1	M	149	GLN
1	M	481	ASN

### 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	A	107	1	10,10,11	0.48	0	8,11,13	1.02	1 (12%)
1	MLY	A	130	1	10,10,11	0.97	1 (10%)	8,11,13	1.32	2 (25%)
1	MLY	A	138	1	10,10,11	1.35	1 (10%)	8,11,13	2.75	1 (12%)
1	MLY	A	19	1	10,10,11	1.18	1 (10%)	8,11,13	0.62	0
1	MLY	A	190	1	10,10,11	1.17	1 (10%)	8,11,13	1.32	1 (12%)
1	MLY	A	236	1	10,10,11	1.08	1 (10%)	8,11,13	1.55	2 (25%)
1	MLY	A	248	1	10,10,11	0.75	0	8,11,13	0.84	0
1	MLY	A	272	1	10,10,11	1.06	1 (10%)	8,11,13	1.32	1 (12%)
1	MLY	A	295	1	10,10,11	1.14	1 (10%)	8,11,13	0.30	0
1	MLY	A	296	1	10,10,11	0.89	1 (10%)	8,11,13	1.20	1 (12%)
1	MLY	A	30	1	10,10,11	0.89	0	8,11,13	0.91	0
1	MLY	A	348	1	10,10,11	0.79	0	8,11,13	1.11	1 (12%)
1	MLY	A	35	1	10,10,11	0.72	0	8,11,13	0.65	0
1	MLY	A	353	1	10,10,11	1.01	0	8,11,13	1.02	1 (12%)
1	MLY	A	367	1	10,10,11	0.89	1 (10%)	8,11,13	0.42	0
1	MLY	A	369	1	10,10,11	0.85	0	8,11,13	0.77	0
1	MLY	A	385	1	10,10,11	0.94	1 (10%)	8,11,13	0.54	0
1	MLY	A	415	1	10,10,11	0.71	0	8,11,13	0.73	0
1	MLY	A	431	1	10,10,11	0.47	0	8,11,13	1.19	1 (12%)
1	MLY	A	436	1	10,10,11	1.02	1 (10%)	8,11,13	1.80	1 (12%)
1	MLY	A	486	1	10,10,11	0.57	0	8,11,13	0.54	0
1	MLY	A	49	1	10,10,11	1.07	1 (10%)	8,11,13	1.24	1 (12%)
1	MLY	A	504	1	10,10,11	0.83	0	8,11,13	0.47	0
1	MLY	A	505	1	10,10,11	1.44	2 (20%)	8,11,13	0.49	0
1	MLY	A	528	1	10,10,11	0.84	0	8,11,13	1.13	1 (12%)
1	MLY	A	55	1	10,10,11	0.96	1 (10%)	8,11,13	1.07	0
1	MLY	A	551	1	10,10,11	0.62	0	8,11,13	0.72	0
1	MLY	A	553	1,4	10,10,11	0.63	0	8,11,13	0.65	0
1	MLY	A	59	1	10,10,11	0.81	0	8,11,13	1.12	1 (12%)
1	MLY	A	598	1	10,10,11	1.16	2 (20%)	8,11,13	1.32	1 (12%)
1	MLY	A	600	1	10,10,11	0.61	0	8,11,13	0.99	1 (12%)
1	MLY	A	613	1	10,10,11	0.65	0	8,11,13	1.10	1 (12%)
1	MLY	A	617	1	10,10,11	0.87	1 (10%)	8,11,13	0.60	0
1	MLY	A	63	1	10,10,11	0.90	0	8,11,13	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	MLY	A	659	1	10,10,11	0.75	0	8,11,13	0.84	0
1	MLY	A	681	1	10,10,11	0.99	1 (10%)	8,11,13	1.44	1 (12%)
1	MLY	A	764	1	10,10,11	0.81	0	8,11,13	0.49	0
1	MLY	A	768	1	10,10,11	0.89	0	8,11,13	1.95	1 (12%)
1	MLY	A	782	1	10,10,11	0.75	0	8,11,13	1.54	1 (12%)
1	MLY	A	827	1	10,10,11	0.99	1 (10%)	8,11,13	0.93	1 (12%)
1	MLY	A	833	1	10,10,11	1.07	1 (10%)	8,11,13	1.10	1 (12%)
1	MLY	A	837	1	10,10,11	0.66	0	8,11,13	0.55	0
1	MLY	A	839	1	10,10,11	0.65	0	8,11,13	1.50	1 (12%)
1	MLY	A	84	1	10,10,11	0.56	0	8,11,13	0.78	0
1	MLY	A	87	1	10,10,11	1.11	1 (10%)	8,11,13	0.58	0
1	MLY	D	107	1	10,10,11	0.51	0	8,11,13	1.02	1 (12%)
1	MLY	D	130	1	10,10,11	0.98	1 (10%)	8,11,13	1.33	2 (25%)
1	MLY	D	138	1	10,10,11	1.35	1 (10%)	8,11,13	2.69	1 (12%)
1	MLY	D	19	1	10,10,11	1.31	2 (20%)	8,11,13	0.63	0
1	MLY	D	190	1	10,10,11	1.13	1 (10%)	8,11,13	1.34	1 (12%)
1	MLY	D	236	1	10,10,11	1.13	1 (10%)	8,11,13	1.55	2 (25%)
1	MLY	D	248	1	10,10,11	0.76	0	8,11,13	0.85	0
1	MLY	D	272	1	10,10,11	1.02	1 (10%)	8,11,13	1.31	1 (12%)
1	MLY	D	295	1	10,10,11	1.10	1 (10%)	8,11,13	0.31	0
1	MLY	D	296	1	10,10,11	0.88	1 (10%)	8,11,13	1.19	1 (12%)
1	MLY	D	30	1	10,10,11	0.89	0	8,11,13	0.92	0
1	MLY	D	348	1	10,10,11	0.75	0	8,11,13	1.07	1 (12%)
1	MLY	D	35	1	10,10,11	0.75	0	8,11,13	0.63	0
1	MLY	D	353	1	10,10,11	0.95	0	8,11,13	1.01	1 (12%)
1	MLY	D	367	1	10,10,11	0.91	1 (10%)	8,11,13	0.41	0
1	MLY	D	369	1	10,10,11	0.85	0	8,11,13	0.77	0
1	MLY	D	385	1	10,10,11	0.92	1 (10%)	8,11,13	0.55	0
1	MLY	D	415	1	10,10,11	0.74	0	8,11,13	0.75	0
1	MLY	D	431	1	10,10,11	0.52	0	8,11,13	1.21	1 (12%)
1	MLY	D	436	1	10,10,11	1.05	1 (10%)	8,11,13	1.75	1 (12%)
1	MLY	D	486	1	10,10,11	0.57	0	8,11,13	0.56	0
1	MLY	D	49	1	10,10,11	1.11	1 (10%)	8,11,13	1.26	1 (12%)
1	MLY	D	504	1	10,10,11	0.82	0	8,11,13	0.44	0
1	MLY	D	505	1	10,10,11	1.42	2 (20%)	8,11,13	0.53	0
1	MLY	D	528	1	10,10,11	0.88	0	8,11,13	1.12	1 (12%)
1	MLY	D	55	1	10,10,11	0.97	1 (10%)	8,11,13	1.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	MLY	D	551	1	10,10,11	0.61	0	8,11,13	0.75	0
1	MLY	D	553	1,4	10,10,11	0.65	0	8,11,13	0.67	0
1	MLY	D	59	1	10,10,11	0.80	0	8,11,13	1.14	1 (12%)
1	MLY	D	598	1	10,10,11	1.12	2 (20%)	8,11,13	1.29	1 (12%)
1	MLY	D	600	1	10,10,11	0.60	0	8,11,13	0.97	1 (12%)
1	MLY	D	613	1	10,10,11	0.63	0	8,11,13	1.08	1 (12%)
1	MLY	D	617	1	10,10,11	0.91	1 (10%)	8,11,13	0.63	0
1	MLY	D	63	1	10,10,11	0.92	0	8,11,13	0.77	0
1	MLY	D	659	1	10,10,11	0.74	0	8,11,13	0.84	0
1	MLY	D	681	1	10,10,11	0.98	1 (10%)	8,11,13	1.42	1 (12%)
1	MLY	D	764	1	10,10,11	0.79	0	8,11,13	0.50	0
1	MLY	D	768	1	10,10,11	0.89	0	8,11,13	1.96	1 (12%)
1	MLY	D	782	1	10,10,11	0.74	0	8,11,13	1.53	1 (12%)
1	MLY	D	827	1	10,10,11	1.00	1 (10%)	8,11,13	0.94	1 (12%)
1	MLY	D	833	1	10,10,11	1.05	1 (10%)	8,11,13	1.14	1 (12%)
1	MLY	D	837	1	10,10,11	0.69	0	8,11,13	0.57	0
1	MLY	D	839	1	10,10,11	0.68	0	8,11,13	1.49	1 (12%)
1	MLY	D	84	1	10,10,11	0.61	0	8,11,13	0.81	0
1	MLY	D	87	1	10,10,11	1.09	1 (10%)	8,11,13	0.62	0
1	MLY	G	107	1	10,10,11	0.48	0	8,11,13	1.00	1 (12%)
1	MLY	G	130	1	10,10,11	0.96	1 (10%)	8,11,13	1.34	2 (25%)
1	MLY	G	138	1	10,10,11	1.35	1 (10%)	8,11,13	2.75	1 (12%)
1	MLY	G	19	1	10,10,11	1.23	1 (10%)	8,11,13	0.65	0
1	MLY	G	190	1	10,10,11	1.15	1 (10%)	8,11,13	1.33	1 (12%)
1	MLY	G	236	1	10,10,11	1.07	1 (10%)	8,11,13	1.55	2 (25%)
1	MLY	G	248	1	10,10,11	0.73	0	8,11,13	0.85	0
1	MLY	G	272	1	10,10,11	1.06	1 (10%)	8,11,13	1.32	1 (12%)
1	MLY	G	295	1	10,10,11	1.13	1 (10%)	8,11,13	0.31	0
1	MLY	G	296	1	10,10,11	0.89	1 (10%)	8,11,13	1.19	1 (12%)
1	MLY	G	30	1	10,10,11	0.87	0	8,11,13	0.91	0
1	MLY	G	348	1	10,10,11	0.78	0	8,11,13	1.07	1 (12%)
1	MLY	G	35	1	10,10,11	0.75	0	8,11,13	0.64	0
1	MLY	G	353	1	10,10,11	1.01	0	8,11,13	1.01	1 (12%)
1	MLY	G	367	1	10,10,11	0.93	1 (10%)	8,11,13	0.44	0
1	MLY	G	369	1	10,10,11	0.85	0	8,11,13	0.78	0
1	MLY	G	385	1	10,10,11	0.94	1 (10%)	8,11,13	0.53	0
1	MLY	G	415	1	10,10,11	0.72	0	8,11,13	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	MLY	G	431	1	10,10,11	0.46	0	8,11,13	1.18	1 (12%)
1	MLY	G	436	1	10,10,11	1.02	1 (10%)	8,11,13	1.78	1 (12%)
1	MLY	G	486	1	10,10,11	0.57	0	8,11,13	0.55	0
1	MLY	G	49	1	10,10,11	1.09	1 (10%)	8,11,13	1.23	1 (12%)
1	MLY	G	504	1	10,10,11	0.83	0	8,11,13	0.45	0
1	MLY	G	505	1	10,10,11	1.44	1 (10%)	8,11,13	0.51	0
1	MLY	G	528	1	10,10,11	0.84	0	8,11,13	1.13	1 (12%)
1	MLY	G	55	1	10,10,11	1.02	1 (10%)	8,11,13	1.09	0
1	MLY	G	551	1	10,10,11	0.63	0	8,11,13	0.73	0
1	MLY	G	553	1,4	10,10,11	0.64	0	8,11,13	0.65	0
1	MLY	G	59	1	10,10,11	0.76	0	8,11,13	1.16	1 (12%)
1	MLY	G	598	1	10,10,11	1.12	2 (20%)	8,11,13	1.33	1 (12%)
1	MLY	G	600	1	10,10,11	0.65	0	8,11,13	0.97	1 (12%)
1	MLY	G	613	1	10,10,11	0.68	0	8,11,13	1.11	1 (12%)
1	MLY	G	617	1	10,10,11	0.88	1 (10%)	8,11,13	0.62	0
1	MLY	G	63	1	10,10,11	0.89	0	8,11,13	0.80	0
1	MLY	G	659	1	10,10,11	0.75	0	8,11,13	0.81	0
1	MLY	G	681	1	10,10,11	1.00	1 (10%)	8,11,13	1.43	1 (12%)
1	MLY	G	764	1	10,10,11	0.74	0	8,11,13	0.50	0
1	MLY	G	768	1	10,10,11	0.89	0	8,11,13	1.93	1 (12%)
1	MLY	G	782	1	10,10,11	0.72	0	8,11,13	1.54	1 (12%)
1	MLY	G	827	1	10,10,11	1.02	1 (10%)	8,11,13	0.94	1 (12%)
1	MLY	G	833	1	10,10,11	1.08	1 (10%)	8,11,13	1.15	1 (12%)
1	MLY	G	837	1	10,10,11	0.66	0	8,11,13	0.54	0
1	MLY	G	839	1	10,10,11	0.68	0	8,11,13	1.52	1 (12%)
1	MLY	G	84	1	10,10,11	0.60	0	8,11,13	0.80	0
1	MLY	G	87	1	10,10,11	1.11	1 (10%)	8,11,13	0.59	0
1	MLY	J	107	1	10,10,11	0.49	0	8,11,13	1.04	1 (12%)
1	MLY	J	130	1	10,10,11	0.92	0	8,11,13	1.33	2 (25%)
1	MLY	J	138	1	10,10,11	1.32	1 (10%)	8,11,13	2.73	1 (12%)
1	MLY	J	19	1	10,10,11	1.28	1 (10%)	8,11,13	0.64	0
1	MLY	J	190	1	10,10,11	1.19	1 (10%)	8,11,13	1.29	1 (12%)
1	MLY	J	236	1	10,10,11	1.14	1 (10%)	8,11,13	1.56	2 (25%)
1	MLY	J	248	1	10,10,11	0.77	0	8,11,13	0.87	0
1	MLY	J	272	1	10,10,11	1.09	1 (10%)	8,11,13	1.30	1 (12%)
1	MLY	J	295	1	10,10,11	1.14	1 (10%)	8,11,13	0.32	0
1	MLY	J	296	1	10,10,11	0.95	1 (10%)	8,11,13	1.18	1 (12%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	MLY	J	30	1	10,10,11	0.85	0	8,11,13	0.92	0
1	MLY	J	348	1	10,10,11	0.75	0	8,11,13	1.06	1 (12%)
1	MLY	J	35	1	10,10,11	0.75	0	8,11,13	0.63	0
1	MLY	J	353	1	10,10,11	0.98	0	8,11,13	1.04	1 (12%)
1	MLY	J	367	1	10,10,11	0.92	1 (10%)	8,11,13	0.42	0
1	MLY	J	369	1	10,10,11	0.85	0	8,11,13	0.78	0
1	MLY	J	385	1	10,10,11	0.94	1 (10%)	8,11,13	0.52	0
1	MLY	J	415	1	10,10,11	0.73	0	8,11,13	0.73	0
1	MLY	J	431	1	10,10,11	0.49	0	8,11,13	1.20	1 (12%)
1	MLY	J	436	1	10,10,11	1.03	1 (10%)	8,11,13	1.75	1 (12%)
1	MLY	J	486	1	10,10,11	0.56	0	8,11,13	0.54	0
1	MLY	J	49	1	10,10,11	1.14	1 (10%)	8,11,13	1.27	1 (12%)
1	MLY	J	504	1	10,10,11	0.78	0	8,11,13	0.46	0
1	MLY	J	505	1	10,10,11	1.48	2 (20%)	8,11,13	0.52	0
1	MLY	J	528	1	10,10,11	0.84	0	8,11,13	1.11	1 (12%)
1	MLY	J	55	1	10,10,11	0.95	1 (10%)	8,11,13	1.12	0
1	MLY	J	551	1	10,10,11	0.64	0	8,11,13	0.75	0
1	MLY	J	553	1	10,10,11	0.63	0	8,11,13	0.63	0
1	MLY	J	59	1	10,10,11	0.81	0	8,11,13	1.15	1 (12%)
1	MLY	J	598	1	10,10,11	1.12	2 (20%)	8,11,13	1.29	1 (12%)
1	MLY	J	600	1	10,10,11	0.62	0	8,11,13	0.98	1 (12%)
1	MLY	J	613	1	10,10,11	0.68	0	8,11,13	1.09	1 (12%)
1	MLY	J	617	1	10,10,11	0.92	1 (10%)	8,11,13	0.60	0
1	MLY	J	63	1	10,10,11	0.89	0	8,11,13	0.78	0
1	MLY	J	659	1	10,10,11	0.74	0	8,11,13	0.84	0
1	MLY	J	681	1	10,10,11	0.95	1 (10%)	8,11,13	1.42	1 (12%)
1	MLY	J	764	1	10,10,11	0.74	0	8,11,13	0.51	0
1	MLY	J	768	1	10,10,11	0.90	0	8,11,13	1.95	1 (12%)
1	MLY	J	782	1	10,10,11	0.72	0	8,11,13	1.53	1 (12%)
1	MLY	J	827	1	10,10,11	1.11	1 (10%)	8,11,13	0.92	1 (12%)
1	MLY	J	833	1	10,10,11	1.09	1 (10%)	8,11,13	1.07	1 (12%)
1	MLY	J	837	1	10,10,11	0.69	0	8,11,13	0.54	0
1	MLY	J	839	1	10,10,11	0.66	0	8,11,13	1.50	1 (12%)
1	MLY	J	84	1	10,10,11	0.57	0	8,11,13	0.80	0
1	MLY	J	87	1	10,10,11	1.12	1 (10%)	8,11,13	0.62	0
1	MLY	M	107	1	10,10,11	0.49	0	8,11,13	1.03	1 (12%)
1	MLY	M	130	1	10,10,11	0.94	1 (10%)	8,11,13	1.33	2 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	MLY	M	138	1	10,10,11	1.33	1 (10%)	8,11,13	2.74	1 (12%)
1	MLY	M	19	1	10,10,11	1.23	1 (10%)	8,11,13	0.64	0
1	MLY	M	190	1	10,10,11	1.18	1 (10%)	8,11,13	1.29	1 (12%)
1	MLY	M	236	1	10,10,11	1.10	1 (10%)	8,11,13	1.56	2 (25%)
1	MLY	M	248	1	10,10,11	0.76	0	8,11,13	0.86	0
1	MLY	M	272	1	10,10,11	1.10	1 (10%)	8,11,13	1.32	1 (12%)
1	MLY	M	295	1	10,10,11	1.14	1 (10%)	8,11,13	0.32	0
1	MLY	M	296	1	10,10,11	0.91	1 (10%)	8,11,13	1.19	1 (12%)
1	MLY	M	30	1	10,10,11	0.86	0	8,11,13	0.93	0
1	MLY	M	348	1	10,10,11	0.75	0	8,11,13	1.08	1 (12%)
1	MLY	M	35	1	10,10,11	0.76	0	8,11,13	0.63	0
1	MLY	M	353	1	10,10,11	1.03	1 (10%)	8,11,13	1.03	1 (12%)
1	MLY	M	367	1	10,10,11	0.90	1 (10%)	8,11,13	0.43	0
1	MLY	M	369	1	10,10,11	0.86	0	8,11,13	0.78	0
1	MLY	M	385	1	10,10,11	0.96	1 (10%)	8,11,13	0.52	0
1	MLY	M	415	1	10,10,11	0.74	0	8,11,13	0.74	0
1	MLY	M	431	1	10,10,11	0.47	0	8,11,13	1.21	1 (12%)
1	MLY	M	436	1	10,10,11	1.05	1 (10%)	8,11,13	1.76	1 (12%)
1	MLY	M	486	1	10,10,11	0.56	0	8,11,13	0.53	0
1	MLY	M	49	1	10,10,11	1.10	1 (10%)	8,11,13	1.25	1 (12%)
1	MLY	M	504	1	10,10,11	0.79	0	8,11,13	0.46	0
1	MLY	M	505	1	10,10,11	1.45	2 (20%)	8,11,13	0.49	0
1	MLY	M	528	1	10,10,11	0.83	0	8,11,13	1.11	1 (12%)
1	MLY	M	55	1	10,10,11	0.97	1 (10%)	8,11,13	1.10	0
1	MLY	M	551	1	10,10,11	0.66	0	8,11,13	0.74	0
1	MLY	M	553	1	10,10,11	0.63	0	8,11,13	0.64	0
1	MLY	M	59	1	10,10,11	0.80	0	8,11,13	1.13	1 (12%)
1	MLY	M	598	1	10,10,11	1.14	2 (20%)	8,11,13	1.32	1 (12%)
1	MLY	M	600	1	10,10,11	0.63	0	8,11,13	0.98	1 (12%)
1	MLY	M	613	1	10,10,11	0.69	0	8,11,13	1.09	1 (12%)
1	MLY	M	617	1	10,10,11	0.88	1 (10%)	8,11,13	0.59	0
1	MLY	M	63	1	10,10,11	0.92	0	8,11,13	0.80	0
1	MLY	M	659	1	10,10,11	0.73	0	8,11,13	0.83	0
1	MLY	M	681	1	10,10,11	0.94	1 (10%)	8,11,13	1.42	1 (12%)
1	MLY	M	764	1	10,10,11	0.75	0	8,11,13	0.51	0
1	MLY	M	768	1	10,10,11	0.91	0	8,11,13	1.92	1 (12%)
1	MLY	M	782	1	10,10,11	0.73	0	8,11,13	1.56	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	MLY	M	827	1	10,10,11	1.03	1 (10%)	8,11,13	0.94	1 (12%)
1	MLY	M	833	1	10,10,11	1.13	1 (10%)	8,11,13	1.08	1 (12%)
1	MLY	M	837	1	10,10,11	0.67	0	8,11,13	0.53	0
1	MLY	M	839	1	10,10,11	0.67	0	8,11,13	1.48	1 (12%)
1	MLY	M	84	1	10,10,11	0.59	0	8,11,13	0.79	0
1	MLY	M	87	1	10,10,11	1.12	1 (10%)	8,11,13	0.62	0
1	MLY	P	107	1	10,10,11	0.48	0	8,11,13	1.03	1 (12%)
1	MLY	P	130	1	10,10,11	0.92	0	8,11,13	1.33	2 (25%)
1	MLY	P	138	1	10,10,11	1.32	1 (10%)	8,11,13	2.72	1 (12%)
1	MLY	P	19	1	10,10,11	1.28	1 (10%)	8,11,13	0.62	0
1	MLY	P	190	1	10,10,11	1.18	1 (10%)	8,11,13	1.29	1 (12%)
1	MLY	P	236	1	10,10,11	1.13	1 (10%)	8,11,13	1.56	2 (25%)
1	MLY	P	248	1	10,10,11	0.77	0	8,11,13	0.86	0
1	MLY	P	272	1	10,10,11	1.06	1 (10%)	8,11,13	1.30	1 (12%)
1	MLY	P	295	1	10,10,11	1.15	1 (10%)	8,11,13	0.33	0
1	MLY	P	296	1	10,10,11	0.88	1 (10%)	8,11,13	1.18	1 (12%)
1	MLY	P	30	1	10,10,11	0.85	0	8,11,13	0.92	0
1	MLY	P	348	1	10,10,11	0.75	0	8,11,13	1.06	1 (12%)
1	MLY	P	35	1	10,10,11	0.75	0	8,11,13	0.64	0
1	MLY	P	353	1	10,10,11	0.97	0	8,11,13	1.03	1 (12%)
1	MLY	P	367	1	10,10,11	0.91	1 (10%)	8,11,13	0.43	0
1	MLY	P	369	1	10,10,11	0.83	0	8,11,13	0.78	0
1	MLY	P	385	1	10,10,11	0.93	1 (10%)	8,11,13	0.52	0
1	MLY	P	415	1	10,10,11	0.71	0	8,11,13	0.74	0
1	MLY	P	431	1	10,10,11	0.50	0	8,11,13	1.20	1 (12%)
1	MLY	P	436	1	10,10,11	1.03	1 (10%)	8,11,13	1.76	1 (12%)
1	MLY	P	486	1	10,10,11	0.55	0	8,11,13	0.54	0
1	MLY	P	49	1	10,10,11	1.15	1 (10%)	8,11,13	1.27	1 (12%)
1	MLY	P	504	1	10,10,11	0.77	0	8,11,13	0.45	0
1	MLY	P	505	1	10,10,11	1.45	2 (20%)	8,11,13	0.51	0
1	MLY	P	528	1	10,10,11	0.84	0	8,11,13	1.12	1 (12%)
1	MLY	P	55	1	10,10,11	0.93	1 (10%)	8,11,13	1.11	0
1	MLY	P	551	1	10,10,11	0.63	0	8,11,13	0.74	0
1	MLY	P	553	1	10,10,11	0.64	0	8,11,13	0.65	0
1	MLY	P	59	1	10,10,11	0.79	0	8,11,13	1.16	1 (12%)
1	MLY	P	598	1	10,10,11	1.15	2 (20%)	8,11,13	1.30	1 (12%)
1	MLY	P	600	1	10,10,11	0.63	0	8,11,13	0.98	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	MLY	P	613	1	10,10,11	0.69	0	8,11,13	1.09	1 (12%)
1	MLY	P	617	1	10,10,11	0.93	1 (10%)	8,11,13	0.60	0
1	MLY	P	63	1	10,10,11	0.89	0	8,11,13	0.78	0
1	MLY	P	659	1	10,10,11	0.76	0	8,11,13	0.84	0
1	MLY	P	681	1	10,10,11	0.98	1 (10%)	8,11,13	1.42	1 (12%)
1	MLY	P	764	1	10,10,11	0.75	0	8,11,13	0.53	0
1	MLY	P	768	1	10,10,11	0.89	0	8,11,13	1.93	1 (12%)
1	MLY	P	782	1	10,10,11	0.72	0	8,11,13	1.56	1 (12%)
1	MLY	P	827	1	10,10,11	1.08	1 (10%)	8,11,13	0.92	1 (12%)
1	MLY	P	833	1	10,10,11	1.09	1 (10%)	8,11,13	1.09	1 (12%)
1	MLY	P	837	1	10,10,11	0.66	0	8,11,13	0.54	0
1	MLY	P	839	1	10,10,11	0.65	0	8,11,13	1.49	1 (12%)
1	MLY	P	84	1	10,10,11	0.61	0	8,11,13	0.80	0
1	MLY	P	87	1	10,10,11	1.11	1 (10%)	8,11,13	0.60	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	-	0/7/9/11	0/0/0/0
1	MLY	A	130	1	-	0/7/9/11	0/0/0/0
1	MLY	A	138	1	-	0/7/9/11	0/0/0/0
1	MLY	A	19	1	-	0/7/9/11	0/0/0/0
1	MLY	A	190	1	-	0/7/9/11	0/0/0/0
1	MLY	A	236	1	-	0/7/9/11	0/0/0/0
1	MLY	A	248	1	-	0/7/9/11	0/0/0/0
1	MLY	A	272	1	-	0/7/9/11	0/0/0/0
1	MLY	A	295	1	-	0/7/9/11	0/0/0/0
1	MLY	A	296	1	-	0/7/9/11	0/0/0/0
1	MLY	A	30	1	-	0/7/9/11	0/0/0/0
1	MLY	A	348	1	-	0/7/9/11	0/0/0/0
1	MLY	A	35	1	-	0/7/9/11	0/0/0/0
1	MLY	A	353	1	-	0/7/9/11	0/0/0/0
1	MLY	A	367	1	-	0/7/9/11	0/0/0/0
1	MLY	A	369	1	-	0/7/9/11	0/0/0/0
1	MLY	A	385	1	-	0/7/9/11	0/0/0/0
1	MLY	A	415	1	-	0/7/9/11	0/0/0/0
1	MLY	A	431	1	-	0/7/9/11	0/0/0/0
1	MLY	A	436	1	-	0/7/9/11	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	A	486	1	-	0/7/9/11	0/0/0/0
1	MLY	A	49	1	-	0/7/9/11	0/0/0/0
1	MLY	A	504	1	-	0/7/9/11	0/0/0/0
1	MLY	A	505	1	-	0/7/9/11	0/0/0/0
1	MLY	A	528	1	-	0/7/9/11	0/0/0/0
1	MLY	A	55	1	-	0/7/9/11	0/0/0/0
1	MLY	A	551	1	-	0/7/9/11	0/0/0/0
1	MLY	A	553	1,4	-	0/7/9/11	0/0/0/0
1	MLY	A	59	1	-	0/7/9/11	0/0/0/0
1	MLY	A	598	1	-	0/7/9/11	0/0/0/0
1	MLY	A	600	1	-	0/7/9/11	0/0/0/0
1	MLY	A	613	1	-	0/7/9/11	0/0/0/0
1	MLY	A	617	1	-	0/7/9/11	0/0/0/0
1	MLY	A	63	1	-	0/7/9/11	0/0/0/0
1	MLY	A	659	1	-	0/7/9/11	0/0/0/0
1	MLY	A	681	1	-	0/7/9/11	0/0/0/0
1	MLY	A	764	1	-	0/7/9/11	0/0/0/0
1	MLY	A	768	1	-	0/7/9/11	0/0/0/0
1	MLY	A	782	1	-	0/7/9/11	0/0/0/0
1	MLY	A	827	1	-	0/7/9/11	0/0/0/0
1	MLY	A	833	1	-	0/7/9/11	0/0/0/0
1	MLY	A	837	1	-	0/7/9/11	0/0/0/0
1	MLY	A	839	1	-	0/7/9/11	0/0/0/0
1	MLY	A	84	1	-	0/7/9/11	0/0/0/0
1	MLY	A	87	1	-	0/7/9/11	0/0/0/0
1	MLY	D	107	1	-	0/7/9/11	0/0/0/0
1	MLY	D	130	1	-	0/7/9/11	0/0/0/0
1	MLY	D	138	1	-	0/7/9/11	0/0/0/0
1	MLY	D	19	1	-	0/7/9/11	0/0/0/0
1	MLY	D	190	1	-	0/7/9/11	0/0/0/0
1	MLY	D	236	1	-	0/7/9/11	0/0/0/0
1	MLY	D	248	1	-	0/7/9/11	0/0/0/0
1	MLY	D	272	1	-	0/7/9/11	0/0/0/0
1	MLY	D	295	1	-	0/7/9/11	0/0/0/0
1	MLY	D	296	1	-	0/7/9/11	0/0/0/0
1	MLY	D	30	1	-	0/7/9/11	0/0/0/0
1	MLY	D	348	1	-	0/7/9/11	0/0/0/0
1	MLY	D	35	1	-	0/7/9/11	0/0/0/0
1	MLY	D	353	1	-	0/7/9/11	0/0/0/0
1	MLY	D	367	1	-	0/7/9/11	0/0/0/0
1	MLY	D	369	1	-	0/7/9/11	0/0/0/0
1	MLY	D	385	1	-	0/7/9/11	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	D	415	1	-	0/7/9/11	0/0/0/0
1	MLY	D	431	1	-	0/7/9/11	0/0/0/0
1	MLY	D	436	1	-	0/7/9/11	0/0/0/0
1	MLY	D	486	1	-	0/7/9/11	0/0/0/0
1	MLY	D	49	1	-	0/7/9/11	0/0/0/0
1	MLY	D	504	1	-	0/7/9/11	0/0/0/0
1	MLY	D	505	1	-	0/7/9/11	0/0/0/0
1	MLY	D	528	1	-	0/7/9/11	0/0/0/0
1	MLY	D	55	1	-	0/7/9/11	0/0/0/0
1	MLY	D	551	1	-	0/7/9/11	0/0/0/0
1	MLY	D	553	1,4	-	0/7/9/11	0/0/0/0
1	MLY	D	59	1	-	0/7/9/11	0/0/0/0
1	MLY	D	598	1	-	0/7/9/11	0/0/0/0
1	MLY	D	600	1	-	0/7/9/11	0/0/0/0
1	MLY	D	613	1	-	0/7/9/11	0/0/0/0
1	MLY	D	617	1	-	0/7/9/11	0/0/0/0
1	MLY	D	63	1	-	0/7/9/11	0/0/0/0
1	MLY	D	659	1	-	0/7/9/11	0/0/0/0
1	MLY	D	681	1	-	0/7/9/11	0/0/0/0
1	MLY	D	764	1	-	0/7/9/11	0/0/0/0
1	MLY	D	768	1	-	0/7/9/11	0/0/0/0
1	MLY	D	782	1	-	0/7/9/11	0/0/0/0
1	MLY	D	827	1	-	0/7/9/11	0/0/0/0
1	MLY	D	833	1	-	0/7/9/11	0/0/0/0
1	MLY	D	837	1	-	0/7/9/11	0/0/0/0
1	MLY	D	839	1	-	0/7/9/11	0/0/0/0
1	MLY	D	84	1	-	0/7/9/11	0/0/0/0
1	MLY	D	87	1	-	0/7/9/11	0/0/0/0
1	MLY	G	107	1	-	0/7/9/11	0/0/0/0
1	MLY	G	130	1	-	0/7/9/11	0/0/0/0
1	MLY	G	138	1	-	0/7/9/11	0/0/0/0
1	MLY	G	19	1	-	0/7/9/11	0/0/0/0
1	MLY	G	190	1	-	0/7/9/11	0/0/0/0
1	MLY	G	236	1	-	0/7/9/11	0/0/0/0
1	MLY	G	248	1	-	0/7/9/11	0/0/0/0
1	MLY	G	272	1	-	0/7/9/11	0/0/0/0
1	MLY	G	295	1	-	0/7/9/11	0/0/0/0
1	MLY	G	296	1	-	0/7/9/11	0/0/0/0
1	MLY	G	30	1	-	0/7/9/11	0/0/0/0
1	MLY	G	348	1	-	0/7/9/11	0/0/0/0
1	MLY	G	35	1	-	0/7/9/11	0/0/0/0
1	MLY	G	353	1	-	0/7/9/11	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	G	367	1	-	0/7/9/11	0/0/0/0
1	MLY	G	369	1	-	0/7/9/11	0/0/0/0
1	MLY	G	385	1	-	0/7/9/11	0/0/0/0
1	MLY	G	415	1	-	0/7/9/11	0/0/0/0
1	MLY	G	431	1	-	0/7/9/11	0/0/0/0
1	MLY	G	436	1	-	0/7/9/11	0/0/0/0
1	MLY	G	486	1	-	0/7/9/11	0/0/0/0
1	MLY	G	49	1	-	0/7/9/11	0/0/0/0
1	MLY	G	504	1	-	0/7/9/11	0/0/0/0
1	MLY	G	505	1	-	0/7/9/11	0/0/0/0
1	MLY	G	528	1	-	0/7/9/11	0/0/0/0
1	MLY	G	55	1	-	0/7/9/11	0/0/0/0
1	MLY	G	551	1	-	0/7/9/11	0/0/0/0
1	MLY	G	553	1,4	-	0/7/9/11	0/0/0/0
1	MLY	G	59	1	-	0/7/9/11	0/0/0/0
1	MLY	G	598	1	-	0/7/9/11	0/0/0/0
1	MLY	G	600	1	-	0/7/9/11	0/0/0/0
1	MLY	G	613	1	-	0/7/9/11	0/0/0/0
1	MLY	G	617	1	-	0/7/9/11	0/0/0/0
1	MLY	G	63	1	-	0/7/9/11	0/0/0/0
1	MLY	G	659	1	-	0/7/9/11	0/0/0/0
1	MLY	G	681	1	-	0/7/9/11	0/0/0/0
1	MLY	G	764	1	-	0/7/9/11	0/0/0/0
1	MLY	G	768	1	-	0/7/9/11	0/0/0/0
1	MLY	G	782	1	-	0/7/9/11	0/0/0/0
1	MLY	G	827	1	-	0/7/9/11	0/0/0/0
1	MLY	G	833	1	-	0/7/9/11	0/0/0/0
1	MLY	G	837	1	-	0/7/9/11	0/0/0/0
1	MLY	G	839	1	-	0/7/9/11	0/0/0/0
1	MLY	G	84	1	-	0/7/9/11	0/0/0/0
1	MLY	G	87	1	-	0/7/9/11	0/0/0/0
1	MLY	J	107	1	-	0/7/9/11	0/0/0/0
1	MLY	J	130	1	-	0/7/9/11	0/0/0/0
1	MLY	J	138	1	-	0/7/9/11	0/0/0/0
1	MLY	J	19	1	-	0/7/9/11	0/0/0/0
1	MLY	J	190	1	-	0/7/9/11	0/0/0/0
1	MLY	J	236	1	-	0/7/9/11	0/0/0/0
1	MLY	J	248	1	-	0/7/9/11	0/0/0/0
1	MLY	J	272	1	-	0/7/9/11	0/0/0/0
1	MLY	J	295	1	-	0/7/9/11	0/0/0/0
1	MLY	J	296	1	-	0/7/9/11	0/0/0/0
1	MLY	J	30	1	-	0/7/9/11	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	J	348	1	-	0/7/9/11	0/0/0/0
1	MLY	J	35	1	-	0/7/9/11	0/0/0/0
1	MLY	J	353	1	-	0/7/9/11	0/0/0/0
1	MLY	J	367	1	-	0/7/9/11	0/0/0/0
1	MLY	J	369	1	-	0/7/9/11	0/0/0/0
1	MLY	J	385	1	-	0/7/9/11	0/0/0/0
1	MLY	J	415	1	-	0/7/9/11	0/0/0/0
1	MLY	J	431	1	-	0/7/9/11	0/0/0/0
1	MLY	J	436	1	-	0/7/9/11	0/0/0/0
1	MLY	J	486	1	-	0/7/9/11	0/0/0/0
1	MLY	J	49	1	-	0/7/9/11	0/0/0/0
1	MLY	J	504	1	-	0/7/9/11	0/0/0/0
1	MLY	J	505	1	-	0/7/9/11	0/0/0/0
1	MLY	J	528	1	-	0/7/9/11	0/0/0/0
1	MLY	J	55	1	-	0/7/9/11	0/0/0/0
1	MLY	J	551	1	-	0/7/9/11	0/0/0/0
1	MLY	J	553	1	-	0/7/9/11	0/0/0/0
1	MLY	J	59	1	-	0/7/9/11	0/0/0/0
1	MLY	J	598	1	-	0/7/9/11	0/0/0/0
1	MLY	J	600	1	-	0/7/9/11	0/0/0/0
1	MLY	J	613	1	-	0/7/9/11	0/0/0/0
1	MLY	J	617	1	-	0/7/9/11	0/0/0/0
1	MLY	J	63	1	-	0/7/9/11	0/0/0/0
1	MLY	J	659	1	-	0/7/9/11	0/0/0/0
1	MLY	J	681	1	-	0/7/9/11	0/0/0/0
1	MLY	J	764	1	-	0/7/9/11	0/0/0/0
1	MLY	J	768	1	-	0/7/9/11	0/0/0/0
1	MLY	J	782	1	-	0/7/9/11	0/0/0/0
1	MLY	J	827	1	-	0/7/9/11	0/0/0/0
1	MLY	J	833	1	-	0/7/9/11	0/0/0/0
1	MLY	J	837	1	-	0/7/9/11	0/0/0/0
1	MLY	J	839	1	-	0/7/9/11	0/0/0/0
1	MLY	J	84	1	-	0/7/9/11	0/0/0/0
1	MLY	J	87	1	-	0/7/9/11	0/0/0/0
1	MLY	M	107	1	-	0/7/9/11	0/0/0/0
1	MLY	M	130	1	-	0/7/9/11	0/0/0/0
1	MLY	M	138	1	-	0/7/9/11	0/0/0/0
1	MLY	M	19	1	-	0/7/9/11	0/0/0/0
1	MLY	M	190	1	-	0/7/9/11	0/0/0/0
1	MLY	M	236	1	-	0/7/9/11	0/0/0/0
1	MLY	M	248	1	-	0/7/9/11	0/0/0/0
1	MLY	M	272	1	-	0/7/9/11	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	M	295	1	-	0/7/9/11	0/0/0/0
1	MLY	M	296	1	-	0/7/9/11	0/0/0/0
1	MLY	M	30	1	-	0/7/9/11	0/0/0/0
1	MLY	M	348	1	-	0/7/9/11	0/0/0/0
1	MLY	M	35	1	-	0/7/9/11	0/0/0/0
1	MLY	M	353	1	-	0/7/9/11	0/0/0/0
1	MLY	M	367	1	-	0/7/9/11	0/0/0/0
1	MLY	M	369	1	-	0/7/9/11	0/0/0/0
1	MLY	M	385	1	-	0/7/9/11	0/0/0/0
1	MLY	M	415	1	-	0/7/9/11	0/0/0/0
1	MLY	M	431	1	-	0/7/9/11	0/0/0/0
1	MLY	M	436	1	-	0/7/9/11	0/0/0/0
1	MLY	M	486	1	-	0/7/9/11	0/0/0/0
1	MLY	M	49	1	-	0/7/9/11	0/0/0/0
1	MLY	M	504	1	-	0/7/9/11	0/0/0/0
1	MLY	M	505	1	-	0/7/9/11	0/0/0/0
1	MLY	M	528	1	-	0/7/9/11	0/0/0/0
1	MLY	M	55	1	-	0/7/9/11	0/0/0/0
1	MLY	M	551	1	-	0/7/9/11	0/0/0/0
1	MLY	M	553	1	-	0/7/9/11	0/0/0/0
1	MLY	M	59	1	-	0/7/9/11	0/0/0/0
1	MLY	M	598	1	-	0/7/9/11	0/0/0/0
1	MLY	M	600	1	-	0/7/9/11	0/0/0/0
1	MLY	M	613	1	-	0/7/9/11	0/0/0/0
1	MLY	M	617	1	-	0/7/9/11	0/0/0/0
1	MLY	M	63	1	-	0/7/9/11	0/0/0/0
1	MLY	M	659	1	-	0/7/9/11	0/0/0/0
1	MLY	M	681	1	-	0/7/9/11	0/0/0/0
1	MLY	M	764	1	-	0/7/9/11	0/0/0/0
1	MLY	M	768	1	-	0/7/9/11	0/0/0/0
1	MLY	M	782	1	-	0/7/9/11	0/0/0/0
1	MLY	M	827	1	-	0/7/9/11	0/0/0/0
1	MLY	M	833	1	-	0/7/9/11	0/0/0/0
1	MLY	M	837	1	-	0/7/9/11	0/0/0/0
1	MLY	M	839	1	-	0/7/9/11	0/0/0/0
1	MLY	M	84	1	-	0/7/9/11	0/0/0/0
1	MLY	M	87	1	-	0/7/9/11	0/0/0/0
1	MLY	P	107	1	-	0/7/9/11	0/0/0/0
1	MLY	P	130	1	-	0/7/9/11	0/0/0/0
1	MLY	P	138	1	-	0/7/9/11	0/0/0/0
1	MLY	P	19	1	-	0/7/9/11	0/0/0/0
1	MLY	P	190	1	-	0/7/9/11	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	P	236	1	-	0/7/9/11	0/0/0/0
1	MLY	P	248	1	-	0/7/9/11	0/0/0/0
1	MLY	P	272	1	-	0/7/9/11	0/0/0/0
1	MLY	P	295	1	-	0/7/9/11	0/0/0/0
1	MLY	P	296	1	-	0/7/9/11	0/0/0/0
1	MLY	P	30	1	-	0/7/9/11	0/0/0/0
1	MLY	P	348	1	-	0/7/9/11	0/0/0/0
1	MLY	P	35	1	-	0/7/9/11	0/0/0/0
1	MLY	P	353	1	-	0/7/9/11	0/0/0/0
1	MLY	P	367	1	-	0/7/9/11	0/0/0/0
1	MLY	P	369	1	-	0/7/9/11	0/0/0/0
1	MLY	P	385	1	-	0/7/9/11	0/0/0/0
1	MLY	P	415	1	-	0/7/9/11	0/0/0/0
1	MLY	P	431	1	-	0/7/9/11	0/0/0/0
1	MLY	P	436	1	-	0/7/9/11	0/0/0/0
1	MLY	P	486	1	-	0/7/9/11	0/0/0/0
1	MLY	P	49	1	-	0/7/9/11	0/0/0/0
1	MLY	P	504	1	-	0/7/9/11	0/0/0/0
1	MLY	P	505	1	-	0/7/9/11	0/0/0/0
1	MLY	P	528	1	-	0/7/9/11	0/0/0/0
1	MLY	P	55	1	-	0/7/9/11	0/0/0/0
1	MLY	P	551	1	-	0/7/9/11	0/0/0/0
1	MLY	P	553	1	-	0/7/9/11	0/0/0/0
1	MLY	P	59	1	-	0/7/9/11	0/0/0/0
1	MLY	P	598	1	-	0/7/9/11	0/0/0/0
1	MLY	P	600	1	-	0/7/9/11	0/0/0/0
1	MLY	P	613	1	-	0/7/9/11	0/0/0/0
1	MLY	P	617	1	-	0/7/9/11	0/0/0/0
1	MLY	P	63	1	-	0/7/9/11	0/0/0/0
1	MLY	P	659	1	-	0/7/9/11	0/0/0/0
1	MLY	P	681	1	-	0/7/9/11	0/0/0/0
1	MLY	P	764	1	-	0/7/9/11	0/0/0/0
1	MLY	P	768	1	-	0/7/9/11	0/0/0/0
1	MLY	P	782	1	-	0/7/9/11	0/0/0/0
1	MLY	P	827	1	-	0/7/9/11	0/0/0/0
1	MLY	P	833	1	-	0/7/9/11	0/0/0/0
1	MLY	P	837	1	-	0/7/9/11	0/0/0/0
1	MLY	P	839	1	-	0/7/9/11	0/0/0/0
1	MLY	P	84	1	-	0/7/9/11	0/0/0/0
1	MLY	P	87	1	-	0/7/9/11	0/0/0/0

The worst 5 of 131 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	138	MLY	CB-CA	-3.72	1.48	1.53
1	D	138	MLY	CB-CA	-3.67	1.48	1.53
1	M	138	MLY	CB-CA	-3.62	1.48	1.53
1	A	138	MLY	CB-CA	-3.61	1.48	1.53
1	J	138	MLY	CB-CA	-3.56	1.48	1.53

The worst 5 of 150 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	138	MLY	CB-CA-C	-7.50	99.29	111.65
1	A	138	MLY	CB-CA-C	-7.49	99.31	111.65
1	M	138	MLY	CB-CA-C	-7.45	99.37	111.65
1	J	138	MLY	CB-CA-C	-7.44	99.39	111.65
1	P	138	MLY	CB-CA-C	-7.42	99.42	111.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

180 monomers are involved in 655 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	107	MLY	3	0
1	A	138	MLY	1	0
1	A	190	MLY	2	0
1	A	248	MLY	2	0
1	A	272	MLY	1	0
1	A	295	MLY	6	0
1	A	296	MLY	3	0
1	A	30	MLY	1	0
1	A	348	MLY	6	0
1	A	415	MLY	1	0
1	A	436	MLY	2	0
1	A	486	MLY	3	0
1	A	49	MLY	3	0
1	A	505	MLY	19	0
1	A	528	MLY	3	0
1	A	55	MLY	1	0
1	A	551	MLY	2	0
1	A	553	MLY	18	3
1	A	59	MLY	3	0
1	A	598	MLY	1	0
1	A	600	MLY	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	617	MLY	1	0
1	A	63	MLY	3	0
1	A	659	MLY	2	0
1	A	764	MLY	10	0
1	A	768	MLY	6	0
1	A	782	MLY	6	0
1	A	827	MLY	1	0
1	A	833	MLY	1	0
1	A	837	MLY	11	0
1	A	839	MLY	8	0
1	A	87	MLY	3	0
1	D	107	MLY	3	0
1	D	138	MLY	1	0
1	D	190	MLY	2	0
1	D	248	MLY	2	0
1	D	272	MLY	1	0
1	D	295	MLY	6	0
1	D	296	MLY	3	0
1	D	30	MLY	1	0
1	D	348	MLY	6	0
1	D	369	MLY	1	0
1	D	415	MLY	1	0
1	D	436	MLY	2	0
1	D	486	MLY	3	0
1	D	49	MLY	3	0
1	D	528	MLY	3	0
1	D	55	MLY	1	0
1	D	551	MLY	2	0
1	D	553	MLY	16	2
1	D	59	MLY	3	0
1	D	598	MLY	1	0
1	D	600	MLY	1	0
1	D	617	MLY	1	0
1	D	63	MLY	4	0
1	D	659	MLY	2	0
1	D	764	MLY	8	0
1	D	782	MLY	52	0
1	D	837	MLY	1	0
1	D	839	MLY	4	0
1	D	87	MLY	2	0
1	G	107	MLY	3	0
1	G	138	MLY	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	G	190	MLY	2	0
1	G	248	MLY	2	0
1	G	272	MLY	1	0
1	G	295	MLY	6	0
1	G	296	MLY	3	0
1	G	30	MLY	1	0
1	G	348	MLY	5	0
1	G	415	MLY	1	0
1	G	436	MLY	2	0
1	G	486	MLY	3	0
1	G	49	MLY	3	0
1	G	505	MLY	19	0
1	G	528	MLY	2	0
1	G	55	MLY	1	0
1	G	553	MLY	26	0
1	G	59	MLY	2	0
1	G	598	MLY	1	0
1	G	600	MLY	1	0
1	G	617	MLY	1	0
1	G	63	MLY	3	0
1	G	659	MLY	2	0
1	G	764	MLY	18	0
1	G	768	MLY	2	0
1	G	782	MLY	1	0
1	G	837	MLY	1	0
1	G	839	MLY	4	0
1	G	84	MLY	28	0
1	G	87	MLY	2	0
1	J	107	MLY	3	0
1	J	138	MLY	1	0
1	J	190	MLY	2	0
1	J	248	MLY	2	0
1	J	272	MLY	1	0
1	J	295	MLY	5	0
1	J	296	MLY	3	0
1	J	30	MLY	1	0
1	J	348	MLY	6	0
1	J	369	MLY	1	0
1	J	415	MLY	1	0
1	J	436	MLY	2	0
1	J	486	MLY	3	0
1	J	49	MLY	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	J	505	MLY	9	0
1	J	528	MLY	3	0
1	J	55	MLY	1	0
1	J	553	MLY	12	0
1	J	59	MLY	3	0
1	J	598	MLY	1	0
1	J	600	MLY	1	0
1	J	617	MLY	1	0
1	J	63	MLY	4	0
1	J	659	MLY	2	0
1	J	764	MLY	1	0
1	J	768	MLY	1	0
1	J	782	MLY	1	0
1	J	837	MLY	1	0
1	J	839	MLY	9	0
1	J	84	MLY	18	0
1	J	87	MLY	3	0
1	M	107	MLY	2	0
1	M	138	MLY	1	0
1	M	190	MLY	2	0
1	M	248	MLY	2	0
1	M	272	MLY	1	0
1	M	295	MLY	6	0
1	M	296	MLY	3	0
1	M	30	MLY	1	0
1	M	348	MLY	5	0
1	M	35	MLY	3	0
1	M	415	MLY	1	0
1	M	436	MLY	2	0
1	M	486	MLY	3	0
1	M	49	MLY	4	0
1	M	528	MLY	3	0
1	M	55	MLY	1	0
1	M	553	MLY	3	0
1	M	59	MLY	2	0
1	M	598	MLY	1	0
1	M	600	MLY	1	0
1	M	617	MLY	1	0
1	M	63	MLY	4	0
1	M	659	MLY	2	0
1	M	764	MLY	1	0
1	M	768	MLY	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	M	782	MLY	4	0
1	M	837	MLY	1	0
1	M	839	MLY	7	0
1	M	87	MLY	2	0
1	P	107	MLY	2	0
1	P	138	MLY	1	0
1	P	190	MLY	2	0
1	P	248	MLY	2	0
1	P	272	MLY	1	0
1	P	295	MLY	6	0
1	P	296	MLY	2	0
1	P	30	MLY	1	0
1	P	348	MLY	4	0
1	P	35	MLY	1	0
1	P	415	MLY	1	0
1	P	436	MLY	2	0
1	P	486	MLY	3	0
1	P	49	MLY	3	0
1	P	505	MLY	2	0
1	P	528	MLY	3	0
1	P	55	MLY	1	0
1	P	553	MLY	3	0
1	P	59	MLY	2	0
1	P	598	MLY	1	0
1	P	600	MLY	1	0
1	P	617	MLY	1	0
1	P	63	MLY	4	0
1	P	659	MLY	2	0
1	P	764	MLY	3	0
1	P	782	MLY	3	0
1	P	837	MLY	1	0
1	P	839	MLY	8	0
1	P	87	MLY	3	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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](#)

There are no chain breaks in this entry.