



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:22 PM BST

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 EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

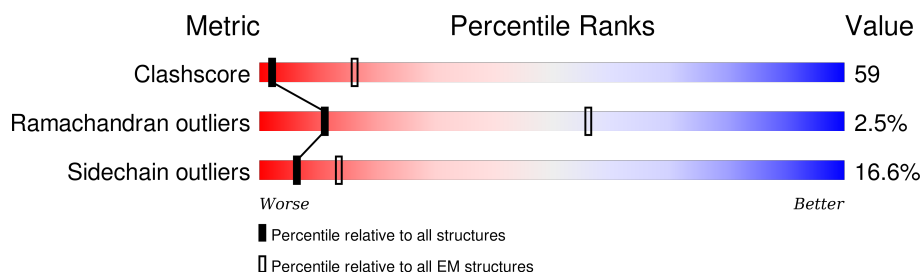
1 Overall quality at a glance

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.















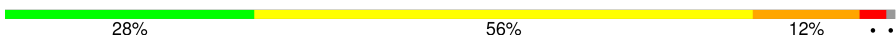



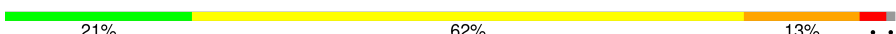
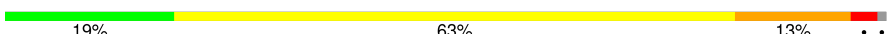





Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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 ≥ 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	 63% 27% 6% .
2	N	145	 65% 26% 6% .
2	Q	145	 65% 26% 6% .
3	C	147	 60% 38% .
3	F	147	 61% 37% .
3	I	147	 61% 37% .
3	L	147	 62% 36% .
3	O	147	 61% 37% .
3	R	147	 60% 37% .
4	1	375	 57% 32% 8% ..
4	2	375	 60% 31% 7% ..
4	3	375	 53% 36% 8% ..
4	4	375	 28% 56% 12% ..
4	5	375	 26% 58% 12% ..
4	6	375	 25% 59% 12% ..
4	7	375	 27% 57% 12% ..
4	8	375	 21% 62% 13% ..
4	9	375	 19% 63% 13% ..
4	V	375	 51% 37% 9% ..
4	W	375	 54% 35% 8% ..
4	X	375	 62% 29% 7% ..
4	Y	375	 62% 29% 7% ..
4	Z	375	 58% 32% 8% ..

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

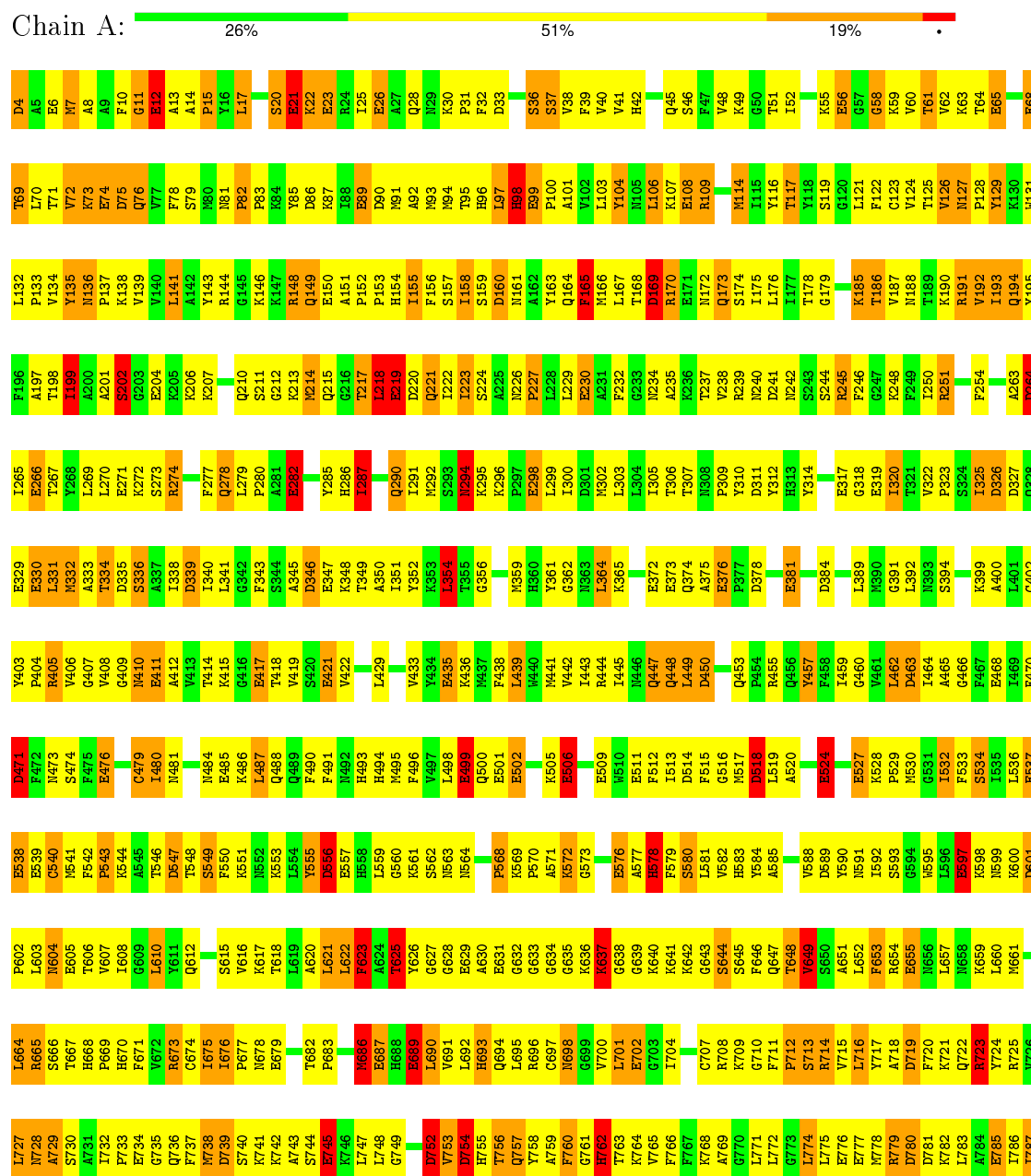
- Molecule 4 is a protein called SKELETAL MUSCLE ACTIN.

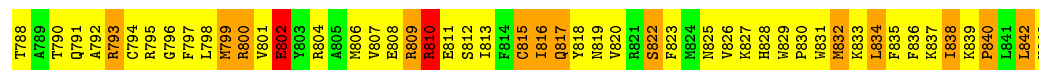
Mol	Chain	Residues	Atoms					AltConf	Trace
4	1	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	2	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	3	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	4	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	5	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20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

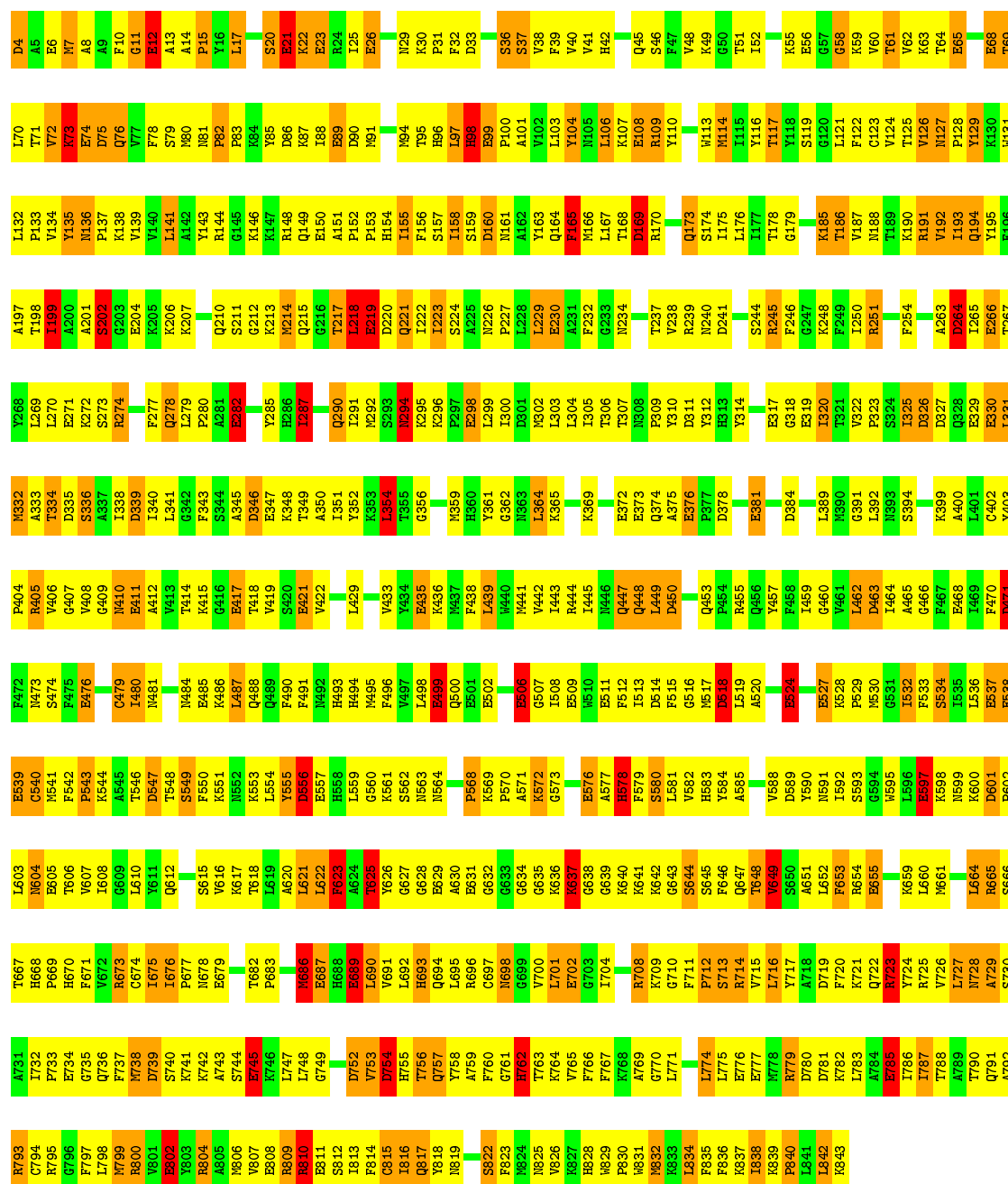
• Molecule 1: SKELETAL MUSCLE MYOSIN II





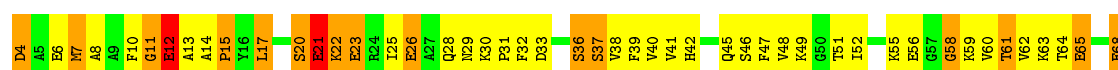
• Molecule 1: SKELETAL MUSCLE MYOSIN II

Chain D: 27% 51% 18%



• Molecule 1: SKELETAL MUSCLE MYOSIN II

Chain G: 25% 51% 19%



E266	L331	C402	F470	E537	D601	L664	N728	A789
T267	M332	Y403	D471	E538	P602	R665	A729	I790
Y268	A333	P404	F472	E539	L603	S666	A730	Q791
L269	T334	R405	L473	C540	M604	T673	A731	A792
L270	D335	V406	S474	M541	T606	H668	I732	G793
E271	S336	G407	F475	F542	T607	P669	I733	R794
K272	A337	V408	E476	D643	V607	H670	E734	R795
S273	L338	G409		K544	L608	P671	G735	G796
R274	D339	M410	C479	A545	G609	V672	Q736	F797
	L340	E411	L480	T546	L611	C674	M737	L798
F277	L341	A412	M481	T547	Q612	L675	M738	M799
D278	G342	V413	N484	T548	S615	P677	D739	R800
L279	F343	K414	E485	S549	V616	B678	S740	V801
P280	S344	K415	K486	F550	K617	E679	K741	E802
A281	A345	G416	L487	K553	T618	B680	A742	Y803
E282	D346	E417	Q488	L554	T619	C681	A743	A805
	E347	V418	Q489	Y555	D620	P683	S744	M806
Y285	K348	V419	F490	D556	A621	L686	E745	V807
H286	T349	S420	F491	E557	L622	B687	K746	B808
L287	A350	V422	M492	B558	F623	E688	L747	E809
	L351	E421	H494	G560	A624	B689	L748	R810
	K353	K429	H495	L559	L624	E690	G749	B811
M292	L354		F496	G562	T625	L690	D752	S812
S293	T355	V433	F497	N564	G627	V691	V753	I813
E294	G356	Y434			E631	G703	D754	F814
	M359	E435			G628	I704	H755	C815
K295		E436			E629	E702	I756	I816
P297	K360	M437	Q500	K567	G630	E703	Q757	Q817
E298	Y361	F438	E501	P568	E634	L695	V758	Q818
L299	K362	L439	E502	K569	G635	G696	A759	N819
L300	L363	M440		P570	G636	C697	F760	V820
D301	L364	M441	K505	A471	K637	B699	G761	R821
K302	K365	L442	E506	K572	V700	G699	T762	S822
L303		L443		E573	G638	L701	K763	N825
K304	K369	R444			G639	E702	V764	V826
L305		L445			K640	E703	V765	V827
T306	E372	M446			K641	I704	F766	K827
T307	E373	Q447			K642	R708	K768	H828
N308	Q374	Q448			S644	K709	A769	H829
P309	A375	L449			G644	G770	P830	P831
Y310	E376	D450			S645	G771	M832	M833
D311	P377				P646	F711	L771	K834
Y312	D378				Q647	F712	L772	V835
H313		Q453			T648	S713	L773	L834
Y314	E381	R455			V649	L774	L775	F835
		A520			S650	R714	E776	K837
		Y457			A651	V715	E777	I838
E317	D384	F458			L652	V716	K778	K839
G318	L389	L459			F653	A717	R779	P840
E319	K390	G460			R654	D719	D780	L841
L320	L391	V461			E655	F720	D781	C123
V322	L392	D462			M656	K721	K782	V124
	K393	D463			L657	T722	L783	T125
T325	S394	L464			M658	Q723	A784	V126
D326		A465			K659	Y724	E785	N127
D327	L398	G466			M660	V725	I786	P128
Q328	K399	F467			L661	V726	I787	Y129
E329	A400	E468						
E330	L401	E469						
	C402	D471						

• Molecule 1: SKELETAL MUSCLE MYOSIN II

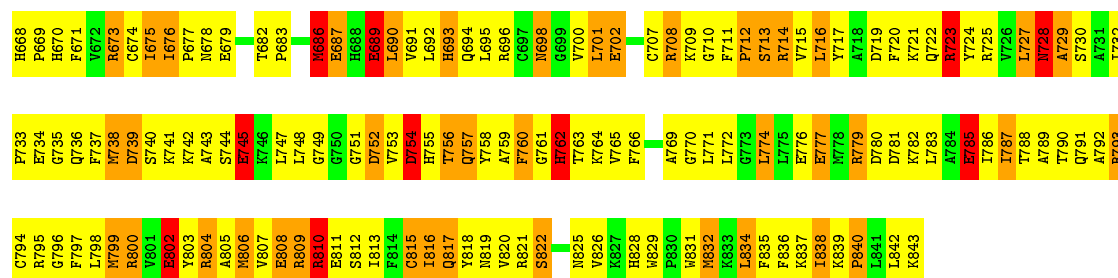
Chain M:  27% 50% 19%

Y403	E329	E266	Y195	W131	T69	D4
P404	E330	T267	F196	L132	L70	A5
R405	L331	Y268	A197	P133	T71	E6
V406	M332	L269	T198	V134	W72	M7
G407	A333	L270	I199	Y135	K73	A8
V408	T334	E271	A200	M136	E74	A9
G409	D335	K272	A201	P137	D75	F10
M410	S336	S273	S202	K138	Q76	G11
E411	A337	R274	G203	V139	V77	E12
A412	L338		E204	V140	F78	A13
D413	D339		K205	L141	S79	A14
T414	I340	Q278	K206	A142	N80	P15
L415	L341	L279	K207	Y143	N81	V16
G416	G342	P280			P82	L17
E417	F343	A281	Q210	G145	P83	
T418	S344	E282	S211	K146	K84	S20
V419	A345		G212	P147	E85	E21
S420	D446	Y285	K213	R148	D86	K22
E421	E347	E286	M214	Q149	K87	E23
V422	K348	L287	Q215	E150	T88	R24
G423	T349	F288	G216	A151	E89	E25
A350	A350	Y289	T217	P152	D90	I26
L351	I351	Q290	L218	F153	N91	
Y352	Y352	T291	E219	H154		N29
K353	K353	M292	D220	I155	N94	K30
L354	L354	S293	Q221	F156	T95	P31
E355	E355	T294	I222	S157	H96	F32
G356	G356	K295	L223	K158	L97	D33
F437		K296	S224	S159	E98	A34
F438		E297	A225	D160	E99	K35
L439	M359	E298	N226	M161	P100	S36
A440	H360	L299	P227	A162	A101	S37
M441	V361	D300	L228	V163	V102	V38
V442	G362	K301	L229	Q164	L103	F39
	K363	D302	E230	F165	Y104	V40
L445	L364	K302	A231	M166	N105	V41
A446	K365	L303	F232	L167	L106	H42
Q447		L304	E233	T168	K107	
Q448	E372	T305	N234	D169	E108	Q45
L449	E373	T306	G233	R170	R109	S46
D450	Q374	T307	T237	E171	Y110	F47
	A375	N308	V238	M172		V48
Q453	E376	P309	R239	Q173	W113	
F454	P377	D310	N240	S174	M114	G50
R455	D378	Y311	D241	L175	I115	T51
Q456		Y312		L176	Y116	I52
Y457	E381	H313	S244	T177	T117	
F458		Y314	R245	I178	Y118	K55
L459	D384	V315	F246	G179	S119	E56
G460		E317	G247			G57
V461	L389	K318	K248	K185	L120	G58
L462	N390	G318	F249	T186	F122	K59
D463	G391	E319	L250	V187	C123	V60
L464	L392	T320	R251	M188	V124	T61
A465	H393	T321		T189	T125	V62
G466	S394	V322	F254	K190	V126	K63
F467				R191	M127	T64
E468	K399	I325	A263	V192	P128	E65
L469	A400	D26	D264	I193	Y129	
F470	F401	D27	D265	G194	E255	F68
E471		G375	T265			

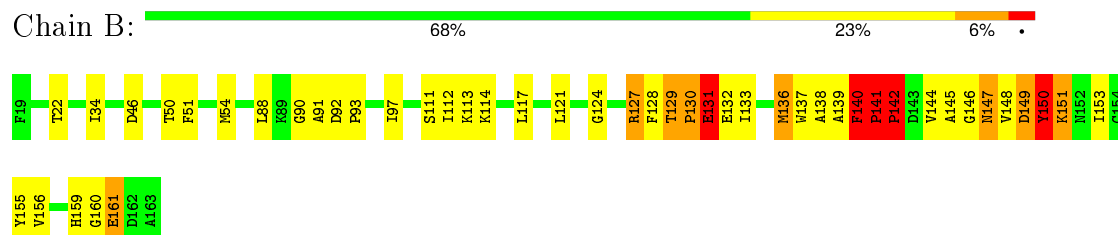


Response	Percentage
Yes, the U.S. is responsible	26%
No, the U.S. is not responsible	50%
Both the U.S. and the hijackers are responsible	20%
Neither the U.S. nor the hijackers are responsible	4%

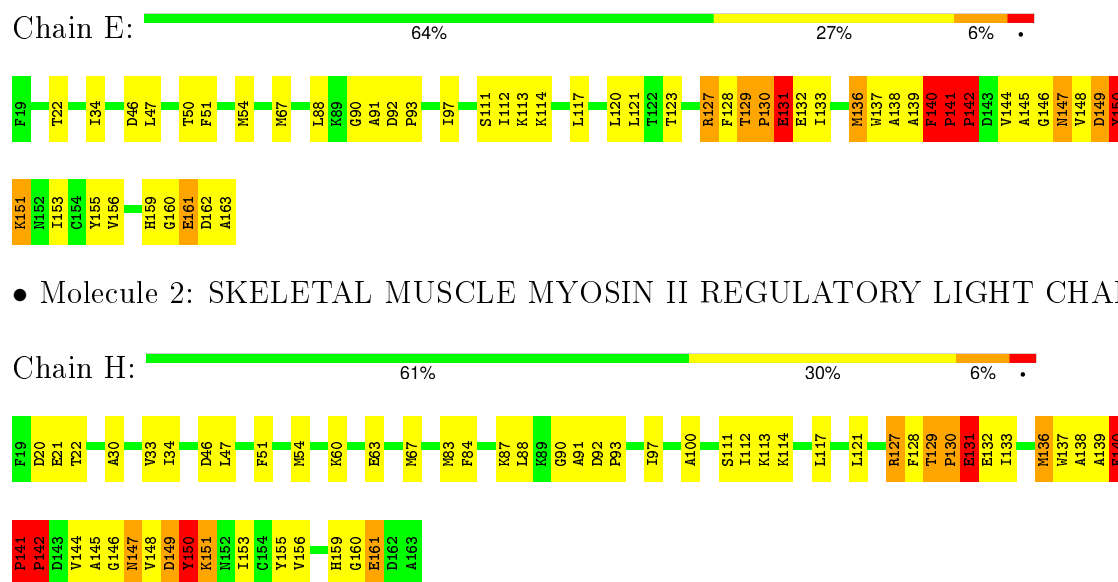




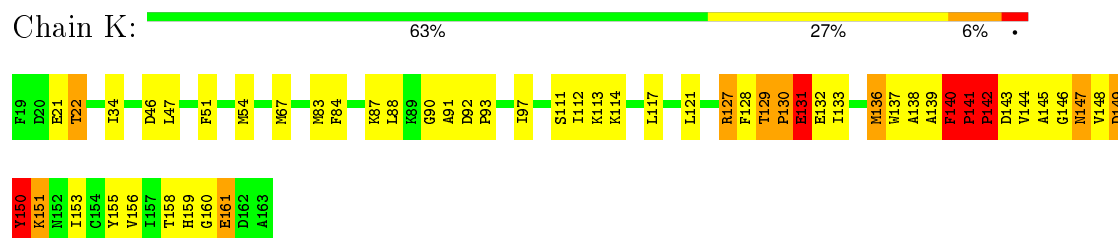
• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN



• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

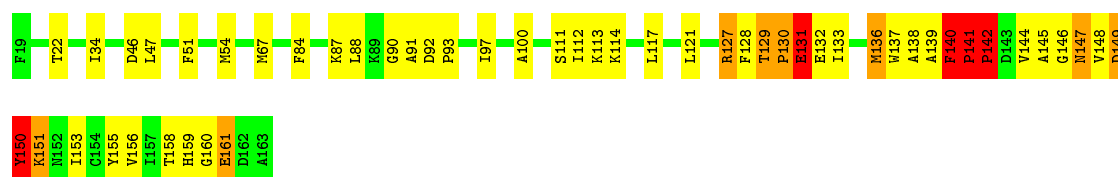


• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

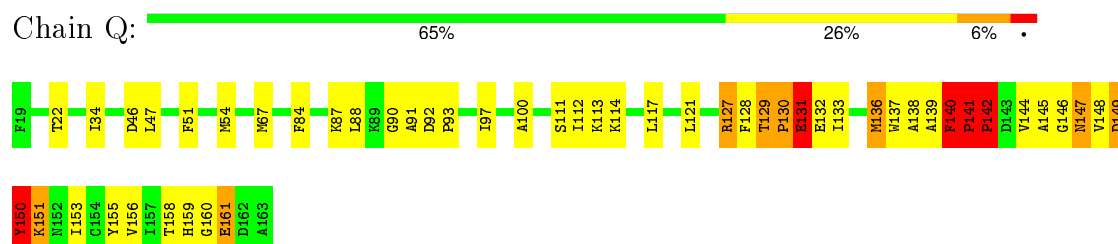


• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

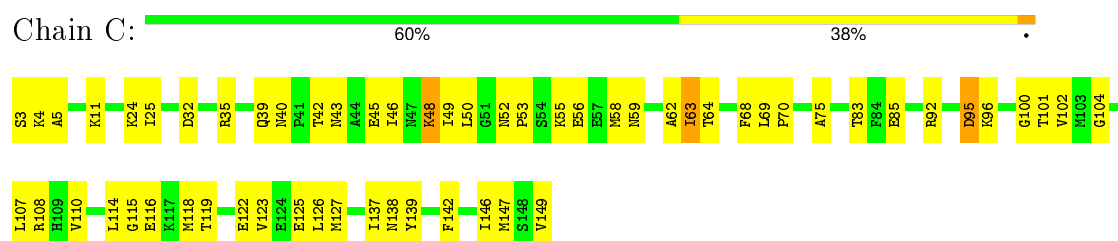




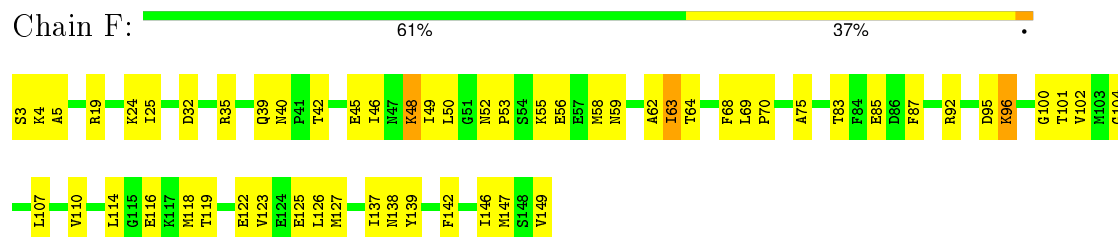
• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN



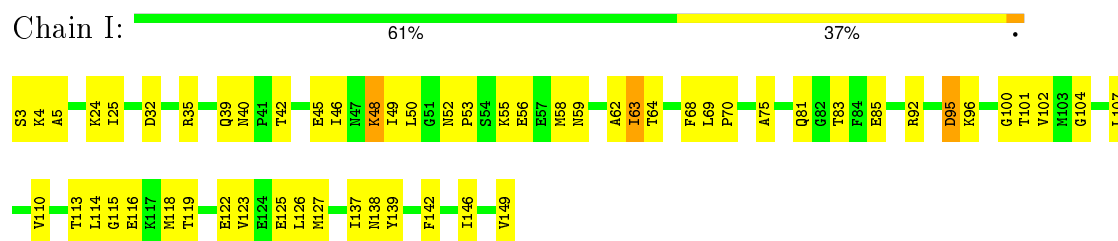
• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN



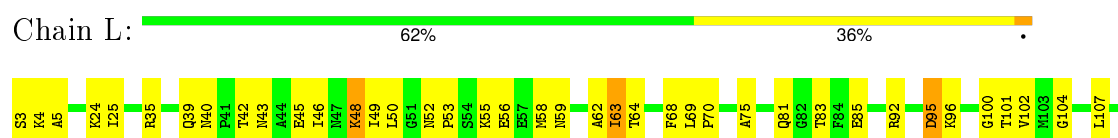
• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN

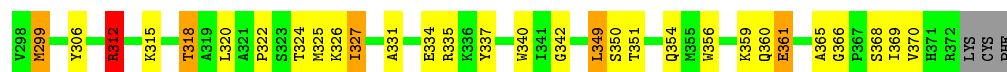


• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN



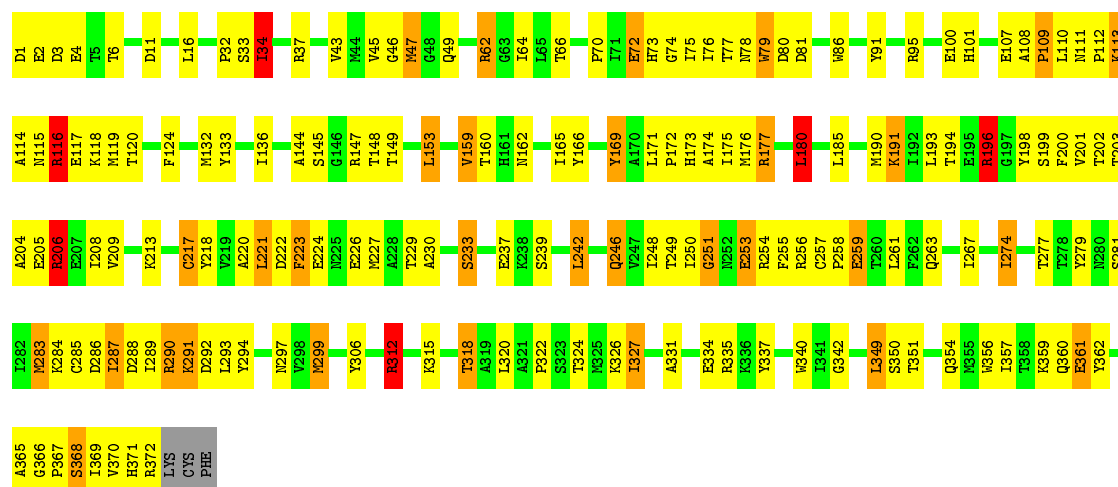
• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN





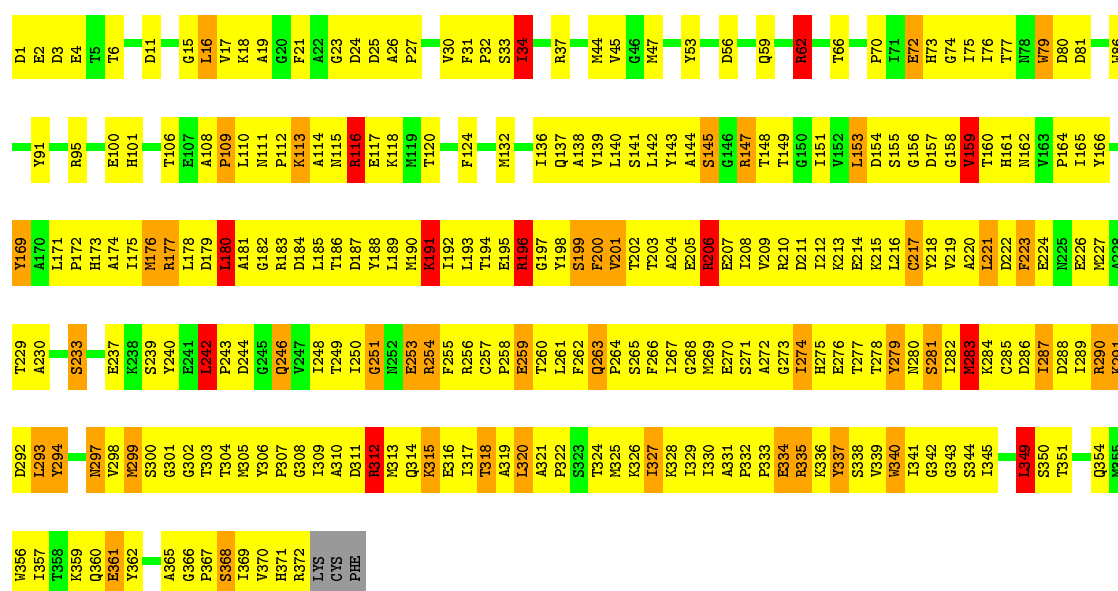
• Molecule 4: SKELETAL MUSCLE ACTIN

Chain 3: 53% 36% 8% ..



• Molecule 4: SKELETAL MUSCLE ACTIN

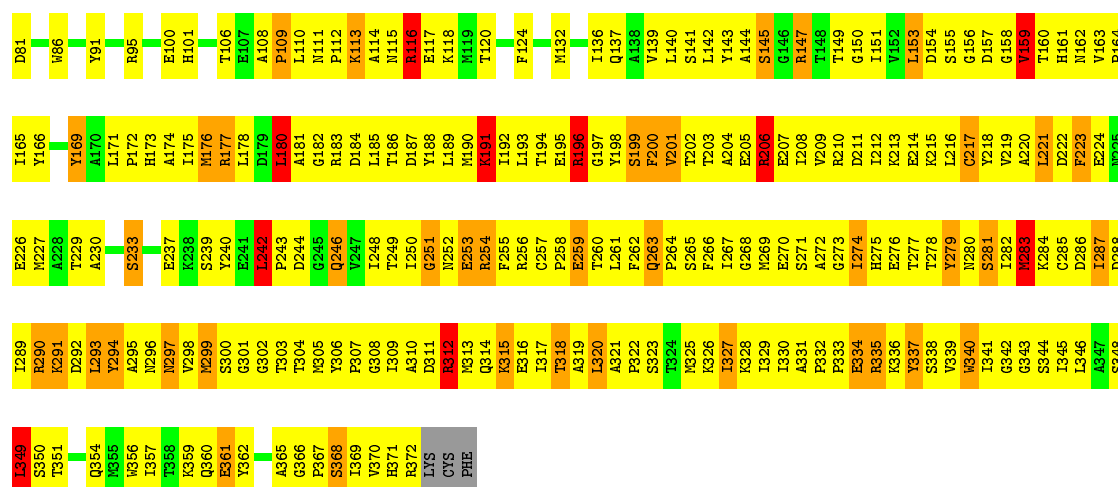
Chain 4: 28% 56% 12% ..



• Molecule 4: SKELETAL MUSCLE ACTIN

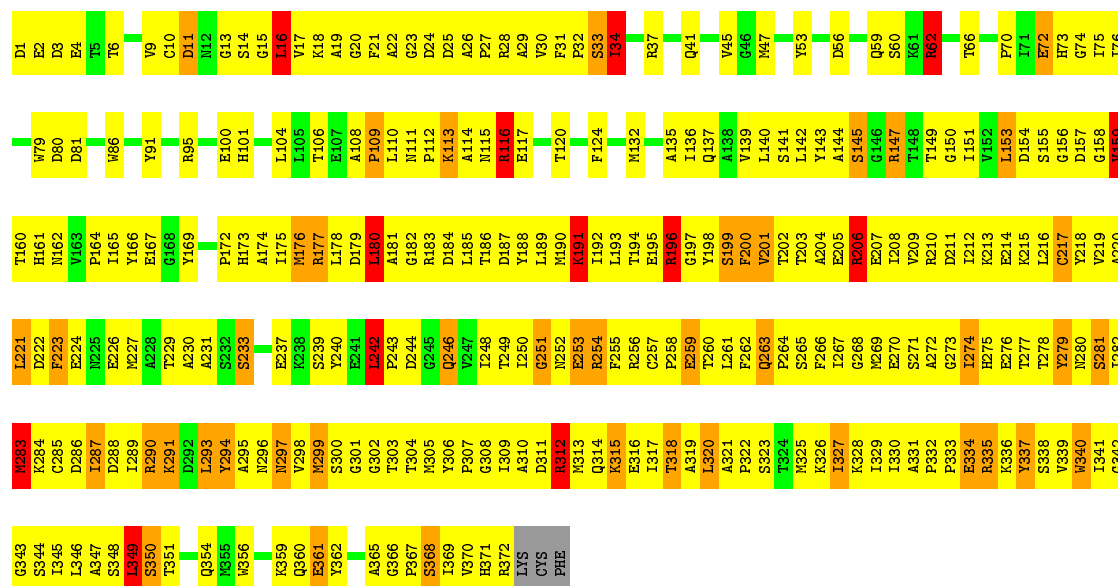
Chain 5: 26% 58% 12% ..





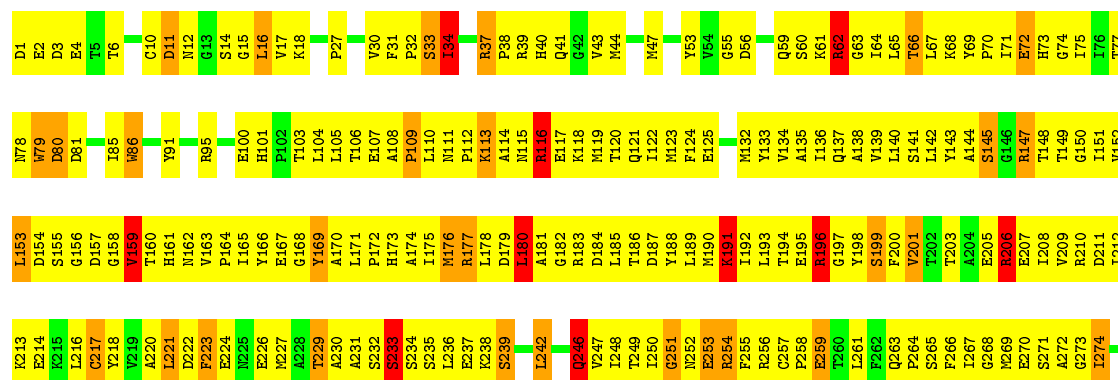
• Molecule 4: SKELETAL MUSCLE ACTIN

Chain 6: 25% 59% 12% ..



• Molecule 4: SKELETAL MUSCLE ACTIN

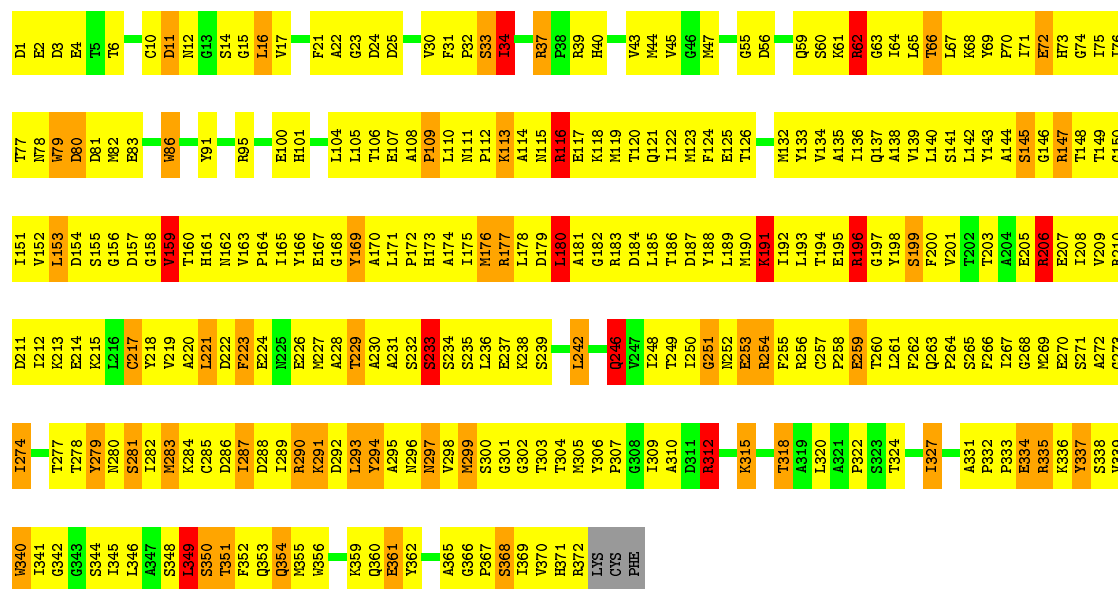
Chain 7: 27% 57% 12% ..





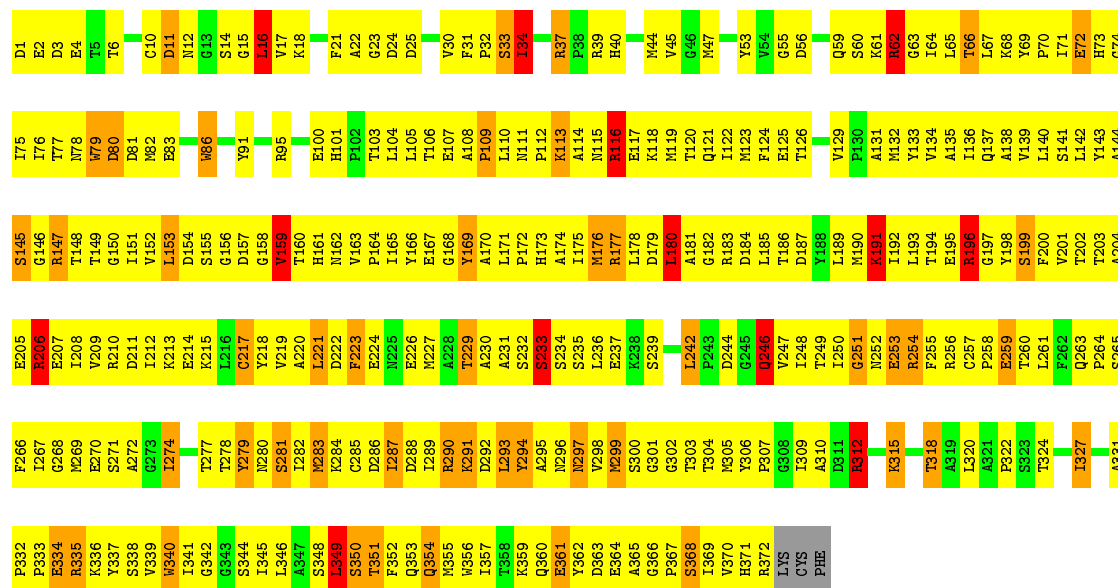
• Molecule 4: SKELETAL MUSCLE ACTIN

Chain 8: 21% 62% 13% ..

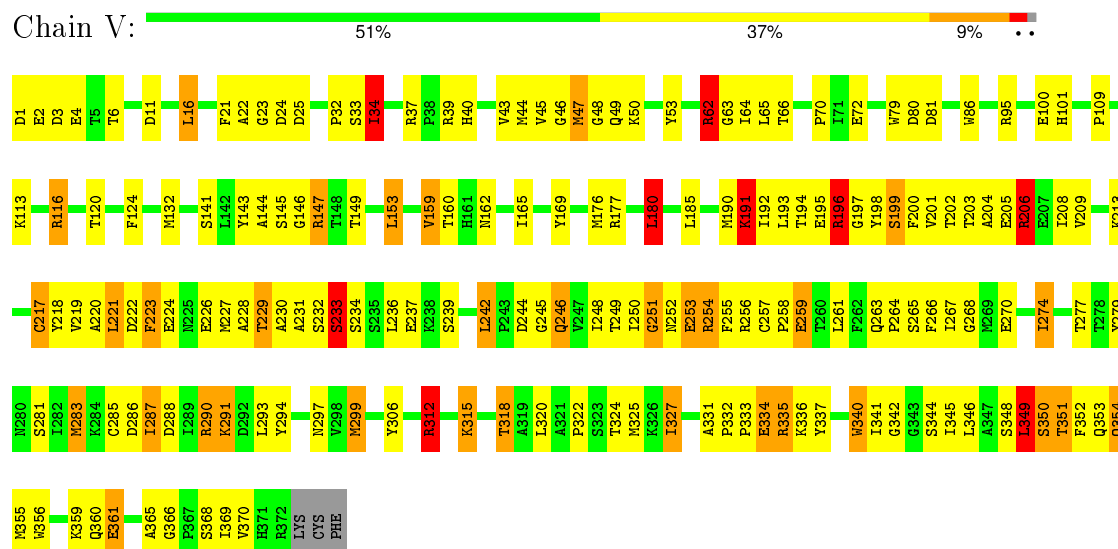


• Molecule 4: SKELETAL MUSCLE ACTIN

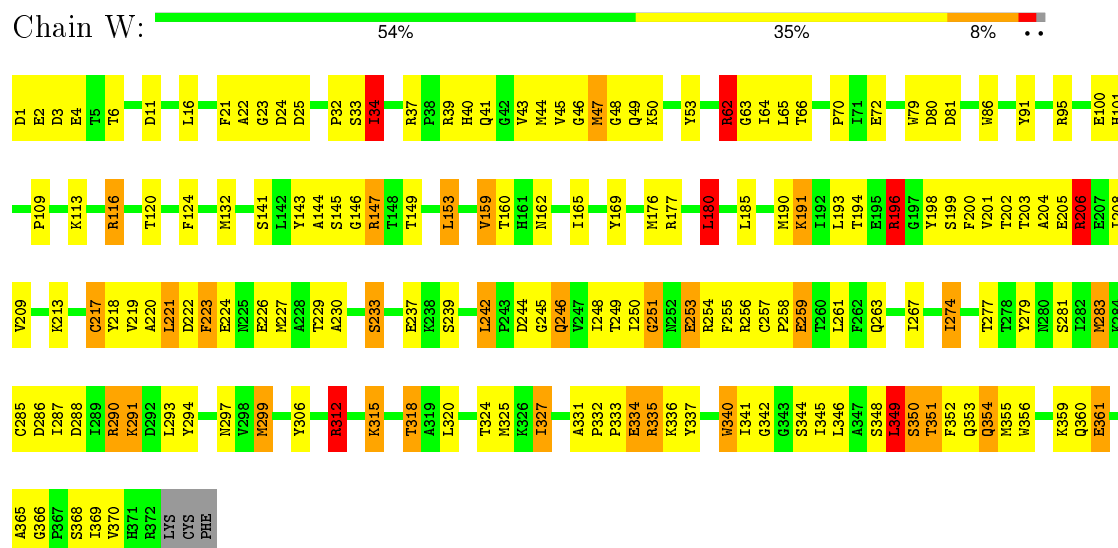
Chain 9: 19% 63% 13% ..



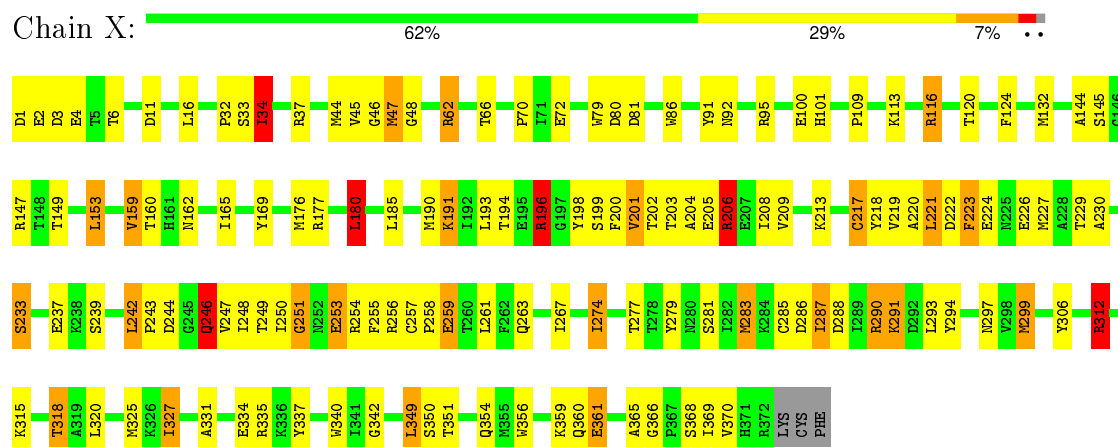
• Molecule 4: SKELETAL MUSCLE ACTIN



• Molecule 4: SKELETAL MUSCLE ACTIN

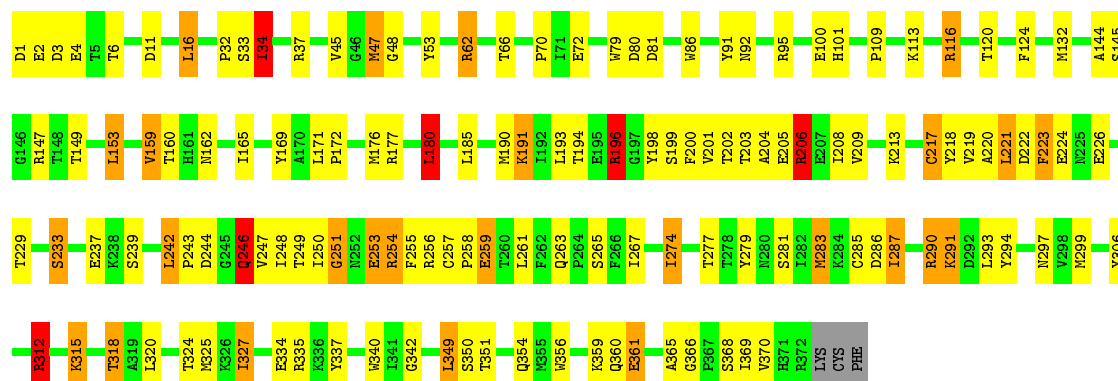


• Molecule 4: SKELETAL MUSCLE ACTIN



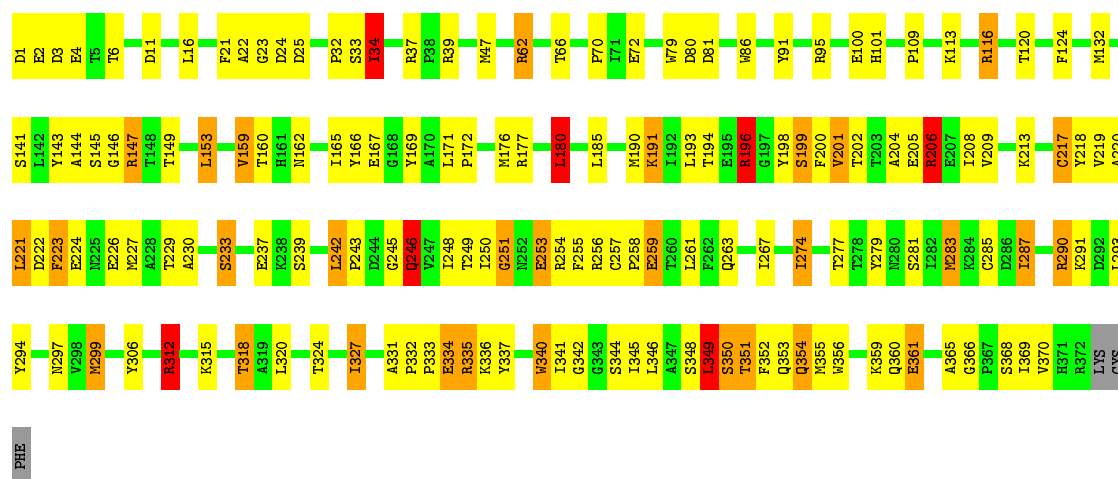
- Molecule 4: SKELETAL MUSCLE ACTIN

Chain Y: 



- Molecule 4: SKELETAL MUSCLE ACTIN

Chain Z: 



4 Experimental information

Property	Value	Source
Reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	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 ⓘ

5.3.1 Protein backbone ⓘ

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%)	5	40
1	D	789/840 (94%)	651 (82%)	112 (14%)	26 (3%)	5	40
1	G	791/840 (94%)	650 (82%)	114 (14%)	27 (3%)	5	40
1	J	791/840 (94%)	652 (82%)	112 (14%)	27 (3%)	5	40
1	M	788/840 (94%)	651 (83%)	110 (14%)	27 (3%)	5	40
1	P	787/840 (94%)	651 (83%)	109 (14%)	27 (3%)	5	40
2	B	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	2	28
2	E	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	2	28
2	H	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	2	28
2	K	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	2	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	N	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	2	28
2	Q	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	2	28
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%)	12	56
4	2	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	12	56
4	3	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	12	56
4	4	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	12	56
4	5	370/375 (99%)	333 (90%)	31 (8%)	6 (2%)	12	56
4	6	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	12	56
4	7	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	12	56
4	8	370/375 (99%)	333 (90%)	31 (8%)	6 (2%)	12	56
4	9	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	12	56
4	V	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	12	56
4	W	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	12	56
4	X	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	12	56
4	Y	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	12	56
4	Z	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	12	56
All	All	11631/12042 (97%)	10138 (87%)	1201 (10%)	292 (2%)	11	46

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	7
1	D	672/672 (100%)	514 (76%)	158 (24%)	1	7
1	G	672/672 (100%)	514 (76%)	158 (24%)	1	7
1	J	672/672 (100%)	513 (76%)	159 (24%)	1	7
1	M	672/672 (100%)	513 (76%)	159 (24%)	1	7
1	P	672/672 (100%)	515 (77%)	157 (23%)	1	7
2	B	120/120 (100%)	119 (99%)	1 (1%)	86	94
2	E	120/120 (100%)	119 (99%)	1 (1%)	86	94
2	H	120/120 (100%)	119 (99%)	1 (1%)	86	94
2	K	120/120 (100%)	119 (99%)	1 (1%)	86	94
2	N	120/120 (100%)	119 (99%)	1 (1%)	86	94
2	Q	120/120 (100%)	119 (99%)	1 (1%)	86	94
3	C	117/117 (100%)	112 (96%)	5 (4%)	35	70
3	F	117/117 (100%)	112 (96%)	5 (4%)	35	70
3	I	117/117 (100%)	112 (96%)	5 (4%)	35	70
3	L	117/117 (100%)	112 (96%)	5 (4%)	35	70
3	O	117/117 (100%)	112 (96%)	5 (4%)	35	70
3	R	117/117 (100%)	112 (96%)	5 (4%)	35	70
4	1	315/318 (99%)	268 (85%)	47 (15%)	4	23
4	2	315/318 (99%)	268 (85%)	47 (15%)	4	23
4	3	315/318 (99%)	269 (85%)	46 (15%)	4	24
4	4	315/318 (99%)	269 (85%)	46 (15%)	4	24
4	5	315/318 (99%)	268 (85%)	47 (15%)	4	23
4	6	315/318 (99%)	268 (85%)	47 (15%)	4	23
4	7	315/318 (99%)	269 (85%)	46 (15%)	4	24
4	8	315/318 (99%)	269 (85%)	46 (15%)	4	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	9	315/318 (99%)	268 (85%)	47 (15%)	4	23
4	V	315/318 (99%)	268 (85%)	47 (15%)	4	23
4	W	315/318 (99%)	269 (85%)	46 (15%)	4	24
4	X	315/318 (99%)	269 (85%)	46 (15%)	4	24
4	Y	315/318 (99%)	268 (85%)	47 (15%)	4	23
4	Z	315/318 (99%)	269 (85%)	46 (15%)	4	24
All	All	9864/9906 (100%)	8226 (83%)	1638 (17%)	6	19

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	8,10,11	0.44	0	9,11,13	0.67	0
1	MLY	A	130	1	8,10,11	0.59	0	9,11,13	1.06	1 (11%)
1	MLY	A	138	1	8,10,11	1.35	1 (12%)	9,11,13	0.81	0
1	MLY	A	19	1	8,10,11	1.12	1 (12%)	9,11,13	0.69	0
1	MLY	A	190	1	8,10,11	1.10	1 (12%)	9,11,13	0.70	0
1	MLY	A	236	1	8,10,11	0.37	0	9,11,13	1.33	1 (11%)
1	MLY	A	248	1	8,10,11	0.73	0	9,11,13	0.91	1 (11%)
1	MLY	A	272	1	8,10,11	1.03	1 (12%)	9,11,13	0.57	0
1	MLY	A	295	1	8,10,11	0.72	0	9,11,13	0.46	0
1	MLY	A	296	1	8,10,11	0.62	0	9,11,13	0.77	0
1	MLY	A	30	1	8,10,11	0.68	0	9,11,13	0.82	0
1	MLY	A	348	1	8,10,11	0.82	0	9,11,13	0.82	0
1	MLY	A	35	1	8,10,11	0.57	0	9,11,13	0.69	0
1	MLY	A	353	1	8,10,11	0.88	0	9,11,13	0.79	0
1	MLY	A	367	1	8,10,11	0.66	0	9,11,13	0.60	0
1	MLY	A	369	1	8,10,11	0.56	0	9,11,13	0.92	1 (11%)
1	MLY	A	385	1	8,10,11	1.01	1 (12%)	9,11,13	0.55	0
1	MLY	A	415	1	8,10,11	0.75	0	9,11,13	0.44	0
1	MLY	A	431	1	8,10,11	0.46	0	9,11,13	0.76	0
1	MLY	A	436	1	8,10,11	1.06	1 (12%)	9,11,13	0.57	0
1	MLY	A	486	1	8,10,11	0.34	0	9,11,13	0.59	0
1	MLY	A	49	1	8,10,11	1.04	1 (12%)	9,11,13	0.98	0
1	MLY	A	504	1	8,10,11	0.80	0	9,11,13	0.50	0
1	MLY	A	505	1	8,10,11	0.89	1 (12%)	9,11,13	0.38	0
1	MLY	A	528	1	8,10,11	0.80	0	9,11,13	1.17	1 (11%)
1	MLY	A	55	1	8,10,11	0.66	0	9,11,13	0.96	0
1	MLY	A	551	1	8,10,11	0.50	0	9,11,13	0.65	0
1	MLY	A	553	1,4	8,10,11	0.62	0	9,11,13	0.59	0
1	MLY	A	59	1	8,10,11	0.78	0	9,11,13	0.75	0
1	MLY	A	598	1	8,10,11	0.86	1 (12%)	9,11,13	0.72	0
1	MLY	A	600	1	8,10,11	0.51	0	9,11,13	0.49	0
1	MLY	A	613	1	8,10,11	0.51	0	9,11,13	0.91	0
1	MLY	A	617	1	8,10,11	0.89	1 (12%)	9,11,13	0.47	0
1	MLY	A	63	1	8,10,11	0.81	0	9,11,13	0.94	0
1	MLY	A	659	1	8,10,11	0.56	0	9,11,13	0.94	0
1	MLY	A	681	1	8,10,11	0.61	0	9,11,13	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	A	764	1	8,10,11	0.70	0	9,11,13	0.55	0
1	MLY	A	768	1	8,10,11	0.65	0	9,11,13	0.86	0
1	MLY	A	782	1	8,10,11	0.51	0	9,11,13	0.93	1 (11%)
1	MLY	A	827	1	8,10,11	0.68	0	9,11,13	0.95	1 (11%)
1	MLY	A	833	1	8,10,11	0.99	1 (12%)	9,11,13	0.57	0
1	MLY	A	837	1	8,10,11	0.54	0	9,11,13	0.57	0
1	MLY	A	839	1	8,10,11	0.67	0	9,11,13	0.78	0
1	MLY	A	84	1	8,10,11	0.45	0	9,11,13	0.79	0
1	MLY	A	87	1	8,10,11	1.15	1 (12%)	9,11,13	0.68	0
1	MLY	D	107	1	8,10,11	0.47	0	9,11,13	0.67	0
1	MLY	D	130	1	8,10,11	0.57	0	9,11,13	1.06	1 (11%)
1	MLY	D	138	1	8,10,11	1.37	1 (12%)	9,11,13	0.81	0
1	MLY	D	19	1	8,10,11	1.22	1 (12%)	9,11,13	0.70	0
1	MLY	D	190	1	8,10,11	1.04	1 (12%)	9,11,13	0.71	0
1	MLY	D	236	1	8,10,11	0.38	0	9,11,13	1.31	1 (11%)
1	MLY	D	248	1	8,10,11	0.73	0	9,11,13	0.93	1 (11%)
1	MLY	D	272	1	8,10,11	0.97	1 (12%)	9,11,13	0.57	0
1	MLY	D	295	1	8,10,11	0.69	0	9,11,13	0.47	0
1	MLY	D	296	1	8,10,11	0.63	0	9,11,13	0.77	0
1	MLY	D	30	1	8,10,11	0.73	0	9,11,13	0.84	1 (11%)
1	MLY	D	348	1	8,10,11	0.78	0	9,11,13	0.80	0
1	MLY	D	35	1	8,10,11	0.59	0	9,11,13	0.67	0
1	MLY	D	353	1	8,10,11	0.87	0	9,11,13	0.78	0
1	MLY	D	367	1	8,10,11	0.64	0	9,11,13	0.62	0
1	MLY	D	369	1	8,10,11	0.54	0	9,11,13	0.92	1 (11%)
1	MLY	D	385	1	8,10,11	0.98	1 (12%)	9,11,13	0.55	0
1	MLY	D	415	1	8,10,11	0.77	0	9,11,13	0.46	0
1	MLY	D	431	1	8,10,11	0.50	0	9,11,13	0.77	0
1	MLY	D	436	1	8,10,11	1.12	1 (12%)	9,11,13	0.58	0
1	MLY	D	486	1	8,10,11	0.35	0	9,11,13	0.61	0
1	MLY	D	49	1	8,10,11	1.09	1 (12%)	9,11,13	1.00	1 (11%)
1	MLY	D	504	1	8,10,11	0.78	0	9,11,13	0.47	0
1	MLY	D	505	1	8,10,11	0.84	1 (12%)	9,11,13	0.40	0
1	MLY	D	528	1	8,10,11	0.85	0	9,11,13	1.17	1 (11%)
1	MLY	D	55	1	8,10,11	0.66	0	9,11,13	0.99	0
1	MLY	D	551	1	8,10,11	0.52	0	9,11,13	0.66	0
1	MLY	D	553	1,4	8,10,11	0.65	0	9,11,13	0.58	0
1	MLY	D	59	1	8,10,11	0.78	0	9,11,13	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	D	598	1	8,10,11	0.83	1 (12%)	9,11,13	0.70	0
1	MLY	D	600	1	8,10,11	0.52	0	9,11,13	0.47	0
1	MLY	D	613	1	8,10,11	0.50	0	9,11,13	0.92	0
1	MLY	D	617	1	8,10,11	0.93	1 (12%)	9,11,13	0.46	0
1	MLY	D	63	1	8,10,11	0.79	0	9,11,13	0.95	0
1	MLY	D	659	1	8,10,11	0.55	0	9,11,13	0.95	0
1	MLY	D	681	1	8,10,11	0.62	0	9,11,13	0.65	0
1	MLY	D	764	1	8,10,11	0.67	0	9,11,13	0.57	0
1	MLY	D	768	1	8,10,11	0.64	0	9,11,13	0.86	0
1	MLY	D	782	1	8,10,11	0.49	0	9,11,13	0.92	1 (11%)
1	MLY	D	827	1	8,10,11	0.63	0	9,11,13	0.96	1 (11%)
1	MLY	D	833	1	8,10,11	0.95	1 (12%)	9,11,13	0.60	0
1	MLY	D	837	1	8,10,11	0.57	0	9,11,13	0.59	0
1	MLY	D	839	1	8,10,11	0.71	0	9,11,13	0.78	0
1	MLY	D	84	1	8,10,11	0.47	0	9,11,13	0.80	0
1	MLY	D	87	1	8,10,11	1.14	1 (12%)	9,11,13	0.68	0
1	MLY	G	107	1	8,10,11	0.45	0	9,11,13	0.66	0
1	MLY	G	130	1	8,10,11	0.59	0	9,11,13	1.08	1 (11%)
1	MLY	G	138	1	8,10,11	1.38	1 (12%)	9,11,13	0.82	0
1	MLY	G	19	1	8,10,11	1.15	1 (12%)	9,11,13	0.71	0
1	MLY	G	190	1	8,10,11	1.08	1 (12%)	9,11,13	0.69	0
1	MLY	G	236	1	8,10,11	0.38	0	9,11,13	1.32	1 (11%)
1	MLY	G	248	1	8,10,11	0.69	0	9,11,13	0.92	1 (11%)
1	MLY	G	272	1	8,10,11	1.00	1 (12%)	9,11,13	0.56	0
1	MLY	G	295	1	8,10,11	0.70	0	9,11,13	0.47	0
1	MLY	G	296	1	8,10,11	0.61	0	9,11,13	0.77	0
1	MLY	G	30	1	8,10,11	0.68	0	9,11,13	0.83	1 (11%)
1	MLY	G	348	1	8,10,11	0.81	0	9,11,13	0.82	0
1	MLY	G	35	1	8,10,11	0.58	0	9,11,13	0.67	0
1	MLY	G	353	1	8,10,11	0.88	0	9,11,13	0.80	0
1	MLY	G	367	1	8,10,11	0.67	0	9,11,13	0.62	0
1	MLY	G	369	1	8,10,11	0.56	0	9,11,13	0.93	1 (11%)
1	MLY	G	385	1	8,10,11	1.01	1 (12%)	9,11,13	0.56	0
1	MLY	G	415	1	8,10,11	0.77	0	9,11,13	0.43	0
1	MLY	G	431	1	8,10,11	0.46	0	9,11,13	0.77	0
1	MLY	G	436	1	8,10,11	1.06	1 (12%)	9,11,13	0.57	0
1	MLY	G	486	1	8,10,11	0.35	0	9,11,13	0.60	0
1	MLY	G	49	1	8,10,11	1.08	1 (12%)	9,11,13	0.97	0
1	MLY	G	504	1	8,10,11	0.79	0	9,11,13	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	G	505	1	8,10,11	0.83	0	9,11,13	0.40	0
1	MLY	G	528	1	8,10,11	0.80	0	9,11,13	1.18	1 (11%)
1	MLY	G	55	1	8,10,11	0.68	0	9,11,13	0.99	0
1	MLY	G	551	1	8,10,11	0.52	0	9,11,13	0.65	0
1	MLY	G	553	1,4	8,10,11	0.63	0	9,11,13	0.58	0
1	MLY	G	59	1	8,10,11	0.74	0	9,11,13	0.78	0
1	MLY	G	598	1	8,10,11	0.83	1 (12%)	9,11,13	0.72	0
1	MLY	G	600	1	8,10,11	0.52	0	9,11,13	0.47	0
1	MLY	G	613	1	8,10,11	0.53	0	9,11,13	0.91	0
1	MLY	G	617	1	8,10,11	0.89	1 (12%)	9,11,13	0.45	0
1	MLY	G	63	1	8,10,11	0.79	0	9,11,13	0.94	0
1	MLY	G	659	1	8,10,11	0.57	0	9,11,13	0.94	0
1	MLY	G	681	1	8,10,11	0.66	0	9,11,13	0.64	0
1	MLY	G	764	1	8,10,11	0.61	0	9,11,13	0.56	0
1	MLY	G	768	1	8,10,11	0.64	0	9,11,13	0.87	0
1	MLY	G	782	1	8,10,11	0.48	0	9,11,13	0.92	1 (11%)
1	MLY	G	827	1	8,10,11	0.64	0	9,11,13	0.96	1 (11%)
1	MLY	G	833	1	8,10,11	0.99	1 (12%)	9,11,13	0.59	0
1	MLY	G	837	1	8,10,11	0.55	0	9,11,13	0.57	0
1	MLY	G	839	1	8,10,11	0.68	0	9,11,13	0.80	0
1	MLY	G	84	1	8,10,11	0.47	0	9,11,13	0.80	0
1	MLY	G	87	1	8,10,11	1.16	1 (12%)	9,11,13	0.68	0
1	MLY	J	107	1	8,10,11	0.45	0	9,11,13	0.67	0
1	MLY	J	130	1	8,10,11	0.54	0	9,11,13	1.07	1 (11%)
1	MLY	J	138	1	8,10,11	1.33	1 (12%)	9,11,13	0.80	0
1	MLY	J	19	1	8,10,11	1.23	1 (12%)	9,11,13	0.71	0
1	MLY	J	190	1	8,10,11	1.11	1 (12%)	9,11,13	0.70	0
1	MLY	J	236	1	8,10,11	0.39	0	9,11,13	1.31	1 (11%)
1	MLY	J	248	1	8,10,11	0.74	0	9,11,13	0.94	1 (11%)
1	MLY	J	272	1	8,10,11	1.04	1 (12%)	9,11,13	0.56	0
1	MLY	J	295	1	8,10,11	0.68	0	9,11,13	0.48	0
1	MLY	J	296	1	8,10,11	0.67	0	9,11,13	0.78	1 (11%)
1	MLY	J	30	1	8,10,11	0.69	0	9,11,13	0.82	0
1	MLY	J	348	1	8,10,11	0.78	0	9,11,13	0.80	0
1	MLY	J	35	1	8,10,11	0.58	0	9,11,13	0.67	0
1	MLY	J	353	1	8,10,11	0.87	0	9,11,13	0.79	0
1	MLY	J	367	1	8,10,11	0.64	0	9,11,13	0.61	0
1	MLY	J	369	1	8,10,11	0.53	0	9,11,13	0.92	1 (11%)
1	MLY	J	385	1	8,10,11	1.00	1 (12%)	9,11,13	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	J	415	1	8,10,11	0.77	0	9,11,13	0.43	0
1	MLY	J	431	1	8,10,11	0.46	0	9,11,13	0.77	0
1	MLY	J	436	1	8,10,11	1.09	1 (12%)	9,11,13	0.56	0
1	MLY	J	486	1	8,10,11	0.33	0	9,11,13	0.61	0
1	MLY	J	49	1	8,10,11	1.10	1 (12%)	9,11,13	1.01	1 (11%)
1	MLY	J	504	1	8,10,11	0.76	0	9,11,13	0.49	0
1	MLY	J	505	1	8,10,11	0.93	1 (12%)	9,11,13	0.39	0
1	MLY	J	528	1	8,10,11	0.82	0	9,11,13	1.15	1 (11%)
1	MLY	J	55	1	8,10,11	0.66	0	9,11,13	1.00	0
1	MLY	J	551	1	8,10,11	0.52	0	9,11,13	0.66	0
1	MLY	J	553	1	8,10,11	0.61	0	9,11,13	0.58	0
1	MLY	J	59	1	8,10,11	0.79	0	9,11,13	0.79	0
1	MLY	J	598	1	8,10,11	0.83	1 (12%)	9,11,13	0.71	0
1	MLY	J	600	1	8,10,11	0.52	0	9,11,13	0.47	0
1	MLY	J	613	1	8,10,11	0.51	0	9,11,13	0.94	0
1	MLY	J	617	1	8,10,11	0.95	1 (12%)	9,11,13	0.46	0
1	MLY	J	63	1	8,10,11	0.78	0	9,11,13	0.94	0
1	MLY	J	659	1	8,10,11	0.54	0	9,11,13	0.93	0
1	MLY	J	681	1	8,10,11	0.62	0	9,11,13	0.63	0
1	MLY	J	764	1	8,10,11	0.63	0	9,11,13	0.58	0
1	MLY	J	768	1	8,10,11	0.65	0	9,11,13	0.86	0
1	MLY	J	782	1	8,10,11	0.50	0	9,11,13	0.95	1 (11%)
1	MLY	J	827	1	8,10,11	0.71	0	9,11,13	0.95	1 (11%)
1	MLY	J	833	1	8,10,11	0.98	1 (12%)	9,11,13	0.57	0
1	MLY	J	837	1	8,10,11	0.53	0	9,11,13	0.58	0
1	MLY	J	839	1	8,10,11	0.68	0	9,11,13	0.75	0
1	MLY	J	84	1	8,10,11	0.46	0	9,11,13	0.80	0
1	MLY	J	87	1	8,10,11	1.16	1 (12%)	9,11,13	0.67	0
1	MLY	M	107	1	8,10,11	0.47	0	9,11,13	0.68	0
1	MLY	M	130	1	8,10,11	0.57	0	9,11,13	1.06	1 (11%)
1	MLY	M	138	1	8,10,11	1.36	1 (12%)	9,11,13	0.81	0
1	MLY	M	19	1	8,10,11	1.17	1 (12%)	9,11,13	0.70	0
1	MLY	M	190	1	8,10,11	1.09	1 (12%)	9,11,13	0.69	0
1	MLY	M	236	1	8,10,11	0.38	0	9,11,13	1.32	1 (11%)
1	MLY	M	248	1	8,10,11	0.73	0	9,11,13	0.94	1 (11%)
1	MLY	M	272	1	8,10,11	1.06	1 (12%)	9,11,13	0.57	0
1	MLY	M	295	1	8,10,11	0.68	0	9,11,13	0.48	0
1	MLY	M	296	1	8,10,11	0.64	0	9,11,13	0.78	1 (11%)
1	MLY	M	30	1	8,10,11	0.68	0	9,11,13	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	M	348	1	8,10,11	0.78	0	9,11,13	0.80	0
1	MLY	M	35	1	8,10,11	0.59	0	9,11,13	0.67	0
1	MLY	M	353	1	8,10,11	0.89	0	9,11,13	0.78	0
1	MLY	M	367	1	8,10,11	0.63	0	9,11,13	0.60	0
1	MLY	M	369	1	8,10,11	0.54	0	9,11,13	0.92	1 (11%)
1	MLY	M	385	1	8,10,11	1.03	1 (12%)	9,11,13	0.54	0
1	MLY	M	415	1	8,10,11	0.79	0	9,11,13	0.44	0
1	MLY	M	431	1	8,10,11	0.42	0	9,11,13	0.78	0
1	MLY	M	436	1	8,10,11	1.11	1 (12%)	9,11,13	0.56	0
1	MLY	M	486	1	8,10,11	0.32	0	9,11,13	0.59	0
1	MLY	M	49	1	8,10,11	1.06	1 (12%)	9,11,13	1.00	0
1	MLY	M	504	1	8,10,11	0.76	0	9,11,13	0.49	0
1	MLY	M	505	1	8,10,11	0.93	1 (12%)	9,11,13	0.38	0
1	MLY	M	528	1	8,10,11	0.82	0	9,11,13	1.16	1 (11%)
1	MLY	M	55	1	8,10,11	0.66	0	9,11,13	0.98	0
1	MLY	M	551	1	8,10,11	0.52	0	9,11,13	0.66	0
1	MLY	M	553	1	8,10,11	0.61	0	9,11,13	0.59	0
1	MLY	M	59	1	8,10,11	0.79	0	9,11,13	0.77	0
1	MLY	M	598	1	8,10,11	0.86	1 (12%)	9,11,13	0.71	0
1	MLY	M	600	1	8,10,11	0.52	0	9,11,13	0.47	0
1	MLY	M	613	1	8,10,11	0.51	0	9,11,13	0.93	0
1	MLY	M	617	1	8,10,11	0.90	1 (12%)	9,11,13	0.45	0
1	MLY	M	63	1	8,10,11	0.81	0	9,11,13	0.95	0
1	MLY	M	659	1	8,10,11	0.55	0	9,11,13	0.92	0
1	MLY	M	681	1	8,10,11	0.62	0	9,11,13	0.63	0
1	MLY	M	764	1	8,10,11	0.64	0	9,11,13	0.58	0
1	MLY	M	768	1	8,10,11	0.66	0	9,11,13	0.87	0
1	MLY	M	782	1	8,10,11	0.51	0	9,11,13	0.95	1 (11%)
1	MLY	M	827	1	8,10,11	0.68	0	9,11,13	0.95	1 (11%)
1	MLY	M	833	1	8,10,11	1.05	1 (12%)	9,11,13	0.59	0
1	MLY	M	837	1	8,10,11	0.52	0	9,11,13	0.57	0
1	MLY	M	839	1	8,10,11	0.69	0	9,11,13	0.77	0
1	MLY	M	84	1	8,10,11	0.47	0	9,11,13	0.80	0
1	MLY	M	87	1	8,10,11	1.16	1 (12%)	9,11,13	0.70	0
1	MLY	P	107	1	8,10,11	0.46	0	9,11,13	0.66	0
1	MLY	P	130	1	8,10,11	0.56	0	9,11,13	1.06	1 (11%)
1	MLY	P	138	1	8,10,11	1.31	1 (12%)	9,11,13	0.78	0
1	MLY	P	19	1	8,10,11	1.22	1 (12%)	9,11,13	0.69	0
1	MLY	P	190	1	8,10,11	1.09	1 (12%)	9,11,13	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	P	236	1	8,10,11	0.39	0	9,11,13	1.32	1 (11%)
1	MLY	P	248	1	8,10,11	0.75	0	9,11,13	0.93	1 (11%)
1	MLY	P	272	1	8,10,11	1.00	1 (12%)	9,11,13	0.56	0
1	MLY	P	295	1	8,10,11	0.72	0	9,11,13	0.48	0
1	MLY	P	296	1	8,10,11	0.61	0	9,11,13	0.78	1 (11%)
1	MLY	P	30	1	8,10,11	0.68	0	9,11,13	0.82	0
1	MLY	P	348	1	8,10,11	0.77	0	9,11,13	0.81	0
1	MLY	P	35	1	8,10,11	0.58	0	9,11,13	0.68	0
1	MLY	P	353	1	8,10,11	0.86	0	9,11,13	0.78	0
1	MLY	P	367	1	8,10,11	0.63	0	9,11,13	0.61	0
1	MLY	P	369	1	8,10,11	0.53	0	9,11,13	0.92	1 (11%)
1	MLY	P	385	1	8,10,11	0.99	1 (12%)	9,11,13	0.54	0
1	MLY	P	415	1	8,10,11	0.75	0	9,11,13	0.43	0
1	MLY	P	431	1	8,10,11	0.46	0	9,11,13	0.78	0
1	MLY	P	436	1	8,10,11	1.09	1 (12%)	9,11,13	0.57	0
1	MLY	P	486	1	8,10,11	0.32	0	9,11,13	0.61	0
1	MLY	P	49	1	8,10,11	1.11	1 (12%)	9,11,13	1.01	1 (11%)
1	MLY	P	504	1	8,10,11	0.74	0	9,11,13	0.49	0
1	MLY	P	505	1	8,10,11	0.92	1 (12%)	9,11,13	0.38	0
1	MLY	P	528	1	8,10,11	0.81	0	9,11,13	1.16	1 (11%)
1	MLY	P	55	1	8,10,11	0.67	0	9,11,13	0.99	0
1	MLY	P	551	1	8,10,11	0.51	0	9,11,13	0.66	0
1	MLY	P	553	1	8,10,11	0.63	0	9,11,13	0.57	0
1	MLY	P	59	1	8,10,11	0.77	0	9,11,13	0.78	0
1	MLY	P	598	1	8,10,11	0.85	1 (12%)	9,11,13	0.71	0
1	MLY	P	600	1	8,10,11	0.52	0	9,11,13	0.48	0
1	MLY	P	613	1	8,10,11	0.50	0	9,11,13	0.93	0
1	MLY	P	617	1	8,10,11	0.95	1 (12%)	9,11,13	0.45	0
1	MLY	P	63	1	8,10,11	0.77	0	9,11,13	0.93	0
1	MLY	P	659	1	8,10,11	0.57	0	9,11,13	0.93	0
1	MLY	P	681	1	8,10,11	0.63	0	9,11,13	0.63	0
1	MLY	P	764	1	8,10,11	0.63	0	9,11,13	0.59	0
1	MLY	P	768	1	8,10,11	0.62	0	9,11,13	0.85	0
1	MLY	P	782	1	8,10,11	0.49	0	9,11,13	0.95	1 (11%)
1	MLY	P	827	1	8,10,11	0.68	0	9,11,13	0.94	1 (11%)
1	MLY	P	833	1	8,10,11	0.99	1 (12%)	9,11,13	0.58	0
1	MLY	P	837	1	8,10,11	0.52	0	9,11,13	0.57	0
1	MLY	P	839	1	8,10,11	0.68	0	9,11,13	0.76	0
1	MLY	P	84	1	8,10,11	0.47	0	9,11,13	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	P	87	1	8,10,11	1.15	1 (12%)	9,11,13	0.67	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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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 71 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	138	MLY	CB-CA	-3.65	1.48	1.53
1	D	138	MLY	CB-CA	-3.60	1.48	1.53
1	M	138	MLY	CB-CA	-3.55	1.48	1.53
1	A	138	MLY	CB-CA	-3.54	1.48	1.53
1	J	138	MLY	CB-CA	-3.49	1.48	1.53

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	236	MLY	O-C-CA	-3.26	116.98	125.72
1	P	236	MLY	O-C-CA	-3.23	117.06	125.72
1	G	236	MLY	O-C-CA	-3.23	117.06	125.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	236	MLY	O-C-CA	-3.22	117.08	125.72
1	J	236	MLY	O-C-CA	-3.21	117.11	125.72

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
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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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
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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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
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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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
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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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.