



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:06 PM BST

PDB ID : 1M8Q  
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 : 2002-07-25  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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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

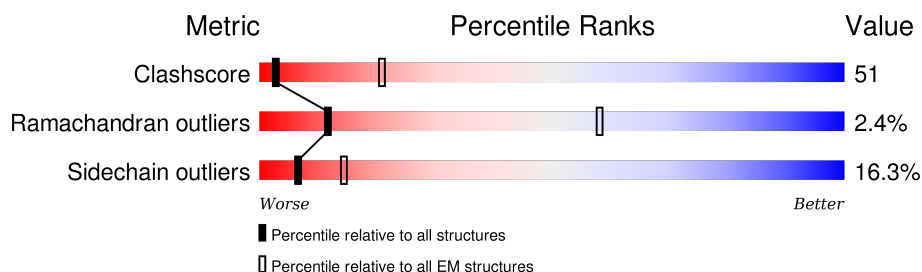
# 1 Overall quality at a glance

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.









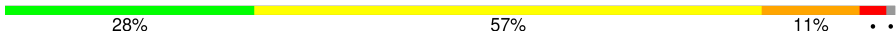
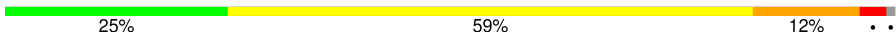
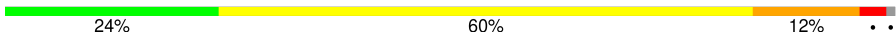
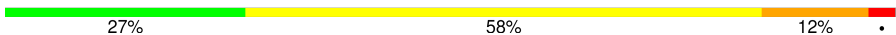
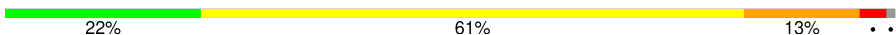
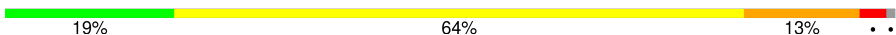





Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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  $\geq 3$ , 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	25% 52% 19% .
1	D	840	27% 51% 19% .
1	G	840	26% 51% 19% .
1	P	840	26% 50% 19% .
2	B	145	63% 28% 6% .
2	E	145	66% 26% 6% .
2	H	145	63% 28% 6% .
2	Q	145	66% 25% 6% .
3	C	147	61% 36% .

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Mol	Chain	Length	Quality of chain
3	F	147	 62% 36% ..
3	I	147	 60% 38% ..
3	R	147	 62% 36% ..
4	0	375	 58% 31% 8% ..
4	1	375	 59% 32% 6% ..
4	2	375	 55% 35% 8% ..
4	3	375	 28% 57% 11% ..
4	4	375	 25% 59% 12% ..
4	5	375	 24% 60% 12% ..
4	7	375	 27% 58% 12% ..
4	8	375	 22% 61% 13% ..
4	9	375	 19% 64% 13% ..
4	V	375	 50% 38% 9% ..
4	W	375	 60% 31% 7% ..
4	X	375	 61% 30% 7% ..
4	Y	375	 63% 29% 6% ..
4	Z	375	 63% 28% 7% ..

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	504	-	-	X	-
1	MLY	A	505	-	-	X	-
1	MLY	A	553	-	-	X	-
1	MLY	A	764	-	-	X	-
1	MLY	A	768	-	-	X	-
1	MLY	A	839	-	-	X	-
1	MLY	D	553	-	-	X	-
1	MLY	D	764	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	MLY	D	782	-	-	X	-
1	MLY	D	839	-	-	X	-
1	MLY	G	553	-	-	X	-
1	MLY	G	768	-	-	X	-
1	MLY	P	764	-	-	X	-
1	MLY	P	839	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 76872 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	P	840	Total	C	N	O	S	0	0
			6797	4382	1135	1243	37		

There are 228 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	MLY	LYS	MODIFIED	UNP P13538
A	30	MLY	LYS	MODIFIED	UNP P13538
A	35	MLY	LYS	MODIFIED	UNP P13538
A	45	GLN	GLU	CONFLICT	UNP P13538
A	49	MLY	LYS	MODIFIED	UNP P13538
A	55	MLY	LYS	MODIFIED	UNP P13538
A	59	MLY	LYS	MODIFIED	UNP P13538
A	63	MLY	LYS	MODIFIED	UNP P13538
A	84	MLY	LYS	MODIFIED	UNP P13538
A	87	MLY	LYS	MODIFIED	UNP P13538
A	107	MLY	LYS	MODIFIED	UNP P13538
A	130	MLY	LYS	MODIFIED	UNP P13538
A	138	MLY	GLU	MODIFIED	UNP P13538
A	190	MLY	LYS	MODIFIED	UNP P13538
A	236	MLY	LYS	MODIFIED	UNP P13538
A	248	MLY	LYS	MODIFIED	UNP P13538
A	272	MLY	LYS	MODIFIED	UNP P13538
A	295	MLY	LYS	MODIFIED	UNP P13538
A	296	MLY	LYS	MODIFIED	UNP P13538
A	317	GLU	GLN	CONFLICT	UNP P13538
A	348	MLY	LYS	MODIFIED	UNP P13538
A	353	MLY	LYS	MODIFIED	UNP P13538

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Chain	Residue	Modelled	Actual	Comment	Reference
A	367	MLY	LYS	MODIFIED	UNP P13538
A	369	MLY	LYS	MODIFIED	UNP P13538
A	385	MLY	LYS	MODIFIED	UNP P13538
A	407	GLY	LYS	CONFLICT	UNP P13538
A	412	ALA	PHE	CONFLICT	UNP P13538
A	415	MLY	LYS	MODIFIED	UNP P13538
A	417	GLU	GLN	CONFLICT	UNP P13538
A	421	GLU	GLN	CONFLICT	UNP P13538
A	431	MLY	LYS	MODIFIED	UNP P13538
A	436	MLY	LYS	MODIFIED	UNP P13538
A	486	MLY	LYS	MODIFIED	UNP P13538
A	504	MLY	LYS	MODIFIED	UNP P13538
A	505	MLY	LYS	MODIFIED	UNP P13538
A	528	MLY	LYS	MODIFIED	UNP P13538
A	551	MLY	LYS	MODIFIED	UNP P13538
A	553	MLY	LYS	MODIFIED	UNP P13538
A	557	GLU	GLN	CONFLICT	UNP P13538
A	598	MLY	LYS	MODIFIED	UNP P13538
A	600	MLY	LYS	MODIFIED	UNP P13538
A	613	MLY	LYS	MODIFIED	UNP P13538
A	617	MLY	LYS	MODIFIED	UNP P13538
A	659	MLY	LYS	MODIFIED	UNP P13538
A	681	MLY	LYS	MODIFIED	UNP P13538
A	750	GLY	SER	CONFLICT	UNP P13538
A	751	GLY	ILE	CONFLICT	UNP P13538
A	759	ALA	ARG	CONFLICT	UNP P13538
A	764	MLY	LYS	MODIFIED	UNP P13538
A	768	MLY	LYS	MODIFIED	UNP P13538
A	782	MLY	LYS	MODIFIED	UNP P13538
A	789	ALA	ARG	MODIFIED	UNP P13538
A	805	ALA	ARG	CONFLICT	UNP P13538
A	827	MLY	LYS	MODIFIED	UNP P13538
A	833	MLY	LYS	MODIFIED	UNP P13538
A	837	MLY	LYS	MODIFIED	UNP P13538
A	839	MLY	LYS	MODIFIED	UNP P13538
D	19	MLY	LYS	MODIFIED	UNP P13538
D	30	MLY	LYS	MODIFIED	UNP P13538
D	35	MLY	LYS	MODIFIED	UNP P13538
D	45	GLN	GLU	CONFLICT	UNP P13538
D	49	MLY	LYS	MODIFIED	UNP P13538
D	55	MLY	LYS	MODIFIED	UNP P13538
D	59	MLY	LYS	MODIFIED	UNP P13538

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Chain	Residue	Modelled	Actual	Comment	Reference
D	63	MLY	LYS	MODIFIED	UNP P13538
D	84	MLY	LYS	MODIFIED	UNP P13538
D	87	MLY	LYS	MODIFIED	UNP P13538
D	107	MLY	LYS	MODIFIED	UNP P13538
D	130	MLY	LYS	MODIFIED	UNP P13538
D	138	MLY	GLU	MODIFIED	UNP P13538
D	190	MLY	LYS	MODIFIED	UNP P13538
D	236	MLY	LYS	MODIFIED	UNP P13538
D	248	MLY	LYS	MODIFIED	UNP P13538
D	272	MLY	LYS	MODIFIED	UNP P13538
D	295	MLY	LYS	MODIFIED	UNP P13538
D	296	MLY	LYS	MODIFIED	UNP P13538
D	317	GLU	GLN	CONFLICT	UNP P13538
D	348	MLY	LYS	MODIFIED	UNP P13538
D	353	MLY	LYS	MODIFIED	UNP P13538
D	367	MLY	LYS	MODIFIED	UNP P13538
D	369	MLY	LYS	MODIFIED	UNP P13538
D	385	MLY	LYS	MODIFIED	UNP P13538
D	407	GLY	LYS	CONFLICT	UNP P13538
D	412	ALA	PHE	CONFLICT	UNP P13538
D	415	MLY	LYS	MODIFIED	UNP P13538
D	417	GLU	GLN	CONFLICT	UNP P13538
D	421	GLU	GLN	CONFLICT	UNP P13538
D	431	MLY	LYS	MODIFIED	UNP P13538
D	436	MLY	LYS	MODIFIED	UNP P13538
D	486	MLY	LYS	MODIFIED	UNP P13538
D	504	MLY	LYS	MODIFIED	UNP P13538
D	505	MLY	LYS	MODIFIED	UNP P13538
D	528	MLY	LYS	MODIFIED	UNP P13538
D	551	MLY	LYS	MODIFIED	UNP P13538
D	553	MLY	LYS	MODIFIED	UNP P13538
D	557	GLU	GLN	CONFLICT	UNP P13538
D	598	MLY	LYS	MODIFIED	UNP P13538
D	600	MLY	LYS	MODIFIED	UNP P13538
D	613	MLY	LYS	MODIFIED	UNP P13538
D	617	MLY	LYS	MODIFIED	UNP P13538
D	659	MLY	LYS	MODIFIED	UNP P13538
D	681	MLY	LYS	MODIFIED	UNP P13538
D	750	GLY	SER	CONFLICT	UNP P13538
D	751	GLY	ILE	CONFLICT	UNP P13538
D	759	ALA	ARG	CONFLICT	UNP P13538
D	764	MLY	LYS	MODIFIED	UNP P13538

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Chain	Residue	Modelled	Actual	Comment	Reference
D	768	MLY	LYS	MODIFIED	UNP P13538
D	782	MLY	LYS	MODIFIED	UNP P13538
D	789	ALA	ARG	CONFLICT	UNP P13538
D	805	ALA	ARG	CONFLICT	UNP P13538
D	827	MLY	LYS	MODIFIED	UNP P13538
D	833	MLY	LYS	MODIFIED	UNP P13538
D	837	MLY	LYS	MODIFIED	UNP P13538
D	839	MLY	LYS	MODIFIED	UNP P13538
G	19	MLY	LYS	MODIFIED	UNP P13538
G	30	MLY	LYS	MODIFIED	UNP P13538
G	35	MLY	LYS	MODIFIED	UNP P13538
G	45	GLN	GLU	CONFLICT	UNP P13538
G	49	MLY	LYS	MODIFIED	UNP P13538
G	55	MLY	LYS	MODIFIED	UNP P13538
G	59	MLY	LYS	MODIFIED	UNP P13538
G	63	MLY	LYS	MODIFIED	UNP P13538
G	84	MLY	LYS	MODIFIED	UNP P13538
G	87	MLY	LYS	MODIFIED	UNP P13538
G	107	MLY	LYS	MODIFIED	UNP P13538
G	130	MLY	LYS	MODIFIED	UNP P13538
G	138	MLY	GLU	MODIFIED	UNP P13538
G	190	MLY	LYS	MODIFIED	UNP P13538
G	236	MLY	LYS	MODIFIED	UNP P13538
G	248	MLY	LYS	MODIFIED	UNP P13538
G	272	MLY	LYS	MODIFIED	UNP P13538
G	295	MLY	LYS	MODIFIED	UNP P13538
G	296	MLY	LYS	MODIFIED	UNP P13538
G	317	GLU	GLN	CONFLICT	UNP P13538
G	348	MLY	LYS	MODIFIED	UNP P13538
G	353	MLY	LYS	MODIFIED	UNP P13538
G	367	MLY	LYS	MODIFIED	UNP P13538
G	369	MLY	LYS	MODIFIED	UNP P13538
G	385	MLY	LYS	MODIFIED	UNP P13538
G	407	GLY	LYS	CONFLICT	UNP P13538
G	412	ALA	PHE	CONFLICT	UNP P13538
G	415	MLY	LYS	MODIFIED	UNP P13538
G	417	GLU	GLN	CONFLICT	UNP P13538
G	421	GLU	GLN	CONFLICT	UNP P13538
G	431	MLY	LYS	MODIFIED	UNP P13538
G	436	MLY	LYS	MODIFIED	UNP P13538
G	486	MLY	LYS	MODIFIED	UNP P13538
G	504	MLY	LYS	MODIFIED	UNP P13538

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Chain	Residue	Modelled	Actual	Comment	Reference
G	505	MLY	LYS	MODIFIED	UNP P13538
G	528	MLY	LYS	MODIFIED	UNP P13538
G	551	MLY	LYS	MODIFIED	UNP P13538
G	553	MLY	LYS	MODIFIED	UNP P13538
G	557	GLU	GLN	CONFLICT	UNP P13538
G	598	MLY	LYS	MODIFIED	UNP P13538
G	600	MLY	LYS	MODIFIED	UNP P13538
G	613	MLY	LYS	MODIFIED	UNP P13538
G	617	MLY	LYS	MODIFIED	UNP P13538
G	659	MLY	LYS	MODIFIED	UNP P13538
G	681	MLY	LYS	MODIFIED	UNP P13538
G	750	GLY	SER	CONFLICT	UNP P13538
G	751	GLY	ILE	CONFLICT	UNP P13538
G	759	ALA	ARG	CONFLICT	UNP P13538
G	764	MLY	LYS	MODIFIED	UNP P13538
G	768	MLY	LYS	MODIFIED	UNP P13538
G	782	MLY	LYS	MODIFIED	UNP P13538
G	789	ALA	ARG	CONFLICT	UNP P13538
G	805	ALA	ARG	CONFLICT	UNP P13538
G	827	MLY	LYS	MODIFIED	UNP P13538
G	833	MLY	LYS	MODIFIED	UNP P13538
G	837	MLY	LYS	MODIFIED	UNP P13538
G	839	MLY	LYS	MODIFIED	UNP P13538
P	19	MLY	LYS	MODIFIED	UNP P13538
P	30	MLY	LYS	MODIFIED	UNP P13538
P	35	MLY	LYS	MODIFIED	UNP P13538
P	45	GLN	GLU	CONFLICT	UNP P13538
P	49	MLY	LYS	MODIFIED	UNP P13538
P	55	MLY	LYS	MODIFIED	UNP P13538
P	59	MLY	LYS	MODIFIED	UNP P13538
P	63	MLY	LYS	MODIFIED	UNP P13538
P	84	MLY	LYS	MODIFIED	UNP P13538
P	87	MLY	LYS	MODIFIED	UNP P13538
P	107	MLY	LYS	MODIFIED	UNP P13538
P	130	MLY	LYS	MODIFIED	UNP P13538
P	138	MLY	GLU	MODIFIED	UNP P13538
P	190	MLY	LYS	MODIFIED	UNP P13538
P	236	MLY	LYS	MODIFIED	UNP P13538
P	248	MLY	LYS	MODIFIED	UNP P13538
P	272	MLY	LYS	MODIFIED	UNP P13538
P	295	MLY	LYS	MODIFIED	UNP P13538
P	296	MLY	LYS	MODIFIED	UNP P13538

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Chain	Residue	Modelled	Actual	Comment	Reference
P	317	GLU	GLN	CONFLICT	UNP P13538
P	348	MLY	LYS	MODIFIED	UNP P13538
P	353	MLY	LYS	MODIFIED	UNP P13538
P	367	MLY	LYS	MODIFIED	UNP P13538
P	369	MLY	LYS	MODIFIED	UNP P13538
P	385	MLY	LYS	MODIFIED	UNP P13538
P	407	GLY	LYS	CONFLICT	UNP P13538
P	412	ALA	PHE	CONFLICT	UNP P13538
P	415	MLY	LYS	MODIFIED	UNP P13538
P	417	GLU	GLN	CONFLICT	UNP P13538
P	421	GLU	GLN	CONFLICT	UNP P13538
P	431	MLY	LYS	MODIFIED	UNP P13538
P	436	MLY	LYS	MODIFIED	UNP P13538
P	486	MLY	LYS	MODIFIED	UNP P13538
P	504	MLY	LYS	MODIFIED	UNP P13538
P	505	MLY	LYS	MODIFIED	UNP P13538
P	528	MLY	LYS	MODIFIED	UNP P13538
P	551	MLY	LYS	MODIFIED	UNP P13538
P	553	MLY	LYS	MODIFIED	UNP P13538
P	557	GLU	GLN	CONFLICT	UNP P13538
P	598	MLY	LYS	MODIFIED	UNP P13538
P	600	MLY	LYS	MODIFIED	UNP P13538
P	613	MLY	LYS	MODIFIED	UNP P13538
P	617	MLY	LYS	MODIFIED	UNP P13538
P	659	MLY	LYS	MODIFIED	UNP P13538
P	681	MLY	LYS	MODIFIED	UNP P13538
P	750	GLY	SER	CONFLICT	UNP P13538
P	751	GLY	ILE	CONFLICT	UNP P13538
P	759	ALA	ARG	CONFLICT	UNP P13538
P	764	MLY	LYS	MODIFIED	UNP P13538
P	768	MLY	LYS	MODIFIED	UNP P13538
P	782	MLY	LYS	MODIFIED	UNP P13538
P	789	ALA	ARG	CONFLICT	UNP P13538
P	805	ALA	ARG	CONFLICT	UNP P13538
P	827	MLY	LYS	MODIFIED	UNP P13538
P	833	MLY	LYS	MODIFIED	UNP P13538
P	837	MLY	LYS	MODIFIED	UNP P13538
P	839	MLY	LYS	MODIFIED	UNP P13538

- 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	Q	145	Total	C	N	O	S	0	0
			1127	717	177	227	6		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	21	GLU	GLN	CONFLICT	UNP P02609
B	23	GLU	GLN	CONFLICT	UNP P02609
B	25	GLU	GLN	CONFLICT	UNP P02609
B	26	ASP	GLU	CONFLICT	UNP P02609
B	38	ALA	ARG	CONFLICT	UNP P02609
B	124	GLY	GLN	CONFLICT	UNP P02609
B	125	GLY	CYS	CONFLICT	UNP P02609
B	126	GLY	ASP	CONFLICT	UNP P02609
B	163	ALA	LYS	CONFLICT	UNP P02609
E	21	GLU	GLN	CONFLICT	UNP P02609
E	23	GLU	GLN	CONFLICT	UNP P02609
E	25	GLU	GLN	CONFLICT	UNP P02609
E	26	ASP	GLU	CONFLICT	UNP P02609
E	38	ALA	ARG	CONFLICT	UNP P02609
E	124	GLY	GLN	CONFLICT	UNP P02609
E	125	GLY	CYS	CONFLICT	UNP P02609
E	126	GLY	ASP	CONFLICT	UNP P02609
E	163	ALA	LYS	CONFLICT	UNP P02609
H	21	GLU	GLN	CONFLICT	UNP P02609
H	23	GLU	GLN	CONFLICT	UNP P02609
H	25	GLU	GLN	CONFLICT	UNP P02609
H	26	ASP	GLU	CONFLICT	UNP P02609
H	38	ALA	ARG	CONFLICT	UNP P02609
H	124	GLY	GLN	CONFLICT	UNP P02609
H	125	GLY	CYS	CONFLICT	UNP P02609
H	126	GLY	ASP	CONFLICT	UNP P02609
H	163	ALA	LYS	CONFLICT	UNP P02609
Q	21	GLU	GLN	CONFLICT	UNP P02609
Q	23	GLU	GLN	CONFLICT	UNP P02609
Q	25	GLU	GLN	CONFLICT	UNP P02609
Q	26	ASP	GLU	CONFLICT	UNP P02609

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	38	ALA	ARG	CONFLICT	UNP P02609
Q	124	GLY	GLN	CONFLICT	UNP P02609
Q	125	GLY	CYS	CONFLICT	UNP P02609
Q	126	GLY	ASP	CONFLICT	UNP P02609
Q	163	ALA	LYS	CONFLICT	UNP P02609

- 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	R	147	Total	C	N	O	S	0	0
			1123	698	188	230	7		

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	5	ALA	GLU	CONFLICT	UNP P02604
C	6	ALA	GLN	CONFLICT	UNP P02604
C	7	ALA	GLN	CONFLICT	UNP P02604
C	27	ALA	LEU	CONFLICT	UNP P02604
C	34	ALA	VAL	CONFLICT	UNP P02604
C	61	ALA	LYS	CONFLICT	UNP P02604
C	105	ALA	LYS	CONFLICT	UNP P02604
F	5	ALA	GLU	CONFLICT	UNP P02604
F	6	ALA	GLN	CONFLICT	UNP P02604
F	7	ALA	GLN	CONFLICT	UNP P02604
F	27	ALA	LEU	CONFLICT	UNP P02604
F	34	ALA	VAL	CONFLICT	UNP P02604
F	61	ALA	LYS	CONFLICT	UNP P02604
F	105	ALA	LYS	CONFLICT	UNP P02604
I	5	ALA	GLU	CONFLICT	UNP P02604
I	6	ALA	GLN	CONFLICT	UNP P02604
I	7	ALA	GLN	CONFLICT	UNP P02604
I	27	ALA	LEU	CONFLICT	UNP P02604
I	34	ALA	VAL	CONFLICT	UNP P02604
I	61	ALA	LYS	CONFLICT	UNP P02604
I	105	ALA	LYS	CONFLICT	UNP P02604

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Chain	Residue	Modelled	Actual	Comment	Reference
R	5	ALA	GLU	CONFLICT	UNP P02604
R	6	ALA	GLN	CONFLICT	UNP P02604
R	7	ALA	GLN	CONFLICT	UNP P02604
R	27	ALA	LEU	CONFLICT	UNP P02604
R	34	ALA	VAL	CONFLICT	UNP P02604
R	61	ALA	LYS	CONFLICT	UNP P02604
R	105	ALA	LYS	CONFLICT	UNP P02604

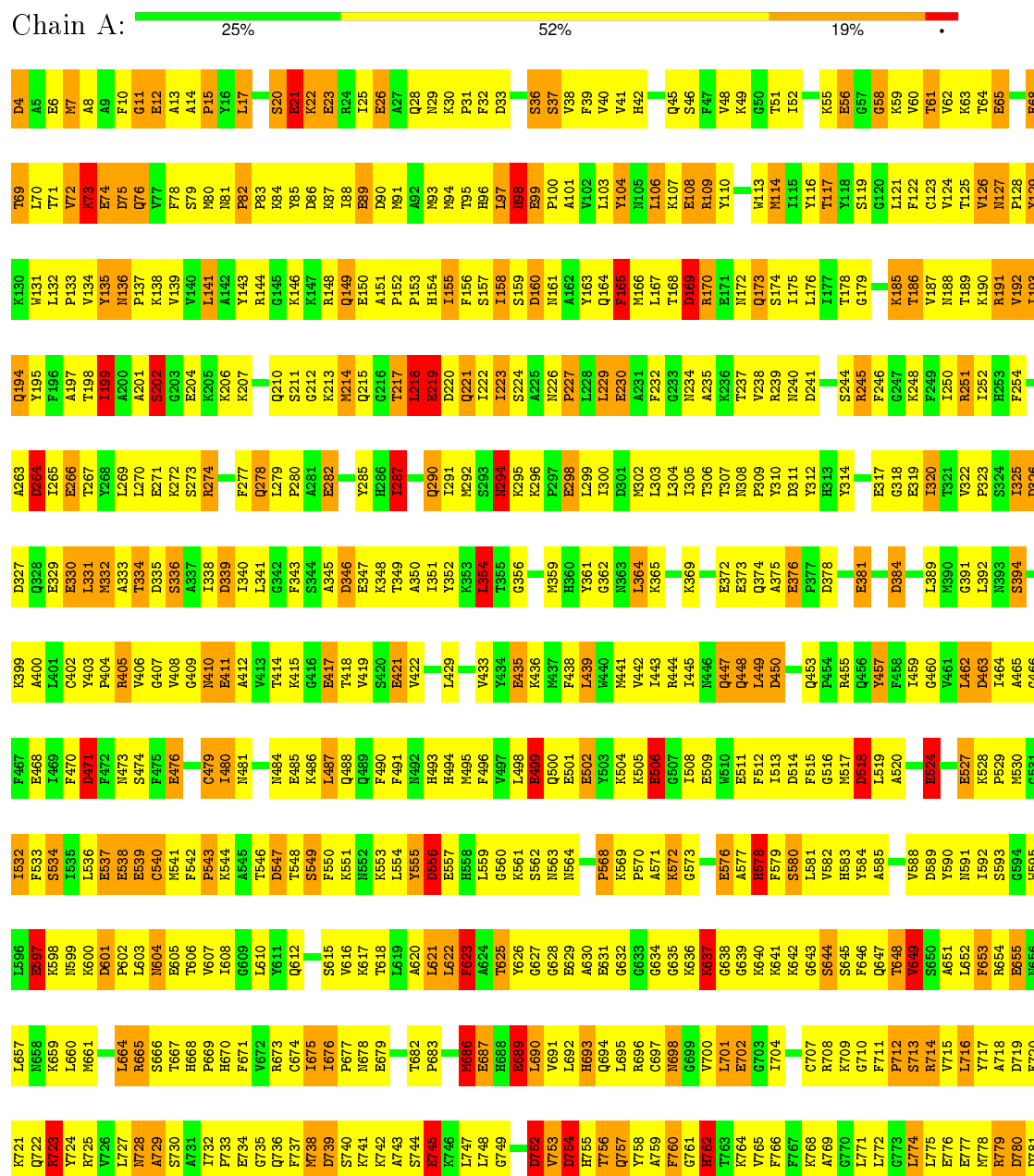
- Molecule 4 is a protein called Skeletal muscle Actin.

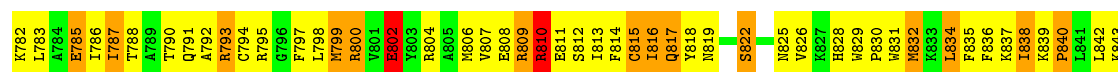
Mol	Chain	Residues	Atoms					AltConf	Trace
4	7	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	8	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	9	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	V	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	W	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
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		
4	0	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
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		

### 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.

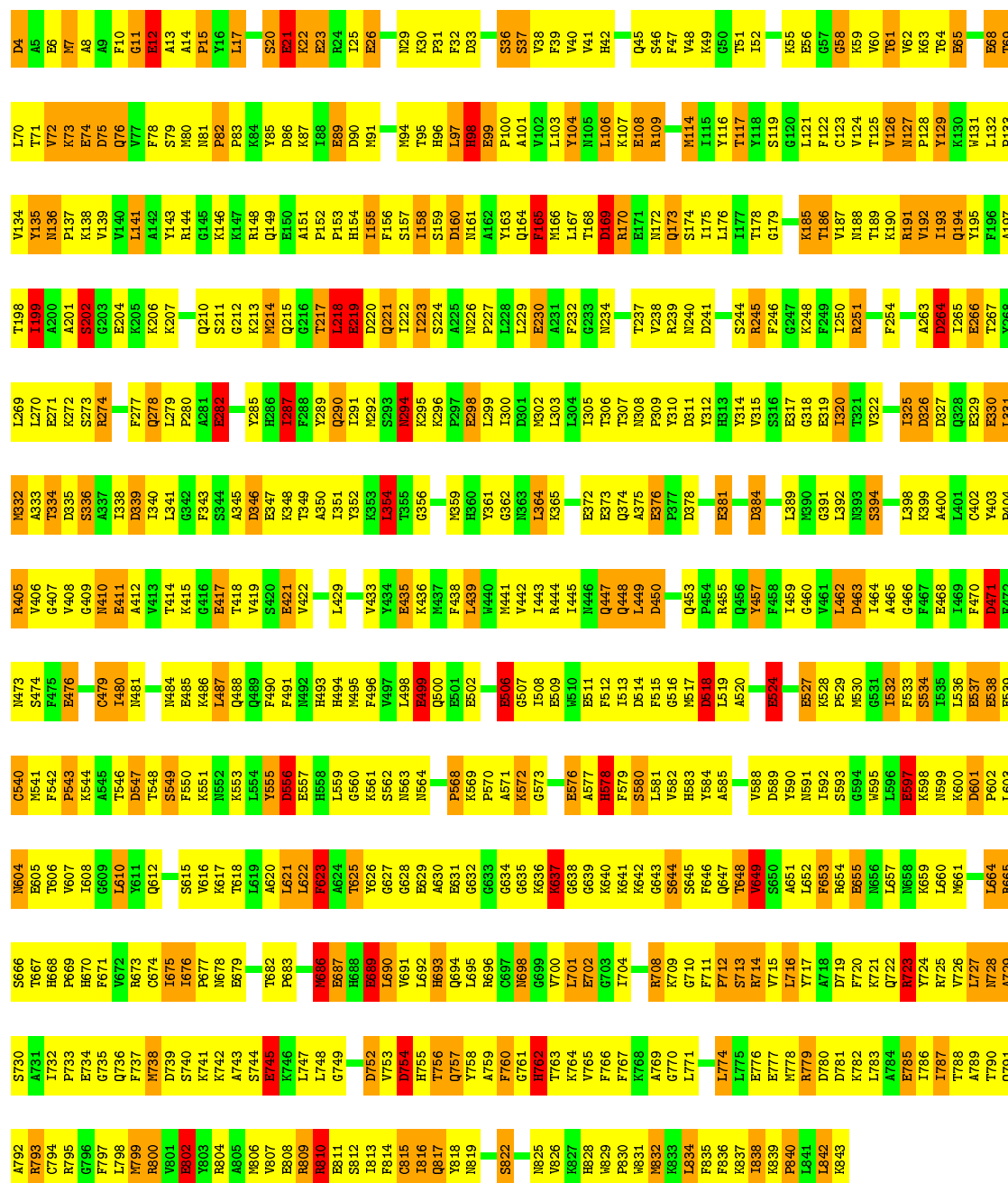
- Molecule 1: Skeletal muscle Myosin II





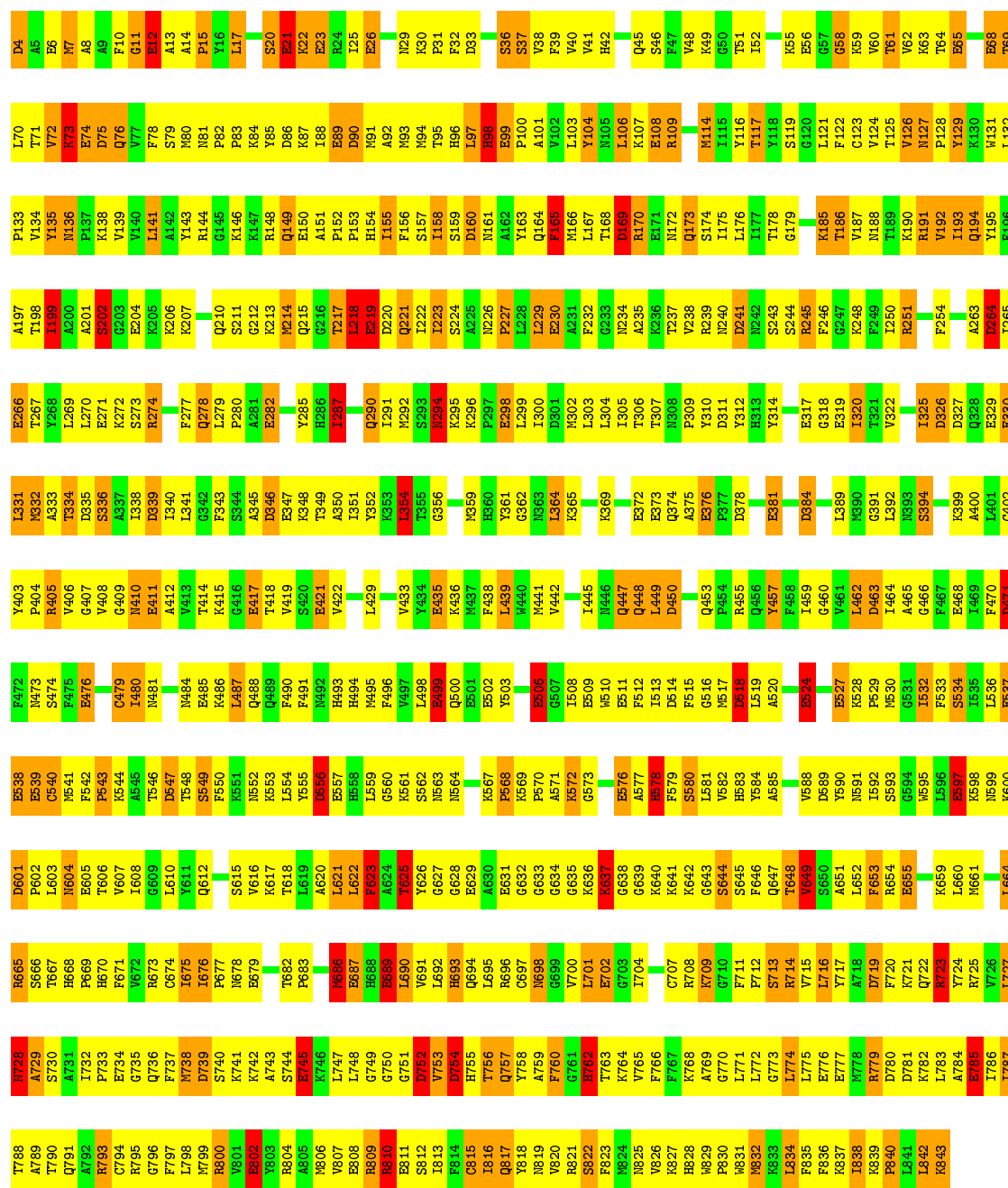
• Molecule 1: Skeletal muscle Myosin II

Chain D: 27% 51% 19%



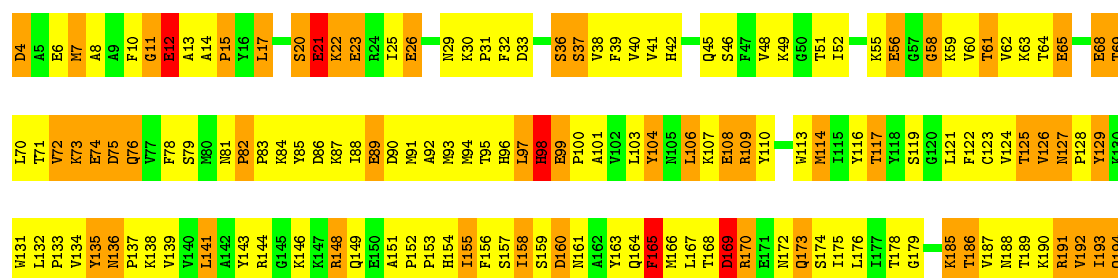
• Molecule 1: Skeletal muscle Myosin II

Chain G: 26% 51% 19%

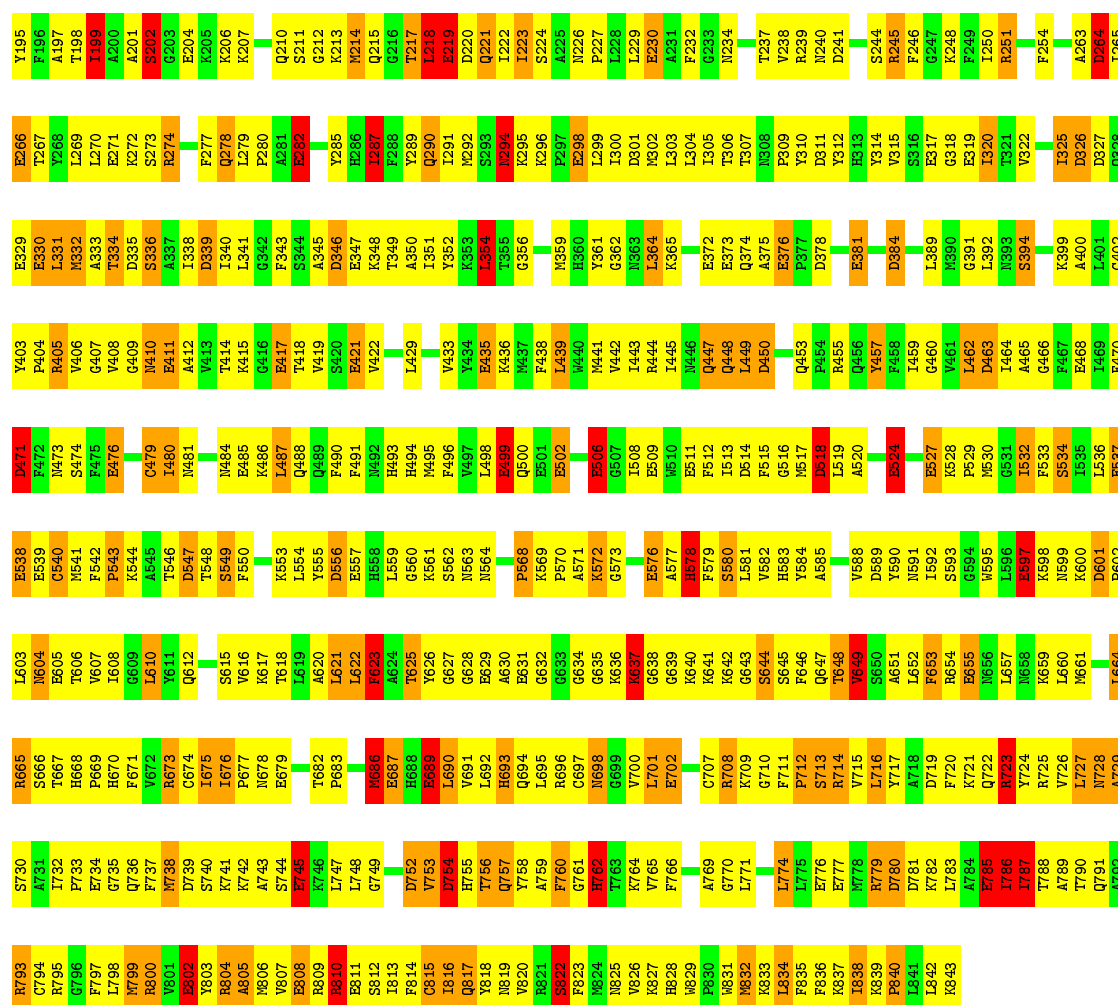


• Molecule 1: Skeletal muscle Myosin II

Chain P: 26% 50% 19%

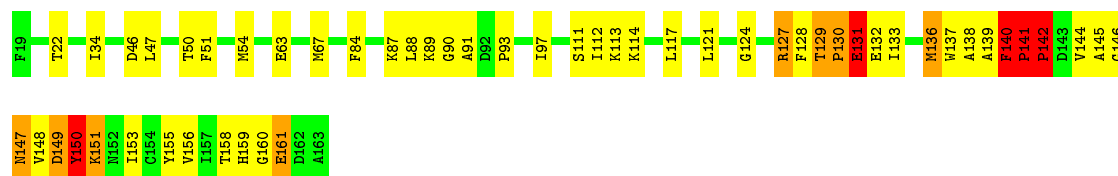






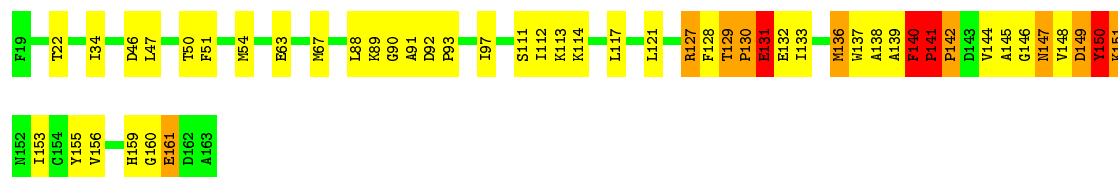
### • Molecule 2: Skeletal muscle Myosin II Regulatory Light Chain

Chain B: 63% 28% 6%

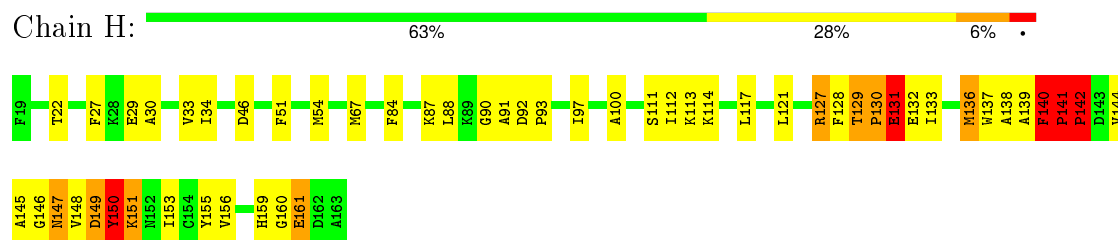


### • Molecule 2: Skeletal muscle Myosin II Regulatory Light Chain

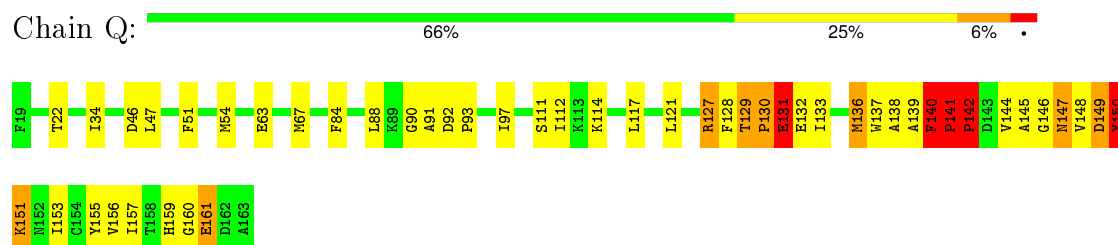
Chain E: 66% 26% 6%



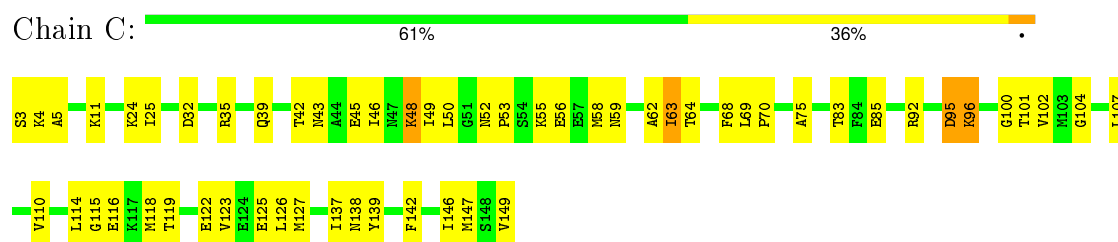
### • Molecule 2: Skeletal muscle Myosin II Regulatory Light Chain



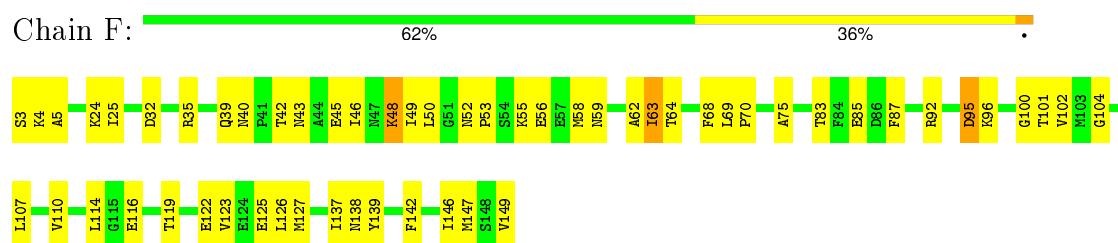
- Molecule 2: Skeletal muscle Myosin II Regulatory Light Chain



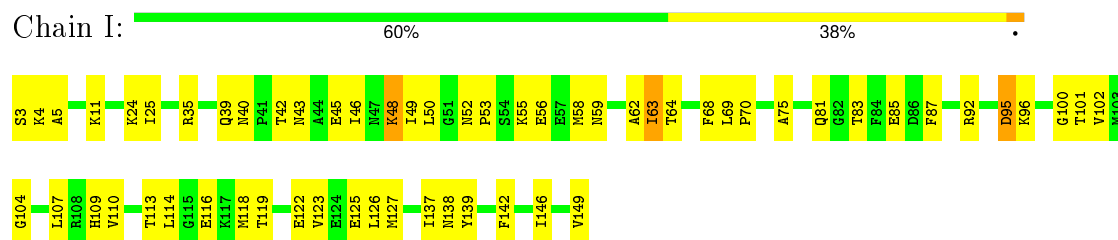
- Molecule 3: Skeletal muscle Myosin II Essential Light Chain



- Molecule 3: Skeletal muscle Myosin II Essential Light Chain

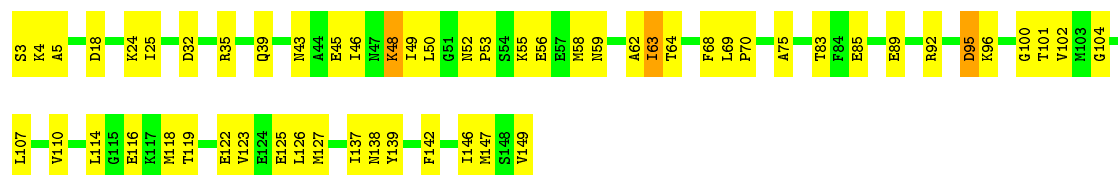


- Molecule 3: Skeletal muscle Myosin II Essential Light Chain



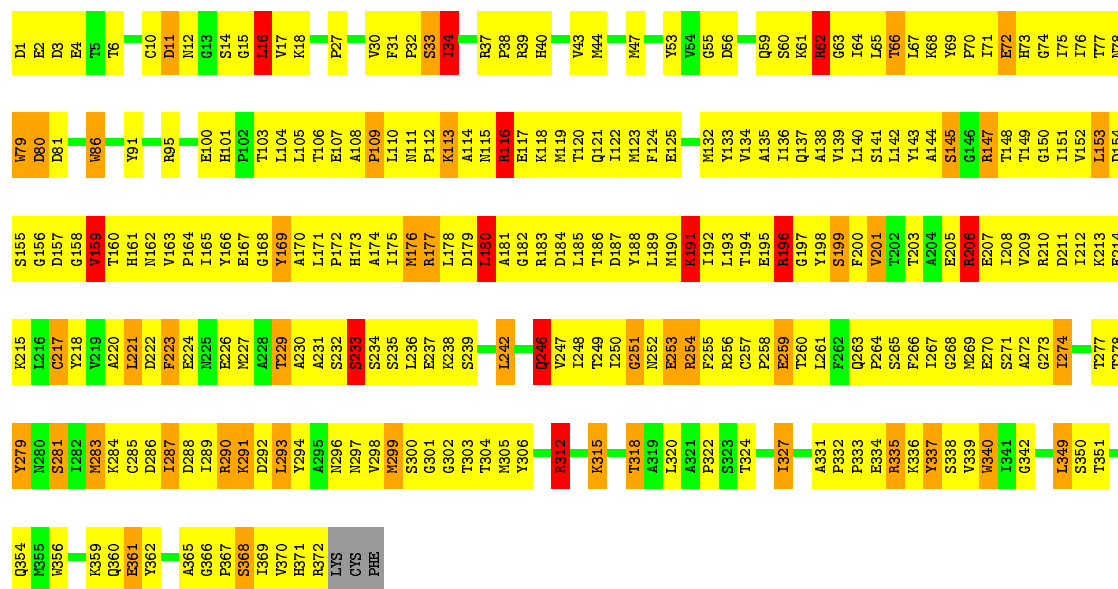
- Molecule 3: Skeletal muscle Myosin II Essential Light Chain





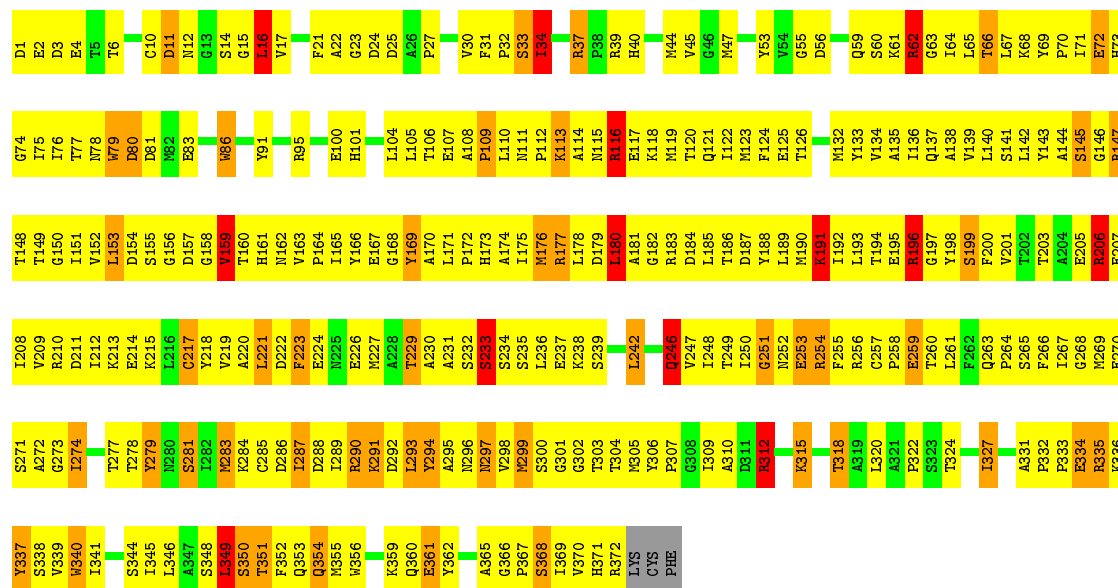
• Molecule 4: Skeletal muscle Actin

Chain 7: 27% 58% 12%

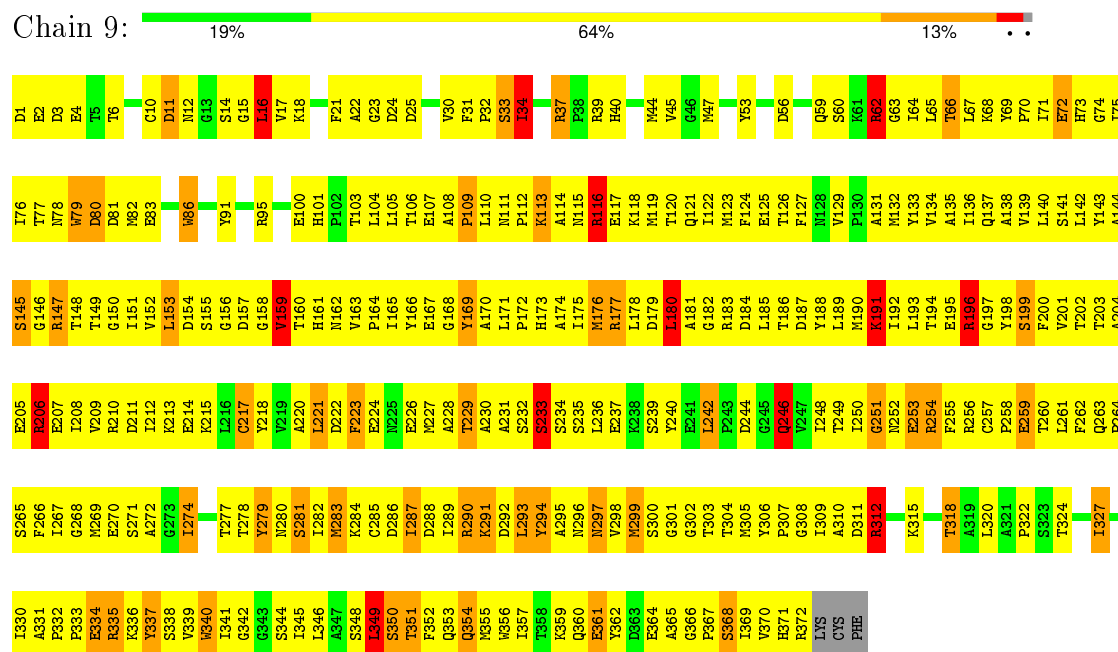


• Molecule 4: Skeletal muscle Actin

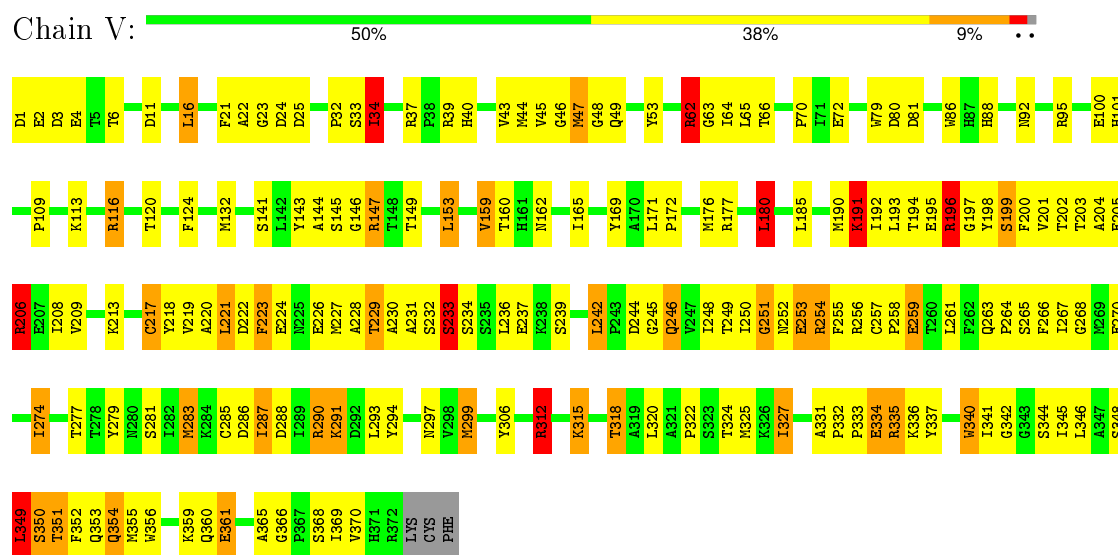
Chain 8: 22% 61% 13%



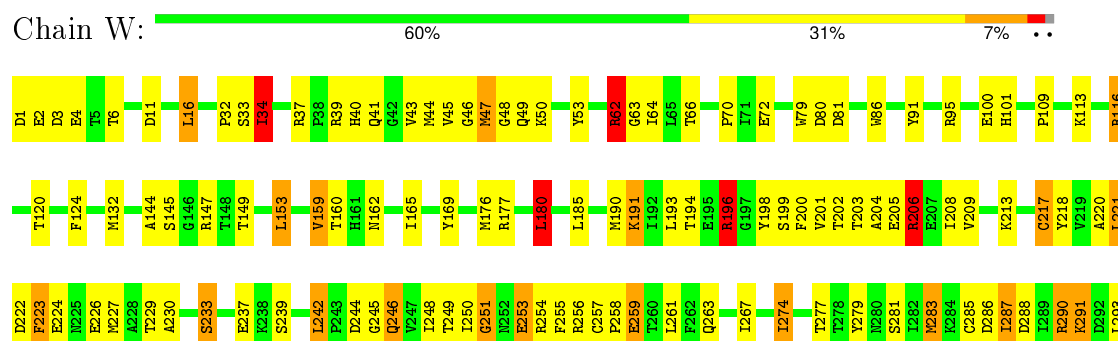
• Molecule 4: Skeletal muscle Actin



• Molecule 4: Skeletal muscle Actin



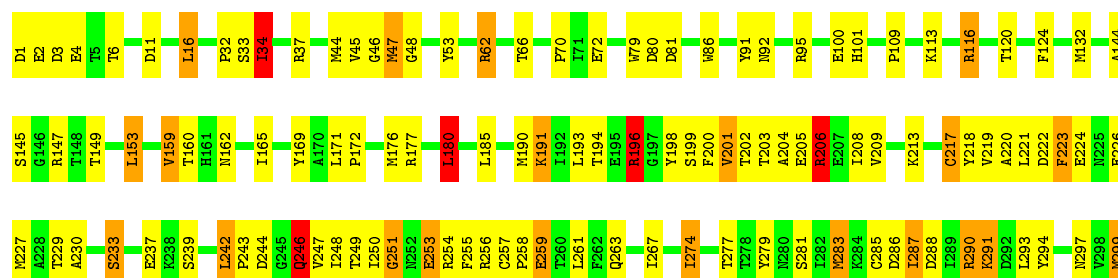
• Molecule 4: Skeletal muscle Actin





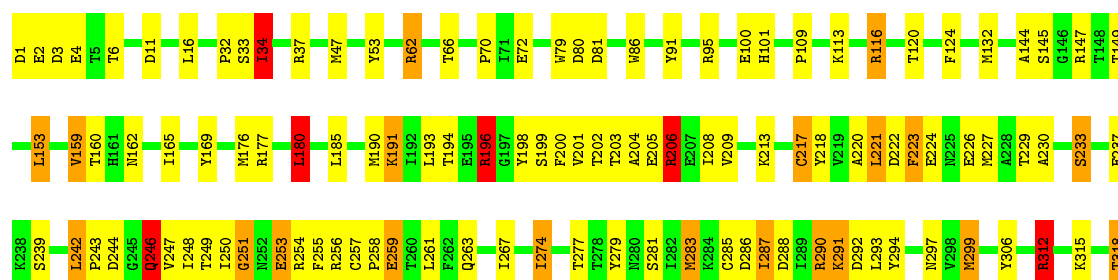
• Molecule 4: Skeletal muscle Actin

Chain X: 61% 30% 7% ..



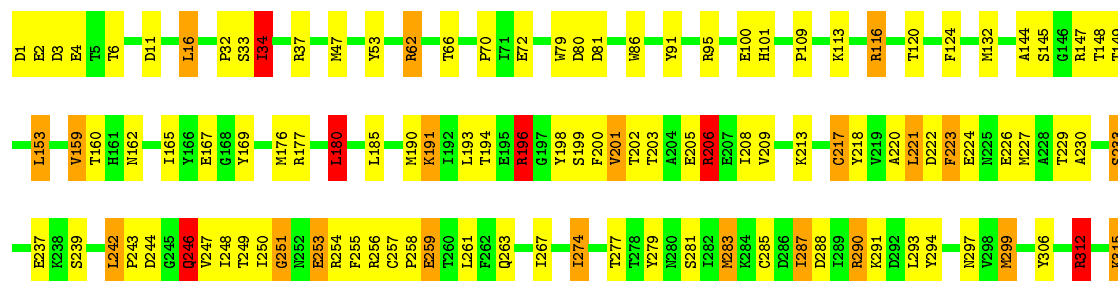
• Molecule 4: Skeletal muscle Actin

Chain Y: 63% 29% 6% ..

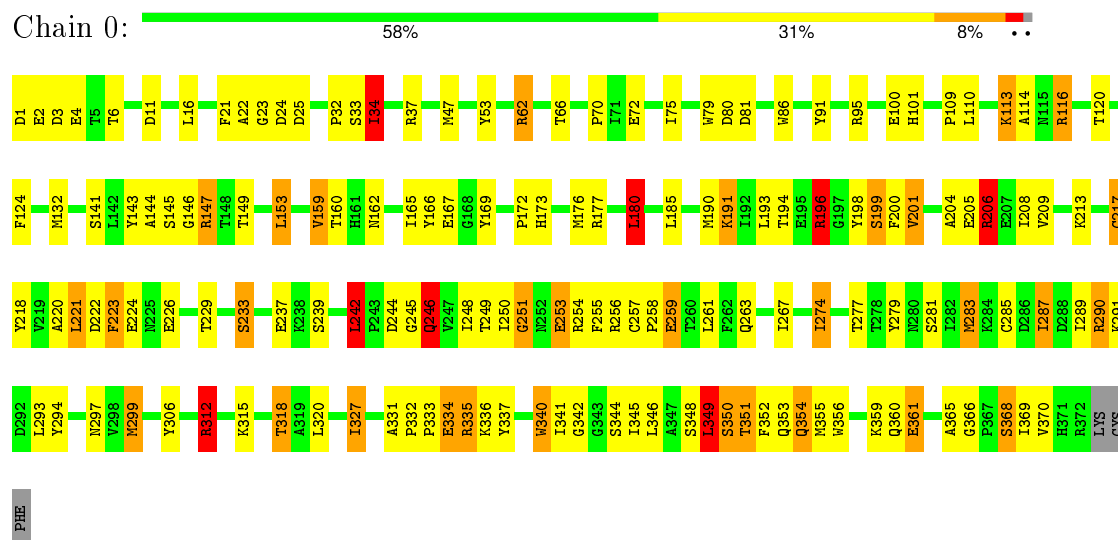


• Molecule 4: Skeletal muscle Actin

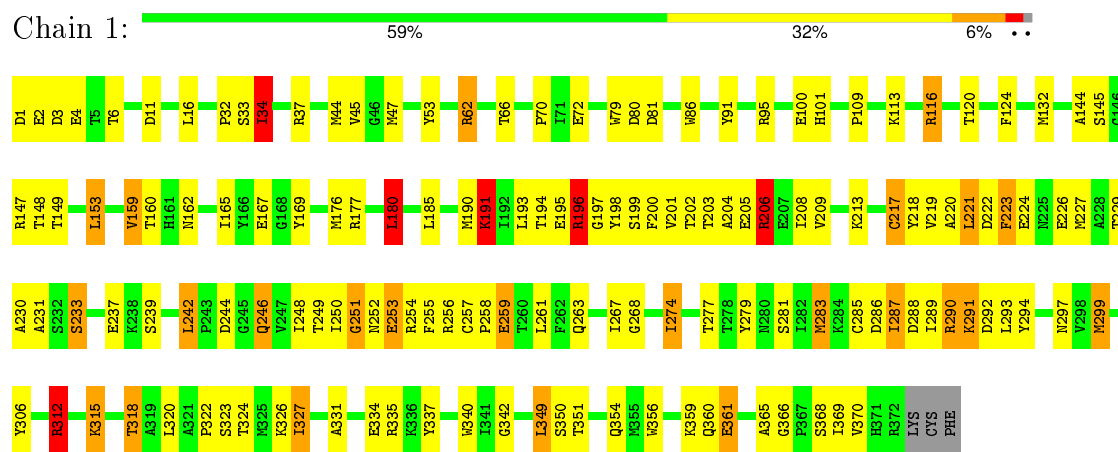
Chain Z: 63% 28% 7% ..



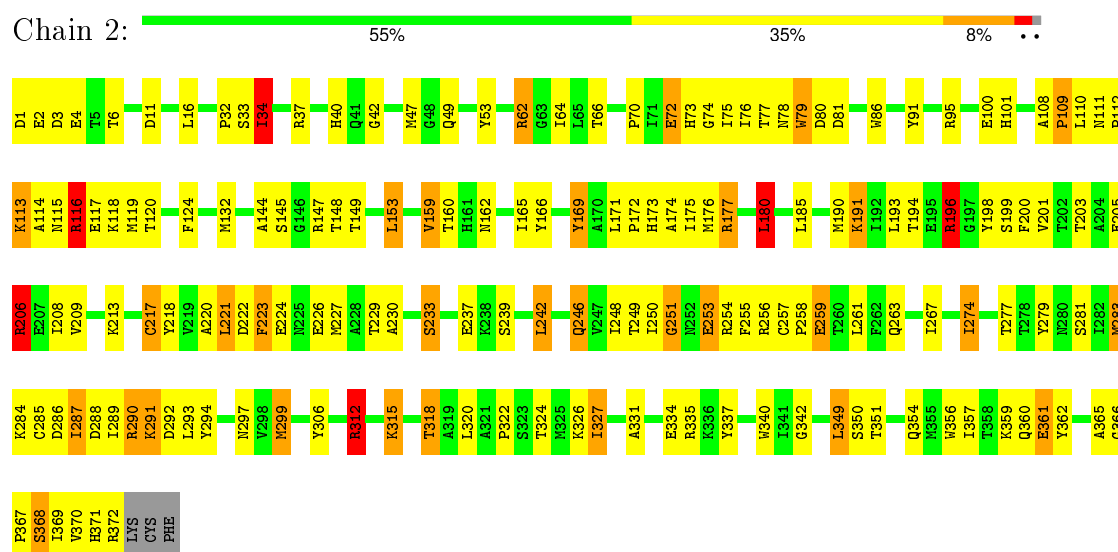
• Molecule 4: Skeletal muscle Actin



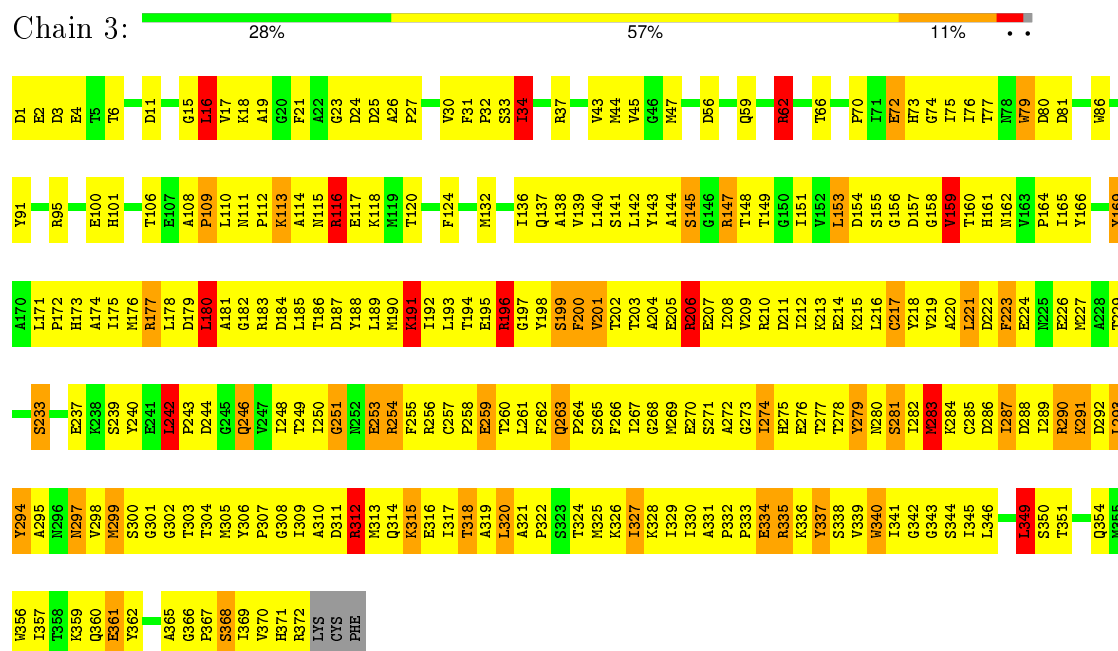
• Molecule 4: Skeletal muscle Actin



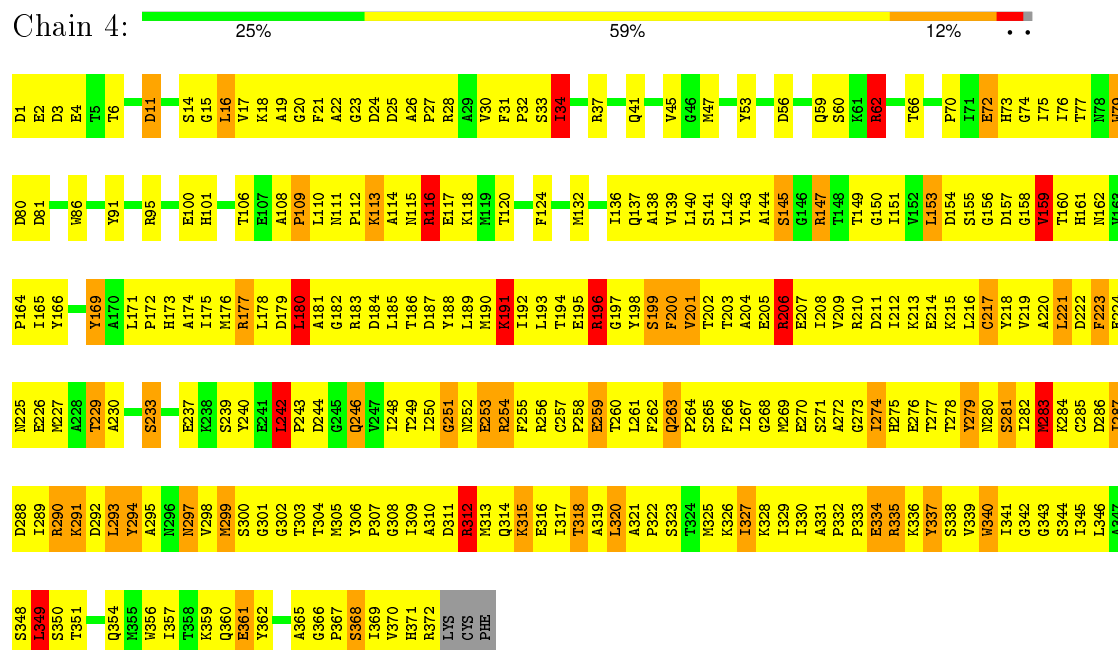
• Molecule 4: Skeletal muscle Actin



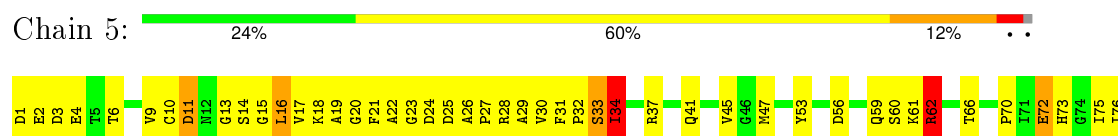
- Molecule 4: Skeletal muscle Actin



- Molecule 4: Skeletal muscle Actin



- Molecule 4: Skeletal muscle Actin



T341	G342	G343	S344	I345	I346	A347	S348	I349	S350	T351	G354	G355	G356	K359	Q360	E361	Y362	A365	G366	P367	S368	I369	V370	H371	R372	LYS	CYS	PHE																															
N280	S281	I282	R283	K284	C285	D286	I287	D288	I289	R290	K291	D292	L293	Y294	A295	N296	N297	V298	M299	S300	G301	G302	T303	T304	K305	V306	P307	G308	I309	T249	A310	D311	R312	M313	Q314	K315	E316	I317	T318	A319	L320	A321	P322																
Y218	V219	A220	L221	D222	F223	E224	R225	E226	N227	A228	T229	A230	A231	S232	S233	E237	V238	S239	Y240	E241	L242	P243	D244	G245	Q246	V247	I248	T249	T250	G251	N252	E253	R254	F255	R256	C257	P258	E259	L261	T260	F262	Q263	P264	S265	F266	I267	G268	N269	E270	S271	A272	G273	I274	E275	E276	T277	Y279		
D157	G158	V159	T160	H161	N162	V163	P164	I165	Y166	E167	G168	Y169	P172	H173	A174	I175	M176	R177	L178	D179	L180	A181	G182	R183	D184	L185	T186	D187	Y188	L189	M190	R191	I192	L193	T194	E195	R196	G197	Y198	S199	F200	V201	T202	T203	A204	E205	A144	S145	G146	I208	V209	R210	D211	I212	I213	K214	L215	L216	C217
W79	D80	D81	W86	Y91	H92	E93	L94	R95	E100	H101	L104	L105	T106	E107	A108	P109	L110	N111	P112	K113	A114	N115	R116	E117	K118	N119	T120	F124	M132	A135	I136	Q137	A138	V139	L140	S141	Y142	Y143	E206	E207	I208	V209	R210	D211	I212	I213	K214	L215	L216	C217									



## 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	none	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	67/6448 (1.0%)	1.82	117/8729 (1.3%)
1	D	1.77	64/6448 (1.0%)	1.82	114/8729 (1.3%)
1	G	1.77	68/6449 (1.1%)	1.86	118/8732 (1.4%)
1	P	1.79	69/6447 (1.1%)	1.84	120/8726 (1.4%)
2	B	1.22	10/1148 (0.9%)	1.61	16/1548 (1.0%)
2	E	1.22	10/1148 (0.9%)	1.62	16/1548 (1.0%)
2	H	1.22	10/1148 (0.9%)	1.62	16/1548 (1.0%)
2	Q	1.22	10/1148 (0.9%)	1.61	16/1548 (1.0%)
3	C	0.80	0/1136	0.95	4/1525 (0.3%)
3	F	0.80	0/1136	0.95	4/1525 (0.3%)
3	I	0.80	0/1136	0.94	4/1525 (0.3%)
3	R	0.80	0/1136	0.95	4/1525 (0.3%)
4	0	0.89	2/2968 (0.1%)	1.64	52/4023 (1.3%)
4	1	0.89	2/2968 (0.1%)	1.64	51/4023 (1.3%)
4	2	0.89	2/2968 (0.1%)	1.64	52/4023 (1.3%)
4	3	0.89	2/2968 (0.1%)	1.64	51/4023 (1.3%)
4	4	0.89	2/2968 (0.1%)	1.64	52/4023 (1.3%)
4	5	0.89	2/2968 (0.1%)	1.64	52/4023 (1.3%)
4	7	0.89	1/2968 (0.0%)	1.64	51/4023 (1.3%)
4	8	0.89	2/2968 (0.1%)	1.64	51/4023 (1.3%)
4	9	0.89	1/2968 (0.0%)	1.64	52/4023 (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	51/4023 (1.3%)
4	X	0.89	2/2968 (0.1%)	1.64	52/4023 (1.3%)
4	Y	0.89	2/2968 (0.1%)	1.64	52/4023 (1.3%)
4	Z	0.89	2/2968 (0.1%)	1.64	52/4023 (1.3%)
All	All	1.27	334/76480 (0.4%)	1.68	1271/103530 (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	6
1	P	1	6
2	B	0	3
2	E	0	3
2	H	0	3
2	Q	0	3
3	C	0	2
3	F	0	2
3	I	0	2
3	R	0	3
4	0	0	1
4	1	0	1
4	2	0	1
4	3	0	1
4	4	0	1
4	5	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	4	55

The worst 5 of 334 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	649	VAL	CB-CG1	53.26	2.64	1.52
1	P	649	VAL	CB-CG1	53.26	2.64	1.52
1	D	649	VAL	CB-CG1	53.20	2.64	1.52
1	A	649	VAL	CB-CG1	53.19	2.64	1.52
1	D	623	PHE	CB-CG	48.20	2.33	1.51

The worst 5 of 1271 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	637	LYS	O-C-N	-58.54	23.69	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	637	LYS	O-C-N	-58.49	23.77	123.20
1	D	637	LYS	O-C-N	-58.47	23.80	123.20
1	A	637	LYS	O-C-N	-58.47	23.81	123.20
1	P	649	VAL	CG1-CB-CG2	-34.04	56.44	110.90

All (4) 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	P	648	THR	CB

5 of 55 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

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	6757	1530	19
1	D	6797	0	6756	1374	22
1	G	6797	0	6760	1438	0
1	P	6797	0	6766	1428	0
2	B	1127	0	1087	268	0
2	E	1127	0	1089	248	0
2	H	1127	0	1086	254	0
2	Q	1127	0	1088	259	0
3	C	1123	0	1084	188	0
3	F	1123	0	1082	179	0
3	I	1123	0	1084	179	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	R	1123	0	1084	182	0
4	0	2906	0	2855	449	0
4	1	2906	0	2864	251	76
4	2	2906	0	2864	122	573
4	3	2906	0	2864	165	3105
4	4	2906	0	2865	99	3232
4	5	2906	0	2865	98	3404
4	7	2906	0	2866	78	3155
4	8	2906	0	2857	316	3225
4	9	2906	0	2855	335	3464
4	V	2906	0	2851	384	416
4	W	2906	0	2860	148	89
4	X	2906	0	2862	197	0
4	Y	2906	0	2860	166	0
4	Z	2906	0	2862	188	0
All	All	76872	0	75773	7833	10390

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 51.

The worst 5 of 7833 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:H:144:VAL:HG13	2:H:153:ILE:CG1	1.17	1.64
1:A:831:TRP:CH2	2:B:34:ILE:HG23	1.18	1.64
1:G:797:PHE:HD1	3:I:149:VAL:CG1	1.11	1.63
1:D:815:CYS:SG	2:E:92:ASP:HB2	1.30	1.63
2:H:144:VAL:HG13	2:H:153:ILE:CD1	1.22	1.63

The worst 5 of 10390 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)
4:9:212:ILE:CG1	4:5:196:ARG:O[1_556]	0.15	2.05
4:9:186:THR:C	4:5:191:LYS:CA[1_556]	0.18	2.02
4:7:11:ASP:OD1	4:3:305:MET:C[1_556]	0.21	1.99
4:9:209:VAL:CG2	4:5:194:THR:C[1_556]	0.21	1.99
4:7:183:ARG:NH2	4:3:186:THR:OG1[1_556]	0.22	1.98

## 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%)	651 (82%)	112 (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	P	787/840 (94%)	648 (82%)	110 (14%)	29 (4%)	4	38
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	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	R	143/147 (97%)	133 (93%)	10 (7%)	0	100	100
4	0	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	12	56
4	1	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	12	56
4	2	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	12	56
4	3	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	12	56
4	4	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	12	56
4	5	370/375 (99%)	333 (90%)	31 (8%)	6 (2%)	12	56
4	7	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	12	56
4	8	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	12	56
4	9	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	12	56
4	V	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	12	56
4	W	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	12	56
4	X	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	12	56
4	Y	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	12	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	Z	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	12	56
All	All	9480/9778 (97%)	8314 (88%)	942 (10%)	224 (2%)	12	47

5 of 224 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%)	513 (76%)	159 (24%)	1	7
1	D	672/672 (100%)	513 (76%)	159 (24%)	1	7
1	G	672/672 (100%)	512 (76%)	160 (24%)	1	7
1	P	672/672 (100%)	514 (76%)	158 (24%)	1	7
2	B	120/120 (100%)	119 (99%)	1 (1%)	86	94
2	E	120/120 (100%)	120 (100%)	0	100	100
2	H	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	R	117/117 (100%)	112 (96%)	5 (4%)	35	70
4	0	315/318 (99%)	269 (85%)	46 (15%)	4	24
4	1	315/318 (99%)	269 (85%)	46 (15%)	4	24
4	2	315/318 (99%)	269 (85%)	46 (15%)	4	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	3	315/318 (99%)	268 (85%)	47 (15%)	4	23
4	4	315/318 (99%)	269 (85%)	46 (15%)	4	24
4	5	315/318 (99%)	269 (85%)	46 (15%)	4	24
4	7	315/318 (99%)	268 (85%)	47 (15%)	4	23
4	8	315/318 (99%)	268 (85%)	47 (15%)	4	23
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%)	268 (85%)	47 (15%)	4	23
4	X	315/318 (99%)	268 (85%)	47 (15%)	4	23
4	Y	315/318 (99%)	269 (85%)	46 (15%)	4	24
4	Z	315/318 (99%)	268 (85%)	47 (15%)	4	23
All	All	8046/8088 (100%)	6735 (84%)	1311 (16%)	6	20

5 of 1311 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	524	GLU
4	8	283	MET
4	3	349	LEU
1	P	621	LEU
4	7	80	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 181 such sidechains are listed below:

Mol	Chain	Res	Type
1	P	188	ASN
3	R	39	GLN
4	3	263	GLN
1	P	253	HIS
1	P	484	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.



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

180 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	1.33	1 (12%)	9,11,13	0.81	0
1	MLY	A	19	1	8,10,11	1.15	1 (12%)	9,11,13	0.68	0
1	MLY	A	190	1	8,10,11	1.09	1 (12%)	9,11,13	0.70	0
1	MLY	A	236	1	8,10,11	0.38	0	9,11,13	1.34	1 (11%)
1	MLY	A	248	1	8,10,11	0.75	0	9,11,13	0.92	1 (11%)
1	MLY	A	272	1	8,10,11	1.02	1 (12%)	9,11,13	0.56	0
1	MLY	A	295	1	8,10,11	0.73	0	9,11,13	0.46	0
1	MLY	A	296	1	8,10,11	0.59	0	9,11,13	0.76	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	0.80	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	0.65	0	9,11,13	0.60	0
1	MLY	A	369	1	8,10,11	0.54	0	9,11,13	0.92	1 (11%)
1	MLY	A	385	1	8,10,11	1.00	1 (12%)	9,11,13	0.55	0
1	MLY	A	415	1	8,10,11	0.74	0	9,11,13	0.44	0
1	MLY	A	431	1	8,10,11	0.48	0	9,11,13	0.76	0
1	MLY	A	436	1	8,10,11	1.05	1 (12%)	9,11,13	0.58	0
1	MLY	A	486	1	8,10,11	0.36	0	9,11,13	0.60	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	0.49	0
1	MLY	A	505	1	8,10,11	0.90	1 (12%)	9,11,13	0.39	0
1	MLY	A	528	1	8,10,11	0.80	0	9,11,13	1.16	1 (11%)
1	MLY	A	55	1	8,10,11	0.65	0	9,11,13	0.96	0
1	MLY	A	551	1	8,10,11	0.51	0	9,11,13	0.64	0
1	MLY	A	553	1,4	8,10,11	0.63	0	9,11,13	0.59	0
1	MLY	A	59	1	8,10,11	0.77	0	9,11,13	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	MLY	A	598	1	8,10,11	0.87	1 (12%)	9,11,13	0.73	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	0.49	0	9,11,13	0.91	0
1	MLY	A	617	1	8,10,11	0.87	1 (12%)	9,11,13	0.46	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	0.58	0	9,11,13	0.95	0
1	MLY	A	681	1	8,10,11	0.60	0	9,11,13	0.63	0
1	MLY	A	764	1	8,10,11	0.68	0	9,11,13	0.56	0
1	MLY	A	768	1	8,10,11	0.65	0	9,11,13	0.85	0
1	MLY	A	782	1	8,10,11	0.50	0	9,11,13	0.93	1 (11%)
1	MLY	A	827	1	8,10,11	0.66	0	9,11,13	0.94	1 (11%)
1	MLY	A	833	1	8,10,11	0.99	1 (12%)	9,11,13	0.58	0
1	MLY	A	837	1	8,10,11	0.55	0	9,11,13	0.56	0
1	MLY	A	839	1	8,10,11	0.67	0	9,11,13	0.80	0
1	MLY	A	84	1	8,10,11	0.46	0	9,11,13	0.80	0
1	MLY	A	87	1	8,10,11	1.14	1 (12%)	9,11,13	0.68	0
1	MLY	D	107	1	8,10,11	0.48	0	9,11,13	0.66	0
1	MLY	D	130	1	8,10,11	0.58	0	9,11,13	1.06	1 (11%)
1	MLY	D	138	1	8,10,11	1.39	1 (12%)	9,11,13	0.82	0
1	MLY	D	19	1	8,10,11	1.21	1 (12%)	9,11,13	0.70	0
1	MLY	D	190	1	8,10,11	1.05	1 (12%)	9,11,13	0.70	0
1	MLY	D	236	1	8,10,11	0.37	0	9,11,13	1.32	1 (11%)
1	MLY	D	248	1	8,10,11	0.71	0	9,11,13	0.93	1 (11%)
1	MLY	D	272	1	8,10,11	1.00	1 (12%)	9,11,13	0.58	0
1	MLY	D	295	1	8,10,11	0.71	0	9,11,13	0.47	0
1	MLY	D	296	1	8,10,11	0.61	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	0.79	0	9,11,13	0.80	0
1	MLY	D	35	1	8,10,11	0.59	0	9,11,13	0.68	0
1	MLY	D	353	1	8,10,11	0.86	0	9,11,13	0.78	0
1	MLY	D	367	1	8,10,11	0.65	0	9,11,13	0.60	0
1	MLY	D	369	1	8,10,11	0.55	0	9,11,13	0.92	1 (11%)
1	MLY	D	385	1	8,10,11	1.00	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	0.47	0	9,11,13	0.78	0
1	MLY	D	436	1	8,10,11	1.11	1 (12%)	9,11,13	0.57	0
1	MLY	D	486	1	8,10,11	0.36	0	9,11,13	0.61	0
1	MLY	D	49	1	8,10,11	1.07	1 (12%)	9,11,13	1.00	0
1	MLY	D	504	1	8,10,11	0.80	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	D	505	1	8,10,11	0.85	1 (12%)	9,11,13	0.40	0
1	MLY	D	528	1	8,10,11	0.81	0	9,11,13	1.17	1 (11%)
1	MLY	D	55	1	8,10,11	0.66	0	9,11,13	0.98	0
1	MLY	D	551	1	8,10,11	0.51	0	9,11,13	0.65	0
1	MLY	D	553	1,4	8,10,11	0.64	0	9,11,13	0.59	0
1	MLY	D	59	1	8,10,11	0.78	0	9,11,13	0.77	0
1	MLY	D	598	1	8,10,11	0.87	1 (12%)	9,11,13	0.70	0
1	MLY	D	600	1	8,10,11	0.51	0	9,11,13	0.47	0
1	MLY	D	613	1	8,10,11	0.50	0	9,11,13	0.91	0
1	MLY	D	617	1	8,10,11	0.93	1 (12%)	9,11,13	0.47	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	0.94	0
1	MLY	D	681	1	8,10,11	0.63	0	9,11,13	0.66	0
1	MLY	D	764	1	8,10,11	0.67	0	9,11,13	0.56	0
1	MLY	D	768	1	8,10,11	0.62	0	9,11,13	0.87	0
1	MLY	D	782	1	8,10,11	0.48	0	9,11,13	0.92	1 (11%)
1	MLY	D	827	1	8,10,11	0.62	0	9,11,13	0.95	1 (11%)
1	MLY	D	833	1	8,10,11	0.96	1 (12%)	9,11,13	0.58	0
1	MLY	D	837	1	8,10,11	0.56	0	9,11,13	0.59	0
1	MLY	D	839	1	8,10,11	0.69	0	9,11,13	0.78	0
1	MLY	D	84	1	8,10,11	0.48	0	9,11,13	0.80	0
1	MLY	D	87	1	8,10,11	1.14	1 (12%)	9,11,13	0.69	0
1	MLY	G	107	1	8,10,11	0.46	0	9,11,13	0.68	0
1	MLY	G	130	1	8,10,11	0.58	0	9,11,13	1.09	1 (11%)
1	MLY	G	138	1	8,10,11	1.35	1 (12%)	9,11,13	0.80	0
1	MLY	G	19	1	8,10,11	1.18	1 (12%)	9,11,13	0.70	0
1	MLY	G	190	1	8,10,11	1.09	1 (12%)	9,11,13	0.69	0
1	MLY	G	236	1	8,10,11	0.37	0	9,11,13	1.32	1 (11%)
1	MLY	G	248	1	8,10,11	0.72	0	9,11,13	0.92	1 (11%)
1	MLY	G	272	1	8,10,11	0.99	1 (12%)	9,11,13	0.55	0
1	MLY	G	295	1	8,10,11	0.73	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	0.59	0	9,11,13	0.68	0
1	MLY	G	353	1	8,10,11	0.86	0	9,11,13	0.80	0
1	MLY	G	367	1	8,10,11	0.66	0	9,11,13	0.61	0
1	MLY	G	369	1	8,10,11	0.53	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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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	0.48	0	9,11,13	0.77	0
1	MLY	G	436	1	8,10,11	1.08	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	1.09	1 (12%)	9,11,13	0.97	0
1	MLY	G	504	1	8,10,11	0.78	0	9,11,13	0.47	0
1	MLY	G	505	1	8,10,11	0.88	1 (12%)	9,11,13	0.40	0
1	MLY	G	528	1	8,10,11	0.81	0	9,11,13	1.17	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	0.51	0	9,11,13	0.66	0
1	MLY	G	553	1,4	8,10,11	0.63	0	9,11,13	0.59	0
1	MLY	G	59	1	8,10,11	0.72	0	9,11,13	0.77	0
1	MLY	G	598	1	8,10,11	0.84	1 (12%)	9,11,13	0.72	0
1	MLY	G	600	1	8,10,11	0.53	0	9,11,13	0.46	0
1	MLY	G	613	1	8,10,11	0.51	0	9,11,13	0.92	0
1	MLY	G	617	1	8,10,11	0.90	1 (12%)	9,11,13	0.45	0
1	MLY	G	63	1	8,10,11	0.80	0	9,11,13	0.94	0
1	MLY	G	659	1	8,10,11	0.57	0	9,11,13	0.93	0
1	MLY	G	681	1	8,10,11	0.64	0	9,11,13	0.64	0
1	MLY	G	764	1	8,10,11	0.64	0	9,11,13	0.57	0
1	MLY	G	768	1	8,10,11	0.61	0	9,11,13	0.88	0
1	MLY	G	782	1	8,10,11	0.47	0	9,11,13	0.93	1 (11%)
1	MLY	G	827	1	8,10,11	0.66	0	9,11,13	0.95	1 (11%)
1	MLY	G	833	1	8,10,11	0.98	1 (12%)	9,11,13	0.60	0
1	MLY	G	837	1	8,10,11	0.54	0	9,11,13	0.56	0
1	MLY	G	839	1	8,10,11	0.69	0	9,11,13	0.78	0
1	MLY	G	84	1	8,10,11	0.46	0	9,11,13	0.80	0
1	MLY	G	87	1	8,10,11	1.18	1 (12%)	9,11,13	0.68	0
1	MLY	P	107	1	8,10,11	0.45	0	9,11,13	0.67	0
1	MLY	P	130	1	8,10,11	0.55	0	9,11,13	1.07	1 (11%)
1	MLY	P	138	1	8,10,11	1.34	1 (12%)	9,11,13	0.80	0
1	MLY	P	19	1	8,10,11	1.18	1 (12%)	9,11,13	0.70	0
1	MLY	P	190	1	8,10,11	1.11	1 (12%)	9,11,13	0.69	0
1	MLY	P	236	1	8,10,11	0.38	0	9,11,13	1.32	1 (11%)
1	MLY	P	248	1	8,10,11	0.74	0	9,11,13	0.94	1 (11%)
1	MLY	P	272	1	8,10,11	1.05	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	0.65	0	9,11,13	0.79	1 (11%)
1	MLY	P	30	1	8,10,11	0.68	0	9,11,13	0.83	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	MLY	P	348	1	8,10,11	0.77	0	9,11,13	0.79	0
1	MLY	P	35	1	8,10,11	0.59	0	9,11,13	0.68	0
1	MLY	P	353	1	8,10,11	0.87	0	9,11,13	0.79	0
1	MLY	P	367	1	8,10,11	0.64	0	9,11,13	0.61	0
1	MLY	P	369	1	8,10,11	0.54	0	9,11,13	0.93	1 (11%)
1	MLY	P	385	1	8,10,11	1.01	1 (12%)	9,11,13	0.55	0
1	MLY	P	415	1	8,10,11	0.77	0	9,11,13	0.44	0
1	MLY	P	431	1	8,10,11	0.45	0	9,11,13	0.77	0
1	MLY	P	436	1	8,10,11	1.10	1 (12%)	9,11,13	0.55	0
1	MLY	P	486	1	8,10,11	0.33	0	9,11,13	0.60	0
1	MLY	P	49	1	8,10,11	1.09	1 (12%)	9,11,13	1.00	0
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	0.89	1 (12%)	9,11,13	0.39	0
1	MLY	P	528	1	8,10,11	0.80	0	9,11,13	1.15	1 (11%)
1	MLY	P	55	1	8,10,11	0.66	0	9,11,13	0.98	0
1	MLY	P	551	1	8,10,11	0.50	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	0.79	0	9,11,13	0.77	0
1	MLY	P	598	1	8,10,11	0.84	1 (12%)	9,11,13	0.70	0
1	MLY	P	600	1	8,10,11	0.54	0	9,11,13	0.48	0
1	MLY	P	613	1	8,10,11	0.50	0	9,11,13	0.94	0
1	MLY	P	617	1	8,10,11	0.93	1 (12%)	9,11,13	0.45	0
1	MLY	P	63	1	8,10,11	0.79	0	9,11,13	0.95	0
1	MLY	P	659	1	8,10,11	0.51	0	9,11,13	0.93	0
1	MLY	P	681	1	8,10,11	0.65	0	9,11,13	0.64	0
1	MLY	P	764	1	8,10,11	0.63	0	9,11,13	0.58	0
1	MLY	P	768	1	8,10,11	0.64	0	9,11,13	0.87	0
1	MLY	P	782	1	8,10,11	0.50	0	9,11,13	0.96	1 (11%)
1	MLY	P	827	1	8,10,11	0.66	0	9,11,13	0.93	1 (11%)
1	MLY	P	833	1	8,10,11	1.04	1 (12%)	9,11,13	0.57	0
1	MLY	P	837	1	8,10,11	0.55	0	9,11,13	0.58	0
1	MLY	P	839	1	8,10,11	0.65	0	9,11,13	0.77	0
1	MLY	P	84	1	8,10,11	0.46	0	9,11,13	0.80	0
1	MLY	P	87	1	8,10,11	1.18	1 (12%)	9,11,13	0.68	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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	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
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

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	138	MLY	CB-CA	-3.66	1.48	1.53
1	G	138	MLY	CB-CA	-3.53	1.48	1.53
1	P	138	MLY	CB-CA	-3.50	1.48	1.53
1	A	138	MLY	CB-CA	-3.47	1.48	1.53
1	D	19	MLY	CB-CA	-3.13	1.49	1.53

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	236	MLY	O-C-CA	-3.27	116.96	125.72
1	D	236	MLY	O-C-CA	-3.24	117.04	125.72
1	G	236	MLY	O-C-CA	-3.23	117.06	125.72
1	P	236	MLY	O-C-CA	-3.23	117.07	125.72
1	D	528	MLY	O-C-CA	-3.10	117.41	125.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

122 monomers are involved in 482 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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	295	MLY	5	0
1	A	296	MLY	3	0
1	A	30	MLY	1	0
1	A	348	MLY	6	0
1	A	369	MLY	1	0
1	A	415	MLY	1	0
1	A	436	MLY	3	0
1	A	486	MLY	3	0
1	A	49	MLY	3	0
1	A	504	MLY	9	0
1	A	505	MLY	38	0
1	A	528	MLY	3	0
1	A	55	MLY	1	0
1	A	551	MLY	2	0
1	A	553	MLY	16	3
1	A	59	MLY	2	0
1	A	598	MLY	1	0
1	A	600	MLY	1	0
1	A	617	MLY	1	0
1	A	63	MLY	4	0
1	A	659	MLY	2	0
1	A	764	MLY	7	0
1	A	768	MLY	14	0
1	A	782	MLY	2	0
1	A	837	MLY	1	0
1	A	839	MLY	15	0
1	A	84	MLY	2	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	415	MLY	1	0
1	D	436	MLY	3	0
1	D	486	MLY	3	0
1	D	49	MLY	3	0
1	D	528	MLY	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	55	MLY	1	0
1	D	551	MLY	2	0
1	D	553	MLY	17	1
1	D	59	MLY	2	0
1	D	598	MLY	1	0
1	D	600	MLY	1	0
1	D	617	MLY	1	0
1	D	63	MLY	3	0
1	D	659	MLY	2	0
1	D	764	MLY	8	0
1	D	782	MLY	16	0
1	D	837	MLY	1	0
1	D	839	MLY	19	0
1	D	87	MLY	3	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	6	0
1	G	369	MLY	1	0
1	G	415	MLY	1	0
1	G	436	MLY	3	0
1	G	486	MLY	3	0
1	G	49	MLY	3	0
1	G	528	MLY	2	0
1	G	55	MLY	1	0
1	G	553	MLY	27	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	4	0
1	G	659	MLY	2	0
1	G	764	MLY	3	0
1	G	768	MLY	34	0
1	G	782	MLY	1	0
1	G	827	MLY	2	0
1	G	837	MLY	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	G	839	MLY	4	0
1	G	84	MLY	5	0
1	G	87	MLY	2	0
1	P	107	MLY	3	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	3	0
1	P	30	MLY	1	0
1	P	348	MLY	5	0
1	P	415	MLY	1	0
1	P	436	MLY	2	0
1	P	486	MLY	3	0
1	P	49	MLY	2	0
1	P	528	MLY	2	0
1	P	55	MLY	1	0
1	P	553	MLY	2	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	1	0
1	P	764	MLY	17	0
1	P	782	MLY	3	0
1	P	827	MLY	4	0
1	P	833	MLY	1	0
1	P	837	MLY	1	0
1	P	839	MLY	7	0
1	P	84	MLY	1	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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.