



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:17 PM BST

PDB ID : 1O1E  
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 : 2002-11-19  
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>

---

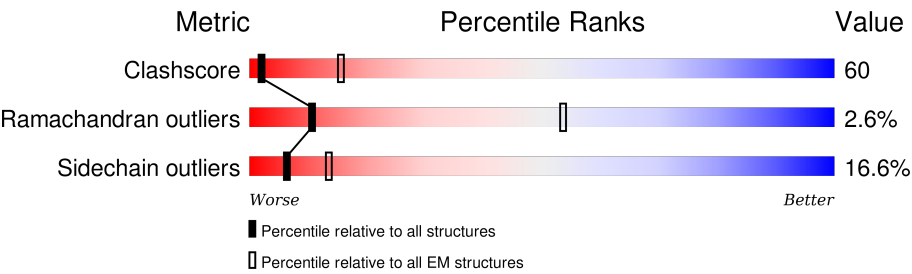
MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk27241

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 70.00 Å.

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




















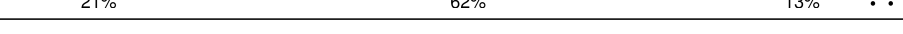
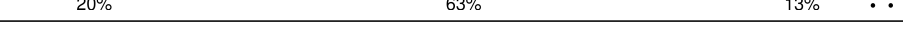




Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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% 51% 19% .
1	D	840	27% 51% 18% .
1	G	840	25% 51% 19% .
1	J	840	26% 50% 20% .
1	M	840	25% 51% 19% .
1	P	840	26% 51% 19% 5%
2	B	145	67% 24% 6% .
2	E	145	63% 28% 6% .
2	H	145	58% 33% 6% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	K	145	 60% 30% 6% .
2	N	145	 66% 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	 60% 38% .
3	O	147	 59% 38% .
3	R	147	 59% 38% .
4	1	375	 57% 31% 9% ..
4	2	375	 59% 32% 6% ..
4	3	375	 53% 36% 8% ..
4	4	375	 29% 55% 12% ..
4	5	375	 23% 60% 12% ..
4	6	375	 26% 59% 11% ..
4	7	375	 27% 56% 12% ..
4	8	375	 21% 62% 13% ..
4	9	375	 20% 63% 13% ..
4	V	375	 50% 39% 8% ..
4	W	375	 54% 35% 8% ..
4	X	375	 61% 30% 7% ..
4	Y	375	 61% 30% 7% ..
4	Z	375	 58% 31% 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	768	-	-	X	-
1	MLY	A	782	-	-	X	-
1	MLY	A	837	-	-	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	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	M	84	-	-	X	-
1	MLY	P	782	-	-	X	-
1	MLY	P	839	-	-	X	-
1	MLY	P	84	-	-	X	-

## 2 Entry composition

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

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

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

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

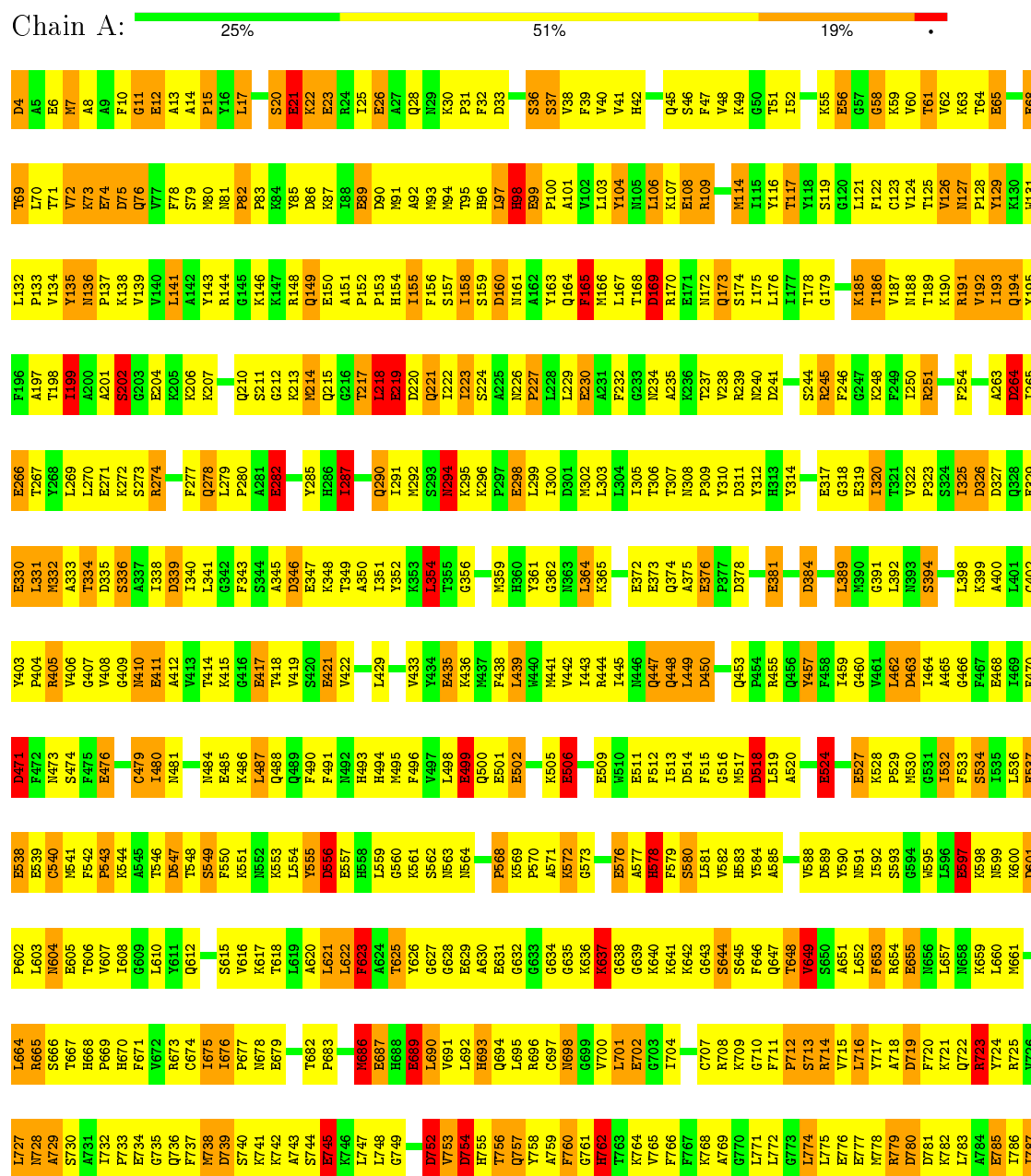
- Molecule 4 is a protein called SKELETAL MUSCLE ACTIN.

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

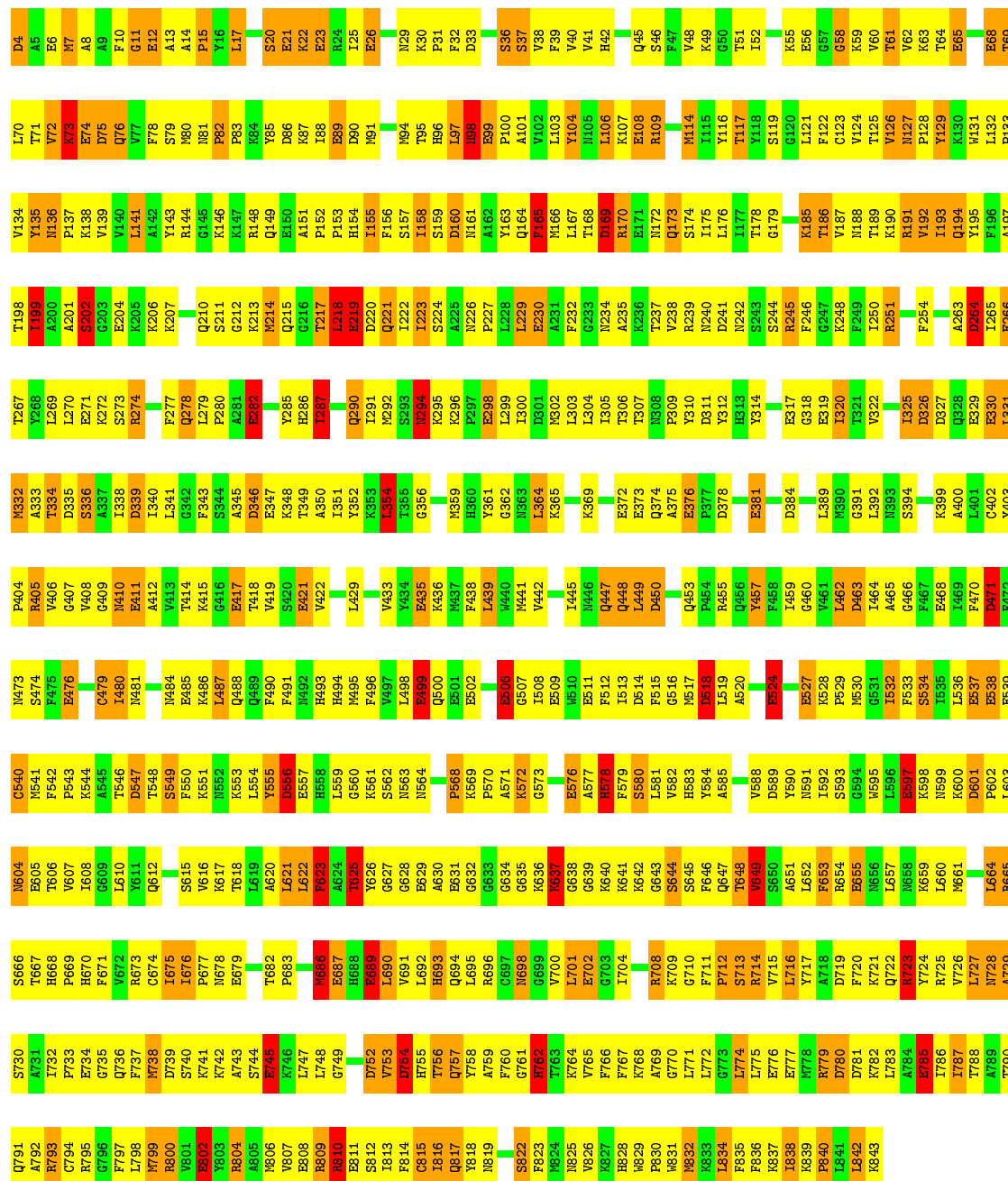
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric 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





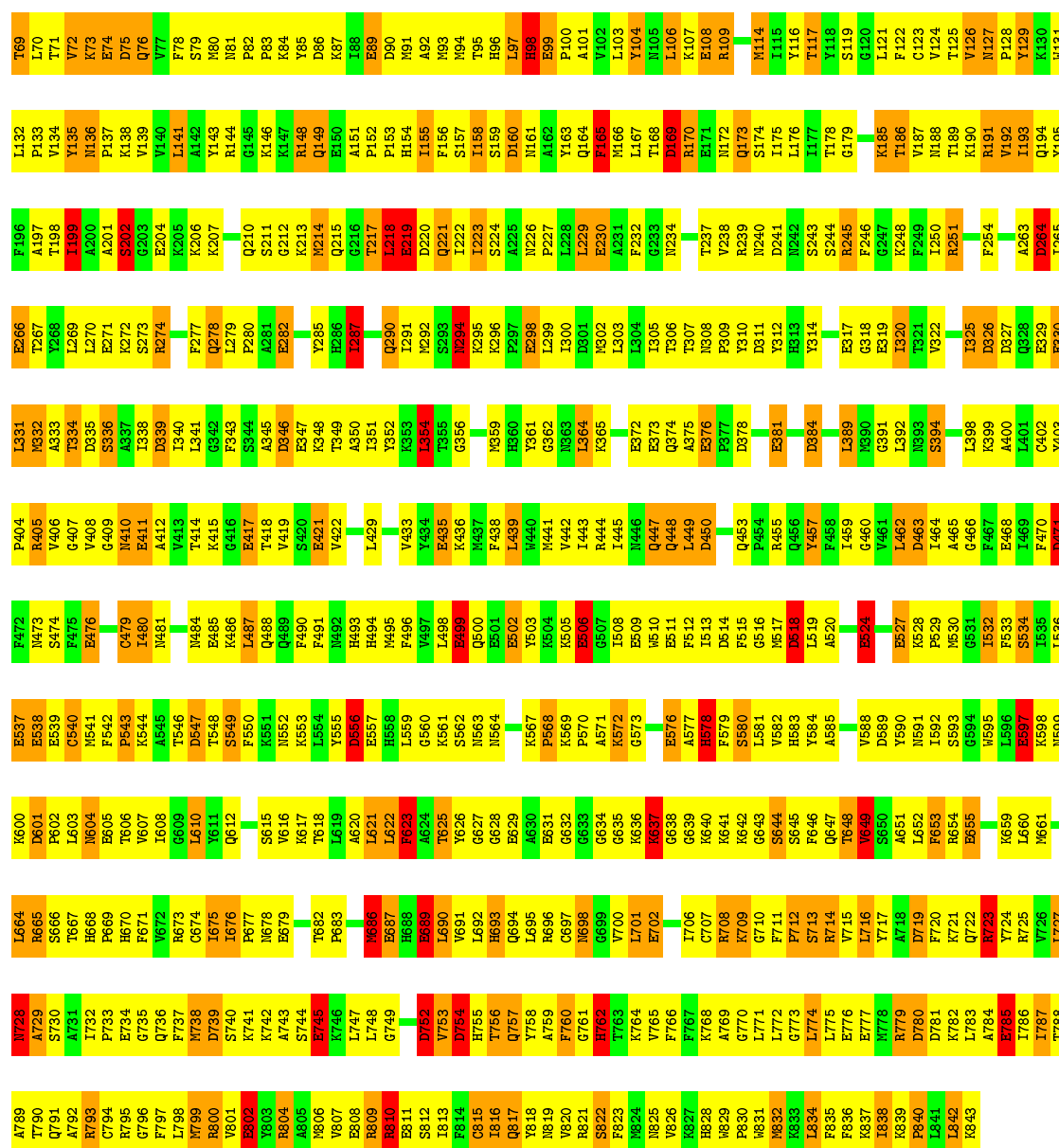
## • Molecule 1: SKELETAL MUSCLE MYOSIN II

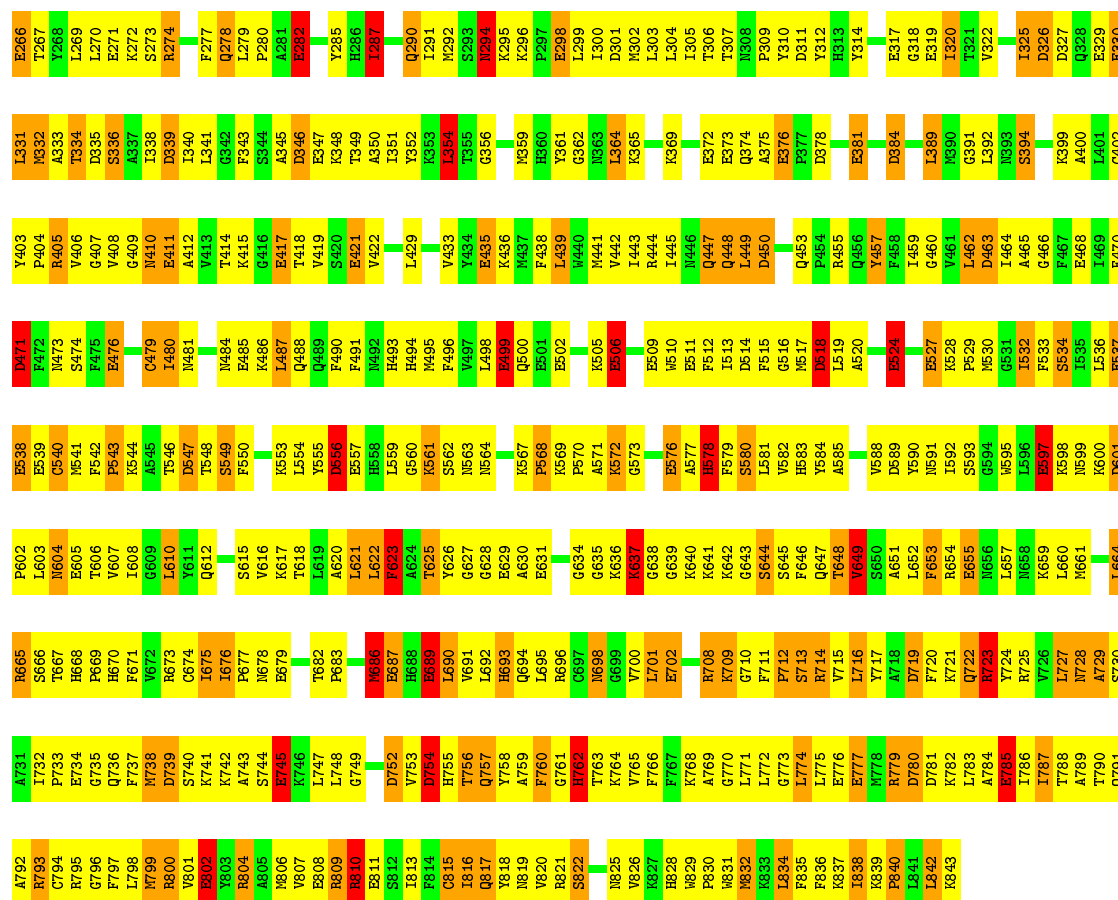


## • Molecule 1: SKELETAL MUSCLE MYOSIN II

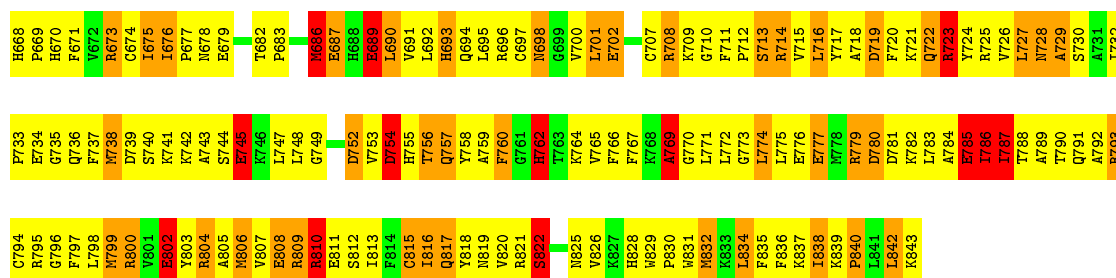




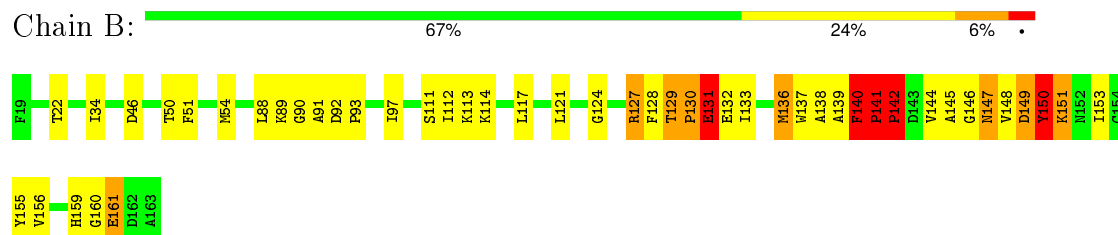




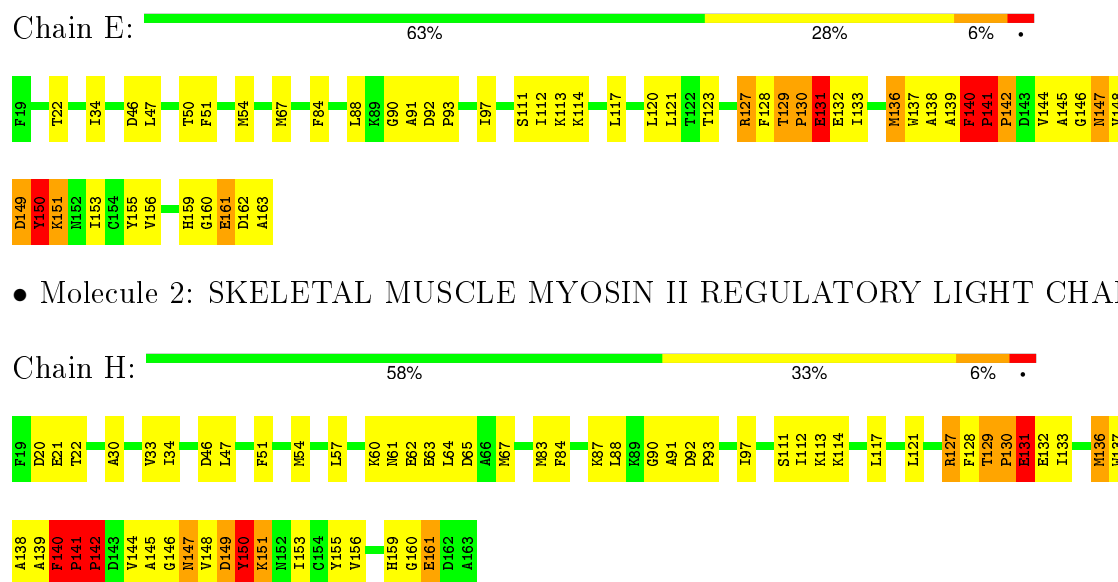




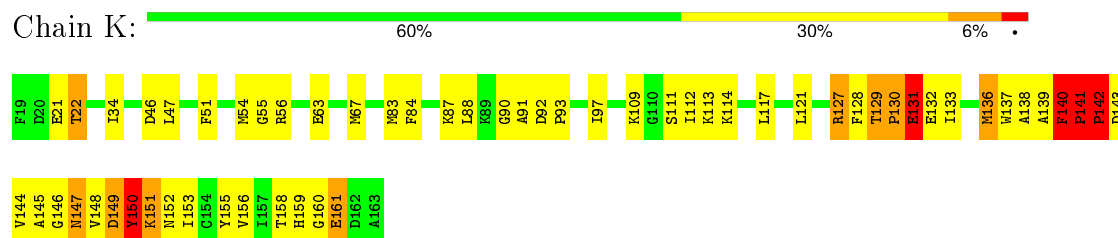
• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN



• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

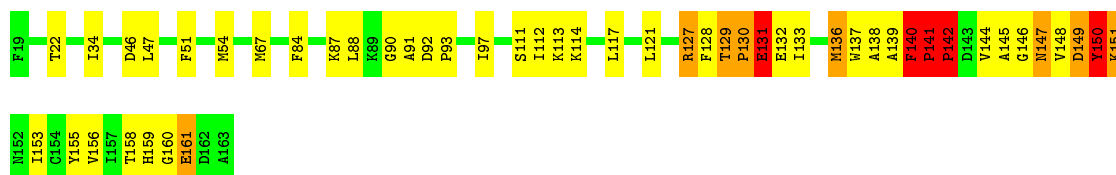


• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN



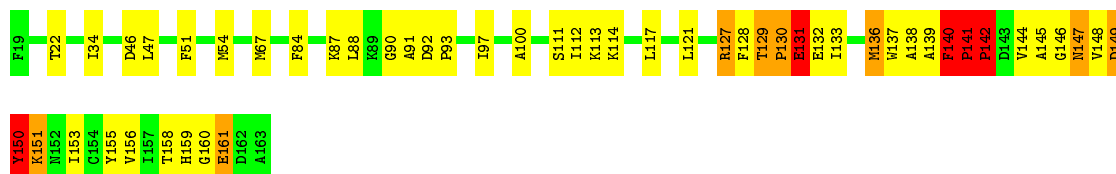
• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN





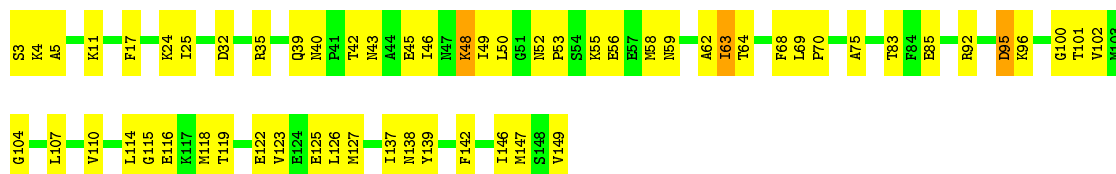
• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

Chain Q: 65% 26% 6%



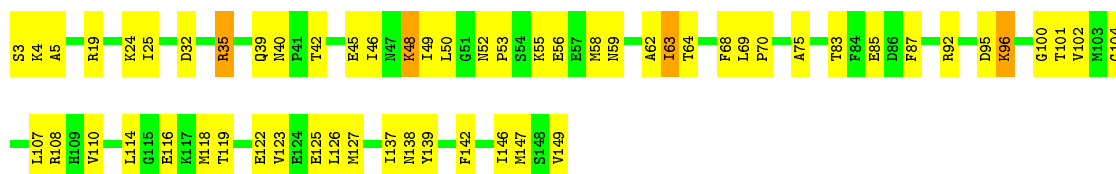
• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN

Chain C: 60% 38%



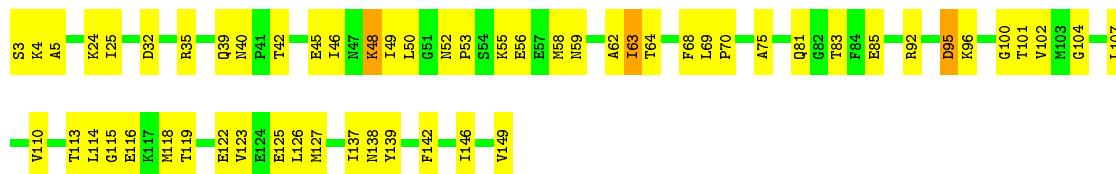
• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN

Chain F: 61% 37%



• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN

Chain I: 61% 37%



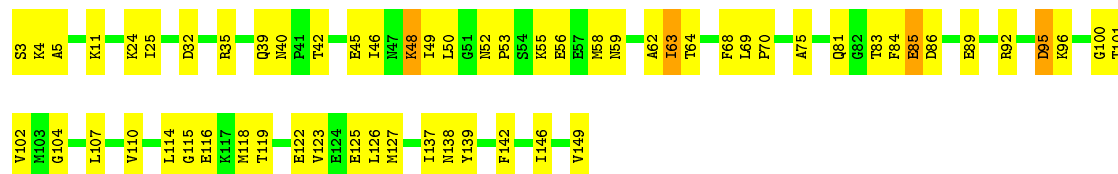
• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN

Chain L: 60% 38%

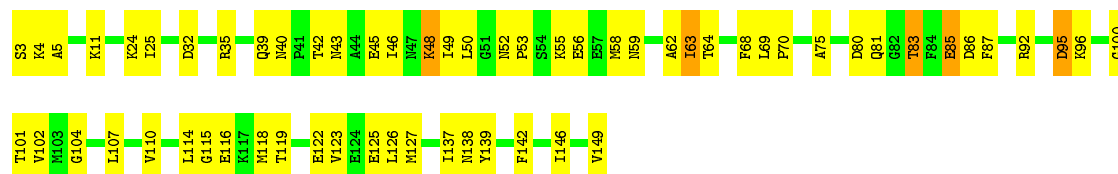




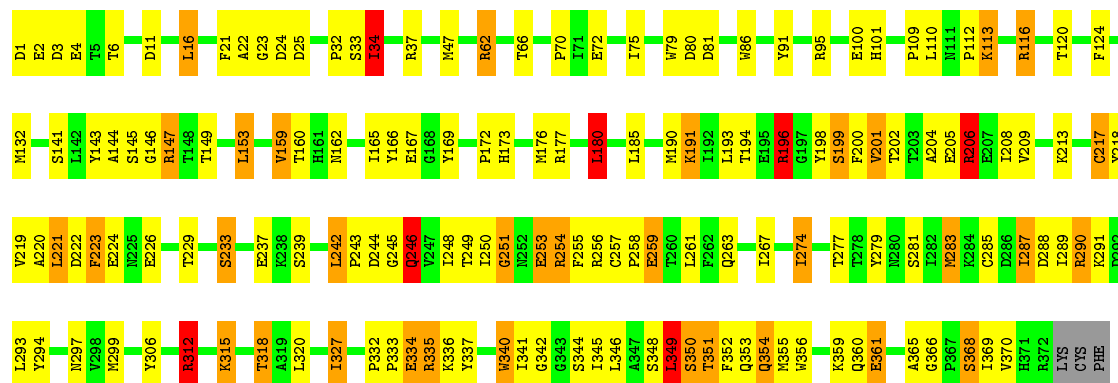
• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN



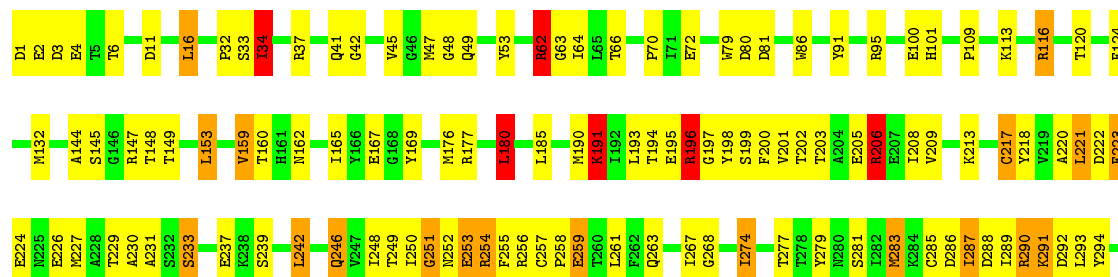
• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN



• Molecule 4: SKELETAL MUSCLE ACTIN

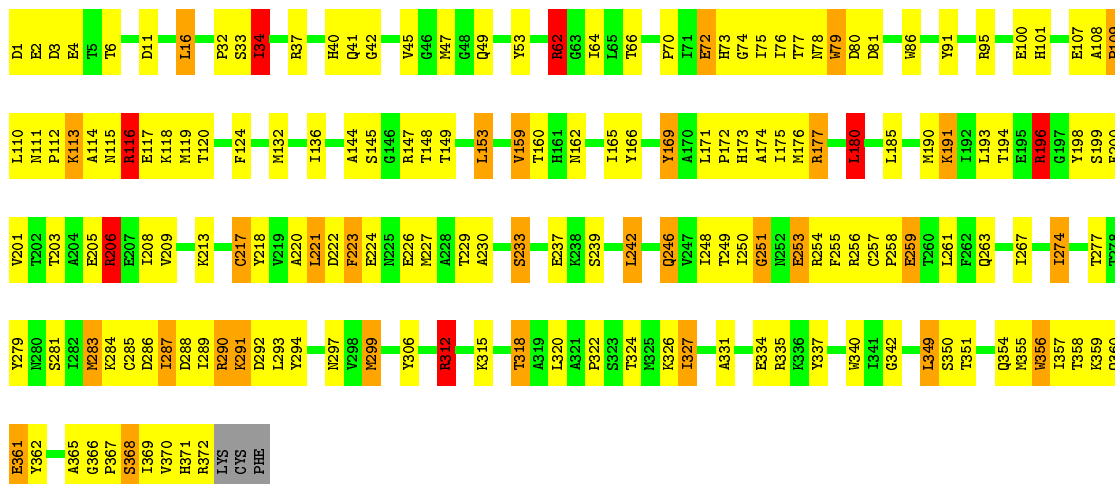


• Molecule 4: SKELETAL MUSCLE ACTIN



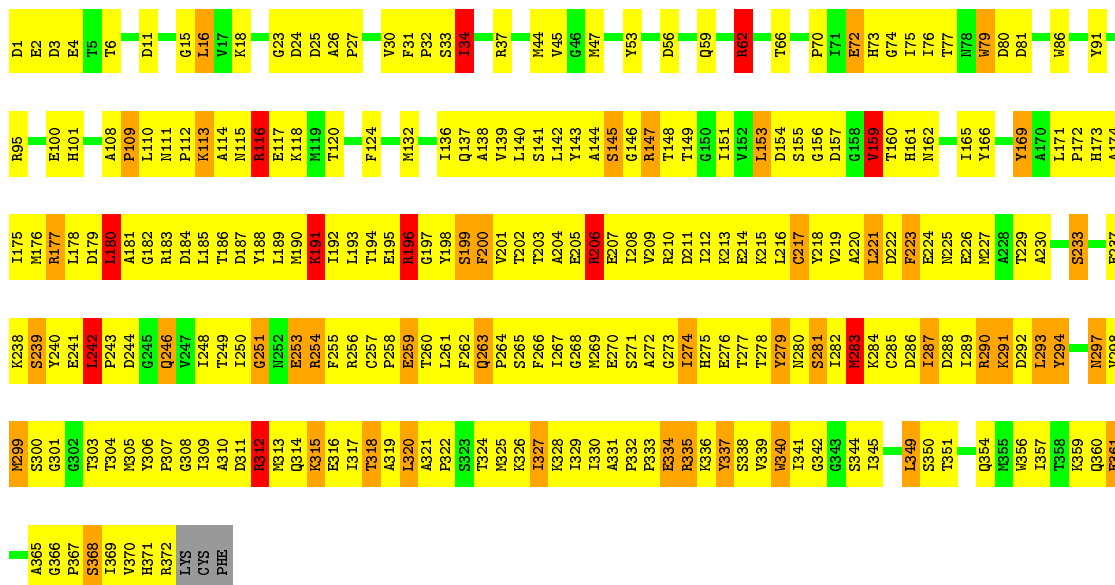
- Molecule 4: SKELETAL MUSCLE ACTIN

Chain 3:  53% 36% 8% 3%



- Molecule 4: SKELETAL MUSCLE ACTIN

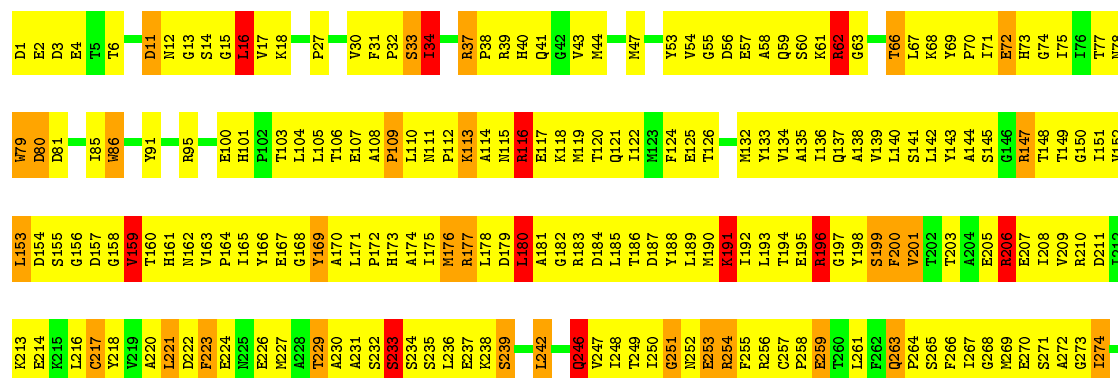
Chain 4:  29% 55% 12% 4%



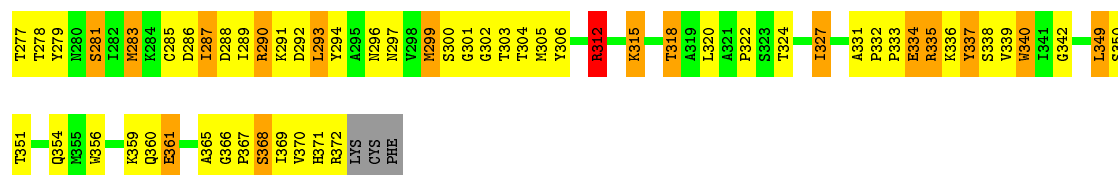
- Molecule 4: SKELETAL MUSCLE ACTIN

Chain 5:  23% 60% 12% . . .



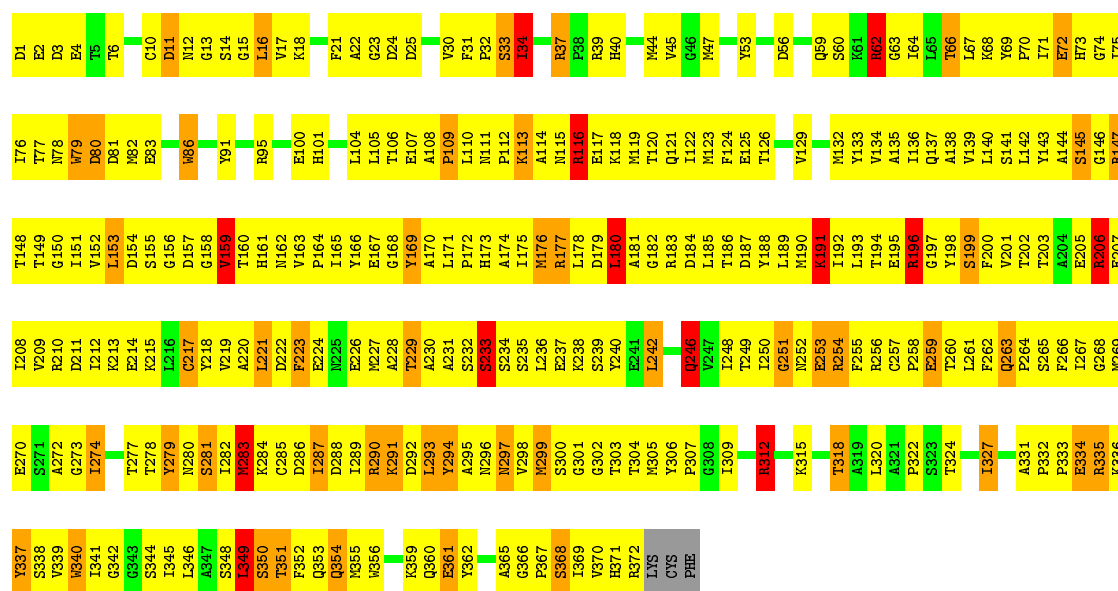






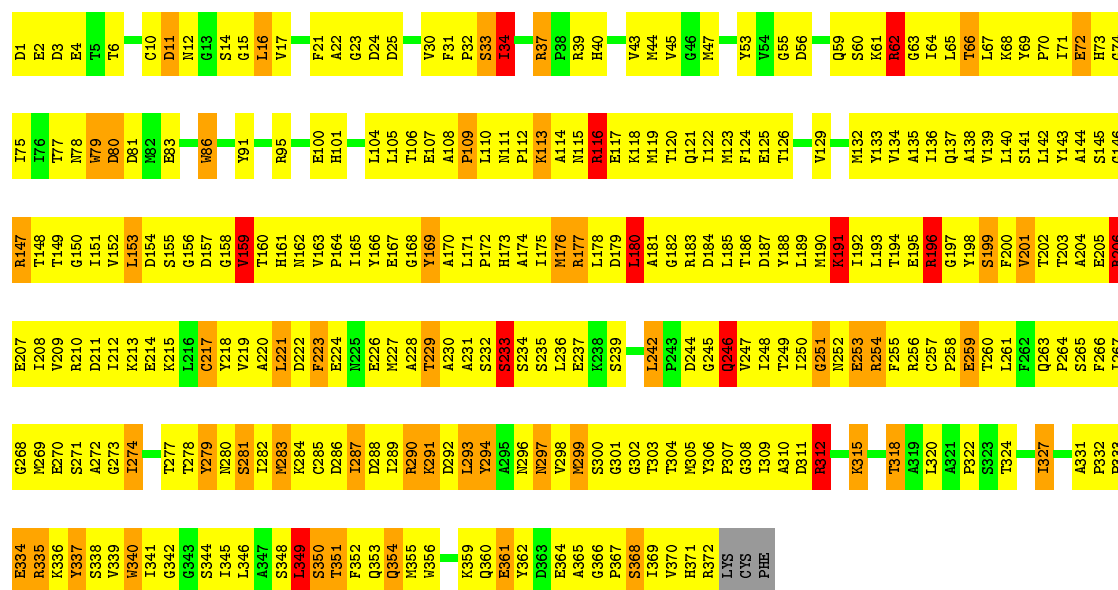
# Molecule 4: SKELETAL MUSCLE ACTIN

Chain 8:

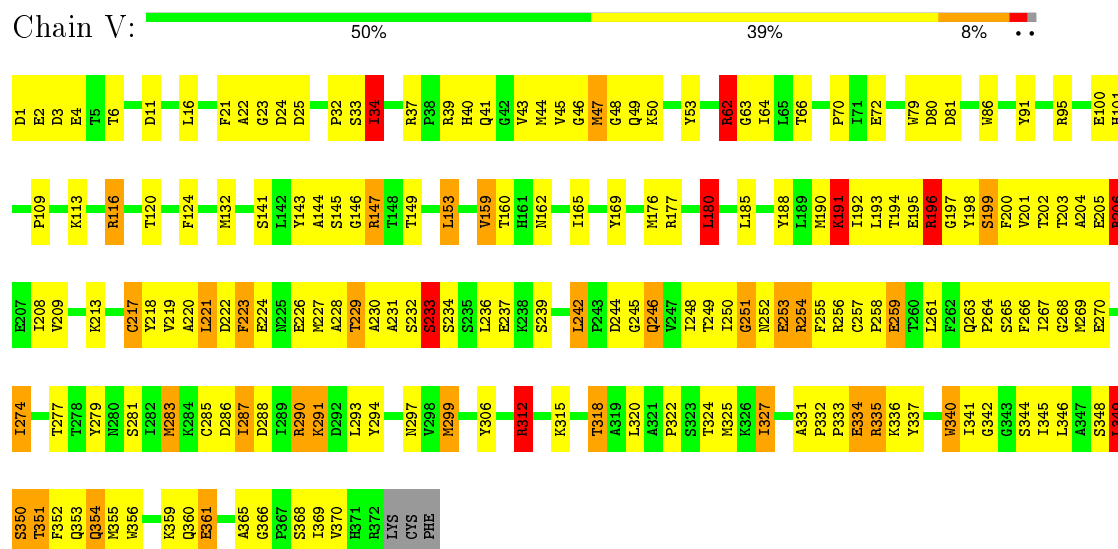


# Molecule 4: SKELETAL MUSCLE ACTIN

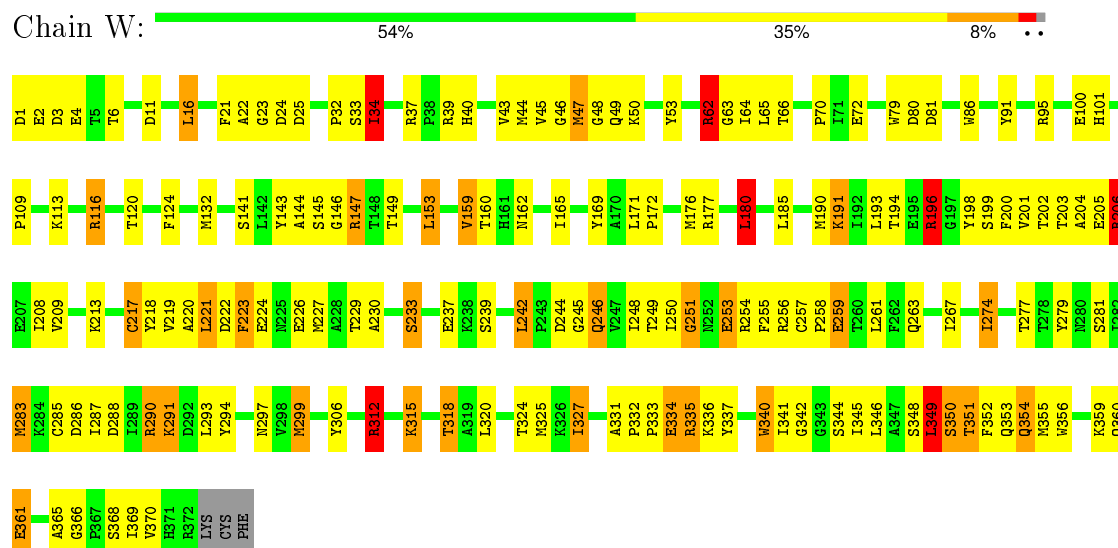
Chain 9:



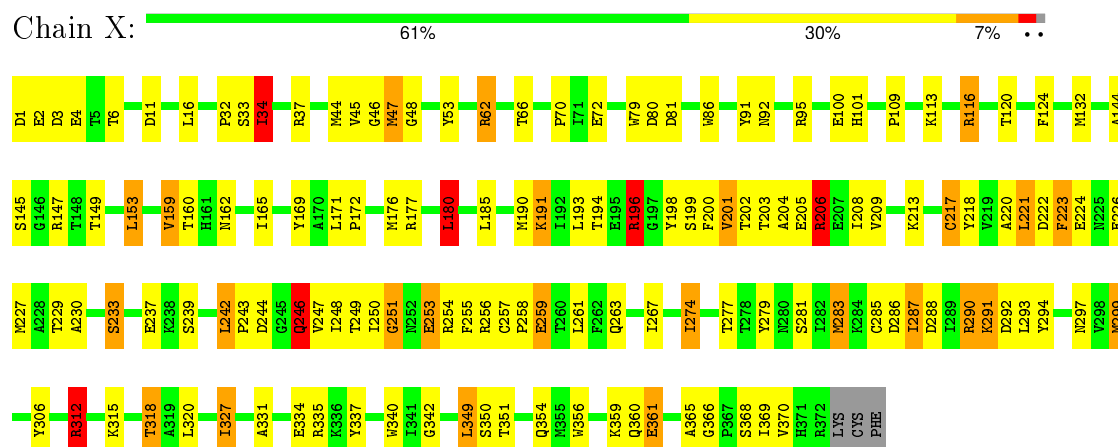
# Molecule 4: SKELETAL MUSCLE ACTIN

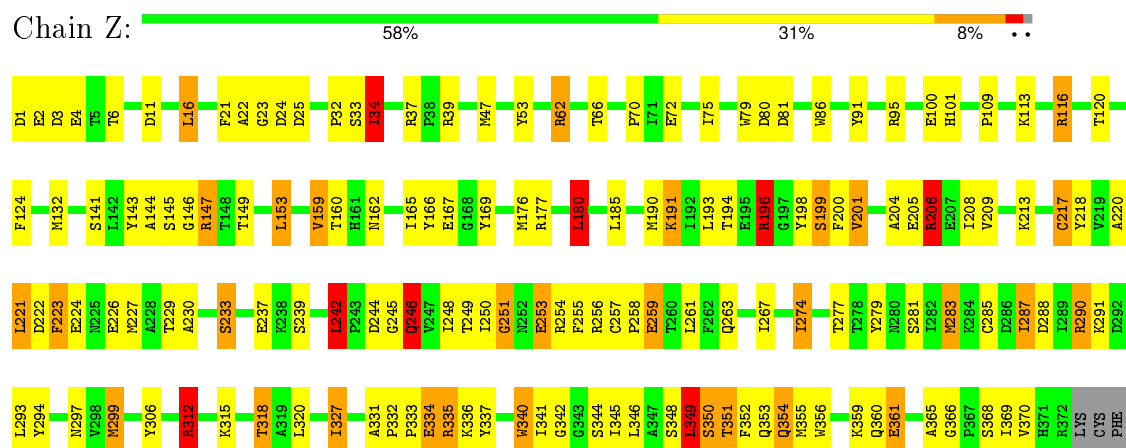


• Molecule 4: SKELETAL MUSCLE ACTIN



• Molecule 4: SKELETAL MUSCLE ACTIN





## 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	67/6448 (1.0%)	1.82	116/8729 (1.3%)
1	D	1.77	64/6448 (1.0%)	1.82	115/8729 (1.3%)
1	G	1.77	66/6449 (1.0%)	1.82	117/8732 (1.3%)
1	J	1.77	67/6449 (1.0%)	1.87	119/8732 (1.4%)
1	M	1.79	68/6449 (1.1%)	1.91	121/8732 (1.4%)
1	P	1.79	69/6449 (1.1%)	1.90	124/8732 (1.4%)
2	B	1.22	10/1148 (0.9%)	1.61	16/1548 (1.0%)
2	E	1.22	10/1148 (0.9%)	1.61	16/1548 (1.0%)
2	H	1.22	9/1148 (0.8%)	1.62	16/1548 (1.0%)
2	K	1.22	10/1148 (0.9%)	1.61	16/1548 (1.0%)
2	N	1.22	10/1148 (0.9%)	1.61	16/1548 (1.0%)
2	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	0.95	4/1525 (0.3%)
3	L	0.79	0/1136	0.94	4/1525 (0.3%)
3	O	0.79	0/1136	0.94	4/1525 (0.3%)
3	R	0.79	0/1136	0.95	4/1525 (0.3%)
4	1	0.89	2/2968 (0.1%)	1.64	51/4023 (1.3%)
4	2	0.89	1/2968 (0.0%)	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	51/4023 (1.3%)
4	5	0.89	2/2968 (0.1%)	1.64	52/4023 (1.3%)
4	6	0.89	2/2968 (0.1%)	1.64	52/4023 (1.3%)
4	7	0.89	1/2968 (0.0%)	1.64	52/4023 (1.3%)
4	8	0.89	1/2968 (0.0%)	1.64	52/4023 (1.3%)
4	9	0.89	2/2968 (0.1%)	1.64	52/4023 (1.3%)
4	V	0.89	2/2968 (0.1%)	1.64	52/4023 (1.3%)
4	W	0.89	1/2968 (0.0%)	1.64	52/4023 (1.3%)
4	X	0.89	1/2968 (0.0%)	1.64	51/4023 (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%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
All	All	1.34	483/93948 (0.5%)	1.69	1555/127146 (1.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	4
1	D	1	4
1	G	1	5
1	J	1	6
1	M	1	9
1	P	1	8
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	3
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	81

The worst 5 of 483 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	649	VAL	CB-CG1	53.27	2.64	1.52
1	M	649	VAL	CB-CG1	53.24	2.64	1.52
1	G	649	VAL	CB-CG1	53.23	2.64	1.52
1	J	649	VAL	CB-CG1	53.20	2.64	1.52
1	D	649	VAL	CB-CG1	53.16	2.64	1.52

The worst 5 of 1555 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	P	637	LYS	O-C-N	-58.47	23.80	123.20
1	M	637	LYS	O-C-N	-58.47	23.81	123.20
1	D	637	LYS	O-C-N	-58.46	23.81	123.20
1	J	637	LYS	O-C-N	-58.43	23.87	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 81 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	6752	1556	32

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	6797	0	6754	1441	7
1	G	6797	0	6757	1537	0
1	J	6797	0	6753	1455	0
1	M	6797	0	6770	1482	0
1	P	6797	0	6773	1487	0
2	B	1127	0	1087	260	0
2	E	1127	0	1086	251	0
2	H	1127	0	1088	298	121
2	K	1127	0	1089	272	121
2	N	1127	0	1088	244	0
2	Q	1127	0	1087	245	0
3	C	1123	0	1084	200	0
3	F	1123	0	1083	172	0
3	I	1123	0	1083	187	0
3	L	1123	0	1082	171	0
3	O	1123	0	1082	233	0
3	R	1123	0	1081	225	0
4	1	2906	0	2855	394	0
4	2	2906	0	2863	227	106
4	3	2906	0	2864	137	617
4	4	2906	0	2863	185	2894
4	5	2906	0	2865	94	3493
4	6	2906	0	2865	102	3173
4	7	2906	0	2866	78	3064
4	8	2906	0	2857	317	3413
4	9	2906	0	2855	346	3244
4	V	2906	0	2851	383	462
4	W	2906	0	2851	390	61
4	X	2906	0	2859	215	0
4	Y	2906	0	2863	161	0
4	Z	2906	0	2855	417	0
All	All	94966	0	93611	11358	10404

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 60.

The worst 5 of 11358 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:797:PHE:CD1	3:F:146:ILE:HG23	1.25	1.69
1:D:792:ALA:HB2	3:F:42:THR:CG2	1.21	1.68

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:831:TRP:CZ3	2:B:50:THR:HG21	1.13	1.64
4:2:287:ILE:CG2	4:4:202:THR:HB	1.23	1.63
4:2:287:ILE:HG23	4:4:202:THR:CB	1.26	1.63

The worst 5 of 10404 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:N	4:7:107:GLU:CD[1_554]	0.09	2.11
4:5:166:TYR:CG	4:V:40:HIS:CE1[1_554]	0.10	2.10
4:4:142:LEU:CG	4:7:372:ARG:O[1_554]	0.10	2.10
4:6:17:VAL:O	4:9:79:TRP:CB[1_554]	0.11	2.09
4:4:198:TYR:CB	4:7:207:GLU:CA[1_554]	0.14	2.06

## 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%)	651 (82%)	112 (14%)	28 (4%)	4	39
1	J	791/840 (94%)	652 (82%)	112 (14%)	27 (3%)	5	40
1	M	791/840 (94%)	651 (82%)	109 (14%)	31 (4%)	4	36
1	P	791/840 (94%)	649 (82%)	110 (14%)	32 (4%)	4	35
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

Continued on next page...

*Continued from previous page...*

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%)	334 (90%)	30 (8%)	6 (2%)	12	56
4	5	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	12	56
4	6	370/375 (99%)	335 (90%)	29 (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%)	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%)	335 (90%)	29 (8%)	6 (2%)	12	56
4	Z	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	12	56
All	All	11638/12042 (97%)	10140 (87%)	1196 (10%)	302 (3%)	11	45

5 of 302 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%)	513 (76%)	159 (24%)	1	7
1	J	672/672 (100%)	514 (76%)	158 (24%)	1	7
1	M	672/672 (100%)	515 (77%)	157 (23%)	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	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%)	268 (85%)	47 (15%)	4	23
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%)	269 (85%)	46 (15%)	4	24
4	7	315/318 (99%)	268 (85%)	47 (15%)	4	23
4	8	315/318 (99%)	269 (85%)	46 (15%)	4	24

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	9	315/318 (99%)	269 (85%)	46 (15%)	4	24
4	V	315/318 (99%)	269 (85%)	46 (15%)	4	24
4	W	315/318 (99%)	268 (85%)	47 (15%)	4	23
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%)	268 (85%)	47 (15%)	4	23
All	All	9864/9906 (100%)	8227 (83%)	1637 (17%)	6	19

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

Mol	Chain	Res	Type
1	M	448	GLN
1	P	506	GLU
4	X	199	SER
1	M	562	SER
1	P	61	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 240 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	194	GLN
1	P	164	GLN
4	W	252	ASN
1	M	290	GLN
1	M	612	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length

(or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	MLY	A	107	1	8,10,11	0.43	0	9,11,13	0.67	0
1	MLY	A	130	1	8,10,11	0.58	0	9,11,13	1.07	1 (11%)
1	MLY	A	138	1	8,10,11	1.35	1 (12%)	9,11,13	0.80	0
1	MLY	A	19	1	8,10,11	1.13	1 (12%)	9,11,13	0.68	0
1	MLY	A	190	1	8,10,11	1.12	1 (12%)	9,11,13	0.70	0
1	MLY	A	236	1	8,10,11	0.36	0	9,11,13	1.34	1 (11%)
1	MLY	A	248	1	8,10,11	0.76	0	9,11,13	0.92	1 (11%)
1	MLY	A	272	1	8,10,11	1.03	1 (12%)	9,11,13	0.56	0
1	MLY	A	295	1	8,10,11	0.75	0	9,11,13	0.46	0
1	MLY	A	296	1	8,10,11	0.58	0	9,11,13	0.76	0
1	MLY	A	30	1	8,10,11	0.66	0	9,11,13	0.82	1 (11%)
1	MLY	A	348	1	8,10,11	0.85	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	0.87	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	0.55	0	9,11,13	0.91	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	0.76	0	9,11,13	0.45	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	1.08	1 (12%)	9,11,13	0.58	0
1	MLY	A	486	1	8,10,11	0.35	0	9,11,13	0.59	0
1	MLY	A	49	1	8,10,11	1.06	1 (12%)	9,11,13	0.97	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	0.92	1 (12%)	9,11,13	0.39	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	0.65	0	9,11,13	0.97	0
1	MLY	A	551	1	8,10,11	0.49	0	9,11,13	0.65	0
1	MLY	A	553	1,4	8,10,11	0.60	0	9,11,13	0.59	0
1	MLY	A	59	1	8,10,11	0.77	0	9,11,13	0.76	0
1	MLY	A	598	1	8,10,11	0.87	1 (12%)	9,11,13	0.72	0
1	MLY	A	600	1	8,10,11	0.51	0	9,11,13	0.48	0
1	MLY	A	613	1	8,10,11	0.49	0	9,11,13	0.92	0
1	MLY	A	617	1	8,10,11	0.86	0	9,11,13	0.46	0
1	MLY	A	63	1	8,10,11	0.84	1 (12%)	9,11,13	0.94	0
1	MLY	A	659	1	8,10,11	0.54	0	9,11,13	0.95	0
1	MLY	A	681	1	8,10,11	0.62	0	9,11,13	0.62	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	0.67	0	9,11,13	0.56	0
1	MLY	A	768	1	8,10,11	0.64	0	9,11,13	0.86	0
1	MLY	A	782	1	8,10,11	0.49	0	9,11,13	0.94	1 (11%)
1	MLY	A	827	1	8,10,11	0.69	0	9,11,13	0.95	1 (11%)
1	MLY	A	833	1	8,10,11	0.98	1 (12%)	9,11,13	0.58	0
1	MLY	A	837	1	8,10,11	0.54	0	9,11,13	0.56	0
1	MLY	A	839	1	8,10,11	0.68	0	9,11,13	0.79	0
1	MLY	A	84	1	8,10,11	0.47	0	9,11,13	0.79	0
1	MLY	A	87	1	8,10,11	1.16	1 (12%)	9,11,13	0.68	0
1	MLY	D	107	1	8,10,11	0.46	0	9,11,13	0.67	0
1	MLY	D	130	1	8,10,11	0.59	0	9,11,13	1.06	1 (11%)
1	MLY	D	138	1	8,10,11	1.40	1 (12%)	9,11,13	0.81	0
1	MLY	D	19	1	8,10,11	1.23	1 (12%)	9,11,13	0.71	0
1	MLY	D	190	1	8,10,11	1.07	1 (12%)	9,11,13	0.70	0
1	MLY	D	236	1	8,10,11	0.35	0	9,11,13	1.32	1 (11%)
1	MLY	D	248	1	8,10,11	0.73	0	9,11,13	0.92	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	0.62	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	0.58	0	9,11,13	0.68	0
1	MLY	D	353	1	8,10,11	0.87	0	9,11,13	0.79	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	0.54	0	9,11,13	0.92	1 (11%)
1	MLY	D	385	1	8,10,11	1.00	1 (12%)	9,11,13	0.56	0
1	MLY	D	415	1	8,10,11	0.79	0	9,11,13	0.46	0
1	MLY	D	431	1	8,10,11	0.49	0	9,11,13	0.77	0
1	MLY	D	436	1	8,10,11	1.14	1 (12%)	9,11,13	0.56	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	1.07	1 (12%)	9,11,13	0.99	0
1	MLY	D	504	1	8,10,11	0.81	0	9,11,13	0.48	0
1	MLY	D	505	1	8,10,11	0.87	1 (12%)	9,11,13	0.40	0
1	MLY	D	528	1	8,10,11	0.83	0	9,11,13	1.16	1 (11%)
1	MLY	D	55	1	8,10,11	0.65	0	9,11,13	0.98	0
1	MLY	D	551	1	8,10,11	0.50	0	9,11,13	0.65	0
1	MLY	D	553	1,4	8,10,11	0.65	0	9,11,13	0.59	0
1	MLY	D	59	1	8,10,11	0.76	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	0.84	1 (12%)	9,11,13	0.69	0
1	MLY	D	600	1	8,10,11	0.50	0	9,11,13	0.47	0
1	MLY	D	613	1	8,10,11	0.47	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	0.94	0
1	MLY	D	659	1	8,10,11	0.52	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	0.68	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	0.93	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	0.58	0
1	MLY	D	837	1	8,10,11	0.54	0	9,11,13	0.58	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	0.44	0	9,11,13	0.67	0
1	MLY	G	130	1	8,10,11	0.60	0	9,11,13	1.09	1 (11%)
1	MLY	G	138	1	8,10,11	1.34	1 (12%)	9,11,13	0.81	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	1.11	1 (12%)	9,11,13	0.70	0
1	MLY	G	236	1	8,10,11	0.36	0	9,11,13	1.32	1 (11%)
1	MLY	G	248	1	8,10,11	0.73	0	9,11,13	0.94	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	0.74	0	9,11,13	0.46	0
1	MLY	G	296	1	8,10,11	0.63	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	0.84	1 (12%)	9,11,13	0.82	0
1	MLY	G	35	1	8,10,11	0.58	0	9,11,13	0.68	0
1	MLY	G	353	1	8,10,11	0.86	0	9,11,13	0.79	0
1	MLY	G	367	1	8,10,11	0.68	0	9,11,13	0.61	0
1	MLY	G	369	1	8,10,11	0.54	0	9,11,13	0.92	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	0.76	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	0.34	0	9,11,13	0.60	0
1	MLY	G	49	1	8,10,11	1.08	1 (12%)	9,11,13	0.98	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	MLY	G	504	1	8,10,11	0.75	0	9,11,13	0.48	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	0.67	0	9,11,13	1.00	0
1	MLY	G	551	1	8,10,11	0.50	0	9,11,13	0.65	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	0.73	0	9,11,13	0.77	0
1	MLY	G	598	1	8,10,11	0.85	1 (12%)	9,11,13	0.71	0
1	MLY	G	600	1	8,10,11	0.52	0	9,11,13	0.46	0
1	MLY	G	613	1	8,10,11	0.50	0	9,11,13	0.91	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	0.56	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	0.56	0
1	MLY	G	768	1	8,10,11	0.63	0	9,11,13	0.87	0
1	MLY	G	782	1	8,10,11	0.47	0	9,11,13	0.92	1 (11%)
1	MLY	G	827	1	8,10,11	0.65	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	0.54	0	9,11,13	0.56	0
1	MLY	G	839	1	8,10,11	0.70	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	1.19	1 (12%)	9,11,13	0.68	0
1	MLY	J	107	1	8,10,11	0.45	0	9,11,13	0.68	0
1	MLY	J	130	1	8,10,11	0.55	0	9,11,13	1.06	1 (11%)
1	MLY	J	138	1	8,10,11	1.35	1 (12%)	9,11,13	0.80	0
1	MLY	J	19	1	8,10,11	1.21	1 (12%)	9,11,13	0.70	0
1	MLY	J	190	1	8,10,11	1.10	1 (12%)	9,11,13	0.69	0
1	MLY	J	236	1	8,10,11	0.36	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	1.05	1 (12%)	9,11,13	0.57	0
1	MLY	J	295	1	8,10,11	0.69	0	9,11,13	0.47	0
1	MLY	J	296	1	8,10,11	0.66	0	9,11,13	0.78	1 (11%)
1	MLY	J	30	1	8,10,11	0.70	0	9,11,13	0.82	0
1	MLY	J	348	1	8,10,11	0.80	0	9,11,13	0.81	0
1	MLY	J	35	1	8,10,11	0.59	0	9,11,13	0.67	0
1	MLY	J	353	1	8,10,11	0.85	0	9,11,13	0.77	0
1	MLY	J	367	1	8,10,11	0.66	0	9,11,13	0.61	0
1	MLY	J	369	1	8,10,11	0.52	0	9,11,13	0.93	1 (11%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	MLY	J	385	1	8,10,11	1.02	1 (12%)	9,11,13	0.55	0
1	MLY	J	415	1	8,10,11	0.79	0	9,11,13	0.45	0
1	MLY	J	431	1	8,10,11	0.47	0	9,11,13	0.78	0
1	MLY	J	436	1	8,10,11	1.10	1 (12%)	9,11,13	0.56	0
1	MLY	J	486	1	8,10,11	0.32	0	9,11,13	0.60	0
1	MLY	J	49	1	8,10,11	1.09	1 (12%)	9,11,13	1.01	1 (11%)
1	MLY	J	504	1	8,10,11	0.74	0	9,11,13	0.49	0
1	MLY	J	505	1	8,10,11	0.94	1 (12%)	9,11,13	0.38	0
1	MLY	J	528	1	8,10,11	0.80	0	9,11,13	1.16	1 (11%)
1	MLY	J	55	1	8,10,11	0.66	0	9,11,13	0.98	0
1	MLY	J	551	1	8,10,11	0.50	0	9,11,13	0.65	0
1	MLY	J	553	1	8,10,11	0.62	0	9,11,13	0.57	0
1	MLY	J	59	1	8,10,11	0.78	0	9,11,13	0.78	0
1	MLY	J	598	1	8,10,11	0.85	1 (12%)	9,11,13	0.70	0
1	MLY	J	600	1	8,10,11	0.53	0	9,11,13	0.47	0
1	MLY	J	613	1	8,10,11	0.49	0	9,11,13	0.94	0
1	MLY	J	617	1	8,10,11	0.93	1 (12%)	9,11,13	0.46	0
1	MLY	J	63	1	8,10,11	0.79	0	9,11,13	0.95	0
1	MLY	J	659	1	8,10,11	0.51	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	0.65	0	9,11,13	0.59	0
1	MLY	J	768	1	8,10,11	0.64	0	9,11,13	0.87	0
1	MLY	J	782	1	8,10,11	0.51	0	9,11,13	0.94	1 (11%)
1	MLY	J	827	1	8,10,11	0.69	0	9,11,13	0.95	1 (11%)
1	MLY	J	833	1	8,10,11	1.01	1 (12%)	9,11,13	0.57	0
1	MLY	J	837	1	8,10,11	0.54	0	9,11,13	0.59	0
1	MLY	J	839	1	8,10,11	0.70	0	9,11,13	0.77	0
1	MLY	J	84	1	8,10,11	0.45	0	9,11,13	0.80	0
1	MLY	J	87	1	8,10,11	1.20	1 (12%)	9,11,13	0.68	0
1	MLY	M	107	1	8,10,11	0.44	0	9,11,13	0.67	0
1	MLY	M	130	1	8,10,11	0.55	0	9,11,13	1.06	1 (11%)
1	MLY	M	138	1	8,10,11	1.33	1 (12%)	9,11,13	0.80	0
1	MLY	M	19	1	8,10,11	1.20	1 (12%)	9,11,13	0.70	0
1	MLY	M	190	1	8,10,11	1.10	1 (12%)	9,11,13	0.70	0
1	MLY	M	236	1	8,10,11	0.36	0	9,11,13	1.32	1 (11%)
1	MLY	M	248	1	8,10,11	0.74	0	9,11,13	0.95	1 (11%)
1	MLY	M	272	1	8,10,11	1.01	1 (12%)	9,11,13	0.57	0
1	MLY	M	295	1	8,10,11	0.69	0	9,11,13	0.48	0
1	MLY	M	296	1	8,10,11	0.66	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	M	30	1	8,10,11	0.68	0	9,11,13	0.82	1 (11%)
1	MLY	M	348	1	8,10,11	0.79	0	9,11,13	0.81	0
1	MLY	M	35	1	8,10,11	0.59	0	9,11,13	0.68	0
1	MLY	M	353	1	8,10,11	0.87	0	9,11,13	0.78	0
1	MLY	M	367	1	8,10,11	0.65	0	9,11,13	0.60	0
1	MLY	M	369	1	8,10,11	0.53	0	9,11,13	0.93	1 (11%)
1	MLY	M	385	1	8,10,11	1.04	1 (12%)	9,11,13	0.54	0
1	MLY	M	415	1	8,10,11	0.77	0	9,11,13	0.44	0
1	MLY	M	431	1	8,10,11	0.46	0	9,11,13	0.77	0
1	MLY	M	436	1	8,10,11	1.08	1 (12%)	9,11,13	0.56	0
1	MLY	M	486	1	8,10,11	0.33	0	9,11,13	0.59	0
1	MLY	M	49	1	8,10,11	1.11	1 (12%)	9,11,13	1.00	0
1	MLY	M	504	1	8,10,11	0.75	0	9,11,13	0.49	0
1	MLY	M	505	1	8,10,11	0.93	1 (12%)	9,11,13	0.39	0
1	MLY	M	528	1	8,10,11	0.80	0	9,11,13	1.17	1 (11%)
1	MLY	M	55	1	8,10,11	0.65	0	9,11,13	0.97	0
1	MLY	M	551	1	8,10,11	0.49	0	9,11,13	0.67	0
1	MLY	M	553	1	8,10,11	0.60	0	9,11,13	0.57	0
1	MLY	M	59	1	8,10,11	0.78	0	9,11,13	0.78	0
1	MLY	M	598	1	8,10,11	0.86	1 (12%)	9,11,13	0.70	0
1	MLY	M	600	1	8,10,11	0.52	0	9,11,13	0.48	0
1	MLY	M	613	1	8,10,11	0.50	0	9,11,13	0.94	0
1	MLY	M	617	1	8,10,11	0.92	1 (12%)	9,11,13	0.46	0
1	MLY	M	63	1	8,10,11	0.83	1 (12%)	9,11,13	0.94	0
1	MLY	M	659	1	8,10,11	0.50	0	9,11,13	0.93	0
1	MLY	M	681	1	8,10,11	0.61	0	9,11,13	0.64	0
1	MLY	M	764	1	8,10,11	0.68	0	9,11,13	0.59	0
1	MLY	M	768	1	8,10,11	0.64	0	9,11,13	0.87	0
1	MLY	M	782	1	8,10,11	0.49	0	9,11,13	0.94	1 (11%)
1	MLY	M	827	1	8,10,11	0.66	0	9,11,13	0.96	1 (11%)
1	MLY	M	833	1	8,10,11	1.05	1 (12%)	9,11,13	0.58	0
1	MLY	M	837	1	8,10,11	0.54	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	0.46	0	9,11,13	0.80	0
1	MLY	M	87	1	8,10,11	1.18	1 (12%)	9,11,13	0.68	0
1	MLY	P	107	1	8,10,11	0.44	0	9,11,13	0.66	0
1	MLY	P	130	1	8,10,11	0.55	0	9,11,13	1.06	1 (11%)
1	MLY	P	138	1	8,10,11	1.33	1 (12%)	9,11,13	0.80	0
1	MLY	P	19	1	8,10,11	1.19	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	190	1	8,10,11	1.14	1 (12%)	9,11,13	0.69	0
1	MLY	P	236	1	8,10,11	0.36	0	9,11,13	1.32	1 (11%)
1	MLY	P	248	1	8,10,11	0.75	0	9,11,13	0.95	1 (11%)
1	MLY	P	272	1	8,10,11	1.06	1 (12%)	9,11,13	0.56	0
1	MLY	P	295	1	8,10,11	0.74	0	9,11,13	0.47	0
1	MLY	P	296	1	8,10,11	0.68	0	9,11,13	0.78	1 (11%)
1	MLY	P	30	1	8,10,11	0.69	0	9,11,13	0.82	1 (11%)
1	MLY	P	348	1	8,10,11	0.82	0	9,11,13	0.80	0
1	MLY	P	35	1	8,10,11	0.59	0	9,11,13	0.67	0
1	MLY	P	353	1	8,10,11	0.86	0	9,11,13	0.79	0
1	MLY	P	367	1	8,10,11	0.65	0	9,11,13	0.61	0
1	MLY	P	369	1	8,10,11	0.55	0	9,11,13	0.93	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	0.76	0	9,11,13	0.45	0
1	MLY	P	431	1	8,10,11	0.46	0	9,11,13	0.77	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	0.33	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	0.48	0
1	MLY	P	505	1	8,10,11	0.95	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	0.66	0	9,11,13	0.98	0
1	MLY	P	551	1	8,10,11	0.49	0	9,11,13	0.65	0
1	MLY	P	553	1	8,10,11	0.63	0	9,11,13	0.58	0
1	MLY	P	59	1	8,10,11	0.77	0	9,11,13	0.77	0
1	MLY	P	598	1	8,10,11	0.81	1 (12%)	9,11,13	0.71	0
1	MLY	P	600	1	8,10,11	0.53	0	9,11,13	0.47	0
1	MLY	P	613	1	8,10,11	0.48	0	9,11,13	0.93	0
1	MLY	P	617	1	8,10,11	0.92	1 (12%)	9,11,13	0.46	0
1	MLY	P	63	1	8,10,11	0.81	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	0.63	0	9,11,13	0.64	0
1	MLY	P	764	1	8,10,11	0.65	0	9,11,13	0.59	0
1	MLY	P	768	1	8,10,11	0.63	0	9,11,13	0.86	0
1	MLY	P	782	1	8,10,11	0.49	0	9,11,13	0.96	1 (11%)
1	MLY	P	827	1	8,10,11	0.67	0	9,11,13	0.95	1 (11%)
1	MLY	P	833	1	8,10,11	1.04	1 (12%)	9,11,13	0.55	0
1	MLY	P	837	1	8,10,11	0.53	0	9,11,13	0.59	0
1	MLY	P	839	1	8,10,11	0.67	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	P	84	1	8,10,11	0.46	0	9,11,13	0.80	0
1	MLY	P	87	1	8,10,11	1.17	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

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	A	63	1	-	0/7/9/11	0/0/0/0
1	MLY	A	659	1	-	0/7/9/11	0/0/0/0
1	MLY	A	681	1	-	0/7/9/11	0/0/0/0
1	MLY	A	764	1	-	0/7/9/11	0/0/0/0
1	MLY	A	768	1	-	0/7/9/11	0/0/0/0
1	MLY	A	782	1	-	0/7/9/11	0/0/0/0
1	MLY	A	827	1	-	0/7/9/11	0/0/0/0
1	MLY	A	833	1	-	0/7/9/11	0/0/0/0
1	MLY	A	837	1	-	0/7/9/11	0/0/0/0
1	MLY	A	839	1	-	0/7/9/11	0/0/0/0
1	MLY	A	84	1	-	0/7/9/11	0/0/0/0
1	MLY	A	87	1	-	0/7/9/11	0/0/0/0
1	MLY	D	107	1	-	0/7/9/11	0/0/0/0
1	MLY	D	130	1	-	0/7/9/11	0/0/0/0
1	MLY	D	138	1	-	0/7/9/11	0/0/0/0
1	MLY	D	19	1	-	0/7/9/11	0/0/0/0
1	MLY	D	190	1	-	0/7/9/11	0/0/0/0
1	MLY	D	236	1	-	0/7/9/11	0/0/0/0
1	MLY	D	248	1	-	0/7/9/11	0/0/0/0
1	MLY	D	272	1	-	0/7/9/11	0/0/0/0
1	MLY	D	295	1	-	0/7/9/11	0/0/0/0
1	MLY	D	296	1	-	0/7/9/11	0/0/0/0
1	MLY	D	30	1	-	0/7/9/11	0/0/0/0
1	MLY	D	348	1	-	0/7/9/11	0/0/0/0
1	MLY	D	35	1	-	0/7/9/11	0/0/0/0
1	MLY	D	353	1	-	0/7/9/11	0/0/0/0
1	MLY	D	367	1	-	0/7/9/11	0/0/0/0
1	MLY	D	369	1	-	0/7/9/11	0/0/0/0
1	MLY	D	385	1	-	0/7/9/11	0/0/0/0
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

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	D	600	1	-	0/7/9/11	0/0/0/0
1	MLY	D	613	1	-	0/7/9/11	0/0/0/0
1	MLY	D	617	1	-	0/7/9/11	0/0/0/0
1	MLY	D	63	1	-	0/7/9/11	0/0/0/0
1	MLY	D	659	1	-	0/7/9/11	0/0/0/0
1	MLY	D	681	1	-	0/7/9/11	0/0/0/0
1	MLY	D	764	1	-	0/7/9/11	0/0/0/0
1	MLY	D	768	1	-	0/7/9/11	0/0/0/0
1	MLY	D	782	1	-	0/7/9/11	0/0/0/0
1	MLY	D	827	1	-	0/7/9/11	0/0/0/0
1	MLY	D	833	1	-	0/7/9/11	0/0/0/0
1	MLY	D	837	1	-	0/7/9/11	0/0/0/0
1	MLY	D	839	1	-	0/7/9/11	0/0/0/0
1	MLY	D	84	1	-	0/7/9/11	0/0/0/0
1	MLY	D	87	1	-	0/7/9/11	0/0/0/0
1	MLY	G	107	1	-	0/7/9/11	0/0/0/0
1	MLY	G	130	1	-	0/7/9/11	0/0/0/0
1	MLY	G	138	1	-	0/7/9/11	0/0/0/0
1	MLY	G	19	1	-	0/7/9/11	0/0/0/0
1	MLY	G	190	1	-	0/7/9/11	0/0/0/0
1	MLY	G	236	1	-	0/7/9/11	0/0/0/0
1	MLY	G	248	1	-	0/7/9/11	0/0/0/0
1	MLY	G	272	1	-	0/7/9/11	0/0/0/0
1	MLY	G	295	1	-	0/7/9/11	0/0/0/0
1	MLY	G	296	1	-	0/7/9/11	0/0/0/0
1	MLY	G	30	1	-	0/7/9/11	0/0/0/0
1	MLY	G	348	1	-	0/7/9/11	0/0/0/0
1	MLY	G	35	1	-	0/7/9/11	0/0/0/0
1	MLY	G	353	1	-	0/7/9/11	0/0/0/0
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

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	G	553	1,4	-	0/7/9/11	0/0/0/0
1	MLY	G	59	1	-	0/7/9/11	0/0/0/0
1	MLY	G	598	1	-	0/7/9/11	0/0/0/0
1	MLY	G	600	1	-	0/7/9/11	0/0/0/0
1	MLY	G	613	1	-	0/7/9/11	0/0/0/0
1	MLY	G	617	1	-	0/7/9/11	0/0/0/0
1	MLY	G	63	1	-	0/7/9/11	0/0/0/0
1	MLY	G	659	1	-	0/7/9/11	0/0/0/0
1	MLY	G	681	1	-	0/7/9/11	0/0/0/0
1	MLY	G	764	1	-	0/7/9/11	0/0/0/0
1	MLY	G	768	1	-	0/7/9/11	0/0/0/0
1	MLY	G	782	1	-	0/7/9/11	0/0/0/0
1	MLY	G	827	1	-	0/7/9/11	0/0/0/0
1	MLY	G	833	1	-	0/7/9/11	0/0/0/0
1	MLY	G	837	1	-	0/7/9/11	0/0/0/0
1	MLY	G	839	1	-	0/7/9/11	0/0/0/0
1	MLY	G	84	1	-	0/7/9/11	0/0/0/0
1	MLY	G	87	1	-	0/7/9/11	0/0/0/0
1	MLY	J	107	1	-	0/7/9/11	0/0/0/0
1	MLY	J	130	1	-	0/7/9/11	0/0/0/0
1	MLY	J	138	1	-	0/7/9/11	0/0/0/0
1	MLY	J	19	1	-	0/7/9/11	0/0/0/0
1	MLY	J	190	1	-	0/7/9/11	0/0/0/0
1	MLY	J	236	1	-	0/7/9/11	0/0/0/0
1	MLY	J	248	1	-	0/7/9/11	0/0/0/0
1	MLY	J	272	1	-	0/7/9/11	0/0/0/0
1	MLY	J	295	1	-	0/7/9/11	0/0/0/0
1	MLY	J	296	1	-	0/7/9/11	0/0/0/0
1	MLY	J	30	1	-	0/7/9/11	0/0/0/0
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

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	J	528	1	-	0/7/9/11	0/0/0/0
1	MLY	J	55	1	-	0/7/9/11	0/0/0/0
1	MLY	J	551	1	-	0/7/9/11	0/0/0/0
1	MLY	J	553	1	-	0/7/9/11	0/0/0/0
1	MLY	J	59	1	-	0/7/9/11	0/0/0/0
1	MLY	J	598	1	-	0/7/9/11	0/0/0/0
1	MLY	J	600	1	-	0/7/9/11	0/0/0/0
1	MLY	J	613	1	-	0/7/9/11	0/0/0/0
1	MLY	J	617	1	-	0/7/9/11	0/0/0/0
1	MLY	J	63	1	-	0/7/9/11	0/0/0/0
1	MLY	J	659	1	-	0/7/9/11	0/0/0/0
1	MLY	J	681	1	-	0/7/9/11	0/0/0/0
1	MLY	J	764	1	-	0/7/9/11	0/0/0/0
1	MLY	J	768	1	-	0/7/9/11	0/0/0/0
1	MLY	J	782	1	-	0/7/9/11	0/0/0/0
1	MLY	J	827	1	-	0/7/9/11	0/0/0/0
1	MLY	J	833	1	-	0/7/9/11	0/0/0/0
1	MLY	J	837	1	-	0/7/9/11	0/0/0/0
1	MLY	J	839	1	-	0/7/9/11	0/0/0/0
1	MLY	J	84	1	-	0/7/9/11	0/0/0/0
1	MLY	J	87	1	-	0/7/9/11	0/0/0/0
1	MLY	M	107	1	-	0/7/9/11	0/0/0/0
1	MLY	M	130	1	-	0/7/9/11	0/0/0/0
1	MLY	M	138	1	-	0/7/9/11	0/0/0/0
1	MLY	M	19	1	-	0/7/9/11	0/0/0/0
1	MLY	M	190	1	-	0/7/9/11	0/0/0/0
1	MLY	M	236	1	-	0/7/9/11	0/0/0/0
1	MLY	M	248	1	-	0/7/9/11	0/0/0/0
1	MLY	M	272	1	-	0/7/9/11	0/0/0/0
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

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	M	49	1	-	0/7/9/11	0/0/0/0
1	MLY	M	504	1	-	0/7/9/11	0/0/0/0
1	MLY	M	505	1	-	0/7/9/11	0/0/0/0
1	MLY	M	528	1	-	0/7/9/11	0/0/0/0
1	MLY	M	55	1	-	0/7/9/11	0/0/0/0
1	MLY	M	551	1	-	0/7/9/11	0/0/0/0
1	MLY	M	553	1	-	0/7/9/11	0/0/0/0
1	MLY	M	59	1	-	0/7/9/11	0/0/0/0
1	MLY	M	598	1	-	0/7/9/11	0/0/0/0
1	MLY	M	600	1	-	0/7/9/11	0/0/0/0
1	MLY	M	613	1	-	0/7/9/11	0/0/0/0
1	MLY	M	617	1	-	0/7/9/11	0/0/0/0
1	MLY	M	63	1	-	0/7/9/11	0/0/0/0
1	MLY	M	659	1	-	0/7/9/11	0/0/0/0
1	MLY	M	681	1	-	0/7/9/11	0/0/0/0
1	MLY	M	764	1	-	0/7/9/11	0/0/0/0
1	MLY	M	768	1	-	0/7/9/11	0/0/0/0
1	MLY	M	782	1	-	0/7/9/11	0/0/0/0
1	MLY	M	827	1	-	0/7/9/11	0/0/0/0
1	MLY	M	833	1	-	0/7/9/11	0/0/0/0
1	MLY	M	837	1	-	0/7/9/11	0/0/0/0
1	MLY	M	839	1	-	0/7/9/11	0/0/0/0
1	MLY	M	84	1	-	0/7/9/11	0/0/0/0
1	MLY	M	87	1	-	0/7/9/11	0/0/0/0
1	MLY	P	107	1	-	0/7/9/11	0/0/0/0
1	MLY	P	130	1	-	0/7/9/11	0/0/0/0
1	MLY	P	138	1	-	0/7/9/11	0/0/0/0
1	MLY	P	19	1	-	0/7/9/11	0/0/0/0
1	MLY	P	190	1	-	0/7/9/11	0/0/0/0
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

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	P	431	1	-	0/7/9/11	0/0/0/0
1	MLY	P	436	1	-	0/7/9/11	0/0/0/0
1	MLY	P	486	1	-	0/7/9/11	0/0/0/0
1	MLY	P	49	1	-	0/7/9/11	0/0/0/0
1	MLY	P	504	1	-	0/7/9/11	0/0/0/0
1	MLY	P	505	1	-	0/7/9/11	0/0/0/0
1	MLY	P	528	1	-	0/7/9/11	0/0/0/0
1	MLY	P	55	1	-	0/7/9/11	0/0/0/0
1	MLY	P	551	1	-	0/7/9/11	0/0/0/0
1	MLY	P	553	1	-	0/7/9/11	0/0/0/0
1	MLY	P	59	1	-	0/7/9/11	0/0/0/0
1	MLY	P	598	1	-	0/7/9/11	0/0/0/0
1	MLY	P	600	1	-	0/7/9/11	0/0/0/0
1	MLY	P	613	1	-	0/7/9/11	0/0/0/0
1	MLY	P	617	1	-	0/7/9/11	0/0/0/0
1	MLY	P	63	1	-	0/7/9/11	0/0/0/0
1	MLY	P	659	1	-	0/7/9/11	0/0/0/0
1	MLY	P	681	1	-	0/7/9/11	0/0/0/0
1	MLY	P	764	1	-	0/7/9/11	0/0/0/0
1	MLY	P	768	1	-	0/7/9/11	0/0/0/0
1	MLY	P	782	1	-	0/7/9/11	0/0/0/0
1	MLY	P	827	1	-	0/7/9/11	0/0/0/0
1	MLY	P	833	1	-	0/7/9/11	0/0/0/0
1	MLY	P	837	1	-	0/7/9/11	0/0/0/0
1	MLY	P	839	1	-	0/7/9/11	0/0/0/0
1	MLY	P	84	1	-	0/7/9/11	0/0/0/0
1	MLY	P	87	1	-	0/7/9/11	0/0/0/0

The worst 5 of 74 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	138	MLY	CB-CA	-3.68	1.48	1.53
1	J	138	MLY	CB-CA	-3.53	1.48	1.53
1	A	138	MLY	CB-CA	-3.53	1.48	1.53
1	G	138	MLY	CB-CA	-3.52	1.48	1.53
1	P	138	MLY	CB-CA	-3.50	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	-3.27	116.94	125.72
1	D	236	MLY	O-C-CA	-3.24	117.03	125.72

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	M	236	MLY	O-C-CA	-3.23	117.06	125.72
1	P	236	MLY	O-C-CA	-3.22	117.08	125.72
1	G	236	MLY	O-C-CA	-3.22	117.08	125.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

182 monomers are involved in 679 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	3	0
1	A	486	MLY	3	0
1	A	49	MLY	4	0
1	A	505	MLY	22	0
1	A	528	MLY	3	0
1	A	55	MLY	1	0
1	A	551	MLY	2	0
1	A	553	MLY	17	1
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	1	0
1	A	764	MLY	9	0
1	A	768	MLY	10	0
1	A	782	MLY	7	0
1	A	827	MLY	2	0
1	A	833	MLY	1	0
1	A	837	MLY	12	0
1	A	839	MLY	4	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	87	MLY	3	0
1	D	107	MLY	3	0
1	D	138	MLY	1	0
1	D	190	MLY	2	0
1	D	248	MLY	2	0
1	D	272	MLY	1	0
1	D	295	MLY	6	0
1	D	296	MLY	3	0
1	D	30	MLY	1	0
1	D	348	MLY	6	0
1	D	369	MLY	1	0
1	D	415	MLY	1	0
1	D	436	MLY	3	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	17	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	7	0
1	D	768	MLY	2	0
1	D	782	MLY	71	0
1	D	837	MLY	1	0
1	D	839	MLY	4	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	5	0
1	G	415	MLY	1	0
1	G	436	MLY	2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	G	486	MLY	3	0
1	G	49	MLY	3	0
1	G	505	MLY	9	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	3	0
1	G	659	MLY	2	0
1	G	764	MLY	4	0
1	G	768	MLY	3	0
1	G	782	MLY	1	0
1	G	837	MLY	1	0
1	G	839	MLY	4	0
1	G	84	MLY	15	0
1	G	87	MLY	3	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	6	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	3	0
1	J	486	MLY	3	0
1	J	49	MLY	3	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	3	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	J	659	MLY	2	0
1	J	764	MLY	1	0
1	J	768	MLY	1	0
1	J	782	MLY	1	0
1	J	837	MLY	1	0
1	J	839	MLY	8	0
1	J	84	MLY	20	0
1	J	87	MLY	3	0
1	M	107	MLY	3	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	415	MLY	1	0
1	M	436	MLY	2	0
1	M	486	MLY	3	0
1	M	49	MLY	2	0
1	M	505	MLY	1	0
1	M	528	MLY	3	0
1	M	55	MLY	1	0
1	M	553	MLY	2	0
1	M	59	MLY	3	0
1	M	598	MLY	1	0
1	M	600	MLY	1	0
1	M	617	MLY	1	0
1	M	63	MLY	3	0
1	M	659	MLY	1	0
1	M	764	MLY	2	0
1	M	768	MLY	3	0
1	M	782	MLY	1	0
1	M	837	MLY	1	0
1	M	839	MLY	7	0
1	M	84	MLY	11	0
1	M	87	MLY	3	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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
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	369	MLY	1	0
1	P	415	MLY	1	0
1	P	436	MLY	3	0
1	P	486	MLY	3	0
1	P	49	MLY	3	0
1	P	528	MLY	3	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	3	0
1	P	659	MLY	2	0
1	P	764	MLY	1	0
1	P	782	MLY	15	0
1	P	837	MLY	1	0
1	P	839	MLY	7	0
1	P	84	MLY	15	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 ⓘ

There are no chain breaks in this entry.