



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:10 PM BST

PDB ID : 1O1C  
EMDB ID: : EMD-1001  
Title : MOLECULAR MODELS OF AVERAGED RIGOR CROSSBRIDGES FROM  
TOMOGRAMS OF INSECT FLIGHT MUSCLE  
Authors : Chen, L.F.; Winkler, H.; Reedy, M.K.; Reedy, M.C.; Taylor, K.A.  
Deposited on : 2002-11-18  
Resolution : 70.00 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could  
stem from errors in the original structure(s) used in the fitting.  
We welcome your comments at [validation@mail.wwpdb.org](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

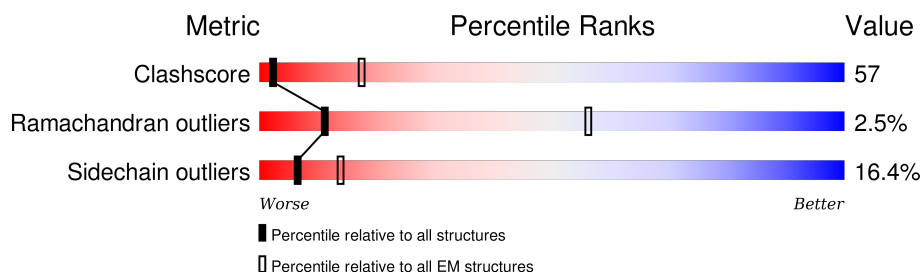
# 1 Overall quality at a glance

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.











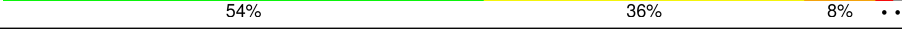

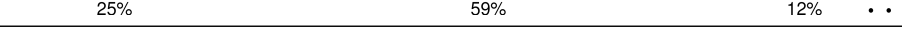
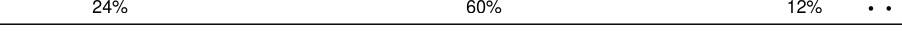

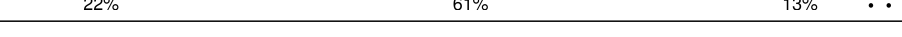
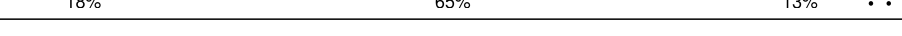



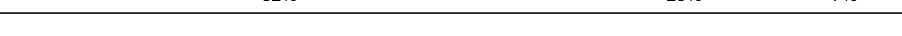

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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	26% 51% 18% .
1	G	840	25% 51% 20% .
1	J	840	26% 51% 19% .
1	P	840	25% 51% 19% .
2	B	145	66% 26% 6% .
2	E	145	64% 27% 6% .
2	H	145	62% 29% 6% .
2	K	145	64% 26% 6% .

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Mol	Chain	Length	Quality of chain
2	Q	145	
3	C	147	
3	F	147	
3	I	147	
3	L	147	
3	R	147	
4	0	375	
4	1	375	
4	2	375	
4	3	375	
4	4	375	
4	5	375	
4	7	375	
4	8	375	
4	9	375	
4	V	375	
4	W	375	
4	X	375	
4	Y	375	
4	Z	375	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	MLY	A	505	-	-	X	-
1	MLY	A	553	-	-	X	-
1	MLY	A	764	-	-	X	-

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

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 85919 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	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	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		

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

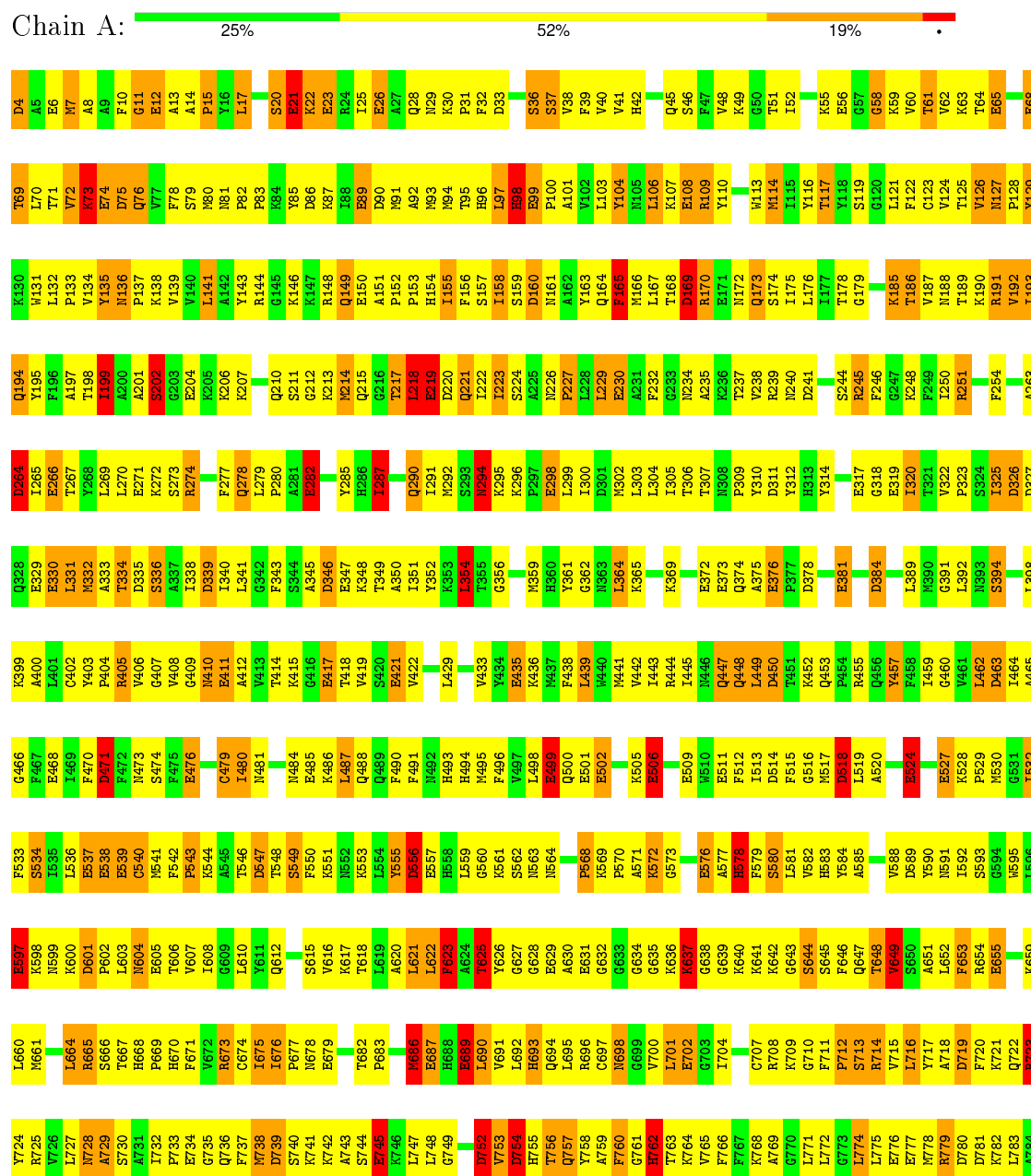
- Molecule 4 is a protein called SKELETAL MUSCLE ACTIN.

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

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

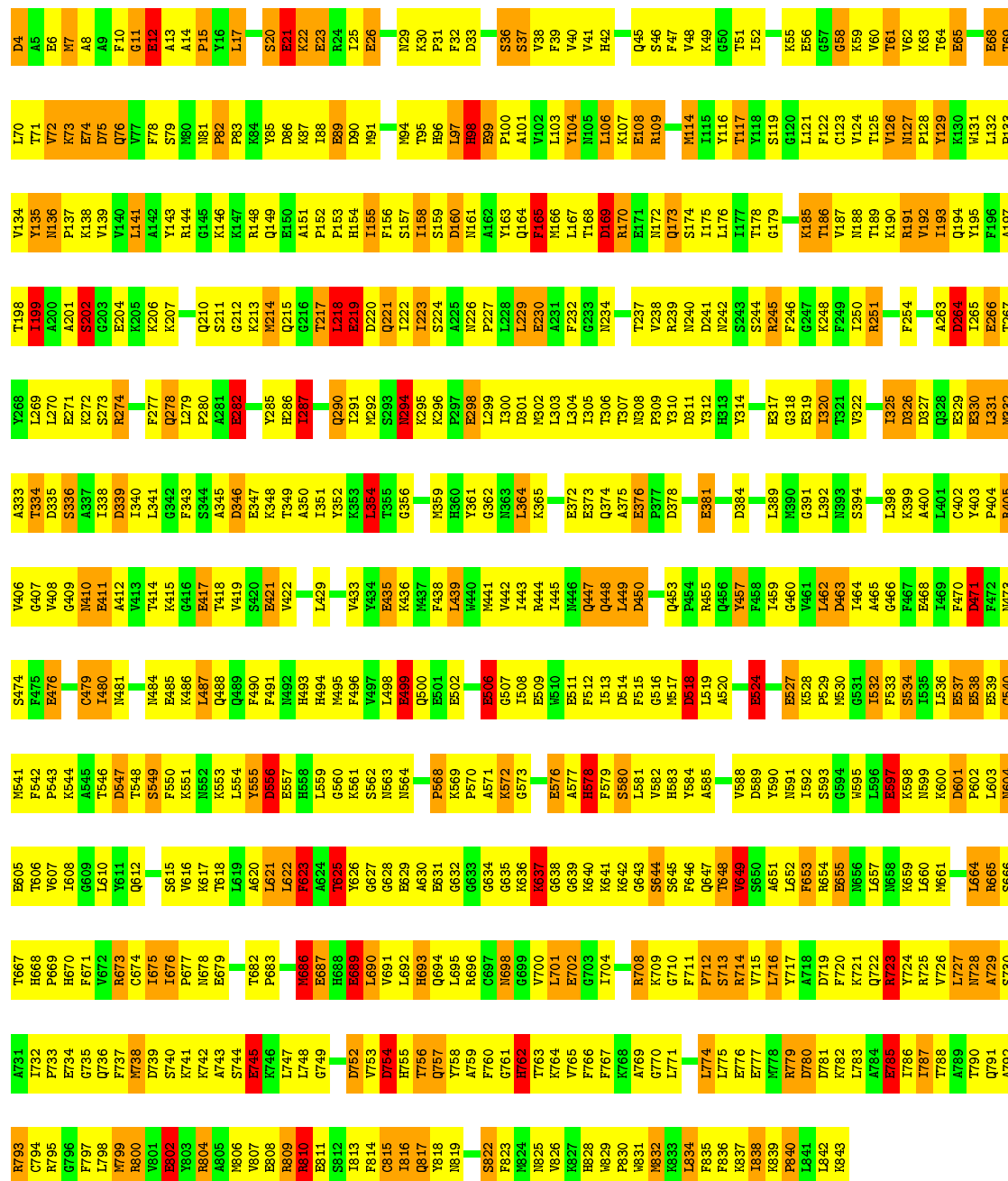
#### • Molecule 1: SKELETAL MUSCLE MYOSIN II





# Molecule 1: SKELETAL MUSCLE MYOSIN II

Chain D: 26% 51% 18%



# Molecule 1: SKELETAL MUSCLE MYOSIN II

Chain G: 25% 51% 20%







Chain J:  26% 51% 19% .

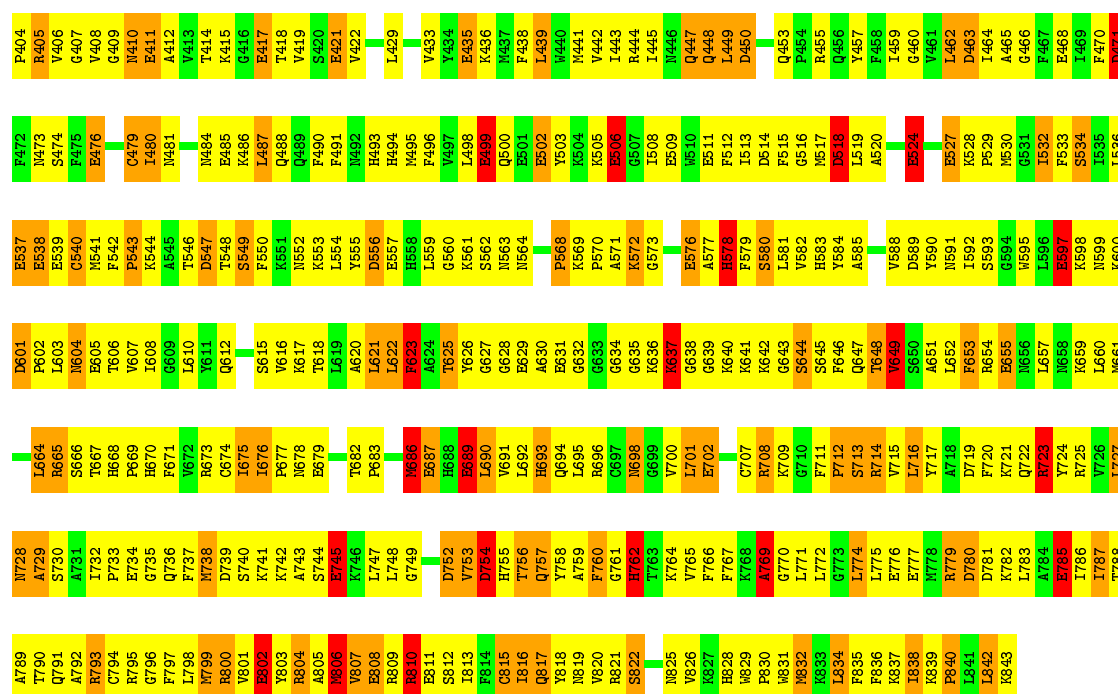


E330	E372	E330	E266	E196
L331	M473	L331	T267	A197
M332	S474	M332	Y268	T198
V406	F475	V406	L269	T199
V408	E476	V408	L270	A200
D335	G409	D335	E271	A201
S336	M410	S336	K272	S202
A337	E411	A337	K273	G203
L338	M412	L338	R274	E204
D339	V413	D339	F277	K205
L340	T414	L340	Q278	K206
L341	K415	L341	L279	K207
G342	K416	G342	P280	Q210
F343	E417	F343	L279	S211
S344	T418	S344	E282	G212
D346	F419	D346	E282	K213
A345	S420	A345	Y285	M214
K348	E421	K348	E286	Q215
T349	V422	T349	L287	G216
L429	L429	L429	Q290	T217
V433	V433	V433	L291	L218
E434	E434	E434	I291	E219
E435	E435	E435	M292	D220
K353	L354	K353	S293	Q221
L355	E436	L355	K294	T222
G356	M437	G356	K295	T223
F359	F438	F359	K296	S224
M360	L440	M360	E298	L226
S361	M441	S361	L299	P227
K362	V442	K362	I300	L228
L364	L443	L364	D301	L229
K365	R444	K365	M302	E230
E372	N446	E372	L304	A231
E373	Q447	E373	I305	F232
A374	Q448	A374	T306	G233
D450	L449	D450	L307	N234
E376	D450	E376	M308	A235
E377	Q453	E377	P309	T237
D378	P454	D378	Y310	V238
E381	R455	E381	D311	R239
D384	Q456	D384	Y312	N240
E384	Y457	E384	E313	D241
E384	F458	E384	Y314	S244
L389	G460	L389	E317	R245
M390	V461	M390	G318	F246
G391	L462	G391	E319	Q247
L392	D463	L392	I320	K248
S394	M464	S394	T321	F249
E399	A465	E399	P323	R251
A400	E466	A400	S324	F254
L401	F467	L401	I325	F254
F470	E468	F470	D326	A263
D471	L469	D471	E327	D264
E509	E509	E509	Q328	T265
E511	E511	E511	E329	E267
F512	F512	F512		
L513	L513	L513		
D514	D514	D514		
F515	F515	F515		
G516	G516	G516		
M517	M517	M517		
D518	D518	D518		
L519	L519	L519		
A520	A520	A520		
E524	E524	E524		
E527	E527	E527		
K528	K528	K528		
P529	P529	P529		
M530	M530	M530		
G531	G531	G531		
L532	L532	L532		
A465	A465	A465		
E466	E466	E466		
F467	F467	F467		
I325	I325	I325		
D326	D326	D326		
E327	E327	E327		
Q328	Q328	Q328		
E265	E265	E265		
E266	E266	E266		
T267	T267	T267		

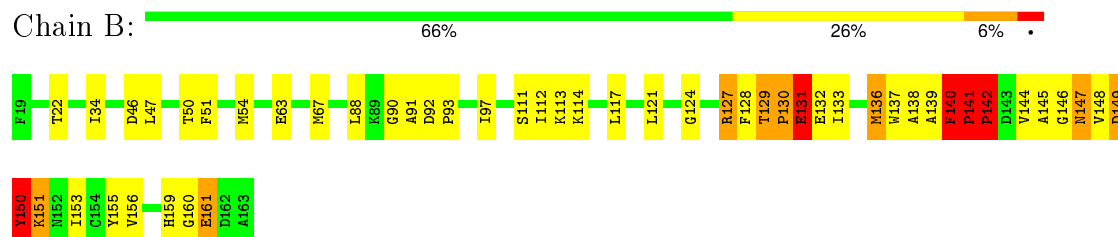
• Molecule 1: SKELETAL MUSCLE MYOSIN II

Chain P:  25% 51% 19%

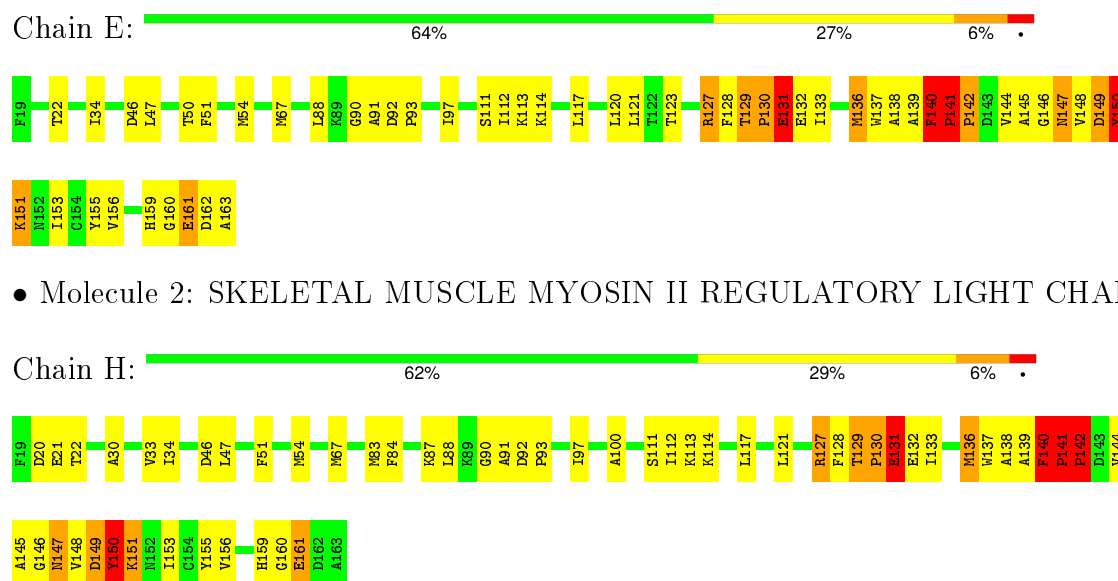
D4	A6	P133	T198	Y268	E330
M7	B7	V134	T199	L269	L331
M8	M7	Y135	A200	L270	M332
A8	A8	M136	E271	E271	A333
A9	A9	P137	S202	K272	D335
D75	D75	K138	G203	S273	T335
Q76	Q76	V139	E204	R274	S336
F77	F77	V140	E205		A337
F78	F78	L141	K206		L338
E12	E12	A13	K207		D339
A14	A14	Y143			L340
N81	N81	R144			L341
P82	P82	G145			G342
P83	P83	K146			F343
K84	K84	K147			S344
Y85	Y85	R148			A345
D86	D86	Q149			D346
K87	K87	E150			E421
I88	I88	A151			F421
E89	E89	P152			V422
D90	D90	P153			L429
M91	M91	H154			V433
A92	A92	I155			E434
M93	M93	F156			E435
M94	M94	S157			L436
T95	T95	T158			M437
F96	F96	S159			F438
L97	L97	D160			L440
H98	H98	M161			M441
E99	E99	A162			V442
P100	P100	Y163			L443
A101	A101	Q164			L444
F165	F165	F165			R444
M166	M166	M166			K446
L167	L167	L167			N446
Y40	Y40	L168			Q447
H42	H42	D169			Q448
Q45	Q45	R170			L449
S46	S46				D450
F47	F47	Q173			E376
V48	V48	S174			E377
K49	K49	I175			Q453
G50	G50	L176			P454
T51	T51	L177			R455
I52	I52	T178			Q456
Y116	Y116	G179			Y457
T117	T117				F458
Y118	Y118	S119			G460
K55	K55	M120			V461
E56	E56	L121			L462
G57	G57	G122			D463
G58	G58	F122			M464
K59	K59	C123			A465
V60	V60	L124			E466
T61	T61	T125			F467
V62	V62	V126			I325
K63	K63	N127			D326
T64	T64	P128			E327
E65	E65	Y129			Q328
		A130			E265
		Y195			E266
		F196			T267
		A197			



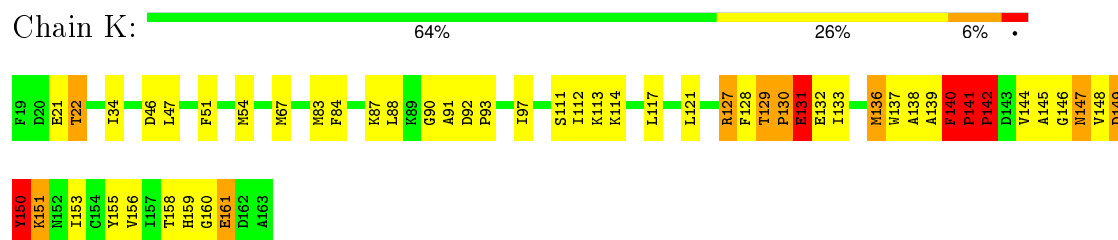
• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN



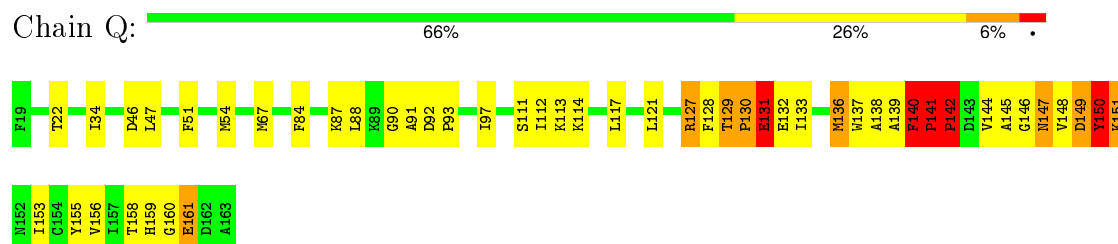
• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN



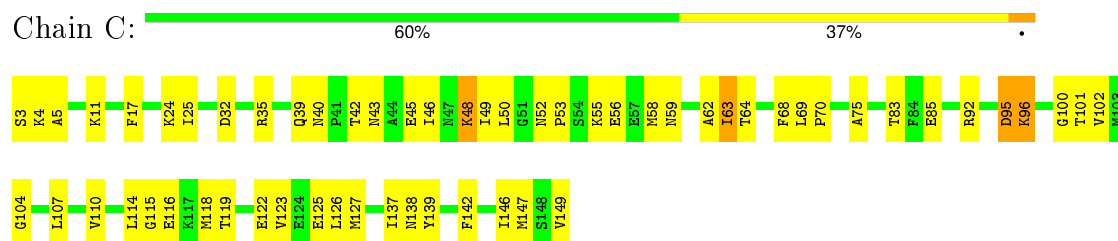
• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN



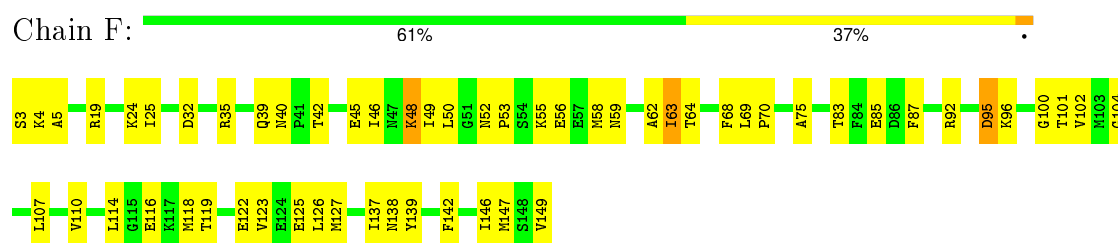
• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN



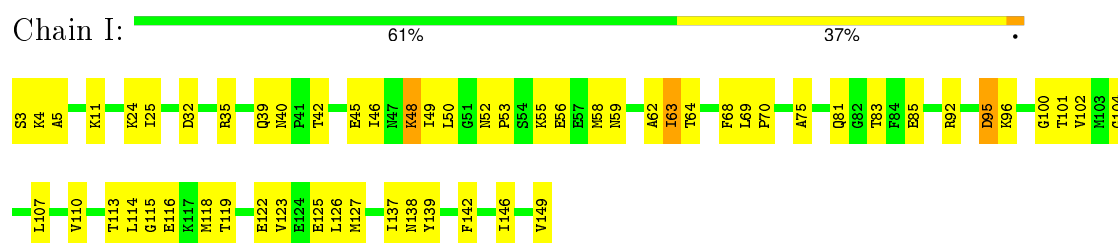
• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN



• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN

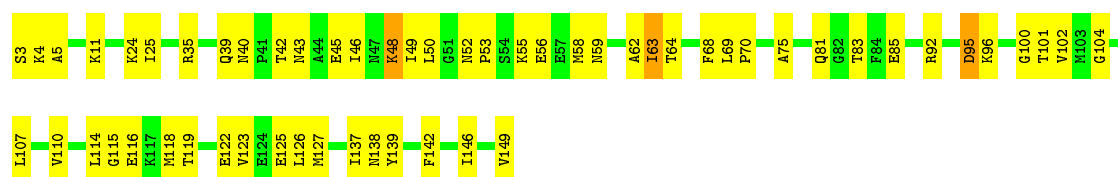


• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN



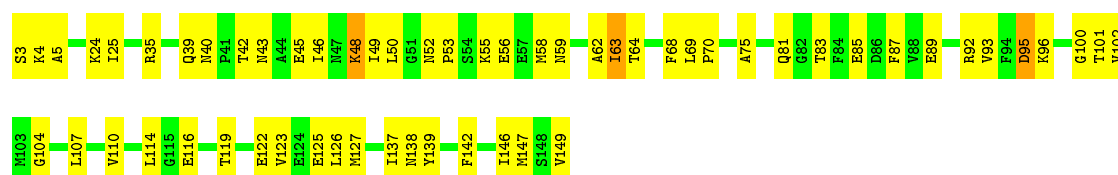
• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN





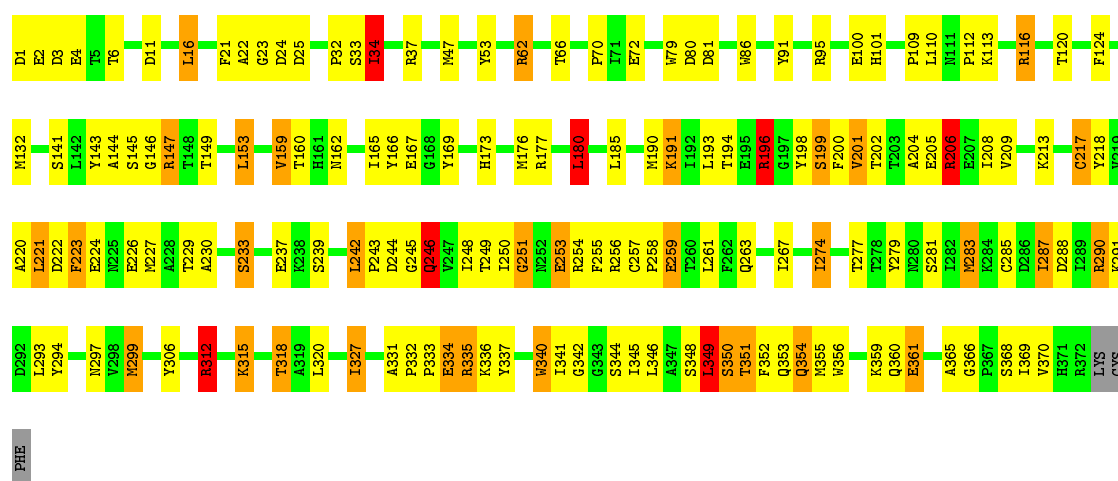
• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN

Chain R: 61% 37% .



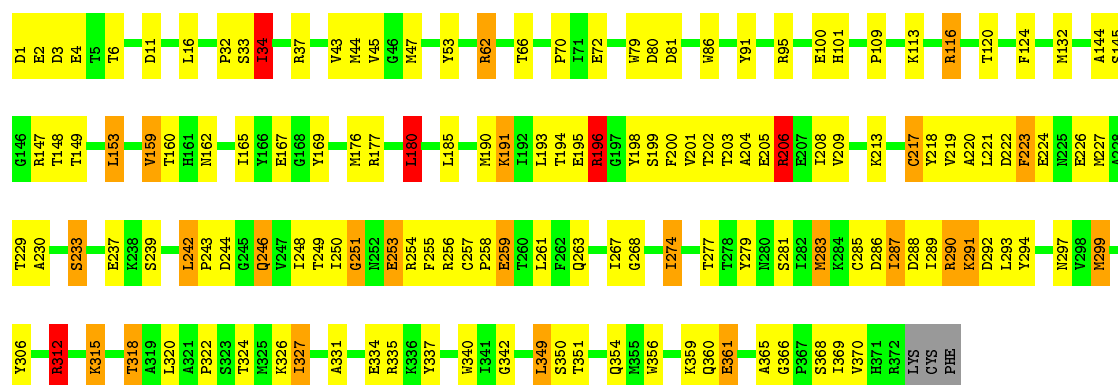
• Molecule 4: SKELETAL MUSCLE ACTIN

Chain 0: 57% 31% 9% ..

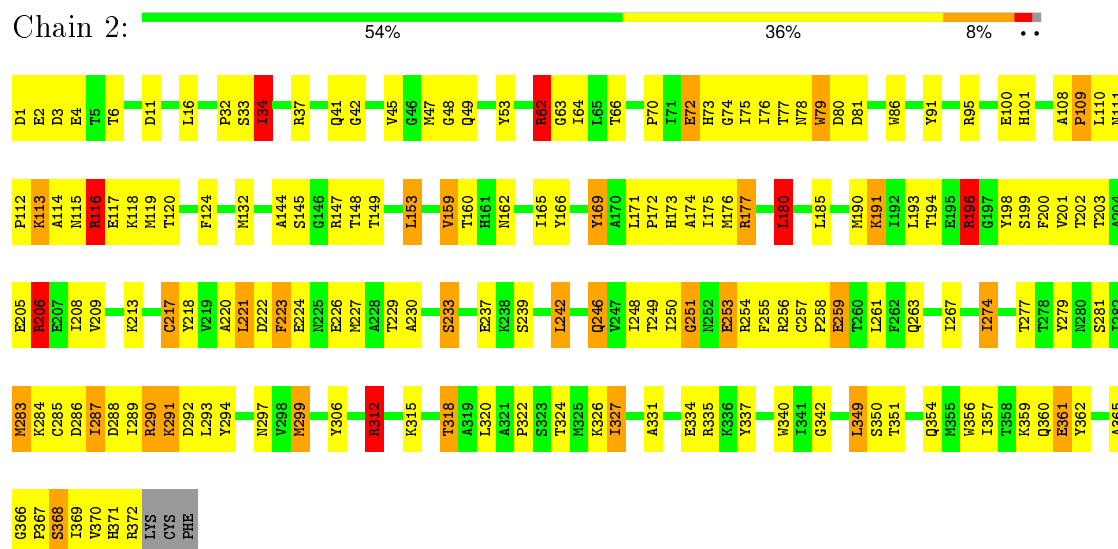


• Molecule 4: SKELETAL MUSCLE ACTIN

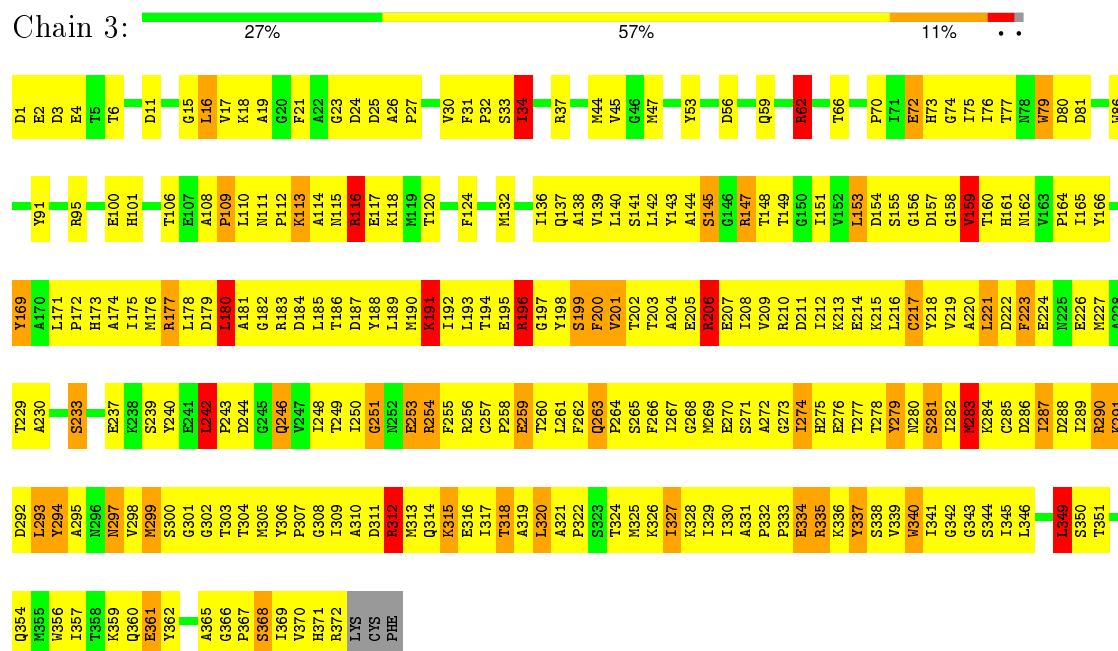
Chain 1: 60% 31% 6% ..



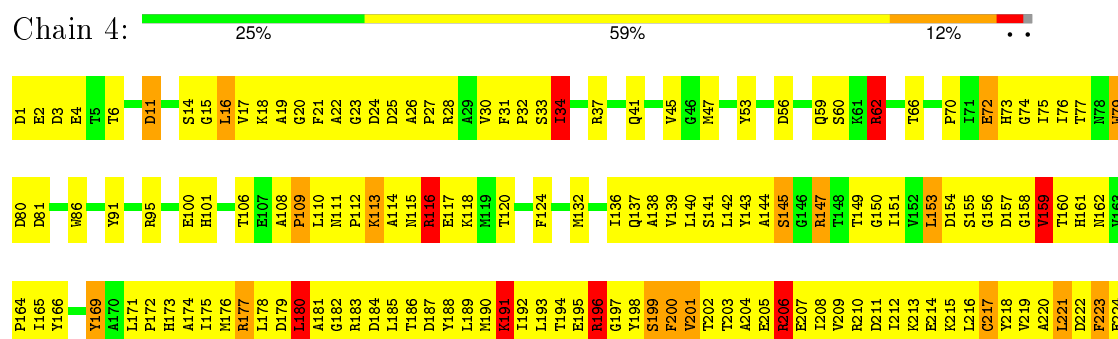
• Molecule 4: SKELETAL MUSCLE ACTIN

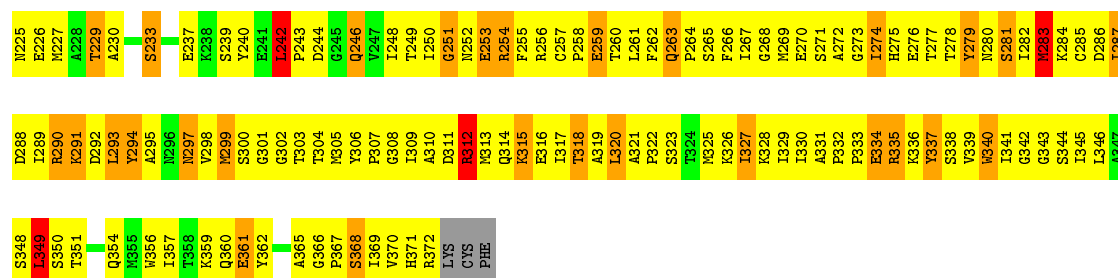


• Molecule 4: SKELETAL MUSCLE ACTIN



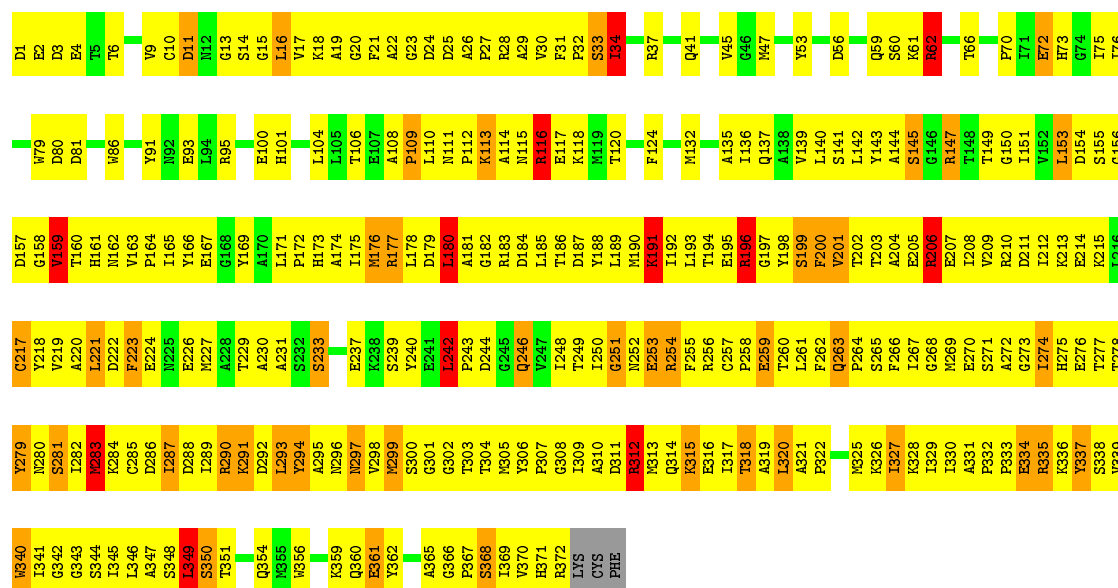
• Molecule 4: SKELETAL MUSCLE ACTIN





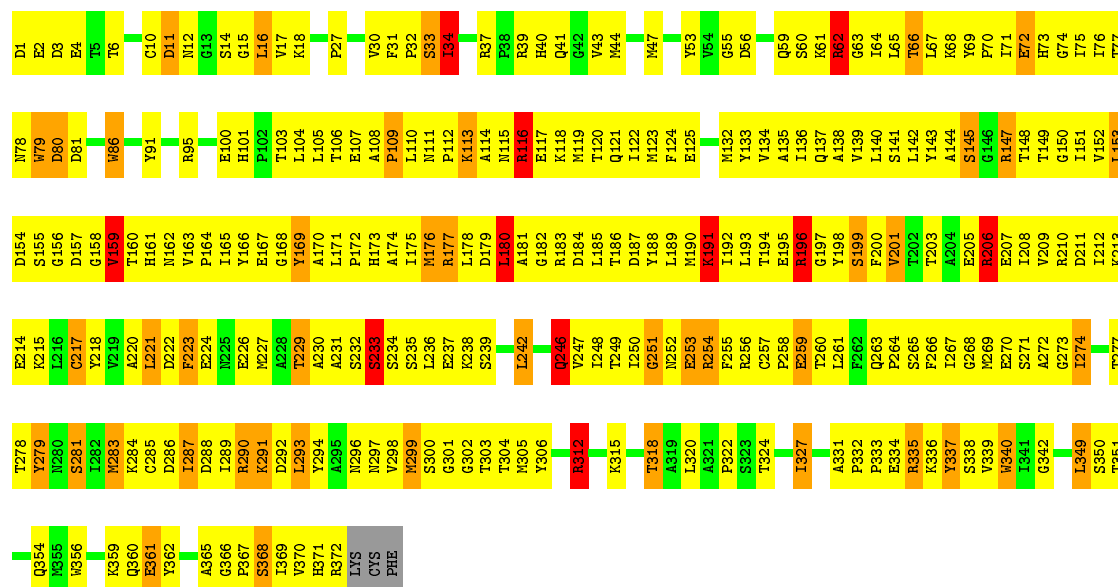
• Molecule 4: SKELETAL MUSCLE ACTIN

Chain 5: 24% 60% 12%

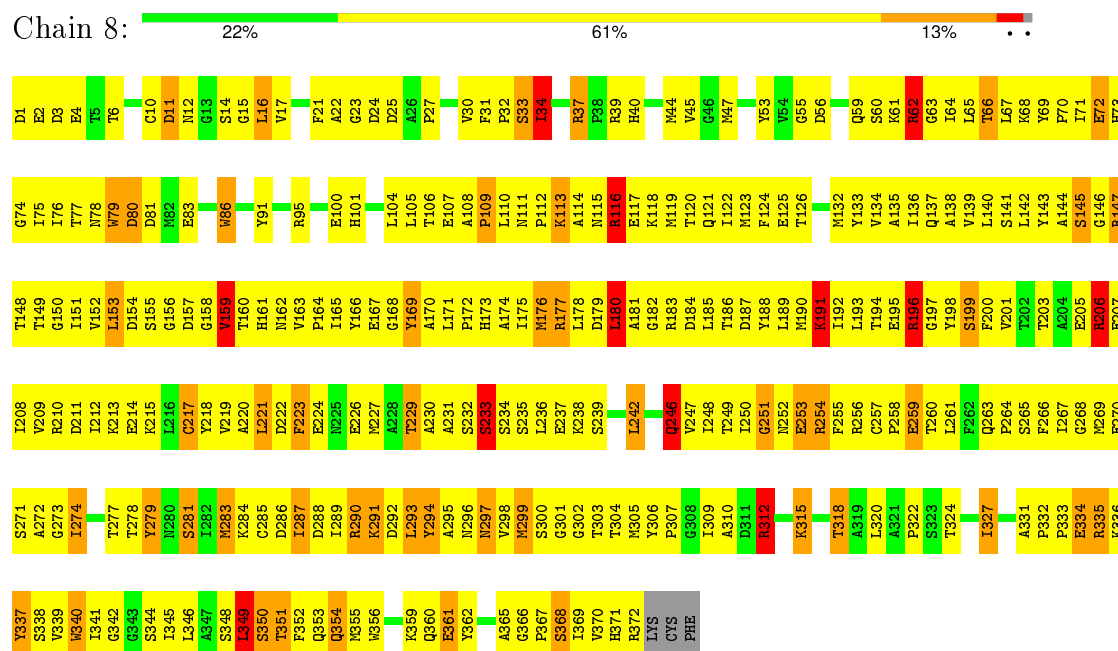


• Molecule 4: SKELETAL MUSCLE ACTIN

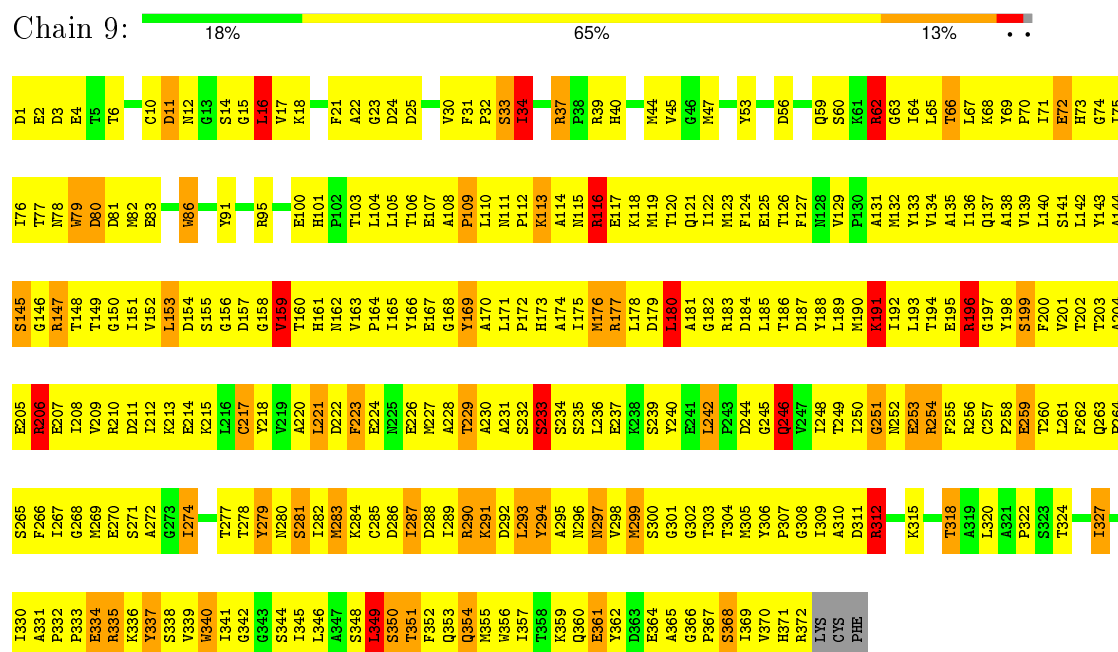
Chain 7: 27% 58% 12%



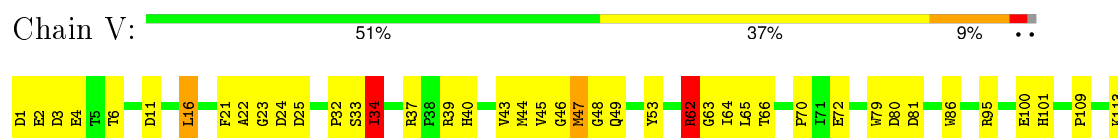
• Molecule 4: SKELETAL MUSCLE ACTIN



• 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%)	1.83	119/8732 (1.4%)
1	J	1.77	66/6449 (1.0%)	1.86	118/8732 (1.4%)
1	P	1.81	66/6449 (1.0%)	1.90	127/8732 (1.5%)
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	17/1548 (1.1%)
2	K	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	R	0.79	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	52/4023 (1.3%)
4	2	0.89	2/2968 (0.1%)	1.64	52/4023 (1.3%)
4	3	0.89	2/2968 (0.1%)	1.64	52/4023 (1.3%)
4	4	0.89	2/2968 (0.1%)	1.64	51/4023 (1.3%)
4	5	0.89	2/2968 (0.1%)	1.64	51/4023 (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	52/4023 (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	50/4023 (1.2%)
4	W	0.89	2/2968 (0.1%)	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	50/4023 (1.2%)
4	Z	0.89	2/2968 (0.1%)	1.64	51/4023 (1.3%)
All	All	1.31	404/85215 (0.5%)	1.68	1415/115341 (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	2	4
1	J	1	6
1	P	1	9
2	B	0	3
2	E	0	3
2	H	0	3
2	K	0	3
2	Q	0	3
3	C	0	2
3	F	0	2
3	I	0	2
3	L	0	2
3	R	0	2
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	6	66

The worst 5 of 404 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	J	649	VAL	CB-CG1	53.25	2.64	1.52
1	A	649	VAL	CB-CG1	53.23	2.64	1.52
1	G	649	VAL	CB-CG1	53.20	2.64	1.52
1	D	649	VAL	CB-CG1	53.20	2.64	1.52

The worst 5 of 1415 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	637	LYS	O-C-N	-58.52	23.71	123.20
1	J	637	LYS	O-C-N	-58.47	23.80	123.20
1	D	637	LYS	O-C-N	-58.46	23.81	123.20
1	P	637	LYS	O-C-N	-58.46	23.82	123.20
1	A	637	LYS	O-C-N	-58.44	23.85	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	75	ASP	CA
1	G	648	THR	CB
1	J	648	THR	CB

5 of 66 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	6754	1510	19
1	D	6797	0	6755	1417	22
1	G	6797	0	6763	1561	0
1	J	6797	0	6754	1418	0
1	P	6797	0	6763	1523	0
2	B	1127	0	1085	239	0
2	E	1127	0	1086	269	0
2	H	1127	0	1088	298	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	1127	0	1088	266	0
2	Q	1127	0	1088	261	0
3	C	1123	0	1083	194	0
3	F	1123	0	1083	168	0
3	I	1123	0	1083	186	0
3	L	1123	0	1083	161	0
3	R	1123	0	1079	229	0
4	0	2906	0	2855	406	0
4	1	2906	0	2864	214	76
4	2	2906	0	2864	174	573
4	3	2906	0	2863	180	3106
4	4	2906	0	2865	98	3233
4	5	2906	0	2865	99	3407
4	7	2906	0	2866	76	3156
4	8	2906	0	2857	321	3226
4	9	2906	0	2855	341	3467
4	V	2906	0	2851	385	416
4	W	2906	0	2851	384	89
4	X	2906	0	2862	212	0
4	Y	2906	0	2863	169	0
4	Z	2906	0	2862	187	0
All	All	85919	0	84678	9656	10395

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 57.

The worst 5 of 9656 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:J:797:PHE:CE1	3:L:146:ILE:HG23	1.21	1.71
1:G:84:MLY:CH1	1:G:724:TYR:HE2	1.03	1.66
1:P:803:TYR:CD1	1:P:807:VAL:HG11	1.22	1.65
1:G:84:MLY:CG	1:G:723:ARG:HD2	1.17	1.64
1:D:798:LEU:HD11	3:F:126:LEU:CD1	1.26	1.63

The worst 5 of 10395 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)
4:5:196:ARG:O	4:9:212:ILE:CG1[1_554]	0.14	2.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:191:LYS:CA	4:9:186:THR:C[1_554]	0.18	2.02
4:3:305:MET:C	4:7:11:ASP:OD1[1_554]	0.21	1.99
4:5:194:THR:C	4:9:209:VAL:CG2[1_554]	0.21	1.99
4:3:186:THR:OG1	4:7:183:ARG:NH2[1_554]	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%)	650 (82%)	113 (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%)	113 (14%)	27 (3%)	5	40
1	J	791/840 (94%)	651 (82%)	113 (14%)	27 (3%)	5	40
1	P	791/840 (94%)	650 (82%)	112 (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	K	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	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%)	334 (90%)	30 (8%)	6 (2%)	12	56
4	2	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	12	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	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	10561/10910 (97%)	9231 (87%)	1071 (10%)	259 (2%)	11	46

5 of 259 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	P	672/672 (100%)	514 (76%)	158 (24%)	1	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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	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	R	117/117 (100%)	112 (96%)	5 (4%)	35	70
4	0	315/318 (99%)	268 (85%)	47 (15%)	4	23
4	1	315/318 (99%)	269 (85%)	46 (15%)	4	24
4	2	315/318 (99%)	269 (85%)	46 (15%)	4	24
4	3	315/318 (99%)	269 (85%)	46 (15%)	4	24
4	4	315/318 (99%)	269 (85%)	46 (15%)	4	24
4	5	315/318 (99%)	269 (85%)	46 (15%)	4	24
4	7	315/318 (99%)	269 (85%)	46 (15%)	4	24
4	8	315/318 (99%)	269 (85%)	46 (15%)	4	24
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%)	269 (85%)	46 (15%)	4	24
All	All	8955/8997 (100%)	7484 (84%)	1471 (16%)	6	19

5 of 1471 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	36	SER
4	0	33	SER
4	X	283	MET
1	P	136	ASN
1	P	471	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 206 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	656	ASN
1	P	563	ASN
4	X	137	GLN
1	J	698	ASN
1	P	188	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

225 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	0.60	0	9,11,13	1.06	1 (11%)
1	MLY	A	138	1	8,10,11	1.34	1 (12%)	9,11,13	0.80	0
1	MLY	A	19	1	8,10,11	1.14	1 (12%)	9,11,13	0.69	0
1	MLY	A	190	1	8,10,11	1.11	1 (12%)	9,11,13	0.70	0
1	MLY	A	236	1	8,10,11	0.37	0	9,11,13	1.33	1 (11%)
1	MLY	A	248	1	8,10,11	0.76	0	9,11,13	0.91	1 (11%)
1	MLY	A	272	1	8,10,11	1.04	1 (12%)	9,11,13	0.57	0
1	MLY	A	295	1	8,10,11	0.74	0	9,11,13	0.46	0
1	MLY	A	296	1	8,10,11	0.62	0	9,11,13	0.77	0
1	MLY	A	30	1	8,10,11	0.67	0	9,11,13	0.82	0
1	MLY	A	348	1	8,10,11	0.83	0	9,11,13	0.81	0
1	MLY	A	35	1	8,10,11	0.56	0	9,11,13	0.70	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	0.64	0	9,11,13	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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	0.56	0
1	MLY	A	415	1	8,10,11	0.74	0	9,11,13	0.45	0
1	MLY	A	431	1	8,10,11	0.46	0	9,11,13	0.77	0
1	MLY	A	436	1	8,10,11	1.09	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	1.05	1 (12%)	9,11,13	0.98	0
1	MLY	A	504	1	8,10,11	0.81	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	1.17	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	0.62	0	9,11,13	0.59	0
1	MLY	A	59	1	8,10,11	0.76	0	9,11,13	0.76	0
1	MLY	A	598	1	8,10,11	0.86	1 (12%)	9,11,13	0.72	0
1	MLY	A	600	1	8,10,11	0.52	0	9,11,13	0.49	0
1	MLY	A	613	1	8,10,11	0.50	0	9,11,13	0.92	0
1	MLY	A	617	1	8,10,11	0.88	1 (12%)	9,11,13	0.47	0
1	MLY	A	63	1	8,10,11	0.83	1 (12%)	9,11,13	0.94	0
1	MLY	A	659	1	8,10,11	0.52	0	9,11,13	0.94	0
1	MLY	A	681	1	8,10,11	0.62	0	9,11,13	0.62	0
1	MLY	A	764	1	8,10,11	0.69	0	9,11,13	0.56	0
1	MLY	A	768	1	8,10,11	0.66	0	9,11,13	0.87	1 (11%)
1	MLY	A	782	1	8,10,11	0.50	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	0.97	1 (12%)	9,11,13	0.58	0
1	MLY	A	837	1	8,10,11	0.54	0	9,11,13	0.57	0
1	MLY	A	839	1	8,10,11	0.66	0	9,11,13	0.79	0
1	MLY	A	84	1	8,10,11	0.45	0	9,11,13	0.79	0
1	MLY	A	87	1	8,10,11	1.16	1 (12%)	9,11,13	0.68	0
1	MLY	D	107	1	8,10,11	0.47	0	9,11,13	0.67	0
1	MLY	D	130	1	8,10,11	0.59	0	9,11,13	1.05	1 (11%)
1	MLY	D	138	1	8,10,11	1.41	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	0.71	0
1	MLY	D	236	1	8,10,11	0.36	0	9,11,13	1.32	1 (11%)
1	MLY	D	248	1	8,10,11	0.71	0	9,11,13	0.92	1 (11%)
1	MLY	D	272	1	8,10,11	1.02	1 (12%)	9,11,13	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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	0.63	0	9,11,13	0.78	0
1	MLY	D	30	1	8,10,11	0.71	0	9,11,13	0.84	1 (11%)
1	MLY	D	348	1	8,10,11	0.78	0	9,11,13	0.81	0
1	MLY	D	35	1	8,10,11	0.59	0	9,11,13	0.67	0
1	MLY	D	353	1	8,10,11	0.86	0	9,11,13	0.79	0
1	MLY	D	367	1	8,10,11	0.63	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	0.55	0
1	MLY	D	415	1	8,10,11	0.77	0	9,11,13	0.45	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	1.13	1 (12%)	9,11,13	0.57	0
1	MLY	D	486	1	8,10,11	0.35	0	9,11,13	0.60	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	0.79	0	9,11,13	0.49	0
1	MLY	D	505	1	8,10,11	0.84	1 (12%)	9,11,13	0.39	0
1	MLY	D	528	1	8,10,11	0.83	0	9,11,13	1.17	1 (11%)
1	MLY	D	55	1	8,10,11	0.64	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	0.64	0	9,11,13	0.58	0
1	MLY	D	59	1	8,10,11	0.78	0	9,11,13	0.76	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	0.52	0	9,11,13	0.47	0
1	MLY	D	613	1	8,10,11	0.49	0	9,11,13	0.91	0
1	MLY	D	617	1	8,10,11	0.92	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	0.94	0
1	MLY	D	681	1	8,10,11	0.58	0	9,11,13	0.64	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	0.49	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	0.98	1 (12%)	9,11,13	0.58	0
1	MLY	D	837	1	8,10,11	0.55	0	9,11,13	0.58	0
1	MLY	D	839	1	8,10,11	0.67	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	0.45	0	9,11,13	0.67	0
1	MLY	G	130	1	8,10,11	0.58	0	9,11,13	1.08	1 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	MLY	G	138	1	8,10,11	1.36	1 (12%)	9,11,13	0.81	0
1	MLY	G	19	1	8,10,11	1.17	1 (12%)	9,11,13	0.69	0
1	MLY	G	190	1	8,10,11	1.09	1 (12%)	9,11,13	0.70	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	0.73	0	9,11,13	0.94	1 (11%)
1	MLY	G	272	1	8,10,11	1.01	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	0.62	0	9,11,13	0.77	0
1	MLY	G	30	1	8,10,11	0.67	0	9,11,13	0.84	1 (11%)
1	MLY	G	348	1	8,10,11	0.83	0	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	0.87	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	0.52	0	9,11,13	0.93	1 (11%)
1	MLY	G	385	1	8,10,11	0.99	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	1.10	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	1.10	1 (12%)	9,11,13	0.97	0
1	MLY	G	504	1	8,10,11	0.77	0	9,11,13	0.49	0
1	MLY	G	505	1	8,10,11	0.88	1 (12%)	9,11,13	0.41	0
1	MLY	G	528	1	8,10,11	0.80	0	9,11,13	1.18	1 (11%)
1	MLY	G	55	1	8,10,11	0.67	0	9,11,13	0.99	0
1	MLY	G	551	1	8,10,11	0.50	0	9,11,13	0.66	0
1	MLY	G	553	1,4	8,10,11	0.64	0	9,11,13	0.58	0
1	MLY	G	59	1	8,10,11	0.75	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	0.53	0	9,11,13	0.47	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	0.46	0
1	MLY	G	63	1	8,10,11	0.80	0	9,11,13	0.95	0
1	MLY	G	659	1	8,10,11	0.53	0	9,11,13	0.94	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	0.65	0	9,11,13	0.58	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	0.64	0	9,11,13	0.97	1 (11%)
1	MLY	G	833	1	8,10,11	0.97	1 (12%)	9,11,13	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	MLY	G	837	1	8,10,11	0.52	0	9,11,13	0.55	0
1	MLY	G	839	1	8,10,11	0.66	0	9,11,13	0.79	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	0.67	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	0.58	0	9,11,13	1.06	1 (11%)
1	MLY	J	138	1	8,10,11	1.34	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	1.11	1 (12%)	9,11,13	0.70	0
1	MLY	J	236	1	8,10,11	0.38	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	1.06	1 (12%)	9,11,13	0.57	0
1	MLY	J	295	1	8,10,11	0.70	0	9,11,13	0.48	0
1	MLY	J	296	1	8,10,11	0.66	0	9,11,13	0.77	1 (11%)
1	MLY	J	30	1	8,10,11	0.68	0	9,11,13	0.82	1 (11%)
1	MLY	J	348	1	8,10,11	0.79	0	9,11,13	0.80	0
1	MLY	J	35	1	8,10,11	0.58	0	9,11,13	0.67	0
1	MLY	J	353	1	8,10,11	0.86	0	9,11,13	0.78	0
1	MLY	J	367	1	8,10,11	0.65	0	9,11,13	0.61	0
1	MLY	J	369	1	8,10,11	0.53	0	9,11,13	0.93	1 (11%)
1	MLY	J	385	1	8,10,11	1.04	1 (12%)	9,11,13	0.55	0
1	MLY	J	415	1	8,10,11	0.79	0	9,11,13	0.44	0
1	MLY	J	431	1	8,10,11	0.45	0	9,11,13	0.78	0
1	MLY	J	436	1	8,10,11	1.08	1 (12%)	9,11,13	0.57	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	1.10	1 (12%)	9,11,13	0.99	0
1	MLY	J	504	1	8,10,11	0.75	0	9,11,13	0.49	0
1	MLY	J	505	1	8,10,11	0.93	1 (12%)	9,11,13	0.37	0
1	MLY	J	528	1	8,10,11	0.81	0	9,11,13	1.16	1 (11%)
1	MLY	J	55	1	8,10,11	0.65	0	9,11,13	0.99	0
1	MLY	J	551	1	8,10,11	0.51	0	9,11,13	0.66	0
1	MLY	J	553	1	8,10,11	0.61	0	9,11,13	0.58	0
1	MLY	J	59	1	8,10,11	0.77	0	9,11,13	0.77	0
1	MLY	J	598	1	8,10,11	0.85	1 (12%)	9,11,13	0.71	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	0.48	0	9,11,13	0.93	0
1	MLY	J	617	1	8,10,11	0.90	1 (12%)	9,11,13	0.46	0
1	MLY	J	63	1	8,10,11	0.80	0	9,11,13	0.94	0
1	MLY	J	659	1	8,10,11	0.54	0	9,11,13	0.93	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	MLY	J	681	1	8,10,11	0.62	0	9,11,13	0.64	0
1	MLY	J	764	1	8,10,11	0.65	0	9,11,13	0.58	0
1	MLY	J	768	1	8,10,11	0.66	0	9,11,13	0.86	0
1	MLY	J	782	1	8,10,11	0.50	0	9,11,13	0.94	1 (11%)
1	MLY	J	827	1	8,10,11	0.71	0	9,11,13	0.95	1 (11%)
1	MLY	J	833	1	8,10,11	1.05	1 (12%)	9,11,13	0.57	0
1	MLY	J	837	1	8,10,11	0.53	0	9,11,13	0.58	0
1	MLY	J	839	1	8,10,11	0.68	0	9,11,13	0.77	0
1	MLY	J	84	1	8,10,11	0.46	0	9,11,13	0.79	0
1	MLY	J	87	1	8,10,11	1.17	1 (12%)	9,11,13	0.68	0
1	MLY	P	107	1	8,10,11	0.45	0	9,11,13	0.68	0
1	MLY	P	130	1	8,10,11	0.56	0	9,11,13	1.06	1 (11%)
1	MLY	P	138	1	8,10,11	1.34	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
1	MLY	P	190	1	8,10,11	1.11	1 (12%)	9,11,13	0.70	0
1	MLY	P	236	1	8,10,11	0.38	0	9,11,13	1.31	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	1.04	1 (12%)	9,11,13	0.56	0
1	MLY	P	295	1	8,10,11	0.71	0	9,11,13	0.48	0
1	MLY	P	296	1	8,10,11	0.63	0	9,11,13	0.78	1 (11%)
1	MLY	P	30	1	8,10,11	0.69	0	9,11,13	0.82	0
1	MLY	P	348	1	8,10,11	0.79	0	9,11,13	0.81	0
1	MLY	P	35	1	8,10,11	0.58	0	9,11,13	0.66	0
1	MLY	P	353	1	8,10,11	0.86	0	9,11,13	0.78	0
1	MLY	P	367	1	8,10,11	0.63	0	9,11,13	0.61	0
1	MLY	P	369	1	8,10,11	0.54	0	9,11,13	0.92	1 (11%)
1	MLY	P	385	1	8,10,11	1.02	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	1.11	1 (12%)	9,11,13	0.56	0
1	MLY	P	486	1	8,10,11	0.32	0	9,11,13	0.61	0
1	MLY	P	49	1	8,10,11	1.11	1 (12%)	9,11,13	1.00	0
1	MLY	P	504	1	8,10,11	0.73	0	9,11,13	0.47	0
1	MLY	P	505	1	8,10,11	0.92	1 (12%)	9,11,13	0.37	0
1	MLY	P	528	1	8,10,11	0.81	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	0.65	0
1	MLY	P	553	1	8,10,11	0.62	0	9,11,13	0.58	0
1	MLY	P	59	1	8,10,11	0.78	0	9,11,13	0.78	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	MLY	P	598	1	8,10,11	0.85	1 (12%)	9,11,13	0.70	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	0.49	0	9,11,13	0.93	0
1	MLY	P	617	1	8,10,11	0.93	1 (12%)	9,11,13	0.46	0
1	MLY	P	63	1	8,10,11	0.79	0	9,11,13	0.94	0
1	MLY	P	659	1	8,10,11	0.52	0	9,11,13	0.94	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	0.66	0	9,11,13	0.86	0
1	MLY	P	782	1	8,10,11	0.50	0	9,11,13	0.95	1 (11%)
1	MLY	P	827	1	8,10,11	0.65	0	9,11,13	0.94	1 (11%)
1	MLY	P	833	1	8,10,11	1.03	1 (12%)	9,11,13	0.58	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	0.69	0	9,11,13	0.76	0
1	MLY	P	84	1	8,10,11	0.45	0	9,11,13	0.79	0
1	MLY	P	87	1	8,10,11	1.21	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	J	296	1	-	0/7/9/11	0/0/0/0
1	MLY	J	30	1	-	0/7/9/11	0/0/0/0
1	MLY	J	348	1	-	0/7/9/11	0/0/0/0
1	MLY	J	35	1	-	0/7/9/11	0/0/0/0
1	MLY	J	353	1	-	0/7/9/11	0/0/0/0
1	MLY	J	367	1	-	0/7/9/11	0/0/0/0
1	MLY	J	369	1	-	0/7/9/11	0/0/0/0
1	MLY	J	385	1	-	0/7/9/11	0/0/0/0
1	MLY	J	415	1	-	0/7/9/11	0/0/0/0
1	MLY	J	431	1	-	0/7/9/11	0/0/0/0
1	MLY	J	436	1	-	0/7/9/11	0/0/0/0
1	MLY	J	486	1	-	0/7/9/11	0/0/0/0
1	MLY	J	49	1	-	0/7/9/11	0/0/0/0
1	MLY	J	504	1	-	0/7/9/11	0/0/0/0
1	MLY	J	505	1	-	0/7/9/11	0/0/0/0
1	MLY	J	528	1	-	0/7/9/11	0/0/0/0
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	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

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

The worst 5 of 61 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	138	MLY	CB-CA	-3.71	1.48	1.53
1	G	138	MLY	CB-CA	-3.57	1.48	1.53
1	P	138	MLY	CB-CA	-3.52	1.48	1.53
1	A	138	MLY	CB-CA	-3.51	1.48	1.53
1	J	138	MLY	CB-CA	-3.51	1.48	1.53

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	236	MLY	O-C-CA	-3.24	117.04	125.72
1	D	236	MLY	O-C-CA	-3.22	117.08	125.72
1	G	236	MLY	O-C-CA	-3.22	117.08	125.72
1	P	236	MLY	O-C-CA	-3.21	117.11	125.72
1	J	236	MLY	O-C-CA	-3.21	117.13	125.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

150 monomers are involved in 617 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	2	0
1	A	30	MLY	1	0
1	A	348	MLY	5	0
1	A	369	MLY	1	0
1	A	415	MLY	1	0
1	A	436	MLY	2	0
1	A	486	MLY	3	0
1	A	49	MLY	3	0
1	A	505	MLY	25	0
1	A	528	MLY	2	0
1	A	55	MLY	1	0
1	A	551	MLY	2	0
1	A	553	MLY	18	3
1	A	59	MLY	2	0
1	A	598	MLY	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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	10	0
1	A	768	MLY	6	0
1	A	782	MLY	7	0
1	A	833	MLY	1	0
1	A	837	MLY	12	0
1	A	839	MLY	8	0
1	A	87	MLY	3	0
1	D	107	MLY	2	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	2	0
1	D	486	MLY	3	0
1	D	49	MLY	3	0
1	D	528	MLY	3	0
1	D	55	MLY	1	0
1	D	551	MLY	1	0
1	D	553	MLY	16	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	7	0
1	D	782	MLY	43	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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	G	248	MLY	2	0
1	G	272	MLY	1	0
1	G	295	MLY	6	0
1	G	296	MLY	2	0
1	G	30	MLY	1	0
1	G	348	MLY	4	0
1	G	369	MLY	1	0
1	G	415	MLY	1	0
1	G	436	MLY	2	0
1	G	486	MLY	3	0
1	G	49	MLY	2	0
1	G	505	MLY	16	0
1	G	528	MLY	3	0
1	G	55	MLY	1	0
1	G	553	MLY	27	0
1	G	59	MLY	3	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	20	0
1	G	768	MLY	2	0
1	G	782	MLY	1	0
1	G	837	MLY	1	0
1	G	839	MLY	4	0
1	G	84	MLY	33	0
1	G	87	MLY	2	0
1	J	107	MLY	2	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	5	0
1	J	415	MLY	1	0
1	J	436	MLY	2	0
1	J	486	MLY	3	0
1	J	49	MLY	2	0
1	J	505	MLY	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	J	528	MLY	3	0
1	J	55	MLY	1	0
1	J	553	MLY	11	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
1	J	659	MLY	2	0
1	J	764	MLY	1	0
1	J	768	MLY	5	0
1	J	782	MLY	1	0
1	J	837	MLY	1	0
1	J	839	MLY	9	0
1	J	84	MLY	18	0
1	J	87	MLY	3	0
1	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	3	0
1	P	505	MLY	8	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	2	0
1	P	764	MLY	1	0
1	P	782	MLY	1	0
1	P	837	MLY	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	P	839	MLY	8	0
1	P	84	MLY	32	0
1	P	87	MLY	3	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.