



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:31 PM BST

PDB ID : 1O1D  
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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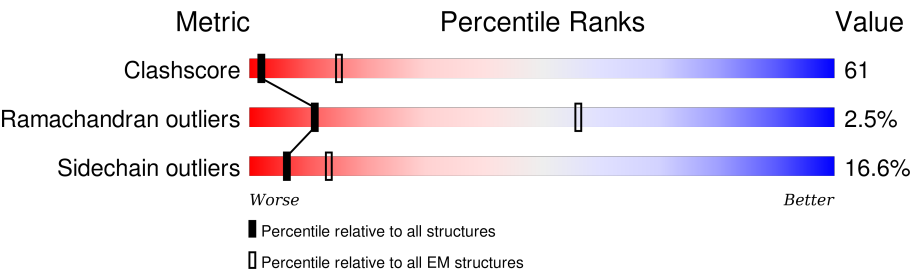
MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk27241

# 1 Overall quality at a glance 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.














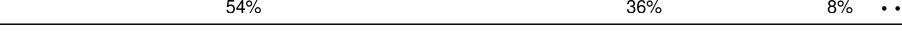

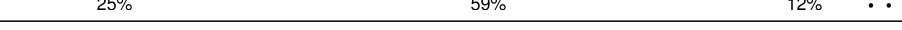


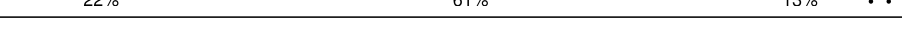
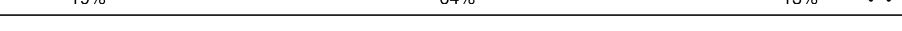



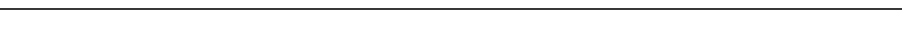

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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	<div><div>25%</div><div>52%</div><div>20%</div><div>.</div></div>
1	D	840	<div><div>26%</div><div>52%</div><div>18%</div><div>.</div></div>
1	G	840	<div><div>25%</div><div>52%</div><div>19%</div><div>.</div></div>
1	J	840	<div><div>26%</div><div>50%</div><div>19%</div><div>.</div></div>
1	M	840	<div><div>25%</div><div>51%</div><div>20%</div><div>.</div></div>
1	P	840	<div><div>26%</div><div>51%</div><div>20%</div><div>.</div></div>
2	B	145	<div><div>65%</div><div>26%</div><div>6%</div><div>.</div></div>
2	E	145	<div><div>64%</div><div>27%</div><div>6%</div><div>.</div></div>
2	H	145	<div><div>63%</div><div>28%</div><div>6%</div><div>.</div></div>

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Mol	Chain	Length	Quality of chain
2	K	145	 63% 27% 6% .
2	N	145	 66% 26% 6% .
2	Q	145	 66% 26% 6% .
3	C	147	 61% 37% .
3	F	147	 60% 38% .
3	I	147	 60% 38% .
3	L	147	 60% 38% .
3	O	147	 60% 37% .
3	R	147	 59% 38% .
4	0	375	 57% 32% 8% ..
4	1	375	 59% 31% 7% ..
4	2	375	 54% 36% 8% ..
4	3	375	 27% 57% 11% ..
4	4	375	 25% 59% 12% ..
4	5	375	 24% 60% 12% ..
4	7	375	 26% 58% 12% ..
4	8	375	 22% 61% 13% ..
4	9	375	 19% 64% 13% ..
4	V	375	 51% 37% 9% ..
4	W	375	 55% 35% 8% ..
4	X	375	 61% 29% 7% ..
4	Y	375	 62% 29% 7% ..
4	Z	375	 57% 32% 8% ..

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	MLY	A	505	-	-	X	-
1	MLY	A	553	-	-	X	-
1	MLY	A	764	-	-	X	-
1	MLY	A	768	-	-	X	-
1	MLY	A	782	-	-	X	-
1	MLY	A	839	-	-	X	-
1	MLY	D	553	-	-	X	-
1	MLY	D	764	-	-	X	-
1	MLY	D	768	-	-	X	-
1	MLY	D	782	-	-	X	-
1	MLY	G	553	-	-	X	-
1	MLY	G	764	-	-	X	-
1	MLY	G	768	-	-	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	35	-	-	X	-
1	MLY	M	505	-	-	X	-
1	MLY	M	553	-	-	X	-
1	MLY	M	782	-	-	X	-
1	MLY	M	839	-	-	X	-
1	MLY	M	84	-	-	X	-
1	MLY	P	764	-	-	X	-
1	MLY	P	839	-	-	X	-

## 2 Entry composition

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

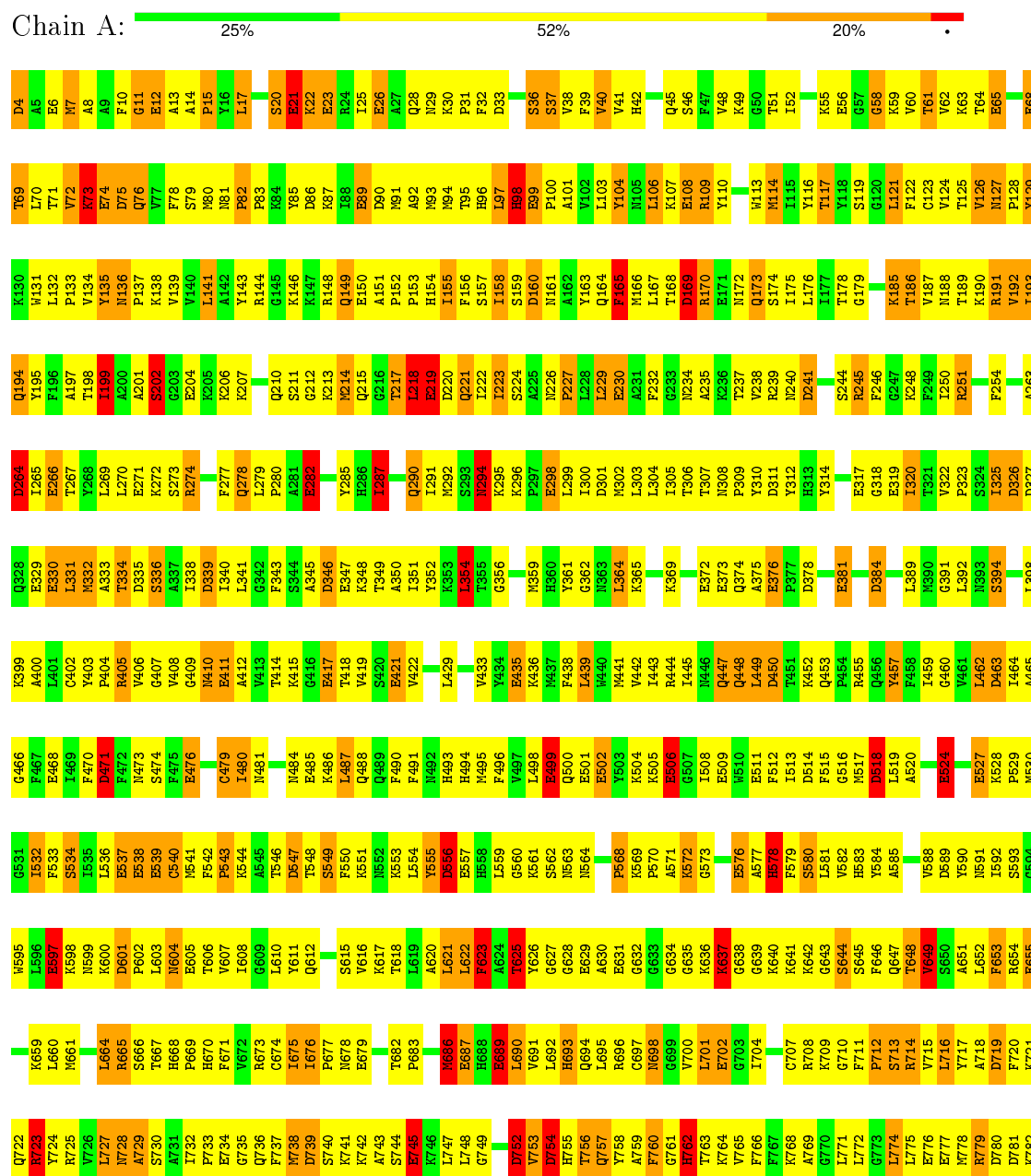
- Molecule 4 is a protein called SKELETAL MUSCLE ACTIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	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

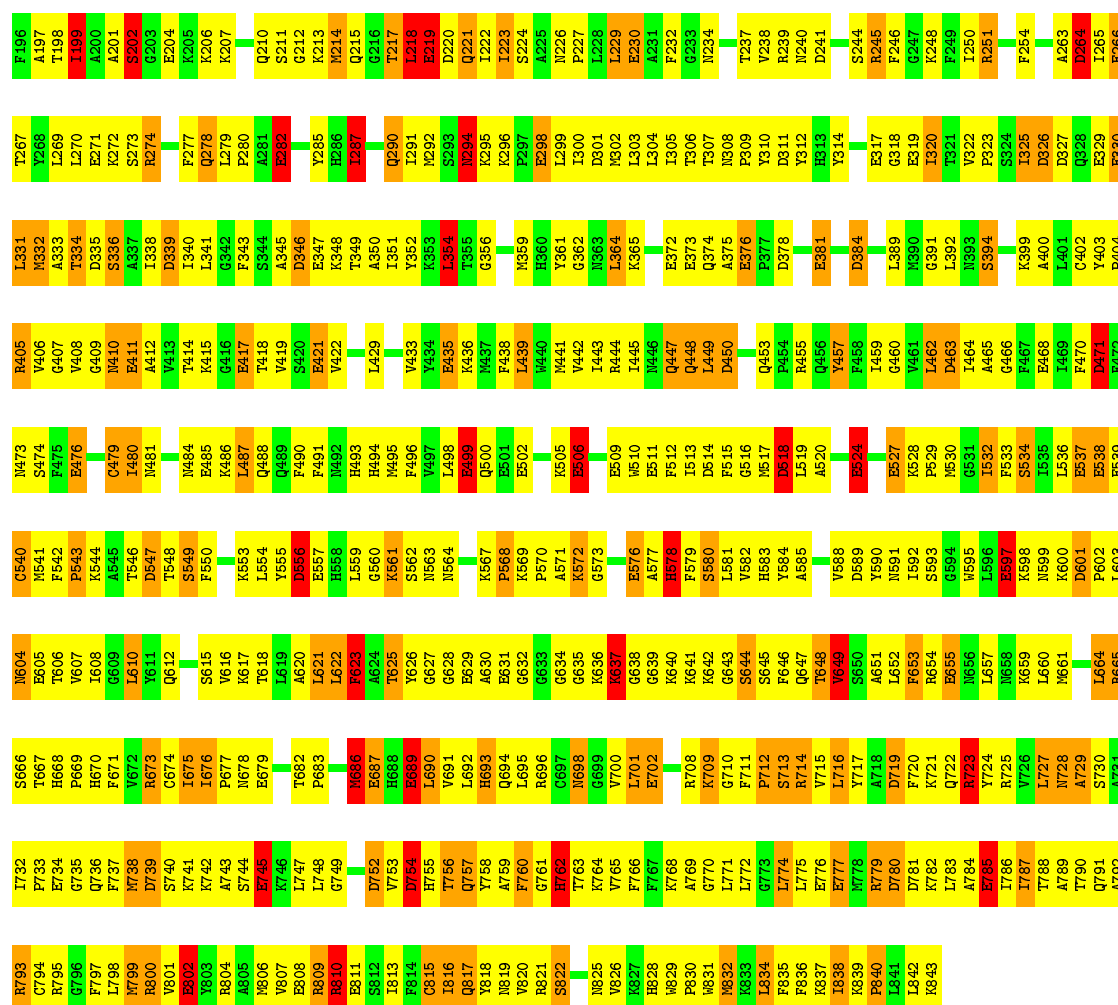


D4	A5	E6	M7	A8	A9	F10	G11	E12	A13	A14	P15	Y16	L17	S20	K21	K22	E23	R24	I25	E26	A27	Q28	N29	K30	P31	F32	D33	S36	S37	F38	V39	V40	V41	H42	Q45	S46	F47	K48	G50	I51	I52	K55	E56	G57	G58	K59	V60	T61	K62	K63	T64	E65	E66
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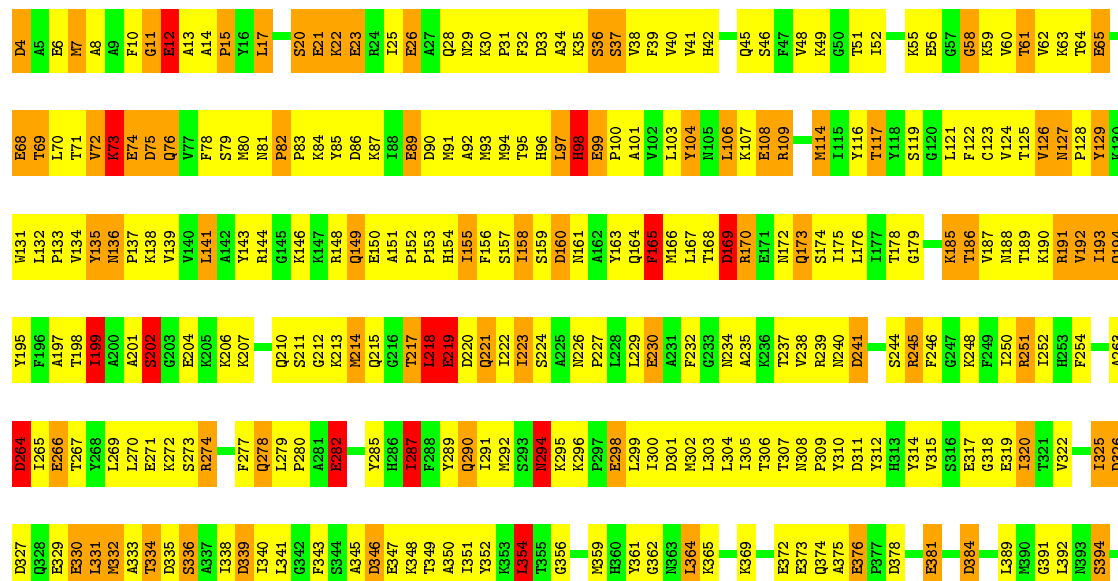
- Molecule 1: SKELETAL MUSCLE MYOSIN II

L132	T69	D4
P133	L70	A5
V134	T71	B6
Y135	V72	M7
M136	K73	A8
P137	E74	A9
K138	D75	F10
V139	Q76	G11
L140	V77	E12
L141	F78	A13
A142	S79	A14
Y143	M80	P15
R144	N81	Y16
K146	P83	L17
K147	K84	S20
R148	Y85	E21
Q149	D86	K22
E150	K87	E23
A151	I88	R24
P152	E89	I25
P153	D90	E26
H154	N91	A27
I155	A92	Q28
F156	M93	I29
K157	M94	K30
I158	T95	P31
S159	H96	F32
D160	L97	D33
M161	H98	S36
A162	E99	S37
Y163	P100	V38
K164	A101	F39
F165	V102	V40
M166	L103	V41
L167	Y104	A42
T168	N105	
D169	L106	Q45
R170	K107	S46
E171	E108	F47
M172	R109	V48
Q173	M114	K49
S174	I115	S50
I175	V116	T51
L177	T117	I52
T178	Y118	
G179	S119	K55
	G120	E56
	L121	S57
K185	F122	S58
M187	K123	K59
R188	V124	V60
T189	T125	T61
K190	V126	V62
R191	N127	K63
V192	P128	T64
I193	Y129	D65
Q194	K130	
	R131	S68

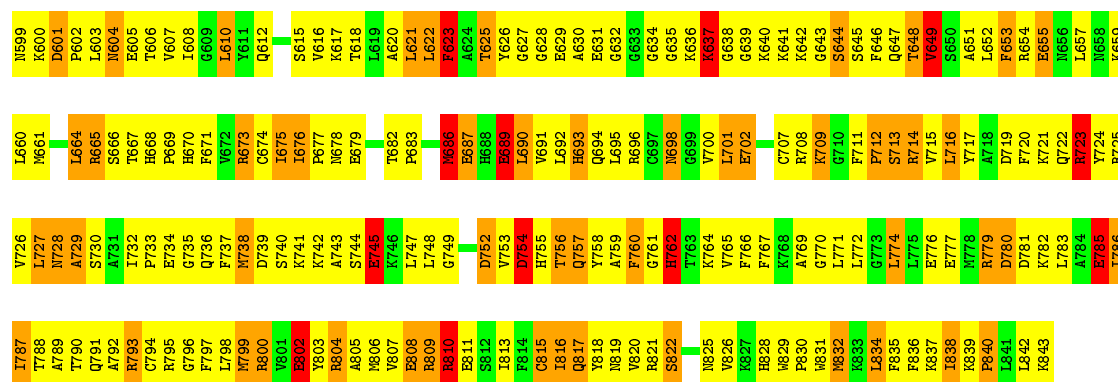


## ● Molecule 1: SKELETAL MUSCLE MYOSIN II

Chain M: 25% 51% 20%

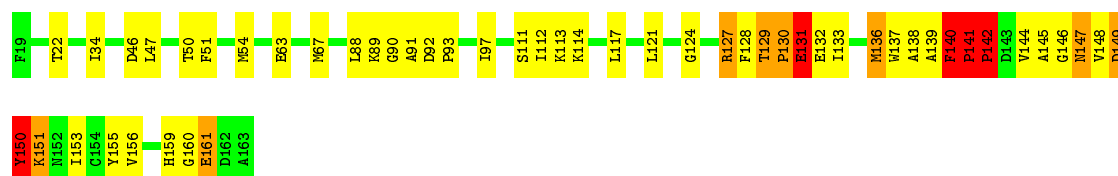






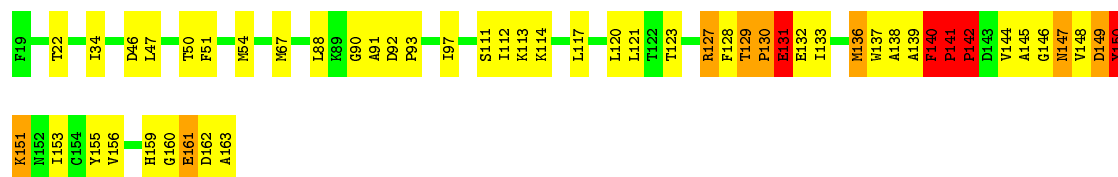
• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

Chain B: 65% 26% 6%



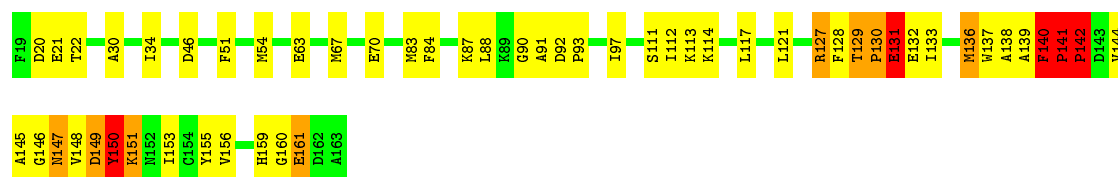
• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

Chain E: 64% 27% 6%



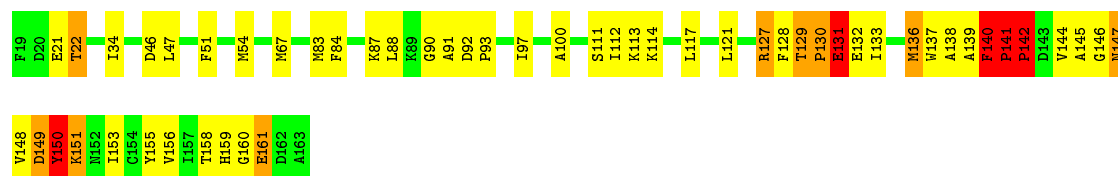
• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

Chain H: 63% 28% 6%

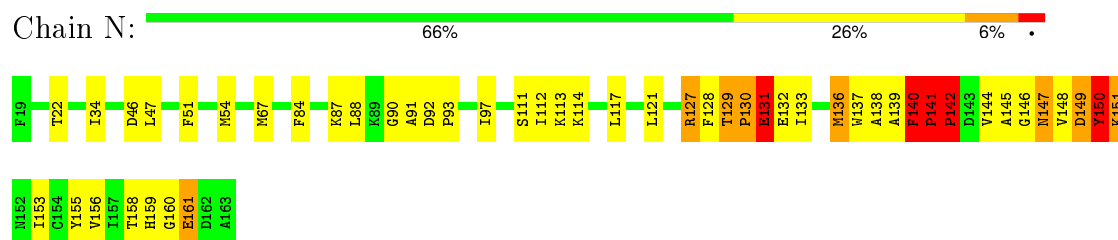


• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

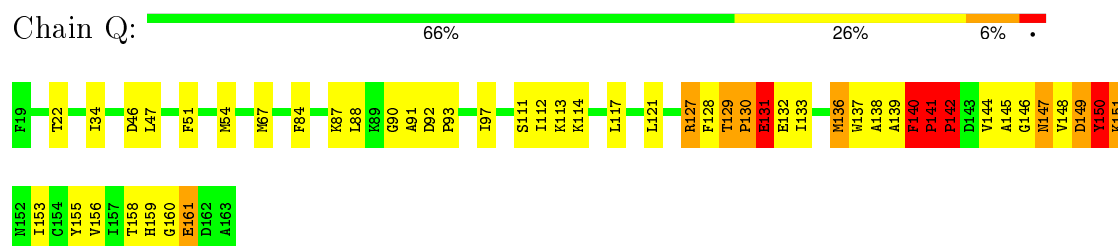
Chain K: 63% 27% 6%



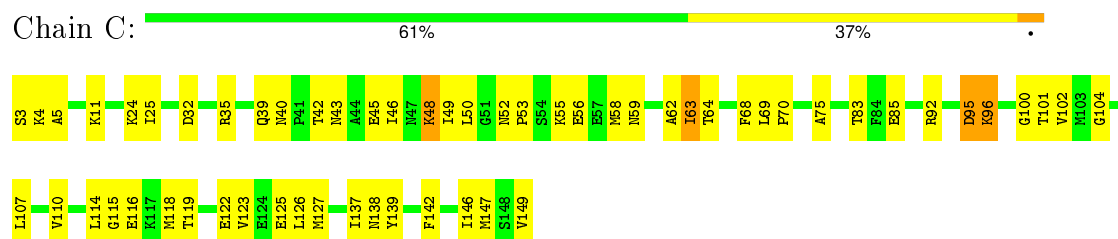
- Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN



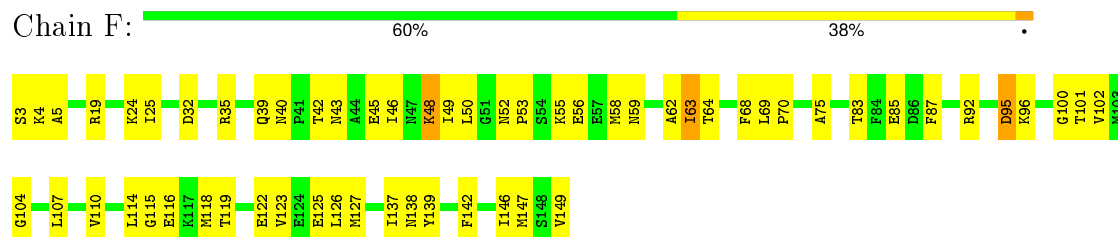
- Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN



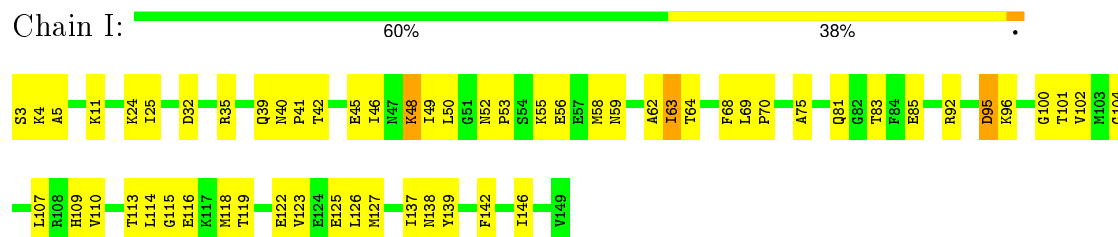
- Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN



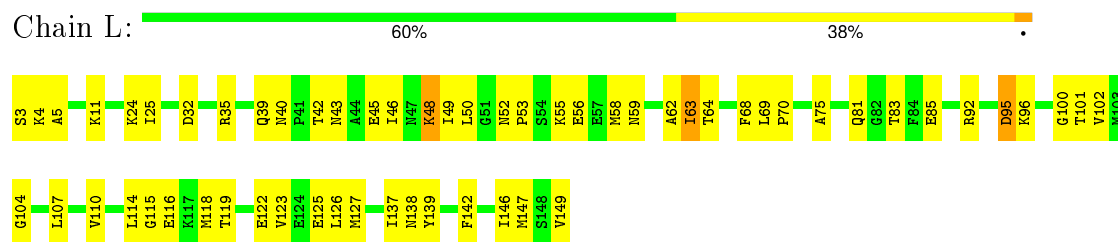
- Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN



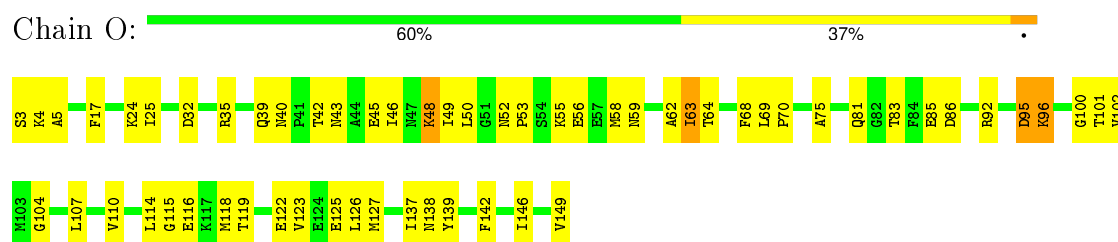
- Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN



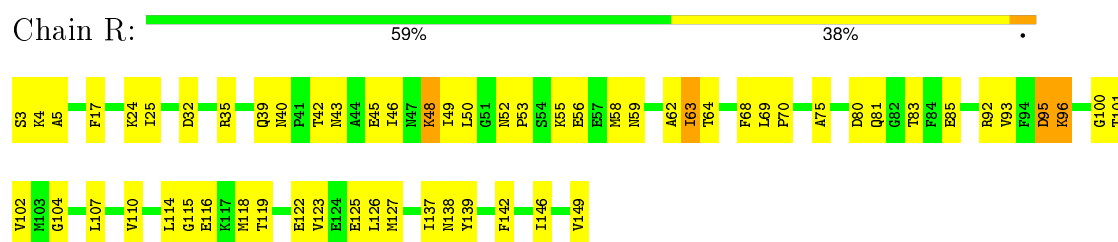
- Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN



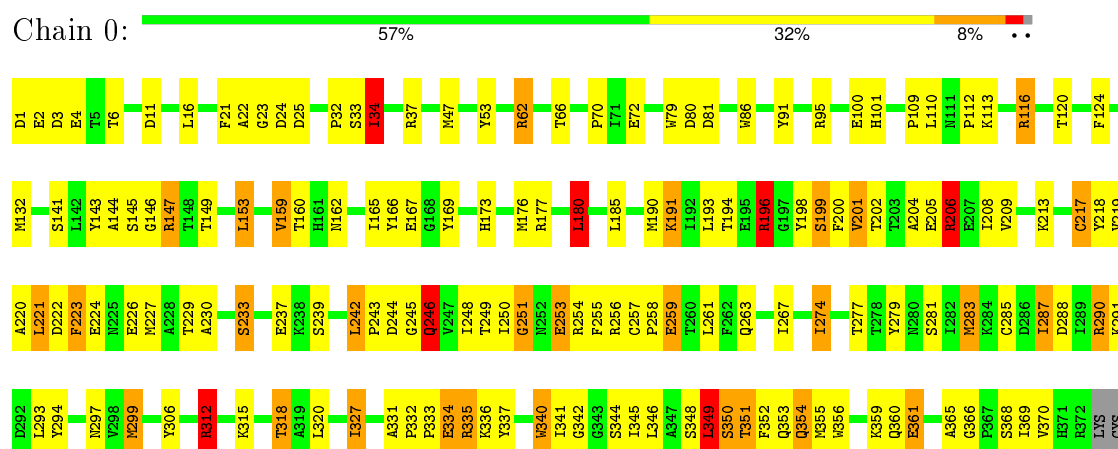
• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN



• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN



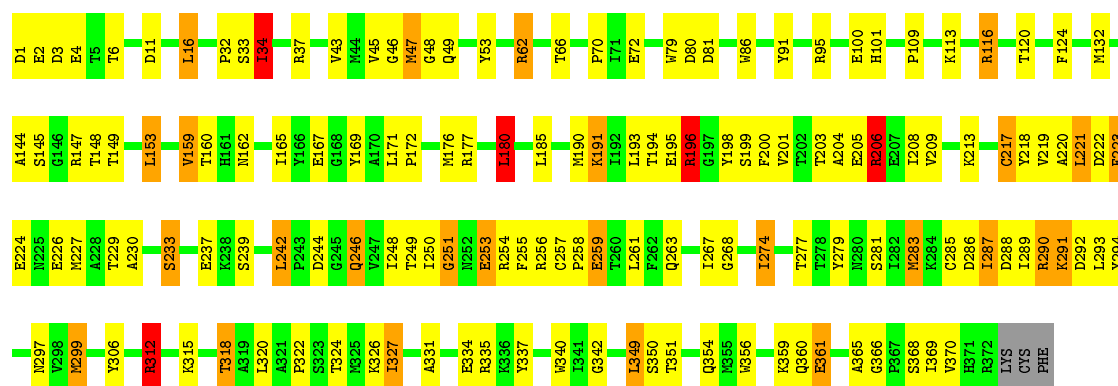
• Molecule 4: SKELETAL MUSCLE ACTIN



PHE

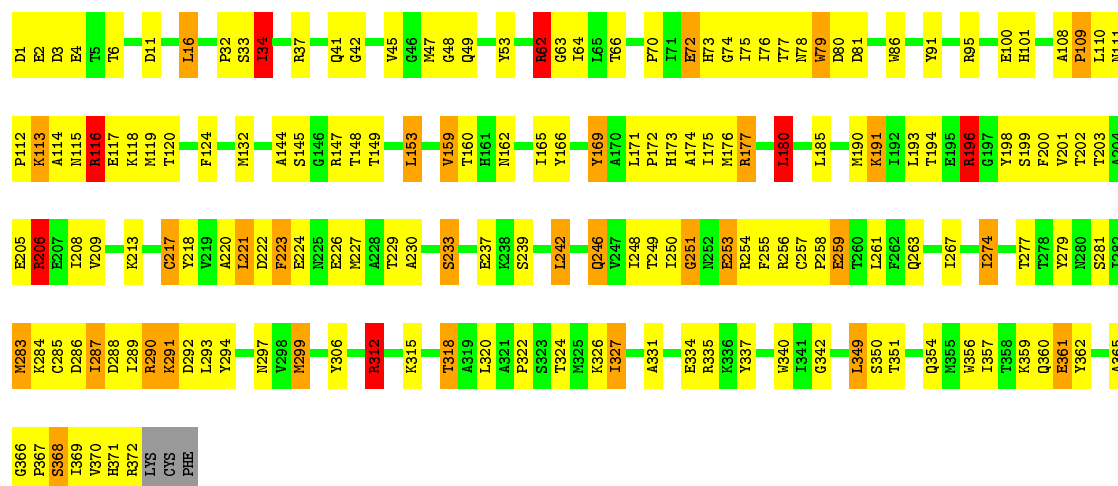
• Molecule 4: SKELETAL MUSCLE ACTIN





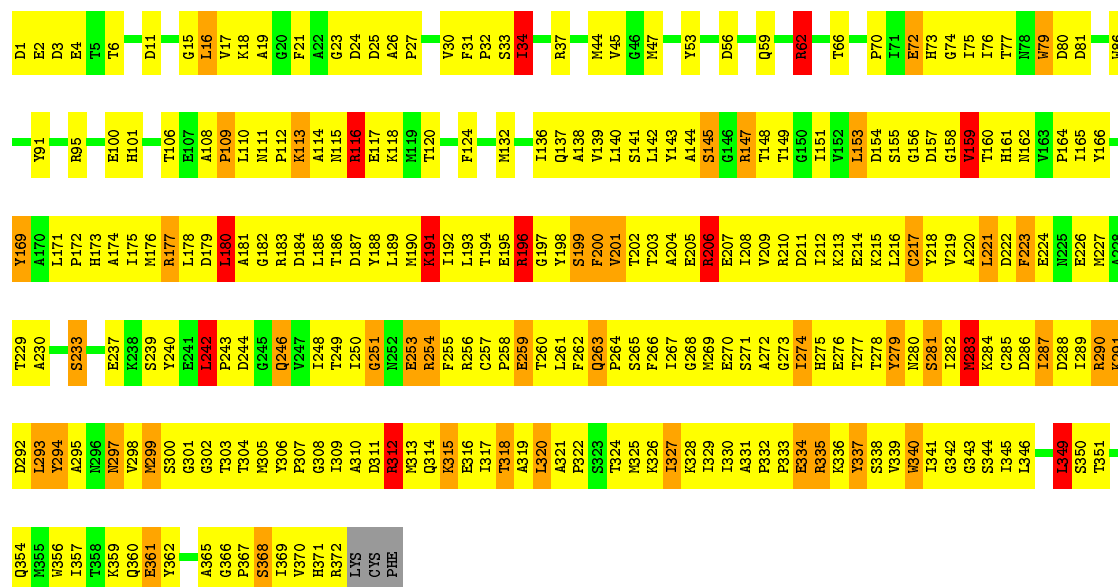
• Molecule 4: SKELETAL MUSCLE ACTIN

Chain 2: 54% 36% 8% ..

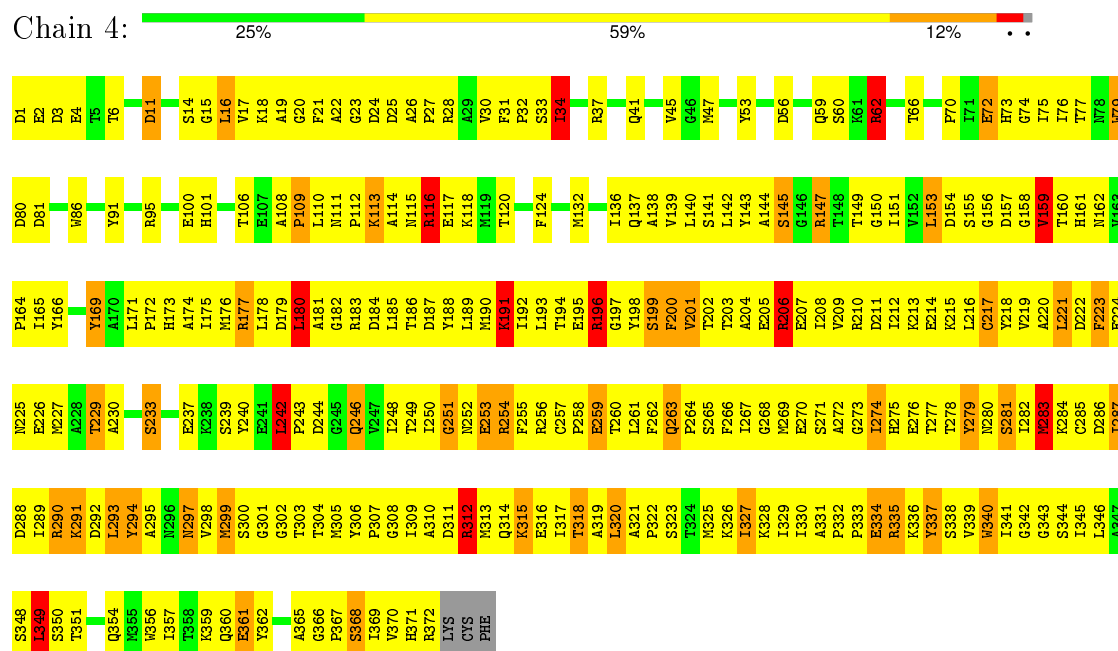


• Molecule 4: SKELETAL MUSCLE ACTIN

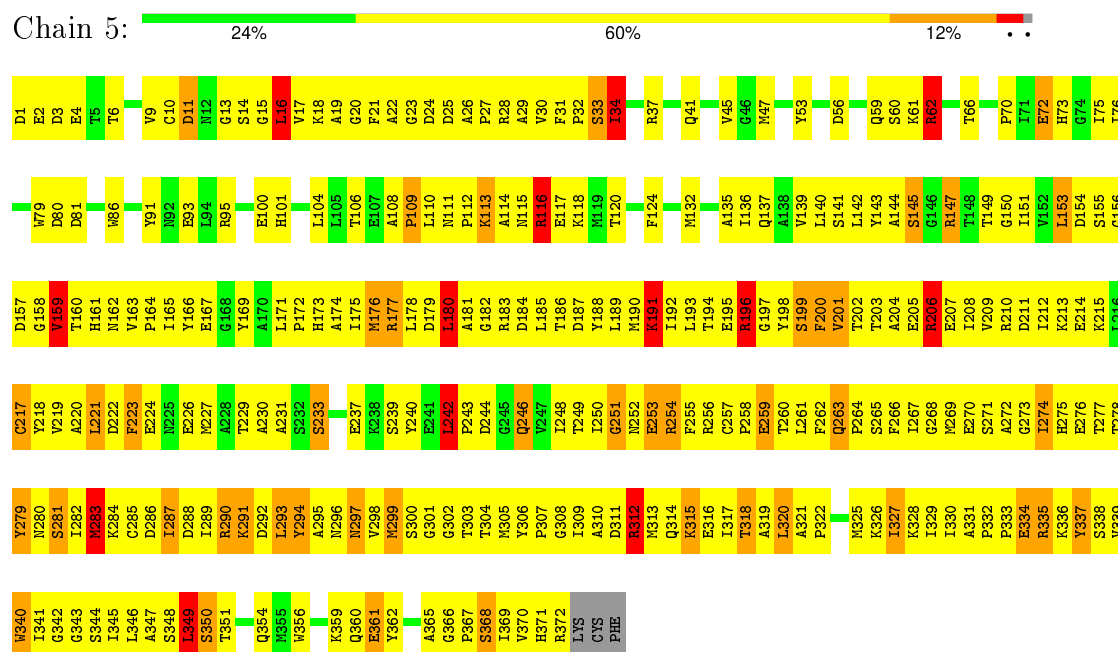
Chain 3: 27% 57% 11% ..



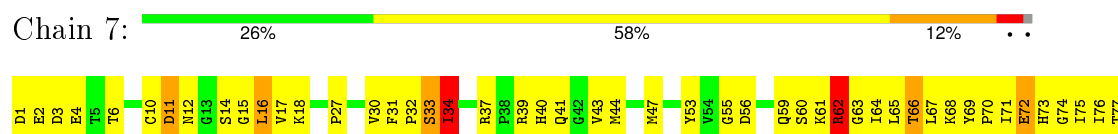
• Molecule 4: SKELETAL MUSCLE ACTIN



• Molecule 4: SKELETAL MUSCLE ACTIN

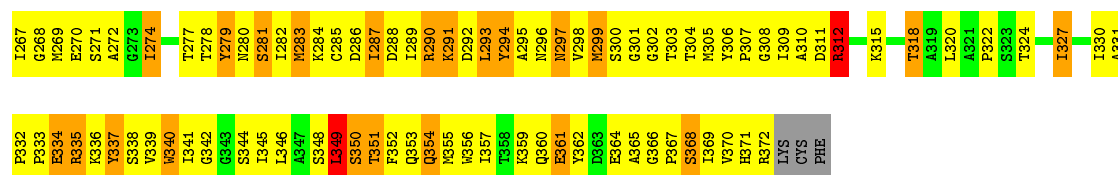


• Molecule 4: SKELETAL MUSCLE ACTIN



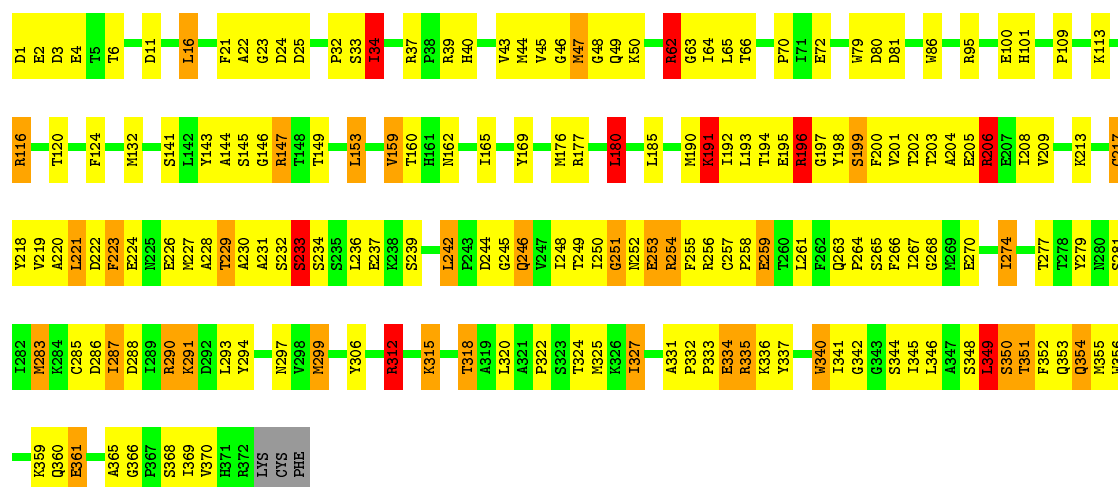






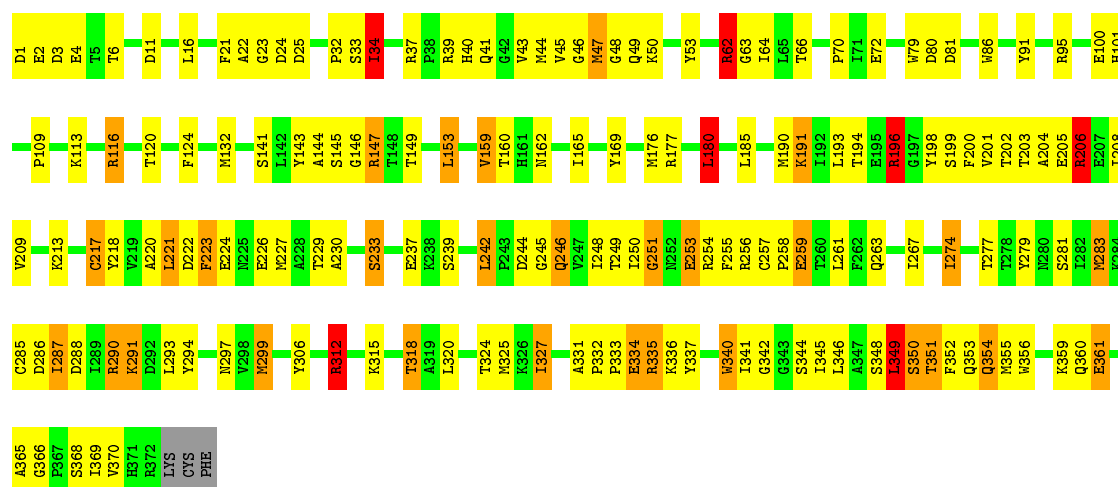
# Molecule 4: SKELETAL MUSCLE ACTIN

## Chain V:



# Molecule 4: SKELETAL MUSCLE ACTIN

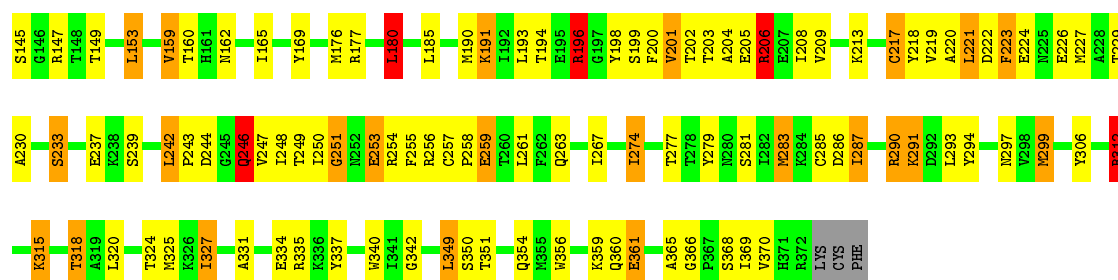
## Chain W:



# Molecule 4: SKELETAL MUSCLE ACTIN

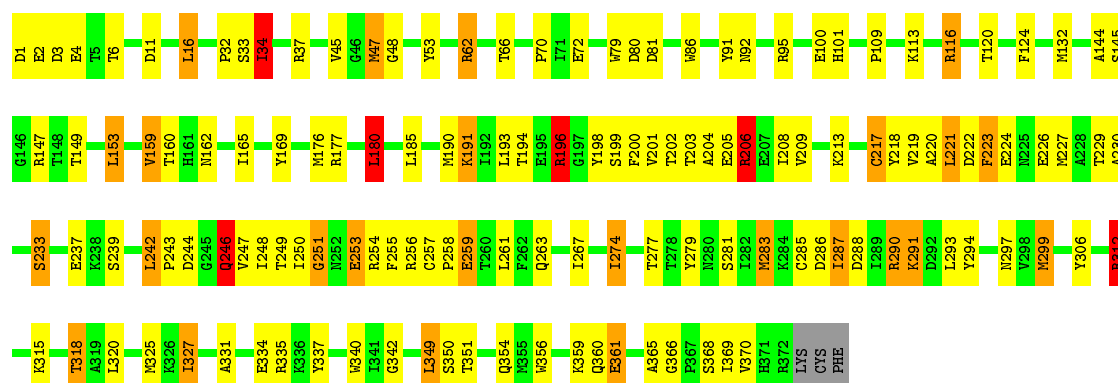
## Chain X:





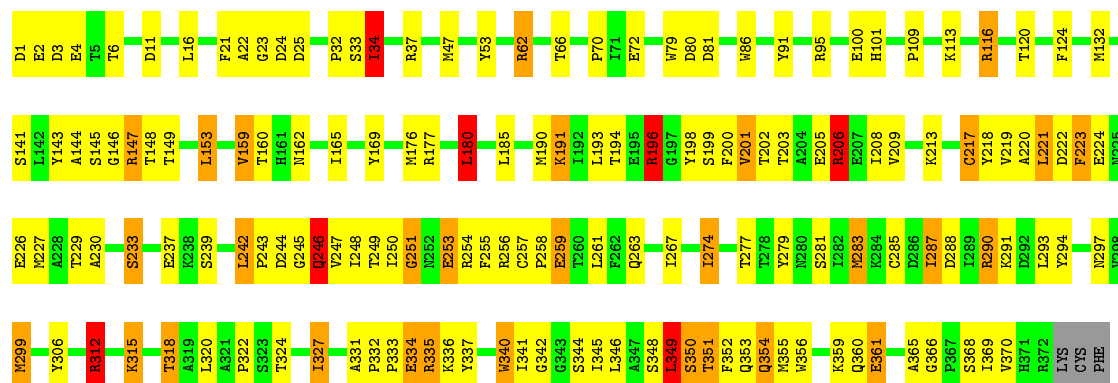
### • Molecule 4: SKELETAL MUSCLE ACTIN

Chain Y: 62% 29% 7% ..



### • Molecule 4: SKELETAL MUSCLE ACTIN

Chain Z: 57% 32% 8% ..



## 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	118/8729 (1.4%)
1	D	1.77	63/6448 (1.0%)	1.82	117/8729 (1.3%)
1	G	1.78	67/6449 (1.0%)	1.83	118/8732 (1.4%)
1	J	1.77	68/6449 (1.1%)	1.87	117/8732 (1.3%)
1	M	1.78	66/6446 (1.0%)	1.83	118/8723 (1.4%)
1	P	1.81	67/6448 (1.0%)	1.87	122/8729 (1.4%)
2	B	1.22	10/1148 (0.9%)	1.61	16/1548 (1.0%)
2	E	1.22	10/1148 (0.9%)	1.62	16/1548 (1.0%)
2	H	1.22	10/1148 (0.9%)	1.62	17/1548 (1.1%)
2	K	1.22	10/1148 (0.9%)	1.61	16/1548 (1.0%)
2	N	1.22	10/1148 (0.9%)	1.62	16/1548 (1.0%)
2	Q	1.22	10/1148 (0.9%)	1.61	16/1548 (1.0%)
3	C	0.80	0/1136	0.95	4/1525 (0.3%)
3	F	0.80	0/1136	0.95	4/1525 (0.3%)
3	I	0.80	0/1136	0.94	4/1525 (0.3%)
3	L	0.79	0/1136	0.94	4/1525 (0.3%)
3	O	0.79	0/1136	0.95	4/1525 (0.3%)
3	R	0.79	0/1136	0.94	4/1525 (0.3%)
4	0	0.89	1/2968 (0.0%)	1.64	51/4023 (1.3%)
4	1	0.89	1/2968 (0.0%)	1.64	51/4023 (1.3%)
4	2	0.89	1/2968 (0.0%)	1.64	52/4023 (1.3%)
4	3	0.89	2/2968 (0.1%)	1.64	51/4023 (1.3%)
4	4	0.89	2/2968 (0.1%)	1.64	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	2/2968 (0.1%)	1.64	51/4023 (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	51/4023 (1.3%)
4	X	0.89	2/2968 (0.1%)	1.64	52/4023 (1.3%)
4	Y	0.89	2/2968 (0.1%)	1.64	51/4023 (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	1.35	482/93944 (0.5%)	1.69	1548/127134 (1.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	4
1	D	1	4
1	G	1	4
1	J	1	6
1	M	1	6
1	P	1	6
2	B	0	3
2	E	0	3
2	H	0	3
2	K	0	3
2	N	0	3
2	Q	0	3
3	C	0	2
3	F	0	2
3	I	0	2
3	L	0	2
3	O	0	2
3	R	0	2
4	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	74

The worst 5 of 482 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	649	VAL	CB-CG1	53.30	2.64	1.52
1	G	649	VAL	CB-CG1	53.30	2.64	1.52
1	M	649	VAL	CB-CG1	53.28	2.64	1.52
1	P	649	VAL	CB-CG1	53.28	2.64	1.52
1	D	649	VAL	CB-CG1	53.20	2.64	1.52

The worst 5 of 1548 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	637	LYS	O-C-N	-58.51	23.73	123.20
1	D	637	LYS	O-C-N	-58.48	23.79	123.20
1	M	637	LYS	O-C-N	-58.47	23.80	123.20
1	J	637	LYS	O-C-N	-58.45	23.83	123.20
1	P	637	LYS	O-C-N	-58.45	23.83	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 74 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	6753	1539	19

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	6797	0	6758	1519	21
1	G	6797	0	6764	1543	0
1	J	6797	0	6760	1449	0
1	M	6797	0	6765	1504	0
1	P	6797	0	6765	1493	0
2	B	1127	0	1085	226	0
2	E	1127	0	1085	249	0
2	H	1127	0	1087	278	0
2	K	1127	0	1088	282	0
2	N	1127	0	1088	238	0
2	Q	1127	0	1088	253	0
3	C	1123	0	1083	200	0
3	F	1123	0	1084	200	0
3	I	1123	0	1082	211	0
3	L	1123	0	1083	168	0
3	O	1123	0	1084	152	0
3	R	1123	0	1084	238	0
4	0	2906	0	2855	404	0
4	1	2906	0	2858	259	76
4	2	2906	0	2864	173	574
4	3	2906	0	2863	178	3105
4	4	2906	0	2865	96	3229
4	5	2906	0	2865	97	3412
4	7	2906	0	2866	79	3158
4	8	2906	0	2857	317	3221
4	9	2906	0	2855	341	3470
4	V	2906	0	2851	390	418
4	W	2906	0	2851	382	89
4	X	2906	0	2862	208	0
4	Y	2906	0	2863	168	0
4	Z	2906	0	2853	410	0
All	All	94966	0	93614	11439	10396

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 61.

The worst 5 of 11439 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	1.26	1.66
1:D:797:PHE:CE2	3:F:126:LEU:HD22	1.31	1.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:797:PHE:CZ	3:I:146:ILE:HD12	1.28	1.66
1:A:505:MLY:HB3	1:A:762:HIS:CD2	1.30	1.65
1:D:508:ILE:HD11	1:D:766:PHE:CE1	1.24	1.65

The worst 5 of 10396 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]	0.16	2.04
4:5:191:LYS:CA	4:9:186:THR:C[1_554]	0.19	2.01
4:5:194:THR:C	4:9:209:VAL:CG2[1_554]	0.21	1.99
4:3:26:ALA:CB	4:7:122:ILE:C[1_554]	0.22	1.98
4:3:305:MET:C	4:7:11:ASP:OD1[1_554]	0.22	1.98

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	789/840 (94%)	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%)	652 (82%)	112 (14%)	27 (3%)	5	40
1	J	791/840 (94%)	652 (82%)	112 (14%)	27 (3%)	5	40
1	M	786/840 (94%)	649 (83%)	111 (14%)	26 (3%)	5	40
1	P	789/840 (94%)	649 (82%)	114 (14%)	26 (3%)	5	40
2	B	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	2	28
2	E	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	2	28
2	H	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	2	28
2	K	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	2	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	N	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	2	28
2	Q	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	2	28
3	C	143/147 (97%)	133 (93%)	10 (7%)	0	100	100
3	F	143/147 (97%)	133 (93%)	10 (7%)	0	100	100
3	I	143/147 (97%)	133 (93%)	10 (7%)	0	100	100
3	L	143/147 (97%)	133 (93%)	10 (7%)	0	100	100
3	O	143/147 (97%)	133 (93%)	10 (7%)	0	100	100
3	R	143/147 (97%)	133 (93%)	10 (7%)	0	100	100
4	0	370/375 (99%)	333 (90%)	31 (8%)	6 (2%)	12	56
4	1	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	12	56
4	2	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	12	56
4	3	370/375 (99%)	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%)	335 (90%)	29 (8%)	6 (2%)	12	56
4	7	370/375 (99%)	335 (90%)	29 (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%)	334 (90%)	30 (8%)	6 (2%)	12	56
4	Z	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	12	56
All	All	11631/12042 (97%)	10138 (87%)	1203 (10%)	290 (2%)	11	46

5 of 290 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%)	510 (76%)	162 (24%)	1	6
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%)	515 (77%)	157 (23%)	1	7
1	M	672/672 (100%)	514 (76%)	158 (24%)	1	7
1	P	672/672 (100%)	514 (76%)	158 (24%)	1	7
2	B	120/120 (100%)	119 (99%)	1 (1%)	86	94
2	E	120/120 (100%)	119 (99%)	1 (1%)	86	94
2	H	120/120 (100%)	119 (99%)	1 (1%)	86	94
2	K	120/120 (100%)	119 (99%)	1 (1%)	86	94
2	N	120/120 (100%)	119 (99%)	1 (1%)	86	94
2	Q	120/120 (100%)	119 (99%)	1 (1%)	86	94
3	C	117/117 (100%)	112 (96%)	5 (4%)	35	70
3	F	117/117 (100%)	112 (96%)	5 (4%)	35	70
3	I	117/117 (100%)	112 (96%)	5 (4%)	35	70
3	L	117/117 (100%)	112 (96%)	5 (4%)	35	70
3	O	117/117 (100%)	112 (96%)	5 (4%)	35	70
3	R	117/117 (100%)	112 (96%)	5 (4%)	35	70
4	0	315/318 (99%)	269 (85%)	46 (15%)	4	24
4	1	315/318 (99%)	268 (85%)	47 (15%)	4	23
4	2	315/318 (99%)	268 (85%)	47 (15%)	4	23
4	3	315/318 (99%)	269 (85%)	46 (15%)	4	24
4	4	315/318 (99%)	269 (85%)	46 (15%)	4	24
4	5	315/318 (99%)	268 (85%)	47 (15%)	4	23
4	7	315/318 (99%)	269 (85%)	46 (15%)	4	24
4	8	315/318 (99%)	268 (85%)	47 (15%)	4	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	9	315/318 (99%)	269 (85%)	46 (15%)	4	24
4	V	315/318 (99%)	268 (85%)	47 (15%)	4	23
4	W	315/318 (99%)	269 (85%)	46 (15%)	4	24
4	X	315/318 (99%)	268 (85%)	47 (15%)	4	23
4	Y	315/318 (99%)	268 (85%)	47 (15%)	4	23
4	Z	315/318 (99%)	269 (85%)	46 (15%)	4	24
All	All	9864/9906 (100%)	8225 (83%)	1639 (17%)	6	19

5 of 1639 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	439	LEU
1	P	495	MET
4	X	196	ARG
1	M	549	SER
1	P	37	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 237 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	127	ASN
1	P	127	ASN
4	W	263	GLN
1	M	194	GLN
1	M	563	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	MLY	A	107	1	8,10,11	0.43	0	9,11,13	0.67	0
1	MLY	A	130	1	8,10,11	0.59	0	9,11,13	1.06	1 (11%)
1	MLY	A	138	1	8,10,11	1.34	1 (12%)	9,11,13	0.80	0
1	MLY	A	19	1	8,10,11	1.14	1 (12%)	9,11,13	0.68	0
1	MLY	A	190	1	8,10,11	1.10	1 (12%)	9,11,13	0.70	0
1	MLY	A	236	1	8,10,11	0.35	0	9,11,13	1.33	1 (11%)
1	MLY	A	248	1	8,10,11	0.74	0	9,11,13	0.92	1 (11%)
1	MLY	A	272	1	8,10,11	1.03	1 (12%)	9,11,13	0.57	0
1	MLY	A	295	1	8,10,11	0.74	0	9,11,13	0.46	0
1	MLY	A	296	1	8,10,11	0.60	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	0.84	0	9,11,13	0.81	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	0.89	0	9,11,13	0.79	0
1	MLY	A	367	1	8,10,11	0.66	0	9,11,13	0.60	0
1	MLY	A	369	1	8,10,11	0.54	0	9,11,13	0.93	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	0.75	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	1.10	1 (12%)	9,11,13	0.57	0
1	MLY	A	486	1	8,10,11	0.35	0	9,11,13	0.60	0
1	MLY	A	49	1	8,10,11	1.04	1 (12%)	9,11,13	0.98	0
1	MLY	A	504	1	8,10,11	0.79	0	9,11,13	0.49	0
1	MLY	A	505	1	8,10,11	0.90	1 (12%)	9,11,13	0.38	0
1	MLY	A	528	1	8,10,11	0.80	0	9,11,13	1.17	1 (11%)
1	MLY	A	55	1	8,10,11	0.66	0	9,11,13	0.97	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	0.85	1 (12%)	9,11,13	0.72	0
1	MLY	A	600	1	8,10,11	0.51	0	9,11,13	0.49	0
1	MLY	A	613	1	8,10,11	0.50	0	9,11,13	0.92	0
1	MLY	A	617	1	8,10,11	0.89	1 (12%)	9,11,13	0.46	0
1	MLY	A	63	1	8,10,11	0.82	0	9,11,13	0.94	0
1	MLY	A	659	1	8,10,11	0.53	0	9,11,13	0.95	0
1	MLY	A	681	1	8,10,11	0.62	0	9,11,13	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	MLY	A	764	1	8,10,11	0.67	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	0.93	1 (11%)
1	MLY	A	827	1	8,10,11	0.68	0	9,11,13	0.95	1 (11%)
1	MLY	A	833	1	8,10,11	0.98	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	0.68	0	9,11,13	0.79	0
1	MLY	A	84	1	8,10,11	0.47	0	9,11,13	0.80	0
1	MLY	A	87	1	8,10,11	1.18	1 (12%)	9,11,13	0.67	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	0.58	0	9,11,13	1.06	1 (11%)
1	MLY	D	138	1	8,10,11	1.40	1 (12%)	9,11,13	0.82	0
1	MLY	D	19	1	8,10,11	1.19	1 (12%)	9,11,13	0.69	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	0.36	0	9,11,13	1.32	1 (11%)
1	MLY	D	248	1	8,10,11	0.74	0	9,11,13	0.92	1 (11%)
1	MLY	D	272	1	8,10,11	0.99	1 (12%)	9,11,13	0.58	0
1	MLY	D	295	1	8,10,11	0.70	0	9,11,13	0.48	0
1	MLY	D	296	1	8,10,11	0.61	0	9,11,13	0.78	0
1	MLY	D	30	1	8,10,11	0.72	0	9,11,13	0.84	1 (11%)
1	MLY	D	348	1	8,10,11	0.80	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	0.85	0	9,11,13	0.79	0
1	MLY	D	367	1	8,10,11	0.62	0	9,11,13	0.60	0
1	MLY	D	369	1	8,10,11	0.54	0	9,11,13	0.91	1 (11%)
1	MLY	D	385	1	8,10,11	0.99	1 (12%)	9,11,13	0.56	0
1	MLY	D	415	1	8,10,11	0.78	0	9,11,13	0.46	0
1	MLY	D	431	1	8,10,11	0.49	0	9,11,13	0.78	0
1	MLY	D	436	1	8,10,11	1.15	1 (12%)	9,11,13	0.58	0
1	MLY	D	486	1	8,10,11	0.35	0	9,11,13	0.61	0
1	MLY	D	49	1	8,10,11	1.08	1 (12%)	9,11,13	0.99	0
1	MLY	D	504	1	8,10,11	0.80	0	9,11,13	0.49	0
1	MLY	D	505	1	8,10,11	0.85	1 (12%)	9,11,13	0.39	0
1	MLY	D	528	1	8,10,11	0.82	0	9,11,13	1.17	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	0.51	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	0.76	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	0.86	1 (12%)	9,11,13	0.70	0
1	MLY	D	600	1	8,10,11	0.51	0	9,11,13	0.47	0
1	MLY	D	613	1	8,10,11	0.49	0	9,11,13	0.92	0
1	MLY	D	617	1	8,10,11	0.95	1 (12%)	9,11,13	0.46	0
1	MLY	D	63	1	8,10,11	0.78	0	9,11,13	0.95	0
1	MLY	D	659	1	8,10,11	0.53	0	9,11,13	0.95	0
1	MLY	D	681	1	8,10,11	0.60	0	9,11,13	0.65	0
1	MLY	D	764	1	8,10,11	0.66	0	9,11,13	0.57	0
1	MLY	D	768	1	8,10,11	0.61	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	0.64	0	9,11,13	0.95	1 (11%)
1	MLY	D	833	1	8,10,11	0.95	1 (12%)	9,11,13	0.59	0
1	MLY	D	837	1	8,10,11	0.56	0	9,11,13	0.59	0
1	MLY	D	839	1	8,10,11	0.69	0	9,11,13	0.78	0
1	MLY	D	84	1	8,10,11	0.48	0	9,11,13	0.80	0
1	MLY	D	87	1	8,10,11	1.16	1 (12%)	9,11,13	0.69	0
1	MLY	G	107	1	8,10,11	0.44	0	9,11,13	0.66	0
1	MLY	G	130	1	8,10,11	0.61	0	9,11,13	1.07	1 (11%)
1	MLY	G	138	1	8,10,11	1.38	1 (12%)	9,11,13	0.81	0
1	MLY	G	19	1	8,10,11	1.17	1 (12%)	9,11,13	0.70	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	0.36	0	9,11,13	1.31	1 (11%)
1	MLY	G	248	1	8,10,11	0.70	0	9,11,13	0.93	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	0.71	0	9,11,13	0.47	0
1	MLY	G	296	1	8,10,11	0.61	0	9,11,13	0.77	0
1	MLY	G	30	1	8,10,11	0.68	0	9,11,13	0.83	1 (11%)
1	MLY	G	348	1	8,10,11	0.83	0	9,11,13	0.82	0
1	MLY	G	35	1	8,10,11	0.59	0	9,11,13	0.68	0
1	MLY	G	353	1	8,10,11	0.86	0	9,11,13	0.79	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	0.55	0	9,11,13	0.92	1 (11%)
1	MLY	G	385	1	8,10,11	1.00	1 (12%)	9,11,13	0.55	0
1	MLY	G	415	1	8,10,11	0.78	0	9,11,13	0.44	0
1	MLY	G	431	1	8,10,11	0.49	0	9,11,13	0.77	0
1	MLY	G	436	1	8,10,11	1.07	1 (12%)	9,11,13	0.58	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	1.07	1 (12%)	9,11,13	0.97	0
1	MLY	G	504	1	8,10,11	0.76	0	9,11,13	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	MLY	G	505	1	8,10,11	0.90	1 (12%)	9,11,13	0.40	0
1	MLY	G	528	1	8,10,11	0.80	0	9,11,13	1.17	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	0.65	0
1	MLY	G	553	1,4	8,10,11	0.62	0	9,11,13	0.59	0
1	MLY	G	59	1	8,10,11	0.72	0	9,11,13	0.78	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	0.51	0	9,11,13	0.92	0
1	MLY	G	617	1	8,10,11	0.91	1 (12%)	9,11,13	0.45	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	0.54	0	9,11,13	0.94	0
1	MLY	G	681	1	8,10,11	0.66	0	9,11,13	0.64	0
1	MLY	G	764	1	8,10,11	0.62	0	9,11,13	0.57	0
1	MLY	G	768	1	8,10,11	0.60	0	9,11,13	0.88	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	0.67	0	9,11,13	0.96	1 (11%)
1	MLY	G	833	1	8,10,11	0.96	1 (12%)	9,11,13	0.59	0
1	MLY	G	837	1	8,10,11	0.53	0	9,11,13	0.55	0
1	MLY	G	839	1	8,10,11	0.71	0	9,11,13	0.79	0
1	MLY	G	84	1	8,10,11	0.46	0	9,11,13	0.81	0
1	MLY	G	87	1	8,10,11	1.17	1 (12%)	9,11,13	0.69	0
1	MLY	J	107	1	8,10,11	0.45	0	9,11,13	0.67	0
1	MLY	J	130	1	8,10,11	0.55	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	1.20	1 (12%)	9,11,13	0.71	0
1	MLY	J	190	1	8,10,11	1.12	1 (12%)	9,11,13	0.70	0
1	MLY	J	236	1	8,10,11	0.36	0	9,11,13	1.32	1 (11%)
1	MLY	J	248	1	8,10,11	0.74	0	9,11,13	0.94	1 (11%)
1	MLY	J	272	1	8,10,11	1.04	1 (12%)	9,11,13	0.58	0
1	MLY	J	295	1	8,10,11	0.69	0	9,11,13	0.48	0
1	MLY	J	296	1	8,10,11	0.66	0	9,11,13	0.77	0
1	MLY	J	30	1	8,10,11	0.68	0	9,11,13	0.82	0
1	MLY	J	348	1	8,10,11	0.76	0	9,11,13	0.81	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	0.77	0
1	MLY	J	367	1	8,10,11	0.64	0	9,11,13	0.60	0
1	MLY	J	369	1	8,10,11	0.54	0	9,11,13	0.93	1 (11%)
1	MLY	J	385	1	8,10,11	1.02	1 (12%)	9,11,13	0.54	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	MLY	J	415	1	8,10,11	0.79	0	9,11,13	0.44	0
1	MLY	J	431	1	8,10,11	0.43	0	9,11,13	0.77	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	1.08	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	0.92	1 (12%)	9,11,13	0.39	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	0.66	0	9,11,13	0.98	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	0.62	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	0.84	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	0.49	0	9,11,13	0.93	0
1	MLY	J	617	1	8,10,11	0.92	1 (12%)	9,11,13	0.45	0
1	MLY	J	63	1	8,10,11	0.81	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	0.61	0	9,11,13	0.64	0
1	MLY	J	764	1	8,10,11	0.64	0	9,11,13	0.59	0
1	MLY	J	768	1	8,10,11	0.64	0	9,11,13	0.85	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	0.70	0	9,11,13	0.94	1 (11%)
1	MLY	J	833	1	8,10,11	1.03	1 (12%)	9,11,13	0.58	0
1	MLY	J	837	1	8,10,11	0.55	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	0.46	0	9,11,13	0.80	0
1	MLY	J	87	1	8,10,11	1.18	1 (12%)	9,11,13	0.67	0
1	MLY	M	107	1	8,10,11	0.46	0	9,11,13	0.67	0
1	MLY	M	130	1	8,10,11	0.59	0	9,11,13	1.07	1 (11%)
1	MLY	M	138	1	8,10,11	1.35	1 (12%)	9,11,13	0.80	0
1	MLY	M	19	1	8,10,11	1.18	1 (12%)	9,11,13	0.70	0
1	MLY	M	190	1	8,10,11	1.11	1 (12%)	9,11,13	0.70	0
1	MLY	M	236	1	8,10,11	0.38	0	9,11,13	1.31	1 (11%)
1	MLY	M	248	1	8,10,11	0.73	0	9,11,13	0.93	1 (11%)
1	MLY	M	272	1	8,10,11	1.03	1 (12%)	9,11,13	0.57	0
1	MLY	M	295	1	8,10,11	0.70	0	9,11,13	0.48	0
1	MLY	M	296	1	8,10,11	0.67	0	9,11,13	0.77	0
1	MLY	M	30	1	8,10,11	0.69	0	9,11,13	0.82	1 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	MLY	M	348	1	8,10,11	0.78	0	9,11,13	0.80	0
1	MLY	M	35	1	8,10,11	0.59	0	9,11,13	0.67	0
1	MLY	M	353	1	8,10,11	0.86	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	0.54	0	9,11,13	0.92	1 (11%)
1	MLY	M	385	1	8,10,11	1.02	1 (12%)	9,11,13	0.55	0
1	MLY	M	415	1	8,10,11	0.79	0	9,11,13	0.44	0
1	MLY	M	431	1	8,10,11	0.45	0	9,11,13	0.78	0
1	MLY	M	436	1	8,10,11	1.11	1 (12%)	9,11,13	0.56	0
1	MLY	M	486	1	8,10,11	0.32	0	9,11,13	0.60	0
1	MLY	M	49	1	8,10,11	1.09	1 (12%)	9,11,13	1.00	0
1	MLY	M	504	1	8,10,11	0.74	0	9,11,13	0.47	0
1	MLY	M	505	1	8,10,11	0.93	1 (12%)	9,11,13	0.38	0
1	MLY	M	528	1	8,10,11	0.80	0	9,11,13	1.16	1 (11%)
1	MLY	M	55	1	8,10,11	0.67	0	9,11,13	0.99	0
1	MLY	M	551	1	8,10,11	0.49	0	9,11,13	0.67	0
1	MLY	M	553	1,4	8,10,11	0.62	0	9,11,13	0.58	0
1	MLY	M	59	1	8,10,11	0.78	0	9,11,13	0.77	0
1	MLY	M	598	1	8,10,11	0.83	1 (12%)	9,11,13	0.71	0
1	MLY	M	600	1	8,10,11	0.52	0	9,11,13	0.47	0
1	MLY	M	613	1	8,10,11	0.49	0	9,11,13	0.93	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	0.81	0	9,11,13	0.95	0
1	MLY	M	659	1	8,10,11	0.52	0	9,11,13	0.93	0
1	MLY	M	681	1	8,10,11	0.60	0	9,11,13	0.63	0
1	MLY	M	764	1	8,10,11	0.67	0	9,11,13	0.58	0
1	MLY	M	768	1	8,10,11	0.62	0	9,11,13	0.87	0
1	MLY	M	782	1	8,10,11	0.50	0	9,11,13	0.94	1 (11%)
1	MLY	M	827	1	8,10,11	0.66	0	9,11,13	0.95	1 (11%)
1	MLY	M	833	1	8,10,11	1.05	1 (12%)	9,11,13	0.59	0
1	MLY	M	837	1	8,10,11	0.51	0	9,11,13	0.58	0
1	MLY	M	839	1	8,10,11	0.68	0	9,11,13	0.77	0
1	MLY	M	84	1	8,10,11	0.47	0	9,11,13	0.80	0
1	MLY	M	87	1	8,10,11	1.17	1 (12%)	9,11,13	0.68	0
1	MLY	P	107	1	8,10,11	0.46	0	9,11,13	0.67	0
1	MLY	P	130	1	8,10,11	0.57	0	9,11,13	1.06	1 (11%)
1	MLY	P	138	1	8,10,11	1.35	1 (12%)	9,11,13	0.81	0
1	MLY	P	19	1	8,10,11	1.20	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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	MLY	P	236	1	8,10,11	0.38	0	9,11,13	1.32	1 (11%)
1	MLY	P	248	1	8,10,11	0.73	0	9,11,13	0.94	1 (11%)
1	MLY	P	272	1	8,10,11	1.05	1 (12%)	9,11,13	0.57	0
1	MLY	P	295	1	8,10,11	0.71	0	9,11,13	0.47	0
1	MLY	P	296	1	8,10,11	0.63	0	9,11,13	0.79	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	0.81	0	9,11,13	0.81	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	0.78	0
1	MLY	P	367	1	8,10,11	0.65	0	9,11,13	0.60	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	0.54	0
1	MLY	P	415	1	8,10,11	0.78	0	9,11,13	0.44	0
1	MLY	P	431	1	8,10,11	0.43	0	9,11,13	0.77	0
1	MLY	P	436	1	8,10,11	1.11	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	1.13	1 (12%)	9,11,13	0.99	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	0.92	1 (12%)	9,11,13	0.38	0
1	MLY	P	528	1	8,10,11	0.81	0	9,11,13	1.16	1 (11%)
1	MLY	P	55	1	8,10,11	0.66	0	9,11,13	0.99	0
1	MLY	P	551	1	8,10,11	0.51	0	9,11,13	0.66	0
1	MLY	P	553	1	8,10,11	0.62	0	9,11,13	0.58	0
1	MLY	P	59	1	8,10,11	0.79	0	9,11,13	0.77	0
1	MLY	P	598	1	8,10,11	0.85	1 (12%)	9,11,13	0.71	0
1	MLY	P	600	1	8,10,11	0.52	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	0.55	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	0.64	0	9,11,13	0.58	0
1	MLY	P	768	1	8,10,11	0.67	0	9,11,13	0.87	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	0.68	0	9,11,13	0.95	1 (11%)
1	MLY	P	833	1	8,10,11	1.02	1 (12%)	9,11,13	0.56	0
1	MLY	P	837	1	8,10,11	0.52	0	9,11,13	0.58	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	0.47	0	9,11,13	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	MLY	P	87	1	8,10,11	1.21	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
1	MLY	A	431	1	-	0/7/9/11	0/0/0/0
1	MLY	A	436	1	-	0/7/9/11	0/0/0/0
1	MLY	A	486	1	-	0/7/9/11	0/0/0/0
1	MLY	A	49	1	-	0/7/9/11	0/0/0/0
1	MLY	A	504	1	-	0/7/9/11	0/0/0/0
1	MLY	A	505	1	-	0/7/9/11	0/0/0/0
1	MLY	A	528	1	-	0/7/9/11	0/0/0/0
1	MLY	A	55	1	-	0/7/9/11	0/0/0/0
1	MLY	A	551	1	-	0/7/9/11	0/0/0/0
1	MLY	A	553	1,4	-	0/7/9/11	0/0/0/0
1	MLY	A	59	1	-	0/7/9/11	0/0/0/0
1	MLY	A	598	1	-	0/7/9/11	0/0/0/0
1	MLY	A	600	1	-	0/7/9/11	0/0/0/0
1	MLY	A	613	1	-	0/7/9/11	0/0/0/0
1	MLY	A	617	1	-	0/7/9/11	0/0/0/0
1	MLY	A	63	1	-	0/7/9/11	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	A	659	1	-	0/7/9/11	0/0/0/0
1	MLY	A	681	1	-	0/7/9/11	0/0/0/0
1	MLY	A	764	1	-	0/7/9/11	0/0/0/0
1	MLY	A	768	1	-	0/7/9/11	0/0/0/0
1	MLY	A	782	1	-	0/7/9/11	0/0/0/0
1	MLY	A	827	1	-	0/7/9/11	0/0/0/0
1	MLY	A	833	1	-	0/7/9/11	0/0/0/0
1	MLY	A	837	1	-	0/7/9/11	0/0/0/0
1	MLY	A	839	1	-	0/7/9/11	0/0/0/0
1	MLY	A	84	1	-	0/7/9/11	0/0/0/0
1	MLY	A	87	1	-	0/7/9/11	0/0/0/0
1	MLY	D	107	1	-	0/7/9/11	0/0/0/0
1	MLY	D	130	1	-	0/7/9/11	0/0/0/0
1	MLY	D	138	1	-	0/7/9/11	0/0/0/0
1	MLY	D	19	1	-	0/7/9/11	0/0/0/0
1	MLY	D	190	1	-	0/7/9/11	0/0/0/0
1	MLY	D	236	1	-	0/7/9/11	0/0/0/0
1	MLY	D	248	1	-	0/7/9/11	0/0/0/0
1	MLY	D	272	1	-	0/7/9/11	0/0/0/0
1	MLY	D	295	1	-	0/7/9/11	0/0/0/0
1	MLY	D	296	1	-	0/7/9/11	0/0/0/0
1	MLY	D	30	1	-	0/7/9/11	0/0/0/0
1	MLY	D	348	1	-	0/7/9/11	0/0/0/0
1	MLY	D	35	1	-	0/7/9/11	0/0/0/0
1	MLY	D	353	1	-	0/7/9/11	0/0/0/0
1	MLY	D	367	1	-	0/7/9/11	0/0/0/0
1	MLY	D	369	1	-	0/7/9/11	0/0/0/0
1	MLY	D	385	1	-	0/7/9/11	0/0/0/0
1	MLY	D	415	1	-	0/7/9/11	0/0/0/0
1	MLY	D	431	1	-	0/7/9/11	0/0/0/0
1	MLY	D	436	1	-	0/7/9/11	0/0/0/0
1	MLY	D	486	1	-	0/7/9/11	0/0/0/0
1	MLY	D	49	1	-	0/7/9/11	0/0/0/0
1	MLY	D	504	1	-	0/7/9/11	0/0/0/0
1	MLY	D	505	1	-	0/7/9/11	0/0/0/0
1	MLY	D	528	1	-	0/7/9/11	0/0/0/0
1	MLY	D	55	1	-	0/7/9/11	0/0/0/0
1	MLY	D	551	1	-	0/7/9/11	0/0/0/0
1	MLY	D	553	1,4	-	0/7/9/11	0/0/0/0
1	MLY	D	59	1	-	0/7/9/11	0/0/0/0
1	MLY	D	598	1	-	0/7/9/11	0/0/0/0
1	MLY	D	600	1	-	0/7/9/11	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	D	613	1	-	0/7/9/11	0/0/0/0
1	MLY	D	617	1	-	0/7/9/11	0/0/0/0
1	MLY	D	63	1	-	0/7/9/11	0/0/0/0
1	MLY	D	659	1	-	0/7/9/11	0/0/0/0
1	MLY	D	681	1	-	0/7/9/11	0/0/0/0
1	MLY	D	764	1	-	0/7/9/11	0/0/0/0
1	MLY	D	768	1	-	0/7/9/11	0/0/0/0
1	MLY	D	782	1	-	0/7/9/11	0/0/0/0
1	MLY	D	827	1	-	0/7/9/11	0/0/0/0
1	MLY	D	833	1	-	0/7/9/11	0/0/0/0
1	MLY	D	837	1	-	0/7/9/11	0/0/0/0
1	MLY	D	839	1	-	0/7/9/11	0/0/0/0
1	MLY	D	84	1	-	0/7/9/11	0/0/0/0
1	MLY	D	87	1	-	0/7/9/11	0/0/0/0
1	MLY	G	107	1	-	0/7/9/11	0/0/0/0
1	MLY	G	130	1	-	0/7/9/11	0/0/0/0
1	MLY	G	138	1	-	0/7/9/11	0/0/0/0
1	MLY	G	19	1	-	0/7/9/11	0/0/0/0
1	MLY	G	190	1	-	0/7/9/11	0/0/0/0
1	MLY	G	236	1	-	0/7/9/11	0/0/0/0
1	MLY	G	248	1	-	0/7/9/11	0/0/0/0
1	MLY	G	272	1	-	0/7/9/11	0/0/0/0
1	MLY	G	295	1	-	0/7/9/11	0/0/0/0
1	MLY	G	296	1	-	0/7/9/11	0/0/0/0
1	MLY	G	30	1	-	0/7/9/11	0/0/0/0
1	MLY	G	348	1	-	0/7/9/11	0/0/0/0
1	MLY	G	35	1	-	0/7/9/11	0/0/0/0
1	MLY	G	353	1	-	0/7/9/11	0/0/0/0
1	MLY	G	367	1	-	0/7/9/11	0/0/0/0
1	MLY	G	369	1	-	0/7/9/11	0/0/0/0
1	MLY	G	385	1	-	0/7/9/11	0/0/0/0
1	MLY	G	415	1	-	0/7/9/11	0/0/0/0
1	MLY	G	431	1	-	0/7/9/11	0/0/0/0
1	MLY	G	436	1	-	0/7/9/11	0/0/0/0
1	MLY	G	486	1	-	0/7/9/11	0/0/0/0
1	MLY	G	49	1	-	0/7/9/11	0/0/0/0
1	MLY	G	504	1	-	0/7/9/11	0/0/0/0
1	MLY	G	505	1	-	0/7/9/11	0/0/0/0
1	MLY	G	528	1	-	0/7/9/11	0/0/0/0
1	MLY	G	55	1	-	0/7/9/11	0/0/0/0
1	MLY	G	551	1	-	0/7/9/11	0/0/0/0
1	MLY	G	553	1,4	-	0/7/9/11	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	G	59	1	-	0/7/9/11	0/0/0/0
1	MLY	G	598	1	-	0/7/9/11	0/0/0/0
1	MLY	G	600	1	-	0/7/9/11	0/0/0/0
1	MLY	G	613	1	-	0/7/9/11	0/0/0/0
1	MLY	G	617	1	-	0/7/9/11	0/0/0/0
1	MLY	G	63	1	-	0/7/9/11	0/0/0/0
1	MLY	G	659	1	-	0/7/9/11	0/0/0/0
1	MLY	G	681	1	-	0/7/9/11	0/0/0/0
1	MLY	G	764	1	-	0/7/9/11	0/0/0/0
1	MLY	G	768	1	-	0/7/9/11	0/0/0/0
1	MLY	G	782	1	-	0/7/9/11	0/0/0/0
1	MLY	G	827	1	-	0/7/9/11	0/0/0/0
1	MLY	G	833	1	-	0/7/9/11	0/0/0/0
1	MLY	G	837	1	-	0/7/9/11	0/0/0/0
1	MLY	G	839	1	-	0/7/9/11	0/0/0/0
1	MLY	G	84	1	-	0/7/9/11	0/0/0/0
1	MLY	G	87	1	-	0/7/9/11	0/0/0/0
1	MLY	J	107	1	-	0/7/9/11	0/0/0/0
1	MLY	J	130	1	-	0/7/9/11	0/0/0/0
1	MLY	J	138	1	-	0/7/9/11	0/0/0/0
1	MLY	J	19	1	-	0/7/9/11	0/0/0/0
1	MLY	J	190	1	-	0/7/9/11	0/0/0/0
1	MLY	J	236	1	-	0/7/9/11	0/0/0/0
1	MLY	J	248	1	-	0/7/9/11	0/0/0/0
1	MLY	J	272	1	-	0/7/9/11	0/0/0/0
1	MLY	J	295	1	-	0/7/9/11	0/0/0/0
1	MLY	J	296	1	-	0/7/9/11	0/0/0/0
1	MLY	J	30	1	-	0/7/9/11	0/0/0/0
1	MLY	J	348	1	-	0/7/9/11	0/0/0/0
1	MLY	J	35	1	-	0/7/9/11	0/0/0/0
1	MLY	J	353	1	-	0/7/9/11	0/0/0/0
1	MLY	J	367	1	-	0/7/9/11	0/0/0/0
1	MLY	J	369	1	-	0/7/9/11	0/0/0/0
1	MLY	J	385	1	-	0/7/9/11	0/0/0/0
1	MLY	J	415	1	-	0/7/9/11	0/0/0/0
1	MLY	J	431	1	-	0/7/9/11	0/0/0/0
1	MLY	J	436	1	-	0/7/9/11	0/0/0/0
1	MLY	J	486	1	-	0/7/9/11	0/0/0/0
1	MLY	J	49	1	-	0/7/9/11	0/0/0/0
1	MLY	J	504	1	-	0/7/9/11	0/0/0/0
1	MLY	J	505	1	-	0/7/9/11	0/0/0/0
1	MLY	J	528	1	-	0/7/9/11	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	J	55	1	-	0/7/9/11	0/0/0/0
1	MLY	J	551	1	-	0/7/9/11	0/0/0/0
1	MLY	J	553	1	-	0/7/9/11	0/0/0/0
1	MLY	J	59	1	-	0/7/9/11	0/0/0/0
1	MLY	J	598	1	-	0/7/9/11	0/0/0/0
1	MLY	J	600	1	-	0/7/9/11	0/0/0/0
1	MLY	J	613	1	-	0/7/9/11	0/0/0/0
1	MLY	J	617	1	-	0/7/9/11	0/0/0/0
1	MLY	J	63	1	-	0/7/9/11	0/0/0/0
1	MLY	J	659	1	-	0/7/9/11	0/0/0/0
1	MLY	J	681	1	-	0/7/9/11	0/0/0/0
1	MLY	J	764	1	-	0/7/9/11	0/0/0/0
1	MLY	J	768	1	-	0/7/9/11	0/0/0/0
1	MLY	J	782	1	-	0/7/9/11	0/0/0/0
1	MLY	J	827	1	-	0/7/9/11	0/0/0/0
1	MLY	J	833	1	-	0/7/9/11	0/0/0/0
1	MLY	J	837	1	-	0/7/9/11	0/0/0/0
1	MLY	J	839	1	-	0/7/9/11	0/0/0/0
1	MLY	J	84	1	-	0/7/9/11	0/0/0/0
1	MLY	J	87	1	-	0/7/9/11	0/0/0/0
1	MLY	M	107	1	-	0/7/9/11	0/0/0/0
1	MLY	M	130	1	-	0/7/9/11	0/0/0/0
1	MLY	M	138	1	-	0/7/9/11	0/0/0/0
1	MLY	M	19	1	-	0/7/9/11	0/0/0/0
1	MLY	M	190	1	-	0/7/9/11	0/0/0/0
1	MLY	M	236	1	-	0/7/9/11	0/0/0/0
1	MLY	M	248	1	-	0/7/9/11	0/0/0/0
1	MLY	M	272	1	-	0/7/9/11	0/0/0/0
1	MLY	M	295	1	-	0/7/9/11	0/0/0/0
1	MLY	M	296	1	-	0/7/9/11	0/0/0/0
1	MLY	M	30	1	-	0/7/9/11	0/0/0/0
1	MLY	M	348	1	-	0/7/9/11	0/0/0/0
1	MLY	M	35	1	-	0/7/9/11	0/0/0/0
1	MLY	M	353	1	-	0/7/9/11	0/0/0/0
1	MLY	M	367	1	-	0/7/9/11	0/0/0/0
1	MLY	M	369	1	-	0/7/9/11	0/0/0/0
1	MLY	M	385	1	-	0/7/9/11	0/0/0/0
1	MLY	M	415	1	-	0/7/9/11	0/0/0/0
1	MLY	M	431	1	-	0/7/9/11	0/0/0/0
1	MLY	M	436	1	-	0/7/9/11	0/0/0/0
1	MLY	M	486	1	-	0/7/9/11	0/0/0/0
1	MLY	M	49	1	-	0/7/9/11	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	M	504	1	-	0/7/9/11	0/0/0/0
1	MLY	M	505	1	-	0/7/9/11	0/0/0/0
1	MLY	M	528	1	-	0/7/9/11	0/0/0/0
1	MLY	M	55	1	-	0/7/9/11	0/0/0/0
1	MLY	M	551	1	-	0/7/9/11	0/0/0/0
1	MLY	M	553	1,4	-	0/7/9/11	0/0/0/0
1	MLY	M	59	1	-	0/7/9/11	0/0/0/0
1	MLY	M	598	1	-	0/7/9/11	0/0/0/0
1	MLY	M	600	1	-	0/7/9/11	0/0/0/0
1	MLY	M	613	1	-	0/7/9/11	0/0/0/0
1	MLY	M	617	1	-	0/7/9/11	0/0/0/0
1	MLY	M	63	1	-	0/7/9/11	0/0/0/0
1	MLY	M	659	1	-	0/7/9/11	0/0/0/0
1	MLY	M	681	1	-	0/7/9/11	0/0/0/0
1	MLY	M	764	1	-	0/7/9/11	0/0/0/0
1	MLY	M	768	1	-	0/7/9/11	0/0/0/0
1	MLY	M	782	1	-	0/7/9/11	0/0/0/0
1	MLY	M	827	1	-	0/7/9/11	0/0/0/0
1	MLY	M	833	1	-	0/7/9/11	0/0/0/0
1	MLY	M	837	1	-	0/7/9/11	0/0/0/0
1	MLY	M	839	1	-	0/7/9/11	0/0/0/0
1	MLY	M	84	1	-	0/7/9/11	0/0/0/0
1	MLY	M	87	1	-	0/7/9/11	0/0/0/0
1	MLY	P	107	1	-	0/7/9/11	0/0/0/0
1	MLY	P	130	1	-	0/7/9/11	0/0/0/0
1	MLY	P	138	1	-	0/7/9/11	0/0/0/0
1	MLY	P	19	1	-	0/7/9/11	0/0/0/0
1	MLY	P	190	1	-	0/7/9/11	0/0/0/0
1	MLY	P	236	1	-	0/7/9/11	0/0/0/0
1	MLY	P	248	1	-	0/7/9/11	0/0/0/0
1	MLY	P	272	1	-	0/7/9/11	0/0/0/0
1	MLY	P	295	1	-	0/7/9/11	0/0/0/0
1	MLY	P	296	1	-	0/7/9/11	0/0/0/0
1	MLY	P	30	1	-	0/7/9/11	0/0/0/0
1	MLY	P	348	1	-	0/7/9/11	0/0/0/0
1	MLY	P	35	1	-	0/7/9/11	0/0/0/0
1	MLY	P	353	1	-	0/7/9/11	0/0/0/0
1	MLY	P	367	1	-	0/7/9/11	0/0/0/0
1	MLY	P	369	1	-	0/7/9/11	0/0/0/0
1	MLY	P	385	1	-	0/7/9/11	0/0/0/0
1	MLY	P	415	1	-	0/7/9/11	0/0/0/0
1	MLY	P	431	1	-	0/7/9/11	0/0/0/0

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

The worst 5 of 72 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	G	138	MLY	CB-CA	-3.63	1.48	1.53
1	P	138	MLY	CB-CA	-3.56	1.48	1.53
1	J	138	MLY	CB-CA	-3.53	1.48	1.53
1	M	138	MLY	CB-CA	-3.53	1.48	1.53

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	236	MLY	O-C-CA	-3.25	117.02	125.72
1	P	236	MLY	O-C-CA	-3.24	117.03	125.72
1	D	236	MLY	O-C-CA	-3.23	117.07	125.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	236	MLY	O-C-CA	-3.22	117.09	125.72
1	M	236	MLY	O-C-CA	-3.21	117.10	125.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

184 monomers are involved in 814 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	107	MLY	2	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	504	MLY	2	0
1	A	505	MLY	35	0
1	A	528	MLY	2	0
1	A	55	MLY	1	0
1	A	551	MLY	2	0
1	A	553	MLY	19	3
1	A	59	MLY	2	0
1	A	598	MLY	1	0
1	A	600	MLY	1	0
1	A	617	MLY	1	0
1	A	63	MLY	3	0
1	A	659	MLY	2	0
1	A	764	MLY	9	0
1	A	768	MLY	18	0
1	A	782	MLY	7	0
1	A	837	MLY	4	0
1	A	839	MLY	8	0
1	A	87	MLY	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	107	MLY	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	9	0
1	D	768	MLY	11	0
1	D	782	MLY	87	0
1	D	827	MLY	2	0
1	D	837	MLY	1	0
1	D	839	MLY	4	0
1	D	87	MLY	3	0
1	G	107	MLY	2	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	5	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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	G	486	MLY	3	0
1	G	49	MLY	2	0
1	G	505	MLY	1	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	4	0
1	G	659	MLY	2	0
1	G	764	MLY	22	0
1	G	768	MLY	7	0
1	G	782	MLY	1	0
1	G	837	MLY	1	0
1	G	839	MLY	4	0
1	G	84	MLY	18	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	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	9	0
1	J	528	MLY	3	0
1	J	55	MLY	1	0
1	J	553	MLY	11	0
1	J	59	MLY	2	0
1	J	598	MLY	1	0
1	J	600	MLY	1	0
1	J	617	MLY	1	0
1	J	63	MLY	4	0
1	J	659	MLY	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	J	764	MLY	2	0
1	J	768	MLY	4	0
1	J	782	MLY	1	0
1	J	837	MLY	1	0
1	J	839	MLY	8	0
1	J	84	MLY	23	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	35	MLY	12	0
1	M	369	MLY	1	0
1	M	415	MLY	1	0
1	M	436	MLY	2	0
1	M	486	MLY	3	0
1	M	49	MLY	3	0
1	M	505	MLY	12	0
1	M	528	MLY	3	0
1	M	55	MLY	1	0
1	M	551	MLY	3	0
1	M	553	MLY	27	0
1	M	59	MLY	2	0
1	M	598	MLY	1	0
1	M	600	MLY	1	0
1	M	617	MLY	1	0
1	M	63	MLY	3	0
1	M	659	MLY	2	0
1	M	764	MLY	6	0
1	M	768	MLY	1	0
1	M	782	MLY	9	0
1	M	837	MLY	1	0
1	M	839	MLY	11	0
1	M	84	MLY	37	0
1	M	87	MLY	3	0
1	P	107	MLY	3	0
1	P	138	MLY	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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	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	3	0
1	P	659	MLY	1	0
1	P	764	MLY	9	0
1	P	782	MLY	2	0
1	P	837	MLY	1	0
1	P	839	MLY	12	0
1	P	84	MLY	5	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.