



wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 11:34 am GMT

PDB ID : 1MVW
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 : 2002-09-26
Resolution : 70.00 Å(reported)

This is a wwPDB/EMDatabank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

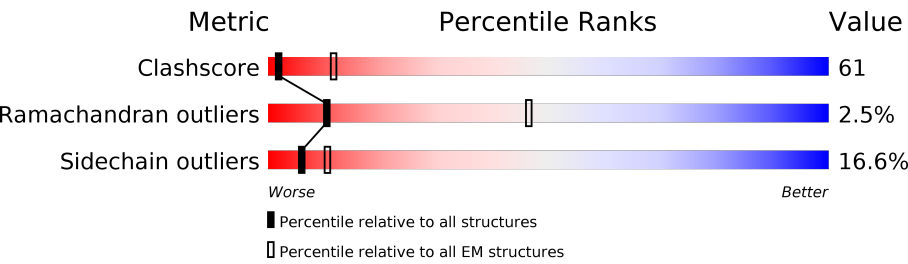
MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : recalc29047

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.















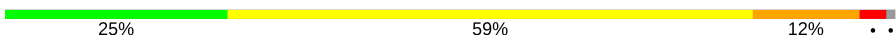



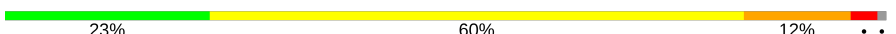
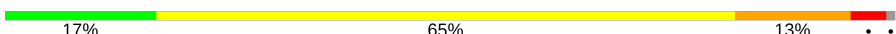





Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	840	<div><div>25%</div><div>51%</div><div>19%</div><div>.</div></div>
1	D	840	<div><div>26%</div><div>51%</div><div>19%</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>25%</div><div>52%</div><div>19%</div><div>.</div></div>
1	M	840	<div><div>26%</div><div>51%</div><div>19%</div><div>.</div></div>
1	P	840	<div><div>26%</div><div>51%</div><div>19%</div><div>.</div></div>
2	B	145	<div><div>66%</div><div>25%</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	 64% 26% 6% .
2	N	145	 65% 26% 6% .
2	Q	145	 65% 26% 6% .
3	C	147	 61% 37% .
3	F	147	 60% 38% .
3	I	147	 61% 37% .
3	L	147	 61% 37% .
3	O	147	 61% 37% .
3	R	147	 61% 37% .
4	1	375	 57% 32% 9% ..
4	2	375	 60% 31% 7% ..
4	3	375	 53% 36% 8% ..
4	4	375	 25% 59% 12% ..
4	5	375	 28% 57% 11% ..
4	6	375	 22% 63% 11% ..
4	7	375	 26% 58% 13% ..
4	8	375	 23% 60% 12% ..
4	9	375	 17% 65% 13% ..
4	V	375	 50% 38% 9% ..
4	W	375	 54% 35% 8% ..
4	X	375	 62% 29% 7% ..
4	Y	375	 62% 28% 7% ..
4	Z	375	 58% 31% 8% ..

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	MLY	A	505	-	-	X	-
1	MLY	A	553	-	-	X	-
1	MLY	A	764	-	-	X	-
1	MLY	A	768	-	-	X	-
1	MLY	A	782	-	-	X	-
1	MLY	A	839	-	-	X	-
1	MLY	D	553	-	-	X	-
1	MLY	D	764	-	-	X	-
1	MLY	D	782	-	-	X	-
1	MLY	G	295	-	-	X	-
1	MLY	G	553	-	-	X	-
1	MLY	G	764	-	-	X	-
1	MLY	G	768	-	-	X	-
1	MLY	G	84	-	-	X	-
1	MLY	J	295	-	-	X	-
1	MLY	J	505	-	-	X	-
1	MLY	J	553	-	-	X	-
1	MLY	J	768	-	-	X	-
1	MLY	J	839	-	-	X	-
1	MLY	J	84	-	-	X	-
1	MLY	M	505	-	-	X	-
1	MLY	M	764	-	-	X	-
1	MLY	M	768	-	-	X	-
1	MLY	M	839	-	-	X	-
1	MLY	P	505	-	-	X	-
1	MLY	P	768	-	-	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		

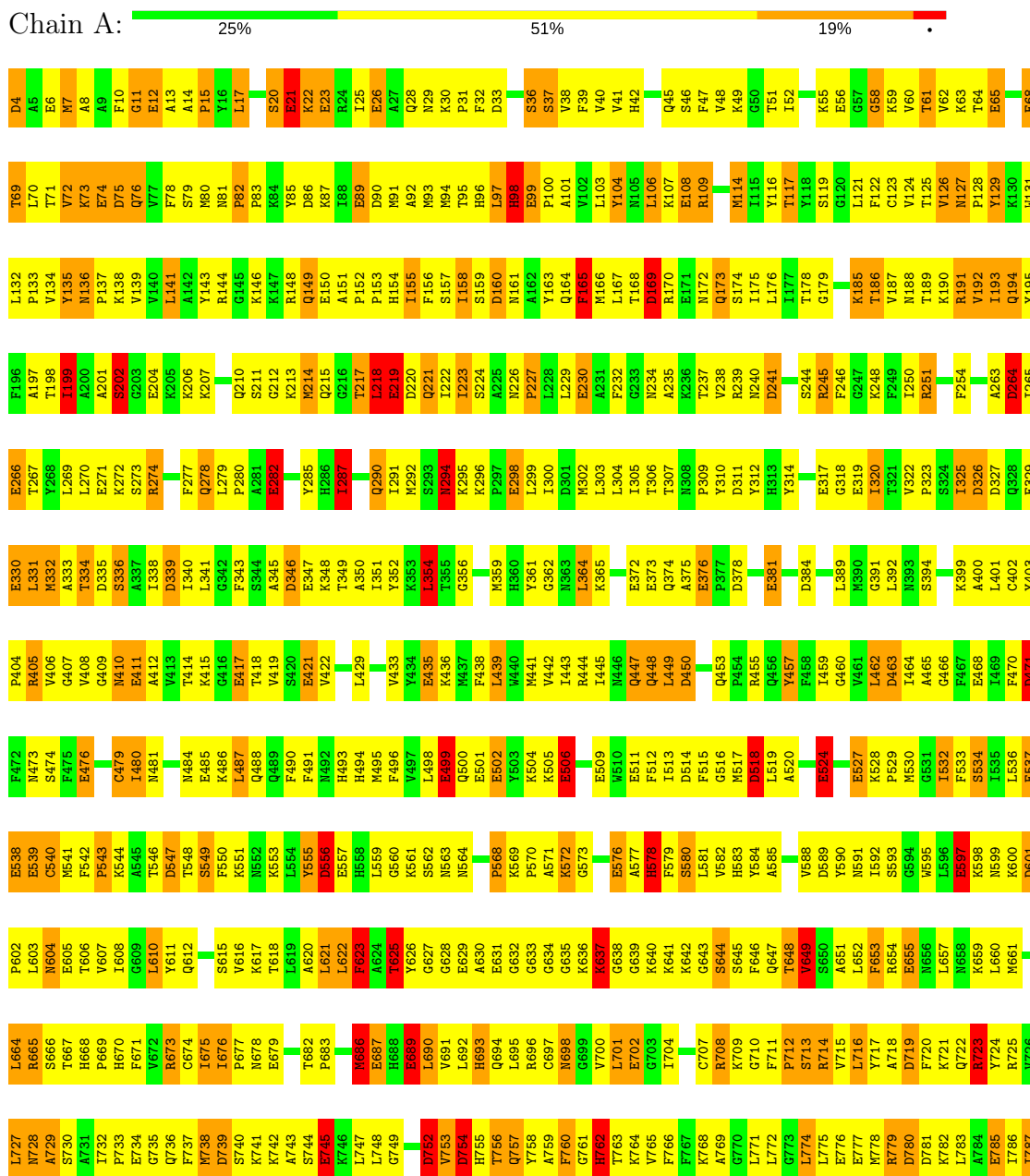
- Molecule 4 is a protein called RABBIT SKELETAL MUSCLE ACTIN.

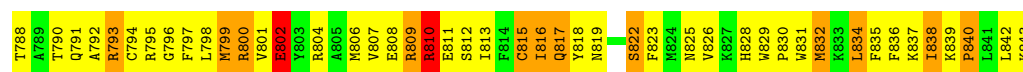
Mol	Chain	Residues	Atoms					AltConf	Trace
4	1	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	2	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	3	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	4	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	5	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	6	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	7	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	8	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	9	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	V	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	W	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	X	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	Y	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	Z	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		

3 Residue-property plots

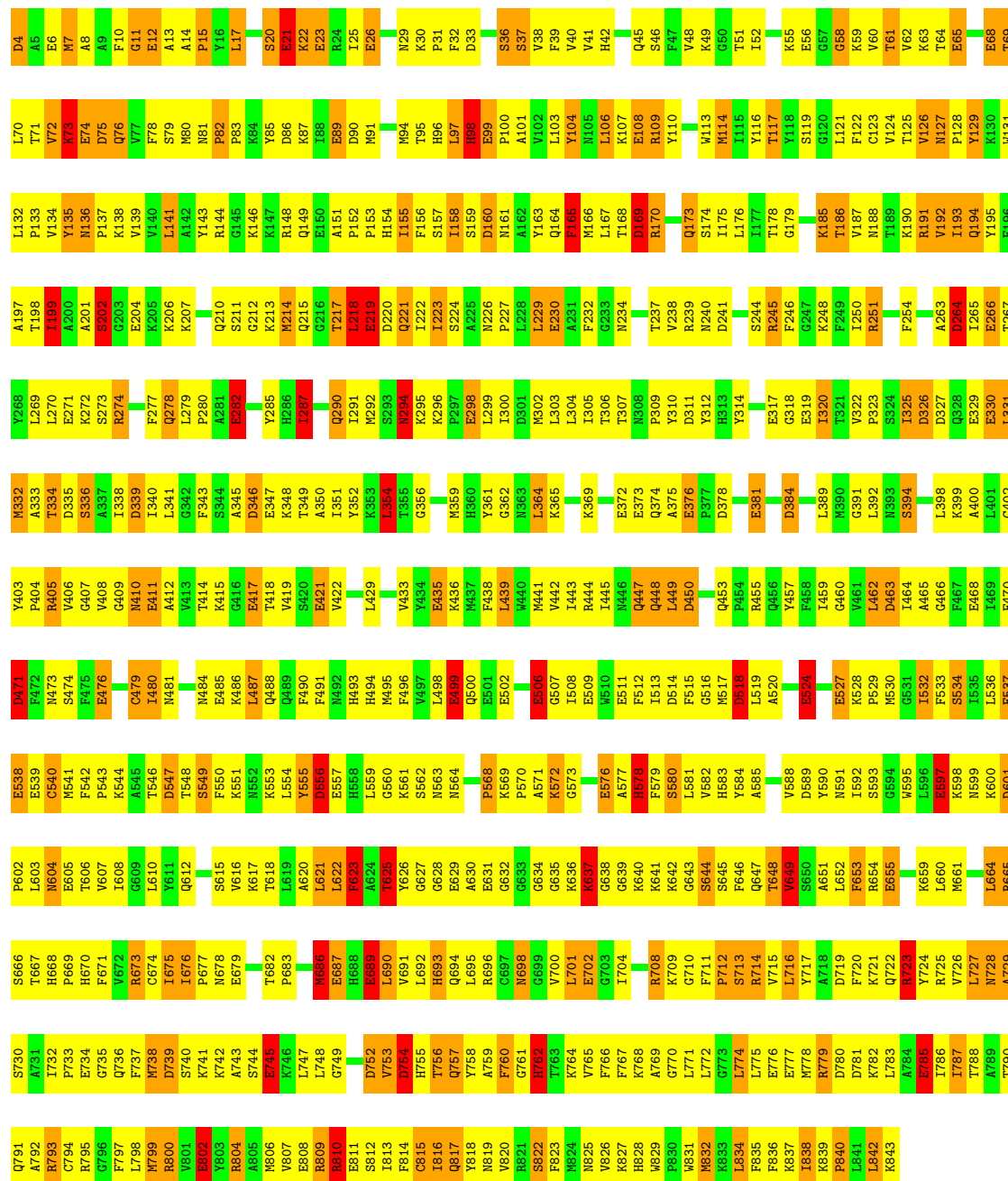
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

• Molecule 1: SKELETAL MUSCLE MYOSIN II



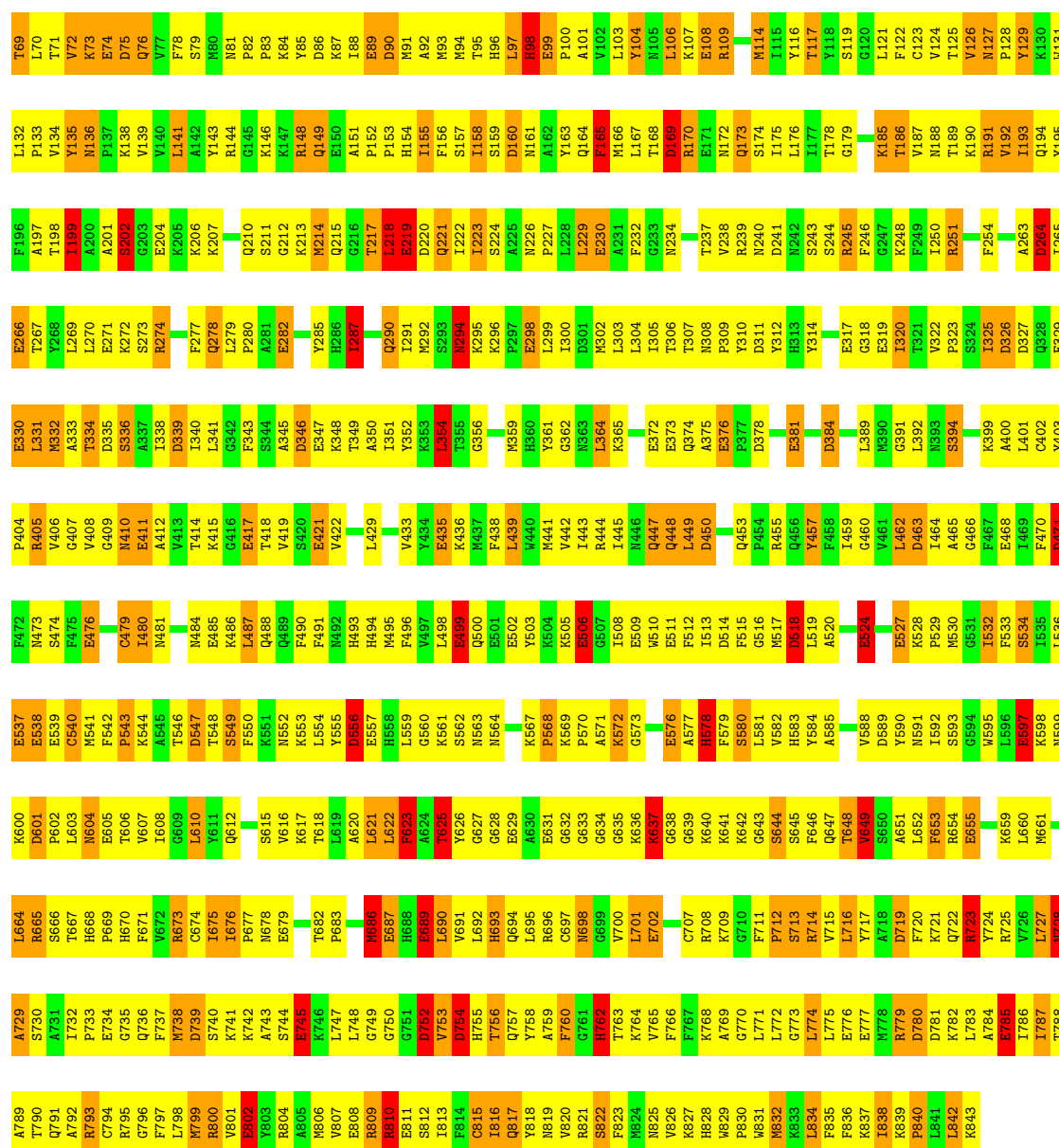


• Molecule 1: SKELETAL MUSCLE MYOSIN II



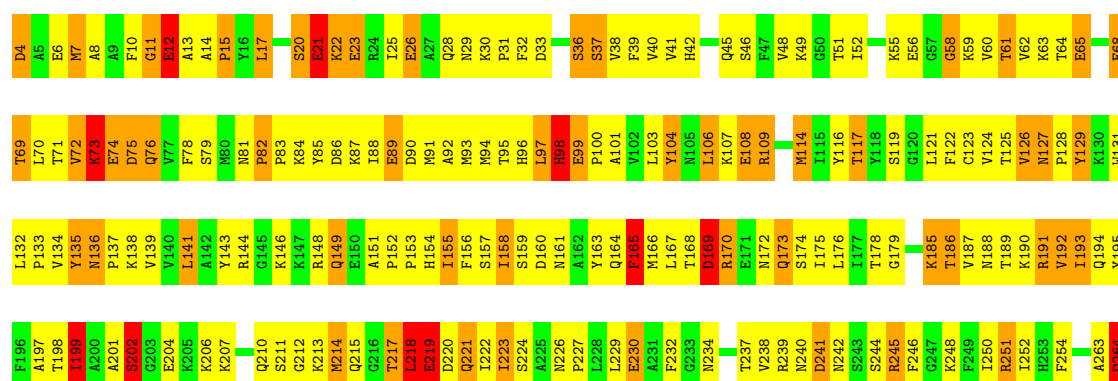
• Molecule 1: SKELETAL MUSCLE MYOSIN II

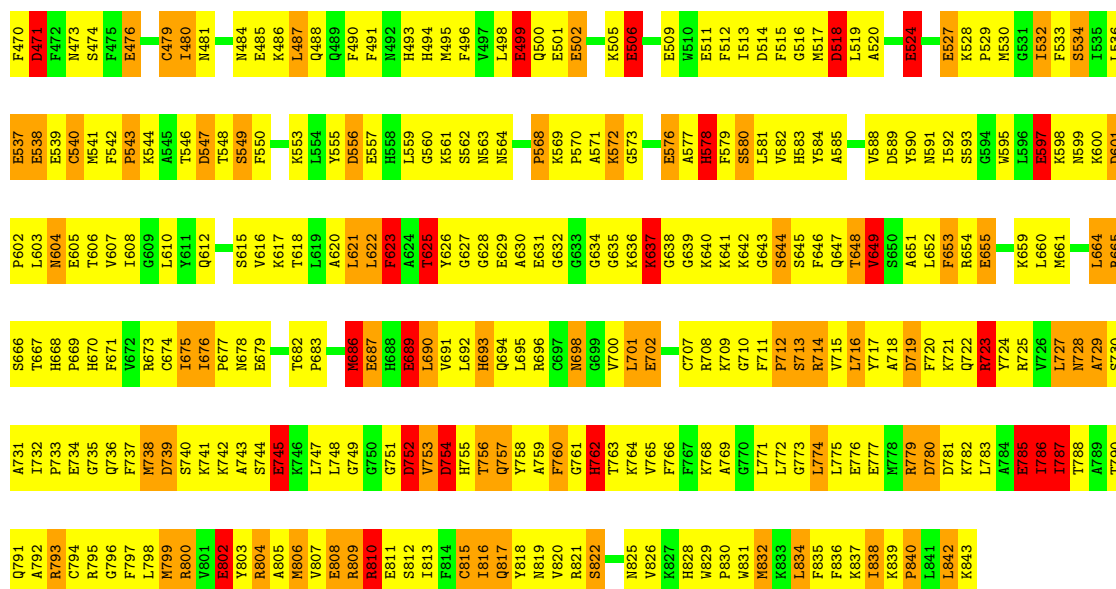




● Molecule 1: SKELETAL MUSCLE MYOSIN II

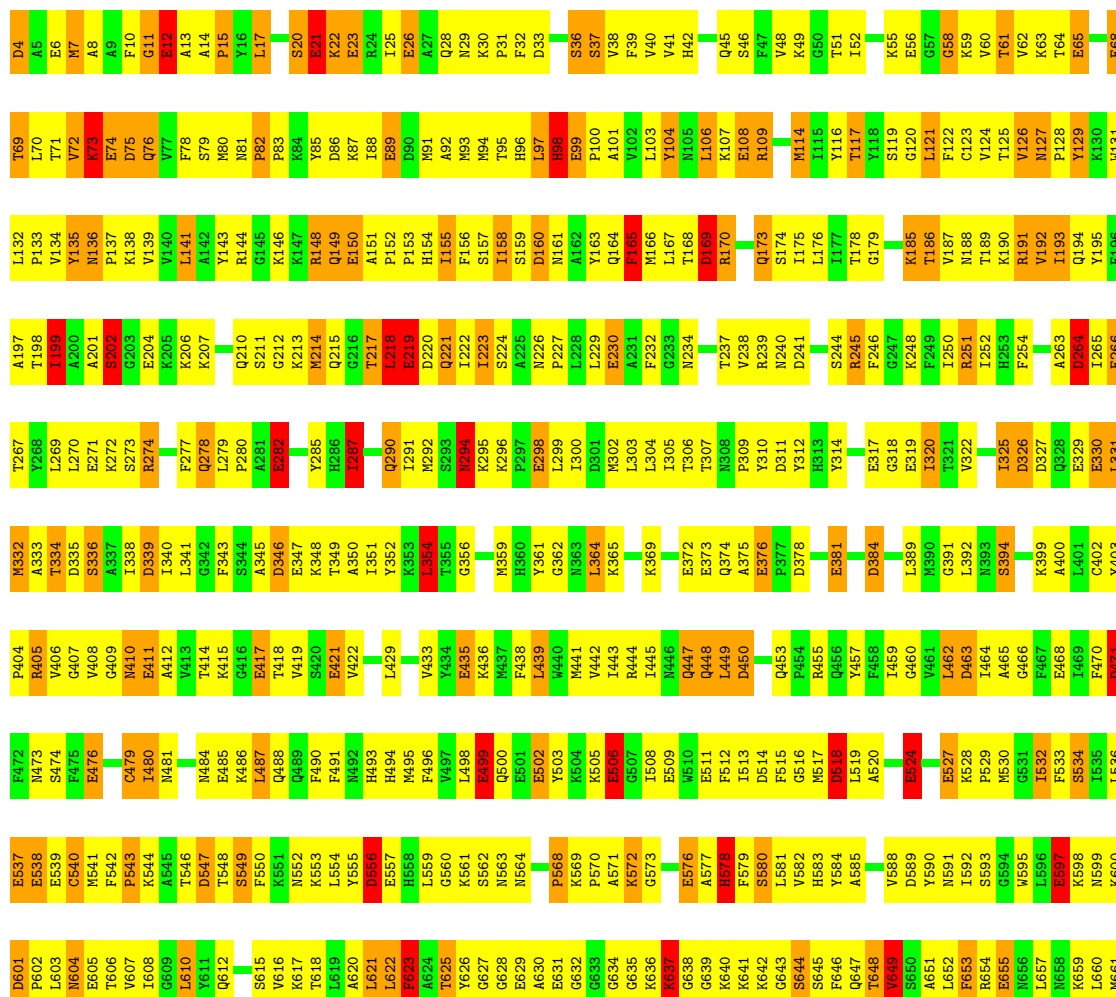
Chain J: 25% 52% 19%

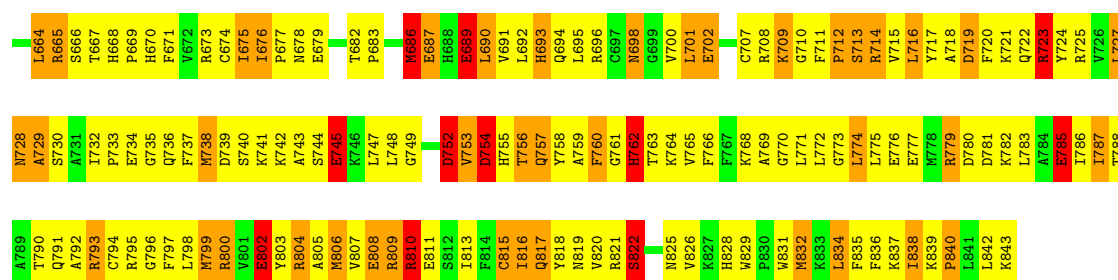




● Molecule 1: SKELETAL MUSCLE MYOSIN II

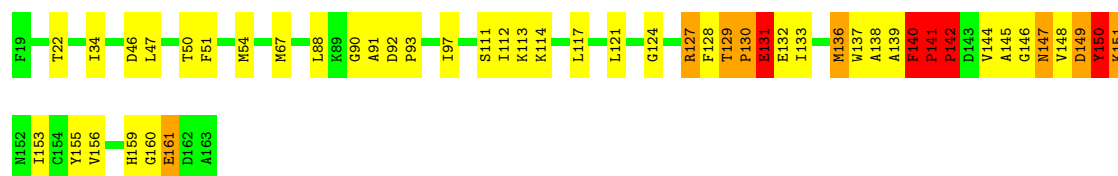
Chain P: 26% 51% 19%





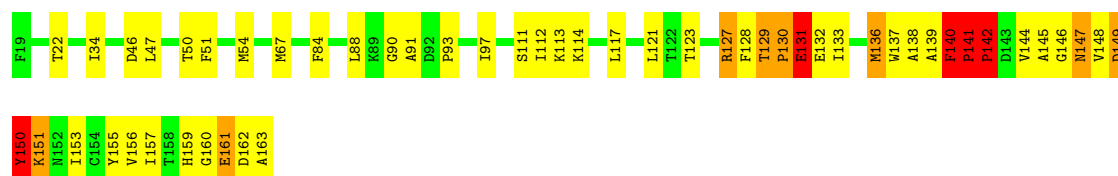
• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY; LIGHT CHAIN

Chain B: 66% 25% 6%



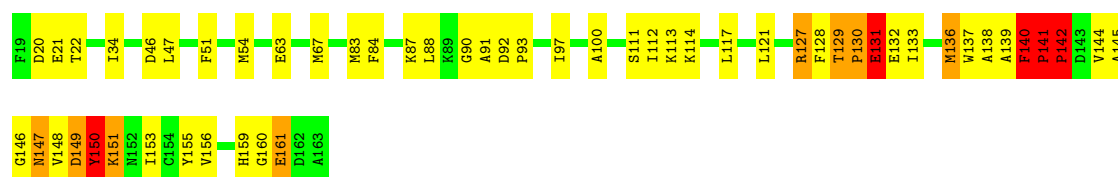
• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY; LIGHT CHAIN

Chain E: 64% 27% 6%



• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY; LIGHT CHAIN

Chain H: 63% 28% 6%



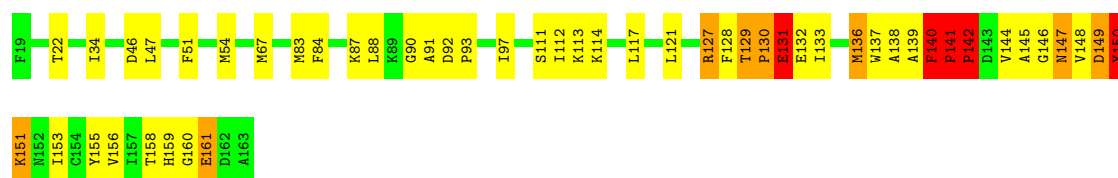
• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY; LIGHT CHAIN

Chain K: 64% 26% 6%



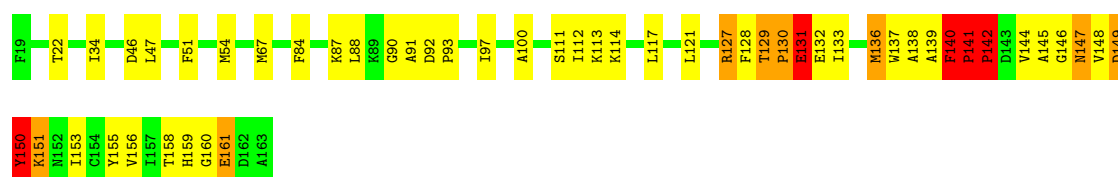
• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY; LIGHT CHAIN

Chain N: 



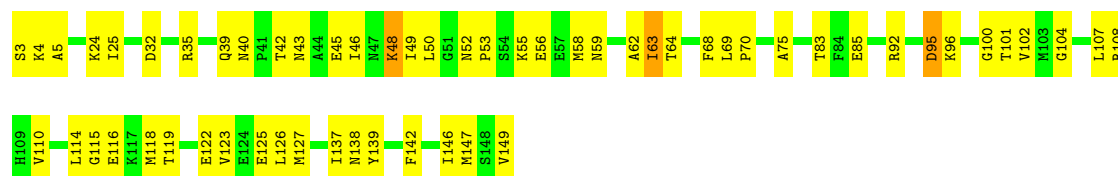
- Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY; LIGHT CHAIN

Chain Q: 



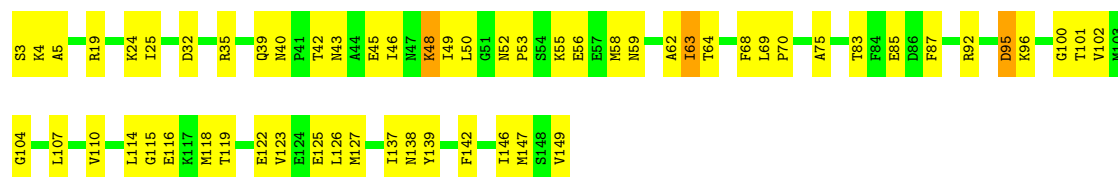
- Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL; LIGHT CHAIN

Chain C: 



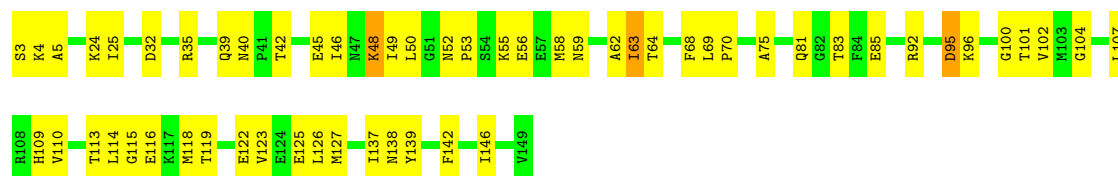
- Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL; LIGHT CHAIN

Chain F: 



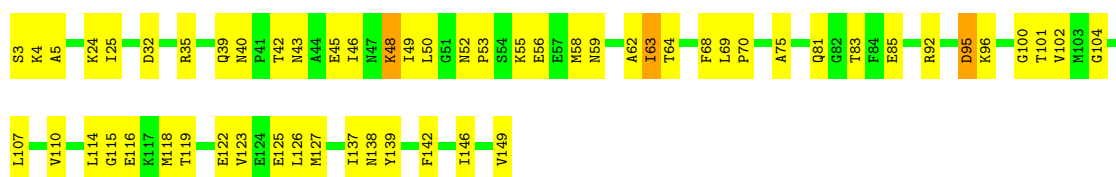
- Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL; LIGHT CHAIN

Chain I: 



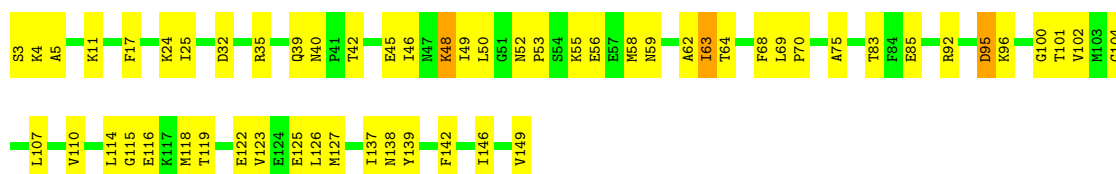
- Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL; LIGHT CHAIN

Chain L: 



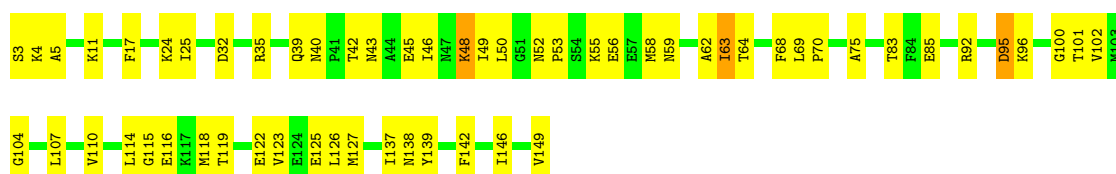
• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL; LIGHT CHAIN

Chain O: 61% 37%



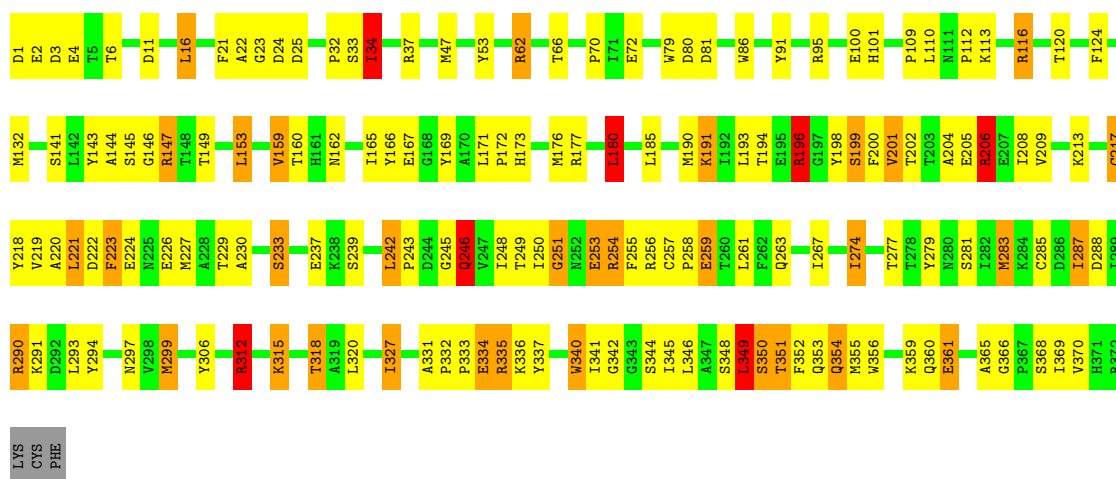
• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL; LIGHT CHAIN

Chain R: 61% 37%



• Molecule 4: RABBIT SKELETAL MUSCLE ACTIN

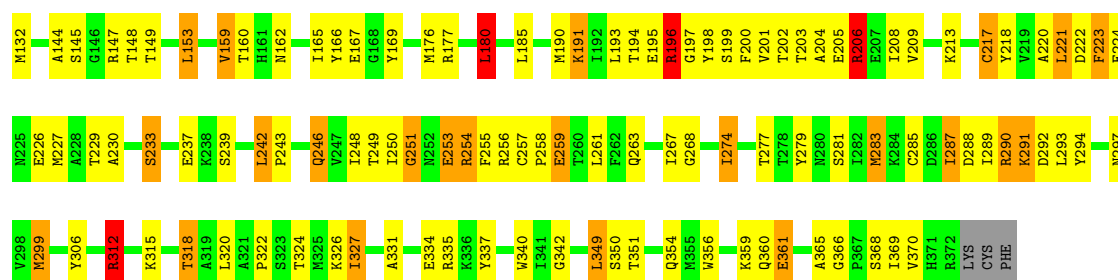
Chain 1: 57% 32% 9%



• Molecule 4: RABBIT SKELETAL MUSCLE ACTIN

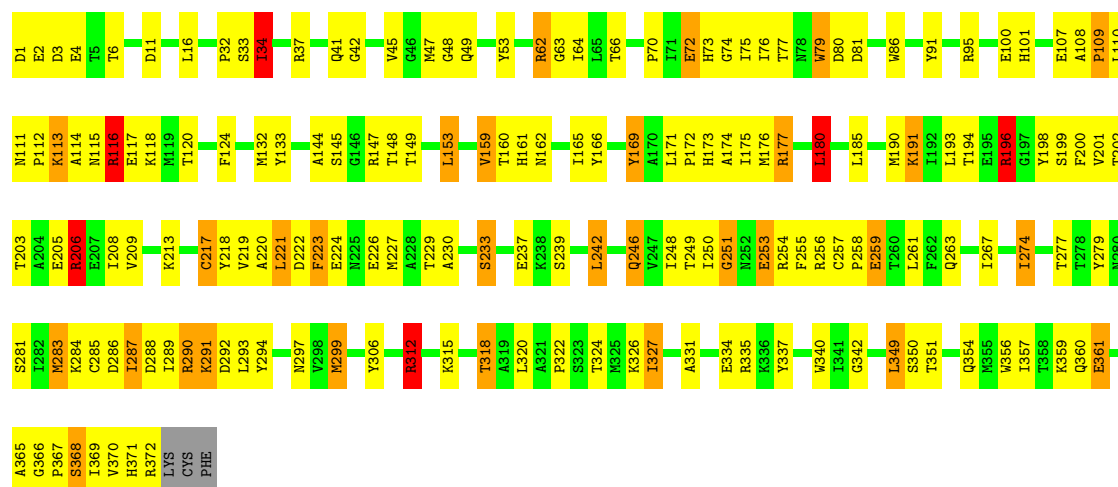
Chain 2: 60% 31% 7%





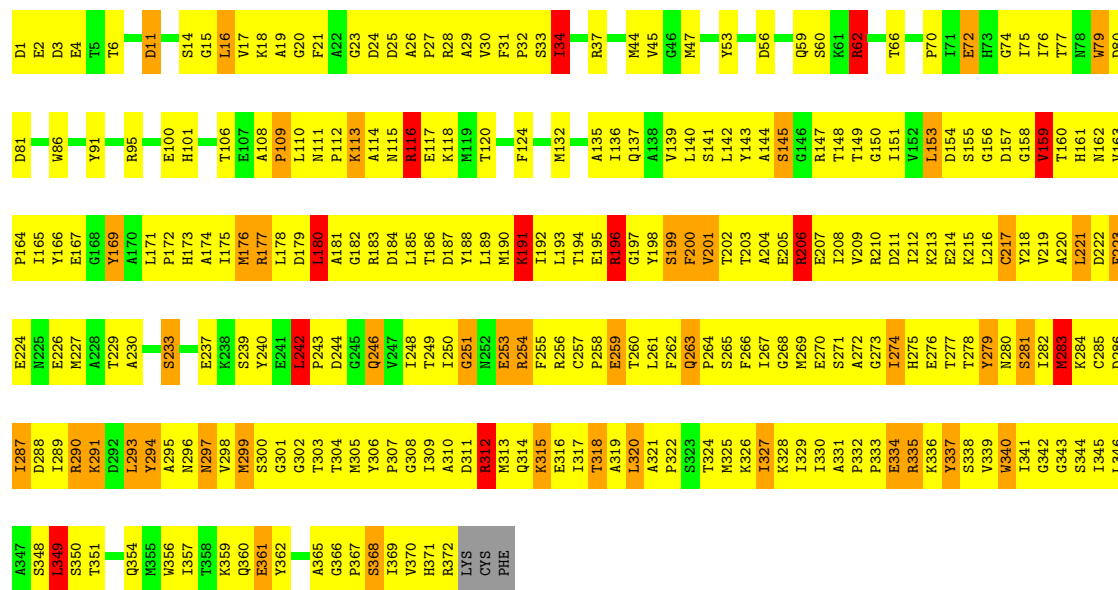
• Molecule 4: RABBIT SKELETAL MUSCLE ACTIN

Chain 3: 53% 36% 8% ..

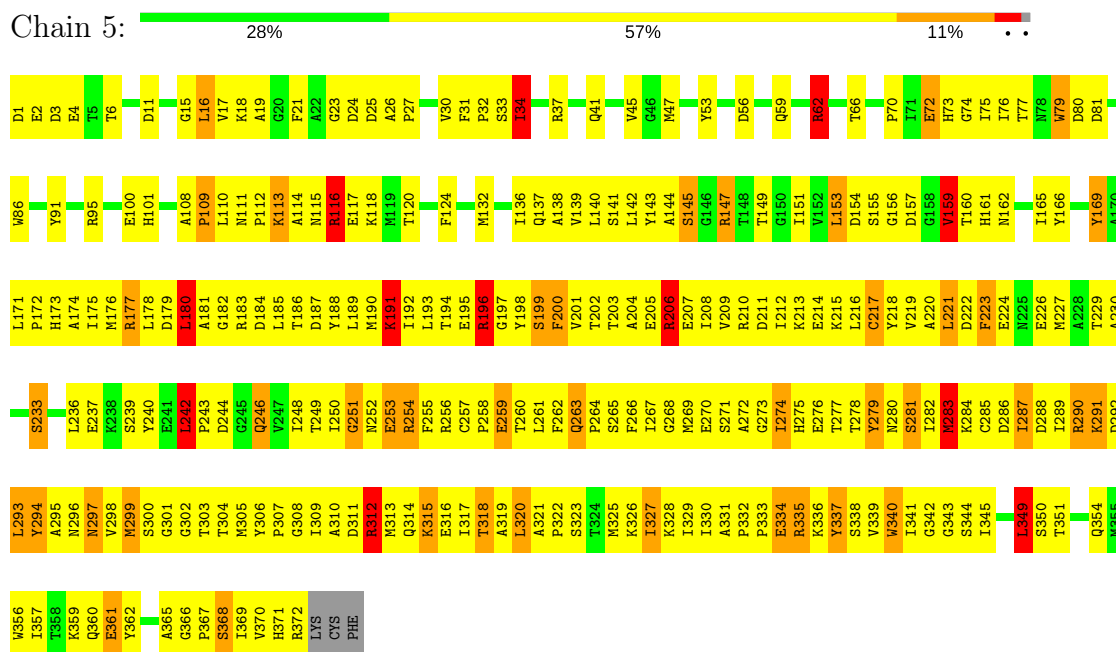


• Molecule 4: RABBIT SKELETAL MUSCLE ACTIN

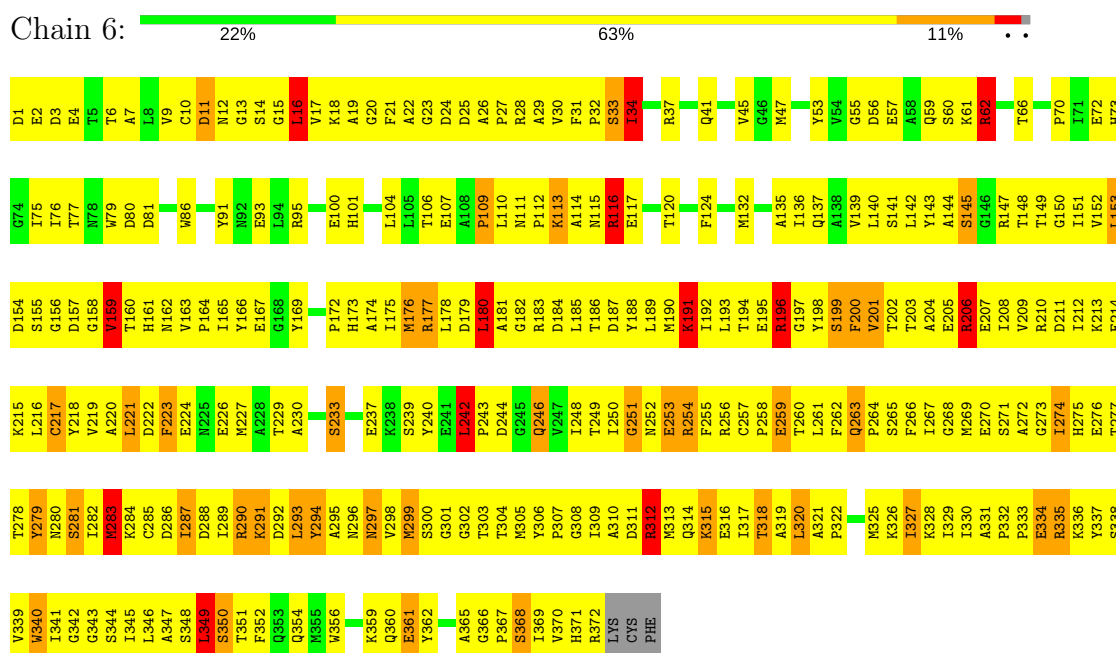
Chain 4: 25% 59% 12% ..



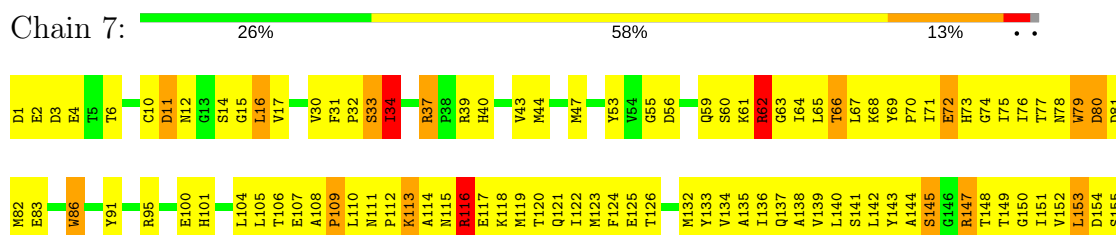
• Molecule 4: RABBIT SKELETAL MUSCLE ACTIN

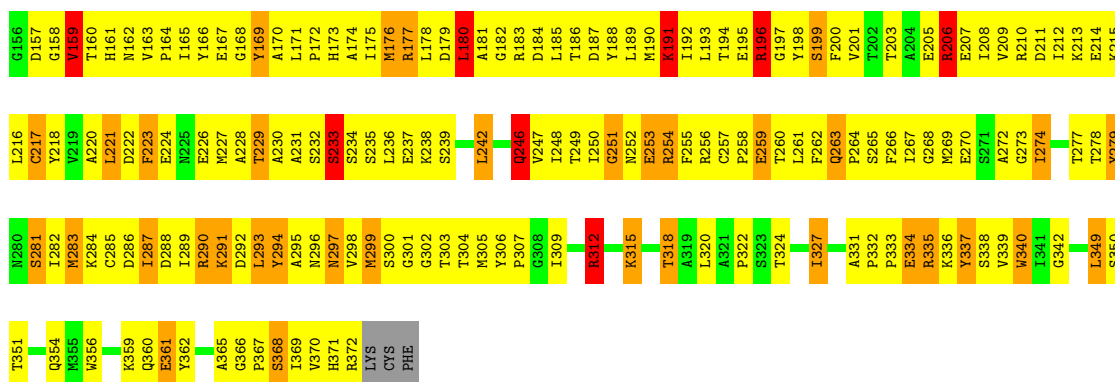


• Molecule 4: RABBIT SKELETAL MUSCLE ACTIN



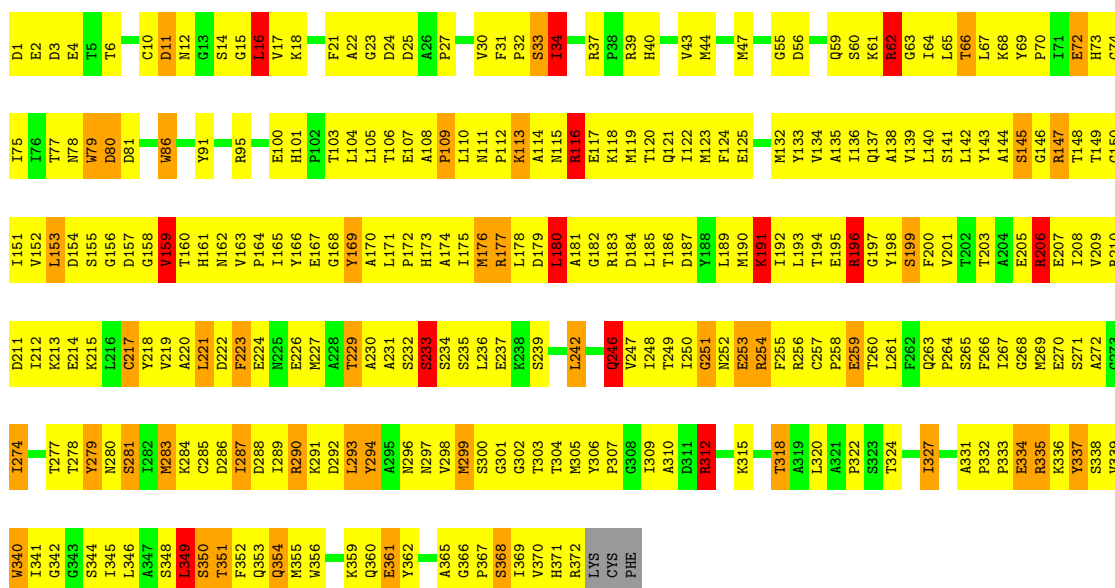
• Molecule 4: RABBIT SKELETAL MUSCLE ACTIN





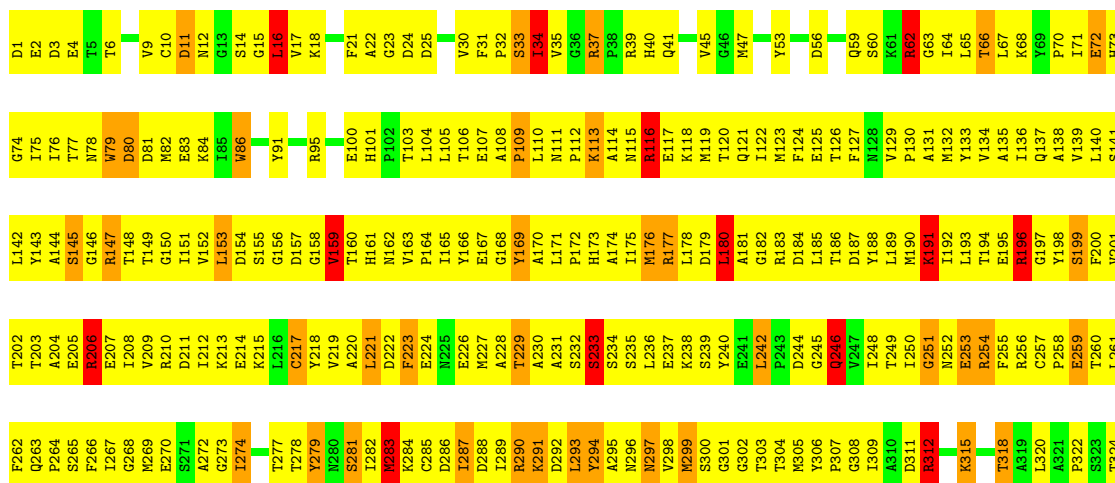
- Molecule 4: RABBIT SKELETAL MUSCLE ACTIN

Chain 8: 23% 60% 12% 5%



- Molecule 4: RABBIT SKELETAL MUSCLE ACTIN

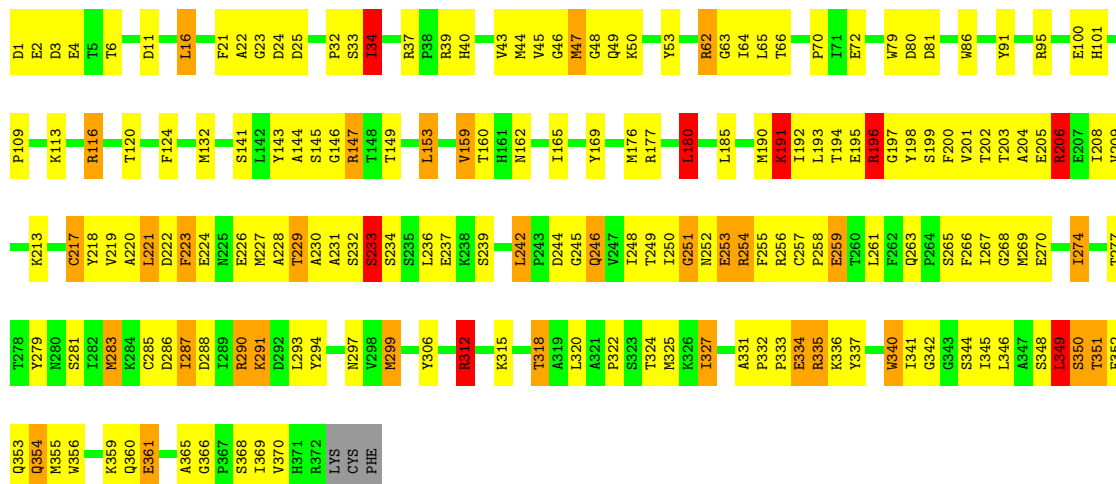
Chain 9: 17% 65% 13% 5%





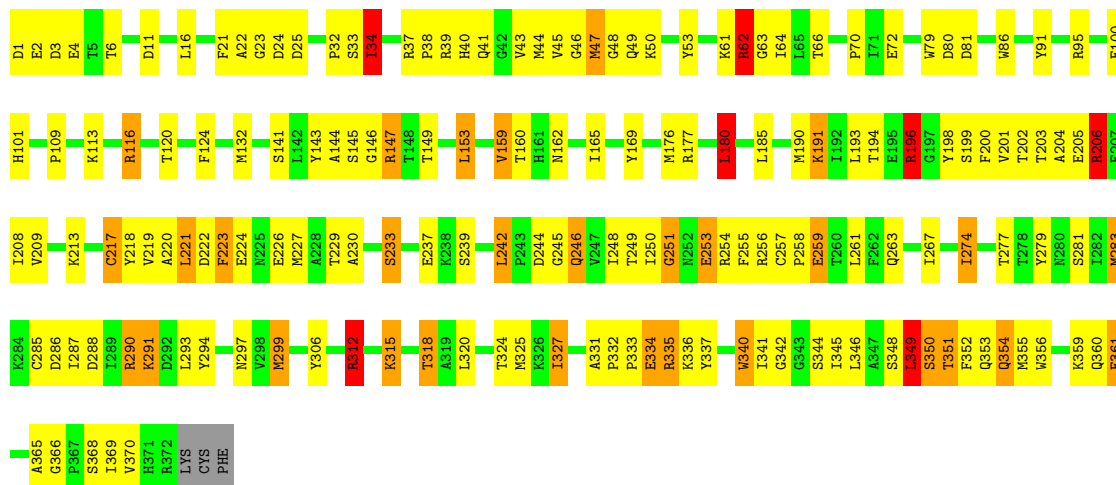
• Molecule 4: RABBIT SKELETAL MUSCLE ACTIN

Chain V: 50% 38% 9% ..



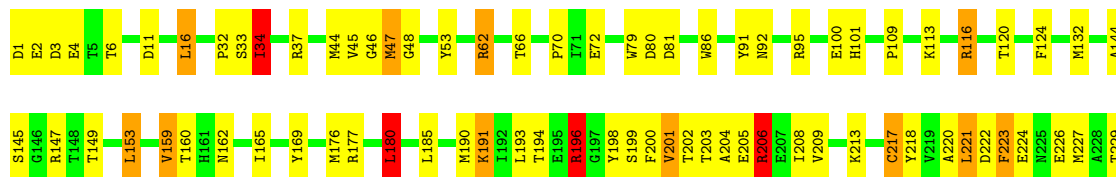
• Molecule 4: RABBIT SKELETAL MUSCLE ACTIN

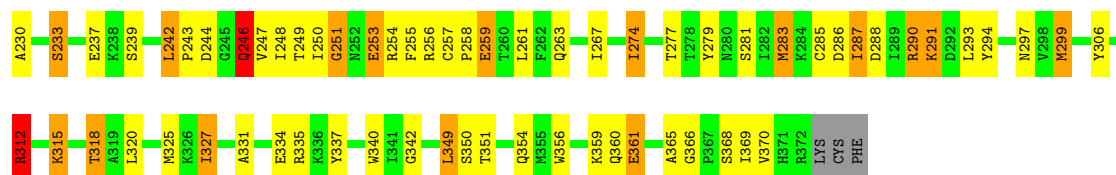
Chain W: 54% 35% 8% ..



• Molecule 4: RABBIT SKELETAL MUSCLE ACTIN

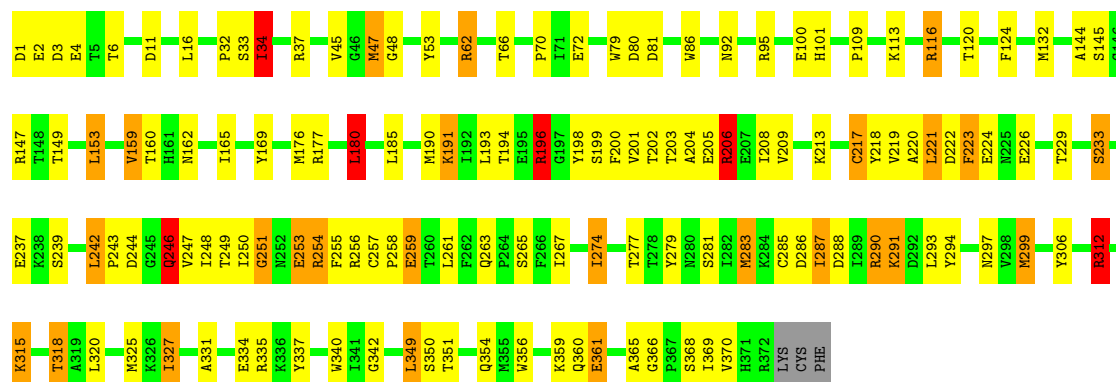
Chain X: 62% 29% 7% ..





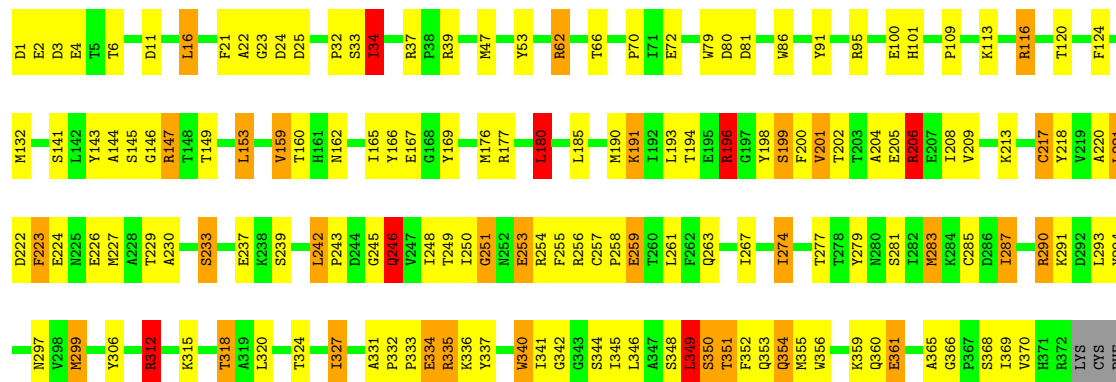
• Molecule 4: RABBIT SKELETAL MUSCLE ACTIN

Chain Y: 62% 28% 7% ..



• Molecule 4: RABBIT SKELETAL MUSCLE ACTIN

Chain Z: 58% 31% 8% ..



4 Experimental information

Property	Value	Source
Reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of tilted images used	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	63/6448 (1.0%)	1.82	114/8729 (1.3%)
1	G	1.77	66/6449 (1.0%)	1.82	118/8732 (1.4%)
1	J	1.78	68/6449 (1.1%)	1.87	118/8732 (1.4%)
1	M	1.78	65/6448 (1.0%)	1.90	122/8729 (1.4%)
1	P	1.82	68/6448 (1.1%)	1.86	119/8729 (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	16/1548 (1.0%)
2	K	1.22	10/1148 (0.9%)	1.61	16/1548 (1.0%)
2	N	1.22	10/1148 (0.9%)	1.61	16/1548 (1.0%)
2	Q	1.22	10/1148 (0.9%)	1.61	16/1548 (1.0%)
3	C	0.80	0/1136	0.95	4/1525 (0.3%)
3	F	0.80	0/1136	0.95	4/1525 (0.3%)
3	I	0.80	0/1136	0.95	4/1525 (0.3%)
3	L	0.79	0/1136	0.94	4/1525 (0.3%)
3	O	0.79	0/1136	0.95	4/1525 (0.3%)
3	R	0.79	0/1136	0.95	4/1525 (0.3%)
4	1	0.89	2/2968 (0.1%)	1.64	51/4023 (1.3%)
4	2	0.89	2/2968 (0.1%)	1.64	50/4023 (1.2%)
4	3	0.89	1/2968 (0.0%)	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	6	0.89	1/2968 (0.0%)	1.64	49/4023 (1.2%)
4	7	0.89	2/2968 (0.1%)	1.64	51/4023 (1.3%)
4	8	0.89	2/2968 (0.1%)	1.64	51/4023 (1.3%)
4	9	0.89	2/2968 (0.1%)	1.64	52/4023 (1.3%)
4	V	0.89	2/2968 (0.1%)	1.64	52/4023 (1.3%)
4	W	0.89	1/2968 (0.0%)	1.64	52/4023 (1.3%)
4	X	0.89	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	51/4023 (1.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
All	All	1.35	482/93946 (0.5%)	1.69	1543/127140 (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	5
1	P	1	4
2	B	0	3
2	E	0	3
2	H	0	3
2	K	0	3
2	N	0	3
2	Q	0	3
3	C	0	2
3	F	0	2
3	I	0	2
3	L	0	2
3	O	0	2
3	R	0	2
4	1	0	1
4	2	0	1
4	3	0	1
4	4	0	1
4	5	0	1
4	6	0	1
4	7	0	1
4	8	0	1
4	9	0	1
4	V	0	1
4	W	0	1
4	X	0	1
4	Y	0	1
4	Z	0	1
All	All	6	71

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	649	VAL	CB-CG1	53.31	2.64	1.52
1	J	649	VAL	CB-CG1	53.28	2.64	1.52
1	G	649	VAL	CB-CG1	53.26	2.64	1.52
1	P	649	VAL	CB-CG1	53.24	2.64	1.52
1	A	649	VAL	CB-CG1	53.20	2.64	1.52

The worst 5 of 1543 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	637	LYS	O-C-N	-58.48	23.78	123.20
1	D	637	LYS	O-C-N	-58.48	23.78	123.20
1	J	637	LYS	O-C-N	-58.47	23.80	123.20
1	M	637	LYS	O-C-N	-58.47	23.81	123.20
1	P	637	LYS	O-C-N	-58.46	23.82	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 71 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	1482	5

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	6797	0	6757	1507	35
1	G	6797	0	6765	1499	0
1	J	6797	0	6761	1459	0
1	M	6797	0	6759	1617	0
1	P	6797	0	6759	1556	0
2	B	1127	0	1085	233	0
2	E	1127	0	1087	278	0
2	H	1127	0	1087	274	0
2	K	1127	0	1089	284	0
2	N	1127	0	1089	261	0
2	Q	1127	0	1088	260	0
3	C	1123	0	1083	188	0
3	F	1123	0	1084	192	0
3	I	1123	0	1082	185	0
3	L	1123	0	1082	159	0
3	O	1123	0	1084	193	0
3	R	1123	0	1083	170	0
4	1	2906	0	2856	425	0
4	2	2906	0	2860	217	73
4	3	2906	0	2864	161	593
4	4	2906	0	2863	181	3275
4	5	2906	0	2865	95	3030
4	6	2906	0	2865	100	3436
4	7	2906	0	2866	76	3348
4	8	2906	0	2857	316	2994
4	9	2906	0	2855	347	3591
4	V	2906	0	2851	381	334
4	W	2906	0	2851	395	100
4	X	2906	0	2863	181	0
4	Y	2906	0	2864	183	0
4	Z	2906	0	2855	379	0
All	All	94966	0	93612	11529	10407

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 11529 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:84:MLY:HD3	1:J:724:TYR:CE2	1.23	1.69
1:D:797:PHE:CE2	3:F:126:LEU:HD22	1.22	1.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:508:ILE:CD1	1:D:766:PHE:CE1	1.74	1.68
1:P:149:GLN:CG	1:P:716:LEU:HD23	1.21	1.68
4:2:287:ILE:CG2	4:4:202:THR:HB	1.23	1.66

The worst 5 of 10407 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)
4:5:297:ASN:OD1	4:8:170:ALA:CA[1_554]	0.08	2.12
4:5:275:HIS:N	4:8:162:ASN:C[1_554]	0.13	2.07
4:5:177:ARG:CZ	4:9:194:THR:CG2[1_554]	0.14	2.06
4:5:26:ALA:CB	4:8:122:ILE:C[1_554]	0.17	2.03
4:6:271:SER:C	4:9:277:THR:OG1[1_554]	0.18	2.02

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	789/840 (94%)	651 (82%)	112 (14%)	26 (3%)	4	35
1	D	789/840 (94%)	651 (82%)	112 (14%)	26 (3%)	4	35
1	G	791/840 (94%)	651 (82%)	113 (14%)	27 (3%)	4	35
1	J	791/840 (94%)	651 (82%)	113 (14%)	27 (3%)	4	35
1	M	789/840 (94%)	650 (82%)	111 (14%)	28 (4%)	4	34
1	P	789/840 (94%)	651 (82%)	111 (14%)	27 (3%)	4	35
2	B	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	2	25
2	E	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	2	25
2	H	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	2	25
2	K	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	2	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	N	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	2	25
2	Q	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	2	25
3	C	143/147 (97%)	133 (93%)	10 (7%)	0	100	100
3	F	143/147 (97%)	133 (93%)	10 (7%)	0	100	100
3	I	143/147 (97%)	133 (93%)	10 (7%)	0	100	100
3	L	143/147 (97%)	133 (93%)	10 (7%)	0	100	100
3	O	143/147 (97%)	133 (93%)	10 (7%)	0	100	100
3	R	143/147 (97%)	133 (93%)	10 (7%)	0	100	100
4	1	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	11	51
4	2	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	11	51
4	3	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	11	51
4	4	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	11	51
4	5	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	11	51
4	6	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	11	51
4	7	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	11	51
4	8	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	11	51
4	9	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	11	51
4	V	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	11	51
4	W	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	11	51
4	X	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	11	51
4	Y	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	11	51
4	Z	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	11	51
All	All	11634/12042 (97%)	10138 (87%)	1203 (10%)	293 (2%)	10	41

5 of 293 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	5
1	D	672/672 (100%)	515 (77%)	157 (23%)	1	5
1	G	672/672 (100%)	513 (76%)	159 (24%)	1	5
1	J	672/672 (100%)	514 (76%)	158 (24%)	1	5
1	M	672/672 (100%)	514 (76%)	158 (24%)	1	5
1	P	672/672 (100%)	514 (76%)	158 (24%)	1	5
2	B	120/120 (100%)	119 (99%)	1 (1%)	85	92
2	E	120/120 (100%)	119 (99%)	1 (1%)	85	92
2	H	120/120 (100%)	119 (99%)	1 (1%)	85	92
2	K	120/120 (100%)	119 (99%)	1 (1%)	85	92
2	N	120/120 (100%)	119 (99%)	1 (1%)	85	92
2	Q	120/120 (100%)	119 (99%)	1 (1%)	85	92
3	C	117/117 (100%)	112 (96%)	5 (4%)	33	64
3	F	117/117 (100%)	112 (96%)	5 (4%)	33	64
3	I	117/117 (100%)	112 (96%)	5 (4%)	33	64
3	L	117/117 (100%)	112 (96%)	5 (4%)	33	64
3	O	117/117 (100%)	112 (96%)	5 (4%)	33	64
3	R	117/117 (100%)	112 (96%)	5 (4%)	33	64
4	1	315/318 (99%)	268 (85%)	47 (15%)	3	20
4	2	315/318 (99%)	269 (85%)	46 (15%)	3	21
4	3	315/318 (99%)	269 (85%)	46 (15%)	3	21
4	4	315/318 (99%)	269 (85%)	46 (15%)	3	21
4	5	315/318 (99%)	269 (85%)	46 (15%)	3	21
4	6	315/318 (99%)	268 (85%)	47 (15%)	3	20
4	7	315/318 (99%)	269 (85%)	46 (15%)	3	21
4	8	315/318 (99%)	268 (85%)	47 (15%)	3	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	9	315/318 (99%)	268 (85%)	47 (15%)	3	20
4	V	315/318 (99%)	268 (85%)	47 (15%)	3	20
4	W	315/318 (99%)	269 (85%)	46 (15%)	3	21
4	X	315/318 (99%)	268 (85%)	47 (15%)	3	20
4	Y	315/318 (99%)	269 (85%)	46 (15%)	3	21
4	Z	315/318 (99%)	268 (85%)	47 (15%)	3	20
All	All	9864/9906 (100%)	8227 (83%)	1637 (17%)	6	16

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

Mol	Chain	Res	Type
1	M	447	GLN
1	P	499	GLU
4	X	196	ARG
1	M	561	LYS
1	P	46	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 238 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	29	ASN
3	O	81	GLN
4	W	263	GLN
1	M	188	ASN
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	10,10,11	0.47	0	8,11,13	1.02	1 (12%)
1	MLY	A	130	1	10,10,11	0.99	1 (10%)	8,11,13	1.34	2 (25%)
1	MLY	A	138	1	10,10,11	1.36	1 (10%)	8,11,13	2.73	1 (12%)
1	MLY	A	19	1	10,10,11	1.20	1 (10%)	8,11,13	0.62	0
1	MLY	A	190	1	10,10,11	1.17	1 (10%)	8,11,13	1.32	1 (12%)
1	MLY	A	236	1	10,10,11	1.10	1 (10%)	8,11,13	1.56	2 (25%)
1	MLY	A	248	1	10,10,11	0.78	0	8,11,13	0.85	0
1	MLY	A	272	1	10,10,11	1.07	1 (10%)	8,11,13	1.31	1 (12%)
1	MLY	A	295	1	10,10,11	1.15	1 (10%)	8,11,13	0.29	0
1	MLY	A	296	1	10,10,11	0.85	1 (10%)	8,11,13	1.20	1 (12%)
1	MLY	A	30	1	10,10,11	0.87	0	8,11,13	0.90	0
1	MLY	A	348	1	10,10,11	0.80	0	8,11,13	1.10	1 (12%)
1	MLY	A	35	1	10,10,11	0.73	0	8,11,13	0.65	0
1	MLY	A	353	1	10,10,11	0.99	0	8,11,13	1.04	1 (12%)
1	MLY	A	367	1	10,10,11	0.88	1 (10%)	8,11,13	0.43	0
1	MLY	A	369	1	10,10,11	0.86	0	8,11,13	0.77	0
1	MLY	A	385	1	10,10,11	0.94	1 (10%)	8,11,13	0.53	0
1	MLY	A	415	1	10,10,11	0.72	0	8,11,13	0.73	0
1	MLY	A	431	1	10,10,11	0.47	0	8,11,13	1.19	1 (12%)
1	MLY	A	436	1	10,10,11	1.01	1 (10%)	8,11,13	1.78	1 (12%)
1	MLY	A	486	1	10,10,11	0.57	0	8,11,13	0.54	0
1	MLY	A	49	1	10,10,11	1.07	1 (10%)	8,11,13	1.24	1 (12%)
1	MLY	A	504	1	10,10,11	0.84	0	8,11,13	0.46	0
1	MLY	A	505	1	10,10,11	1.44	2 (20%)	8,11,13	0.51	0
1	MLY	A	528	1	10,10,11	0.84	0	8,11,13	1.13	1 (12%)
1	MLY	A	55	1	10,10,11	0.94	1 (10%)	8,11,13	1.10	0
1	MLY	A	551	1	10,10,11	0.60	0	8,11,13	0.72	0
1	MLY	A	553	1,4	10,10,11	0.67	0	8,11,13	0.65	0
1	MLY	A	59	1	10,10,11	0.79	0	8,11,13	1.14	1 (12%)
1	MLY	A	598	1	10,10,11	1.15	2 (20%)	8,11,13	1.30	1 (12%)
1	MLY	A	600	1	10,10,11	0.63	0	8,11,13	0.98	1 (12%)
1	MLY	A	613	1	10,10,11	0.63	0	8,11,13	1.10	1 (12%)
1	MLY	A	617	1	10,10,11	0.86	1 (10%)	8,11,13	0.58	0
1	MLY	A	63	1	10,10,11	0.93	1 (10%)	8,11,13	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	A	659	1	10,10,11	0.73	0	8,11,13	0.84	0
1	MLY	A	681	1	10,10,11	0.99	1 (10%)	8,11,13	1.44	1 (12%)
1	MLY	A	764	1	10,10,11	0.81	0	8,11,13	0.50	0
1	MLY	A	768	1	10,10,11	0.89	0	8,11,13	1.97	1 (12%)
1	MLY	A	782	1	10,10,11	0.74	0	8,11,13	1.53	1 (12%)
1	MLY	A	827	1	10,10,11	1.01	1 (10%)	8,11,13	0.94	1 (12%)
1	MLY	A	833	1	10,10,11	1.06	1 (10%)	8,11,13	1.13	1 (12%)
1	MLY	A	837	1	10,10,11	0.68	0	8,11,13	0.54	0
1	MLY	A	839	1	10,10,11	0.66	0	8,11,13	1.50	1 (12%)
1	MLY	A	84	1	10,10,11	0.58	0	8,11,13	0.80	0
1	MLY	A	87	1	10,10,11	1.10	1 (10%)	8,11,13	0.59	0
1	MLY	D	107	1	10,10,11	0.50	0	8,11,13	1.04	1 (12%)
1	MLY	D	130	1	10,10,11	0.94	1 (10%)	8,11,13	1.33	2 (25%)
1	MLY	D	138	1	10,10,11	1.36	1 (10%)	8,11,13	2.70	1 (12%)
1	MLY	D	19	1	10,10,11	1.28	1 (10%)	8,11,13	0.64	0
1	MLY	D	190	1	10,10,11	1.15	1 (10%)	8,11,13	1.32	1 (12%)
1	MLY	D	236	1	10,10,11	1.11	1 (10%)	8,11,13	1.55	2 (25%)
1	MLY	D	248	1	10,10,11	0.76	0	8,11,13	0.85	0
1	MLY	D	272	1	10,10,11	1.05	1 (10%)	8,11,13	1.31	1 (12%)
1	MLY	D	295	1	10,10,11	1.11	1 (10%)	8,11,13	0.33	0
1	MLY	D	296	1	10,10,11	0.88	1 (10%)	8,11,13	1.20	1 (12%)
1	MLY	D	30	1	10,10,11	0.89	0	8,11,13	0.94	0
1	MLY	D	348	1	10,10,11	0.76	0	8,11,13	1.07	1 (12%)
1	MLY	D	35	1	10,10,11	0.74	0	8,11,13	0.63	0
1	MLY	D	353	1	10,10,11	0.96	0	8,11,13	1.01	1 (12%)
1	MLY	D	367	1	10,10,11	0.91	1 (10%)	8,11,13	0.41	0
1	MLY	D	369	1	10,10,11	0.83	0	8,11,13	0.76	0
1	MLY	D	385	1	10,10,11	0.93	1 (10%)	8,11,13	0.55	0
1	MLY	D	415	1	10,10,11	0.75	0	8,11,13	0.76	0
1	MLY	D	431	1	10,10,11	0.49	0	8,11,13	1.19	1 (12%)
1	MLY	D	436	1	10,10,11	1.07	1 (10%)	8,11,13	1.75	1 (12%)
1	MLY	D	486	1	10,10,11	0.57	0	8,11,13	0.56	0
1	MLY	D	49	1	10,10,11	1.11	1 (10%)	8,11,13	1.26	1 (12%)
1	MLY	D	504	1	10,10,11	0.81	0	8,11,13	0.46	0
1	MLY	D	505	1	10,10,11	1.43	2 (20%)	8,11,13	0.51	0
1	MLY	D	528	1	10,10,11	0.86	0	8,11,13	1.13	1 (12%)
1	MLY	D	55	1	10,10,11	0.98	1 (10%)	8,11,13	1.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	D	551	1	10,10,11	0.59	0	8,11,13	0.74	0
1	MLY	D	553	1,4	10,10,11	0.65	0	8,11,13	0.67	0
1	MLY	D	59	1	10,10,11	0.80	0	8,11,13	1.14	1 (12%)
1	MLY	D	598	1	10,10,11	1.17	2 (20%)	8,11,13	1.29	1 (12%)
1	MLY	D	600	1	10,10,11	0.59	0	8,11,13	0.97	1 (12%)
1	MLY	D	613	1	10,10,11	0.65	0	8,11,13	1.08	1 (12%)
1	MLY	D	617	1	10,10,11	0.91	1 (10%)	8,11,13	0.60	0
1	MLY	D	63	1	10,10,11	0.90	0	8,11,13	0.78	0
1	MLY	D	659	1	10,10,11	0.74	0	8,11,13	0.84	0
1	MLY	D	681	1	10,10,11	0.94	1 (10%)	8,11,13	1.42	1 (12%)
1	MLY	D	764	1	10,10,11	0.80	0	8,11,13	0.50	0
1	MLY	D	768	1	10,10,11	0.86	0	8,11,13	1.95	1 (12%)
1	MLY	D	782	1	10,10,11	0.74	0	8,11,13	1.53	1 (12%)
1	MLY	D	827	1	10,10,11	0.96	1 (10%)	8,11,13	0.93	1 (12%)
1	MLY	D	833	1	10,10,11	1.07	1 (10%)	8,11,13	1.12	1 (12%)
1	MLY	D	837	1	10,10,11	0.67	0	8,11,13	0.56	0
1	MLY	D	839	1	10,10,11	0.64	0	8,11,13	1.49	1 (12%)
1	MLY	D	84	1	10,10,11	0.61	0	8,11,13	0.80	0
1	MLY	D	87	1	10,10,11	1.07	1 (10%)	8,11,13	0.61	0
1	MLY	G	107	1	10,10,11	0.48	0	8,11,13	1.02	1 (12%)
1	MLY	G	130	1	10,10,11	0.98	1 (10%)	8,11,13	1.34	2 (25%)
1	MLY	G	138	1	10,10,11	1.35	1 (10%)	8,11,13	2.74	1 (12%)
1	MLY	G	19	1	10,10,11	1.21	1 (10%)	8,11,13	0.64	0
1	MLY	G	190	1	10,10,11	1.18	1 (10%)	8,11,13	1.32	1 (12%)
1	MLY	G	236	1	10,10,11	1.08	1 (10%)	8,11,13	1.55	2 (25%)
1	MLY	G	248	1	10,10,11	0.75	0	8,11,13	0.86	0
1	MLY	G	272	1	10,10,11	1.06	1 (10%)	8,11,13	1.32	1 (12%)
1	MLY	G	295	1	10,10,11	1.14	1 (10%)	8,11,13	0.31	0
1	MLY	G	296	1	10,10,11	0.88	1 (10%)	8,11,13	1.19	1 (12%)
1	MLY	G	30	1	10,10,11	0.87	0	8,11,13	0.91	0
1	MLY	G	348	1	10,10,11	0.79	0	8,11,13	1.07	1 (12%)
1	MLY	G	35	1	10,10,11	0.75	0	8,11,13	0.65	0
1	MLY	G	353	1	10,10,11	1.00	0	8,11,13	1.02	1 (12%)
1	MLY	G	367	1	10,10,11	0.91	1 (10%)	8,11,13	0.44	0
1	MLY	G	369	1	10,10,11	0.83	0	8,11,13	0.78	0
1	MLY	G	385	1	10,10,11	0.93	1 (10%)	8,11,13	0.54	0
1	MLY	G	415	1	10,10,11	0.71	0	8,11,13	0.73	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	G	431	1	10,10,11	0.48	0	8,11,13	1.17	1 (12%)
1	MLY	G	436	1	10,10,11	1.03	1 (10%)	8,11,13	1.77	1 (12%)
1	MLY	G	486	1	10,10,11	0.55	0	8,11,13	0.54	0
1	MLY	G	49	1	10,10,11	1.11	1 (10%)	8,11,13	1.24	1 (12%)
1	MLY	G	504	1	10,10,11	0.83	0	8,11,13	0.44	0
1	MLY	G	505	1	10,10,11	1.43	2 (20%)	8,11,13	0.51	0
1	MLY	G	528	1	10,10,11	0.84	0	8,11,13	1.13	1 (12%)
1	MLY	G	55	1	10,10,11	0.98	1 (10%)	8,11,13	1.11	0
1	MLY	G	551	1	10,10,11	0.61	0	8,11,13	0.73	0
1	MLY	G	553	1,4	10,10,11	0.66	0	8,11,13	0.64	0
1	MLY	G	59	1	10,10,11	0.76	0	8,11,13	1.16	1 (12%)
1	MLY	G	598	1	10,10,11	1.13	2 (20%)	8,11,13	1.30	1 (12%)
1	MLY	G	600	1	10,10,11	0.61	0	8,11,13	0.95	1 (12%)
1	MLY	G	613	1	10,10,11	0.64	0	8,11,13	1.10	1 (12%)
1	MLY	G	617	1	10,10,11	0.89	1 (10%)	8,11,13	0.61	0
1	MLY	G	63	1	10,10,11	0.91	1 (10%)	8,11,13	0.79	0
1	MLY	G	659	1	10,10,11	0.74	0	8,11,13	0.83	0
1	MLY	G	681	1	10,10,11	0.97	1 (10%)	8,11,13	1.43	1 (12%)
1	MLY	G	764	1	10,10,11	0.78	0	8,11,13	0.51	0
1	MLY	G	768	1	10,10,11	0.92	0	8,11,13	1.95	1 (12%)
1	MLY	G	782	1	10,10,11	0.73	0	8,11,13	1.52	1 (12%)
1	MLY	G	827	1	10,10,11	1.02	1 (10%)	8,11,13	0.93	1 (12%)
1	MLY	G	833	1	10,10,11	1.09	1 (10%)	8,11,13	1.15	1 (12%)
1	MLY	G	837	1	10,10,11	0.68	0	8,11,13	0.51	0
1	MLY	G	839	1	10,10,11	0.67	0	8,11,13	1.50	1 (12%)
1	MLY	G	84	1	10,10,11	0.59	0	8,11,13	0.80	0
1	MLY	G	87	1	10,10,11	1.15	1 (10%)	8,11,13	0.61	0
1	MLY	J	107	1	10,10,11	0.46	0	8,11,13	1.02	1 (12%)
1	MLY	J	130	1	10,10,11	0.90	0	8,11,13	1.33	2 (25%)
1	MLY	J	138	1	10,10,11	1.35	1 (10%)	8,11,13	2.73	1 (12%)
1	MLY	J	19	1	10,10,11	1.25	1 (10%)	8,11,13	0.63	0
1	MLY	J	190	1	10,10,11	1.19	1 (10%)	8,11,13	1.29	1 (12%)
1	MLY	J	236	1	10,10,11	1.12	1 (10%)	8,11,13	1.56	2 (25%)
1	MLY	J	248	1	10,10,11	0.76	0	8,11,13	0.86	0
1	MLY	J	272	1	10,10,11	1.07	1 (10%)	8,11,13	1.32	1 (12%)
1	MLY	J	295	1	10,10,11	1.13	1 (10%)	8,11,13	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	J	296	1	10,10,11	0.91	1 (10%)	8,11,13	1.18	1 (12%)
1	MLY	J	30	1	10,10,11	0.86	0	8,11,13	0.94	0
1	MLY	J	348	1	10,10,11	0.76	0	8,11,13	1.07	1 (12%)
1	MLY	J	35	1	10,10,11	0.75	0	8,11,13	0.64	0
1	MLY	J	353	1	10,10,11	0.99	0	8,11,13	1.02	1 (12%)
1	MLY	J	367	1	10,10,11	0.90	1 (10%)	8,11,13	0.43	0
1	MLY	J	369	1	10,10,11	0.86	0	8,11,13	0.78	0
1	MLY	J	385	1	10,10,11	0.95	1 (10%)	8,11,13	0.52	0
1	MLY	J	415	1	10,10,11	0.73	0	8,11,13	0.74	0
1	MLY	J	431	1	10,10,11	0.49	0	8,11,13	1.19	1 (12%)
1	MLY	J	436	1	10,10,11	1.02	1 (10%)	8,11,13	1.77	1 (12%)
1	MLY	J	486	1	10,10,11	0.58	0	8,11,13	0.55	0
1	MLY	J	49	1	10,10,11	1.15	1 (10%)	8,11,13	1.27	1 (12%)
1	MLY	J	504	1	10,10,11	0.77	0	8,11,13	0.45	0
1	MLY	J	505	1	10,10,11	1.46	2 (20%)	8,11,13	0.49	0
1	MLY	J	528	1	10,10,11	0.82	0	8,11,13	1.11	1 (12%)
1	MLY	J	55	1	10,10,11	0.94	1 (10%)	8,11,13	1.11	0
1	MLY	J	551	1	10,10,11	0.60	0	8,11,13	0.74	0
1	MLY	J	553	1	10,10,11	0.65	0	8,11,13	0.64	0
1	MLY	J	59	1	10,10,11	0.80	0	8,11,13	1.14	1 (12%)
1	MLY	J	598	1	10,10,11	1.16	2 (20%)	8,11,13	1.29	1 (12%)
1	MLY	J	600	1	10,10,11	0.63	0	8,11,13	0.97	1 (12%)
1	MLY	J	613	1	10,10,11	0.66	0	8,11,13	1.09	1 (12%)
1	MLY	J	617	1	10,10,11	0.92	1 (10%)	8,11,13	0.59	0
1	MLY	J	63	1	10,10,11	0.89	0	8,11,13	0.79	0
1	MLY	J	659	1	10,10,11	0.73	0	8,11,13	0.83	0
1	MLY	J	681	1	10,10,11	0.93	1 (10%)	8,11,13	1.42	1 (12%)
1	MLY	J	764	1	10,10,11	0.77	0	8,11,13	0.52	0
1	MLY	J	768	1	10,10,11	0.87	0	8,11,13	1.94	1 (12%)
1	MLY	J	782	1	10,10,11	0.74	0	8,11,13	1.54	1 (12%)
1	MLY	J	827	1	10,10,11	1.08	1 (10%)	8,11,13	0.93	1 (12%)
1	MLY	J	833	1	10,10,11	1.12	1 (10%)	8,11,13	1.09	1 (12%)
1	MLY	J	837	1	10,10,11	0.66	0	8,11,13	0.55	0
1	MLY	J	839	1	10,10,11	0.66	0	8,11,13	1.52	1 (12%)
1	MLY	J	84	1	10,10,11	0.58	0	8,11,13	0.79	0
1	MLY	J	87	1	10,10,11	1.12	1 (10%)	8,11,13	0.61	0
1	MLY	M	107	1	10,10,11	0.48	0	8,11,13	1.04	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	M	130	1	10,10,11	0.93	0	8,11,13	1.33	2 (25%)
1	MLY	M	138	1	10,10,11	1.34	1 (10%)	8,11,13	2.72	1 (12%)
1	MLY	M	19	1	10,10,11	1.25	1 (10%)	8,11,13	0.63	0
1	MLY	M	190	1	10,10,11	1.18	1 (10%)	8,11,13	1.28	1 (12%)
1	MLY	M	236	1	10,10,11	1.11	1 (10%)	8,11,13	1.56	2 (25%)
1	MLY	M	248	1	10,10,11	0.76	0	8,11,13	0.87	0
1	MLY	M	272	1	10,10,11	1.09	1 (10%)	8,11,13	1.31	1 (12%)
1	MLY	M	295	1	10,10,11	1.12	1 (10%)	8,11,13	0.32	0
1	MLY	M	296	1	10,10,11	0.89	1 (10%)	8,11,13	1.18	1 (12%)
1	MLY	M	30	1	10,10,11	0.85	0	8,11,13	0.92	0
1	MLY	M	348	1	10,10,11	0.76	0	8,11,13	1.07	1 (12%)
1	MLY	M	35	1	10,10,11	0.76	0	8,11,13	0.64	0
1	MLY	M	353	1	10,10,11	0.98	0	8,11,13	1.02	1 (12%)
1	MLY	M	367	1	10,10,11	0.88	1 (10%)	8,11,13	0.42	0
1	MLY	M	369	1	10,10,11	0.84	0	8,11,13	0.76	0
1	MLY	M	385	1	10,10,11	0.94	1 (10%)	8,11,13	0.53	0
1	MLY	M	415	1	10,10,11	0.75	0	8,11,13	0.74	0
1	MLY	M	431	1	10,10,11	0.49	0	8,11,13	1.20	1 (12%)
1	MLY	M	436	1	10,10,11	1.06	1 (10%)	8,11,13	1.75	1 (12%)
1	MLY	M	486	1	10,10,11	0.57	0	8,11,13	0.55	0
1	MLY	M	49	1	10,10,11	1.15	1 (10%)	8,11,13	1.25	1 (12%)
1	MLY	M	504	1	10,10,11	0.77	0	8,11,13	0.46	0
1	MLY	M	505	1	10,10,11	1.43	2 (20%)	8,11,13	0.50	0
1	MLY	M	528	1	10,10,11	0.82	0	8,11,13	1.11	1 (12%)
1	MLY	M	55	1	10,10,11	0.95	1 (10%)	8,11,13	1.11	0
1	MLY	M	551	1	10,10,11	0.62	0	8,11,13	0.74	0
1	MLY	M	553	1	10,10,11	0.64	0	8,11,13	0.64	0
1	MLY	M	59	1	10,10,11	0.80	0	8,11,13	1.13	1 (12%)
1	MLY	M	598	1	10,10,11	1.15	2 (20%)	8,11,13	1.29	1 (12%)
1	MLY	M	600	1	10,10,11	0.64	0	8,11,13	0.99	1 (12%)
1	MLY	M	613	1	10,10,11	0.66	0	8,11,13	1.09	1 (12%)
1	MLY	M	617	1	10,10,11	0.90	1 (10%)	8,11,13	0.60	0
1	MLY	M	63	1	10,10,11	0.91	0	8,11,13	0.80	0
1	MLY	M	659	1	10,10,11	0.71	0	8,11,13	0.83	0
1	MLY	M	681	1	10,10,11	0.96	1 (10%)	8,11,13	1.43	1 (12%)
1	MLY	M	764	1	10,10,11	0.79	0	8,11,13	0.50	0
1	MLY	M	768	1	10,10,11	0.86	0	8,11,13	1.93	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	M	782	1	10,10,11	0.72	0	8,11,13	1.55	1 (12%)
1	MLY	M	827	1	10,10,11	1.03	1 (10%)	8,11,13	0.92	1 (12%)
1	MLY	M	833	1	10,10,11	1.13	1 (10%)	8,11,13	1.06	1 (12%)
1	MLY	M	837	1	10,10,11	0.66	0	8,11,13	0.54	0
1	MLY	M	839	1	10,10,11	0.65	0	8,11,13	1.49	1 (12%)
1	MLY	M	84	1	10,10,11	0.59	0	8,11,13	0.79	0
1	MLY	M	87	1	10,10,11	1.11	1 (10%)	8,11,13	0.62	0
1	MLY	P	107	1	10,10,11	0.48	0	8,11,13	1.03	1 (12%)
1	MLY	P	130	1	10,10,11	0.92	0	8,11,13	1.32	2 (25%)
1	MLY	P	138	1	10,10,11	1.32	1 (10%)	8,11,13	2.74	1 (12%)
1	MLY	P	19	1	10,10,11	1.23	1 (10%)	8,11,13	0.64	0
1	MLY	P	190	1	10,10,11	1.21	1 (10%)	8,11,13	1.28	1 (12%)
1	MLY	P	236	1	10,10,11	1.11	1 (10%)	8,11,13	1.56	2 (25%)
1	MLY	P	248	1	10,10,11	0.76	0	8,11,13	0.87	0
1	MLY	P	272	1	10,10,11	1.10	1 (10%)	8,11,13	1.33	1 (12%)
1	MLY	P	295	1	10,10,11	1.14	1 (10%)	8,11,13	0.32	0
1	MLY	P	296	1	10,10,11	0.92	1 (10%)	8,11,13	1.18	1 (12%)
1	MLY	P	30	1	10,10,11	0.85	0	8,11,13	0.93	0
1	MLY	P	348	1	10,10,11	0.77	0	8,11,13	1.08	1 (12%)
1	MLY	P	35	1	10,10,11	0.73	0	8,11,13	0.64	0
1	MLY	P	353	1	10,10,11	0.97	0	8,11,13	1.02	1 (12%)
1	MLY	P	367	1	10,10,11	0.88	1 (10%)	8,11,13	0.41	0
1	MLY	P	369	1	10,10,11	0.84	0	8,11,13	0.77	0
1	MLY	P	385	1	10,10,11	0.95	1 (10%)	8,11,13	0.53	0
1	MLY	P	415	1	10,10,11	0.75	0	8,11,13	0.74	0
1	MLY	P	431	1	10,10,11	0.48	0	8,11,13	1.21	1 (12%)
1	MLY	P	436	1	10,10,11	1.02	1 (10%)	8,11,13	1.76	1 (12%)
1	MLY	P	486	1	10,10,11	0.57	0	8,11,13	0.55	0
1	MLY	P	49	1	10,10,11	1.12	1 (10%)	8,11,13	1.27	1 (12%)
1	MLY	P	504	1	10,10,11	0.76	0	8,11,13	0.45	0
1	MLY	P	505	1	10,10,11	1.46	2 (20%)	8,11,13	0.48	0
1	MLY	P	528	1	10,10,11	0.82	0	8,11,13	1.12	1 (12%)
1	MLY	P	55	1	10,10,11	0.93	1 (10%)	8,11,13	1.10	0
1	MLY	P	551	1	10,10,11	0.61	0	8,11,13	0.73	0
1	MLY	P	553	1	10,10,11	0.63	0	8,11,13	0.63	0
1	MLY	P	59	1	10,10,11	0.79	0	8,11,13	1.15	1 (12%)
1	MLY	P	598	1	10,10,11	1.16	2 (20%)	8,11,13	1.29	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	P	600	1	10,10,11	0.63	0	8,11,13	0.96	1 (12%)
1	MLY	P	613	1	10,10,11	0.67	0	8,11,13	1.09	1 (12%)
1	MLY	P	617	1	10,10,11	0.93	1 (10%)	8,11,13	0.60	0
1	MLY	P	63	1	10,10,11	0.92	0	8,11,13	0.79	0
1	MLY	P	659	1	10,10,11	0.74	0	8,11,13	0.83	0
1	MLY	P	681	1	10,10,11	0.92	1 (10%)	8,11,13	1.42	1 (12%)
1	MLY	P	764	1	10,10,11	0.76	0	8,11,13	0.53	0
1	MLY	P	768	1	10,10,11	0.88	0	8,11,13	1.94	1 (12%)
1	MLY	P	782	1	10,10,11	0.72	0	8,11,13	1.55	1 (12%)
1	MLY	P	827	1	10,10,11	1.01	1 (10%)	8,11,13	0.92	1 (12%)
1	MLY	P	833	1	10,10,11	1.13	1 (10%)	8,11,13	1.09	1 (12%)
1	MLY	P	837	1	10,10,11	0.63	0	8,11,13	0.55	0
1	MLY	P	839	1	10,10,11	0.65	0	8,11,13	1.50	1 (12%)
1	MLY	P	84	1	10,10,11	0.57	0	8,11,13	0.79	0
1	MLY	P	87	1	10,10,11	1.11	1 (10%)	8,11,13	0.60	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	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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	P	19	1	-	0/7/9/11	0/0/0/0
1	MLY	P	190	1	-	0/7/9/11	0/0/0/0
1	MLY	P	236	1	-	0/7/9/11	0/0/0/0
1	MLY	P	248	1	-	0/7/9/11	0/0/0/0
1	MLY	P	272	1	-	0/7/9/11	0/0/0/0
1	MLY	P	295	1	-	0/7/9/11	0/0/0/0
1	MLY	P	296	1	-	0/7/9/11	0/0/0/0
1	MLY	P	30	1	-	0/7/9/11	0/0/0/0
1	MLY	P	348	1	-	0/7/9/11	0/0/0/0
1	MLY	P	35	1	-	0/7/9/11	0/0/0/0
1	MLY	P	353	1	-	0/7/9/11	0/0/0/0
1	MLY	P	367	1	-	0/7/9/11	0/0/0/0
1	MLY	P	369	1	-	0/7/9/11	0/0/0/0
1	MLY	P	385	1	-	0/7/9/11	0/0/0/0
1	MLY	P	415	1	-	0/7/9/11	0/0/0/0
1	MLY	P	431	1	-	0/7/9/11	0/0/0/0
1	MLY	P	436	1	-	0/7/9/11	0/0/0/0
1	MLY	P	486	1	-	0/7/9/11	0/0/0/0
1	MLY	P	49	1	-	0/7/9/11	0/0/0/0
1	MLY	P	504	1	-	0/7/9/11	0/0/0/0
1	MLY	P	505	1	-	0/7/9/11	0/0/0/0
1	MLY	P	528	1	-	0/7/9/11	0/0/0/0
1	MLY	P	55	1	-	0/7/9/11	0/0/0/0
1	MLY	P	551	1	-	0/7/9/11	0/0/0/0
1	MLY	P	553	1	-	0/7/9/11	0/0/0/0
1	MLY	P	59	1	-	0/7/9/11	0/0/0/0
1	MLY	P	598	1	-	0/7/9/11	0/0/0/0
1	MLY	P	600	1	-	0/7/9/11	0/0/0/0
1	MLY	P	613	1	-	0/7/9/11	0/0/0/0
1	MLY	P	617	1	-	0/7/9/11	0/0/0/0
1	MLY	P	63	1	-	0/7/9/11	0/0/0/0
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 131 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	-3.65	1.48	1.53
1	J	138	MLY	CB-CA	-3.63	1.48	1.53
1	A	138	MLY	CB-CA	-3.59	1.48	1.53
1	M	138	MLY	CB-CA	-3.58	1.48	1.53

The worst 5 of 150 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	138	MLY	CB-CA-C	-7.46	99.35	111.65
1	G	138	MLY	CB-CA-C	-7.46	99.36	111.65
1	J	138	MLY	CB-CA-C	-7.45	99.38	111.65
1	A	138	MLY	CB-CA-C	-7.43	99.41	111.65
1	M	138	MLY	CB-CA-C	-7.43	99.41	111.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

183 monomers are involved in 776 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	3	0
1	A	30	MLY	1	0
1	A	348	MLY	6	0
1	A	415	MLY	1	0
1	A	436	MLY	2	0
1	A	486	MLY	3	0
1	A	49	MLY	4	0
1	A	504	MLY	1	0
1	A	505	MLY	26	0
1	A	528	MLY	3	0
1	A	55	MLY	1	0
1	A	551	MLY	2	0
1	A	553	MLY	17	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	59	MLY	3	0
1	A	598	MLY	1	0
1	A	600	MLY	1	0
1	A	617	MLY	1	0
1	A	63	MLY	3	0
1	A	659	MLY	2	0
1	A	764	MLY	11	0
1	A	768	MLY	12	0
1	A	782	MLY	8	0
1	A	837	MLY	3	0
1	A	839	MLY	8	0
1	A	87	MLY	3	0
1	D	107	MLY	3	0
1	D	138	MLY	1	0
1	D	190	MLY	2	0
1	D	248	MLY	2	0
1	D	272	MLY	1	0
1	D	295	MLY	6	0
1	D	296	MLY	2	0
1	D	30	MLY	1	0
1	D	348	MLY	5	0
1	D	369	MLY	1	0
1	D	415	MLY	1	0
1	D	436	MLY	2	0
1	D	486	MLY	3	0
1	D	49	MLY	3	0
1	D	528	MLY	3	0
1	D	55	MLY	1	0
1	D	551	MLY	2	0
1	D	553	MLY	18	0
1	D	59	MLY	3	0
1	D	598	MLY	1	0
1	D	600	MLY	1	0
1	D	617	MLY	1	0
1	D	63	MLY	3	0
1	D	659	MLY	2	0
1	D	764	MLY	8	0
1	D	768	MLY	1	0
1	D	782	MLY	67	0
1	D	827	MLY	3	0
1	D	837	MLY	1	0
1	D	839	MLY	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	87	MLY	2	0
1	G	107	MLY	3	0
1	G	138	MLY	1	0
1	G	190	MLY	2	0
1	G	248	MLY	2	0
1	G	272	MLY	1	0
1	G	295	MLY	7	0
1	G	296	MLY	3	0
1	G	30	MLY	1	0
1	G	348	MLY	6	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	1	0
1	G	528	MLY	2	0
1	G	55	MLY	1	0
1	G	553	MLY	27	0
1	G	59	MLY	2	0
1	G	598	MLY	1	0
1	G	600	MLY	1	0
1	G	617	MLY	1	0
1	G	63	MLY	3	0
1	G	659	MLY	2	0
1	G	764	MLY	19	0
1	G	768	MLY	9	0
1	G	782	MLY	1	0
1	G	827	MLY	1	0
1	G	837	MLY	1	0
1	G	839	MLY	4	0
1	G	84	MLY	22	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	7	0
1	J	296	MLY	3	0
1	J	30	MLY	1	0
1	J	348	MLY	6	0
1	J	369	MLY	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	J	415	MLY	1	0
1	J	436	MLY	2	0
1	J	486	MLY	3	0
1	J	49	MLY	2	0
1	J	505	MLY	9	0
1	J	528	MLY	3	0
1	J	55	MLY	1	0
1	J	553	MLY	12	0
1	J	59	MLY	2	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	5	0
1	J	768	MLY	8	0
1	J	782	MLY	1	0
1	J	837	MLY	1	0
1	J	839	MLY	13	0
1	J	84	MLY	36	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	5	0
1	M	296	MLY	3	0
1	M	30	MLY	1	0
1	M	348	MLY	5	0
1	M	415	MLY	1	0
1	M	436	MLY	2	0
1	M	486	MLY	3	0
1	M	49	MLY	4	0
1	M	505	MLY	28	0
1	M	528	MLY	3	0
1	M	55	MLY	1	0
1	M	553	MLY	3	0
1	M	59	MLY	3	0
1	M	598	MLY	1	0
1	M	600	MLY	1	0
1	M	617	MLY	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	M	63	MLY	4	0
1	M	659	MLY	2	0
1	M	764	MLY	8	0
1	M	768	MLY	9	0
1	M	782	MLY	1	0
1	M	837	MLY	1	0
1	M	839	MLY	12	0
1	M	87	MLY	2	0
1	P	107	MLY	3	0
1	P	138	MLY	1	0
1	P	190	MLY	2	0
1	P	248	MLY	2	0
1	P	272	MLY	1	0
1	P	295	MLY	6	0
1	P	296	MLY	3	0
1	P	30	MLY	1	0
1	P	348	MLY	6	0
1	P	369	MLY	1	0
1	P	415	MLY	1	0
1	P	436	MLY	3	0
1	P	486	MLY	3	0
1	P	49	MLY	3	0
1	P	505	MLY	21	0
1	P	528	MLY	3	0
1	P	55	MLY	1	0
1	P	553	MLY	2	0
1	P	59	MLY	2	0
1	P	598	MLY	1	0
1	P	600	MLY	1	0
1	P	617	MLY	1	0
1	P	63	MLY	3	0
1	P	659	MLY	2	0
1	P	764	MLY	6	0
1	P	768	MLY	14	0
1	P	782	MLY	1	0
1	P	837	MLY	1	0
1	P	839	MLY	12	0
1	P	87	MLY	3	0

5.5 Carbohydrates

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.