



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 11:23 am GMT

PDB ID : 1O1F
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 : 2002-11-15
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

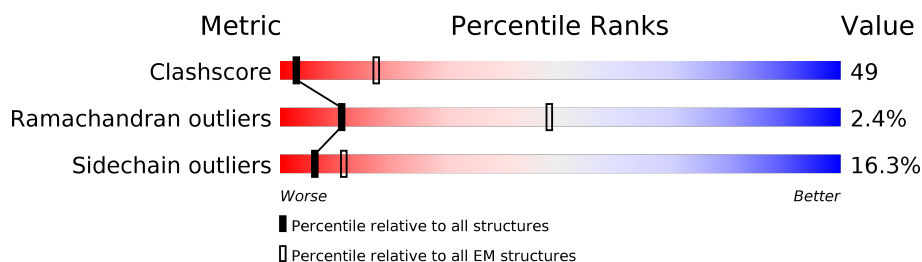
1 Overall quality at a glance

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.






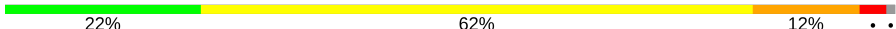
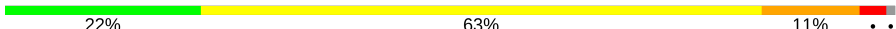
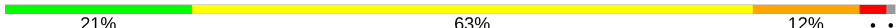











Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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	26% 51% 19% .
1	D	840	26% 51% 19% .
1	G	840	25% 52% 19% .
1	J	840	25% 51% 19% .
2	B	145	66% 26% 6% .
2	E	145	63% 28% 6% .
2	H	145	63% 28% 6% .
2	K	145	65% 26% 6% .
3	C	147	61% 37% .

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Mol	Chain	Length	Quality of chain
3	F	147	 61% 38% .
3	I	147	 61% 37% .
3	L	147	 61% 37% .
4	0	375	 22% 62% 12% ..
4	1	375	 22% 63% 11% ..
4	2	375	 21% 63% 12% ..
4	3	375	 57% 34% 6% ..
4	4	375	 56% 34% 8% ..
4	5	375	 58% 32% 8% ..
4	6	375	 56% 33% 9% ..
4	7	375	 56% 34% 8% ..
4	8	375	 60% 30% 7% ..
4	V	375	 59% 32% 7% ..
4	W	375	 57% 32% 8% ..
4	X	375	 23% 61% 12% ..
4	Y	375	 23% 61% 11% ..
4	Z	375	 23% 61% 11% ..

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	839	-	-	X	-
1	MLY	D	553	-	-	X	-
1	MLY	D	782	-	-	X	-
1	MLY	D	839	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	MLY	G	553	-	-	X	-
1	MLY	G	764	-	-	X	-
1	MLY	G	768	-	-	X	-
1	MLY	G	84	-	-	X	-
1	MLY	J	553	-	-	X	-
1	MLY	J	764	-	-	X	-
1	MLY	J	768	-	-	X	-
1	MLY	J	84	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 76872 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

- 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		

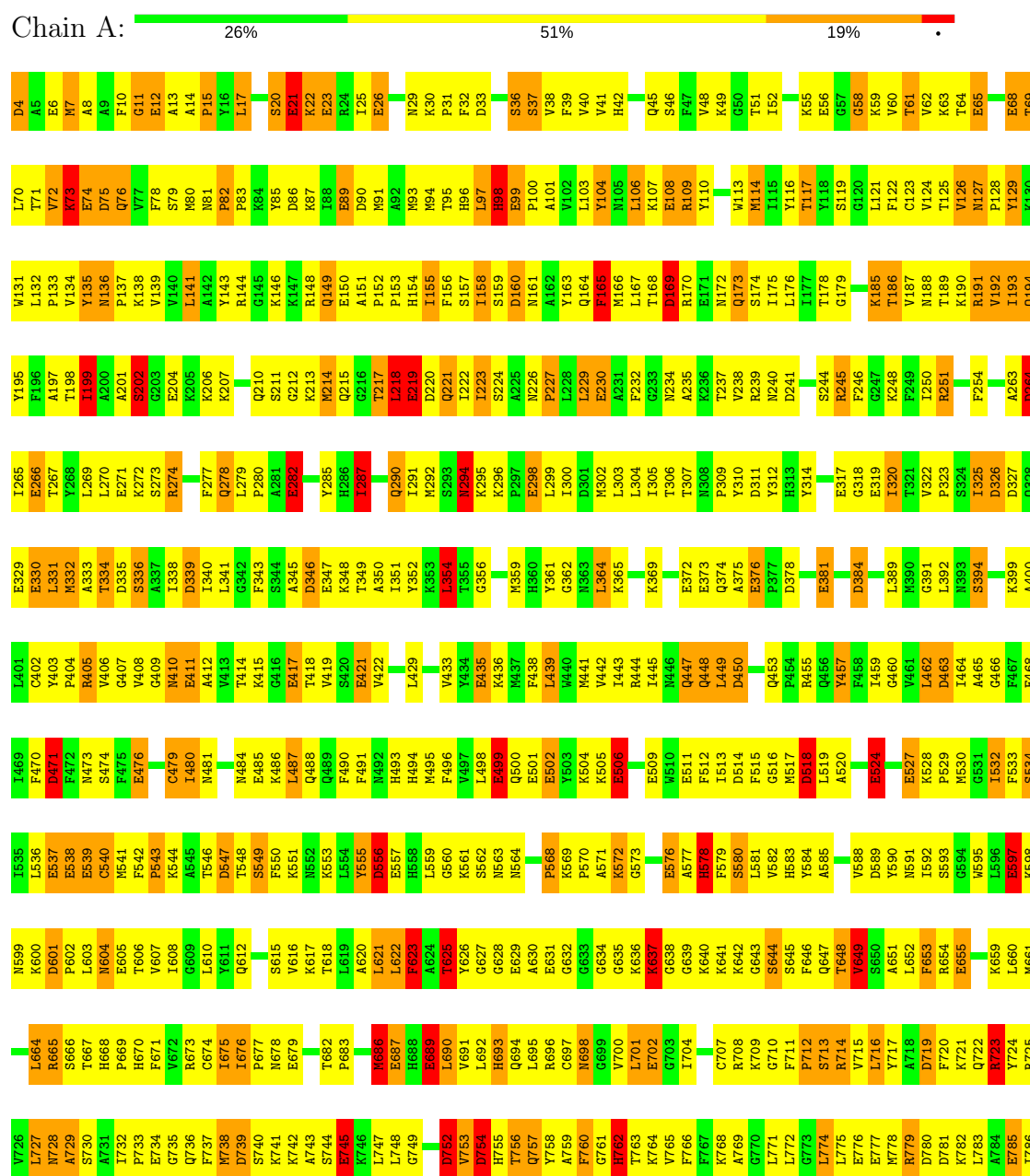
- Molecule 4 is a protein called SKELETAL MUSCLE ACTIN.

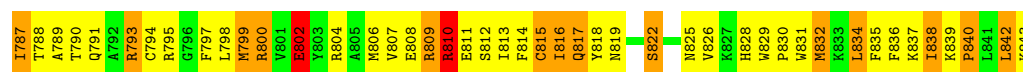
Mol	Chain	Residues	Atoms					AltConf	Trace
4	0	372	Total 2906	C 1836	N 489	O 561	S 20	0	0
4	1	372	Total 2906	C 1836	N 489	O 561	S 20	0	0
4	2	372	Total 2906	C 1836	N 489	O 561	S 20	0	0
4	3	372	Total 2906	C 1836	N 489	O 561	S 20	0	0
4	4	372	Total 2906	C 1836	N 489	O 561	S 20	0	0
4	5	372	Total 2906	C 1836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

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

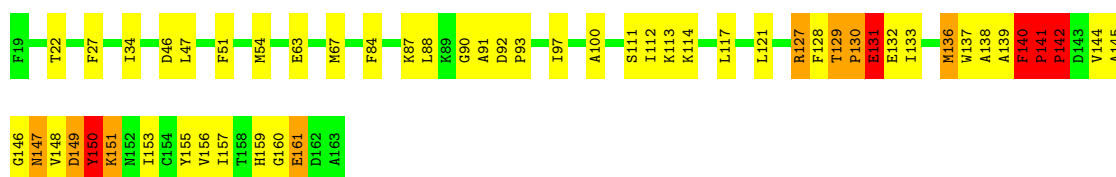




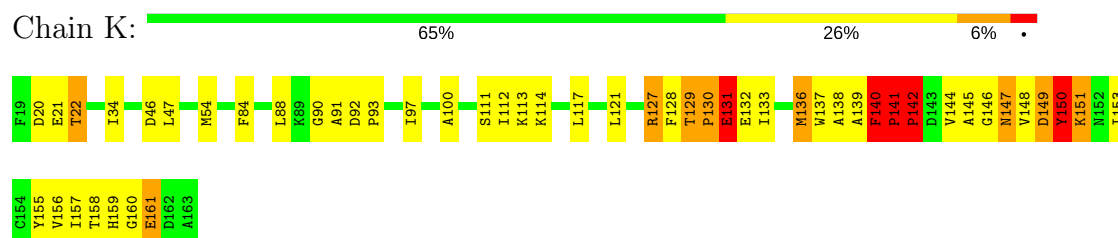


Response	Percentage
Yes, the U.S. should take action to protect the environment	25%
No, the U.S. should focus on the economy	51%
It's not the U.S.'s responsibility	19%
Don't know	5%

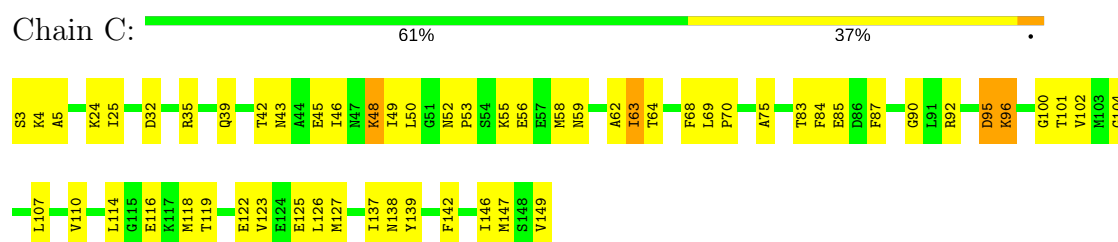




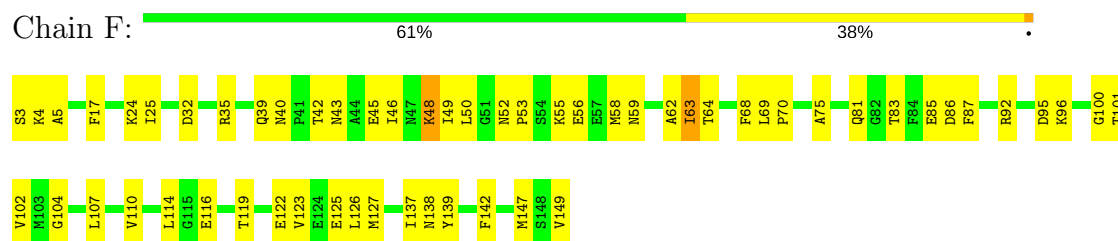
• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN



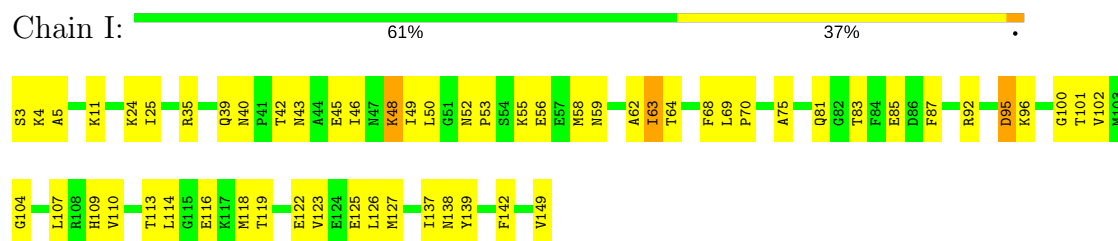
• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN



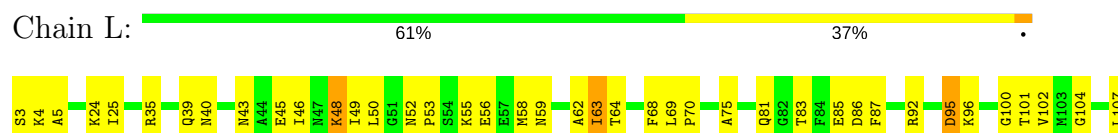
• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN



• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN



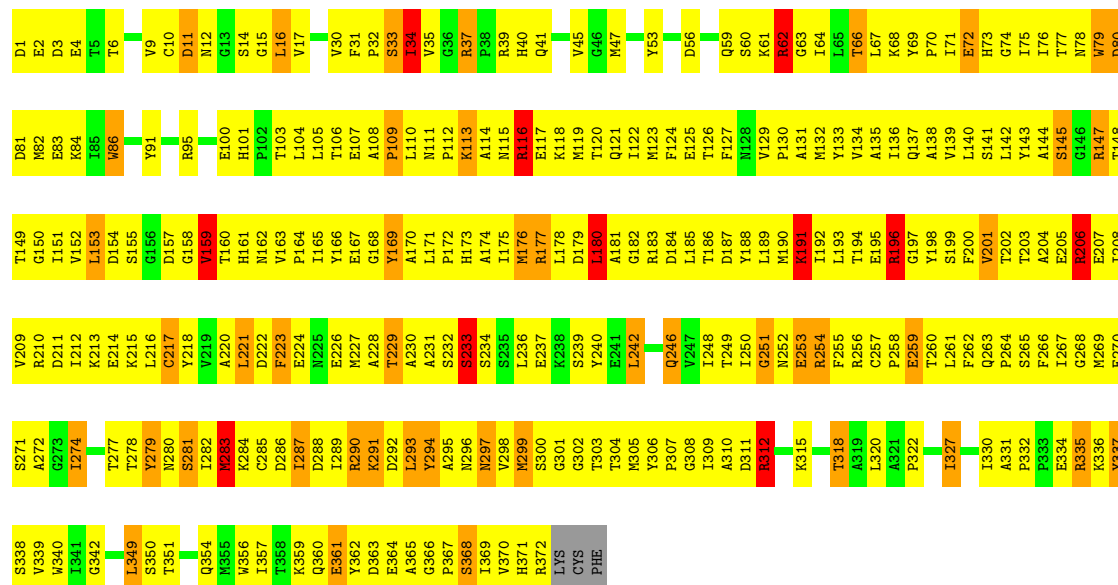
• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN





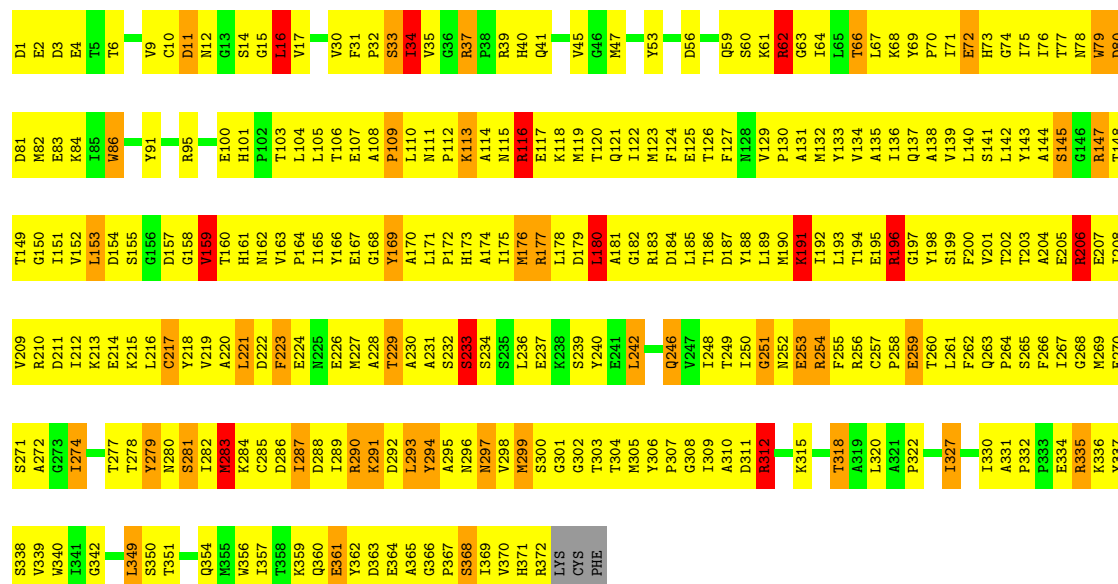
● Molecule 4: SKELETAL MUSCLE ACTIN

Chain 0: 22% 62% 12% . .



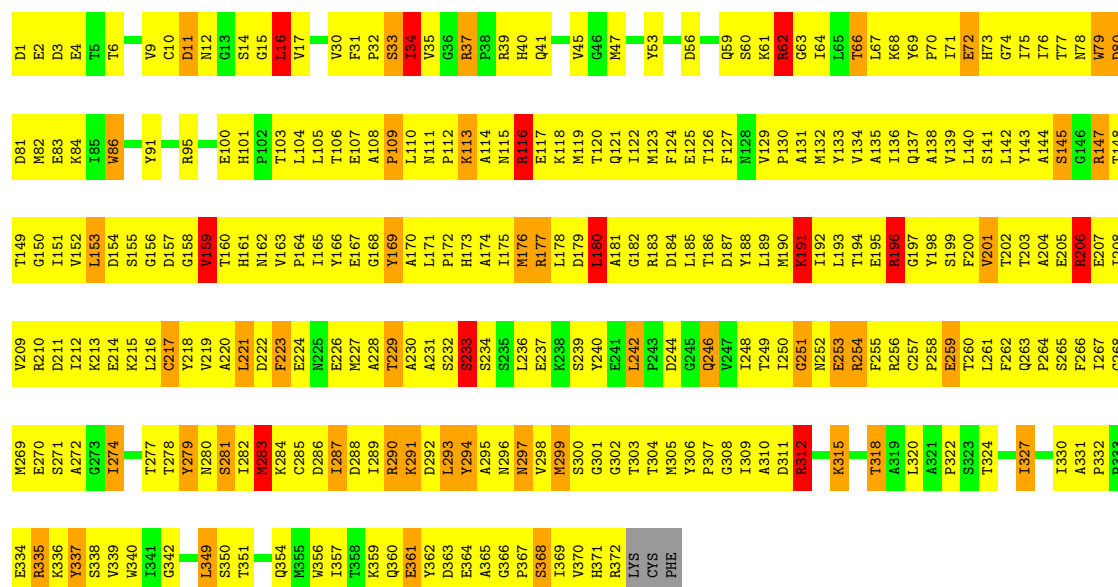
● Molecule 4: SKELETAL MUSCLE ACTIN

Chain 1: 22% 63% 11% . .



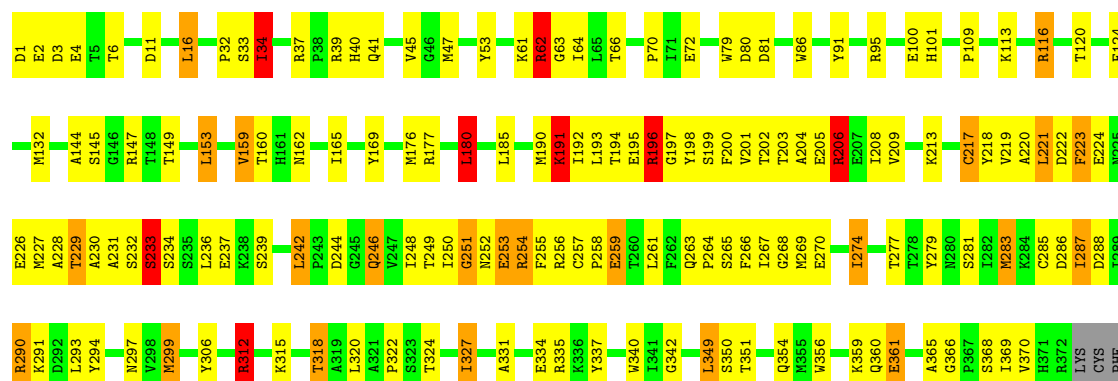
● Molecule 4: SKELETAL MUSCLE ACTIN

Chain 2: 21% 63% 12% . .



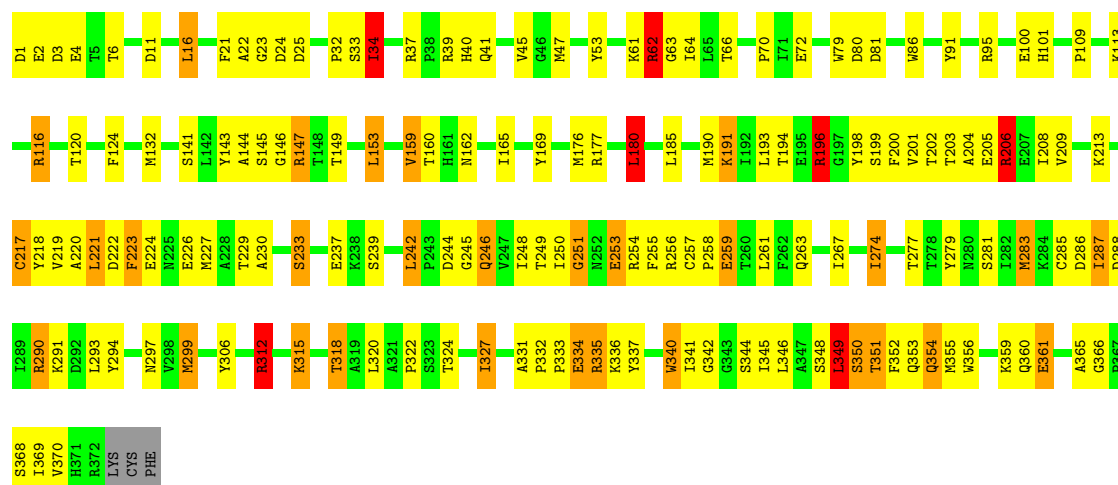
• Molecule 4: SKELETAL MUSCLE ACTIN

Chain 3: 57% 34% 6% ..

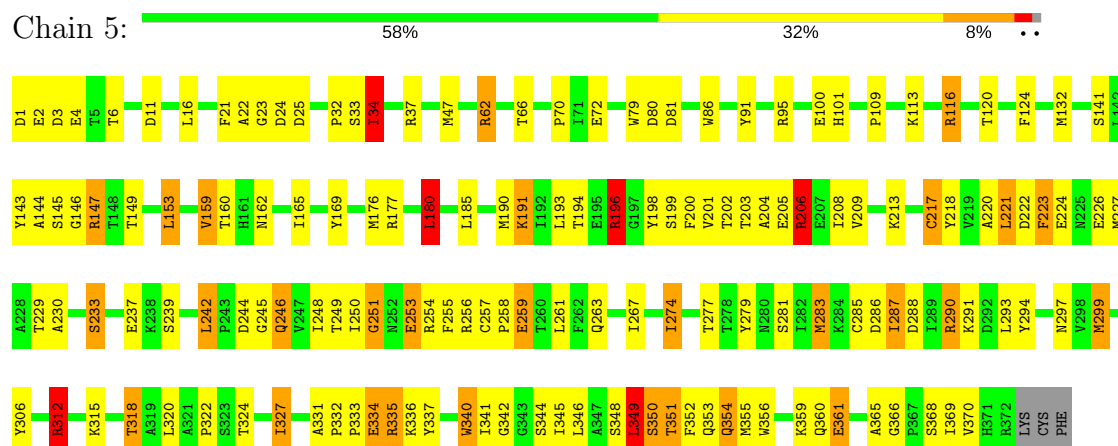


• Molecule 4: SKELETAL MUSCLE ACTIN

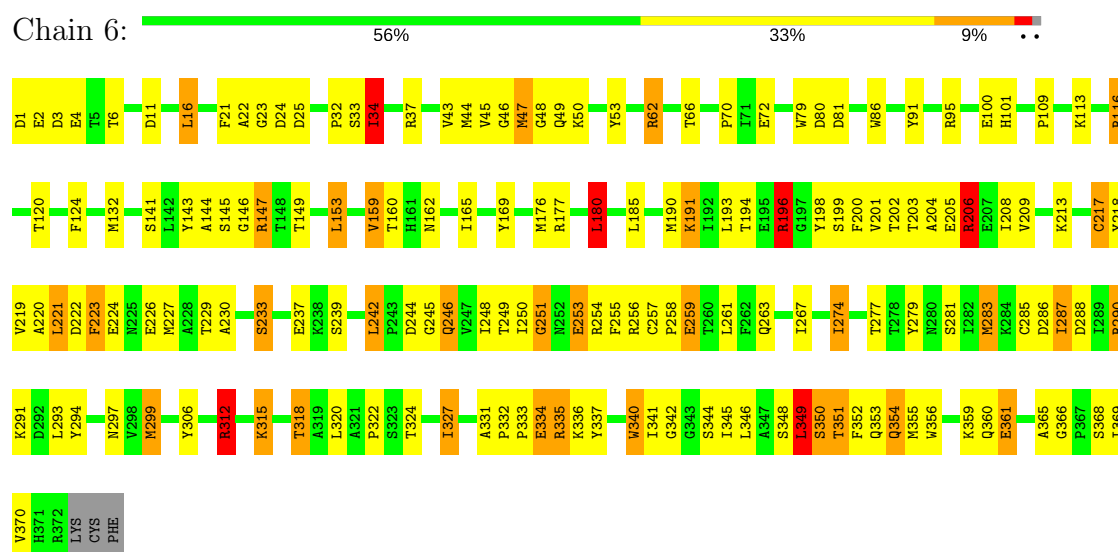
Chain 4: 56% 34% 8% ..



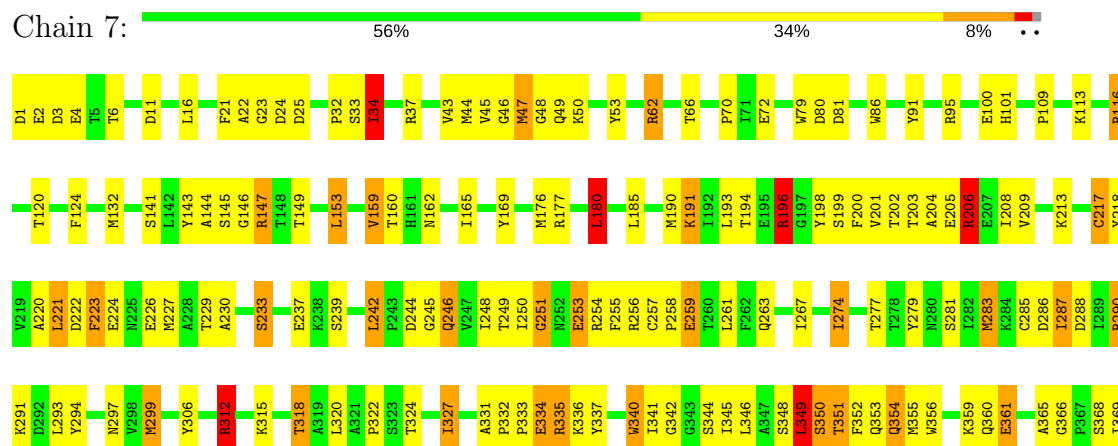
● Molecule 4: SKELETAL MUSCLE ACTIN



● Molecule 4: SKELETAL MUSCLE ACTIN



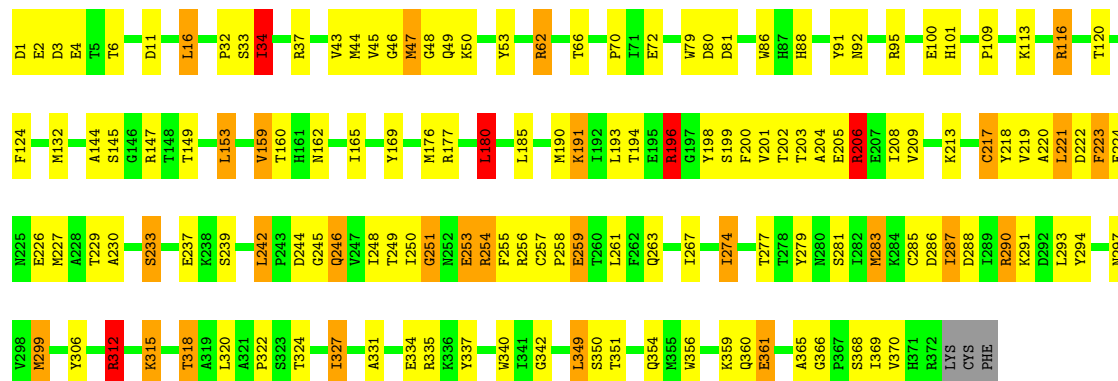
● Molecule 4: SKELETAL MUSCLE ACTIN





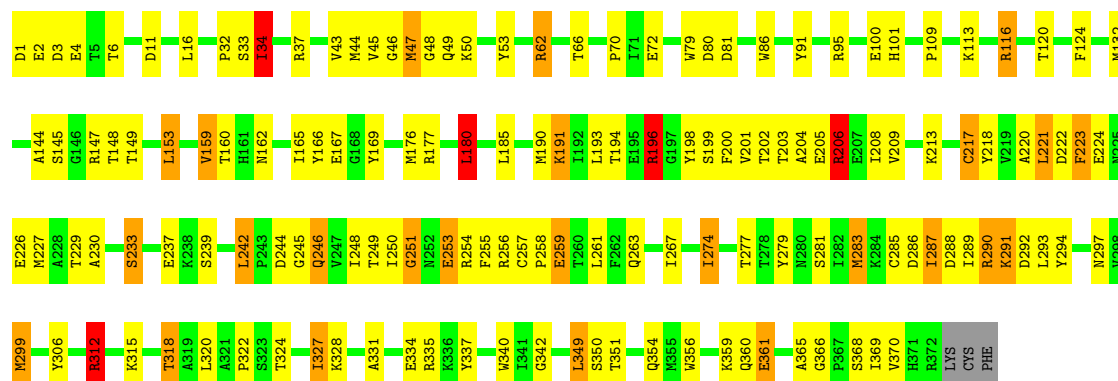
• Molecule 4: SKELETAL MUSCLE ACTIN

Chain 8: 60% 30% 7% ..



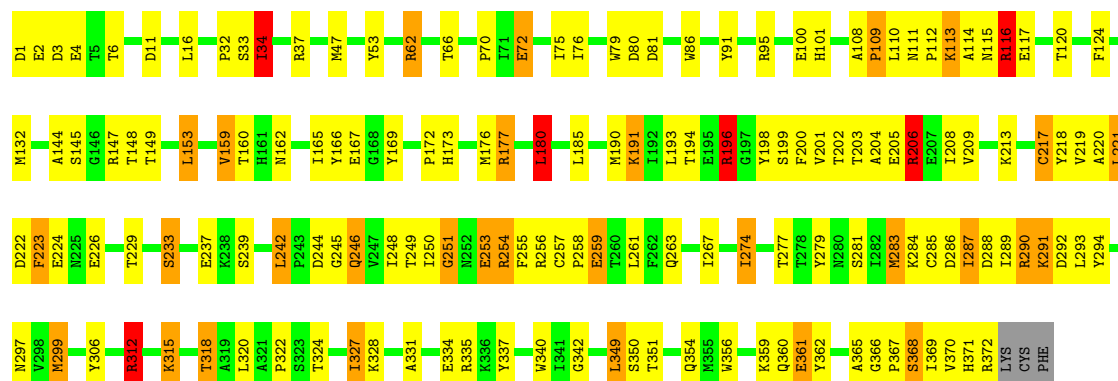
• Molecule 4: SKELETAL MUSCLE ACTIN

Chain V: 59% 32% 7% ..

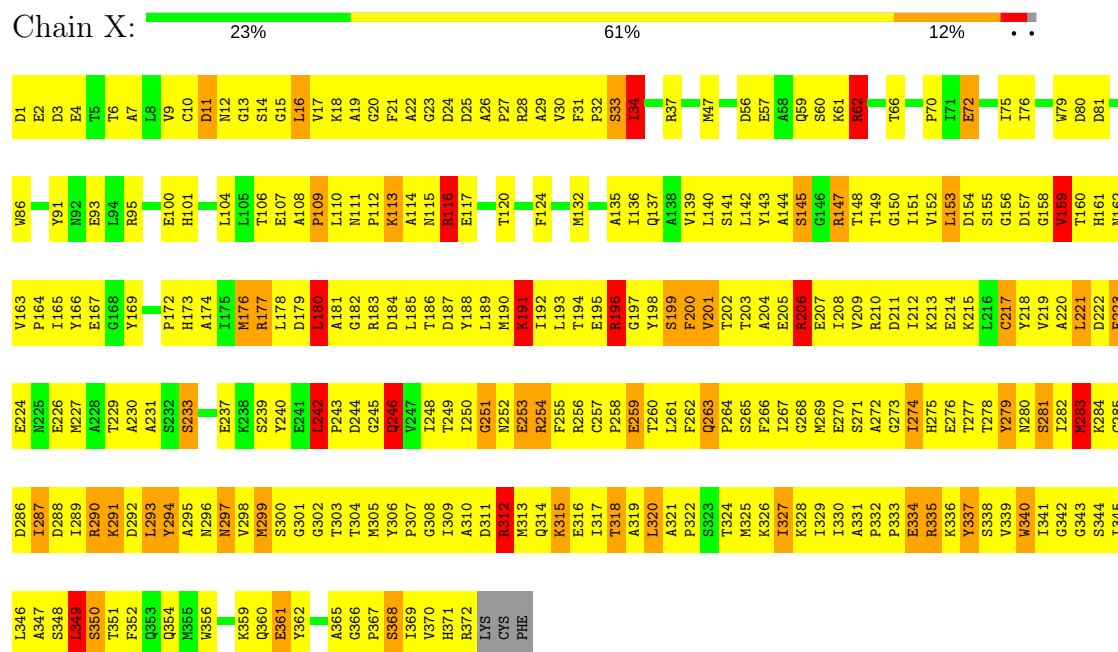


• Molecule 4: SKELETAL MUSCLE ACTIN

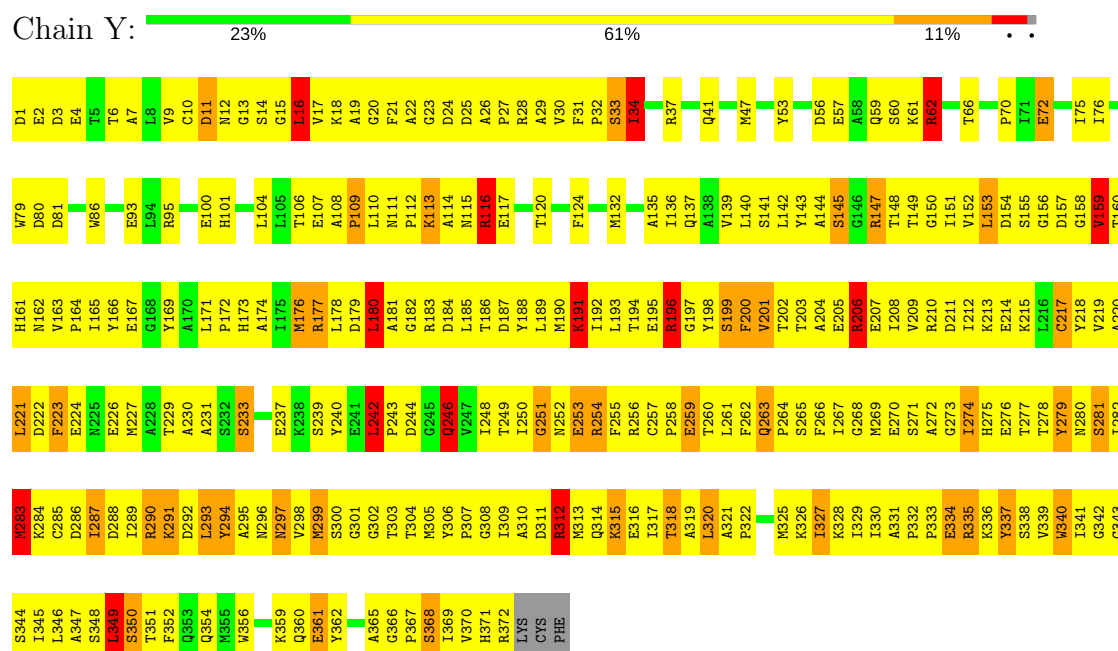
Chain W: 57% 32% 8% ..



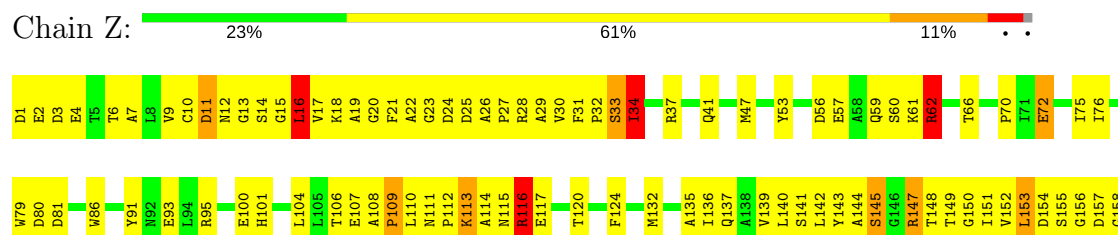
• Molecule 4: SKELETAL MUSCLE ACTIN



- Molecule 4: SKELETAL MUSCLE ACTIN



- Molecule 4: SKELETAL MUSCLE ACTIN



G343	I282	A220	V188
S344	R283	L221	T160
I345	K284	D222	H161
L346	C285	F223	N162
A347	D286	E224	V163
S348	I287	N225	P164
L349	D288	E226	I165
S350	I289	M227	Y166
T351	R290	A228	E167
F352	K291	T229	G168
Q353	D292	A230	Y169
Q354	L293	A231	
K355	Y294	S232	P172
W356	A295	S233	H173
	N296		A174
	N297	E237	I175
K359	V298	R238	M176
Q360	M299	S239	R177
E361	S300	Y240	L178
Y362	G301	E241	D179
	G302	L242	L180
A365	T303	P243	A181
G366	T304	D244	G182
P367	N305	G245	R183
S368	N306	Q246	D184
I369	Y306	V247	L185
V370	P307	I248	T186
H371	G308	T249	D187
R372	I309	I250	Y188
LYS	A310	G251	L189
CYS	D311	N252	M190
PHE	R312	E253	R191
	K313	R254	I192
	Q314	F255	L193
	K315	R256	T194
	E316	C257	E195
	I317	P258	R196
	T318	E259	G197
	A319	T260	Y198
	L320	L261	S199
	A321	F262	F200
	P322	Q263	V201
		P264	T202
	M325	S265	T203
	K326	F266	A204
	I327	I267	E205
	K328	G268	R206
	I329	M269	E207
	I330	E270	I208
	A331	S271	V209
	P332	A272	R210
	P333	G273	D211
	E334	I274	I212
	R335	H275	K213
	K336	E276	E214
	Y337	T277	K215
	S338	T278	L216
	V339	Y279	C217
	W340	N280	Y218
	I341	S281	V219
	G342		

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	114/8729 (1.3%)
1	D	1.77	65/6448 (1.0%)	1.82	114/8729 (1.3%)
1	G	1.77	67/6448 (1.0%)	1.82	116/8729 (1.3%)
1	J	1.90	68/6449 (1.1%)	1.84	118/8732 (1.4%)
2	B	1.22	10/1148 (0.9%)	1.61	16/1548 (1.0%)
2	E	1.22	10/1148 (0.9%)	1.61	16/1548 (1.0%)
2	H	1.22	10/1148 (0.9%)	1.62	16/1548 (1.0%)
2	K	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%)
4	0	0.89	1/2968 (0.0%)	1.64	52/4023 (1.3%)
4	1	0.89	2/2968 (0.1%)	1.64	50/4023 (1.2%)
4	2	0.89	1/2968 (0.0%)	1.64	52/4023 (1.3%)
4	3	0.89	1/2968 (0.0%)	1.64	51/4023 (1.3%)
4	4	0.89	1/2968 (0.0%)	1.64	51/4023 (1.3%)
4	5	0.89	2/2968 (0.1%)	1.64	51/4023 (1.3%)
4	6	0.89	2/2968 (0.1%)	1.64	52/4023 (1.3%)
4	7	0.89	2/2968 (0.1%)	1.64	52/4023 (1.3%)
4	8	0.89	2/2968 (0.1%)	1.64	51/4023 (1.3%)
4	V	0.89	1/2968 (0.0%)	1.64	52/4023 (1.3%)
4	W	0.89	2/2968 (0.1%)	1.64	51/4023 (1.3%)
4	X	0.89	2/2968 (0.1%)	1.64	51/4023 (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%)
All	All	1.29	330/76481 (0.4%)	1.67	1261/103533 (1.2%)

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

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	4
1	D	1	4
1	G	2	4
1	J	1	6
2	B	0	3
2	E	0	3
2	H	0	3
2	K	0	3
3	C	0	2
3	F	0	2
3	I	0	2
3	L	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	6	0	1
4	7	0	1
4	8	0	1
4	V	0	1
4	W	0	1
4	X	0	1
4	Y	0	1
4	Z	0	1
All	All	5	52

The worst 5 of 330 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	709	LYS	C-N	-55.36	0.33	1.33
1	J	649	VAL	CB-CG1	53.26	2.64	1.52
1	G	649	VAL	CB-CG1	53.23	2.64	1.52
1	D	649	VAL	CB-CG1	53.18	2.64	1.52
1	A	649	VAL	CB-CG1	53.16	2.64	1.52

The worst 5 of 1261 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	637	LYS	O-C-N	-58.53	23.69	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	637	LYS	O-C-N	-58.47	23.80	123.20
1	D	637	LYS	O-C-N	-58.47	23.81	123.20
1	A	637	LYS	O-C-N	-58.45	23.83	123.20
1	J	649	VAL	CG1-CB-CG2	-34.02	56.47	110.90

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	648	THR	CB
1	D	648	THR	CB
1	G	75	ASP	CA
1	G	648	THR	CB
1	J	648	THR	CB

5 of 52 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	623	PHE	Sidechain
1	A	637	LYS	Mainchain
1	A	649	VAL	Mainchain
1	A	98	HIS	Mainchain
2	B	22	THR	Mainchain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6797	0	6752	1414	0
1	D	6797	0	6761	1431	0
1	G	6797	0	6754	1380	0
1	J	6797	0	6760	1429	0
2	B	1127	0	1086	252	0
2	E	1127	0	1087	320	0
2	H	1127	0	1087	228	0
2	K	1127	0	1087	227	0
3	C	1123	0	1084	181	0
3	F	1123	0	1082	139	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	1123	0	1084	169	0
3	L	1123	0	1084	165	0
4	0	2906	0	2866	75	3476
4	1	2906	0	2866	77	3458
4	2	2906	0	2864	102	3464
4	3	2906	0	2864	100	410
4	4	2906	0	2855	345	94
4	5	2906	0	2855	340	0
4	6	2906	0	2852	382	0
4	7	2906	0	2852	377	0
4	8	2906	0	2861	150	0
4	V	2906	0	2861	142	95
4	W	2906	0	2864	107	400
4	X	2906	0	2864	105	3474
4	Y	2906	0	2865	78	3456
4	Z	2906	0	2865	78	3477
All	All	76872	0	75762	7444	10902

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 49.

The worst 5 of 7444 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:G:797:PHE:CD1	3:I:149:VAL:HG11	1.20	1.68
2:E:144:VAL:HG13	2:E:153:ILE:CD1	1.22	1.66
1:G:798:LEU:CD1	3:I:126:LEU:HD21	1.20	1.65
1:A:725:ARG:HE	1:A:733:PRO:CB	1.09	1.64
1:D:725:ARG:HE	1:D:733:PRO:CB	1.09	1.64

The worst 5 of 10902 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)
4:2:206:ARG:CG	4:Z:200:PHE:CA[1_556]	0.14	2.06
4:0:206:ARG:CG	4:X:200:PHE:CA[1_556]	0.14	2.06
4:0:186:THR:OG1	4:X:189:LEU:O[1_556]	0.15	2.05
4:2:186:THR:OG1	4:Z:189:LEU:O[1_556]	0.16	2.04
4:1:32:PRO:CD	4:Y:211:ASP:CG[1_556]	0.17	2.03

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	789/840 (94%)	650 (82%)	113 (14%)	26 (3%)	4	35
1	D	789/840 (94%)	651 (82%)	112 (14%)	26 (3%)	4	35
1	G	789/840 (94%)	649 (82%)	113 (14%)	27 (3%)	4	35
1	J	791/840 (94%)	651 (82%)	112 (14%)	28 (4%)	4	34
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
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
4	0	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	11	51
4	1	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	11	51
4	2	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	11	51
4	3	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	11	51
4	4	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	11	51
4	5	370/375 (99%)	335 (90%)	29 (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%)	335 (90%)	29 (8%)	6 (2%)	11	51
4	V	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	11	51
4	W	370/375 (99%)	334 (90%)	30 (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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	Z	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	11	51
All	All	9482/9778 (97%)	8319 (88%)	940 (10%)	223 (2%)	11	42

5 of 223 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%)	514 (76%)	158 (24%)	1	5
1	J	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
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
4	0	315/318 (99%)	269 (85%)	46 (15%)	3	21
4	1	315/318 (99%)	268 (85%)	47 (15%)	3	20
4	2	315/318 (99%)	268 (85%)	47 (15%)	3	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	3	315/318 (99%)	268 (85%)	47 (15%)	3	20
4	4	315/318 (99%)	268 (85%)	47 (15%)	3	20
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
4	V	315/318 (99%)	269 (85%)	46 (15%)	3	21
4	W	315/318 (99%)	269 (85%)	46 (15%)	3	21
4	X	315/318 (99%)	269 (85%)	46 (15%)	3	21
4	Y	315/318 (99%)	268 (85%)	47 (15%)	3	20
4	Z	315/318 (99%)	268 (85%)	47 (15%)	3	20
All	All	8046/8088 (100%)	6737 (84%)	1309 (16%)	6	17

5 of 1309 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	532	ILE
4	1	291	LYS
4	X	351	THR
1	J	625	THR
4	0	109	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 184 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	194	GLN
3	L	39	GLN
4	X	263	GLN
1	J	253	HIS
1	J	563	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	MLY	A	107	1	10,10,11	0.46	0	8,11,13	1.02	1 (12%)
1	MLY	A	130	1	10,10,11	0.99	1 (10%)	8,11,13	1.33	2 (25%)
1	MLY	A	138	1	10,10,11	1.36	1 (10%)	8,11,13	2.72	1 (12%)
1	MLY	A	19	1	10,10,11	1.19	1 (10%)	8,11,13	0.62	0
1	MLY	A	190	1	10,10,11	1.18	1 (10%)	8,11,13	1.31	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	0.77	0	8,11,13	0.85	0
1	MLY	A	272	1	10,10,11	1.08	1 (10%)	8,11,13	1.32	1 (12%)
1	MLY	A	295	1	10,10,11	1.16	1 (10%)	8,11,13	0.31	0
1	MLY	A	296	1	10,10,11	0.84	1 (10%)	8,11,13	1.20	1 (12%)
1	MLY	A	30	1	10,10,11	0.88	0	8,11,13	0.91	0
1	MLY	A	348	1	10,10,11	0.79	0	8,11,13	1.10	1 (12%)
1	MLY	A	35	1	10,10,11	0.72	0	8,11,13	0.65	0
1	MLY	A	353	1	10,10,11	0.98	0	8,11,13	1.03	1 (12%)
1	MLY	A	367	1	10,10,11	0.89	1 (10%)	8,11,13	0.42	0
1	MLY	A	369	1	10,10,11	0.85	0	8,11,13	0.77	0
1	MLY	A	385	1	10,10,11	0.94	1 (10%)	8,11,13	0.52	0
1	MLY	A	415	1	10,10,11	0.71	0	8,11,13	0.73	0
1	MLY	A	431	1	10,10,11	0.49	0	8,11,13	1.19	1 (12%)
1	MLY	A	436	1	10,10,11	1.02	1 (10%)	8,11,13	1.79	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	1.10	1 (10%)	8,11,13	1.24	1 (12%)
1	MLY	A	504	1	10,10,11	0.83	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	1.12	1 (12%)
1	MLY	A	55	1	10,10,11	0.94	1 (10%)	8,11,13	1.09	0
1	MLY	A	551	1	10,10,11	0.61	0	8,11,13	0.72	0
1	MLY	A	553	1,4	10,10,11	0.65	0	8,11,13	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	A	59	1	10,10,11	0.80	0	8,11,13	1.13	1 (12%)
1	MLY	A	598	1	10,10,11	1.15	2 (20%)	8,11,13	1.31	1 (12%)
1	MLY	A	600	1	10,10,11	0.59	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	0.88	1 (10%)	8,11,13	0.60	0
1	MLY	A	63	1	10,10,11	0.91	0	8,11,13	0.79	0
1	MLY	A	659	1	10,10,11	0.73	0	8,11,13	0.85	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	0.86	0	8,11,13	1.96	1 (12%)
1	MLY	A	782	1	10,10,11	0.74	0	8,11,13	1.54	1 (12%)
1	MLY	A	827	1	10,10,11	1.00	1 (10%)	8,11,13	0.93	1 (12%)
1	MLY	A	833	1	10,10,11	1.08	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	1,2	10,10,11	0.65	0	8,11,13	1.50	1 (12%)
1	MLY	A	84	1	10,10,11	0.56	0	8,11,13	0.79	0
1	MLY	A	87	1	10,10,11	1.11	1 (10%)	8,11,13	0.59	0
1	MLY	D	107	1	10,10,11	0.49	0	8,11,13	1.03	1 (12%)
1	MLY	D	130	1	10,10,11	0.98	1 (10%)	8,11,13	1.34	2 (25%)
1	MLY	D	138	1	10,10,11	1.39	1 (10%)	8,11,13	2.70	1 (12%)
1	MLY	D	19	1	10,10,11	1.28	1 (10%)	8,11,13	0.63	0
1	MLY	D	190	1	10,10,11	1.15	1 (10%)	8,11,13	1.33	1 (12%)
1	MLY	D	236	1	10,10,11	1.12	1 (10%)	8,11,13	1.55	2 (25%)
1	MLY	D	248	1	10,10,11	0.77	0	8,11,13	0.85	0
1	MLY	D	272	1	10,10,11	1.07	1 (10%)	8,11,13	1.32	1 (12%)
1	MLY	D	295	1	10,10,11	1.13	1 (10%)	8,11,13	0.33	0
1	MLY	D	296	1	10,10,11	0.86	0	8,11,13	1.20	1 (12%)
1	MLY	D	30	1	10,10,11	0.88	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	0.76	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	0.90	1 (10%)	8,11,13	0.42	0
1	MLY	D	369	1	10,10,11	0.85	0	8,11,13	0.77	0
1	MLY	D	385	1	10,10,11	0.93	1 (10%)	8,11,13	0.54	0
1	MLY	D	415	1	10,10,11	0.73	0	8,11,13	0.77	0
1	MLY	D	431	1	10,10,11	0.48	0	8,11,13	1.20	1 (12%)
1	MLY	D	436	1	10,10,11	1.07	1 (10%)	8,11,13	1.76	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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	1.24	1 (12%)
1	MLY	D	504	1	10,10,11	0.82	0	8,11,13	0.46	0
1	MLY	D	505	1	10,10,11	1.42	2 (20%)	8,11,13	0.51	0
1	MLY	D	528	1	10,10,11	0.86	0	8,11,13	1.12	1 (12%)
1	MLY	D	55	1	10,10,11	0.96	1 (10%)	8,11,13	1.07	0
1	MLY	D	551	1	10,10,11	0.60	0	8,11,13	0.74	0
1	MLY	D	553	1,4	10,10,11	0.64	0	8,11,13	0.67	0
1	MLY	D	59	1	10,10,11	0.80	0	8,11,13	1.13	1 (12%)
1	MLY	D	598	1	10,10,11	1.18	2 (20%)	8,11,13	1.28	1 (12%)
1	MLY	D	600	1	10,10,11	0.58	0	8,11,13	0.98	1 (12%)
1	MLY	D	613	1	10,10,11	0.61	0	8,11,13	1.08	1 (12%)
1	MLY	D	617	1	10,10,11	0.90	1 (10%)	8,11,13	0.61	0
1	MLY	D	63	1	10,10,11	0.91	0	8,11,13	0.79	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	0.96	1 (10%)	8,11,13	1.43	1 (12%)
1	MLY	D	764	1	10,10,11	0.78	0	8,11,13	0.50	0
1	MLY	D	768	1	10,10,11	0.85	0	8,11,13	1.96	1 (12%)
1	MLY	D	782	1	10,10,11	0.76	0	8,11,13	1.53	1 (12%)
1	MLY	D	827	1	10,10,11	0.98	1 (10%)	8,11,13	0.93	1 (12%)
1	MLY	D	833	1	10,10,11	1.06	1 (10%)	8,11,13	1.11	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	0.66	0	8,11,13	1.49	1 (12%)
1	MLY	D	84	1	10,10,11	0.60	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	0.46	0	8,11,13	1.01	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	1.31	1 (10%)	8,11,13	2.74	1 (12%)
1	MLY	G	19	1	10,10,11	1.23	1 (10%)	8,11,13	0.65	0
1	MLY	G	190	1	10,10,11	1.19	1 (10%)	8,11,13	1.33	1 (12%)
1	MLY	G	236	1	10,10,11	1.09	1 (10%)	8,11,13	1.55	2 (25%)
1	MLY	G	248	1	10,10,11	0.74	0	8,11,13	0.87	0
1	MLY	G	272	1	10,10,11	1.07	1 (10%)	8,11,13	1.32	1 (12%)
1	MLY	G	295	1	10,10,11	1.15	1 (10%)	8,11,13	0.31	0
1	MLY	G	296	1	10,10,11	0.85	0	8,11,13	1.19	1 (12%)
1	MLY	G	30	1	10,10,11	0.88	0	8,11,13	0.92	0
1	MLY	G	348	1	10,10,11	0.80	1 (10%)	8,11,13	1.09	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	G	35	1	10,10,11	0.74	0	8,11,13	0.64	0
1	MLY	G	353	1	10,10,11	0.99	0	8,11,13	1.01	1 (12%)
1	MLY	G	367	1	10,10,11	0.92	1 (10%)	8,11,13	0.43	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	0.55	0
1	MLY	G	415	1	10,10,11	0.70	0	8,11,13	0.75	0
1	MLY	G	431	1	10,10,11	0.50	0	8,11,13	1.17	1 (12%)
1	MLY	G	436	1	10,10,11	1.03	1 (10%)	8,11,13	1.78	1 (12%)
1	MLY	G	486	1	10,10,11	0.56	0	8,11,13	0.55	0
1	MLY	G	49	1	10,10,11	1.10	1 (10%)	8,11,13	1.23	1 (12%)
1	MLY	G	504	1	10,10,11	0.81	0	8,11,13	0.45	0
1	MLY	G	505	1	10,10,11	1.44	2 (20%)	8,11,13	0.51	0
1	MLY	G	528	1	10,10,11	0.83	0	8,11,13	1.13	1 (12%)
1	MLY	G	55	1	10,10,11	0.98	1 (10%)	8,11,13	1.10	0
1	MLY	G	551	1	10,10,11	0.60	0	8,11,13	0.73	0
1	MLY	G	553	1,4	10,10,11	0.64	0	8,11,13	0.66	0
1	MLY	G	59	1	10,10,11	0.77	0	8,11,13	1.17	1 (12%)
1	MLY	G	598	1	10,10,11	1.12	2 (20%)	8,11,13	1.31	1 (12%)
1	MLY	G	600	1	10,10,11	0.63	0	8,11,13	0.97	1 (12%)
1	MLY	G	613	1	10,10,11	0.65	0	8,11,13	1.10	1 (12%)
1	MLY	G	617	1	10,10,11	0.88	1 (10%)	8,11,13	0.61	0
1	MLY	G	63	1	10,10,11	0.92	1 (10%)	8,11,13	0.79	0
1	MLY	G	659	1	10,10,11	0.75	0	8,11,13	0.82	0
1	MLY	G	681	1	10,10,11	0.98	1 (10%)	8,11,13	1.42	1 (12%)
1	MLY	G	764	1	10,10,11	0.76	0	8,11,13	0.51	0
1	MLY	G	768	1	10,10,11	0.88	0	8,11,13	1.95	1 (12%)
1	MLY	G	782	1	10,10,11	0.72	0	8,11,13	1.54	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	0.65	0	8,11,13	0.52	0
1	MLY	G	839	1	10,10,11	0.68	0	8,11,13	1.51	1 (12%)
1	MLY	G	84	1	10,10,11	0.61	0	8,11,13	0.80	0
1	MLY	G	87	1	10,10,11	1.12	1 (10%)	8,11,13	0.59	0
1	MLY	J	107	1	10,10,11	0.48	0	8,11,13	1.03	1 (12%)
1	MLY	J	130	1	10,10,11	0.93	0	8,11,13	1.34	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	1.24	1 (10%)	8,11,13	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	J	190	1	10,10,11	1.19	1 (10%)	8,11,13	1.30	1 (12%)
1	MLY	J	236	1	10,10,11	1.12	1 (10%)	8,11,13	1.55	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	1.11	1 (10%)	8,11,13	1.31	1 (12%)
1	MLY	J	295	1	10,10,11	1.14	1 (10%)	8,11,13	0.33	0
1	MLY	J	296	1	10,10,11	0.90	1 (10%)	8,11,13	1.18	1 (12%)
1	MLY	J	30	1	10,10,11	0.85	0	8,11,13	0.93	0
1	MLY	J	348	1	10,10,11	0.76	0	8,11,13	1.06	1 (12%)
1	MLY	J	35	1	10,10,11	0.74	0	8,11,13	0.64	0
1	MLY	J	353	1	10,10,11	0.96	0	8,11,13	1.02	1 (12%)
1	MLY	J	367	1	10,10,11	0.88	1 (10%)	8,11,13	0.42	0
1	MLY	J	369	1	10,10,11	0.85	0	8,11,13	0.77	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	0.74	0	8,11,13	0.75	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	1.76	1 (12%)
1	MLY	J	486	1	10,10,11	0.56	0	8,11,13	0.55	0
1	MLY	J	49	1	10,10,11	1.12	1 (10%)	8,11,13	1.25	1 (12%)
1	MLY	J	504	1	10,10,11	0.79	0	8,11,13	0.45	0
1	MLY	J	505	1	10,10,11	1.47	2 (20%)	8,11,13	0.50	0
1	MLY	J	528	1	10,10,11	0.82	0	8,11,13	1.12	1 (12%)
1	MLY	J	55	1	10,10,11	0.93	1 (10%)	8,11,13	1.10	0
1	MLY	J	551	1	10,10,11	0.61	0	8,11,13	0.74	0
1	MLY	J	553	1,4	10,10,11	0.64	0	8,11,13	0.63	0
1	MLY	J	59	1	10,10,11	0.80	0	8,11,13	1.15	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	0.64	0	8,11,13	0.97	1 (12%)
1	MLY	J	613	1	10,10,11	0.67	0	8,11,13	1.09	1 (12%)
1	MLY	J	617	1	10,10,11	0.90	1 (10%)	8,11,13	0.59	0
1	MLY	J	63	1	10,10,11	0.91	0	8,11,13	0.79	0
1	MLY	J	659	1	10,10,11	0.71	0	8,11,13	0.84	0
1	MLY	J	681	1	10,10,11	0.94	1 (10%)	8,11,13	1.43	1 (12%)
1	MLY	J	764	1	10,10,11	0.76	0	8,11,13	0.52	0
1	MLY	J	768	1	10,10,11	0.88	0	8,11,13	1.93	1 (12%)
1	MLY	J	782	1	10,10,11	0.73	0	8,11,13	1.55	1 (12%)
1	MLY	J	827	1	10,10,11	1.04	1 (10%)	8,11,13	0.92	1 (12%)
1	MLY	J	833	1	10,10,11	1.13	1 (10%)	8,11,13	1.07	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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	0.67	0	8,11,13	1.50	1 (12%)
1	MLY	J	84	1	10,10,11	0.58	0	8,11,13	0.80	0
1	MLY	J	87	1	10,10,11	1.13	1 (10%)	8,11,13	0.61	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	1,2	-	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	1,4	-	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

The worst 5 of 87 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	138	MLY	CB-CA	-3.76	1.48	1.53
1	J	138	MLY	CB-CA	-3.62	1.48	1.53
1	A	138	MLY	CB-CA	-3.57	1.48	1.53
1	G	138	MLY	CB-CA	-3.52	1.48	1.53
1	D	19	MLY	CB-CA	-3.20	1.49	1.53

The worst 5 of 100 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	138	MLY	CB-CA-C	-7.47	99.33	111.65
1	J	138	MLY	CB-CA-C	-7.45	99.38	111.65
1	A	138	MLY	CB-CA-C	-7.40	99.45	111.65
1	D	138	MLY	CB-CA-C	-7.34	99.56	111.65
1	A	768	MLY	CB-CA-C	-5.21	103.06	111.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

124 monomers are involved in 525 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	107	MLY	3	0
1	A	138	MLY	1	0
1	A	190	MLY	2	0
1	A	248	MLY	2	0
1	A	272	MLY	1	0
1	A	295	MLY	6	0
1	A	296	MLY	2	0
1	A	30	MLY	1	0
1	A	348	MLY	5	0
1	A	369	MLY	1	0
1	A	415	MLY	1	0
1	A	436	MLY	2	0
1	A	486	MLY	3	0
1	A	49	MLY	3	0
1	A	504	MLY	4	0
1	A	505	MLY	11	0
1	A	528	MLY	2	0
1	A	55	MLY	1	0
1	A	551	MLY	2	0
1	A	553	MLY	17	0
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	7	0
1	A	768	MLY	14	0
1	A	782	MLY	1	0
1	A	837	MLY	1	0
1	A	839	MLY	15	0
1	A	87	MLY	3	0
1	D	107	MLY	2	0
1	D	138	MLY	1	0
1	D	190	MLY	2	0
1	D	248	MLY	2	0
1	D	272	MLY	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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	0
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	2	0
1	D	768	MLY	6	0
1	D	782	MLY	32	0
1	D	837	MLY	1	0
1	D	839	MLY	16	0
1	D	87	MLY	3	0
1	G	107	MLY	3	0
1	G	138	MLY	1	0
1	G	190	MLY	2	0
1	G	248	MLY	2	0
1	G	272	MLY	1	0
1	G	295	MLY	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
1	G	486	MLY	3	0
1	G	49	MLY	2	0
1	G	528	MLY	3	0
1	G	55	MLY	1	0
1	G	551	MLY	2	0
1	G	553	MLY	16	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	G	59	MLY	3	0
1	G	598	MLY	1	0
1	G	600	MLY	1	0
1	G	617	MLY	1	0
1	G	63	MLY	3	0
1	G	659	MLY	2	0
1	G	764	MLY	12	0
1	G	768	MLY	15	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	18	0
1	G	87	MLY	2	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	528	MLY	3	0
1	J	55	MLY	1	0
1	J	551	MLY	1	0
1	J	553	MLY	17	0
1	J	59	MLY	3	0
1	J	598	MLY	1	0
1	J	600	MLY	1	0
1	J	617	MLY	1	0
1	J	63	MLY	4	0
1	J	659	MLY	2	0
1	J	764	MLY	26	0
1	J	768	MLY	41	0
1	J	782	MLY	1	0
1	J	827	MLY	1	0
1	J	837	MLY	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	J	839	MLY	5	0
1	J	84	MLY	25	0
1	J	87	MLY	3	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.