



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:44 PM BST

PDB ID : 1O18
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 : 2002-11-04
Resolution : 70.00 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

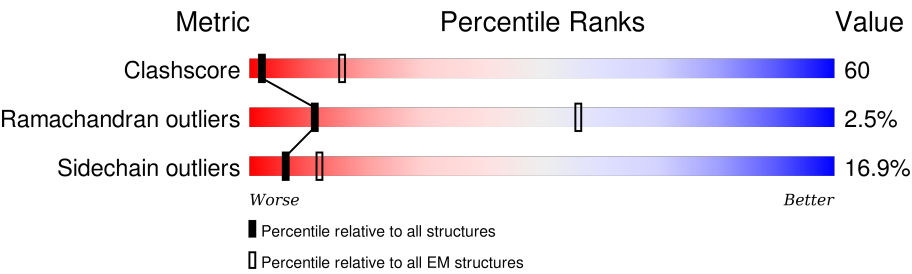
MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

1 Overall quality at a glance i

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

The reported resolution of this entry is 70.00 Å.

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













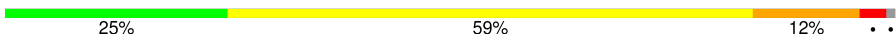
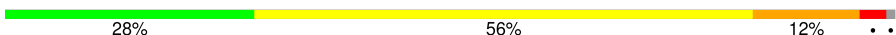
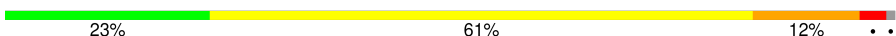


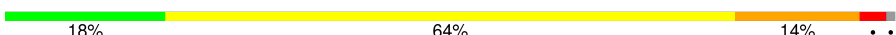





Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 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	27% 50% 19% .
1	D	840	26% 51% 19% .
1	G	840	25% 52% 19% .
1	J	840	26% 51% 19% .
1	M	840	25% 51% 19% .
1	P	840	26% 50% 19% .
2	E	145	65% 26% 6% .
2	H	145	63% 28% 6% .
2	K	145	64% 26% 6% .

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Mol	Chain	Length	Quality of chain
2	N	145	
2	Q	145	
3	F	147	
3	I	147	
3	L	147	
3	O	147	
3	R	147	
4	1	375	
4	2	375	
4	3	375	
4	4	375	
4	5	375	
4	6	375	
4	7	375	
4	8	375	
4	9	375	
4	V	375	
4	W	375	
4	X	375	
4	Y	375	
4	Z	375	

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

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

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

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 92716 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	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	F	147	Total	C	N	O	S	0	0
			1123	698	188	230	7		

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

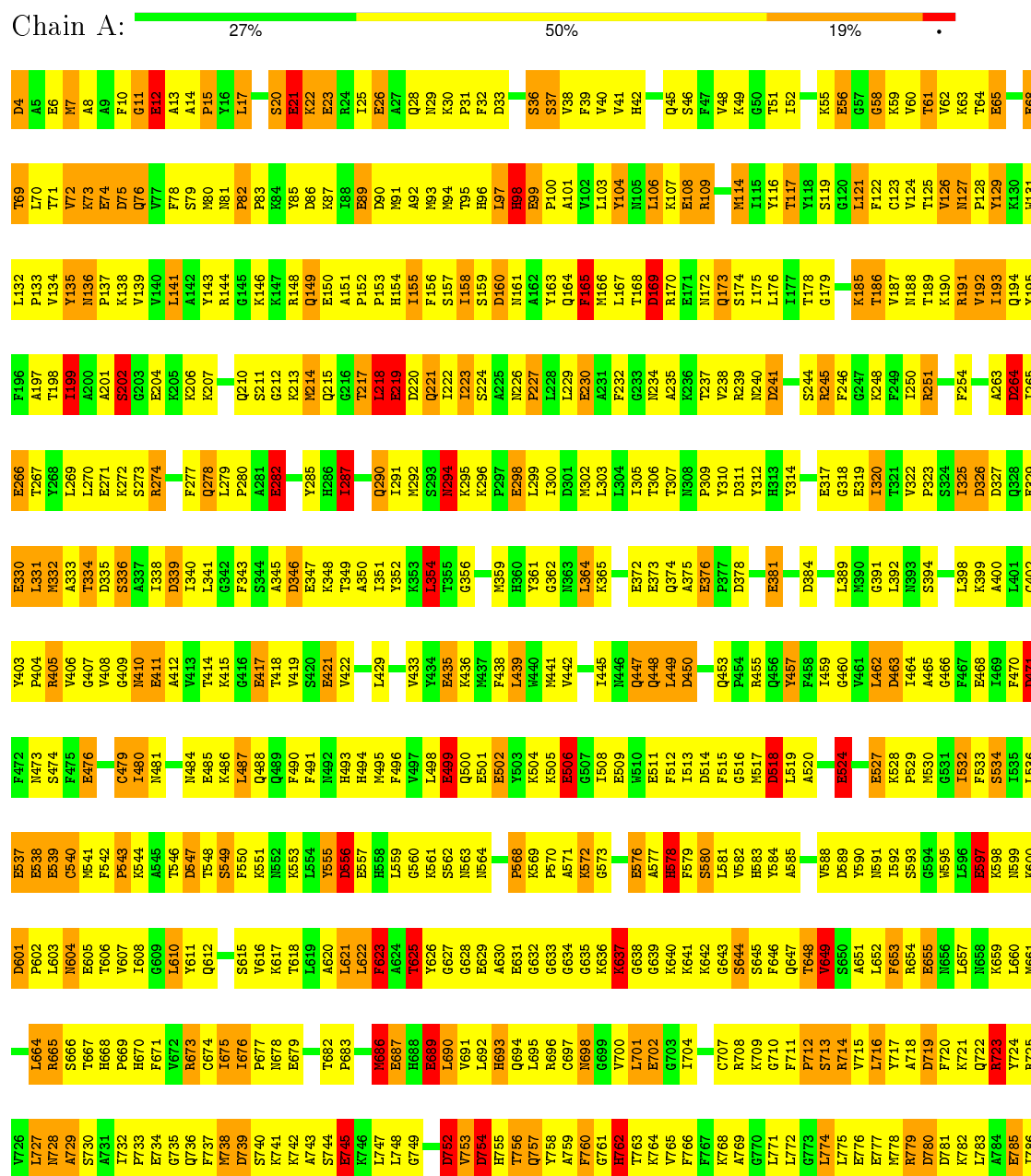
- Molecule 4 is a protein called SKELETAL MUSCLE ACTIN.

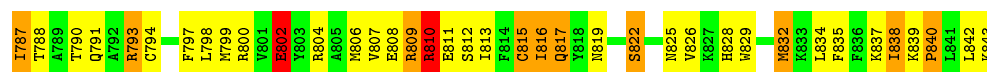
Mol	Chain	Residues	Atoms					AltConf	Trace
4	1	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	2	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	3	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	4	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	5	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20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

3 Residue-property plots

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

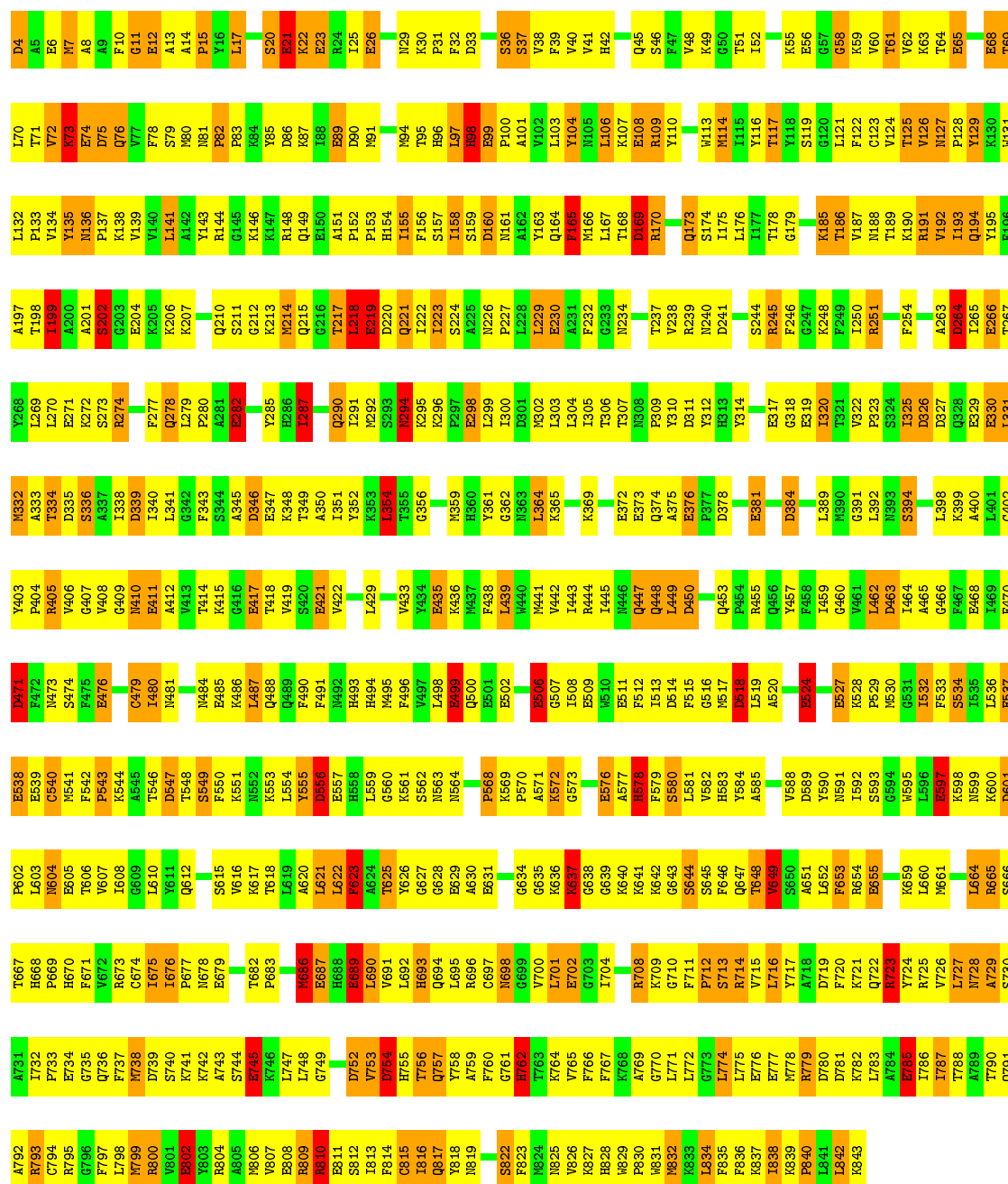
• Molecule 1: SKELETAL MUSCLE MYOSIN II





• Molecule 1: SKELETAL MUSCLE MYOSIN II

Chain D: 26% 51% 19%



• Molecule 1: SKELETAL MUSCLE MYOSIN II

Chain G: 25% 52% 19%

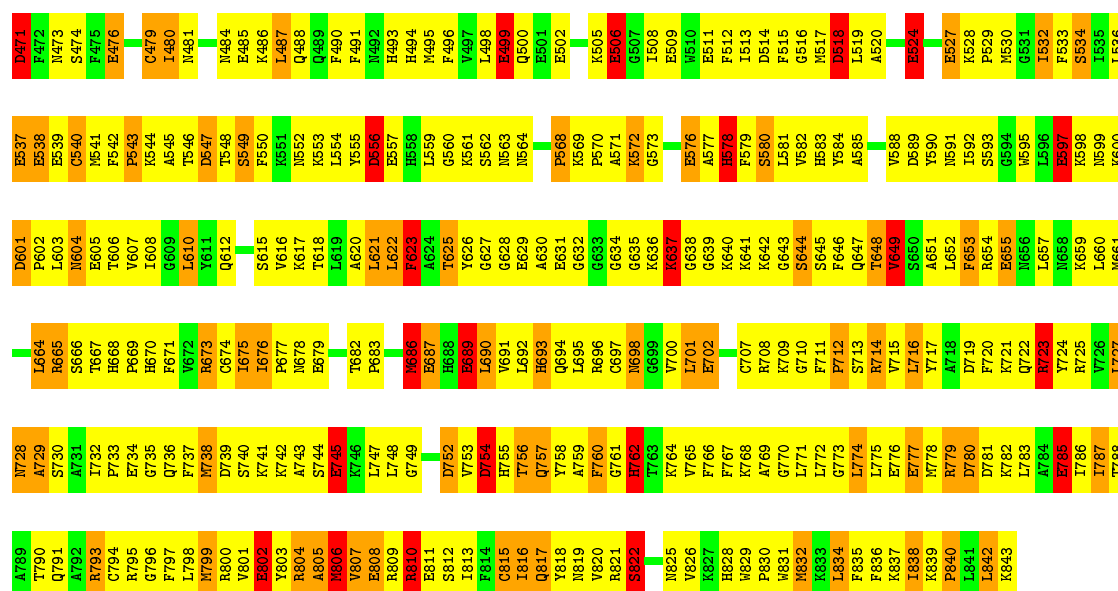




Response	Percentage
Yes, the U.S. should take action to protect the environment	26%
No, the U.S. should focus on the economy	51%
It's not the U.S.'s responsibility	19%
Don't know	4%

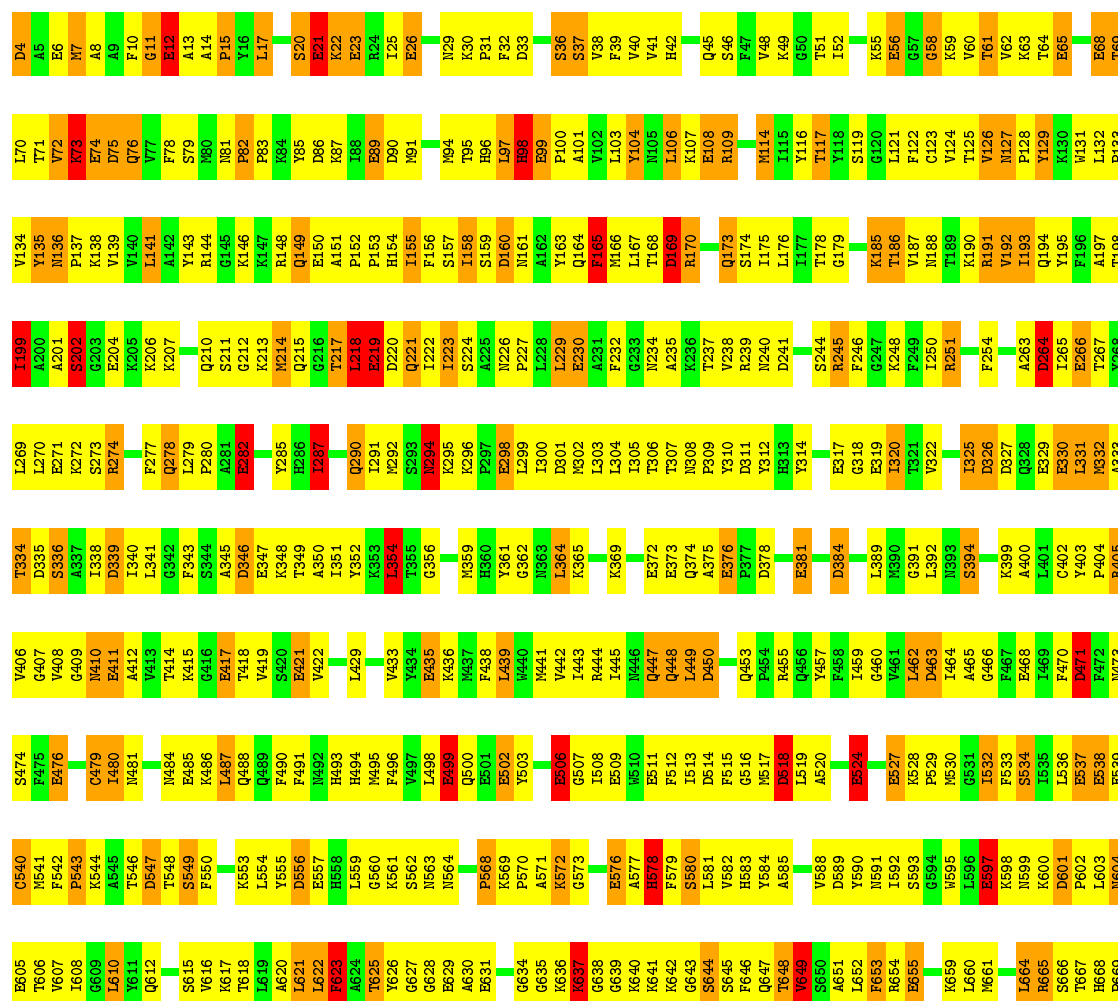


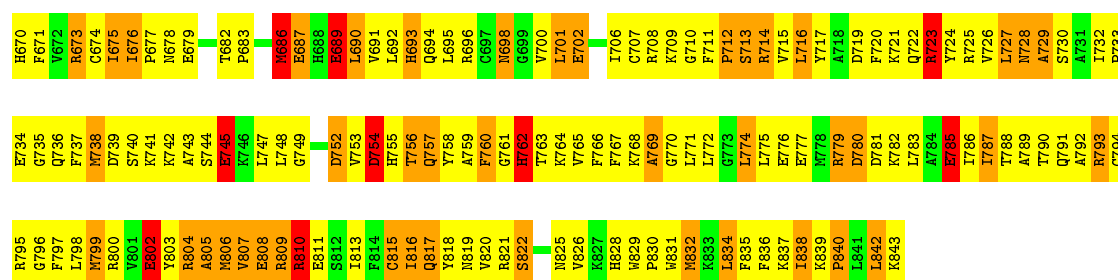
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L404	C403	P404	E331	E332	M333	L271	E271	E272	T277
L405	C404	R405	E333	E334	M334	L272	E272	E273	T278
L406	C405	S406	E335	E336	M335	L273	E273	E274	T279
L407	C406	T407	E337	E338	M336	L274	E274	E275	T280
L408	C407	V408	E339	E340	M337	L275	E275	E276	T281
L409	C408	W409	E341	E342	M338	L276	E276	E277	T282
L410	C409	X410	E343	E344	M339	L277	E277	E278	T283
L411	C410	Y411	E345	E346	M340	L278	E278	E279	T284
L412	C411	Z412	E347	E348	M341	L279	E279	E280	T285
L413	C412	A413	E349	E350	M342	L280	E280	E281	T286
L414	C413	B414	E351	E352	M343	L281	E281	E282	T287
L415	C414	C415	E353	E354	M344	L282	E282	E283	T288
L416	C415	D416	E355	E356	M345	L283	E283	E284	T289
L417	C416	E417	E357	E358	M346	L284	E284	E285	T290
L418	C417	F418	E359	E360	M347	L285	E285	E286	T291
L419	C418	G419	E361	E362	M348	L286	E286	E287	T292
L420	C419	H420	E363	E364	M349	L287	E287	E288	T293
L421	C420	I421	E365	E366	M350	L288	E288	E289	T294
L422	C421	J422	E367	E368	M351	L289	E289	E290	T295
L423	C422	K423	E369	E370	M352	L290	E290	E291	T296
L424	C423	L424	E371	E372	M353	L291	E291	E292	T297
L425	C424	M425	E373	E374	M354	L292	E292	E293	T298
L426	C425	N426	E375	E376	M355	L293	E293	E294	T299
L427	C426	O427	E377	E378	M356	L294	E294	E295	T300
L428	C427	P428	E379	E380	M357	L295	E295	E296	T301
L429	C428	Q429	E381	E382	M358	L296	E296	E297	T302
L430	C429	R430	E383	E384	M359	L297	E297	E298	T303
L431	C430	S431	E385	E386	M360	L298	E298	E299	T304
L432	C431	T432	E387	E388	M361	L299	E299	E300	T305
L433	C432	U433	E389	E390	M362	L300	E300	E301	T306
L434	C433	V434	E391	E392	M363	L301	E301	E302	T307
L435	C434	W435	E393	E394	M364	L302	E302	E303	T308
L436	C435	X436	E395	E396	M365	L303	E303	E304	T309
L437	C436	Y437	E397	E398	M366	L304	E304	E305	T310
L438	C437	Z438	E399	E400	M367	L305	E305	E306	T311
L439	C438	A439	E401	E402	M368	L306	E306	E307	T312
L440	C439	B440	E403	E404	M369	L307	E307	E308	T313
L441	C440	C441	E405	E406	M370	L308	E308	E309	T314
L442	C441	D442	E407	E408	M371	L309	E309	E310	T315
L443	C442	E443	E409	E410	M372	L310	E310	E311	T316
L444	C443	F444	E411	E412	M373	L311	E311	E312	T317
L445	C444	G445	E413	E414	M374	L312	E312	E313	T318
L446	C445	H446	E415	E416	M375	L313	E313	E314	T319
L447	C446	I447	E417	E418	M376	L314	E314	E315	T320
L448	C447	J448	E419	E420	M377	L315	E315	E316	T321
L449	C448	K449	E421	E422	M378	L316	E316	E317	T322
L450	C449	L450	E423	E424	M379	L317	E317	E318	T323
L451	C450	M451	E425	E426	M380	L318	E318	E319	T324
L452	C451	N452	E427	E428	M381	L319	E319	E320	T325
L453	C452	O453	E429	E430	M382	L320	E320	E321	T326
L454	C453	P454	E431	E432	M383	L321	E321	E322	T327
L455	C454	Q455	E433	E434	M384	L322	E322	E323	T328
L456	C455	R456	E435	E436	M385	L323	E323	E324	T329
L457	C456	S457	E437	E438	M386	L324	E324	E325	T330
L458	C457	T458	E439	E440	M387	L325	E325	E326	T331
L459	C458	U459	E441	E442	M388	L326	E326	E327	T332
L460	C459	V460	E443	E444	M389	L327	E327	E328	T333
L461	C460	W461	E445	E446	M390	L328	E328	E329	T334
L462	C461	X462	E447	E448	M391	L329	E329	E330	T335
L463	C462	Y463	E449	E450	M392	L330	E330	E331	T336
L464	C463	Z464	E451	E452	M393	L331	E331	E332	T337
L465	C464	A465	E453	E454	M394	L332	E332	E333	T338
L466	C465	B466	E455	E456	M395	L333	E333	E334	T339
L467	C466	C467	E457	E458	M396	L334	E334	E335	T340
L468	C467	D468	E459	E460	M397	L335	E335	E336	T341
L469	C468	E469	E461	E462	M398	L336	E336	E337	T342
L470	C469	F470	E463	E464	M399	L337	E337	E338	T343
L471	C470	G471	E465	E466	M400	L338	E338	E339	T344
L472	C471	H472	E467	E468	M401	L339	E339	E340	T345
L473	C472	I473	E469	E470	M402	L340	E340	E341	T346
L474	C473	J474	E471	E472	M403	L341	E341	E342	T347
L475	C474	K475	E473	E474	M404	L342	E342	E343	T348
L476	C475	L476	E475	E476	M405	L343	E343	E344	T349
L477	C476	M477	E477	E478	M406	L344	E344	E345	T350
L478	C477	N478	E479	E480	M407	L345	E345	E346	T351
L479	C478	O479	E481	E482	M408	L346	E346	E347	T352
L480	C479	P480	E483	E484	M409	L347	E347	E348	T353
L481	C480	Q481	E485	E486	M410	L348	E348	E349	T354
L482	C481	R482	E487	E488	M411	L349	E349	E350	T355
L483	C482	S483	E489	E490	M412	L350	E350	E351	T356
L484	C483	T484	E491	E492	M413	L351	E351	E352	T357
L485	C484	U485	E493	E494	M414	L352	E352	E353	T358
L486	C485	V486	E495	E496	M415	L353	E353	E354	T359
L487	C486	W487	E497	E498	M416	L354	E354	E355	T360
L488	C487	X488	E499	E500	M417	L355	E355	E356	T361
L489	C488	Y489	E501	E502	M418	L356	E356	E357	T362
L490	C489	Z490	E503	E504	M419	L357	E357	E358	T363
L491	C490	A491	E505	E506	M420	L358	E358	E359	T364
L492	C491	B492	E507	E508	M421	L359	E359	E360	T365
L493	C492	C493	E509	E510	M422	L360	E360	E361	T366
L494	C493	D494	E511	E512	M423	L361	E361	E362	T367
L495	C494	E495	E513	E514	M424	L362	E362	E363	T368
L496	C495	F496	E515	E516	M425	L363	E363	E364	T369
L497	C496	G497	E517	E518	M426	L364	E364	E365	T370
L498	C497	H498	E519	E520	M427	L365	E365	E366	T371
L499	C498	I499	E521	E522	M428	L366	E366	E367	T372
L500	C499	J500	E523	E524	M429	L367	E367	E368	T373
L501	C500	K501	E525	E526	M430	L368	E368	E369	T374
L502	C501	L502	E527	E528	M431	L369	E369	E370	T375
L503	C502	M503	E529	E530	M432	L370	E370	E371	T376
L504	C503	N504	E531	E532	M433	L371	E371	E372	T377
L505	C504	O505	E533	E534	M434	L372	E372	E373	T378
L506	C505	P506	E535	E536	M435	L373	E373	E374	T379
L507	C506	Q507	E537	E538	M436	L374	E374	E375	T380
L508	C507	R508	E539	E540	M437	L375	E375	E376	T381
L509	C508	S509	E541	E542	M438	L376	E376	E377	T382
L510	C509	T510	E543	E544	M439	L377	E377	E378	T383
L511	C510	U511	E545	E546	M440	L378	E378	E379	T384
L512	C511	V512	E547	E548	M441	L379	E379	E380	T385
L513	C512	W513	E549	E550	M442	L380	E380	E381	T386
L514	C513	X514	E551	E552	M443	L381	E381	E382	T387
L515	C514	Y515	E553	E554	M444	L382	E382	E383	T388
L516	C515	Z516	E555	E556	M445	L383	E383	E384	T389
L517	C516	A517	E557	E558	M446	L384	E384	E385	T390
L518	C517	B518	E559	E560	M447	L385	E385	E386	T391
L519	C518	C519	E561	E562	M448	L386	E386	E387	T392
L520	C519	D520	E563	E564	M449	L387	E387	E388	T393
L521	C520	E521	E565	E566	M450	L388	E388	E389	T394
L522	C521	F522	E567	E568	M451	L389	E389	E390	T395
L523	C522	G523	E569	E570	M452	L390	E390	E391	T396
L524	C523	H524	E571	E572	M453	L391	E391	E392	T397
L525	C524	I525	E573	E574	M454	L392	E392	E393	T398
L526	C525	J526	E575	E576	M455	L393	E393	E394	T399
L527	C526	K527	E577	E578	M456	L394	E394	E395	T400
L528	C527	L528	E579	E580	M457	L395	E395	E396	T401
L529	C528	M529	E581	E582	M458	L396	E396	E397	T402
L530	C529	N530	E583	E584	M459	L397	E397	E398	T403
L531	C530	O531	E585	E586	M460	L398	E398	E399	T404
L532	C531	P532	E587	E588	M461	L399	E399	E400	T405
L533	C532	Q533	E589	E590	M462	L400	E400	E401	T406
L534	C533	R534	E591	E592	M463	L401	E401	E402	T407
L535	C534	S535	E593	E594	M464	L402	E402	E403	T408
L536	C535	T536	E595	E596	M465	L403	E403	E404	T409
L537	C536	U537	E597	E598	M466	L404	E404	E405	T410
L538	C537	V538	E599	E600	M467	L405	E405	E406	T411
L539	C538	W539	E601	E602	M468	L406	E406	E407	T412
L540	C539	X540	E603	E604	M469	L407	E407	E408	T413
L541	C540	Y541	E605	E606	M470	L408	E408	E409	T414
L542	C541	Z542	E607	E608	M471	L409	E409	E410	T415
L543	C542	A543	E609	E610	M472	L410	E410	E411	T416
L544	C543	B544	E611	E612	M473	L411	E411	E412	T417
L545	C544	C545	E613	E614	M474	L412	E412	E413	T418
L546	C545	D546	E615	E616	M475	L413	E413	E414	



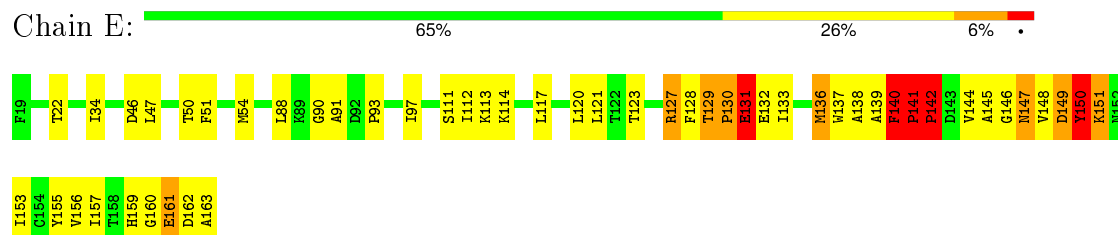
• Molecule 1: SKELETAL MUSCLE MYOSIN II

Chain P: 26% 50% 19%

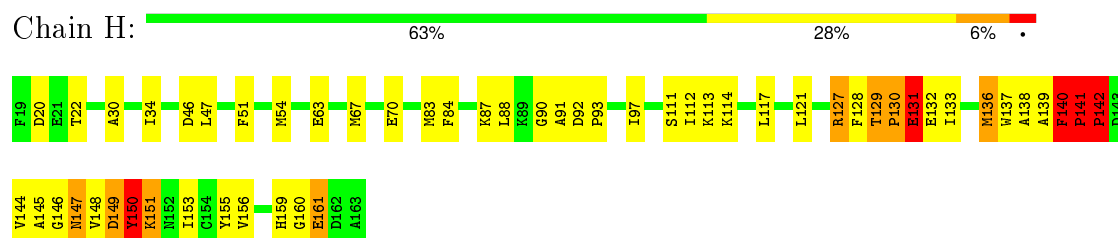




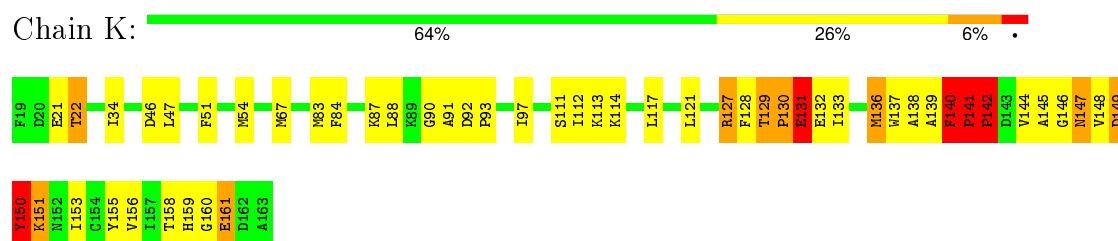
• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN



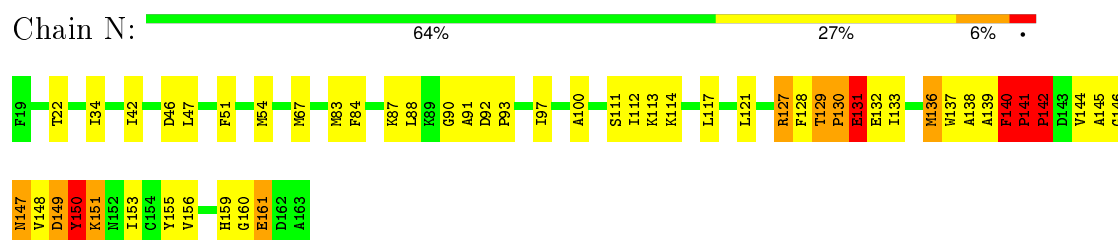
• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN



• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

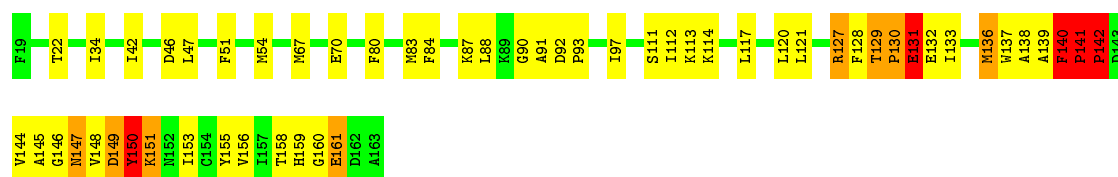


• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN



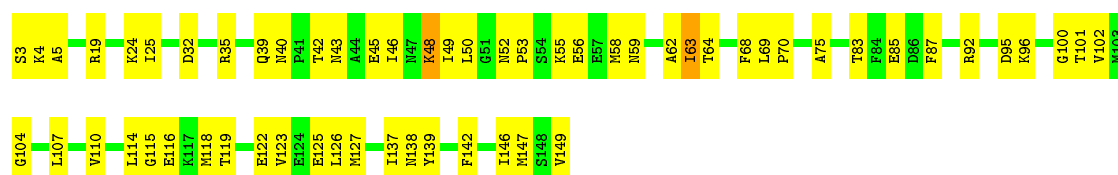
• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN





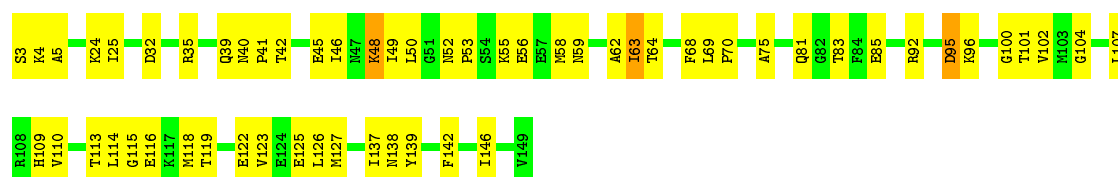
• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN

Chain F: 60% 39%



• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN

Chain I: 61% 37%



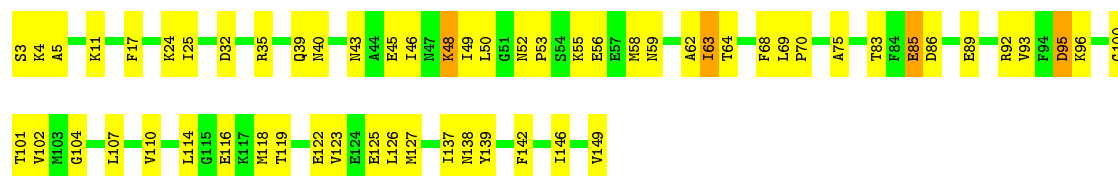
• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN

Chain L: 61% 37%



• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN

Chain O: 60% 37%

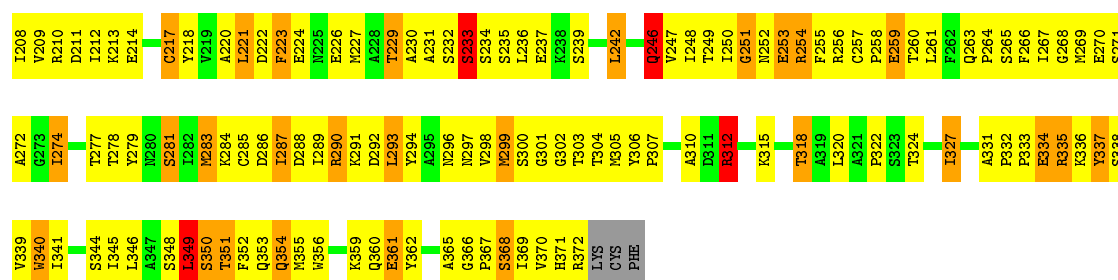


• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN

Chain R: 61% 37%

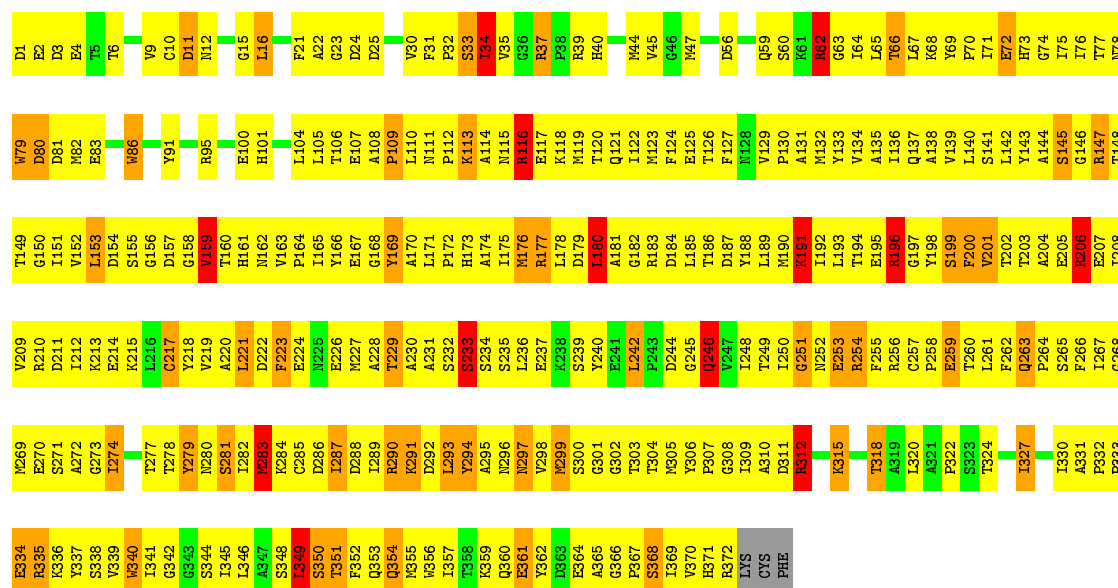






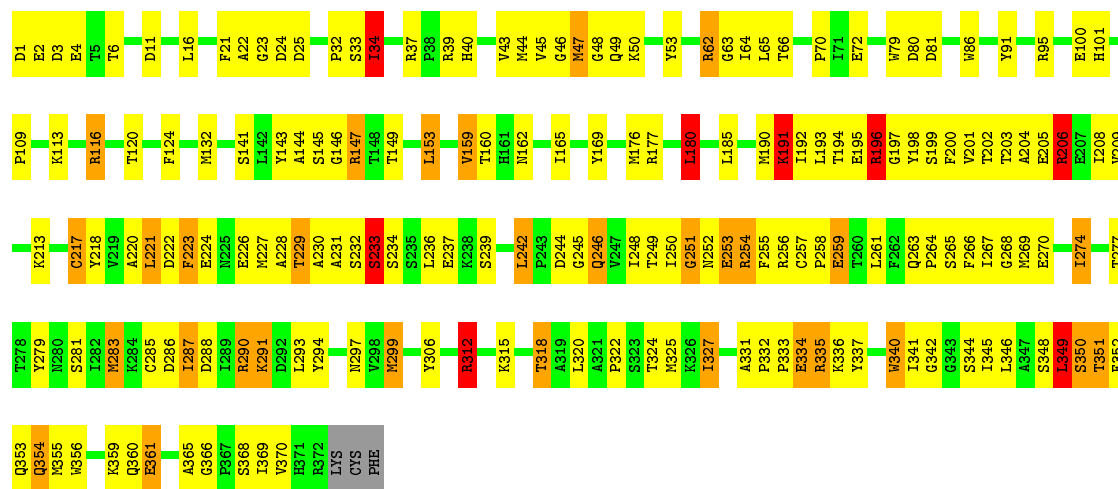
• Molecule 4: SKELETAL MUSCLE ACTIN

Chain 9: 18% 64% 14%

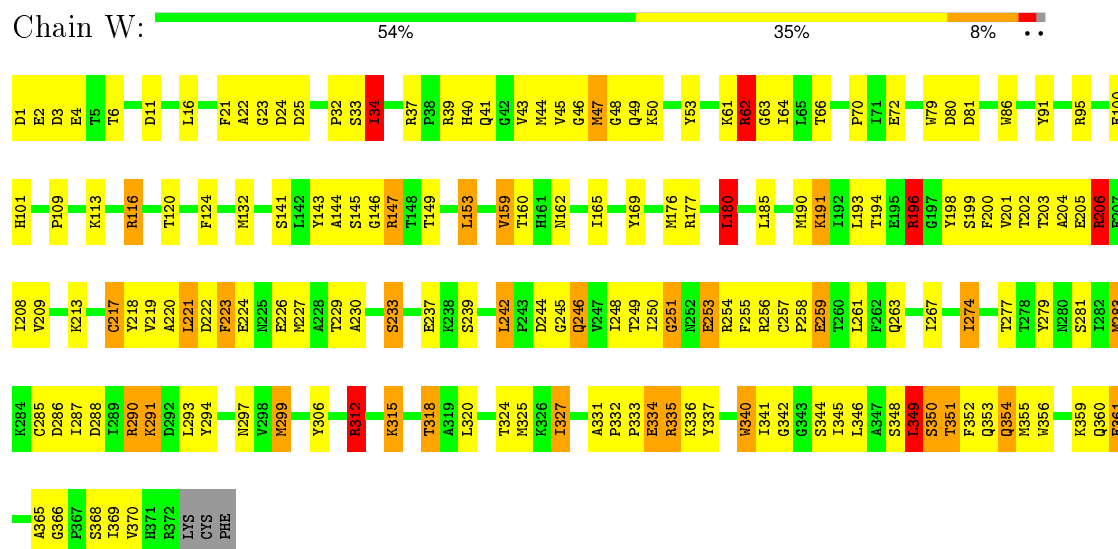


• Molecule 4: SKELETAL MUSCLE ACTIN

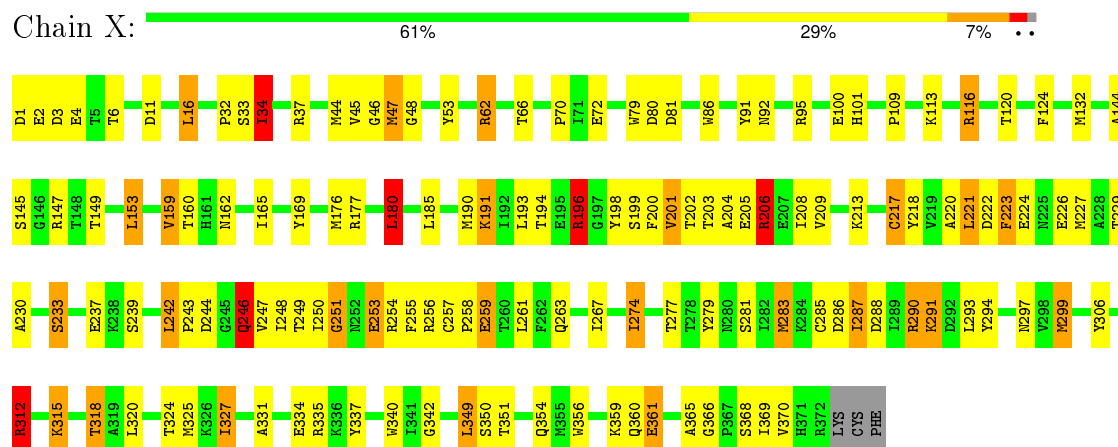
Chain V: 50% 38% 8%



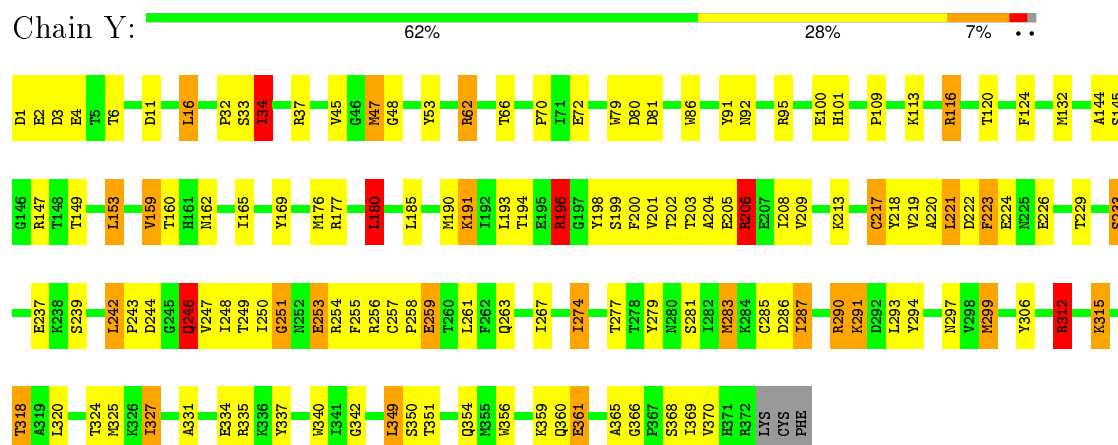
• Molecule 4: SKELETAL MUSCLE ACTIN



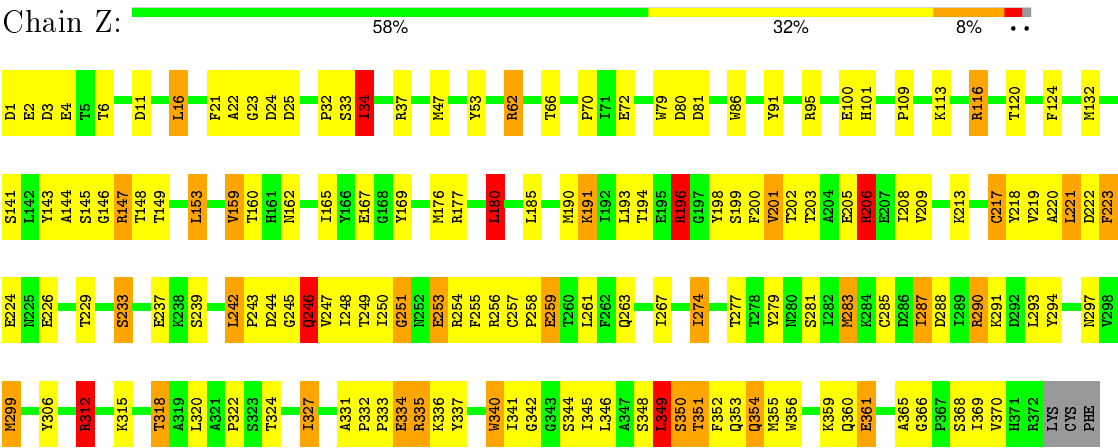
• Molecule 4: SKELETAL MUSCLE ACTIN



• Molecule 4: SKELETAL MUSCLE ACTIN



• Molecule 4: SKELETAL MUSCLE ACTIN



4 Experimental information

Property	Value	Source
Reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	Not provided	Depositor
Voltage (kV)	Not provided	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	KODAK S0163 FILM	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MLY

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
1	A	1.77	69/6448 (1.1%)	1.82	116/8729 (1.3%)
1	D	1.77	64/6448 (1.0%)	1.82	114/8729 (1.3%)
1	G	1.77	67/6449 (1.0%)	1.83	118/8732 (1.4%)
1	J	1.78	68/6449 (1.1%)	1.87	118/8732 (1.4%)
1	M	1.79	70/6447 (1.1%)	1.91	120/8726 (1.4%)
1	P	1.78	69/6448 (1.1%)	1.92	125/8729 (1.4%)
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	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	0.80	0/1136	0.95	4/1525 (0.3%)
3	O	0.79	0/1136	0.95	4/1525 (0.3%)
3	R	0.80	1/1136 (0.1%)	0.94	4/1525 (0.3%)
4	1	0.89	2/2968 (0.1%)	1.64	52/4023 (1.3%)
4	2	0.89	2/2968 (0.1%)	1.64	52/4023 (1.3%)
4	3	0.89	2/2968 (0.1%)	1.64	51/4023 (1.3%)
4	4	0.89	2/2968 (0.1%)	1.64	51/4023 (1.3%)
4	5	0.89	2/2968 (0.1%)	1.64	52/4023 (1.3%)
4	6	0.89	2/2968 (0.1%)	1.64	51/4023 (1.3%)
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	50/4023 (1.2%)
4	V	0.89	2/2968 (0.1%)	1.64	51/4023 (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	52/4023 (1.3%)
4	Z	0.89	2/2968 (0.1%)	1.64	51/4023 (1.3%)
All	All	1.35	486/91661 (0.5%)	1.70	1528/124064 (1.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	4
1	D	1	4
1	G	2	4
1	J	1	6
1	M	1	7
1	P	1	8
2	E	0	3
2	H	0	3
2	K	0	3
2	N	0	3
2	Q	0	3
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	7	72

The worst 5 of 486 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	649	VAL	CB-CG1	53.35	2.64	1.52
1	M	649	VAL	CB-CG1	53.33	2.64	1.52
1	P	649	VAL	CB-CG1	53.30	2.64	1.52
1	J	649	VAL	CB-CG1	53.28	2.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	649	VAL	CB-CG1	53.24	2.64	1.52

The worst 5 of 1528 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	637	LYS	O-C-N	-58.53	23.70	123.20
1	M	637	LYS	O-C-N	-58.50	23.75	123.20
1	A	637	LYS	O-C-N	-58.48	23.79	123.20
1	D	637	LYS	O-C-N	-58.48	23.79	123.20
1	J	637	LYS	O-C-N	-58.47	23.81	123.20

5 of 7 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 72 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
1	D	98	HIS	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	6760	1300	14
1	D	6797	0	6758	1469	25
1	G	6797	0	6764	1552	0
1	J	6797	0	6761	1442	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	M	6797	0	6767	1465	0
1	P	6797	0	6765	1500	0
2	E	1127	0	1086	259	0
2	H	1127	0	1088	273	0
2	K	1127	0	1088	284	0
2	N	1127	0	1089	283	0
2	Q	1127	0	1089	287	0
3	F	1123	0	1084	191	0
3	I	1123	0	1082	210	0
3	L	1123	0	1082	164	0
3	O	1123	0	1084	193	0
3	R	1123	0	1083	201	0
4	1	2906	0	2856	417	0
4	2	2906	0	2861	253	65
4	3	2906	0	2863	169	563
4	4	2906	0	2863	182	3212
4	5	2906	0	2865	94	3078
4	6	2906	0	2865	96	3458
4	7	2906	0	2866	78	3207
4	8	2906	0	2857	313	3137
4	9	2906	0	2855	349	3521
4	V	2906	0	2851	380	380
4	W	2906	0	2851	395	92
4	X	2906	0	2862	210	0
4	Y	2906	0	2863	189	0
4	Z	2906	0	2853	424	0
All	All	92716	0	91461	10967	10376

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 60.

The worst 5 of 10967 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:A:757:GLN:HB3	1:A:771:LEU:CD1	1.23	1.67
4:2:287:ILE:CG2	4:4:202:THR:HB	1.23	1.66
1:A:505:MLY:HB3	1:A:762:HIS:CD2	1.28	1.64
2:E:144:VAL:HG13	2:E:153:ILE:CG1	1.17	1.64
2:H:144:VAL:HG13	2:H:153:ILE:CD1	1.22	1.64

The worst 5 of 10376 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)
4:6:109:PRO:C	4:V:195:GLU:OE2[1_554]	0.13	2.07
4:4:16:LEU:CA	4:7:77:THR:C[1_554]	0.13	2.07
4:6:347:ALA:C	4:9:366:GLY:CA[1_554]	0.13	2.07
4:6:288:ASP:CB	4:W:62:ARG:O[1_554]	0.14	2.06
4:5:299:MET:CE	4:8:136:ILE:O[1_554]	0.15	2.05

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	789/840 (94%)	650 (82%)	113 (14%)	26 (3%)	5	40
1	D	789/840 (94%)	650 (82%)	113 (14%)	26 (3%)	5	40
1	G	791/840 (94%)	651 (82%)	113 (14%)	27 (3%)	5	40
1	J	791/840 (94%)	651 (82%)	113 (14%)	27 (3%)	5	40
1	M	787/840 (94%)	648 (82%)	110 (14%)	29 (4%)	4	38
1	P	789/840 (94%)	650 (82%)	112 (14%)	27 (3%)	5	40
2	E	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	2	28
2	H	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	2	28
2	K	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	2	28
2	N	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	2	28
2	Q	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	2	28
3	F	143/147 (97%)	133 (93%)	10 (7%)	0	100	100
3	I	143/147 (97%)	133 (93%)	10 (7%)	0	100	100
3	L	143/147 (97%)	133 (93%)	10 (7%)	0	100	100
3	O	143/147 (97%)	133 (93%)	10 (7%)	0	100	100
3	R	143/147 (97%)	133 (93%)	10 (7%)	0	100	100
4	1	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	12	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	2	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	12	56
4	3	370/375 (99%)	333 (90%)	31 (8%)	6 (2%)	12	56
4	4	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	12	56
4	5	370/375 (99%)	333 (90%)	31 (8%)	6 (2%)	12	56
4	6	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	12	56
4	7	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	12	56
4	8	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	12	56
4	9	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	12	56
4	V	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	12	56
4	W	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	12	56
4	X	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	12	56
4	Y	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	12	56
4	Z	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	12	56
All	All	11346/11750 (97%)	9872 (87%)	1188 (10%)	286 (2%)	11	46

5 of 286 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	LYS
1	A	202	SER
1	A	572	LYS
1	A	712	PRO
1	A	729	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	672/672 (100%)	512 (76%)	160 (24%)	1	7
1	D	672/672 (100%)	513 (76%)	159 (24%)	1	7
1	G	672/672 (100%)	514 (76%)	158 (24%)	1	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	672/672 (100%)	514 (76%)	158 (24%)	1	7
1	M	672/672 (100%)	514 (76%)	158 (24%)	1	7
1	P	672/672 (100%)	515 (77%)	157 (23%)	1	7
2	E	120/120 (100%)	119 (99%)	1 (1%)	86	94
2	H	120/120 (100%)	119 (99%)	1 (1%)	86	94
2	K	120/120 (100%)	119 (99%)	1 (1%)	86	94
2	N	120/120 (100%)	119 (99%)	1 (1%)	86	94
2	Q	120/120 (100%)	119 (99%)	1 (1%)	86	94
3	F	117/117 (100%)	112 (96%)	5 (4%)	35	70
3	I	117/117 (100%)	112 (96%)	5 (4%)	35	70
3	L	117/117 (100%)	112 (96%)	5 (4%)	35	70
3	O	117/117 (100%)	112 (96%)	5 (4%)	35	70
3	R	117/117 (100%)	112 (96%)	5 (4%)	35	70
4	1	315/318 (99%)	268 (85%)	47 (15%)	4	23
4	2	315/318 (99%)	268 (85%)	47 (15%)	4	23
4	3	315/318 (99%)	269 (85%)	46 (15%)	4	24
4	4	315/318 (99%)	269 (85%)	46 (15%)	4	24
4	5	315/318 (99%)	269 (85%)	46 (15%)	4	24
4	6	315/318 (99%)	269 (85%)	46 (15%)	4	24
4	7	315/318 (99%)	269 (85%)	46 (15%)	4	24
4	8	315/318 (99%)	269 (85%)	46 (15%)	4	24
4	9	315/318 (99%)	269 (85%)	46 (15%)	4	24
4	V	315/318 (99%)	269 (85%)	46 (15%)	4	24
4	W	315/318 (99%)	269 (85%)	46 (15%)	4	24
4	X	315/318 (99%)	268 (85%)	47 (15%)	4	23
4	Y	315/318 (99%)	268 (85%)	47 (15%)	4	23
4	Z	315/318 (99%)	268 (85%)	47 (15%)	4	23
All	All	9627/9669 (100%)	7998 (83%)	1629 (17%)	6	18

5 of 1629 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	448	GLN

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Mol	Chain	Res	Type
1	P	506	GLU
4	X	201	VAL
1	M	562	SER
1	P	61	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 236 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	188	ASN
1	P	149	GLN
4	W	263	GLN
1	M	253	HIS
1	M	564	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	MLY	A	107	1	8,10,11	0.45	0	9,11,13	0.67	0
1	MLY	A	130	1	8,10,11	0.59	0	9,11,13	1.07	1 (11%)
1	MLY	A	138	1	8,10,11	1.36	1 (12%)	9,11,13	0.80	0
1	MLY	A	19	1	8,10,11	1.13	1 (12%)	9,11,13	0.68	0
1	MLY	A	190	1	8,10,11	1.10	1 (12%)	9,11,13	0.70	0
1	MLY	A	236	1	8,10,11	0.38	0	9,11,13	1.34	1 (11%)
1	MLY	A	248	1	8,10,11	0.72	0	9,11,13	0.92	1 (11%)
1	MLY	A	272	1	8,10,11	1.01	1 (12%)	9,11,13	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	A	295	1	8,10,11	0.73	0	9,11,13	0.47	0
1	MLY	A	296	1	8,10,11	0.58	0	9,11,13	0.76	0
1	MLY	A	30	1	8,10,11	0.68	0	9,11,13	0.82	0
1	MLY	A	348	1	8,10,11	0.82	0	9,11,13	0.81	0
1	MLY	A	35	1	8,10,11	0.58	0	9,11,13	0.69	0
1	MLY	A	353	1	8,10,11	0.89	0	9,11,13	0.80	0
1	MLY	A	367	1	8,10,11	0.64	0	9,11,13	0.60	0
1	MLY	A	369	1	8,10,11	0.55	0	9,11,13	0.92	1 (11%)
1	MLY	A	385	1	8,10,11	1.00	1 (12%)	9,11,13	0.55	0
1	MLY	A	415	1	8,10,11	0.75	0	9,11,13	0.44	0
1	MLY	A	431	1	8,10,11	0.46	0	9,11,13	0.76	0
1	MLY	A	436	1	8,10,11	1.09	1 (12%)	9,11,13	0.56	0
1	MLY	A	486	1	8,10,11	0.34	0	9,11,13	0.60	0
1	MLY	A	49	1	8,10,11	1.04	1 (12%)	9,11,13	0.98	0
1	MLY	A	504	1	8,10,11	0.82	0	9,11,13	0.48	0
1	MLY	A	505	1	8,10,11	0.89	1 (12%)	9,11,13	0.38	0
1	MLY	A	528	1	8,10,11	0.81	0	9,11,13	1.16	1 (11%)
1	MLY	A	55	1	8,10,11	0.66	0	9,11,13	0.97	0
1	MLY	A	551	1	8,10,11	0.51	0	9,11,13	0.65	0
1	MLY	A	553	1,4	8,10,11	0.65	0	9,11,13	0.60	0
1	MLY	A	59	1	8,10,11	0.77	0	9,11,13	0.76	0
1	MLY	A	598	1	8,10,11	0.87	1 (12%)	9,11,13	0.73	0
1	MLY	A	600	1	8,10,11	0.50	0	9,11,13	0.48	0
1	MLY	A	613	1	8,10,11	0.52	0	9,11,13	0.91	0
1	MLY	A	617	1	8,10,11	0.89	1 (12%)	9,11,13	0.46	0
1	MLY	A	63	1	8,10,11	0.80	0	9,11,13	0.94	0
1	MLY	A	659	1	8,10,11	0.55	0	9,11,13	0.94	0
1	MLY	A	681	1	8,10,11	0.63	0	9,11,13	0.63	0
1	MLY	A	764	1	8,10,11	0.67	0	9,11,13	0.55	0
1	MLY	A	768	1	8,10,11	0.65	0	9,11,13	0.85	0
1	MLY	A	782	1	8,10,11	0.51	0	9,11,13	0.93	1 (11%)
1	MLY	A	827	1	8,10,11	0.68	0	9,11,13	0.95	1 (11%)
1	MLY	A	833	1	8,10,11	0.95	1 (12%)	9,11,13	0.58	0
1	MLY	A	837	1	8,10,11	0.58	0	9,11,13	0.57	0
1	MLY	A	839	1	8,10,11	0.66	0	9,11,13	0.79	0
1	MLY	A	84	1	8,10,11	0.46	0	9,11,13	0.80	0
1	MLY	A	87	1	8,10,11	1.15	1 (12%)	9,11,13	0.68	0
1	MLY	D	107	1	8,10,11	0.47	0	9,11,13	0.67	0
1	MLY	D	130	1	8,10,11	0.55	0	9,11,13	1.06	1 (11%)
1	MLY	D	138	1	8,10,11	1.38	1 (12%)	9,11,13	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	D	19	1	8,10,11	1.20	1 (12%)	9,11,13	0.70	0
1	MLY	D	190	1	8,10,11	1.05	1 (12%)	9,11,13	0.70	0
1	MLY	D	236	1	8,10,11	0.37	0	9,11,13	1.31	1 (11%)
1	MLY	D	248	1	8,10,11	0.73	0	9,11,13	0.92	1 (11%)
1	MLY	D	272	1	8,10,11	0.97	1 (12%)	9,11,13	0.57	0
1	MLY	D	295	1	8,10,11	0.69	0	9,11,13	0.48	0
1	MLY	D	296	1	8,10,11	0.62	0	9,11,13	0.77	0
1	MLY	D	30	1	8,10,11	0.72	0	9,11,13	0.84	1 (11%)
1	MLY	D	348	1	8,10,11	0.75	0	9,11,13	0.81	0
1	MLY	D	35	1	8,10,11	0.60	0	9,11,13	0.67	0
1	MLY	D	353	1	8,10,11	0.86	0	9,11,13	0.78	0
1	MLY	D	367	1	8,10,11	0.64	0	9,11,13	0.60	0
1	MLY	D	369	1	8,10,11	0.54	0	9,11,13	0.91	1 (11%)
1	MLY	D	385	1	8,10,11	0.98	1 (12%)	9,11,13	0.56	0
1	MLY	D	415	1	8,10,11	0.77	0	9,11,13	0.46	0
1	MLY	D	431	1	8,10,11	0.49	0	9,11,13	0.77	0
1	MLY	D	436	1	8,10,11	1.14	1 (12%)	9,11,13	0.57	0
1	MLY	D	486	1	8,10,11	0.35	0	9,11,13	0.61	0
1	MLY	D	49	1	8,10,11	1.07	1 (12%)	9,11,13	0.99	0
1	MLY	D	504	1	8,10,11	0.81	0	9,11,13	0.48	0
1	MLY	D	505	1	8,10,11	0.85	1 (12%)	9,11,13	0.39	0
1	MLY	D	528	1	8,10,11	0.82	0	9,11,13	1.16	1 (11%)
1	MLY	D	55	1	8,10,11	0.66	0	9,11,13	0.98	0
1	MLY	D	551	1	8,10,11	0.52	0	9,11,13	0.65	0
1	MLY	D	553	1,4	8,10,11	0.63	0	9,11,13	0.59	0
1	MLY	D	59	1	8,10,11	0.80	0	9,11,13	0.78	0
1	MLY	D	598	1	8,10,11	0.86	1 (12%)	9,11,13	0.69	0
1	MLY	D	600	1	8,10,11	0.51	0	9,11,13	0.47	0
1	MLY	D	613	1	8,10,11	0.51	0	9,11,13	0.91	0
1	MLY	D	617	1	8,10,11	0.91	1 (12%)	9,11,13	0.47	0
1	MLY	D	63	1	8,10,11	0.79	0	9,11,13	0.95	0
1	MLY	D	659	1	8,10,11	0.56	0	9,11,13	0.94	0
1	MLY	D	681	1	8,10,11	0.61	0	9,11,13	0.65	0
1	MLY	D	764	1	8,10,11	0.63	0	9,11,13	0.56	0
1	MLY	D	768	1	8,10,11	0.64	0	9,11,13	0.87	0
1	MLY	D	782	1	8,10,11	0.49	0	9,11,13	0.92	1 (11%)
1	MLY	D	827	1	8,10,11	0.64	0	9,11,13	0.96	1 (11%)
1	MLY	D	833	1	8,10,11	0.94	1 (12%)	9,11,13	0.59	0
1	MLY	D	837	1	8,10,11	0.55	0	9,11,13	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	D	839	1	8,10,11	0.67	0	9,11,13	0.78	0
1	MLY	D	84	1	8,10,11	0.46	0	9,11,13	0.79	0
1	MLY	D	87	1	8,10,11	1.12	1 (12%)	9,11,13	0.69	0
1	MLY	G	107	1	8,10,11	0.45	0	9,11,13	0.66	0
1	MLY	G	130	1	8,10,11	0.62	0	9,11,13	1.08	1 (11%)
1	MLY	G	138	1	8,10,11	1.34	1 (12%)	9,11,13	0.80	0
1	MLY	G	19	1	8,10,11	1.16	1 (12%)	9,11,13	0.70	0
1	MLY	G	190	1	8,10,11	1.09	1 (12%)	9,11,13	0.69	0
1	MLY	G	236	1	8,10,11	0.38	0	9,11,13	1.32	1 (11%)
1	MLY	G	248	1	8,10,11	0.71	0	9,11,13	0.94	1 (11%)
1	MLY	G	272	1	8,10,11	0.99	1 (12%)	9,11,13	0.56	0
1	MLY	G	295	1	8,10,11	0.72	0	9,11,13	0.47	0
1	MLY	G	296	1	8,10,11	0.58	0	9,11,13	0.77	0
1	MLY	G	30	1	8,10,11	0.68	0	9,11,13	0.83	1 (11%)
1	MLY	G	348	1	8,10,11	0.80	0	9,11,13	0.82	0
1	MLY	G	35	1	8,10,11	0.58	0	9,11,13	0.67	0
1	MLY	G	353	1	8,10,11	0.89	0	9,11,13	0.79	0
1	MLY	G	367	1	8,10,11	0.65	0	9,11,13	0.62	0
1	MLY	G	369	1	8,10,11	0.54	0	9,11,13	0.93	1 (11%)
1	MLY	G	385	1	8,10,11	1.02	1 (12%)	9,11,13	0.55	0
1	MLY	G	415	1	8,10,11	0.77	0	9,11,13	0.42	0
1	MLY	G	431	1	8,10,11	0.46	0	9,11,13	0.77	0
1	MLY	G	436	1	8,10,11	1.09	1 (12%)	9,11,13	0.56	0
1	MLY	G	486	1	8,10,11	0.34	0	9,11,13	0.60	0
1	MLY	G	49	1	8,10,11	1.07	1 (12%)	9,11,13	0.98	0
1	MLY	G	504	1	8,10,11	0.77	0	9,11,13	0.48	0
1	MLY	G	505	1	8,10,11	0.88	1 (12%)	9,11,13	0.41	0
1	MLY	G	528	1	8,10,11	0.81	0	9,11,13	1.17	1 (11%)
1	MLY	G	55	1	8,10,11	0.68	0	9,11,13	0.99	0
1	MLY	G	551	1	8,10,11	0.52	0	9,11,13	0.66	0
1	MLY	G	553	1,4	8,10,11	0.63	0	9,11,13	0.58	0
1	MLY	G	59	1	8,10,11	0.74	0	9,11,13	0.77	0
1	MLY	G	598	1	8,10,11	0.84	1 (12%)	9,11,13	0.71	0
1	MLY	G	600	1	8,10,11	0.51	0	9,11,13	0.46	0
1	MLY	G	613	1	8,10,11	0.54	0	9,11,13	0.92	0
1	MLY	G	617	1	8,10,11	0.88	1 (12%)	9,11,13	0.45	0
1	MLY	G	63	1	8,10,11	0.79	0	9,11,13	0.94	0
1	MLY	G	659	1	8,10,11	0.57	0	9,11,13	0.94	0
1	MLY	G	681	1	8,10,11	0.68	0	9,11,13	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	G	764	1	8,10,11	0.62	0	9,11,13	0.57	0
1	MLY	G	768	1	8,10,11	0.63	0	9,11,13	0.88	0
1	MLY	G	782	1	8,10,11	0.47	0	9,11,13	0.92	1 (11%)
1	MLY	G	827	1	8,10,11	0.67	0	9,11,13	0.96	1 (11%)
1	MLY	G	833	1	8,10,11	0.96	1 (12%)	9,11,13	0.60	0
1	MLY	G	837	1	8,10,11	0.53	0	9,11,13	0.56	0
1	MLY	G	839	1	8,10,11	0.67	0	9,11,13	0.77	0
1	MLY	G	84	1	8,10,11	0.46	0	9,11,13	0.80	0
1	MLY	G	87	1	8,10,11	1.17	1 (12%)	9,11,13	0.68	0
1	MLY	J	107	1	8,10,11	0.47	0	9,11,13	0.68	0
1	MLY	J	130	1	8,10,11	0.56	0	9,11,13	1.06	1 (11%)
1	MLY	J	138	1	8,10,11	1.32	1 (12%)	9,11,13	0.79	0
1	MLY	J	19	1	8,10,11	1.19	1 (12%)	9,11,13	0.71	0
1	MLY	J	190	1	8,10,11	1.09	1 (12%)	9,11,13	0.69	0
1	MLY	J	236	1	8,10,11	0.39	0	9,11,13	1.32	1 (11%)
1	MLY	J	248	1	8,10,11	0.72	0	9,11,13	0.94	1 (11%)
1	MLY	J	272	1	8,10,11	1.03	1 (12%)	9,11,13	0.57	0
1	MLY	J	295	1	8,10,11	0.67	0	9,11,13	0.48	0
1	MLY	J	296	1	8,10,11	0.66	0	9,11,13	0.78	1 (11%)
1	MLY	J	30	1	8,10,11	0.69	0	9,11,13	0.83	1 (11%)
1	MLY	J	348	1	8,10,11	0.79	0	9,11,13	0.81	0
1	MLY	J	35	1	8,10,11	0.60	0	9,11,13	0.67	0
1	MLY	J	353	1	8,10,11	0.87	0	9,11,13	0.78	0
1	MLY	J	367	1	8,10,11	0.65	0	9,11,13	0.61	0
1	MLY	J	369	1	8,10,11	0.54	0	9,11,13	0.93	1 (11%)
1	MLY	J	385	1	8,10,11	1.03	1 (12%)	9,11,13	0.54	0
1	MLY	J	415	1	8,10,11	0.79	0	9,11,13	0.44	0
1	MLY	J	431	1	8,10,11	0.45	0	9,11,13	0.77	0
1	MLY	J	436	1	8,10,11	1.08	1 (12%)	9,11,13	0.56	0
1	MLY	J	486	1	8,10,11	0.33	0	9,11,13	0.60	0
1	MLY	J	49	1	8,10,11	1.09	1 (12%)	9,11,13	1.01	1 (11%)
1	MLY	J	504	1	8,10,11	0.74	0	9,11,13	0.49	0
1	MLY	J	505	1	8,10,11	0.93	1 (12%)	9,11,13	0.38	0
1	MLY	J	528	1	8,10,11	0.80	0	9,11,13	1.15	1 (11%)
1	MLY	J	55	1	8,10,11	0.67	0	9,11,13	0.98	0
1	MLY	J	551	1	8,10,11	0.51	0	9,11,13	0.66	0
1	MLY	J	553	1	8,10,11	0.60	0	9,11,13	0.59	0
1	MLY	J	59	1	8,10,11	0.78	0	9,11,13	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	J	598	1	8,10,11	0.85	1 (12%)	9,11,13	0.70	0
1	MLY	J	600	1	8,10,11	0.52	0	9,11,13	0.48	0
1	MLY	J	613	1	8,10,11	0.51	0	9,11,13	0.93	0
1	MLY	J	617	1	8,10,11	0.92	1 (12%)	9,11,13	0.46	0
1	MLY	J	63	1	8,10,11	0.77	0	9,11,13	0.95	0
1	MLY	J	659	1	8,10,11	0.53	0	9,11,13	0.93	0
1	MLY	J	681	1	8,10,11	0.62	0	9,11,13	0.63	0
1	MLY	J	764	1	8,10,11	0.63	0	9,11,13	0.58	0
1	MLY	J	768	1	8,10,11	0.66	0	9,11,13	0.87	0
1	MLY	J	782	1	8,10,11	0.51	0	9,11,13	0.94	1 (11%)
1	MLY	J	827	1	8,10,11	0.68	0	9,11,13	0.94	1 (11%)
1	MLY	J	833	1	8,10,11	1.03	1 (12%)	9,11,13	0.58	0
1	MLY	J	837	1	8,10,11	0.54	0	9,11,13	0.59	0
1	MLY	J	839	1	8,10,11	0.70	0	9,11,13	0.76	0
1	MLY	J	84	1	8,10,11	0.45	0	9,11,13	0.79	0
1	MLY	J	87	1	8,10,11	1.16	1 (12%)	9,11,13	0.69	0
1	MLY	M	107	1	8,10,11	0.46	0	9,11,13	0.67	0
1	MLY	M	130	1	8,10,11	0.57	0	9,11,13	1.05	1 (11%)
1	MLY	M	138	1	8,10,11	1.36	1 (12%)	9,11,13	0.80	0
1	MLY	M	19	1	8,10,11	1.20	1 (12%)	9,11,13	0.71	0
1	MLY	M	190	1	8,10,11	1.10	1 (12%)	9,11,13	0.70	0
1	MLY	M	236	1	8,10,11	0.39	0	9,11,13	1.31	1 (11%)
1	MLY	M	248	1	8,10,11	0.72	0	9,11,13	0.94	1 (11%)
1	MLY	M	272	1	8,10,11	1.05	1 (12%)	9,11,13	0.57	0
1	MLY	M	295	1	8,10,11	0.68	0	9,11,13	0.48	0
1	MLY	M	296	1	8,10,11	0.66	0	9,11,13	0.77	1 (11%)
1	MLY	M	30	1	8,10,11	0.71	0	9,11,13	0.83	0
1	MLY	M	348	1	8,10,11	0.77	0	9,11,13	0.80	0
1	MLY	M	35	1	8,10,11	0.59	0	9,11,13	0.67	0
1	MLY	M	353	1	8,10,11	0.87	0	9,11,13	0.79	0
1	MLY	M	367	1	8,10,11	0.64	0	9,11,13	0.60	0
1	MLY	M	369	1	8,10,11	0.54	0	9,11,13	0.92	1 (11%)
1	MLY	M	385	1	8,10,11	1.02	1 (12%)	9,11,13	0.54	0
1	MLY	M	415	1	8,10,11	0.80	0	9,11,13	0.45	0
1	MLY	M	431	1	8,10,11	0.45	0	9,11,13	0.77	0
1	MLY	M	436	1	8,10,11	1.09	1 (12%)	9,11,13	0.55	0
1	MLY	M	486	1	8,10,11	0.34	0	9,11,13	0.60	0
1	MLY	M	49	1	8,10,11	1.07	1 (12%)	9,11,13	0.99	0
1	MLY	M	504	1	8,10,11	0.76	0	9,11,13	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	M	505	1	8,10,11	0.90	1 (12%)	9,11,13	0.38	0
1	MLY	M	528	1	8,10,11	0.83	0	9,11,13	1.15	1 (11%)
1	MLY	M	55	1	8,10,11	0.66	0	9,11,13	0.98	0
1	MLY	M	551	1	8,10,11	0.51	0	9,11,13	0.67	0
1	MLY	M	553	1	8,10,11	0.62	0	9,11,13	0.58	0
1	MLY	M	59	1	8,10,11	0.78	0	9,11,13	0.77	0
1	MLY	M	598	1	8,10,11	0.86	1 (12%)	9,11,13	0.71	0
1	MLY	M	600	1	8,10,11	0.51	0	9,11,13	0.47	0
1	MLY	M	613	1	8,10,11	0.50	0	9,11,13	0.94	0
1	MLY	M	617	1	8,10,11	0.93	1 (12%)	9,11,13	0.45	0
1	MLY	M	63	1	8,10,11	0.80	0	9,11,13	0.95	0
1	MLY	M	659	1	8,10,11	0.54	0	9,11,13	0.93	0
1	MLY	M	681	1	8,10,11	0.63	0	9,11,13	0.64	0
1	MLY	M	764	1	8,10,11	0.65	0	9,11,13	0.58	0
1	MLY	M	768	1	8,10,11	0.65	0	9,11,13	0.87	0
1	MLY	M	782	1	8,10,11	0.51	0	9,11,13	0.95	1 (11%)
1	MLY	M	827	1	8,10,11	0.65	0	9,11,13	0.94	1 (11%)
1	MLY	M	833	1	8,10,11	1.02	1 (12%)	9,11,13	0.57	0
1	MLY	M	837	1	8,10,11	0.55	0	9,11,13	0.58	0
1	MLY	M	839	1	8,10,11	0.72	0	9,11,13	0.76	0
1	MLY	M	84	1	8,10,11	0.46	0	9,11,13	0.80	0
1	MLY	M	87	1	8,10,11	1.16	1 (12%)	9,11,13	0.69	0
1	MLY	P	107	1	8,10,11	0.46	0	9,11,13	0.66	0
1	MLY	P	130	1	8,10,11	0.56	0	9,11,13	1.06	1 (11%)
1	MLY	P	138	1	8,10,11	1.35	1 (12%)	9,11,13	0.79	0
1	MLY	P	19	1	8,10,11	1.21	1 (12%)	9,11,13	0.70	0
1	MLY	P	190	1	8,10,11	1.11	1 (12%)	9,11,13	0.70	0
1	MLY	P	236	1	8,10,11	0.39	0	9,11,13	1.32	1 (11%)
1	MLY	P	248	1	8,10,11	0.74	0	9,11,13	0.93	1 (11%)
1	MLY	P	272	1	8,10,11	1.03	1 (12%)	9,11,13	0.57	0
1	MLY	P	295	1	8,10,11	0.70	0	9,11,13	0.47	0
1	MLY	P	296	1	8,10,11	0.63	0	9,11,13	0.77	0
1	MLY	P	30	1	8,10,11	0.69	0	9,11,13	0.82	0
1	MLY	P	348	1	8,10,11	0.78	0	9,11,13	0.81	0
1	MLY	P	35	1	8,10,11	0.59	0	9,11,13	0.67	0
1	MLY	P	353	1	8,10,11	0.87	0	9,11,13	0.78	0
1	MLY	P	367	1	8,10,11	0.64	0	9,11,13	0.61	0
1	MLY	P	369	1	8,10,11	0.53	0	9,11,13	0.92	1 (11%)
1	MLY	P	385	1	8,10,11	1.00	1 (12%)	9,11,13	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	P	415	1	8,10,11	0.76	0	9,11,13	0.43	0
1	MLY	P	431	1	8,10,11	0.47	0	9,11,13	0.78	0
1	MLY	P	436	1	8,10,11	1.09	1 (12%)	9,11,13	0.56	0
1	MLY	P	486	1	8,10,11	0.32	0	9,11,13	0.61	0
1	MLY	P	49	1	8,10,11	1.10	1 (12%)	9,11,13	1.01	1 (11%)
1	MLY	P	504	1	8,10,11	0.75	0	9,11,13	0.49	0
1	MLY	P	505	1	8,10,11	0.92	1 (12%)	9,11,13	0.37	0
1	MLY	P	528	1	8,10,11	0.82	0	9,11,13	1.16	1 (11%)
1	MLY	P	55	1	8,10,11	0.67	0	9,11,13	0.99	0
1	MLY	P	551	1	8,10,11	0.50	0	9,11,13	0.65	0
1	MLY	P	553	1	8,10,11	0.62	0	9,11,13	0.58	0
1	MLY	P	59	1	8,10,11	0.76	0	9,11,13	0.77	0
1	MLY	P	598	1	8,10,11	0.85	1 (12%)	9,11,13	0.71	0
1	MLY	P	600	1	8,10,11	0.53	0	9,11,13	0.48	0
1	MLY	P	613	1	8,10,11	0.50	0	9,11,13	0.93	0
1	MLY	P	617	1	8,10,11	0.92	1 (12%)	9,11,13	0.46	0
1	MLY	P	63	1	8,10,11	0.76	0	9,11,13	0.94	0
1	MLY	P	659	1	8,10,11	0.55	0	9,11,13	0.93	0
1	MLY	P	681	1	8,10,11	0.64	0	9,11,13	0.65	0
1	MLY	P	764	1	8,10,11	0.65	0	9,11,13	0.59	0
1	MLY	P	768	1	8,10,11	0.65	0	9,11,13	0.86	0
1	MLY	P	782	1	8,10,11	0.52	0	9,11,13	0.95	1 (11%)
1	MLY	P	827	1	8,10,11	0.64	0	9,11,13	0.94	1 (11%)
1	MLY	P	833	1	8,10,11	1.02	1 (12%)	9,11,13	0.57	0
1	MLY	P	837	1	8,10,11	0.52	0	9,11,13	0.58	0
1	MLY	P	839	1	8,10,11	0.71	0	9,11,13	0.78	0
1	MLY	P	84	1	8,10,11	0.46	0	9,11,13	0.79	0
1	MLY	P	87	1	8,10,11	1.18	1 (12%)	9,11,13	0.68	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	A	107	1	-	0/7/9/11	0/0/0/0
1	MLY	A	130	1	-	0/7/9/11	0/0/0/0
1	MLY	A	138	1	-	0/7/9/11	0/0/0/0
1	MLY	A	19	1	-	0/7/9/11	0/0/0/0
1	MLY	A	190	1	-	0/7/9/11	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	A	236	1	-	0/7/9/11	0/0/0/0
1	MLY	A	248	1	-	0/7/9/11	0/0/0/0
1	MLY	A	272	1	-	0/7/9/11	0/0/0/0
1	MLY	A	295	1	-	0/7/9/11	0/0/0/0
1	MLY	A	296	1	-	0/7/9/11	0/0/0/0
1	MLY	A	30	1	-	0/7/9/11	0/0/0/0
1	MLY	A	348	1	-	0/7/9/11	0/0/0/0
1	MLY	A	35	1	-	0/7/9/11	0/0/0/0
1	MLY	A	353	1	-	0/7/9/11	0/0/0/0
1	MLY	A	367	1	-	0/7/9/11	0/0/0/0
1	MLY	A	369	1	-	0/7/9/11	0/0/0/0
1	MLY	A	385	1	-	0/7/9/11	0/0/0/0
1	MLY	A	415	1	-	0/7/9/11	0/0/0/0
1	MLY	A	431	1	-	0/7/9/11	0/0/0/0
1	MLY	A	436	1	-	0/7/9/11	0/0/0/0
1	MLY	A	486	1	-	0/7/9/11	0/0/0/0
1	MLY	A	49	1	-	0/7/9/11	0/0/0/0
1	MLY	A	504	1	-	0/7/9/11	0/0/0/0
1	MLY	A	505	1	-	0/7/9/11	0/0/0/0
1	MLY	A	528	1	-	0/7/9/11	0/0/0/0
1	MLY	A	55	1	-	0/7/9/11	0/0/0/0
1	MLY	A	551	1	-	0/7/9/11	0/0/0/0
1	MLY	A	553	1,4	-	0/7/9/11	0/0/0/0
1	MLY	A	59	1	-	0/7/9/11	0/0/0/0
1	MLY	A	598	1	-	0/7/9/11	0/0/0/0
1	MLY	A	600	1	-	0/7/9/11	0/0/0/0
1	MLY	A	613	1	-	0/7/9/11	0/0/0/0
1	MLY	A	617	1	-	0/7/9/11	0/0/0/0
1	MLY	A	63	1	-	0/7/9/11	0/0/0/0
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	D	138	1	-	0/7/9/11	0/0/0/0
1	MLY	D	19	1	-	0/7/9/11	0/0/0/0
1	MLY	D	190	1	-	0/7/9/11	0/0/0/0
1	MLY	D	236	1	-	0/7/9/11	0/0/0/0
1	MLY	D	248	1	-	0/7/9/11	0/0/0/0
1	MLY	D	272	1	-	0/7/9/11	0/0/0/0
1	MLY	D	295	1	-	0/7/9/11	0/0/0/0
1	MLY	D	296	1	-	0/7/9/11	0/0/0/0
1	MLY	D	30	1	-	0/7/9/11	0/0/0/0
1	MLY	D	348	1	-	0/7/9/11	0/0/0/0
1	MLY	D	35	1	-	0/7/9/11	0/0/0/0
1	MLY	D	353	1	-	0/7/9/11	0/0/0/0
1	MLY	D	367	1	-	0/7/9/11	0/0/0/0
1	MLY	D	369	1	-	0/7/9/11	0/0/0/0
1	MLY	D	385	1	-	0/7/9/11	0/0/0/0
1	MLY	D	415	1	-	0/7/9/11	0/0/0/0
1	MLY	D	431	1	-	0/7/9/11	0/0/0/0
1	MLY	D	436	1	-	0/7/9/11	0/0/0/0
1	MLY	D	486	1	-	0/7/9/11	0/0/0/0
1	MLY	D	49	1	-	0/7/9/11	0/0/0/0
1	MLY	D	504	1	-	0/7/9/11	0/0/0/0
1	MLY	D	505	1	-	0/7/9/11	0/0/0/0
1	MLY	D	528	1	-	0/7/9/11	0/0/0/0
1	MLY	D	55	1	-	0/7/9/11	0/0/0/0
1	MLY	D	551	1	-	0/7/9/11	0/0/0/0
1	MLY	D	553	1,4	-	0/7/9/11	0/0/0/0
1	MLY	D	59	1	-	0/7/9/11	0/0/0/0
1	MLY	D	598	1	-	0/7/9/11	0/0/0/0
1	MLY	D	600	1	-	0/7/9/11	0/0/0/0
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	D	87	1	-	0/7/9/11	0/0/0/0
1	MLY	G	107	1	-	0/7/9/11	0/0/0/0
1	MLY	G	130	1	-	0/7/9/11	0/0/0/0
1	MLY	G	138	1	-	0/7/9/11	0/0/0/0
1	MLY	G	19	1	-	0/7/9/11	0/0/0/0
1	MLY	G	190	1	-	0/7/9/11	0/0/0/0
1	MLY	G	236	1	-	0/7/9/11	0/0/0/0
1	MLY	G	248	1	-	0/7/9/11	0/0/0/0
1	MLY	G	272	1	-	0/7/9/11	0/0/0/0
1	MLY	G	295	1	-	0/7/9/11	0/0/0/0
1	MLY	G	296	1	-	0/7/9/11	0/0/0/0
1	MLY	G	30	1	-	0/7/9/11	0/0/0/0
1	MLY	G	348	1	-	0/7/9/11	0/0/0/0
1	MLY	G	35	1	-	0/7/9/11	0/0/0/0
1	MLY	G	353	1	-	0/7/9/11	0/0/0/0
1	MLY	G	367	1	-	0/7/9/11	0/0/0/0
1	MLY	G	369	1	-	0/7/9/11	0/0/0/0
1	MLY	G	385	1	-	0/7/9/11	0/0/0/0
1	MLY	G	415	1	-	0/7/9/11	0/0/0/0
1	MLY	G	431	1	-	0/7/9/11	0/0/0/0
1	MLY	G	436	1	-	0/7/9/11	0/0/0/0
1	MLY	G	486	1	-	0/7/9/11	0/0/0/0
1	MLY	G	49	1	-	0/7/9/11	0/0/0/0
1	MLY	G	504	1	-	0/7/9/11	0/0/0/0
1	MLY	G	505	1	-	0/7/9/11	0/0/0/0
1	MLY	G	528	1	-	0/7/9/11	0/0/0/0
1	MLY	G	55	1	-	0/7/9/11	0/0/0/0
1	MLY	G	551	1	-	0/7/9/11	0/0/0/0
1	MLY	G	553	1,4	-	0/7/9/11	0/0/0/0
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	G	837	1	-	0/7/9/11	0/0/0/0
1	MLY	G	839	1	-	0/7/9/11	0/0/0/0
1	MLY	G	84	1	-	0/7/9/11	0/0/0/0
1	MLY	G	87	1	-	0/7/9/11	0/0/0/0
1	MLY	J	107	1	-	0/7/9/11	0/0/0/0
1	MLY	J	130	1	-	0/7/9/11	0/0/0/0
1	MLY	J	138	1	-	0/7/9/11	0/0/0/0
1	MLY	J	19	1	-	0/7/9/11	0/0/0/0
1	MLY	J	190	1	-	0/7/9/11	0/0/0/0
1	MLY	J	236	1	-	0/7/9/11	0/0/0/0
1	MLY	J	248	1	-	0/7/9/11	0/0/0/0
1	MLY	J	272	1	-	0/7/9/11	0/0/0/0
1	MLY	J	295	1	-	0/7/9/11	0/0/0/0
1	MLY	J	296	1	-	0/7/9/11	0/0/0/0
1	MLY	J	30	1	-	0/7/9/11	0/0/0/0
1	MLY	J	348	1	-	0/7/9/11	0/0/0/0
1	MLY	J	35	1	-	0/7/9/11	0/0/0/0
1	MLY	J	353	1	-	0/7/9/11	0/0/0/0
1	MLY	J	367	1	-	0/7/9/11	0/0/0/0
1	MLY	J	369	1	-	0/7/9/11	0/0/0/0
1	MLY	J	385	1	-	0/7/9/11	0/0/0/0
1	MLY	J	415	1	-	0/7/9/11	0/0/0/0
1	MLY	J	431	1	-	0/7/9/11	0/0/0/0
1	MLY	J	436	1	-	0/7/9/11	0/0/0/0
1	MLY	J	486	1	-	0/7/9/11	0/0/0/0
1	MLY	J	49	1	-	0/7/9/11	0/0/0/0
1	MLY	J	504	1	-	0/7/9/11	0/0/0/0
1	MLY	J	505	1	-	0/7/9/11	0/0/0/0
1	MLY	J	528	1	-	0/7/9/11	0/0/0/0
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	J	782	1	-	0/7/9/11	0/0/0/0
1	MLY	J	827	1	-	0/7/9/11	0/0/0/0
1	MLY	J	833	1	-	0/7/9/11	0/0/0/0
1	MLY	J	837	1	-	0/7/9/11	0/0/0/0
1	MLY	J	839	1	-	0/7/9/11	0/0/0/0
1	MLY	J	84	1	-	0/7/9/11	0/0/0/0
1	MLY	J	87	1	-	0/7/9/11	0/0/0/0
1	MLY	M	107	1	-	0/7/9/11	0/0/0/0
1	MLY	M	130	1	-	0/7/9/11	0/0/0/0
1	MLY	M	138	1	-	0/7/9/11	0/0/0/0
1	MLY	M	19	1	-	0/7/9/11	0/0/0/0
1	MLY	M	190	1	-	0/7/9/11	0/0/0/0
1	MLY	M	236	1	-	0/7/9/11	0/0/0/0
1	MLY	M	248	1	-	0/7/9/11	0/0/0/0
1	MLY	M	272	1	-	0/7/9/11	0/0/0/0
1	MLY	M	295	1	-	0/7/9/11	0/0/0/0
1	MLY	M	296	1	-	0/7/9/11	0/0/0/0
1	MLY	M	30	1	-	0/7/9/11	0/0/0/0
1	MLY	M	348	1	-	0/7/9/11	0/0/0/0
1	MLY	M	35	1	-	0/7/9/11	0/0/0/0
1	MLY	M	353	1	-	0/7/9/11	0/0/0/0
1	MLY	M	367	1	-	0/7/9/11	0/0/0/0
1	MLY	M	369	1	-	0/7/9/11	0/0/0/0
1	MLY	M	385	1	-	0/7/9/11	0/0/0/0
1	MLY	M	415	1	-	0/7/9/11	0/0/0/0
1	MLY	M	431	1	-	0/7/9/11	0/0/0/0
1	MLY	M	436	1	-	0/7/9/11	0/0/0/0
1	MLY	M	486	1	-	0/7/9/11	0/0/0/0
1	MLY	M	49	1	-	0/7/9/11	0/0/0/0
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	M	681	1	-	0/7/9/11	0/0/0/0
1	MLY	M	764	1	-	0/7/9/11	0/0/0/0
1	MLY	M	768	1	-	0/7/9/11	0/0/0/0
1	MLY	M	782	1	-	0/7/9/11	0/0/0/0
1	MLY	M	827	1	-	0/7/9/11	0/0/0/0
1	MLY	M	833	1	-	0/7/9/11	0/0/0/0
1	MLY	M	837	1	-	0/7/9/11	0/0/0/0
1	MLY	M	839	1	-	0/7/9/11	0/0/0/0
1	MLY	M	84	1	-	0/7/9/11	0/0/0/0
1	MLY	M	87	1	-	0/7/9/11	0/0/0/0
1	MLY	P	107	1	-	0/7/9/11	0/0/0/0
1	MLY	P	130	1	-	0/7/9/11	0/0/0/0
1	MLY	P	138	1	-	0/7/9/11	0/0/0/0
1	MLY	P	19	1	-	0/7/9/11	0/0/0/0
1	MLY	P	190	1	-	0/7/9/11	0/0/0/0
1	MLY	P	236	1	-	0/7/9/11	0/0/0/0
1	MLY	P	248	1	-	0/7/9/11	0/0/0/0
1	MLY	P	272	1	-	0/7/9/11	0/0/0/0
1	MLY	P	295	1	-	0/7/9/11	0/0/0/0
1	MLY	P	296	1	-	0/7/9/11	0/0/0/0
1	MLY	P	30	1	-	0/7/9/11	0/0/0/0
1	MLY	P	348	1	-	0/7/9/11	0/0/0/0
1	MLY	P	35	1	-	0/7/9/11	0/0/0/0
1	MLY	P	353	1	-	0/7/9/11	0/0/0/0
1	MLY	P	367	1	-	0/7/9/11	0/0/0/0
1	MLY	P	369	1	-	0/7/9/11	0/0/0/0
1	MLY	P	385	1	-	0/7/9/11	0/0/0/0
1	MLY	P	415	1	-	0/7/9/11	0/0/0/0
1	MLY	P	431	1	-	0/7/9/11	0/0/0/0
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	P	617	1	-	0/7/9/11	0/0/0/0
1	MLY	P	63	1	-	0/7/9/11	0/0/0/0
1	MLY	P	659	1	-	0/7/9/11	0/0/0/0
1	MLY	P	681	1	-	0/7/9/11	0/0/0/0
1	MLY	P	764	1	-	0/7/9/11	0/0/0/0
1	MLY	P	768	1	-	0/7/9/11	0/0/0/0
1	MLY	P	782	1	-	0/7/9/11	0/0/0/0
1	MLY	P	827	1	-	0/7/9/11	0/0/0/0
1	MLY	P	833	1	-	0/7/9/11	0/0/0/0
1	MLY	P	837	1	-	0/7/9/11	0/0/0/0
1	MLY	P	839	1	-	0/7/9/11	0/0/0/0
1	MLY	P	84	1	-	0/7/9/11	0/0/0/0
1	MLY	P	87	1	-	0/7/9/11	0/0/0/0

The worst 5 of 72 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	138	MLY	CB-CA	-3.61	1.48	1.53
1	M	138	MLY	CB-CA	-3.56	1.48	1.53
1	A	138	MLY	CB-CA	-3.56	1.48	1.53
1	P	138	MLY	CB-CA	-3.54	1.48	1.53
1	G	138	MLY	CB-CA	-3.51	1.48	1.53

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	236	MLY	O-C-CA	-3.29	116.90	125.72
1	G	236	MLY	O-C-CA	-3.23	117.07	125.72
1	P	236	MLY	O-C-CA	-3.23	117.07	125.72
1	J	236	MLY	O-C-CA	-3.22	117.08	125.72
1	D	236	MLY	O-C-CA	-3.21	117.10	125.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

180 monomers are involved in 709 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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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	3	0
1	A	504	MLY	3	0
1	A	505	MLY	35	0
1	A	528	MLY	3	0
1	A	55	MLY	1	0
1	A	551	MLY	2	0
1	A	553	MLY	17	2
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	9	0
1	A	768	MLY	18	0
1	A	782	MLY	7	0
1	A	837	MLY	3	0
1	A	839	MLY	4	0
1	A	87	MLY	3	0
1	D	107	MLY	2	0
1	D	138	MLY	1	0
1	D	190	MLY	2	0
1	D	248	MLY	2	0
1	D	272	MLY	1	0
1	D	295	MLY	5	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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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	10	0
1	D	782	MLY	89	0
1	D	827	MLY	2	0
1	D	837	MLY	1	0
1	D	839	MLY	4	0
1	D	87	MLY	3	0
1	G	107	MLY	2	0
1	G	138	MLY	1	0
1	G	190	MLY	2	0
1	G	248	MLY	2	0
1	G	272	MLY	1	0
1	G	295	MLY	7	0
1	G	296	MLY	3	0
1	G	30	MLY	1	0
1	G	348	MLY	5	0
1	G	415	MLY	1	0
1	G	436	MLY	2	0
1	G	486	MLY	3	0
1	G	49	MLY	3	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	20	0
1	G	768	MLY	5	0
1	G	782	MLY	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	G	837	MLY	1	0
1	G	839	MLY	4	0
1	G	84	MLY	21	0
1	G	87	MLY	3	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	5	0
1	J	296	MLY	3	0
1	J	30	MLY	1	0
1	J	348	MLY	5	0
1	J	369	MLY	1	0
1	J	415	MLY	1	0
1	J	436	MLY	2	0
1	J	486	MLY	3	0
1	J	49	MLY	2	0
1	J	505	MLY	9	0
1	J	528	MLY	3	0
1	J	55	MLY	1	0
1	J	553	MLY	12	0
1	J	59	MLY	3	0
1	J	598	MLY	1	0
1	J	600	MLY	1	0
1	J	617	MLY	1	0
1	J	63	MLY	3	0
1	J	659	MLY	2	0
1	J	764	MLY	2	0
1	J	768	MLY	6	0
1	J	782	MLY	1	0
1	J	837	MLY	1	0
1	J	839	MLY	8	0
1	J	84	MLY	27	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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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	3	0
1	M	505	MLY	1	0
1	M	528	MLY	2	0
1	M	55	MLY	1	0
1	M	553	MLY	12	0
1	M	59	MLY	2	0
1	M	598	MLY	1	0
1	M	600	MLY	1	0
1	M	617	MLY	1	0
1	M	63	MLY	4	0
1	M	659	MLY	1	0
1	M	764	MLY	1	0
1	M	768	MLY	3	0
1	M	782	MLY	3	0
1	M	837	MLY	1	0
1	M	839	MLY	8	0
1	M	87	MLY	3	0
1	P	107	MLY	2	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	5	0
1	P	296	MLY	2	0
1	P	30	MLY	1	0
1	P	348	MLY	4	0
1	P	369	MLY	1	0
1	P	415	MLY	1	0
1	P	436	MLY	2	0
1	P	486	MLY	3	0
1	P	49	MLY	2	0
1	P	528	MLY	3	0
1	P	55	MLY	1	0
1	P	553	MLY	3	0
1	P	59	MLY	3	0
1	P	598	MLY	1	0
1	P	600	MLY	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	P	617	MLY	1	0
1	P	63	MLY	4	0
1	P	659	MLY	2	0
1	P	764	MLY	9	0
1	P	768	MLY	2	0
1	P	782	MLY	1	0
1	P	837	MLY	1	0
1	P	839	MLY	9	0
1	P	87	MLY	2	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.