wwPDB EM Validation Summary Report (i)

Dec 18, 2023 – 11:50 PM EST

PDB ID	:	1O19
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)
Based on initial models	:	1ATN, 2MYS

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

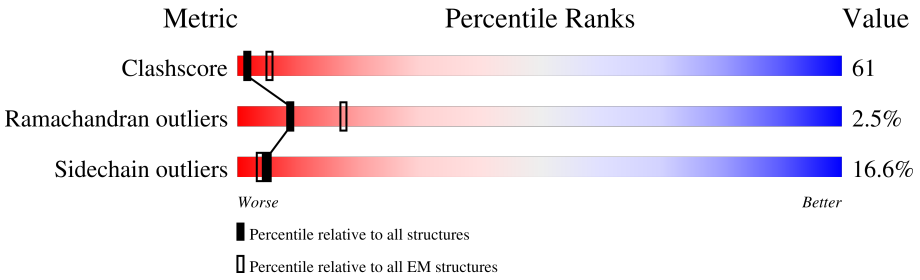
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	840	100% 25% 51% 20% ·
1	D	840	100% 25% 50% 20% ·
1	G	840	100% 24% 51% 20% ·
1	J	840	99% 26% 50% 20% ·
1	M	840	100% 26% 50% 21% ·
1	S	840	100% 25% 51% 20% ·
2	B	145	100% 66% 26% 6% ·
2	E	145	90% 64% 27% 6% ·

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Mol	Chain	Length	Quality of chain
2	H	145	100% 64% 27% 6%
2	K	145	100% 64% 26% 6%
2	N	145	100% 64% 27% 6%
2	T	145	100% 65% 26% 6%
3	C	147	100% 60% 37%
3	F	147	96% 60% 38%
3	I	147	100% 61% 37%
3	L	147	82% 61% 37%
3	O	147	100% 61% 37%
3	U	147	100% 57% 40%
4	1	375	99% 62% 29% 6%
4	2	375	96% 55% 34% 9%
4	3	375	99% 62% 30% 6%
4	4	375	99% 62% 30% 6%
4	5	375	99% 63% 29% 6%
4	6	375	99% 64% 28% 6%
4	7	375	99% 64% 27% 6%
4	8	375	99% 58% 31% 8%
4	9	375	99% 58% 32% 8%
4	V	375	99% 55% 34% 8%
4	W	375	99% 55% 33% 9%
4	X	375	93% 61% 30% 7%
4	Y	375	99% 61% 30% 7%
4	Z	375	99% 57% 32% 8%

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	MLY	A	505	-	-	X	-
1	MLY	A	553	-	-	X	-
1	MLY	A	764	-	-	X	-
1	MLY	A	768	-	-	X	-
1	MLY	A	782	-	-	X	-
1	MLY	A	839	-	-	X	-
1	MLY	D	553	-	-	X	-
1	MLY	D	782	-	-	X	-
1	MLY	D	839	-	-	X	-
1	MLY	G	295	-	-	X	-
1	MLY	G	553	-	-	X	-
1	MLY	G	764	-	-	X	-
1	MLY	G	768	-	-	X	-
1	MLY	G	84	-	-	X	-
1	MLY	J	295	-	-	X	-
1	MLY	J	505	-	-	X	-
1	MLY	J	553	-	-	X	-
1	MLY	J	764	-	-	X	-
1	MLY	J	768	-	-	X	-
1	MLY	J	839	-	-	X	-
1	MLY	J	84	-	-	X	-
1	MLY	M	35	-	-	X	-
1	MLY	M	553	-	-	X	-
1	MLY	M	839	-	-	X	-
1	MLY	M	84	-	-	X	-
1	MLY	S	505	-	-	X	-
1	MLY	S	764	-	-	X	-
1	MLY	S	839	-	-	X	-
1	MLY	S	84	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 94966 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

- Molecule 2 is a protein called SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	145	Total	C	N	O	S	0	0
			1127	717	177	227	6		
2	E	145	Total	C	N	O	S	0	0
			1127	717	177	227	6		
2	H	145	Total	C	N	O	S	0	0
			1127	717	177	227	6		
2	K	145	Total	C	N	O	S	0	0
			1127	717	177	227	6		
2	N	145	Total	C	N	O	S	0	0
			1127	717	177	227	6		
2	T	145	Total	C	N	O	S	0	0
			1127	717	177	227	6		

- Molecule 3 is a protein called SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN.

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

- Molecule 4 is a protein called SKELETAL MUSCLE ACTIN.

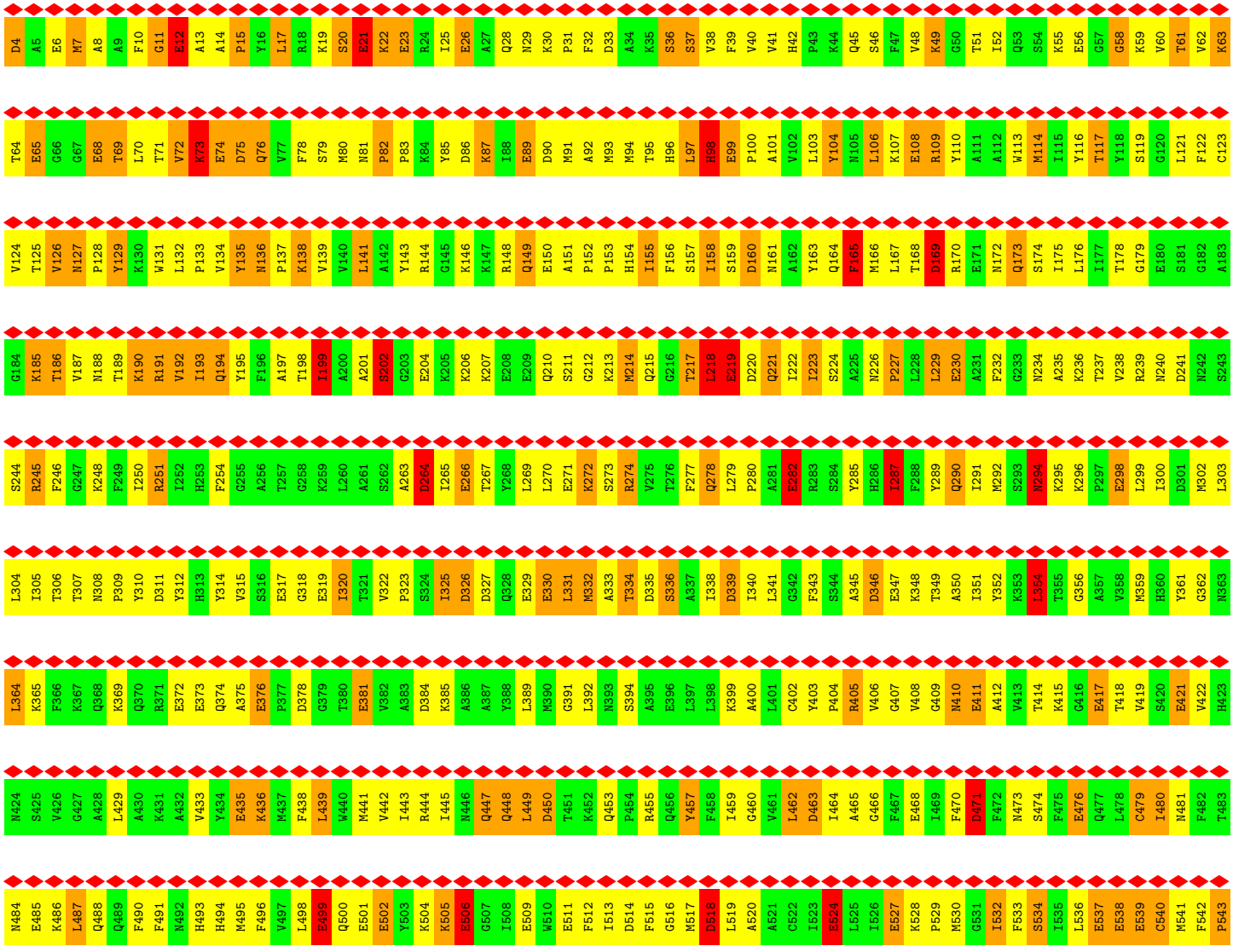
Mol	Chain	Residues	Atoms					AltConf	Trace
4	1	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	2	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	3	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	4	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	5	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
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		

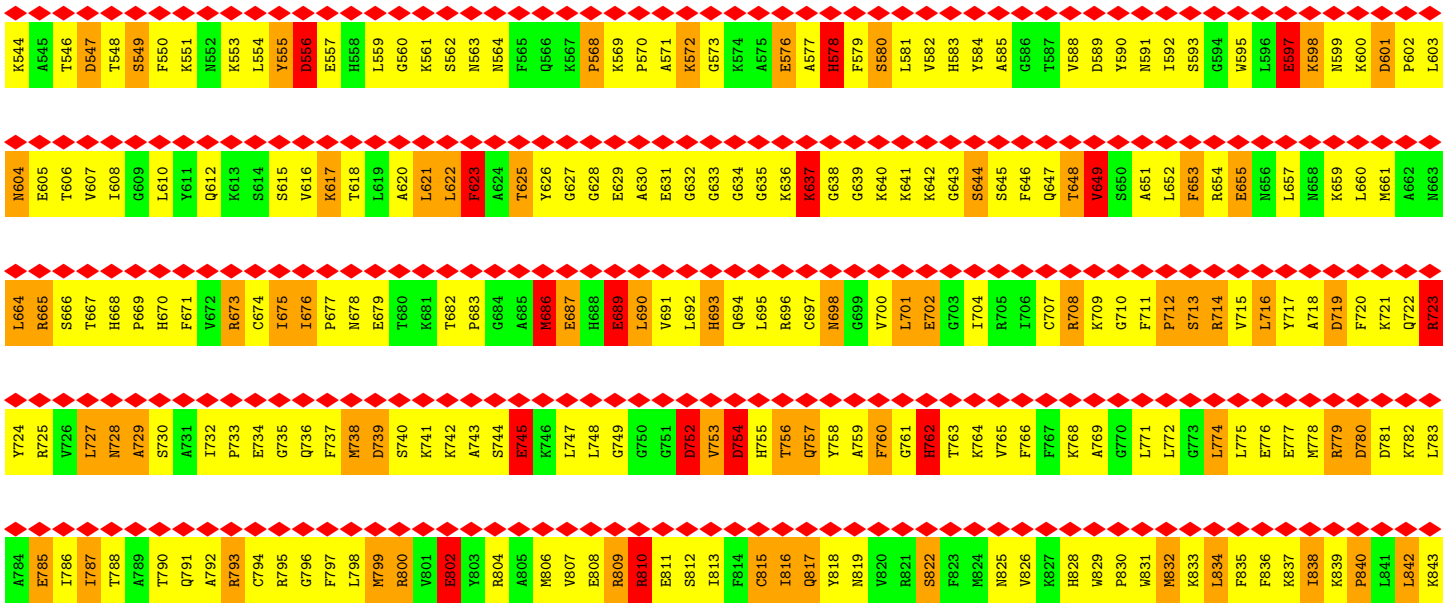
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 and atom inclusion in map density. 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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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

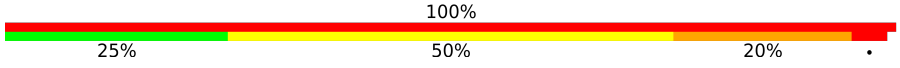
Chain A:

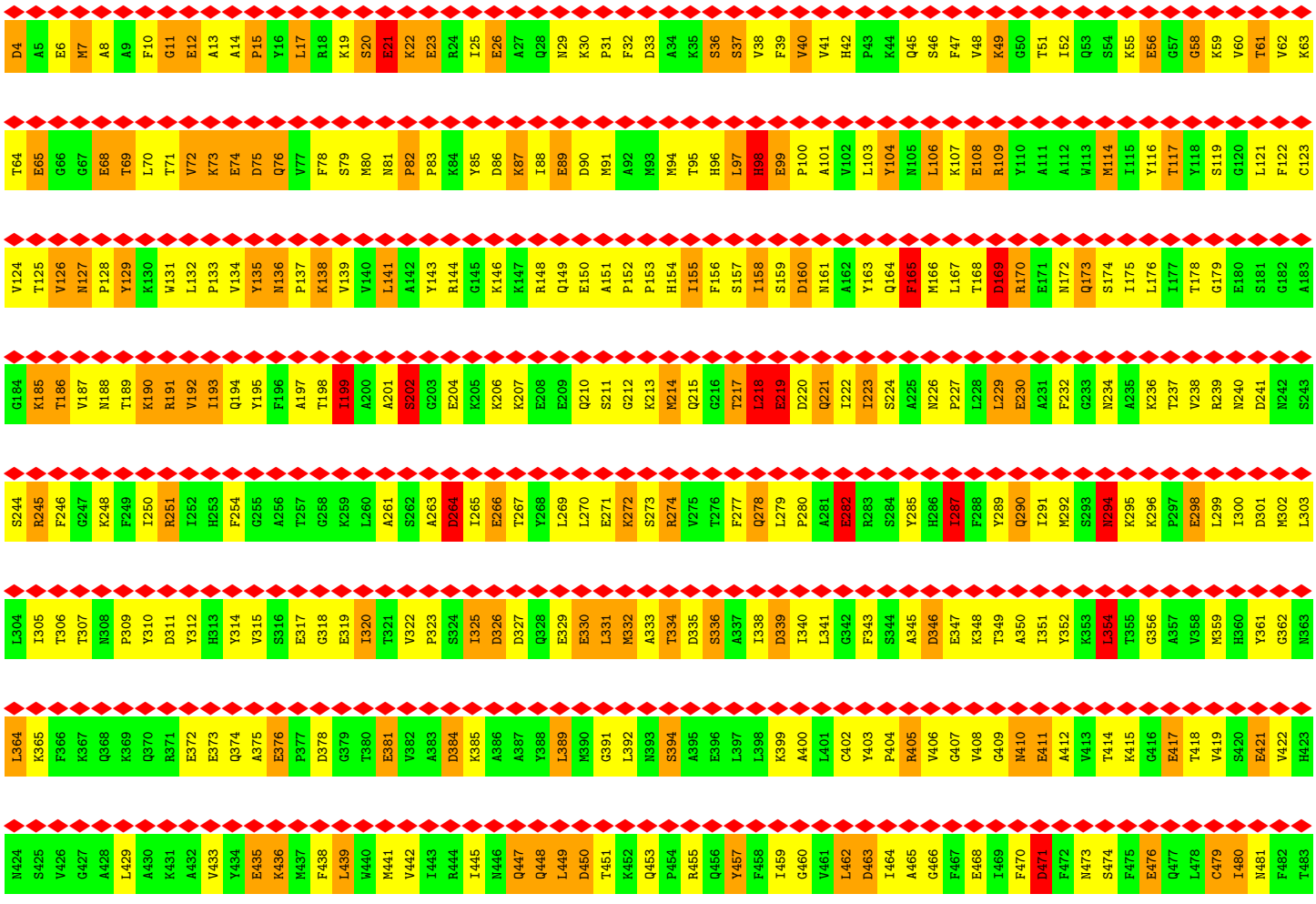


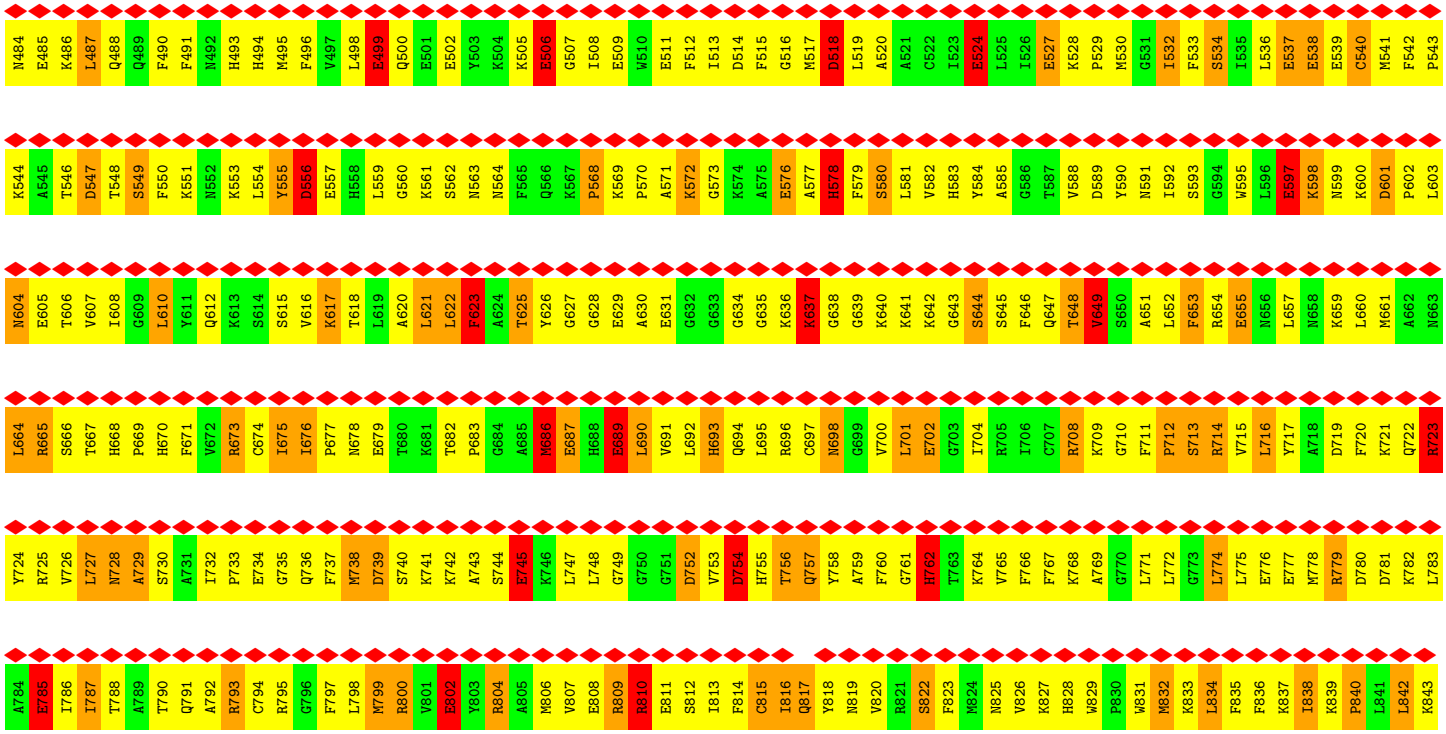


- Molecule 1: SKELETAL MUSCLE MYOSIN II

Chain D:

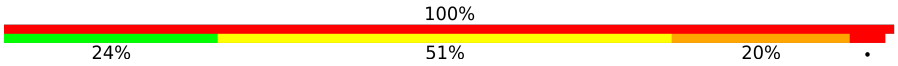


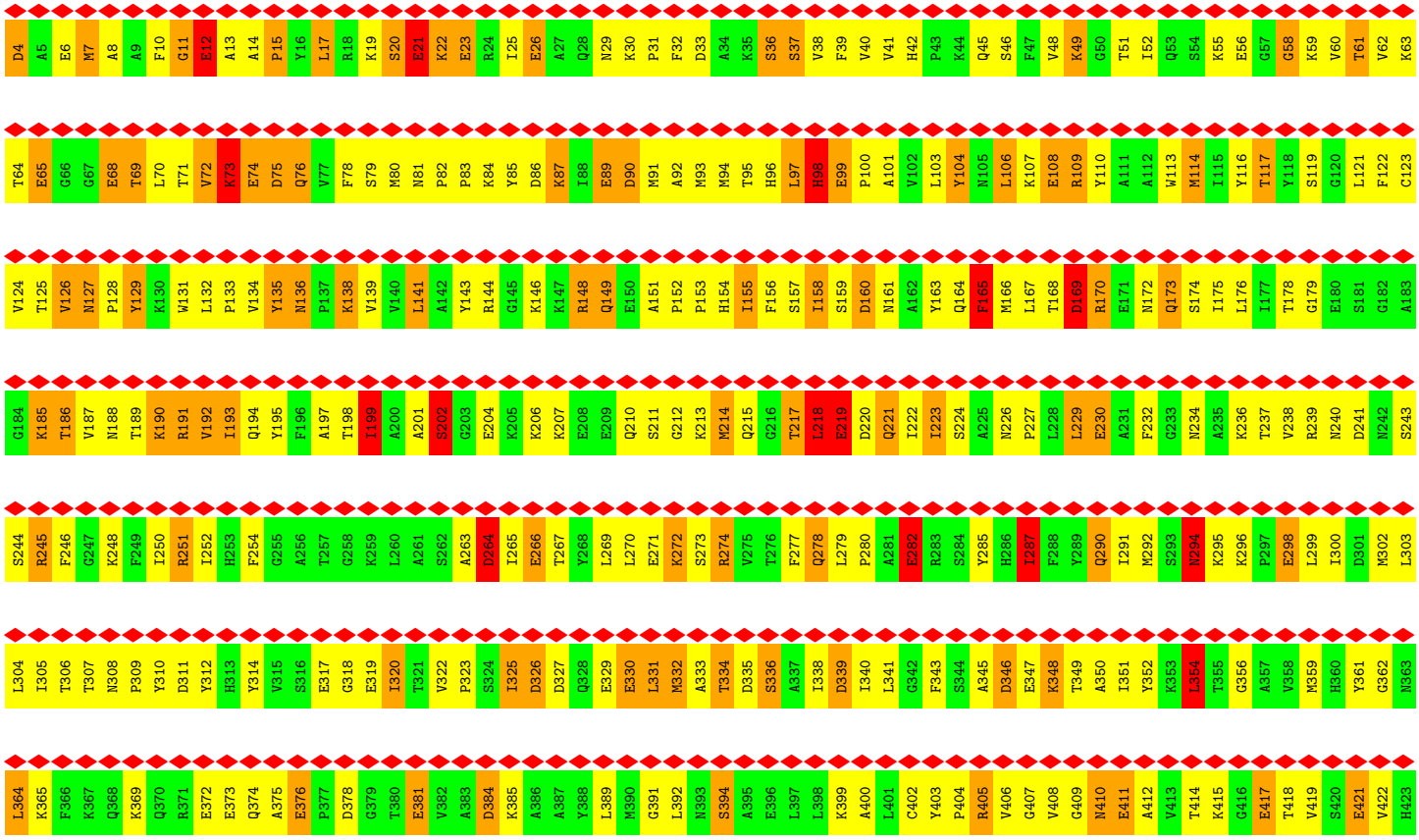


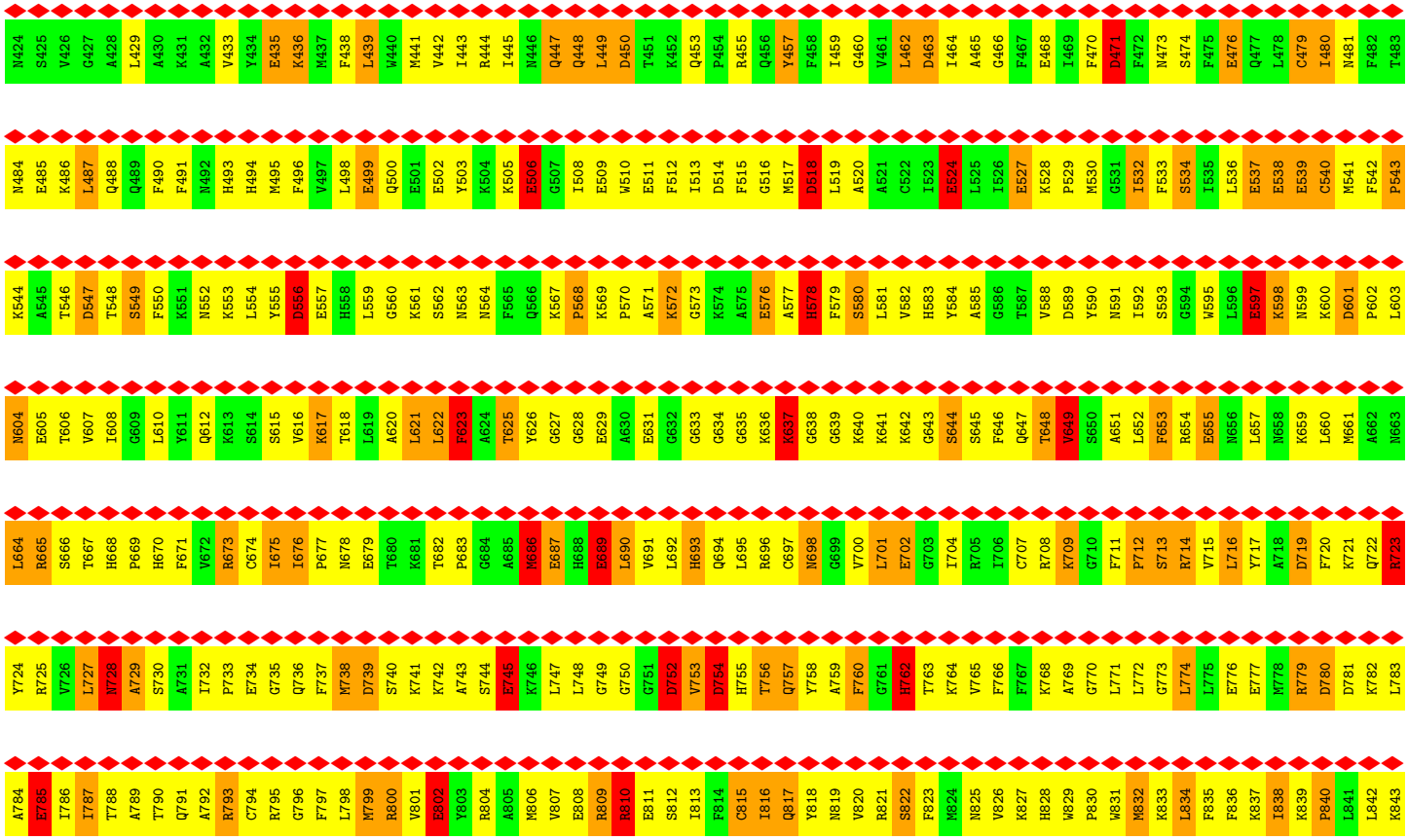


• Molecule 1: SKELETAL MUSCLE MYOSIN II

Chain G:

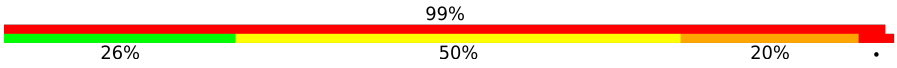


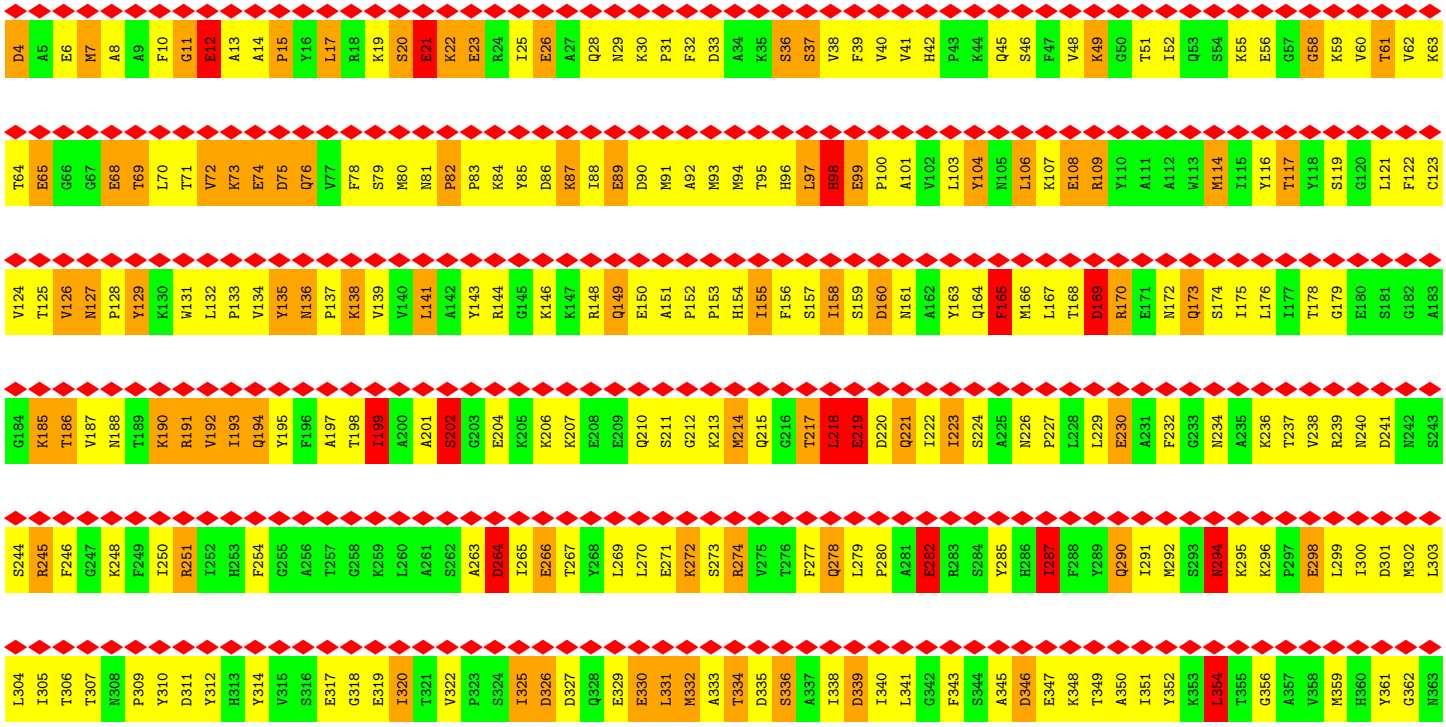


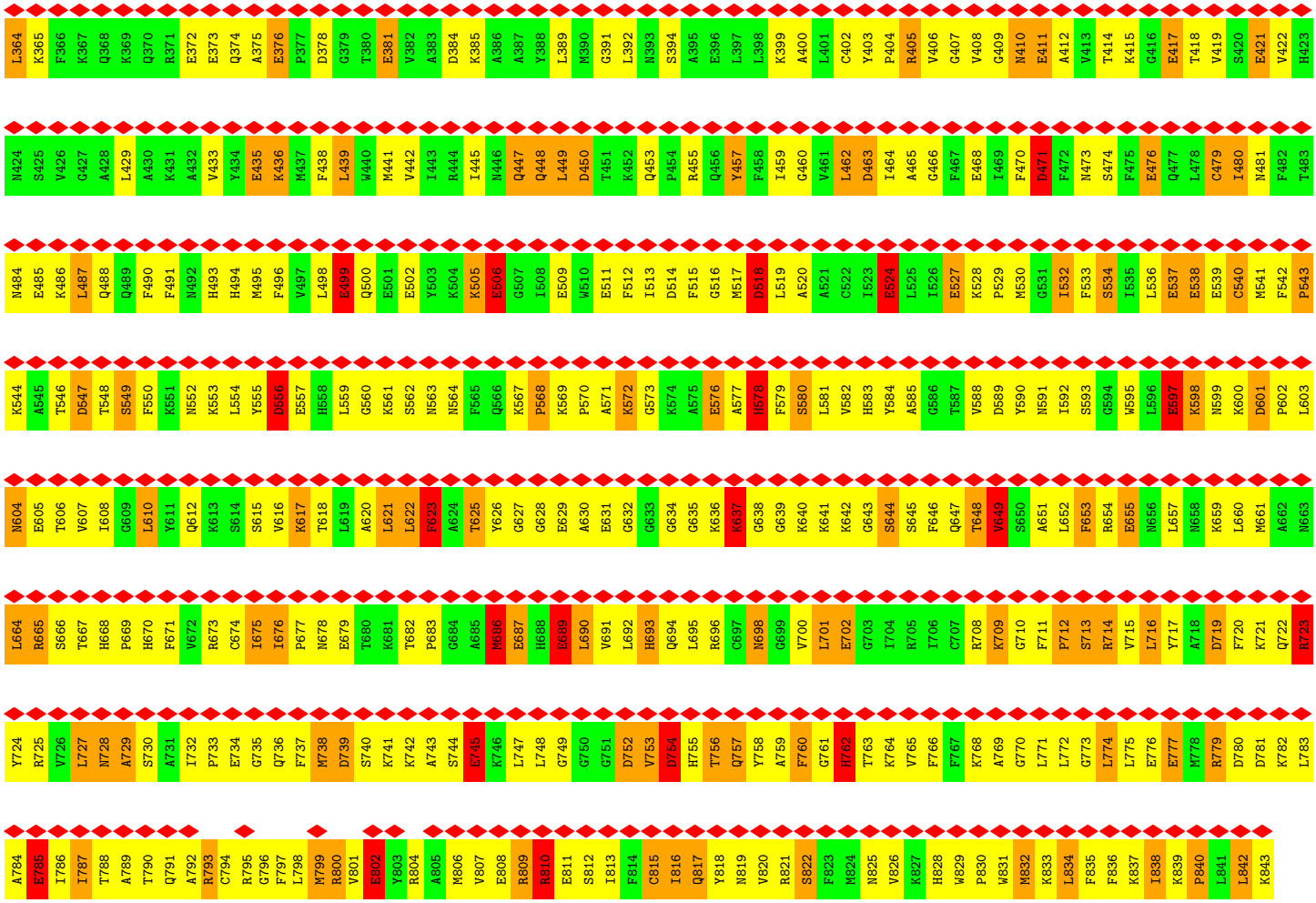


• Molecule 1: SKELETAL MUSCLE MYOSIN II

Chain J:

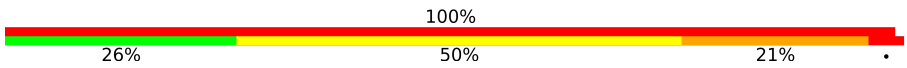


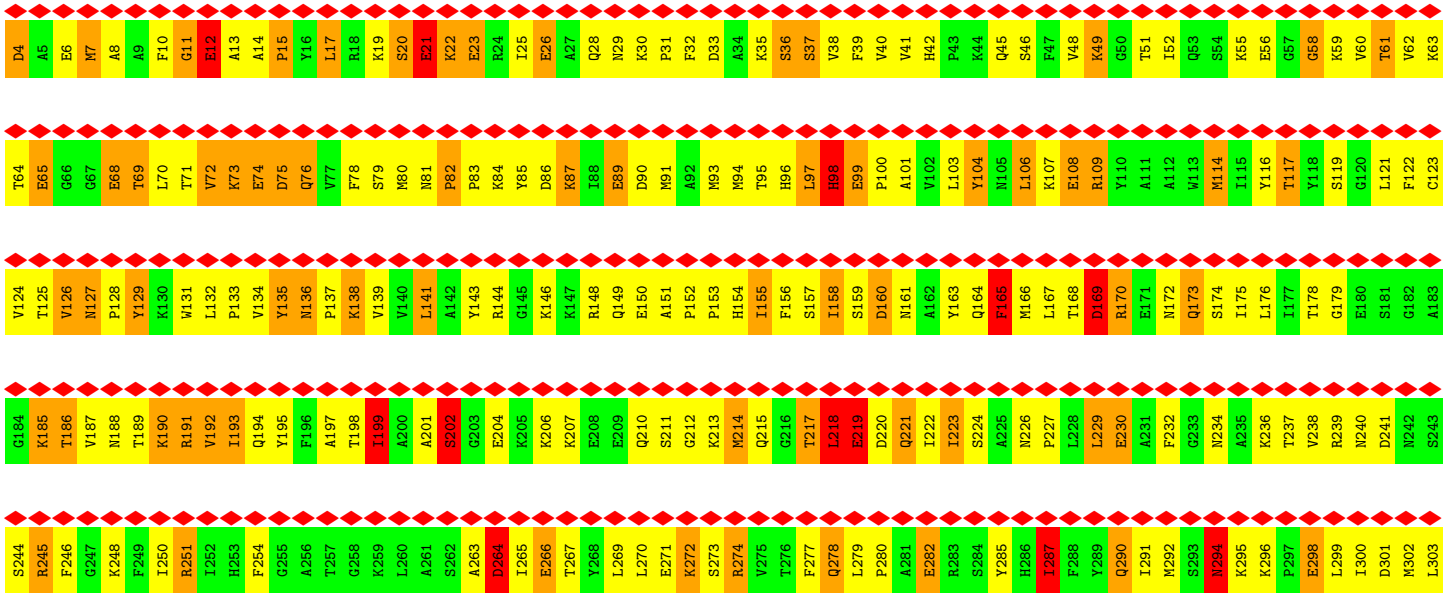


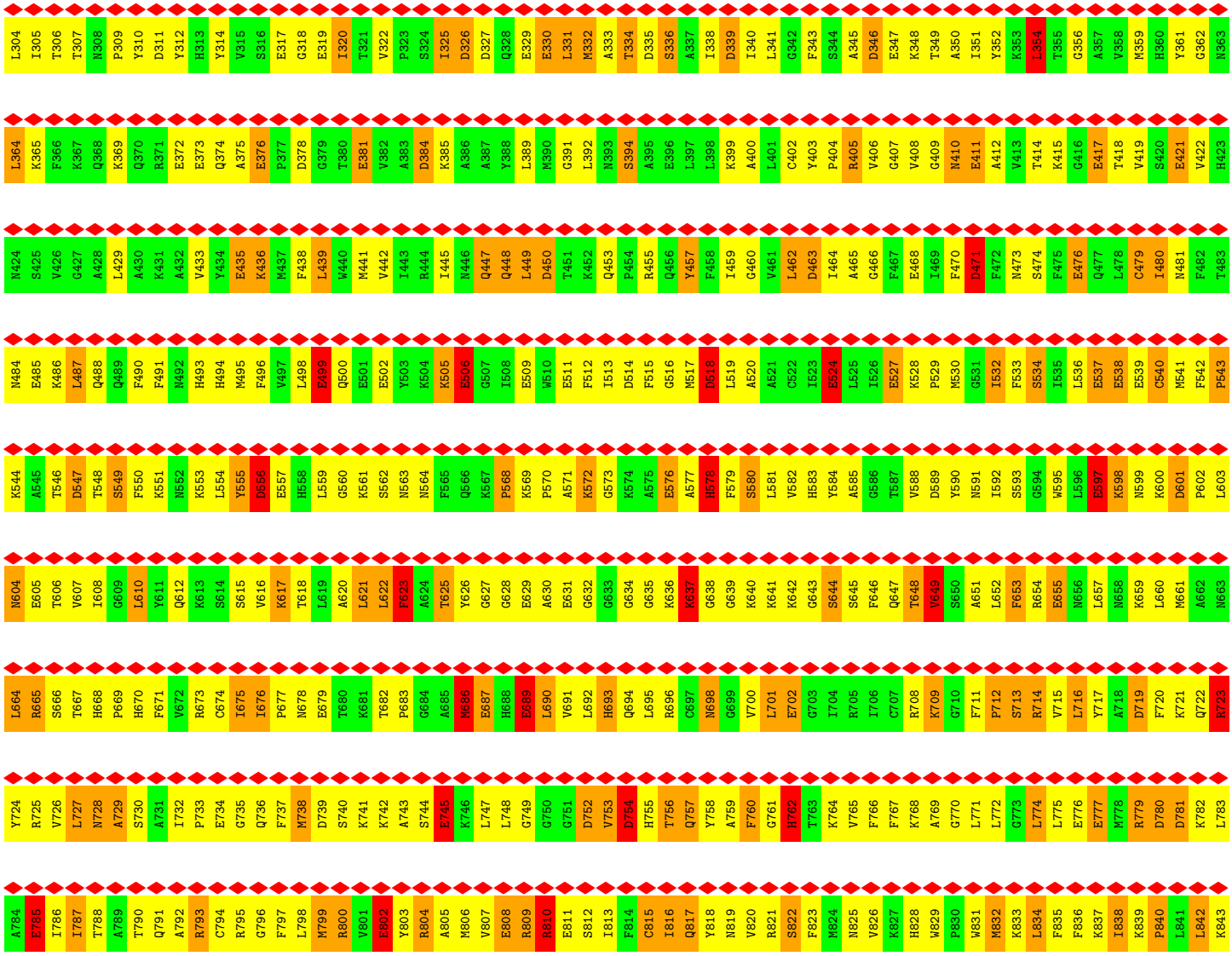


• Molecule 1: SKELETAL MUSCLE MYOSIN II

Chain M:

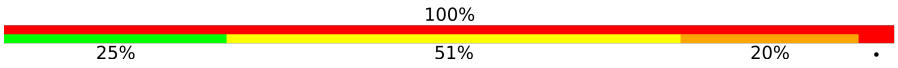


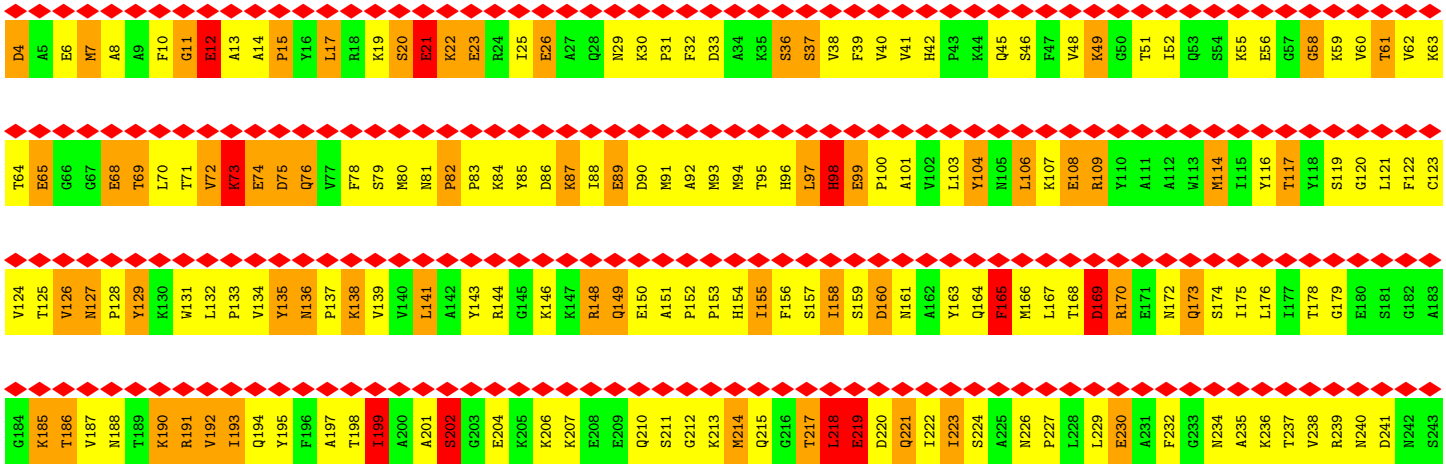


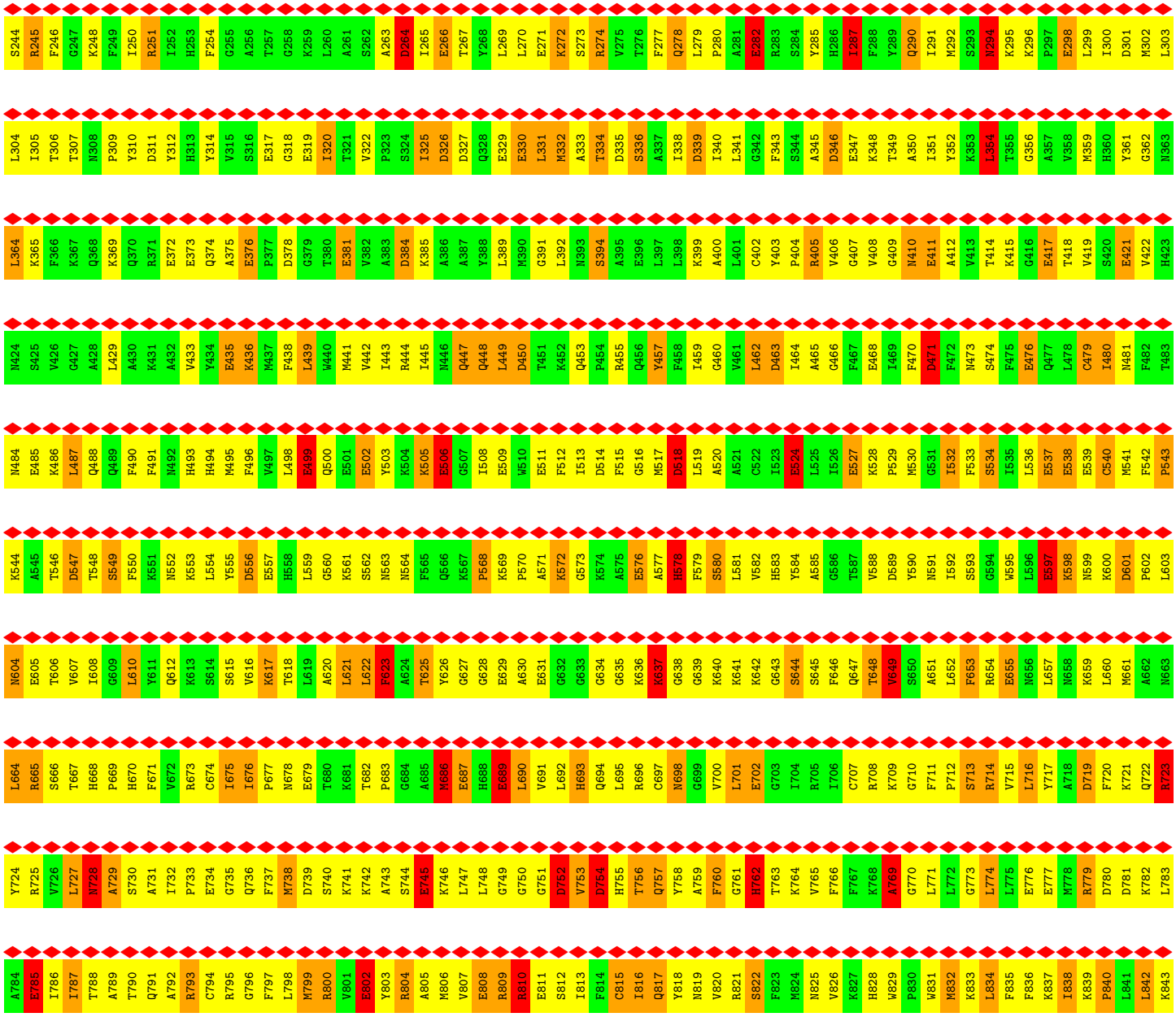


• Molecule 1: SKELETAL MUSCLE MYOSIN II

Chain S:

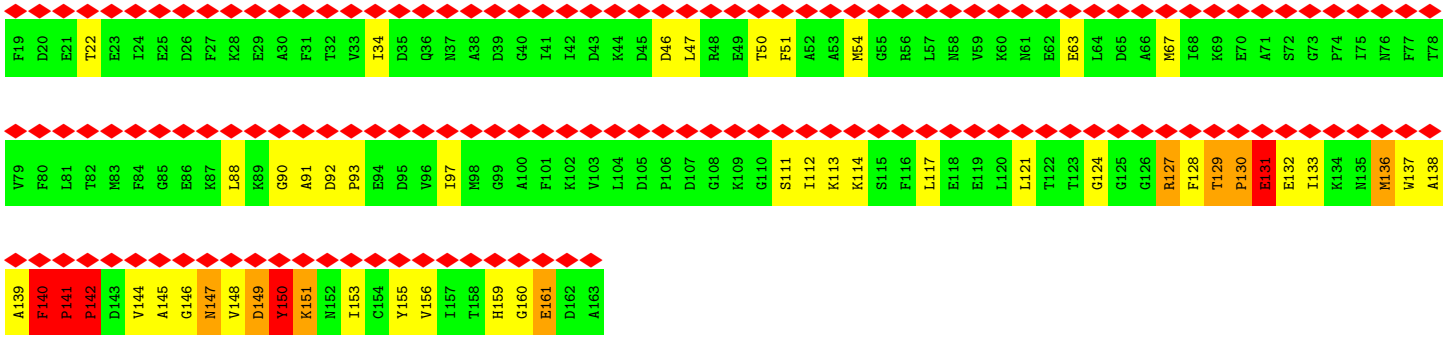






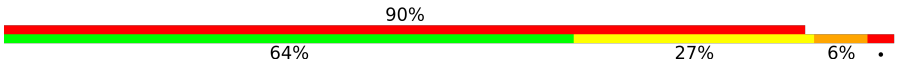
• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

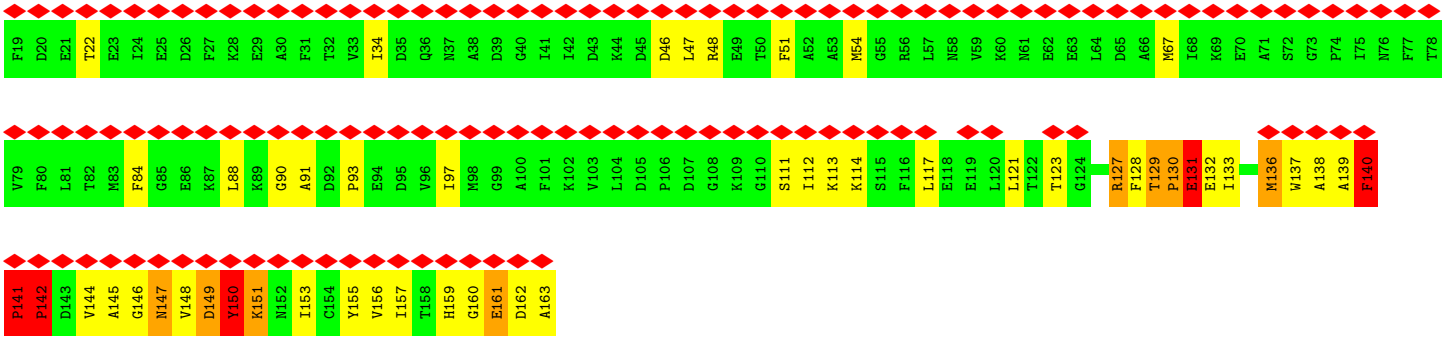
Chain B:



• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

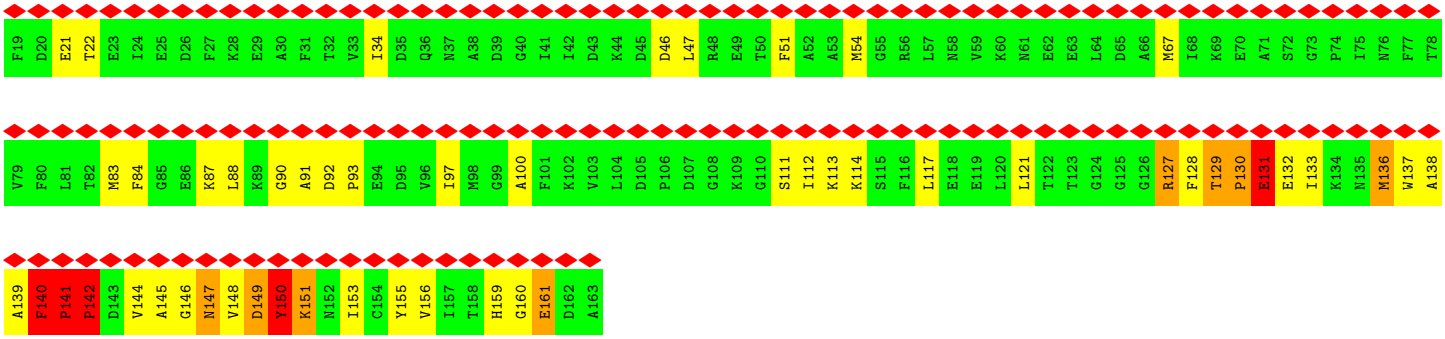
Chain E:





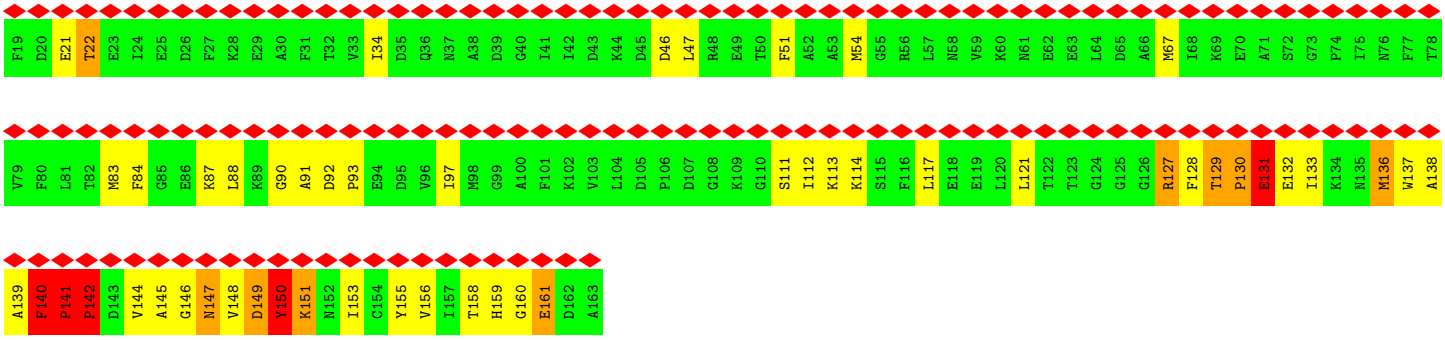
• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

Chain H:



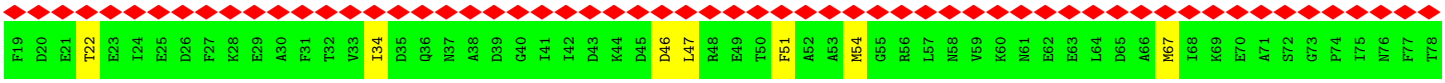
• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

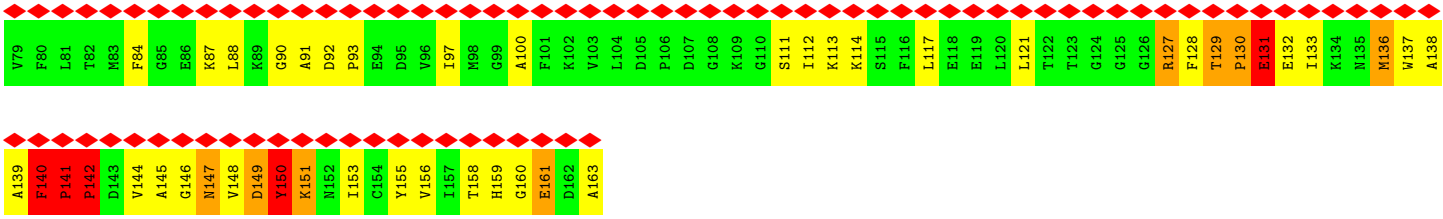
Chain K:



• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

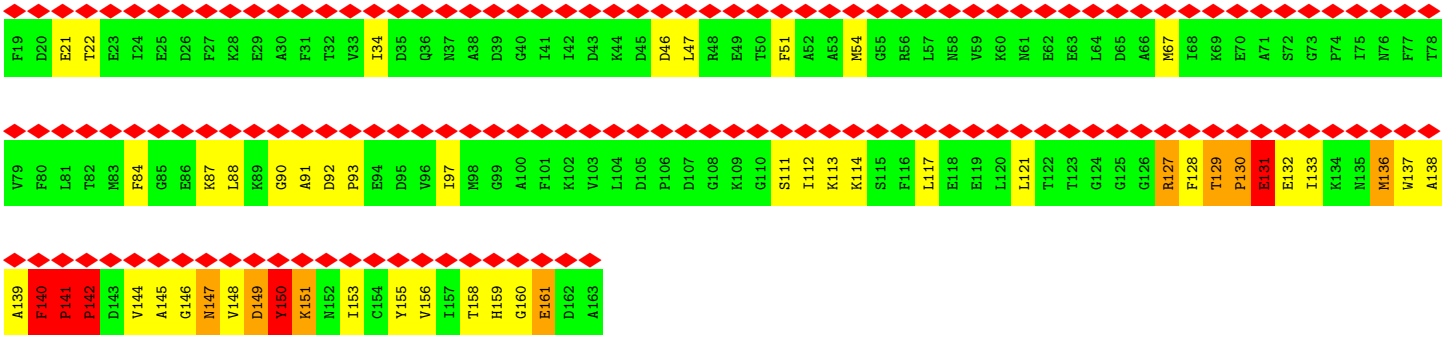
Chain N:





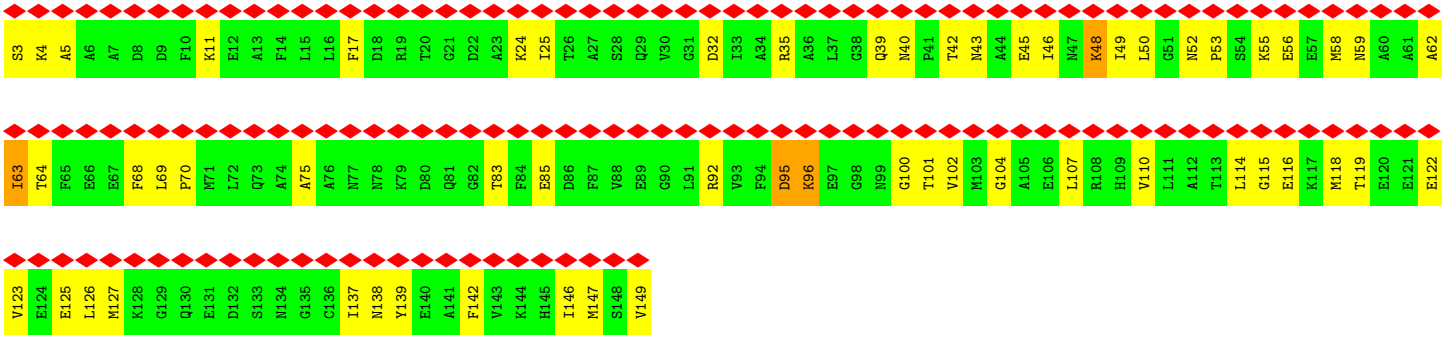
• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

Chain T:



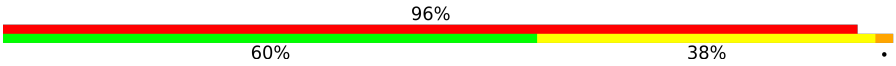
• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN

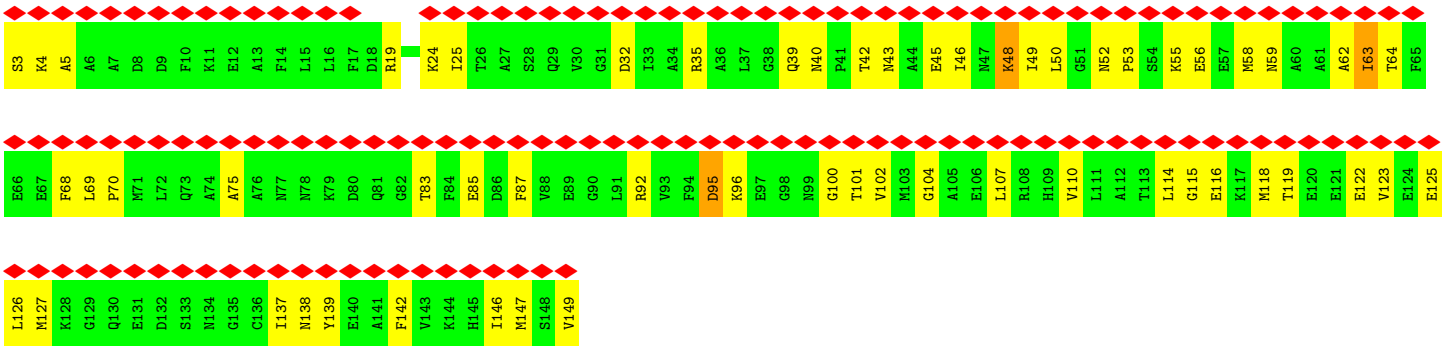
Chain C:



• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN

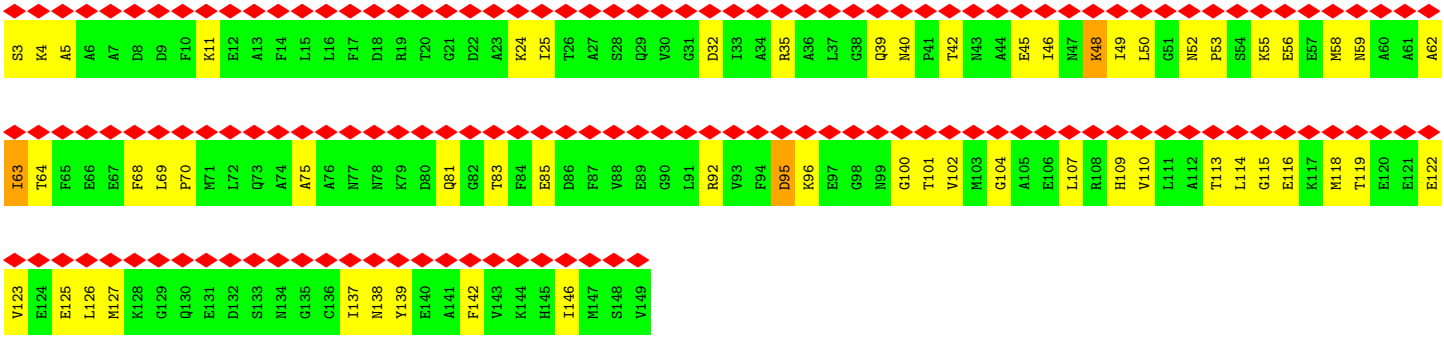
Chain F:





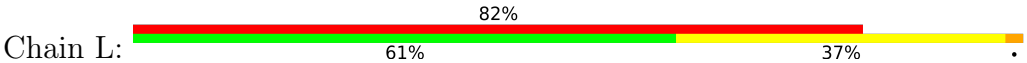
• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN

Chain I:



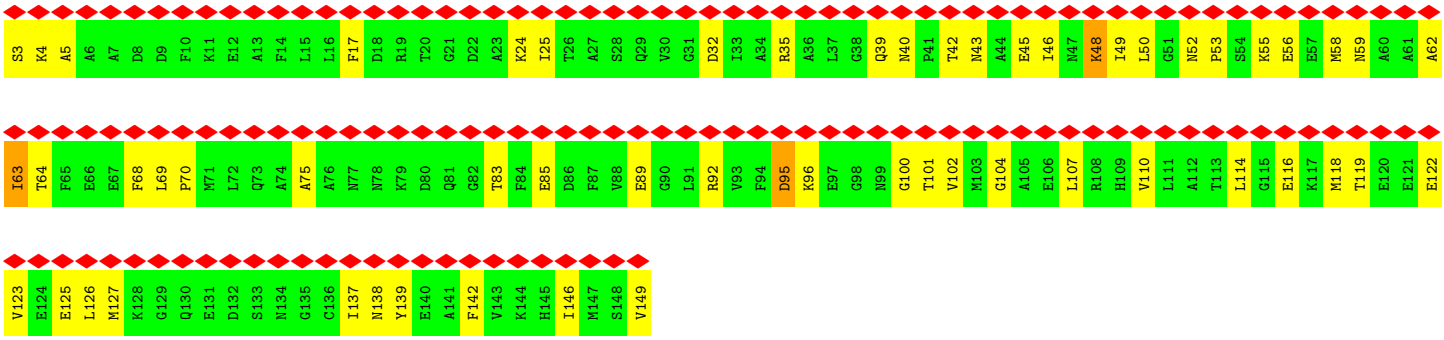
• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN

Chain L:



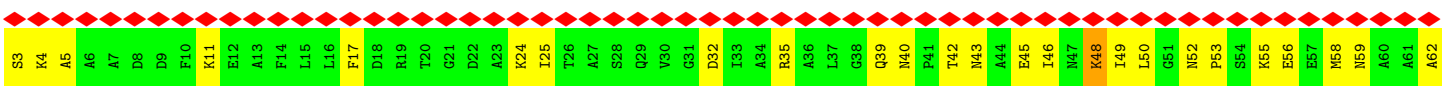
• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN

Chain O:



• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN

Chain U:



I63 T64 F65 E66 E67 F68 L69 P70 M71 L72 Q73 A74 A75 A76 N77 N78 K79 D80 Q81 G82 T83 F84 E85 D86 F87 V88 E89 G90 L91 R92 V93 F94 D95 K96 E97 G98 N99 G100 T101 V102 M103 G104 A105 E106 L107 R108 H109 V110 L111 A112 T113 L114 G115 E116 K117 M118 T119 E120 E121 E122

V123 E124 E125 L126 M127 K128 G129 Q130 E131 D132 S133 N134 G135 C136 I137 N138 Y139 E140 A141 F142 V143 K144 H145 I146 M147 S148 V149

• Molecule 4: SKELETAL MUSCLE ACTIN

Chain 1: 99% 62% 29% 6%

D1 E2 D3 E4 T5 T6 A7 L8 V9 C10 D11 N12 G13 S14 G15 L16 V17 K18 A19 G20 F21 A22 G23 D24 D25 A26 P27 R28 A29 V30 F31 P32 S33 I34 V35 G36 R37 P38 R39 H40 Q41 G42 V43 M44 V45 G46 M47 G48 Q49 K50 D51 S52 Y53 V54 G55 D56 E57 A58 Q59 S60

K61 R62 G63 I64 L65 T66 L67 K68 Y69 P70 I71 E72 H73 G74 I75 I76 T77 N78 W79 D80 D81 M82 E83 K84 I85 W86 H87 H88 T89 F90 Y91 N92 E93 L94 R95 V96 A97 P98 E99 E100 H101 P102 T103 L104 L105 T106 E107 A108 P109 L110 N111 P112 K113 A114 N115 R116 E117 K118 M119 T120

Q121 I122 M123 F124 E125 T126 F127 N128 V129 P130 A131 M132 Y133 V134 A135 I136 Q137 A138 V139 L140 S141 L142 Y143 A144 S145 G146 R147 T148 T149 G150 I151 V152 L153 D154 S155 G156 D157 G158 V159 T160 H161 N162 V163 P164 I165 Y166 E167 G168 Y169 A170 L171 P172 H173 A174 I175 M176 R177 L178 D179 L180

A181 G182 R183 D184 L185 T186 D187 Y188 L189 M190 K191 I192 L193 T194 E195 R196 G197 Y198 S199 F200 V201 T202 T203 A204 E205 R206 E207 I208 V209 R210 D211 I212 K213 E214 K215 L216 C217 Y218 V219 A220 L221 D222 F223 E224 N225 E226 M227 A228 T229 A230 A231 S232 S233 S234 S235 L236 E237 K238 S239 Y240

E241 L242 P243 D244 G245 Q246 V247 I248 T249 I250 G251 N252 E253 R254 F255 R256 C257 P258 E259 T260 L261 F262 Q263 P264 S265 F266 I267 G268 M269 E270 S271 A272 G273 I274 H275 E276 T277 T278 Y279 N280 S281 I282 M283 K284 C285 D286 I287 D288 I289 R290 K291 D292 L293 Y294 A295 N296 N297 V298 M299 S300

G301 G302 T303 T304 M305 Y306 P307 G308 I309 A310 D311 R312 M313 Q314 K315 E316 I317 T318 A319 L320 A321 P322 S323 T324 M325 K326 I327 K328 I329 I330 A331 P332 P333 E334 R335 K336 Y337 S338 V339 W340 I341 G342 G343 S344 I345 L346 A347 S348 L349 S350 T351 F352 Q353 Q354 M355 W356 I357 T358 K359 Q360

E361 Y362 D363 E364 A365 G366 P367 S368 I369 V370 H371 R372 LYS CYS PHE

• Molecule 4: SKELETAL MUSCLE ACTIN

Chain 2: 96% 55% 34% 9%

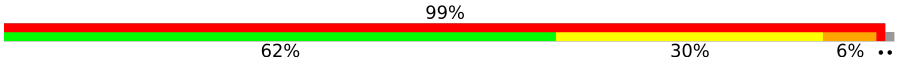
D1 E2 D3 E4 T5 T6 A7 L8 V9 C10 D11 N12 G13 S14 G15 L16 V17 K18 A19 G20 F21 A22 G23 D24 D25 A26 P27 R28 A29 V30 F31 P32 S33 I34 V35 G36 R37 P38 R39 H40 Q41 G42 V43 M44 V45 G46 M47 G48 Q49 K50 D51 S52 Y53 V54 G55 D56 E57 A58 Q59 S60

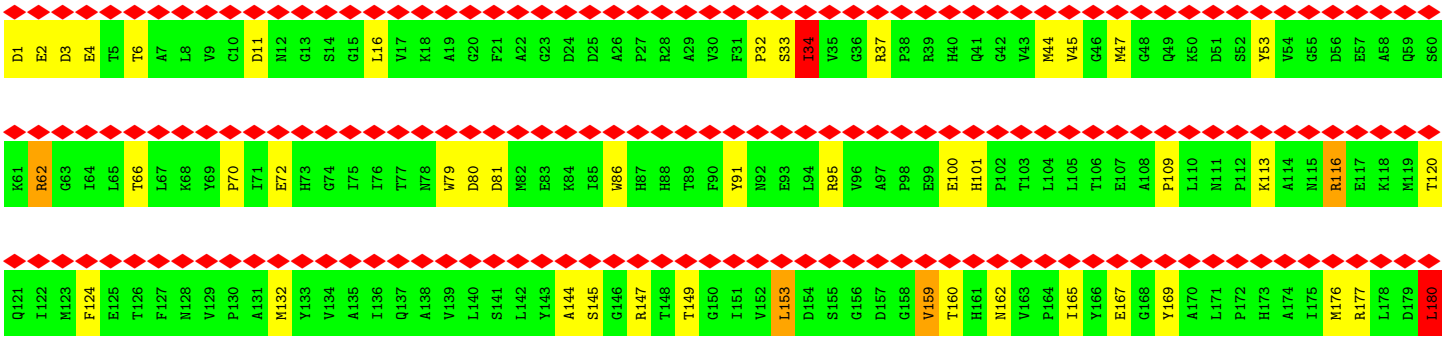
K61 R62 G63 I64 L65 T66 L67 K68 Y69 P70 I71 E72 H73 G74 I75 I76 T77 N78 W79 D80 D81 M82 E83 K84 I85 W86 H87 H88 T89 F90 Y91 N92 E93 L94 R95 V96 A97 P98 E99 E100 H101 P102 T103 L104 L105 T106 E107 A108 P109 L110 N111 P112 K113 A114 N115 R116 E117 K118 M119 T120

Q121 I122 M123 F124 E125 T126 F127 N128 V129 P130 A131 M132 Y133 V134 A135 I136 Q137 A138 V139 L140 S141 L142 Y143 A144 S145 G146 R147 T148 T149 G150 I151 V152 L153 D154 S155 G156 D157 G158 V159 T160 H161 N162 V163 P164 I165 Y166 E167 G168 Y169 A170 L171 P172 H173 A174 I175 M176 R177 L178 D179 L180

• Molecule 4: SKELETAL MUSCLE ACTIN

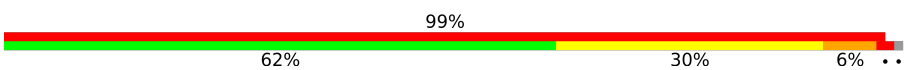
Chain 3:

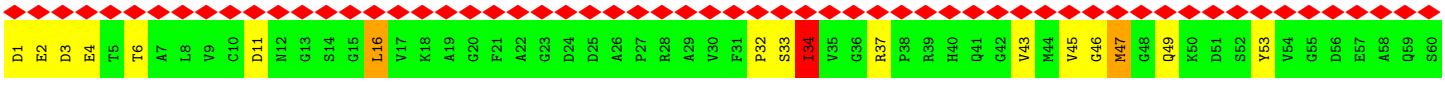


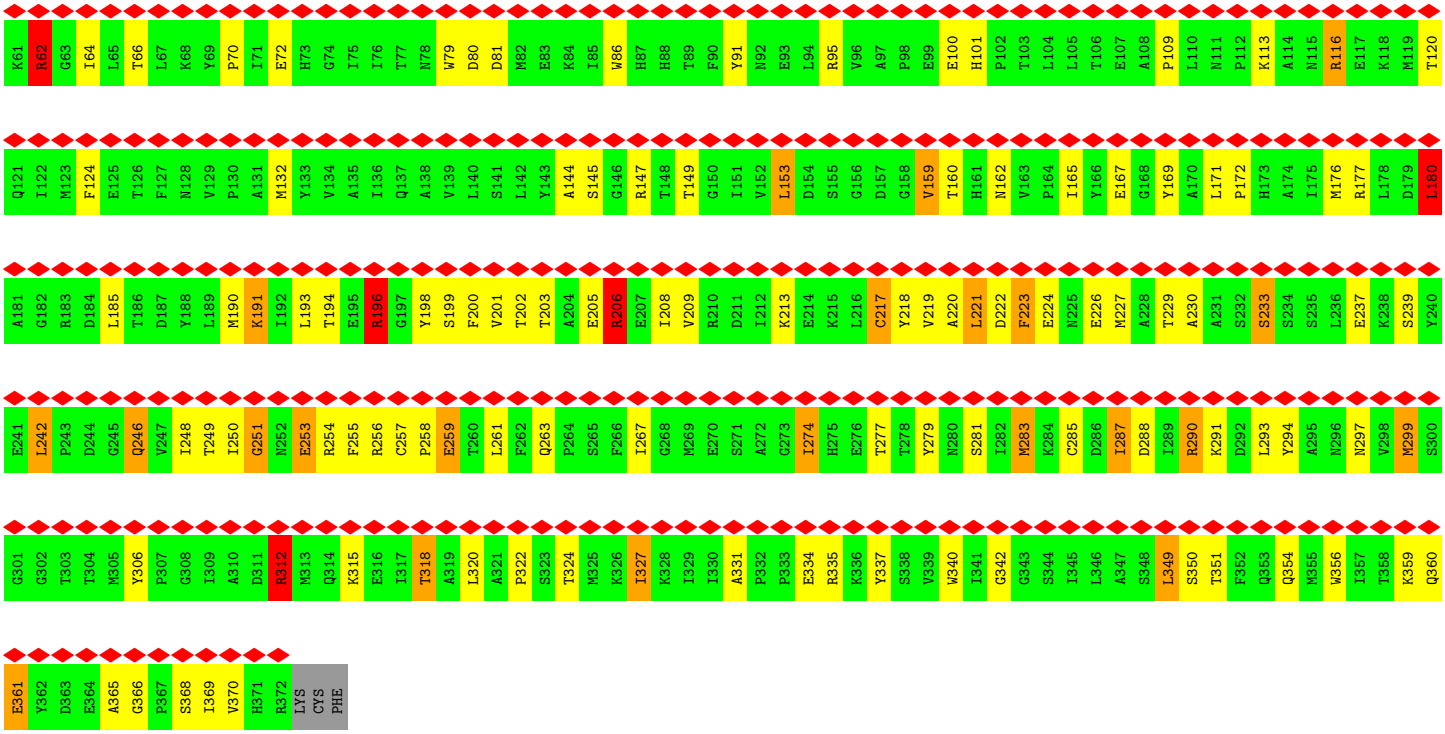


• Molecule 4: SKELETAL MUSCLE ACTIN

Chain 4:

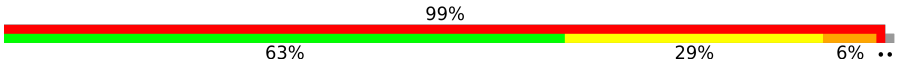


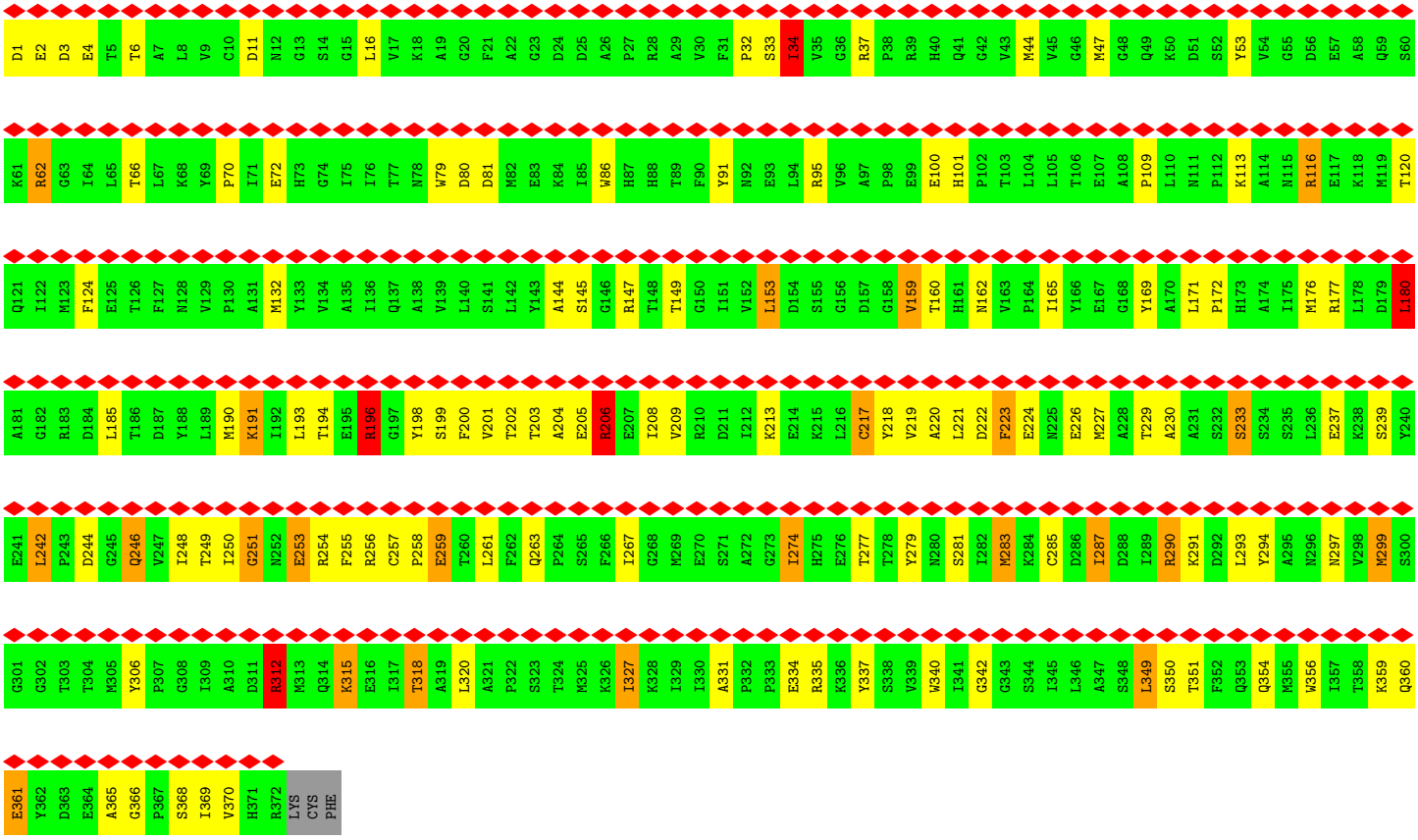




- Molecule 4: SKELETAL MUSCLE ACTIN

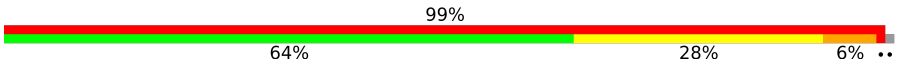
Chain 5:

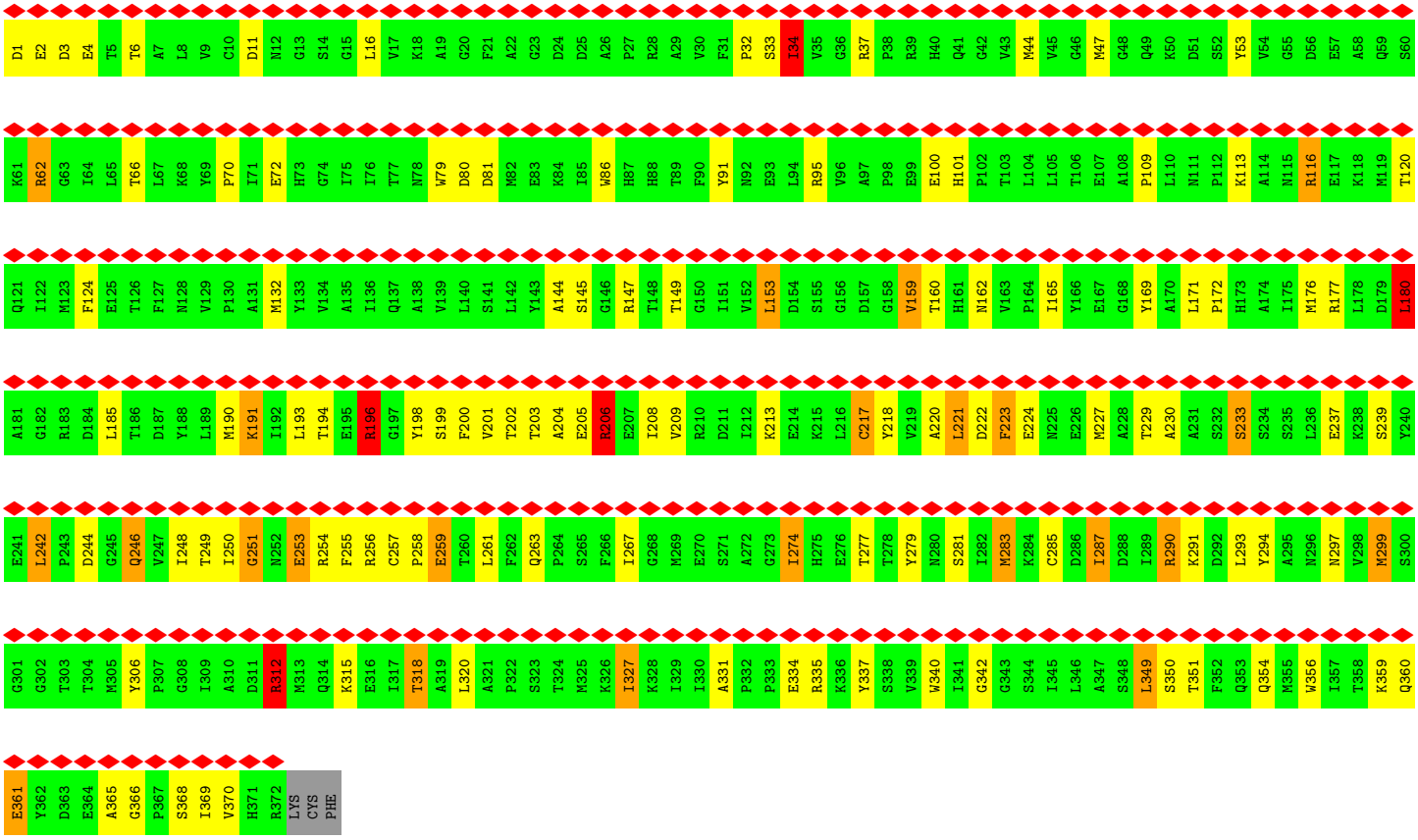




• Molecule 4: SKELETAL MUSCLE ACTIN

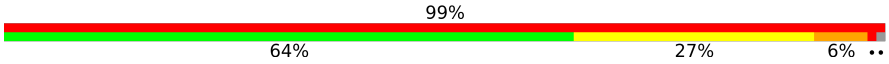
Chain 6:

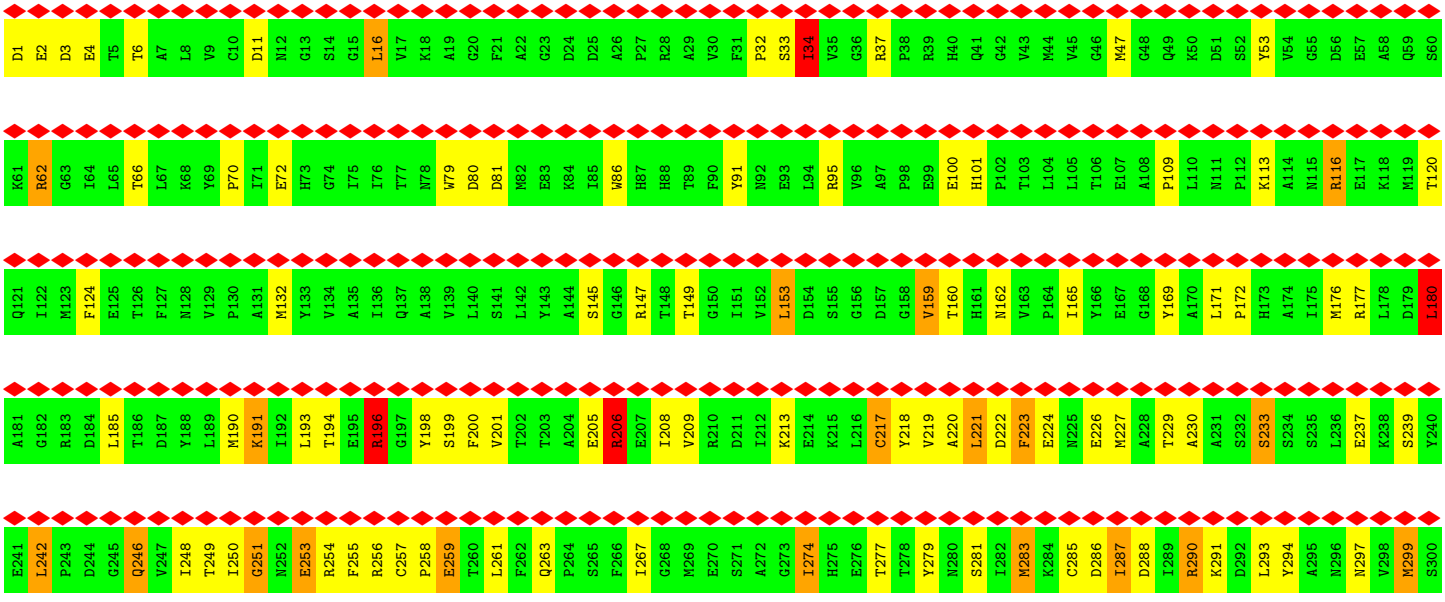


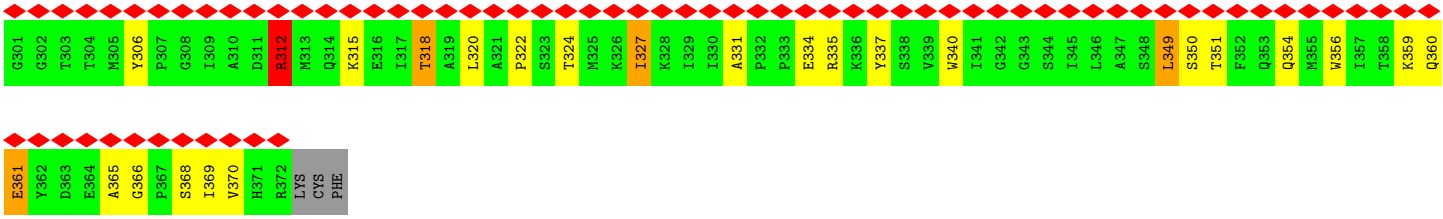


• Molecule 4: SKELETAL MUSCLE ACTIN

Chain 7:

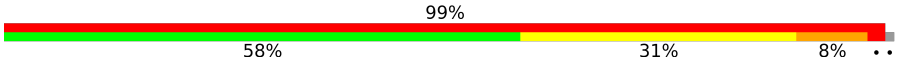


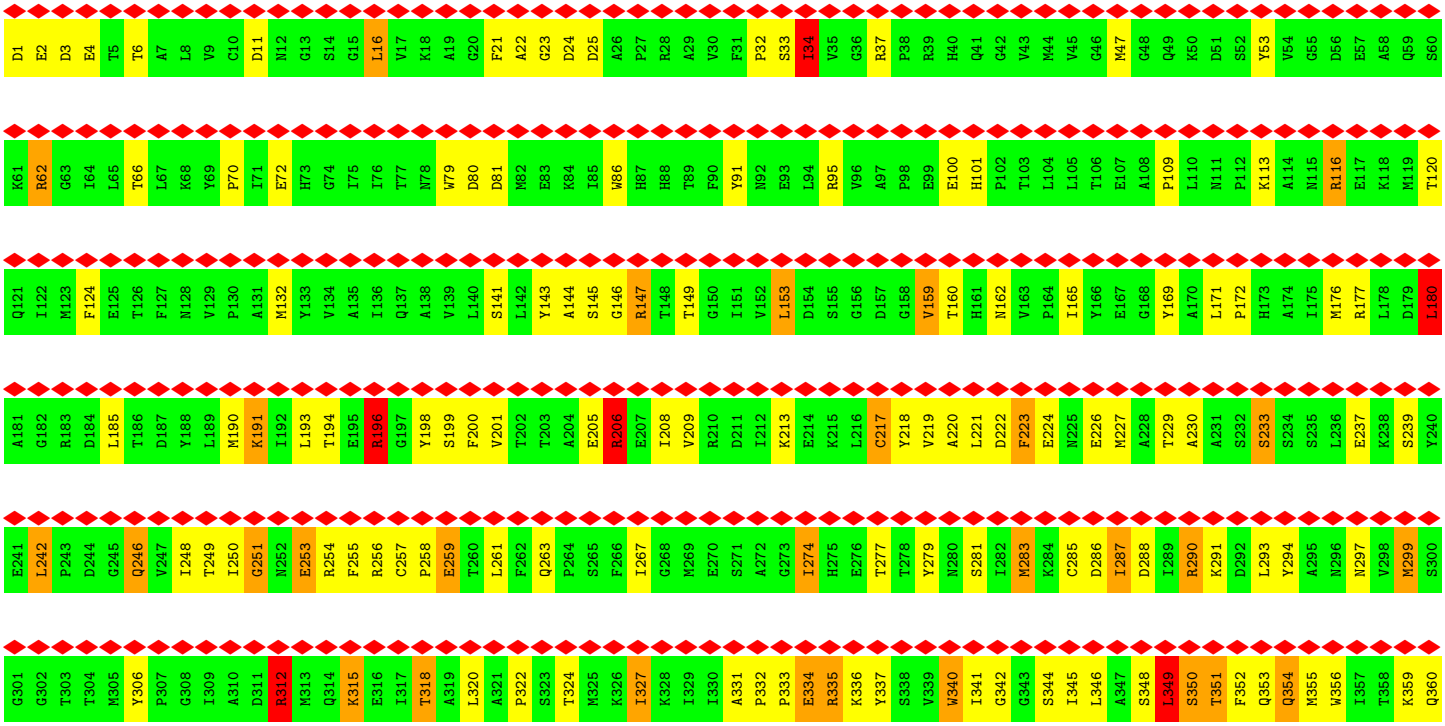




• Molecule 4: SKELETAL MUSCLE ACTIN

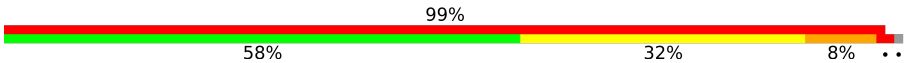
Chain 8:

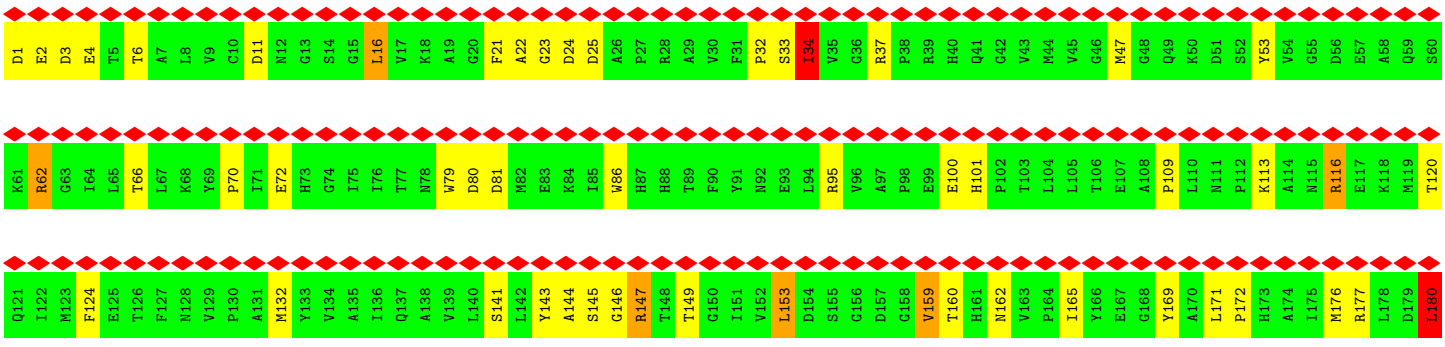




• Molecule 4: SKELETAL MUSCLE ACTIN

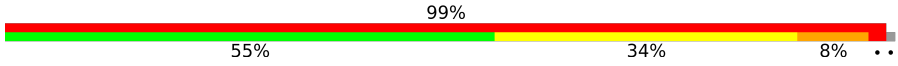
Chain 9:

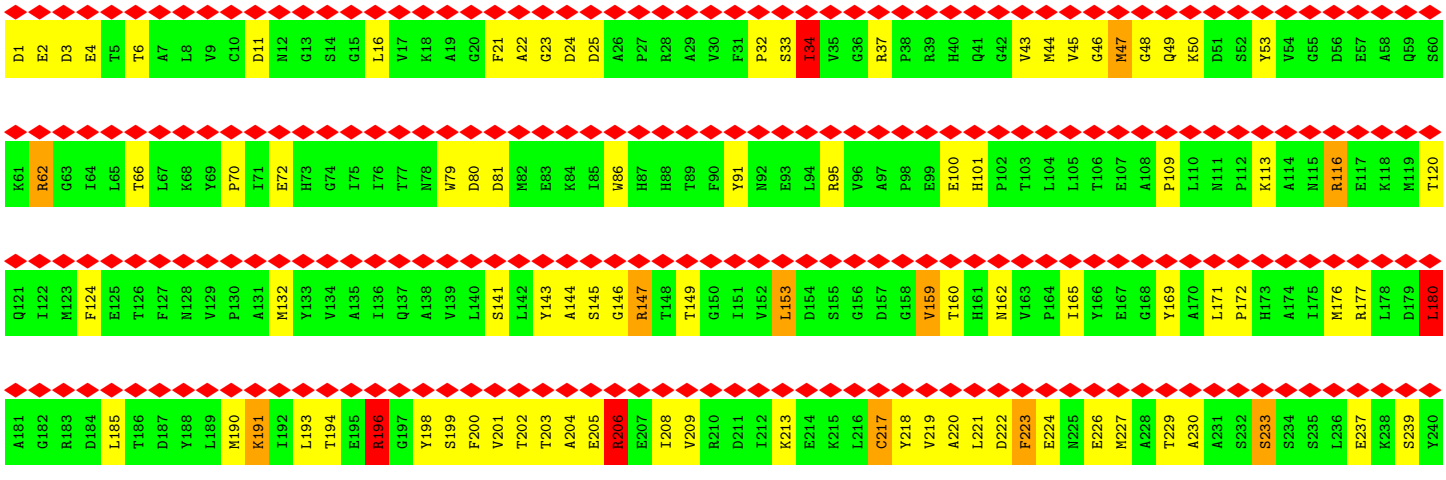




• Molecule 4: SKELETAL MUSCLE ACTIN

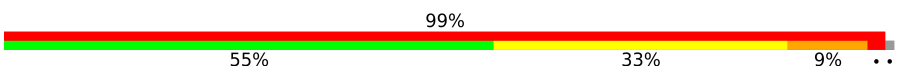
Chain V:

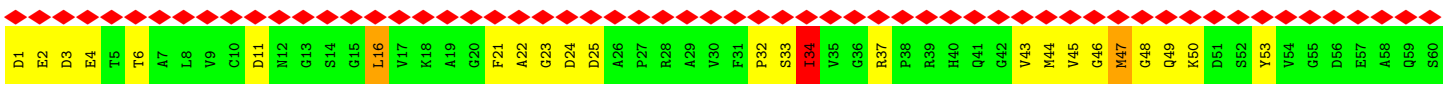


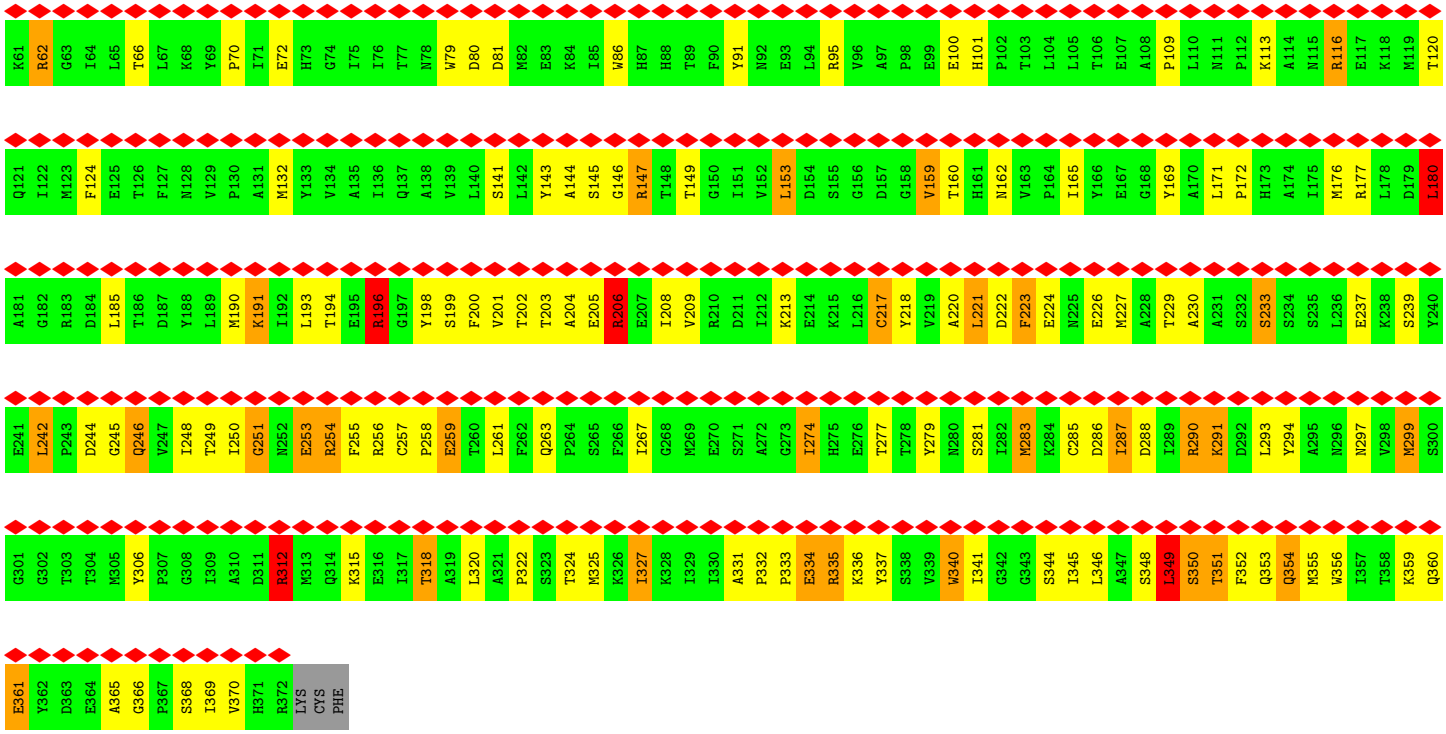


• Molecule 4: SKELETAL MUSCLE ACTIN

Chain W:

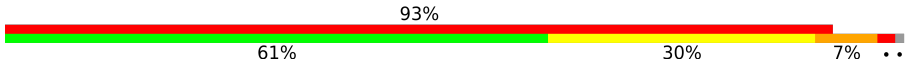


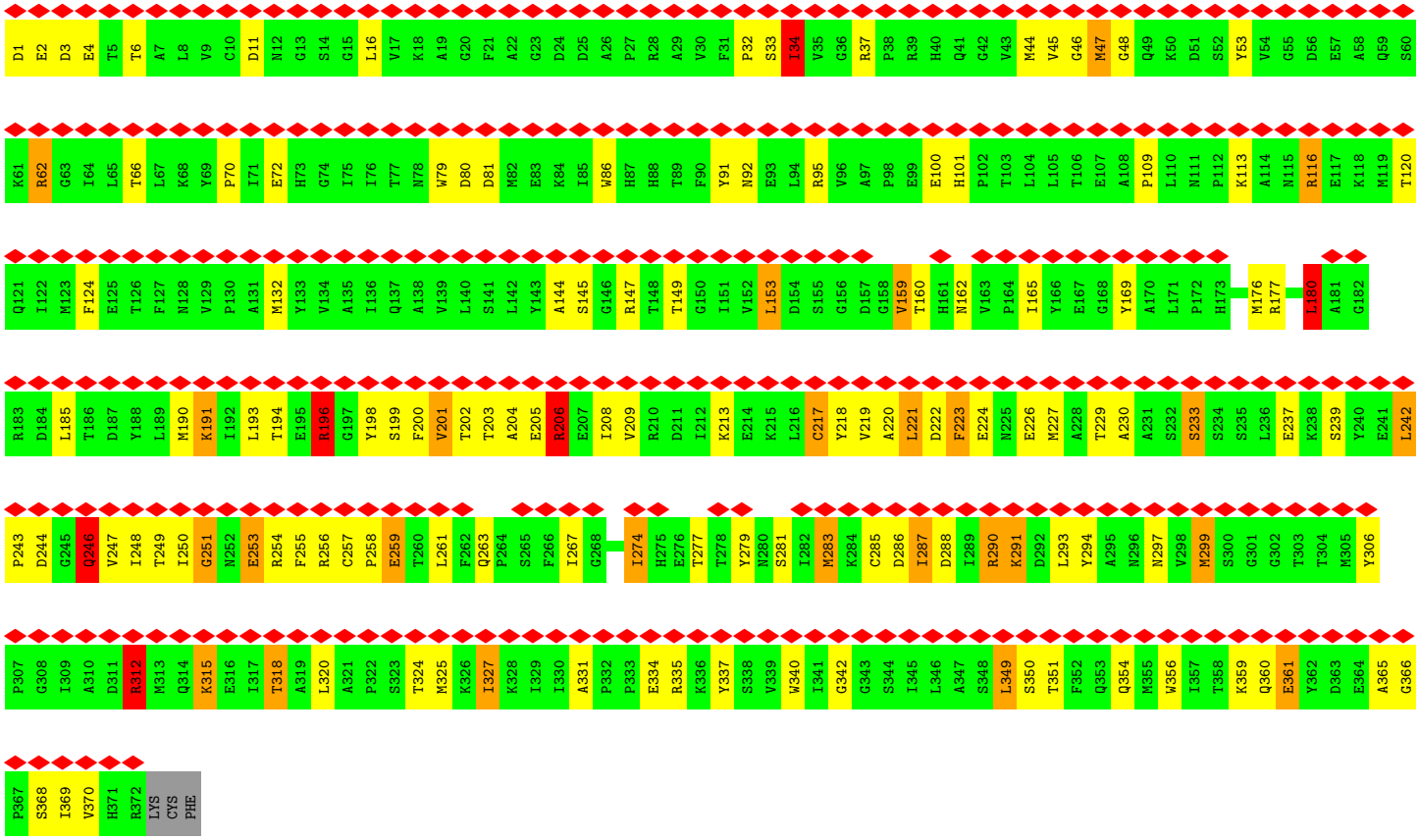




• Molecule 4: SKELETAL MUSCLE ACTIN

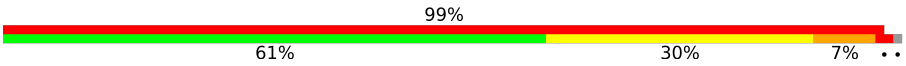
Chain X:

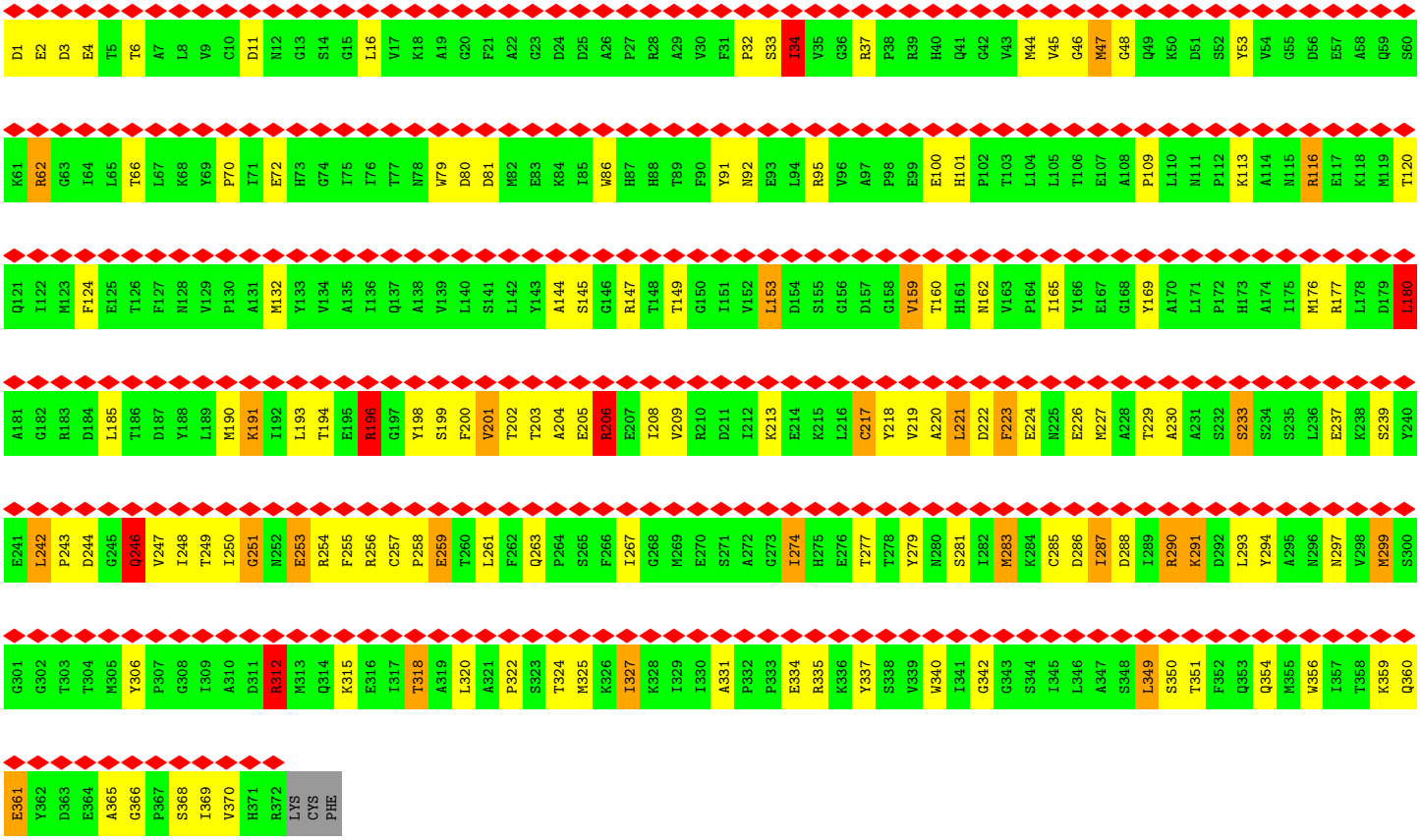




• Molecule 4: SKELETAL MUSCLE ACTIN

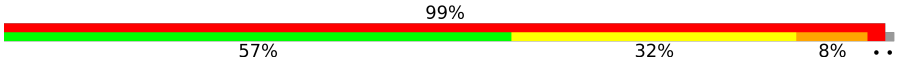
Chain Y:

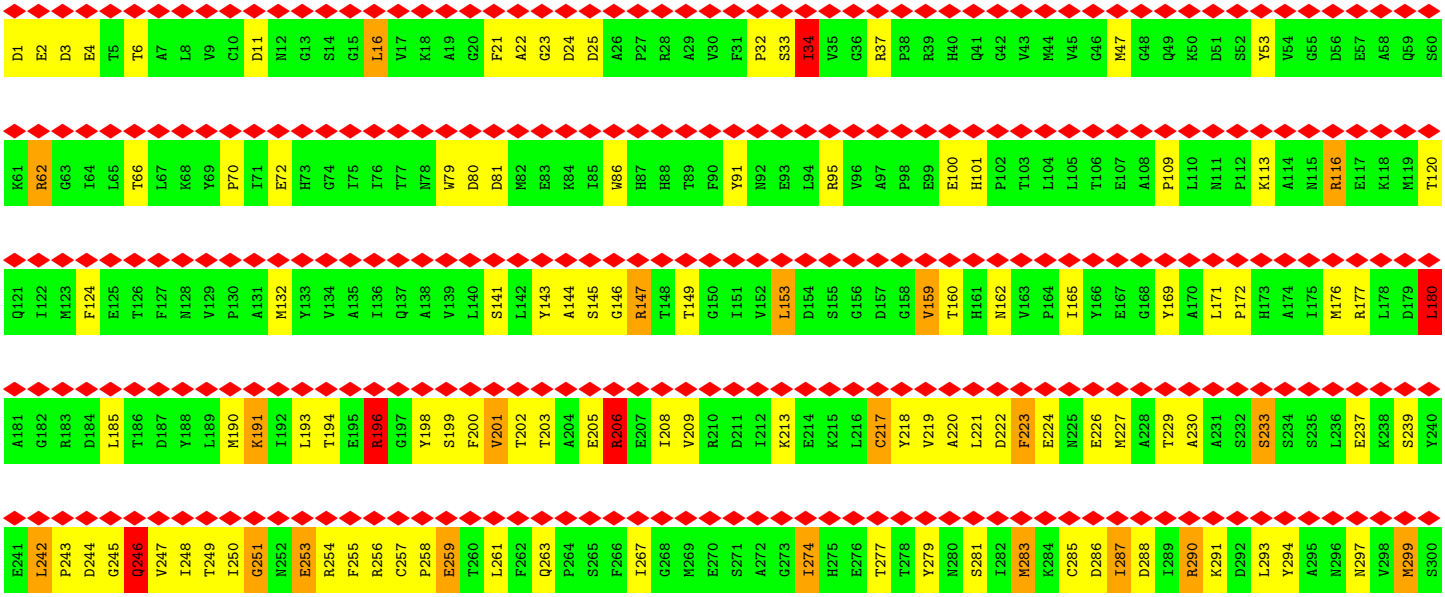


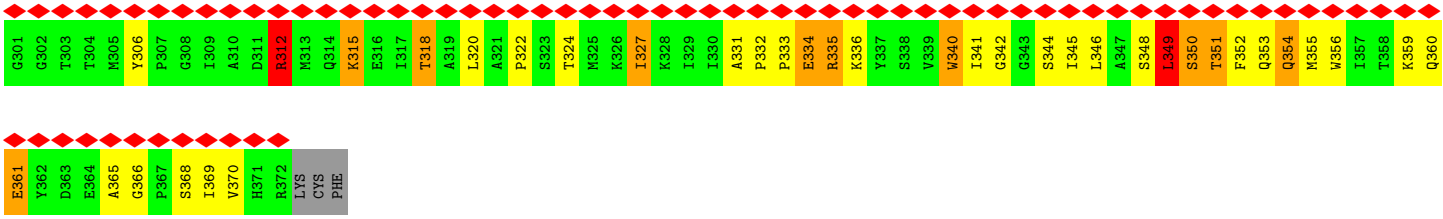


• Molecule 4: SKELETAL MUSCLE ACTIN

Chain Z:






G301 G302 T303 T304 M305 Y306 P307 G308 I309 A310 D311 R312 M313 Q314 K315 E316 I317 T318 A319 L320 A321 P322 S323 T324 M325 K326 I327 K328 I329 I330 A331 P332 P333 E334 R335 K336 Y337 S338 V339 W340 I341 G342 G343 S344 I345 L346 A347 S348 L349 S350 T351 F352 Q353 Q354 M355 W356 I357 T358 K359 Q360
E361 Y362 D363 E364 A365 G366 P367 S368 I369 V370 H371 R372 LYS CYS PHE

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of tilted images used	Not provided	
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	FEI/PHILIPS EM400	Depositor
Voltage (kV)	100	Depositor
Electron dose ($e^-/Å^2$)	Not provided	
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	17000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum voxel value	366.680	Depositor
Minimum voxel value	-417.992	Depositor
Average voxel value	1.860	Depositor
Voxel value standard deviation	47.792	Depositor
Recommended contour level	81.2	Depositor
Tomogram size (Å)	9280, 9280, 464	wwPDB
Tomogram dimensions	600, 600, 30	wwPDB
Tomogram angles (°)	90, 90, 90	wwPDB
Grid spacing (Å)	15.4667, 15.4667, 15.4667	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.77	68/6448 (1.1%)	1.82	116/8729 (1.3%)
1	D	1.77	66/6448 (1.0%)	1.82	115/8729 (1.3%)
1	G	1.77	67/6449 (1.0%)	1.82	118/8732 (1.4%)
1	J	1.79	68/6449 (1.1%)	1.87	118/8732 (1.4%)
1	M	1.77	66/6447 (1.0%)	1.83	119/8726 (1.4%)
1	S	1.78	69/6446 (1.1%)	1.85	119/8723 (1.4%)
2	B	1.22	10/1148 (0.9%)	1.61	16/1548 (1.0%)
2	E	1.21	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	T	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	0.95	4/1525 (0.3%)
3	O	0.79	0/1136	0.95	4/1525 (0.3%)
3	U	0.80	0/1136	0.95	4/1525 (0.3%)
4	1	0.89	2/2968 (0.1%)	1.64	51/4023 (1.3%)
4	2	0.89	2/2968 (0.1%)	1.64	52/4023 (1.3%)
4	3	0.89	2/2968 (0.1%)	1.64	52/4023 (1.3%)
4	4	0.89	2/2968 (0.1%)	1.64	50/4023 (1.2%)
4	5	0.89	2/2968 (0.1%)	1.64	51/4023 (1.3%)
4	6	0.89	1/2968 (0.0%)	1.64	52/4023 (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	52/4023 (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	1/2968 (0.0%)	1.64	52/4023 (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	50/4023 (1.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
All	All	1.34	490/93943 (0.5%)	1.68	1542/127131 (1.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	4
1	D	1	4
1	G	1	5
1	J	1	6
1	M	1	7
1	S	1	7
2	B	0	3
2	E	0	3
2	H	0	3
2	K	0	3
2	N	0	3
2	T	0	3
3	C	0	2
3	F	0	2
3	I	0	2
3	L	0	2
3	O	0	2
3	U	0	2
4	1	0	1
4	2	0	1
4	3	0	1
4	4	0	1
4	5	0	1
4	6	0	1
4	7	0	1
4	8	0	1
4	9	0	1
4	V	0	1
4	W	0	1
4	X	0	1
4	Y	0	1
4	Z	0	1
All	All	6	77

The worst 5 of 490 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	649	VAL	CB-CG1	53.33	2.64	1.52
1	S	649	VAL	CB-CG1	53.30	2.64	1.52
1	M	649	VAL	CB-CG1	53.28	2.64	1.52
1	G	649	VAL	CB-CG1	53.26	2.64	1.52
1	D	649	VAL	CB-CG1	53.22	2.64	1.52

The worst 5 of 1542 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	637	LYS	O-C-N	-58.53	23.70	123.20
1	D	637	LYS	O-C-N	-58.47	23.79	123.20
1	M	637	LYS	O-C-N	-58.47	23.80	123.20
1	S	637	LYS	O-C-N	-58.47	23.80	123.20
1	J	637	LYS	O-C-N	-58.47	23.81	123.20

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	648	THR	CB
1	D	648	THR	CB
1	G	648	THR	CB
1	J	648	THR	CB
1	M	648	THR	CB

5 of 77 planarity outliers are listed below:

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

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6797	0	6755	1473	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	6797	0	6759	1500	0
1	G	6797	0	6762	1471	0
1	J	6797	0	6761	1483	0
1	M	6797	0	6766	1434	0
1	S	6797	0	6764	1607	0
2	B	1127	0	1085	237	0
2	E	1127	0	1088	272	0
2	H	1127	0	1087	258	0
2	K	1127	0	1088	282	0
2	N	1127	0	1088	252	0
2	T	1127	0	1089	262	0
3	C	1123	0	1083	191	0
3	F	1123	0	1084	187	0
3	I	1123	0	1082	184	0
3	L	1123	0	1083	163	0
3	O	1123	0	1084	164	0
3	U	1123	0	1084	292	0
4	1	2906	0	2862	156	0
4	2	2906	0	2853	428	0
4	3	2906	0	2865	219	0
4	4	2906	0	2862	199	0
4	5	2906	0	2866	124	0
4	6	2906	0	2866	117	0
4	7	2906	0	2866	77	0
4	8	2906	0	2857	321	0
4	9	2906	0	2855	339	0
4	V	2906	0	2851	383	0
4	W	2906	0	2851	388	0
4	X	2906	0	2862	210	0
4	Y	2906	0	2861	167	0
4	Z	2906	0	2854	390	0
All	All	94966	0	93623	11394	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 61.

The worst 5 of 11394 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:D:797:PHE:CE2	3:F:126:LEU:HD22	1.17	1.68
4:1:287:ILE:CG1	4:3:203:THR:H	1.06	1.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:783:LEU:CG	1:S:786:ILE:HD11	1.24	1.68
1:D:813:ILE:HG23	2:E:128:PHE:CZ	1.23	1.66
4:4:287:ILE:HG23	4:6:202:THR:CB	1.20	1.65

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	789/840 (94%)	651 (82%)	112 (14%)	26 (3%)	4	26
1	D	789/840 (94%)	651 (82%)	112 (14%)	26 (3%)	4	26
1	G	791/840 (94%)	652 (82%)	112 (14%)	27 (3%)	3	26
1	J	791/840 (94%)	652 (82%)	112 (14%)	27 (3%)	3	26
1	M	787/840 (94%)	649 (82%)	112 (14%)	26 (3%)	4	26
1	S	785/840 (94%)	648 (82%)	110 (14%)	27 (3%)	3	26
2	B	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	2	19
2	E	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	2	19
2	H	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	2	19
2	K	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	2	19
2	N	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	2	19
2	T	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	2	19
3	C	143/147 (97%)	133 (93%)	10 (7%)	0	100	100
3	F	143/147 (97%)	133 (93%)	10 (7%)	0	100	100
3	I	143/147 (97%)	133 (93%)	10 (7%)	0	100	100
3	L	143/147 (97%)	133 (93%)	10 (7%)	0	100	100
3	O	143/147 (97%)	133 (93%)	10 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	U	143/147 (97%)	133 (93%)	10 (7%)	0	100	100
4	1	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	9	44
4	2	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	9	44
4	3	370/375 (99%)	333 (90%)	31 (8%)	6 (2%)	9	44
4	4	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	9	44
4	5	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	9	44
4	6	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	9	44
4	7	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	9	44
4	8	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	9	44
4	9	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	9	44
4	V	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	9	44
4	W	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	9	44
4	X	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	9	44
4	Y	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	9	44
4	Z	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	9	44
All	All	11628/12042 (97%)	10139 (87%)	1198 (10%)	291 (2%)	9	32

5 of 291 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 (i)

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%)	0	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	672/672 (100%)	513 (76%)	159 (24%)	1 4
1	G	672/672 (100%)	513 (76%)	159 (24%)	1 4
1	J	672/672 (100%)	515 (77%)	157 (23%)	1 4
1	M	672/672 (100%)	514 (76%)	158 (24%)	1 4
1	S	672/672 (100%)	515 (77%)	157 (23%)	1 4
2	B	120/120 (100%)	119 (99%)	1 (1%)	81 89
2	E	120/120 (100%)	119 (99%)	1 (1%)	81 89
2	H	120/120 (100%)	119 (99%)	1 (1%)	81 89
2	K	120/120 (100%)	119 (99%)	1 (1%)	81 89
2	N	120/120 (100%)	119 (99%)	1 (1%)	81 89
2	T	120/120 (100%)	119 (99%)	1 (1%)	81 89
3	C	117/117 (100%)	112 (96%)	5 (4%)	29 53
3	F	117/117 (100%)	112 (96%)	5 (4%)	29 53
3	I	117/117 (100%)	112 (96%)	5 (4%)	29 53
3	L	117/117 (100%)	112 (96%)	5 (4%)	29 53
3	O	117/117 (100%)	112 (96%)	5 (4%)	29 53
3	U	117/117 (100%)	112 (96%)	5 (4%)	29 53
4	1	315/318 (99%)	269 (85%)	46 (15%)	3 15
4	2	315/318 (99%)	268 (85%)	47 (15%)	3 15
4	3	315/318 (99%)	269 (85%)	46 (15%)	3 15
4	4	315/318 (99%)	268 (85%)	47 (15%)	3 15
4	5	315/318 (99%)	269 (85%)	46 (15%)	3 15
4	6	315/318 (99%)	269 (85%)	46 (15%)	3 15
4	7	315/318 (99%)	268 (85%)	47 (15%)	3 15
4	8	315/318 (99%)	268 (85%)	47 (15%)	3 15
4	9	315/318 (99%)	268 (85%)	47 (15%)	3 15
4	V	315/318 (99%)	269 (85%)	46 (15%)	3 15
4	W	315/318 (99%)	268 (85%)	47 (15%)	3 15
4	X	315/318 (99%)	269 (85%)	46 (15%)	3 15
4	Y	315/318 (99%)	269 (85%)	46 (15%)	3 15
4	Z	315/318 (99%)	268 (85%)	47 (15%)	3 15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9864/9906 (100%)	8227 (83%)	1637 (17%)	5 12

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

Mol	Chain	Res	Type
1	S	561	LYS
4	4	229	THR
4	Z	116	ARG
1	S	714	ARG
1	S	549	SER

Sometimes 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	221	GLN
4	X	137	GLN
1	S	424	ASN
4	X	41	GLN
4	8	41	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	9,10,11	0.47	0	6,11,13	0.33	0
1	MLY	S	272	1	9,10,11	0.99	1 (11%)	6,11,13	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	MLY	A	617	1	9,10,11	0.96	1 (11%)	6,11,13	0.34	0
1	MLY	A	486	1	9,10,11	0.65	0	6,11,13	0.38	0
1	MLY	M	827	1	9,10,11	0.73	0	6,11,13	0.48	0
1	MLY	A	659	1	9,10,11	0.84	0	6,11,13	0.59	0
1	MLY	G	436	1	9,10,11	1.04	1 (11%)	6,11,13	0.48	0
1	MLY	D	505	1	9,10,11	0.86	1 (11%)	6,11,13	0.35	0
1	MLY	M	19	1	9,10,11	1.16	1 (11%)	6,11,13	0.57	0
1	MLY	S	833	1	9,10,11	1.18	1 (11%)	6,11,13	0.31	0
1	MLY	A	553	1,4	9,10,11	0.68	0	6,11,13	0.55	0
1	MLY	D	431	1	9,10,11	0.53	0	6,11,13	0.45	0
1	MLY	D	598	1	9,10,11	0.91	1 (11%)	6,11,13	0.43	0
1	MLY	J	369	1	9,10,11	0.69	0	6,11,13	0.46	0
1	MLY	G	236	1	9,10,11	0.79	1 (11%)	6,11,13	0.48	0
1	MLY	M	768	1	9,10,11	0.76	0	6,11,13	0.42	0
1	MLY	S	839	1	9,10,11	0.69	0	6,11,13	0.77	0
1	MLY	S	369	1	9,10,11	0.70	0	6,11,13	0.46	0
1	MLY	A	837	1	9,10,11	0.60	0	6,11,13	0.54	0
1	MLY	D	63	1	9,10,11	0.91	0	6,11,13	0.46	0
1	MLY	D	837	1	9,10,11	0.61	0	6,11,13	0.57	0
1	MLY	G	30	1	9,10,11	0.88	0	6,11,13	0.30	0
1	MLY	G	190	1	9,10,11	1.26	1 (11%)	6,11,13	0.51	0
1	MLY	M	55	1	9,10,11	0.73	0	6,11,13	0.78	0
1	MLY	S	19	1	9,10,11	1.17	1 (11%)	6,11,13	0.57	0
1	MLY	J	833	1	9,10,11	1.19	1 (11%)	6,11,13	0.31	0
1	MLY	A	19	1	9,10,11	1.12	1 (11%)	6,11,13	0.58	0
1	MLY	J	49	1	9,10,11	1.08	1 (11%)	6,11,13	0.74	0
1	MLY	M	190	1	9,10,11	1.24	1 (11%)	6,11,13	0.53	0
1	MLY	S	431	1	9,10,11	0.51	0	6,11,13	0.44	0
1	MLY	M	236	1	9,10,11	0.80	1 (11%)	6,11,13	0.47	0
1	MLY	M	30	1	9,10,11	0.89	0	6,11,13	0.32	0
1	MLY	A	248	1	9,10,11	0.83	0	6,11,13	0.61	0
1	MLY	G	839	1	9,10,11	0.71	0	6,11,13	0.80	0
1	MLY	J	617	1	9,10,11	0.96	1 (11%)	6,11,13	0.33	0
1	MLY	J	107	1	9,10,11	0.49	0	6,11,13	0.34	0
1	MLY	D	87	1	9,10,11	1.15	1 (11%)	6,11,13	0.45	0
1	MLY	D	528	1	9,10,11	0.91	0	6,11,13	0.64	0
1	MLY	D	138	1	9,10,11	1.39	1 (11%)	6,11,13	0.86	0
1	MLY	G	681	1	9,10,11	0.62	0	6,11,13	0.45	0
1	MLY	J	659	1	9,10,11	0.82	0	6,11,13	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	MLY	M	782	1	9,10,11	0.78	0	6,11,13	0.36	0
1	MLY	A	764	1	9,10,11	0.84	0	6,11,13	0.36	0
1	MLY	S	107	1	9,10,11	0.48	0	6,11,13	0.35	0
1	MLY	S	436	1	9,10,11	1.04	1 (11%)	6,11,13	0.49	0
1	MLY	D	272	1	9,10,11	0.95	1 (11%)	6,11,13	0.58	0
1	MLY	S	768	1	9,10,11	0.75	0	6,11,13	0.42	0
1	MLY	J	598	1	9,10,11	0.88	1 (11%)	6,11,13	0.43	0
1	MLY	G	369	1	9,10,11	0.70	0	6,11,13	0.46	0
1	MLY	G	84	1	9,10,11	0.49	0	6,11,13	0.80	0
1	MLY	G	504	1	9,10,11	0.88	0	6,11,13	0.22	0
1	MLY	D	613	1	9,10,11	0.58	0	6,11,13	0.63	0
1	MLY	J	84	1	9,10,11	0.49	0	6,11,13	0.80	0
1	MLY	J	63	1	9,10,11	0.89	0	6,11,13	0.43	0
1	MLY	M	505	1	9,10,11	0.93	1 (11%)	6,11,13	0.33	0
1	MLY	G	55	1	9,10,11	0.73	0	6,11,13	0.79	0
1	MLY	S	190	1	9,10,11	1.25	1 (11%)	6,11,13	0.52	0
1	MLY	D	59	1	9,10,11	0.86	0	6,11,13	0.49	0
1	MLY	M	613	1	9,10,11	0.56	0	6,11,13	0.64	0
1	MLY	S	63	1	9,10,11	0.88	0	6,11,13	0.43	0
1	MLY	G	833	1	9,10,11	1.17	2 (22%)	6,11,13	0.33	0
1	MLY	M	84	1	9,10,11	0.50	0	6,11,13	0.80	0
1	MLY	M	600	1	9,10,11	0.53	0	6,11,13	0.37	0
1	MLY	J	295	1	9,10,11	0.78	0	6,11,13	0.35	0
1	MLY	S	367	1	9,10,11	0.63	0	6,11,13	0.38	0
1	MLY	A	190	1	9,10,11	1.26	1 (11%)	6,11,13	0.51	0
1	MLY	J	248	1	9,10,11	0.84	0	6,11,13	0.62	0
1	MLY	M	431	1	9,10,11	0.53	0	6,11,13	0.44	0
1	MLY	G	138	1	9,10,11	1.35	1 (11%)	6,11,13	0.84	0
1	MLY	S	528	1	9,10,11	0.89	0	6,11,13	0.66	0
1	MLY	S	681	1	9,10,11	0.63	0	6,11,13	0.46	0
1	MLY	G	87	1	9,10,11	1.22	1 (11%)	6,11,13	0.43	0
1	MLY	S	55	1	9,10,11	0.73	0	6,11,13	0.77	0
1	MLY	J	505	1	9,10,11	0.93	1 (11%)	6,11,13	0.34	0
1	MLY	M	107	1	9,10,11	0.48	0	6,11,13	0.34	0
1	MLY	J	35	1	9,10,11	0.72	0	6,11,13	0.38	0
1	MLY	M	617	1	9,10,11	0.97	1 (11%)	6,11,13	0.33	0
1	MLY	A	296	1	9,10,11	0.62	0	6,11,13	0.36	0
1	MLY	A	385	1	9,10,11	0.99	1 (11%)	6,11,13	0.43	0
1	MLY	D	35	1	9,10,11	0.73	0	6,11,13	0.37	0
1	MLY	D	107	1	9,10,11	0.51	0	6,11,13	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	MLY	M	486	1	9,10,11	0.64	0	6,11,13	0.40	0
1	MLY	D	617	1	9,10,11	0.96	1 (11%)	6,11,13	0.34	0
1	MLY	J	59	1	9,10,11	0.87	0	6,11,13	0.49	0
1	MLY	G	837	1	9,10,11	0.59	0	6,11,13	0.53	0
1	MLY	M	553	1,4	9,10,11	0.68	0	6,11,13	0.53	0
1	MLY	M	436	1	9,10,11	1.07	1 (11%)	6,11,13	0.50	0
1	MLY	D	553	1,4	9,10,11	0.68	0	6,11,13	0.55	0
1	MLY	S	49	1	9,10,11	1.11	1 (11%)	6,11,13	0.74	0
1	MLY	A	87	1	9,10,11	1.20	1 (11%)	6,11,13	0.42	0
1	MLY	A	504	1	9,10,11	0.90	0	6,11,13	0.24	0
1	MLY	D	504	1	9,10,11	0.88	0	6,11,13	0.21	0
1	MLY	M	369	1	9,10,11	0.70	0	6,11,13	0.45	0
1	MLY	D	839	1	9,10,11	0.67	0	6,11,13	0.79	0
1	MLY	D	369	1	9,10,11	0.69	0	6,11,13	0.44	0
1	MLY	G	295	1	9,10,11	0.78	0	6,11,13	0.33	0
1	MLY	A	600	1	9,10,11	0.50	0	6,11,13	0.37	0
1	MLY	G	248	1	9,10,11	0.81	0	6,11,13	0.63	0
1	MLY	A	138	1	9,10,11	1.33	1 (11%)	6,11,13	0.84	0
1	MLY	S	617	1	9,10,11	0.98	1 (11%)	6,11,13	0.34	0
1	MLY	A	367	1	9,10,11	0.63	0	6,11,13	0.36	0
1	MLY	M	272	1	9,10,11	1.02	1 (11%)	6,11,13	0.56	0
1	MLY	J	431	1	9,10,11	0.53	0	6,11,13	0.45	0
1	MLY	A	436	1	9,10,11	1.04	1 (11%)	6,11,13	0.49	0
1	MLY	G	49	1	9,10,11	1.08	1 (11%)	6,11,13	0.74	0
1	MLY	M	295	1	9,10,11	0.78	0	6,11,13	0.34	0
1	MLY	M	248	1	9,10,11	0.82	0	6,11,13	0.62	0
1	MLY	G	35	1	9,10,11	0.72	0	6,11,13	0.39	0
1	MLY	G	272	1	9,10,11	0.97	1 (11%)	6,11,13	0.54	0
1	MLY	S	764	1	9,10,11	0.83	0	6,11,13	0.38	0
1	MLY	M	87	1	9,10,11	1.20	1 (11%)	6,11,13	0.43	0
1	MLY	A	236	1	9,10,11	0.80	1 (11%)	6,11,13	0.50	0
1	MLY	A	30	1	9,10,11	0.88	0	6,11,13	0.32	0
1	MLY	G	59	1	9,10,11	0.84	0	6,11,13	0.50	0
1	MLY	J	768	1	9,10,11	0.77	0	6,11,13	0.42	0
1	MLY	M	35	1	9,10,11	0.71	0	6,11,13	0.39	0
1	MLY	D	768	1	9,10,11	0.73	0	6,11,13	0.40	0
1	MLY	A	295	1	9,10,11	0.80	0	6,11,13	0.33	0
1	MLY	J	504	1	9,10,11	0.85	0	6,11,13	0.24	0
1	MLY	S	295	1	9,10,11	0.77	0	6,11,13	0.34	0
1	MLY	J	87	1	9,10,11	1.20	1 (11%)	6,11,13	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	MLY	S	348	1	9,10,11	0.80	0	6,11,13	0.47	0
1	MLY	S	782	1	9,10,11	0.77	0	6,11,13	0.37	0
1	MLY	S	248	1	9,10,11	0.82	0	6,11,13	0.62	0
1	MLY	A	827	1	9,10,11	0.72	0	6,11,13	0.46	0
1	MLY	A	839	1	9,10,11	0.68	0	6,11,13	0.81	0
1	MLY	M	59	1	9,10,11	0.88	0	6,11,13	0.49	0
1	MLY	D	600	1	9,10,11	0.51	0	6,11,13	0.37	0
1	MLY	S	827	1	9,10,11	0.72	0	6,11,13	0.49	0
1	MLY	A	782	1	9,10,11	0.79	0	6,11,13	0.37	0
1	MLY	D	367	1	9,10,11	0.61	0	6,11,13	0.38	0
1	MLY	G	431	1	9,10,11	0.52	0	6,11,13	0.46	0
1	MLY	M	504	1	9,10,11	0.85	0	6,11,13	0.23	0
1	MLY	J	353	1	9,10,11	0.86	0	6,11,13	0.78	0
1	MLY	G	130	1	9,10,11	0.78	0	6,11,13	0.75	0
1	MLY	S	505	1	9,10,11	0.92	1 (11%)	6,11,13	0.33	0
1	MLY	G	505	1	9,10,11	0.88	1 (11%)	6,11,13	0.35	0
1	MLY	G	782	1	9,10,11	0.77	0	6,11,13	0.35	0
1	MLY	D	353	1	9,10,11	0.85	0	6,11,13	0.79	0
1	MLY	D	295	1	9,10,11	0.78	0	6,11,13	0.36	0
1	MLY	A	369	1	9,10,11	0.71	0	6,11,13	0.46	0
1	MLY	D	248	1	9,10,11	0.86	0	6,11,13	0.62	0
1	MLY	J	415	1	9,10,11	0.77	0	6,11,13	0.18	0
1	MLY	D	681	1	9,10,11	0.59	0	6,11,13	0.45	0
1	MLY	A	59	1	9,10,11	0.87	0	6,11,13	0.49	0
1	MLY	G	617	1	9,10,11	0.95	1 (11%)	6,11,13	0.35	0
1	MLY	D	415	1	9,10,11	0.79	0	6,11,13	0.19	0
1	MLY	S	84	1	9,10,11	0.50	0	6,11,13	0.80	0
1	MLY	S	296	1	9,10,11	0.68	0	6,11,13	0.36	0
1	MLY	A	63	1	9,10,11	0.92	1 (11%)	6,11,13	0.44	0
1	MLY	A	598	1	9,10,11	0.91	1 (11%)	6,11,13	0.44	0
1	MLY	J	486	1	9,10,11	0.63	0	6,11,13	0.40	0
1	MLY	A	551	1	9,10,11	0.52	0	6,11,13	0.19	0
1	MLY	G	659	1	9,10,11	0.85	0	6,11,13	0.59	0
1	MLY	G	553	1,4	9,10,11	0.67	0	6,11,13	0.55	0
1	MLY	M	764	1	9,10,11	0.83	0	6,11,13	0.38	0
1	MLY	S	385	1	9,10,11	1.01	1 (11%)	6,11,13	0.44	0
1	MLY	D	486	1	9,10,11	0.66	0	6,11,13	0.38	0
1	MLY	S	353	1	9,10,11	0.86	0	6,11,13	0.78	0
1	MLY	M	659	1	9,10,11	0.81	0	6,11,13	0.57	0
1	MLY	G	613	1	9,10,11	0.59	0	6,11,13	0.63	0
1	MLY	G	600	1	9,10,11	0.52	0	6,11,13	0.37	0
1	MLY	J	55	1	9,10,11	0.73	0	6,11,13	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	MLY	S	504	1	9,10,11	0.85	0	6,11,13	0.23	0
1	MLY	S	600	1	9,10,11	0.53	0	6,11,13	0.37	0
1	MLY	S	837	1	9,10,11	0.58	0	6,11,13	0.54	0
1	MLY	J	837	1	9,10,11	0.59	0	6,11,13	0.56	0
1	MLY	M	367	1	9,10,11	0.62	0	6,11,13	0.36	0
1	MLY	S	486	1	9,10,11	0.63	0	6,11,13	0.40	0
1	MLY	A	348	1	9,10,11	0.82	0	6,11,13	0.48	0
1	MLY	A	681	1	9,10,11	0.59	0	6,11,13	0.46	0
1	MLY	G	353	1	9,10,11	0.86	0	6,11,13	0.80	0
1	MLY	J	528	1	9,10,11	0.88	0	6,11,13	0.65	0
1	MLY	A	833	1	9,10,11	1.15	1 (11%)	6,11,13	0.32	0
1	MLY	J	130	1	9,10,11	0.77	0	6,11,13	0.75	0
1	MLY	D	130	1	9,10,11	0.80	0	6,11,13	0.74	0
1	MLY	G	598	1	9,10,11	0.90	1 (11%)	6,11,13	0.42	0
1	MLY	A	84	1	9,10,11	0.49	0	6,11,13	0.79	0
1	MLY	G	528	1	9,10,11	0.91	0	6,11,13	0.66	0
1	MLY	J	190	1	9,10,11	1.25	1 (11%)	6,11,13	0.53	0
1	MLY	D	436	1	9,10,11	1.09	1 (11%)	6,11,13	0.50	0
1	MLY	J	551	1	9,10,11	0.54	0	6,11,13	0.19	0
1	MLY	G	486	1	9,10,11	0.65	0	6,11,13	0.39	0
1	MLY	J	764	1	9,10,11	0.83	0	6,11,13	0.37	0
1	MLY	S	30	1	9,10,11	0.89	0	6,11,13	0.32	0
1	MLY	A	55	1	9,10,11	0.71	0	6,11,13	0.79	0
1	MLY	D	551	1	9,10,11	0.54	0	6,11,13	0.20	0
1	MLY	S	59	1	9,10,11	0.86	0	6,11,13	0.50	0
1	MLY	S	551	1	9,10,11	0.53	0	6,11,13	0.19	0
1	MLY	M	415	1	9,10,11	0.78	0	6,11,13	0.19	0
1	MLY	D	385	1	9,10,11	0.97	1 (11%)	6,11,13	0.44	0
1	MLY	D	236	1	9,10,11	0.79	1 (11%)	6,11,13	0.48	0
1	MLY	D	659	1	9,10,11	0.84	0	6,11,13	0.60	0
1	MLY	J	839	1	9,10,11	0.68	0	6,11,13	0.77	0
1	MLY	J	348	1	9,10,11	0.82	0	6,11,13	0.47	0
1	MLY	D	190	1	9,10,11	1.21	1 (11%)	6,11,13	0.54	0
1	MLY	J	681	1	9,10,11	0.59	0	6,11,13	0.46	0
1	MLY	J	782	1	9,10,11	0.79	0	6,11,13	0.36	0
1	MLY	A	528	1	9,10,11	0.88	0	6,11,13	0.67	0
1	MLY	A	49	1	9,10,11	1.06	1 (11%)	6,11,13	0.74	0
1	MLY	D	348	1	9,10,11	0.82	0	6,11,13	0.47	0
1	MLY	G	107	1	9,10,11	0.48	0	6,11,13	0.34	0
1	MLY	G	19	1	9,10,11	1.15	1 (11%)	6,11,13	0.58	0
1	MLY	M	839	1	9,10,11	0.71	0	6,11,13	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	MLY	D	827	1	9,10,11	0.67	0	6,11,13	0.48	0
1	MLY	A	272	1	9,10,11	1.00	1 (11%)	6,11,13	0.56	0
1	MLY	G	385	1	9,10,11	0.99	1 (11%)	6,11,13	0.44	0
1	MLY	S	415	1	9,10,11	0.77	0	6,11,13	0.18	0
1	MLY	S	598	1	9,10,11	0.89	1 (11%)	6,11,13	0.43	0
1	MLY	D	84	1	9,10,11	0.51	0	6,11,13	0.80	0
1	MLY	G	551	1	9,10,11	0.53	0	6,11,13	0.19	0
1	MLY	S	553	1	9,10,11	0.67	0	6,11,13	0.53	0
1	MLY	G	764	1	9,10,11	0.81	0	6,11,13	0.35	0
1	MLY	M	130	1	9,10,11	0.78	0	6,11,13	0.74	0
1	MLY	D	55	1	9,10,11	0.72	0	6,11,13	0.79	0
1	MLY	G	63	1	9,10,11	0.90	0	6,11,13	0.43	0
1	MLY	M	49	1	9,10,11	1.08	1 (11%)	6,11,13	0.75	0
1	MLY	M	528	1	9,10,11	0.89	0	6,11,13	0.64	0
1	MLY	J	385	1	9,10,11	1.01	1 (11%)	6,11,13	0.44	0
1	MLY	M	598	1	9,10,11	0.91	1 (11%)	6,11,13	0.43	0
1	MLY	J	296	1	9,10,11	0.69	0	6,11,13	0.36	0
1	MLY	D	296	1	9,10,11	0.64	0	6,11,13	0.38	0
1	MLY	M	551	1	9,10,11	0.53	0	6,11,13	0.19	0
1	MLY	J	553	1,4	9,10,11	0.67	0	6,11,13	0.54	0
1	MLY	A	431	1	9,10,11	0.51	0	6,11,13	0.44	0
1	MLY	G	768	1	9,10,11	0.74	0	6,11,13	0.42	0
1	MLY	M	385	1	9,10,11	1.02	1 (11%)	6,11,13	0.44	0
1	MLY	G	348	1	9,10,11	0.87	1 (11%)	6,11,13	0.48	0
1	MLY	D	49	1	9,10,11	1.08	1 (11%)	6,11,13	0.75	0
1	MLY	J	367	1	9,10,11	0.61	0	6,11,13	0.37	0
1	MLY	S	87	1	9,10,11	1.23	1 (11%)	6,11,13	0.43	0
1	MLY	J	827	1	9,10,11	0.75	0	6,11,13	0.48	0
1	MLY	S	138	1	9,10,11	1.33	1 (11%)	6,11,13	0.83	0
1	MLY	G	367	1	9,10,11	0.66	0	6,11,13	0.38	0
1	MLY	J	138	1	9,10,11	1.34	1 (11%)	6,11,13	0.83	0
1	MLY	M	348	1	9,10,11	0.79	0	6,11,13	0.47	0
1	MLY	J	613	1	9,10,11	0.57	0	6,11,13	0.64	0
1	MLY	A	35	1	9,10,11	0.71	0	6,11,13	0.38	0
1	MLY	D	764	1	9,10,11	0.86	0	6,11,13	0.36	0
1	MLY	S	35	1	9,10,11	0.72	0	6,11,13	0.38	0
1	MLY	S	659	1	9,10,11	0.81	0	6,11,13	0.57	0
1	MLY	M	681	1	9,10,11	0.60	0	6,11,13	0.46	0
1	MLY	S	613	1	9,10,11	0.56	0	6,11,13	0.63	0
1	MLY	A	768	1	9,10,11	0.76	0	6,11,13	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	MLY	J	436	1	9,10,11	1.05	1 (11%)	6,11,13	0.50	0
1	MLY	S	130	1	9,10,11	0.78	0	6,11,13	0.75	0
1	MLY	D	833	1	9,10,11	1.15	2 (22%)	6,11,13	0.32	0
1	MLY	A	613	1	9,10,11	0.57	0	6,11,13	0.63	0
1	MLY	M	353	1	9,10,11	0.85	0	6,11,13	0.79	0
1	MLY	G	296	1	9,10,11	0.65	0	6,11,13	0.37	0
1	MLY	G	415	1	9,10,11	0.77	0	6,11,13	0.19	0
1	MLY	J	236	1	9,10,11	0.79	1 (11%)	6,11,13	0.47	0
1	MLY	M	837	1	9,10,11	0.59	0	6,11,13	0.56	0
1	MLY	M	63	1	9,10,11	0.91	0	6,11,13	0.43	0
1	MLY	J	30	1	9,10,11	0.89	0	6,11,13	0.32	0
1	MLY	J	19	1	9,10,11	1.18	1 (11%)	6,11,13	0.57	0
1	MLY	S	236	1	9,10,11	0.78	1 (11%)	6,11,13	0.47	0
1	MLY	D	30	1	9,10,11	0.92	0	6,11,13	0.32	0
1	MLY	D	19	1	9,10,11	1.19	1 (11%)	6,11,13	0.56	0
1	MLY	M	833	1	9,10,11	1.17	1 (11%)	6,11,13	0.31	0
1	MLY	A	353	1	9,10,11	0.86	0	6,11,13	0.79	0
1	MLY	J	600	1	9,10,11	0.53	0	6,11,13	0.37	0
1	MLY	M	296	1	9,10,11	0.71	0	6,11,13	0.36	0
1	MLY	A	130	1	9,10,11	0.80	0	6,11,13	0.74	0
1	MLY	D	782	1	9,10,11	0.79	0	6,11,13	0.34	0
1	MLY	G	827	1	9,10,11	0.71	0	6,11,13	0.49	0
1	MLY	A	505	1	9,10,11	0.88	1 (11%)	6,11,13	0.33	0
1	MLY	J	272	1	9,10,11	0.99	1 (11%)	6,11,13	0.56	0
1	MLY	A	415	1	9,10,11	0.76	0	6,11,13	0.19	0
1	MLY	M	138	1	9,10,11	1.34	1 (11%)	6,11,13	0.83	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	-	2/8/9/11	-
1	MLY	S	272	1	-	3/8/9/11	-
1	MLY	A	617	1	-	1/8/9/11	-
1	MLY	A	486	1	-	2/8/9/11	-
1	MLY	M	827	1	-	0/8/9/11	-
1	MLY	A	659	1	-	3/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	G	436	1	-	4/8/9/11	-
1	MLY	D	505	1	-	5/8/9/11	-
1	MLY	M	19	1	-	4/8/9/11	-
1	MLY	S	833	1	-	6/8/9/11	-
1	MLY	A	553	1,4	-	4/8/9/11	-
1	MLY	D	431	1	-	4/8/9/11	-
1	MLY	D	598	1	-	5/8/9/11	-
1	MLY	J	369	1	-	2/8/9/11	-
1	MLY	G	236	1	-	3/8/9/11	-
1	MLY	M	768	1	-	4/8/9/11	-
1	MLY	S	839	1	-	3/8/9/11	-
1	MLY	S	369	1	-	2/8/9/11	-
1	MLY	A	837	1	-	5/8/9/11	-
1	MLY	D	63	1	-	4/8/9/11	-
1	MLY	D	837	1	-	5/8/9/11	-
1	MLY	G	30	1	-	2/8/9/11	-
1	MLY	G	190	1	-	5/8/9/11	-
1	MLY	M	55	1	-	6/8/9/11	-
1	MLY	S	19	1	-	4/8/9/11	-
1	MLY	J	833	1	-	6/8/9/11	-
1	MLY	A	19	1	-	4/8/9/11	-
1	MLY	J	49	1	-	3/8/9/11	-
1	MLY	M	190	1	-	5/8/9/11	-
1	MLY	S	431	1	-	4/8/9/11	-
1	MLY	M	236	1	-	3/8/9/11	-
1	MLY	M	30	1	-	2/8/9/11	-
1	MLY	A	248	1	-	6/8/9/11	-
1	MLY	G	839	1	-	3/8/9/11	-
1	MLY	J	617	1	-	1/8/9/11	-
1	MLY	J	107	1	-	2/8/9/11	-
1	MLY	D	87	1	-	2/8/9/11	-
1	MLY	D	528	1	-	4/8/9/11	-
1	MLY	D	138	1	-	4/8/9/11	-
1	MLY	G	681	1	-	4/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	J	659	1	-	3/8/9/11	-
1	MLY	M	782	1	-	6/8/9/11	-
1	MLY	A	764	1	-	2/8/9/11	-
1	MLY	S	107	1	-	2/8/9/11	-
1	MLY	S	436	1	-	4/8/9/11	-
1	MLY	D	272	1	-	3/8/9/11	-
1	MLY	S	768	1	-	4/8/9/11	-
1	MLY	J	598	1	-	5/8/9/11	-
1	MLY	G	369	1	-	2/8/9/11	-
1	MLY	G	84	1	-	4/8/9/11	-
1	MLY	G	504	1	-	4/8/9/11	-
1	MLY	D	613	1	-	4/8/9/11	-
1	MLY	J	84	1	-	4/8/9/11	-
1	MLY	J	63	1	-	4/8/9/11	-
1	MLY	M	505	1	-	5/8/9/11	-
1	MLY	G	55	1	-	6/8/9/11	-
1	MLY	S	190	1	-	5/8/9/11	-
1	MLY	D	59	1	-	3/8/9/11	-
1	MLY	M	613	1	-	4/8/9/11	-
1	MLY	S	63	1	-	4/8/9/11	-
1	MLY	G	833	1	-	6/8/9/11	-
1	MLY	M	84	1	-	4/8/9/11	-
1	MLY	M	600	1	-	3/8/9/11	-
1	MLY	J	295	1	-	2/8/9/11	-
1	MLY	S	367	1	-	2/8/9/11	-
1	MLY	A	190	1	-	5/8/9/11	-
1	MLY	J	248	1	-	6/8/9/11	-
1	MLY	M	431	1	-	4/8/9/11	-
1	MLY	G	138	1	-	4/8/9/11	-
1	MLY	S	528	1	-	4/8/9/11	-
1	MLY	S	681	1	-	4/8/9/11	-
1	MLY	G	87	1	-	2/8/9/11	-
1	MLY	S	55	1	-	6/8/9/11	-
1	MLY	J	505	1	-	5/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	M	107	1	-	2/8/9/11	-
1	MLY	J	35	1	-	3/8/9/11	-
1	MLY	M	617	1	-	1/8/9/11	-
1	MLY	A	296	1	-	4/8/9/11	-
1	MLY	A	385	1	-	2/8/9/11	-
1	MLY	D	35	1	-	3/8/9/11	-
1	MLY	D	107	1	-	2/8/9/11	-
1	MLY	M	486	1	-	2/8/9/11	-
1	MLY	D	617	1	-	1/8/9/11	-
1	MLY	J	59	1	-	3/8/9/11	-
1	MLY	G	837	1	-	5/8/9/11	-
1	MLY	M	553	1,4	-	4/8/9/11	-
1	MLY	M	436	1	-	4/8/9/11	-
1	MLY	D	553	1,4	-	5/8/9/11	-
1	MLY	S	49	1	-	3/8/9/11	-
1	MLY	A	87	1	-	2/8/9/11	-
1	MLY	A	504	1	-	4/8/9/11	-
1	MLY	D	504	1	-	4/8/9/11	-
1	MLY	M	369	1	-	2/8/9/11	-
1	MLY	D	839	1	-	3/8/9/11	-
1	MLY	D	369	1	-	2/8/9/11	-
1	MLY	G	295	1	-	2/8/9/11	-
1	MLY	A	600	1	-	3/8/9/11	-
1	MLY	G	248	1	-	6/8/9/11	-
1	MLY	A	138	1	-	4/8/9/11	-
1	MLY	S	617	1	-	1/8/9/11	-
1	MLY	A	367	1	-	2/8/9/11	-
1	MLY	M	272	1	-	3/8/9/11	-
1	MLY	J	431	1	-	4/8/9/11	-
1	MLY	A	436	1	-	4/8/9/11	-
1	MLY	G	49	1	-	3/8/9/11	-
1	MLY	M	295	1	-	2/8/9/11	-
1	MLY	M	248	1	-	6/8/9/11	-
1	MLY	G	35	1	-	3/8/9/11	-
1	MLY	G	272	1	-	3/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	S	764	1	-	2/8/9/11	-
1	MLY	M	87	1	-	2/8/9/11	-
1	MLY	A	236	1	-	3/8/9/11	-
1	MLY	A	30	1	-	2/8/9/11	-
1	MLY	G	59	1	-	3/8/9/11	-
1	MLY	J	768	1	-	4/8/9/11	-
1	MLY	M	35	1	-	3/8/9/11	-
1	MLY	D	768	1	-	4/8/9/11	-
1	MLY	A	295	1	-	2/8/9/11	-
1	MLY	J	504	1	-	4/8/9/11	-
1	MLY	S	295	1	-	2/8/9/11	-
1	MLY	J	87	1	-	2/8/9/11	-
1	MLY	S	348	1	-	5/8/9/11	-
1	MLY	S	782	1	-	6/8/9/11	-
1	MLY	S	248	1	-	6/8/9/11	-
1	MLY	A	827	1	-	0/8/9/11	-
1	MLY	A	839	1	-	3/8/9/11	-
1	MLY	M	59	1	-	3/8/9/11	-
1	MLY	D	600	1	-	3/8/9/11	-
1	MLY	S	827	1	-	0/8/9/11	-
1	MLY	A	782	1	-	6/8/9/11	-
1	MLY	D	367	1	-	2/8/9/11	-
1	MLY	G	431	1	-	4/8/9/11	-
1	MLY	M	504	1	-	4/8/9/11	-
1	MLY	J	353	1	-	4/8/9/11	-
1	MLY	G	130	1	-	5/8/9/11	-
1	MLY	S	505	1	-	5/8/9/11	-
1	MLY	G	505	1	-	5/8/9/11	-
1	MLY	G	782	1	-	6/8/9/11	-
1	MLY	D	353	1	-	4/8/9/11	-
1	MLY	D	295	1	-	2/8/9/11	-
1	MLY	A	369	1	-	2/8/9/11	-
1	MLY	D	248	1	-	6/8/9/11	-
1	MLY	J	415	1	-	3/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	D	681	1	-	4/8/9/11	-
1	MLY	A	59	1	-	3/8/9/11	-
1	MLY	G	617	1	-	1/8/9/11	-
1	MLY	D	415	1	-	3/8/9/11	-
1	MLY	S	84	1	-	4/8/9/11	-
1	MLY	S	296	1	-	4/8/9/11	-
1	MLY	A	63	1	-	4/8/9/11	-
1	MLY	A	598	1	-	5/8/9/11	-
1	MLY	J	486	1	-	2/8/9/11	-
1	MLY	A	551	1	-	3/8/9/11	-
1	MLY	G	659	1	-	3/8/9/11	-
1	MLY	G	553	1,4	-	4/8/9/11	-
1	MLY	M	764	1	-	2/8/9/11	-
1	MLY	S	385	1	-	2/8/9/11	-
1	MLY	D	486	1	-	2/8/9/11	-
1	MLY	S	353	1	-	4/8/9/11	-
1	MLY	M	659	1	-	3/8/9/11	-
1	MLY	G	613	1	-	4/8/9/11	-
1	MLY	G	600	1	-	3/8/9/11	-
1	MLY	J	55	1	-	6/8/9/11	-
1	MLY	S	504	1	-	4/8/9/11	-
1	MLY	S	600	1	-	3/8/9/11	-
1	MLY	S	837	1	-	5/8/9/11	-
1	MLY	J	837	1	-	5/8/9/11	-
1	MLY	M	367	1	-	2/8/9/11	-
1	MLY	S	486	1	-	2/8/9/11	-
1	MLY	A	348	1	-	5/8/9/11	-
1	MLY	A	681	1	-	4/8/9/11	-
1	MLY	G	353	1	-	4/8/9/11	-
1	MLY	J	528	1	-	5/8/9/11	-
1	MLY	A	833	1	-	6/8/9/11	-
1	MLY	J	130	1	-	5/8/9/11	-
1	MLY	D	130	1	-	5/8/9/11	-
1	MLY	G	598	1	-	5/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	A	84	1	-	4/8/9/11	-
1	MLY	G	528	1	-	4/8/9/11	-
1	MLY	J	190	1	-	5/8/9/11	-
1	MLY	D	436	1	-	4/8/9/11	-
1	MLY	J	551	1	-	3/8/9/11	-
1	MLY	G	486	1	-	2/8/9/11	-
1	MLY	J	764	1	-	2/8/9/11	-
1	MLY	S	30	1	-	2/8/9/11	-
1	MLY	A	55	1	-	6/8/9/11	-
1	MLY	D	551	1	-	3/8/9/11	-
1	MLY	S	59	1	-	3/8/9/11	-
1	MLY	S	551	1	-	3/8/9/11	-
1	MLY	M	415	1	-	3/8/9/11	-
1	MLY	D	385	1	-	2/8/9/11	-
1	MLY	D	236	1	-	3/8/9/11	-
1	MLY	D	659	1	-	3/8/9/11	-
1	MLY	J	839	1	-	3/8/9/11	-
1	MLY	J	348	1	-	5/8/9/11	-
1	MLY	D	190	1	-	5/8/9/11	-
1	MLY	J	681	1	-	4/8/9/11	-
1	MLY	J	782	1	-	6/8/9/11	-
1	MLY	A	528	1	-	5/8/9/11	-
1	MLY	A	49	1	-	3/8/9/11	-
1	MLY	D	348	1	-	5/8/9/11	-
1	MLY	G	107	1	-	2/8/9/11	-
1	MLY	G	19	1	-	4/8/9/11	-
1	MLY	M	839	1	-	3/8/9/11	-
1	MLY	D	827	1	-	0/8/9/11	-
1	MLY	A	272	1	-	3/8/9/11	-
1	MLY	G	385	1	-	2/8/9/11	-
1	MLY	S	415	1	-	3/8/9/11	-
1	MLY	S	598	1	-	5/8/9/11	-
1	MLY	D	84	1	-	4/8/9/11	-
1	MLY	G	551	1	-	3/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	S	553	1	-	4/8/9/11	-
1	MLY	G	764	1	-	2/8/9/11	-
1	MLY	M	130	1	-	5/8/9/11	-
1	MLY	D	55	1	-	6/8/9/11	-
1	MLY	G	63	1	-	4/8/9/11	-
1	MLY	M	49	1	-	3/8/9/11	-
1	MLY	M	528	1	-	5/8/9/11	-
1	MLY	J	385	1	-	2/8/9/11	-
1	MLY	M	598	1	-	5/8/9/11	-
1	MLY	J	296	1	-	4/8/9/11	-
1	MLY	D	296	1	-	4/8/9/11	-
1	MLY	M	551	1	-	3/8/9/11	-
1	MLY	J	553	1,4	-	4/8/9/11	-
1	MLY	A	431	1	-	4/8/9/11	-
1	MLY	G	768	1	-	4/8/9/11	-
1	MLY	M	385	1	-	2/8/9/11	-
1	MLY	G	348	1	-	5/8/9/11	-
1	MLY	D	49	1	-	3/8/9/11	-
1	MLY	J	367	1	-	2/8/9/11	-
1	MLY	S	87	1	-	2/8/9/11	-
1	MLY	J	827	1	-	0/8/9/11	-
1	MLY	S	138	1	-	4/8/9/11	-
1	MLY	G	367	1	-	2/8/9/11	-
1	MLY	J	138	1	-	4/8/9/11	-
1	MLY	M	348	1	-	5/8/9/11	-
1	MLY	J	613	1	-	4/8/9/11	-
1	MLY	A	35	1	-	3/8/9/11	-
1	MLY	D	764	1	-	2/8/9/11	-
1	MLY	S	35	1	-	3/8/9/11	-
1	MLY	S	659	1	-	3/8/9/11	-
1	MLY	M	681	1	-	4/8/9/11	-
1	MLY	S	613	1	-	4/8/9/11	-
1	MLY	A	768	1	-	4/8/9/11	-
1	MLY	J	436	1	-	4/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	S	130	1	-	5/8/9/11	-
1	MLY	D	833	1	-	6/8/9/11	-
1	MLY	A	613	1	-	4/8/9/11	-
1	MLY	M	353	1	-	4/8/9/11	-
1	MLY	G	296	1	-	4/8/9/11	-
1	MLY	G	415	1	-	3/8/9/11	-
1	MLY	J	236	1	-	3/8/9/11	-
1	MLY	M	837	1	-	5/8/9/11	-
1	MLY	M	63	1	-	4/8/9/11	-
1	MLY	J	30	1	-	2/8/9/11	-
1	MLY	J	19	1	-	4/8/9/11	-
1	MLY	S	236	1	-	3/8/9/11	-
1	MLY	D	30	1	-	2/8/9/11	-
1	MLY	D	19	1	-	4/8/9/11	-
1	MLY	M	833	1	-	6/8/9/11	-
1	MLY	A	353	1	-	4/8/9/11	-
1	MLY	J	600	1	-	3/8/9/11	-
1	MLY	M	296	1	-	4/8/9/11	-
1	MLY	A	130	1	-	5/8/9/11	-
1	MLY	D	782	1	-	6/8/9/11	-
1	MLY	G	827	1	-	0/8/9/11	-
1	MLY	A	505	1	-	5/8/9/11	-
1	MLY	J	272	1	-	3/8/9/11	-
1	MLY	A	415	1	-	3/8/9/11	-
1	MLY	M	138	1	-	4/8/9/11	-

The worst 5 of 82 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	138	MLY	CB-CA	-3.81	1.48	1.53
1	G	138	MLY	CB-CA	-3.70	1.48	1.53
1	J	138	MLY	CB-CA	-3.67	1.48	1.53
1	M	138	MLY	CB-CA	-3.66	1.48	1.53
1	S	138	MLY	CB-CA	-3.62	1.48	1.53

There are no bond angle outliers.

There are no chirality outliers.

5 of 958 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	19	MLY	C-CA-CB-CG
1	A	49	MLY	N-CA-CB-CG
1	A	49	MLY	C-CA-CB-CG
1	A	55	MLY	N-CA-CB-CG
1	A	55	MLY	C-CA-CB-CG

There are no ring outliers.

186 monomers are involved in 820 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	107	MLY	2	0
1	S	272	MLY	1	0
1	A	617	MLY	1	0
1	A	486	MLY	3	0
1	A	659	MLY	2	0
1	G	436	MLY	2	0
1	A	553	MLY	17	0
1	D	598	MLY	1	0
1	M	768	MLY	1	0
1	S	839	MLY	15	0
1	S	369	MLY	1	0
1	A	837	MLY	1	0
1	D	63	MLY	4	0
1	D	837	MLY	1	0
1	G	30	MLY	1	0
1	G	190	MLY	2	0
1	M	55	MLY	1	0
1	J	49	MLY	4	0
1	M	190	MLY	2	0
1	M	30	MLY	1	0
1	A	248	MLY	2	0
1	G	839	MLY	4	0
1	J	617	MLY	1	0
1	J	107	MLY	3	0
1	D	87	MLY	3	0
1	D	528	MLY	3	0
1	D	138	MLY	1	0
1	J	659	MLY	2	0
1	M	782	MLY	3	0
1	A	764	MLY	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	S	107	MLY	3	0
1	S	436	MLY	2	0
1	D	272	MLY	1	0
1	J	598	MLY	1	0
1	G	369	MLY	1	0
1	G	84	MLY	16	0
1	J	84	MLY	43	0
1	J	63	MLY	4	0
1	M	505	MLY	2	0
1	G	55	MLY	1	0
1	S	190	MLY	2	0
1	D	59	MLY	2	0
1	S	63	MLY	3	0
1	M	84	MLY	23	0
1	M	600	MLY	1	0
1	J	295	MLY	7	0
1	A	190	MLY	2	0
1	J	248	MLY	2	0
1	G	138	MLY	1	0
1	S	528	MLY	3	0
1	G	87	MLY	3	0
1	S	55	MLY	1	0
1	J	505	MLY	9	0
1	M	107	MLY	4	0
1	M	617	MLY	1	0
1	A	296	MLY	3	0
1	D	107	MLY	3	0
1	M	486	MLY	3	0
1	D	617	MLY	1	0
1	J	59	MLY	2	0
1	G	837	MLY	1	0
1	M	553	MLY	17	0
1	M	436	MLY	2	0
1	D	553	MLY	16	0
1	S	49	MLY	3	0
1	A	87	MLY	3	0
1	A	504	MLY	4	0
1	M	369	MLY	1	0
1	D	839	MLY	7	0
1	G	295	MLY	7	0
1	A	600	MLY	1	0
1	G	248	MLY	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	138	MLY	1	0
1	S	617	MLY	1	0
1	M	272	MLY	1	0
1	A	436	MLY	3	0
1	G	49	MLY	3	0
1	M	295	MLY	6	0
1	M	248	MLY	2	0
1	G	272	MLY	1	0
1	S	764	MLY	31	0
1	M	87	MLY	3	0
1	A	30	MLY	1	0
1	G	59	MLY	2	0
1	J	768	MLY	9	0
1	M	35	MLY	13	0
1	D	768	MLY	1	0
1	A	295	MLY	6	0
1	S	295	MLY	6	0
1	J	87	MLY	3	0
1	S	348	MLY	6	0
1	S	782	MLY	1	0
1	S	248	MLY	2	0
1	A	839	MLY	9	0
1	M	59	MLY	2	0
1	D	600	MLY	1	0
1	A	782	MLY	8	0
1	S	505	MLY	8	0
1	G	782	MLY	1	0
1	D	295	MLY	6	0
1	A	369	MLY	1	0
1	D	248	MLY	2	0
1	J	415	MLY	1	0
1	A	59	MLY	2	0
1	G	617	MLY	1	0
1	D	415	MLY	1	0
1	S	84	MLY	14	0
1	S	296	MLY	3	0
1	A	63	MLY	3	0
1	A	598	MLY	1	0
1	J	486	MLY	3	0
1	A	551	MLY	2	0
1	G	659	MLY	2	0
1	G	553	MLY	26	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	M	764	MLY	5	0
1	D	486	MLY	3	0
1	M	659	MLY	2	0
1	G	600	MLY	1	0
1	J	55	MLY	1	0
1	S	600	MLY	1	0
1	S	837	MLY	1	0
1	J	837	MLY	1	0
1	S	486	MLY	3	0
1	A	348	MLY	5	0
1	J	528	MLY	3	0
1	G	598	MLY	1	0
1	G	528	MLY	3	0
1	J	190	MLY	2	0
1	D	436	MLY	3	0
1	G	486	MLY	3	0
1	J	764	MLY	7	0
1	S	30	MLY	1	0
1	A	55	MLY	1	0
1	D	551	MLY	2	0
1	S	59	MLY	2	0
1	M	415	MLY	1	0
1	D	659	MLY	2	0
1	J	839	MLY	15	0
1	J	348	MLY	5	0
1	D	190	MLY	2	0
1	J	782	MLY	1	0
1	A	528	MLY	3	0
1	A	49	MLY	3	0
1	D	348	MLY	6	0
1	G	107	MLY	2	0
1	M	839	MLY	7	0
1	D	827	MLY	3	0
1	A	272	MLY	1	0
1	S	415	MLY	1	0
1	S	598	MLY	1	0
1	S	553	MLY	3	0
1	G	764	MLY	8	0
1	D	55	MLY	1	0
1	G	63	MLY	4	0
1	M	49	MLY	3	0
1	M	528	MLY	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	M	598	MLY	1	0
1	J	296	MLY	3	0
1	D	296	MLY	3	0
1	M	551	MLY	1	0
1	J	553	MLY	27	0
1	G	768	MLY	9	0
1	G	348	MLY	4	0
1	D	49	MLY	3	0
1	S	87	MLY	3	0
1	S	138	MLY	1	0
1	J	138	MLY	1	0
1	M	348	MLY	6	0
1	D	764	MLY	6	0
1	S	659	MLY	2	0
1	A	768	MLY	12	0
1	J	436	MLY	2	0
1	G	296	MLY	2	0
1	G	415	MLY	1	0
1	M	837	MLY	1	0
1	M	63	MLY	4	0
1	J	30	MLY	1	0
1	D	30	MLY	1	0
1	J	600	MLY	1	0
1	M	296	MLY	3	0
1	D	782	MLY	71	0
1	G	827	MLY	1	0
1	A	505	MLY	24	0
1	J	272	MLY	1	0
1	A	415	MLY	1	0
1	M	138	MLY	1	0

5.5 Carbohydrates (i)

There are no monosaccharides 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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	S	8
1	M	5
1	J	4
1	D	4
1	A	4
1	G	3
3	C	1
3	F	1
3	I	1
3	L	1
3	O	1
3	U	1
2	H	1
2	B	1
2	E	1
2	K	1
2	N	1
2	T	1

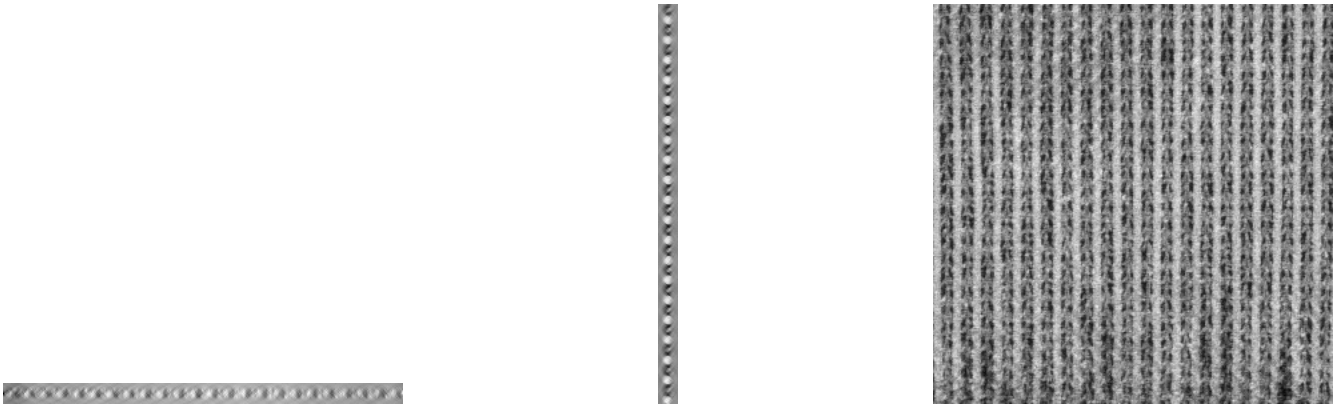
The worst 5 of 40 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	J	769:ALA	C	770:GLY	N	5.58
1	D	769:ALA	C	770:GLY	N	5.32
1	G	769:ALA	C	770:GLY	N	4.88
1	M	769:ALA	C	770:GLY	N	3.92
1	A	709:LYS	C	710:GLY	N	3.14

6 Tomogram visualisation

This section contains visualisations of the EMDB entry EMD-1001. These allow visual inspection of the internal detail of the tomogram and identification of artifacts.

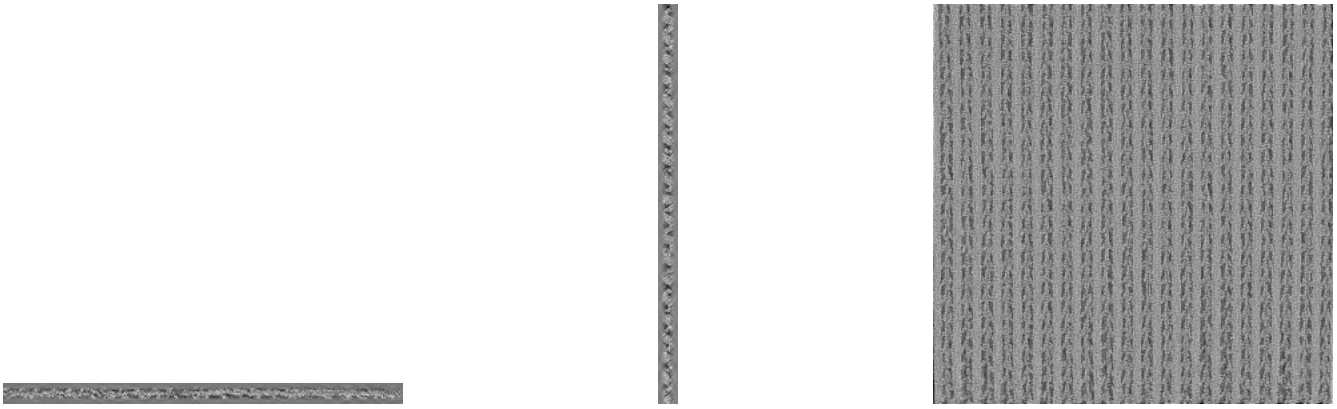
6.1 Orthogonal projections



X Y Z

The images above show the tomogram projected in three orthogonal directions.

6.2 Central slices



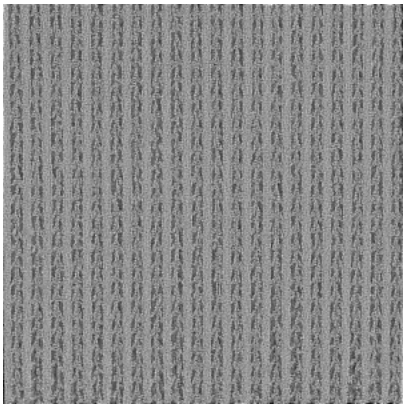
X Index: 300 Y Index: 300 Z Index: 15

The images above show central slices of the tomogram in three orthogonal directions.

6.3 Largest variance slices (i)

X Index: 598

Y Index: 598

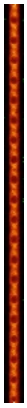


Z Index: 15

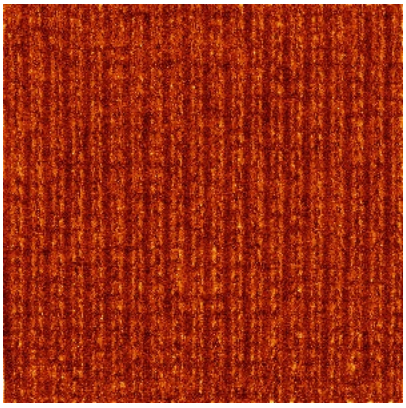
The images above show the largest variance slices of the tomogram in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

X



Y



Z

The images above show the tomogram projected in three orthogonal directions.

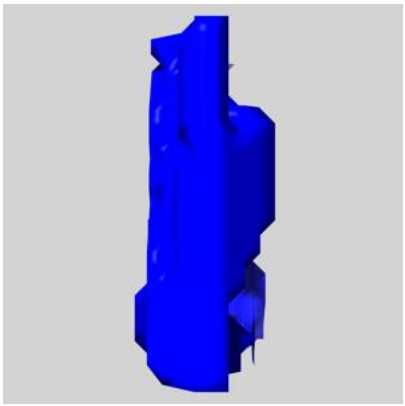
6.5 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

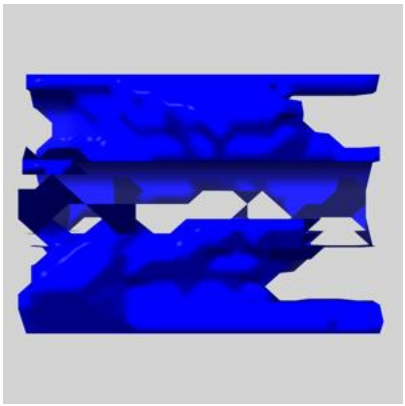
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

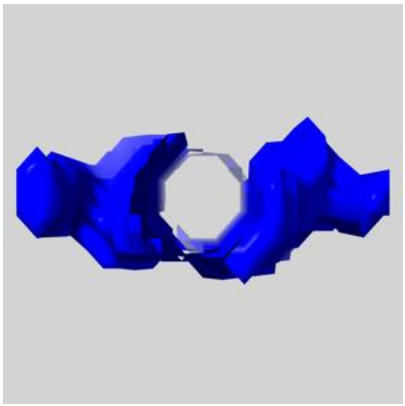
6.5.1 emd_1001_msk_25.map (i)



X

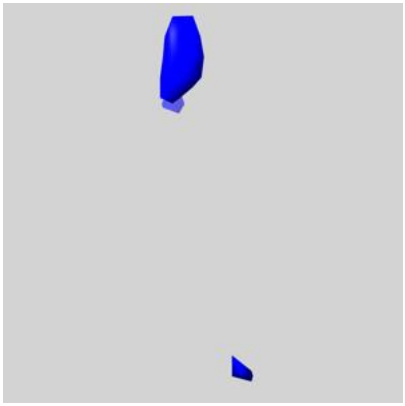


Y

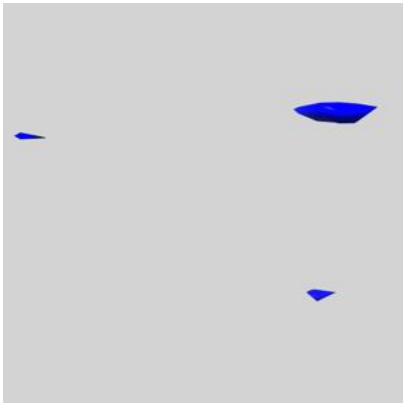


Z

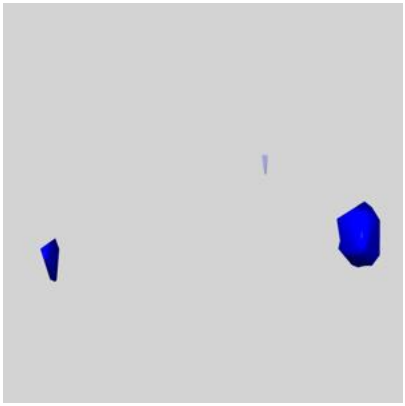
6.5.2 emd_1001_msk_24.map (i)



X

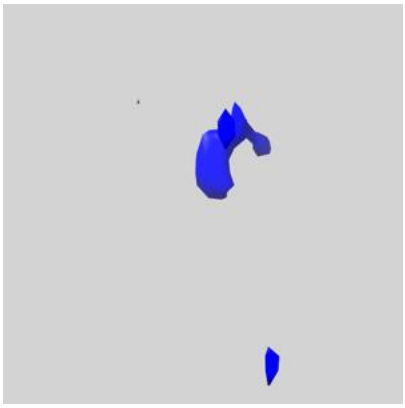


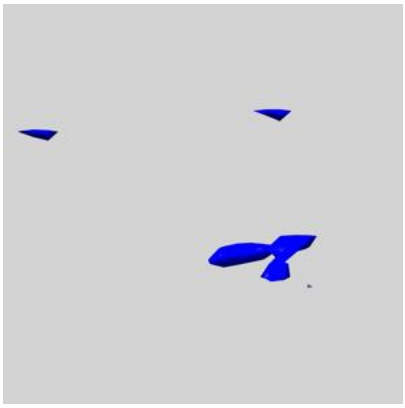
Y

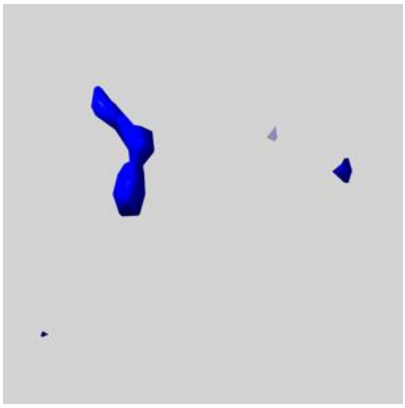


Z

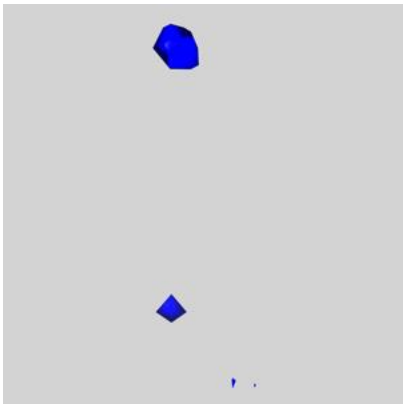
6.5.3 emd_1001_msk_23.map

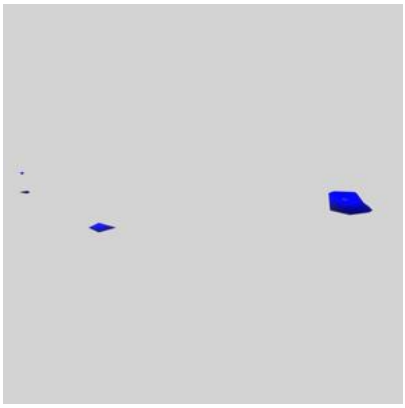

X

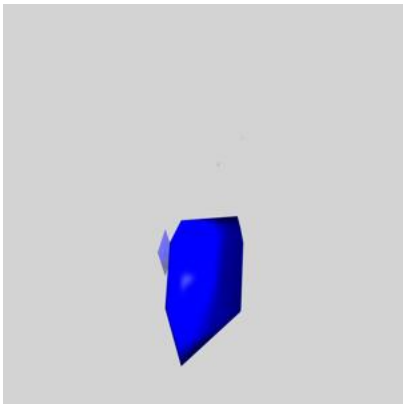

Y


Z

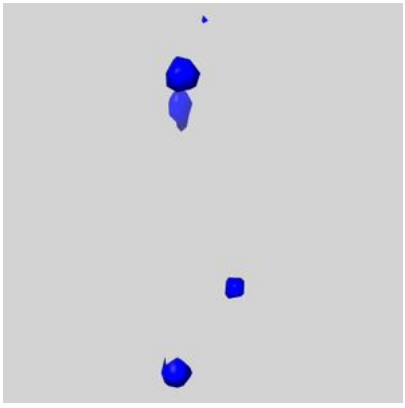
6.5.4 emd_1001_msk_22.map

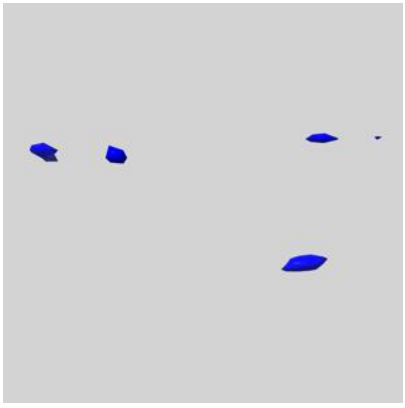

X

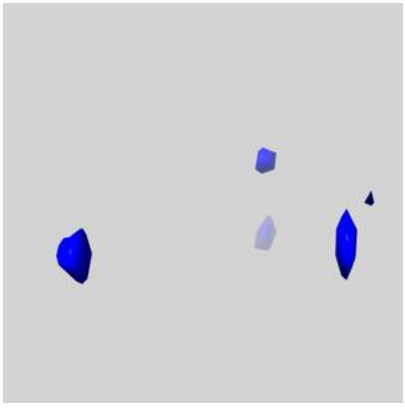

Y


Z

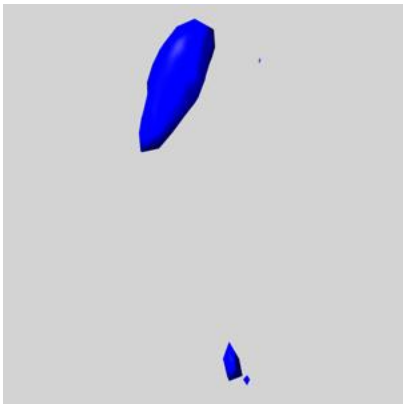
6.5.5 emd_1001_msk_21.map


X

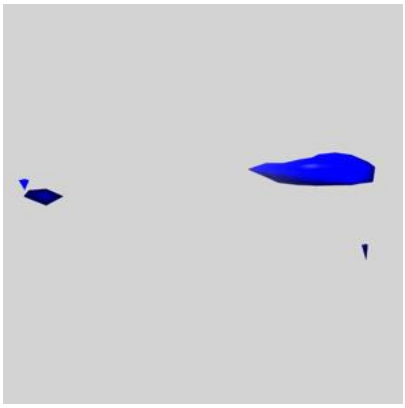

Y


Z

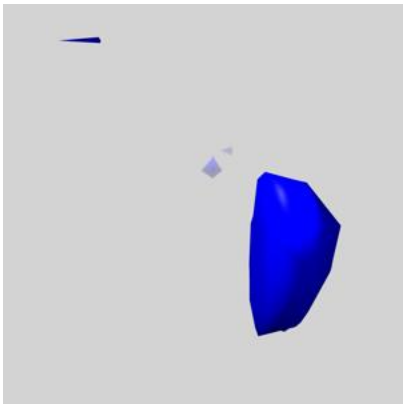
6.5.6 emd_1001_msk_20.map



X

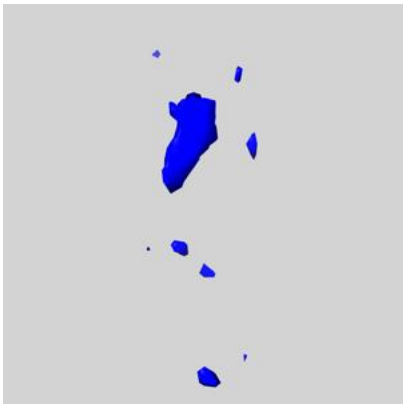


Y

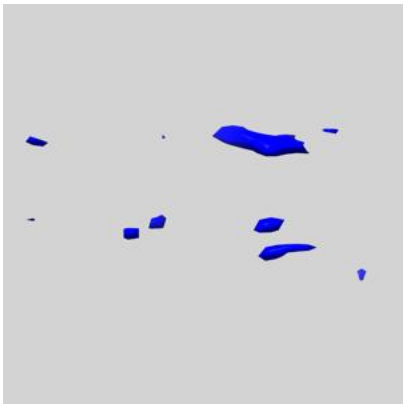


Z

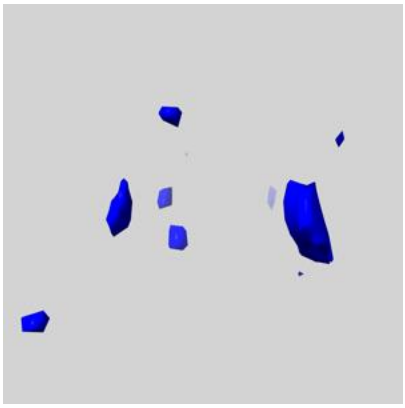
6.5.7 emd_1001_msk_19.map



X

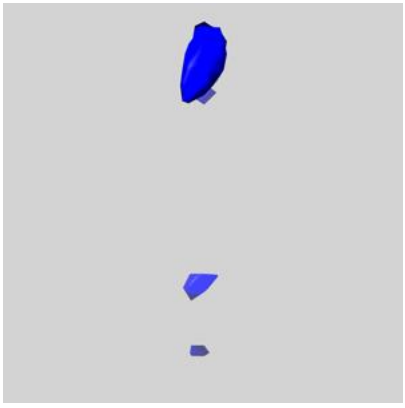


Y

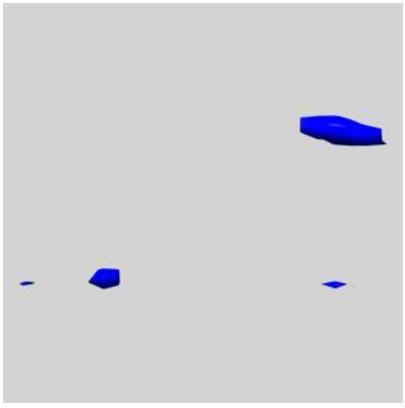


Z

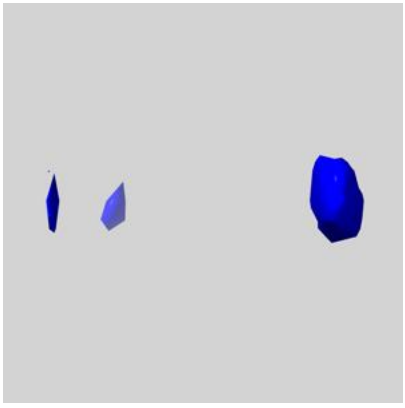
6.5.8 emd_1001_msk_18.map



X

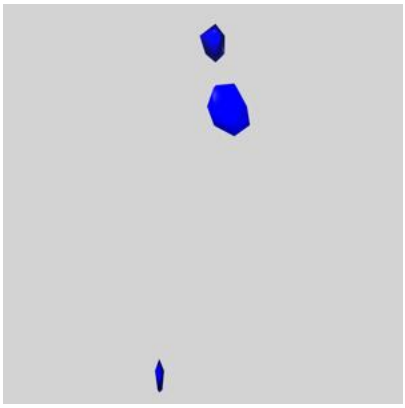


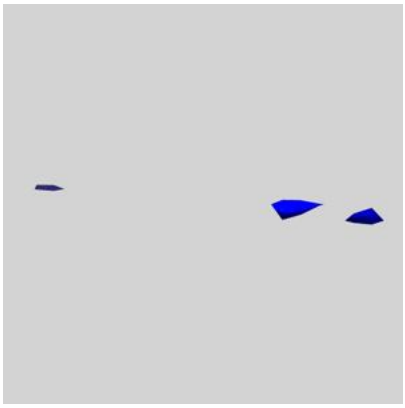
Y

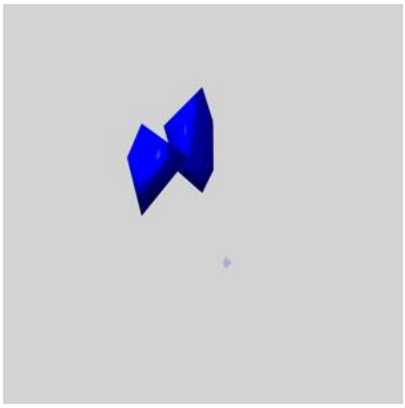


Z

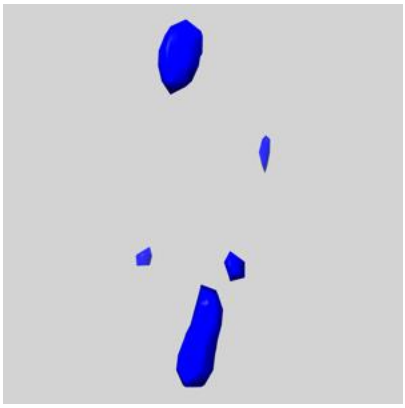
6.5.9 emd_1001_msk_17.map

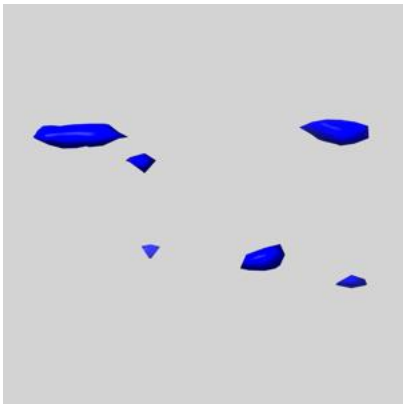

X

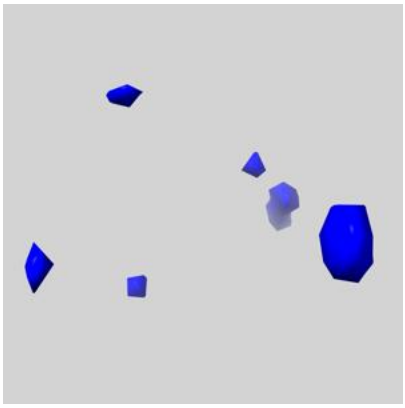

Y


Z

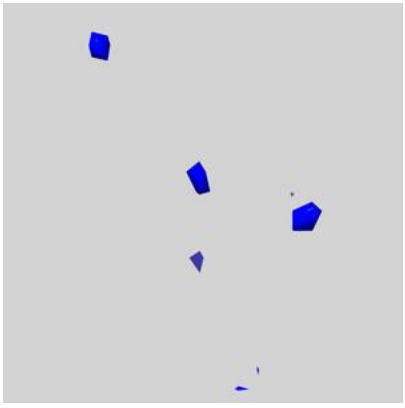
6.5.10 emd_1001_msk_16.map

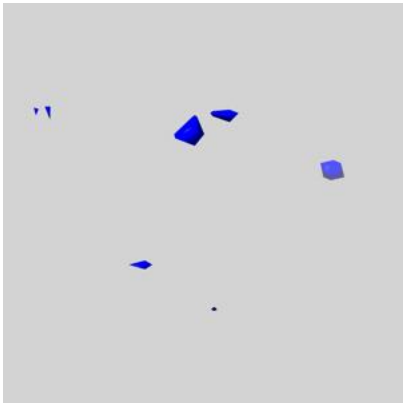

X

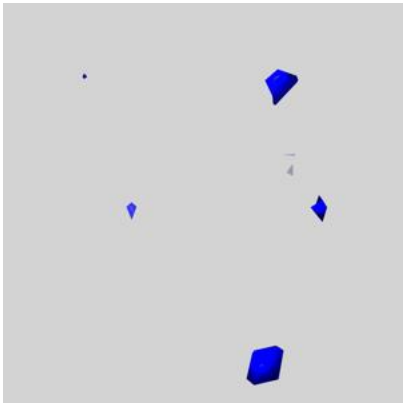

Y


Z

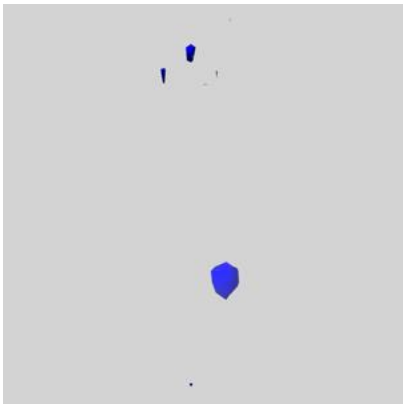
6.5.11 emd_1001_msk_15.map


X

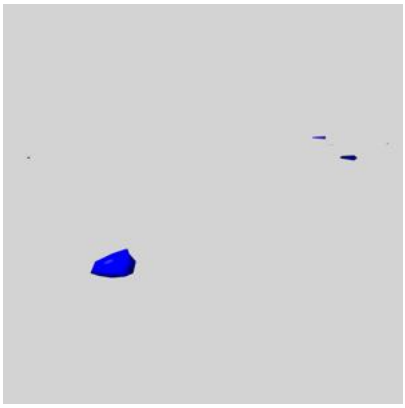

Y


Z

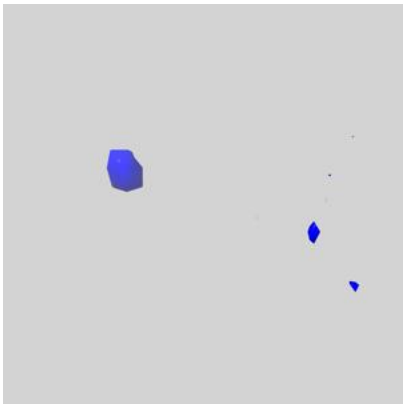
6.5.12 emd_1001_msk_14.map



X

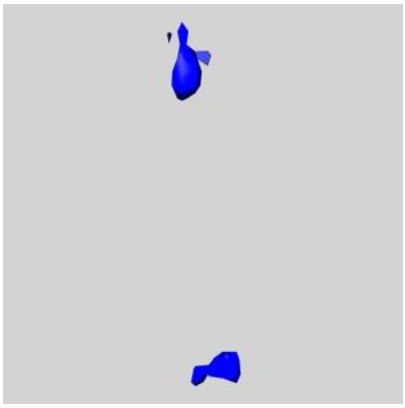


Y

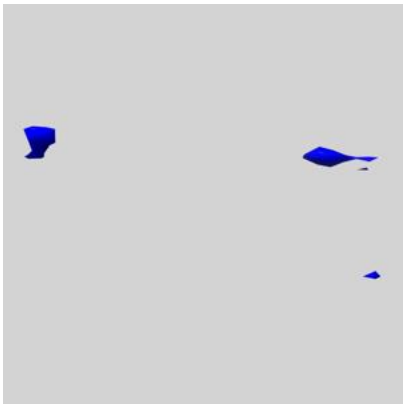


Z

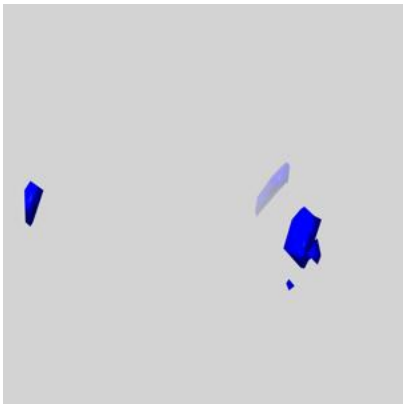
6.5.13 emd_1001_msk_13.map



X

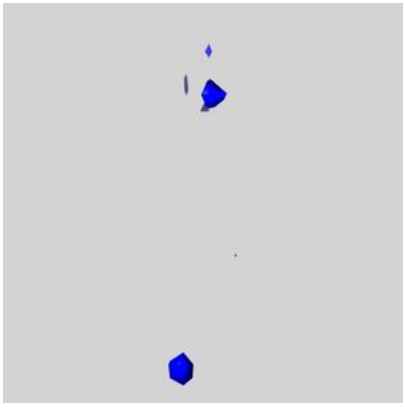


Y

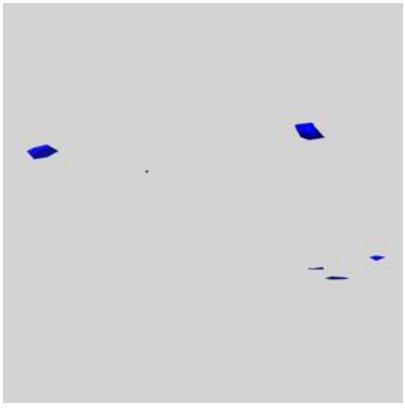


Z

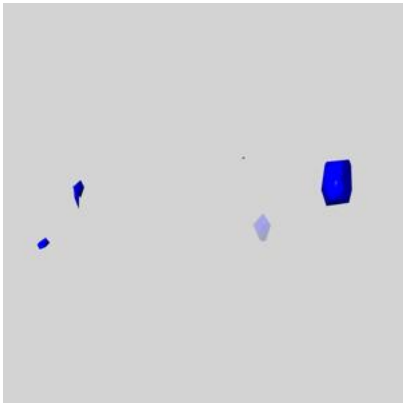
6.5.14 emd_1001_msk_12.map



X

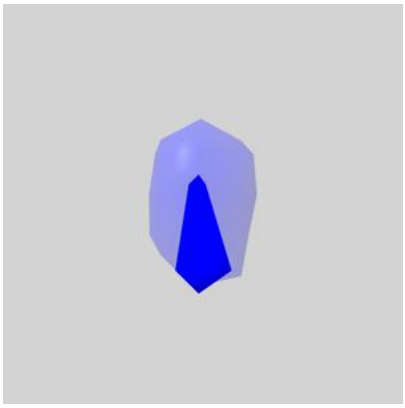


Y

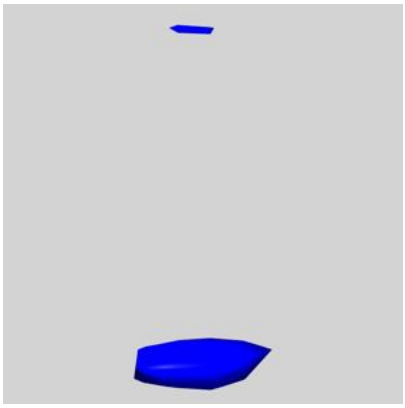


Z

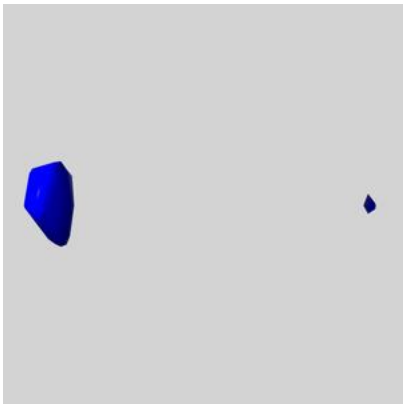
6.5.15 emd_1001_msk_11.map



X

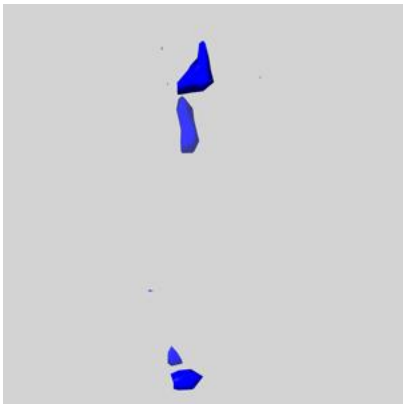


Y

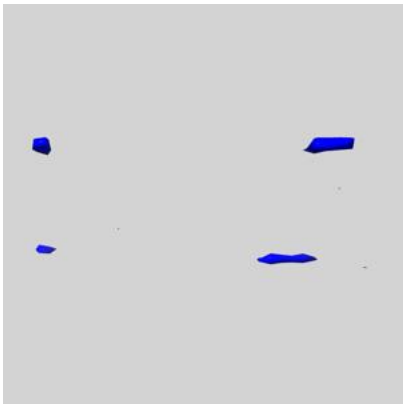


Z

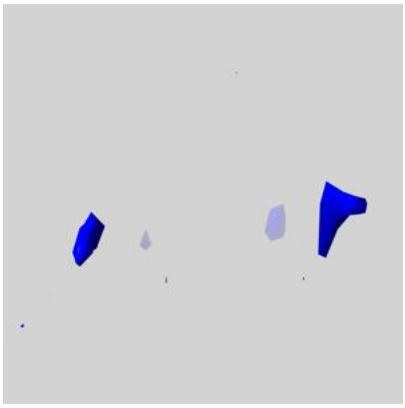
6.5.16 emd_1001_msk_10.map



X

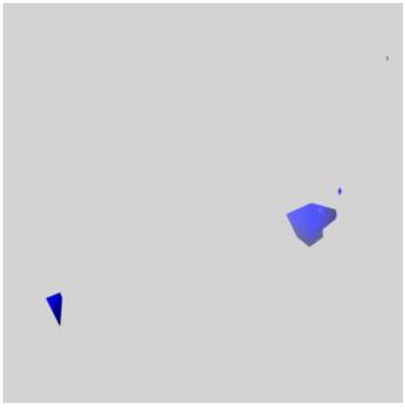


Y

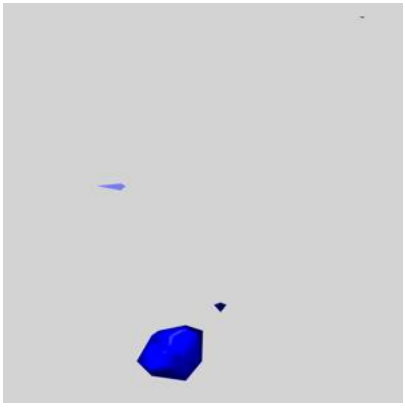


Z

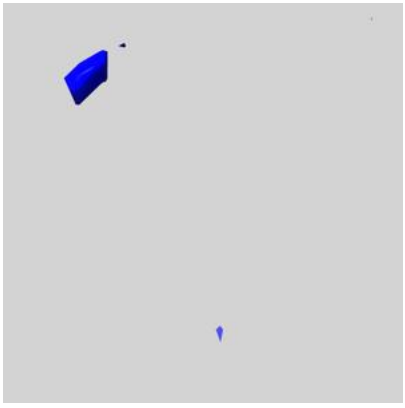
6.5.17 emd_1001_msk_9.map



X

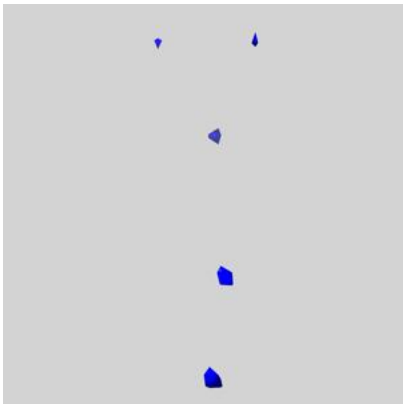


Y

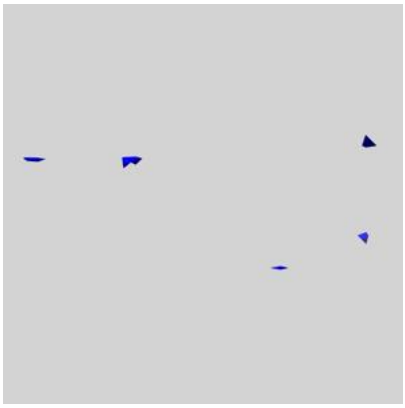


Z

6.5.18 emd_1001_msk_8.map



X



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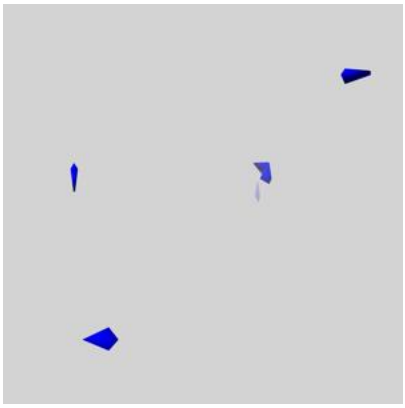

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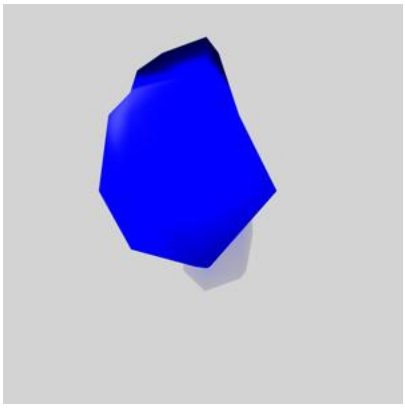
6.5.19 emd_1001_msk_7.map



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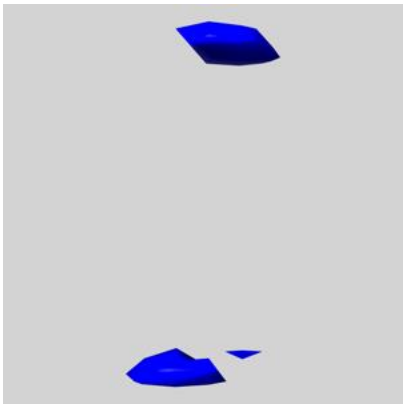

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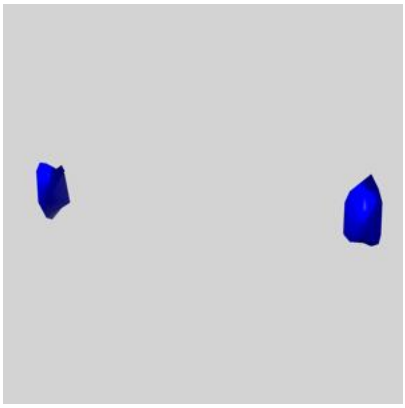

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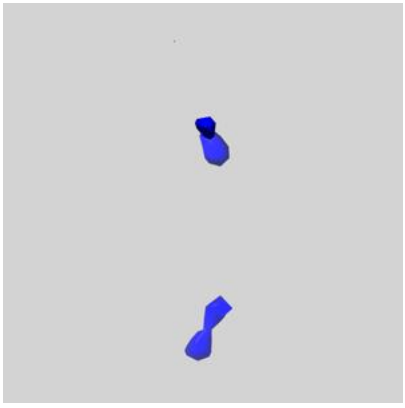
6.5.20 emd_1001_msk_6.map



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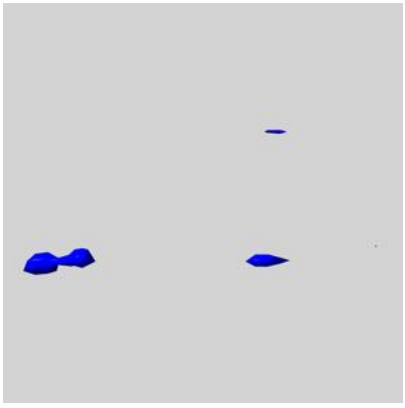

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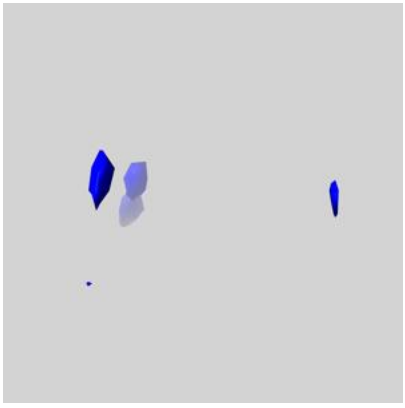

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6.5.21 emd_1001_msk_5.map


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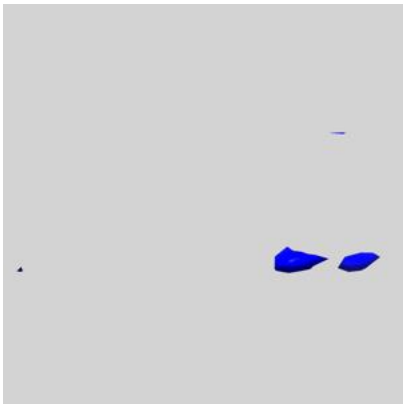
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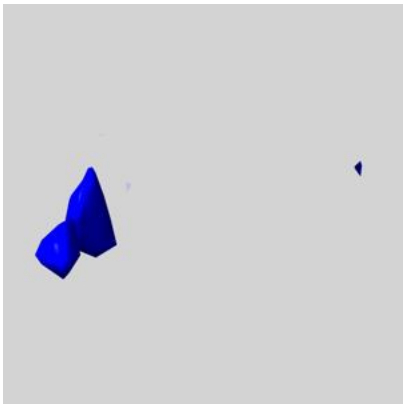
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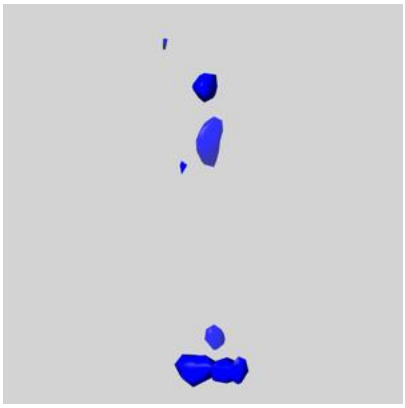
6.5.22 emd_1001_msk_4.map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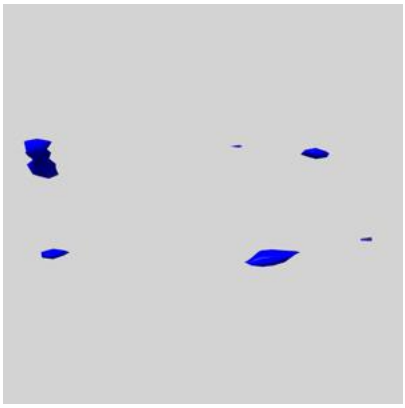
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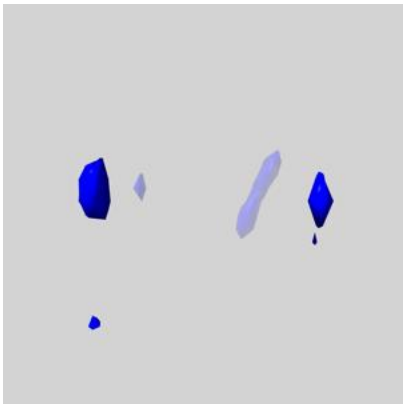
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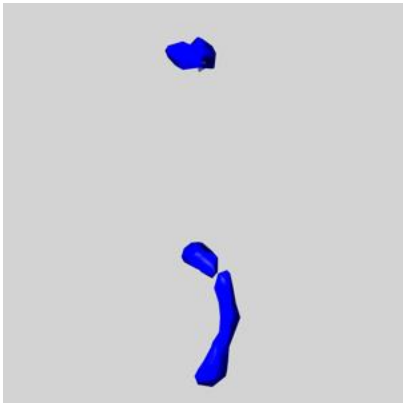
6.5.23 emd_1001_msk_3.map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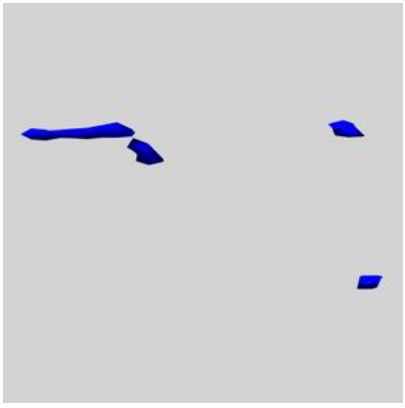
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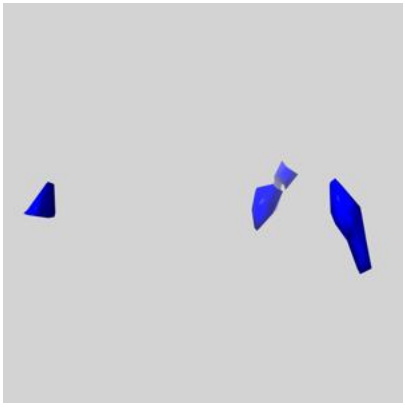
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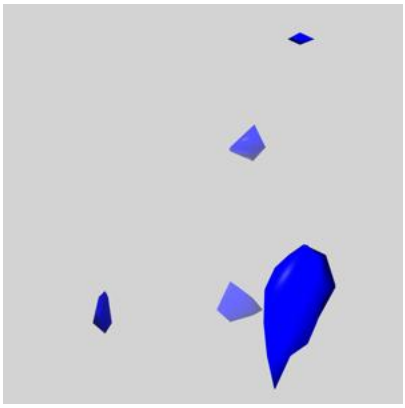
6.5.24 emd_1001_msk_2.map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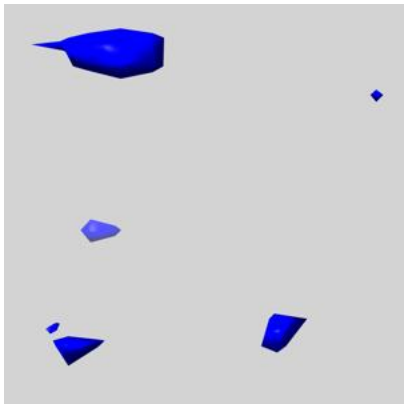
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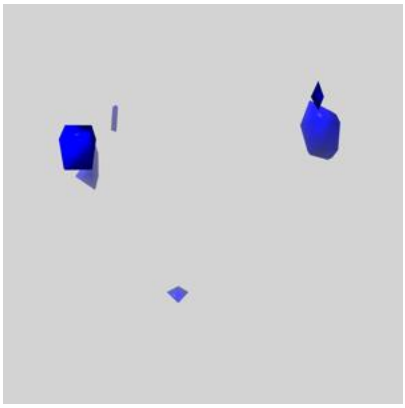
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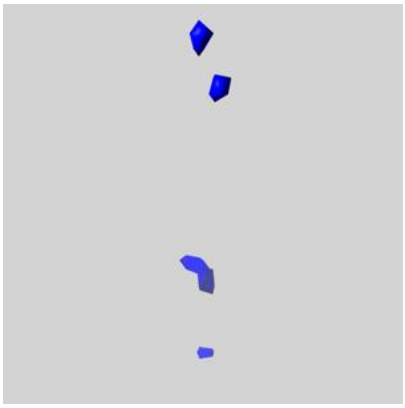
6.5.25 emd_1001_msk_1.map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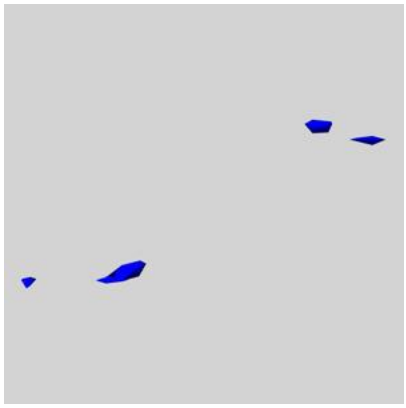
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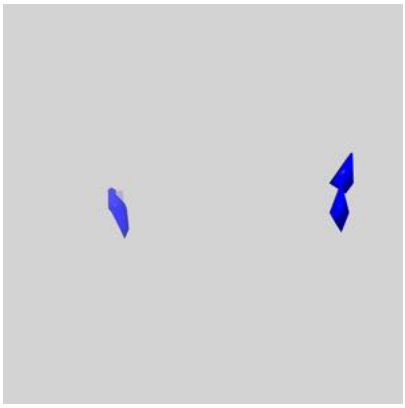
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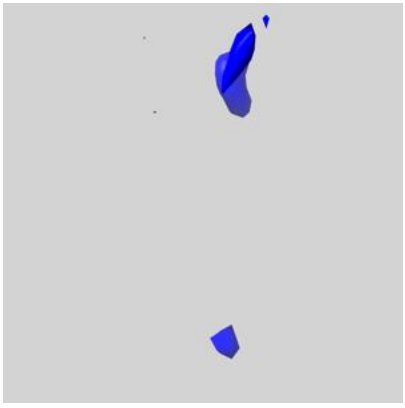
6.5.26 emd_1001_msk_26.map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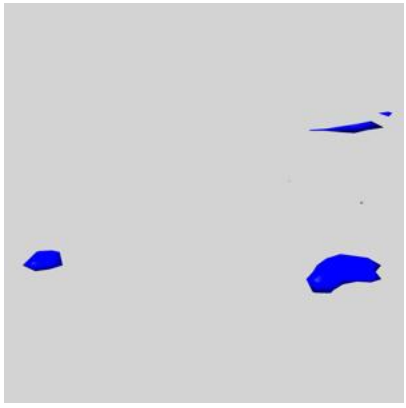
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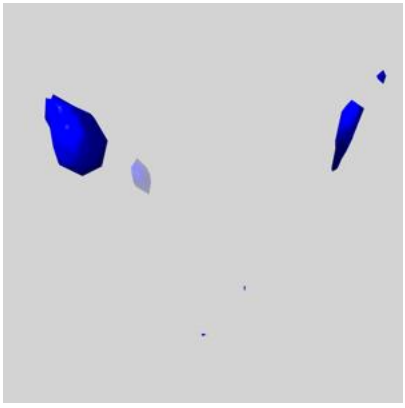
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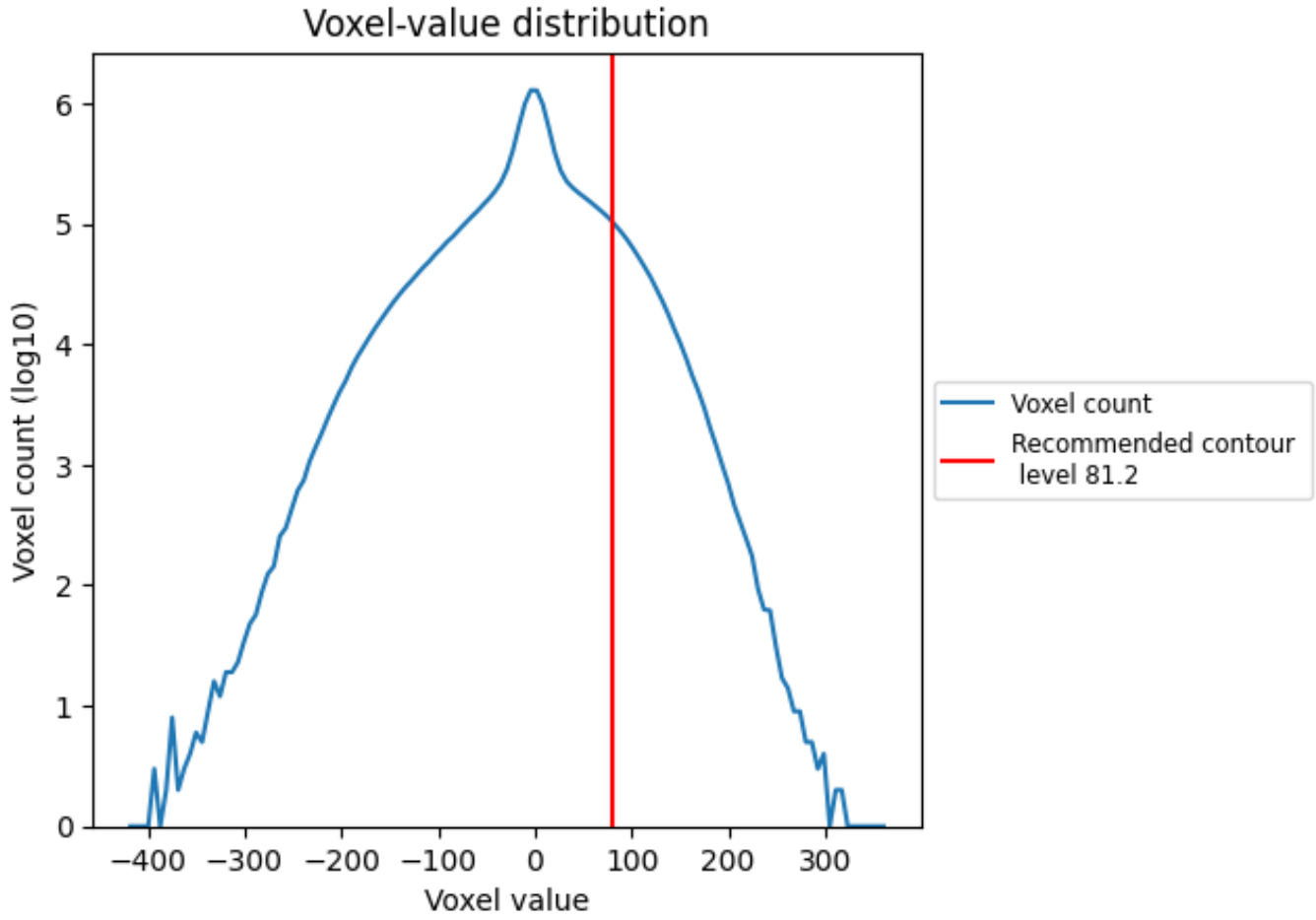
7 Tomogram analysis (i)

This section contains the results of statistical analysis of the tomogram.

7.1 Voxel-value distribution (i)



The voxel-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic.

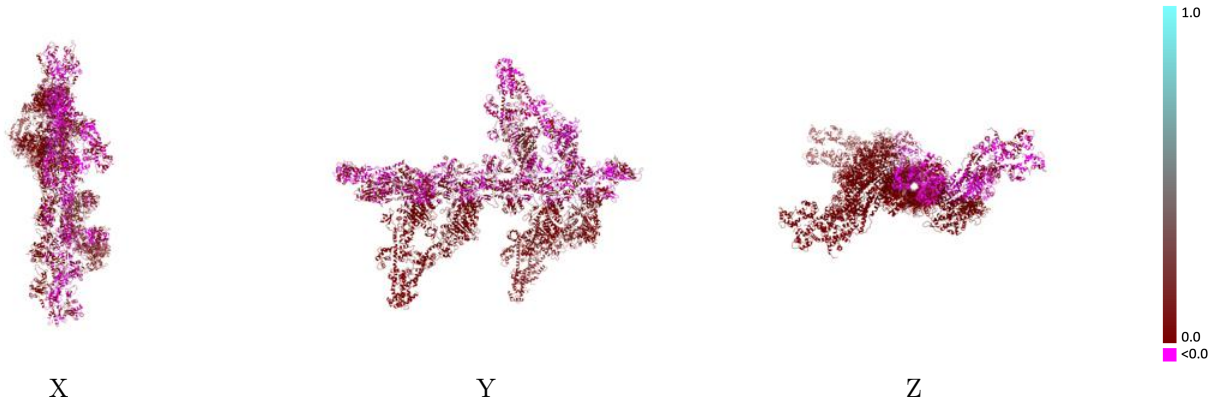
8 Map-model fit

This section contains information regarding the fit between EMDB map EMD-1001 and PDB model 1O19. Per-residue inclusion information can be found in section 3 on page 7.

8.1 Map-model overlay

This section was not generated.

8.2 Q-score mapped to coordinate model

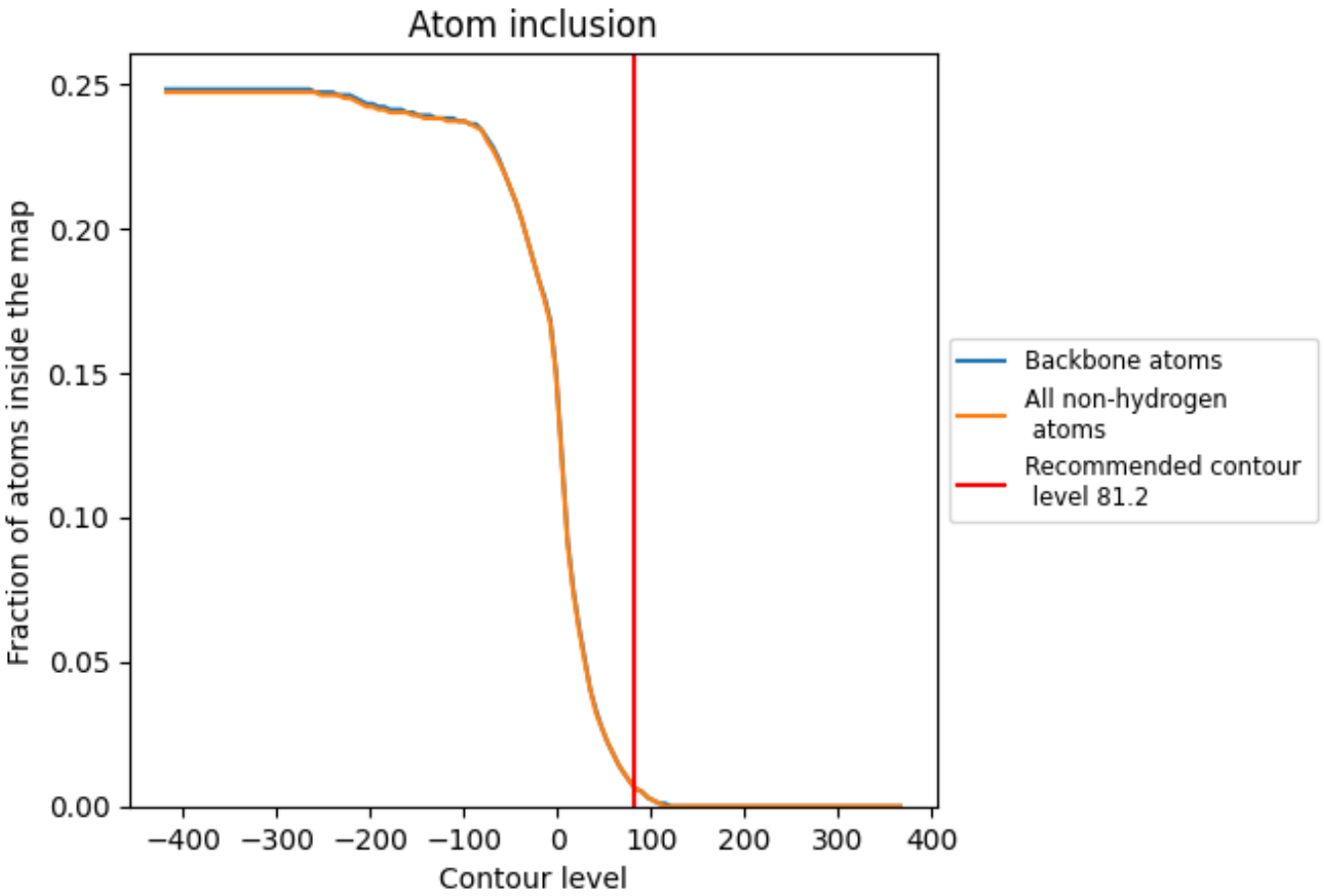


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

8.3 Atom inclusion mapped to coordinate model

This section was not generated.

8.4 Atom inclusion (i)



At the recommended contour level, 1% of all backbone atoms, 1% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (81.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.0070	0.0020
1	0.0000	0.0050
2	0.0280	0.0120
3	0.0000	-0.0070
4	0.0000	0.0150
5	0.0000	-0.0040
6	0.0000	0.0040
7	0.0000	-0.0010
8	0.0000	0.0020
9	0.0000	-0.0020
A	0.0000	0.0000
B	0.0000	0.0000
C	0.0000	0.0000
D	0.0020	-0.0030
E	0.1030	0.0240
F	0.0400	-0.0110
G	0.0000	-0.0000
H	0.0000	0.0000
I	0.0000	0.0000
J	0.0110	0.0070
K	0.0000	-0.0200
L	0.1700	0.0250
M	0.0000	0.0000
N	0.0000	0.0000
O	0.0000	0.0000
S	0.0000	0.0020
T	0.0000	0.0000
U	0.0000	0.0000
V	0.0000	0.0070
W	0.0000	-0.0040
X	0.0540	0.0060
Y	0.0000	0.0050
Z	0.0000	-0.0080