wwPDB EM Validation Summary Report (i)

Dec 18, 2023 – 04:26 PM EST

PDB ID	:	1O1B
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:

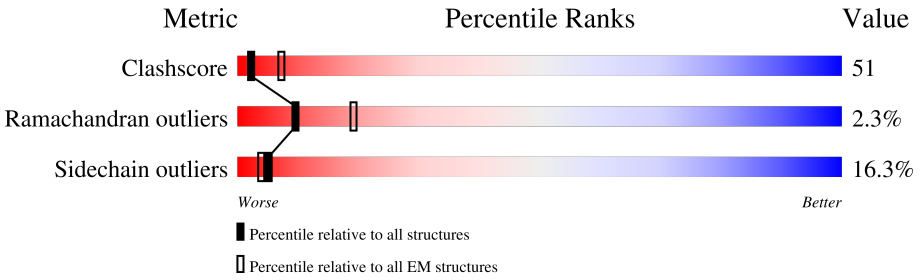
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (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% 26% 50% 20% ·
1	D	840	100% 25% 51% 20% ·
1	G	840	100% 24% 52% 20% ·
1	J	840	99% 25% 51% 20% ·
2	B	145	100% 66% 25% 6% ·
2	E	145	100% 63% 28% 6% ·
2	H	145	100% 63% 28% 6% ·
2	K	145	92% 65% 26% 6% ·

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Mol	Chain	Length	Quality of chain
3	C	147	100% 61% 37%
3	F	147	78% 61% 37%
3	I	147	100% 61% 37%
3	L	147	93% 61% 37%
4	0	375	99% 62% 29% 6%
4	1	375	99% 61% 30% 7%
4	2	375	99% 63% 28% 6%
4	3	375	99% 62% 29% 6%
4	4	375	99% 63% 29% 6%
4	5	375	99% 64% 27% 6%
4	7	375	99% 64% 28% 6%
4	8	375	99% 59% 31% 8%
4	9	375	99% 58% 32% 8%
4	V	375	99% 55% 33% 9%
4	W	375	99% 56% 33% 8%
4	X	375	93% 61% 29% 7%
4	Y	375	99% 62% 29% 7%
4	Z	375	87% 61% 30% 6%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	MLY	A	505	-	-	X	-
1	MLY	A	553	-	-	X	-
1	MLY	A	764	-	-	X	-
1	MLY	A	768	-	-	X	-
1	MLY	A	839	-	-	X	-
1	MLY	D	553	-	-	X	-
1	MLY	D	768	-	-	X	-

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

2 Entry composition (i)

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

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

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

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

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

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

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

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

- Molecule 4 is a protein called SKELETAL MUSCLE ACTIN.

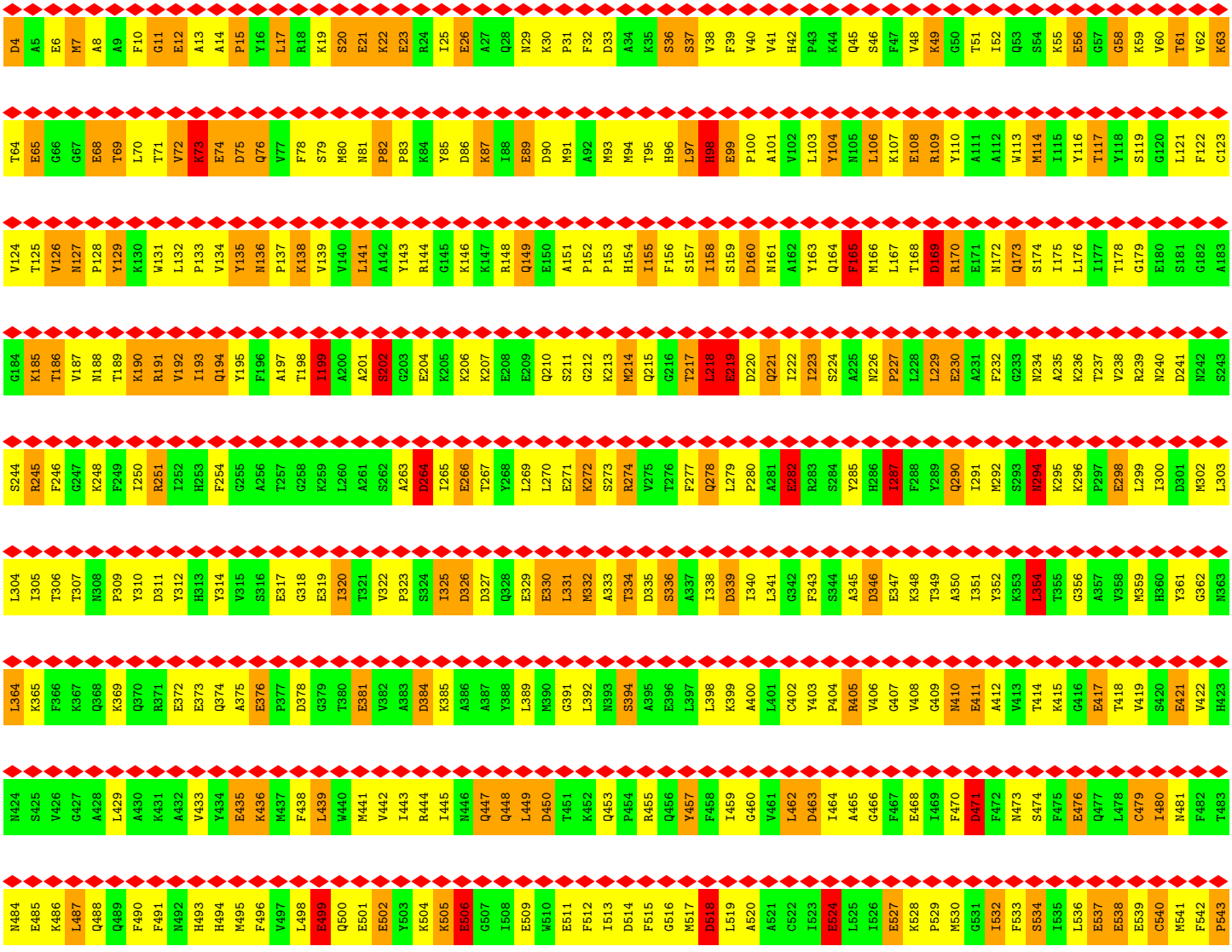
Mol	Chain	Residues	Atoms					AltConf	Trace
4	0	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	1	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	2	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	3	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	4	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20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

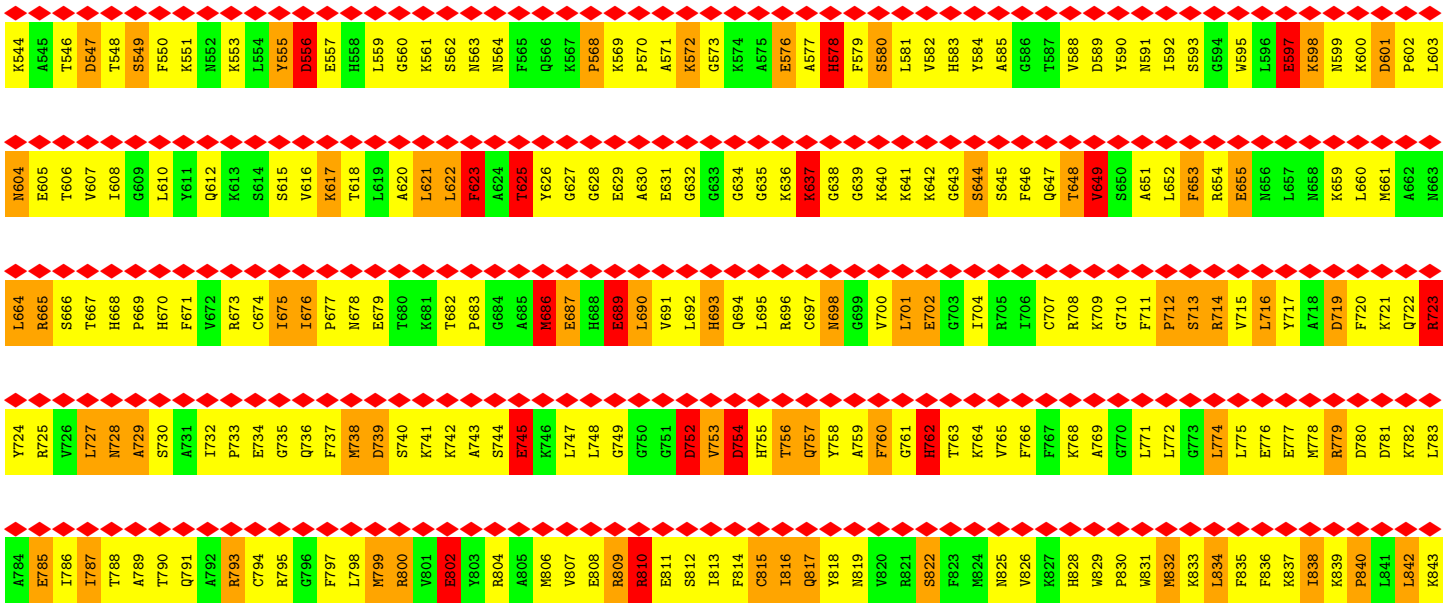
3 Residue-property plots (i)

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

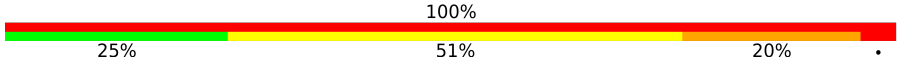
Chain A:

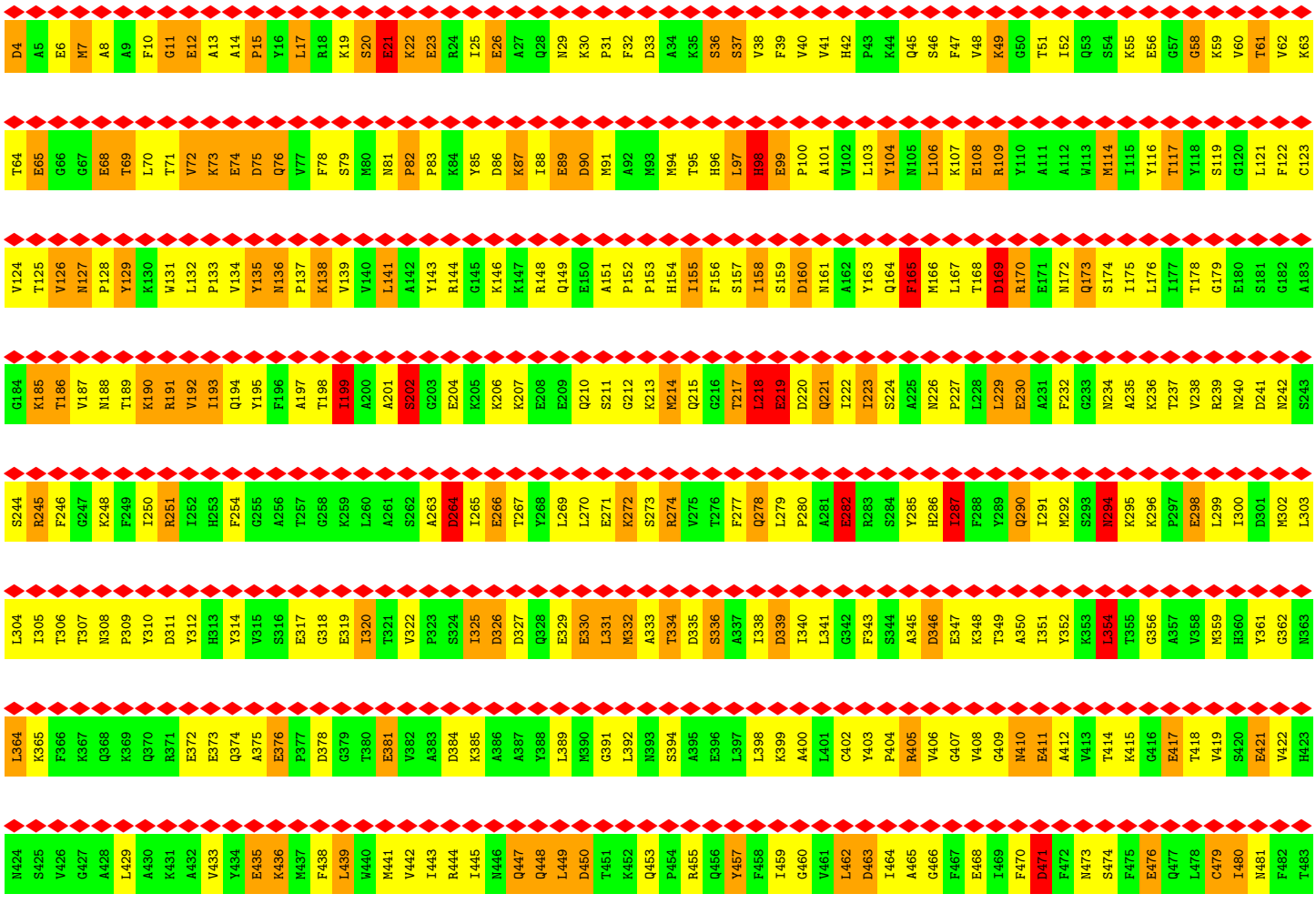


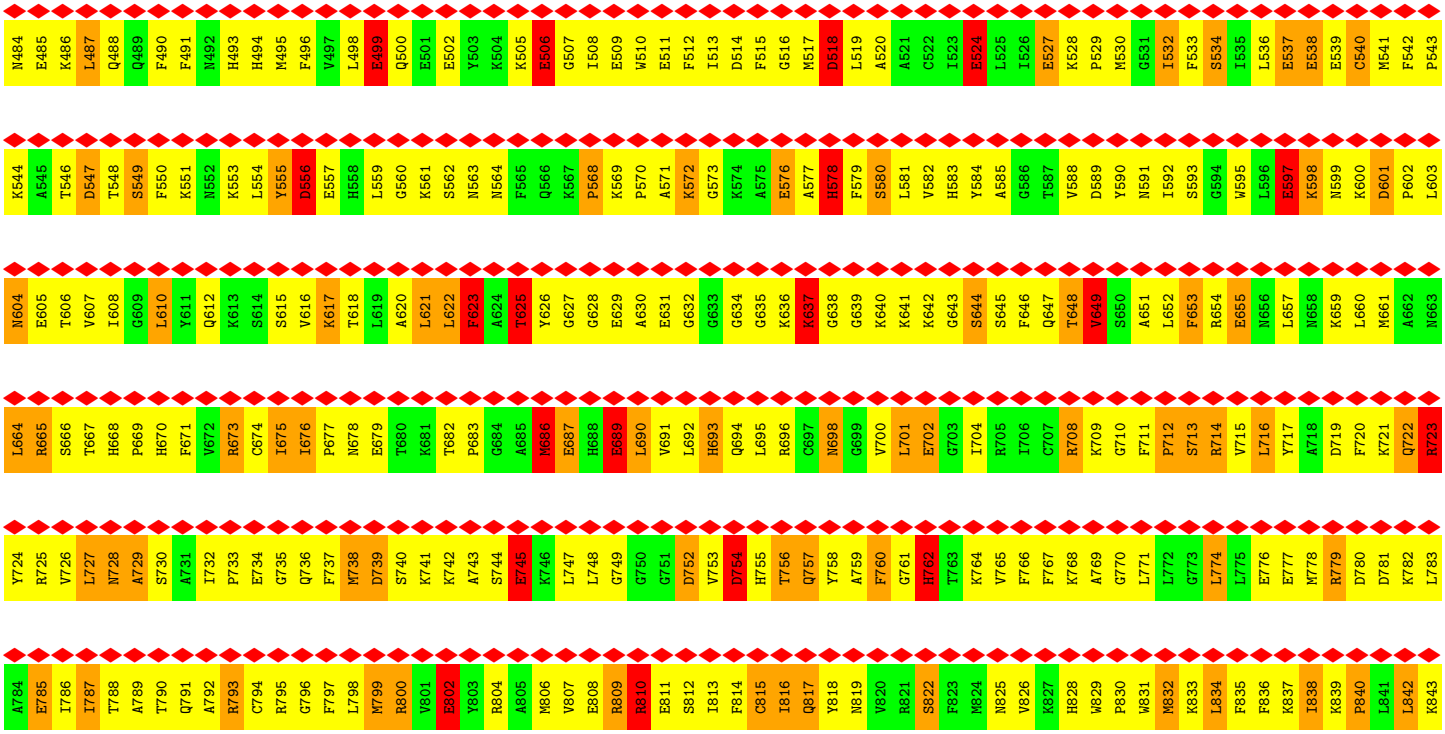


- Molecule 1: SKELETAL MUSCLE MYOSIN II

Chain D:

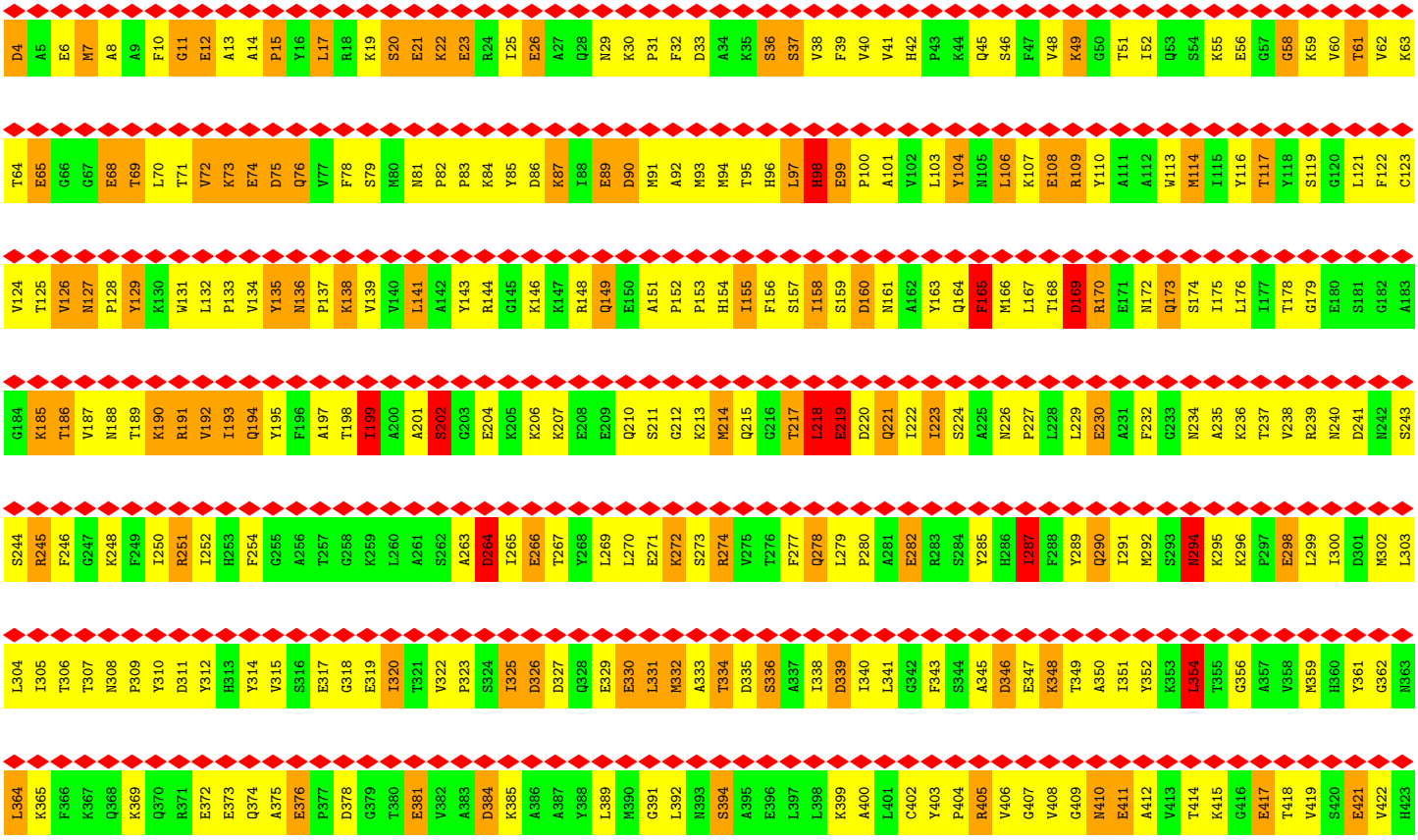


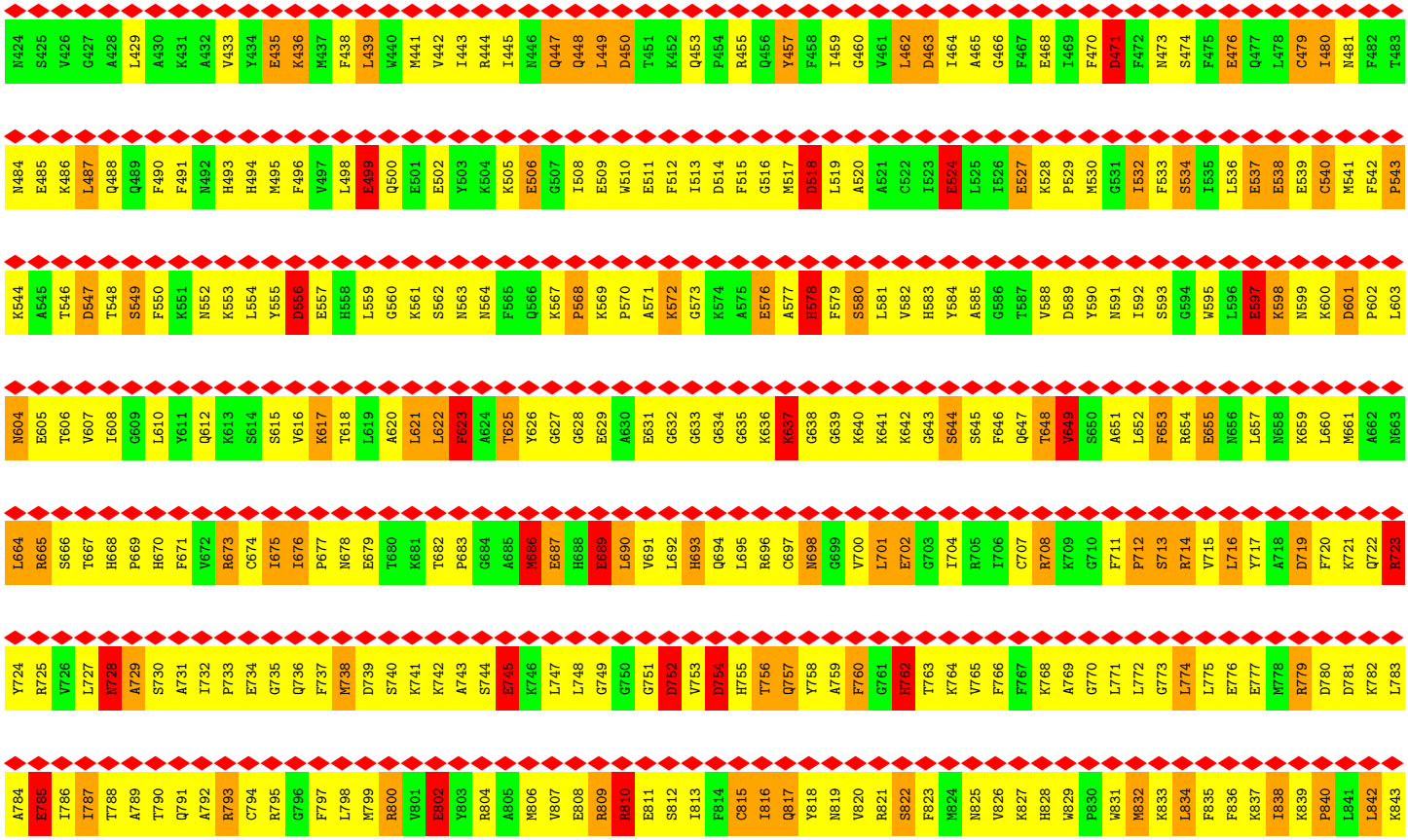




• Molecule 1: SKELETAL MUSCLE MYOSIN II

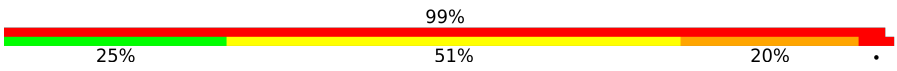
Chain G:

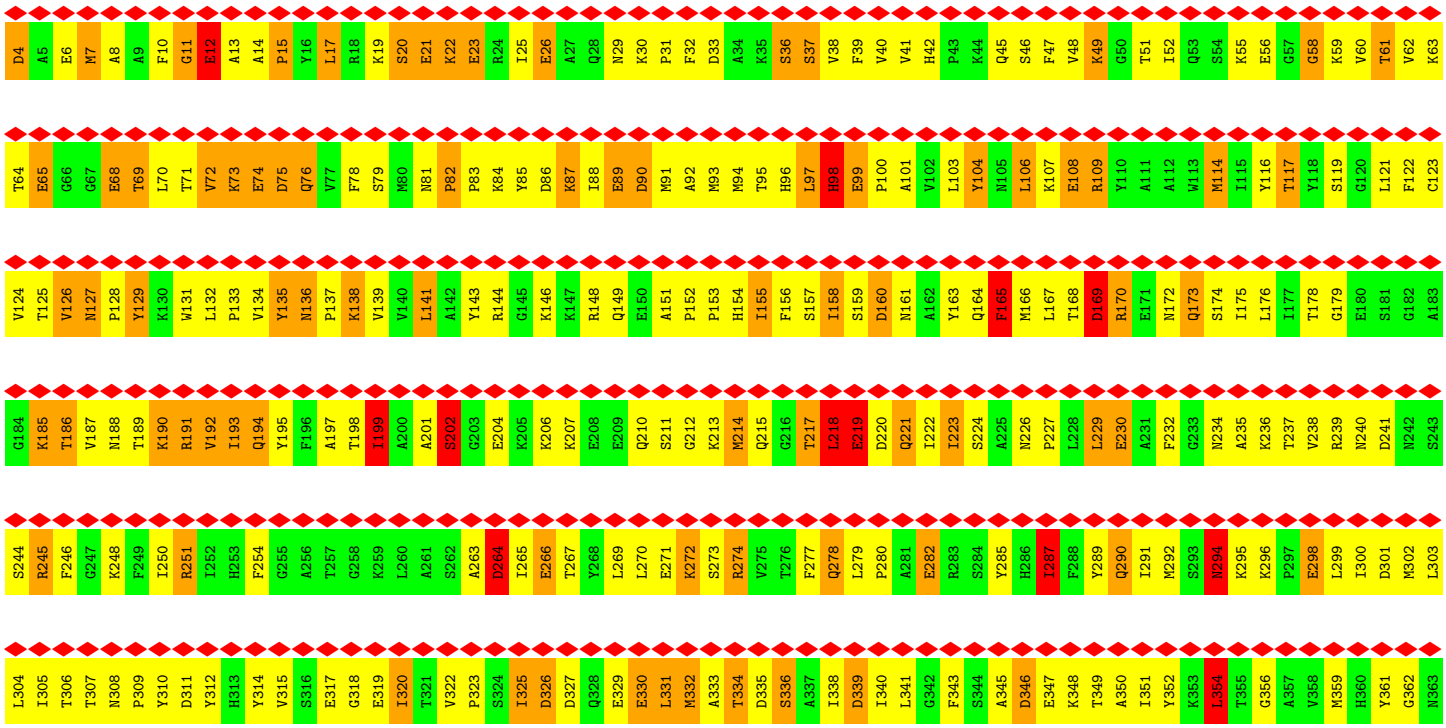


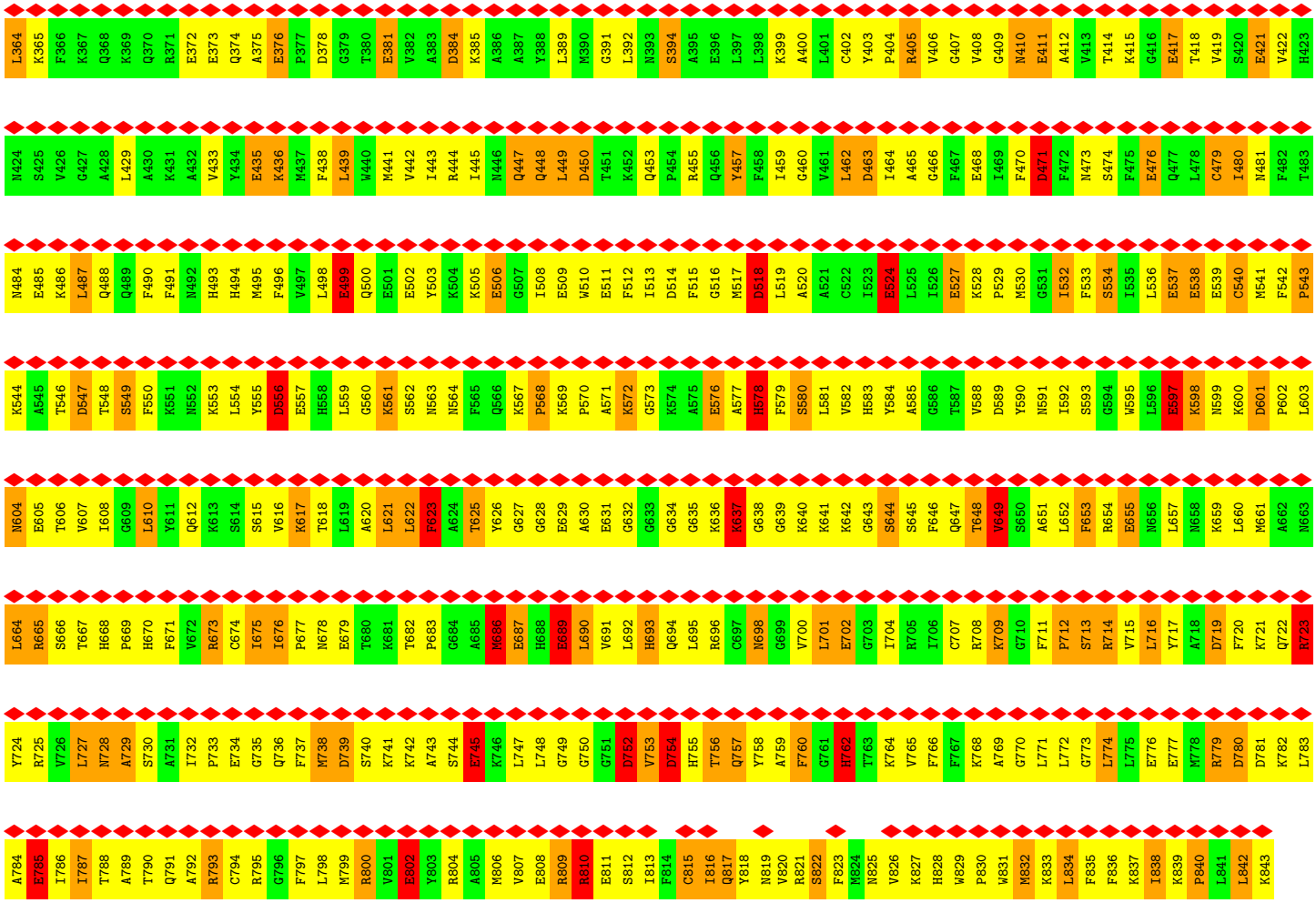


• Molecule 1: SKELETAL MUSCLE MYOSIN II

Chain J:

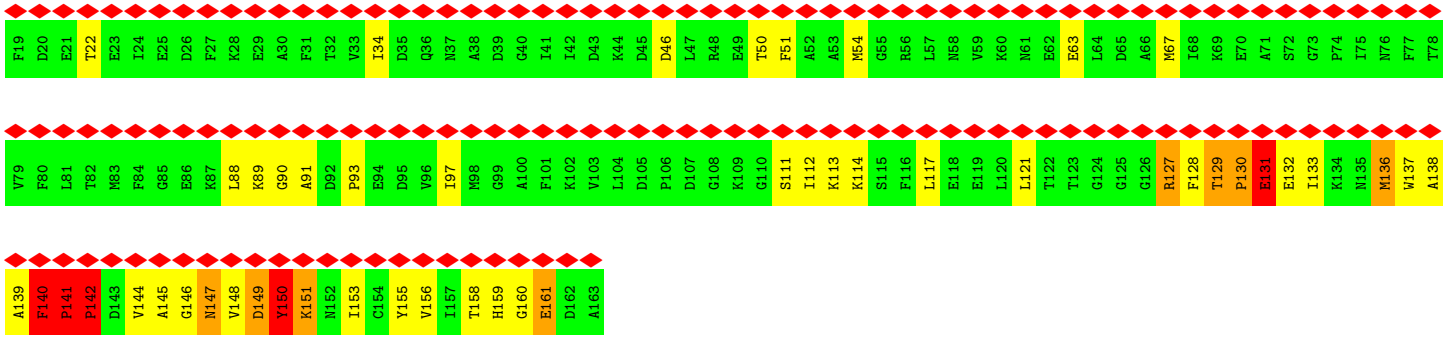






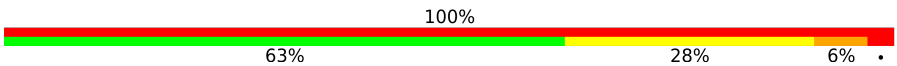
• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

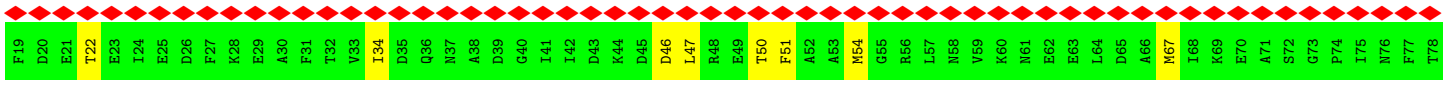
Chain B:

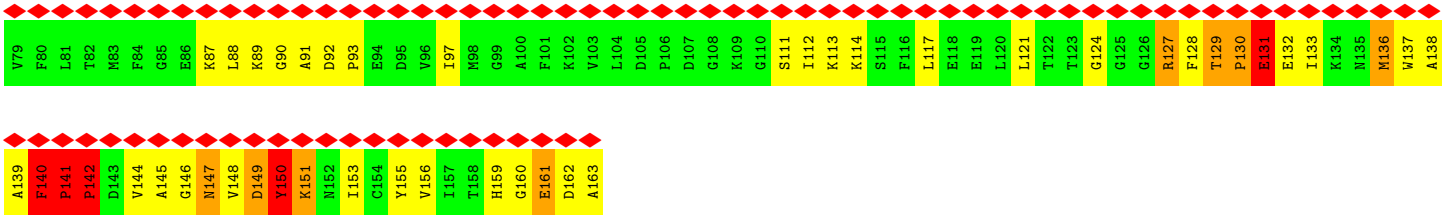


• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

Chain E:

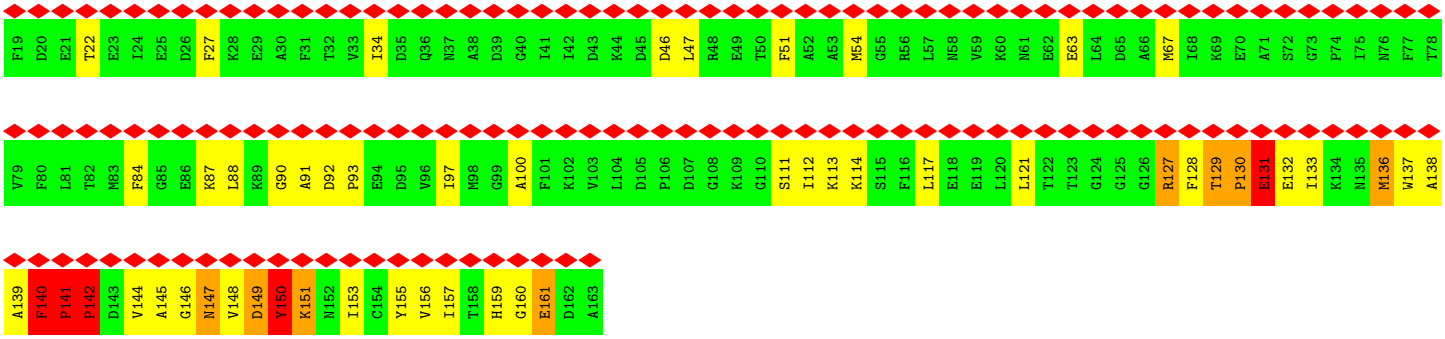






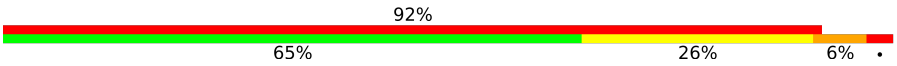
• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

Chain H:



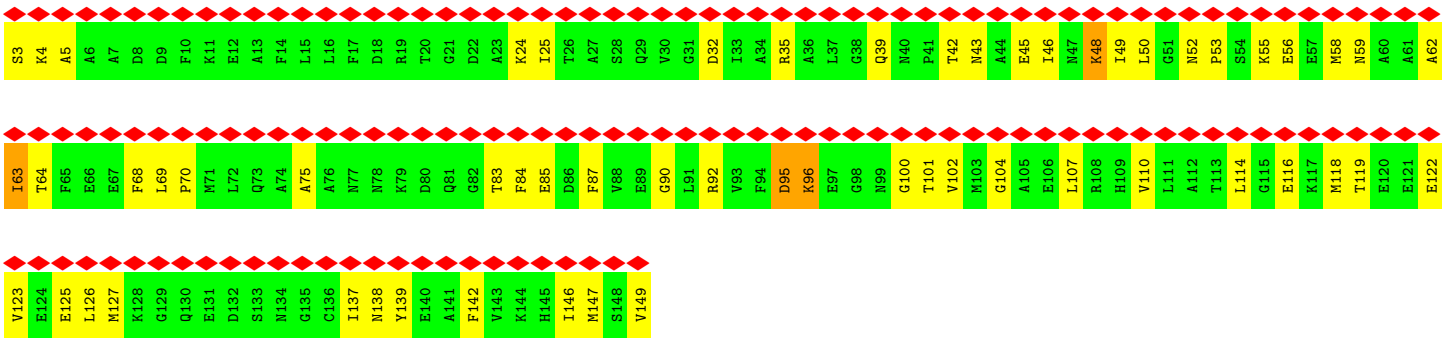
• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

Chain K:



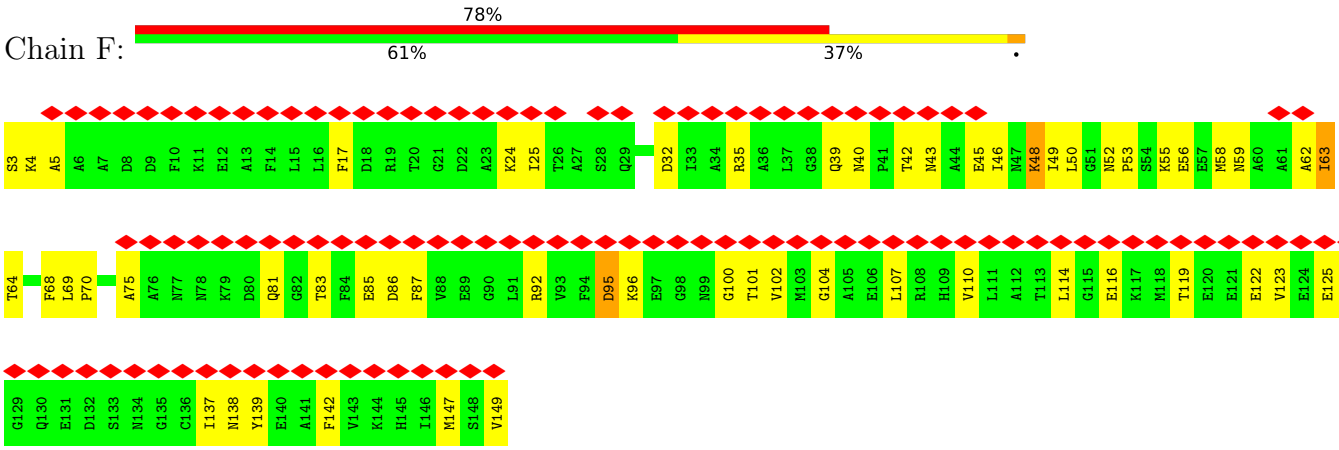
• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN

Chain C:



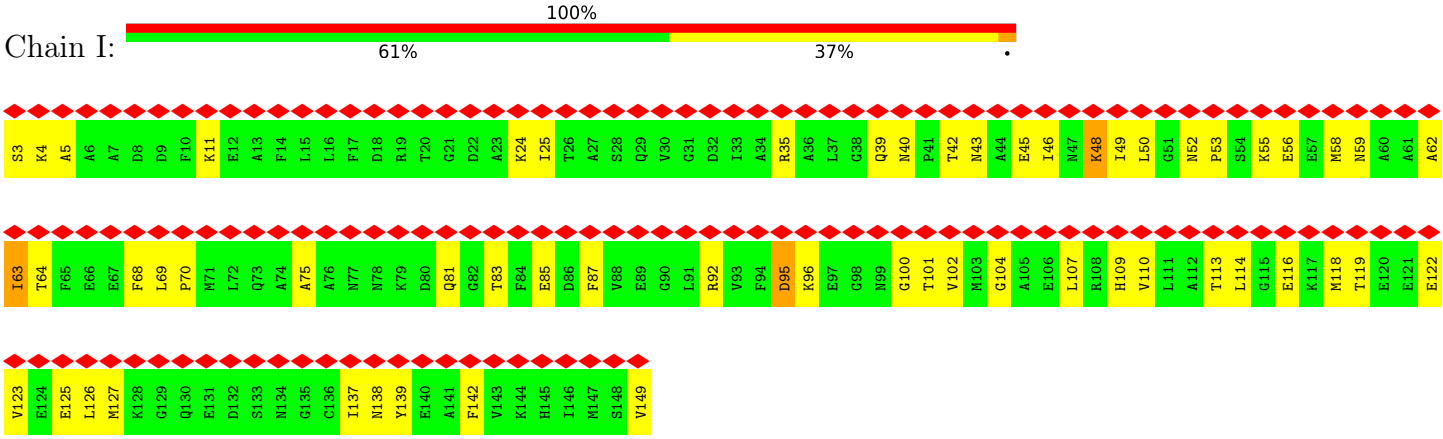
• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN

Chain F:



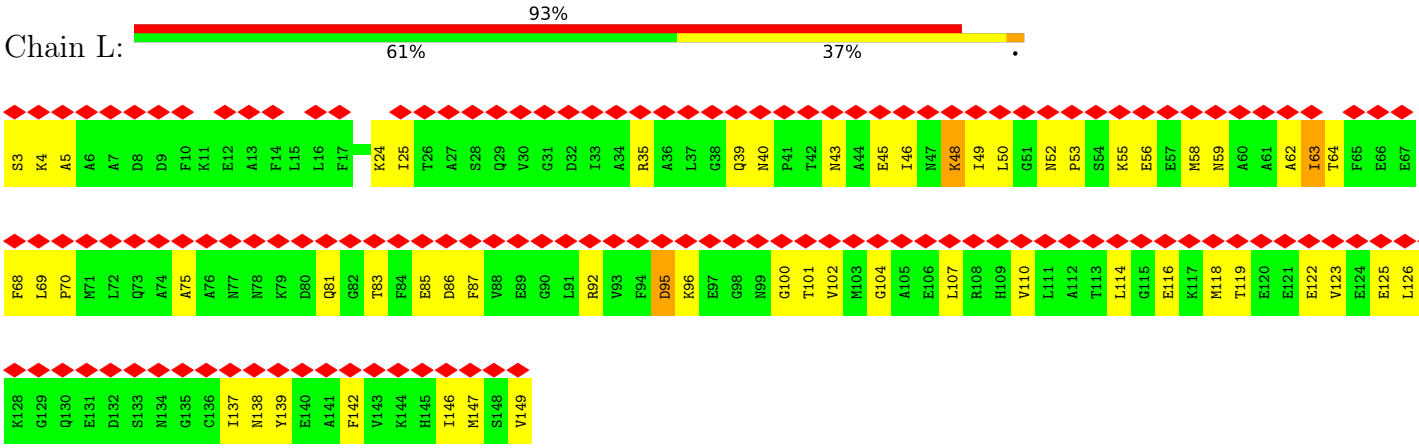
• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN

Chain I:



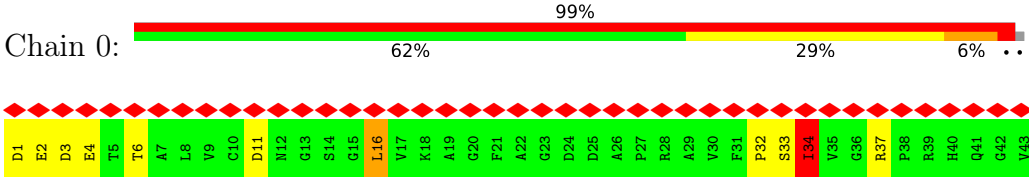
• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN

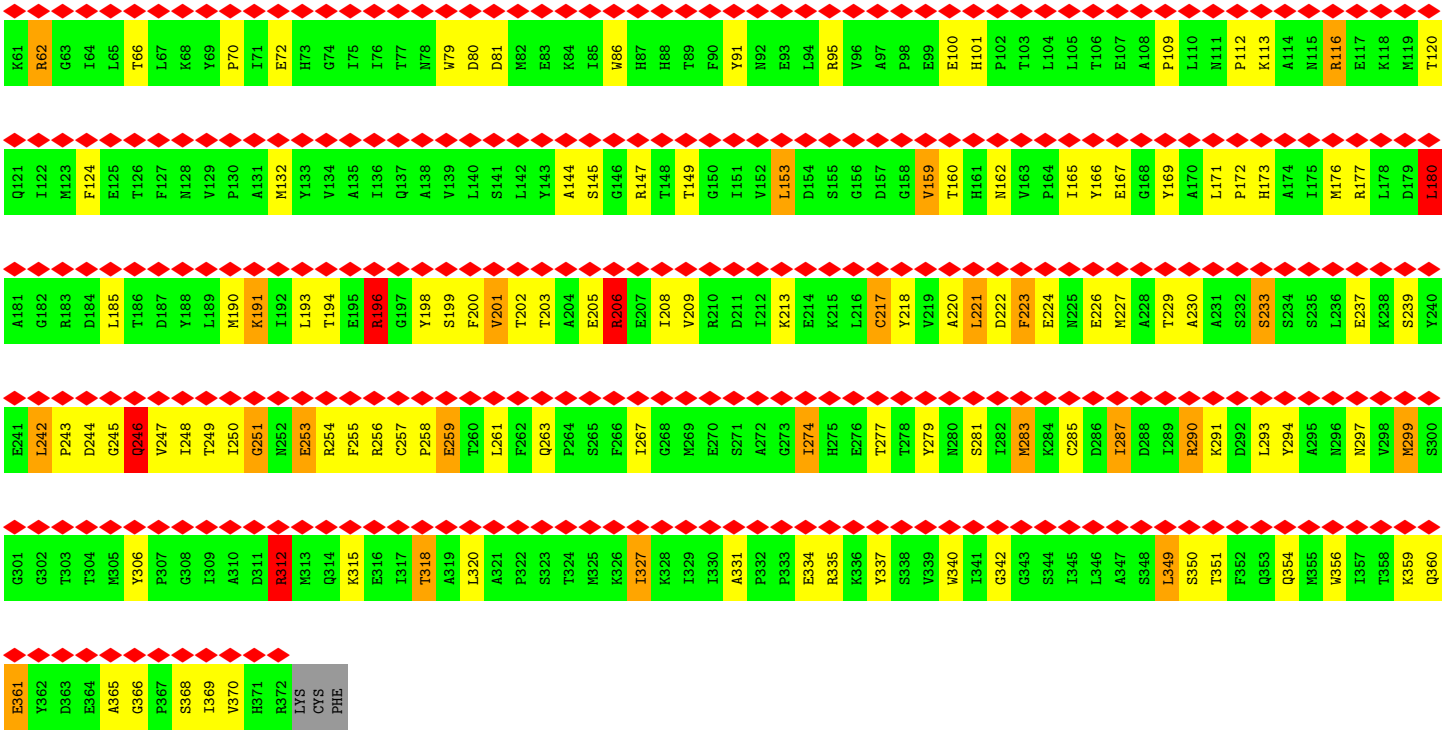
Chain L:



• Molecule 4: SKELETAL MUSCLE ACTIN

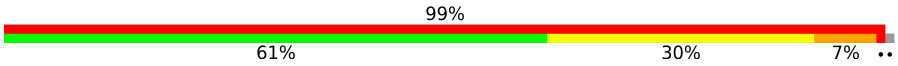
Chain 0:

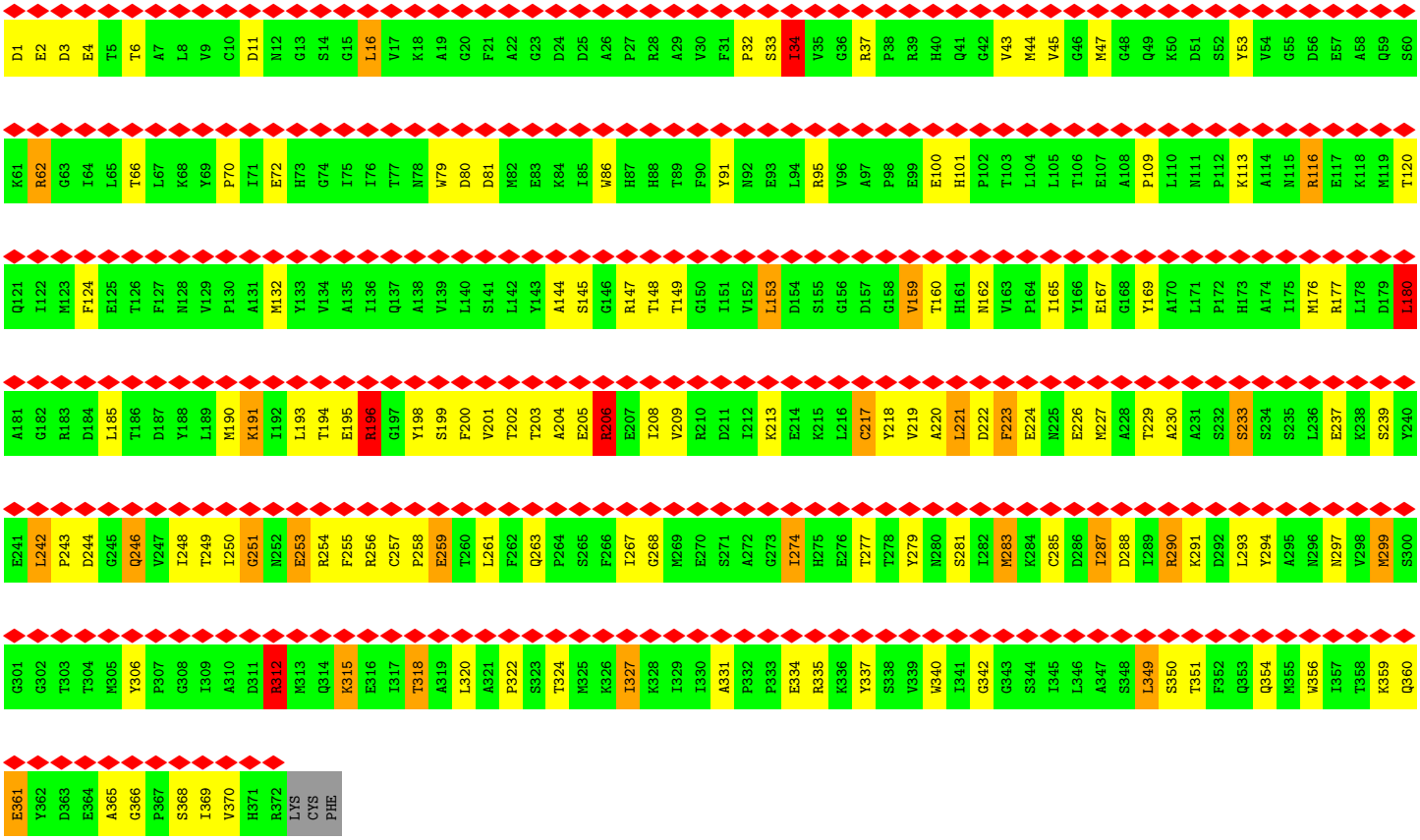




- Molecule 4: SKELETAL MUSCLE ACTIN

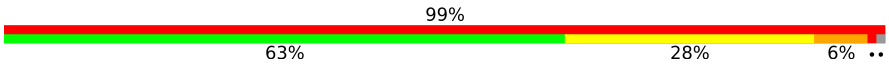
Chain 1:

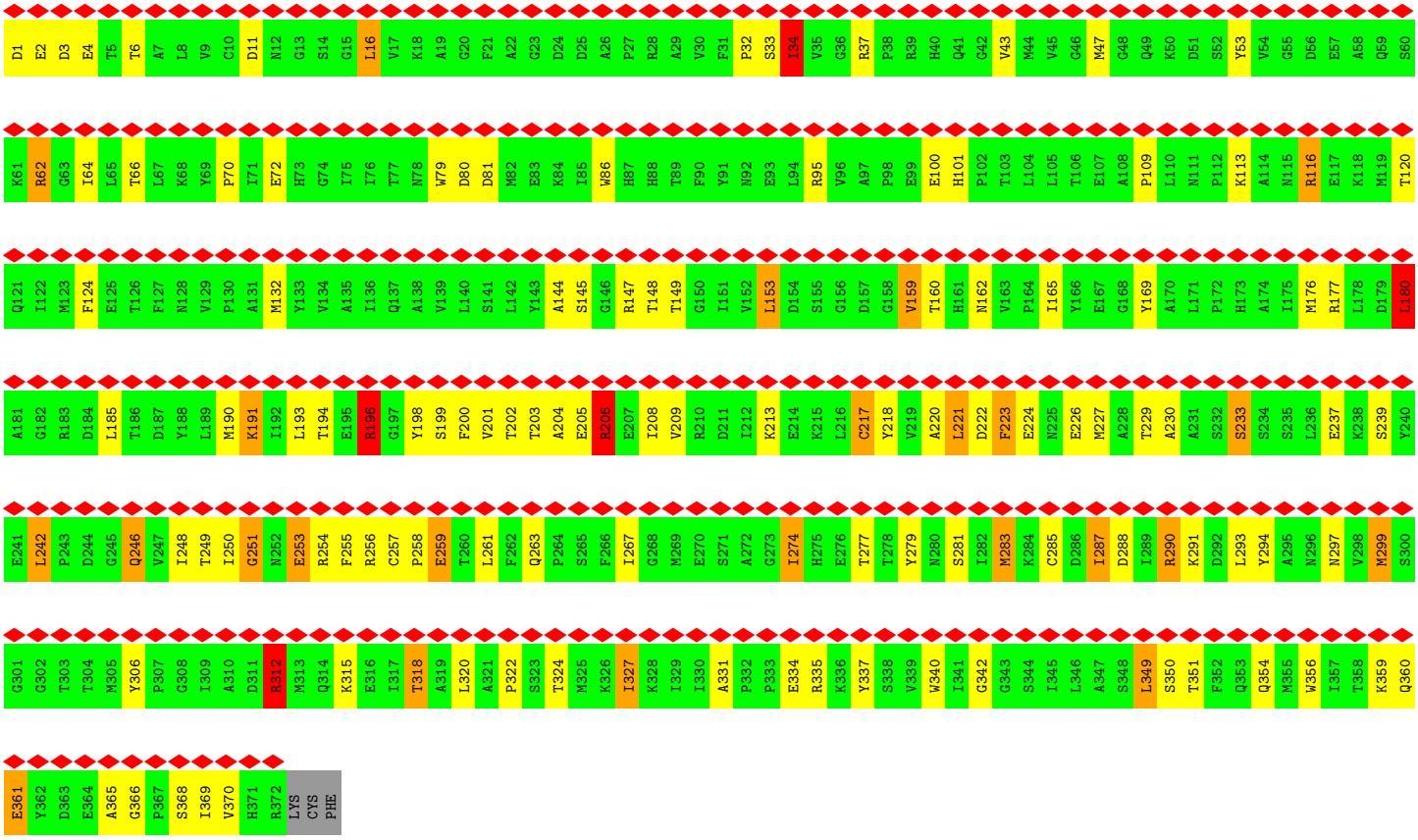




• Molecule 4: SKELETAL MUSCLE ACTIN

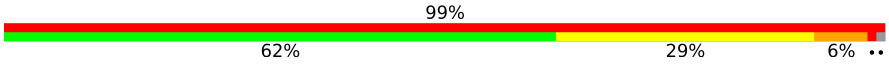
Chain 2:

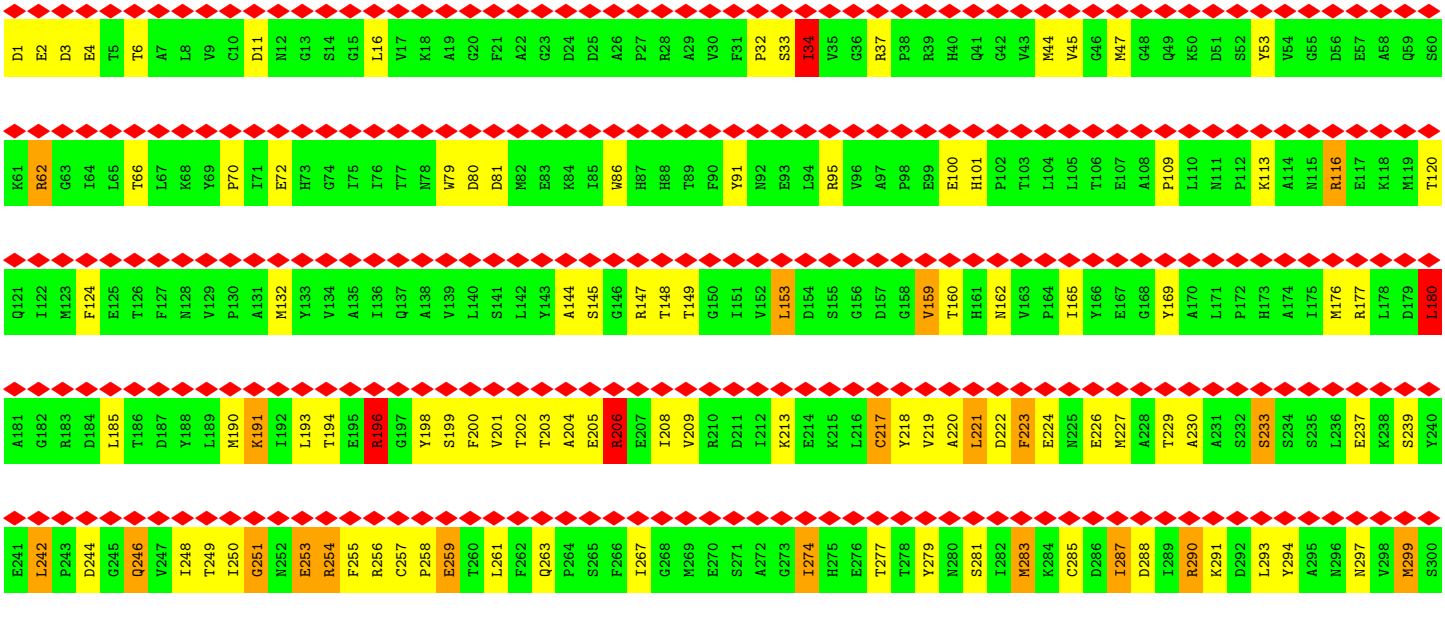


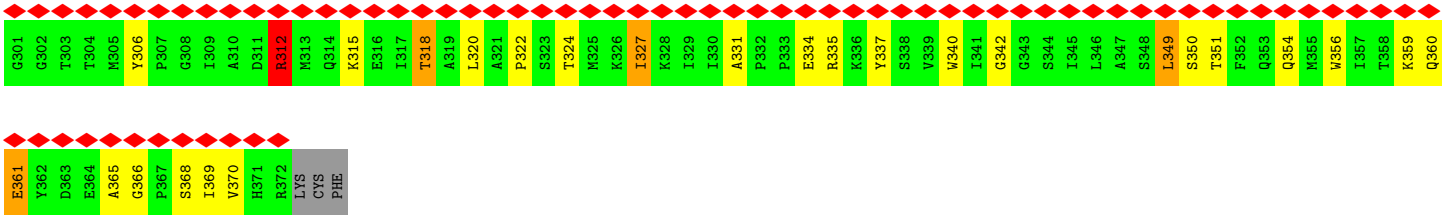


• Molecule 4: SKELETAL MUSCLE ACTIN

Chain 3:

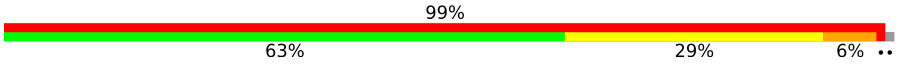


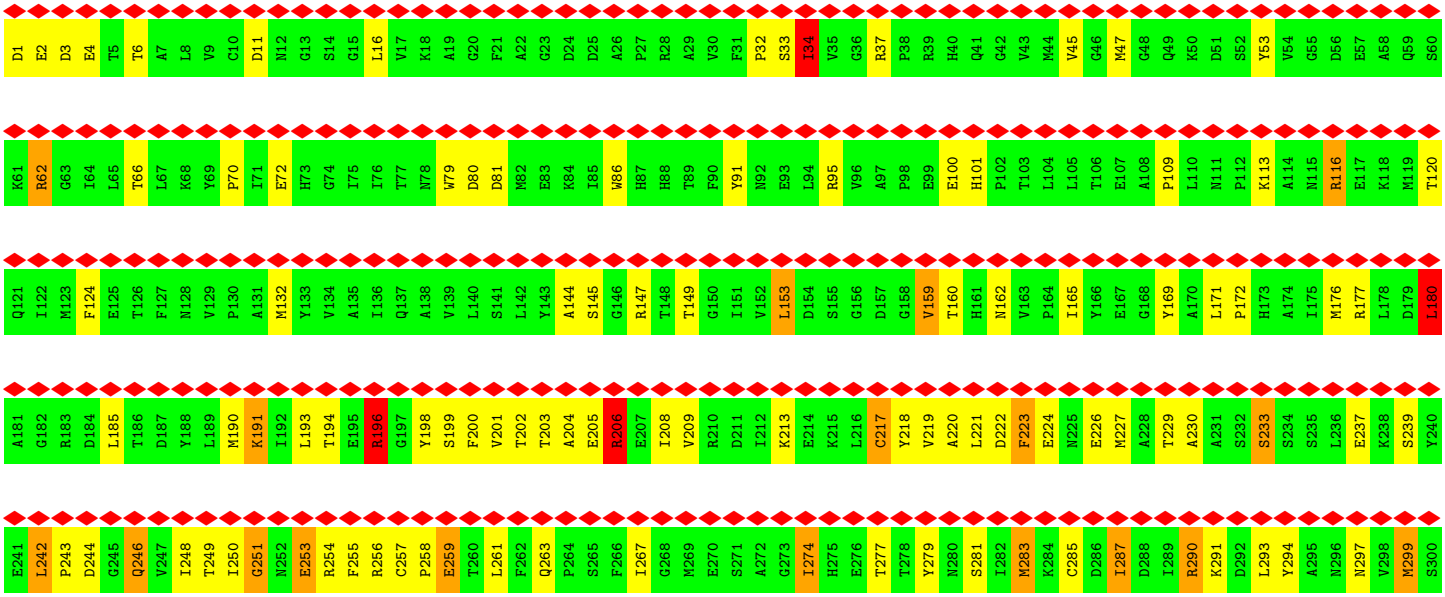




• Molecule 4: SKELETAL MUSCLE ACTIN

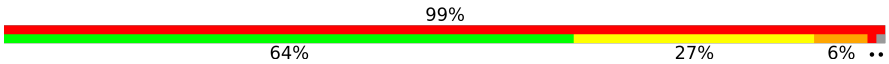
Chain 4:

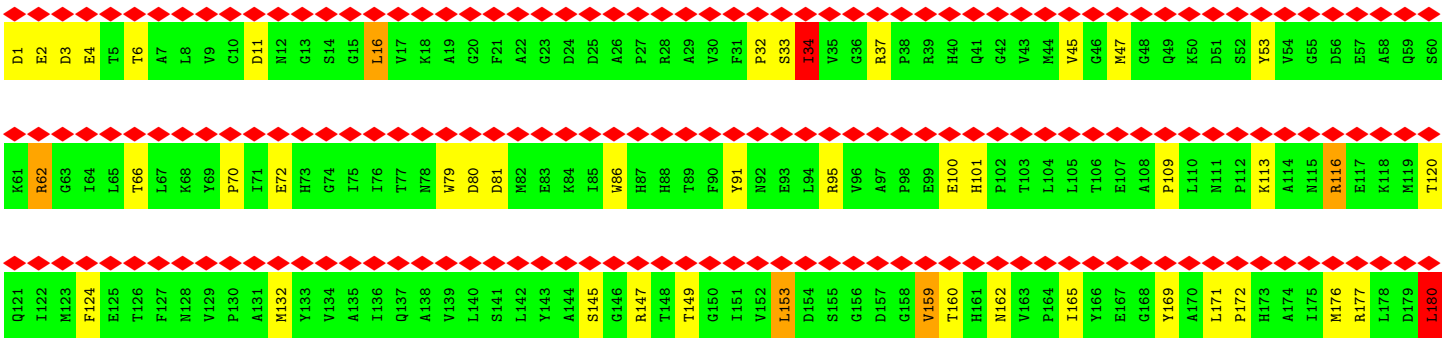




• Molecule 4: SKELETAL MUSCLE ACTIN

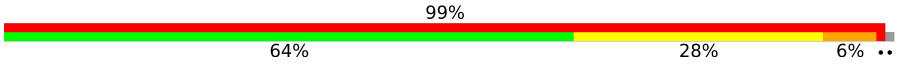
Chain 5:

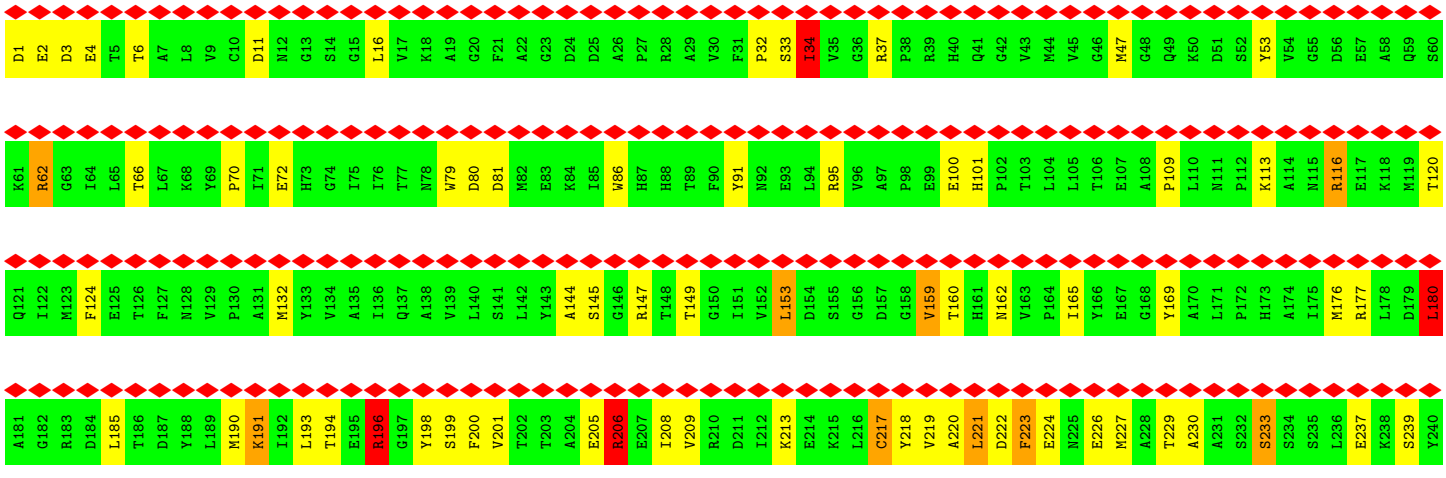




• Molecule 4: SKELETAL MUSCLE ACTIN

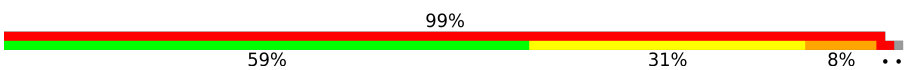
Chain 7:

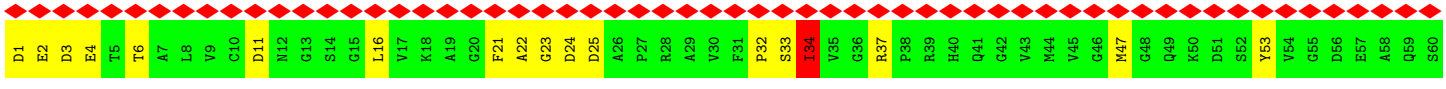


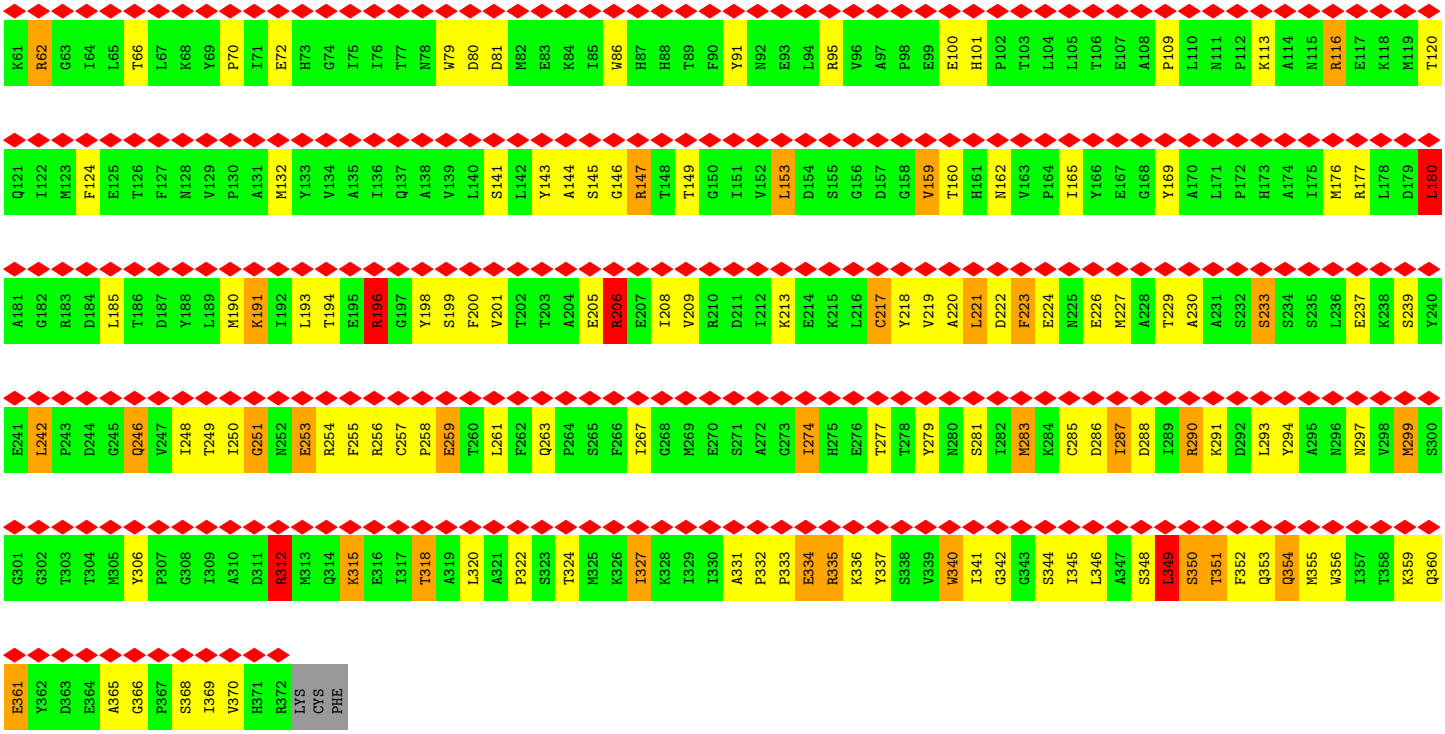


• Molecule 4: SKELETAL MUSCLE ACTIN

Chain 8:

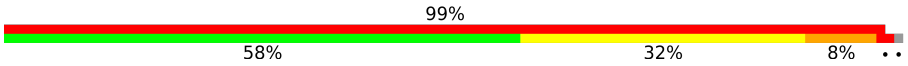


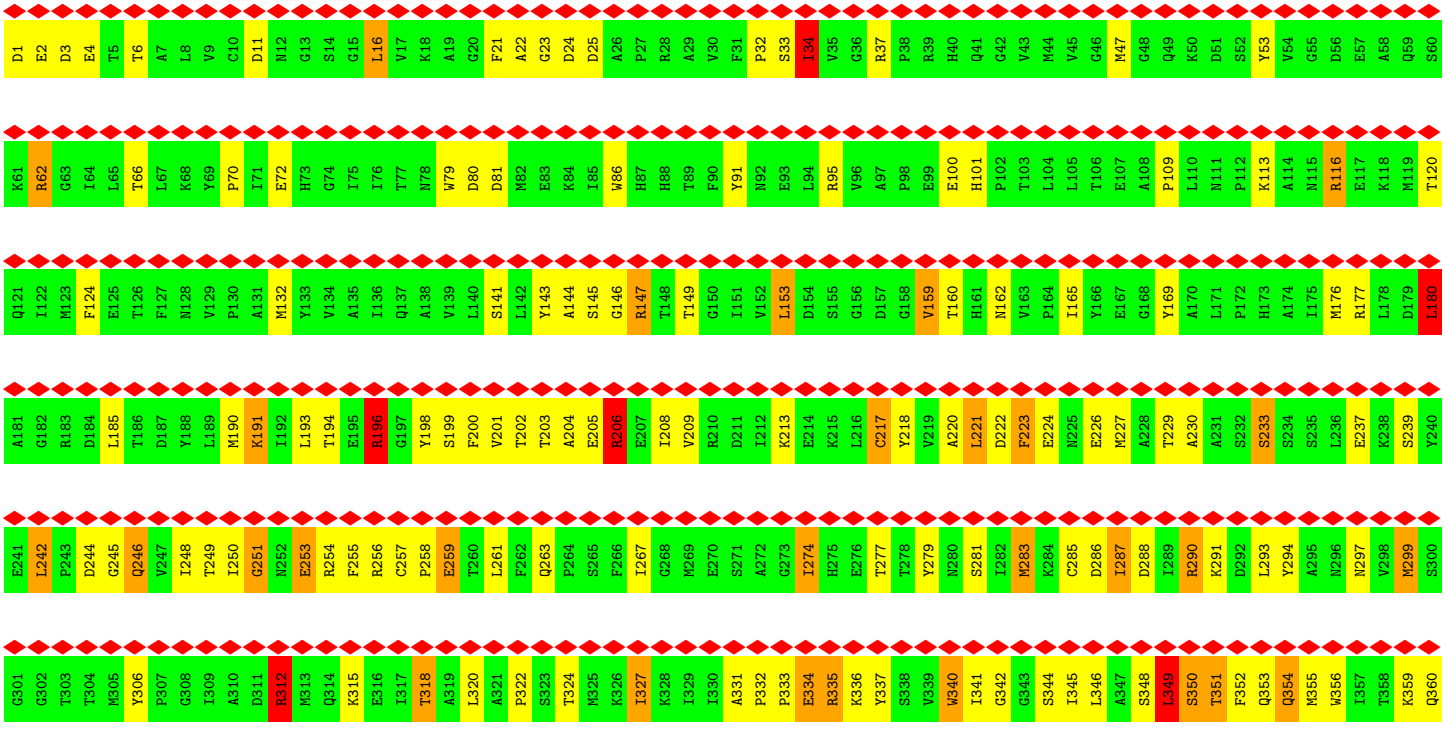




- Molecule 4: SKELETAL MUSCLE ACTIN

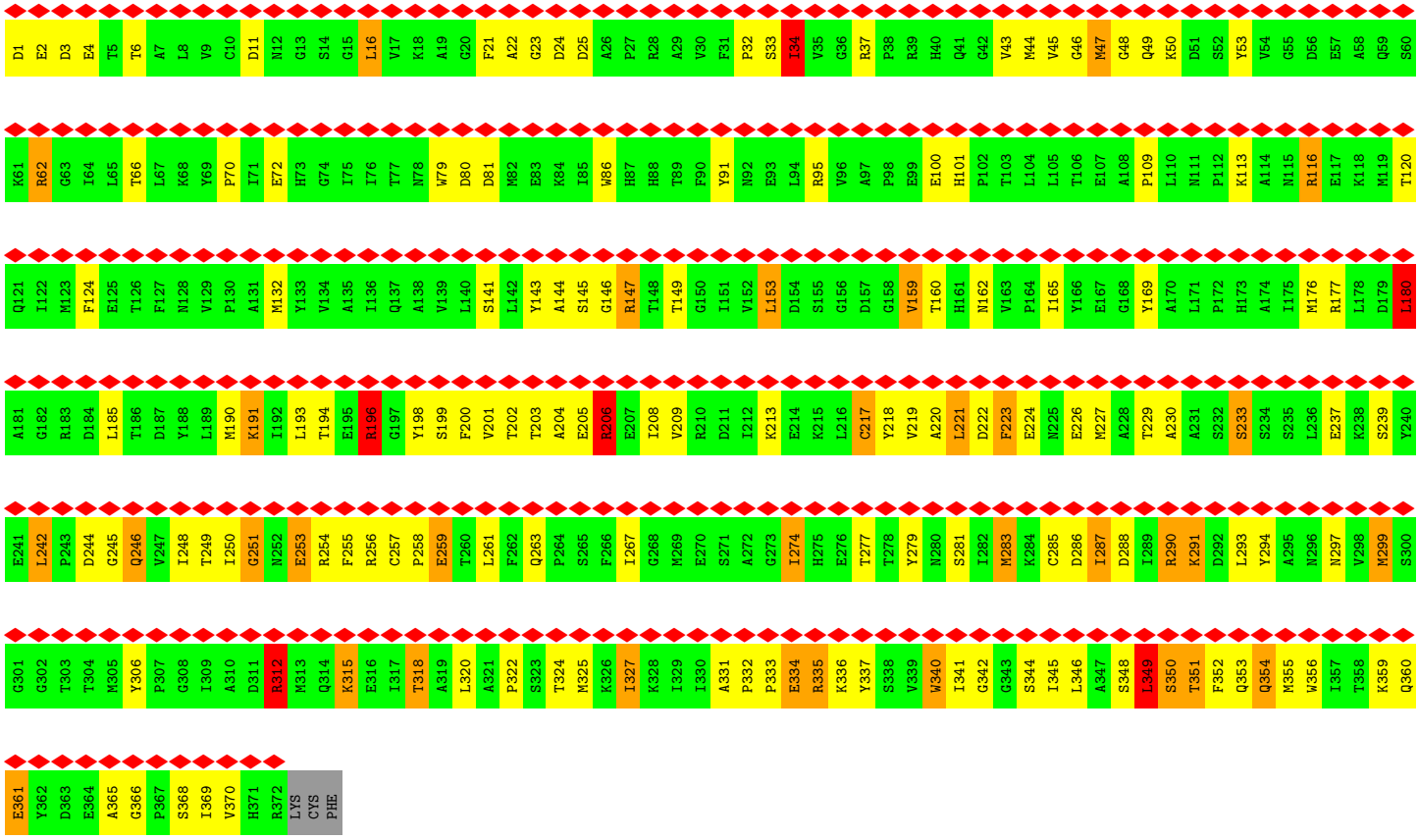
Chain 9:





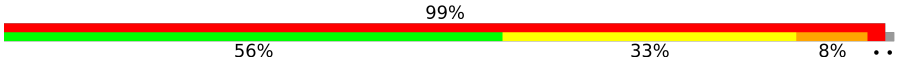
• Molecule 4: SKELETAL MUSCLE ACTIN

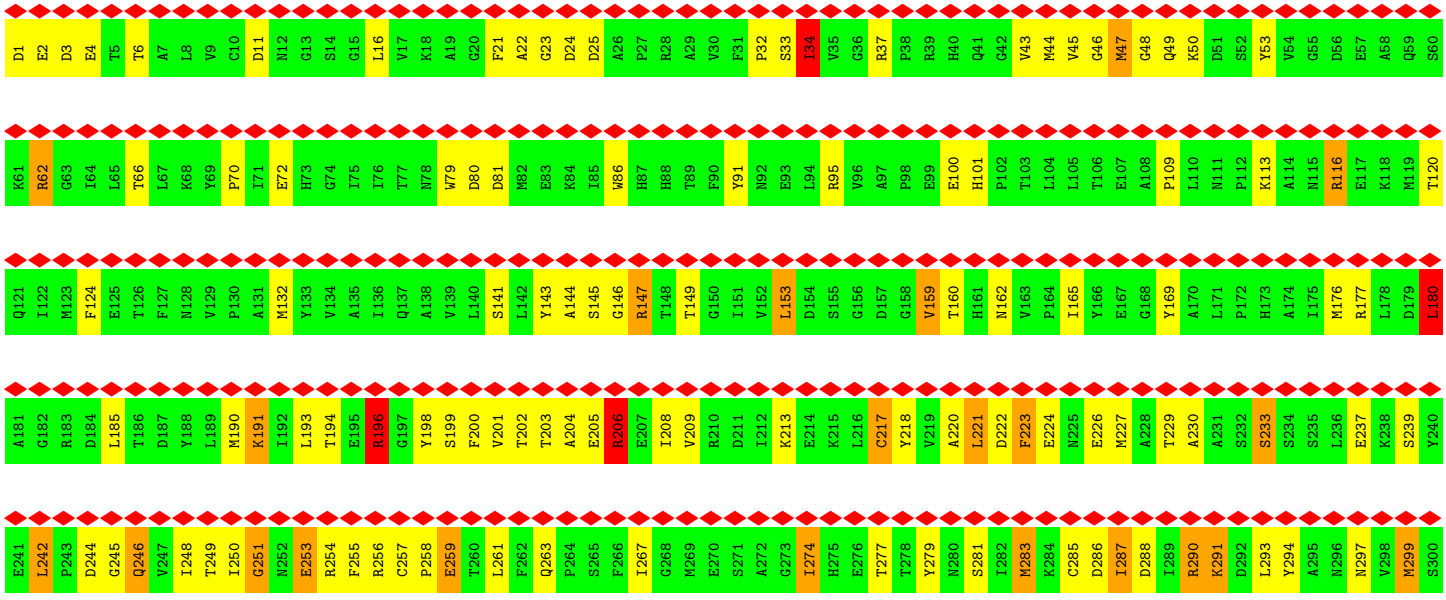
Chain V:

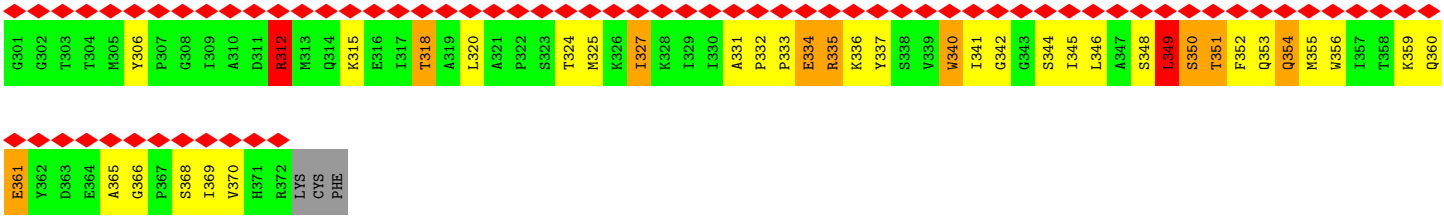


• Molecule 4: SKELETAL MUSCLE ACTIN

Chain W:

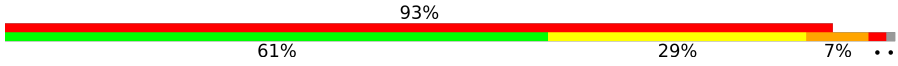


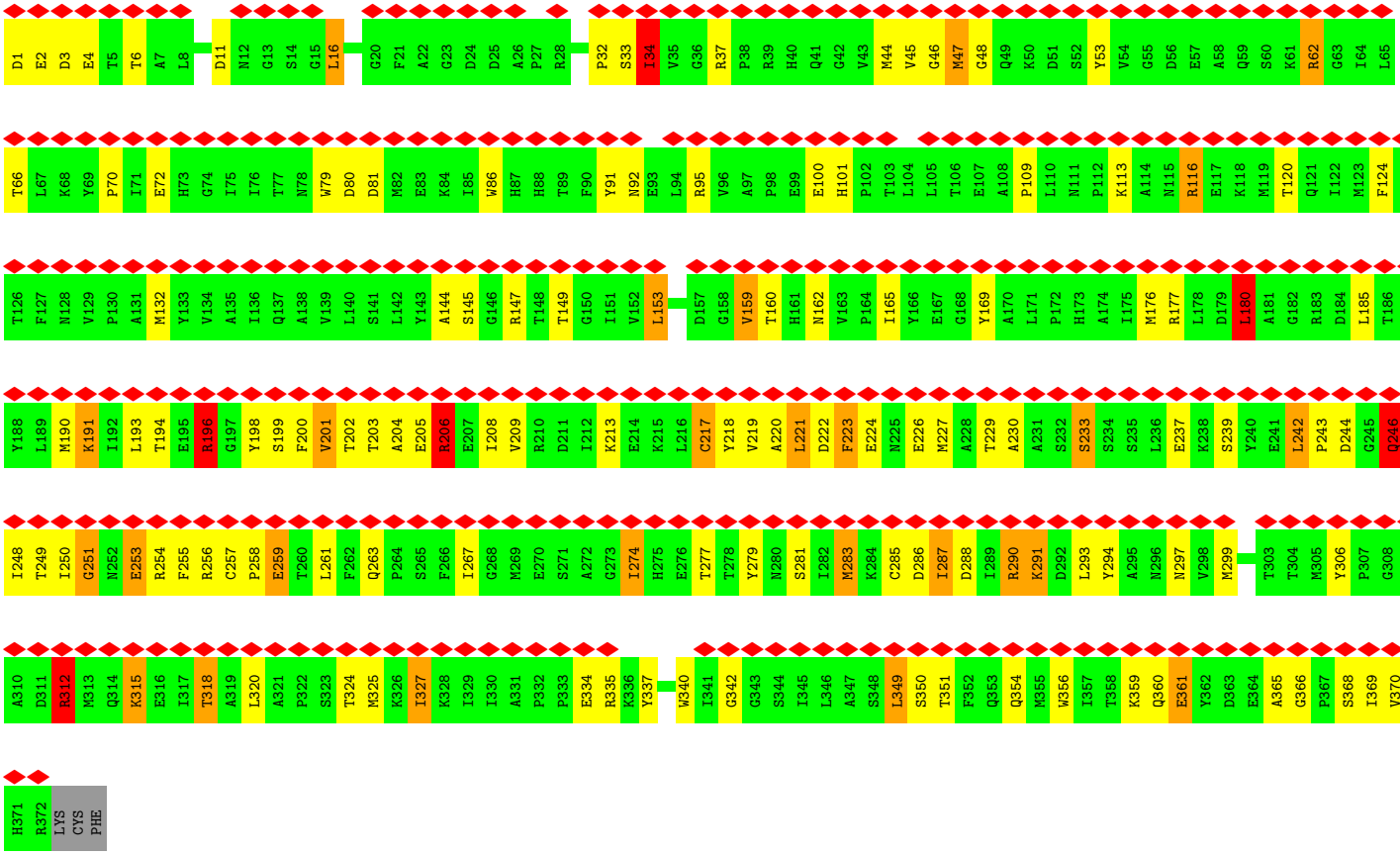




• Molecule 4: SKELETAL MUSCLE ACTIN

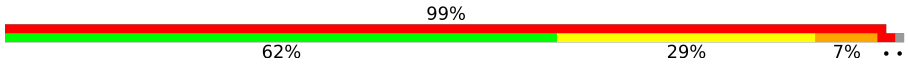
Chain X:

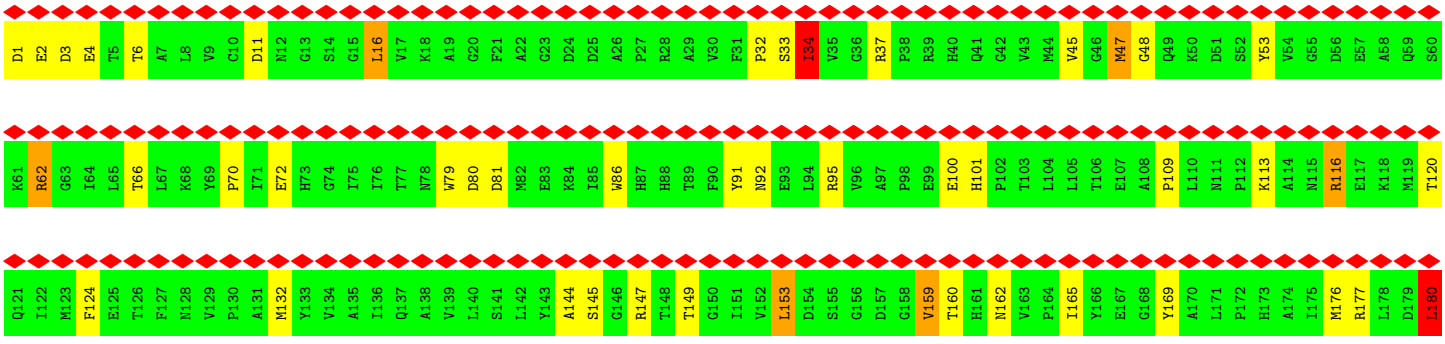




• Molecule 4: SKELETAL MUSCLE ACTIN

Chain Y:





- Molecule 4: SKELETAL MUSCLE ACTIN

Chain Z:

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	65/6448 (1.0%)	1.82	117/8729 (1.3%)
1	D	1.77	65/6448 (1.0%)	1.82	115/8729 (1.3%)
1	G	1.77	64/6448 (1.0%)	1.82	116/8729 (1.3%)
1	J	1.90	65/6449 (1.0%)	1.84	120/8732 (1.4%)
2	B	1.22	10/1148 (0.9%)	1.61	16/1548 (1.0%)
2	E	1.22	10/1148 (0.9%)	1.62	16/1548 (1.0%)
2	H	1.22	10/1148 (0.9%)	1.62	17/1548 (1.1%)
2	K	1.22	10/1148 (0.9%)	1.61	16/1548 (1.0%)
3	C	0.80	0/1136	0.95	4/1525 (0.3%)
3	F	0.80	0/1136	0.95	4/1525 (0.3%)
3	I	0.80	0/1136	0.94	4/1525 (0.3%)
3	L	0.79	0/1136	0.95	4/1525 (0.3%)
4	0	0.89	1/2968 (0.0%)	1.64	51/4023 (1.3%)
4	1	0.89	1/2968 (0.0%)	1.64	52/4023 (1.3%)
4	2	0.90	2/2968 (0.1%)	1.64	51/4023 (1.3%)
4	3	0.89	2/2968 (0.1%)	1.64	52/4023 (1.3%)
4	4	0.90	1/2968 (0.0%)	1.64	52/4023 (1.3%)
4	5	0.89	1/2968 (0.0%)	1.64	52/4023 (1.3%)
4	7	0.89	1/2968 (0.0%)	1.64	52/4023 (1.3%)
4	8	0.89	2/2968 (0.1%)	1.64	50/4023 (1.2%)
4	9	0.89	1/2968 (0.0%)	1.64	52/4023 (1.3%)
4	V	0.89	1/2968 (0.0%)	1.64	52/4023 (1.3%)
4	W	0.89	2/2968 (0.1%)	1.64	52/4023 (1.3%)
4	X	0.89	1/2968 (0.0%)	1.64	51/4023 (1.3%)
4	Y	0.89	2/2968 (0.1%)	1.64	51/4023 (1.3%)
4	Z	0.89	2/2968 (0.1%)	1.64	51/4023 (1.3%)
All	All	1.29	319/76481 (0.4%)	1.67	1270/103533 (1.2%)

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

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	4
1	D	1	4
1	G	1	4
1	J	1	6
2	B	0	3
2	E	0	3
2	H	0	3
2	K	0	3
3	C	0	2
3	F	0	2
3	I	0	2
3	L	0	2
4	0	0	1
4	1	0	1
4	2	0	1
4	3	0	1
4	4	0	1
4	5	0	1
4	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	4	52

The worst 5 of 319 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	709	LYS	C-N	-55.30	0.33	1.33
1	G	649	VAL	CB-CG1	53.23	2.64	1.52
1	J	649	VAL	CB-CG1	53.22	2.64	1.52
1	D	649	VAL	CB-CG1	53.14	2.64	1.52
1	A	649	VAL	CB-CG1	53.14	2.64	1.52

The worst 5 of 1270 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	637	LYS	O-C-N	-58.52	23.72	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	637	LYS	O-C-N	-58.47	23.80	123.20
1	J	637	LYS	O-C-N	-58.47	23.81	123.20
1	A	637	LYS	O-C-N	-58.43	23.87	123.20
1	J	649	VAL	CG1-CB-CG2	-34.01	56.48	110.90

All (4) 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

5 of 52 planarity outliers are listed below:

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

5.2 Too-close contacts (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	6752	1412	0
1	D	6797	0	6761	1437	0
1	G	6797	0	6760	1397	0
1	J	6797	0	6766	1420	0
2	B	1127	0	1086	251	0
2	E	1127	0	1087	320	0
2	H	1127	0	1087	227	0
2	K	1127	0	1087	230	0
3	C	1123	0	1084	177	0
3	F	1123	0	1082	142	0
3	I	1123	0	1084	167	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	1123	0	1084	166	0
4	0	2906	0	2865	176	0
4	1	2906	0	2865	202	0
4	2	2906	0	2865	137	0
4	3	2906	0	2863	180	0
4	4	2906	0	2865	96	0
4	5	2906	0	2865	98	0
4	7	2906	0	2866	78	0
4	8	2906	0	2857	320	0
4	9	2906	0	2855	340	0
4	V	2906	0	2851	385	0
4	W	2906	0	2851	383	0
4	X	2906	0	2862	213	0
4	Y	2906	0	2863	186	0
4	Z	2906	0	2862	189	0
All	All	76872	0	75775	7716	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 51.

The worst 5 of 7716 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:797:PHE:CD1	3:I:149:VAL:HG11	1.21	1.69
2:E:144:VAL:HG13	2:E:153:ILE:CD1	1.22	1.66
1:A:725:ARG:HE	1:A:733:PRO:CB	1.09	1.64
1:D:725:ARG:HE	1:D:733:PRO:CB	1.09	1.64
1:G:798:LEU:CD1	3:I:126:LEU:HD21	1.22	1.64

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%)	650 (82%)	113 (14%)	26 (3%)	4	26
1	D	789/840 (94%)	650 (82%)	113 (14%)	26 (3%)	4	26
1	G	789/840 (94%)	650 (82%)	112 (14%)	27 (3%)	3	26
1	J	791/840 (94%)	652 (82%)	112 (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
3	C	143/147 (97%)	133 (93%)	10 (7%)	0	100	100
3	F	143/147 (97%)	133 (93%)	10 (7%)	0	100	100
3	I	143/147 (97%)	133 (93%)	10 (7%)	0	100	100
3	L	143/147 (97%)	133 (93%)	10 (7%)	0	100	100
4	0	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	9	44
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%)	334 (90%)	30 (8%)	6 (2%)	9	44
4	4	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	9	44
4	5	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	9	44
4	7	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	9	44
4	8	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	9	44
4	9	370/375 (99%)	333 (90%)	31 (8%)	6 (2%)	9	44
4	V	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	9	44
4	W	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	9	44
4	X	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	9	44
4	Y	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	9	44
4	Z	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	9	44
All	All	9482/9778 (97%)	8316 (88%)	944 (10%)	222 (2%)	9	34

5 of 222 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	LYS
1	A	202	SER
1	A	572	LYS

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Mol	Chain	Res	Type
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
1	D	672/672 (100%)	514 (76%)	158 (24%)	1 4
1	G	672/672 (100%)	513 (76%)	159 (24%)	1 4
1	J	672/672 (100%)	513 (76%)	159 (24%)	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
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
4	0	315/318 (99%)	268 (85%)	47 (15%)	3 15
4	1	315/318 (99%)	268 (85%)	47 (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%)	269 (85%)	46 (15%)	3 15
4	5	315/318 (99%)	268 (85%)	47 (15%)	3 15
4	7	315/318 (99%)	269 (85%)	46 (15%)	3 15
4	8	315/318 (99%)	269 (85%)	46 (15%)	3 15
4	9	315/318 (99%)	268 (85%)	47 (15%)	3 15
4	V	315/318 (99%)	268 (85%)	47 (15%)	3 15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	W	315/318 (99%)	269 (85%)	46 (15%)	3	15
4	X	315/318 (99%)	268 (85%)	47 (15%)	3	15
4	Y	315/318 (99%)	268 (85%)	47 (15%)	3	15
4	Z	315/318 (99%)	269 (85%)	46 (15%)	3	15
All	All	8046/8088 (100%)	6734 (84%)	1312 (16%)	5	13

5 of 1312 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	5	312	ARG
4	W	229	THR
4	7	191	LYS
4	5	299	MET
4	9	109	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 185 such sidechains are listed below:

Mol	Chain	Res	Type
4	1	263	GLN
4	7	137	GLN
4	2	137	GLN
4	4	92	ASN
4	8	252	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	MLY	A	59	1	9,10,11	0.87	0	6,11,13	0.49	0
1	MLY	J	55	1	9,10,11	0.72	0	6,11,13	0.78	0
1	MLY	D	528	1	9,10,11	0.91	0	6,11,13	0.65	0
1	MLY	G	272	1	9,10,11	0.97	1 (11%)	6,11,13	0.53	0
1	MLY	J	659	1	9,10,11	0.81	0	6,11,13	0.58	0
1	MLY	D	63	1	9,10,11	0.91	0	6,11,13	0.45	0
1	MLY	A	353	1	9,10,11	0.87	0	6,11,13	0.78	0
1	MLY	A	348	1	9,10,11	0.84	0	6,11,13	0.48	0
1	MLY	D	436	1	9,10,11	1.12	1 (11%)	6,11,13	0.49	0
1	MLY	G	63	1	9,10,11	0.91	0	6,11,13	0.44	0
1	MLY	D	415	1	9,10,11	0.79	0	6,11,13	0.20	0
1	MLY	G	551	1	9,10,11	0.51	0	6,11,13	0.20	0
1	MLY	G	681	1	9,10,11	0.62	0	6,11,13	0.44	0
1	MLY	A	236	1	9,10,11	0.79	1 (11%)	6,11,13	0.48	0
1	MLY	J	63	1	9,10,11	0.92	0	6,11,13	0.43	0
1	MLY	G	130	1	9,10,11	0.80	0	6,11,13	0.76	0
1	MLY	A	30	1	9,10,11	0.88	0	6,11,13	0.31	0
1	MLY	G	367	1	9,10,11	0.64	0	6,11,13	0.39	0
1	MLY	G	369	1	9,10,11	0.70	0	6,11,13	0.47	0
1	MLY	G	431	1	9,10,11	0.54	0	6,11,13	0.47	0
1	MLY	J	600	1	9,10,11	0.53	0	6,11,13	0.37	0
1	MLY	J	130	1	9,10,11	0.78	0	6,11,13	0.76	0
1	MLY	J	528	1	9,10,11	0.87	0	6,11,13	0.66	0
1	MLY	G	19	1	9,10,11	1.15	1 (11%)	6,11,13	0.57	0
1	MLY	G	782	1	9,10,11	0.79	0	6,11,13	0.35	0
1	MLY	J	272	1	9,10,11	1.03	1 (11%)	6,11,13	0.56	0
1	MLY	D	553	4,1	9,10,11	0.67	0	6,11,13	0.55	0
1	MLY	G	486	1	9,10,11	0.65	0	6,11,13	0.39	0
1	MLY	G	505	1	9,10,11	0.91	1 (11%)	6,11,13	0.34	0
1	MLY	J	84	1	9,10,11	0.51	0	6,11,13	0.80	0
1	MLY	J	551	1	9,10,11	0.51	0	6,11,13	0.19	0
1	MLY	J	839	1	9,10,11	0.69	0	6,11,13	0.77	0
1	MLY	A	63	1	9,10,11	0.92	1 (11%)	6,11,13	0.43	0
1	MLY	G	107	1	9,10,11	0.48	0	6,11,13	0.33	0
1	MLY	G	35	1	9,10,11	0.72	0	6,11,13	0.39	0
1	MLY	J	19	1	9,10,11	1.18	1 (11%)	6,11,13	0.57	0
1	MLY	J	782	1	9,10,11	0.78	0	6,11,13	0.36	0
1	MLY	A	87	1	9,10,11	1.21	1 (11%)	6,11,13	0.41	0
1	MLY	A	55	1	9,10,11	0.71	0	6,11,13	0.79	0
1	MLY	A	600	1	9,10,11	0.52	0	6,11,13	0.38	0
1	MLY	G	837	1	9,10,11	0.61	0	6,11,13	0.52	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	1.09	1 (11%)	6,11,13	0.50	0
1	MLY	D	613	1	9,10,11	0.57	0	6,11,13	0.64	0
1	MLY	D	190	1	9,10,11	1.21	1 (11%)	6,11,13	0.53	0
1	MLY	A	764	1	9,10,11	0.85	0	6,11,13	0.36	0
1	MLY	A	367	1	9,10,11	0.63	0	6,11,13	0.37	0
1	MLY	G	248	1	9,10,11	0.83	0	6,11,13	0.63	0
1	MLY	A	431	1	9,10,11	0.52	0	6,11,13	0.44	0
1	MLY	A	369	1	9,10,11	0.71	0	6,11,13	0.45	0
1	MLY	D	617	1	9,10,11	0.97	1 (11%)	6,11,13	0.34	0
1	MLY	D	84	1	9,10,11	0.52	0	6,11,13	0.80	0
1	MLY	D	296	1	9,10,11	0.66	0	6,11,13	0.36	0
1	MLY	D	598	1	9,10,11	0.92	1 (11%)	6,11,13	0.44	0
1	MLY	G	348	1	9,10,11	0.86	1 (11%)	6,11,13	0.48	0
1	MLY	G	600	1	9,10,11	0.52	0	6,11,13	0.37	0
1	MLY	J	248	1	9,10,11	0.83	0	6,11,13	0.62	0
1	MLY	A	504	1	9,10,11	0.90	0	6,11,13	0.25	0
1	MLY	J	348	1	9,10,11	0.83	0	6,11,13	0.47	0
1	MLY	A	272	1	9,10,11	1.03	1 (11%)	6,11,13	0.56	0
1	MLY	J	385	1	9,10,11	1.03	1 (11%)	6,11,13	0.44	0
1	MLY	G	30	1	9,10,11	0.88	0	6,11,13	0.30	0
1	MLY	A	681	1	9,10,11	0.61	0	6,11,13	0.46	0
1	MLY	D	272	1	9,10,11	0.99	1 (11%)	6,11,13	0.57	0
1	MLY	D	295	1	9,10,11	0.80	0	6,11,13	0.35	0
1	MLY	J	30	1	9,10,11	0.89	0	6,11,13	0.31	0
1	MLY	D	551	1	9,10,11	0.53	0	6,11,13	0.19	0
1	MLY	G	190	1	9,10,11	1.25	1 (11%)	6,11,13	0.52	0
1	MLY	A	49	1	9,10,11	1.03	1 (11%)	6,11,13	0.74	0
1	MLY	D	833	1	9,10,11	1.14	1 (11%)	6,11,13	0.32	0
1	MLY	J	367	1	9,10,11	0.62	0	6,11,13	0.37	0
1	MLY	D	385	1	9,10,11	0.98	1 (11%)	6,11,13	0.43	0
1	MLY	J	369	1	9,10,11	0.69	0	6,11,13	0.44	0
1	MLY	J	431	1	9,10,11	0.53	0	6,11,13	0.45	0
1	MLY	G	385	1	9,10,11	1.00	1 (11%)	6,11,13	0.44	0
1	MLY	D	19	1	9,10,11	1.21	1 (11%)	6,11,13	0.57	0
1	MLY	G	295	1	9,10,11	0.80	0	6,11,13	0.34	0
1	MLY	A	528	1	9,10,11	0.89	0	6,11,13	0.67	0
1	MLY	A	385	1	9,10,11	1.01	1 (11%)	6,11,13	0.43	0
1	MLY	J	295	1	9,10,11	0.79	0	6,11,13	0.34	0
1	MLY	D	839	1	9,10,11	0.70	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	G	659	1	9,10,11	0.83	0	6,11,13	0.59	0
1	MLY	D	49	1	9,10,11	1.09	1 (11%)	6,11,13	0.74	0
1	MLY	A	436	1	9,10,11	1.06	1 (11%)	6,11,13	0.50	0
1	MLY	G	764	1	9,10,11	0.82	0	6,11,13	0.36	0
1	MLY	D	87	1	9,10,11	1.20	1 (11%)	6,11,13	0.44	0
1	MLY	A	296	1	9,10,11	0.62	0	6,11,13	0.35	0
1	MLY	D	681	1	9,10,11	0.59	0	6,11,13	0.46	0
1	MLY	G	59	1	9,10,11	0.85	0	6,11,13	0.50	0
1	MLY	J	415	1	9,10,11	0.79	0	6,11,13	0.19	0
1	MLY	A	486	1	9,10,11	0.65	0	6,11,13	0.38	0
1	MLY	J	87	1	9,10,11	1.22	1 (11%)	6,11,13	0.44	0
1	MLY	A	295	1	9,10,11	0.84	0	6,11,13	0.32	0
1	MLY	J	617	1	9,10,11	0.98	1 (11%)	6,11,13	0.33	0
1	MLY	J	837	1	9,10,11	0.60	0	6,11,13	0.55	0
1	MLY	D	768	1	9,10,11	0.72	0	6,11,13	0.41	0
1	MLY	J	59	1	9,10,11	0.86	0	6,11,13	0.50	0
1	MLY	D	130	1	9,10,11	0.80	0	6,11,13	0.74	0
1	MLY	D	486	1	9,10,11	0.64	0	6,11,13	0.39	0
1	MLY	D	367	1	9,10,11	0.63	0	6,11,13	0.38	0
1	MLY	D	369	1	9,10,11	0.70	0	6,11,13	0.44	0
1	MLY	D	431	1	9,10,11	0.53	0	6,11,13	0.46	0
1	MLY	G	504	1	9,10,11	0.88	0	6,11,13	0.22	0
1	MLY	G	768	1	9,10,11	0.74	0	6,11,13	0.42	0
1	MLY	J	107	1	9,10,11	0.47	0	6,11,13	0.34	0
1	MLY	A	553	4,1	9,10,11	0.68	0	6,11,13	0.55	0
1	MLY	D	782	1	9,10,11	0.77	0	6,11,13	0.34	0
1	MLY	J	190	1	9,10,11	1.26	1 (11%)	6,11,13	0.52	0
1	MLY	J	768	1	9,10,11	0.75	0	6,11,13	0.42	0
1	MLY	A	659	1	9,10,11	0.84	0	6,11,13	0.60	0
1	MLY	J	49	1	9,10,11	1.09	1 (11%)	6,11,13	0.75	0
1	MLY	D	505	1	9,10,11	0.87	1 (11%)	6,11,13	0.35	0
1	MLY	G	415	1	9,10,11	0.77	0	6,11,13	0.19	0
1	MLY	G	87	1	9,10,11	1.27	1 (11%)	6,11,13	0.43	0
1	MLY	G	613	1	9,10,11	0.58	0	6,11,13	0.64	0
1	MLY	A	415	1	9,10,11	0.76	0	6,11,13	0.19	0
1	MLY	J	504	1	9,10,11	0.83	0	6,11,13	0.23	0
1	MLY	D	55	1	9,10,11	0.72	0	6,11,13	0.79	0
1	MLY	D	107	1	9,10,11	0.50	0	6,11,13	0.33	0
1	MLY	G	833	1	9,10,11	1.19	2 (22%)	6,11,13	0.32	0
1	MLY	G	49	1	9,10,11	1.10	1 (11%)	6,11,13	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	MLY	J	833	1	9,10,11	1.19	1 (11%)	6,11,13	0.30	0
1	MLY	G	296	1	9,10,11	0.65	0	6,11,13	0.38	0
1	MLY	G	236	1	9,10,11	0.78	1 (11%)	6,11,13	0.48	0
1	MLY	G	598	1	9,10,11	0.90	1 (11%)	6,11,13	0.43	0
1	MLY	A	839	1,2	9,10,11	0.70	0	6,11,13	0.81	0
1	MLY	A	617	1	9,10,11	0.94	1 (11%)	6,11,13	0.34	0
1	MLY	J	505	1	9,10,11	0.92	1 (11%)	6,11,13	0.34	0
1	MLY	A	84	1	9,10,11	0.49	0	6,11,13	0.79	0
1	MLY	D	353	1	9,10,11	0.85	0	6,11,13	0.79	0
1	MLY	G	528	1	9,10,11	0.90	0	6,11,13	0.66	0
1	MLY	J	681	1	9,10,11	0.60	0	6,11,13	0.46	0
1	MLY	J	553	1	9,10,11	0.67	0	6,11,13	0.53	0
1	MLY	A	19	1	9,10,11	1.14	1 (11%)	6,11,13	0.56	0
1	MLY	G	436	1	9,10,11	1.05	1 (11%)	6,11,13	0.49	0
1	MLY	A	782	1	9,10,11	0.78	0	6,11,13	0.36	0
1	MLY	G	827	1	9,10,11	0.70	0	6,11,13	0.49	0
1	MLY	J	827	1	9,10,11	0.74	0	6,11,13	0.49	0
1	MLY	A	505	1	9,10,11	0.91	1 (11%)	6,11,13	0.32	0
1	MLY	J	764	1	9,10,11	0.84	0	6,11,13	0.37	0
1	MLY	A	837	1	9,10,11	0.61	0	6,11,13	0.53	0
1	MLY	D	35	1	9,10,11	0.72	0	6,11,13	0.38	0
1	MLY	A	613	1	9,10,11	0.55	0	6,11,13	0.63	0
1	MLY	D	348	1	9,10,11	0.82	0	6,11,13	0.47	0
1	MLY	A	551	1	9,10,11	0.51	0	6,11,13	0.19	0
1	MLY	D	600	1	9,10,11	0.51	0	6,11,13	0.37	0
1	MLY	D	764	1	9,10,11	0.86	0	6,11,13	0.35	0
1	MLY	G	353	1	9,10,11	0.85	0	6,11,13	0.80	0
1	MLY	A	107	1	9,10,11	0.46	0	6,11,13	0.33	0
1	MLY	J	486	1	9,10,11	0.63	0	6,11,13	0.38	0
1	MLY	A	833	1	9,10,11	1.15	1 (11%)	6,11,13	0.33	0
1	MLY	D	30	1	9,10,11	0.90	0	6,11,13	0.31	0
1	MLY	A	138	1	9,10,11	1.35	1 (11%)	6,11,13	0.84	0
1	MLY	G	553	4,1	9,10,11	0.66	0	6,11,13	0.55	0
1	MLY	G	839	1	9,10,11	0.70	0	6,11,13	0.79	0
1	MLY	A	598	1	9,10,11	0.90	1 (11%)	6,11,13	0.44	0
1	MLY	A	827	1	9,10,11	0.73	0	6,11,13	0.45	0
1	MLY	D	504	1	9,10,11	0.88	0	6,11,13	0.20	0
1	MLY	J	353	1	9,10,11	0.87	0	6,11,13	0.78	0
1	MLY	A	248	1	9,10,11	0.83	0	6,11,13	0.61	0
1	MLY	D	827	1	9,10,11	0.67	0	6,11,13	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	MLY	D	248	1	9,10,11	0.83	0	6,11,13	0.62	0
1	MLY	D	236	1	9,10,11	0.80	1 (11%)	6,11,13	0.47	0
1	MLY	J	35	1	9,10,11	0.72	0	6,11,13	0.38	0
1	MLY	D	659	1	9,10,11	0.84	0	6,11,13	0.59	0
1	MLY	J	613	1	9,10,11	0.54	0	6,11,13	0.64	0
1	MLY	A	190	1	9,10,11	1.29	2 (22%)	6,11,13	0.51	0
1	MLY	G	617	1	9,10,11	0.98	1 (11%)	6,11,13	0.34	0
1	MLY	A	130	1	9,10,11	0.81	0	6,11,13	0.75	0
1	MLY	G	84	1	9,10,11	0.50	0	6,11,13	0.80	0
1	MLY	A	768	1	9,10,11	0.76	0	6,11,13	0.41	0
1	MLY	D	837	1	9,10,11	0.60	0	6,11,13	0.57	0
1	MLY	J	236	1	9,10,11	0.79	1 (11%)	6,11,13	0.47	0
1	MLY	D	59	1	9,10,11	0.87	0	6,11,13	0.49	0
1	MLY	J	296	1	9,10,11	0.71	0	6,11,13	0.36	0
1	MLY	J	598	1	9,10,11	0.90	1 (11%)	6,11,13	0.44	0
1	MLY	A	35	1	9,10,11	0.72	0	6,11,13	0.38	0
1	MLY	G	138	1	9,10,11	1.34	1 (11%)	6,11,13	0.84	0
1	MLY	G	55	1	9,10,11	0.73	0	6,11,13	0.80	0
1	MLY	J	138	1	9,10,11	1.34	1 (11%)	6,11,13	0.84	0
1	MLY	D	138	1	9,10,11	1.40	1 (11%)	6,11,13	0.85	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	59	1	-	3/8/9/11	-
1	MLY	J	55	1	-	6/8/9/11	-
1	MLY	D	528	1	-	4/8/9/11	-
1	MLY	G	272	1	-	3/8/9/11	-
1	MLY	J	659	1	-	3/8/9/11	-
1	MLY	D	63	1	-	4/8/9/11	-
1	MLY	A	353	1	-	4/8/9/11	-
1	MLY	A	348	1	-	5/8/9/11	-
1	MLY	D	436	1	-	4/8/9/11	-
1	MLY	G	63	1	-	4/8/9/11	-
1	MLY	D	415	1	-	3/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	G	551	1	-	3/8/9/11	-
1	MLY	G	681	1	-	4/8/9/11	-
1	MLY	A	236	1	-	3/8/9/11	-
1	MLY	J	63	1	-	4/8/9/11	-
1	MLY	G	130	1	-	5/8/9/11	-
1	MLY	A	30	1	-	2/8/9/11	-
1	MLY	G	367	1	-	2/8/9/11	-
1	MLY	G	369	1	-	2/8/9/11	-
1	MLY	G	431	1	-	4/8/9/11	-
1	MLY	J	600	1	-	3/8/9/11	-
1	MLY	J	130	1	-	5/8/9/11	-
1	MLY	J	528	1	-	4/8/9/11	-
1	MLY	G	19	1	-	4/8/9/11	-
1	MLY	G	782	1	-	6/8/9/11	-
1	MLY	J	272	1	-	3/8/9/11	-
1	MLY	D	553	4,1	-	5/8/9/11	-
1	MLY	G	486	1	-	2/8/9/11	-
1	MLY	G	505	1	-	5/8/9/11	-
1	MLY	J	84	1	-	4/8/9/11	-
1	MLY	J	551	1	-	3/8/9/11	-
1	MLY	J	839	1	-	3/8/9/11	-
1	MLY	A	63	1	-	4/8/9/11	-
1	MLY	G	107	1	-	2/8/9/11	-
1	MLY	G	35	1	-	3/8/9/11	-
1	MLY	J	19	1	-	4/8/9/11	-
1	MLY	J	782	1	-	6/8/9/11	-
1	MLY	A	87	1	-	2/8/9/11	-
1	MLY	A	55	1	-	6/8/9/11	-
1	MLY	A	600	1	-	3/8/9/11	-
1	MLY	G	837	1	-	5/8/9/11	-
1	MLY	J	436	1	-	4/8/9/11	-
1	MLY	D	613	1	-	4/8/9/11	-
1	MLY	D	190	1	-	5/8/9/11	-
1	MLY	A	764	1	-	2/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	A	367	1	-	2/8/9/11	-
1	MLY	G	248	1	-	6/8/9/11	-
1	MLY	A	431	1	-	4/8/9/11	-
1	MLY	A	369	1	-	2/8/9/11	-
1	MLY	D	617	1	-	1/8/9/11	-
1	MLY	D	84	1	-	4/8/9/11	-
1	MLY	D	296	1	-	4/8/9/11	-
1	MLY	D	598	1	-	5/8/9/11	-
1	MLY	G	348	1	-	5/8/9/11	-
1	MLY	G	600	1	-	3/8/9/11	-
1	MLY	J	248	1	-	6/8/9/11	-
1	MLY	A	504	1	-	4/8/9/11	-
1	MLY	J	348	1	-	5/8/9/11	-
1	MLY	A	272	1	-	3/8/9/11	-
1	MLY	J	385	1	-	2/8/9/11	-
1	MLY	G	30	1	-	2/8/9/11	-
1	MLY	A	681	1	-	4/8/9/11	-
1	MLY	D	272	1	-	3/8/9/11	-
1	MLY	D	295	1	-	2/8/9/11	-
1	MLY	J	30	1	-	2/8/9/11	-
1	MLY	D	551	1	-	3/8/9/11	-
1	MLY	G	190	1	-	5/8/9/11	-
1	MLY	A	49	1	-	3/8/9/11	-
1	MLY	D	833	1	-	6/8/9/11	-
1	MLY	J	367	1	-	2/8/9/11	-
1	MLY	D	385	1	-	2/8/9/11	-
1	MLY	J	369	1	-	2/8/9/11	-
1	MLY	J	431	1	-	4/8/9/11	-
1	MLY	G	385	1	-	2/8/9/11	-
1	MLY	D	19	1	-	4/8/9/11	-
1	MLY	G	295	1	-	2/8/9/11	-
1	MLY	A	528	1	-	5/8/9/11	-
1	MLY	A	385	1	-	2/8/9/11	-
1	MLY	J	295	1	-	2/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	D	839	1	-	3/8/9/11	-
1	MLY	G	659	1	-	3/8/9/11	-
1	MLY	D	49	1	-	3/8/9/11	-
1	MLY	A	436	1	-	4/8/9/11	-
1	MLY	G	764	1	-	2/8/9/11	-
1	MLY	D	87	1	-	2/8/9/11	-
1	MLY	A	296	1	-	4/8/9/11	-
1	MLY	D	681	1	-	4/8/9/11	-
1	MLY	G	59	1	-	3/8/9/11	-
1	MLY	J	415	1	-	3/8/9/11	-
1	MLY	A	486	1	-	2/8/9/11	-
1	MLY	J	87	1	-	2/8/9/11	-
1	MLY	A	295	1	-	2/8/9/11	-
1	MLY	J	617	1	-	1/8/9/11	-
1	MLY	J	837	1	-	5/8/9/11	-
1	MLY	D	768	1	-	4/8/9/11	-
1	MLY	J	59	1	-	3/8/9/11	-
1	MLY	D	130	1	-	5/8/9/11	-
1	MLY	D	486	1	-	2/8/9/11	-
1	MLY	D	367	1	-	2/8/9/11	-
1	MLY	D	369	1	-	2/8/9/11	-
1	MLY	D	431	1	-	4/8/9/11	-
1	MLY	G	504	1	-	4/8/9/11	-
1	MLY	G	768	1	-	4/8/9/11	-
1	MLY	J	107	1	-	2/8/9/11	-
1	MLY	A	553	4,1	-	4/8/9/11	-
1	MLY	D	782	1	-	6/8/9/11	-
1	MLY	J	190	1	-	5/8/9/11	-
1	MLY	J	768	1	-	4/8/9/11	-
1	MLY	A	659	1	-	3/8/9/11	-
1	MLY	J	49	1	-	3/8/9/11	-
1	MLY	D	505	1	-	5/8/9/11	-
1	MLY	G	415	1	-	3/8/9/11	-
1	MLY	G	87	1	-	2/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	G	613	1	-	4/8/9/11	-
1	MLY	A	415	1	-	3/8/9/11	-
1	MLY	J	504	1	-	4/8/9/11	-
1	MLY	D	55	1	-	6/8/9/11	-
1	MLY	D	107	1	-	2/8/9/11	-
1	MLY	G	833	1	-	6/8/9/11	-
1	MLY	G	49	1	-	3/8/9/11	-
1	MLY	J	833	1	-	6/8/9/11	-
1	MLY	G	296	1	-	4/8/9/11	-
1	MLY	G	236	1	-	3/8/9/11	-
1	MLY	G	598	1	-	5/8/9/11	-
1	MLY	A	839	1,2	-	3/8/9/11	-
1	MLY	A	617	1	-	1/8/9/11	-
1	MLY	J	505	1	-	5/8/9/11	-
1	MLY	A	84	1	-	4/8/9/11	-
1	MLY	D	353	1	-	4/8/9/11	-
1	MLY	G	528	1	-	4/8/9/11	-
1	MLY	J	681	1	-	4/8/9/11	-
1	MLY	J	553	1	-	4/8/9/11	-
1	MLY	A	19	1	-	4/8/9/11	-
1	MLY	G	436	1	-	4/8/9/11	-
1	MLY	A	782	1	-	6/8/9/11	-
1	MLY	G	827	1	-	0/8/9/11	-
1	MLY	J	827	1	-	0/8/9/11	-
1	MLY	A	505	1	-	5/8/9/11	-
1	MLY	J	764	1	-	2/8/9/11	-
1	MLY	A	837	1	-	5/8/9/11	-
1	MLY	D	35	1	-	3/8/9/11	-
1	MLY	A	613	1	-	4/8/9/11	-
1	MLY	D	348	1	-	5/8/9/11	-
1	MLY	A	551	1	-	3/8/9/11	-
1	MLY	D	600	1	-	3/8/9/11	-
1	MLY	D	764	1	-	2/8/9/11	-
1	MLY	G	353	1	-	4/8/9/11	-
1	MLY	A	107	1	-	2/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	J	486	1	-	2/8/9/11	-
1	MLY	A	833	1	-	6/8/9/11	-
1	MLY	D	30	1	-	2/8/9/11	-
1	MLY	A	138	1	-	4/8/9/11	-
1	MLY	G	553	4,1	-	4/8/9/11	-
1	MLY	G	839	1	-	3/8/9/11	-
1	MLY	A	598	1	-	5/8/9/11	-
1	MLY	A	827	1	-	0/8/9/11	-
1	MLY	D	504	1	-	4/8/9/11	-
1	MLY	J	353	1	-	4/8/9/11	-
1	MLY	A	248	1	-	6/8/9/11	-
1	MLY	D	827	1	-	0/8/9/11	-
1	MLY	D	248	1	-	6/8/9/11	-
1	MLY	D	236	1	-	3/8/9/11	-
1	MLY	J	35	1	-	3/8/9/11	-
1	MLY	D	659	1	-	3/8/9/11	-
1	MLY	J	613	1	-	4/8/9/11	-
1	MLY	A	190	1	-	5/8/9/11	-
1	MLY	G	617	1	-	1/8/9/11	-
1	MLY	A	130	1	-	5/8/9/11	-
1	MLY	G	84	1	-	4/8/9/11	-
1	MLY	A	768	1	-	4/8/9/11	-
1	MLY	D	837	1	-	5/8/9/11	-
1	MLY	J	236	1	-	3/8/9/11	-
1	MLY	D	59	1	-	3/8/9/11	-
1	MLY	J	296	1	-	4/8/9/11	-
1	MLY	J	598	1	-	5/8/9/11	-
1	MLY	A	35	1	-	3/8/9/11	-
1	MLY	G	138	1	-	4/8/9/11	-
1	MLY	G	55	1	-	6/8/9/11	-
1	MLY	J	138	1	-	4/8/9/11	-
1	MLY	D	138	1	-	4/8/9/11	-

The worst 5 of 56 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	138	MLY	CB-CA	-3.85	1.48	1.53
1	A	138	MLY	CB-CA	-3.68	1.48	1.53
1	J	138	MLY	CB-CA	-3.66	1.48	1.53
1	G	138	MLY	CB-CA	-3.65	1.48	1.53
1	G	87	MLY	CB-CA	-3.33	1.49	1.53

There are no bond angle outliers.

There are no chirality outliers.

5 of 638 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.

122 monomers are involved in 520 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	59	MLY	2	0
1	J	55	MLY	1	0
1	D	528	MLY	3	0
1	G	272	MLY	1	0
1	J	659	MLY	2	0
1	D	63	MLY	3	0
1	A	348	MLY	5	0
1	D	436	MLY	2	0
1	G	63	MLY	3	0
1	D	415	MLY	1	0
1	J	63	MLY	4	0
1	A	30	MLY	1	0
1	G	369	MLY	1	0
1	J	600	MLY	1	0
1	J	528	MLY	3	0
1	G	782	MLY	1	0
1	J	272	MLY	1	0
1	D	553	MLY	16	0
1	G	486	MLY	3	0
1	J	84	MLY	25	0
1	J	839	MLY	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	63	MLY	3	0
1	G	107	MLY	3	0
1	J	782	MLY	1	0
1	A	87	MLY	3	0
1	A	55	MLY	1	0
1	A	600	MLY	1	0
1	G	837	MLY	1	0
1	J	436	MLY	2	0
1	D	190	MLY	2	0
1	A	764	MLY	7	0
1	G	248	MLY	2	0
1	A	369	MLY	1	0
1	D	617	MLY	1	0
1	D	296	MLY	3	0
1	D	598	MLY	1	0
1	G	348	MLY	4	0
1	G	600	MLY	1	0
1	J	248	MLY	2	0
1	A	504	MLY	4	0
1	J	348	MLY	5	0
1	A	272	MLY	1	0
1	G	30	MLY	1	0
1	D	272	MLY	1	0
1	D	295	MLY	6	0
1	J	30	MLY	1	0
1	D	551	MLY	1	0
1	G	190	MLY	2	0
1	A	49	MLY	3	0
1	G	295	MLY	6	0
1	A	528	MLY	2	0
1	J	295	MLY	6	0
1	D	839	MLY	16	0
1	G	659	MLY	2	0
1	D	49	MLY	3	0
1	A	436	MLY	2	0
1	G	764	MLY	11	0
1	D	87	MLY	3	0
1	A	296	MLY	2	0
1	G	59	MLY	3	0
1	J	415	MLY	1	0
1	A	486	MLY	3	0
1	J	87	MLY	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	295	MLY	6	0
1	J	617	MLY	1	0
1	J	837	MLY	1	0
1	D	768	MLY	7	0
1	J	59	MLY	3	0
1	D	486	MLY	3	0
1	G	768	MLY	13	0
1	J	107	MLY	3	0
1	A	553	MLY	17	0
1	D	782	MLY	31	0
1	J	190	MLY	2	0
1	J	768	MLY	40	0
1	A	659	MLY	2	0
1	J	49	MLY	2	0
1	G	415	MLY	1	0
1	G	87	MLY	2	0
1	A	415	MLY	1	0
1	D	55	MLY	1	0
1	D	107	MLY	2	0
1	G	49	MLY	2	0
1	G	296	MLY	2	0
1	G	598	MLY	1	0
1	A	839	MLY	15	0
1	A	617	MLY	1	0
1	G	528	MLY	3	0
1	J	553	MLY	11	0
1	G	436	MLY	2	0
1	A	782	MLY	1	0
1	G	827	MLY	1	0
1	J	827	MLY	1	0
1	A	505	MLY	11	0
1	J	764	MLY	22	0
1	A	837	MLY	1	0
1	D	348	MLY	6	0
1	A	551	MLY	2	0
1	D	600	MLY	1	0
1	D	764	MLY	2	0
1	A	107	MLY	3	0
1	J	486	MLY	3	0
1	D	30	MLY	1	0
1	A	138	MLY	1	0
1	G	553	MLY	27	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	G	839	MLY	4	0
1	A	598	MLY	1	0
1	A	248	MLY	2	0
1	D	248	MLY	2	0
1	D	659	MLY	2	0
1	A	190	MLY	2	0
1	G	617	MLY	1	0
1	G	84	MLY	18	0
1	A	768	MLY	14	0
1	D	837	MLY	1	0
1	D	59	MLY	2	0
1	J	296	MLY	3	0
1	J	598	MLY	1	0
1	G	138	MLY	1	0
1	G	55	MLY	1	0
1	J	138	MLY	1	0
1	D	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	G	4
1	J	4
1	D	4
1	A	4

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Mol	Chain	Number of breaks
3	C	1
3	F	1
3	I	1
3	L	1
2	B	1
2	E	1
2	H	1
2	K	1

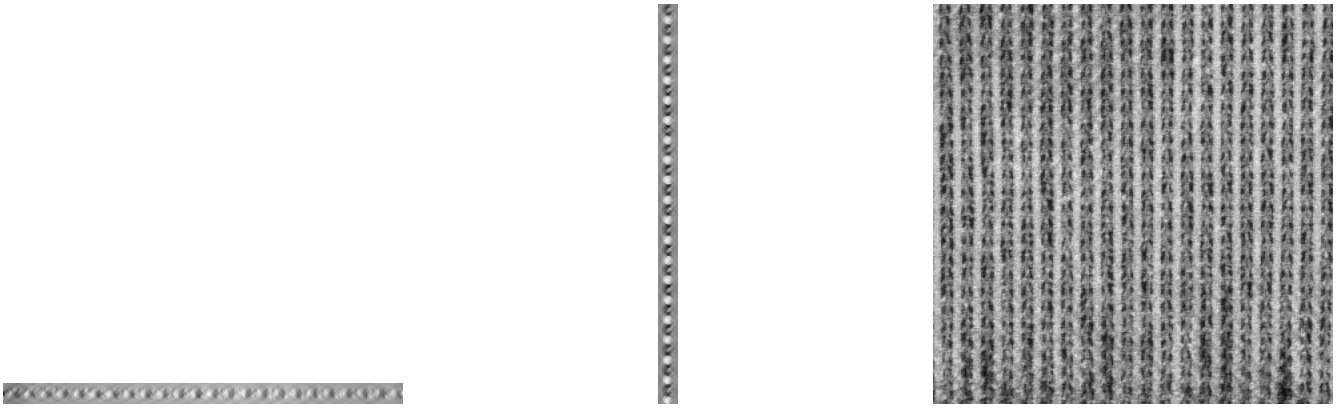
The worst 5 of 24 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	769:ALA	C	770:GLY	N	4.88
1	J	769:ALA	C	770:GLY	N	4.64
1	D	769:ALA	C	770:GLY	N	4.52
1	D	709:LYS	C	710:GLY	N	3.32
1	A	709:LYS	C	710:GLY	N	3.27

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.

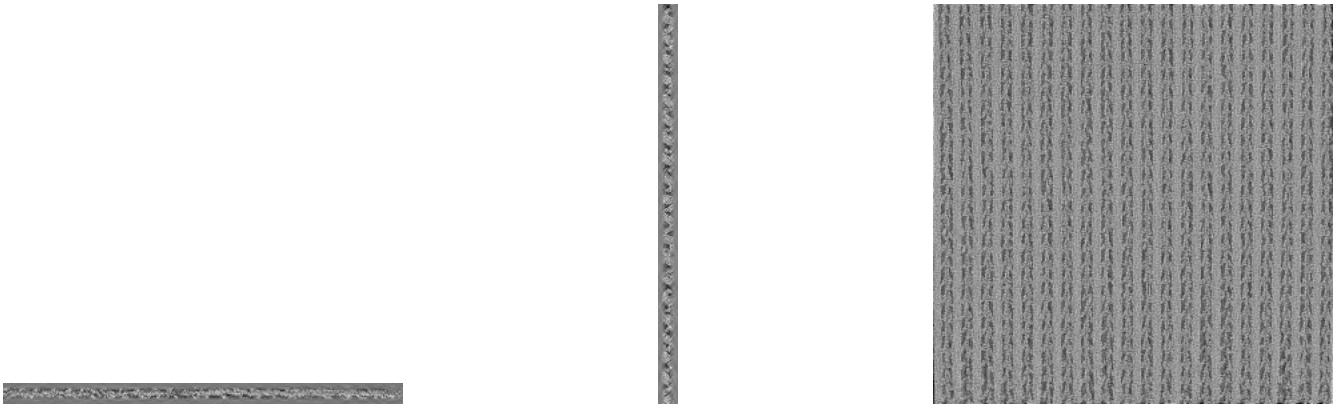
6.1 Orthogonal projections



X Y Z

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

6.2 Central slices



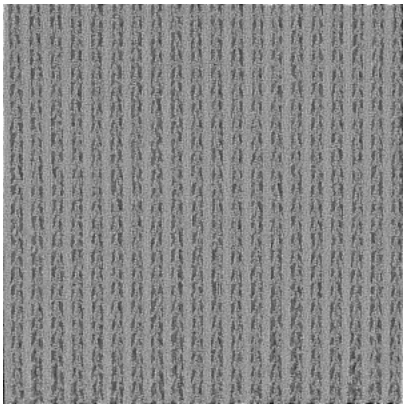
X Index: 300 Y Index: 300 Z Index: 15

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

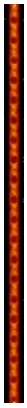


Z Index: 15

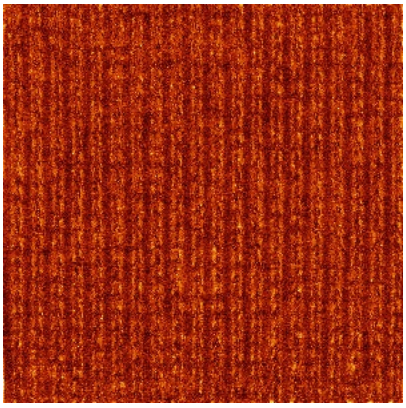
The images above show the largest variance slices of the tomogram in three orthogonal directions.

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

X



Y



Z

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

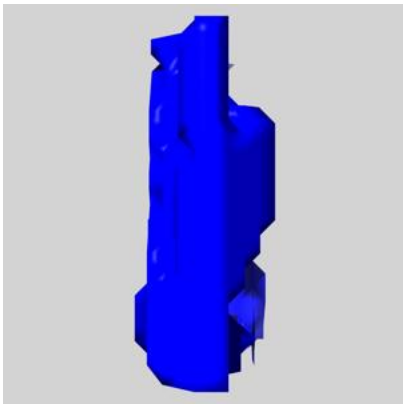
6.5 Mask visualisation

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

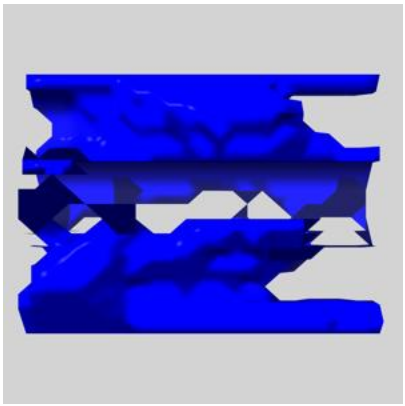
A mask typically either:

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

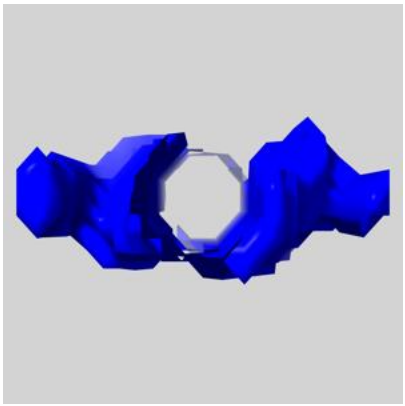
6.5.1 emd_1001_msk_25.map



X

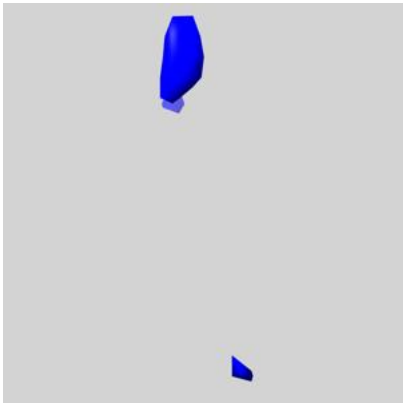


Y

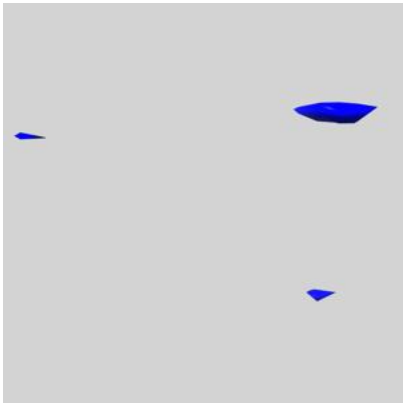


Z

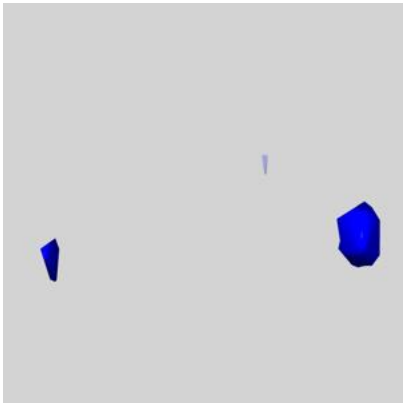
6.5.2 emd_1001_msk_24.map



X

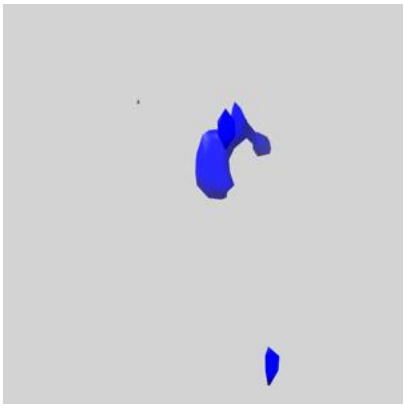


Y

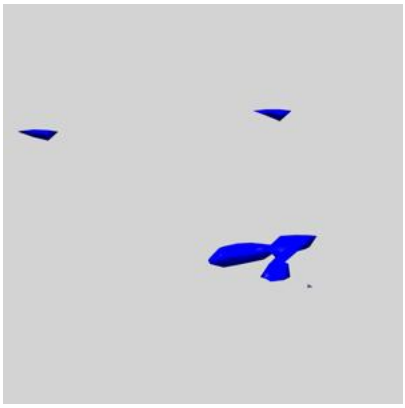


Z

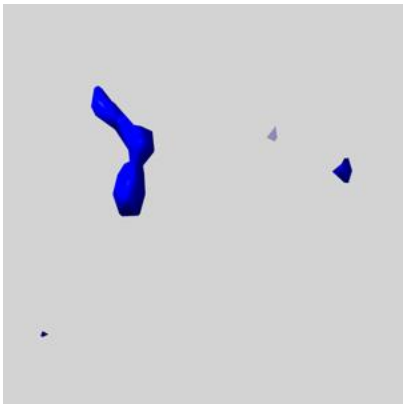
6.5.3 emd_1001_msk_23.map



X

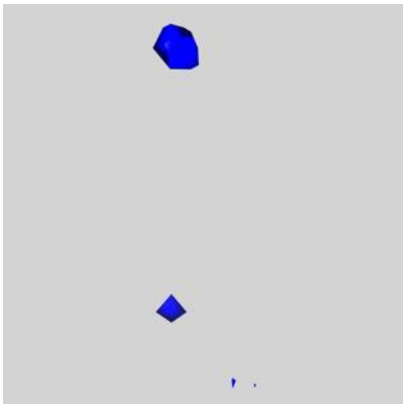


Y

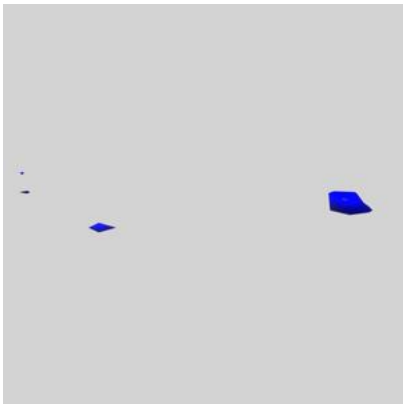


Z

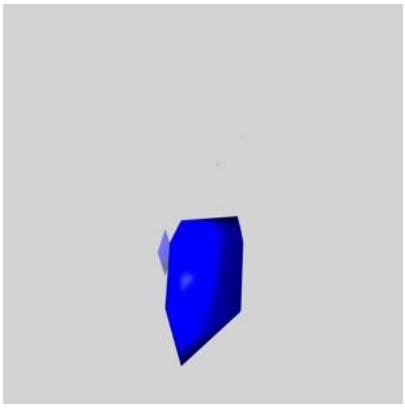
6.5.4 emd_1001_msk_22.map



X

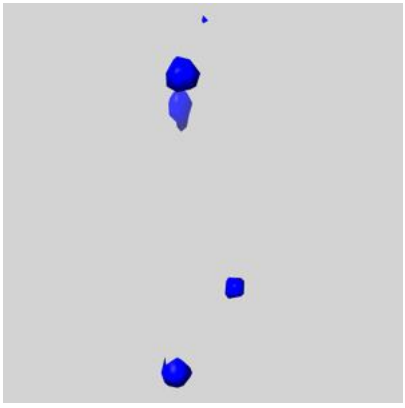


Y

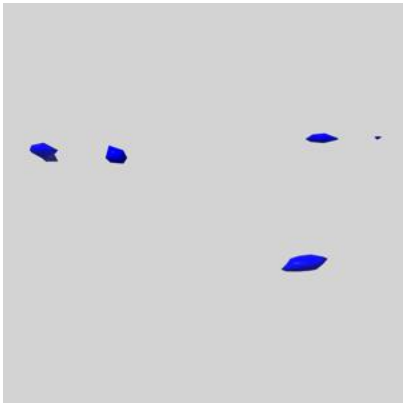


Z

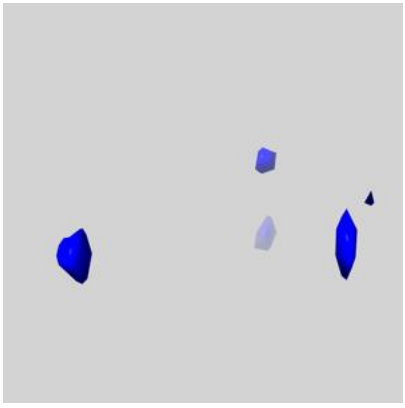
6.5.5 emd_1001_msk_21.map



X

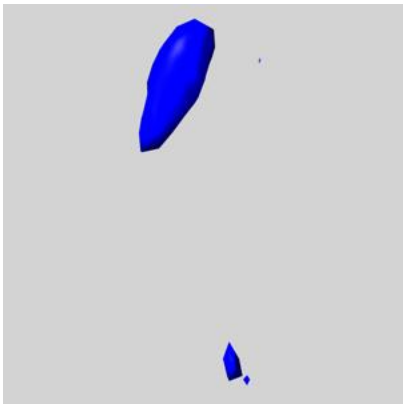


Y



Z

6.5.6 emd_1001_msk_20.map



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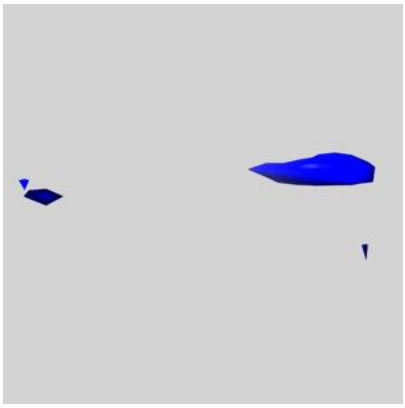

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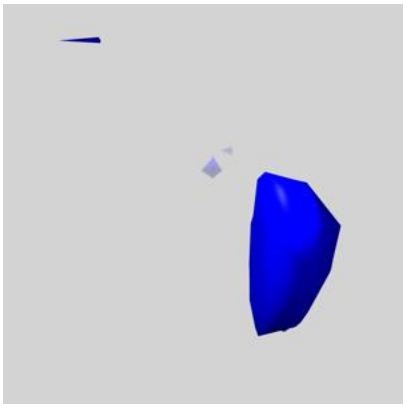

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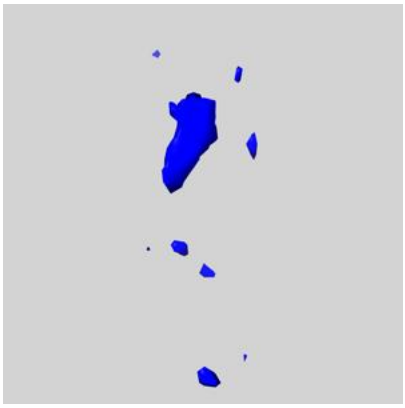
6.5.7 emd_1001_msk_19.map



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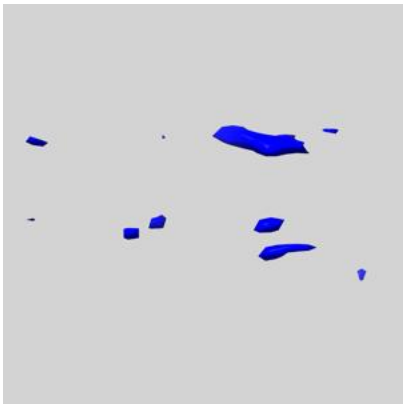

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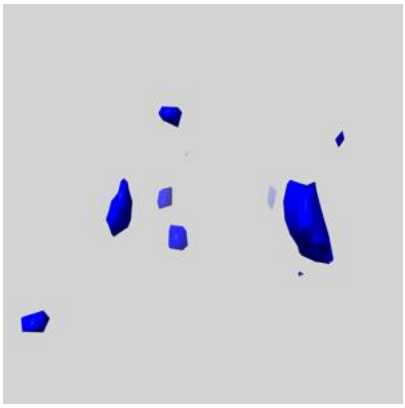

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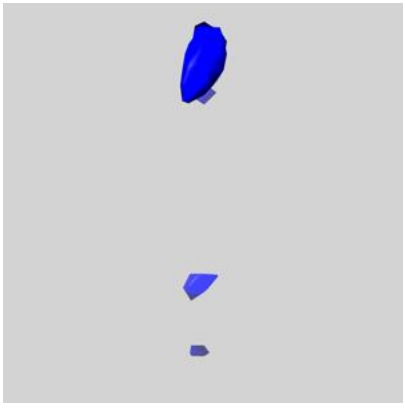
6.5.8 emd_1001_msk_18.map



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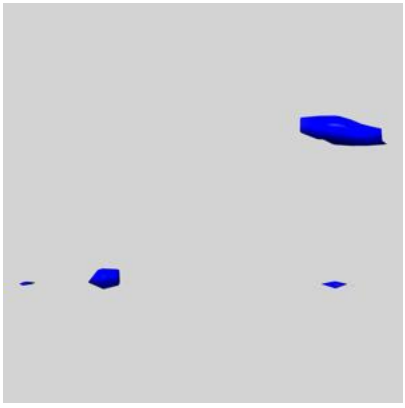

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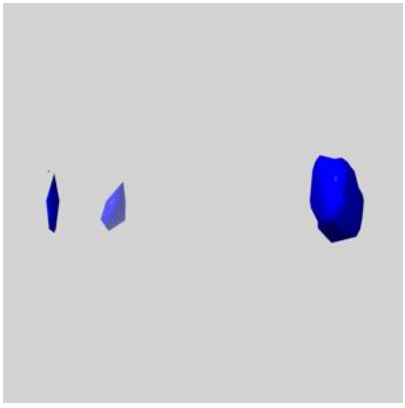
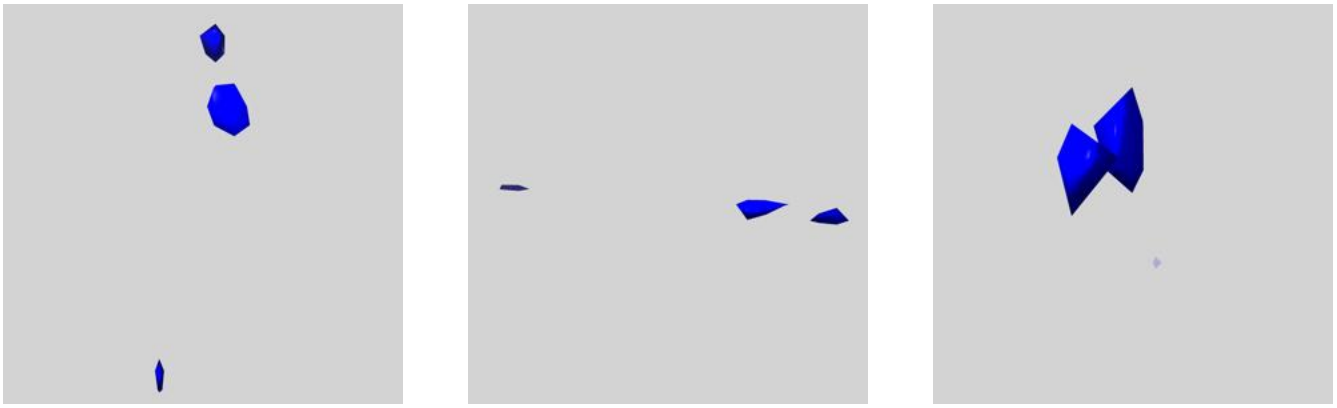


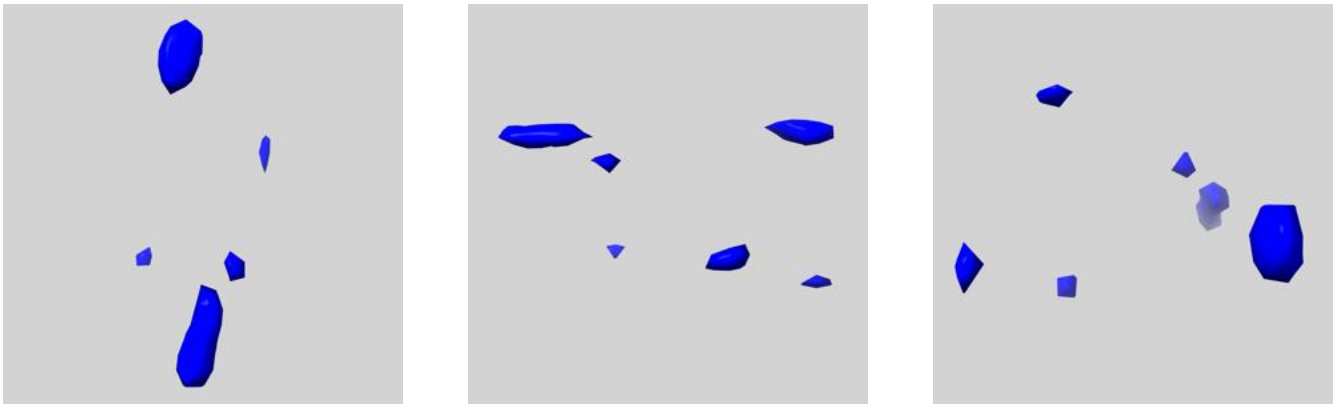
Z

6.5.9 emd_1001_msk_17.map



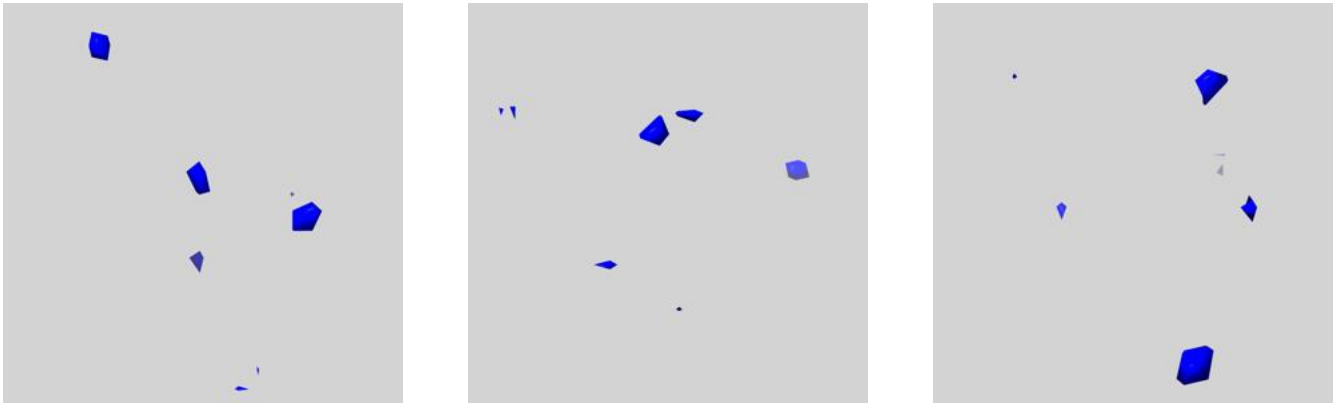
X Y Z

6.5.10 emd_1001_msk_16.map



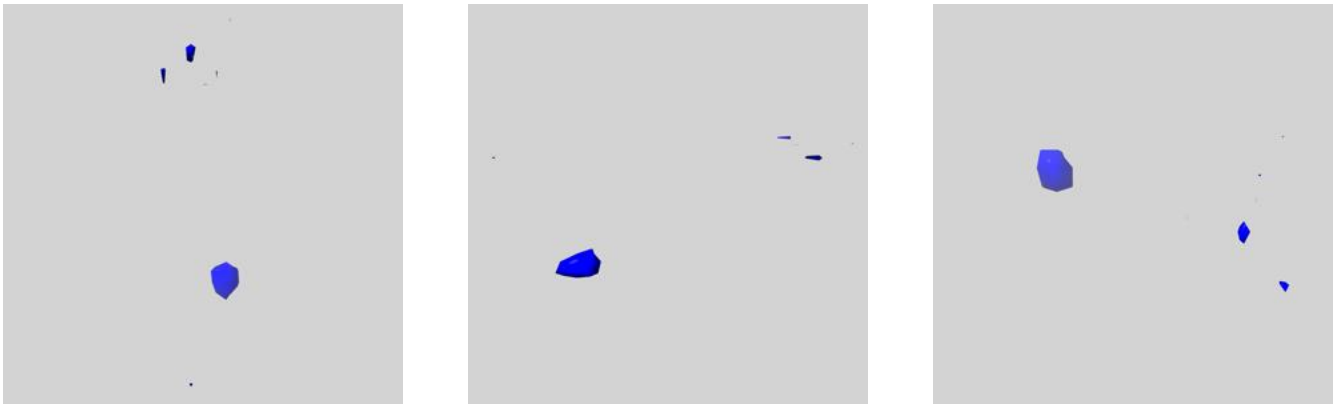
X Y Z

6.5.11 emd_1001_msk_15.map



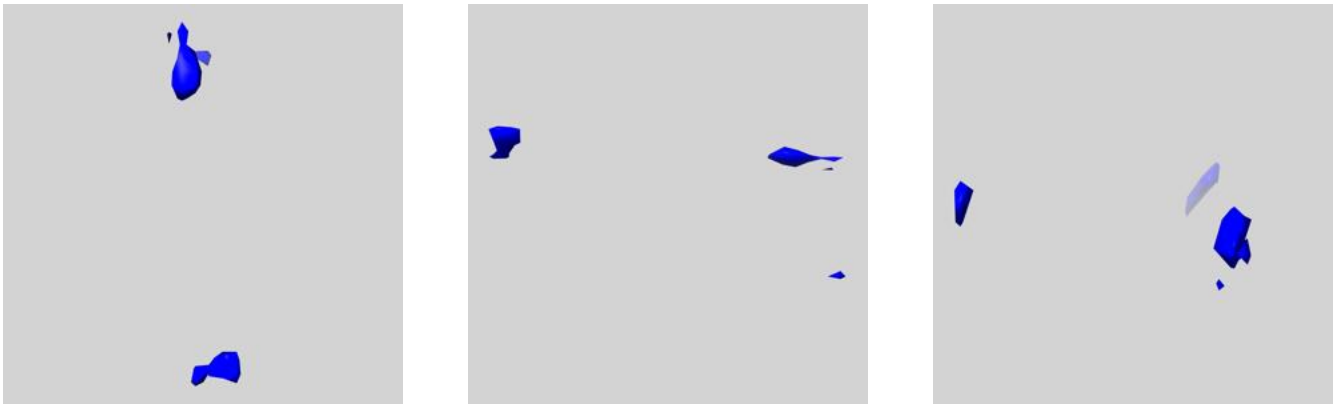
X Y Z

6.5.12 emd_1001_msk_14.map



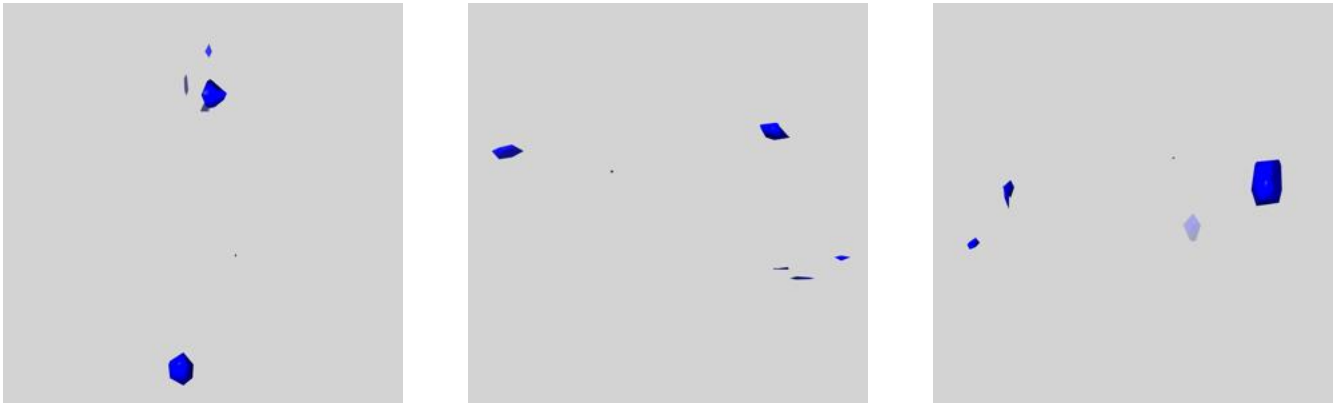
X Y Z

6.5.13 emd_1001_msk_13.map



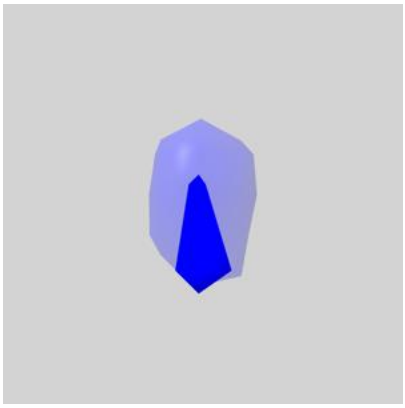
X Y Z

6.5.14 emd_1001_msk_12.map

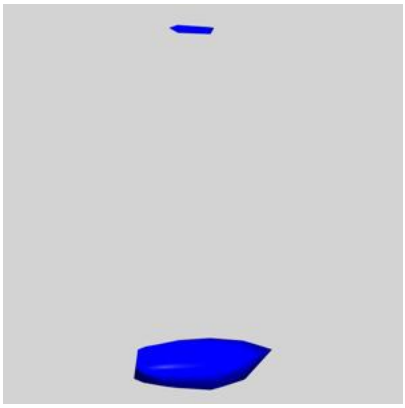


X Y Z

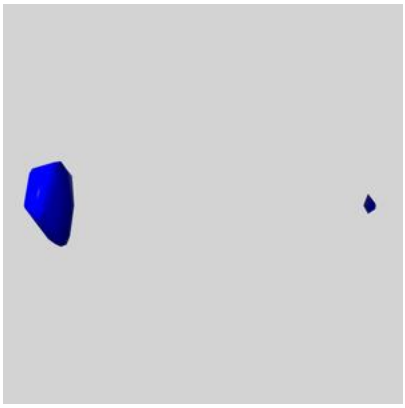
6.5.15 emd_1001_msk_11.map



X

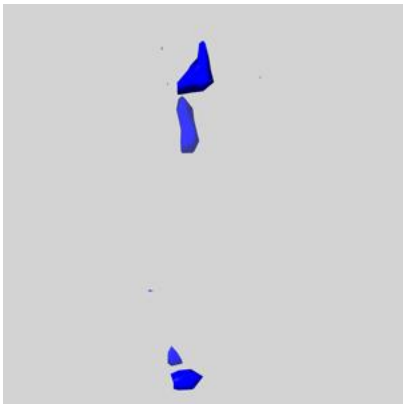


Y

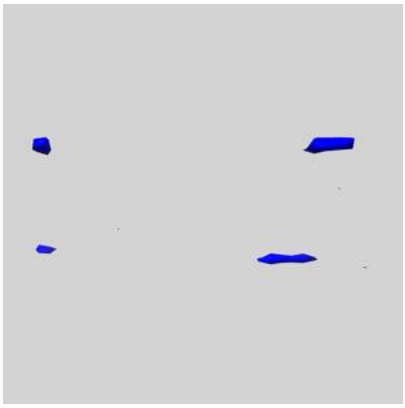


Z

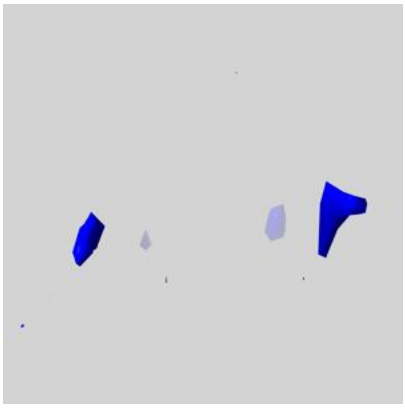
6.5.16 emd_1001_msk_10.map



X

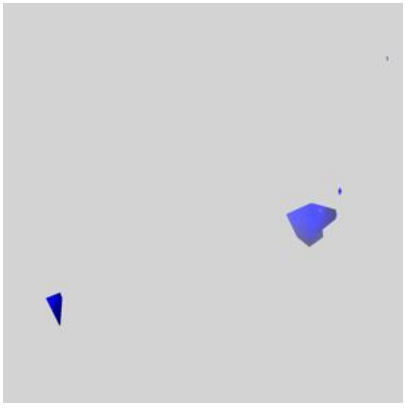


Y

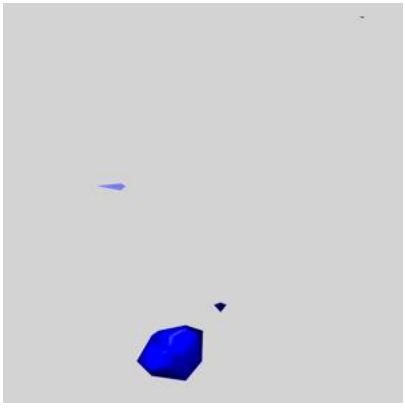


Z

6.5.17 emd_1001_msk_9.map



X



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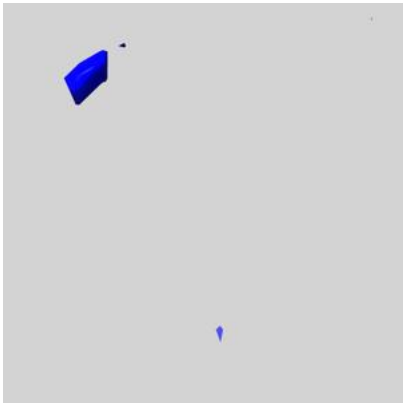

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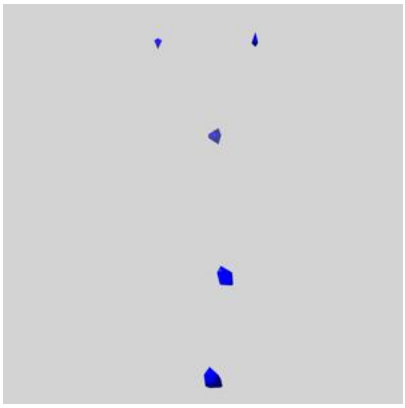
6.5.18 emd_1001_msk_8.map



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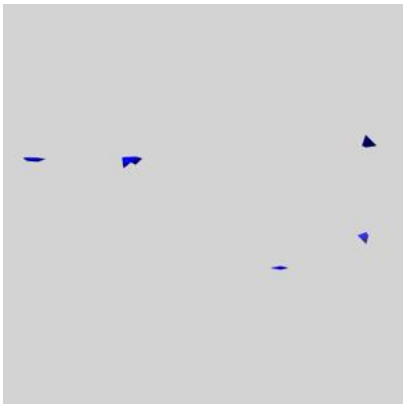

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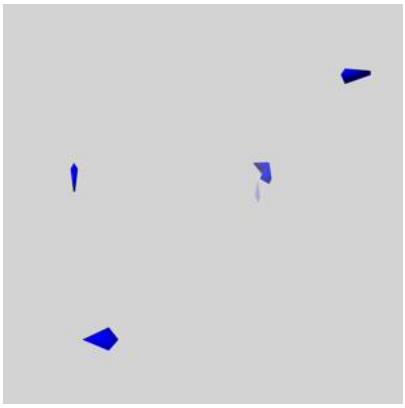

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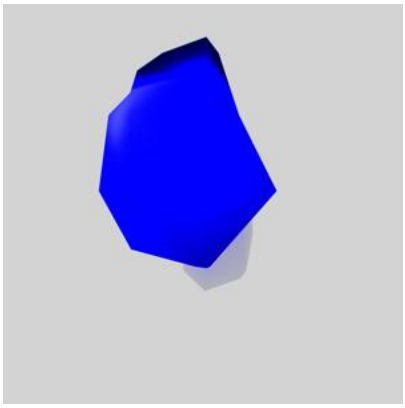
6.5.19 emd_1001_msk_7.map



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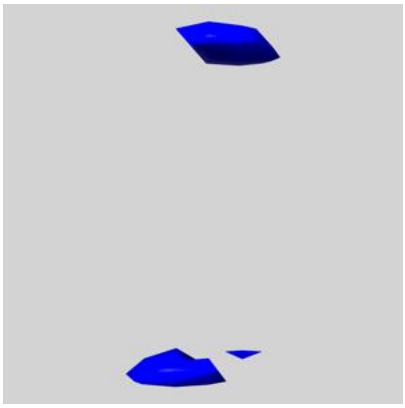

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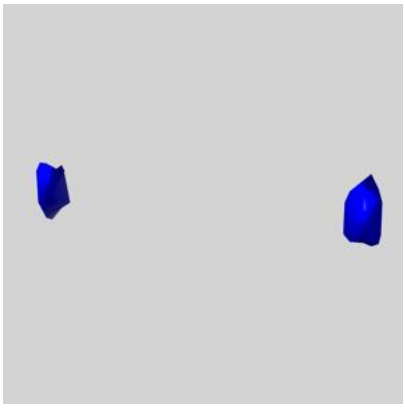

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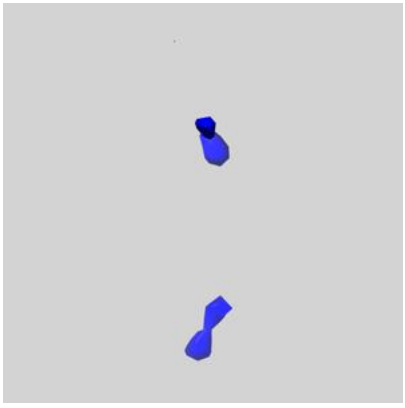
6.5.20 emd_1001_msk_6.map



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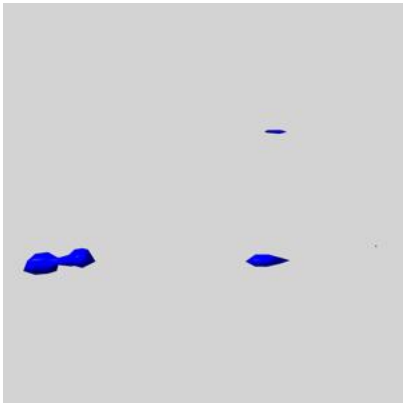

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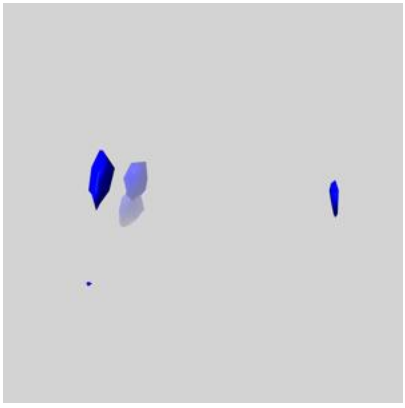

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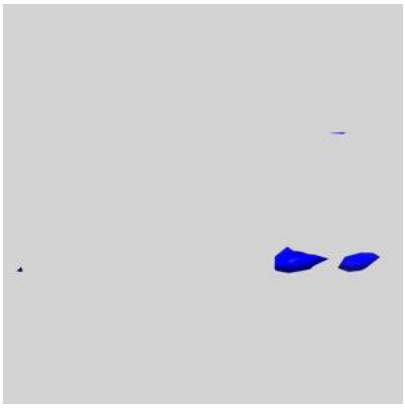
6.5.21 emd_1001_msk_5.map


X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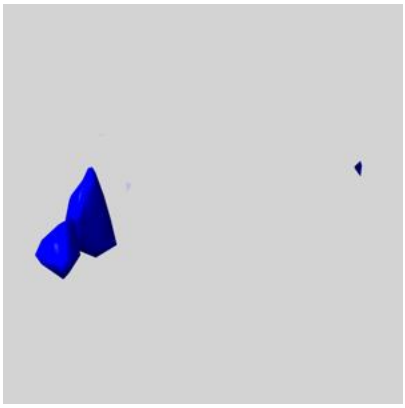
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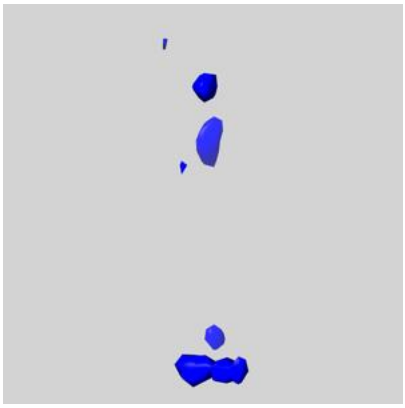
6.5.22 emd_1001_msk_4.map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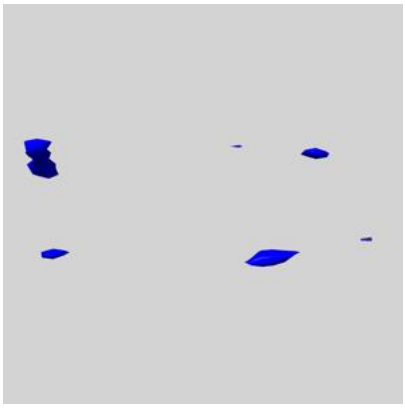
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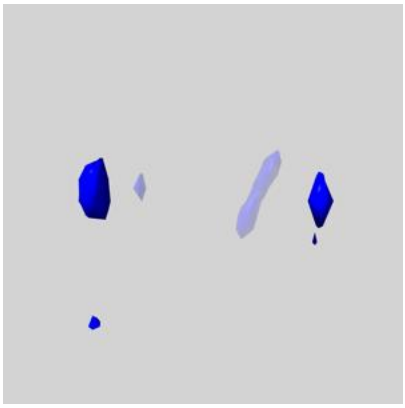
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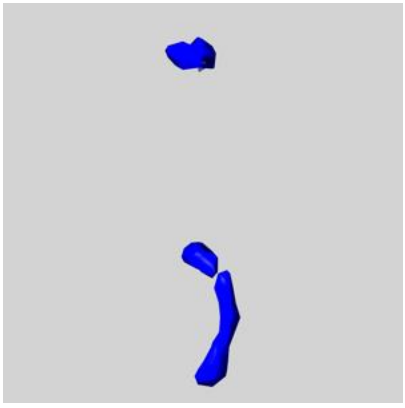
6.5.23 emd_1001_msk_3.map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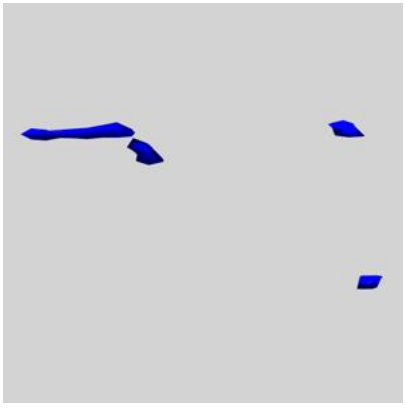
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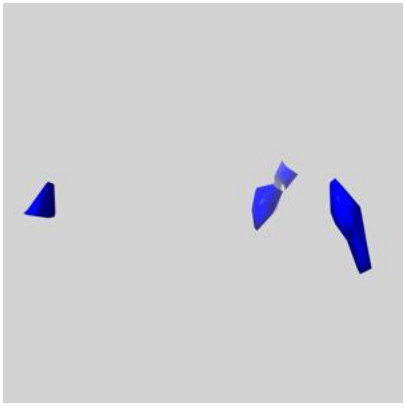
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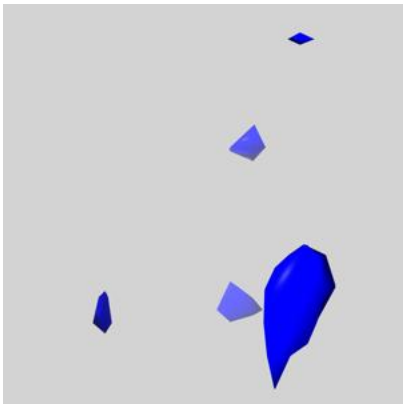
6.5.24 emd_1001_msk_2.map



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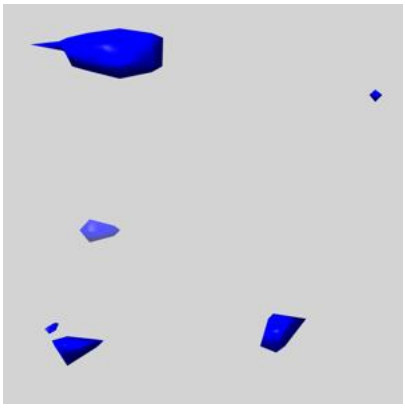

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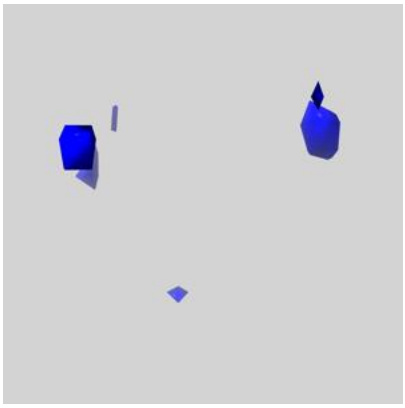

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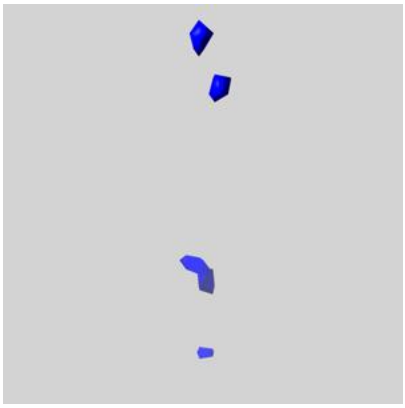
6.5.25 emd_1001_msk_1.map



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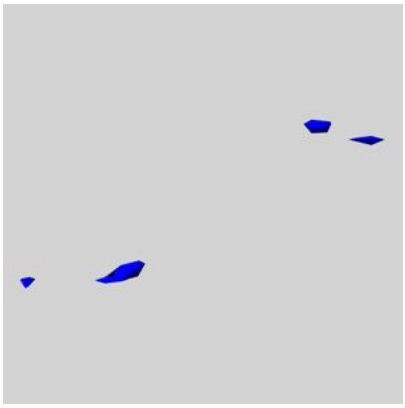

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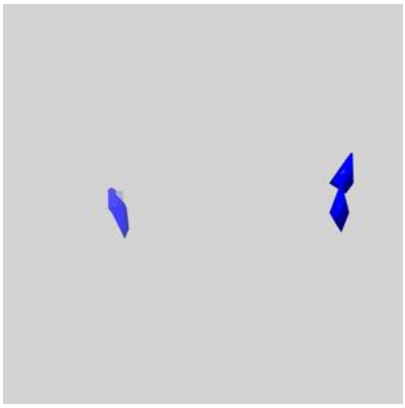

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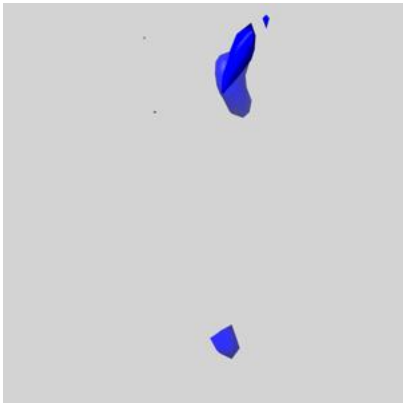
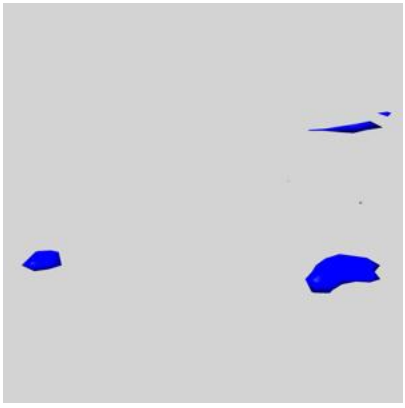
6.5.26 emd_1001_msk_26.map



X



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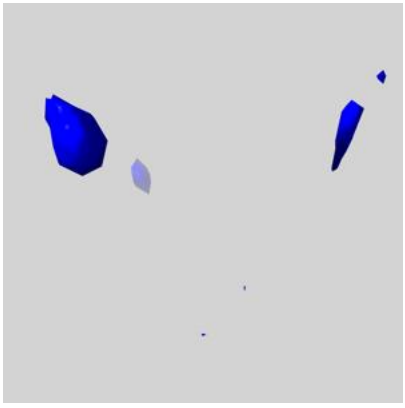
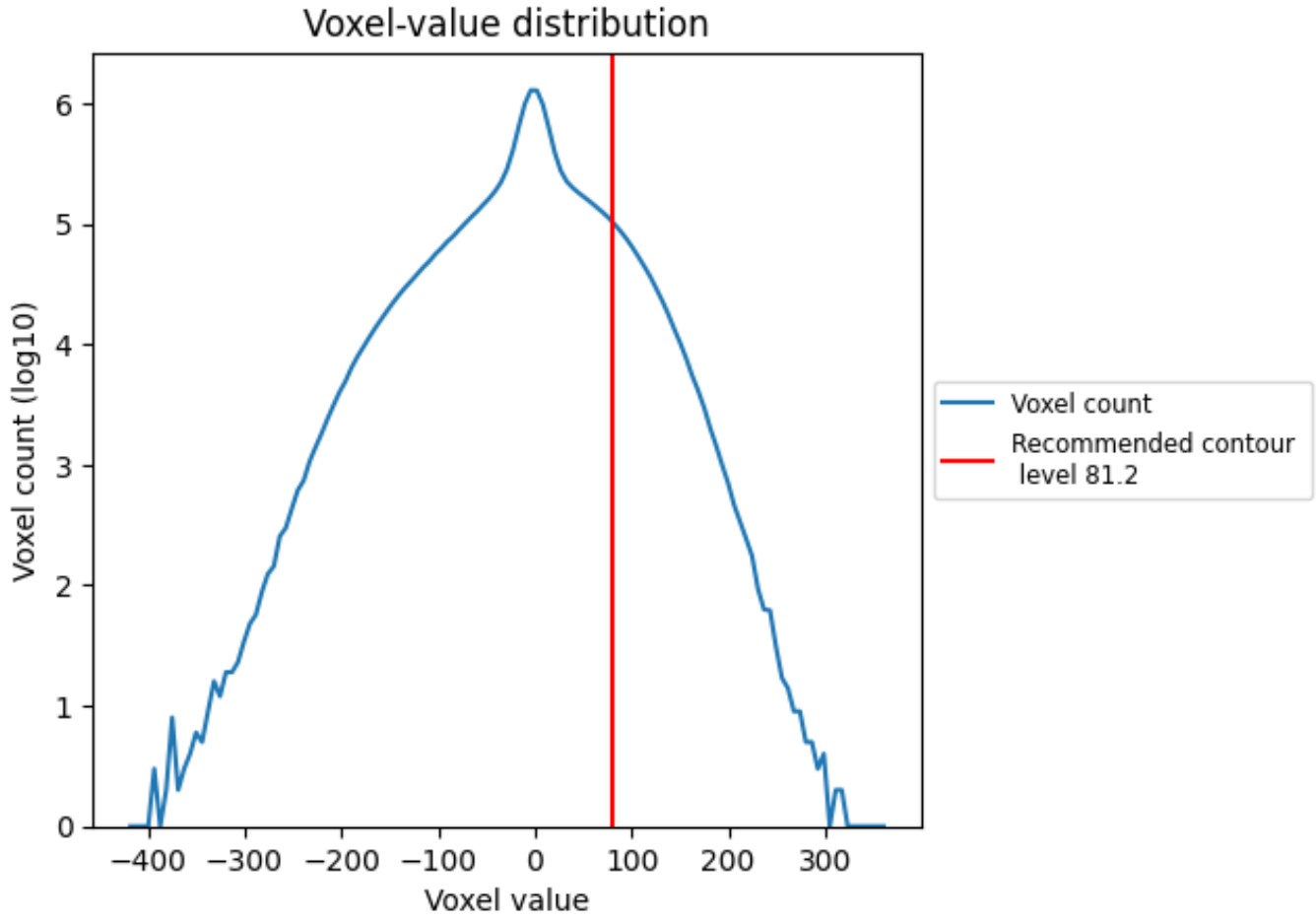


Z

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.

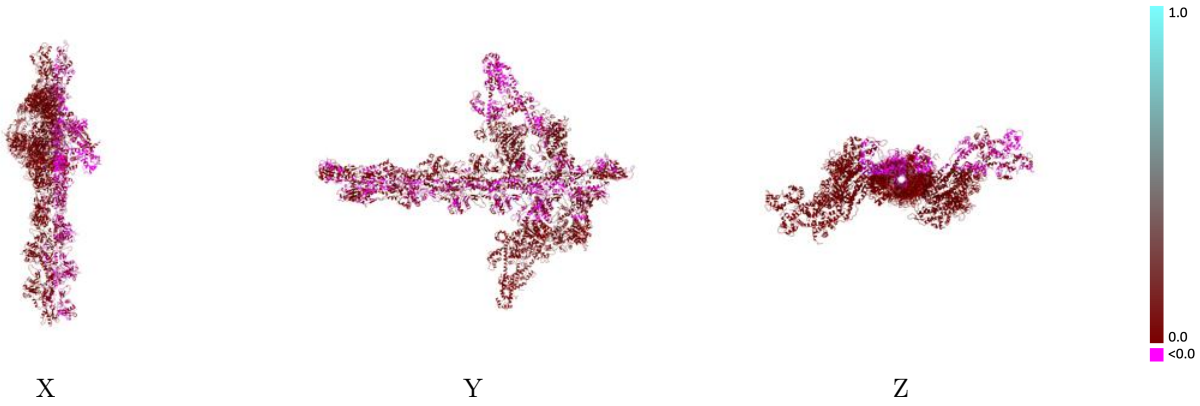
8 Map-model fit

This section contains information regarding the fit between EMDB map EMD-1001 and PDB model 1O1B. 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

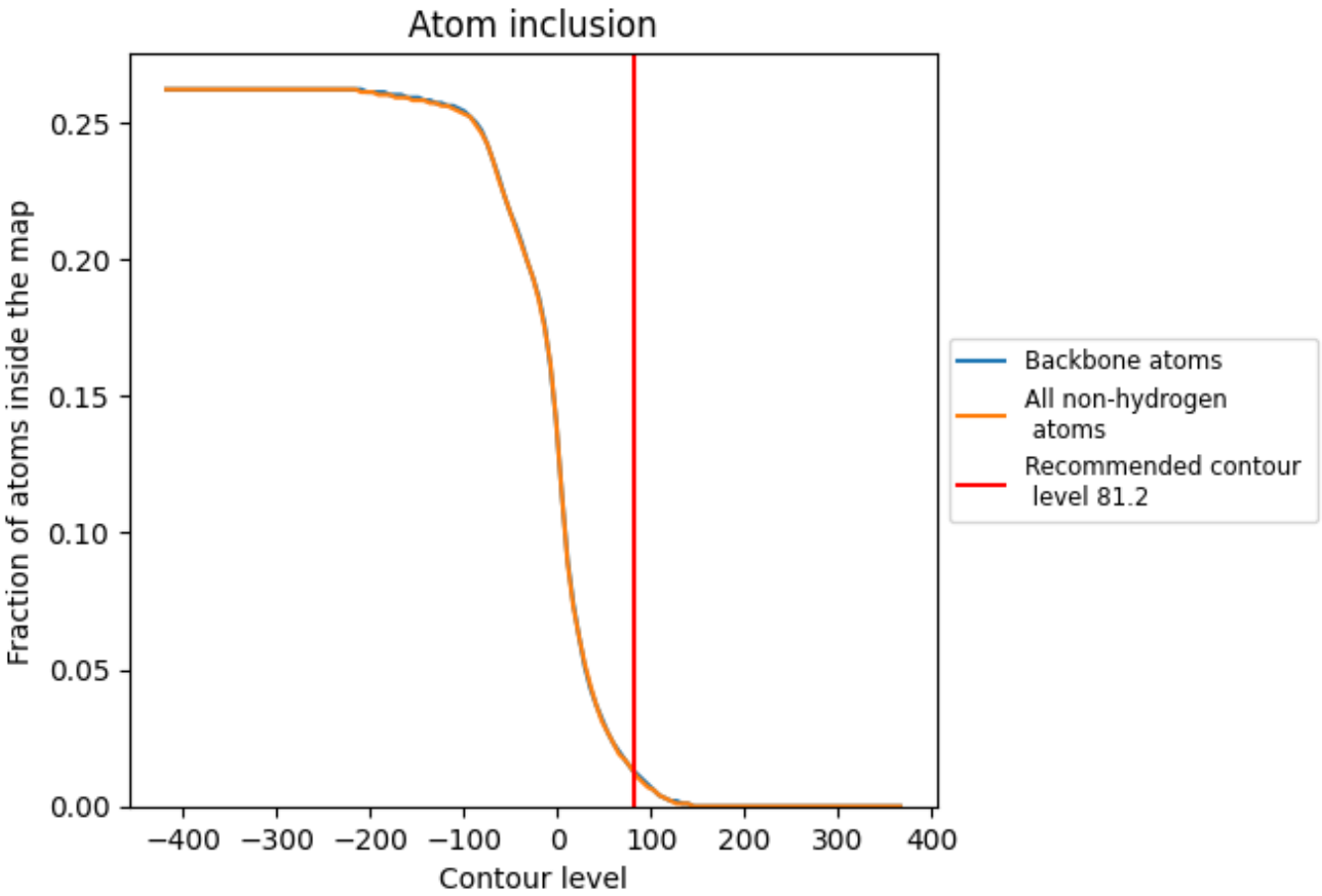


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	0.0130	-0.0010
0	0.0000	-0.0010
1	0.0000	0.0020
2	0.0000	-0.0030
3	0.0000	-0.0150
4	0.0000	-0.0030
5	0.0000	-0.0060
7	0.0000	0.0070
8	0.0000	-0.0010
9	0.0000	0.0010
A	0.0000	-0.0030
B	0.0000	0.0000
C	0.0000	0.0000
D	0.0000	0.0060
E	0.0000	-0.0440
F	0.2030	0.0400
G	0.0000	-0.0040
H	0.0000	0.0000
I	0.0000	0.0000
J	0.0090	-0.0010
K	0.0620	0.0150
L	0.0780	-0.0100
V	0.0000	-0.0180
W	0.0000	-0.0000
X	0.0610	-0.0010
Y	0.0000	0.0020
Z	0.1200	0.0110