



wwPDB EM Validation Summary Report ⓘ

Nov 19, 2022 – 01:48 PM EST

PDB ID : 3B5U
EMDB ID : EMD-1088
Title : Actin filament model from extended form of acromsomal bundle in the Limulus sperm
Authors : Cong, Y.; Topf, M.; Sali, A.; Matsudaira, P.; Dougherty, M.; Chiu, W.; Schmid, M.F.
Deposited on : 2007-10-26
Resolution : 9.50 Å(reported)
Based on initial model : ?

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 ⓘ 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 ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev43
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) : 2.31.3

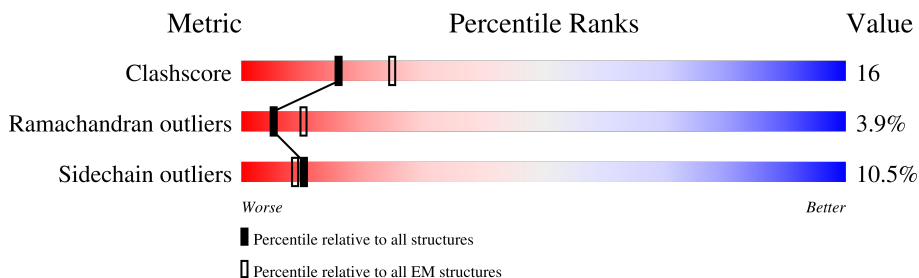
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON CRYSTALLOGRAPHY

The reported resolution of this entry is 9.50 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 $\leq 5\%$. 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	377	93% 57% 36% 5% ..
1	B	377	89% 58% 34% 6% ..
1	C	377	88% 66% 27% 6% .
1	D	377	92% 57% 33% 9% ..
1	E	377	91% 60% 29% 9% ..
1	F	377	90% 58% 34% 6% ..
1	G	377	93% 65% 29% 6% .
1	H	377	97% 69% 27% ..

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Mol	Chain	Length	Quality of chain
1	I	377	<p>98% 61% 33% 6%</p>
1	J	377	<p>95% 60% 31% 6%</p>
1	K	377	<p>96% 61% 31% 6%</p>
1	L	377	<p>95% 56% 36% 6%</p>
1	M	377	<p>92% 64% 28% 6%</p>
1	N	377	<p>92% 57% 32% 9%</p>

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 41062 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.

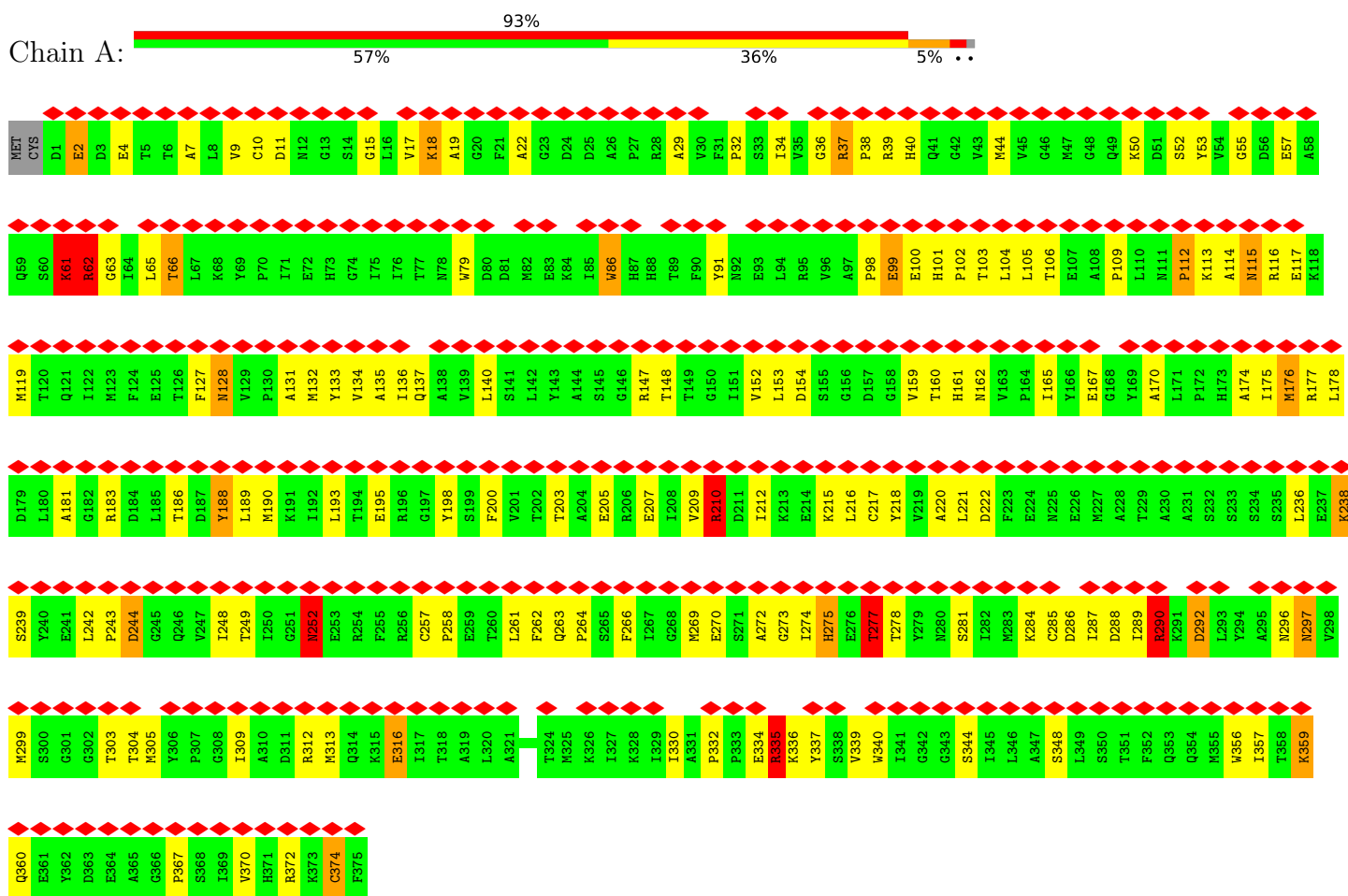
- Molecule 1 is a protein called Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	375	2933	1854	493	565	21	0	0
1	B	375	2933	1854	493	565	21	0	0
1	C	375	2933	1854	493	565	21	0	0
1	D	375	2933	1854	493	565	21	0	0
1	E	375	2933	1854	493	565	21	0	0
1	F	375	2933	1854	493	565	21	0	0
1	G	375	2933	1854	493	565	21	0	0
1	H	375	2933	1854	493	565	21	0	0
1	I	375	2933	1854	493	565	21	0	0
1	J	375	2933	1854	493	565	21	0	0
1	K	375	2933	1854	493	565	21	0	0
1	L	375	2933	1854	493	565	21	0	0
1	M	375	2933	1854	493	565	21	0	0
1	N	375	2933	1854	493	565	21	0	0

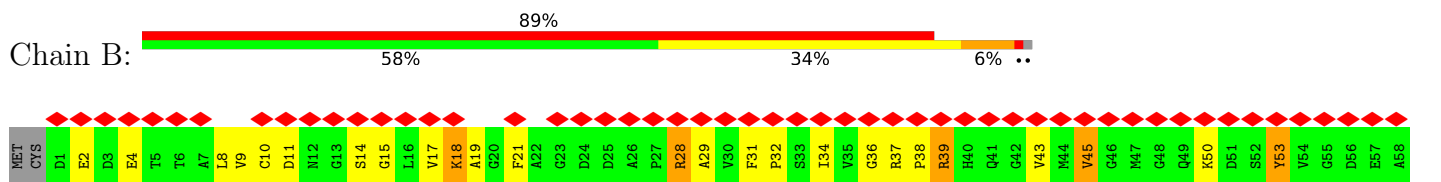
3 Residue-property plots

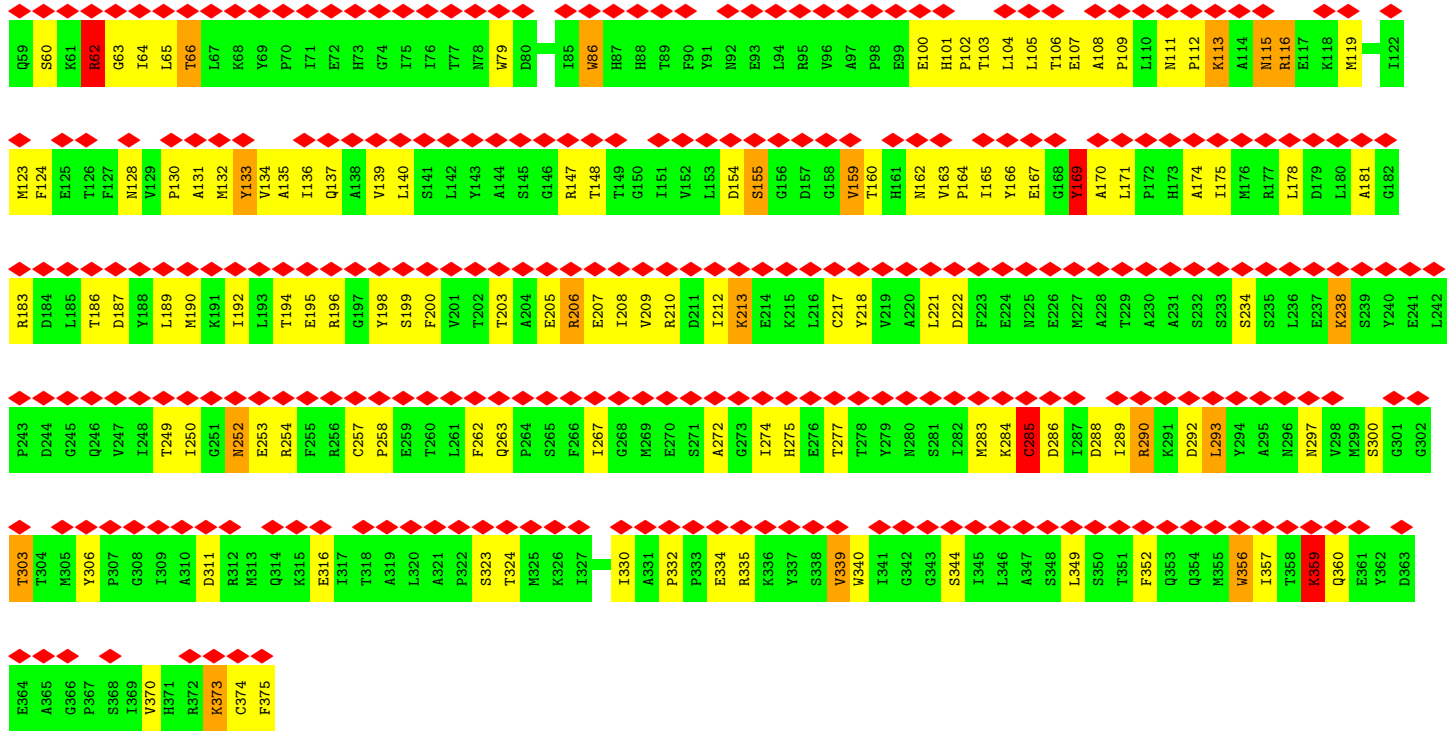
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Actin, alpha skeletal muscle

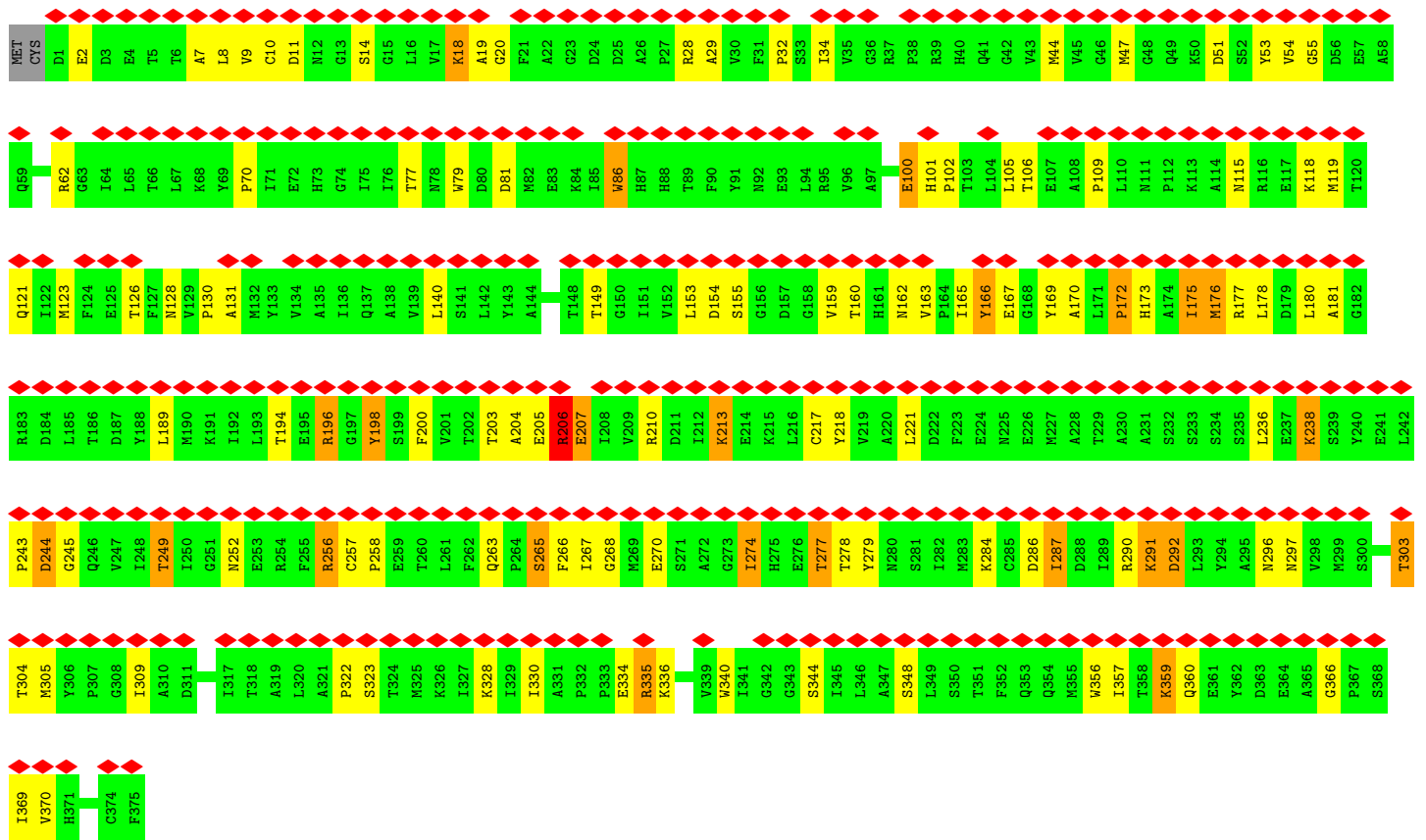
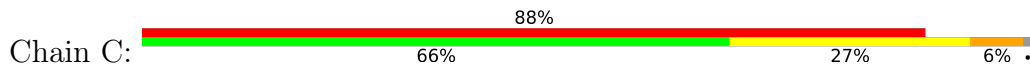


- Molecule 1: Actin, alpha skeletal muscle

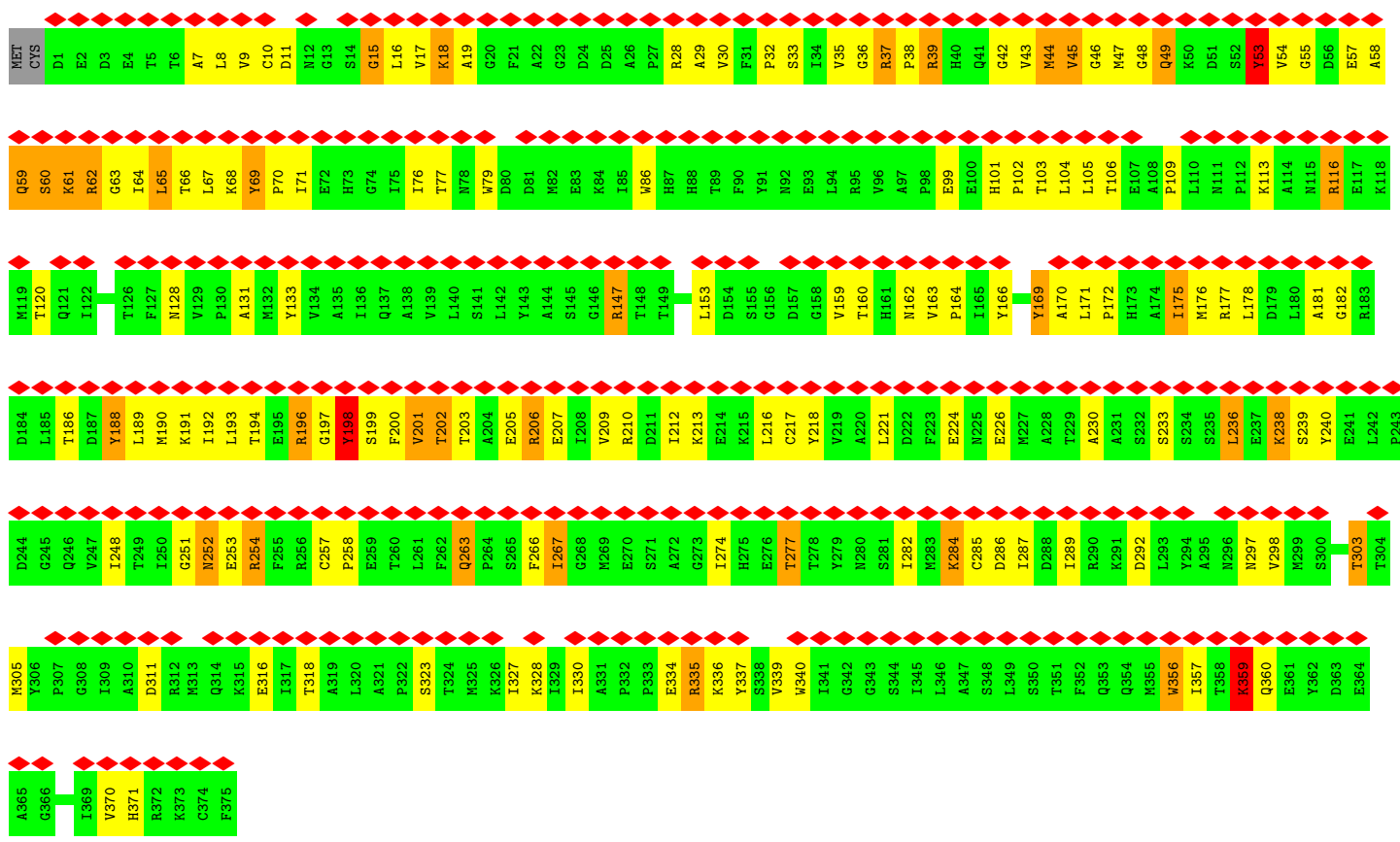
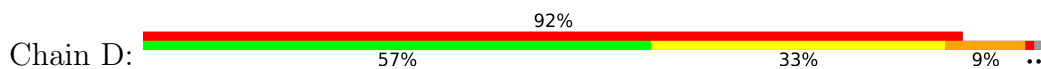




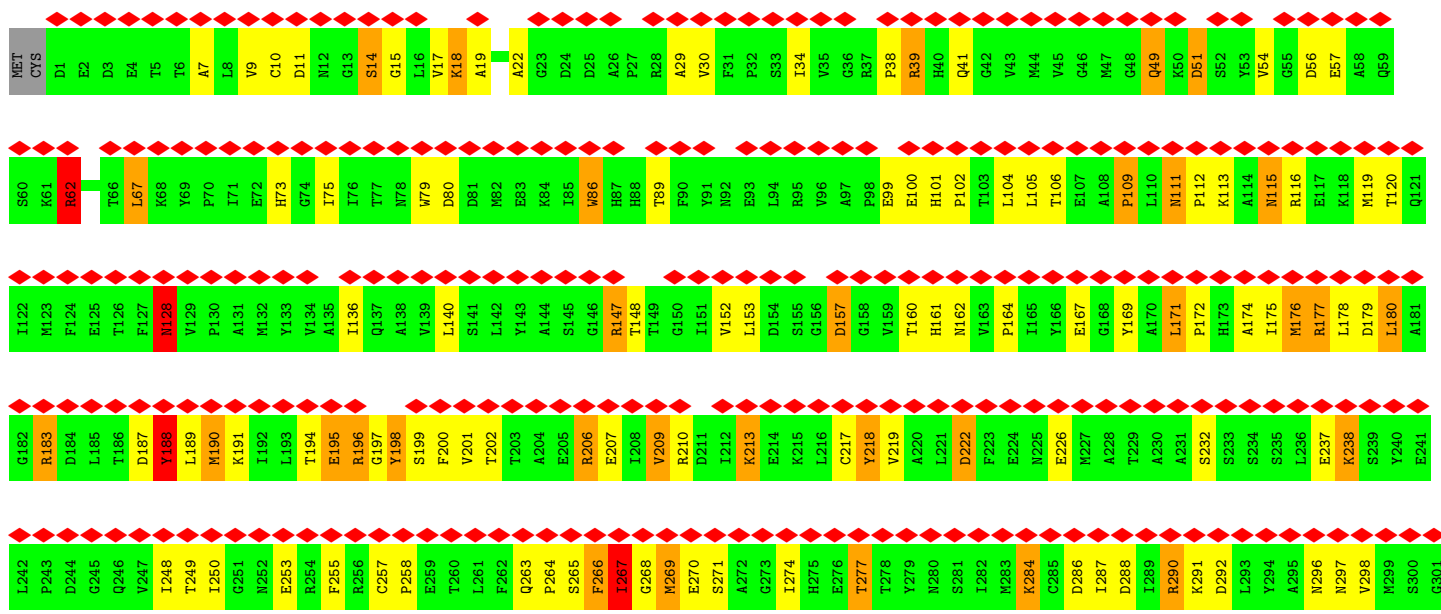
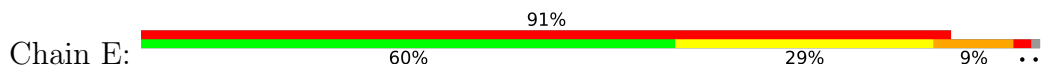
• Molecule 1: Actin, alpha skeletal muscle

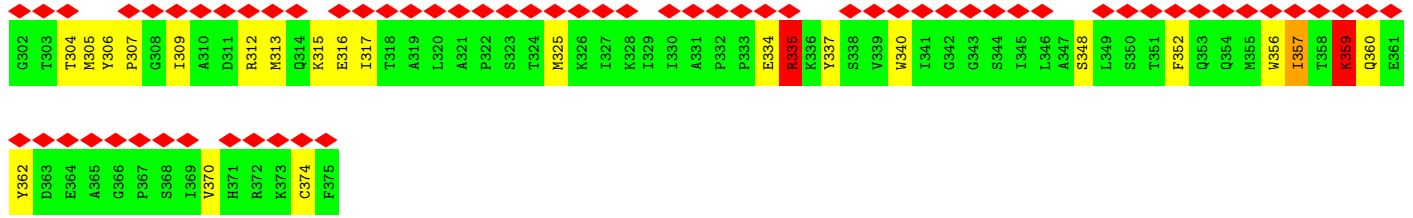


• Molecule 1: Actin, alpha skeletal muscle

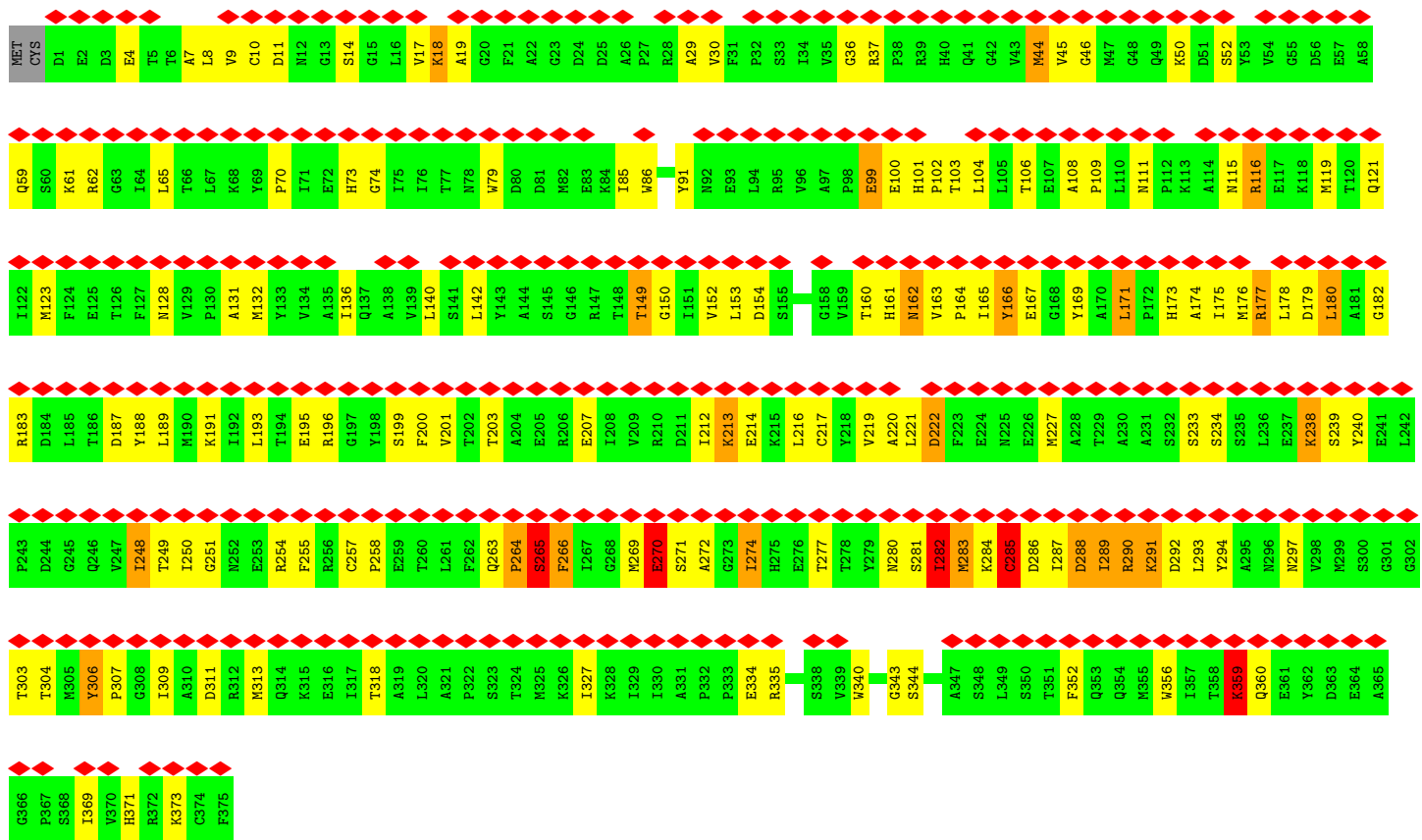
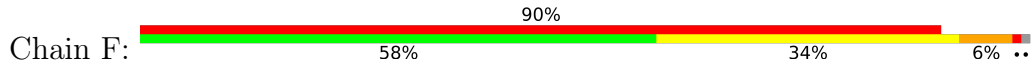


• Molecule 1: Actin, alpha skeletal muscle

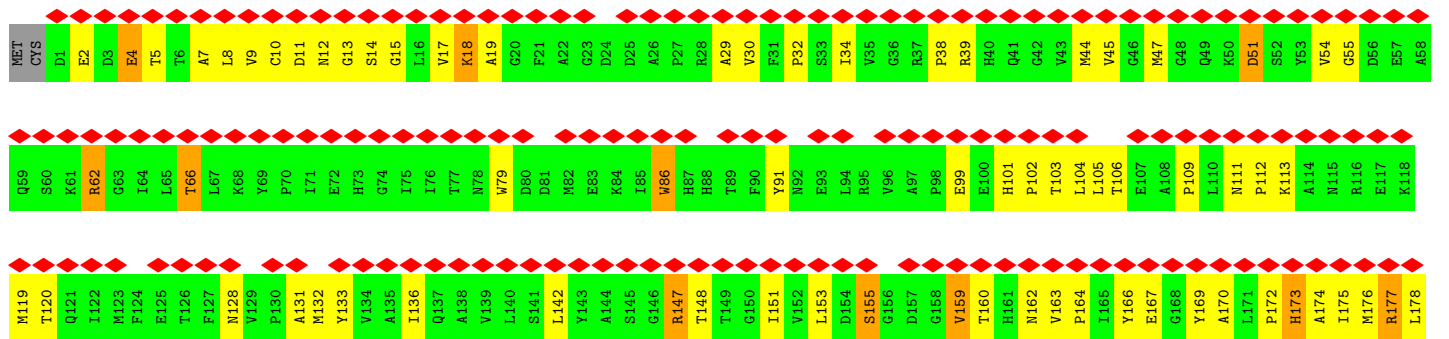
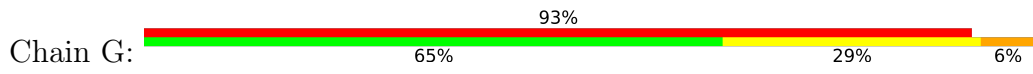


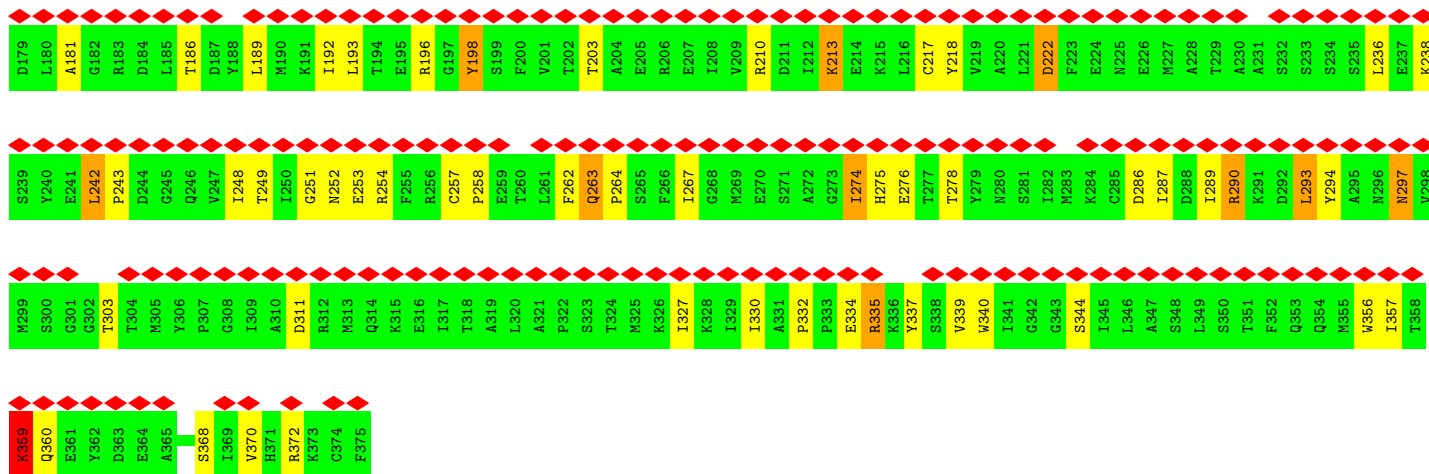


• Molecule 1: Actin, alpha skeletal muscle

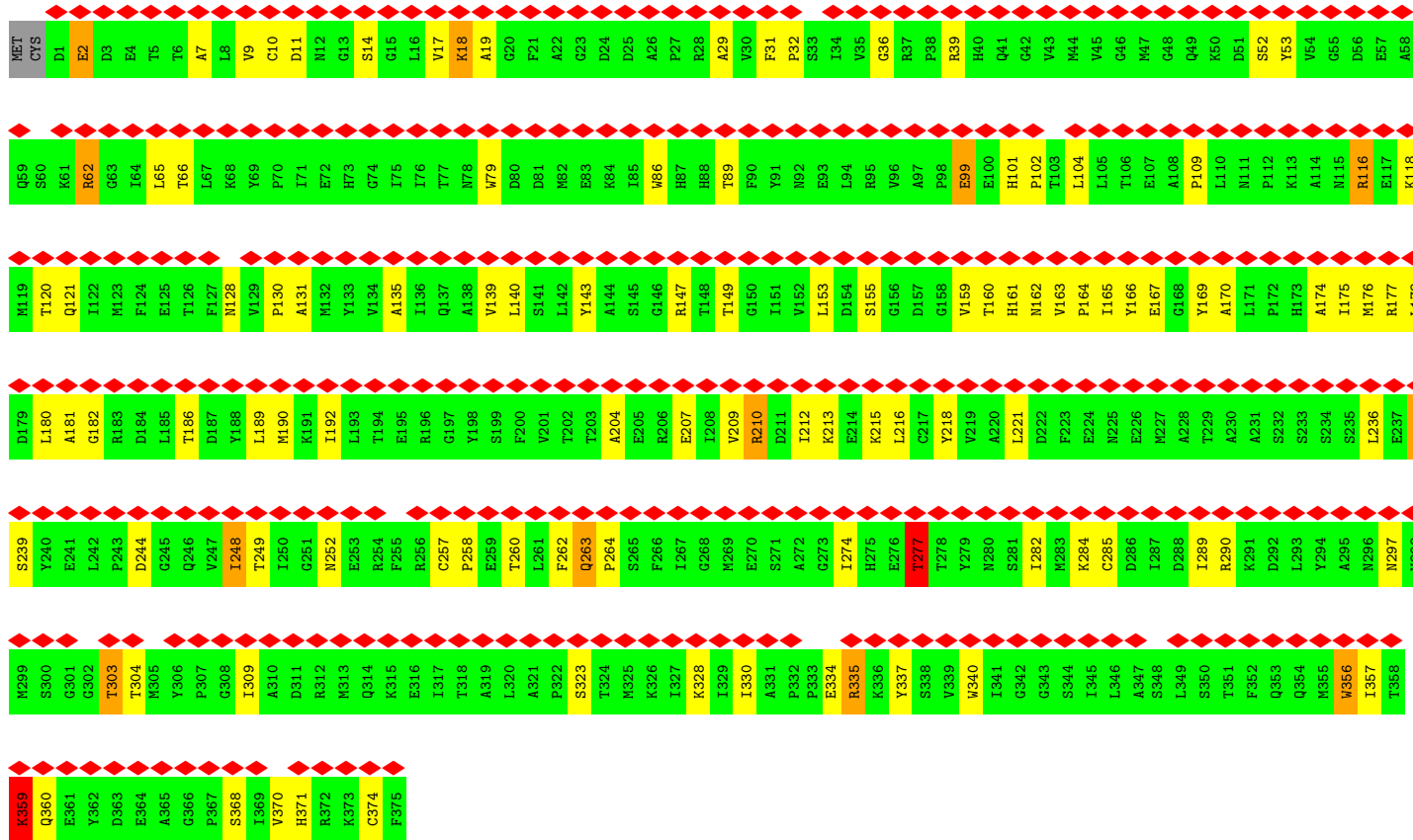


• Molecule 1: Actin, alpha skeletal muscle

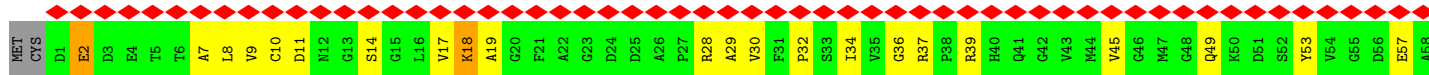


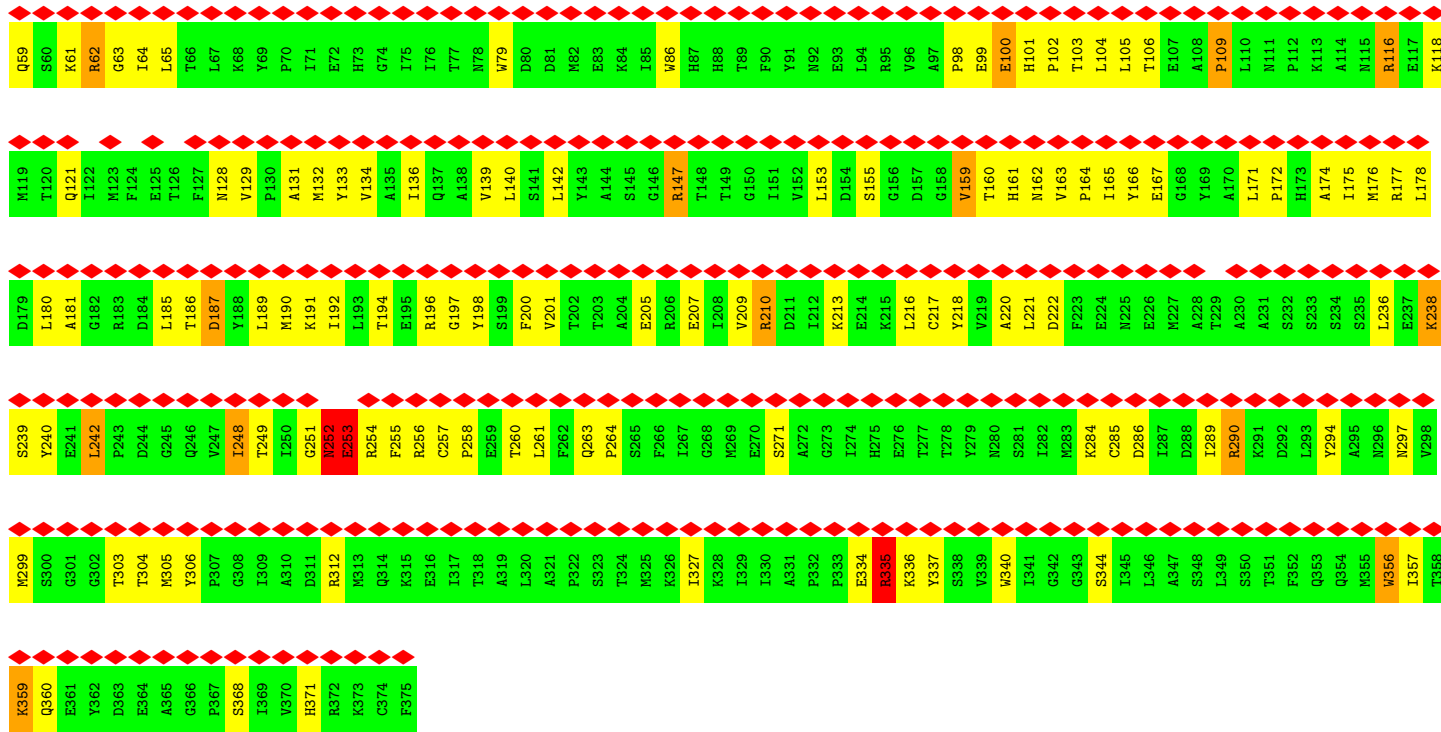


• Molecule 1: Actin, alpha skeletal muscle

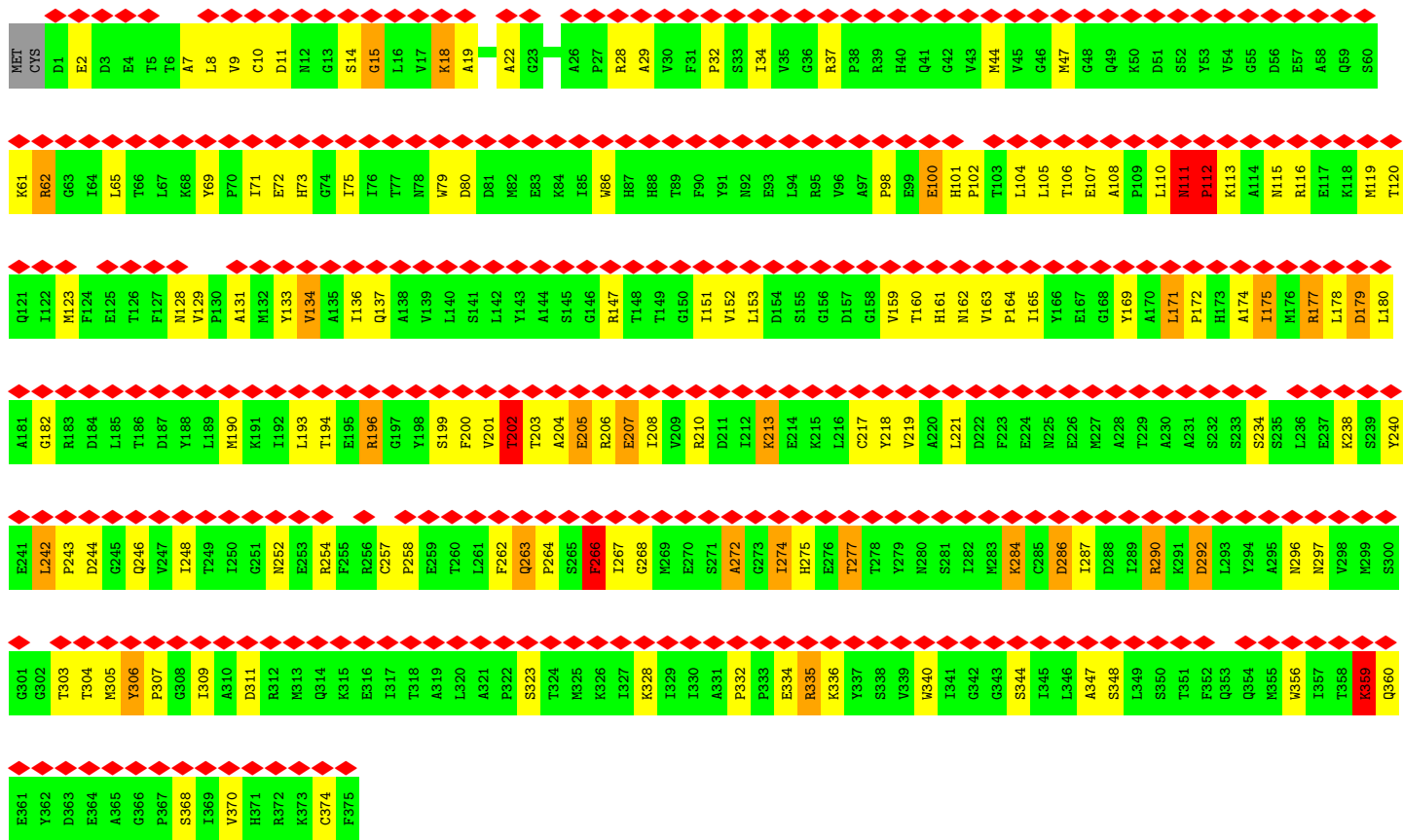


• Molecule 1: Actin, alpha skeletal muscle

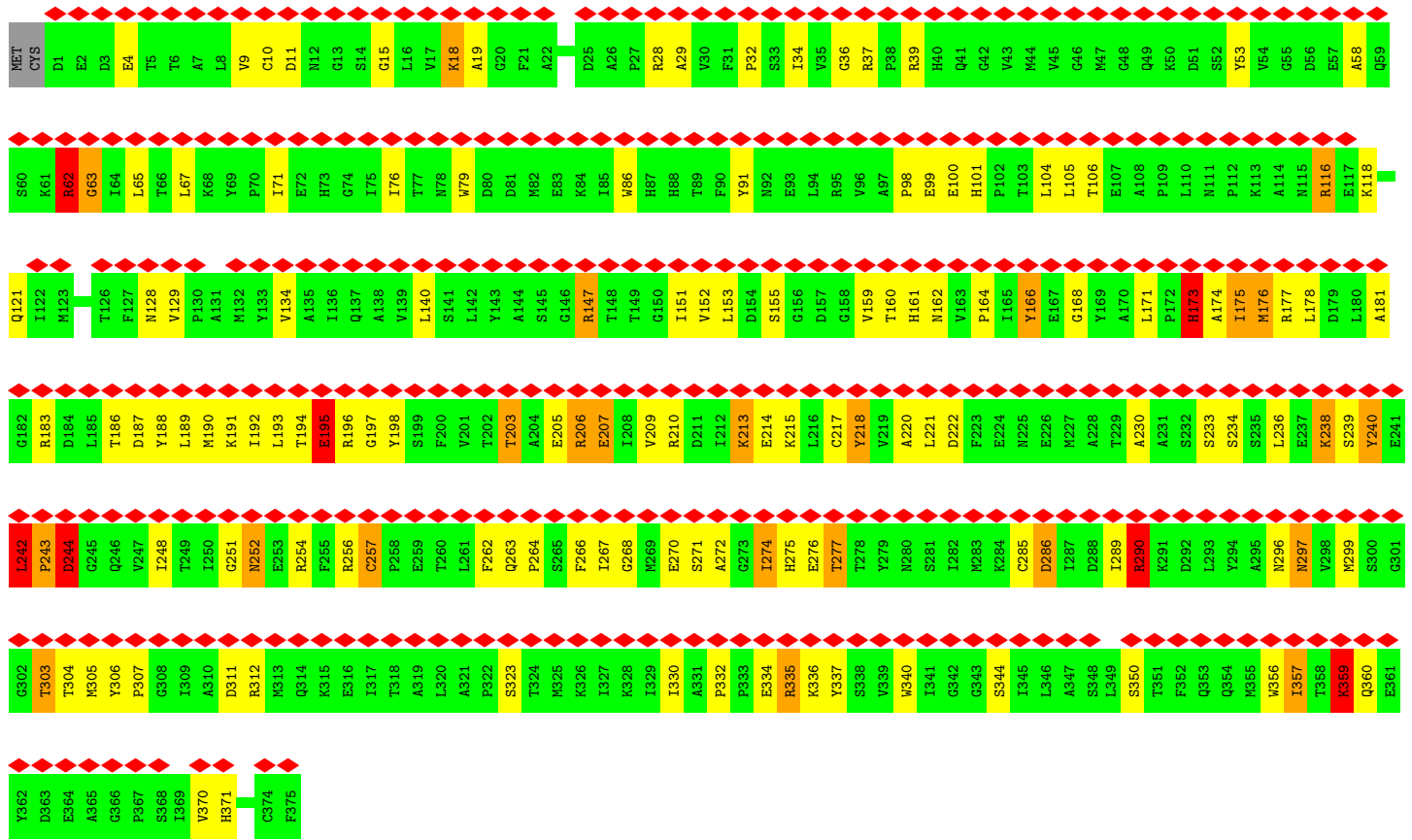
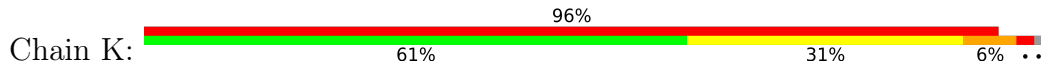




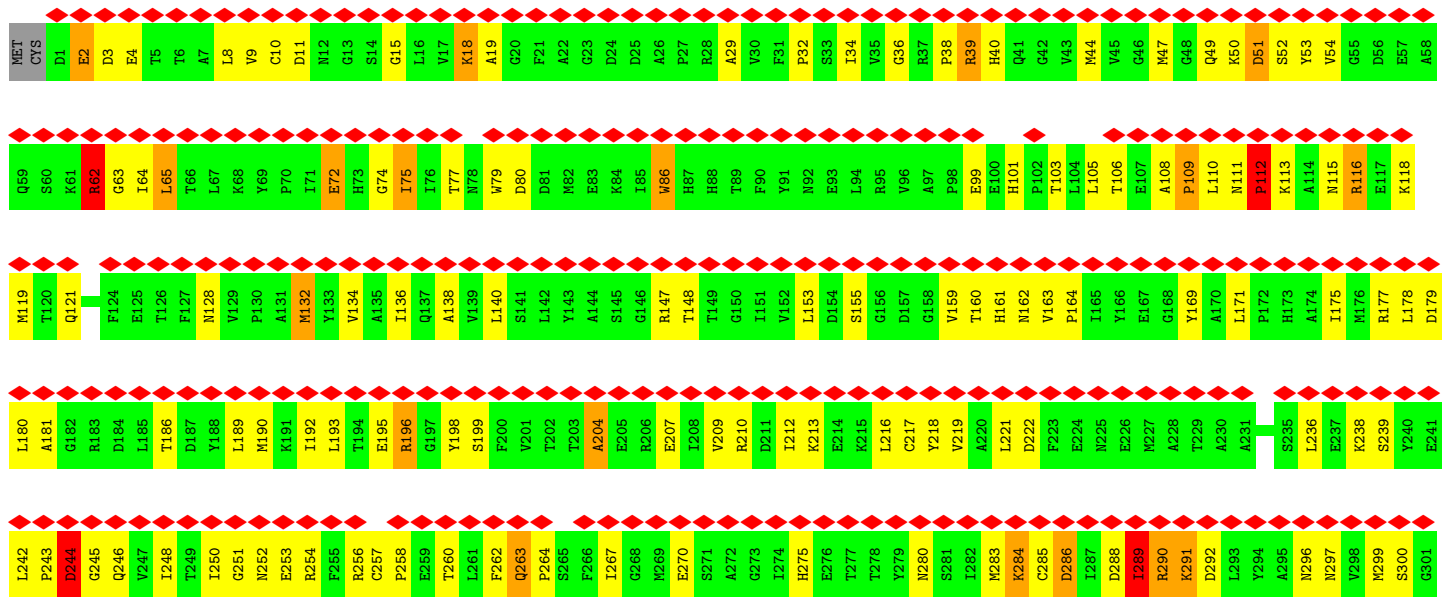
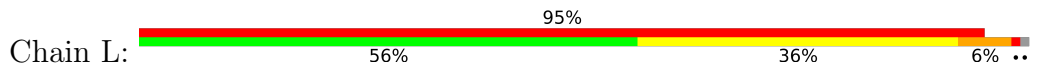
• Molecule 1: Actin, alpha skeletal muscle

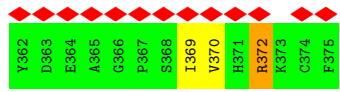
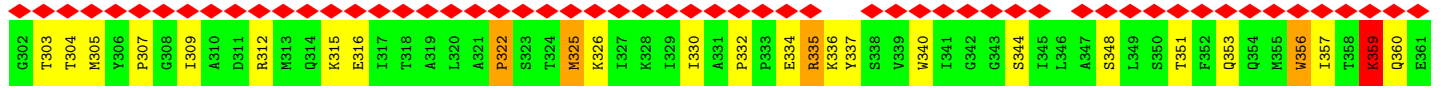


• Molecule 1: Actin, alpha skeletal muscle

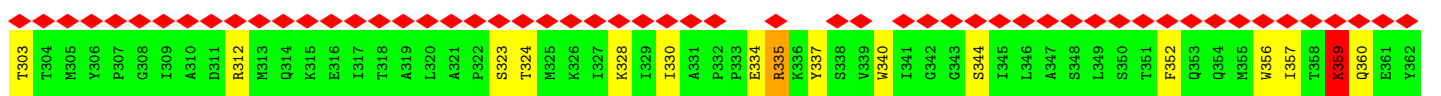
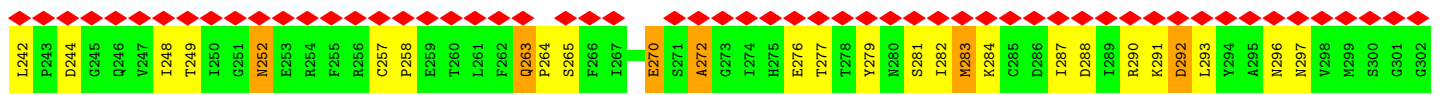
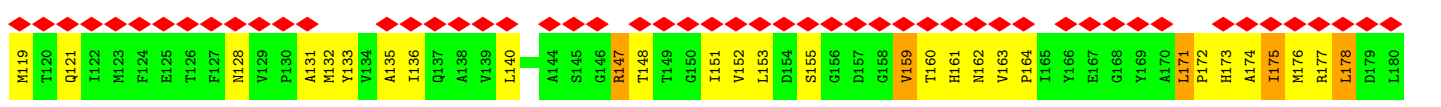
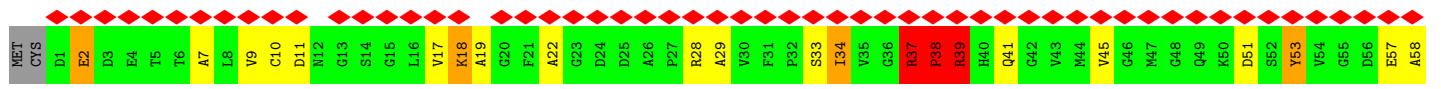
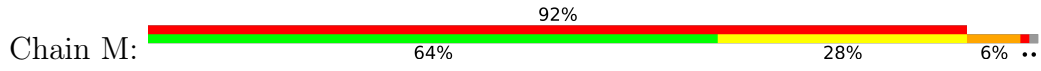


• Molecule 1: Actin, alpha skeletal muscle

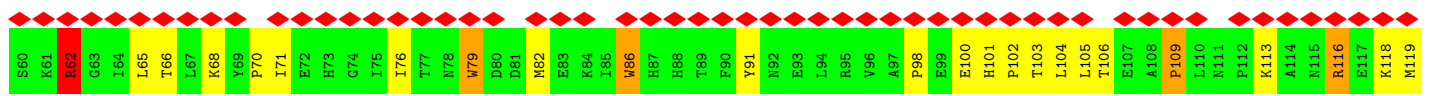
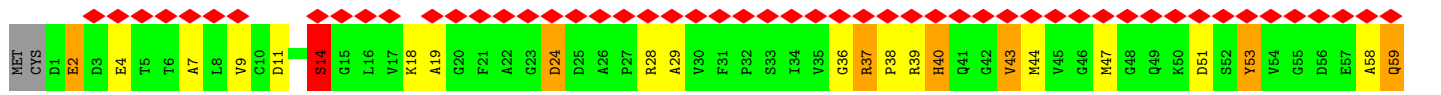
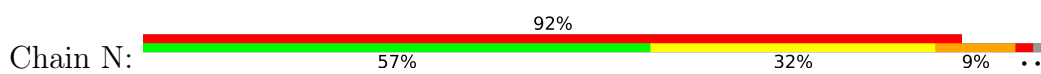




• Molecule 1: Actin, alpha skeletal muscle



• Molecule 1: Actin, alpha skeletal muscle



L180	A181	G182	R183	D184	L185	T186	D187	Y188	L189	M190	K191	L192	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	L287	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	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	K373	C374	F375																																													

4 Experimental information

Property	Value	Source
EM reconstruction method	CRYSTALLOGRAPHY	Depositor
Imposed symmetry	3D CRYSTAL, a =Not provided Å, b =Not provided Å, c =Not provided Å, α =Not provided°, β =Not provided°, γ =Not provided°, space group=Not provided	Depositor
Number of images used	Not provided	
Resolution determination method	DIFFRACTION PATTERN/LAYERLINES	Depositor
CTF correction method	Not provided	
Microscope	JEOL 4000EX	Depositor
Voltage (kV)	400	Depositor
Electron dose ($e^-/\text{Å}^2$)	15	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	40000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	977.199	Depositor
Minimum map value	-974.403	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	215.097	Depositor
Recommended contour level	430.0	Depositor
Map size (Å)	255.99936, 148.00015, 765.7977	wwPDB
Map dimensions	576, 192, 112	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.33333, 1.32143, 1.32951	Depositor

5 Model quality i

5.1 Standard geometry i

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	0.69	0/2996	1.34	21/4058 (0.5%)
1	B	0.68	0/2996	1.35	23/4058 (0.6%)
1	C	0.64	0/2996	1.30	22/4058 (0.5%)
1	D	0.66	0/2996	1.42	33/4058 (0.8%)
1	E	0.65	0/2996	1.40	30/4058 (0.7%)
1	F	0.64	0/2996	1.34	19/4058 (0.5%)
1	G	0.65	0/2996	1.29	23/4058 (0.6%)
1	H	0.67	0/2996	1.32	20/4058 (0.5%)
1	I	0.67	0/2996	1.29	24/4058 (0.6%)
1	J	1.60	6/2996 (0.2%)	1.32	22/4058 (0.5%)
1	K	2.88	3/2996 (0.1%)	1.40	36/4058 (0.9%)
1	L	1.19	5/2996 (0.2%)	1.39	28/4058 (0.7%)
1	M	0.69	0/2996	1.40	27/4058 (0.7%)
1	N	0.69	0/2996	1.39	32/4058 (0.8%)
All	All	1.11	14/41944 (0.0%)	1.35	360/56812 (0.6%)

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	0	8
1	B	0	11
1	C	0	7
1	D	0	11
1	E	0	10
1	F	0	8
1	G	0	3
1	H	0	6
1	I	0	9
1	J	0	8
1	K	0	12

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	13
1	M	0	7
1	N	0	10
All	All	0	123

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	195	GLU	CB-CG	122.37	3.84	1.52
1	K	173	HIS	CB-CG	91.74	3.15	1.50
1	J	266	PHE	CG-CD2	38.22	1.96	1.38
1	J	266	PHE	CG-CD1	37.55	1.95	1.38
1	J	266	PHE	CE2-CZ	30.64	1.95	1.37

The worst 5 of 360 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	173	HIS	CA-CB-CG	16.70	141.98	113.60
1	E	177	ARG	NE-CZ-NH2	11.76	126.18	120.30
1	M	183	ARG	NE-CZ-NH2	-11.55	114.53	120.30
1	D	116	ARG	NE-CZ-NH1	10.44	125.52	120.30
1	N	196	ARG	NE-CZ-NH2	-10.23	115.19	120.30

There are no chirality outliers.

5 of 123 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	188	TYR	Sidechain
1	A	210	ARG	Sidechain
1	A	37	ARG	Sidechain
1	A	62	ARG	Sidechain
1	A	91	TYR	Sidechain

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	2933	0	2894	113	0
1	B	2933	0	2894	110	0
1	C	2933	0	2894	98	0
1	D	2933	0	2894	241	0
1	E	2933	0	2894	109	0
1	F	2933	0	2894	270	0
1	G	2933	0	2894	67	0
1	H	2933	0	2894	85	0
1	I	2933	0	2894	76	0
1	J	2933	0	2894	105	0
1	K	2933	0	2894	120	0
1	L	2933	0	2894	114	0
1	M	2933	0	2894	69	0
1	N	2933	0	2894	82	0
All	All	41062	0	40516	1305	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 16.

The worst 5 of 1305 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:44:MET:CG	1:F:293:LEU:CD2	1.79	1.58
1:J:266:PHE:CZ	1:J:266:PHE:CE2	1.95	1.52
1:J:266:PHE:CD1	1:J:266:PHE:CE1	1.94	1.52
1:J:266:PHE:CD1	1:J:266:PHE:CG	1.95	1.52
1:J:266:PHE:CZ	1:J:266:PHE:CE1	1.95	1.51

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	373/377 (99%)	297 (80%)	63 (17%)	13 (4%)	3	25
1	B	373/377 (99%)	298 (80%)	58 (16%)	17 (5%)	2	21
1	C	373/377 (99%)	310 (83%)	55 (15%)	8 (2%)	7	36
1	D	373/377 (99%)	310 (83%)	49 (13%)	14 (4%)	3	24
1	E	373/377 (99%)	303 (81%)	56 (15%)	14 (4%)	3	24
1	F	373/377 (99%)	291 (78%)	62 (17%)	20 (5%)	2	19
1	G	373/377 (99%)	315 (84%)	46 (12%)	12 (3%)	4	26
1	H	373/377 (99%)	308 (83%)	55 (15%)	10 (3%)	5	31
1	I	373/377 (99%)	318 (85%)	45 (12%)	10 (3%)	5	31
1	J	373/377 (99%)	308 (83%)	48 (13%)	17 (5%)	2	21
1	K	373/377 (99%)	323 (87%)	33 (9%)	17 (5%)	2	21
1	L	373/377 (99%)	311 (83%)	44 (12%)	18 (5%)	2	21
1	M	373/377 (99%)	300 (80%)	54 (14%)	19 (5%)	2	19
1	N	373/377 (99%)	307 (82%)	51 (14%)	15 (4%)	3	23
All	All	5222/5278 (99%)	4299 (82%)	719 (14%)	204 (4%)	5	23

5 of 204 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
1	A	236	LEU
1	A	252	ASN
1	A	272	ALA
1	B	113	LYS

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	318/320 (99%)	284 (89%)	34 (11%)	6	23
1	B	318/320 (99%)	285 (90%)	33 (10%)	7	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	318/320 (99%)	281 (88%)	37 (12%)	5	21
1	D	318/320 (99%)	284 (89%)	34 (11%)	6	23
1	E	318/320 (99%)	282 (89%)	36 (11%)	6	21
1	F	318/320 (99%)	287 (90%)	31 (10%)	8	27
1	G	318/320 (99%)	294 (92%)	24 (8%)	13	38
1	H	318/320 (99%)	291 (92%)	27 (8%)	10	33
1	I	318/320 (99%)	288 (91%)	30 (9%)	8	28
1	J	318/320 (99%)	277 (87%)	41 (13%)	4	18
1	K	318/320 (99%)	289 (91%)	29 (9%)	9	29
1	L	318/320 (99%)	286 (90%)	32 (10%)	7	25
1	M	318/320 (99%)	286 (90%)	32 (10%)	7	25
1	N	318/320 (99%)	271 (85%)	47 (15%)	3	15
All	All	4452/4480 (99%)	3985 (90%)	467 (10%)	10	24

5 of 467 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	99	GLU
1	N	218	TYR
1	J	2	GLU
1	N	180	LEU
1	M	128	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	275	HIS
1	I	263	GLN
1	H	111	ASN
1	H	263	GLN
1	K	263	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](#)

There are no non-standard protein/DNA/RNA residues in this entry.

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](#)

There are no chain breaks in this entry.

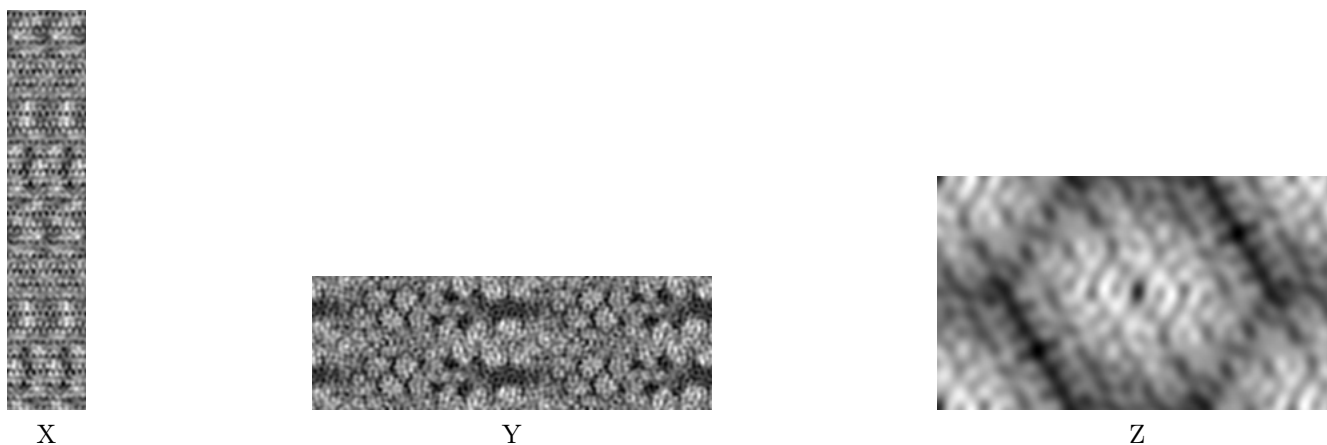
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-1088. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

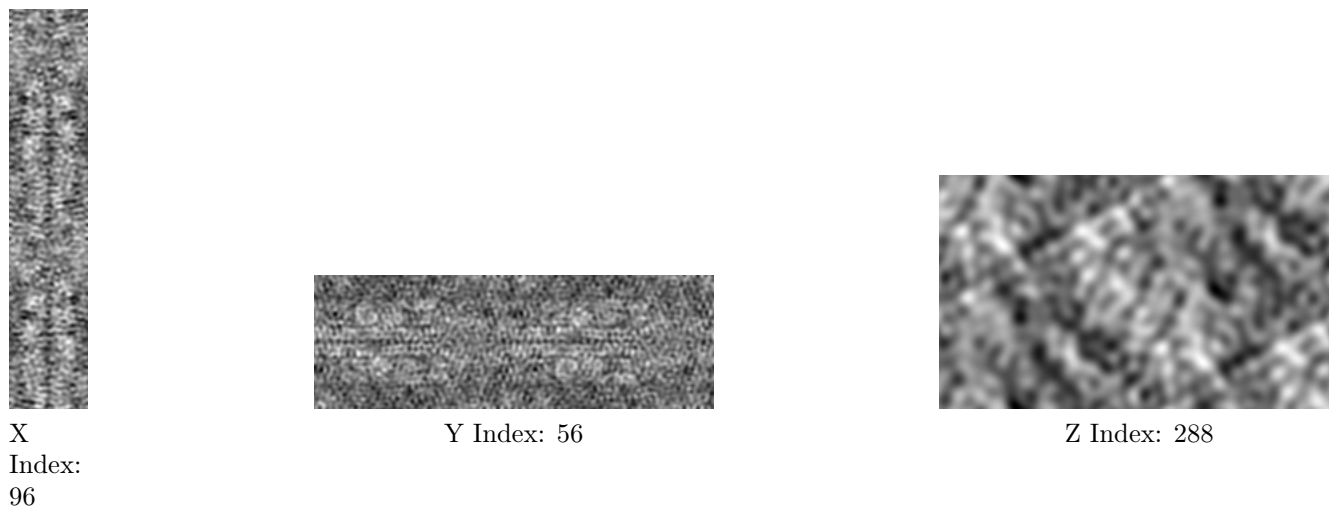
6.1.1 Primary map



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

6.2 Central slices [i](#)

6.2.1 Primary map



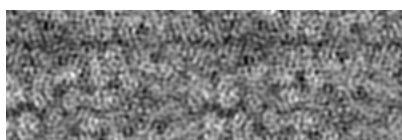
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X
Index:
123



Y Index: 84



Z Index: 413

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 430.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

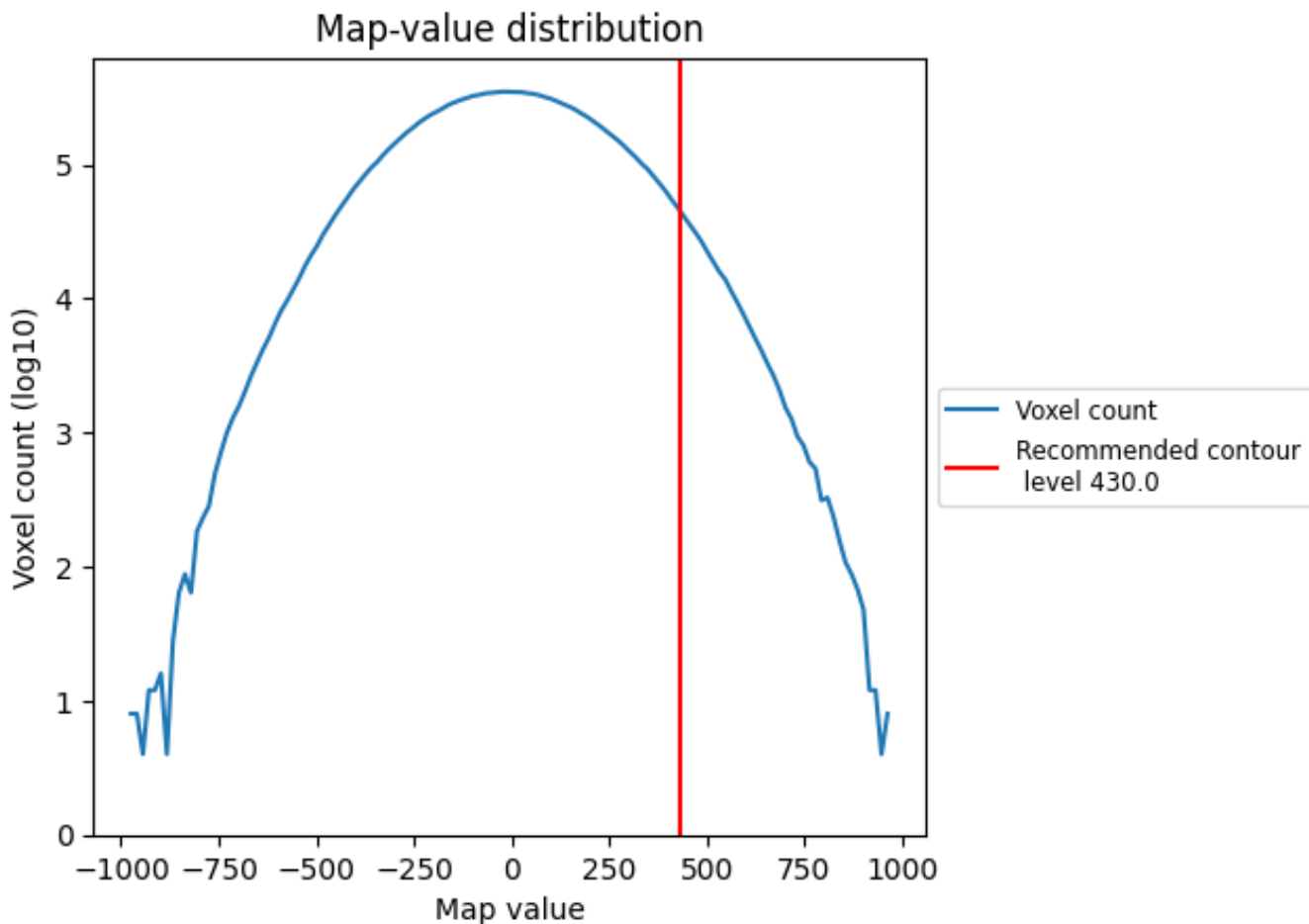
6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

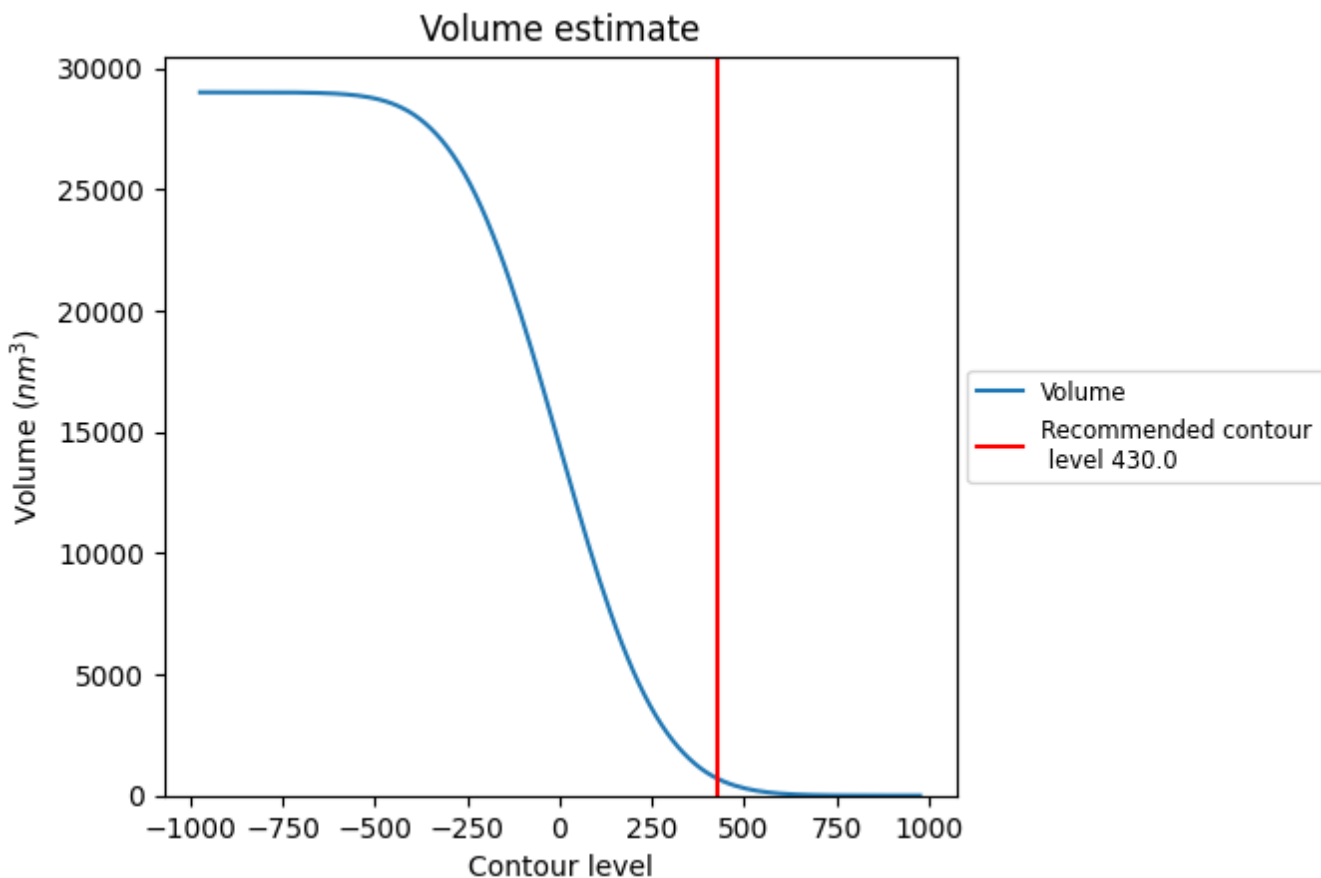
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate [i](#)



The volume at the recommended contour level is 687 nm³; this corresponds to an approximate mass of 621 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

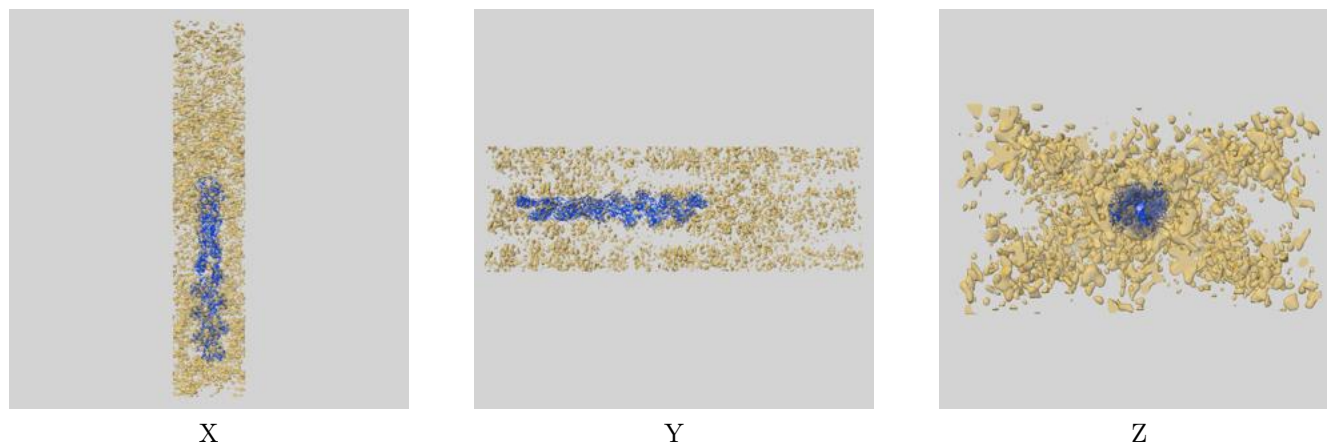
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

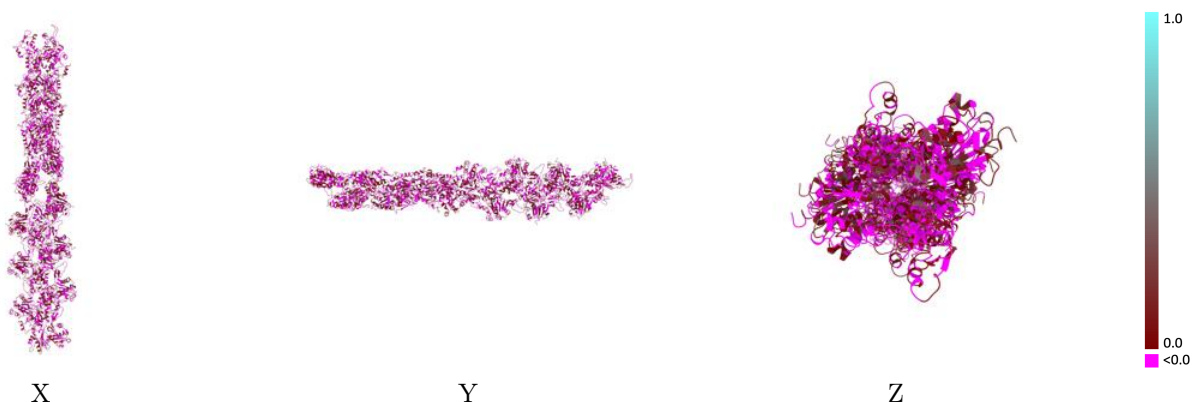
This section contains information regarding the fit between EMDB map EMD-1088 and PDB model 3B5U. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)



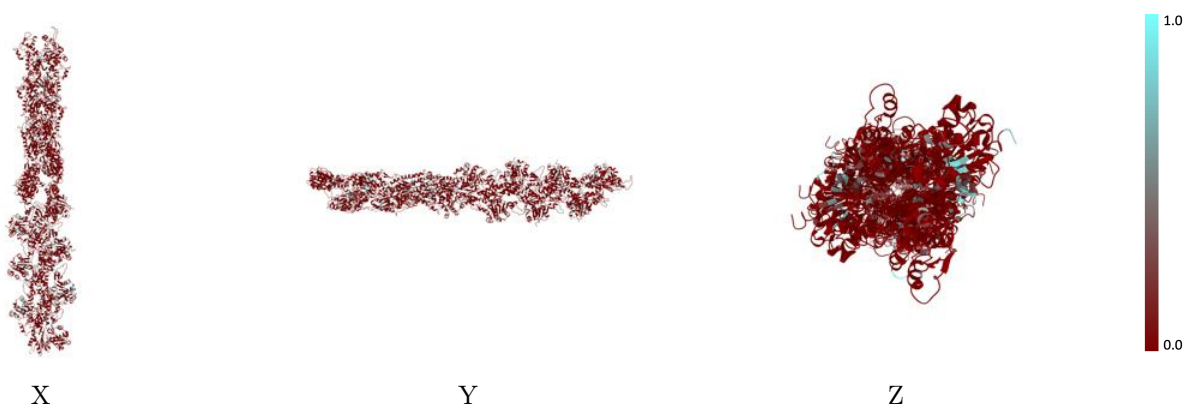
The images above show the 3D surface view of the map at the recommended contour level 430.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



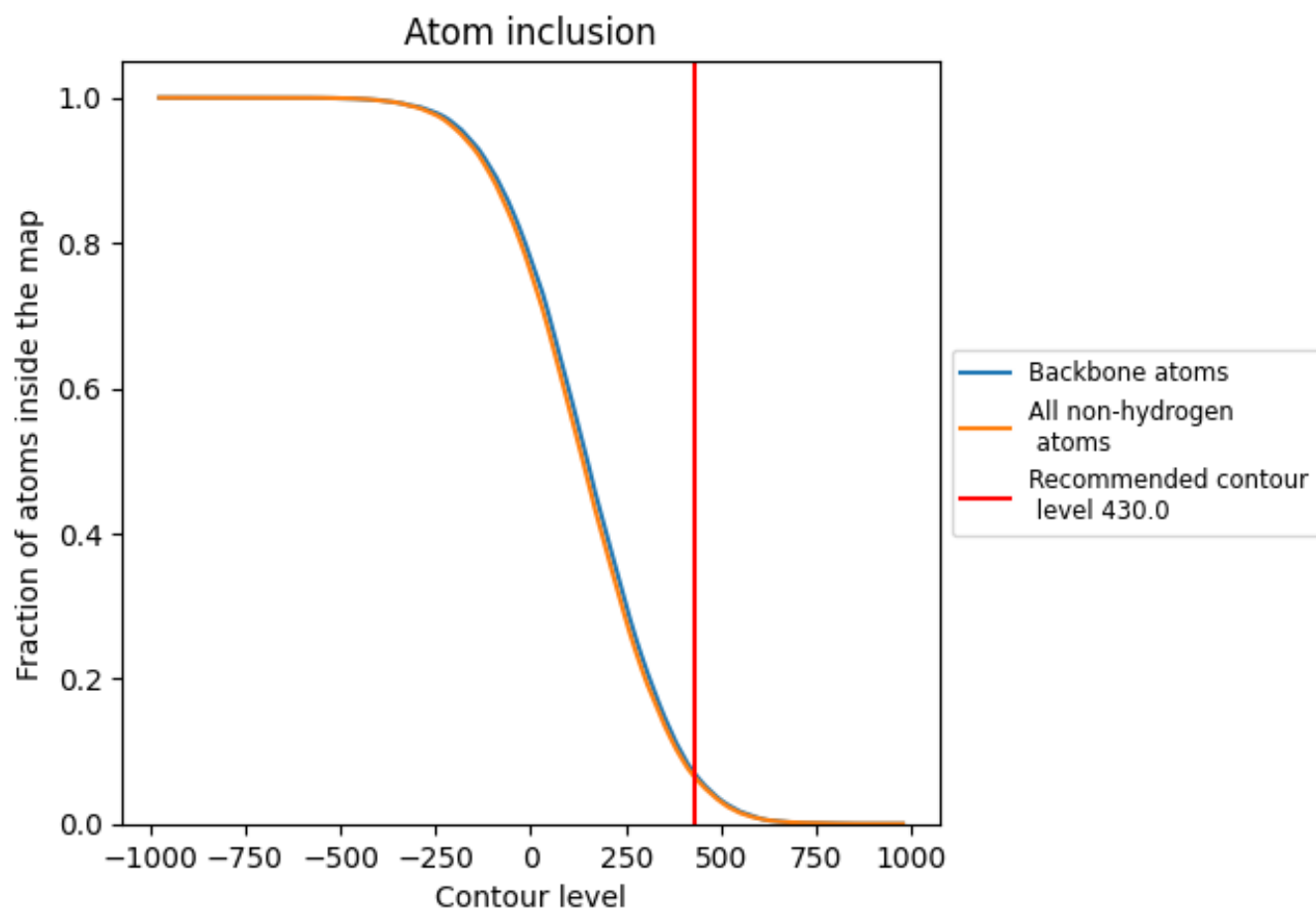
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (430.0).































9.4 Atom inclusion [i](#)



At the recommended contour level, 7% of all backbone atoms, 6% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (430.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.0648	 0.0230
A	 0.0598	 0.0150
B	 0.0959	 0.0190
C	 0.1130	 0.0330
D	 0.0772	 0.0110
E	 0.0796	 0.0250
F	 0.0855	 0.0240
G	 0.0650	 0.0290
H	 0.0302	 0.0040
I	 0.0209	 0.0280
J	 0.0393	 0.0190
K	 0.0393	 0.0280
L	 0.0521	 0.0390
M	 0.0719	 0.0240
N	 0.0768	 0.0190

