wwPDB EM Validation Summary Report (i)

Nov 16, 2022 – 11:45 AM JST

PDB ID	:	6LTJ
EMDB ID	:	EMD-0974
Title	:	Structure of nucleosome-bound human BAF complex
Authors	:	He, S.; Wu, Z.; Tian, Y.; Yu, Z.; Yu, J.; Wang, X.; Li, J.; Liu, B.; Xu, Y.
Deposited on	:	2020-01-22
Resolution	:	3.70 Å(reported)

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:

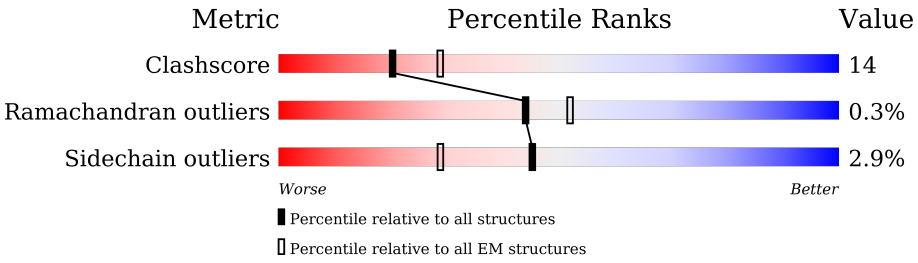
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 3.70 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	136	35% 50% 17% 33%
1	E	136	29% 49% 18% 33%
2	B	103	30% 61% 15% 24%
2	F	103	33% 58% 17% 25%
3	C	130	29% 62% 12% 27%
3	G	130	34% 57% 16% 27%
4	D	126	33% 61% 9% 30%
4	H	126	38% 60% 11% 29%

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Mol	Chain	Length	Quality of chain
5	I	1647	23% 19% 13% 67%
6	J	407	33% 57% 23% 18%
7	K	375	58% 54% 29% 15%
8	L	1295	20% 27% 9% 64%
9	M	336	38% 61% 22% 16%
10	N	1214	11% 14% 7% 79%
10	O	1214	10% 19% 7% 73%
11	P	515	23% 30% 16% 54%
12	Q	411	7% 17% 9% 74%
13	R	292	11% 17% 7% 76%
14	X	119	34% 45% 55%
15	Y	119	29% 39% 61%

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 34283 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 Histone H3.3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	91	Total	C	N	O	S	0	0
			739	466	141	130	2		
1	E	91	Total	C	N	O	S	0	0
			739	466	141	130	2		

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	78	Total	C	N	O	S	0	0
			622	393	120	108	1		
2	F	77	Total	C	N	O	S	0	0
			614	389	119	105	1		

- Molecule 3 is a protein called Histone H2A type 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	95	Total	C	N	O	0	0
			726	455	142	129		
3	G	95	Total	C	N	O	0	0
			727	457	142	128		

- Molecule 4 is a protein called Histone H2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	88	Total	C	N	O	S	0	0
			682	430	121	129	2		
4	H	90	Total	C	N	O	S	0	0
			700	441	124	133	2		

- Molecule 5 is a protein called Transcription activator BRG1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	551	Total	C	N	O	S	0	0
			4606	2932	841	809	24		

- Molecule 6 is a protein called Actin-like protein 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	334	Total	C	N	O	S	0	0
			2612	1656	441	495	20		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	418	PRO	-	expression tag	UNP O96019

- Molecule 7 is a protein called Actin, cytoplasmic 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	317	Total	C	N	O	S	0	0
			2482	1575	409	480	18		

- Molecule 8 is a protein called AT-rich interactive domain-containing protein 1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	466	Total	C	N	O	S	0	0
			3670	2341	620	688	21		

- Molecule 9 is a protein called SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily B member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	283	Total	C	N	O	S	0	0
			2277	1437	388	440	12		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	163	GLY	-	linker	UNP Q12824
M	164	GLY	-	linker	UNP Q12824
M	165	SER	-	linker	UNP Q12824
M	166	GLY	-	linker	UNP Q12824
M	167	GLY	-	linker	UNP Q12824
M	168	SER	-	linker	UNP Q12824

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Chain	Residue	Modelled	Actual	Comment	Reference
M	169	GLY	-	linker	UNP Q12824
M	170	GLY	-	linker	UNP Q12824
M	171	SER	-	linker	UNP Q12824

- Molecule 10 is a protein called SWI/SNF complex subunit SMARCC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	N	261	Total	C	N	O	S	0	0
			2120	1346	374	388	12		
10	O	325	Total	C	N	O	S	0	0
			2632	1676	458	485	13		

- Molecule 11 is a protein called SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily D member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	P	239	Total	C	N	O	S	0	0
			2015	1281	362	361	11		

- Molecule 12 is a protein called SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily E member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Q	105	Total	C	N	O	S	0	0
			860	530	161	165	4		

- Molecule 13 is a protein called Zinc finger protein ubi-d4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	R	70	Total	C	N	O	S	0	0
			580	361	112	102	5		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	101	GLY	-	linker	UNP Q92785
R	102	GLY	-	linker	UNP Q92785
R	103	SER	-	linker	UNP Q92785
R	104	GLY	-	linker	UNP Q92785
R	105	GLY	-	linker	UNP Q92785
R	106	SER	-	linker	UNP Q92785

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Chain	Residue	Modelled	Actual	Comment	Reference
R	107	GLY	-	linker	UNP Q92785
R	108	GLY	-	linker	UNP Q92785
R	109	SER	-	linker	UNP Q92785

- Molecule 14 is a DNA chain called DNA (119-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	X	119	Total	C	N	O	P	0	0
			2424	1150	440	715	119		

- Molecule 15 is a DNA chain called DNA (119-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Y	119	Total	C	N	O	P	0	0
			2455	1160	463	713	119		

- Molecule 16 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

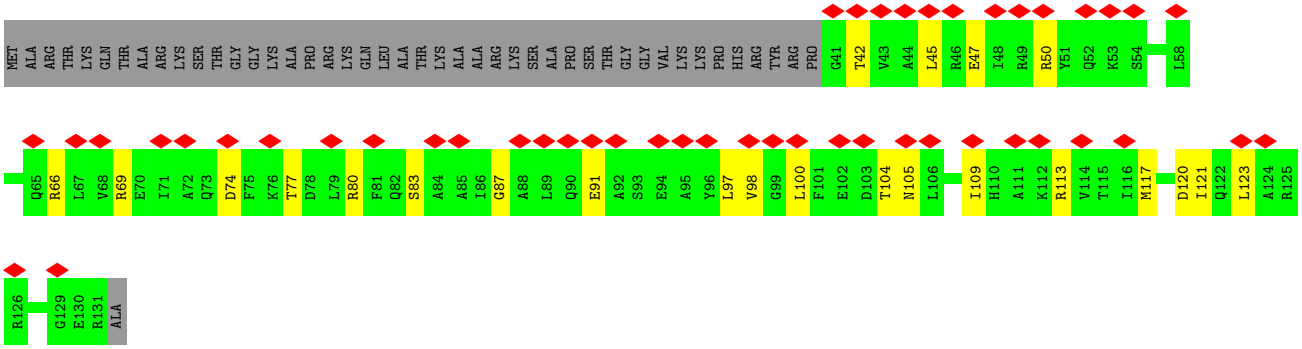
Mol	Chain	Residues	Atoms		AltConf
16	L	1	Total	Zn	0
			1	1	

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.

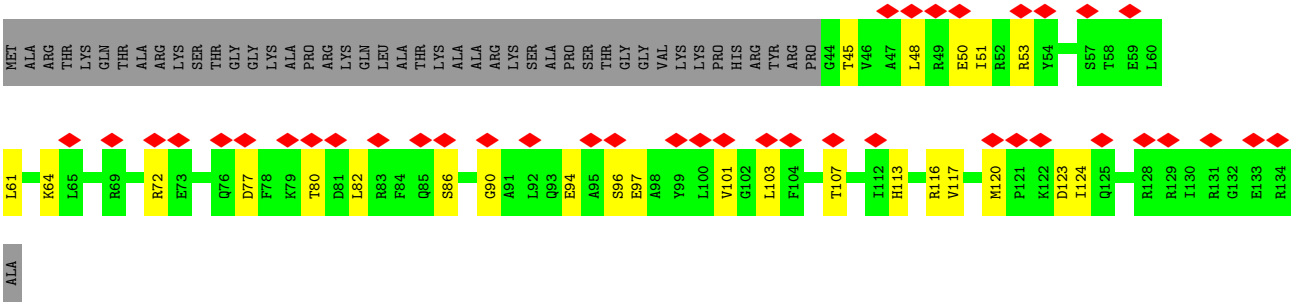
• Molecule 1: Histone H3.3

Chain A:



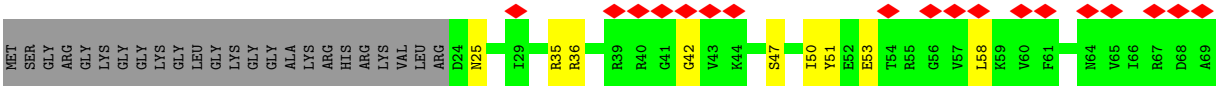
• Molecule 1: Histone H3.3

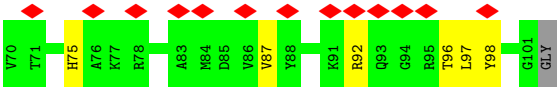
Chain E:



• Molecule 2: Histone H4

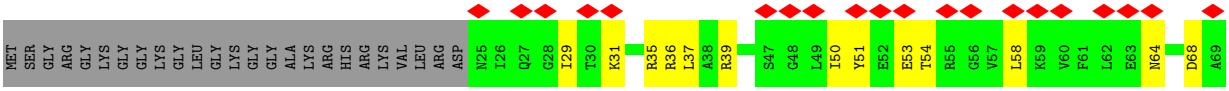
Chain B:

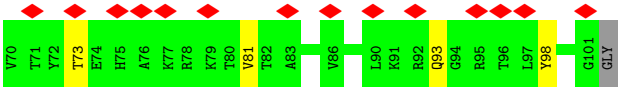




• Molecule 2: Histone H4

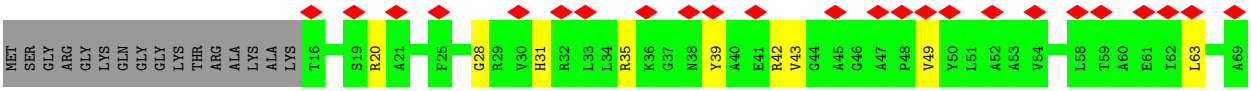
Chain F:

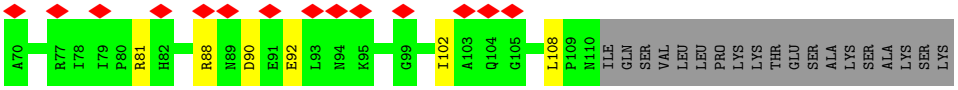




• Molecule 3: Histone H2A type 1

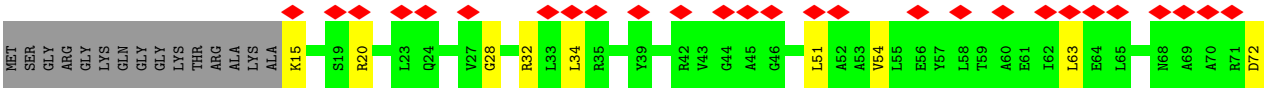
Chain C:

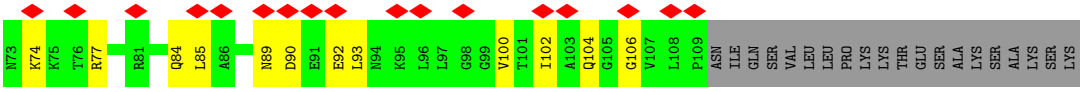




• Molecule 3: Histone H2A type 1

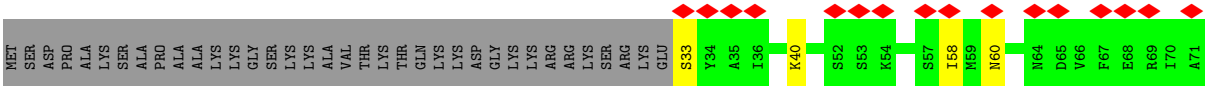
Chain G:

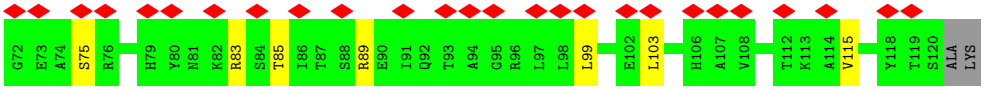




• Molecule 4: Histone H2B

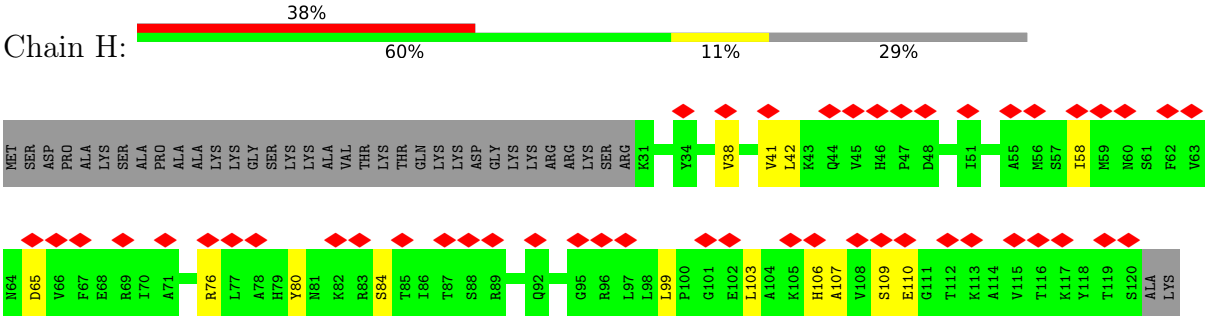
Chain D:





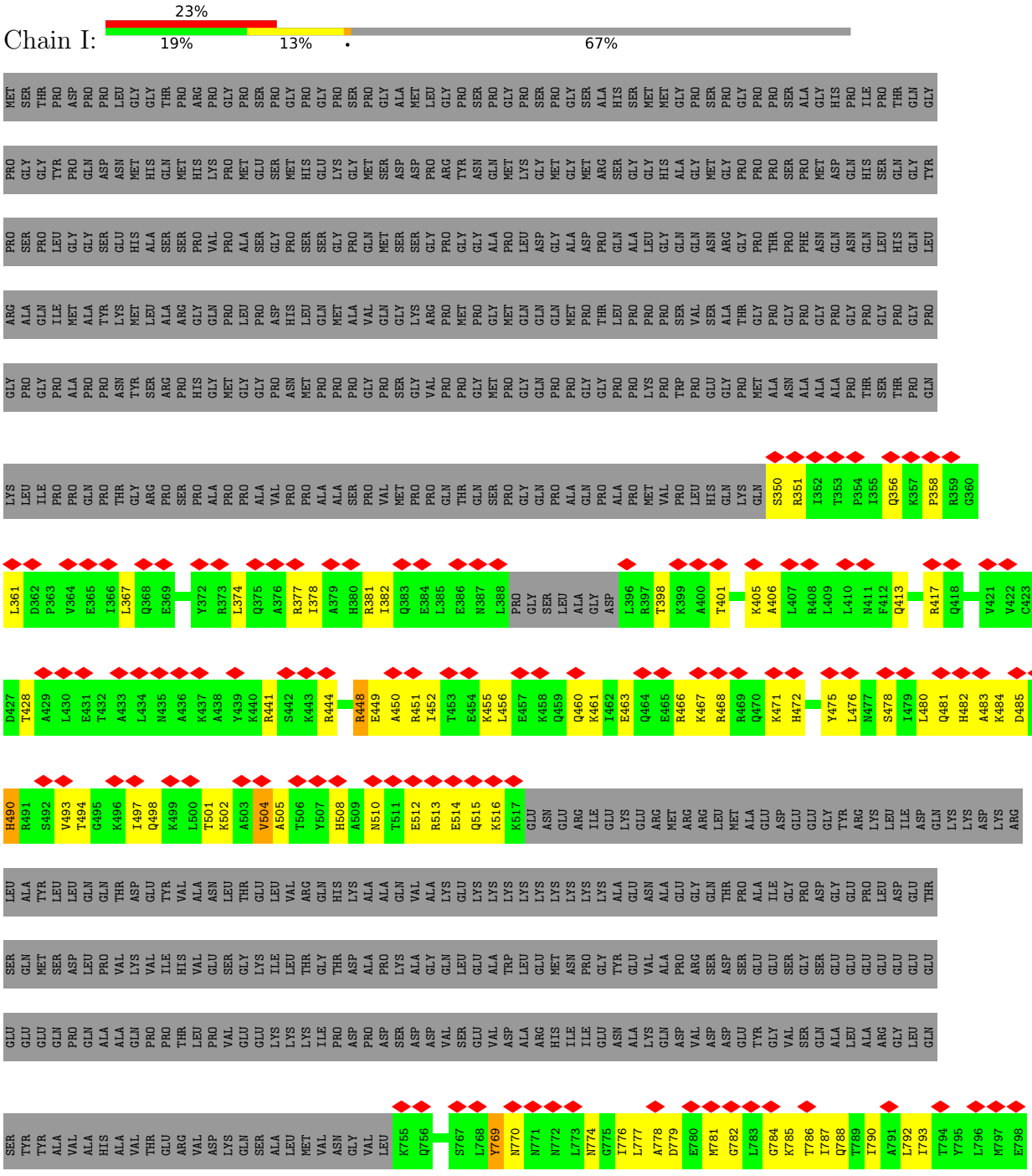
• Molecule 4: Histone H2B

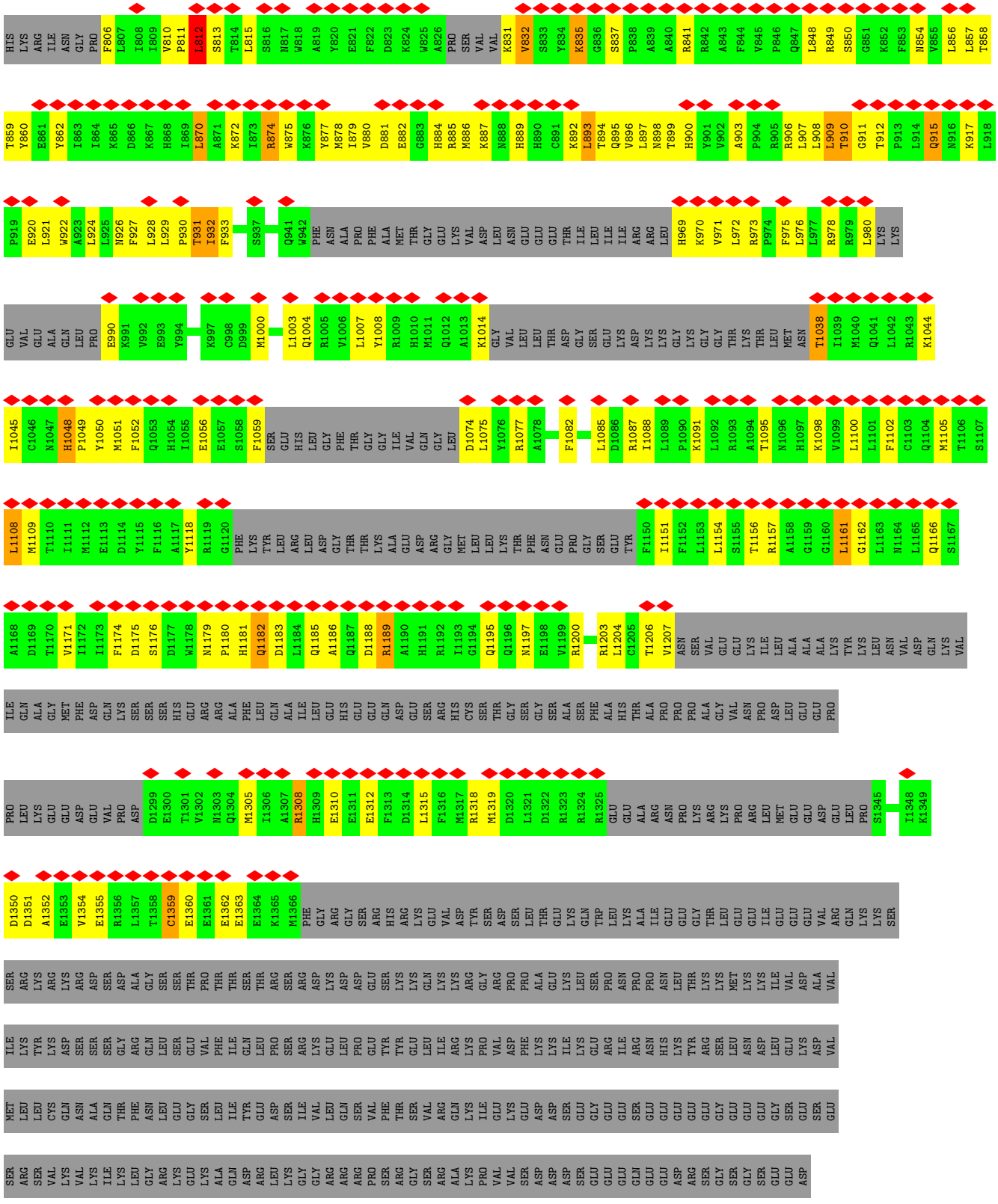
Chain H:



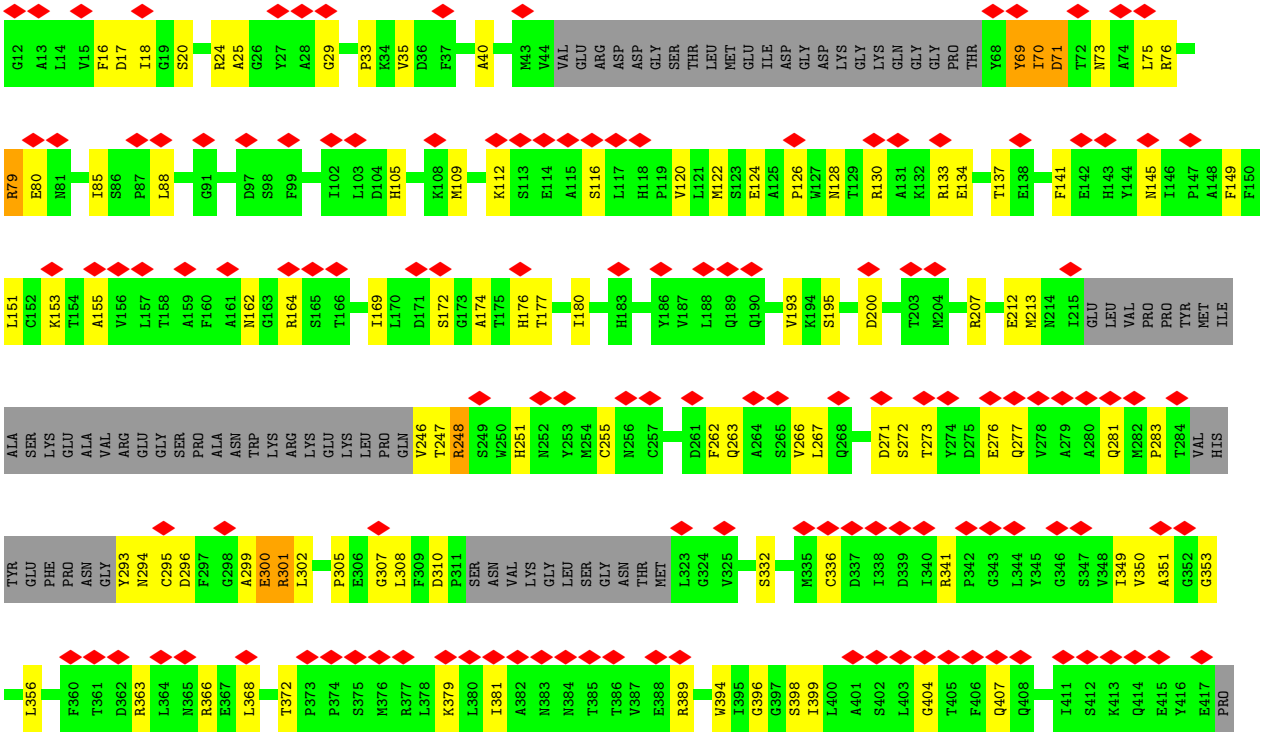
• Molecule 5: Transcription activator BRG1

Chain I:



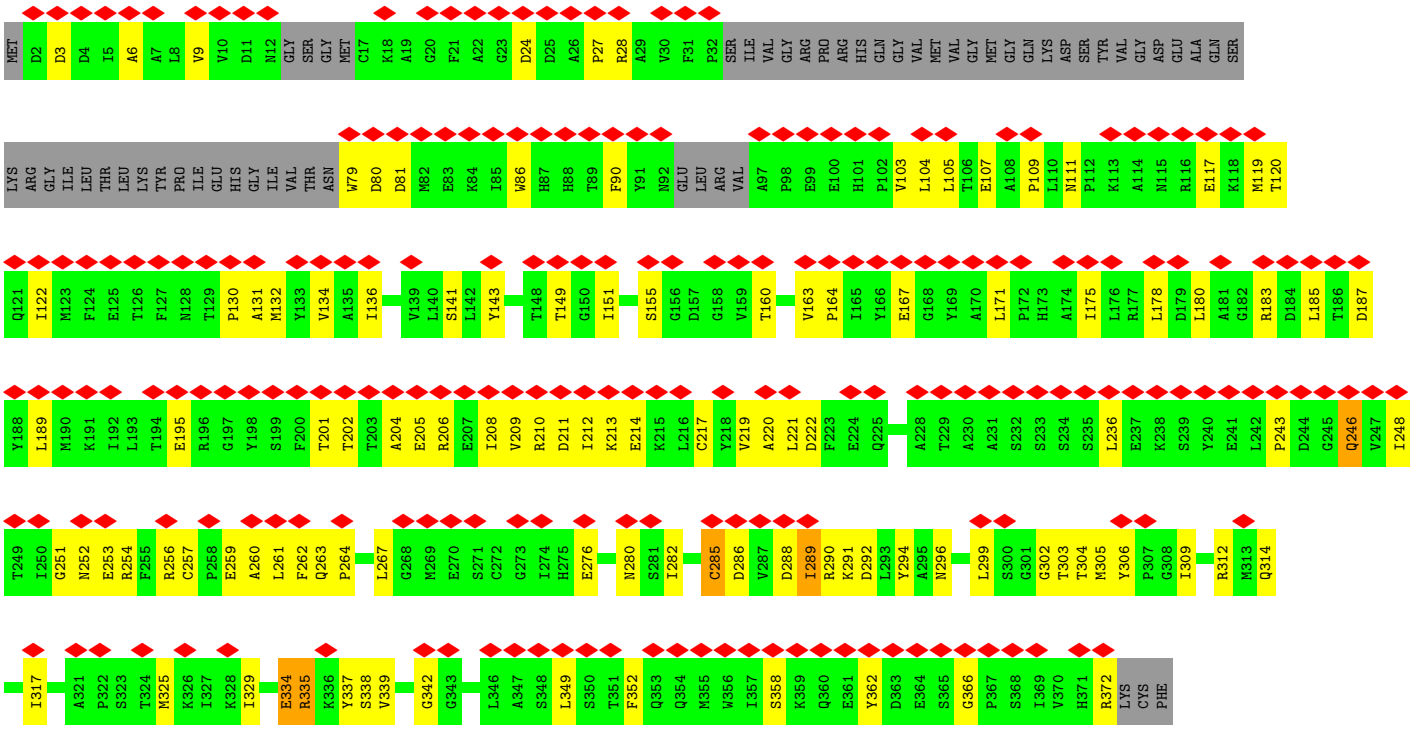


• Molecule 6: Actin-like protein 6A



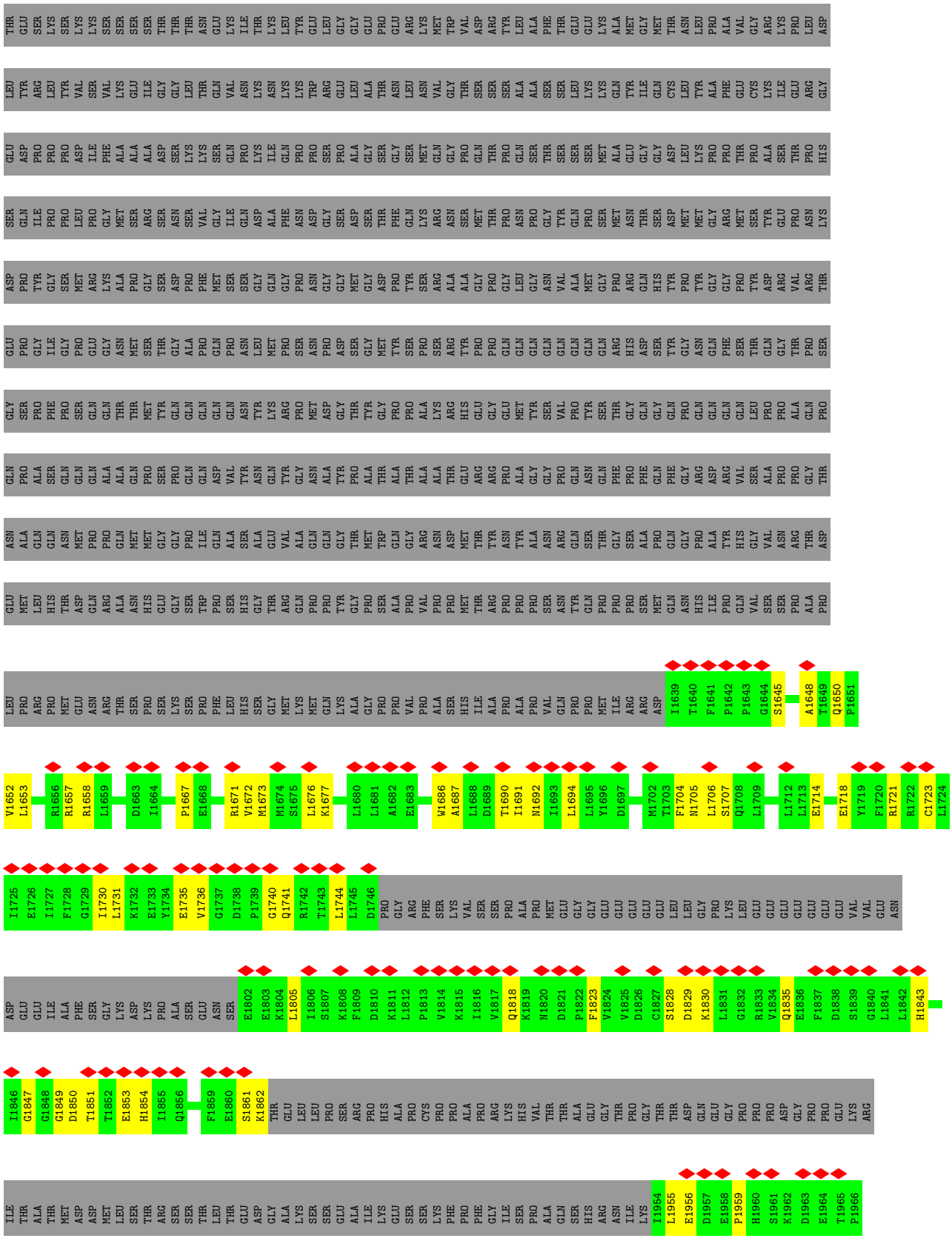
• Molecule 7: Actin, cytoplasmic 1

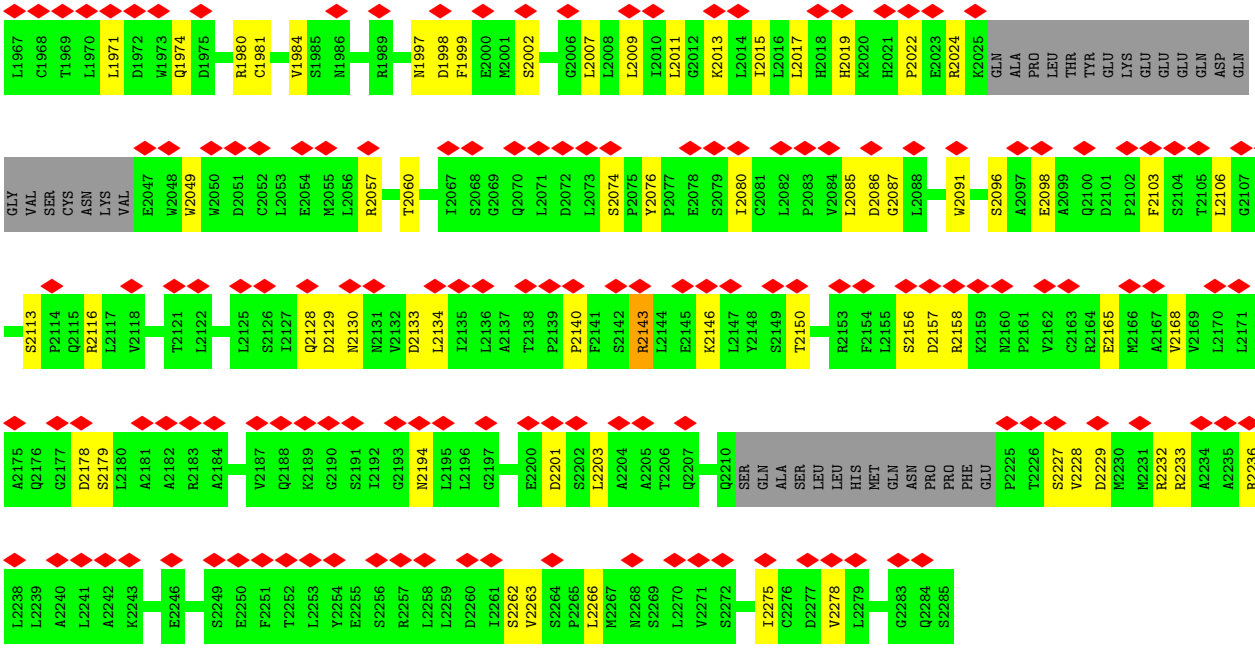
Chain K:



• Molecule 8: AT-rich interactive domain-containing protein 1A

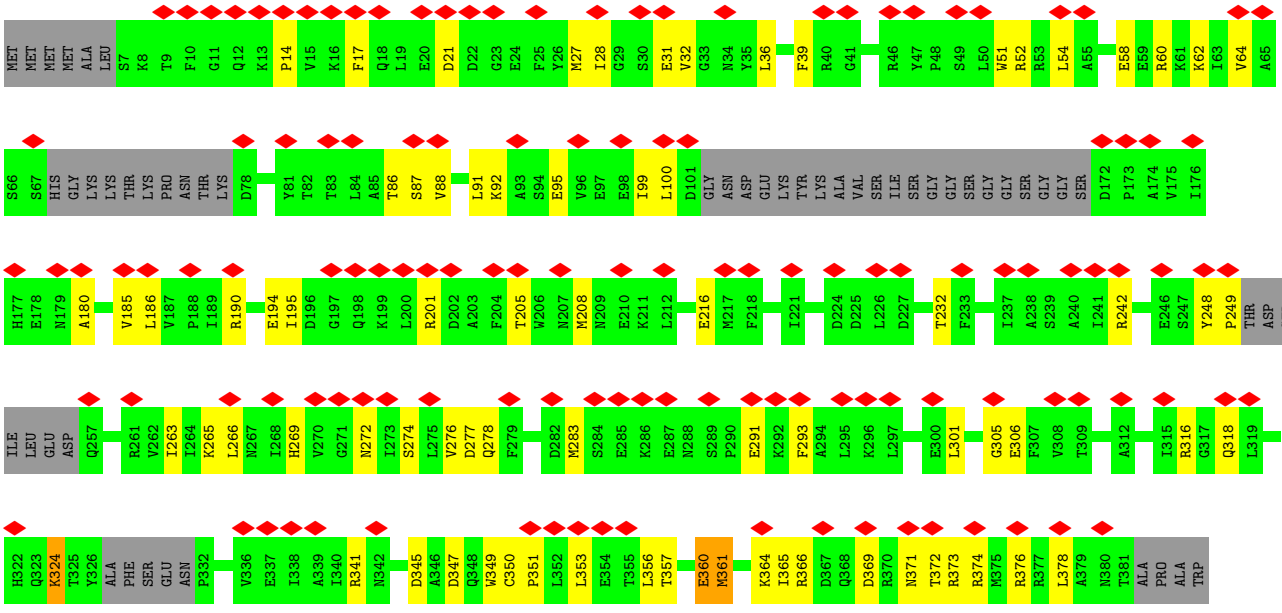
Chain L:





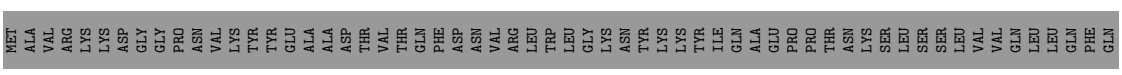
• Molecule 9: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily B member 1

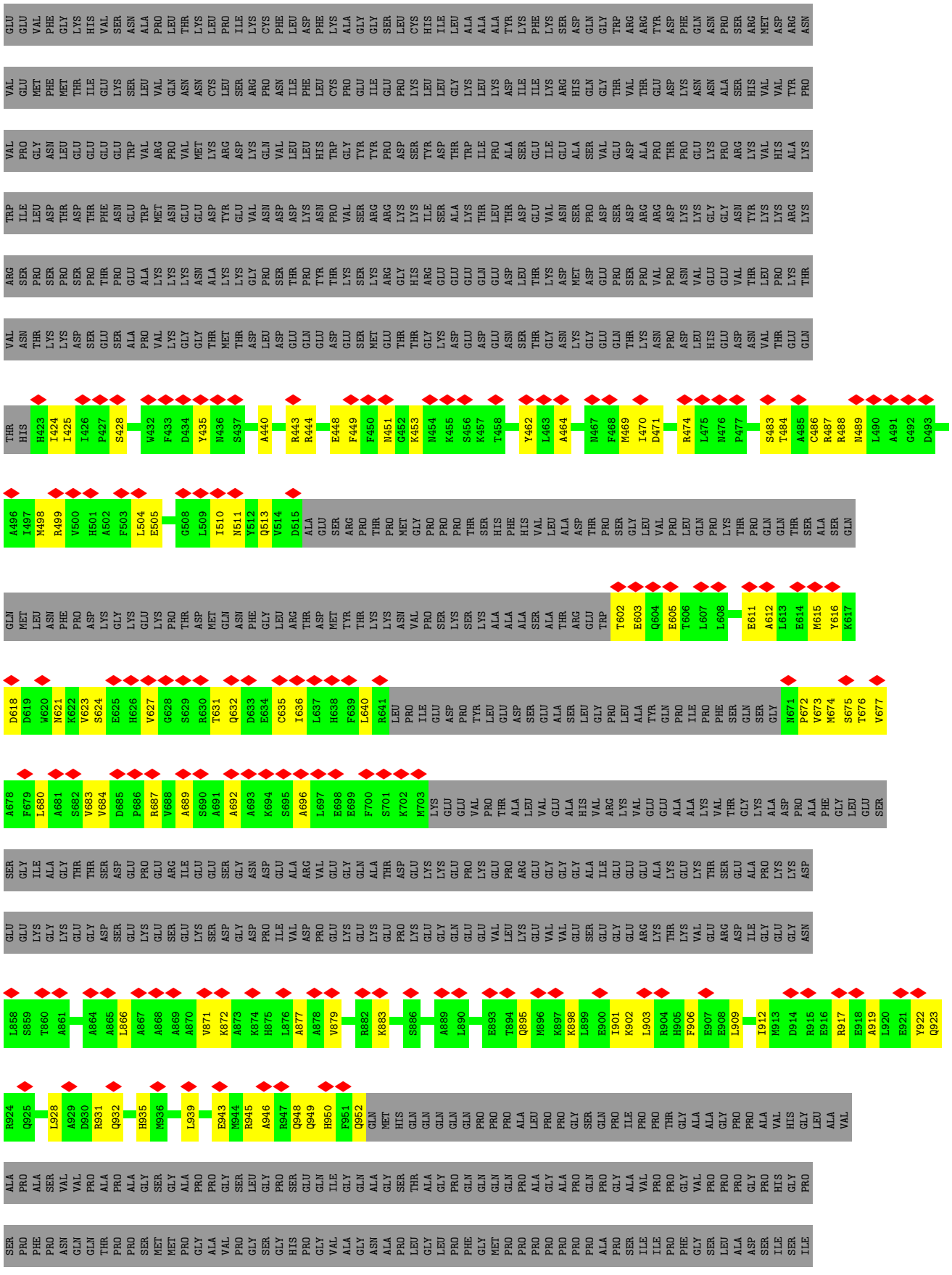
Chain M:

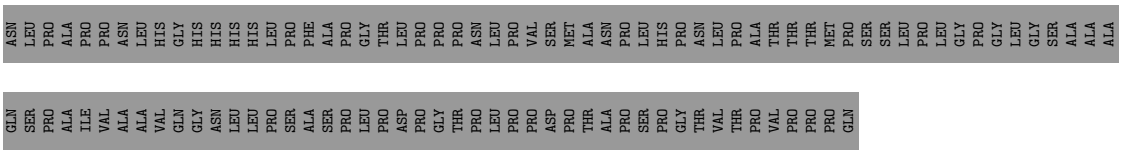


• Molecule 10: SWI/SNF complex subunit SMARCC2

Chain N:

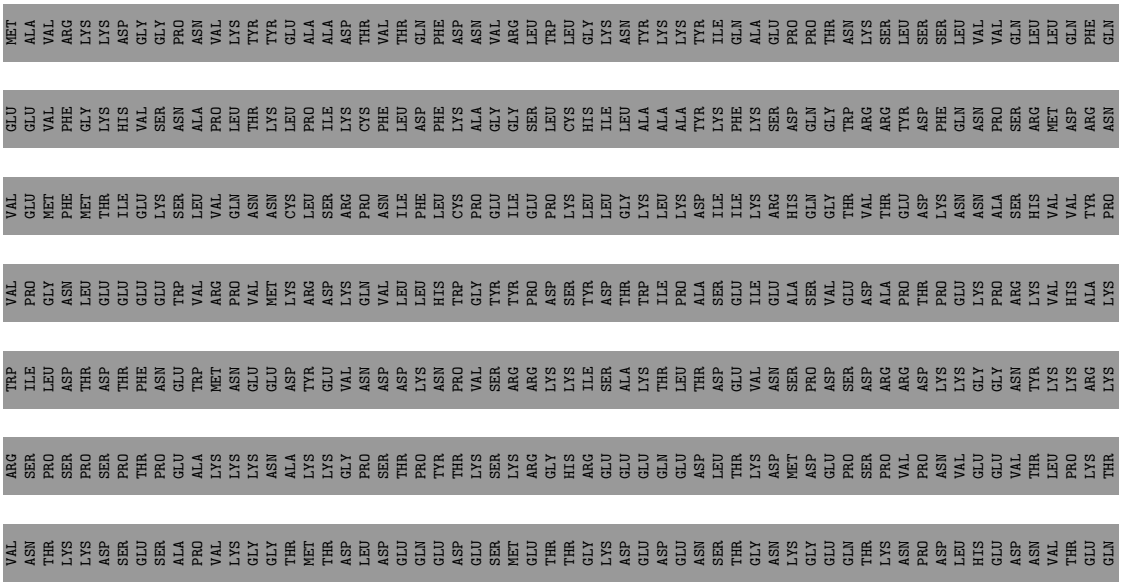


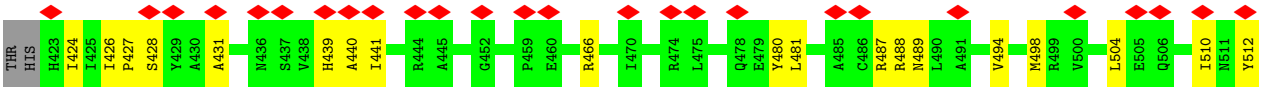

THR HIS H423 I424 I425 I426 P427 S428 W432 F433 D434 Y435 N436 S437 A440 R443 R444 E448 F449 F450 N451 C452 K453 N454 K455 S456 K457 T458 Y462 L463 A464 N467 F468 M469 I470 D471 R474 L475 N476 P477 S483 T484 A485 C486 R487 R488 N489 L490 A491 G492 D493
A496 I497 M498 R499 V500 H501 A502 F503 L504 E505 G508 L509 I510 N511 Y512 Q513 V514 D515
T602 E603 Q604 E605 T606 L607 L608 E611 A612 L613 E614 M615 Y616 K617
D618 D619 W620 N621 K622 V623 S624 E625 H626 V627 G628 S629 R630 T631 Q632 D633 E634 C635 I636 L637 H638 F639 L640 R641 N671 P672 V673 M674 S675 T676 V677
A678 F679 L680 A681 S682 V683 V684 D685 P686 R687 V688 A689 S690 A691 A692 A693 K694 S695 A696 L697 E698 E699 F700 S701 K702 M703
L858 S859 T860 A861 A864 A865 L866 A867 A868 A869 A870 V871 K872 A873 K874 H875 L876 A877 A878 V879 R882 K883 S886 A889 L890 E893 T894 Q895 M896 K897 K898 L899 E900 I901 K902 L903 R904 H905 F906 E907 E908 L909 I912 M913 D914 R915 E916 R917 E918 A919 L920 E921 Y922 Q923
R924 Q925 L928 A929 D930 R931 Q932 H935 M936 L939 E943 M944 R945 A946 R947 Q948 Q949 H950 F951 Q952

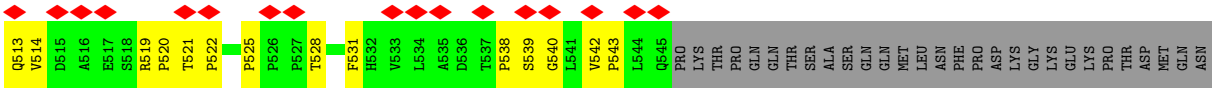


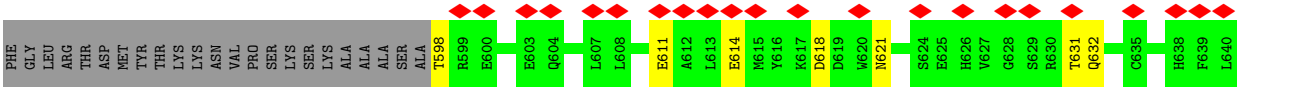
• Molecule 10: SWI/SNF complex subunit SMARCC2

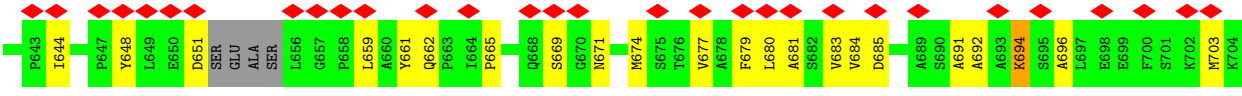
Chain O:

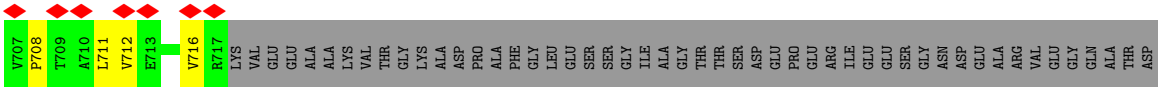


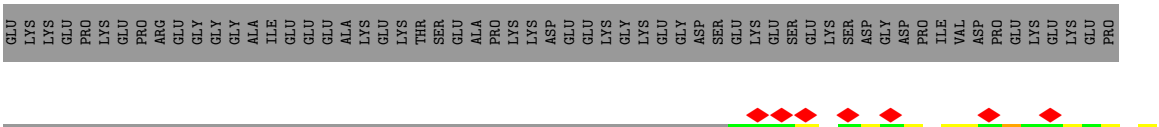


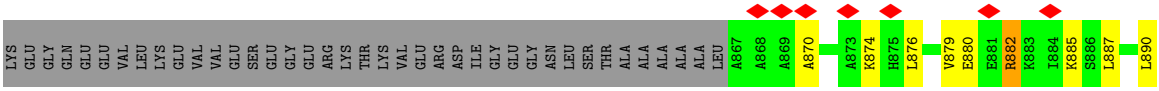


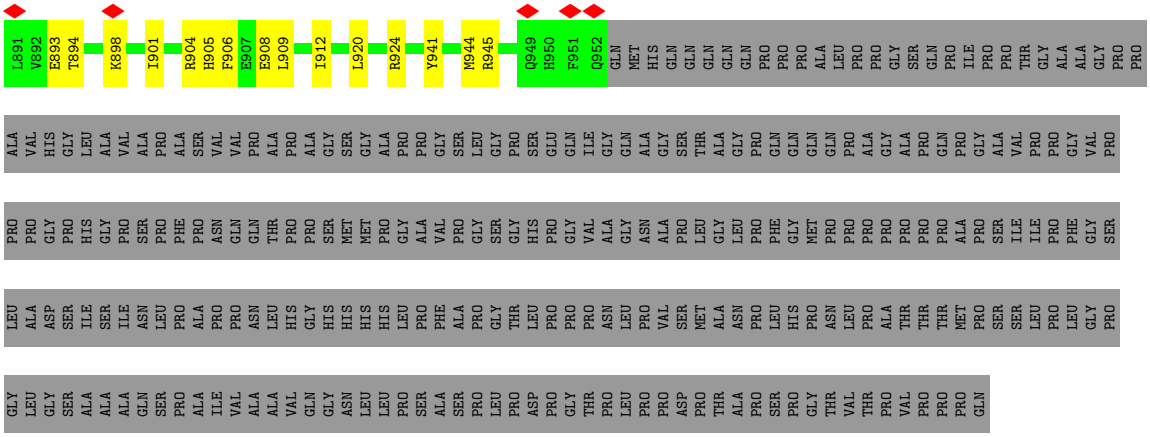






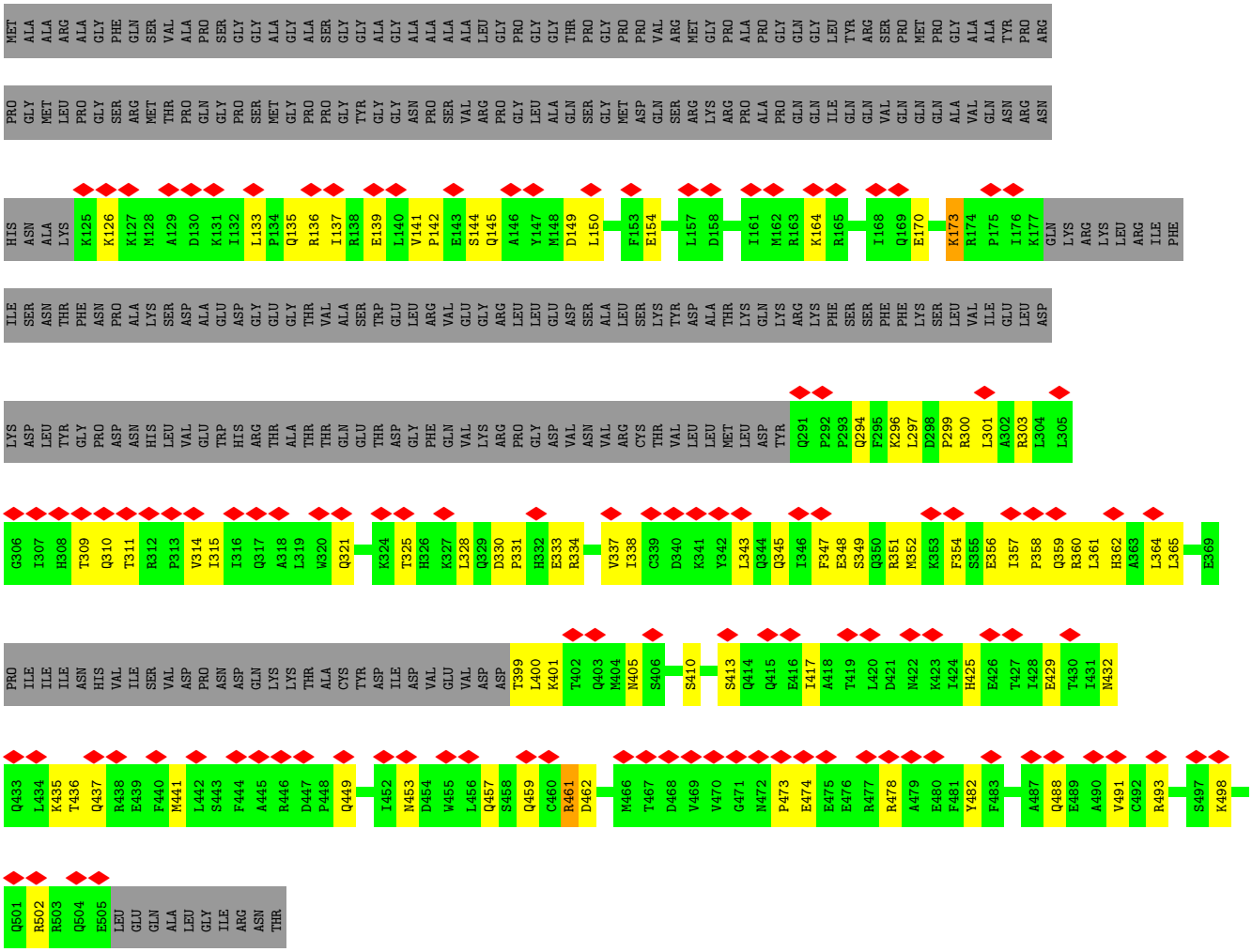






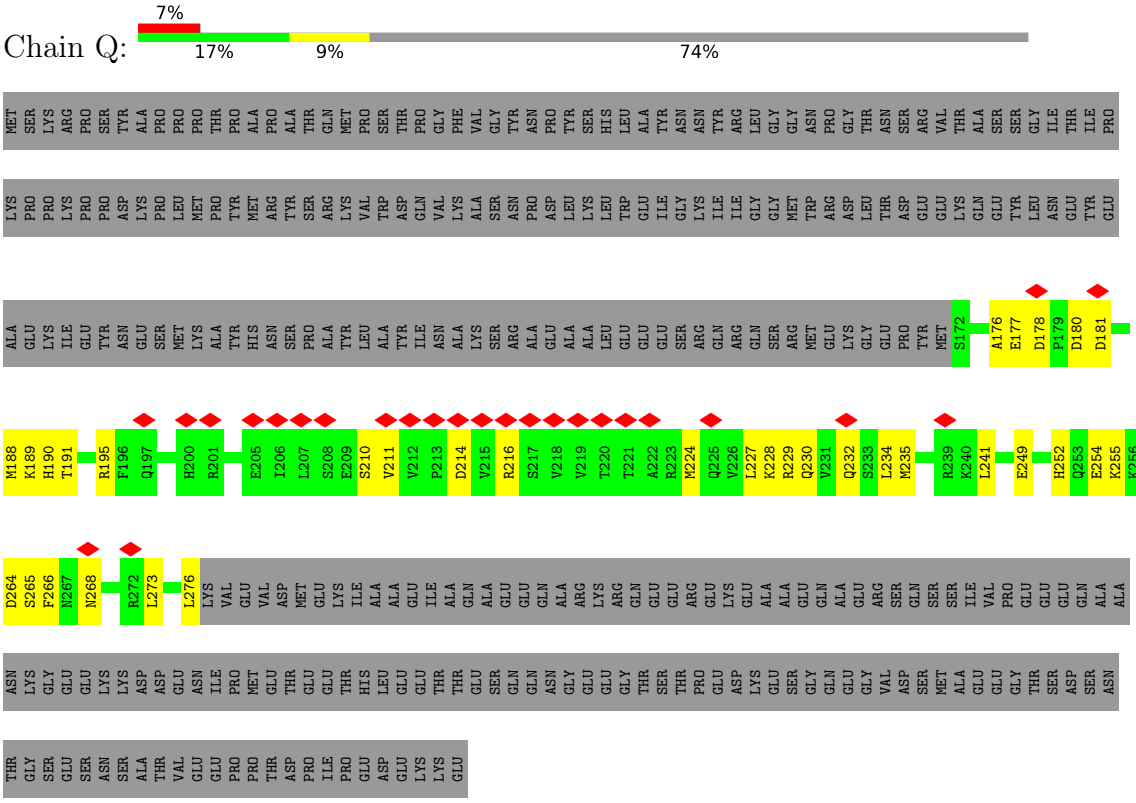
• Molecule 11: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily D member 1

Chain P:



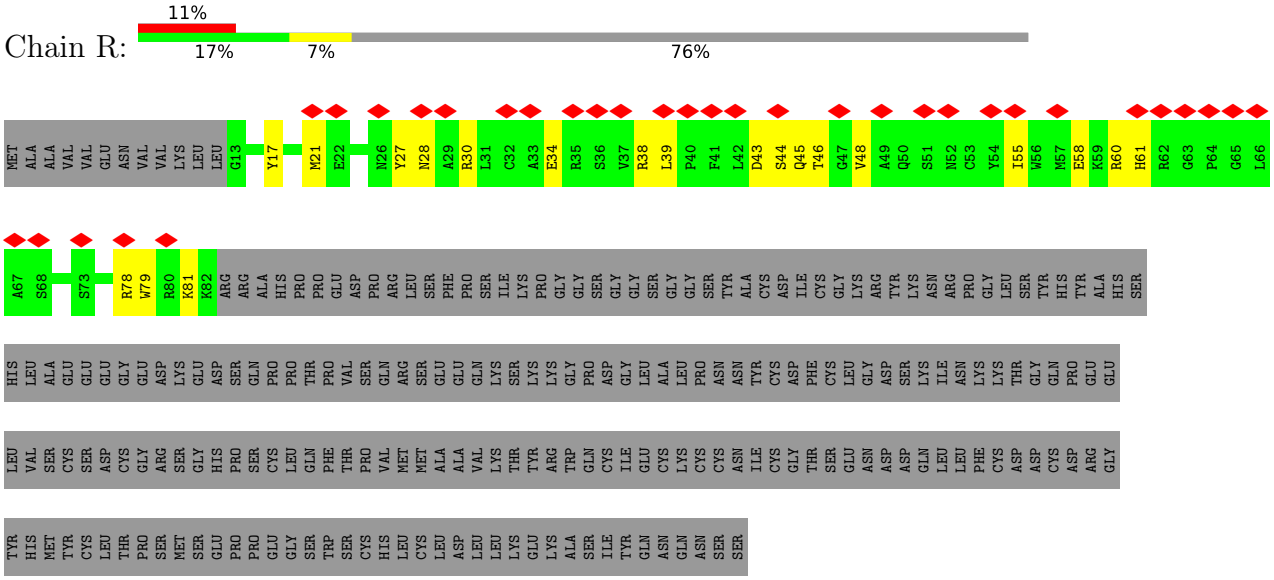
• Molecule 12: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily E member 1

Chain Q:



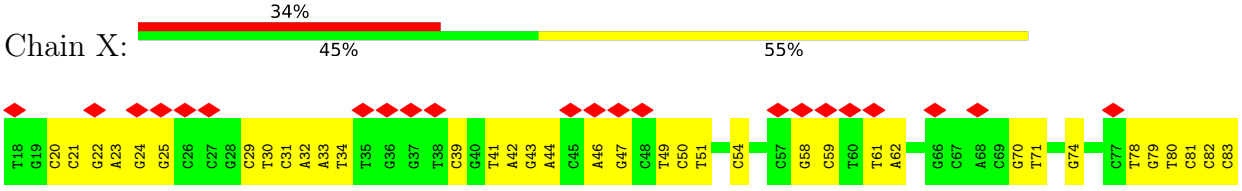
• Molecule 13: Zinc finger protein ubi-d4

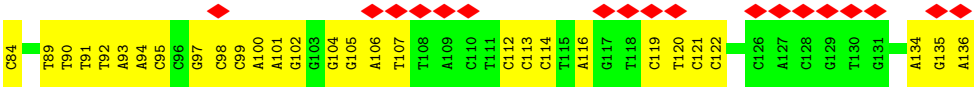
Chain R:



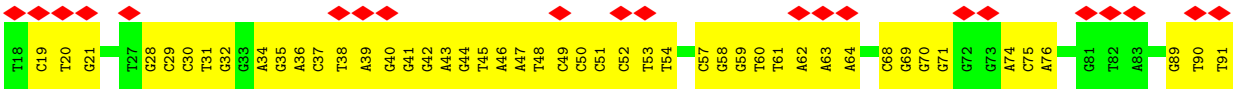
• Molecule 14: DNA (119-MER)

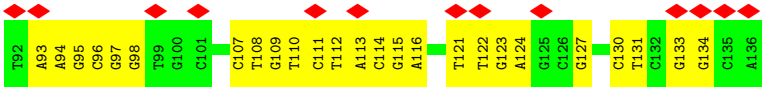
Chain X:





• Molecule 15: DNA (119-MER)





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	320658	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.306	Depositor
Minimum map value	-1.288	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.107	Depositor
Recommended contour level	0.48	Depositor
Map size (Å)	532.48, 532.48, 532.48	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.74	0/747	0.67	0/1001
1	E	0.74	0/747	0.67	0/1001
2	B	0.78	0/629	0.70	0/843
2	F	0.81	0/621	0.77	0/832
3	C	0.73	0/735	0.68	0/993
3	G	0.72	0/736	0.66	0/993
4	D	0.74	0/693	0.64	0/934
4	H	0.75	0/711	0.62	0/957
5	I	0.51	0/4682	0.75	0/6281
6	J	0.46	0/2667	0.67	0/3615
7	K	0.42	0/2535	0.62	0/3436
8	L	0.32	0/3739	0.46	0/5070
9	M	0.37	0/2317	0.52	0/3129
10	N	0.34	0/2158	0.46	0/2908
10	O	0.33	0/2692	0.46	0/3646
11	P	0.31	0/2055	0.45	0/2764
12	Q	0.29	0/871	0.45	0/1168
13	R	0.36	0/595	0.47	0/799
14	X	0.98	0/2715	1.05	0/4184
15	Y	0.97	0/2757	0.99	0/4257
All	All	0.59	0/35402	0.69	0/48811

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	739	0	778	17	0
1	E	739	0	778	17	0
2	B	622	0	660	11	0
2	F	614	0	656	14	0
3	C	726	0	761	12	0
3	G	727	0	768	31	0
4	D	682	0	697	10	0
4	H	700	0	716	11	0
5	I	4606	0	4726	197	0
6	J	2612	0	2557	71	0
7	K	2482	0	2432	71	0
8	L	3670	0	3724	85	0
9	M	2277	0	2248	84	0
10	N	2120	0	2116	80	0
10	O	2632	0	2606	87	0
11	P	2015	0	2046	68	0
12	Q	860	0	864	30	0
13	R	580	0	557	19	0
14	X	2424	0	1335	69	0
15	Y	2455	0	1334	85	0
16	L	1	0	0	0	0
All	All	34283	0	32359	904	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 14.

The worst 5 of 904 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)
3:G:74:LYS:HZ1	9:M:195:ILE:HG21	1.08	1.16
3:G:74:LYS:NZ	9:M:195:ILE:HG21	1.68	1.05
3:G:74:LYS:NZ	9:M:232:THR:HG23	1.74	1.02
6:J:305:PRO:O	6:J:308:LEU:HB2	1.61	1.00
6:J:248:ARG:HA	6:J:248:ARG:CZ	1.92	0.99

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	89/136 (65%)	87 (98%)	2 (2%)	0	100	100
1	E	89/136 (65%)	87 (98%)	2 (2%)	0	100	100
2	B	76/103 (74%)	73 (96%)	3 (4%)	0	100	100
2	F	75/103 (73%)	74 (99%)	1 (1%)	0	100	100
3	C	93/130 (72%)	88 (95%)	5 (5%)	0	100	100
3	G	93/130 (72%)	90 (97%)	3 (3%)	0	100	100
4	D	86/126 (68%)	82 (95%)	4 (5%)	0	100	100
4	H	88/126 (70%)	84 (96%)	4 (4%)	0	100	100
5	I	527/1647 (32%)	445 (84%)	75 (14%)	7 (1%)	12	47
6	J	324/407 (80%)	288 (89%)	34 (10%)	2 (1%)	25	62
7	K	309/375 (82%)	290 (94%)	18 (6%)	1 (0%)	41	74
8	L	456/1295 (35%)	434 (95%)	22 (5%)	0	100	100
9	M	273/336 (81%)	263 (96%)	10 (4%)	0	100	100
10	N	253/1214 (21%)	247 (98%)	6 (2%)	0	100	100
10	O	317/1214 (26%)	304 (96%)	13 (4%)	0	100	100
11	P	233/515 (45%)	220 (94%)	13 (6%)	0	100	100
12	Q	103/411 (25%)	96 (93%)	7 (7%)	0	100	100
13	R	68/292 (23%)	61 (90%)	7 (10%)	0	100	100
All	All	3552/8696 (41%)	3313 (93%)	229 (6%)	10 (0%)	44	74

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	I	811	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	I	874	ARG
5	I	1050	TYR
5	I	1162	GLY
7	K	288	ASP

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	77/110 (70%)	71 (92%)	6 (8%)	12 42
1	E	77/110 (70%)	71 (92%)	6 (8%)	12 42
2	B	64/79 (81%)	63 (98%)	1 (2%)	62 80
2	F	63/79 (80%)	63 (100%)	0	100 100
3	C	73/100 (73%)	73 (100%)	0	100 100
3	G	73/100 (73%)	73 (100%)	0	100 100
4	D	74/104 (71%)	74 (100%)	0	100 100
4	H	76/104 (73%)	76 (100%)	0	100 100
5	I	501/1422 (35%)	459 (92%)	42 (8%)	11 40
6	J	287/348 (82%)	272 (95%)	15 (5%)	23 55
7	K	270/318 (85%)	260 (96%)	10 (4%)	34 61
8	L	418/1117 (37%)	415 (99%)	3 (1%)	84 91
9	M	252/294 (86%)	248 (98%)	4 (2%)	62 80
10	N	222/1030 (22%)	222 (100%)	0	100 100
10	O	282/1030 (27%)	279 (99%)	3 (1%)	73 85
11	P	223/442 (50%)	220 (99%)	3 (1%)	69 83
12	Q	98/361 (27%)	98 (100%)	0	100 100
13	R	59/253 (23%)	59 (100%)	0	100 100
All	All	3189/7401 (43%)	3096 (97%)	93 (3%)	45 66

5 of 93 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	J	71	ASP
7	K	206	ARG
6	J	80	GLU
6	J	293	TYR
7	K	285	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 57 such sidechains are listed below:

Mol	Chain	Res	Type
8	L	1858	HIS
13	R	61	HIS
10	N	604	GLN
12	Q	268	ASN
11	P	432	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)

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)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

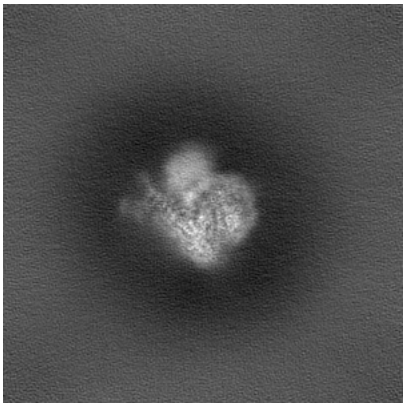
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-0974. These allow visual inspection of the internal detail of the map and identification of artifacts.

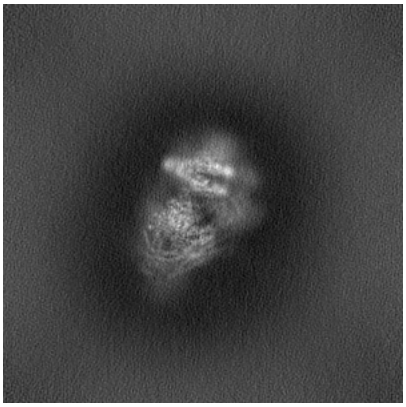
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

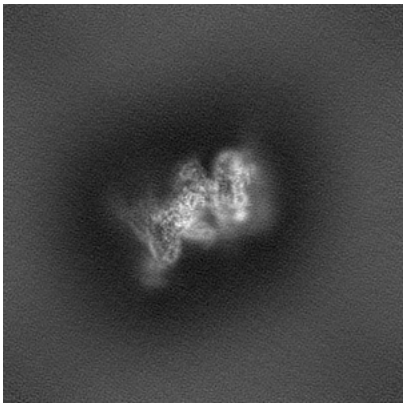
6.1.1 Primary map



X



Y

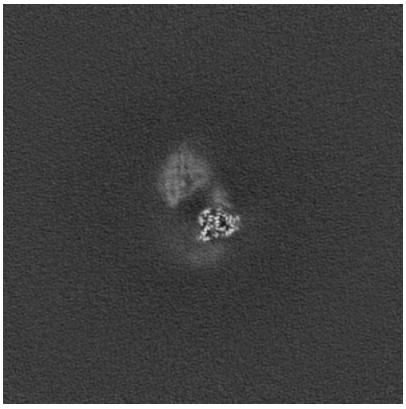


Z

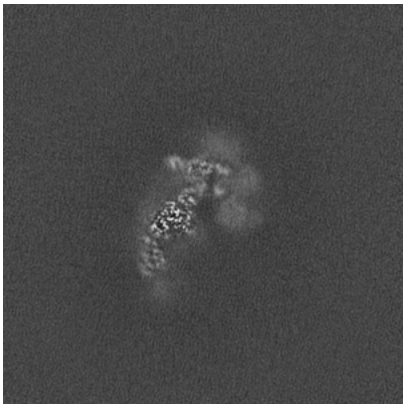
The images above show the map projected in three orthogonal directions.

6.2 Central slices

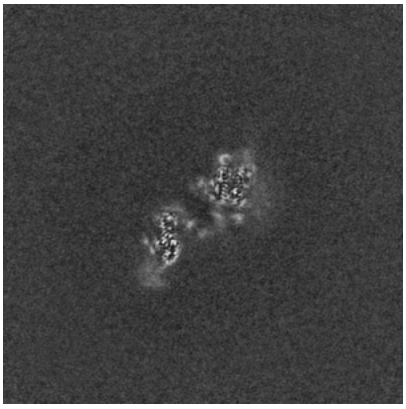
6.2.1 Primary map



X Index: 256



Y Index: 256

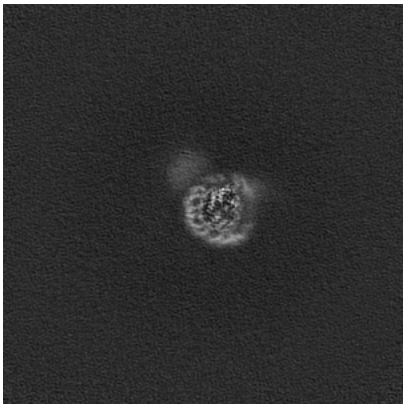


Z Index: 256

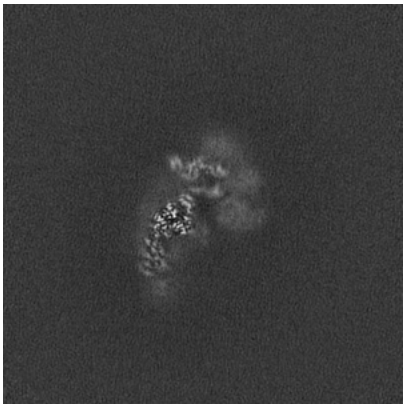
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

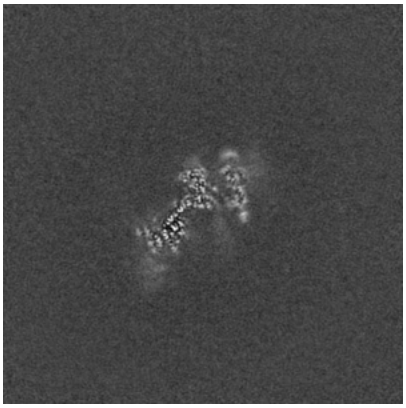
6.3.1 Primary map



X Index: 304



Y Index: 253



Z Index: 238

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 0.48. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

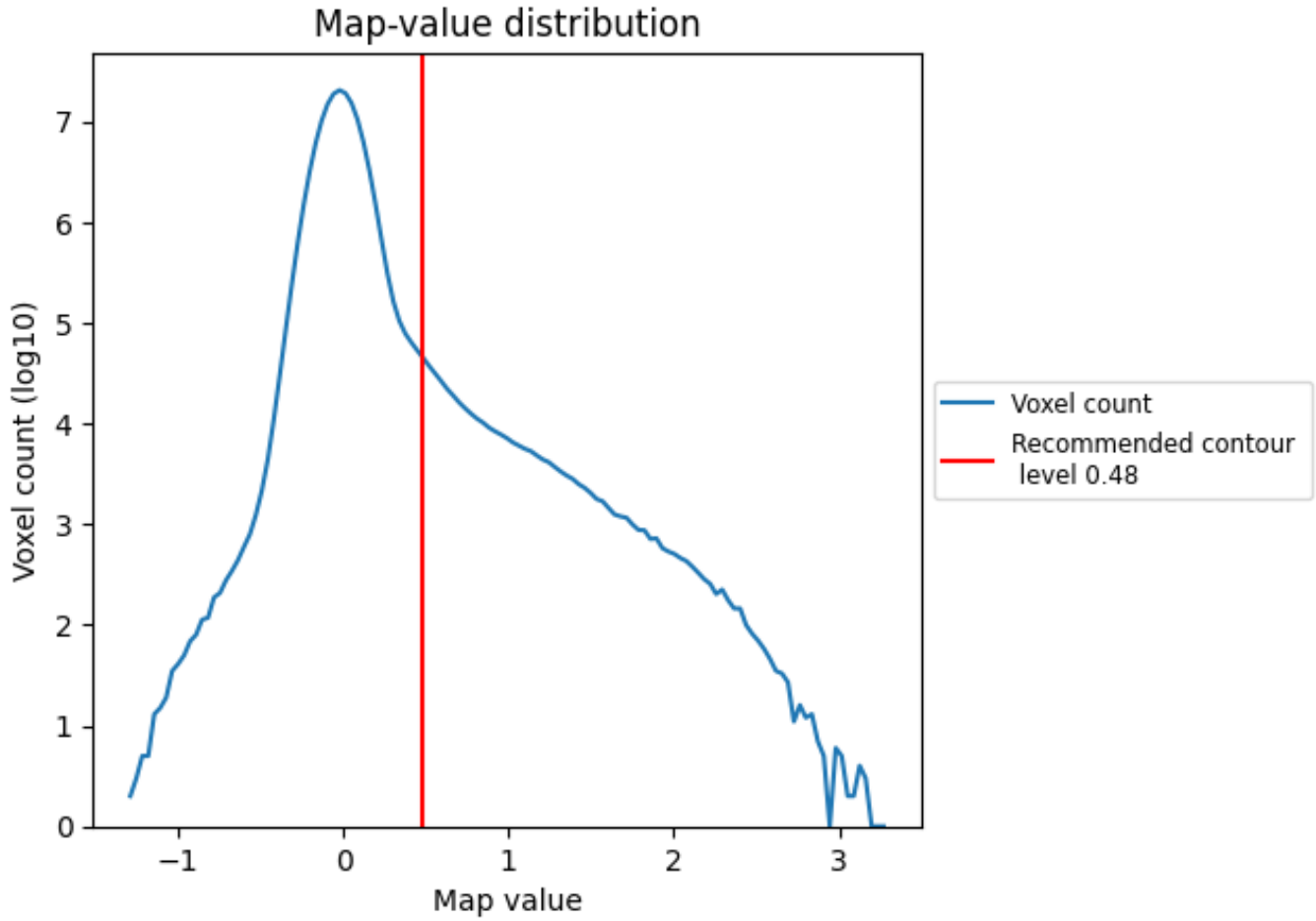
6.5 Mask visualisation (i)

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

7 Map analysis

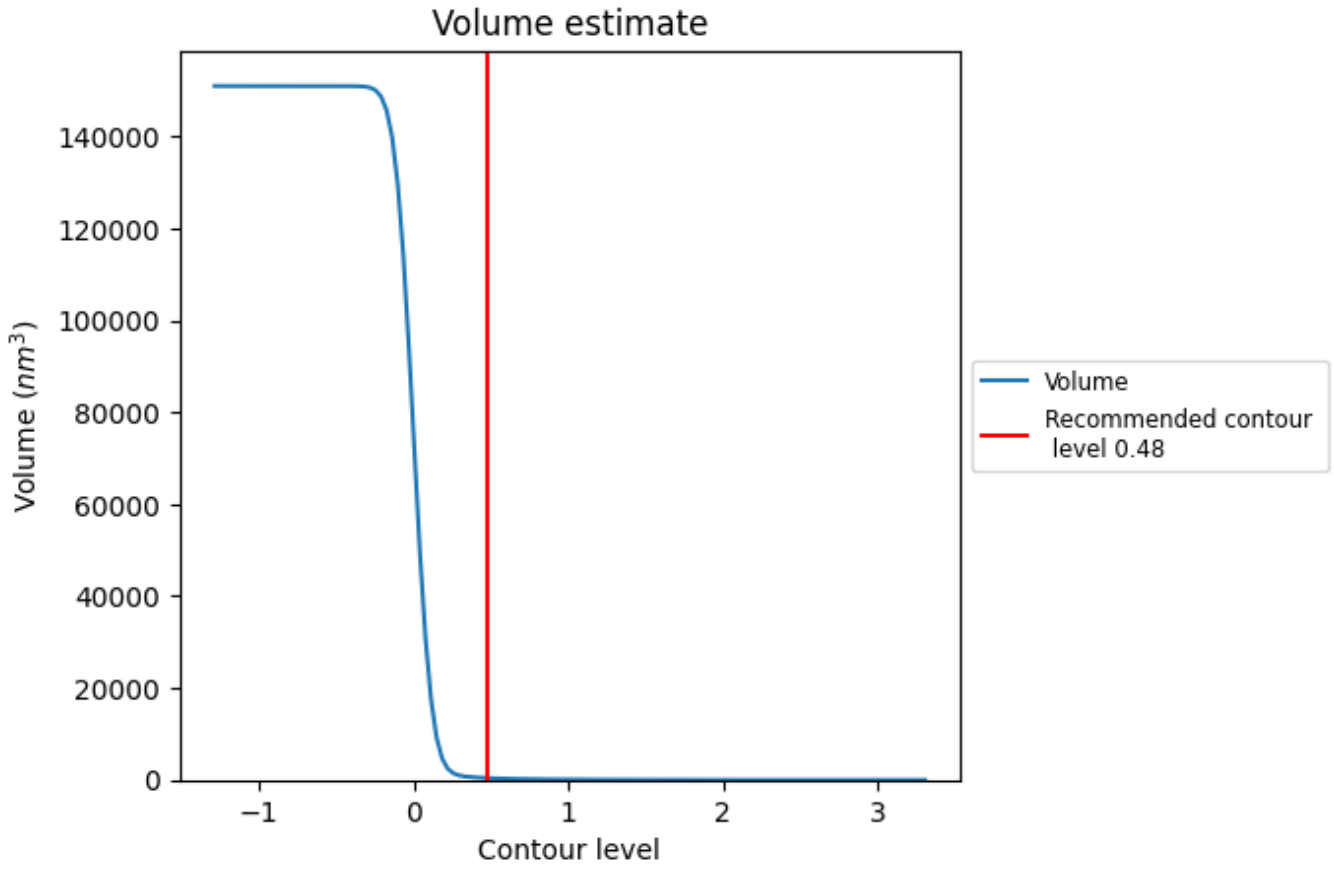
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

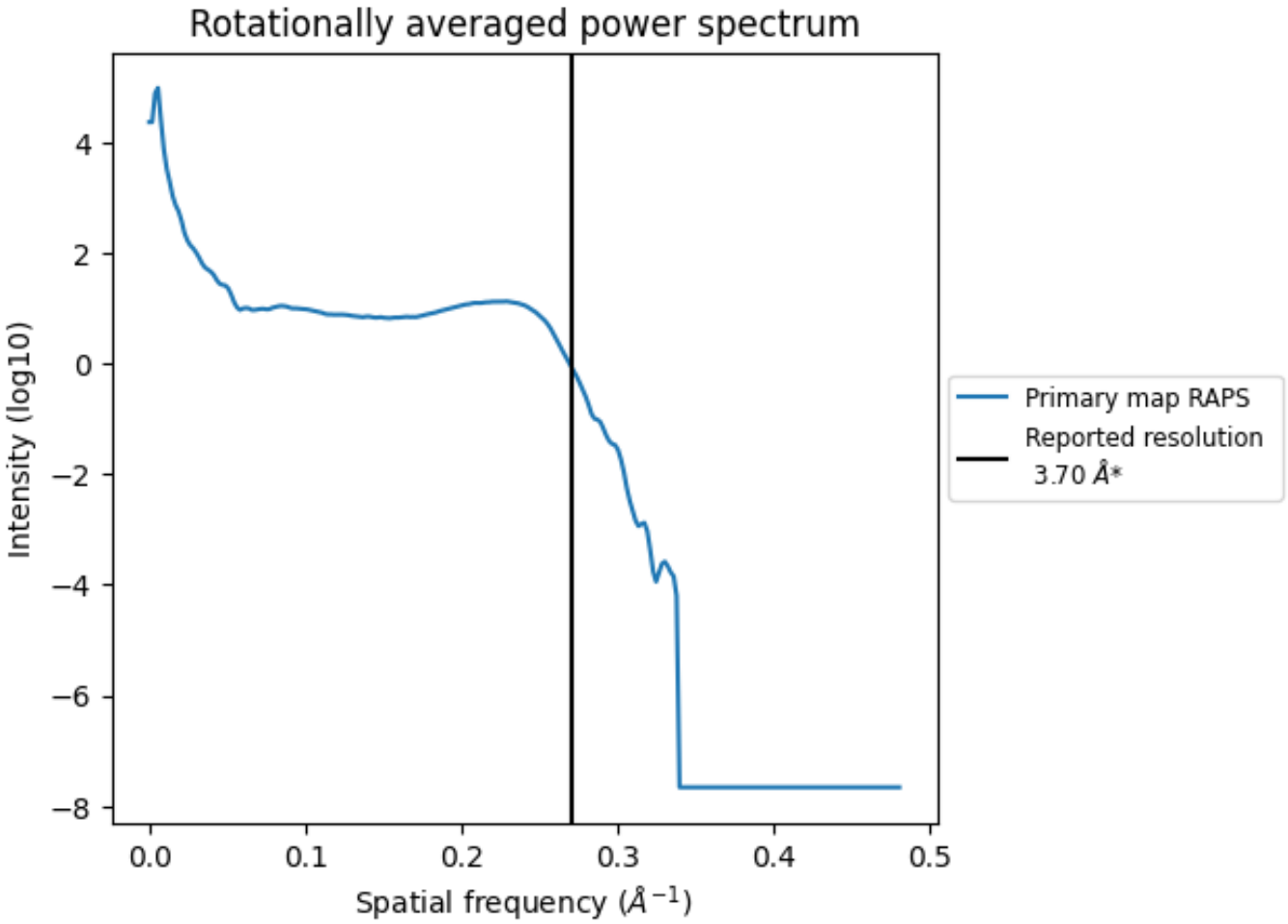
7.2 Volume estimate



The volume at the recommended contour level is 404 nm^3; this corresponds to an approximate mass of 365 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)



*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

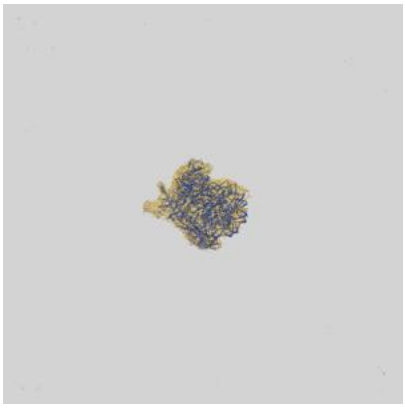
8 Fourier-Shell correlation (i)

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

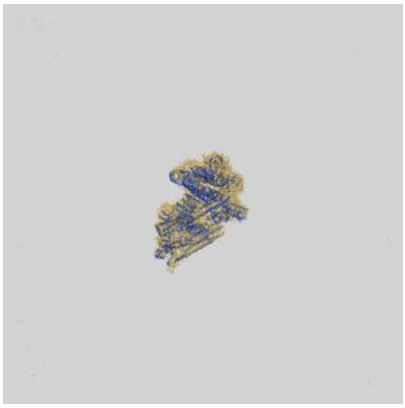
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-0974 and PDB model 6LTJ. Per-residue inclusion information can be found in section 3 on page 8.

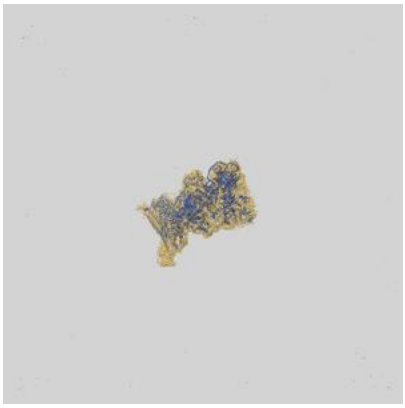
9.1 Map-model overlay



X



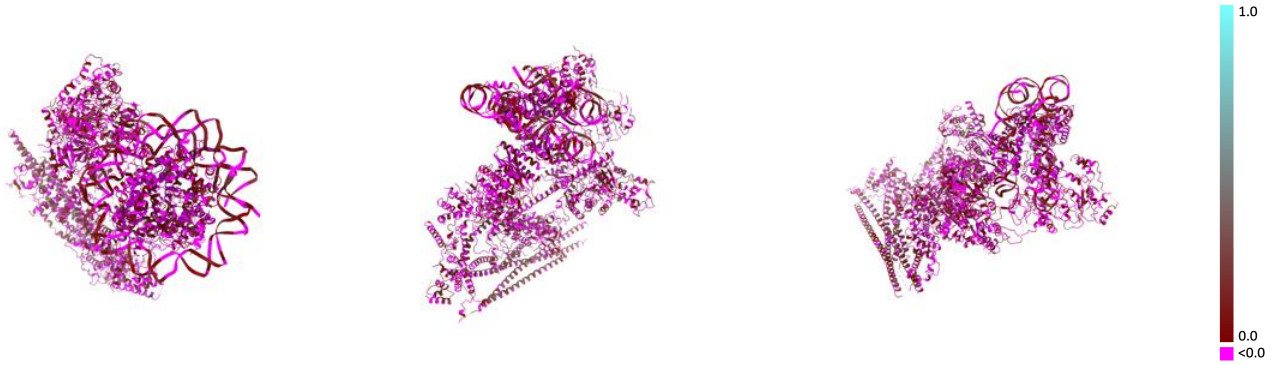
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.48 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.

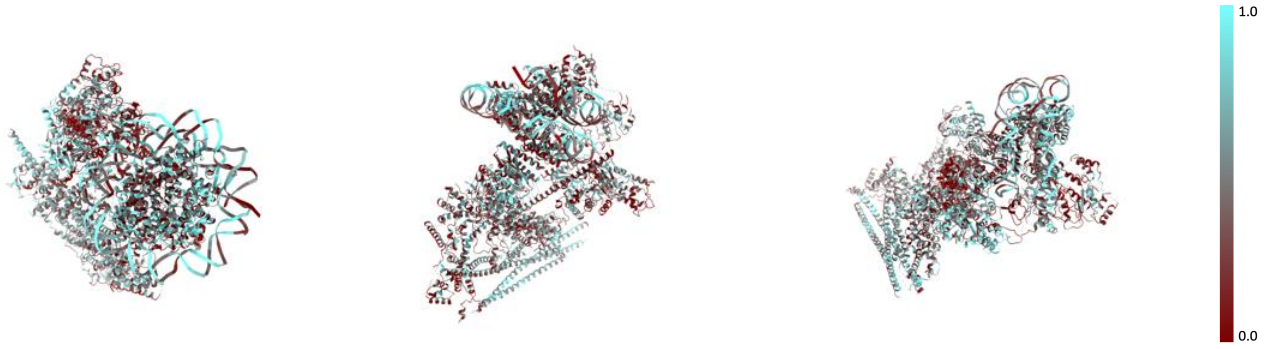
9.2 Q-score mapped to coordinate model



X Y Z

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.

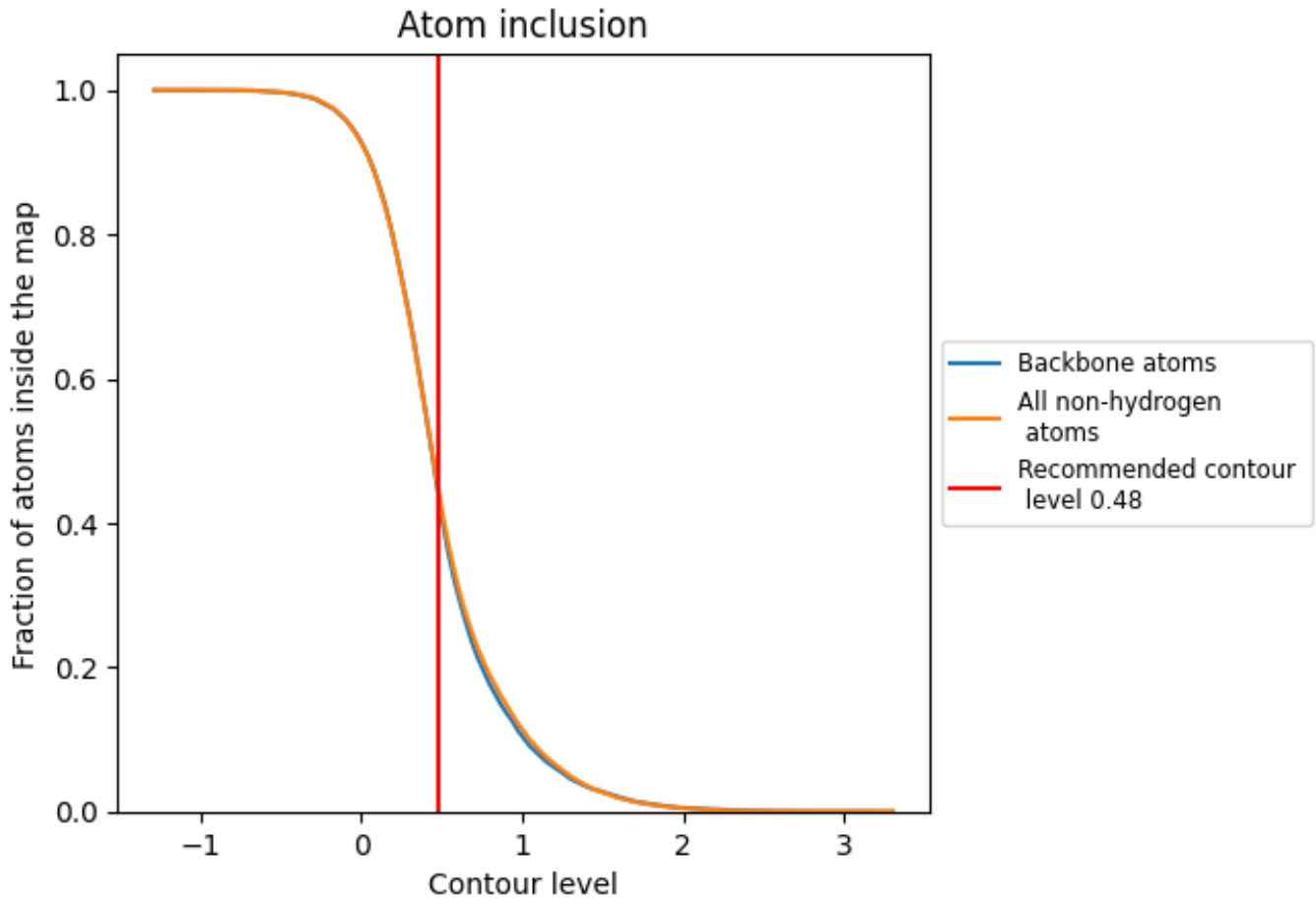
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.48).

9.4 Atom inclusion (i)



At the recommended contour level, 44% of all backbone atoms, 44% 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 (0.48) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4426	0.0070
A	0.4516	-0.0070
B	0.4967	-0.0090
C	0.5021	-0.0140
D	0.4633	-0.0280
E	0.4614	-0.0760
F	0.4678	0.0050
G	0.4389	-0.0310
H	0.3810	-0.0530
I	0.2940	-0.0020
J	0.5415	0.0100
K	0.2803	0.0300
L	0.3891	-0.0050
M	0.4574	-0.0130
N	0.4206	0.0210
O	0.5194	0.0290
P	0.4481	0.0110
Q	0.5507	0.0880
R	0.4299	-0.0440
X	0.5644	0.0270
Y	0.5845	0.0320