wwPDB EM Validation Summary Report

Nov 19, 2022 – 08:35 pm GMT

PDB ID	:	6EM1
EMDB ID	:	EMD-3893
Title	:	State C (Nsa1-TAP Flag-Ytm1) - Visualizing the assembly pathway of nucleolar pre-60S ribosomes
Authors	:	Kater, L.; Cheng, J.; Barrio-Garcia, C.; Hurt, E.; Beckmann, R.
Deposited on	:	2017-10-01
Resolution	:	3.60 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 ⓘ 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:

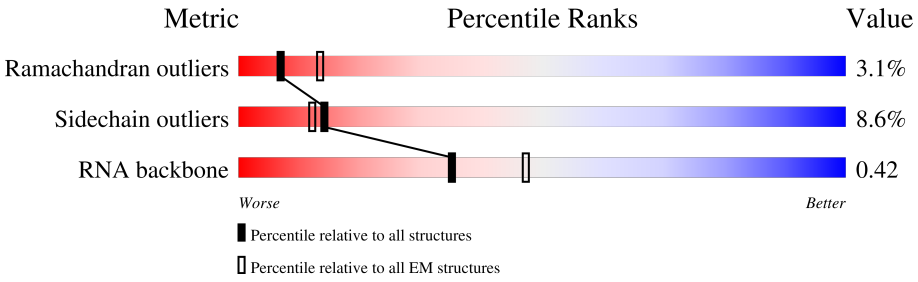
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 3.60 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	x	295	72% 17% 9%
2	F	244	91% 8%
3	3	306	44% 12% 43%
4	4	278	6% 64% 14% 22%
5	5	463	7% 78% 5% 17%
6	A	291	32% 45% 50%
7	b	647	37% 59% 6% 35%
8	J	427	13% 15% 85%

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Mol	Chain	Length	Quality of chain
9	r	261	6% 26% 72%
10	s	520	5% 95%
11	u	199	25% 55% 42%
12	v	231	52% 5% 44%
13	W	236	58% 93% 5%
14	y	245	47% 88% 8%
15	z	106	47% 52% 48%
16	B	387	9% 78% 8% 14%
17	C	362	80% 15% 5%
18	e	130	83% 13%
19	E	176	81% 5% 14%
20	f	107	86% 12%
21	G	256	54% 9% 38%
22	h	120	5% 88% 10%
23	H	191	9% 91% 8%
24	i	100	10% 64% 10% 26%
25	j	88	69% 10% 19%
26	L	199	49% 6% 46%
27	M	138	92% 5%
28	N	204	7% 74% 13% 13%
29	O	199	42% 47% 10%
30	P	184	65% 9% 26%
31	Q	186	65% 6% 30%
32	S	172	5% 87% 11%
33	V	137	58% 90% 8%

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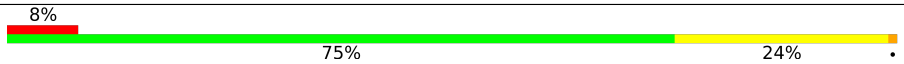
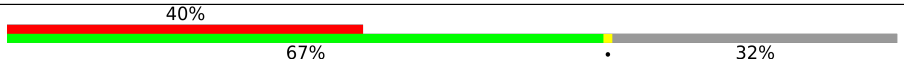
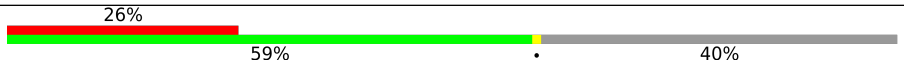
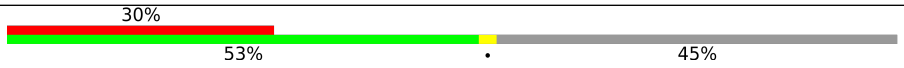
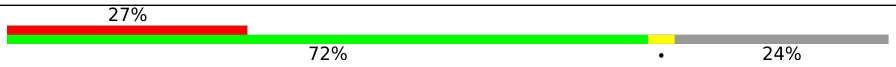
Mol	Chain	Length	Quality of chain
34	Y	127	
35	1	3396	
36	2	158	
37	6	232	
38	K	376	
39	m	807	
40	D	505	
41	o	220	
42	n	605	
43	t	322	

2 Entry composition (i)

There are 44 unique types of molecules in this entry. The entry contains 99980 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 Ribosome production factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	x	267	2268	1444	413	407	4	0	0

- Molecule 2 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	F	241	1936	1246	351	338	1	0	0

- Molecule 3 is a protein called Protein MAK16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	3	173	1434	901	274	250	9	0	0

- Molecule 4 is a protein called Ribosomal RNA-processing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	4	217	1853	1208	319	323	3	0	0

- Molecule 5 is a protein called Ribosome biogenesis protein NSA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	5	385	3055	1957	514	573	11	0	0

- Molecule 6 is a protein called Ribosome biogenesis protein BRX1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	A	145	1211	780	218	210	3	0	0

- Molecule 7 is a protein called Nucleolar GTP-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	b	421	Total	C	N	O	S	0	0
			3410	2180	585	627	18		

- Molecule 8 is a protein called rRNA-processing protein EBP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	66	Total	C	N	O	S	0	0
			549	341	97	110	1		

- Molecule 9 is a protein called Ribosome biogenesis protein NSA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	r	73	Total	C	N	O	S	0	0
			628	388	133	106	1		

- Molecule 10 is a protein called Nuclear GTP-binding protein NUG1.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	s	27	Total	C	N	O	0	0
			224	136	51	37		

- Molecule 11 is a protein called Ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	u	116	Total	C	N	O	S	0	0
			976	612	200	155	9		

- Molecule 12 is a protein called Nucleolar protein 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	v	130	Total	C	N	O	S	0	0
			1087	678	211	195	3		

- Molecule 13 is a protein called Ribosome assembly factor MRT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	W	232	Total	C	N	O	S	0	0
			1870	1184	321	360	5		

- Molecule 14 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	y	225	Total	C	N	O	S	0	0
			1701	1056	295	343	7		

- Molecule 15 is a protein called UPF0642 protein YBL028C.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	z	55	Total	C	N	O	0	0
			444	273	88	83		

- Molecule 16 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	B	333	Total	C	N	O	S	0	0
			2646	1680	490	470	6		

- Molecule 17 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	C	343	Total	C	N	O	S	0	0
			2611	1643	499	466	3		

- Molecule 18 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	e	125	Total	C	N	O	S	0	0
			1009	641	203	164	1		

- Molecule 19 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	E	151	Total	C	N	O	S	0	0
			1205	780	215	209	1		

- Molecule 20 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	f	106	Total	C	N	O	S	0	0
			850	540	165	144	1		

- Molecule 21 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	G	159	Total	C	N	O	S	0	0
			1231	794	209	226	2		

- Molecule 22 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	h	119	Total	C	N	O	S	0	0
			969	615	186	167	1		

- Molecule 23 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	H	190	Total	C	N	O	S	0	0
			1510	957	273	276	4		

- Molecule 24 is a protein called 60S ribosomal protein L36-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	i	74	Total	C	N	O	S	0	0
			594	367	125	101	1		

- Molecule 25 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	j	71	Total	C	N	O	S	0	0
			566	344	123	94	5		

- Molecule 26 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	L	108	Total	C	N	O	0	0
			864	541	180	143		

- Molecule 27 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	M	134	Total	C	N	O	S	0	0
			1041	668	197	174	2		

- Molecule 28 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	N	177	Total	C	N	O	S	0	0
			1513	948	320	244	1		

- Molecule 29 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	O	197	Total	C	N	O	S	0	0
			1555	1003	289	262	1		

- Molecule 30 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	P	137	Total	C	N	O	0	0
			1062	666	198	198		

- Molecule 31 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Q	131	Total	C	N	O	S	0	0
			1009	645	190	173	1		

- Molecule 32 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	S	170	Total	C	N	O	S	0	0
			1432	922	265	242	3		

- Molecule 33 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	V	126	Total	C	N	O	S	0	0
			936	588	176	165	7		

- Molecule 34 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	Y	125	Total	C	N	O	0	0
			984	620	191	173		

- Molecule 35 is a RNA chain called 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	1	1785	Total	C	N	O	P	0	0
			38221	17064	6918	12454	1785		

- Molecule 36 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	2	158	Total	C	N	O	P	0	0
			3353	1500	586	1109	158		

- Molecule 37 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	6	65	Total	C	N	O	P	0	0
			1370	614	228	463	65		

- Molecule 38 is a protein called Proteasome-interacting protein CIC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	K	257	Total	C	N	O	S	0	0
			2073	1337	341	392	3		

- Molecule 39 is a protein called Ribosome biogenesis protein ERB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	m	161	Total	C	N	O	S	0	0
			1362	867	238	253	4		

- Molecule 40 is a protein called ATP-dependent RNA helicase HAS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	D	194	Total	C	N	O	S	0	0
			1590	1030	268	287	5		

- Molecule 41 is a protein called Ribosome biogenesis protein 15.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	o	133	Total	C	N	O	S	0	0
			1107	716	198	189	4		

- Molecule 42 is a protein called Pescadillo homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	n	334	Total	C	N	O	S	0	0
			2734	1787	457	482	8		

- Molecule 43 is a protein called Ribosome biogenesis protein RLP7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	t	244	Total	C	N	O	S	0	0
			1935	1233	345	354	3		

- Molecule 44 is ZINC ION (three-letter code: ZN) (formula: Zn).

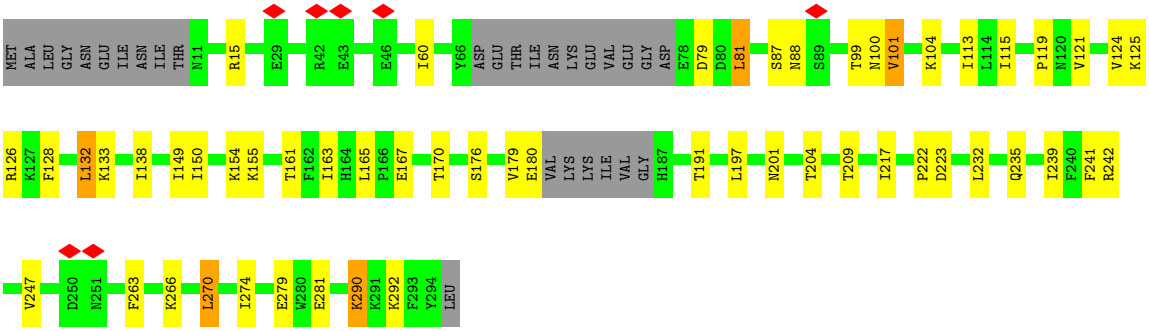
Mol	Chain	Residues	Atoms		AltConf
44	u	1	Total	Zn	0
			1	1	
44	j	1	Total	Zn	0
			1	1	

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: Ribosome production factor 1

Chain x:

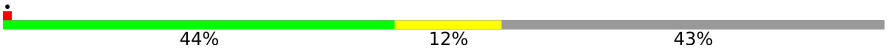


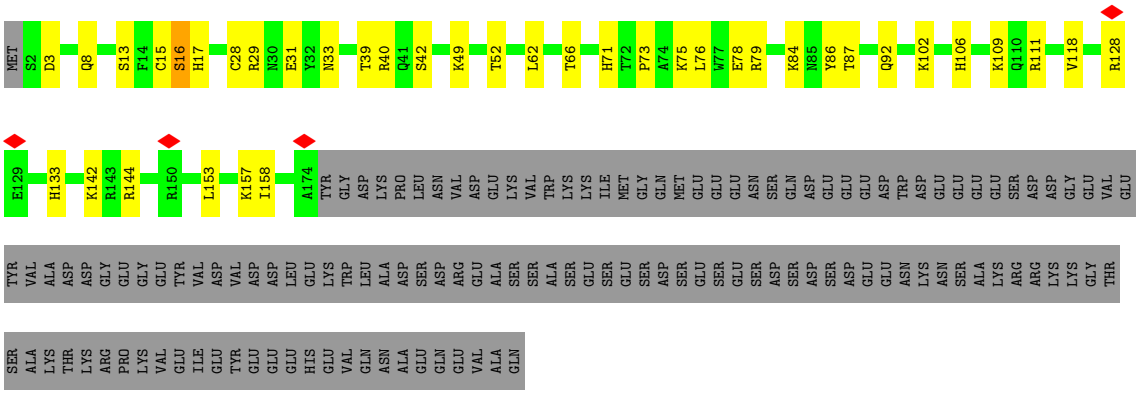
• Molecule 2: 60S ribosomal protein L7-A

Chain F:

• Molecule 3: Protein MAK16

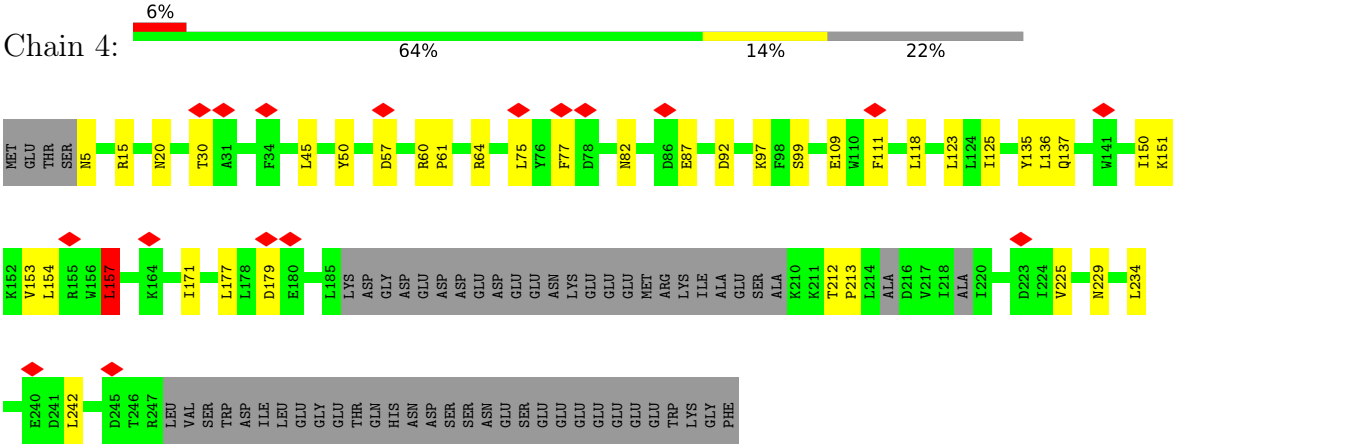
Chain 3:





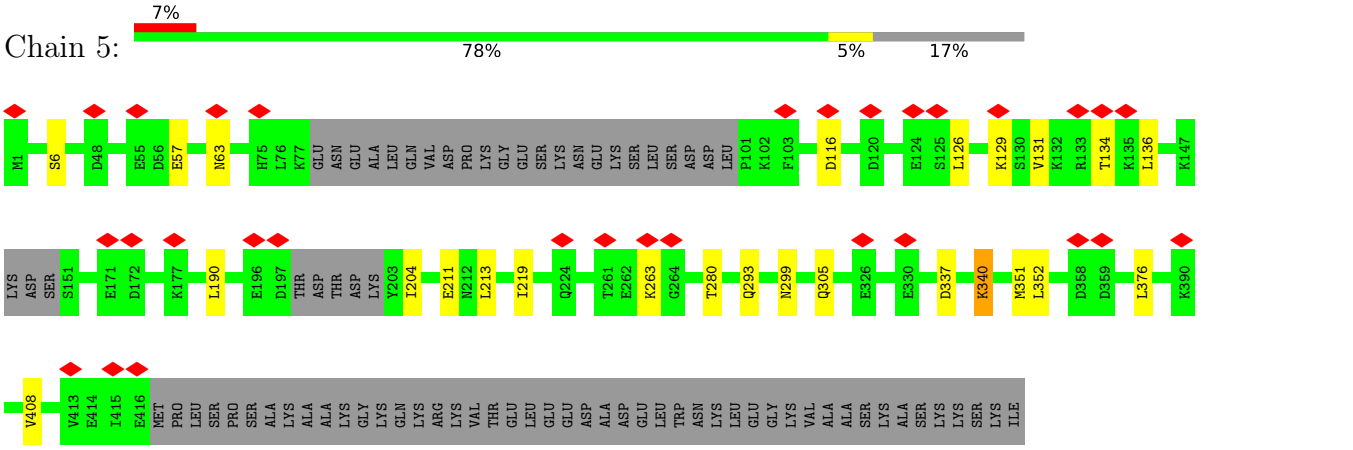
• Molecule 4: Ribosomal RNA-processing protein 1

Chain 4:



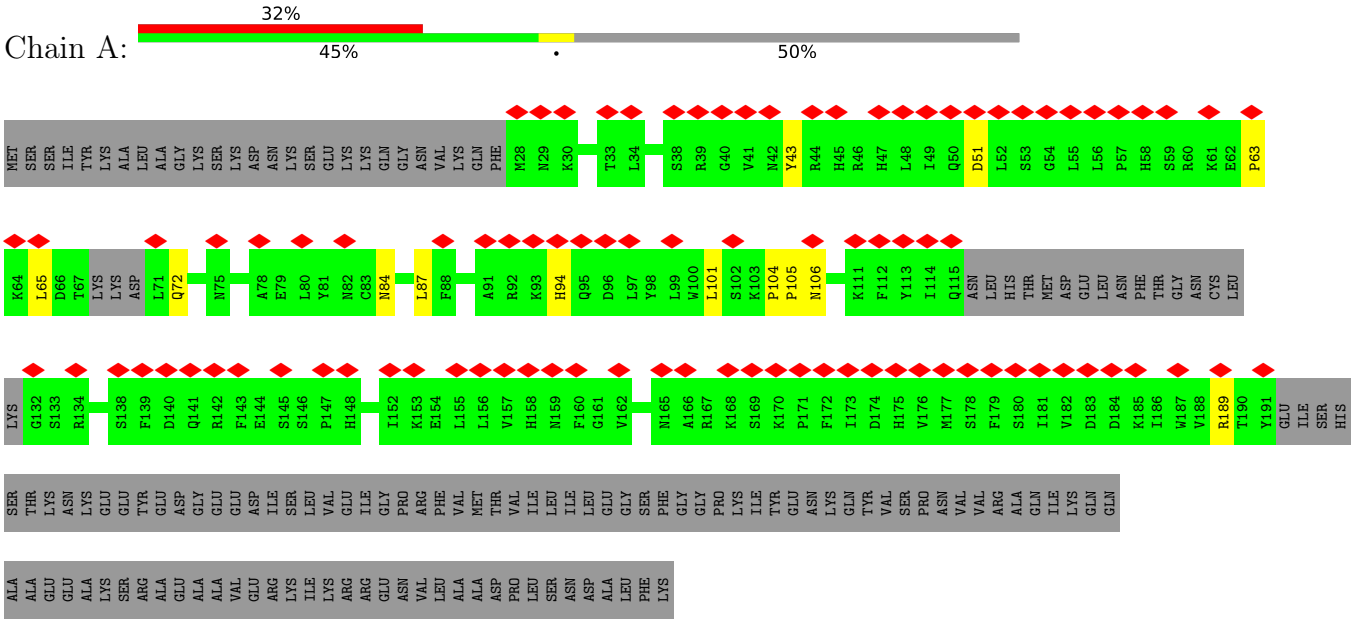
• Molecule 5: Ribosome biogenesis protein NSA1

Chain 5:



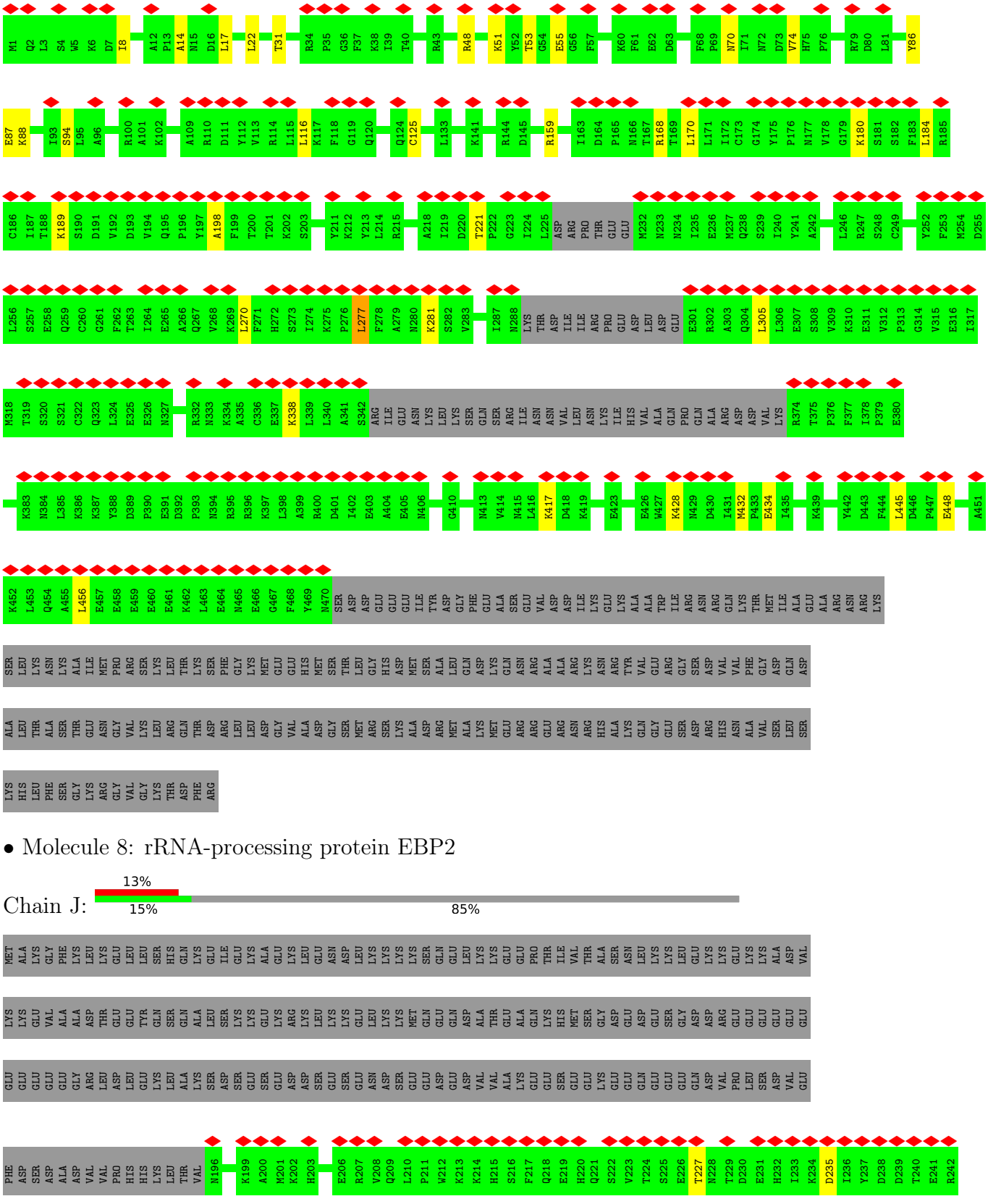
• Molecule 6: Ribosome biogenesis protein BRX1

Chain A:



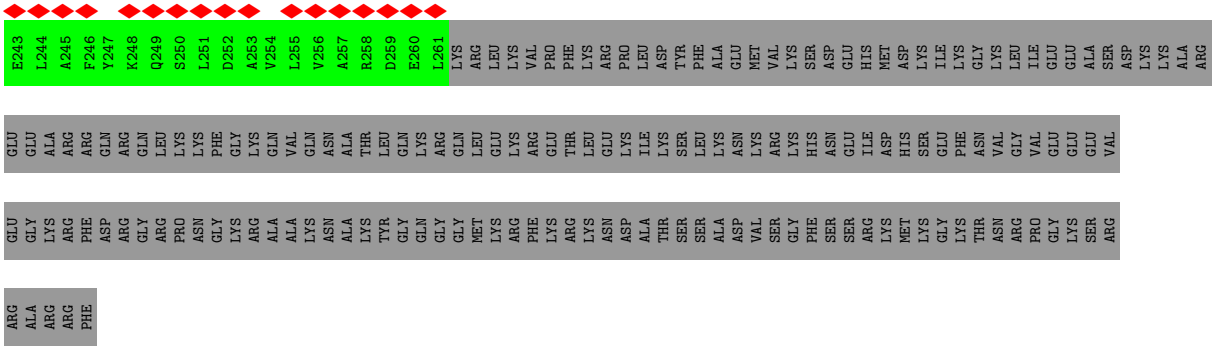
• Molecule 7: Nucleolar GTP-binding protein 1

Chain b:

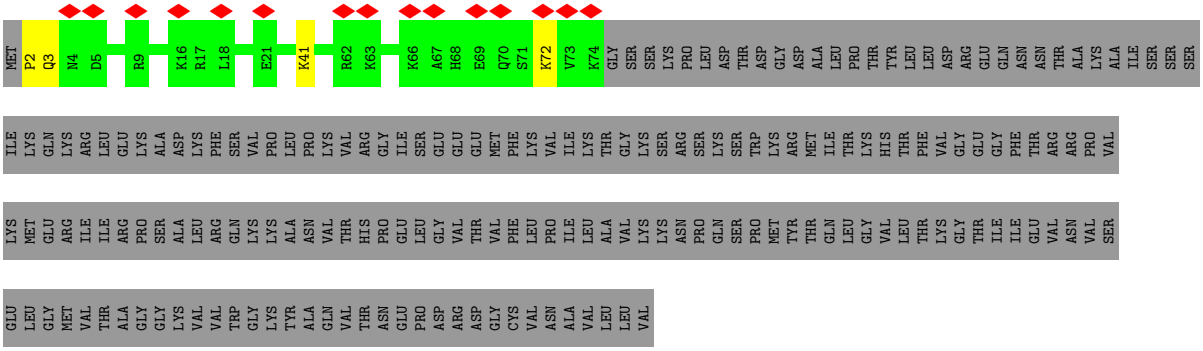


• Molecule 8: rRNA-processing protein EBP2

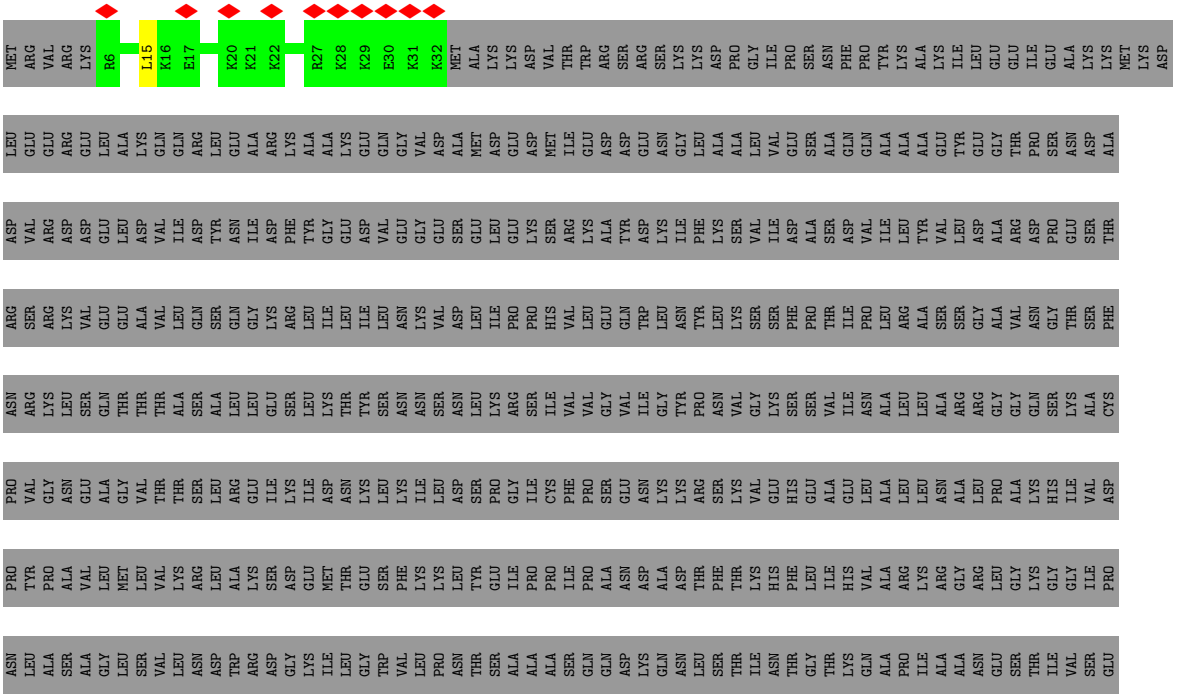
Chain J:

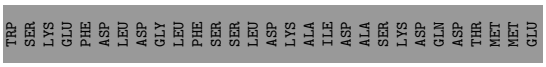


• Molecule 9: Ribosome biogenesis protein NSA2



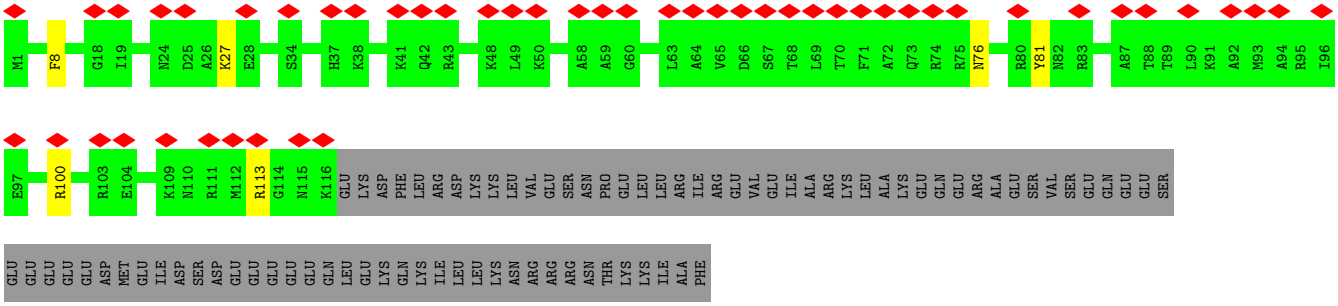
• Molecule 10: Nuclear GTP-binding protein NUG1





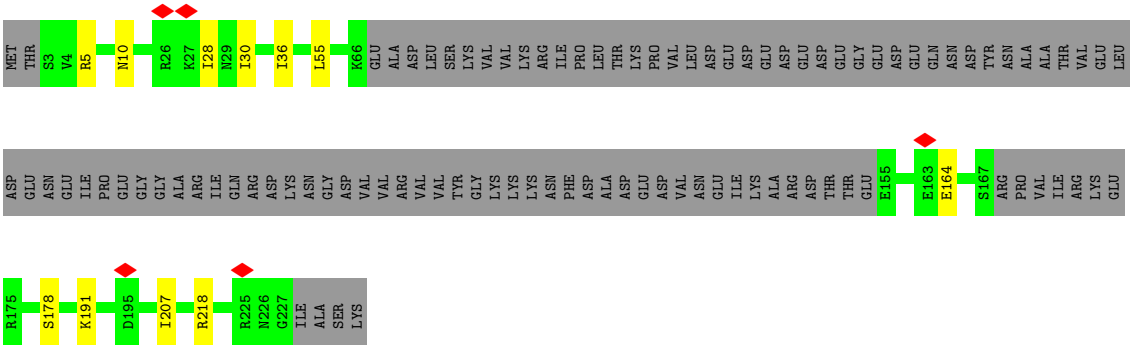
• Molecule 11: Ribosome biogenesis protein RLP24

Chain u:



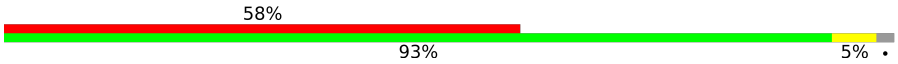
• Molecule 12: Nucleolar protein 16

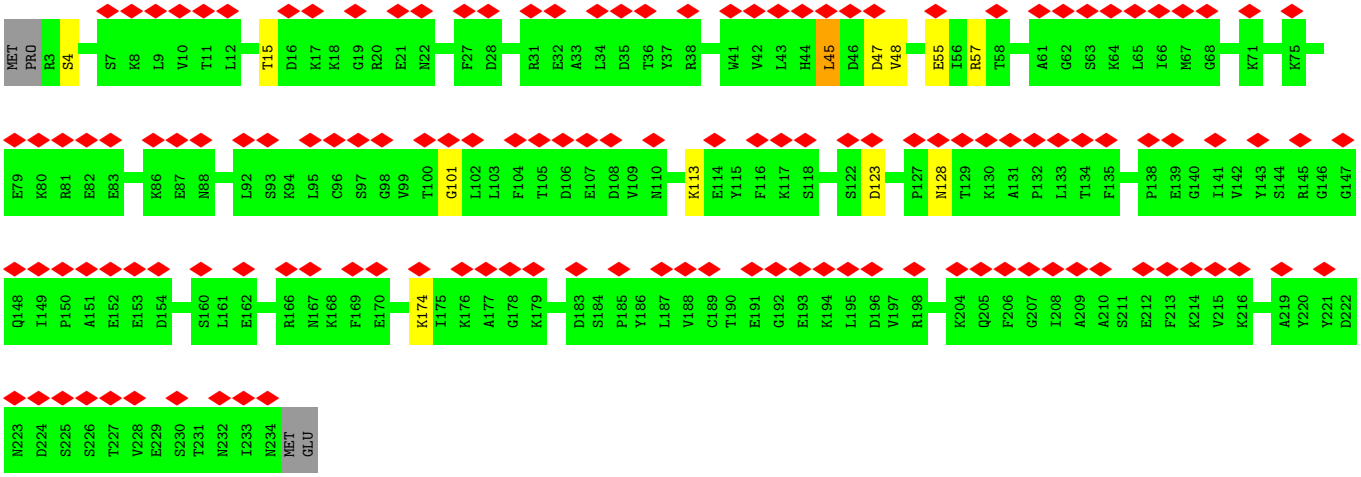
Chain v:



• Molecule 13: Ribosome assembly factor MRT4

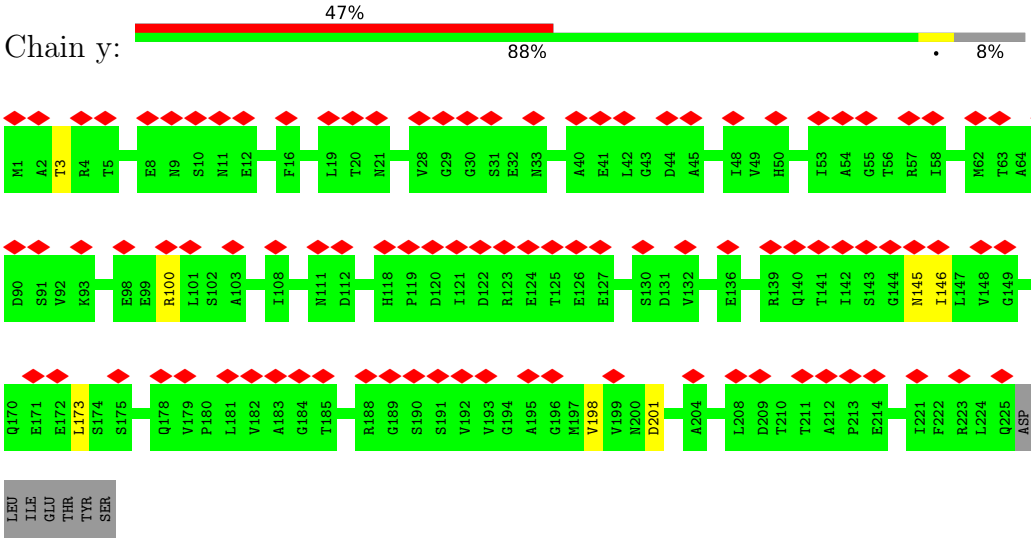
Chain W:





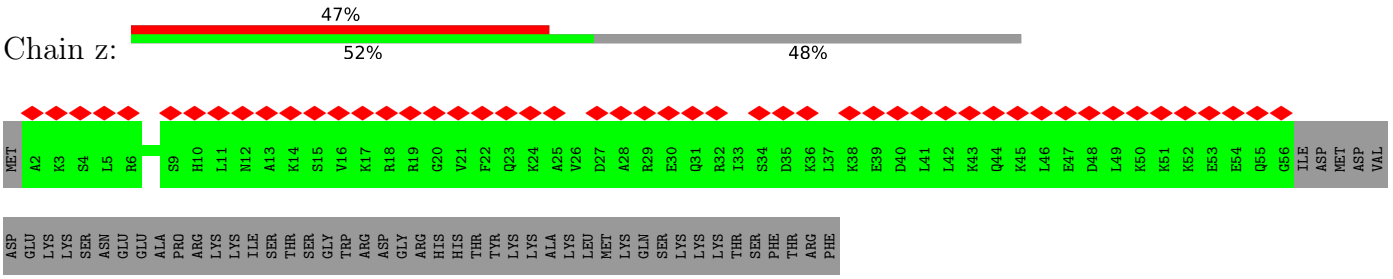
• Molecule 14: Eukaryotic translation initiation factor 6

Chain y:



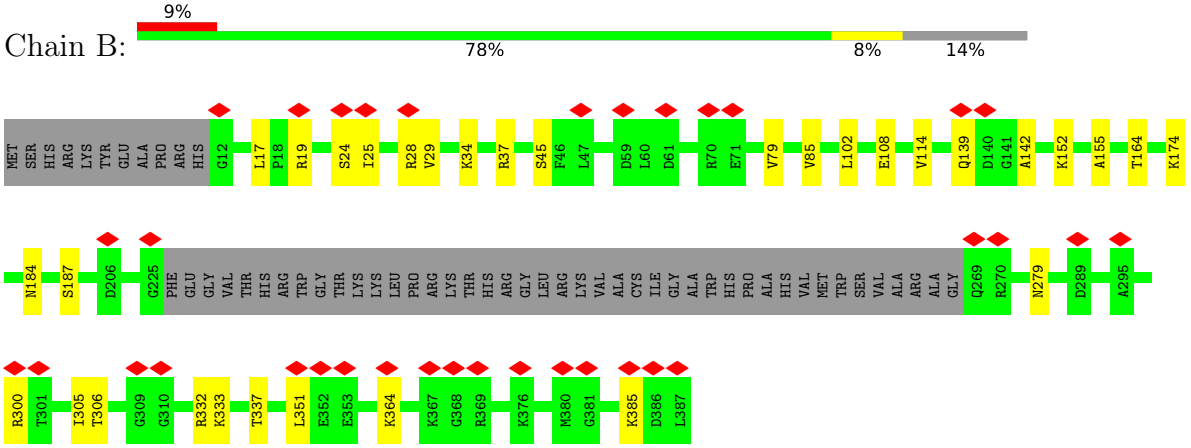
• Molecule 15: UPF0642 protein YBL028C

Chain z:



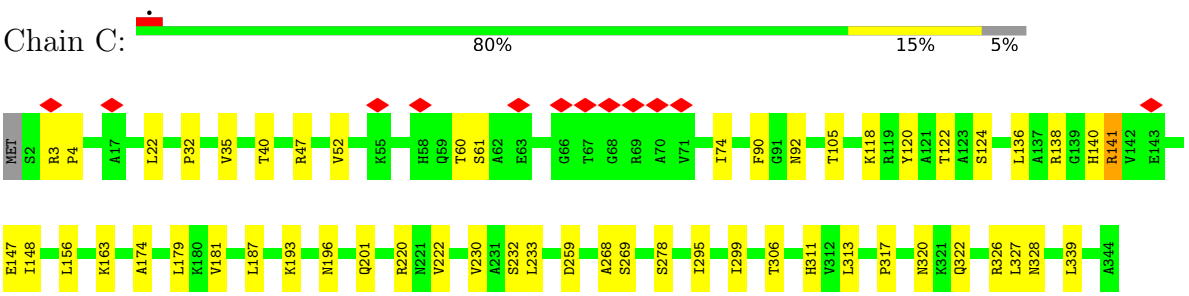
• Molecule 16: 60S ribosomal protein L3

Chain B:



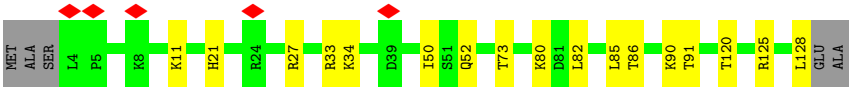
• Molecule 17: 60S ribosomal protein L4-A

Chain C:



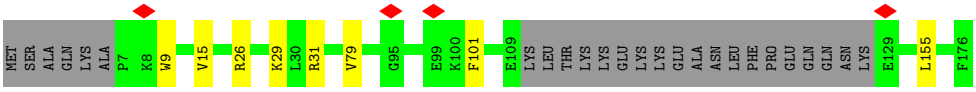
• Molecule 18: 60S ribosomal protein L32

Chain e:



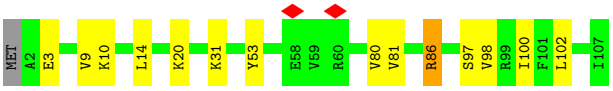
• Molecule 19: 60S ribosomal protein L6-A

Chain E:



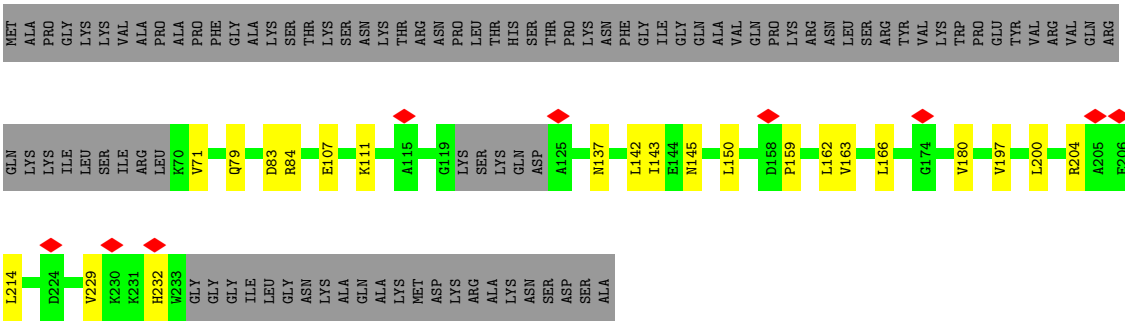
• Molecule 20: 60S ribosomal protein L33-A

Chain f:



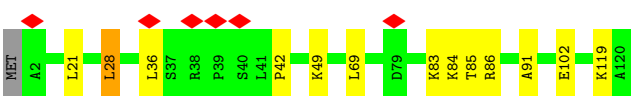
• Molecule 21: 60S ribosomal protein L8-A

Chain G:



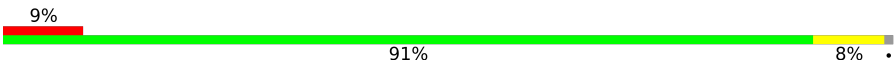
• Molecule 22: 60S ribosomal protein L35-A

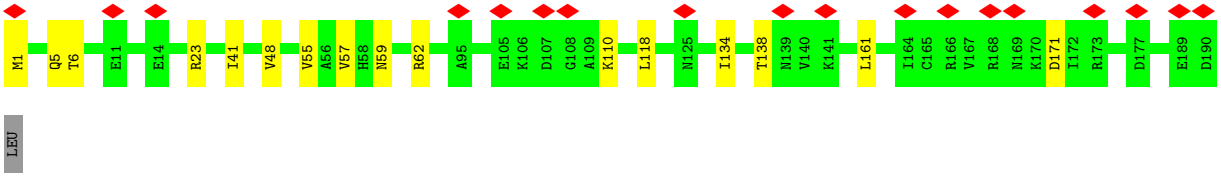
Chain h:



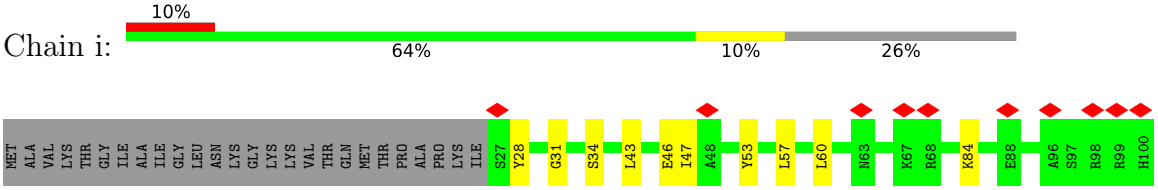
• Molecule 23: 60S ribosomal protein L9-A

Chain H:

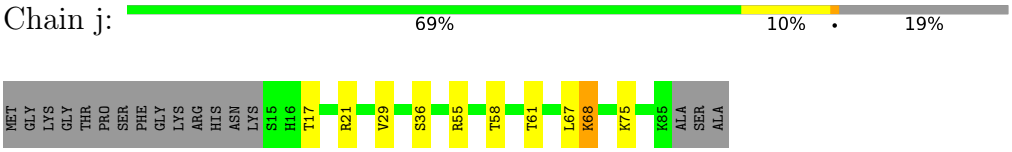




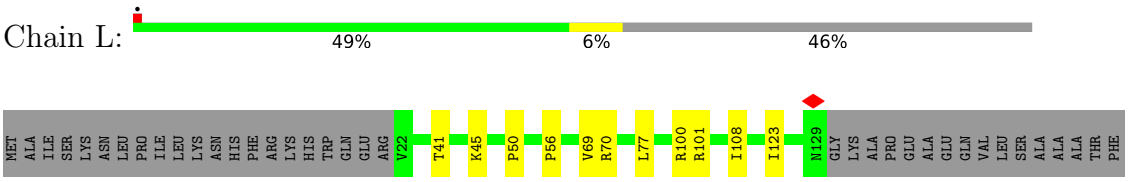
• Molecule 24: 60S ribosomal protein L36-B



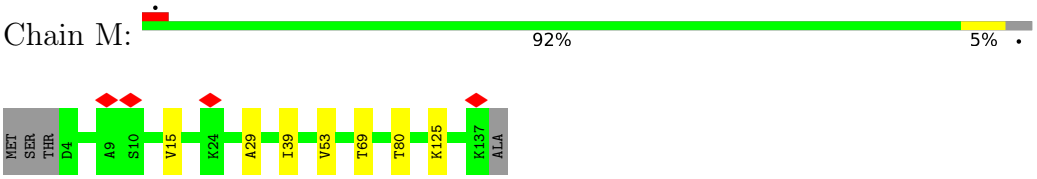
• Molecule 25: 60S ribosomal protein L37-A



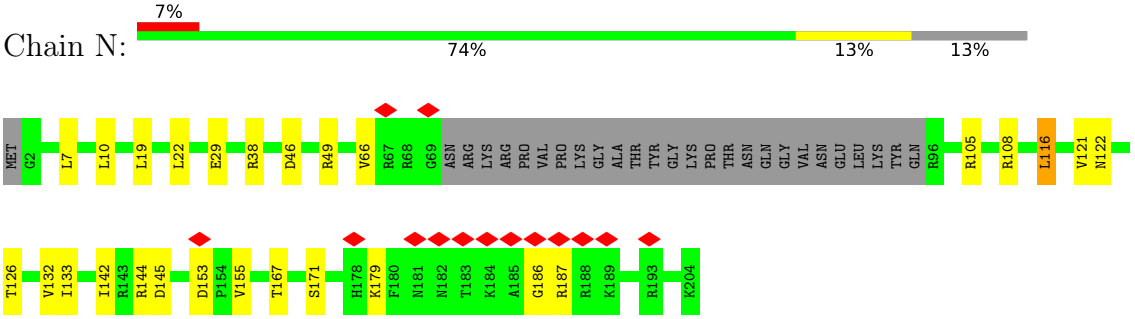
• Molecule 26: 60S ribosomal protein L13-A



• Molecule 27: 60S ribosomal protein L14-A

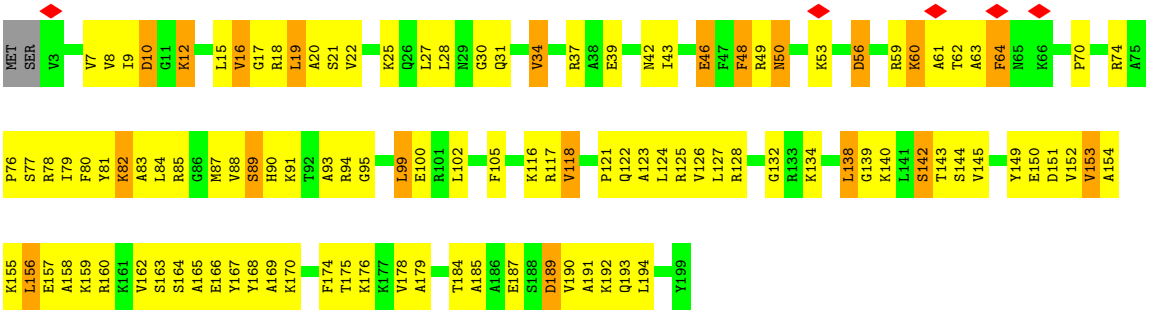


• Molecule 28: 60S ribosomal protein L15-A



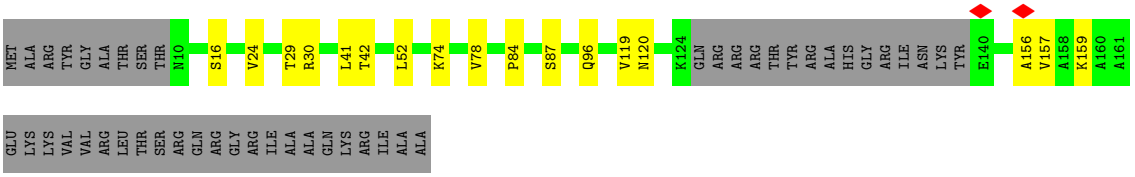
• Molecule 29: 60S ribosomal protein L16-A

Chain O:



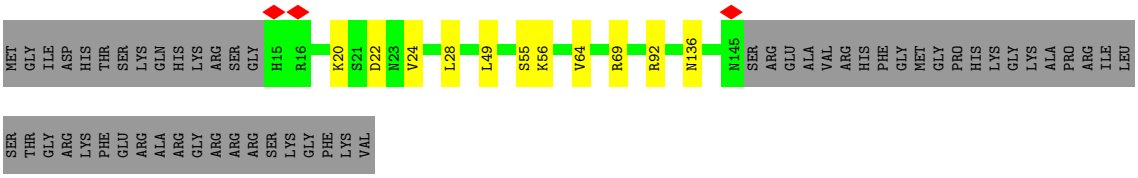
• Molecule 30: 60S ribosomal protein L17-A

Chain P:



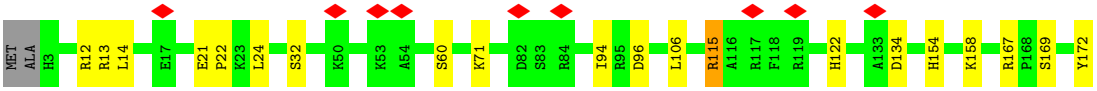
• Molecule 31: 60S ribosomal protein L18-A

Chain Q:



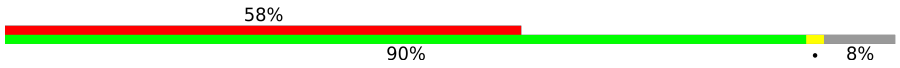
• Molecule 32: 60S ribosomal protein L20-A

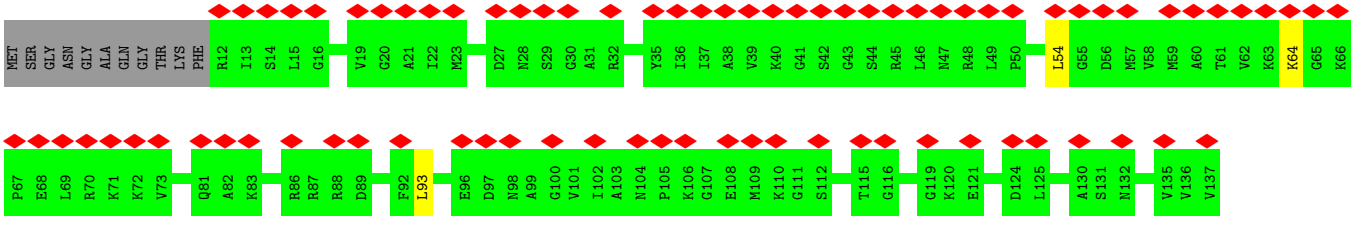
Chain S:



• Molecule 33: 60S ribosomal protein L23-A

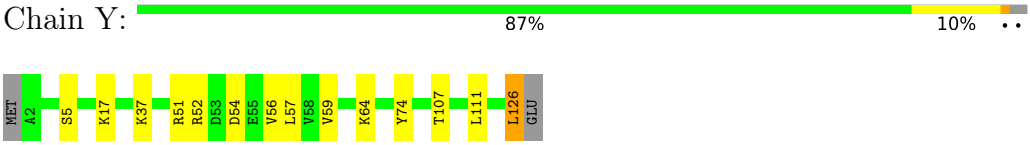
Chain V:





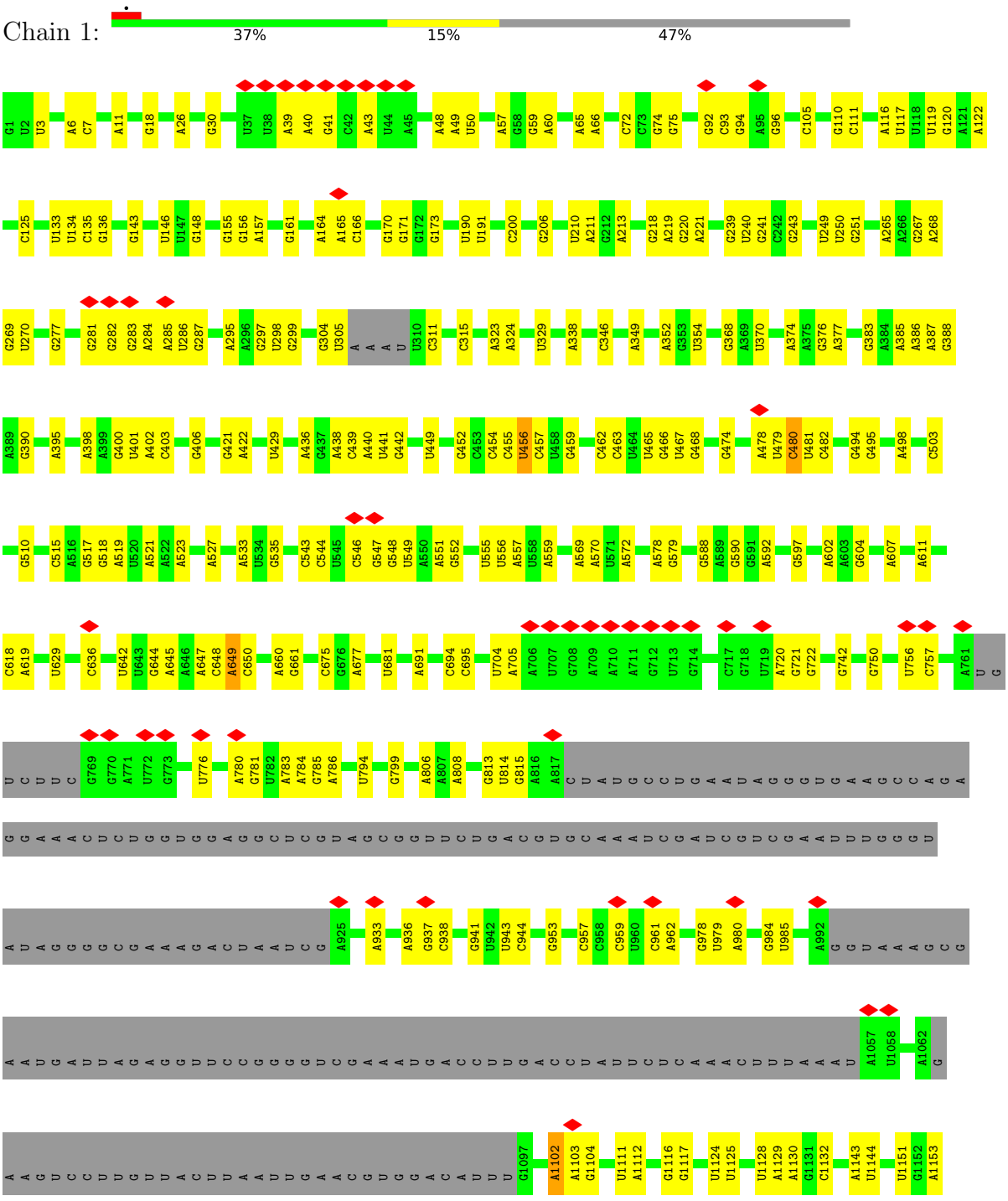
• Molecule 34: 60S ribosomal protein L26-A

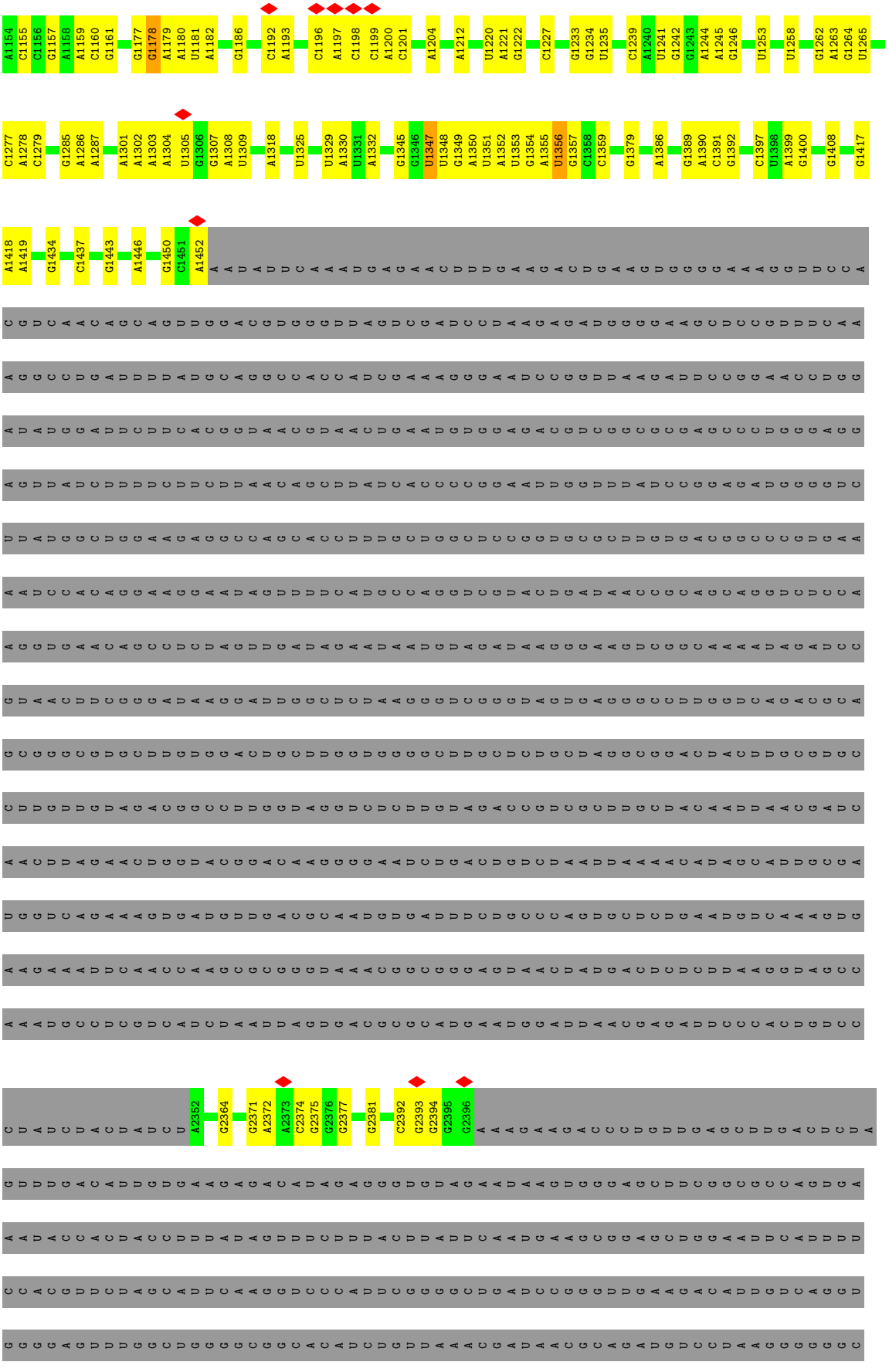
Chain Y:

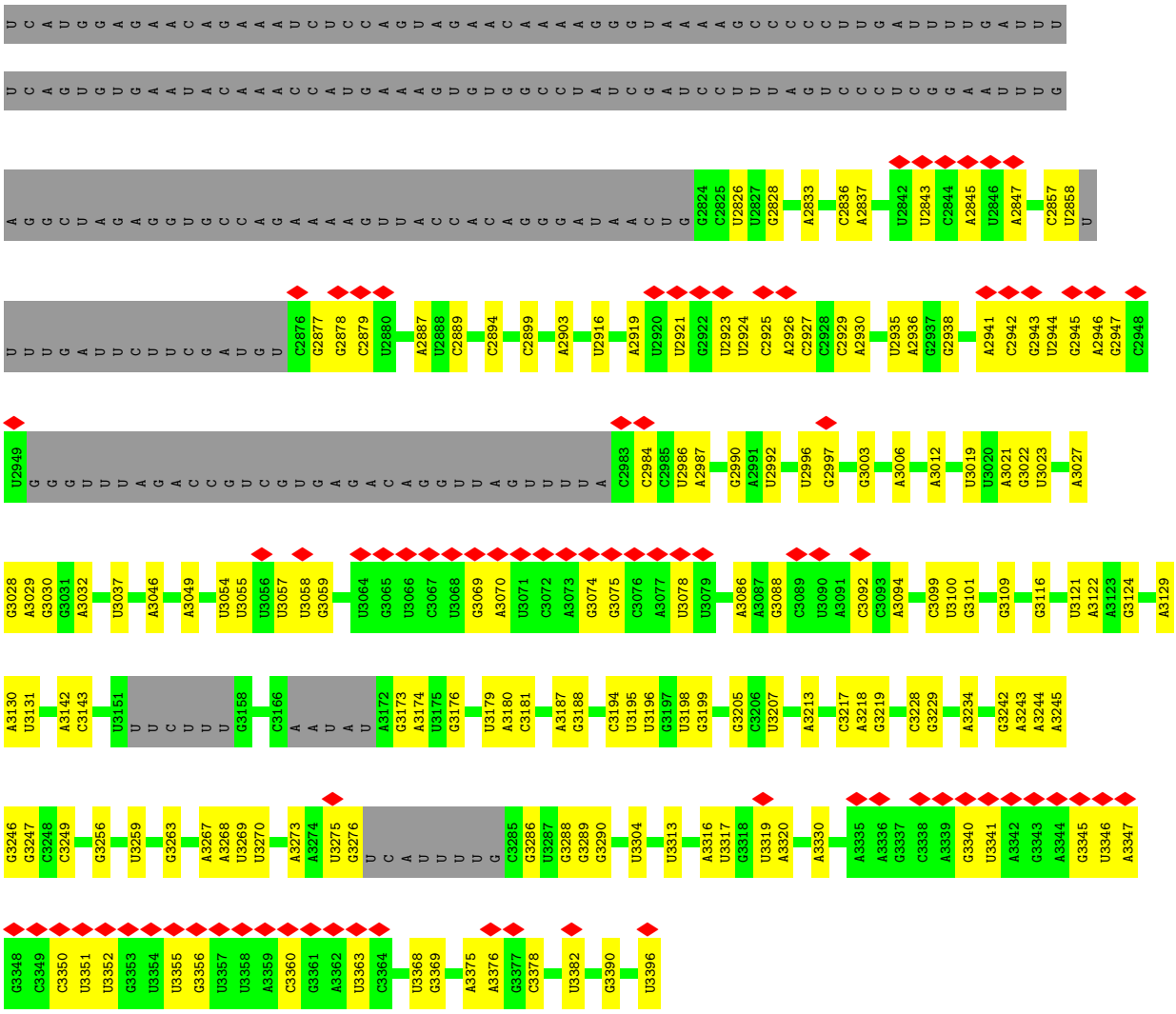


• Molecule 35: 25S ribosomal RNA

Chain 1:

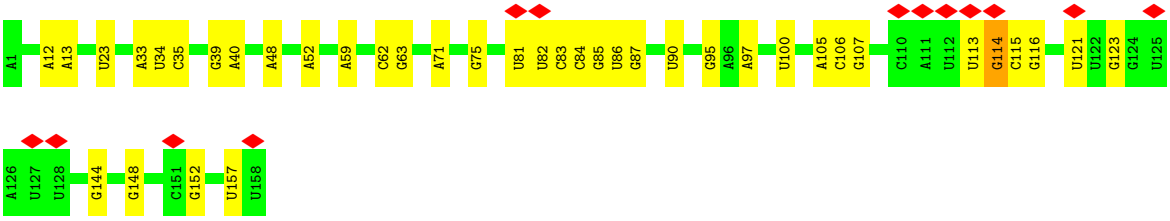



A1154 C1155 C1156 G1157 A1158 A1159 C1160 G1161 G1177 G1178 A1179 A1180 U1181 A1182 G1186 C1192 A1193 C1196 A1197 C1198 C1199 A1200 C1201 A1204 A1212 U1220 A1221 G1222 C1227 G1233 G1234 U1235 C1239 A1240 U1241 G1242 G1243 A1244 A1245 G1246 U1253 U1258 G1262 A1263 G1264 U1265
C1277 A1278 C1279 G1285 A1286 A1287 A1301 A1302 A1303 A1304 U1305 G1306 G1307 A1308 U1309 A1318 U1325 U1329 A1330 U1331 A1332 G1345 G1346 U1347 U1348 G1349 A1350 U1351 A1352 U1353 G1354 A1355 U1356 G1357 C1358 C1359 G1379 A1386 G1389 A1390 C1391 G1392 C1397 U1398 A1399 G1400 G1408 G1417
A1418 A1419 G1434 C1437 G1443 A1446 G1450 C1451 A1452
C2352 G2364 G2371 A2372 A2373 C2374 G2375 G2376 G2377 G2381 C2392 G2393 G2394 G2395 G2396



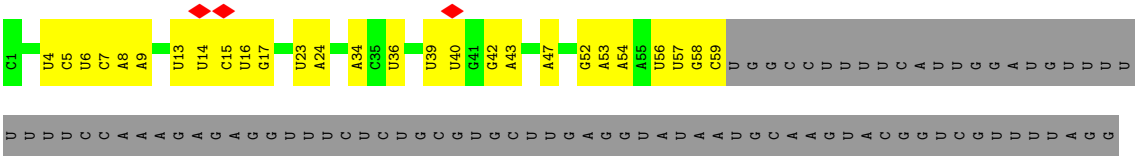
• Molecule 36: 5.8S ribosomal RNA

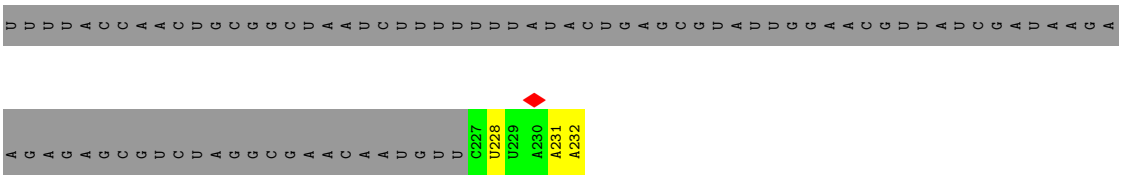
Chain 2:



• Molecule 37: 5.8S ribosomal RNA

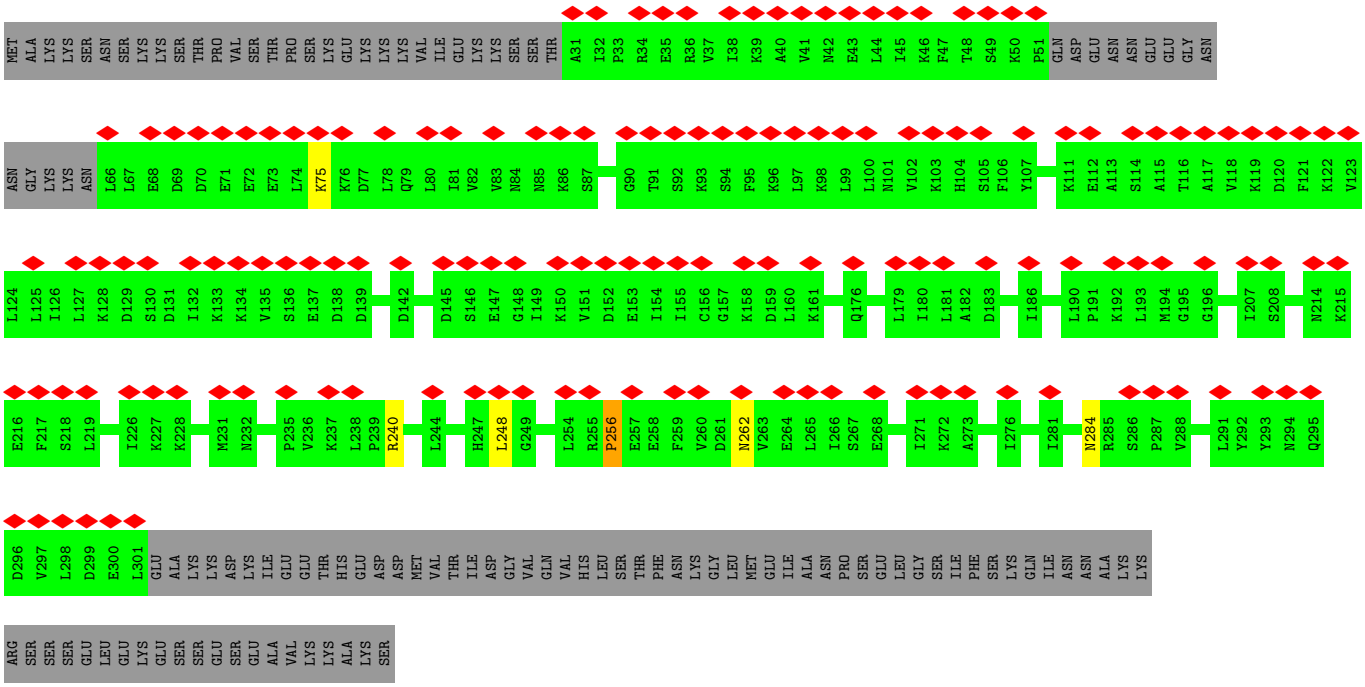
Chain 6:





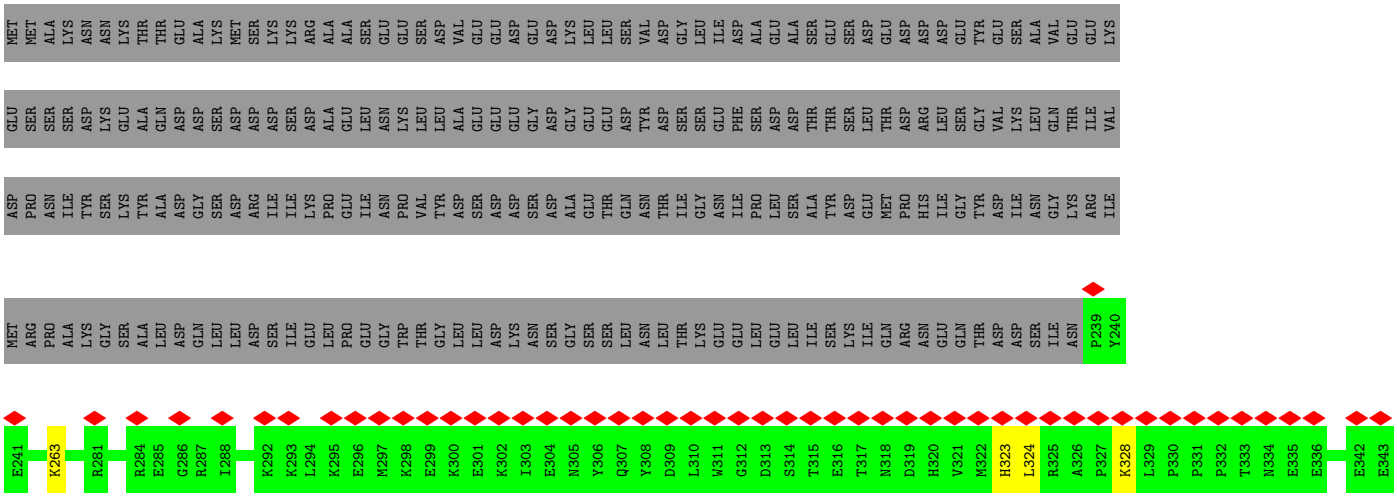
• Molecule 38: Proteasome-interacting protein CIC1

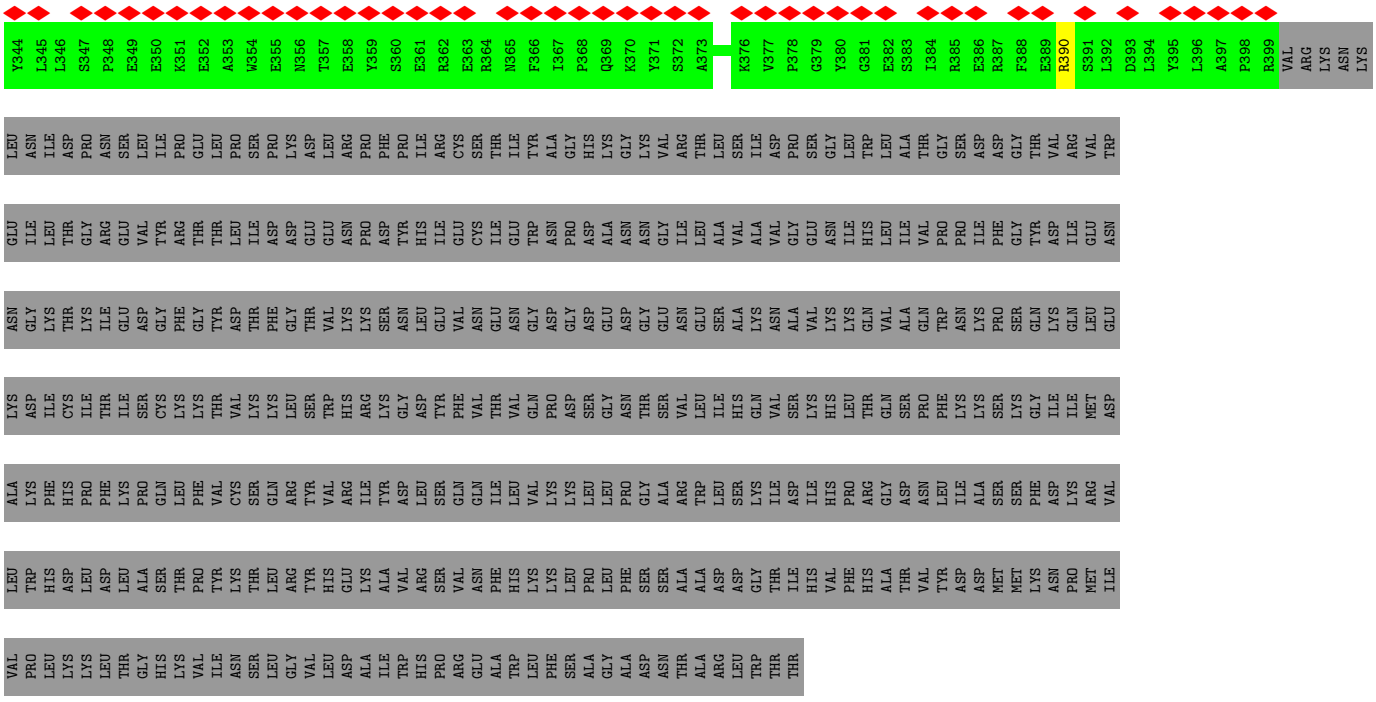
Chain K:



• Molecule 39: Ribosome biogenesis protein ERB1

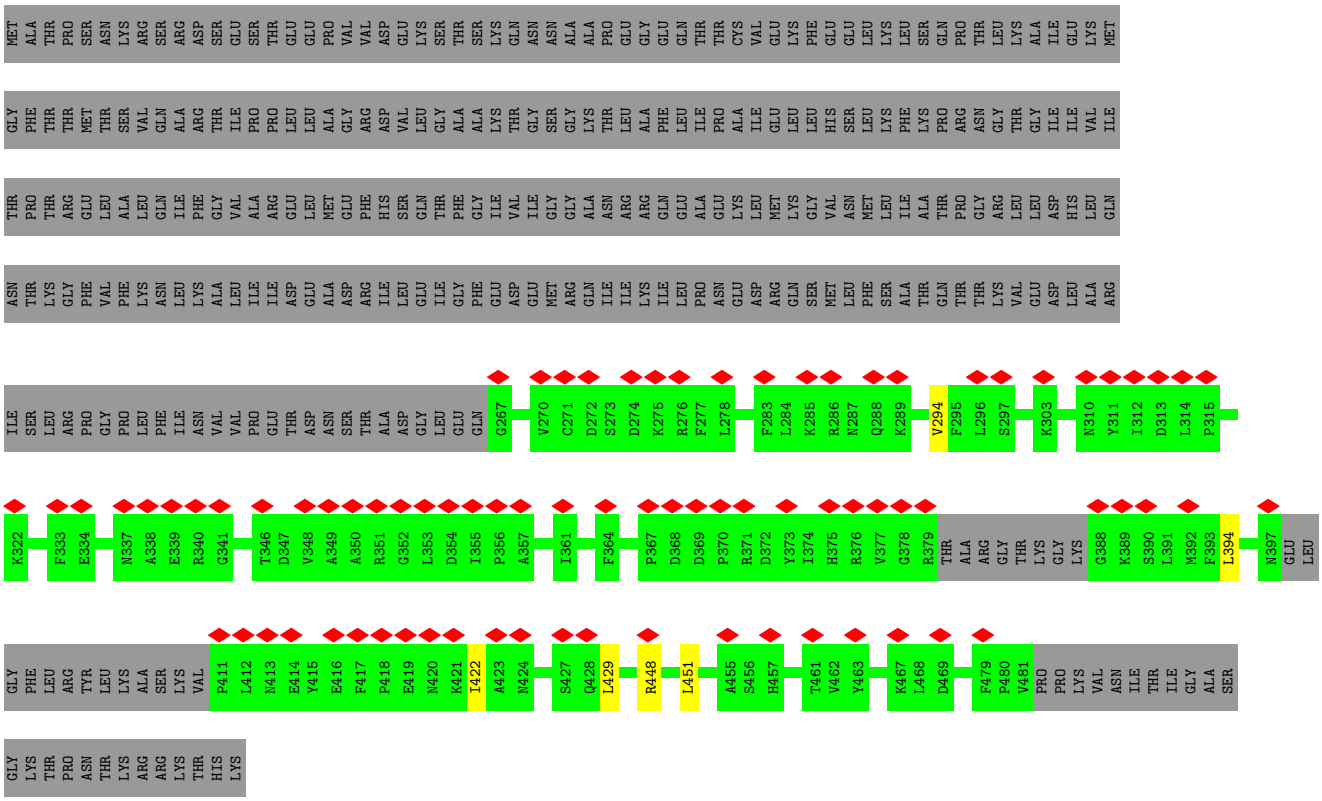
Chain m:





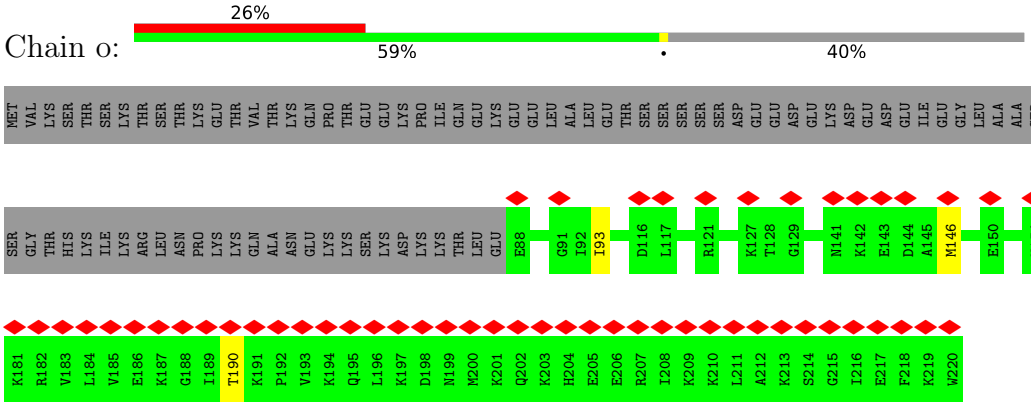
• Molecule 40: ATP-dependent RNA helicase HAS1

Chain D:



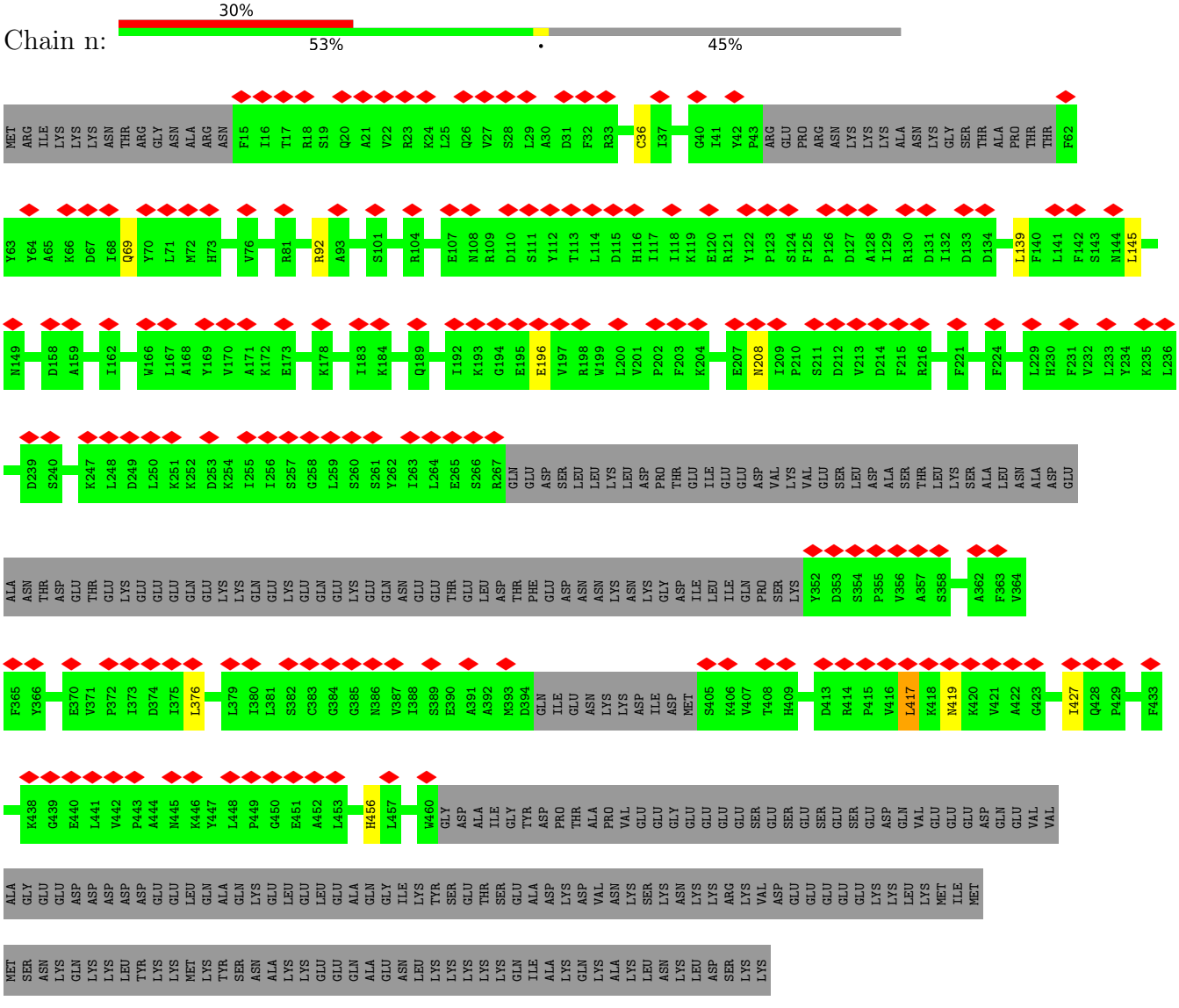
• Molecule 41: Ribosome biogenesis protein 15

Chain o:



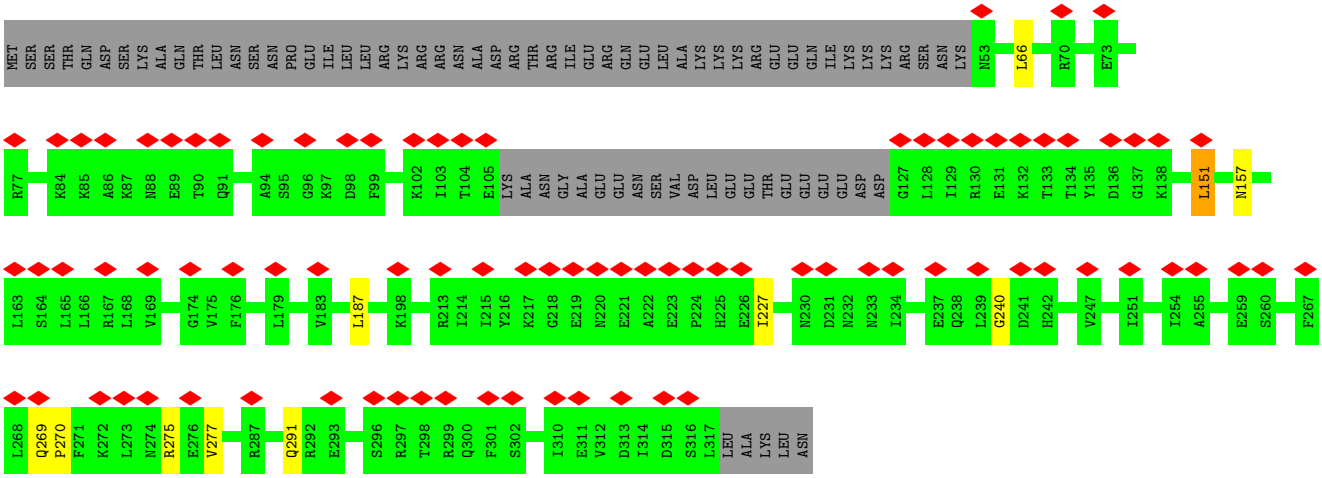
• Molecule 42: Pescadillo homolog

Chain n:



• Molecule 43: Ribosome biogenesis protein RLP7

Chain t:


MET SER SER THR GLN ASP SER LYS ALA GLN THR LEU ASN SER ASN PRO GLU ILE LEU LEU ARG LYS ARG ARG ASN ALA ASP ARG THR ARG ILE GLU ARG GLN GLU LEU ALA LYS LYS LYS ARG GLU GLU GLN ILE LYS LYS LYS ARG SER ASN LYS N53 L66 R70 E73
R77 K84 K85 A86 K87 N88 E89 T90 Q91 A94 S95 G96 K97 D98 F99 K102 I103 T104 E105 LYS ALA ASN GLY ALA GLU GLU ASN SER VAL ASP LEU GLU GLU THR GLU GLU GLU GLU ASP ASP G127 L128 I129 R130 E131 K132 T133 T134 Y135 D136 G137 K138 L151 N157
L163 S164 L165 L166 R167 L168 V169 G174 V175 F176 L179 V183 L187 K198 R213 I214 I215 Y216 K217 G218 E219 N220 E221 A222 E223 P224 H225 E226 I227 N230 D231 N232 N233 I234 E237 Q238 L239 G240 D241 H242 V247 I251 I254 A255 E259 S260 F267
L268 Q269 P270 F271 K272 L273 N274 R275 E276 V277 R287 Q291 R292 E293 S296 R297 T298 R299 Q300 F301 S302 I310 E311 V312 D313 I314 D315 S316 L317 LEU ALA LYS LEU ASN

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	156937	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 ($e^-/Å^2$)	27	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.194	Depositor
Minimum map value	-0.082	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.032	Depositor
Map size (Å)	455.28, 455.28, 455.28	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.084, 1.084, 1.084	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: 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	x	0.55	1/2312 (0.0%)	0.80	1/3097 (0.0%)
2	F	0.49	0/1974	0.73	2/2654 (0.1%)
3	3	0.64	0/1461	0.93	2/1958 (0.1%)
4	4	0.47	0/1895	0.81	2/2549 (0.1%)
5	5	0.44	0/3109	0.68	0/4187
6	A	0.47	0/1243	0.64	0/1679
7	b	0.43	0/3474	0.64	1/4683 (0.0%)
8	J	0.44	0/559	0.58	0/754
9	r	0.41	0/638	0.61	0/837
10	s	0.44	0/224	0.64	0/288
11	u	0.42	0/996	0.61	0/1324
12	v	0.46	0/1100	0.63	0/1456
13	W	0.42	0/1902	0.62	1/2564 (0.0%)
14	y	0.41	0/1722	0.63	0/2343
15	z	0.39	0/445	0.60	0/585
16	B	0.44	0/2699	0.70	1/3626 (0.0%)
17	C	0.56	0/2660	0.86	4/3601 (0.1%)
18	e	0.56	0/1030	0.82	2/1379 (0.1%)
19	E	0.47	0/1226	0.72	0/1648
20	f	0.56	0/868	0.79	0/1168
21	G	0.44	0/1252	0.71	0/1695
22	h	0.42	0/978	0.70	1/1301 (0.1%)
23	H	0.43	0/1531	0.65	0/2062
24	i	0.41	0/599	0.70	0/793
25	j	0.55	0/578	0.85	0/767
26	L	0.51	0/877	0.84	0/1179
27	M	0.42	0/1056	0.69	0/1421
28	N	0.56	2/1544 (0.1%)	0.78	3/2065 (0.1%)
29	O	0.70	1/1585 (0.1%)	0.88	2/2128 (0.1%)
30	P	0.49	0/1080	0.70	0/1455
31	Q	0.47	0/1024	0.74	0/1385
32	S	0.47	0/1468	0.69	0/1973

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	V	0.41	0/950	0.61	0/1279
34	Y	0.59	1/995 (0.1%)	0.77	0/1329
35	1	0.35	0/42777	0.69	10/66679 (0.0%)
36	2	0.35	0/3740	0.69	1/5808 (0.0%)
37	6	0.27	0/1527	0.75	0/2371
38	K	0.42	0/2107	0.65	0/2845
39	m	0.40	0/1401	0.64	0/1895
40	D	0.44	0/1626	0.65	0/2193
41	o	0.42	0/1129	0.65	0/1502
42	n	0.42	0/2802	0.62	1/3791 (0.0%)
43	t	0.40	0/1961	0.65	0/2639
All	All	0.42	5/106124 (0.0%)	0.70	34/152935 (0.0%)

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
3	3	0	1
4	4	0	3
All	All	0	4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	Y	126	LEU	C-O	11.24	1.44	1.23
29	O	100	GLU	CD-OE2	8.32	1.34	1.25
28	N	105	ARG	CZ-NH1	7.06	1.42	1.33
1	x	180	GLU	C-O	5.37	1.33	1.23
28	N	105	ARG	NE-CZ	5.00	1.39	1.33

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	1	649	A	C2'-C3'-O3'	8.99	129.27	109.50
29	O	19	LEU	CA-CB-CG	-8.57	95.58	115.30
17	C	313	LEU	CA-CB-CG	8.43	134.69	115.30
35	1	1347	U	C4'-C3'-O3'	7.64	128.28	113.00
28	N	105	ARG	NE-CZ-NH1	7.48	124.04	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	3	118	VAL	Peptide
4	4	135	TYR	Peptide
4	4	136	LEU	Mainchain
4	4	225	VAL	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	x	259/295 (88%)	203 (78%)	44 (17%)	12 (5%)	2 23
2	F	239/244 (98%)	212 (89%)	23 (10%)	4 (2%)	9 45
3	3	171/306 (56%)	122 (71%)	38 (22%)	11 (6%)	1 17
4	4	209/278 (75%)	173 (83%)	26 (12%)	10 (5%)	2 22
5	5	377/463 (81%)	338 (90%)	33 (9%)	6 (2%)	9 46
6	A	139/291 (48%)	122 (88%)	12 (9%)	5 (4%)	3 29
7	b	413/647 (64%)	381 (92%)	27 (6%)	5 (1%)	13 51
8	J	64/427 (15%)	58 (91%)	4 (6%)	2 (3%)	4 32
9	r	71/261 (27%)	65 (92%)	4 (6%)	2 (3%)	5 34
10	s	25/520 (5%)	25 (100%)	0	0	100 100
11	u	114/199 (57%)	109 (96%)	4 (4%)	1 (1%)	17 57
12	v	124/231 (54%)	115 (93%)	9 (7%)	0	100 100
13	W	230/236 (98%)	213 (93%)	15 (6%)	2 (1%)	17 57
14	y	223/245 (91%)	210 (94%)	13 (6%)	0	100 100

Continued on next page...

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	z	53/106 (50%)	49 (92%)	4 (8%)	0	100	100
16	B	329/387 (85%)	289 (88%)	30 (9%)	10 (3%)	4	33
17	C	341/362 (94%)	295 (86%)	30 (9%)	16 (5%)	2	22
18	e	123/130 (95%)	113 (92%)	9 (7%)	1 (1%)	19	59
19	E	147/176 (84%)	131 (89%)	16 (11%)	0	100	100
20	f	104/107 (97%)	98 (94%)	4 (4%)	2 (2%)	8	42
21	G	155/256 (60%)	134 (86%)	17 (11%)	4 (3%)	5	35
22	h	117/120 (98%)	104 (89%)	8 (7%)	5 (4%)	2	24
23	H	188/191 (98%)	167 (89%)	20 (11%)	1 (0%)	29	68
24	i	72/100 (72%)	66 (92%)	4 (6%)	2 (3%)	5	34
25	j	69/88 (78%)	62 (90%)	5 (7%)	2 (3%)	4	33
26	L	106/199 (53%)	97 (92%)	7 (7%)	2 (2%)	8	42
27	M	132/138 (96%)	121 (92%)	9 (7%)	2 (2%)	10	47
28	N	173/204 (85%)	150 (87%)	22 (13%)	1 (1%)	25	64
29	O	195/199 (98%)	66 (34%)	44 (23%)	85 (44%)	0	0
30	P	133/184 (72%)	118 (89%)	13 (10%)	2 (2%)	10	47
31	Q	129/186 (69%)	117 (91%)	12 (9%)	0	100	100
32	S	168/172 (98%)	143 (85%)	18 (11%)	7 (4%)	3	25
33	V	124/137 (90%)	113 (91%)	11 (9%)	0	100	100
34	Y	123/127 (97%)	110 (89%)	11 (9%)	2 (2%)	9	46
38	K	253/376 (67%)	231 (91%)	20 (8%)	2 (1%)	19	59
39	m	159/807 (20%)	144 (91%)	14 (9%)	1 (1%)	25	64
40	D	188/505 (37%)	167 (89%)	21 (11%)	0	100	100
41	o	131/220 (60%)	121 (92%)	9 (7%)	1 (1%)	19	59
42	n	326/605 (54%)	302 (93%)	22 (7%)	2 (1%)	25	64
43	t	240/322 (74%)	214 (89%)	20 (8%)	6 (2%)	5	36
All	All	6936/11047 (63%)	6068 (88%)	652 (9%)	216 (3%)	7	32

5 of 216 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	x	119	PRO
1	x	128	PHE

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Mol	Chain	Res	Type
1	x	222	PRO
2	F	160	ARG
2	F	164	SER

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	x	252/276 (91%)	206 (82%)	46 (18%)	1 10
2	F	204/205 (100%)	191 (94%)	13 (6%)	17 52
3	3	155/274 (57%)	129 (83%)	26 (17%)	2 14
4	4	203/257 (79%)	177 (87%)	26 (13%)	4 24
5	5	343/410 (84%)	323 (94%)	20 (6%)	20 55
6	A	137/263 (52%)	129 (94%)	8 (6%)	20 55
7	b	377/573 (66%)	345 (92%)	32 (8%)	10 41
8	J	61/383 (16%)	61 (100%)	0	100 100
9	r	65/229 (28%)	63 (97%)	2 (3%)	40 71
10	s	24/445 (5%)	23 (96%)	1 (4%)	30 63
11	u	101/180 (56%)	96 (95%)	5 (5%)	24 59
12	v	116/205 (57%)	105 (90%)	11 (10%)	8 37
13	W	209/213 (98%)	199 (95%)	10 (5%)	25 60
14	y	193/211 (92%)	184 (95%)	9 (5%)	26 61
15	z	48/95 (50%)	48 (100%)	0	100 100
16	B	280/323 (87%)	259 (92%)	21 (8%)	13 45
17	C	273/289 (94%)	238 (87%)	35 (13%)	4 24
18	e	108/111 (97%)	94 (87%)	14 (13%)	4 24
19	E	131/153 (86%)	123 (94%)	8 (6%)	18 53
20	f	90/91 (99%)	77 (86%)	13 (14%)	3 20
21	G	128/208 (62%)	110 (86%)	18 (14%)	3 21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
22	h	104/105 (99%)	96 (92%)	8 (8%)	13 45
23	H	170/171 (99%)	155 (91%)	15 (9%)	10 40
24	i	61/81 (75%)	53 (87%)	8 (13%)	4 23
25	j	59/71 (83%)	50 (85%)	9 (15%)	2 18
26	L	87/159 (55%)	78 (90%)	9 (10%)	7 34
27	M	106/109 (97%)	101 (95%)	5 (5%)	26 61
28	N	153/176 (87%)	128 (84%)	25 (16%)	2 15
29	O	160/162 (99%)	114 (71%)	46 (29%)	0 2
30	P	109/146 (75%)	94 (86%)	15 (14%)	3 22
31	Q	107/151 (71%)	96 (90%)	11 (10%)	7 34
32	S	155/156 (99%)	141 (91%)	14 (9%)	9 39
33	V	98/105 (93%)	95 (97%)	3 (3%)	40 71
34	Y	108/110 (98%)	96 (89%)	12 (11%)	6 31
38	K	238/346 (69%)	233 (98%)	5 (2%)	53 78
39	m	150/723 (21%)	146 (97%)	4 (3%)	44 73
40	D	175/440 (40%)	169 (97%)	6 (3%)	37 69
41	o	118/199 (59%)	116 (98%)	2 (2%)	60 82
42	n	302/548 (55%)	292 (97%)	10 (3%)	38 69
43	t	216/287 (75%)	210 (97%)	6 (3%)	43 72
All	All	6174/9639 (64%)	5643 (91%)	531 (9%)	14 41

5 of 531 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
31	Q	55	SER
32	S	115	ARG
31	Q	49	LEU
42	n	208	ASN
13	W	55	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 71 such sidechains are listed below:

Mol	Chain	Res	Type
32	S	62	ASN

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Mol	Chain	Res	Type
32	S	142	GLN
41	o	113	GLN
12	v	33	ASN
8	J	228	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
35	1	1772/3396 (52%)	498 (28%)	49 (2%)
36	2	152/158 (96%)	36 (23%)	6 (3%)
37	6	63/232 (27%)	30 (47%)	2 (3%)
All	All	1987/3786 (52%)	564 (28%)	57 (2%)

5 of 564 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
35	1	3	U
35	1	6	A
35	1	7	C
35	1	11	A
35	1	18	G

5 of 57 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
35	1	1307	G
37	6	16	U
35	1	2392	C
36	2	114	G
36	2	39	G

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 2 ligands modelled in this entry, 2 are 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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
36	2	6
1	x	1

The worst 5 of 7 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	124:G	O3'	125:U	P	7.11
1	2	110:C	O3'	111:A	P	6.92
1	2	125:U	O3'	126:A	P	6.42
1	2	113:U	O3'	114:G	P	4.42
1	2	126:A	O3'	127:U	P	3.70

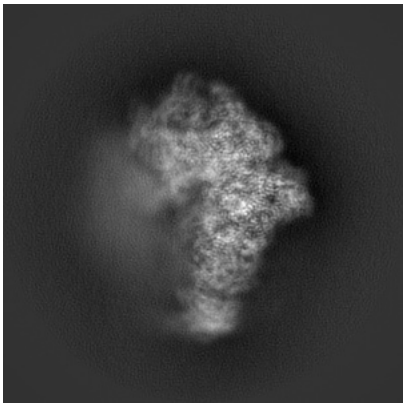
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-3893. These allow visual inspection of the internal detail of the map and identification of artifacts.

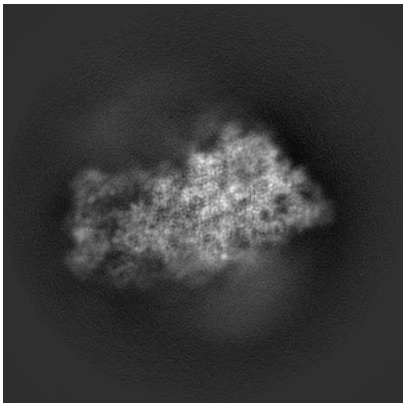
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

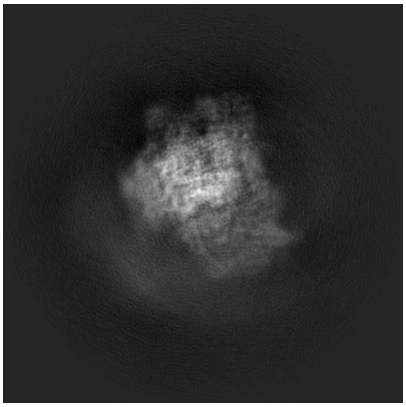
6.1.1 Primary map



X



Y

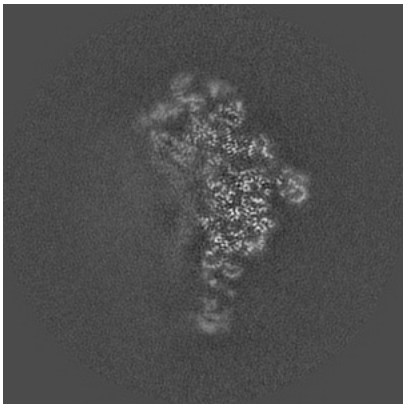


Z

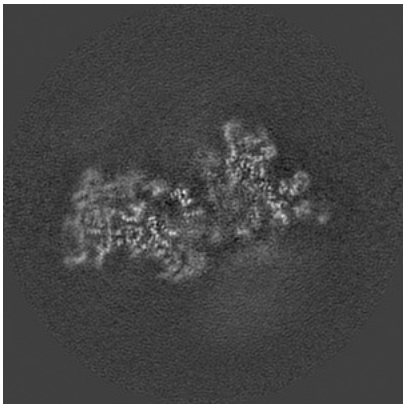
The images above show the map projected in three orthogonal directions.

6.2 Central slices

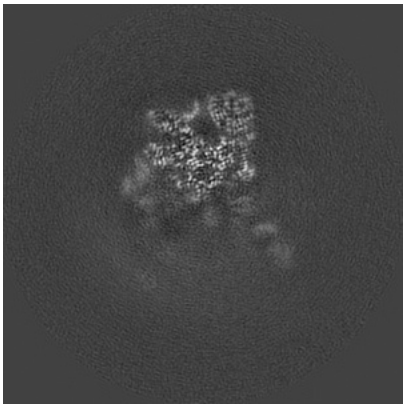
6.2.1 Primary map



X Index: 210



Y Index: 210

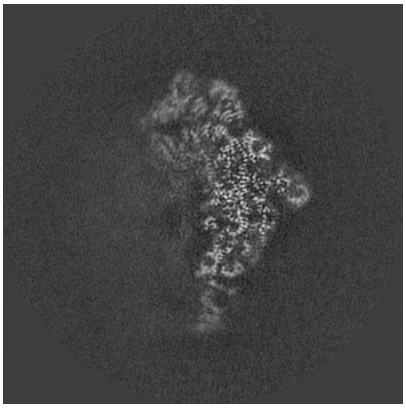


Z Index: 210

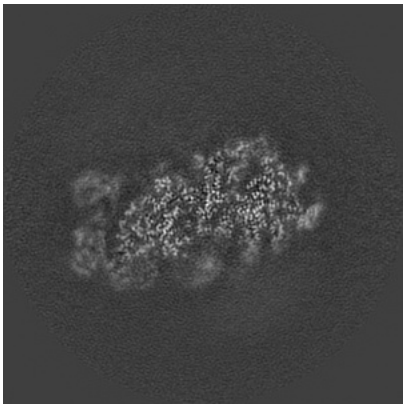
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

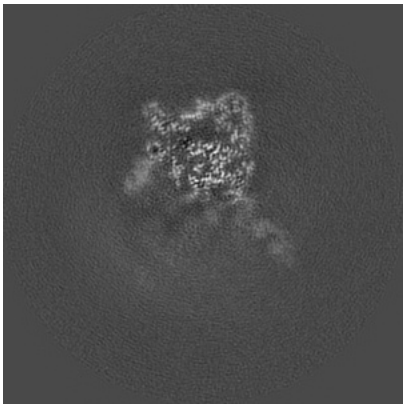
6.3.1 Primary map



X Index: 205



Y Index: 235



Z Index: 215

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

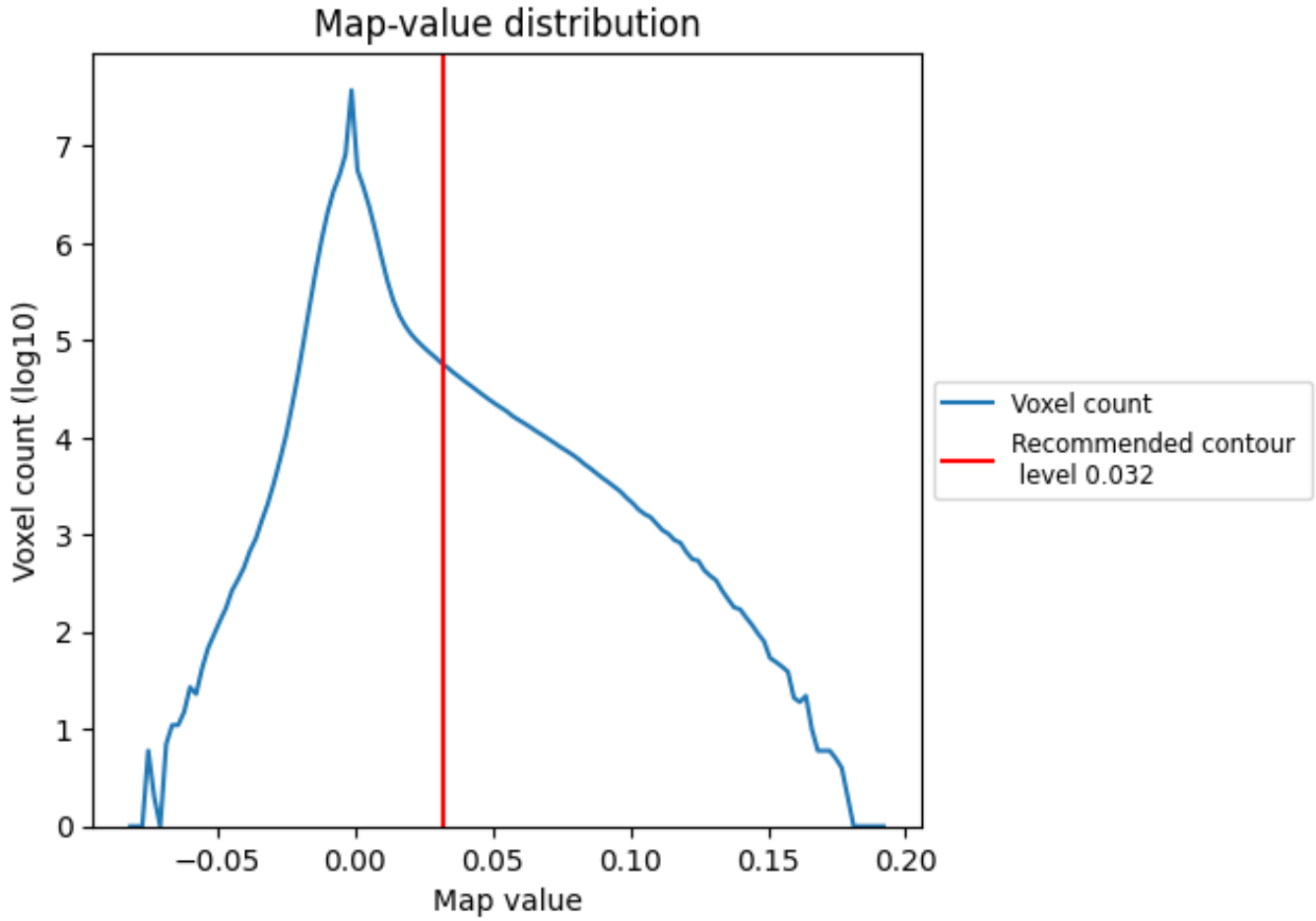
6.5 Mask visualisation (i)

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

7 Map analysis

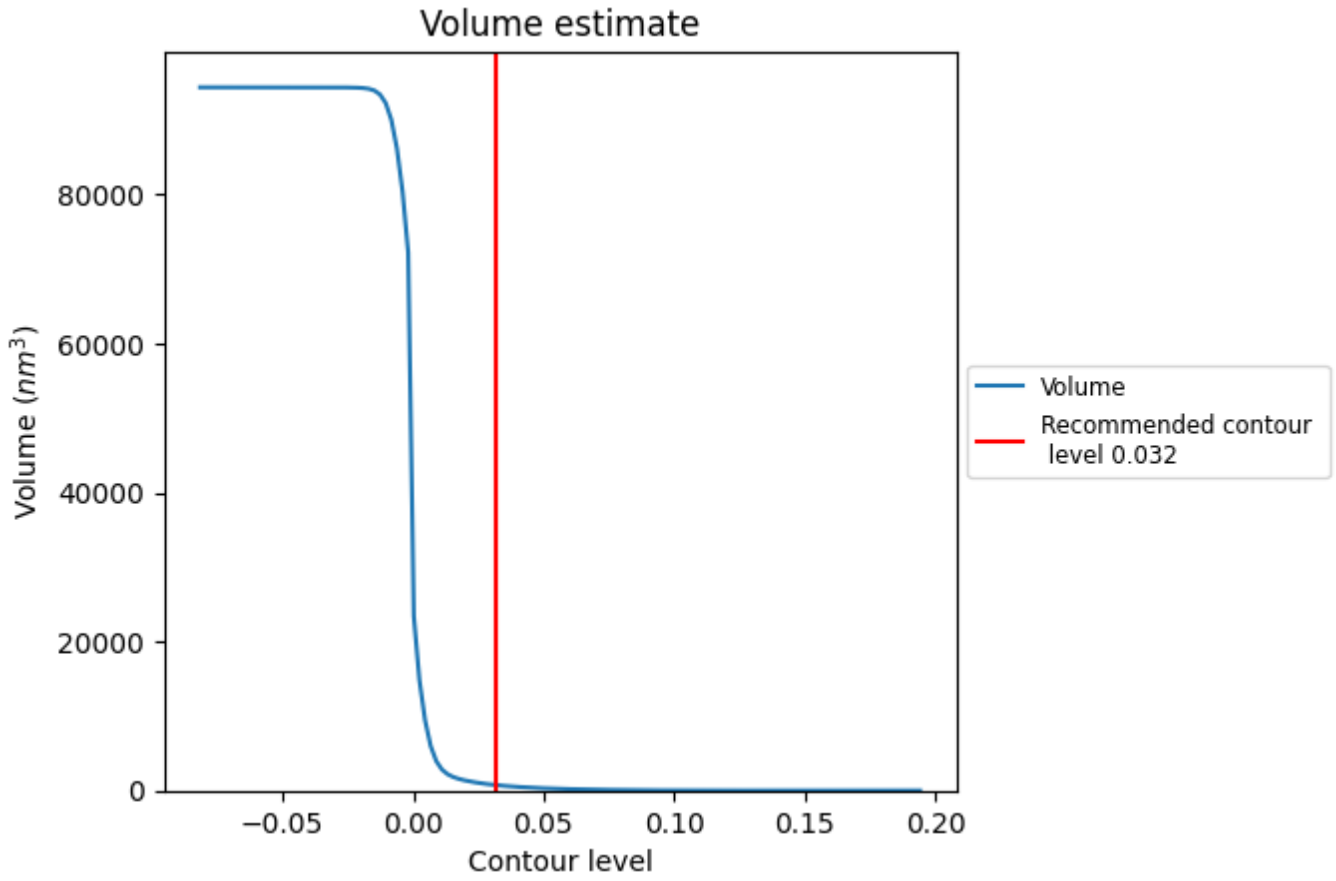
This section contains the results of statistical analysis of the map.

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.

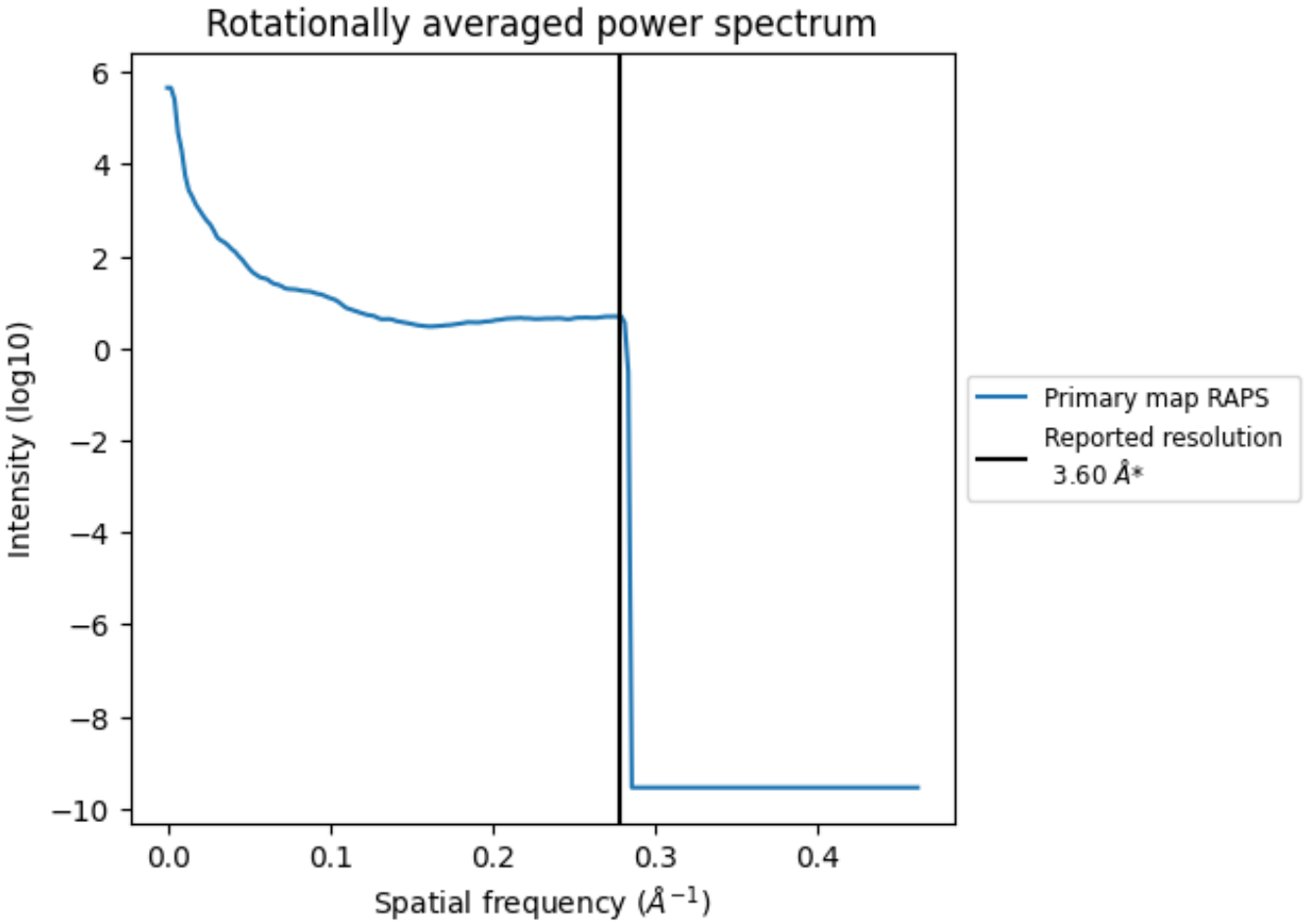
7.2 Volume estimate (i)



The volume at the recommended contour level is 727 nm^3; this corresponds to an approximate mass of 657 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)

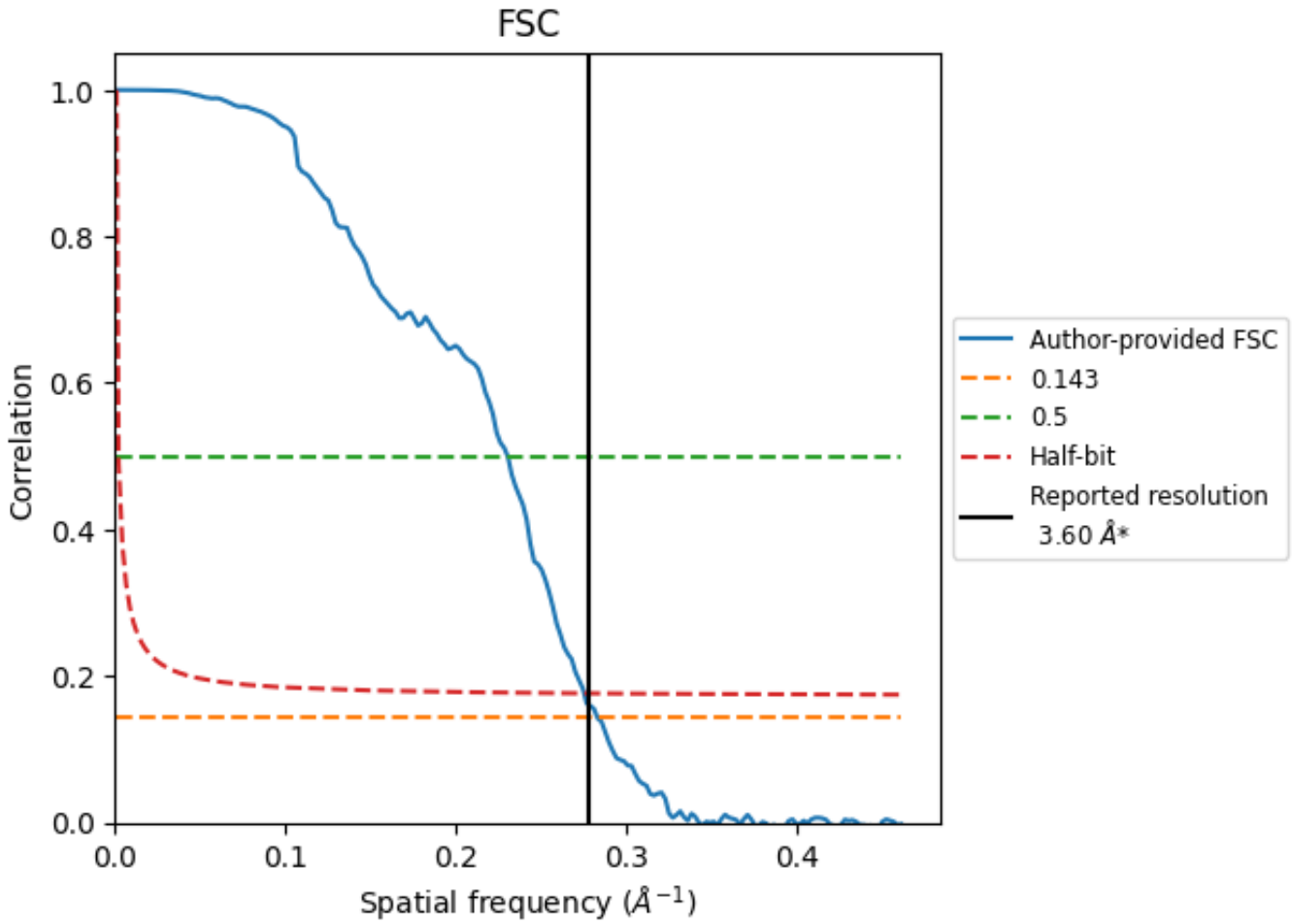


*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8.2 Resolution estimates (i)

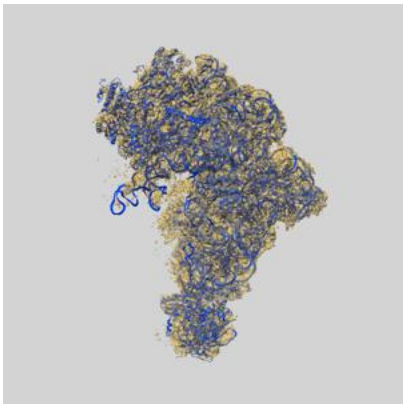
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.53	4.34	3.63
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

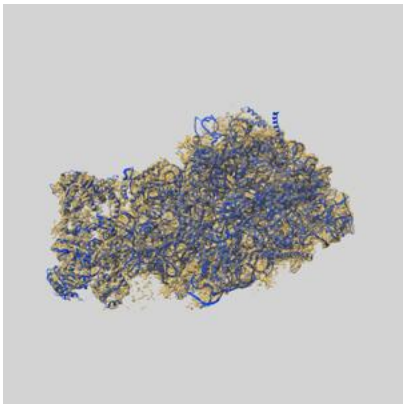
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-3893 and PDB model 6EM1. Per-residue inclusion information can be found in section 3 on page 12.

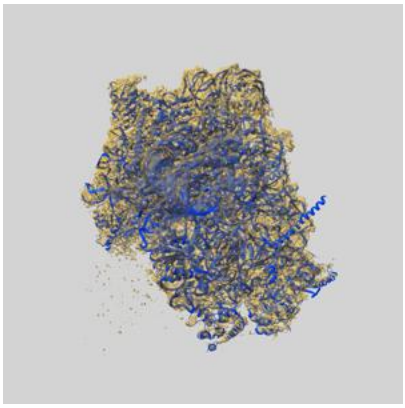
9.1 Map-model overlay



X



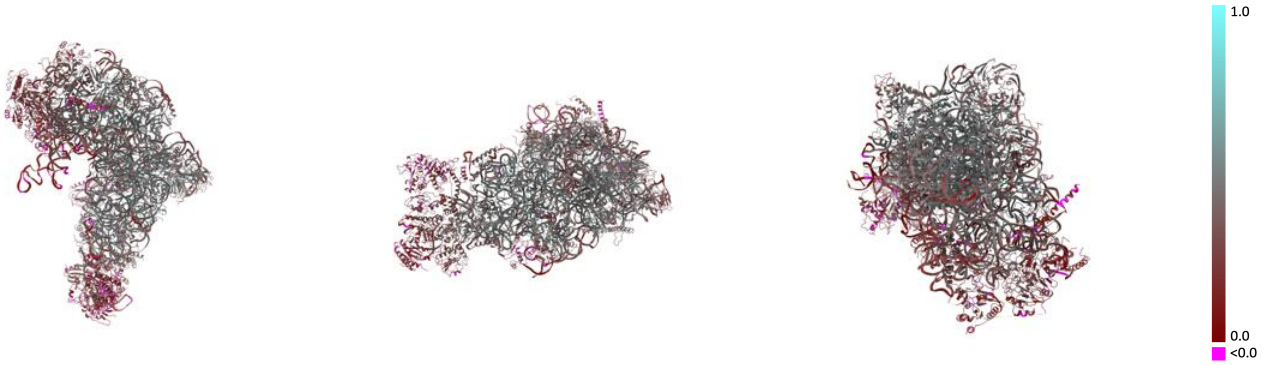
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.032 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.

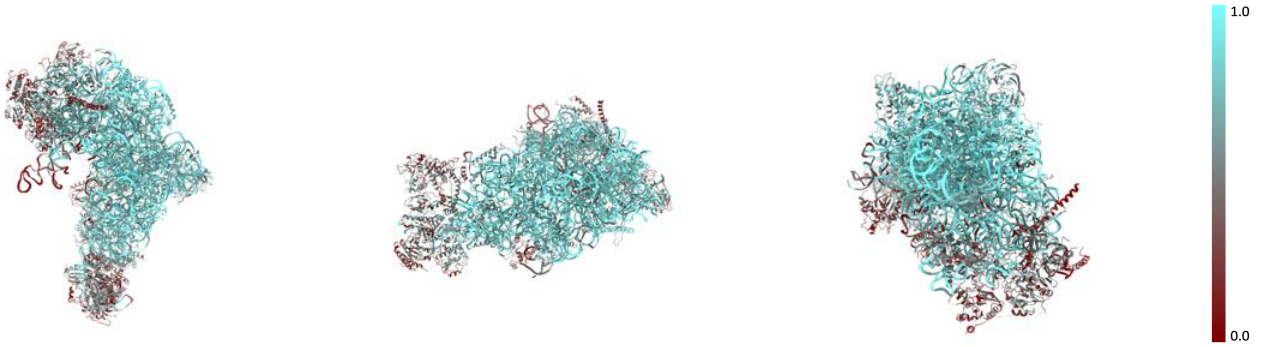
9.2 Q-score mapped to coordinate model (i)



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.

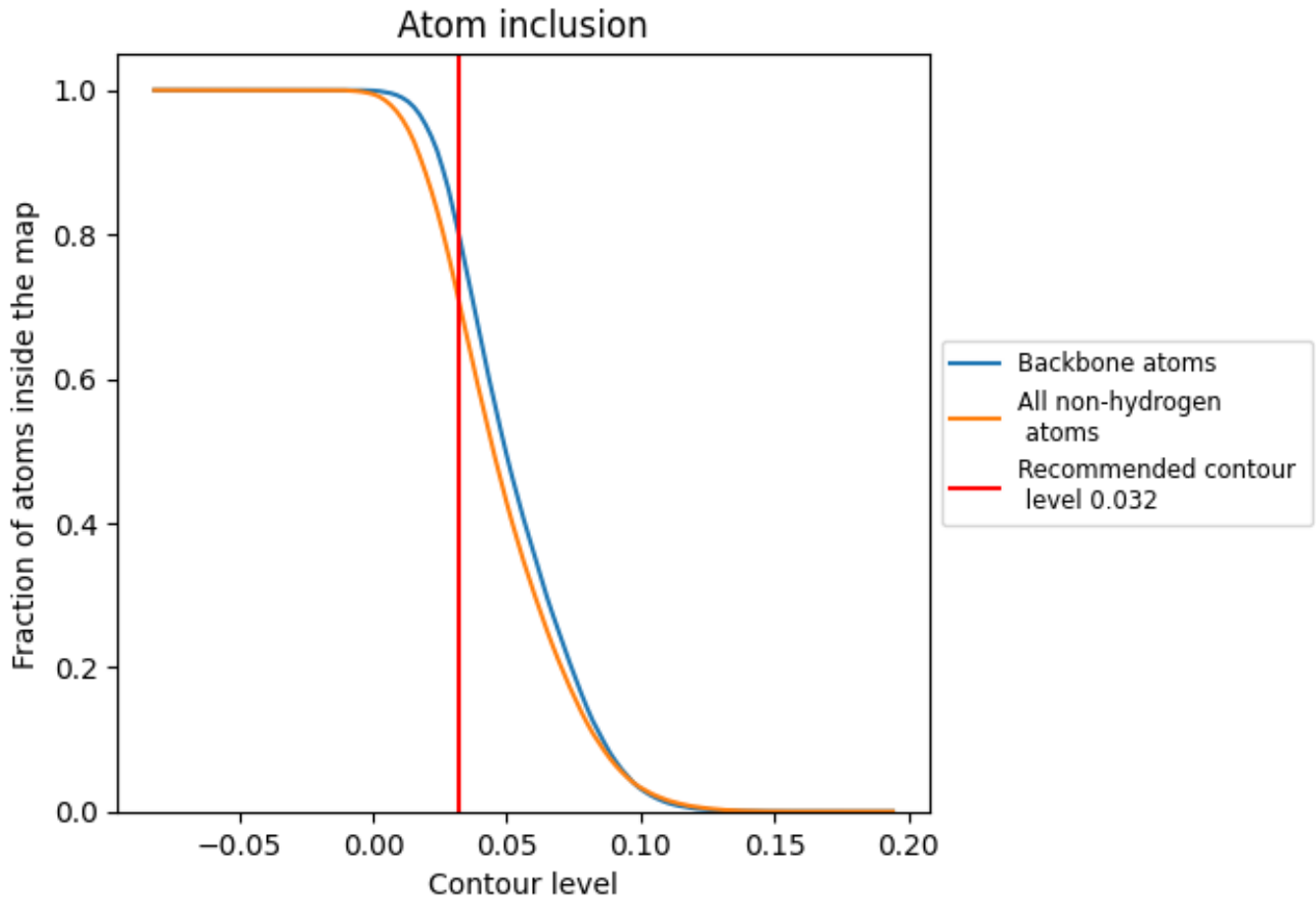
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.032).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 71% 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 (0.032) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7100	0.3710
1	0.8377	0.3920
2	0.8580	0.3980
3	0.8313	0.4580
4	0.7420	0.4000
5	0.7030	0.4290
6	0.7168	0.2680
A	0.3170	0.1750
B	0.7088	0.3950
C	0.8086	0.4990
D	0.4480	0.2520
E	0.7981	0.4470
F	0.8268	0.4720
G	0.6985	0.4080
H	0.6646	0.4000
J	0.2352	0.1530
K	0.3468	0.1930
L	0.8468	0.4730
M	0.7988	0.4490
N	0.7563	0.4530
O	0.8514	0.5070
P	0.7877	0.4650
Q	0.8169	0.4720
S	0.7696	0.4260
V	0.3322	0.2520
W	0.3569	0.2620
Y	0.8495	0.4930
b	0.3505	0.2650
e	0.7965	0.5070
f	0.8307	0.5010
h	0.7402	0.4260
i	0.6285	0.3250
j	0.8453	0.4920
m	0.3136	0.1840
n	0.3765	0.1670

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Chain	Atom inclusion	Q-score
o	0.4424	0.2170
r	0.5733	0.3780
s	0.4259	0.3860
t	0.4686	0.2110
u	0.4701	0.2300
v	0.7426	0.4300
x	0.7759	0.4350
y	0.3906	0.2320
z	0.1129	0.1010