Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 08:13 pm GMT

PDB ID	:	5OQL
EMDB ID	:	EMD-3847
Title	:	Cryo-EM structure of the 90S pre-ribosome from Chaetomium thermophilum
Authors	:	Cheng, J.; Kellner, N.; Berninghausen, O.; Hurt, E.; Beckmann, R.
Deposited on	:	2017-08-12
Resolution	:	3.20 Å(reported)

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

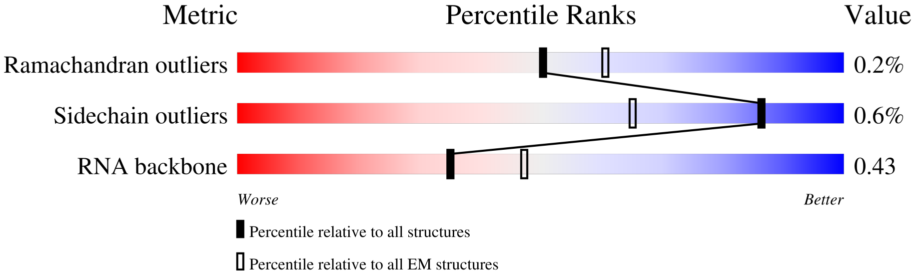
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

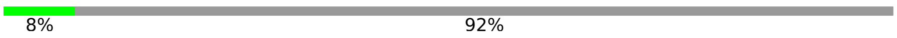
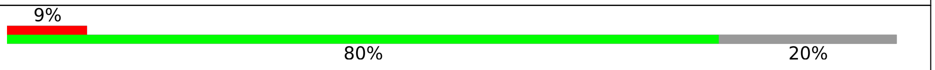
The reported resolution of this entry is 3.20 Å.

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	A	904	
2	B	907	
3	C	648	
4	D	884	
5	E	414	
6	F	558	
7	G	1802	
8	H	270	

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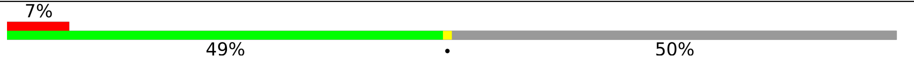
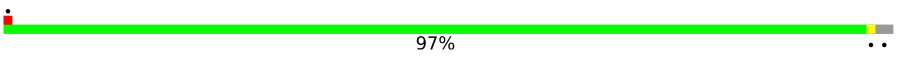
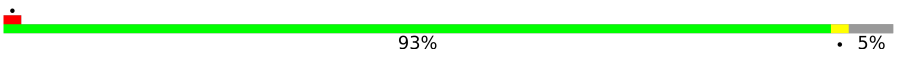
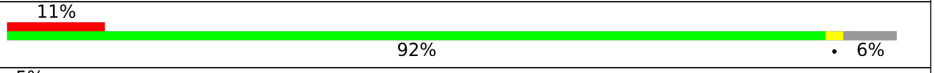
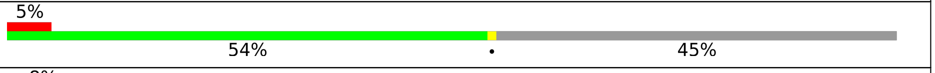
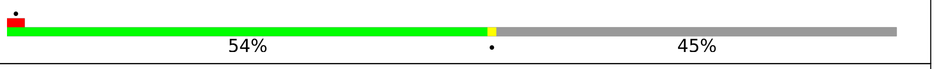
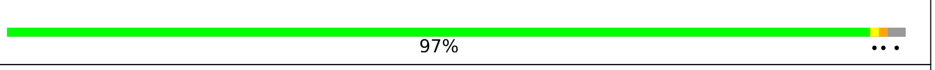
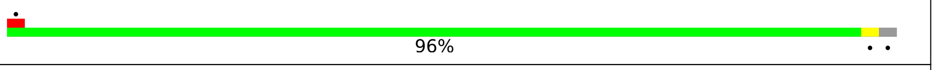
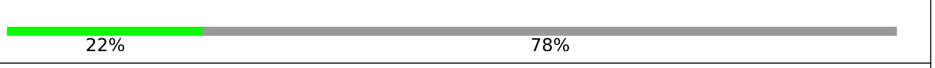
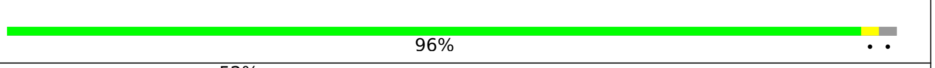
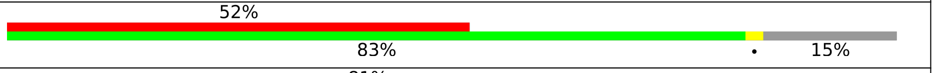
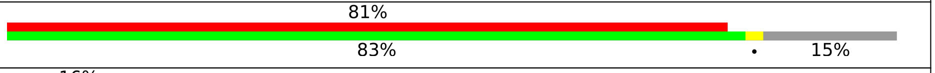
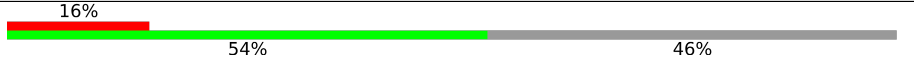
Mol	Chain	Length	Quality of chain
9	I	962	
10	J	912	
11	K	938	
12	L	557	
13	M	960	
14	N	618	
15	O	1049	
16	P	194	
17	Q	391	
18	R	313	
18	S	313	
19	T	523	
20	U	582	
21	V	127	
21	W	127	
22	X	630	
23	Y	411	
24	Z	1163	
25	a	183	
26	b	297	
27	c	785	
28	d	446	
29	e	252	
29	f	252	
30	g	322	

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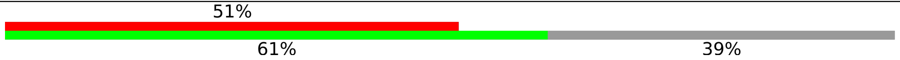
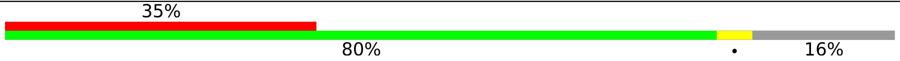
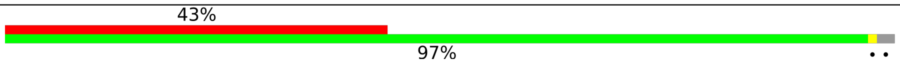
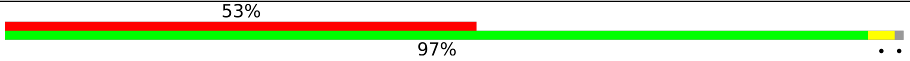
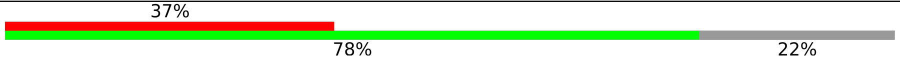
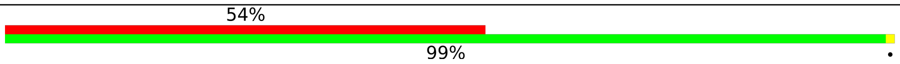
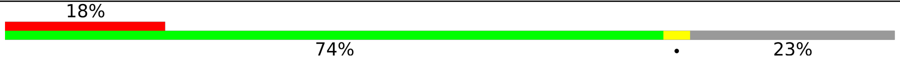
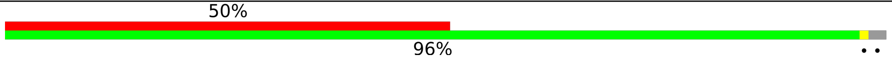
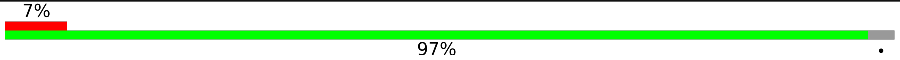
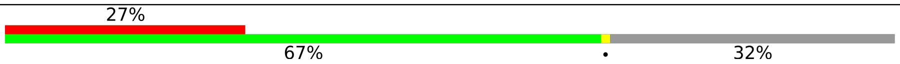
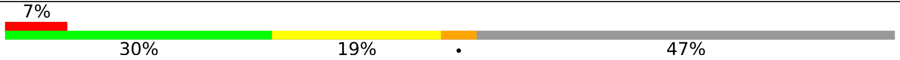
Mol	Chain	Length	Quality of chain
31	h	259	
32	i	1073	
32	j	1073	
33	k	203	
34	l	255	
35	m	264	
36	n	212	
37	o	239	
38	p	203	
39	q	202	
40	r	190	
41	s	151	
42	t	150	
43	u	143	
44	v	161	
45	w	130	
46	x	145	
47	y	136	
48	z	68	
49	0	311	
50	1	2568	
51	2	274	

2 Entry composition

There are 52 unique types of molecules in this entry. The entry contains 135120 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 Periodic tryptophan protein 2-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	827	Total	C	N	O	S	0	0
			6242	4029	1114	1077	22		

- Molecule 2 is a protein called Utp2.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	69	Total	C	N	O	0	0
			537	338	121	78		

- Molecule 3 is a protein called Utp3.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	74	Total	C	N	O	0	0
			588	371	120	97		

- Molecule 4 is a protein called Utp4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	292	Total	C	N	O	S	0	0
			2170	1383	403	373	11		

- Molecule 5 is a protein called Utp6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	331	Total	C	N	O	S	0	0
			2591	1674	504	399	14		

- Molecule 6 is a protein called Utp7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	429	Total	C	N	O	S	0	0
			3282	2103	611	557	11		

- Molecule 7 is a protein called Utp10.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	363	Total 2772	C 1784	N 501	O 473	S 14	0	0

- Molecule 8 is a protein called U3 small nucleolar RNA-associated protein 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	190	Total 1456	C 915	N 306	O 230	S 5	0	0

- Molecule 9 is a protein called Utp12.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	155	Total 1230	C 788	N 222	O 214	S 6	0	0

- Molecule 10 is a protein called Utp13.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	J	151	Total 1201	C 765	N 214	O 222	0	0

- Molecule 11 is a protein called Utp14.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	147	Total 1139	C 725	N 215	O 194	S 5	0	0

- Molecule 12 is a protein called Utp15.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	280	Total 2070	C 1320	N 379	O 363	S 8	0	0

- Molecule 13 is a protein called Utp17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	284	Total 2134	C 1386	N 364	O 378	S 6	0	0

- Molecule 14 is a protein called Utp18.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	443	Total 3435	C 2181	N 646	O 598	S 10	0	0

- Molecule 15 is a protein called Putative U3 snoRNP protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	864	Total 6446	C 4152	N 1189	O 1079	S 26	0	0

- Molecule 16 is a protein called Utp24.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	190	Total 1460	C 928	N 281	O 241	S 10	0	0

- Molecule 17 is a protein called Utp30.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Q	182	Total 905	C 541	N 182	O 182	0	0

- Molecule 18 is a protein called Nop1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	242	Total 1778	C 1149	N 327	O 293	S 9	0	0
18	S	237	Total 1816	C 1154	N 318	O 335	S 9	0	0

- Molecule 19 is a protein called Putative nucleolar protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	387	Total 2866	C 1836	N 527	O 492	S 11	0	0

- Molecule 20 is a protein called Nop58.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	405	Total 3035	C 1954	N 539	O 532	S 10	0	0

- Molecule 21 is a protein called Snu13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	V	121	879	557	165	154	3	0	0
21	W	120	864	550	161	150	3	0	0

- Molecule 22 is a protein called Rrp9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	X	347	2686	1707	486	481	12	0	0

- Molecule 23 is a protein called RNA 3'-terminal phosphate cyclase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	Y	345	2594	1648	465	472	9	0	0

- Molecule 24 is a protein called Bms1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	Z	639	4848	3145	903	782	18	0	0

- Molecule 25 is a protein called Imp3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	a	179	1434	918	283	226	7	0	0

- Molecule 26 is a protein called Putative U3 small nucleolar ribonucleoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	b	291	2279	1445	437	389	8	0	0

- Molecule 27 is a protein called Putative U3 small nucleolar ribonucleoprotein protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	c	175	1387	869	269	244	5	0	0

- Molecule 28 is a protein called Sof1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	d	439	3436	2158	663	600	15	0	0

- Molecule 29 is a protein called Emg1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	e	215	1683	1067	293	313	10	0	0
29	f	215	1683	1067	293	313	10	0	0

- Molecule 30 is a protein called KRR1 small subunit processome component.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	g	174	1393	890	250	244	9	0	0

- Molecule 31 is a protein called Pre-rRNA-processing protein PNO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	h	167	1288	817	234	231	6	0	0

- Molecule 32 is a protein called RNA cytidine acetyltransferase.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
32	i	659	3254	1936	659	659	0	0
32	j	677	3342	1988	677	677	0	0

- Molecule 33 is a protein called Fcf2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	k	117	930	589	179	158	4	0	0

- Molecule 34 is a protein called 40S ribosomal protein S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	l	214	1735	1105	322	303	5	0	0

- Molecule 35 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	m	258	Total	C	N	O	S	0	0
			2057	1305	386	359	7		

- Molecule 36 is a protein called 40S ribosomal protein s5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	n	192	Total	C	N	O	S	0	0
			1447	918	277	245	7		

- Molecule 37 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	o	237	Total	C	N	O	S	0	0
			1911	1192	384	330	5		

- Molecule 38 is a protein called 40S ribosomal protein S7-like protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	p	159	Total	C	N	O	0	0
			1279	810	237	232		

- Molecule 39 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	q	201	Total	C	N	O	S	0	0
			1622	1009	330	282	1		

- Molecule 40 is a protein called 40S ribosomal protein s9-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	r	159	Total	C	N	O	S	0	0
			1242	801	255	184	2		

- Molecule 41 is a protein called 40S ribosomal protein S13-like protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	s	49	Total	C	N	O	0	0
			416	270	82	64		

- Molecule 42 is a protein called 40S ribosomal protein S14-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	t	115	Total 791	C 492	N 154	O 141	S 4	0	0

- Molecule 43 is a protein called 40S ribosomal protein S16-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	u	126	Total 943	C 613	N 177	O 151	S 2	0	0

- Molecule 44 is a protein called 40S ribosomal protein S11-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	v	157	Total 1286	C 825	N 248	O 208	S 5	0	0

- Molecule 45 is a protein called 40S ribosomal protein S22-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	w	126	Total 985	C 632	N 184	O 164	S 5	0	0

- Molecule 46 is a protein called 40S ribosomal protein s23-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	x	94	Total 684	C 445	N 129	O 108	S 2	0	0

- Molecule 47 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	y	93	Total 752	C 481	N 140	O 129	S 2	0	0

- Molecule 48 is a protein called 40S ribosomal protein S28-like protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	z	61	Total 455	C 284	N 97	O 74	0	0

- Molecule 49 is a protein called Faf1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	0	92	694	426	144	120	4	0	0

- Molecule 50 is a RNA chain called 35S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
50	1	1350	28796	12851	5157	9440	1348	0	0

- Molecule 51 is a RNA chain called U3 snoRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
51	2	230	4891	2182	856	1623	230	0	0

- Molecule 52 is ZINC ION (three-letter code: ZN) (formula: Zn).

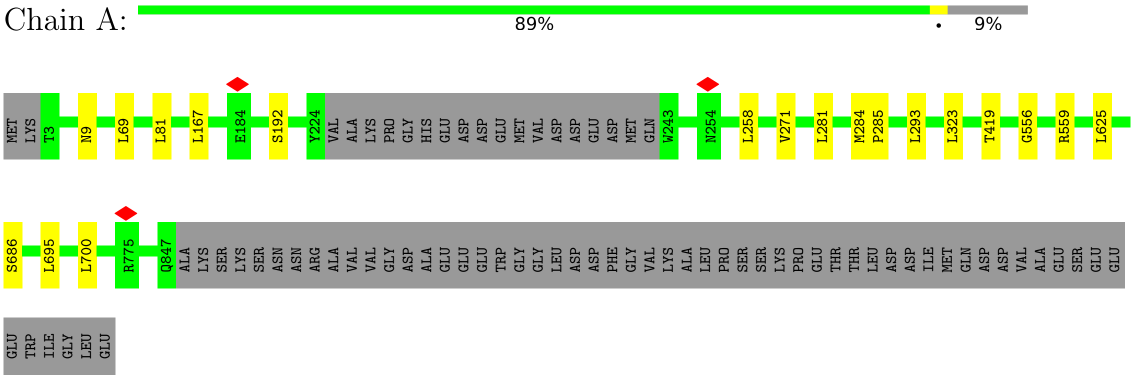
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
52	P	1	1	1	0

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.

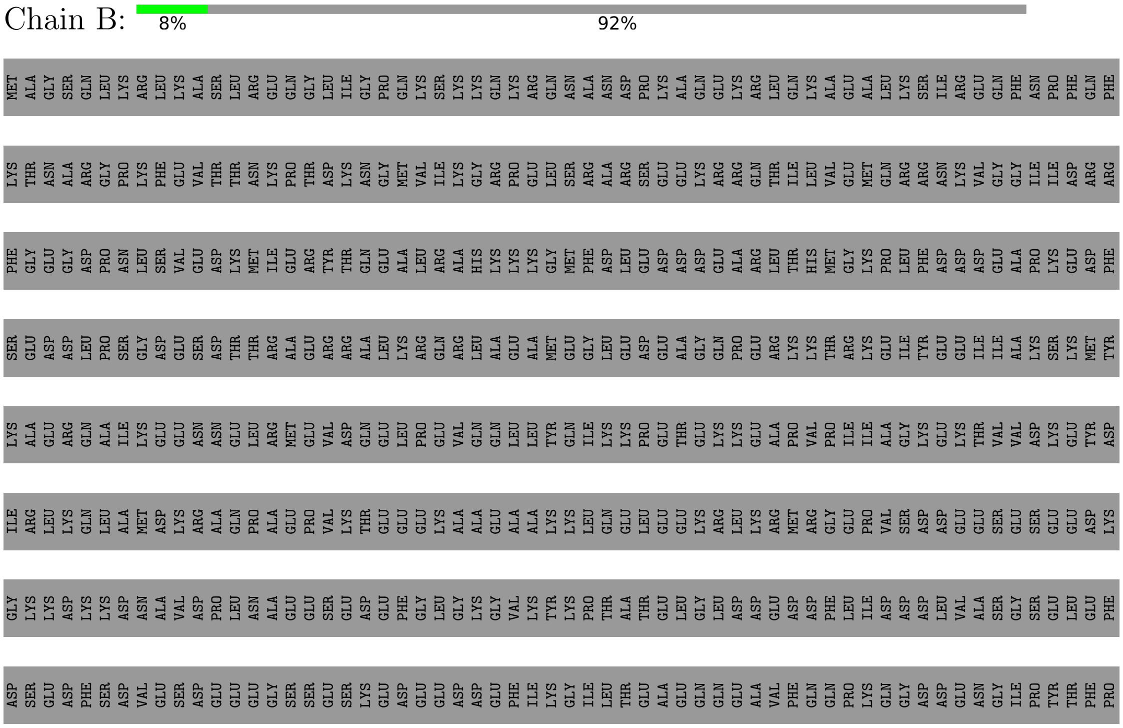
- Molecule 1: Periodic tryptophan protein 2-like protein

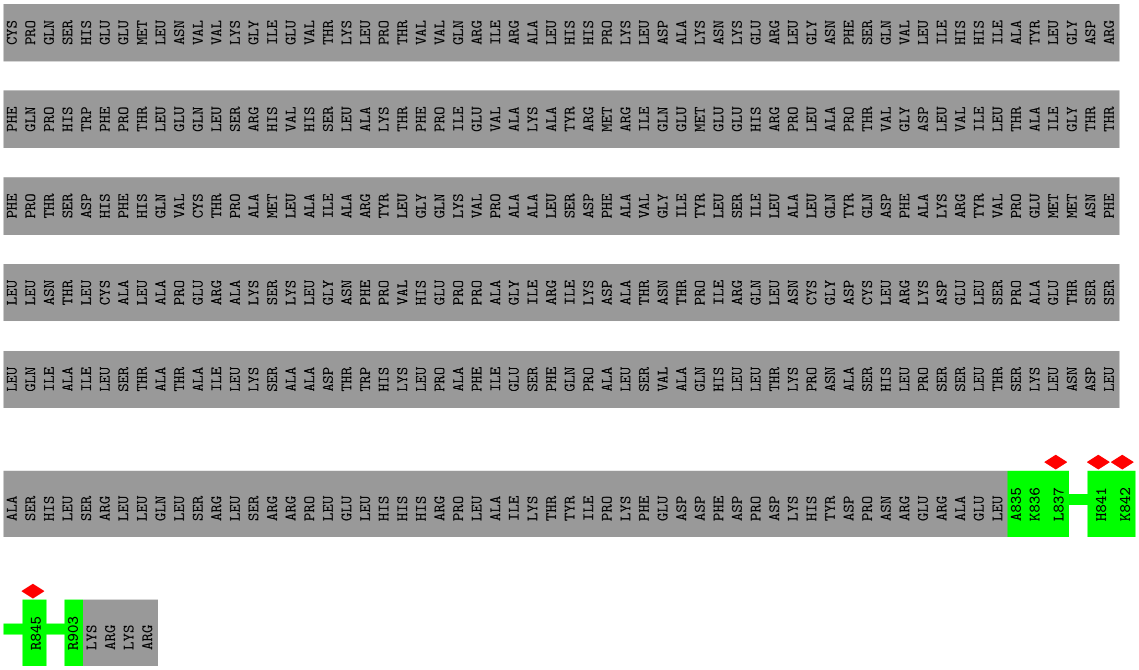
Chain A:



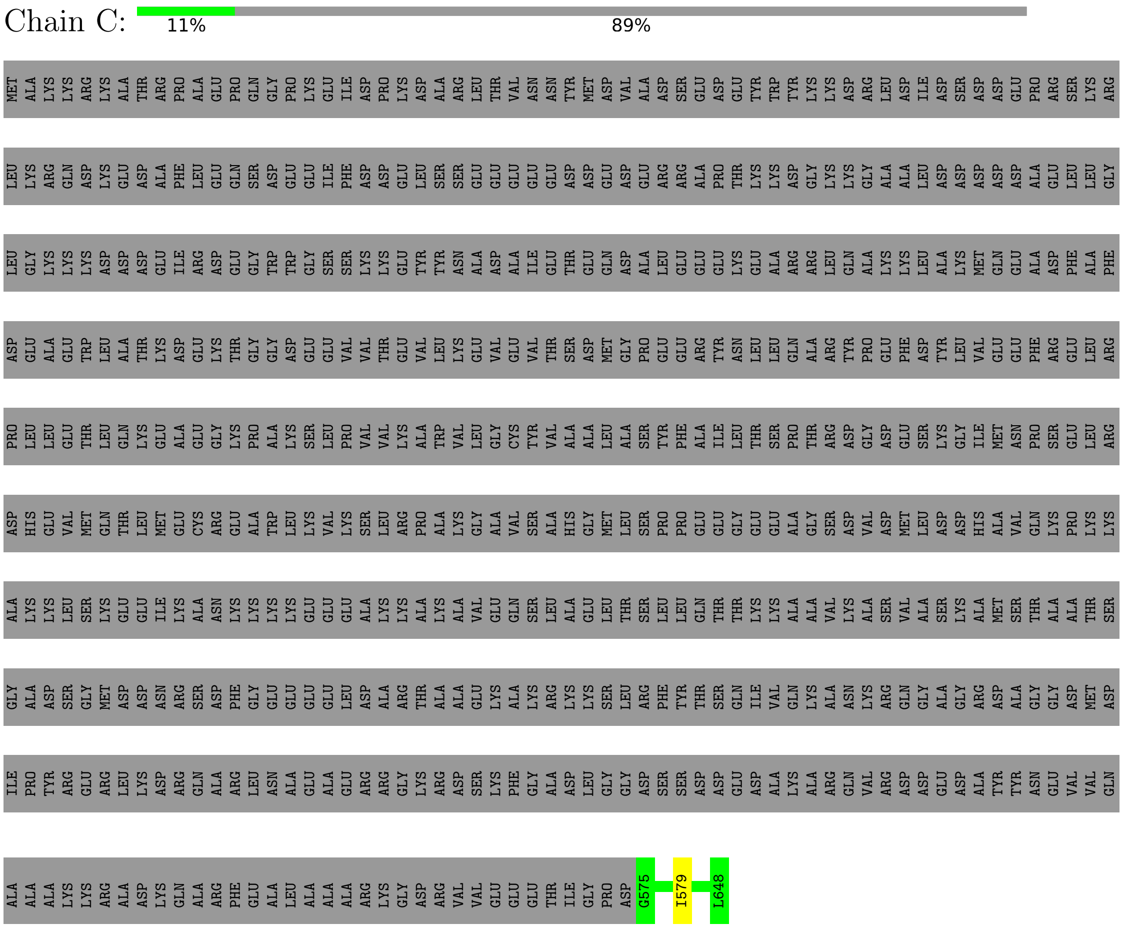
- Molecule 2: Utp2

Chain B:

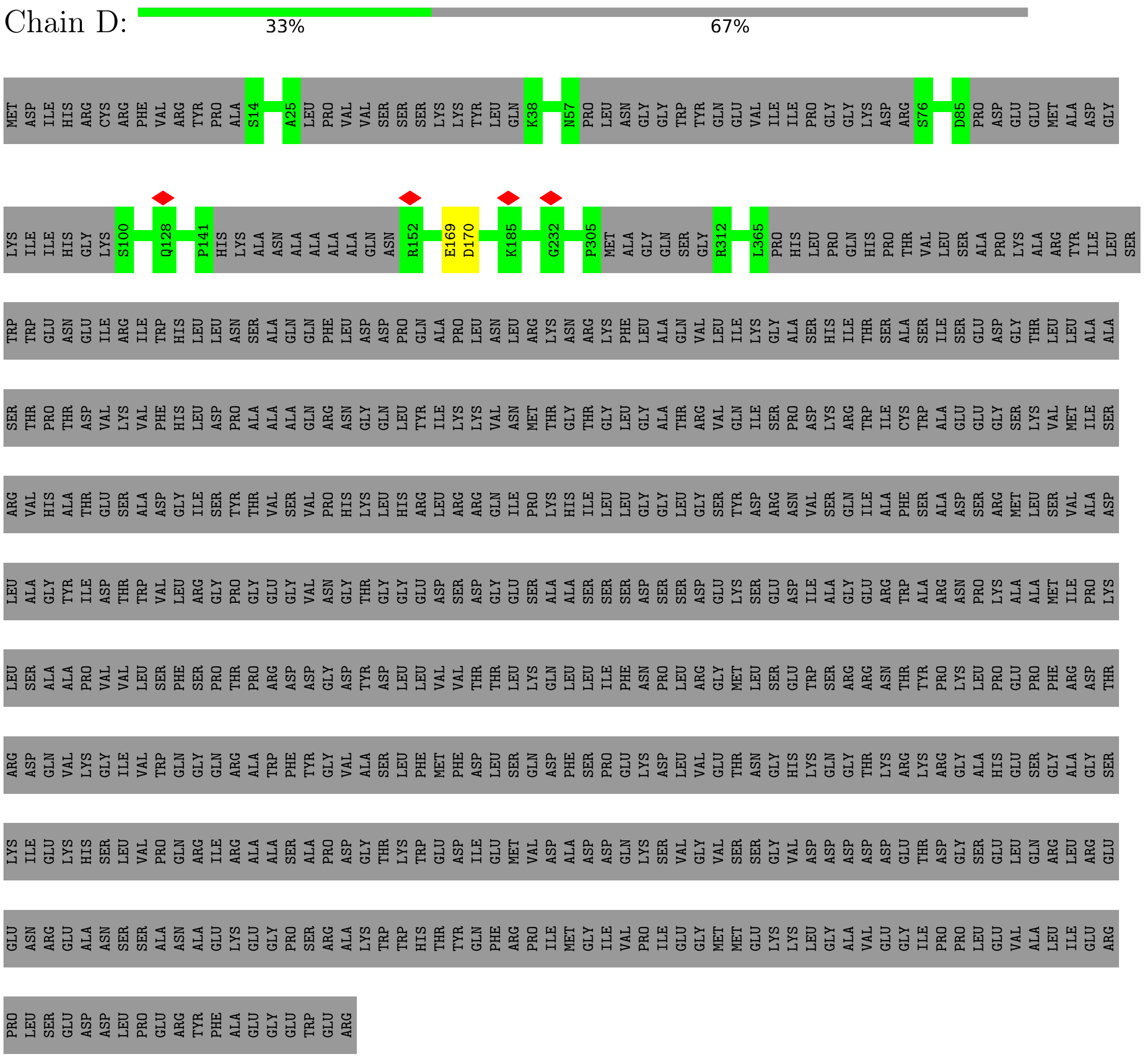




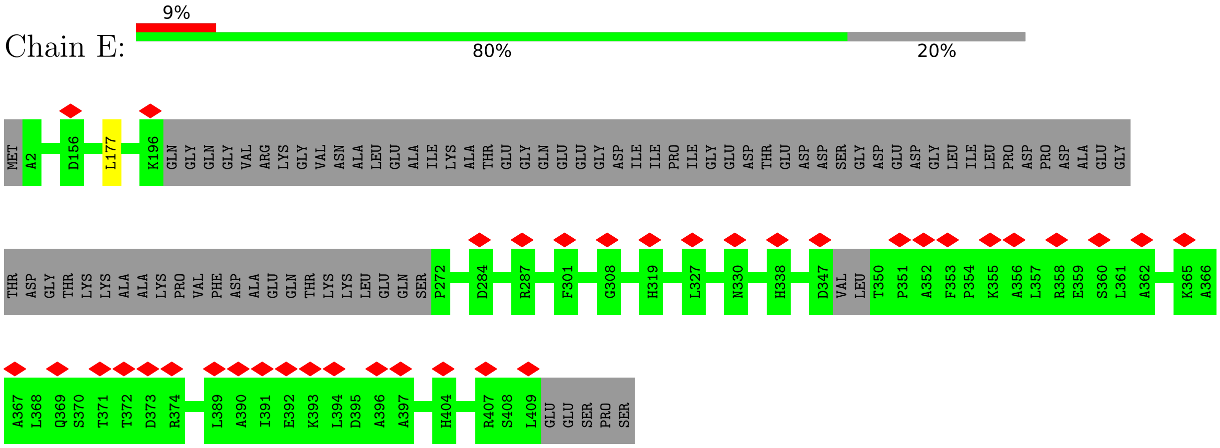
- Molecule 3: Utp3



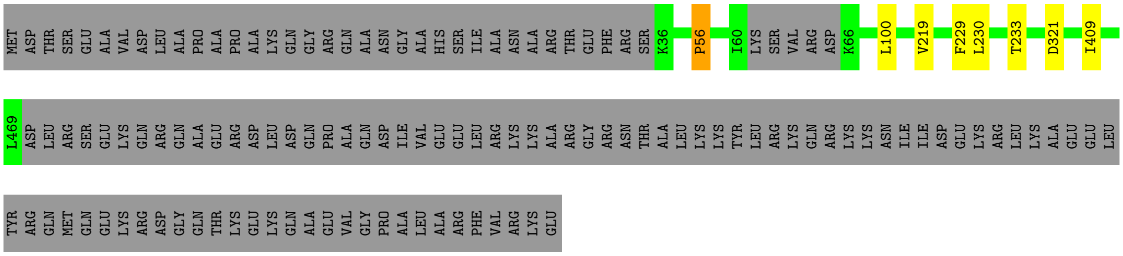
- Molecule 4: Utp4



- Molecule 5: Utp6

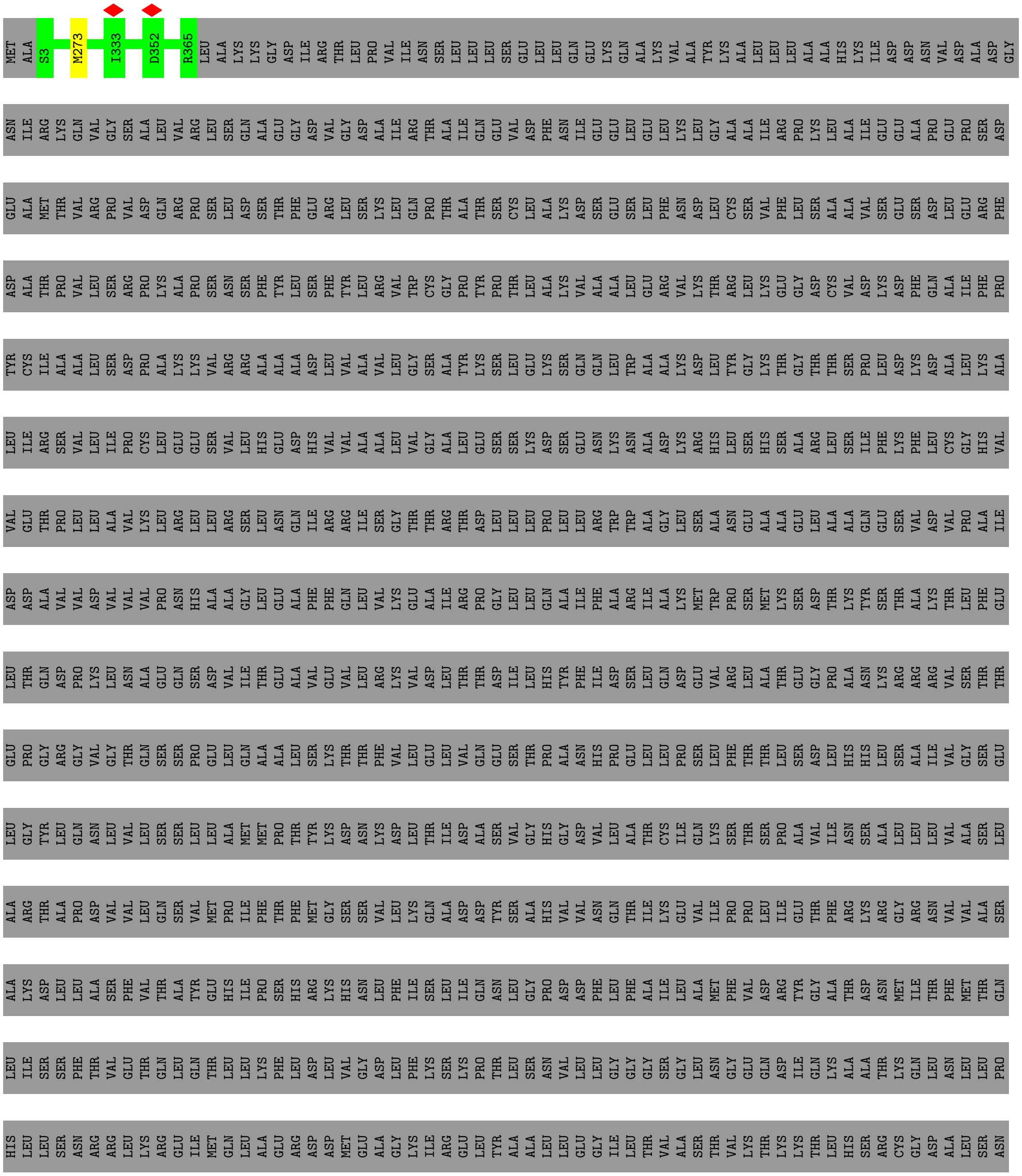


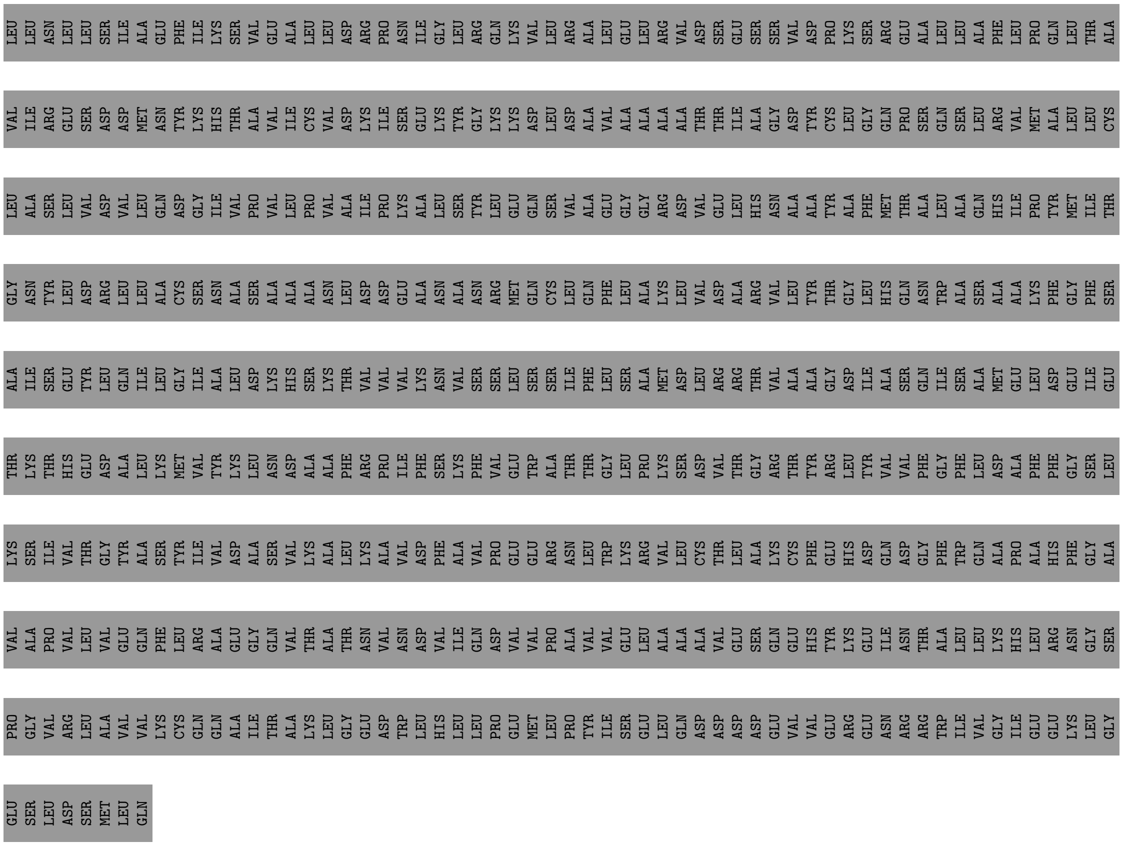
- Molecule 6: Utp7



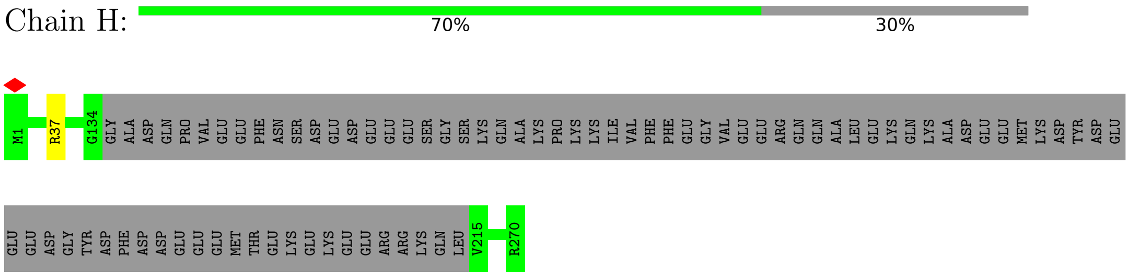
- Molecule 7: Utp10

Chain G:

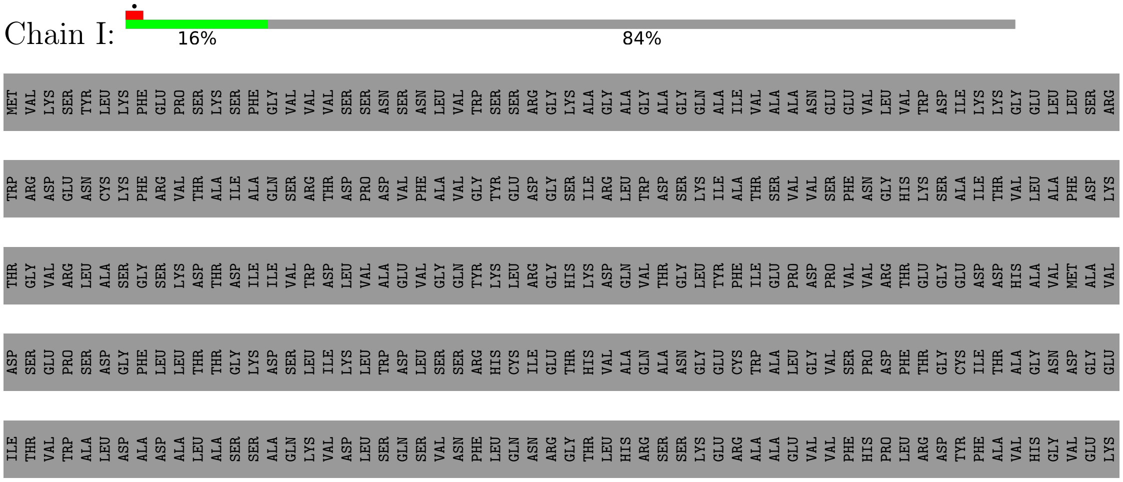


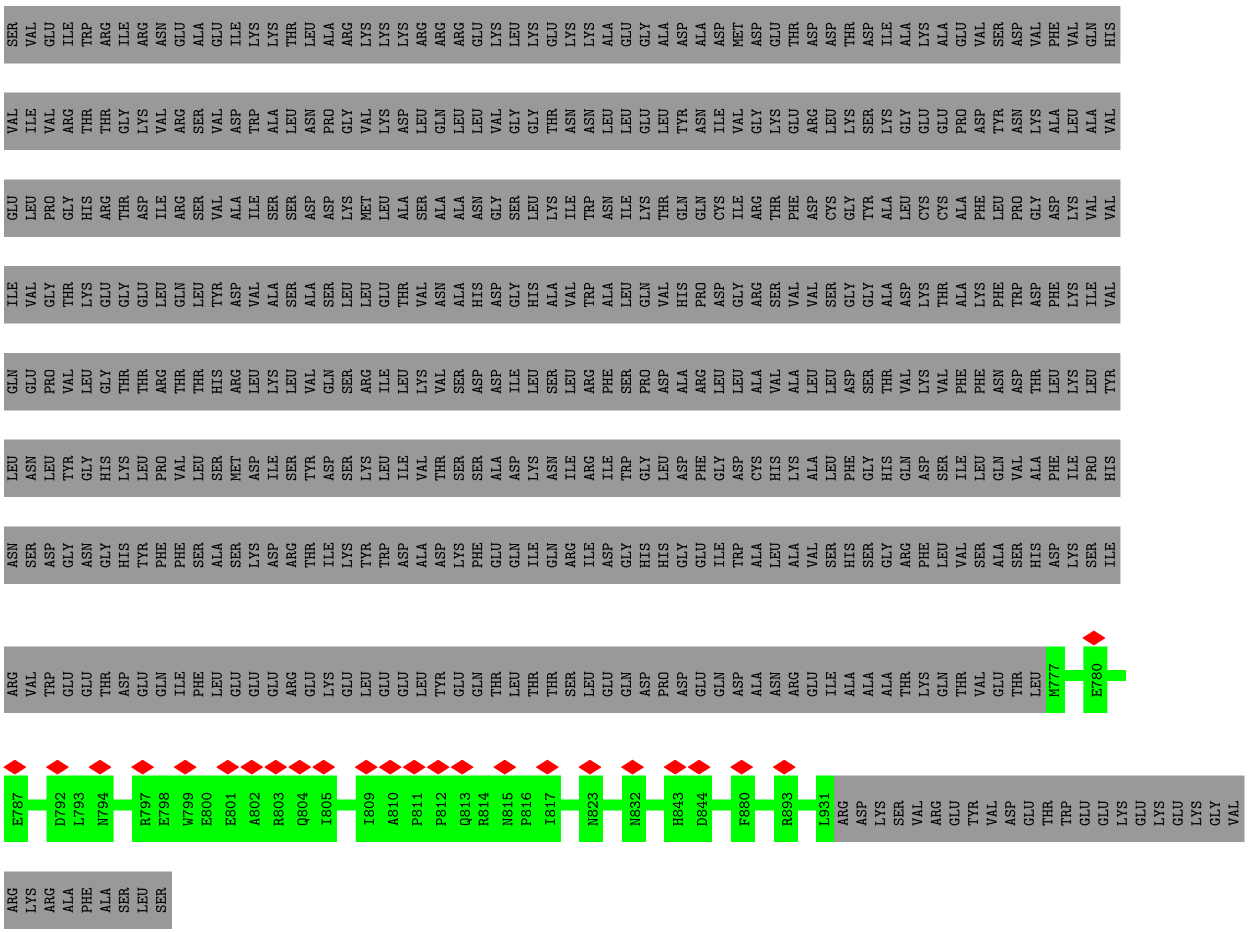


• Molecule 8: U3 small nucleolar RNA-associated protein 11



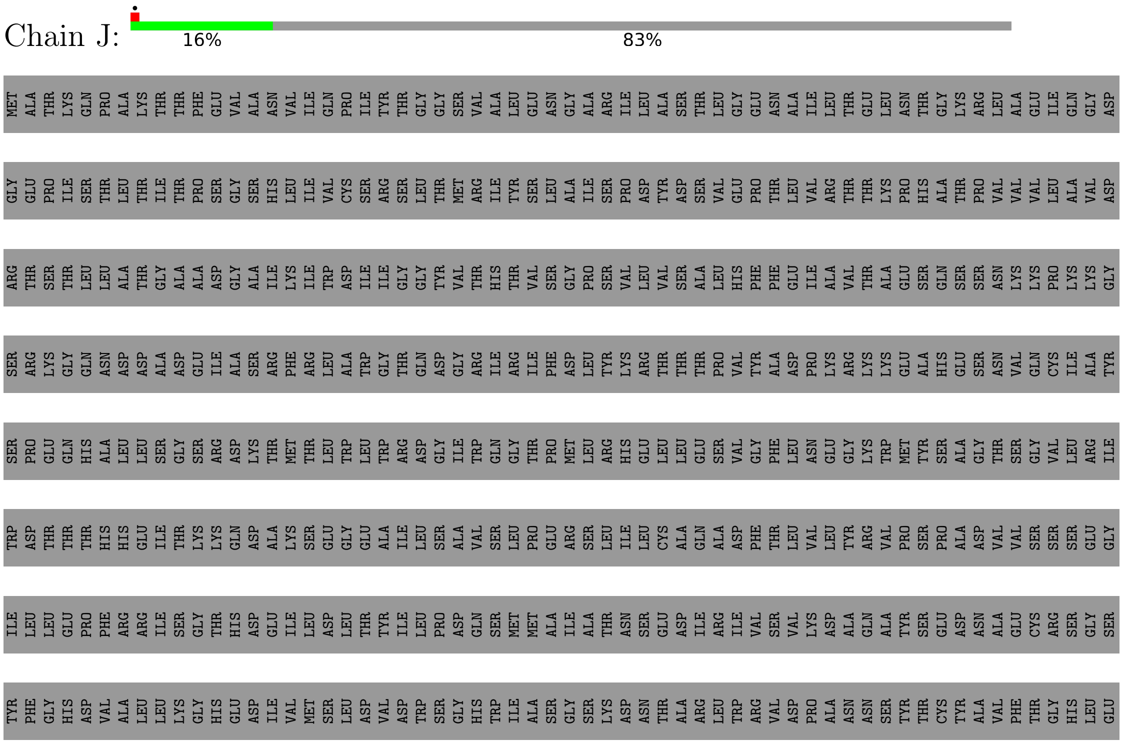
• Molecule 9: Utp12

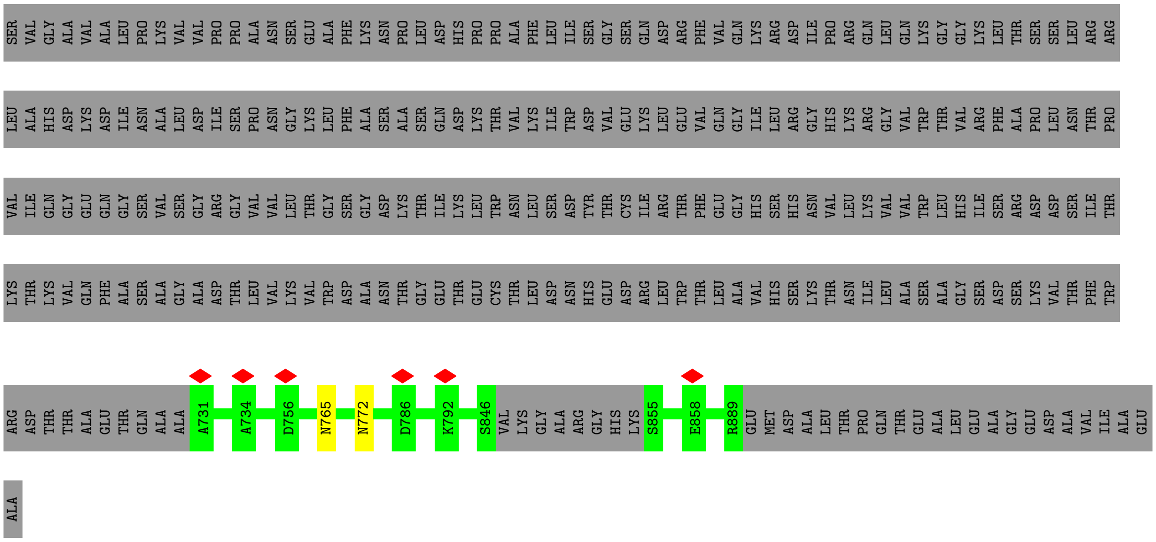




- Molecule 10: Utp13

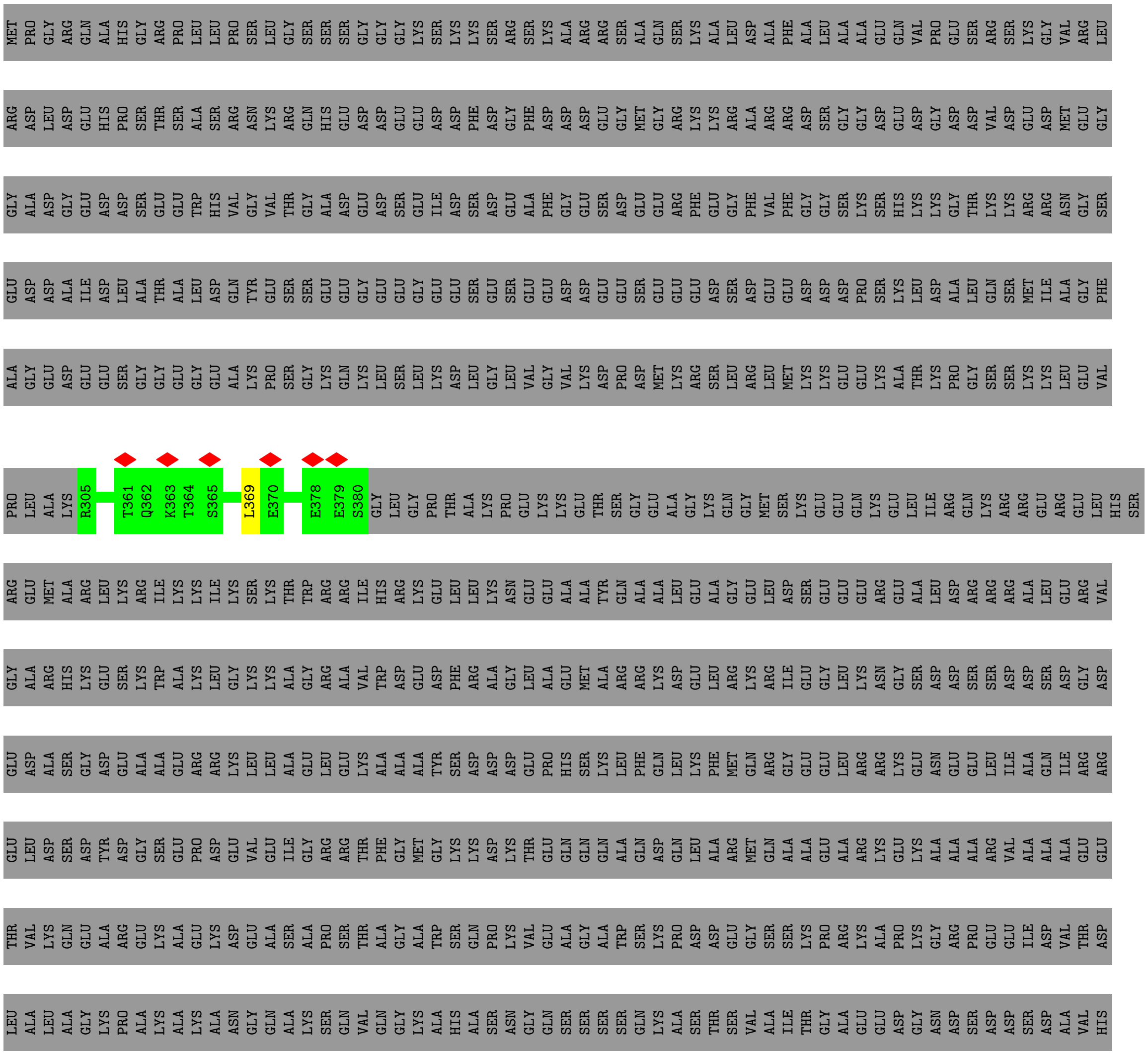
Chain J:

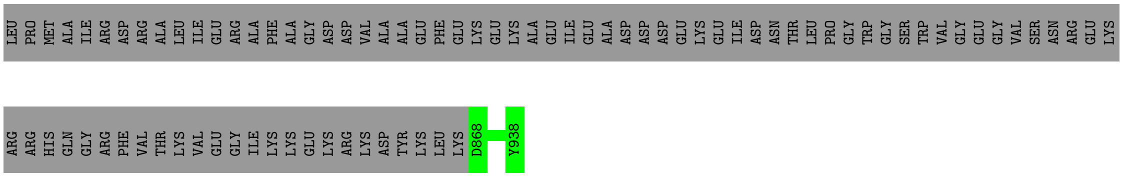




- Molecule 11: Utp14

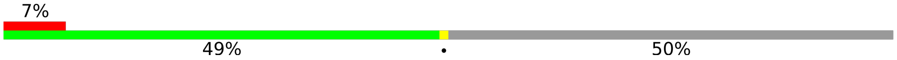
Chain K:

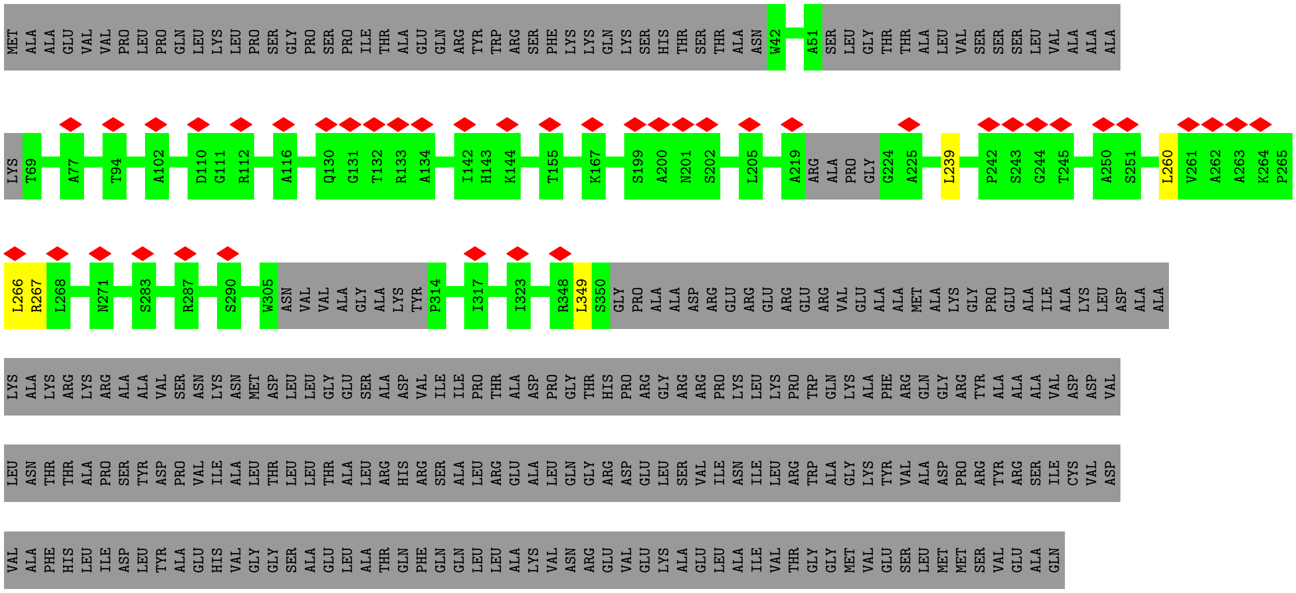




- Molecule 12: Utp15

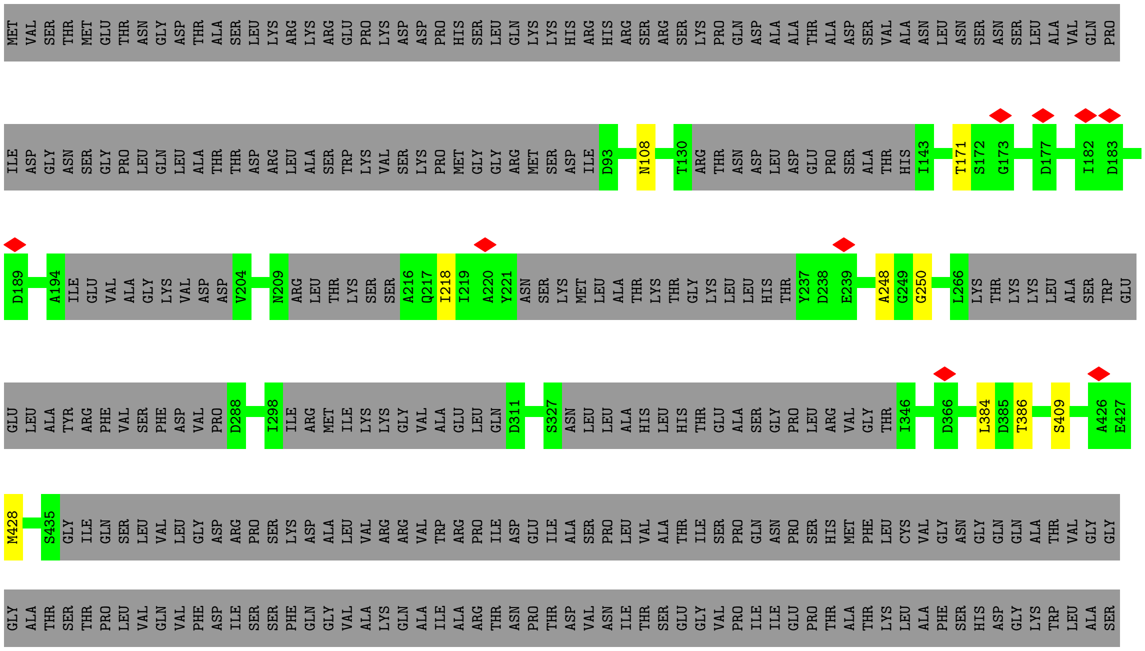
Chain L:

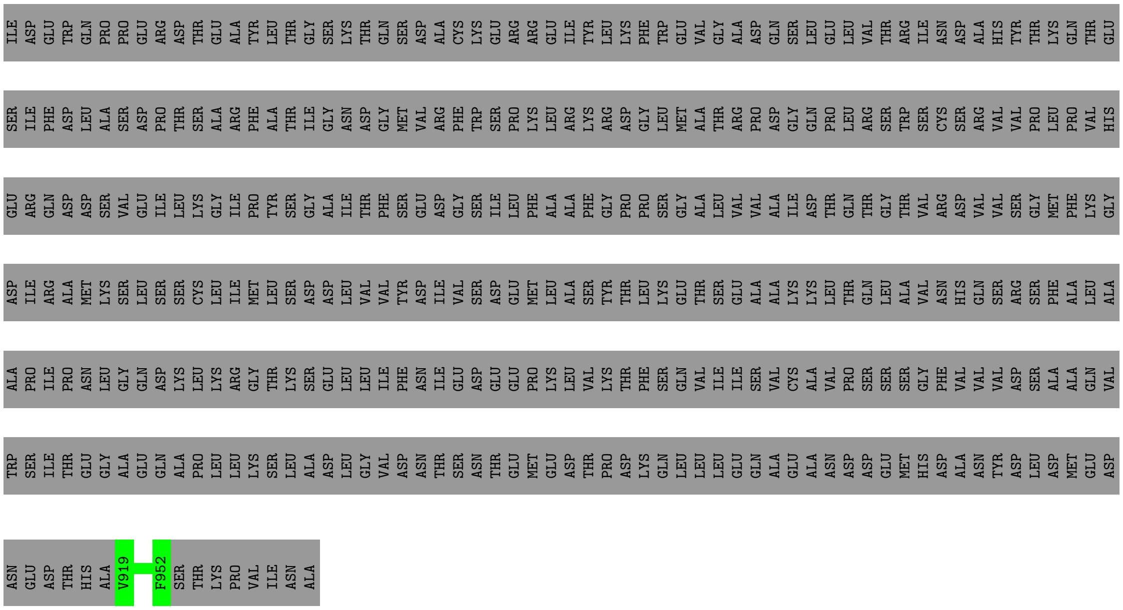




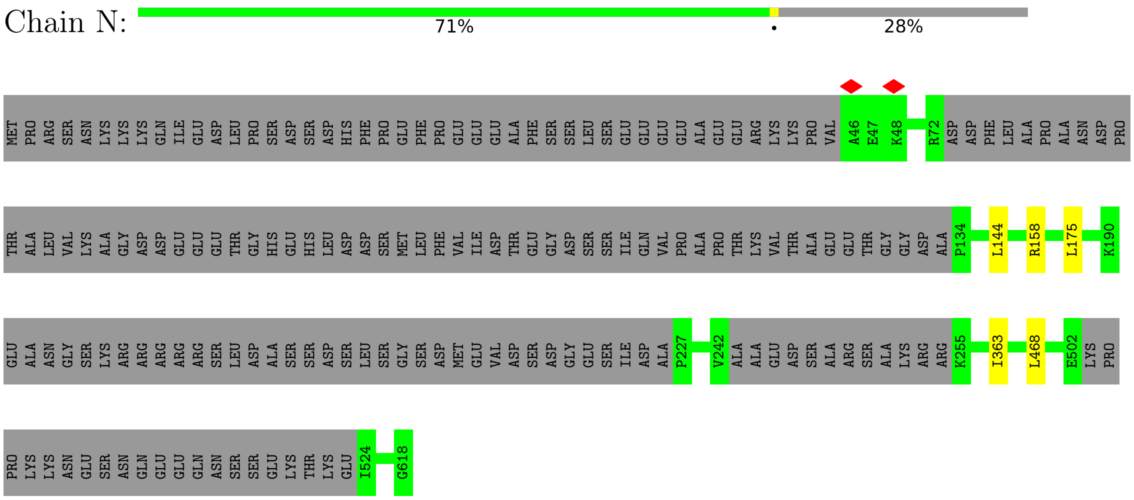
- Molecule 13: Utp17

Chain M:

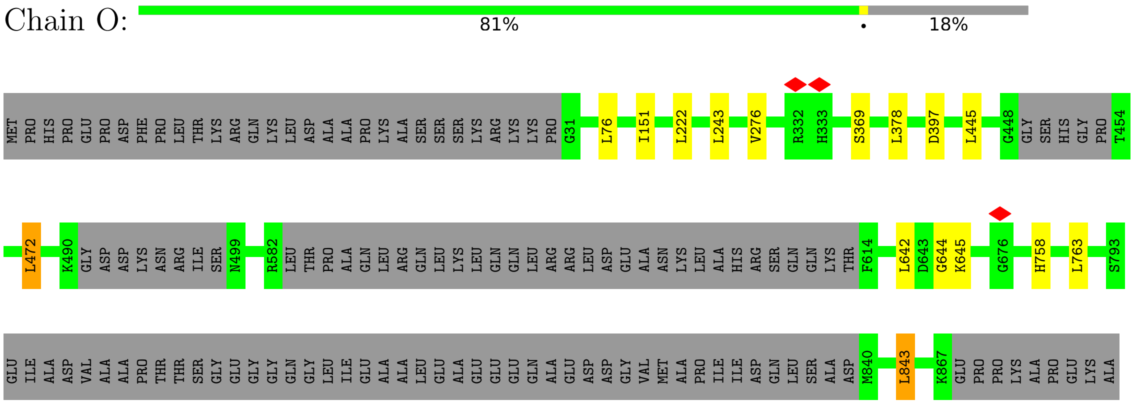


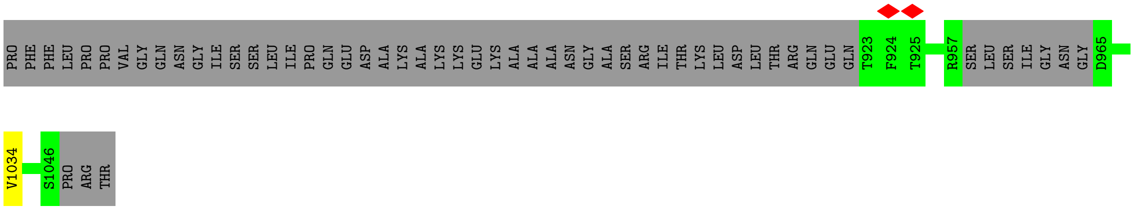


- Molecule 14: Utp18



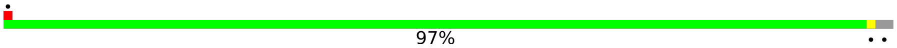
- Molecule 15: Putative U3 snoRNP protein

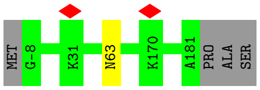




- Molecule 16: Utp24

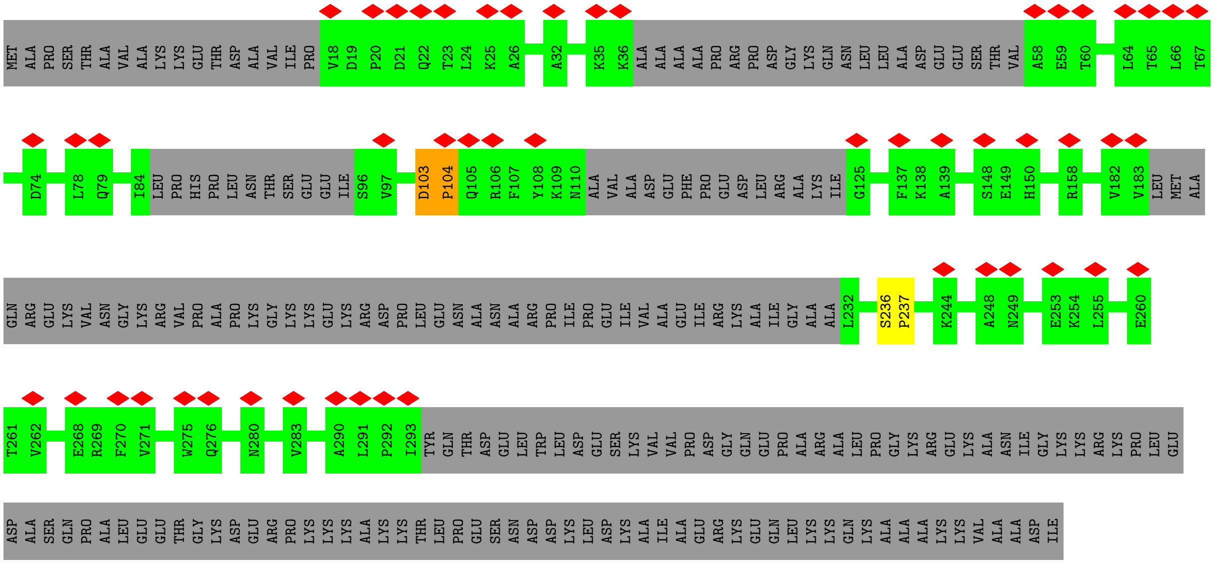
Chain P:





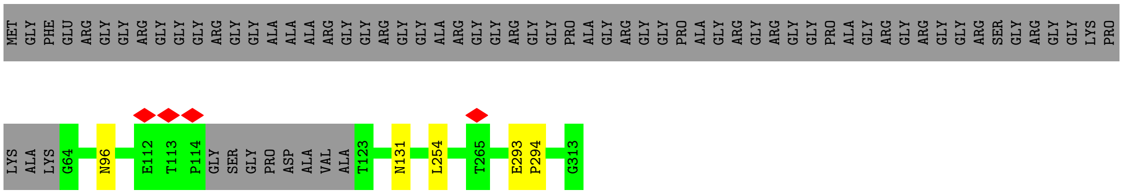
- Molecule 17: Utp30

Chain Q:



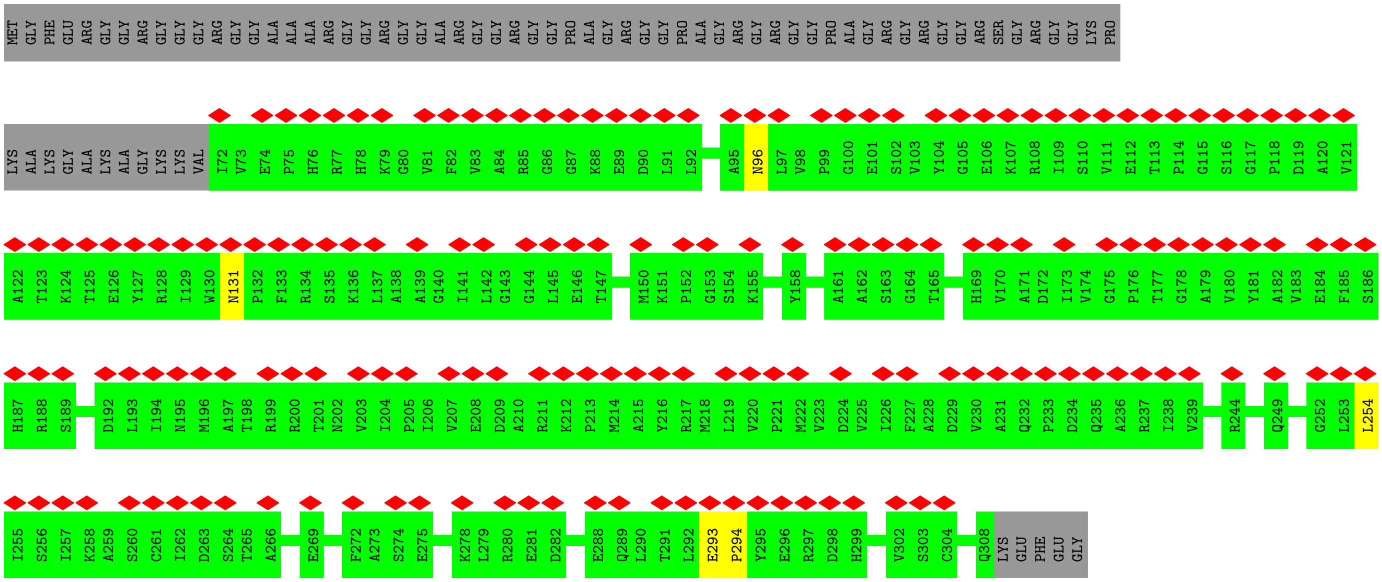
- Molecule 18: Nop1

Chain R:



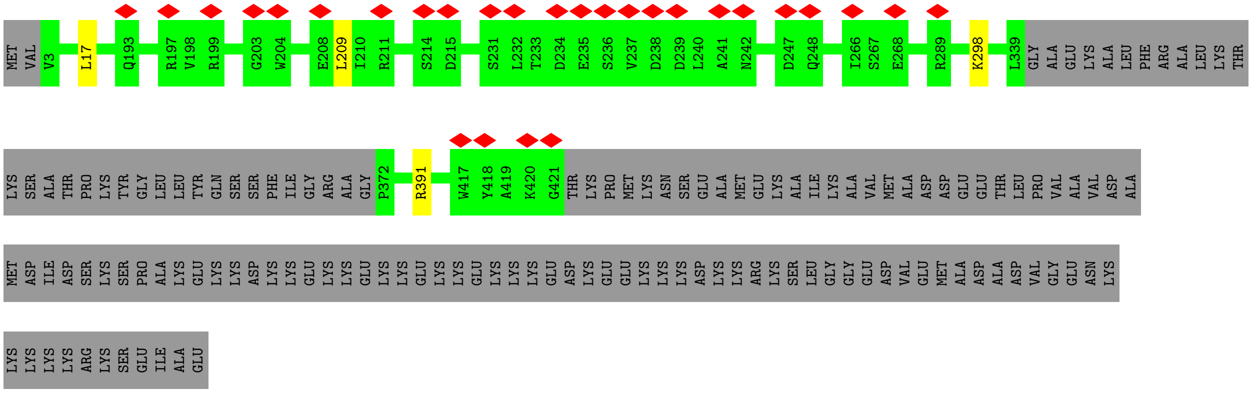
- Molecule 18: Nop1

Chain S:



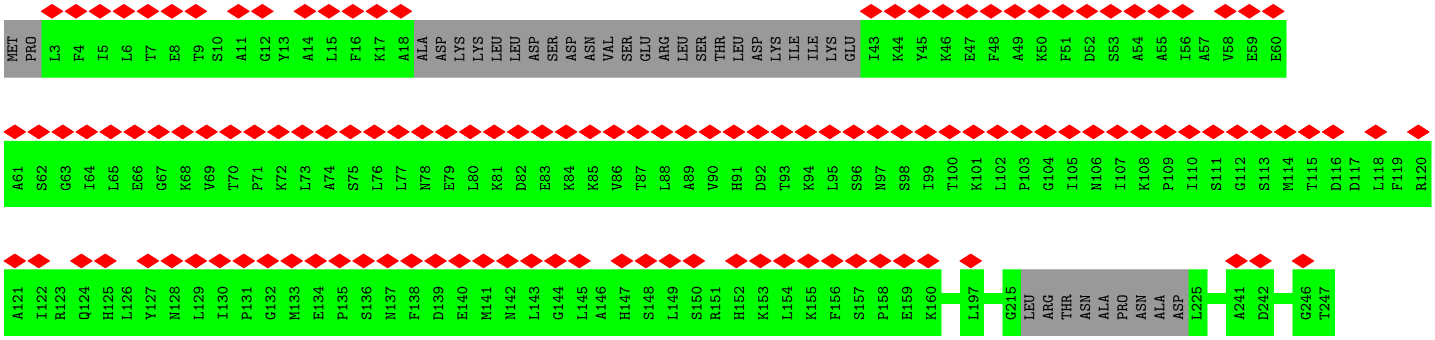
- Molecule 19: Putative nucleolar protein

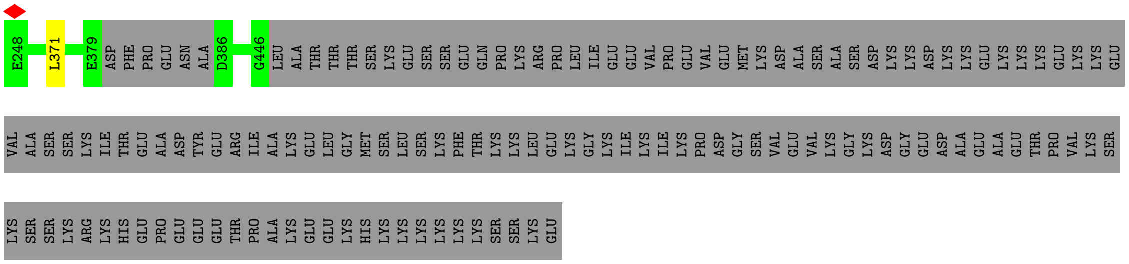
Chain T:



- Molecule 20: Nop58

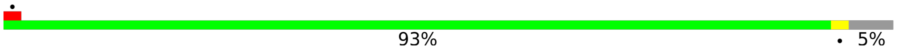
Chain U:

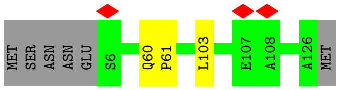




- Molecule 21: Snu13

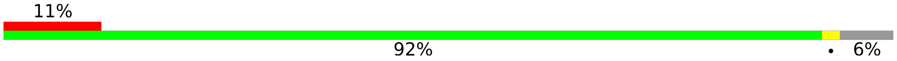
Chain V:

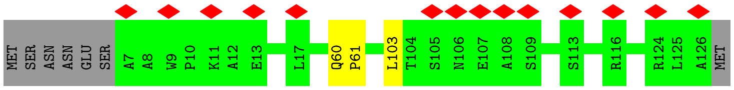




- Molecule 21: Snu13

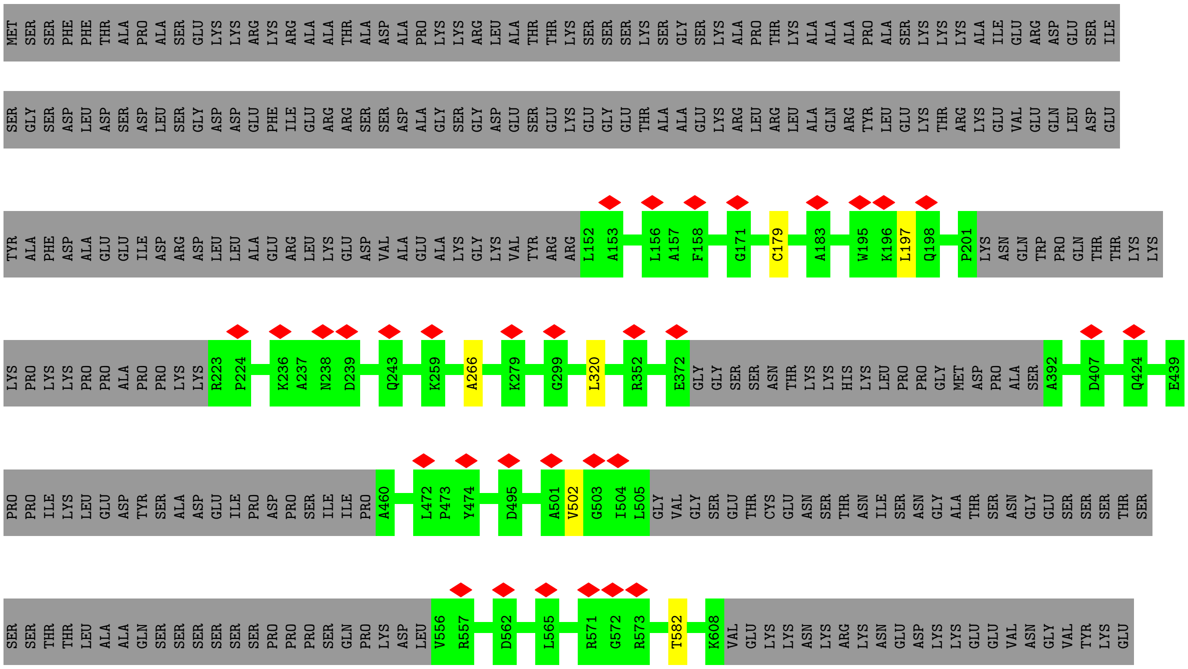
Chain W:





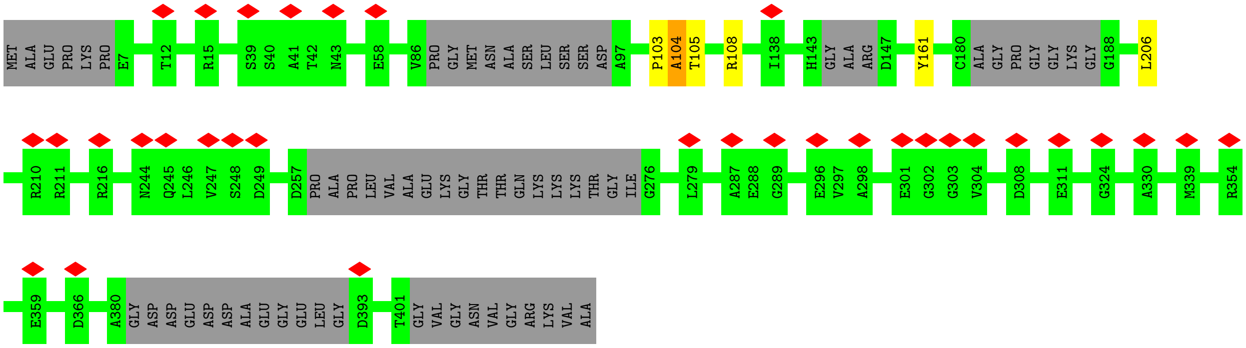
- Molecule 22: Rrp9

Chain X:



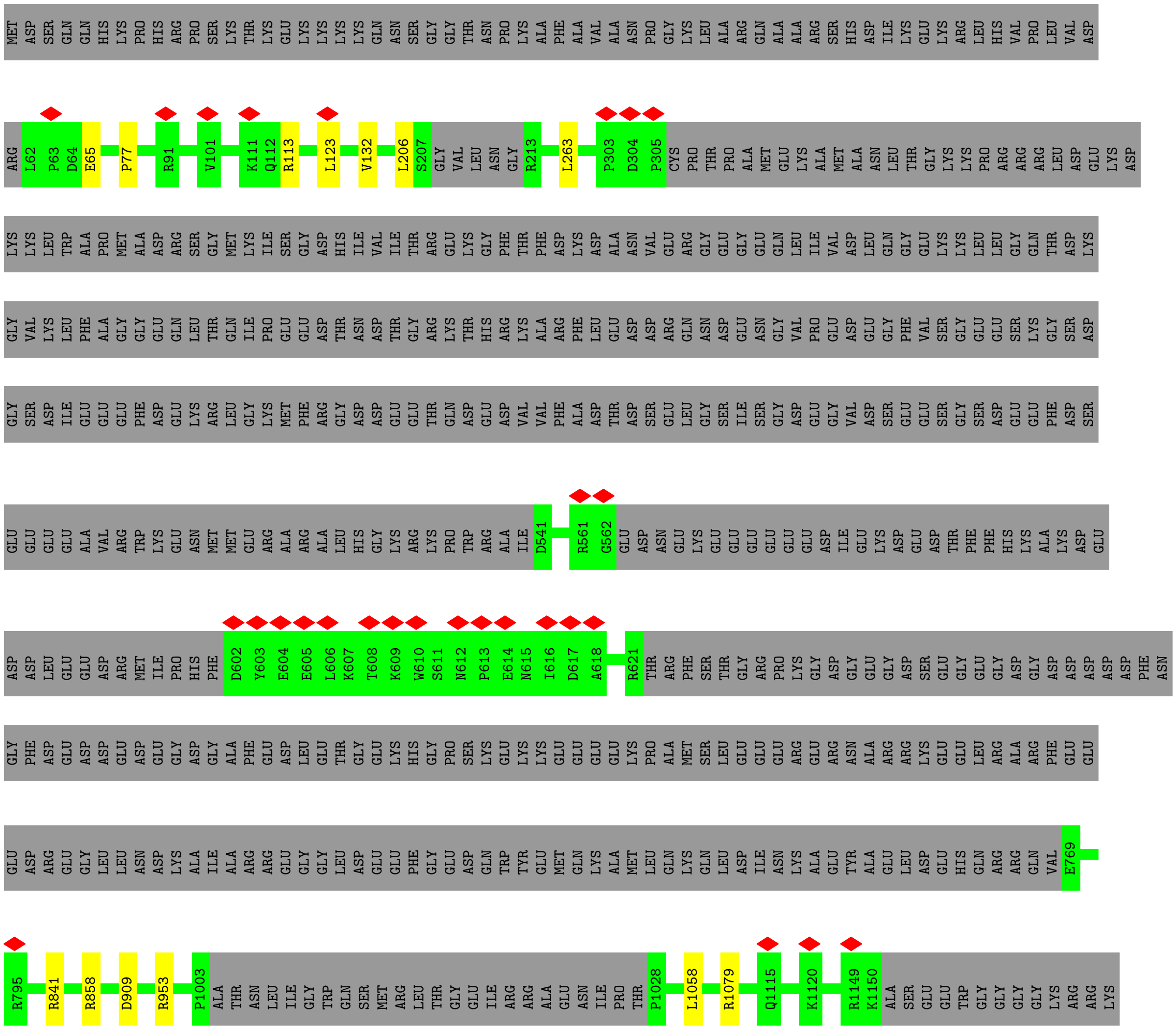
- Molecule 23: RNA 3'-terminal phosphate cyclase-like protein

Chain Y:



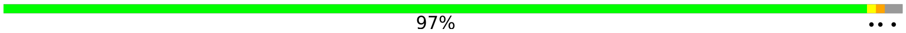
- Molecule 24: Bms1

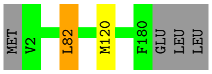
Chain Z:



- Molecule 25: Imp3

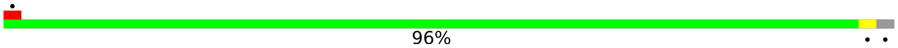
Chain a:

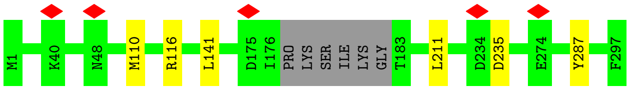




• Molecule 26: Putative U3 small nucleolar ribonucleoprotein

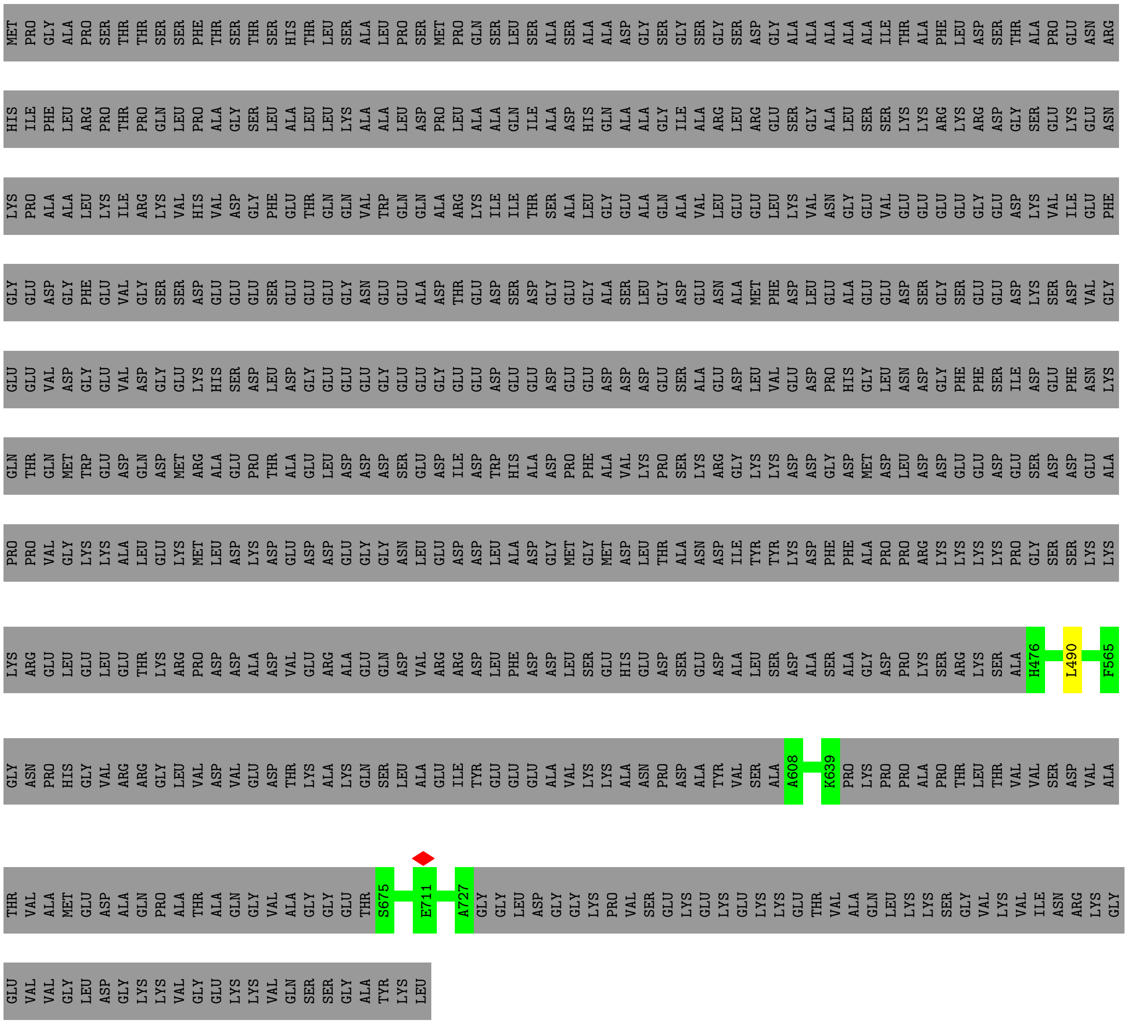
Chain b:





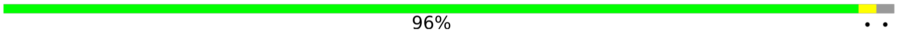
• Molecule 27: Putative U3 small nucleolar ribonucleoprotein protein

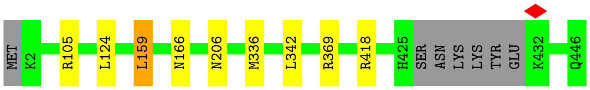
Chain c:



• Molecule 28: Sof1

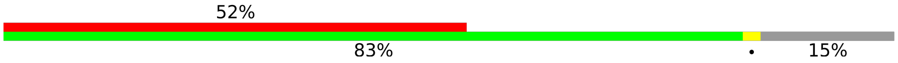
Chain d:

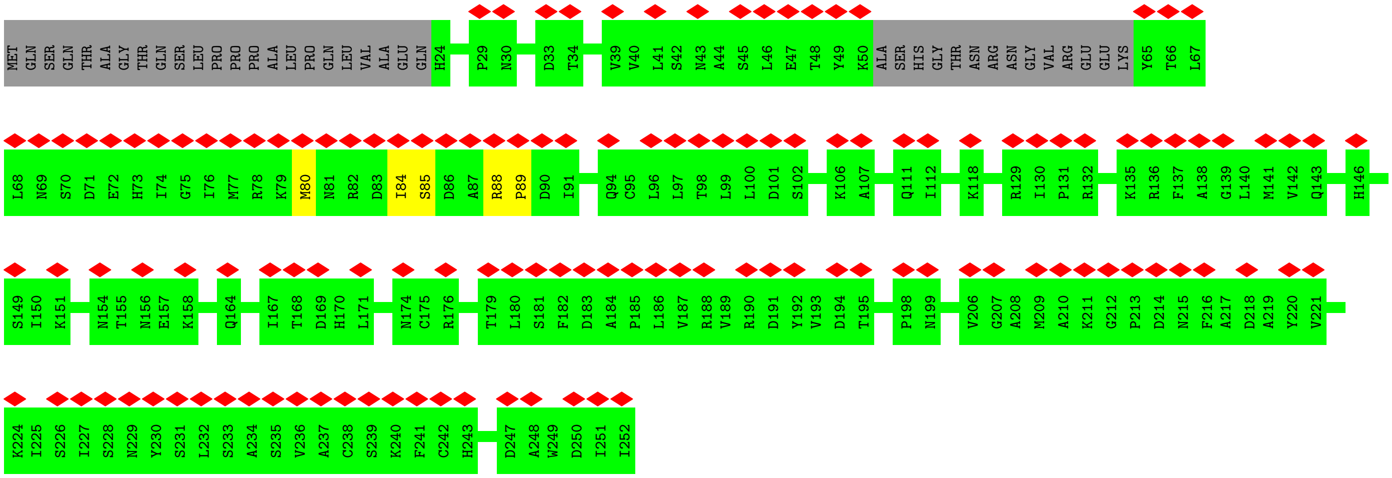




- Molecule 29: Emg1

Chain e:



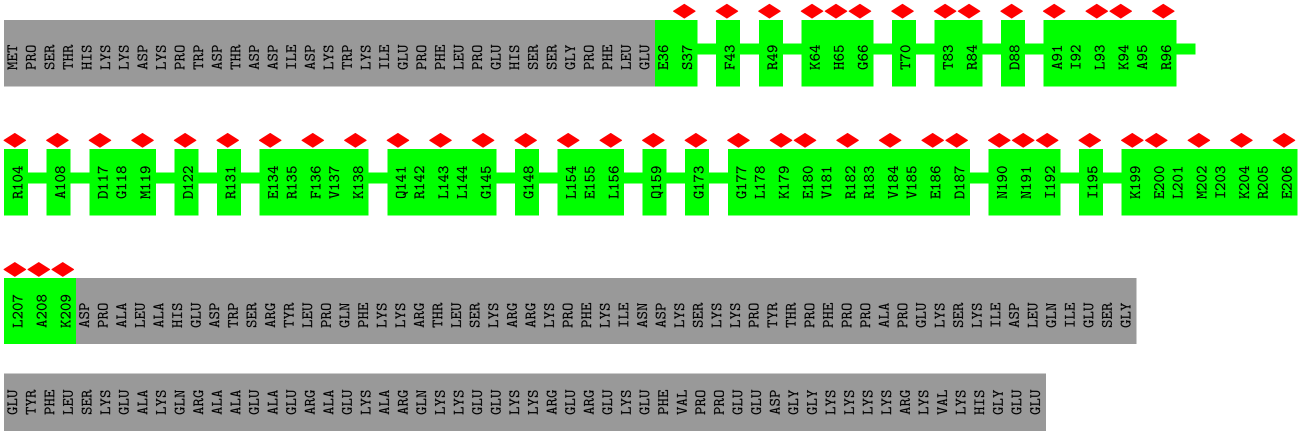


- Molecule 29: Emg1

Chain f:

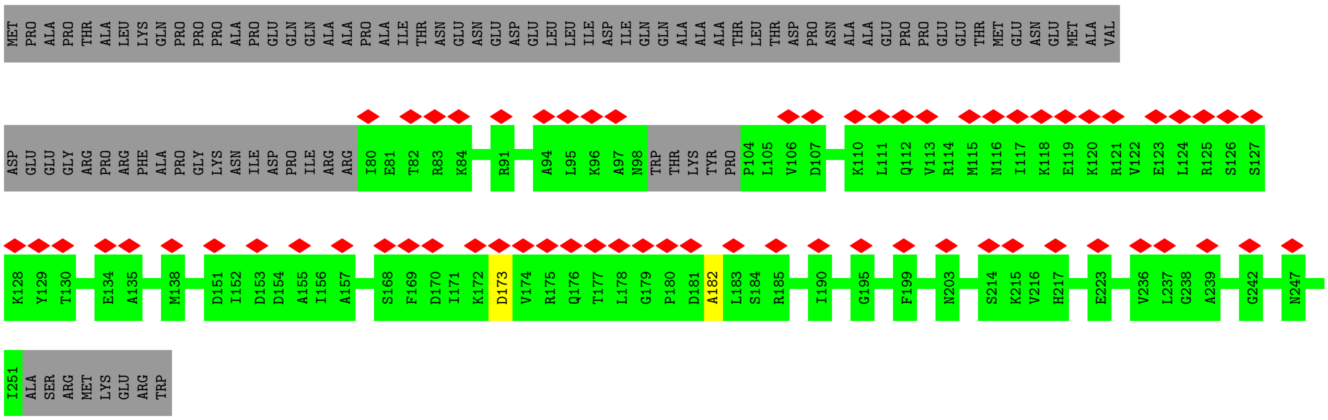
- Molecule 30: KRR1 small subunit processome component

Chain g:



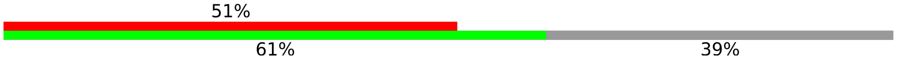
- Molecule 31: Pre-rRNA-processing protein PNO1

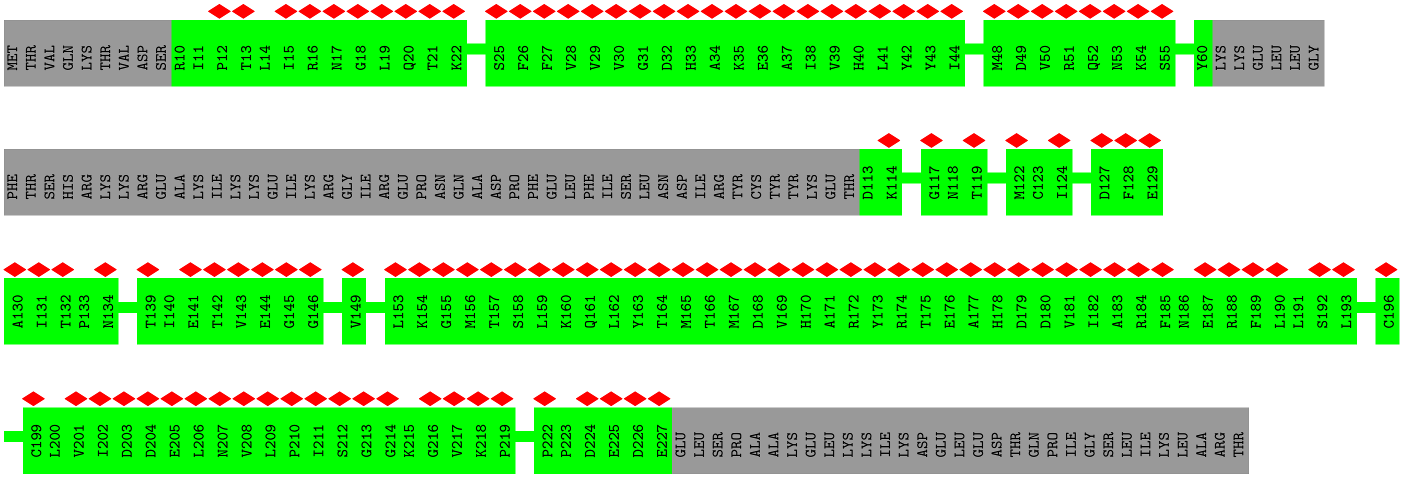
Chain h:

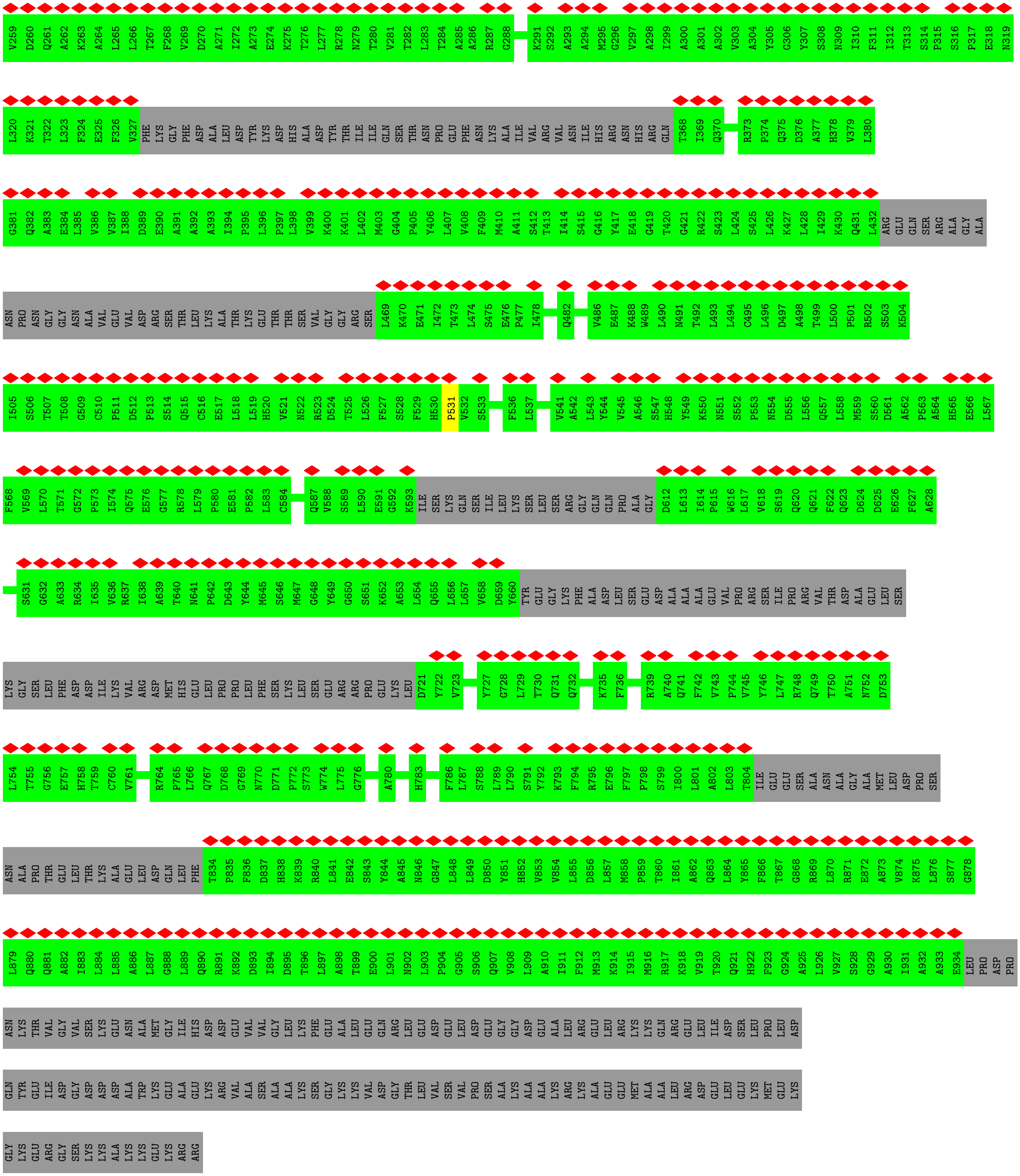


- Molecule 32: RNA cytidine acetyltransferase

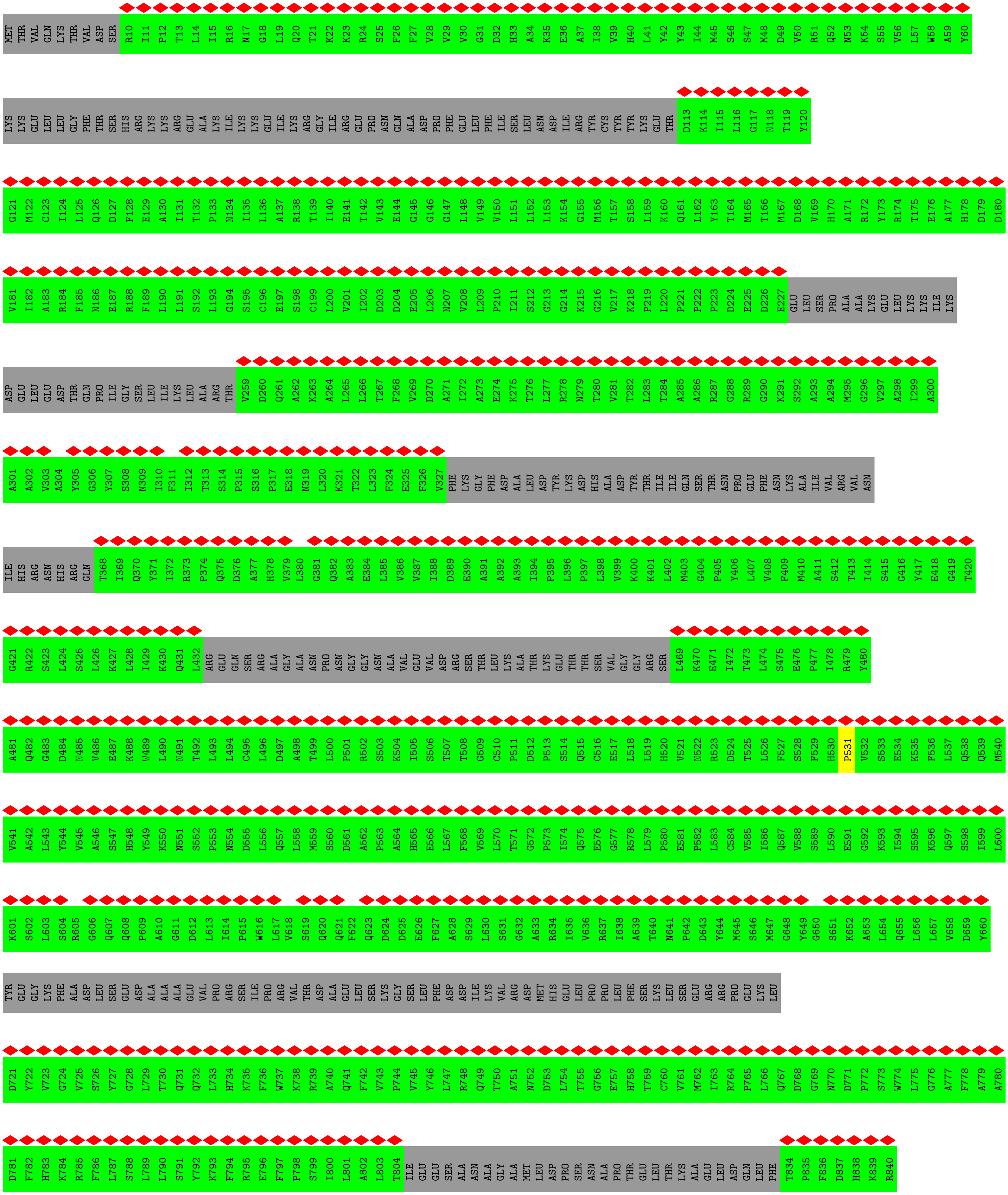
Chain i:







- Molecule 32: RNA cytidine acetyltransferase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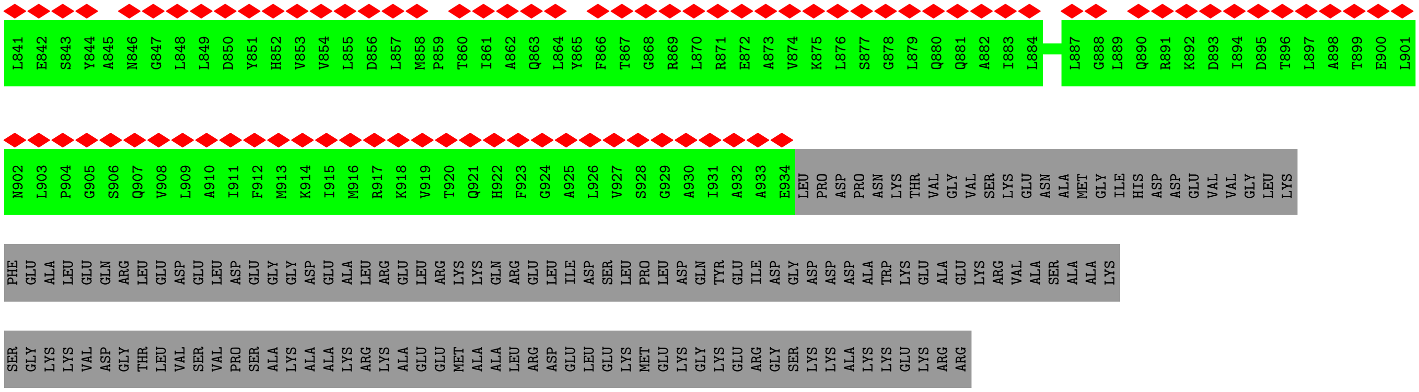
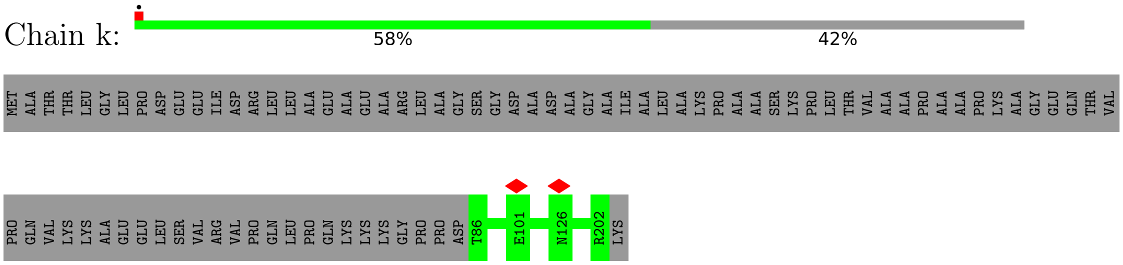
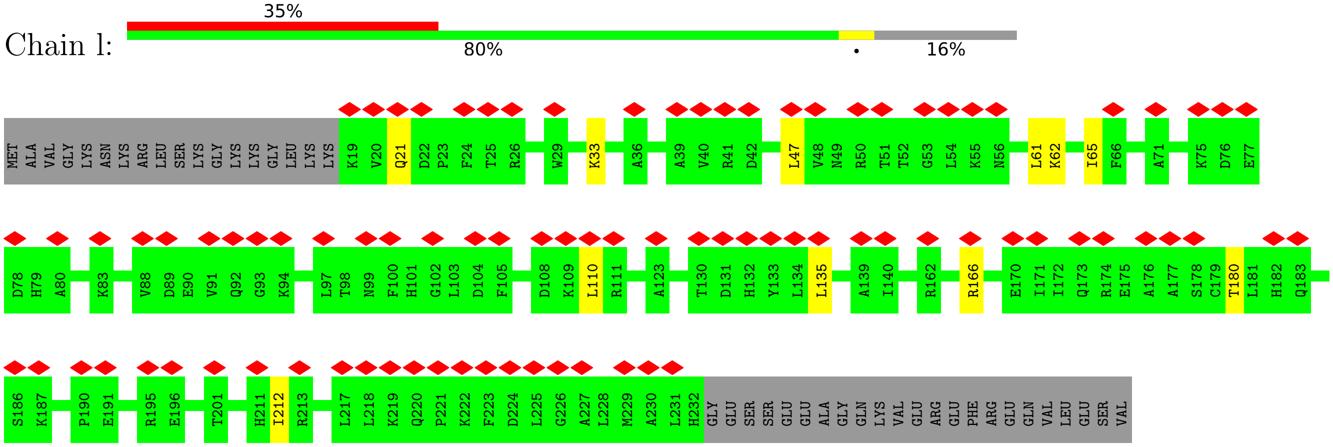
LYS LYS GLU LEU LEU GLY PHE THR SER HIS ARG LYS LYS ARG GLU ALA LYS ILE LYS LYS GLU ILE LYS ARG GLY ILE ARG GLU PRO ASN GLN ALA ASP PRO PHE GLU LEU PHE ILE SER LEU ASN ASP ILE ARG TYR CYS TYR TYR LYS GLU THR D113 K114 I115 L116 G117 N118 T119 Y120
G121 M122 C123 I124 L125 Q126 D127 F128 E129 A130 I131 T132 P133 N134 I135 L136 A137 R138 T139 I140 E141 T142 V143 E144 G145 G146 G147 L148 V149 V150 L151 L152 L153 K154 G155 M156 T157 S158 L159 K160 Q161 L162 Y163 T164 M165 T166 M167 D168 V169 H170 A171 R172 Y173 R174 T175 E176 A177 H178 D179 D180
V181 I182 A183 R184 F185 N186 E187 R188 F189 L190 L191 S192 L193 G194 S195 C196 E197 S198 C199 L200 V201 I202 D203 D204 E205 L206 N207 V208 L209 P210 I211 S212 G213 G214 K215 G216 V217 K218 P219 L220 P221 P222 P223 D224 E225 D226 E227 GLU LEU SER PRO ALA ALA LYS GLU LEU LYS LYS ILE LYS
ASP GLU LEU GLU ASP THR GLN PRO ILE GLY SER LEU ILE LYS LEU ALA ARG THR V259 D260 Q261 A262 K263 A264 L265 L266 T267 F268 V269 D270 A271 I272 A273 E274 K275 T276 L277 R278 N279 T280 V281 T282 L283 T284 A285 A286 R287 G288 R289 G290 K291 S292 A293 A294 M295 G296 V297 A298 I299 A300
A301 A302 V303 A304 Y305 G306 Y307 S308 N309 I310 F311 I312 T313 S314 P315 S316 P317 E318 N319 L320 K321 T322 L323 F324 E325 F326 V327 PHE LYS GLY PHE ASP ALA LEU ASP TYR LYS ASP HIS ALA ASP TYR THR ILE ILE GLN SER THR ASN PRO GLU PHE ASN LYS ALA ILE VAL ARG VAL ASN
ILE HIS ARG ASN HIS ARG GLN T368 I369 Q370 Y371 I372 R373 P374 Q375 D376 A377 H378 V379 L380 G381 Q382 A383 E384 L385 V386 V387 I388 D389 E390 A391 A392 A393 I394 P395 L396 P397 L398 V399 K400 K401 L402 M403 G404 P405 Y406 L407 V408 F409 M410 A411 S412 T413 I414 S415 G416 Y417 E418 G419 T420
G421 R422 S423 L424 S425 L426 K427 L428 I429 K430 Q431 L432 ARG GLU GLN SER ARG ALA GLY ALA ASN PRO ASN GLY GLY ASN ALA VAL GLU VAL ASP ARG SER THR LEU LYS ALA THR LYS GLU THR THR SER VAL GLY GLY ARG SER L469 K470 E471 I472 T473 L474 S475 E476 P477 I478 R479 Y480
A481 Q482 G483 D484 N485 V486 E487 K488 W489 L490 N491 T492 L493 L494 C495 L496 D497 A498 T499 L500 P501 R502 S503 K504 I505 S506 T507 T508 G509 C510 P511 D512 P513 S514 Q515 C516 E517 L518 L519 H520 V521 N522 R523 D524 T525 L526 F527 S528 F529 H530 P531 V532 S533 E534 K535 F536 L537 Q538 Q539 M540
V541 A542 L543 Y544 V545 A546 S547 H548 Y549 K550 N551 S552 P553 N554 D555 L556 Q557 L558 M559 S560 D561 A562 P563 A564 H565 E566 L567 F568 V569 L570 T571 G572 P573 I574 Q575 E576 G577 R578 L579 P580 E581 P582 L583 C584 V585 I586 Q587 V588 S589 L590 E591 G592 K593 I594 S595 K596 Q597 S598 I599 L600
K601 S602 L603 S604 R605 G606 Q607 Q608 P609 A610 G611 D612 L613 I614 P615 W616 L617 V618 S619 Q620 Q621 F622 Q623 D624 D625 E626 F627 A628 S629 L630 S631 G632 A633 R634 I635 V636 R637 I638 A639 T640 N641 P642 D643 Y644 M645 S646 M647 G648 Y649 G650 S651 K652 A653 L654 Q655 L656 L657 V658 D659 Y660
TYR GLU GLY LYS PHE ALA ASP LEU SER GLU ASP ALA ALA ALA GLU VAL PRO ARG SER ILE PRO ARG VAL THR ASP ALA GLU LEU SER LYS GLY SER LEU PHE ASP ASP ILE LYS VAL ARG ASP MET HIS GLU LEU PRO PRO LEU PHE SER LYS LEU SER GLU ARG ARG PRO GLU LYS LEU
D721 Y722 V723 G724 V725 S726 Y727 G728 L729 T730 Q731 Q732 L733 H734 K735 F736 W737 K738 R739 A740 Q741 F742 V743 P744 V745 Y746 L747 R748 Q749 T750 A751 N752 D753 L754 T755 G756 E757 H758 T759 C760 V761 M762 I763 R764 P765 L766 Q767 D768 G769 N770 D771 P772 S773 W774 L775 G776 A777 F778 A779 A780
D781 F782 H783 K784 R785 F786 L787 S788 L789 L790 S791 Y792 K793 F794 R795 E796 F797 P798 S799 I800 L801 A802 L803 T804 ILE GLU GLU SER ALA ASN ALA GLY ALA MET LEU ASP PRO SER ASN ALA PRO THR GLU LEU THR LYS ALA GLU LEU ASP GLN LEU PHE T834 P835 F836 D837 H838 K839 R840



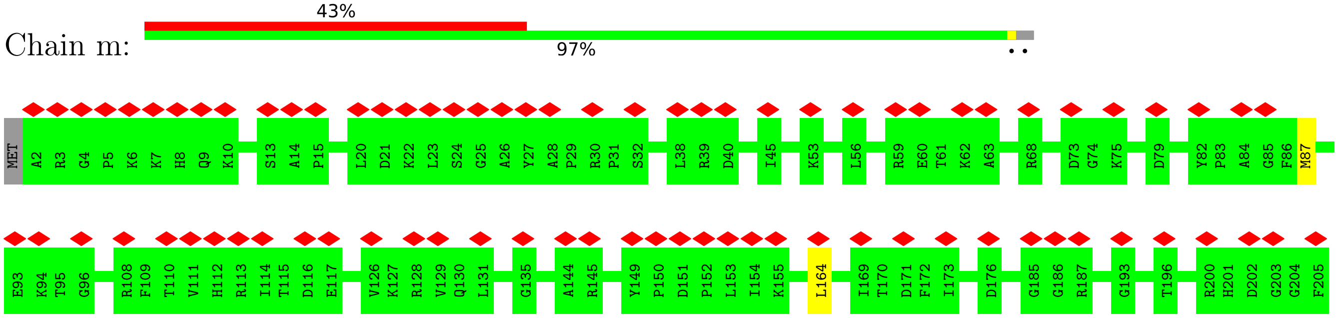
- Molecule 33: Fcf2

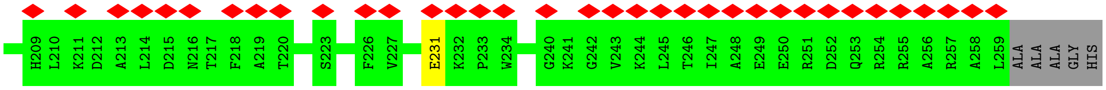


- Molecule 34: 40S ribosomal protein S1



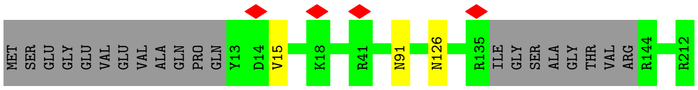
- Molecule 35: 40S ribosomal protein S4





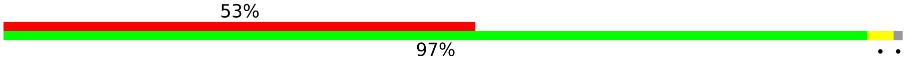
- Molecule 36: 40S ribosomal protein s5-like protein

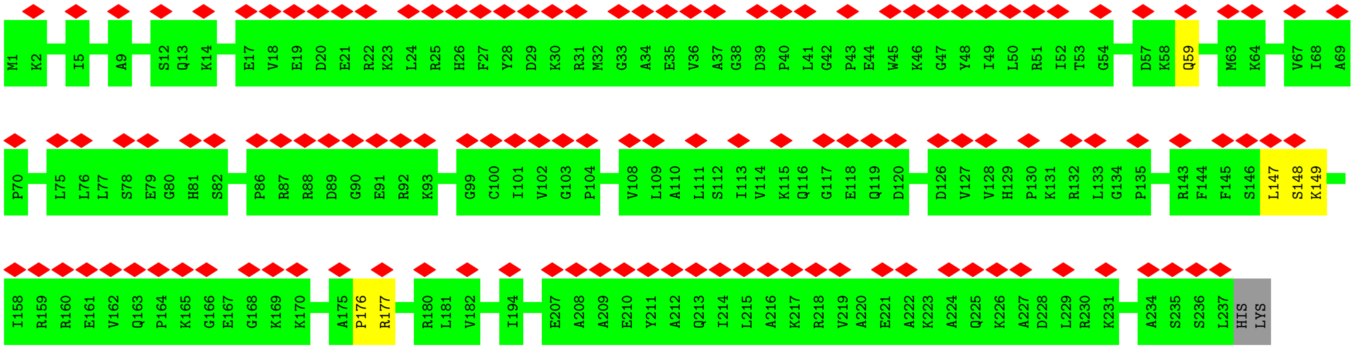
Chain n:



- Molecule 37: 40S ribosomal protein S6

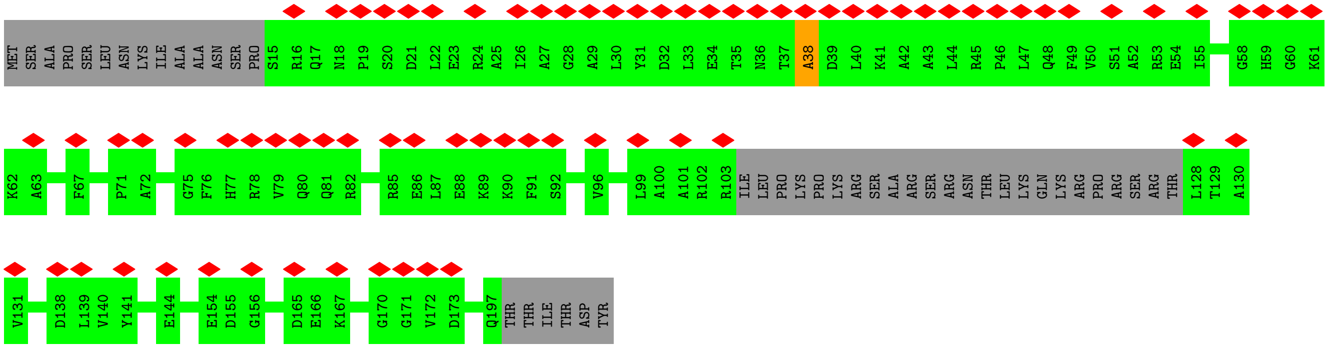
Chain o:





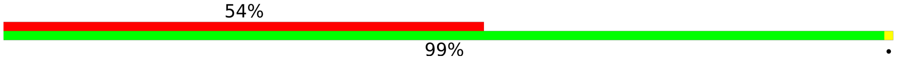
- Molecule 38: 40S ribosomal protein S7-like protein

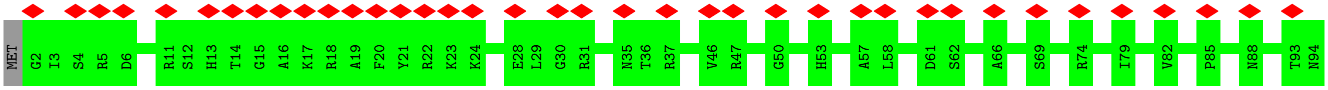
Chain p:

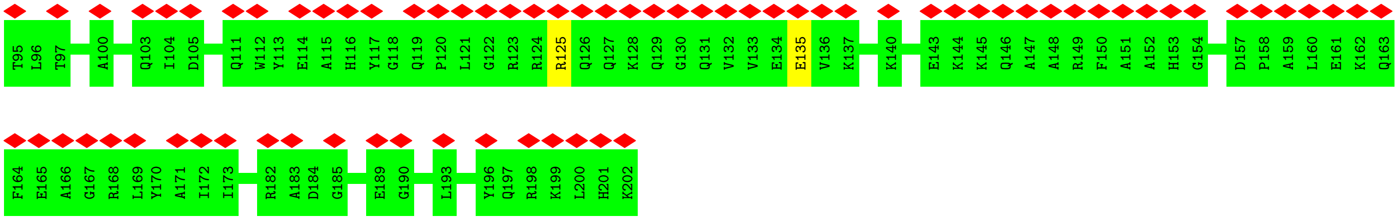


- Molecule 39: 40S ribosomal protein S8

Chain q:

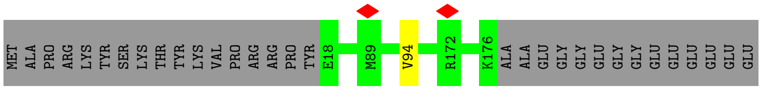






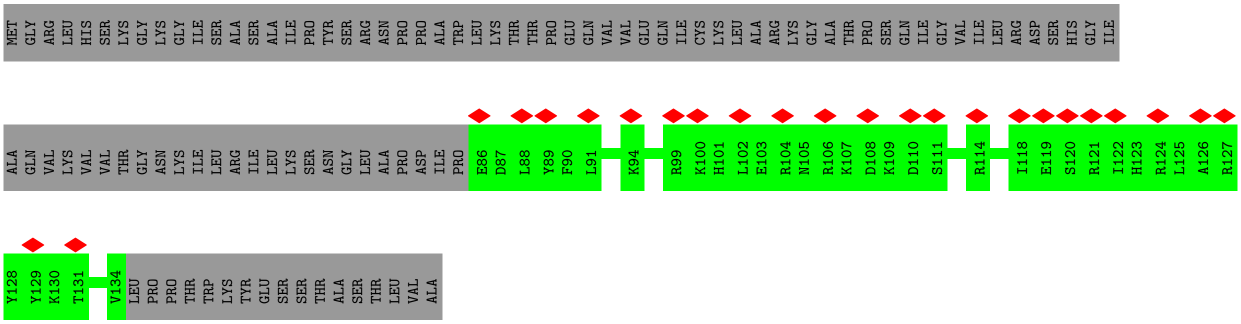
- Molecule 40: 40S ribosomal protein s9-like protein

Chain r:



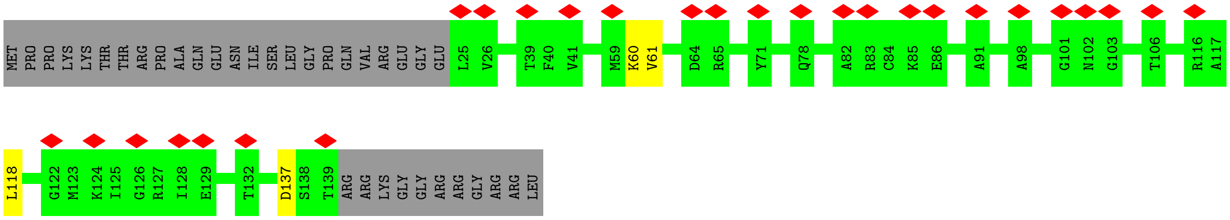
- Molecule 41: 40S ribosomal protein S13-like protein

Chain s:



- Molecule 42: 40S ribosomal protein S14-like protein

Chain t:

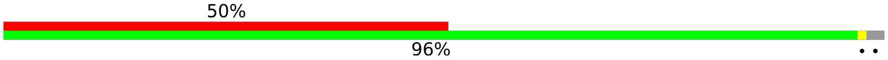


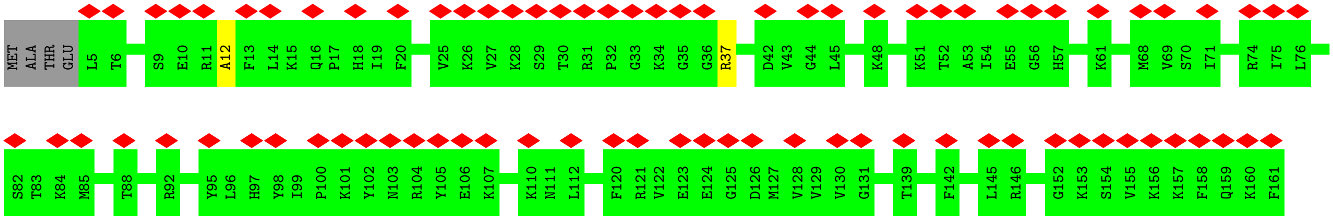
- Molecule 43: 40S ribosomal protein S16-like protein

Chain u:

- Molecule 44: 40S ribosomal protein S11-like protein

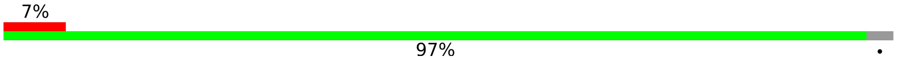
Chain v:

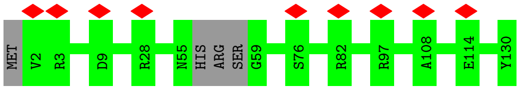




- Molecule 45: 40S ribosomal protein S22-like protein

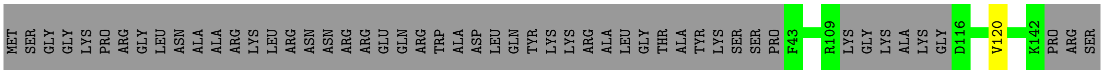
Chain w:





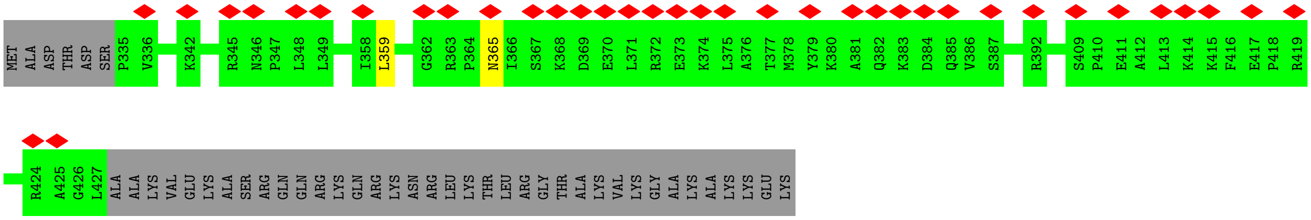
- Molecule 46: 40S ribosomal protein s23-like protein

Chain x:



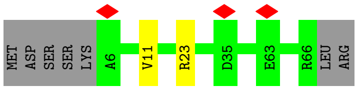
- Molecule 47: 40S ribosomal protein S24

Chain y:



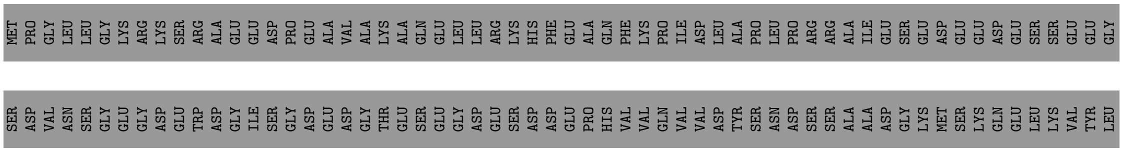
- Molecule 48: 40S ribosomal protein S28-like protein

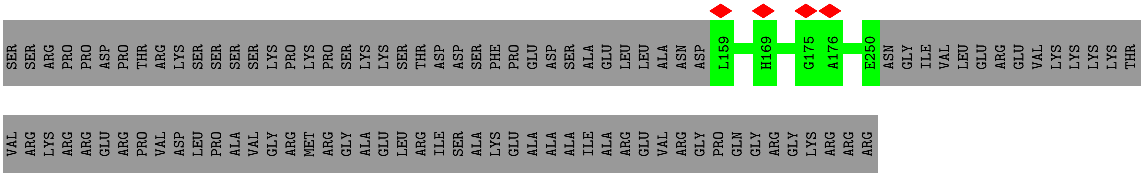
Chain z:



- Molecule 49: Faf1

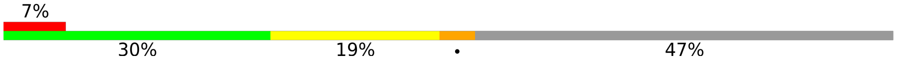
Chain 0:

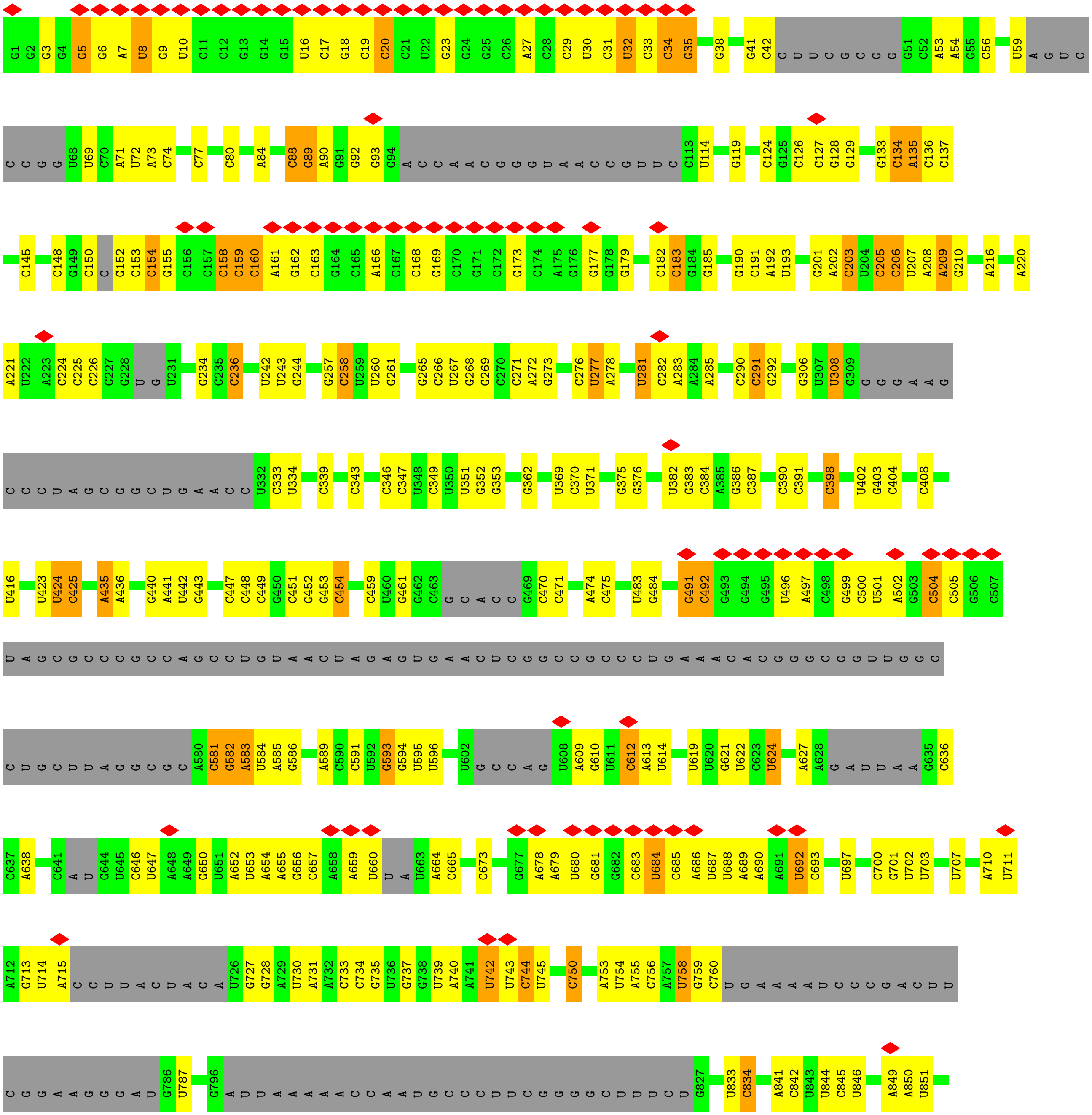


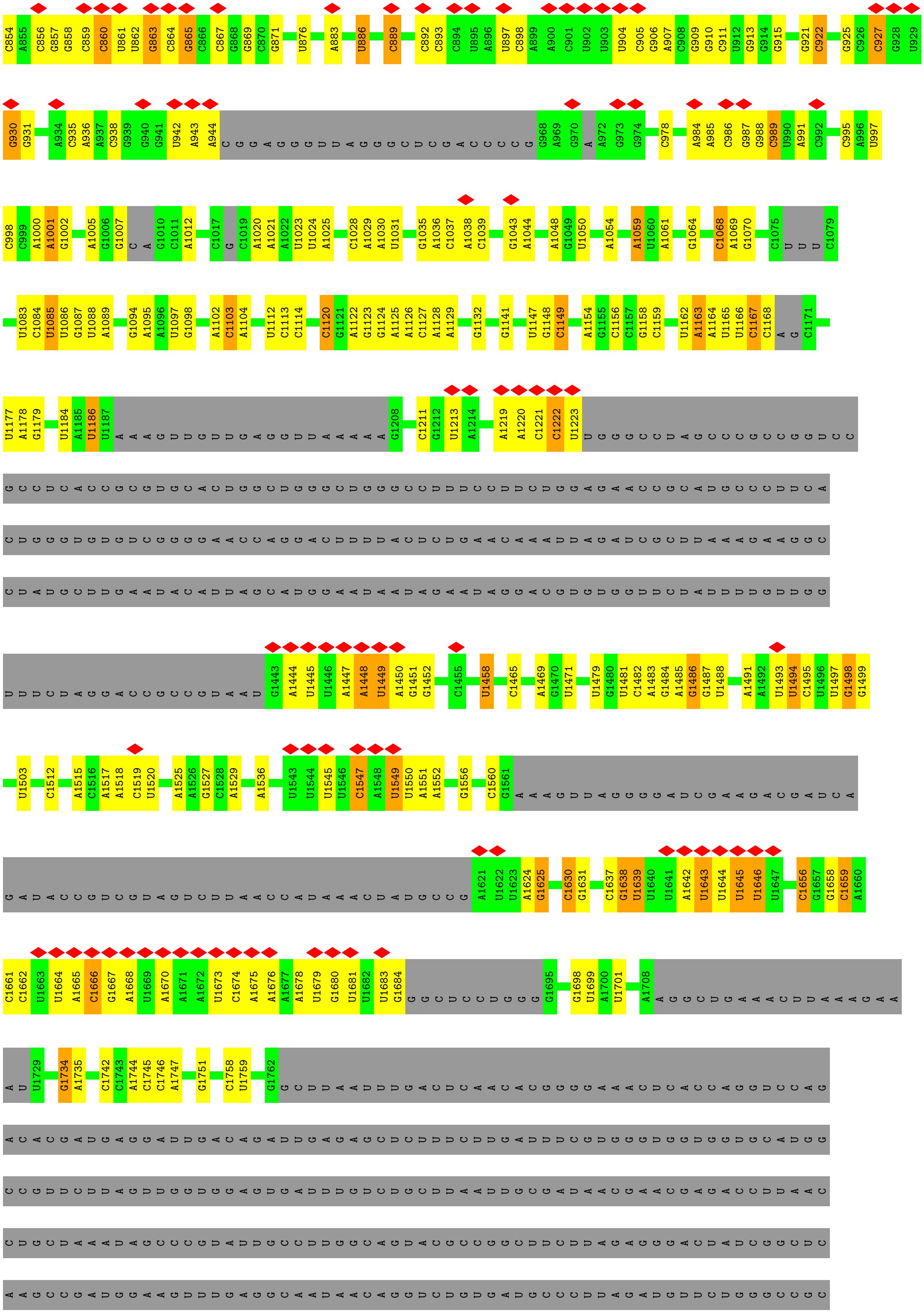


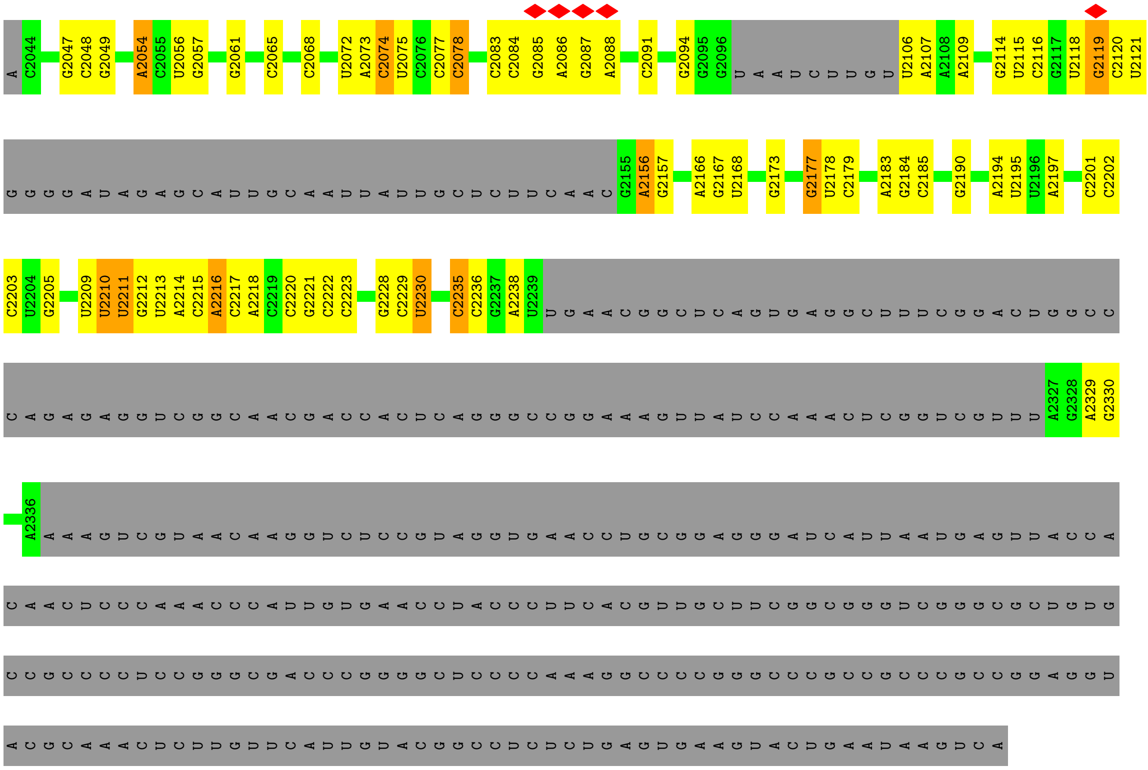
- Molecule 50: 35S rRNA

Chain 1:



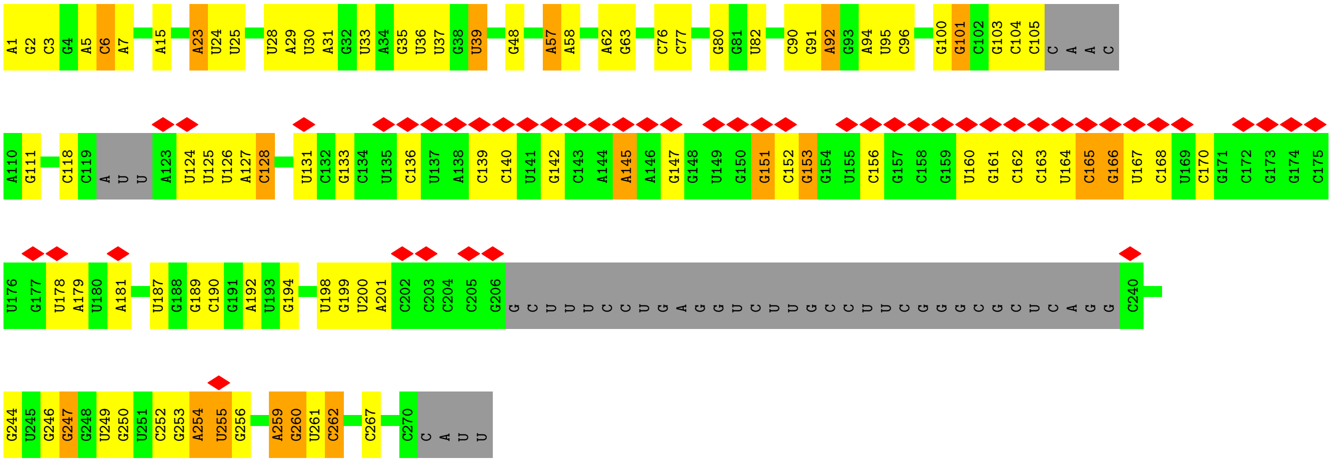



C854 A855 C856 G857 G858 C859 C860 U861 U862 G863 C864 G865 C866 C867 G868 G869 C870 G871 U876 A883 U886 C889 C892 C893 C894 U895 A896 U897 C898 A899 A900 C901 U902 U903 U904 C905 G906 A907 C908 G909 G910 C911 U912 G913 G914 G915 G921 C922 G925 C926 C927 G928 U929
G930 G931 A934 C935 A936 A937 C938 G939 G940 G941 U942 A943 A944 C G G A G G G U U A G G G C U C G A C C C C G G968 A969 G970 A A972 G973 G974 C978 A984 A985 C986 G987 G988 C989 U990 A991 C992 C995 A996 U997
C998 C999 A1000 A1001 G1002 A1005 G1006 G1007 C A G1010 C1011 A1012 C1017 G C1019 A1020 A1021 A1022 U1023 U1024 A1025 C1028 A1029 A1030 U1031 G1035 A1036 C1037 A1038 C1039 G1043 A1044 A1048 G1049 U1050 A1054 A1059 U1060 A1061 G1064 C1068 A1069 G1070 C1075 U U U C1079
U1083 C1084 U1085 U1086 G1087 U1088 A1089 G1094 A1095 A1096 U1097 G1098 A1102 C1103 A1104 U1112 C1113 C1114 C1120 G1121 A1122 G1123 G1124 A1125 A1126 C1127 A1128 A1129 G1132 G1141 U1147 G1148 C1149 A1154 G1155 C1156 C1157 G1158 C1159 U1162 A1163 A1164 U1165 U1166 C1167 C1168 A G C1171
U1177 A1178 G1179 U1184 A1185 U1186 U1187 A A A G U U G U U G A G G U U A A A A A G1208 C1211 G1212 U1213 A1214 A1219 A1220 C1221 C1222 U1223 U G G G C C U A G C C C G C C G G U C C
G C C U C A C C G C G U G C A C U G G C U G G G C U G G G C C U U U C C U U C U G G A G A A C C G C A U G C C C U U C A
C U G G G U G U G U C G G G G A A C C A G G A C U U U U A C U C U G A A C A A A U U A G A U C G C U U A A A G A A G G C
C U A U G C U U G A A U A C A U U A G C A U G G A A U A A U A G A A U A G G A C G U G U G G U U C U A U U U U G U U G G
U U U C U A G G A C C G C C G U A A U G1443 A1444 U1445 U1446 A1447 A1448 U1449 A1450 G1451 G1452 C1455 U1458 C1465 A1469 G1470 U1471 U1479 G1480 U1481 C1482 A1483 G1484 A1485 G1486 G1487 U1488 A1491 A1492 U1493 U1494 C1495 U1496 U1497 G1498 G1499
U1503 C1512 A1515 C1516 A1517 A1518 C1519 U1520 A1525 A1526 G1527 C1528 A1529 A1536 U1543 U1544 U1545 U1546 C1547 A1548 U1549 U1550 A1551 A1552 G1556 C1560 G1561 A A A G U U A G G G G A U C G A A G A C G A U C A
G A U A C C G U C G U A G U C U U A A C C A U A A A C U A U G C C G A1621 U1622 U1623 A1624 G1625 C1630 G1631 C1637 G1638 U1639 U1640 U1641 A1642 U1643 U1644 U1645 U1646 U1647 C1656 G1657 G1658 C1659 A1660
C1661 C1662 U1663 U1664 A1665 C1666 G1667 A1668 U1669 A1670 A1671 A1672 U1673 C1674 A1675 A1676 A1677 A1678 U1679 G1680 U1681 U1682 U1683 G1684 G G C U C C U G G G G1695 G1698 U1699 A1700 U1701 A1708 A G G C U G A A A C U U A A A G A A
A U U1729 G1734 A1735 C1742 C1743 A1744 C1745 C1746 A1747 G1751 C1758 U1759 G1762 G C U U A A U U U G A C U C A A C A C G G G G A A A C U C A C C A G G U C C A G
A C A C G A U G A G G A U U G A C A G A U U G A G A G C U C U U U C U U G A U U U C G U G G G U G G U G G U G C A U G G
C C G U U C U U A G U U G G U G G A G U G A U U U G U C U G C U U A A U U G C G A U A A C G A A C G A G A C C U U A A C
C U G C U A A A U A G C C C G U A U U G C C U U G G C A G U A C G C C G G C U U C U U A G A G G G A C U A U C G G C U C
A A G C C G A U G G A A G U U U G A G G C A A U A A C A G G U C U G U G A U G C C C U U A G A U G U U C U G G G C C G C



- Molecule 51: U3 snoRNA

Chain 2:



4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	231121	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 $(e^-/\text{Å}^2)$	2.4	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	0.596	Depositor
Minimum map value	-0.325	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	520.32, 520.32, 520.32	wwPDB
Map dimensions	480, 480, 480	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	A	0.50	0/6395	0.75	10/8703 (0.1%)
2	B	0.33	0/541	0.46	0/713
3	C	0.38	0/595	0.56	0/786
4	D	0.37	0/2209	0.66	0/2986
5	E	0.37	0/2657	0.55	1/3596 (0.0%)
6	F	0.51	0/3353	0.73	1/4544 (0.0%)
7	G	0.41	0/2828	0.65	1/3841 (0.0%)
8	H	0.42	0/1468	0.60	0/1946
9	I	0.34	0/1251	0.62	0/1696
10	J	0.38	0/1221	0.65	0/1662
11	K	0.39	0/1161	0.64	1/1570 (0.1%)
12	L	0.33	0/2117	0.69	3/2887 (0.1%)
13	M	0.37	0/2179	0.72	2/2972 (0.1%)
14	N	0.42	0/3508	0.64	2/4742 (0.0%)
15	O	0.45	0/6604	0.76	10/8981 (0.1%)
16	P	0.43	0/1483	0.70	0/1998
17	Q	0.25	0/900	0.49	0/1249
18	R	0.39	0/1814	0.59	0/2456
18	S	0.40	0/1853	0.59	0/2511
19	T	0.36	0/2911	0.66	1/3937 (0.0%)
20	U	0.35	0/3085	0.65	1/4169 (0.0%)
21	V	0.38	0/891	0.67	1/1214 (0.1%)
21	W	0.38	0/876	0.67	1/1195 (0.1%)
22	X	0.36	0/2739	0.69	1/3699 (0.0%)
23	Y	0.33	0/2638	0.63	1/3580 (0.0%)
24	Z	0.39	0/4960	0.66	4/6710 (0.1%)
25	a	0.49	0/1462	0.71	2/1967 (0.1%)
26	b	0.48	0/2324	0.73	4/3144 (0.1%)
27	c	0.36	0/1405	0.59	1/1879 (0.1%)
28	d	0.50	0/3506	0.72	3/4739 (0.1%)
29	e	0.28	0/1714	0.53	0/2325
29	f	0.28	0/1714	0.53	0/2325

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
30	g	0.32	0/1412	0.61	0/1897
31	h	0.28	0/1304	0.61	0/1751
32	i	0.25	0/3246	0.45	0/4507
32	j	0.24	0/3335	0.45	0/4632
33	k	0.41	0/945	0.60	0/1264
34	l	0.31	0/1764	0.73	4/2377 (0.2%)
35	m	0.29	0/2097	0.63	1/2821 (0.0%)
36	n	0.41	0/1468	0.63	0/1987
37	o	0.32	0/1942	0.67	1/2595 (0.0%)
38	p	0.34	0/1298	0.69	1/1750 (0.1%)
39	q	0.28	0/1655	0.57	0/2213
40	r	0.38	0/1259	0.63	0/1687
41	s	0.26	0/422	0.48	0/561
42	t	0.31	0/801	0.62	1/1087 (0.1%)
43	u	0.48	0/958	0.70	0/1293
44	v	0.31	0/1315	0.59	0/1760
45	w	0.36	0/1001	0.63	0/1345
46	x	0.42	0/693	0.59	0/928
47	y	0.28	0/766	0.65	1/1027 (0.1%)
48	z	0.42	0/458	0.67	0/617
49	0	0.32	0/702	0.58	0/939
50	1	0.54	2/32166 (0.0%)	1.31	444/50073 (0.9%)
51	2	0.62	0/5459	1.45	76/8498 (0.9%)
All	All	0.44	2/140828 (0.0%)	0.91	580/198331 (0.3%)

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	4
4	D	0	1
6	F	0	3
12	L	0	1
13	M	0	4
14	N	0	1
15	O	0	5
17	Q	0	3
18	R	0	1
18	S	0	1
21	V	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
21	W	0	1
22	X	0	4
23	Y	0	2
24	Z	0	3
26	b	0	1
28	d	0	1
29	e	0	3
29	f	0	3
31	h	0	2
32	i	0	1
32	j	0	1
34	l	0	5
35	m	0	2
37	o	0	2
38	p	0	1
39	q	0	1
42	t	0	1
43	u	0	1
44	v	0	2
46	x	0	1
47	y	0	1
All	All	0	64

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	1	435	A	N9-C4	-5.50	1.34	1.37
50	1	2194	A	C2-N3	-5.21	1.28	1.33

All (580) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	2	2	G	O5'-P-OP1	-32.85	71.28	110.70
51	2	2	G	OP1-P-OP2	-26.67	79.59	119.60
50	1	18	G	N1-C6-O6	-19.83	108.00	119.90
51	2	2	G	O5'-P-OP2	19.02	133.53	110.70
50	1	18	G	C5-C6-O6	16.50	138.50	128.60
51	2	1	A	OP1-P-O3'	13.73	135.41	105.20
50	1	258	C	N1-C2-O2	13.69	127.11	118.90
50	1	1547	C	N1-C2-O2	13.39	126.93	118.90
50	1	758	U	N3-C2-O2	-12.77	113.26	122.20
51	2	1	A	OP2-P-O3'	-11.57	79.73	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	1	758	U	C2-N1-C1’	11.38	131.35	117.70
50	1	683	C	C2-N1-C1’	10.99	130.89	118.80
50	1	8	U	C2-N1-C1’	10.93	130.82	117.70
50	1	2074	C	N1-C2-O2	10.57	125.24	118.90
50	1	8	U	N1-C2-O2	10.51	130.16	122.80
51	2	165	C	N1-C2-O2	10.33	125.10	118.90
50	1	160	C	N3-C2-O2	-10.27	114.71	121.90
50	1	1149	C	N1-C2-O2	10.27	125.06	118.90
50	1	258	C	N3-C2-O2	-10.17	114.78	121.90
50	1	1550	U	C2-N1-C1’	10.11	129.83	117.70
50	1	750	C	N1-C2-O2	10.10	124.96	118.90
50	1	291	C	N1-C2-O2	10.06	124.94	118.90
50	1	203	C	N1-C2-O2	10.02	124.91	118.90
50	1	2168	U	N3-C2-O2	-9.96	115.23	122.20
50	1	8	U	N3-C2-O2	-9.95	115.24	122.20
50	1	1661	C	N3-C2-O2	-9.89	114.98	121.90
50	1	2074	C	C2-N1-C1’	9.80	129.58	118.80
51	2	6	C	C6-N1-C2	-9.80	116.38	120.30
50	1	1547	C	C2-N1-C1’	9.68	129.44	118.80
50	1	758	U	N1-C2-O2	9.67	129.57	122.80
51	2	6	C	C5-C6-N1	9.55	125.77	121.00
50	1	1662	C	N3-C2-O2	-9.49	115.26	121.90
51	2	259	A	O4’-C1’-N9	9.48	115.78	108.20
15	O	222	LEU	C-N-CA	9.47	145.38	121.70
50	1	258	C	C2-N1-C1’	9.44	129.19	118.80
50	1	20	C	N3-C4-N4	-9.41	111.41	118.00
50	1	159	C	N3-C2-O2	-9.40	115.32	121.90
50	1	1661	C	N1-C2-O2	9.39	124.53	118.90
50	1	683	C	C6-N1-C2	-9.35	116.56	120.30
50	1	927	C	N3-C2-O2	-9.33	115.37	121.90
50	1	1163	A	P-O3’-C3’	9.25	130.79	119.70
50	1	2210	U	N3-C2-O2	-9.21	115.75	122.20
50	1	2168	U	N1-C2-O2	9.14	129.20	122.80
50	1	291	C	C2-N1-C1’	9.13	128.84	118.80
50	1	595	U	N3-C2-O2	-9.12	115.82	122.20
50	1	1547	C	N3-C2-O2	-9.03	115.58	121.90
51	2	165	C	C6-N1-C2	-9.02	116.69	120.30
50	1	1149	C	C2-N1-C1’	8.79	128.47	118.80
50	1	595	U	N1-C2-O2	8.75	128.92	122.80
50	1	158	C	N1-C2-O2	8.69	124.11	118.90
51	2	165	C	C2-N1-C1’	8.69	128.35	118.80
50	1	1149	C	N3-C2-O2	-8.67	115.83	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	1	449	C	N3-C2-O2	-8.65	115.85	121.90
50	1	750	C	N3-C2-O2	-8.64	115.85	121.90
50	1	1666	C	C5-C6-N1	8.58	125.29	121.00
50	1	148	C	N3-C2-O2	-8.58	115.90	121.90
51	2	165	C	N3-C2-O2	-8.56	115.91	121.90
50	1	203	C	N3-C2-O2	-8.52	115.93	121.90
50	1	42	C	N1-C2-O2	8.52	124.01	118.90
50	1	291	C	N3-C2-O2	-8.52	115.94	121.90
50	1	505	C	N3-C2-O2	-8.51	115.94	121.90
51	2	3	C	C5-C6-N1	8.49	125.25	121.00
50	1	595	U	C2-N1-C1’	8.48	127.88	117.70
50	1	922	C	N3-C2-O2	-8.45	115.98	121.90
51	2	3	C	C6-N1-C2	-8.42	116.93	120.30
50	1	581	C	N1-C2-O2	8.36	123.91	118.90
50	1	1666	C	N1-C2-O2	8.36	123.91	118.90
50	1	160	C	N1-C2-O2	8.34	123.91	118.90
50	1	750	C	C2-N1-C1’	8.30	127.93	118.80
50	1	80	C	N3-C2-O2	-8.18	116.18	121.90
50	1	942	U	N3-C2-O2	-8.17	116.48	122.20
50	1	683	C	C5-C6-N1	8.12	125.06	121.00
50	1	20	C	C5-C4-N4	8.06	125.85	120.20
50	1	1645	U	C2-N1-C1’	8.03	127.33	117.70
50	1	2235	C	C2-N1-C1’	8.02	127.62	118.80
50	1	2074	C	N3-C2-O2	-7.98	116.31	121.90
50	1	471	C	N3-C2-O2	-7.97	116.32	121.90
50	1	1149	C	C6-N1-C2	-7.97	117.11	120.30
50	1	2217	C	N1-C2-O2	7.94	123.66	118.90
50	1	581	C	N3-C2-O2	-7.91	116.36	121.90
51	2	57	A	O4’-C1’-N9	7.87	114.49	108.20
50	1	1486	G	C4-N9-C1’	7.86	136.72	126.50
50	1	1645	U	N3-C2-O2	-7.84	116.71	122.20
50	1	2216	A	C8-N9-C4	-7.84	102.66	105.80
50	1	206	C	C2-N1-C1’	7.82	127.40	118.80
51	2	267	C	N3-C2-O2	-7.81	116.43	121.90
50	1	1630	C	N3-C2-O2	-7.81	116.44	121.90
50	1	18	G	C4-N9-C1’	7.78	136.62	126.50
50	1	1666	C	C2-N1-C1’	7.78	127.36	118.80
51	2	128	C	O4’-C1’-N1	7.76	114.41	108.20
15	O	378	LEU	CA-CB-CG	7.75	133.13	115.30
50	1	2084	C	N3-C2-O2	-7.74	116.48	121.90
51	2	152	C	C6-N1-C2	-7.70	117.22	120.30
50	1	583	A	O5’-P-OP1	-7.69	98.78	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	81	LEU	CA-CB-CG	7.67	132.94	115.30
50	1	989	C	C2-N1-C1'	7.67	127.24	118.80
28	d	159	LEU	CB-CG-CD2	-7.67	97.97	111.00
50	1	860	C	C2-N1-C1'	-7.65	110.38	118.80
50	1	1114	C	N1-C2-O2	7.65	123.49	118.90
50	1	203	C	C2-N1-C1'	7.63	127.20	118.80
51	2	161	G	N3-C4-N9	7.63	130.58	126.00
50	1	505	C	N1-C2-O2	7.61	123.46	118.90
51	2	128	C	C6-N1-C2	-7.58	117.27	120.30
50	1	889	C	N1-C2-O2	7.57	123.44	118.90
50	1	1165	U	N1-C2-O2	7.57	128.10	122.80
50	1	2217	C	C2-N1-C1'	7.57	127.12	118.80
50	1	582	G	OP1-P-O3'	7.55	121.82	105.20
50	1	56	C	N1-C2-O2	7.51	123.41	118.90
50	1	995	C	N3-C2-O2	-7.51	116.64	121.90
1	A	293	LEU	CA-CB-CG	7.49	132.51	115.30
50	1	1759	U	C5-C6-N1	7.48	126.44	122.70
50	1	1222	C	C2-N1-C1'	7.47	127.02	118.80
50	1	2048	C	C6-N1-C2	-7.45	117.32	120.30
50	1	1159	C	N1-C2-O2	7.45	123.37	118.90
50	1	1163	A	OP2-P-O3'	7.43	121.56	105.20
50	1	291	C	C6-N1-C2	-7.42	117.33	120.30
50	1	148	C	C6-N1-C2	-7.41	117.34	120.30
50	1	1165	U	C2-N1-C1'	7.39	126.57	117.70
50	1	18	G	C2-N3-C4	7.38	115.59	111.90
50	1	683	C	N1-C2-O2	7.37	123.32	118.90
50	1	2084	C	C6-N1-C2	-7.36	117.36	120.30
50	1	8	U	C6-N1-C1'	-7.34	110.92	121.20
50	1	1550	U	N1-C2-O2	7.29	127.90	122.80
28	d	124	LEU	CA-CB-CG	7.27	132.02	115.30
50	1	1486	G	N3-C4-C5	-7.27	124.97	128.60
13	M	428	MET	C-N-CA	7.25	139.83	121.70
51	2	152	C	C5-C6-N1	7.25	124.62	121.00
50	1	1549	U	N3-C4-C5	7.24	118.94	114.60
50	1	1167	C	N1-C2-O2	7.21	123.23	118.90
50	1	673	C	C6-N1-C2	-7.21	117.42	120.30
50	1	1547	C	C5-C6-N1	7.18	124.59	121.00
51	2	80	G	N3-C4-N9	-7.16	121.70	126.00
50	1	159	C	N1-C2-O2	7.14	123.18	118.90
50	1	911	C	C5-C6-N1	7.13	124.57	121.00
51	2	165	C	C5-C6-N1	7.13	124.57	121.00
50	1	308	U	N1-C2-O2	7.13	127.79	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	2	247	G	O5'-P-OP1	7.13	119.25	110.70
50	1	308	U	N3-C2-O2	-7.13	117.21	122.20
50	1	281	U	P-O3'-C3'	7.10	128.22	119.70
50	1	2074	C	C6-N1-C1'	-7.10	112.28	120.80
50	1	927	C	N1-C2-O2	7.07	123.14	118.90
50	1	978	C	N3-C2-O2	-7.07	116.95	121.90
50	1	750	C	C6-N1-C2	-7.05	117.48	120.30
50	1	42	C	N3-C2-O2	-7.05	116.97	121.90
50	1	1625	G	N3-C4-N9	7.05	130.23	126.00
50	1	2230	U	C2-N1-C1'	7.02	126.13	117.70
50	1	209	A	P-O3'-C3'	7.02	128.12	119.70
50	1	1630	C	N1-C2-O2	7.01	123.10	118.90
22	X	320	LEU	CA-CB-CG	7.00	131.39	115.30
50	1	2209	U	N3-C2-O2	-7.00	117.30	122.20
51	2	255	U	P-O3'-C3'	6.99	128.09	119.70
50	1	160	C	C6-N1-C2	-6.97	117.51	120.30
50	1	692	U	N1-C2-O2	6.97	127.68	122.80
50	1	1165	U	N3-C2-O2	-6.97	117.32	122.20
50	1	1550	U	N3-C2-O2	-6.97	117.32	122.20
51	2	161	G	C4-N9-C1'	6.96	135.55	126.50
50	1	758	U	C6-N1-C2	-6.96	116.83	121.00
50	1	1645	U	N1-C2-O2	6.93	127.65	122.80
50	1	491	G	N3-C4-C5	-6.92	125.14	128.60
50	1	1547	C	C6-N1-C2	-6.92	117.53	120.30
50	1	1167	C	C2-N1-C1'	6.92	126.41	118.80
50	1	665	C	C5-C6-N1	6.91	124.46	121.00
50	1	1747	A	C6-N1-C2	-6.90	114.46	118.60
50	1	32	U	N3-C2-O2	-6.90	117.37	122.20
51	2	252	C	N3-C2-O2	-6.90	117.07	121.90
50	1	1448	A	C5-C6-N1	6.90	121.15	117.70
50	1	683	C	C6-N1-C1'	-6.89	112.53	120.80
50	1	886	U	C2-N1-C1'	6.88	125.96	117.70
50	1	18	G	N3-C4-C5	-6.87	125.17	128.60
50	1	369	U	N3-C2-O2	-6.86	117.40	122.20
50	1	258	C	C6-N1-C1'	-6.85	112.58	120.80
50	1	152	G	N9-C1'-C2'	-6.85	104.47	112.00
51	2	103	G	N3-C4-N9	6.81	130.09	126.00
50	1	34	C	P-O3'-C3'	6.80	127.86	119.70
50	1	692	U	N3-C2-O2	-6.80	117.44	122.20
51	2	23	A	P-O3'-C3'	6.80	127.86	119.70
50	1	593	G	P-O3'-C3'	6.78	127.84	119.70
50	1	491	G	C4-N9-C1'	6.78	135.31	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	1	1550	U	C6-N1-C1'	-6.78	111.71	121.20
50	1	1498	G	C4-N9-C1'	6.77	135.30	126.50
50	1	1103	C	N1-C2-O2	6.76	122.96	118.90
51	2	166	G	N3-C4-C5	-6.74	125.23	128.60
50	1	1479	U	N1-C2-O2	6.74	127.52	122.80
50	1	860	C	C6-N1-C1'	6.71	128.86	120.80
50	1	758	U	C6-N1-C1'	-6.71	111.81	121.20
50	1	1113	C	N1-C2-O2	6.71	122.92	118.90
50	1	32	U	N1-C2-O2	6.70	127.49	122.80
15	O	76	LEU	CB-CG-CD1	-6.70	99.62	111.00
50	1	909	G	N3-C4-N9	6.68	130.01	126.00
50	1	448	C	N3-C2-O2	-6.68	117.23	121.90
50	1	886	U	C5-C6-N1	6.67	126.04	122.70
50	1	2091	C	C2-N1-C1'	6.66	126.12	118.80
50	1	582	G	P-O3'-C3'	6.65	127.68	119.70
51	2	23	A	O4'-C1'-N9	6.64	113.52	108.20
50	1	2210	U	C2-N1-C1'	6.63	125.66	117.70
50	1	1549	U	N3-C4-O4	-6.62	114.77	119.40
50	1	1625	G	N3-C4-C5	-6.62	125.29	128.60
5	E	177	LEU	CB-CG-CD2	-6.59	99.80	111.00
50	1	2065	C	N1-C2-O2	6.58	122.84	118.90
51	2	252	C	C6-N1-C2	-6.56	117.67	120.30
50	1	925	G	C6-C5-N7	-6.54	126.47	130.40
50	1	995	C	N1-C2-O2	6.54	122.82	118.90
50	1	5	G	N3-C4-N9	-6.53	122.08	126.00
50	1	2210	U	N1-C2-O2	6.53	127.37	122.80
50	1	1471	U	C2-N1-C1'	6.52	125.53	117.70
50	1	1639	U	C2-N1-C1'	6.52	125.52	117.70
50	1	1493	U	N1-C2-O2	6.52	127.36	122.80
50	1	1222	C	N1-C2-O2	6.52	122.81	118.90
1	A	323	LEU	CA-CB-CG	6.50	130.25	115.30
15	O	472	LEU	CA-CB-CG	6.50	130.24	115.30
50	1	154	C	C5-C6-N1	6.50	124.25	121.00
50	1	203	C	C6-N1-C2	-6.50	117.70	120.30
50	1	1114	C	N3-C2-O2	-6.49	117.35	121.90
50	1	56	C	N3-C2-O2	-6.49	117.36	121.90
50	1	1547	C	C6-N1-C1'	-6.49	113.01	120.80
50	1	277	U	P-O3'-C3'	6.48	127.48	119.70
50	1	281	U	OP1-P-O3'	6.47	119.44	105.20
21	W	103	LEU	CA-CB-CG	6.46	130.17	115.30
51	2	260	G	N3-C4-C5	-6.46	125.37	128.60
37	o	147	LEU	CA-CB-CG	6.45	130.13	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	2	260	G	C4-N9-C1’	6.45	134.88	126.50
21	V	103	LEU	CA-CB-CG	6.44	130.11	115.30
50	1	925	G	N3-C4-N9	6.44	129.86	126.00
50	1	1479	U	C2-N1-C1’	6.43	125.42	117.70
51	2	153	G	C4-N9-C1’	6.43	134.86	126.50
50	1	886	U	N1-C2-O2	6.43	127.30	122.80
50	1	18	G	C8-N9-C4	-6.42	103.83	106.40
50	1	154	C	C6-N1-C2	-6.40	117.74	120.30
50	1	471	C	C6-N1-C2	-6.40	117.74	120.30
50	1	2119	G	C4-N9-C1’	6.39	134.81	126.50
50	1	1001	A	P-O3’-C3’	6.38	127.36	119.70
50	1	34	C	OP1-P-O3’	6.38	119.23	105.20
1	A	700	LEU	CA-CB-CG	6.38	129.96	115.30
50	1	470	C	N1-C2-O2	6.37	122.72	118.90
50	1	183	C	N1-C2-O2	6.36	122.72	118.90
50	1	1451	G	N3-C2-N2	6.36	124.35	119.90
51	2	166	G	N3-C4-N9	6.36	129.81	126.00
50	1	135	A	P-O3’-C3’	6.35	127.32	119.70
51	2	128	C	C5-C6-N1	6.35	124.17	121.00
51	2	254	A	O4’-C1’-N9	6.33	113.26	108.20
50	1	1493	U	N3-C2-O2	-6.30	117.79	122.20
50	1	1666	C	C6-N1-C2	-6.28	117.79	120.30
50	1	665	C	N1-C2-O2	6.28	122.67	118.90
50	1	1486	G	N3-C4-N9	6.28	129.77	126.00
50	1	1498	G	N3-C4-N9	6.28	129.77	126.00
51	2	153	G	C8-N9-C4	-6.27	103.89	106.40
50	1	2230	U	N1-C2-O2	6.27	127.19	122.80
51	2	161	G	C6-C5-N7	-6.26	126.64	130.40
51	2	260	G	N3-C4-N9	6.24	129.75	126.00
50	1	2195	U	N3-C2-O2	-6.23	117.84	122.20
50	1	206	C	N1-C2-O2	6.23	122.64	118.90
50	1	159	C	C6-N1-C2	-6.21	117.81	120.30
11	K	369	LEU	CA-CB-CG	6.20	129.56	115.30
50	1	665	C	C6-N1-C2	-6.20	117.82	120.30
50	1	1746	C	N1-C2-O2	6.18	122.61	118.90
50	1	5	G	C4-N9-C1’	-6.18	118.47	126.50
50	1	2177	G	P-O3’-C3’	6.17	127.11	119.70
50	1	225	C	C2-N1-C1’	6.17	125.59	118.80
51	2	101	G	N3-C4-N9	-6.17	122.30	126.00
50	1	1103	C	C2-N1-C1’	6.16	125.58	118.80
50	1	2203	C	C6-N1-C2	-6.16	117.84	120.30
50	1	842	C	N1-C2-O2	6.15	122.59	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	1	56	C	C6-N1-C2	-6.14	117.84	120.30
38	p	38	ALA	C-N-CA	6.14	137.06	121.70
50	1	2119	G	N3-C4-N9	6.14	129.69	126.00
50	1	5	G	C8-N9-C1'	6.14	134.98	127.00
50	1	88	C	P-O3'-C3'	6.12	127.04	119.70
50	1	205	C	P-O3'-C3'	6.11	127.03	119.70
50	1	2156	A	P-O3'-C3'	6.11	127.03	119.70
50	1	867	C	C6-N1-C2	-6.11	117.86	120.30
12	L	260	LEU	CA-CB-CG	6.10	129.33	115.30
50	1	133	G	N3-C2-N2	-6.10	115.63	119.90
50	1	1458	U	N1-C2-O2	6.09	127.07	122.80
51	2	140	C	C2-N1-C1'	6.09	125.50	118.80
50	1	622	U	N3-C2-O2	-6.09	117.94	122.20
50	1	271	C	N3-C2-O2	-6.08	117.64	121.90
50	1	492	C	N1-C2-O2	6.08	122.55	118.90
50	1	1486	G	C8-N9-C1'	-6.07	119.11	127.00
51	2	161	G	C8-N9-C1'	-6.07	119.11	127.00
50	1	225	C	N1-C2-O2	6.07	122.54	118.90
27	c	490	LEU	CB-CG-CD1	-6.06	100.69	111.00
50	1	1149	C	C5-C6-N1	6.06	124.03	121.00
50	1	491	G	N3-C4-N9	6.06	129.64	126.00
51	2	156	C	C2-N1-C1'	6.05	125.46	118.80
50	1	930	G	C4-N9-C1'	6.05	134.37	126.50
51	2	153	G	N7-C8-N9	6.05	116.12	113.10
1	A	625	LEU	CA-CB-CG	6.05	129.21	115.30
51	2	156	C	C5-C6-N1	6.04	124.02	121.00
50	1	1662	C	N1-C2-O2	6.03	122.52	118.90
50	1	153	C	C5-C6-N1	6.02	124.01	121.00
50	1	2203	C	N1-C2-O2	6.01	122.51	118.90
50	1	1120	C	C2-N1-C1'	6.01	125.41	118.80
50	1	2209	U	N1-C2-O2	6.01	127.01	122.80
50	1	154	C	C2-N1-C1'	6.01	125.41	118.80
50	1	665	C	C2-N1-C1'	6.01	125.41	118.80
51	2	145	A	N7-C8-N9	6.00	116.80	113.80
50	1	145	C	N1-C2-O2	5.99	122.49	118.90
50	1	1113	C	N3-C2-O2	-5.98	117.72	121.90
50	1	447	C	N3-C2-O2	-5.98	117.72	121.90
26	b	141	LEU	CA-CB-CG	5.97	129.04	115.30
50	1	2217	C	C6-N1-C1'	-5.97	113.63	120.80
50	1	1498	G	C8-N9-C1'	-5.97	119.24	127.00
50	1	989	C	N1-C2-O2	5.97	122.48	118.90
50	1	2078	C	N3-C2-O2	-5.97	117.72	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	1	2168	U	C5-C6-N1	5.97	125.68	122.70
50	1	18	G	C8-N9-C1’	-5.96	119.25	127.00
50	1	733	C	C2-N1-C1’	5.96	125.36	118.80
50	1	2230	U	N3-C2-O2	-5.96	118.03	122.20
50	1	88	C	C5-C6-N1	5.96	123.98	121.00
50	1	29	C	C6-N1-C2	-5.95	117.92	120.30
50	1	1494	U	N3-C2-O2	-5.95	118.04	122.20
50	1	744	C	C5-C6-N1	5.94	123.97	121.00
51	2	80	G	N9-C4-C5	5.94	107.78	105.40
1	A	323	LEU	CB-CG-CD2	-5.94	100.91	111.00
51	2	82	U	N1-C2-O2	5.94	126.96	122.80
50	1	978	C	C6-N1-C2	-5.93	117.93	120.30
50	1	1503	U	N1-C2-O2	5.93	126.95	122.80
34	l	47	LEU	CA-CB-CG	5.91	128.90	115.30
50	1	206	C	N3-C2-O2	-5.91	117.76	121.90
15	O	642	LEU	CA-CB-CG	5.91	128.89	115.30
25	a	82	LEU	CA-CB-CG	5.89	128.85	115.30
51	2	161	G	N3-C4-C5	-5.89	125.66	128.60
50	1	2216	A	N7-C8-N9	5.88	116.74	113.80
50	1	369	U	N1-C2-O2	5.88	126.92	122.80
50	1	291	C	C6-N1-C1’	-5.84	113.79	120.80
50	1	684	U	P-O3’-C3’	5.84	126.71	119.70
50	1	859	C	C6-N1-C2	-5.83	117.97	120.30
50	1	1159	C	N3-C2-O2	-5.83	117.82	121.90
50	1	291	C	C5-C6-N1	5.83	123.92	121.00
50	1	742	U	P-O3’-C3’	5.83	126.69	119.70
50	1	2235	C	C6-N1-C2	-5.81	117.98	120.30
50	1	1630	C	C6-N1-C2	-5.80	117.98	120.30
50	1	114	U	N1-C2-O2	5.80	126.86	122.80
19	T	17	LEU	CA-CB-CG	5.79	128.63	115.30
24	Z	263	LEU	CA-CB-CG	5.79	128.62	115.30
50	1	33	C	C5-C6-N1	5.79	123.89	121.00
50	1	2083	C	N1-C2-O2	5.79	122.37	118.90
50	1	2084	C	C6-N1-C1’	5.78	127.73	120.80
50	1	657	C	C2-N1-C1’	5.77	125.15	118.80
50	1	2074	C	C6-N1-C2	-5.77	117.99	120.30
50	1	1486	G	C8-N9-C4	-5.76	104.10	106.40
50	1	371	U	N1-C2-O2	5.76	126.83	122.80
50	1	1449	U	N3-C2-O2	-5.76	118.17	122.20
50	1	129	G	C5-C6-O6	5.75	132.05	128.60
50	1	158	C	N3-C2-O2	-5.75	117.87	121.90
51	2	267	C	C6-N1-C2	-5.75	118.00	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	2	92	A	C2-N3-C4	5.75	113.47	110.60
14	N	175	LEU	CA-CB-CG	5.75	128.51	115.30
50	1	1745	C	C5-C6-N1	5.75	123.87	121.00
50	1	154	C	N1-C2-O2	5.74	122.35	118.90
50	1	461	G	N3-C4-N9	5.74	129.44	126.00
51	2	39	U	N3-C2-O2	-5.74	118.19	122.20
50	1	371	U	N3-C2-O2	-5.73	118.19	122.20
50	1	886	U	N3-C2-O2	-5.73	118.19	122.20
50	1	2116	C	N1-C2-O2	5.73	122.34	118.90
50	1	2195	U	N1-C2-O2	5.73	126.81	122.80
51	2	103	G	N3-C4-C5	-5.73	125.74	128.60
50	1	1646	U	N1-C2-O2	5.72	126.81	122.80
50	1	2179	C	C2-N1-C1’	5.72	125.09	118.80
50	1	1734	G	P-O3’-C3’	5.72	126.56	119.70
50	1	1479	U	N3-C2-O2	-5.71	118.20	122.20
50	1	398	C	C6-N1-C2	-5.71	118.02	120.30
51	2	145	A	C5-N7-C8	-5.70	101.05	103.90
50	1	1646	U	N3-C2-O2	-5.70	118.21	122.20
50	1	1498	G	N3-C4-C5	-5.69	125.75	128.60
50	1	657	C	N1-C2-O2	5.69	122.32	118.90
50	1	581	C	C6-N1-C2	-5.69	118.02	120.30
50	1	158	C	C2-N1-C1’	5.67	125.04	118.80
50	1	183	C	C6-N1-C2	-5.67	118.03	120.30
50	1	925	G	C4-N9-C1’	5.67	133.87	126.50
50	1	925	G	C8-N9-C1’	-5.67	119.63	127.00
15	O	763	LEU	CA-CB-CG	5.66	128.33	115.30
50	1	1495	C	C5-C6-N1	5.66	123.83	121.00
50	1	504	C	C2-N3-C4	5.66	122.73	119.90
50	1	1745	C	C6-N1-C2	-5.66	118.04	120.30
50	1	876	U	N1-C2-O2	5.65	126.75	122.80
50	1	1503	U	N3-C2-O2	-5.65	118.25	122.20
50	1	271	C	N1-C2-O2	5.65	122.29	118.90
24	Z	206	LEU	CA-CB-CG	5.64	128.28	115.30
50	1	35	G	O5’-P-OP1	-5.64	100.62	105.70
50	1	56	C	C2-N1-C1’	5.64	125.01	118.80
50	1	683	C	N3-C2-O2	-5.64	117.95	121.90
50	1	177	G	C4-N9-C1’	5.64	133.83	126.50
50	1	1745	C	N1-C2-O2	5.64	122.28	118.90
50	1	8	U	C5-C6-N1	5.63	125.52	122.70
42	t	118	LEU	CA-CB-CG	5.63	128.25	115.30
50	1	1512	C	C6-N1-C2	-5.63	118.05	120.30
51	2	156	C	C6-N1-C2	-5.62	118.05	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	1	145	C	N3-C2-O2	-5.62	117.96	121.90
26	b	110	MET	C-N-CA	-5.62	107.66	121.70
50	1	491	G	C8-N9-C1’	-5.61	119.71	127.00
50	1	1666	C	N3-C2-O2	-5.60	117.98	121.90
50	1	1448	A	C6-N1-C2	-5.60	115.24	118.60
50	1	922	C	N1-C2-O2	5.59	122.25	118.90
50	1	1560	C	C6-N1-C2	-5.59	118.06	120.30
51	2	262	C	C2-N1-C1’	5.59	124.95	118.80
50	1	225	C	C6-N1-C2	-5.59	118.06	120.30
12	L	239	LEU	CA-CB-CG	5.57	128.11	115.30
50	1	447	C	C6-N1-C2	-5.57	118.07	120.30
50	1	308	U	C2-N1-C1’	5.56	124.38	117.70
50	1	860	C	N3-C2-O2	-5.55	118.02	121.90
50	1	1211	C	C5-C6-N1	5.55	123.78	121.00
50	1	2217	C	N3-C2-O2	-5.55	118.02	121.90
50	1	909	G	C4-N9-C1’	5.54	133.70	126.50
50	1	2179	C	N1-C2-O2	5.54	122.22	118.90
50	1	865	G	N1-C2-N2	-5.53	111.22	116.20
28	d	369	ARG	NE-CZ-NH1	-5.53	117.53	120.30
15	O	843	LEU	CA-CB-CG	5.53	128.02	115.30
50	1	624	U	N3-C2-O2	-5.53	118.33	122.20
50	1	2091	C	N1-C2-O2	5.52	122.21	118.90
50	1	681	G	C4-N9-C1’	5.52	133.67	126.50
50	1	1085	U	P-O3’-C3’	5.51	126.31	119.70
50	1	1479	U	C5-C6-N1	5.51	125.45	122.70
50	1	2119	G	C8-N9-C1’	-5.50	119.85	127.00
50	1	449	C	N1-C2-O2	5.49	122.19	118.90
51	2	92	A	C4-N9-C1’	5.48	136.16	126.30
51	2	166	G	C4-N9-C1’	5.48	133.62	126.50
50	1	2078	C	C6-N1-C1’	5.46	127.36	120.80
50	1	163	C	C2-N1-C1’	5.46	124.81	118.80
1	A	258	LEU	CB-CG-CD2	-5.46	101.72	111.00
50	1	2177	G	OP2-P-O3’	5.46	117.21	105.20
35	m	164	LEU	CA-CB-CG	5.45	127.84	115.30
50	1	454	C	C2-N1-C1’	5.45	124.80	118.80
50	1	88	C	C6-N1-C2	-5.45	118.12	120.30
50	1	2235	C	N1-C2-O2	5.44	122.16	118.90
50	1	2065	C	N3-C2-O2	-5.44	118.09	121.90
50	1	867	C	N1-C2-O2	5.44	122.16	118.90
51	2	77	C	C5-C6-N1	5.43	123.72	121.00
51	2	80	G	C5-C6-O6	5.43	131.86	128.60
50	1	114	U	N3-C2-O2	-5.43	118.40	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	1	206	C	C6-N1-C1'	-5.43	114.29	120.80
13	M	384	LEU	CA-CB-CG	5.43	127.78	115.30
50	1	2229	C	N1-C2-O2	5.42	122.15	118.90
50	1	2235	C	C6-N1-C1'	-5.42	114.30	120.80
50	1	2203	C	N3-C2-O2	-5.42	118.11	121.90
50	1	1458	U	N3-C2-O2	-5.41	118.42	122.20
51	2	156	C	N1-C2-O2	5.41	122.14	118.90
50	1	1656	C	C6-N1-C2	-5.41	118.14	120.30
50	1	2211	U	N1-C2-O2	5.41	126.58	122.80
50	1	595	U	C5-C6-N1	5.40	125.40	122.70
50	1	114	U	C2-N1-C1'	5.40	124.18	117.70
50	1	922	C	C6-N1-C2	-5.40	118.14	120.30
26	b	211	LEU	CA-CB-CG	5.39	127.71	115.30
34	l	110	LEU	CA-CB-CG	5.39	127.70	115.30
50	1	1149	C	C6-N1-C1'	-5.39	114.33	120.80
1	A	695	LEU	CA-CB-CG	5.39	127.70	115.30
50	1	750	C	C6-N1-C1'	-5.38	114.34	120.80
50	1	909	G	C8-N9-C1'	-5.38	120.01	127.00
50	1	343	C	C6-N1-C2	-5.38	118.15	120.30
50	1	1059	A	C2-N3-C4	5.37	113.29	110.60
50	1	2074	C	C5-C6-N1	5.37	123.69	121.00
50	1	942	U	N1-C2-O2	5.37	126.56	122.80
50	1	865	G	N3-C2-N2	5.36	123.65	119.90
50	1	32	U	C2-N1-C1'	5.36	124.13	117.70
51	2	105	C	C6-N1-C2	-5.36	118.16	120.30
15	O	445	LEU	CA-CB-CG	5.36	127.62	115.30
34	l	33	LYS	C-N-CA	5.36	135.09	121.70
50	1	408	C	C6-N1-C2	-5.36	118.16	120.30
50	1	989	C	C6-N1-C1'	-5.35	114.38	120.80
50	1	369	U	C2-N1-C1'	5.35	124.12	117.70
50	1	183	C	C5-C6-N1	5.33	123.67	121.00
50	1	451	C	C5-C6-N1	5.33	123.67	121.00
50	1	595	U	C6-N1-C2	-5.33	117.80	121.00
50	1	1745	C	C2-N1-C1'	5.32	124.66	118.80
50	1	787	U	N3-C2-O2	-5.32	118.47	122.20
50	1	89	G	P-O3'-C3'	5.31	126.07	119.70
50	1	236	C	C6-N1-C2	-5.31	118.18	120.30
50	1	997	U	N3-C2-O2	-5.31	118.48	122.20
50	1	1471	U	C5-C6-N1	5.31	125.36	122.70
14	N	468	LEU	CA-CB-CG	5.31	127.51	115.30
50	1	5	G	C6-C5-N7	5.31	133.58	130.40
50	1	163	C	N1-C2-O2	5.31	122.08	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	1	1664	U	C5-C6-N1	5.30	125.35	122.70
51	2	139	C	C6-N1-C2	-5.30	118.18	120.30
50	1	496	U	N3-C2-O2	-5.30	118.49	122.20
51	2	260	G	C8-N9-C1'	-5.29	120.12	127.00
51	2	166	G	C2-N3-C4	5.29	114.55	111.90
50	1	930	G	C8-N9-C1'	-5.29	120.12	127.00
50	1	308	U	C5-C6-N1	5.29	125.34	122.70
15	O	243	LEU	CA-CB-CG	5.29	127.46	115.30
50	1	80	C	N1-C2-O2	5.29	122.07	118.90
23	Y	206	LEU	CA-CB-CG	5.28	127.45	115.30
50	1	54	A	N7-C8-N9	5.28	116.44	113.80
50	1	504	C	C2-N1-C1'	5.28	124.60	118.80
50	1	1659	C	N3-C4-C5	-5.27	119.79	121.90
50	1	1167	C	C6-N1-C1'	-5.27	114.47	120.80
50	1	1222	C	C6-N1-C2	-5.27	118.19	120.30
50	1	619	U	N3-C2-O2	-5.26	118.52	122.20
50	1	390	C	C6-N1-C2	-5.26	118.20	120.30
50	1	876	U	N3-C2-O2	-5.26	118.52	122.20
50	1	1746	C	N3-C2-O2	-5.25	118.22	121.90
51	2	82	U	N3-C2-O2	-5.25	118.52	122.20
50	1	1068	C	C6-N1-C2	-5.25	118.20	120.30
50	1	989	C	C5-C6-N1	5.25	123.62	121.00
50	1	860	C	O4'-C1'-N1	5.25	112.40	108.20
50	1	258	C	C6-N1-C2	-5.24	118.20	120.30
50	1	1645	U	C6-N1-C2	-5.24	117.86	121.00
50	1	1449	U	N1-C2-O2	5.24	126.46	122.80
50	1	371	U	C2-N1-C1'	5.23	123.98	117.70
50	1	80	C	C6-N1-C2	-5.23	118.21	120.30
50	1	226	C	C6-N1-C2	-5.23	118.21	120.30
50	1	707	U	C2-N1-C1'	5.22	123.97	117.70
34	1	135	LEU	CA-CB-CG	5.22	127.30	115.30
50	1	134	C	N3-C2-O2	-5.22	118.25	121.90
50	1	1547	C	C2-N3-C4	5.21	122.51	119.90
50	1	2119	G	N3-C4-C5	-5.21	126.00	128.60
50	1	1560	C	N3-C2-O2	-5.21	118.25	121.90
50	1	889	C	C5-C6-N1	5.20	123.60	121.00
50	1	925	G	N9-C4-C5	-5.20	103.32	105.40
50	1	89	G	OP1-P-O3'	5.20	116.63	105.20
50	1	681	G	N3-C4-N9	5.20	129.12	126.00
50	1	889	C	C6-N1-C2	-5.20	118.22	120.30
51	2	131	U	N1-C2-O2	5.20	126.44	122.80
51	2	76	C	N1-C2-O2	5.19	122.02	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	1	834	C	C6-N1-C2	-5.19	118.22	120.30
50	1	1167	C	N3-C2-O2	-5.19	118.27	121.90
50	1	915	G	C5-C6-O6	5.19	131.71	128.60
50	1	206	C	C6-N1-C2	-5.19	118.22	120.30
50	1	1184	U	C5-C6-N1	5.18	125.29	122.70
50	1	1666	C	C4-C5-C6	-5.18	114.81	117.40
50	1	387	C	C6-N1-C2	-5.17	118.23	120.30
1	A	281	LEU	CA-CB-CG	5.17	127.18	115.30
50	1	863	G	C8-N9-C4	-5.17	104.33	106.40
50	1	454	C	N1-C2-O2	5.16	122.00	118.90
50	1	1494	U	N1-C2-O2	5.16	126.41	122.80
50	1	681	G	N3-C4-C5	-5.16	126.02	128.60
50	1	1747	A	C5-C6-N1	5.16	120.28	117.70
50	1	425	C	C6-N1-C2	-5.16	118.24	120.30
50	1	2238	A	C2-N3-C4	5.15	113.18	110.60
26	b	235	ASP	CB-CG-OD1	5.15	122.94	118.30
50	1	1638	G	P-O3'-C3'	5.15	125.88	119.70
51	2	6	C	C2-N1-C1'	5.15	124.46	118.80
50	1	2054	A	N1-C6-N6	-5.15	115.51	118.60
50	1	612	C	P-O3'-C3'	5.14	125.87	119.70
50	1	673	C	C2-N1-C1'	5.14	124.46	118.80
50	1	636	C	C2-N1-C1'	5.13	124.44	118.80
51	2	151	G	N3-C4-N9	5.13	129.08	126.00
6	F	100	LEU	CA-CB-CG	5.13	127.10	115.30
50	1	842	C	N3-C2-O2	-5.13	118.31	121.90
50	1	938	C	C6-N1-C2	-5.12	118.25	120.30
50	1	889	C	C2-N1-C1'	5.12	124.43	118.80
51	2	3	C	C2-N1-C1'	5.11	124.42	118.80
51	2	96	C	C6-N1-C2	-5.11	118.25	120.30
20	U	371	LEU	CA-CB-CG	5.11	127.06	115.30
50	1	425	C	N1-C2-O2	5.11	121.96	118.90
50	1	370	C	N1-C2-O2	5.10	121.96	118.90
50	1	1222	C	N3-C2-O2	-5.10	118.33	121.90
25	a	120	MET	CA-CB-CG	5.10	121.96	113.30
50	1	369	U	C6-N1-C2	-5.10	117.94	121.00
50	1	909	G	N3-C4-C5	-5.09	126.06	128.60
51	2	131	U	N3-C2-O2	-5.09	118.64	122.20
50	1	88	C	C2-N1-C1'	5.08	124.39	118.80
50	1	1186	U	C5-C6-N1	5.08	125.24	122.70
50	1	1050	U	N3-C2-O2	-5.08	118.64	122.20
50	1	1465	C	C5-C6-N1	5.08	123.54	121.00
50	1	1643	U	C2-N1-C1'	5.08	123.79	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	1	758	U	C5-C6-N1	5.07	125.23	122.70
50	1	258	C	C5-C6-N1	5.07	123.53	121.00
12	L	349	LEU	CA-CB-CG	5.07	126.95	115.30
50	1	424	U	P-O3'-C3'	5.07	125.78	119.70
50	1	2106	U	N1-C2-O2	5.07	126.35	122.80
50	1	1120	C	C6-N1-C2	-5.06	118.28	120.30
50	1	1112	U	N3-C2-O2	-5.06	118.66	122.20
50	1	1495	C	C6-N1-C2	-5.06	118.28	120.30
1	A	69	LEU	CA-CB-CG	5.06	126.93	115.30
24	Z	1058	LEU	CA-CB-CG	5.05	126.91	115.30
47	y	359	LEU	CA-CB-CG	5.05	126.91	115.30
51	2	260	G	C2-N3-C4	5.04	114.42	111.90
24	Z	123	LEU	CA-CB-CG	-5.04	103.72	115.30
7	G	273	MET	CB-CG-SD	-5.03	97.30	112.40
15	O	76	LEU	CA-CB-CG	5.03	126.88	115.30
50	1	989	C	C6-N1-C2	-5.03	118.29	120.30
50	1	404	C	C2-N1-C1'	5.02	124.33	118.80
50	1	889	C	N3-C2-O2	-5.02	118.39	121.90
50	1	470	C	C2-N1-C1'	5.02	124.32	118.80
50	1	133	G	N3-C4-N9	-5.01	122.99	126.00
50	1	376	G	N3-C2-N2	-5.01	116.40	119.90
50	1	1222	C	C6-N1-C1'	-5.01	114.79	120.80
50	1	56	C	C5-C6-N1	5.00	123.50	121.00
50	1	148	C	N1-C2-N3	5.00	122.70	119.20

There are no chirality outliers.

All (64) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	192	SER	Peptide
1	A	284	MET	Peptide
1	A	556	GLY	Peptide
1	A	686	SER	Peptide
4	D	169	GLU	Peptide
6	F	229	PHE	Peptide
6	F	321	ASP	Peptide
6	F	56	PRO	Peptide
12	L	266	LEU	Peptide
13	M	218	ILE	Peptide
13	M	248	ALA	Peptide
13	M	250	GLY	Peptide
13	M	386	THR	Peptide

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Mol	Chain	Res	Type	Group
14	N	363	ILE	Peptide
15	O	369	SER	Peptide
15	O	397	ASP	Peptide
15	O	472	LEU	Peptide
15	O	644	GLY	Peptide
15	O	758	HIS	Peptide
17	Q	103	ASP	Peptide
17	Q	104	PRO	Peptide
17	Q	236	SER	Peptide
18	R	293	GLU	Peptide
18	S	293	GLU	Peptide
21	V	60	GLN	Peptide
21	W	60	GLN	Peptide
22	X	179	CYS	Peptide
22	X	197	LEU	Peptide
22	X	266	ALA	Peptide
22	X	502	VAL	Peptide
23	Y	104	ALA	Peptide
23	Y	161	TYR	Peptide
24	Z	132	VAL	Peptide
24	Z	65	GLU	Peptide
24	Z	909	ASP	Peptide
26	b	287	TYR	Peptide
28	d	336	MET	Peptide
29	e	80	MET	Peptide
29	e	84	ILE	Peptide
29	e	88	ARG	Peptide
29	f	80	MET	Peptide
29	f	84	ILE	Peptide
29	f	88	ARG	Peptide
31	h	173	ASP	Peptide
31	h	182	ALA	Peptide
32	i	531	PRO	Peptide
32	j	531	PRO	Peptide
34	l	180	THR	Peptide
34	l	21	GLN	Peptide
34	l	212	ILE	Peptide
34	l	61	LEU	Peptide
34	l	65	ILE	Peptide
35	m	231	GLU	Peptide
35	m	87	MET	Peptide
37	o	148	SER	Peptide

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Mol	Chain	Res	Type	Group
37	o	59	GLN	Peptide
38	p	38	ALA	Peptide
39	q	135	GLU	Peptide
42	t	137	ASP	Peptide
43	u	41	PRO	Peptide
44	v	12	ALA	Peptide
44	v	37	ARG	Peptide
46	x	120	VAL	Peptide
47	y	365	ASN	Peptide

5.2 Too-close contacts ⓘ

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	823/904 (91%)	739 (90%)	83 (10%)	1 (0%)	51	83
2	B	67/907 (7%)	66 (98%)	1 (2%)	0	100	100
3	C	72/648 (11%)	64 (89%)	8 (11%)	0	100	100
4	D	280/884 (32%)	256 (91%)	23 (8%)	1 (0%)	34	69
5	E	325/414 (78%)	312 (96%)	13 (4%)	0	100	100
6	F	425/558 (76%)	390 (92%)	34 (8%)	1 (0%)	47	79
7	G	361/1802 (20%)	340 (94%)	21 (6%)	0	100	100
8	H	186/270 (69%)	178 (96%)	8 (4%)	0	100	100
9	I	153/962 (16%)	141 (92%)	12 (8%)	0	100	100
10	J	147/912 (16%)	139 (95%)	8 (5%)	0	100	100
11	K	143/938 (15%)	130 (91%)	13 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	L	272/557 (49%)	237 (87%)	35 (13%)	0	100	100
13	M	266/960 (28%)	222 (84%)	43 (16%)	1 (0%)	34	69
14	N	433/618 (70%)	404 (93%)	29 (7%)	0	100	100
15	O	850/1049 (81%)	768 (90%)	82 (10%)	0	100	100
16	P	188/194 (97%)	173 (92%)	15 (8%)	0	100	100
17	Q	172/391 (44%)	146 (85%)	23 (13%)	3 (2%)	9	42
18	R	238/313 (76%)	222 (93%)	15 (6%)	1 (0%)	34	69
18	S	235/313 (75%)	221 (94%)	13 (6%)	1 (0%)	34	69
19	T	383/523 (73%)	352 (92%)	31 (8%)	0	100	100
20	U	397/582 (68%)	375 (94%)	22 (6%)	0	100	100
21	V	119/127 (94%)	105 (88%)	13 (11%)	1 (1%)	19	58
21	W	118/127 (93%)	104 (88%)	13 (11%)	1 (1%)	19	58
22	X	337/630 (54%)	294 (87%)	42 (12%)	1 (0%)	41	74
23	Y	333/411 (81%)	300 (90%)	30 (9%)	3 (1%)	17	56
24	Z	627/1163 (54%)	582 (93%)	44 (7%)	1 (0%)	47	79
25	a	177/183 (97%)	162 (92%)	15 (8%)	0	100	100
26	b	287/297 (97%)	263 (92%)	24 (8%)	0	100	100
27	c	169/785 (22%)	160 (95%)	9 (5%)	0	100	100
28	d	435/446 (98%)	390 (90%)	45 (10%)	0	100	100
29	e	211/252 (84%)	199 (94%)	10 (5%)	2 (1%)	17	56
29	f	211/252 (84%)	199 (94%)	10 (5%)	2 (1%)	17	56
30	g	172/322 (53%)	164 (95%)	8 (5%)	0	100	100
31	h	163/259 (63%)	154 (94%)	9 (6%)	0	100	100
32	i	643/1073 (60%)	569 (88%)	74 (12%)	0	100	100
32	j	663/1073 (62%)	588 (89%)	75 (11%)	0	100	100
33	k	115/203 (57%)	101 (88%)	14 (12%)	0	100	100
34	l	212/255 (83%)	184 (87%)	27 (13%)	1 (0%)	29	67
35	m	256/264 (97%)	219 (86%)	37 (14%)	0	100	100
36	n	188/212 (89%)	170 (90%)	17 (9%)	1 (0%)	29	67
37	o	235/239 (98%)	202 (86%)	31 (13%)	2 (1%)	17	56
38	p	155/203 (76%)	137 (88%)	18 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	q	199/202 (98%)	187 (94%)	12 (6%)	0	100	100
40	r	157/190 (83%)	152 (97%)	5 (3%)	0	100	100
41	s	47/151 (31%)	45 (96%)	2 (4%)	0	100	100
42	t	113/150 (75%)	95 (84%)	16 (14%)	2 (2%)	8	41
43	u	124/143 (87%)	113 (91%)	11 (9%)	0	100	100
44	v	155/161 (96%)	134 (86%)	21 (14%)	0	100	100
45	w	122/130 (94%)	113 (93%)	9 (7%)	0	100	100
46	x	90/145 (62%)	79 (88%)	11 (12%)	0	100	100
47	y	91/136 (67%)	82 (90%)	9 (10%)	0	100	100
48	z	59/68 (87%)	51 (86%)	8 (14%)	0	100	100
49	0	90/311 (29%)	82 (91%)	8 (9%)	0	100	100
All	All	13489/25262 (53%)	12254 (91%)	1209 (9%)	26 (0%)	50	79

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
29	e	85	SER
29	f	85	SER
34	l	62	LYS
23	Y	105	THR
36	n	91	ASN
6	F	56	PRO
37	o	176	PRO
42	t	61	VAL
4	D	170	ASP
13	M	409	SER
17	Q	103	ASP
17	Q	104	PRO
21	V	61	PRO
21	W	61	PRO
22	X	582	THR
37	o	149	LYS
42	t	60	LYS
23	Y	104	ALA
24	Z	77	PRO
18	R	294	PRO
18	S	294	PRO
1	A	285	PRO

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Mol	Chain	Res	Type
23	Y	103	PRO
29	e	89	PRO
29	f	89	PRO
17	Q	237	PRO

5.3.2 Protein sidechains ⓘ

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	633/775 (82%)	628 (99%)	5 (1%)	81	93
2	B	43/788 (6%)	43 (100%)	0	100	100
3	C	61/536 (11%)	60 (98%)	1 (2%)	62	84
4	D	222/738 (30%)	222 (100%)	0	100	100
5	E	248/341 (73%)	248 (100%)	0	100	100
6	F	326/474 (69%)	322 (99%)	4 (1%)	71	88
7	G	289/1526 (19%)	289 (100%)	0	100	100
8	H	135/227 (60%)	134 (99%)	1 (1%)	84	94
9	I	134/821 (16%)	134 (100%)	0	100	100
10	J	129/770 (17%)	127 (98%)	2 (2%)	62	84
11	K	115/765 (15%)	115 (100%)	0	100	100
12	L	218/456 (48%)	217 (100%)	1 (0%)	88	95
13	M	219/817 (27%)	217 (99%)	2 (1%)	78	91
14	N	351/524 (67%)	349 (99%)	2 (1%)	86	94
15	O	638/863 (74%)	633 (99%)	5 (1%)	81	93
16	P	147/168 (88%)	146 (99%)	1 (1%)	84	94
18	R	175/228 (77%)	172 (98%)	3 (2%)	60	83
18	S	195/228 (86%)	192 (98%)	3 (2%)	65	85
19	T	287/435 (66%)	284 (99%)	3 (1%)	76	90
20	U	307/489 (63%)	307 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	V	91/108 (84%)	91 (100%)	0	100	100
21	W	88/108 (82%)	88 (100%)	0	100	100
22	X	273/525 (52%)	273 (100%)	0	100	100
23	Y	275/320 (86%)	274 (100%)	1 (0%)	91	95
24	Z	466/1009 (46%)	461 (99%)	5 (1%)	73	88
25	a	147/169 (87%)	146 (99%)	1 (1%)	84	94
26	b	238/266 (90%)	237 (100%)	1 (0%)	91	95
27	c	138/642 (22%)	138 (100%)	0	100	100
28	d	354/383 (92%)	348 (98%)	6 (2%)	60	83
29	e	193/223 (86%)	193 (100%)	0	100	100
29	f	193/223 (86%)	193 (100%)	0	100	100
30	g	153/287 (53%)	153 (100%)	0	100	100
31	h	138/215 (64%)	138 (100%)	0	100	100
33	k	95/167 (57%)	95 (100%)	0	100	100
34	l	189/223 (85%)	188 (100%)	1 (0%)	88	95
35	m	219/221 (99%)	219 (100%)	0	100	100
36	n	144/178 (81%)	142 (99%)	2 (1%)	67	86
37	o	202/204 (99%)	201 (100%)	1 (0%)	88	95
38	p	137/177 (77%)	137 (100%)	0	100	100
39	q	163/164 (99%)	162 (99%)	1 (1%)	86	94
40	r	122/162 (75%)	121 (99%)	1 (1%)	81	93
41	s	43/130 (33%)	43 (100%)	0	100	100
42	t	74/117 (63%)	74 (100%)	0	100	100
43	u	92/115 (80%)	92 (100%)	0	100	100
44	v	140/143 (98%)	140 (100%)	0	100	100
45	w	103/113 (91%)	103 (100%)	0	100	100
46	x	68/116 (59%)	68 (100%)	0	100	100
47	y	81/115 (70%)	81 (100%)	0	100	100
48	z	46/61 (75%)	44 (96%)	2 (4%)	29	64
49	0	68/260 (26%)	68 (100%)	0	100	100
All	All	9605/19113 (50%)	9550 (99%)	55 (1%)	86	94

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	167	LEU
1	A	271	VAL
1	A	419	THR
1	A	559	ARG
3	C	579	ILE
6	F	219	VAL
6	F	230	LEU
6	F	233	THR
6	F	409	ILE
8	H	37	ARG
10	J	765	ASN
10	J	772	ASN
12	L	267	ARG
13	M	108	ASN
13	M	171	THR
14	N	144	LEU
14	N	158	ARG
15	O	151	ILE
15	O	276	VAL
15	O	645	LYS
15	O	843	LEU
15	O	1034	VAL
16	P	63	ASN
18	R	96	ASN
18	R	131	ASN
18	R	254	LEU
18	S	96	ASN
18	S	131	ASN
18	S	254	LEU
19	T	209	LEU
19	T	298	LYS
19	T	391	ARG
23	Y	108	ARG
24	Z	113	ARG
24	Z	841	ARG
24	Z	858	ARG
24	Z	953	ARG
24	Z	1079	ARG
25	a	82	LEU
26	b	116	ARG
28	d	105	ARG

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Mol	Chain	Res	Type
28	d	159	LEU
28	d	166	ASN
28	d	206	ASN
28	d	342	LEU
28	d	418	ARG
34	l	166	ARG
36	n	15	VAL
36	n	126	ASN
37	o	177	ARG
39	q	125	ARG
40	r	94	VAL
48	z	11	VAL
48	z	23	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (120) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	28	HIS
1	A	78	GLN
1	A	253	GLN
1	A	337	GLN
1	A	524	GLN
1	A	846	ASN
4	D	128	GLN
5	E	154	ASN
5	E	319	HIS
6	F	96	GLN
6	F	175	GLN
6	F	205	HIS
6	F	221	HIS
6	F	266	GLN
6	F	267	ASN
6	F	270	ASN
6	F	274	HIS
6	F	277	GLN
6	F	322	ASN
6	F	378	GLN
6	F	427	ASN
7	G	77	GLN
7	G	226	ASN
7	G	295	GLN

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Mol	Chain	Res	Type
7	G	318	HIS
7	G	349	HIS
8	H	13	HIS
9	I	835	GLN
10	J	765	ASN
10	J	772	ASN
10	J	776	ASN
11	K	338	HIS
11	K	371	GLN
11	K	916	GLN
12	L	103	HIS
12	L	333	HIS
13	M	108	ASN
13	M	167	HIS
13	M	401	ASN
14	N	351	ASN
14	N	370	GLN
14	N	411	GLN
14	N	584	GLN
15	O	197	ASN
15	O	334	ASN
15	O	577	GLN
15	O	621	HIS
15	O	740	HIS
16	P	63	ASN
16	P	149	ASN
18	R	96	ASN
18	R	131	ASN
18	R	249	GLN
18	R	308	GLN
18	S	96	ASN
18	S	131	ASN
18	S	299	HIS
19	T	5	ASN
19	T	54	ASN
19	T	176	HIS
19	T	321	HIS
20	U	147	HIS
20	U	167	HIS
20	U	288	ASN
20	U	336	HIS
20	U	364	GLN

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Mol	Chain	Res	Type
20	U	404	ASN
21	V	67	HIS
21	W	67	HIS
22	X	561	ASN
23	Y	316	GLN
24	Z	159	ASN
24	Z	239	ASN
25	a	16	HIS
25	a	135	HIS
26	b	210	HIS
26	b	275	ASN
26	b	295	ASN
28	d	13	GLN
28	d	21	GLN
28	d	111	ASN
28	d	166	ASN
28	d	206	ASN
28	d	207	GLN
28	d	327	GLN
29	e	93	HIS
29	e	111	GLN
29	e	243	HIS
29	f	93	HIS
29	f	94	GLN
29	f	111	GLN
31	h	137	GLN
33	k	179	HIS
34	l	21	GLN
34	l	99	ASN
34	l	118	GLN
34	l	124	ASN
34	l	232	HIS
35	m	36	HIS
35	m	98	ASN
36	n	126	ASN
37	o	13	GLN
37	o	179	GLN
37	o	185	GLN
37	o	189	HIS
38	p	95	HIS
39	q	84	HIS
39	q	153	HIS

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Mol	Chain	Res	Type
39	q	179	GLN
43	u	15	ASN
43	u	77	GLN
44	v	16	GLN
44	v	111	ASN
45	w	8	HIS
45	w	12	ASN
45	w	42	GLN
45	w	113	HIS
46	x	89	ASN
47	y	385	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
50	1	1319/2568 (51%)	478 (36%)	27 (2%)
51	2	226/274 (82%)	76 (33%)	5 (2%)
All	All	1545/2842 (54%)	554 (35%)	32 (2%)

All (554) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
50	1	3	G
50	1	5	G
50	1	6	G
50	1	7	A
50	1	8	U
50	1	9	G
50	1	10	U
50	1	16	U
50	1	17	C
50	1	19	C
50	1	20	C
50	1	23	G
50	1	27	A
50	1	30	U
50	1	31	C
50	1	32	U
50	1	35	G
50	1	38	G
50	1	41	G

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Mol	Chain	Res	Type
50	1	53	A
50	1	59	U
50	1	69	U
50	1	71	A
50	1	72	U
50	1	73	A
50	1	74	C
50	1	77	C
50	1	84	A
50	1	89	G
50	1	90	A
50	1	92	G
50	1	93	G
50	1	119	G
50	1	124	C
50	1	126	C
50	1	127	C
50	1	128	G
50	1	134	C
50	1	136	C
50	1	137	C
50	1	150	C
50	1	154	C
50	1	155	G
50	1	158	C
50	1	159	C
50	1	160	C
50	1	161	A
50	1	162	G
50	1	166	A
50	1	168	C
50	1	169	G
50	1	173	G
50	1	179	G
50	1	182	C
50	1	183	C
50	1	185	G
50	1	190	G
50	1	191	C
50	1	192	A
50	1	193	U
50	1	201	G

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Mol	Chain	Res	Type
50	1	202	A
50	1	203	C
50	1	205	C
50	1	206	C
50	1	207	U
50	1	208	A
50	1	209	A
50	1	210	G
50	1	216	A
50	1	220	A
50	1	221	A
50	1	224	C
50	1	234	G
50	1	236	C
50	1	242	U
50	1	243	U
50	1	244	G
50	1	257	G
50	1	258	C
50	1	260	U
50	1	261	G
50	1	265	G
50	1	266	C
50	1	267	U
50	1	268	G
50	1	269	G
50	1	272	A
50	1	273	G
50	1	276	C
50	1	277	U
50	1	278	A
50	1	281	U
50	1	282	C
50	1	283	A
50	1	285	A
50	1	290	C
50	1	291	C
50	1	292	G
50	1	306	G
50	1	308	U
50	1	333	C
50	1	334	U

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Mol	Chain	Res	Type
50	1	339	C
50	1	346	C
50	1	347	C
50	1	349	C
50	1	351	U
50	1	352	G
50	1	353	G
50	1	362	G
50	1	375	G
50	1	382	U
50	1	383	G
50	1	384	C
50	1	386	G
50	1	391	C
50	1	398	C
50	1	402	U
50	1	403	G
50	1	416	U
50	1	423	U
50	1	424	U
50	1	425	C
50	1	435	A
50	1	436	A
50	1	440	G
50	1	441	A
50	1	442	U
50	1	443	G
50	1	452	G
50	1	453	G
50	1	454	C
50	1	459	C
50	1	474	A
50	1	475	C
50	1	483	U
50	1	484	G
50	1	491	G
50	1	492	C
50	1	497	A
50	1	499	G
50	1	500	C
50	1	501	U
50	1	502	A

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Mol	Chain	Res	Type
50	1	504	C
50	1	581	C
50	1	582	G
50	1	583	A
50	1	584	U
50	1	585	A
50	1	586	G
50	1	589	A
50	1	591	C
50	1	594	G
50	1	596	U
50	1	609	A
50	1	610	G
50	1	612	C
50	1	613	A
50	1	614	U
50	1	621	G
50	1	624	U
50	1	627	A
50	1	638	A
50	1	646	C
50	1	647	U
50	1	650	G
50	1	652	A
50	1	653	U
50	1	654	A
50	1	655	A
50	1	656	G
50	1	659	A
50	1	660	U
50	1	664	A
50	1	678	A
50	1	679	A
50	1	680	U
50	1	684	U
50	1	685	C
50	1	686	A
50	1	687	U
50	1	688	U
50	1	689	A
50	1	690	A
50	1	692	U

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Mol	Chain	Res	Type
50	1	693	C
50	1	697	U
50	1	700	C
50	1	701	G
50	1	702	U
50	1	703	U
50	1	710	A
50	1	711	U
50	1	713	G
50	1	714	U
50	1	715	A
50	1	727	G
50	1	728	G
50	1	730	U
50	1	731	A
50	1	734	C
50	1	735	G
50	1	737	G
50	1	739	U
50	1	740	A
50	1	742	U
50	1	743	U
50	1	744	C
50	1	745	U
50	1	750	C
50	1	753	A
50	1	754	U
50	1	755	A
50	1	756	C
50	1	758	U
50	1	759	G
50	1	760	C
50	1	833	U
50	1	834	C
50	1	841	A
50	1	844	U
50	1	845	C
50	1	846	U
50	1	849	A
50	1	850	A
50	1	851	U
50	1	854	C

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Mol	Chain	Res	Type
50	1	856	C
50	1	857	G
50	1	858	G
50	1	860	C
50	1	861	U
50	1	862	U
50	1	863	G
50	1	864	C
50	1	865	G
50	1	869	G
50	1	871	G
50	1	883	A
50	1	886	U
50	1	889	C
50	1	892	C
50	1	893	C
50	1	897	U
50	1	898	C
50	1	904	U
50	1	905	C
50	1	906	G
50	1	907	A
50	1	910	G
50	1	913	G
50	1	921	G
50	1	922	C
50	1	927	C
50	1	930	G
50	1	931	G
50	1	935	C
50	1	936	A
50	1	943	A
50	1	944	A
50	1	984	A
50	1	985	A
50	1	986	C
50	1	987	G
50	1	988	G
50	1	989	C
50	1	991	A
50	1	998	C
50	1	1000	A

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Mol	Chain	Res	Type
50	1	1001	A
50	1	1002	G
50	1	1005	A
50	1	1007	G
50	1	1012	A
50	1	1020	A
50	1	1021	A
50	1	1023	U
50	1	1024	U
50	1	1025	A
50	1	1028	C
50	1	1029	A
50	1	1030	A
50	1	1031	U
50	1	1035	G
50	1	1036	A
50	1	1037	C
50	1	1038	A
50	1	1039	C
50	1	1043	G
50	1	1044	A
50	1	1048	A
50	1	1054	A
50	1	1059	A
50	1	1061	A
50	1	1064	G
50	1	1069	A
50	1	1070	G
50	1	1083	U
50	1	1084	C
50	1	1085	U
50	1	1086	U
50	1	1087	G
50	1	1088	U
50	1	1089	A
50	1	1094	G
50	1	1095	A
50	1	1097	U
50	1	1098	G
50	1	1102	A
50	1	1103	C
50	1	1104	A

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Mol	Chain	Res	Type
50	1	1120	C
50	1	1122	A
50	1	1123	G
50	1	1124	G
50	1	1125	A
50	1	1126	A
50	1	1127	C
50	1	1128	A
50	1	1129	A
50	1	1132	G
50	1	1141	G
50	1	1147	U
50	1	1148	G
50	1	1149	C
50	1	1154	A
50	1	1156	C
50	1	1158	G
50	1	1162	U
50	1	1163	A
50	1	1164	A
50	1	1166	U
50	1	1167	C
50	1	1168	C
50	1	1177	U
50	1	1178	A
50	1	1179	G
50	1	1186	U
50	1	1213	U
50	1	1219	A
50	1	1220	A
50	1	1221	C
50	1	1222	C
50	1	1223	U
50	1	1444	A
50	1	1445	U
50	1	1447	A
50	1	1448	A
50	1	1449	U
50	1	1450	A
50	1	1452	G
50	1	1458	U
50	1	1469	A

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Mol	Chain	Res	Type
50	1	1481	U
50	1	1482	C
50	1	1483	A
50	1	1484	G
50	1	1486	G
50	1	1487	G
50	1	1488	U
50	1	1491	A
50	1	1494	U
50	1	1497	U
50	1	1498	G
50	1	1499	G
50	1	1515	A
50	1	1517	A
50	1	1518	A
50	1	1519	C
50	1	1520	U
50	1	1525	A
50	1	1527	G
50	1	1529	A
50	1	1536	A
50	1	1545	U
50	1	1547	C
50	1	1549	U
50	1	1551	A
50	1	1552	A
50	1	1556	G
50	1	1624	A
50	1	1625	G
50	1	1630	C
50	1	1631	G
50	1	1637	C
50	1	1638	G
50	1	1639	U
50	1	1642	A
50	1	1643	U
50	1	1644	U
50	1	1645	U
50	1	1646	U
50	1	1656	C
50	1	1658	G
50	1	1659	C

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Mol	Chain	Res	Type
50	1	1665	A
50	1	1666	C
50	1	1667	G
50	1	1668	A
50	1	1670	A
50	1	1673	U
50	1	1674	C
50	1	1675	A
50	1	1676	A
50	1	1678	A
50	1	1679	U
50	1	1680	G
50	1	1681	U
50	1	1683	U
50	1	1684	G
50	1	1698	G
50	1	1699	U
50	1	1701	U
50	1	1735	A
50	1	1742	C
50	1	1744	A
50	1	1751	G
50	1	1758	C
50	1	2047	G
50	1	2049	G
50	1	2054	A
50	1	2056	U
50	1	2057	G
50	1	2061	G
50	1	2068	C
50	1	2072	U
50	1	2073	A
50	1	2074	C
50	1	2075	U
50	1	2077	C
50	1	2078	C
50	1	2085	G
50	1	2086	A
50	1	2087	G
50	1	2088	A
50	1	2094	G
50	1	2107	A

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Mol	Chain	Res	Type
50	1	2109	A
50	1	2114	G
50	1	2115	U
50	1	2118	U
50	1	2119	G
50	1	2120	C
50	1	2121	U
50	1	2156	A
50	1	2157	G
50	1	2166	A
50	1	2167	G
50	1	2173	G
50	1	2178	U
50	1	2183	A
50	1	2184	G
50	1	2185	C
50	1	2190	G
50	1	2197	A
50	1	2201	C
50	1	2202	C
50	1	2205	G
50	1	2210	U
50	1	2211	U
50	1	2212	G
50	1	2213	U
50	1	2214	A
50	1	2215	C
50	1	2216	A
50	1	2218	A
50	1	2220	C
50	1	2221	G
50	1	2222	C
50	1	2223	C
50	1	2228	G
50	1	2230	U
50	1	2235	C
50	1	2236	C
50	1	2329	A
50	1	2330	G
51	2	5	A
51	2	6	C
51	2	7	A

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Mol	Chain	Res	Type
51	2	15	A
51	2	23	A
51	2	24	U
51	2	25	U
51	2	28	U
51	2	29	A
51	2	30	U
51	2	31	A
51	2	33	U
51	2	36	U
51	2	37	U
51	2	39	U
51	2	48	G
51	2	57	A
51	2	58	A
51	2	62	A
51	2	63	G
51	2	90	C
51	2	91	G
51	2	92	A
51	2	94	A
51	2	95	U
51	2	100	G
51	2	101	G
51	2	104	C
51	2	111	G
51	2	118	C
51	2	124	U
51	2	125	U
51	2	126	U
51	2	127	A
51	2	128	C
51	2	133	G
51	2	136	C
51	2	142	G
51	2	145	A
51	2	147	G
51	2	151	G
51	2	153	G
51	2	160	U
51	2	162	C
51	2	163	C

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Mol	Chain	Res	Type
51	2	164	U
51	2	165	C
51	2	166	G
51	2	167	U
51	2	168	C
51	2	170	C
51	2	178	U
51	2	179	A
51	2	181	A
51	2	187	U
51	2	189	G
51	2	190	C
51	2	192	A
51	2	194	G
51	2	198	U
51	2	199	G
51	2	200	U
51	2	201	A
51	2	244	G
51	2	246	G
51	2	247	G
51	2	249	U
51	2	250	G
51	2	253	G
51	2	254	A
51	2	255	U
51	2	256	G
51	2	259	A
51	2	260	G
51	2	261	U
51	2	262	C

All (32) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
50	1	34	C
50	1	88	C
50	1	89	G
50	1	135	A
50	1	205	C
50	1	209	A
50	1	277	U

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Mol	Chain	Res	Type
50	1	281	U
50	1	424	U
50	1	582	G
50	1	585	A
50	1	593	G
50	1	612	C
50	1	684	U
50	1	742	U
50	1	1001	A
50	1	1068	C
50	1	1085	U
50	1	1087	G
50	1	1128	A
50	1	1163	A
50	1	1481	U
50	1	1485	A
50	1	1638	G
50	1	1734	G
50	1	2156	A
50	1	2177	G
51	2	6	C
51	2	23	A
51	2	35	G
51	2	246	G
51	2	255	U

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

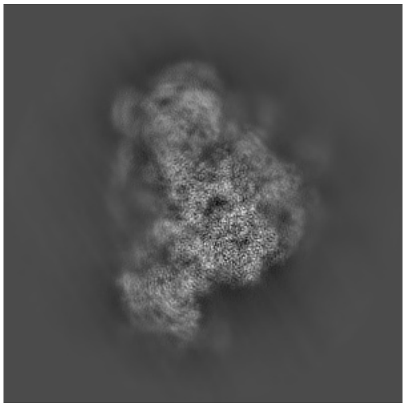
6 Map visualisation

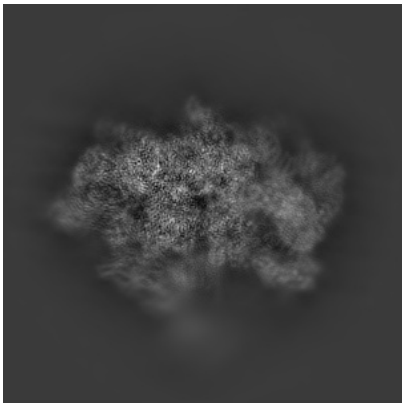
This section contains visualisations of the EMDB entry EMD-3847. These allow visual inspection of the internal detail of the map and identification of artifacts.

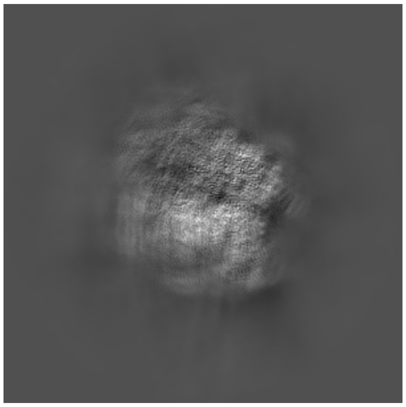
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

6.1.1 Primary map


X

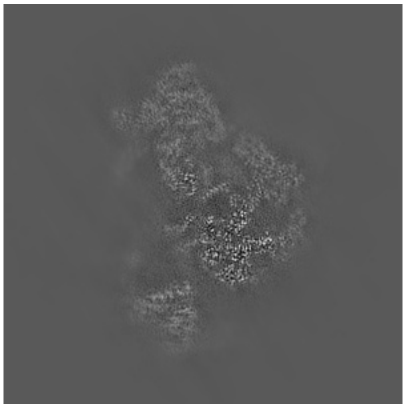

Y

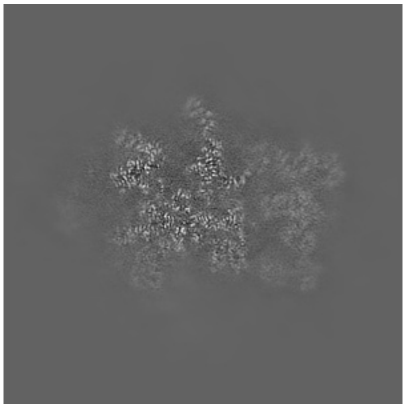

Z

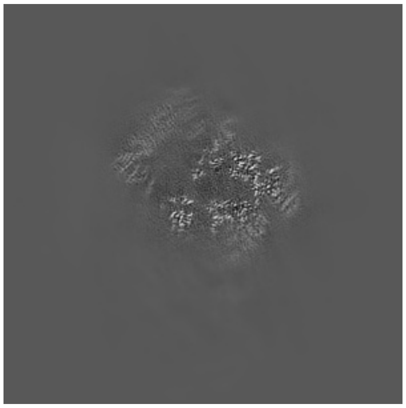
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map


X Index: 240

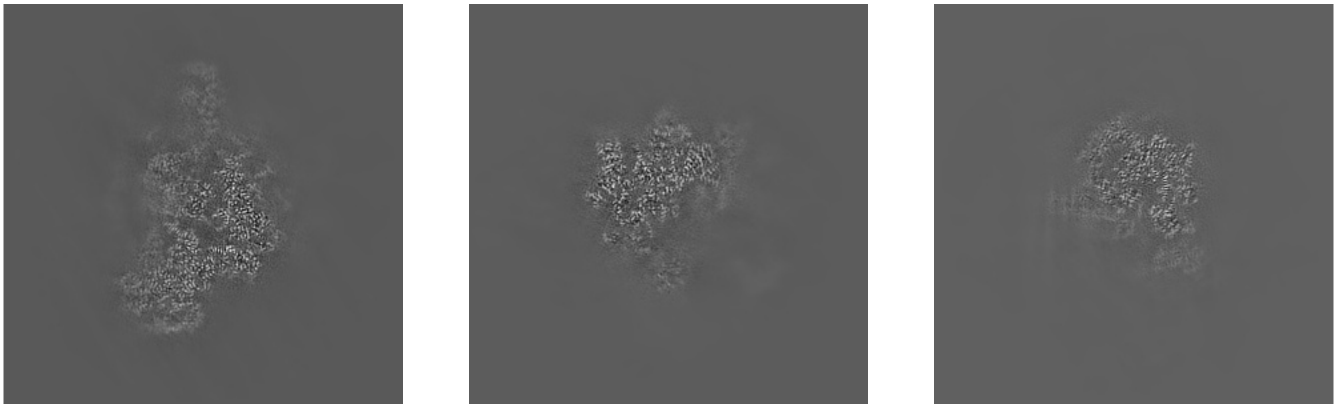

Y Index: 240


Z Index: 240

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

6.3 Largest variance slices

6.3.1 Primary map



X Index: 279 Y Index: 281 Z Index: 183

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

6.4 Orthogonal surface views

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

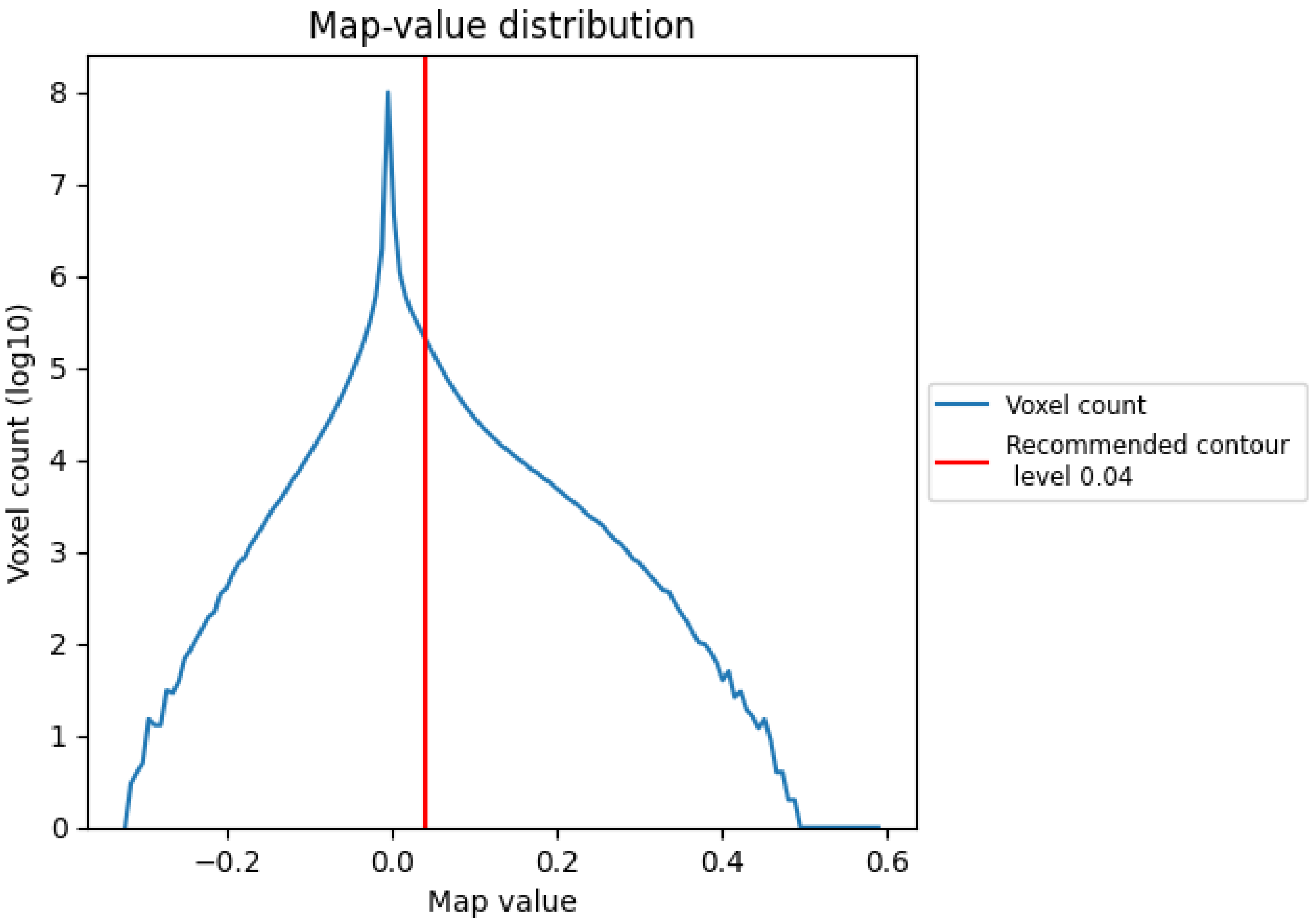
6.5 Mask visualisation ⓘ

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

7 Map analysis ⓘ

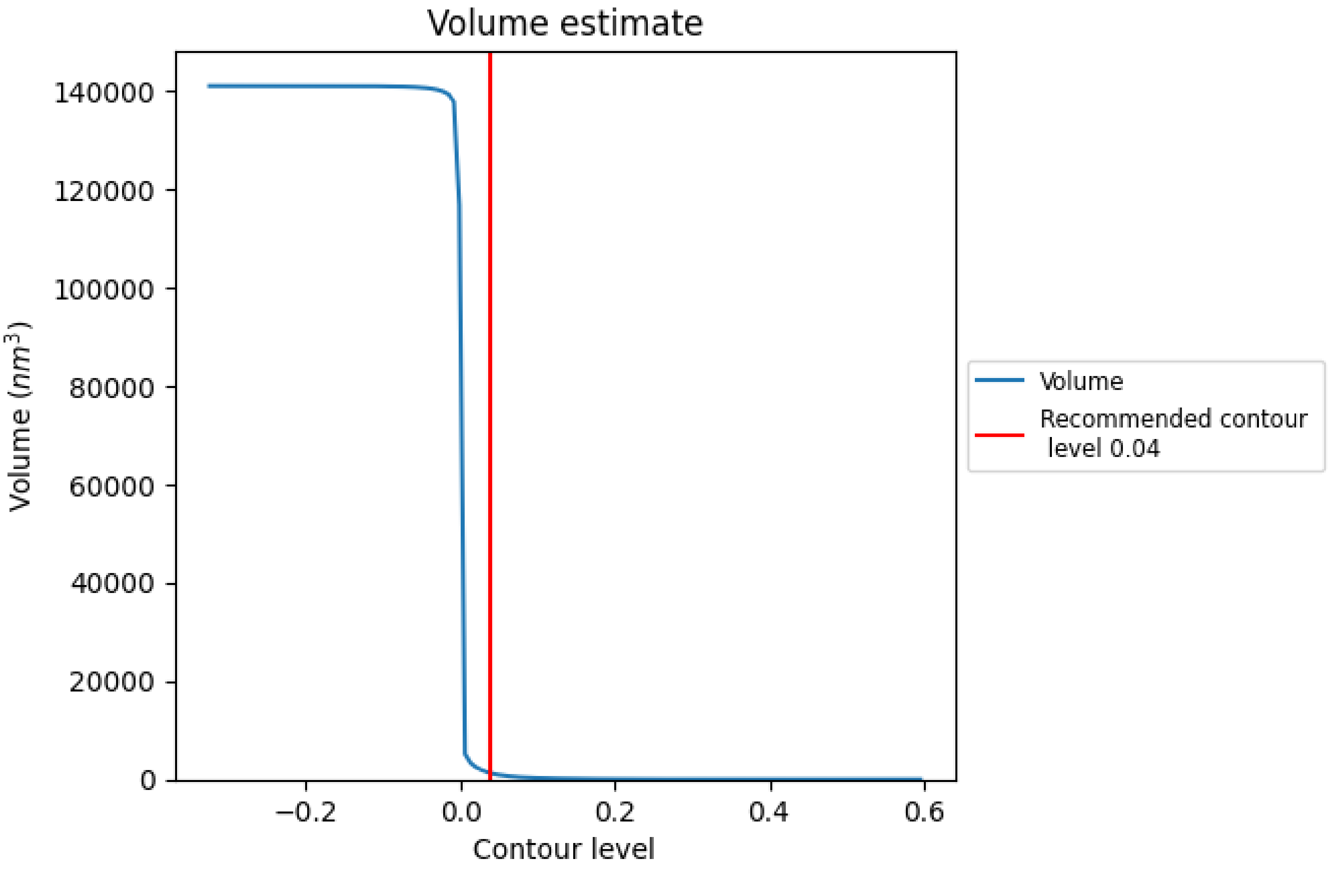
This section contains the results of statistical analysis of the map.

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.

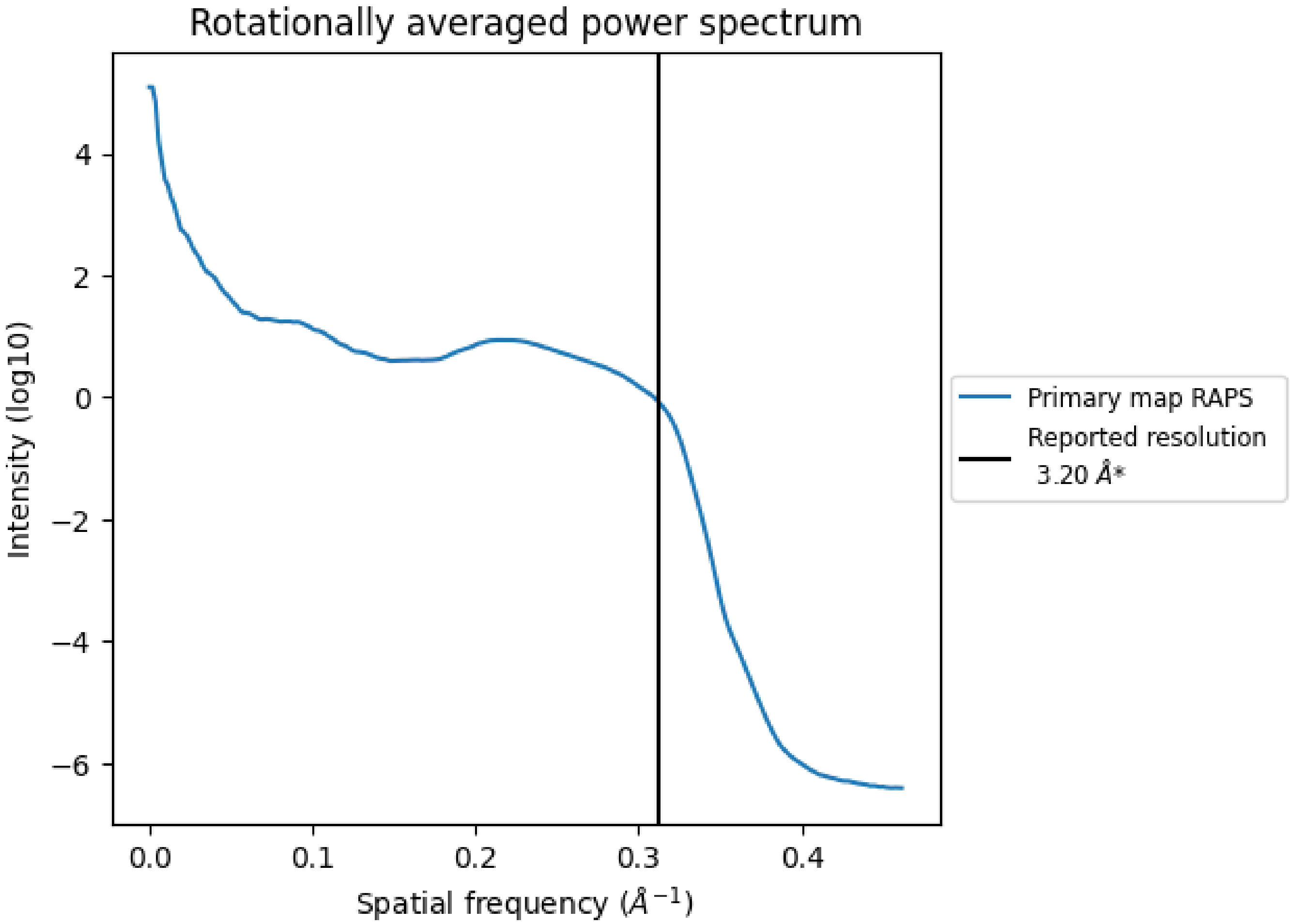
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 1269 nm^3; this corresponds to an approximate mass of 1146 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 ⓘ

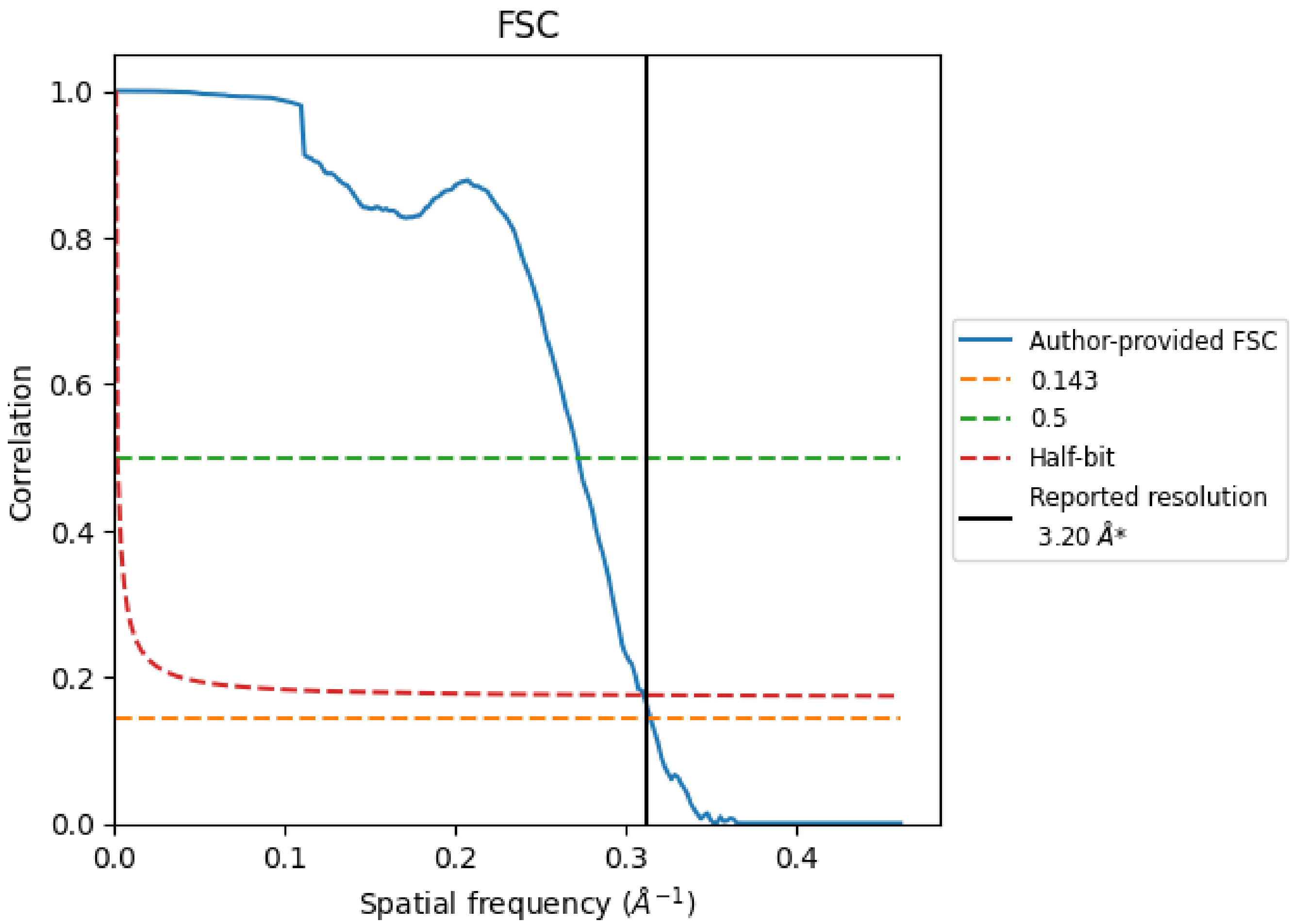


*Reported resolution corresponds to spatial frequency of 0.312 $Å^{-1}$

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 0.312 $Å^{-1}$

8.2 Resolution estimates ⓘ

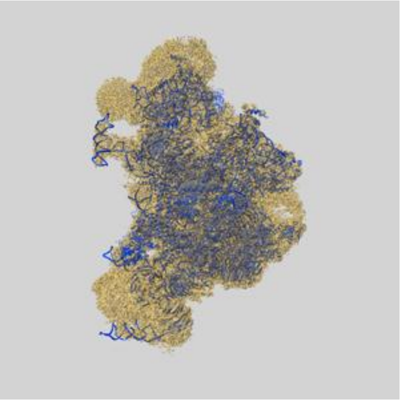
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.18	3.68	3.22
Unmasked-calculated*	-	-	-

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

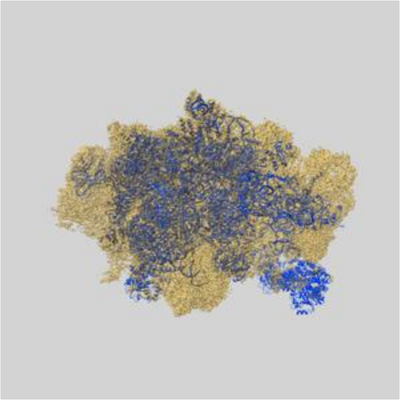
9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-3847 and PDB model 5OQL. Per-residue inclusion information can be found in section 3 on page 13.

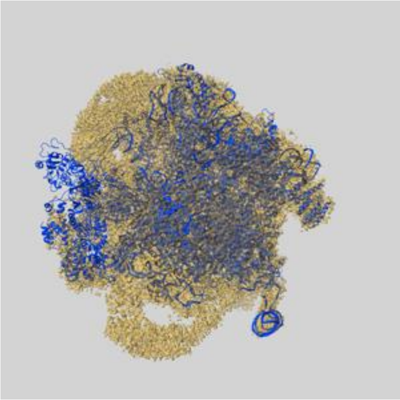
9.1 Map-model overlay ⓘ



X



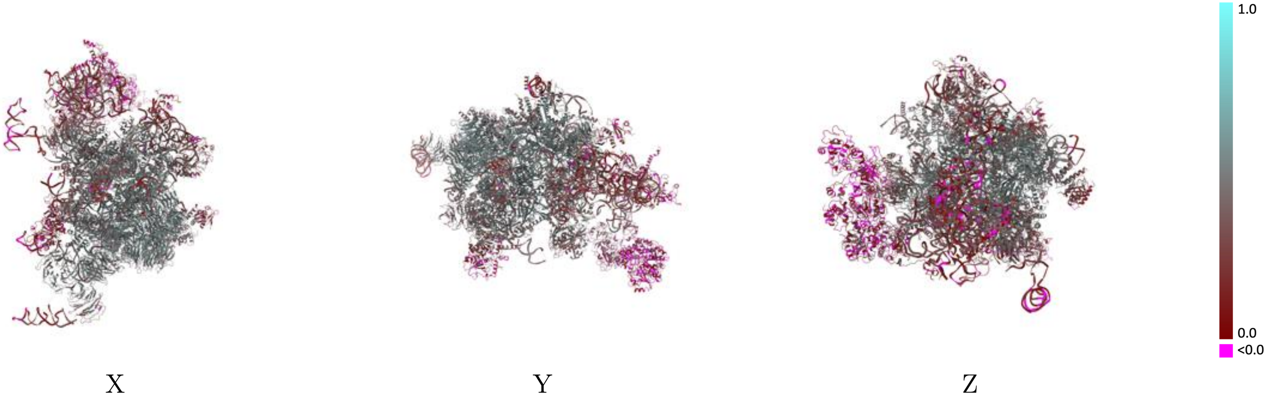
Y



Z

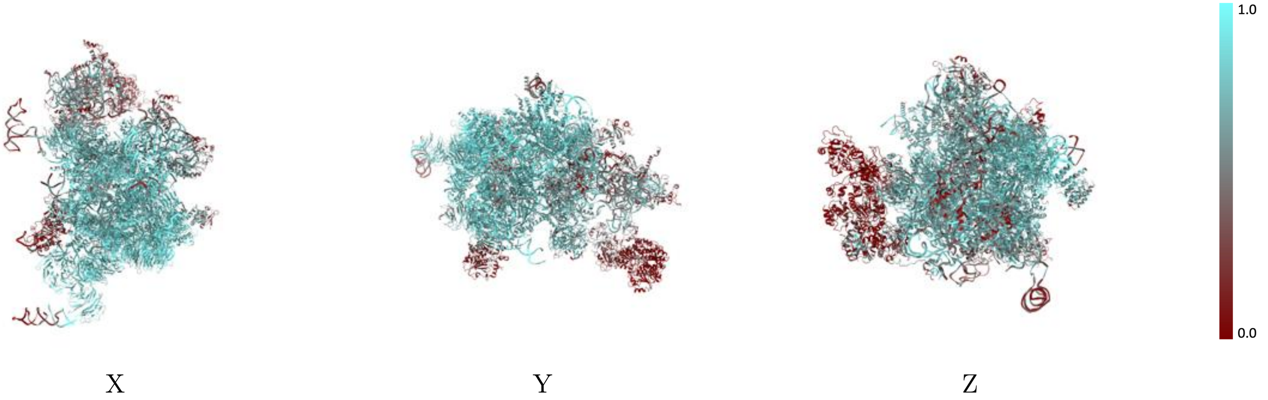
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ



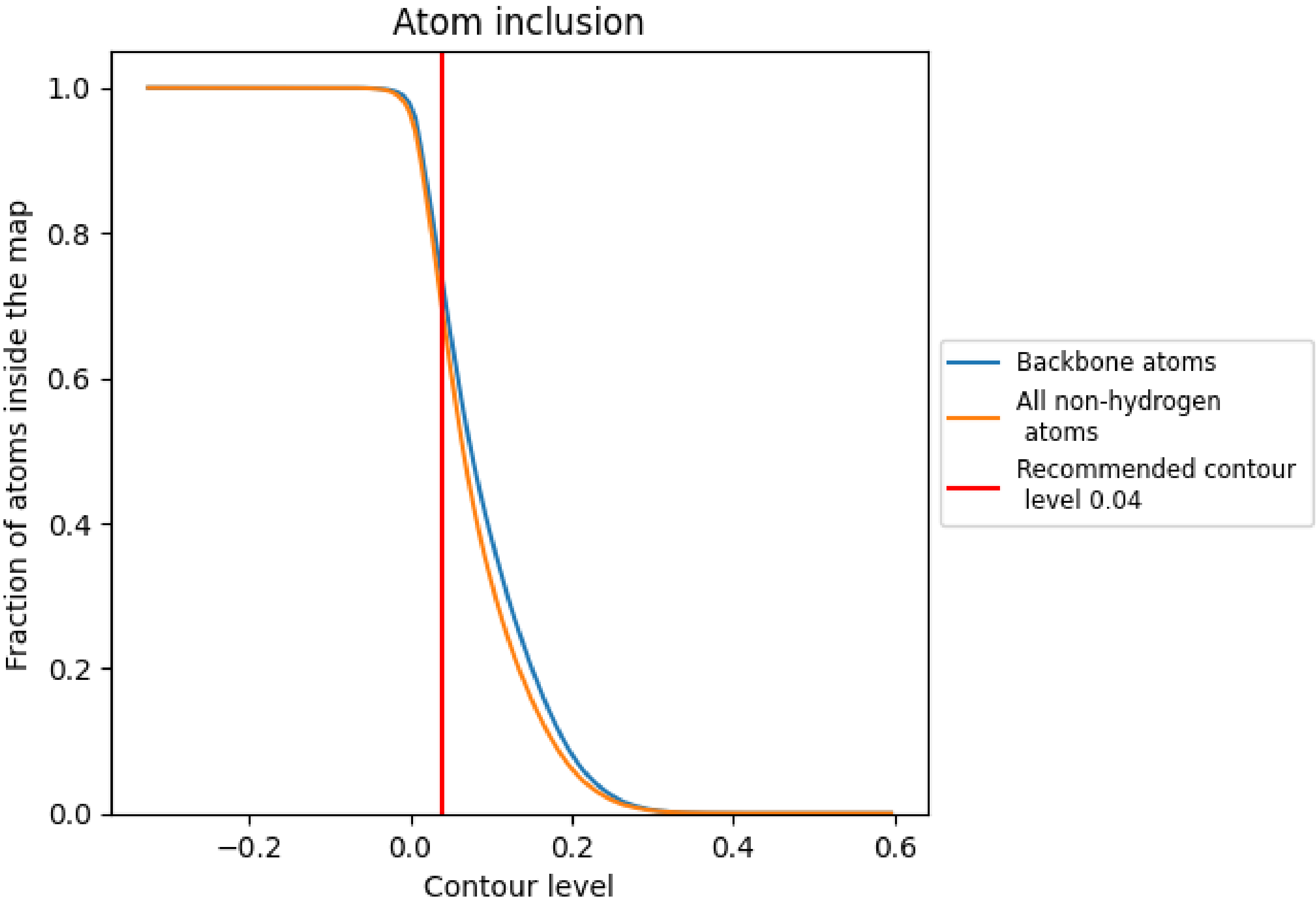
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 ⓘ



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 (0.04).

9.4 Atom inclusion ⓘ



At the recommended contour level, 73% of all backbone atoms, 69% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6914	0.3820
0	0.7120	0.4640
1	0.7329	0.3550
2	0.7236	0.3600
A	0.8650	0.4950
B	0.7524	0.4400
C	0.8252	0.4940
D	0.8141	0.4580
E	0.7666	0.3920
F	0.8921	0.5210
G	0.8691	0.4970
H	0.8379	0.4990
I	0.6944	0.3900
J	0.7809	0.4010
K	0.8401	0.4800
L	0.6571	0.3730
M	0.8073	0.4230
N	0.8741	0.5100
O	0.8819	0.5000
P	0.8121	0.4790
Q	0.6088	0.3400
R	0.8712	0.5060
S	0.2729	0.2150
T	0.7630	0.4080
U	0.5738	0.3530
V	0.8014	0.4560
W	0.6851	0.3740
X	0.6945	0.3800
Y	0.6758	0.3870
Z	0.8123	0.4610
a	0.8957	0.5260
b	0.8093	0.4820
c	0.7776	0.4460
d	0.8735	0.5080
e	0.3277	0.2480

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Chain	Atom inclusion	Q-score
f	0.0895	0.0800
g	0.5353	0.3700
h	0.4822	0.2610
i	0.2136	0.1550
j	0.0386	0.0820
k	0.8276	0.4800
l	0.4555	0.2900
m	0.4329	0.2260
n	0.8196	0.4630
o	0.4029	0.1770
p	0.4306	0.2430
q	0.3828	0.1720
r	0.8208	0.4630
s	0.4436	0.2070
t	0.5712	0.3280
u	0.8698	0.5000
v	0.3863	0.1660
w	0.7536	0.4290
x	0.8430	0.4850
y	0.4615	0.2300
z	0.7816	0.4430