Full wwPDB EM Validation Report ⓘ

Nov 14, 2022 – 03:50 AM EST

PDB ID	:	6VZJ
EMDB ID	:	EMD-21494
Title	:	Escherichia coli transcription-translation complex A1 (TTC-A1) containing mRNA with a 15 nt long spacer, fMet-tRNAs at E-site and P-site, and lacking transcription factor NusG
Authors	:	Molodtsov, V.; Wang, C.; Su, M.; Ebright, R.H.
Deposited on	:	2020-02-28
Resolution	:	4.10 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

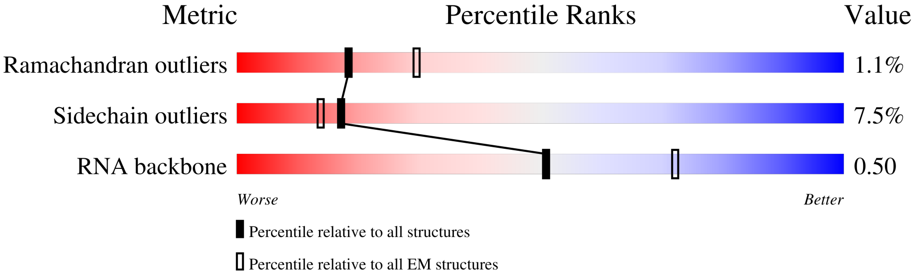
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance ⓘ

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

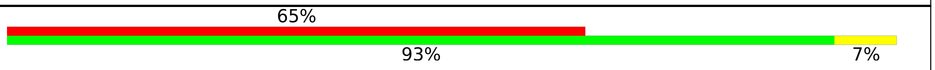
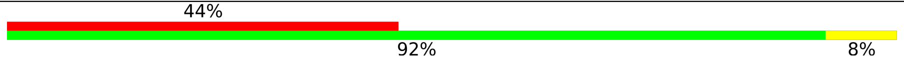
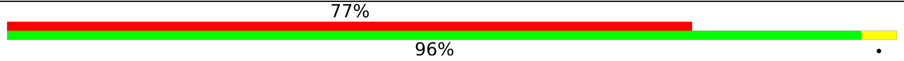
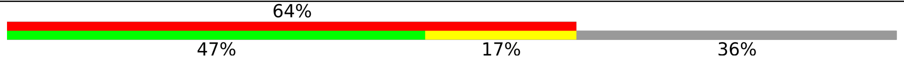
The reported resolution of this entry is 4.10 Å.

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	0	103	
2	1	110	
3	2	100	
4	3	104	
5	4	94	
6	5	36	
7	6	36	
8	7	32	

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Mol	Chain	Length	Quality of chain
9	9	165	88% 54% 33% • 10%
10	A	76	95% 58% 38% •
10	B	76	99% 46% 49% 5%
11	AA	1342	99% 89% 8% ••
12	AC	329	70% 64% 5% 30%
12	AD	329	69% 69% • 31%
13	AE	1407	95% 89% 5% • 5%
14	C	75	67% 85% • 12%
15	D	1542	27% 78% 20% ••
16	E	87	76% 93% 6% •
17	F	71	82% 94% • •
18	G	241	72% 90% • 7%
19	H	557	46% 41% • • 54%
20	I	233	76% 86% • 11%
21	J	205	84% 97% •
22	K	167	50% 89% 5% 7%
23	L	135	67% 72% • • 23%
24	M	151	83% 95% 5% •
25	N	129	69% 98% •
26	O	127	84% 95% 5%
27	P	99	90% 90% 10%
28	Q	117	83% 96% •
29	R	123	45% 93% 6% •
30	S	101	80% 95% • •
31	T	89	66% 85% 13% •

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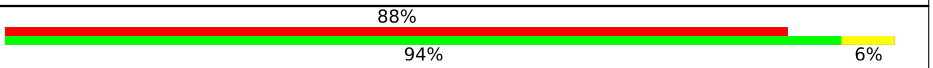
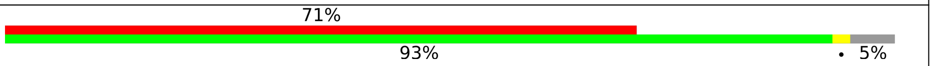
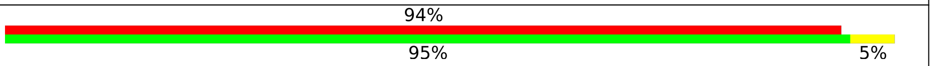
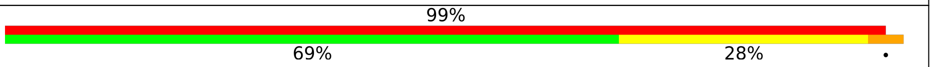
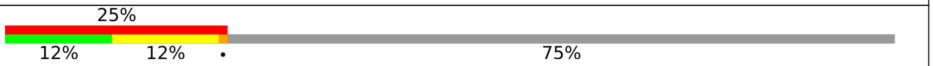
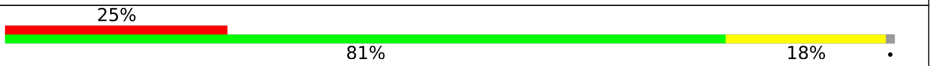
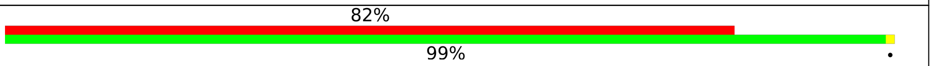
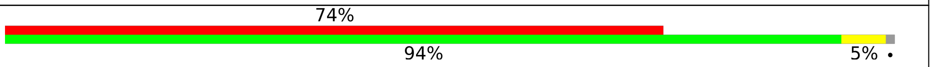
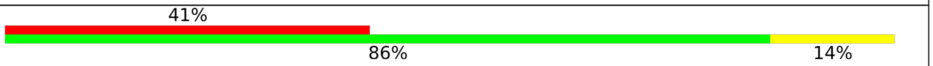
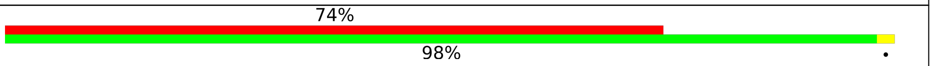
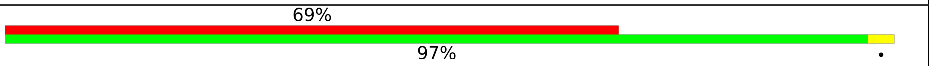
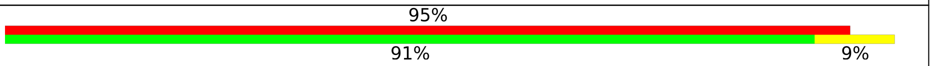
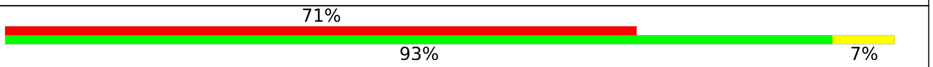
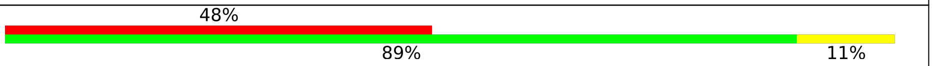
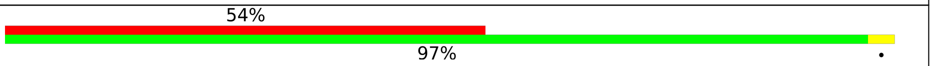
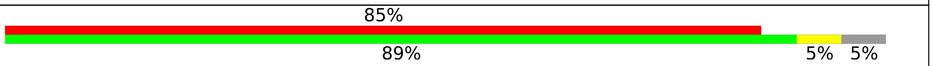
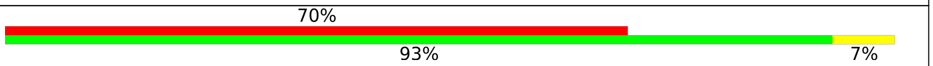
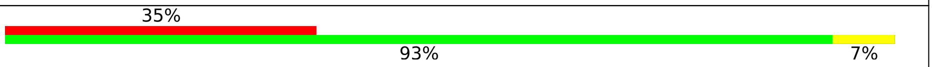
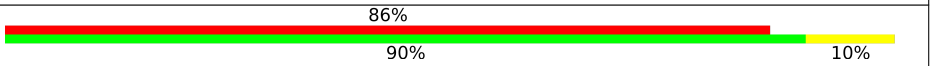
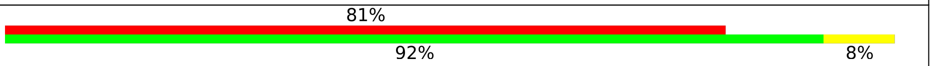
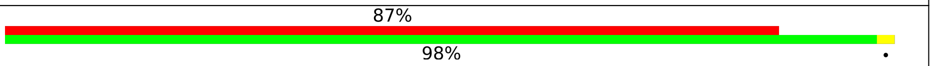
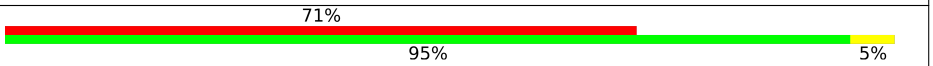
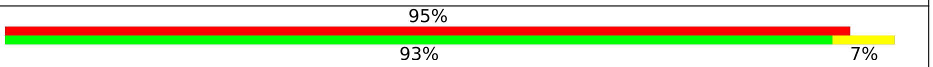
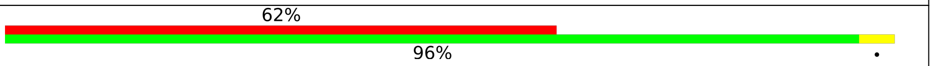
Mol	Chain	Length	Quality of chain
32	U	82	 88% 94% 6%
33	V	84	 71% 93% • 5%
34	W	83	 94% 95% 5%
35	X	116	 89% 90% 10%
36	Y	141	 99% 69% 28% •
37	Z	121	 25% 12% 12% • 75%
38	a	2904	 25% 81% 18% •
39	b	76	 82% 99% •
40	c	78	 74% 94% 5% •
41	d	120	 41% 86% 14%
42	e	62	 74% 98% •
43	f	58	 69% 97% •
44	g	66	 95% 91% 9%
45	h	271	 71% 93% 7%
46	i	56	 48% 89% 11%
47	j	209	 54% 97% •
48	k	55	 85% 89% 5% 5%
49	l	201	 70% 93% 7%
50	m	46	 35% 93% 7%
51	n	177	 86% 90% 10%
52	o	64	 81% 92% 8%
53	p	175	 87% 98% •
54	q	38	 71% 95% 5%
55	r	149	 95% 93% 7%
56	s	142	 62% 96% •

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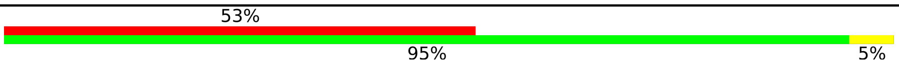
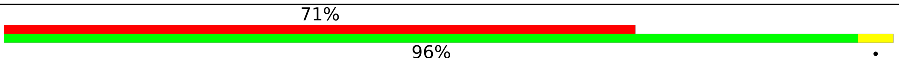
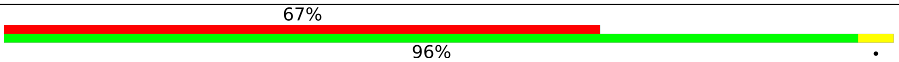
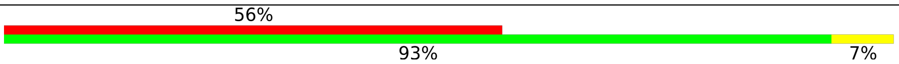
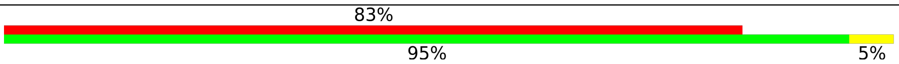
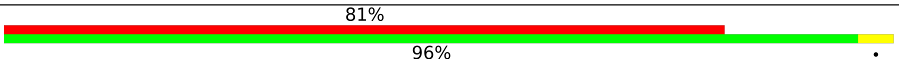
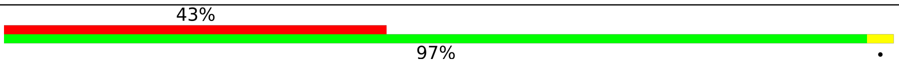
Mol	Chain	Length	Quality of chain
57	t	123	
58	u	144	
59	v	136	
60	w	119	
61	x	116	
62	y	114	
63	z	117	

2 Entry composition

There are 65 unique types of molecules in this entry. The entry contains 299095 atoms, of which 123940 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 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	0	103	1655	516	839	153	145	2	0	0

- Molecule 2 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	1	110	1779	532	922	166	156	3	0	0

- Molecule 3 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	2	94	1557	470	811	140	134	2	0	0

- Molecule 4 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
4	3	103	1632	498	844	148	142	0	0

- Molecule 5 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	4	94	1533	479	780	137	134	3	0	0

- Molecule 6 is a DNA chain called NT DNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
6	5	23	732	225	260	87	137	23	0	0

- Molecule 7 is a DNA chain called T DNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
7	6	27	847	259	305	89	167	27	0	0

- Molecule 8 is a RNA chain called mRNA with 27 nt long spacer.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
8	7	32	769	300	97	100	240	32	0	0

- Molecule 9 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	9	148	1117	705	196	209	7	0	0

- Molecule 10 is a RNA chain called E-site and P-site tRNA (fMet).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
10	A	76	2446	723	826	295	527	75	0	0
10	B	76	2433	723	813	295	527	75	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	U	deletion	GB 1848959854
B	?	-	U	deletion	GB 1848959854

- Molecule 11 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
11	AA	1322	20851	6539	10426	1817	2026	43	0	0

- Molecule 12 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
12	AC	230	3599	1112	1813	317	351	6	0	0

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Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
12	AD	228	3556	1100	1789	312	349	6	0	0

- Molecule 13 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
13	AE	1335	21000	6526	10612	1854	1958	50	0	0

- Molecule 14 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
14	C	66	1103	344	559	102	97	1	0	0

- Molecule 15 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
15	D	1524	49126	14585	16423	6003	10591	1524	0	0

- Molecule 16 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
16	E	86	1388	414	719	138	114	3	0	0

- Molecule 17 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
17	F	70	1218	366	629	125	97	1	0	0

- Molecule 18 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
18	G	225	3545	1113	1785	316	323	8	0	0

- Molecule 19 is a protein called 30S ribosomal protein S1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
19	H	259	3184	1073	1454	305	349	3	0	0

- Molecule 20 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
20	I	208	3346	1036	1710	307	290	3	0	0

- Molecule 21 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
21	J	205	3350	1026	1707	315	298	4	0	0

- Molecule 22 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
22	K	156	2348	717	1196	217	212	6	0	0

- Molecule 23 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
23	L	104	1694	536	846	153	152	7	0	0

- Molecule 24 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
24	M	151	2416	735	1235	227	215	4	0	0

- Molecule 25 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
25	N	129	2010	616	1031	173	184	6	0	0

- Molecule 26 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
26	O	127	2092	634	1070	206	179	3	0	0

- Molecule 27 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
27	P	99	1621	495	831	151	143	1	0	0

- Molecule 28 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
28	Q	117	1764	540	887	174	160	3	0	0

- Molecule 29 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
29	R	121	1940	580	1001	194	161	4	0	0

- Molecule 30 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
30	S	100	1649	499	844	164	139	3	0	0

- Molecule 31 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
31	T	88	1448	439	734	144	130	1	0	0

- Molecule 32 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
32	U	82	1315	406	666	128	114	1	0	0

- Molecule 33 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
33	V	80	1339	411	691	121	113	3	0	0

- Molecule 34 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
34	W	83	1351	424	688	126	111	2	0	0

- Molecule 35 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
35	X	116	1864	558	964	181	158	3	0	0

- Molecule 36 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	Y	141	1032	651	179	196	6	0	0

- Molecule 37 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	Z	30	227	144	33	47	3	0	0

- Molecule 38 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
38	a	2880	92918	27587	31077	11398	19976	2880	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	887	A	U	conflict	GB 937521852

- Molecule 39 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
39	b	76	1181	360	599	117	104	1	0	0

- Molecule 40 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
40	c	77	1277	388	652	129	106	2	0	0

- Molecule 41 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
41	d	120	3870	1144	1301	468	837	120	0	0

- Molecule 42 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
42	e	62	1032	308	531	98	94	1	0	0

- Molecule 43 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
43	f	58	936	281	488	87	78	2	0	0

- Molecule 44 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
44	g	66	1042	323	520	99	94	6	0	0

- Molecule 45 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
45	h	271	4236	1288	2154	423	364	7	0	0

- Molecule 46 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms						AltConf	Trace
46	i	56	Total 903	C 269	H 459	N 94	O 80	S 1	0	0

- Molecule 47 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms						AltConf	Trace
47	j	209	Total 3182	C 979	H 1617	N 288	O 294	S 4	0	0

- Molecule 48 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	k	52	Total 890	C 275	H 464	N 78	O 73	0	0

- Molecule 49 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms						AltConf	Trace
49	l	201	Total 3171	C 974	H 1619	N 283	O 290	S 5	0	0

- Molecule 50 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms						AltConf	Trace
50	m	46	Total 795	C 228	H 418	N 90	O 57	S 2	0	0

- Molecule 51 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms						AltConf	Trace
51	n	177	Total 2853	C 899	H 1443	N 249	O 256	S 6	0	0

- Molecule 52 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms						AltConf	Trace
52	o	64	Total 1076	C 323	H 572	N 105	O 74	S 2	0	0

- Molecule 53 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
53	p	175	2671	826	1358	241	244	2	0	0

- Molecule 54 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
54	q	38	645	185	343	65	48	4	0	0

- Molecule 55 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
55	r	149	2259	699	1148	197	214	1	0	0

- Molecule 56 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
56	s	142	2291	714	1162	212	199	4	0	0

- Molecule 57 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
57	t	123	1969	593	1023	181	166	6	0	0

- Molecule 58 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
58	u	144	2182	654	1129	207	190	2	0	0

- Molecule 59 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
59	v	136	2231	686	1157	205	177	6	0	0

- Molecule 60 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
60	w	119	1945	588	994	195	163	5	0	0

- Molecule 61 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
61	x	116	1815	552	923	178	162	0	0

- Molecule 62 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
62	y	114	1879	574	962	179	163	1	0	0

- Molecule 63 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
63	z	117	1967	604	1020	192	151	0	0

- Molecule 64 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
64	AE	1	1	1	0

- Molecule 65 is ZINC ION (three-letter code: ZN) (formula: Zn).

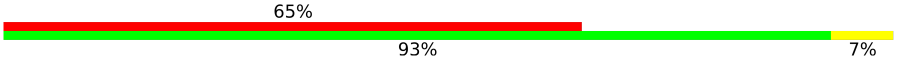
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
65	AE	2	2	2	0

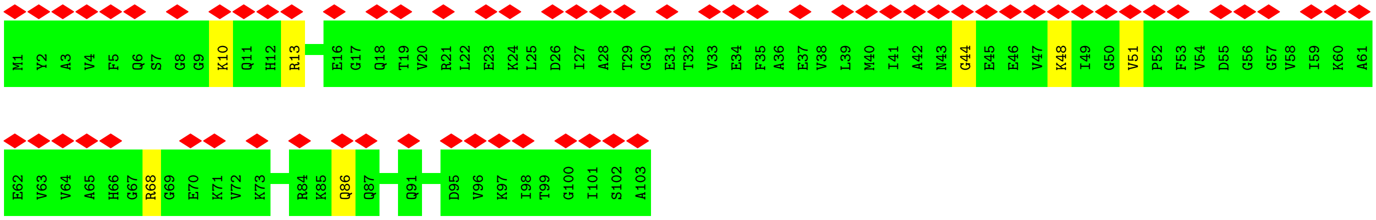
3 Residue-property plots ⓘ

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: 50S ribosomal protein L21

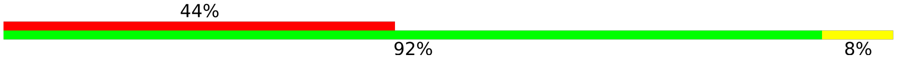
Chain 0:

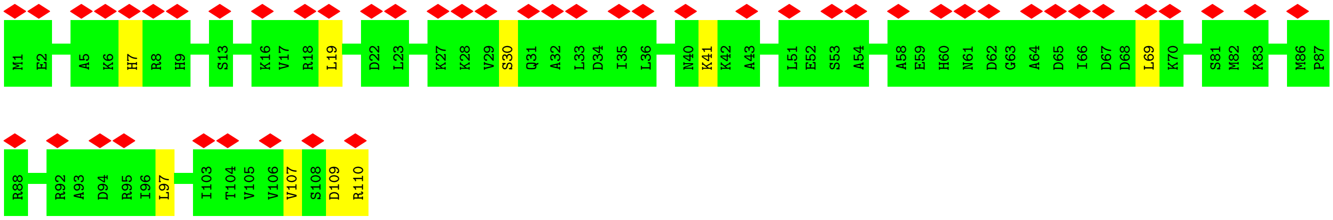




- Molecule 2: 50S ribosomal protein L22

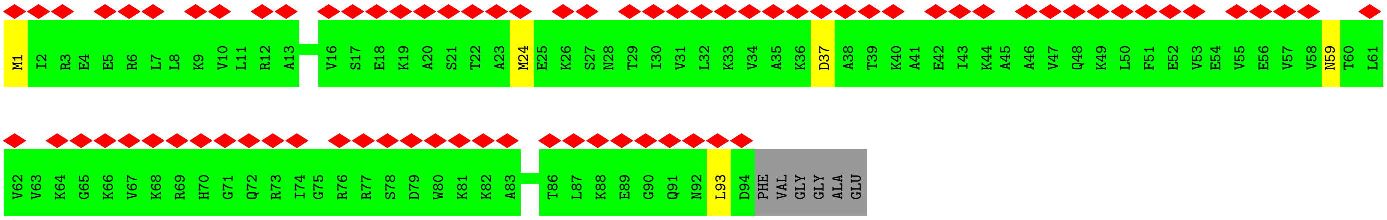
Chain 1:





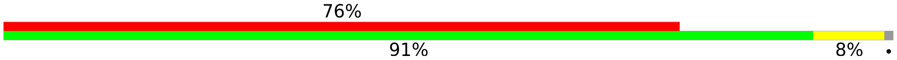
- Molecule 3: 50S ribosomal protein L23

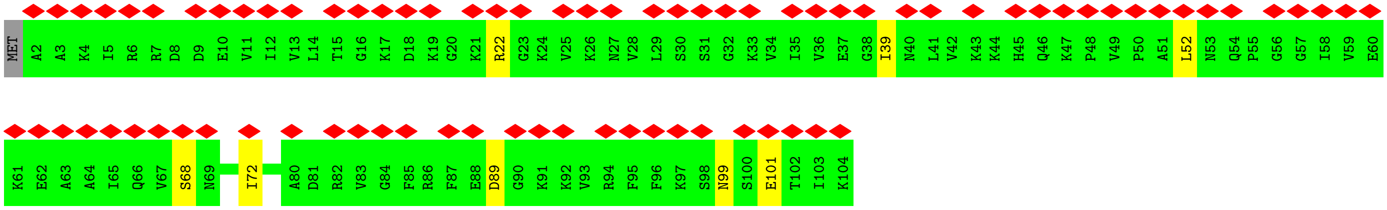
Chain 2:



- Molecule 4: 50S ribosomal protein L24

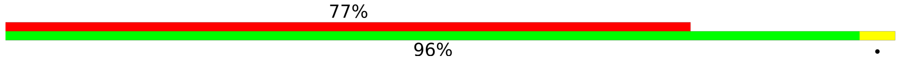
Chain 3:

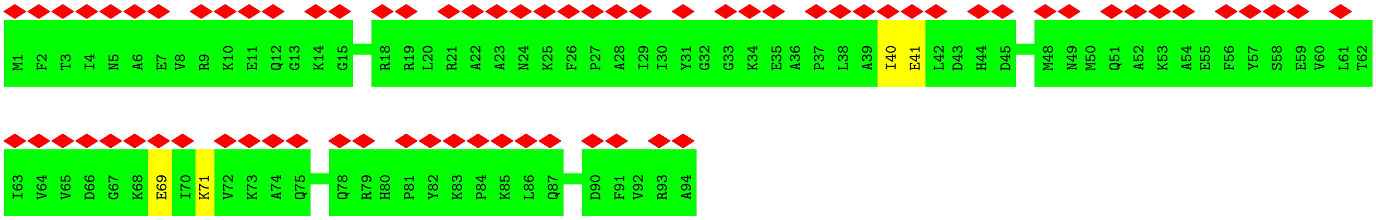




- Molecule 5: 50S ribosomal protein L25

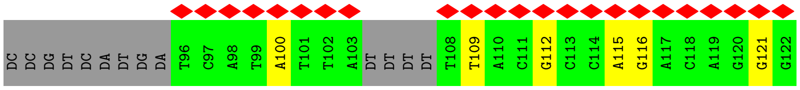
Chain 4:





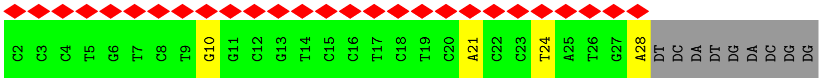
- Molecule 6: NT DNA

Chain 5:



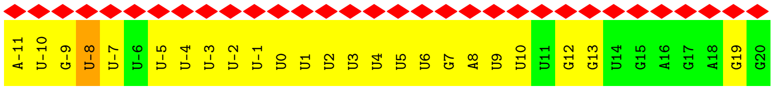
- Molecule 7: T DNA

Chain 6:



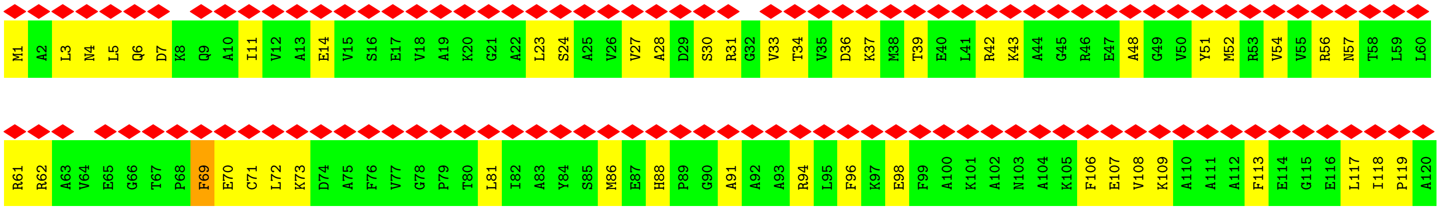
- Molecule 8: mRNA with 27 nt long spacer

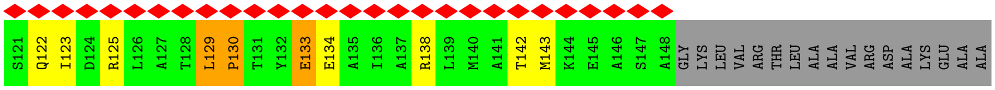
Chain 7:



- Molecule 9: 50S ribosomal protein L10

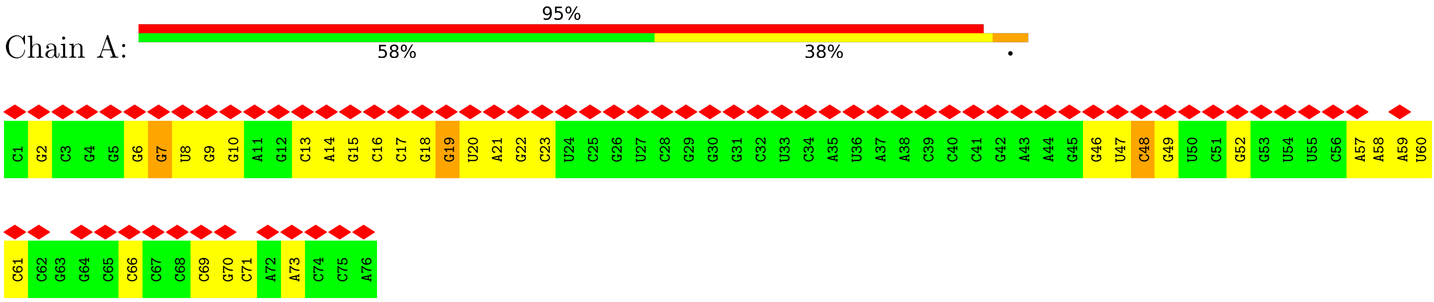
Chain 9:





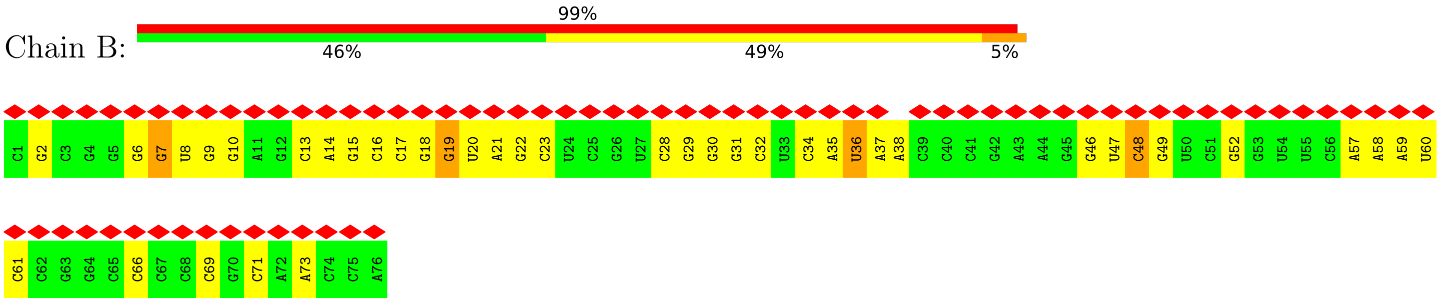
- Molecule 10: E-site and P-site tRNA (fMet)

Chain A:



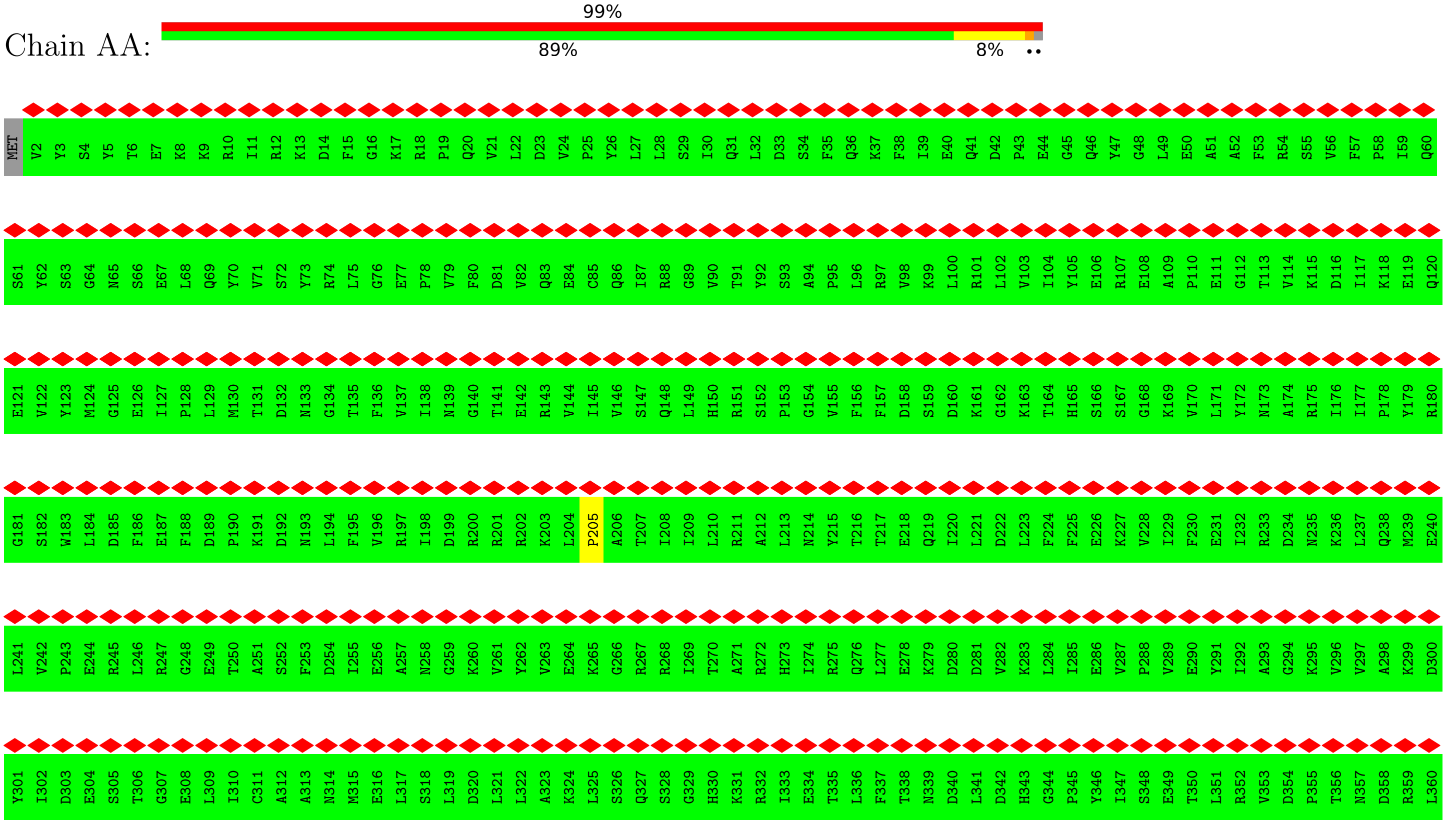
- Molecule 10: E-site and P-site tRNA (fMet)

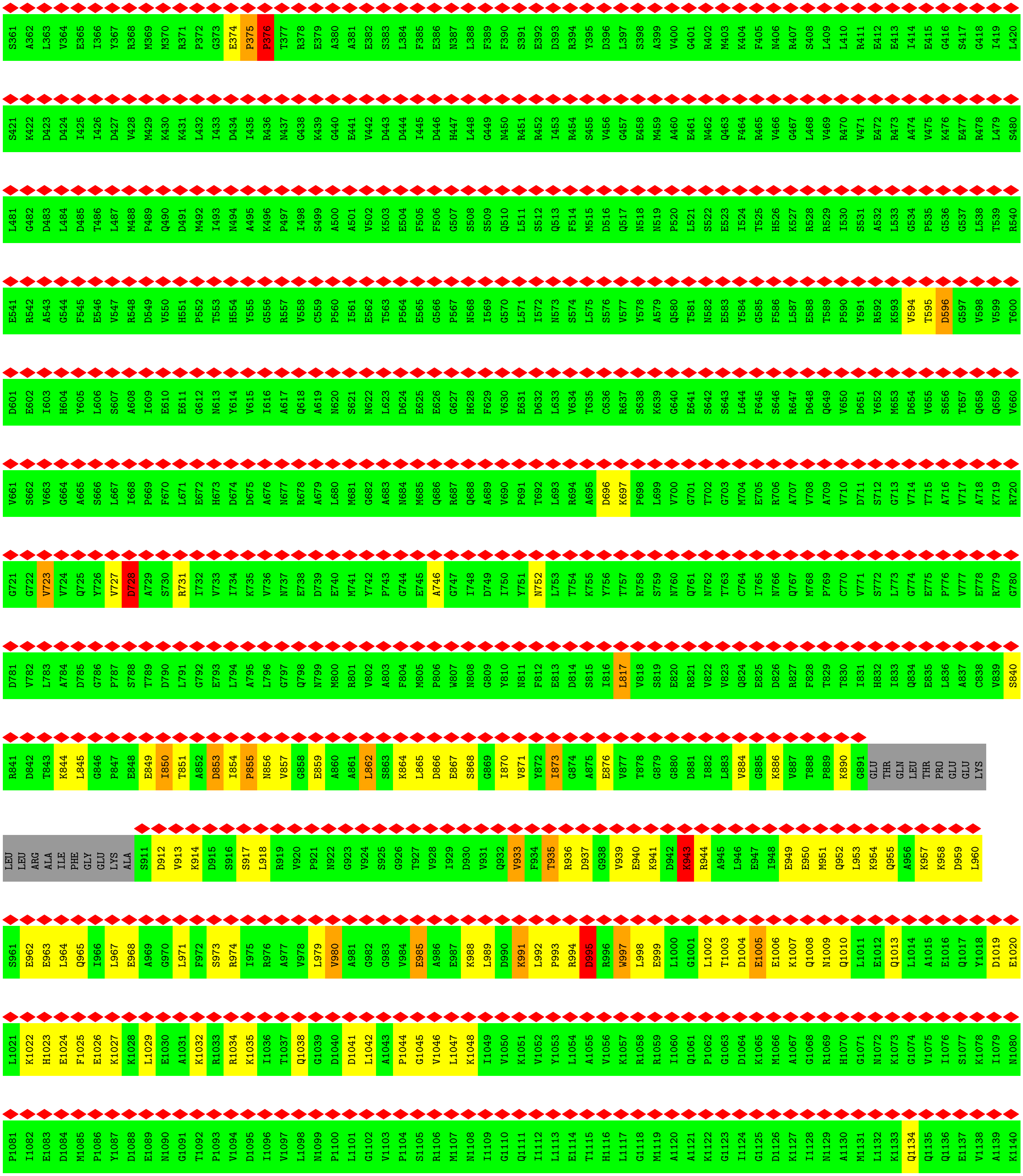
Chain B:



- Molecule 11: DNA-directed RNA polymerase subunit beta

Chain AA:





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S421 K422 D423 D424 I425 I426 D427 V428 M429 K430 K431 L432 I433 D434 I435 R436 N437 G438 K439 G440 E441 V442 D443 D444 I445 D446 H447 L448 G449 N450 R451 R452 I453 R454 S455 V456 G457 E458 M459 A460 E461 N462 Q463 F464 R465 V466 G467 L468 V469 R470 V471 E472 R473 A474 V475 K476 E477 R478 L479 S480

L481 G482 D483 L484 D485 T486 L487 M488 P489 Q490 D491 M492 I493 N494 A495 K496 P497 I498 S499 A500 A501 V502 K503 E504 F505 F506 G507 S508 S509 Q510 L511 S512 Q513 F514 M515 D516 Q517 N518 N519 P520 L521 S522 E523 I524 T525 H526 K527 R528 R529 I530 S531 A532 L533 G534 P535 G536 G537 L538 T539 R540

E541 R542 A543 G544 F545 E546 V547 R548 D549 V550 H551 P552 T553 H554 Y555 G556 R557 V558 C559 P560 I561 E562 T563 P564 E565 G566 P567 N568 I569 G570 L571 I572 N573 S574 L575 S576 V577 Y578 A579 Q580 T581 N582 E583 Y584 G585 F586 L587 E588 T589 P590 Y591 R592 K593 V594 T595 D596 G597 V598 V599 T600

D601 E602 I603 H604 Y605 L606 S607 A608 I609 E610 E611 G612 N613 Y614 V615 I616 A617 Q618 A619 N620 S621 N622 L623 D624 E625 E626 G627 H628 F629 V630 E631 D632 L633 V634 T635 C636 R637 S638 K639 G640 E641 S642 S643 L644 F645 S646 R647 D648 Q649 V650 D651 Y652 M653 D654 V655 S656 T657 Q658 Q659 V660

V661 S662 V663 G664 A665 S666 L667 I668 P669 F670 L671 E672 H673 D674 D675 A676 N677 R678 A679 L680 M681 G682 A683 N684 M685 Q686 R687 Q688 A689 V690 P691 T692 L693 R694 A695 D696 K697 P698 L699 V700 G701 T702 G703 M704 E705 R706 A707 V708 A709 V710 D711 S712 G713 V714 T715 A716 V717 A718 K719 R720

G721 G722 V723 V724 Q725 Y726 V727 D728 A729 S730 R731 I732 V733 I734 K735 V736 N737 E738 D739 E740 M741 Y742 P743 G744 E745 A746 G747 I748 D749 I750 Y751 N752 L753 T754 K755 Y756 T757 R758 S759 N760 Q761 N762 T763 C764 I765 N766 Q767 M768 P769 C770 V771 S772 L773 G774 E775 P776 V777 E778 R779 G780

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LEU LEU ARG ALA ILE PHE GLY GLU LYS ALA S911 D912 V913 K914 D915 S916 S917 L918 R919 V920 P921 N922 G923 V924 S925 G926 T927 V928 I929 D930 V931 Q932 V933 F934 T935 R936 D937 G938 V939 E940 K941 D942 K943 R944 A945 L946 E947 I948 E949 E950 M951 Q952 L953 K954 Q955 A956 K957 K958 D959 L960

S961 E962 E963 L964 Q965 I966 L967 E968 A969 G970 L971 F972 S973 R974 I975 R976 A977 V978 L979 V980 A981 G982 G983 V984 E985 A986 E987 K988 L989 D990 K991 L992 P993 R994 D995 R996 W997 L998 E999 L1000 G1001 L1002 T1003 D1004 E1005 E1006 K1007 Q1008 N1009 Q1010 L1011 E1012 Q1013 L1014 A1015 E1016 Q1017 Y1018 D1019 E1020

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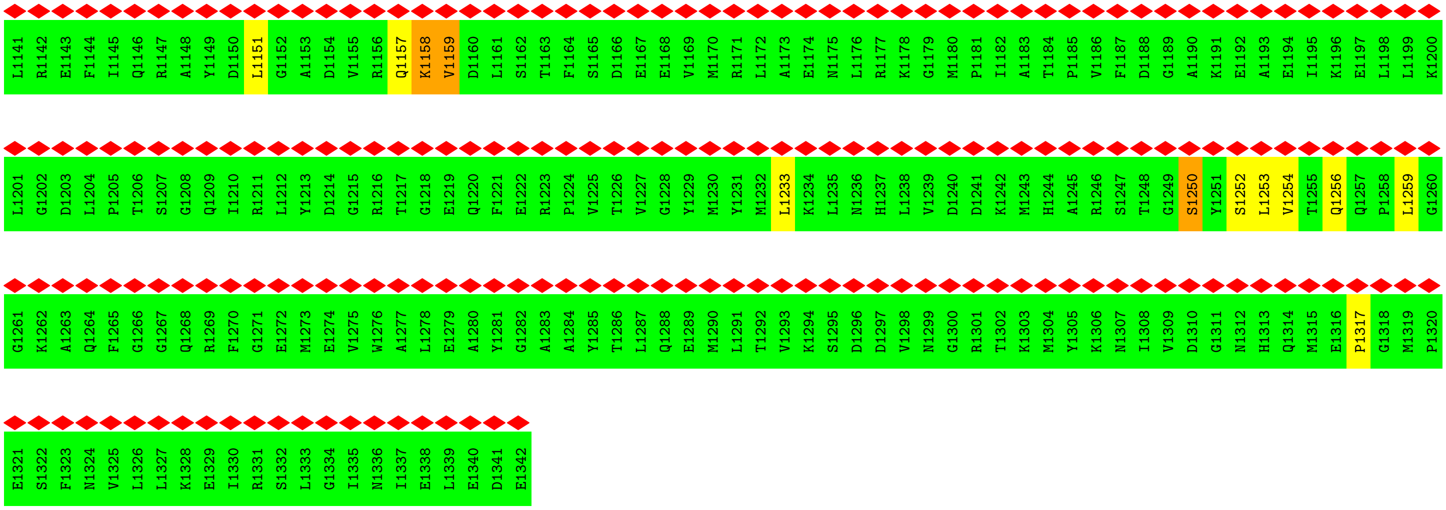
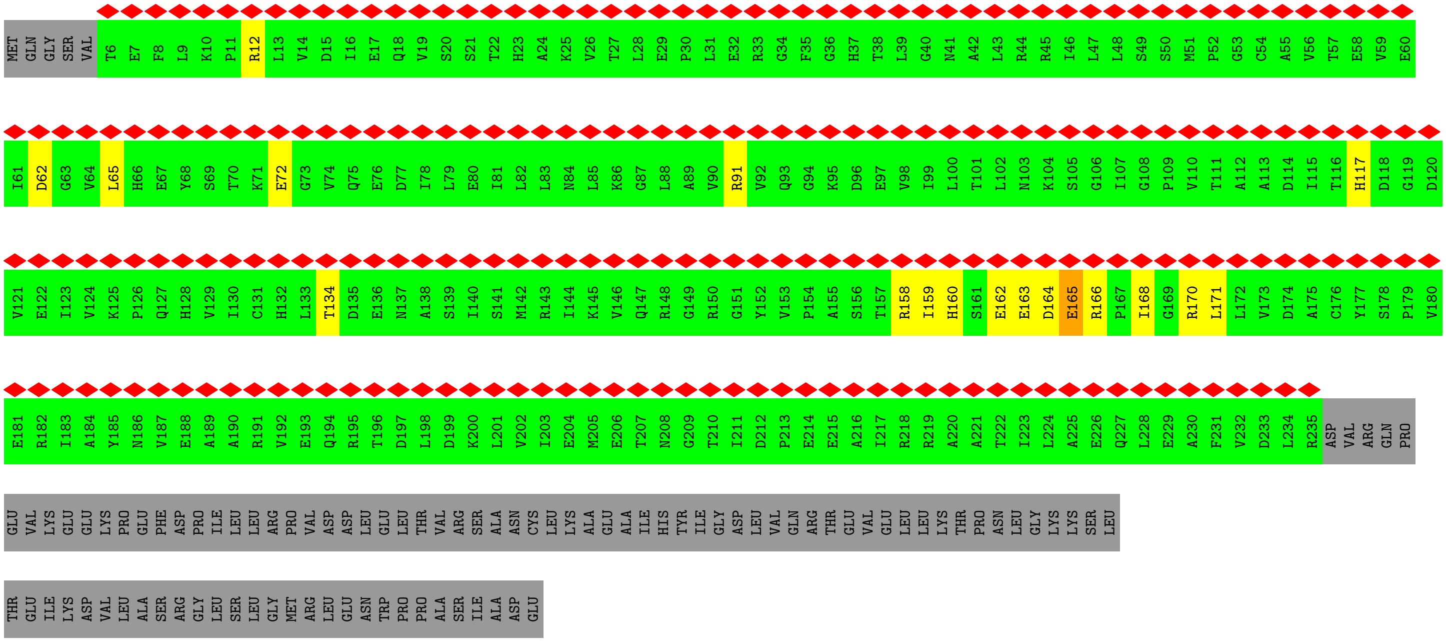
P1081 I1082 E1083 D1084 M1085 P1086 Y1087 D1088 E1089 N1090 G1091 T1092 P1093 V1094 D1095 I1096 V1097 L1098 N1099 P1100 L1101 G1102 V1103 P1104 S1105 R1106 M1107 N1108 I1109 G1110 Q1111 I1112 L1113 E1114 T1115 H1116 L1117 G1118 M1119 A1120 A1121 K1122 G1123 I1124 G1125 D1126 K1127 I1128 N1129 A1130 M1131 L1132 K1133 Q1134 Q1135 Q1136 E1137 V1138 A1139 K1140



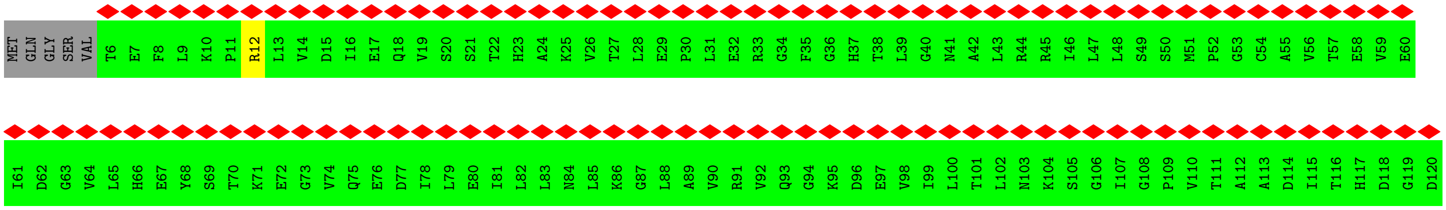
- Molecule 12: DNA-directed RNA polymerase subunit alpha

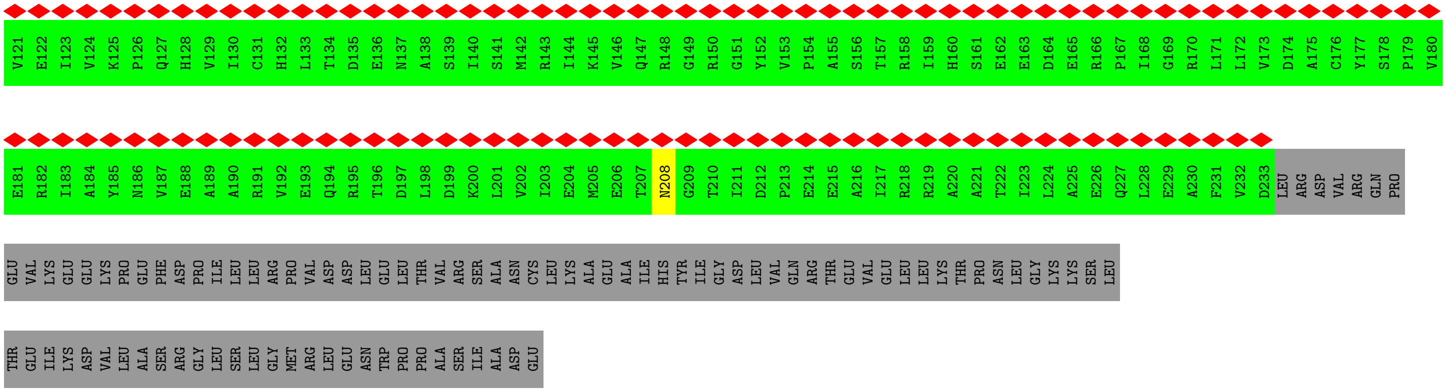
Chain AC:



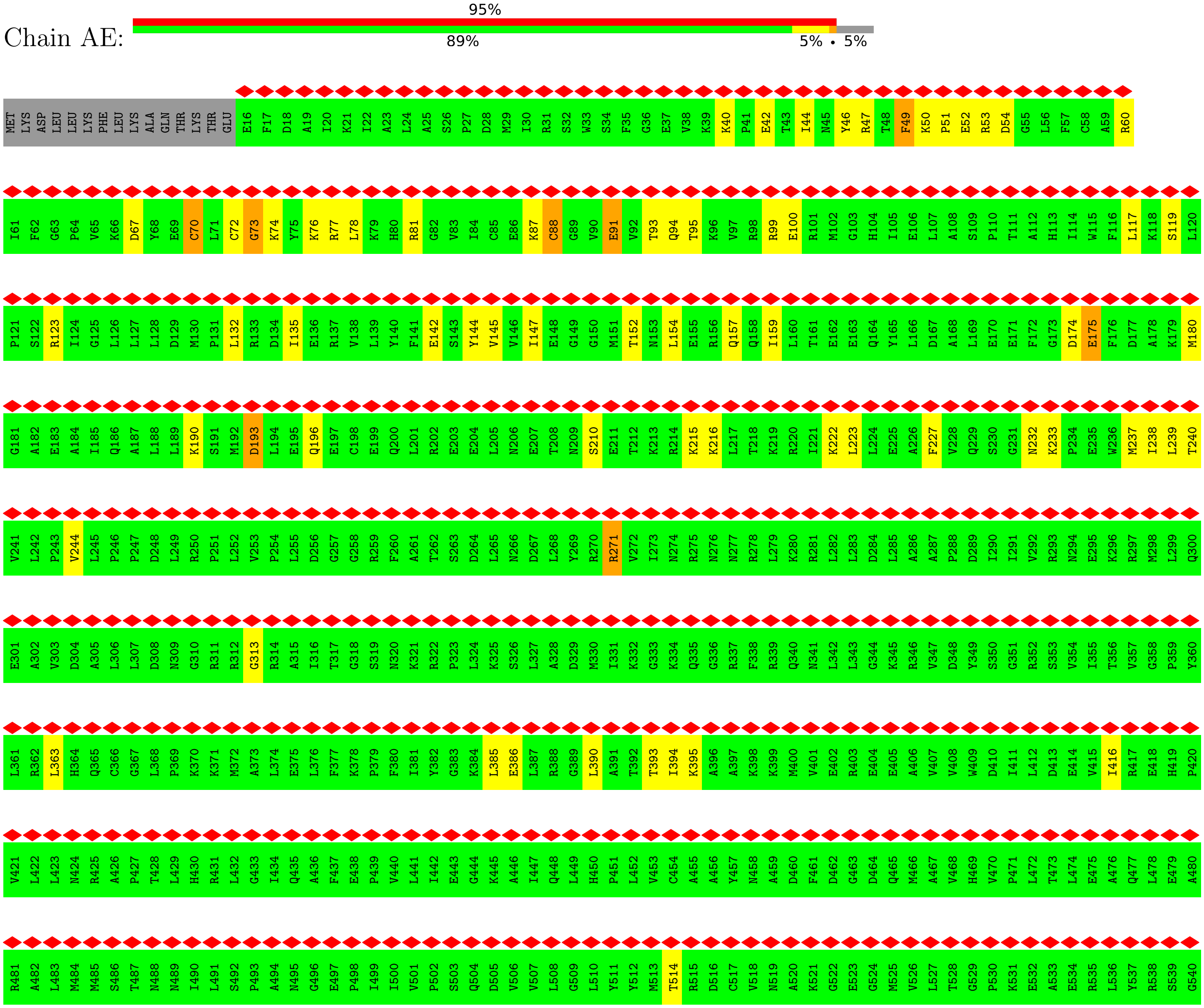
- Molecule 12: DNA-directed RNA polymerase subunit alpha

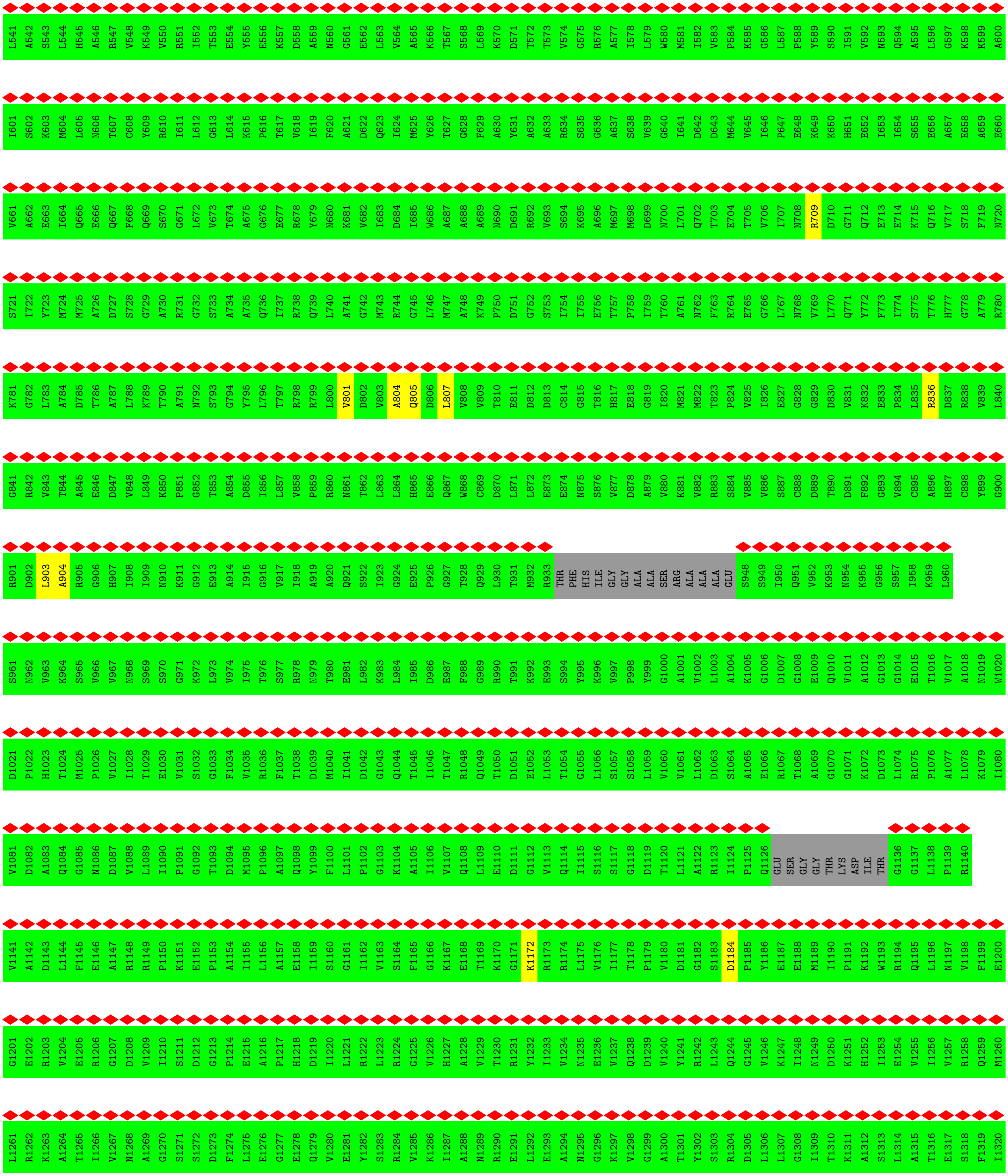
Chain AD:





- Molecule 13: DNA-directed RNA polymerase subunit beta'

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S961 N962 V963 K964 S965 V966 V967 N968 S969 S970 G971 K972 L973 V974 I975 T976 S977 R978 N979 T980 E981 L982 K983 L984 I985 D986 E987 F988 G989 R990 T991 K992 E993 S994 Y995 K996 V997 P998 Y999 G1000 A1001 V1002 L1003 A1004 K1005 G1006 D1007 G1008 E1009 Q1010 V1011 A1012 G1013 G1014 E1015 T1016 V1017 A1018 N1019 W1020
D1021 P1022 H1023 T1024 M1025 P1026 V1027 I1028 T1029 E1030 V1031 S1032 G1033 F1034 V1035 R1036 F1037 T1038 D1039 M1040 I1041 D1042 G1043 Q1044 T1045 I1046 T1047 R1048 Q1049 T1050 D1051 E1052 L1053 T1054 G1055 L1056 S1057 S1058 L1059 V1060 V1061 L1062 D1063 S1064 A1065 E1066 R1067 T1068 A1069 G1070 G1071 K1072 D1073 L1074 R1075 P1076 A1077 L1078 K1079 I1080
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G1201 E1202 R1203 V1204 E1205 R1206 G1207 D1208 V1209 I1210 S1211 D1212 G1213 P1214 E1215 A1216 P1217 H1218 D1219 I1220 L1221 R1222 L1223 R1224 G1225 V1226 H1227 A1228 V1229 T1230 R1231 Y1232 I1233 V1234 N1235 E1236 V1237 Q1238 D1239 V1240 Y1241 R1242 L1243 Q1244 G1245 V1246 K1247 I1248 N1249 D1250 K1251 H1252 I1253 E1254 V1255 I1256 V1257 R1258 Q1259 M1260
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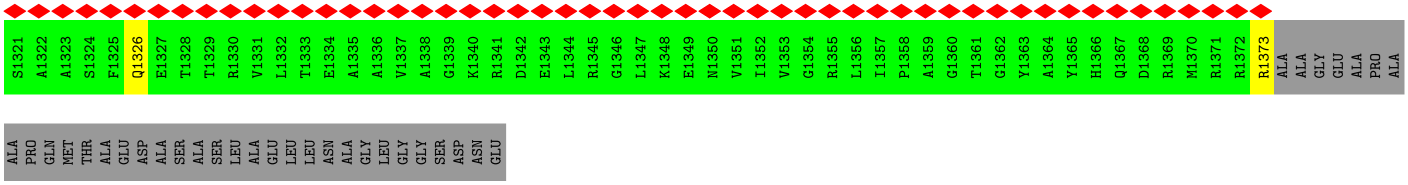
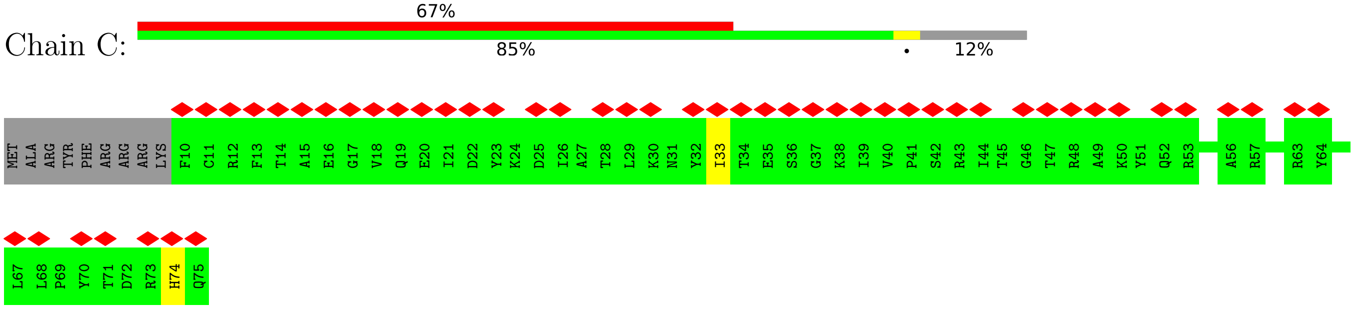
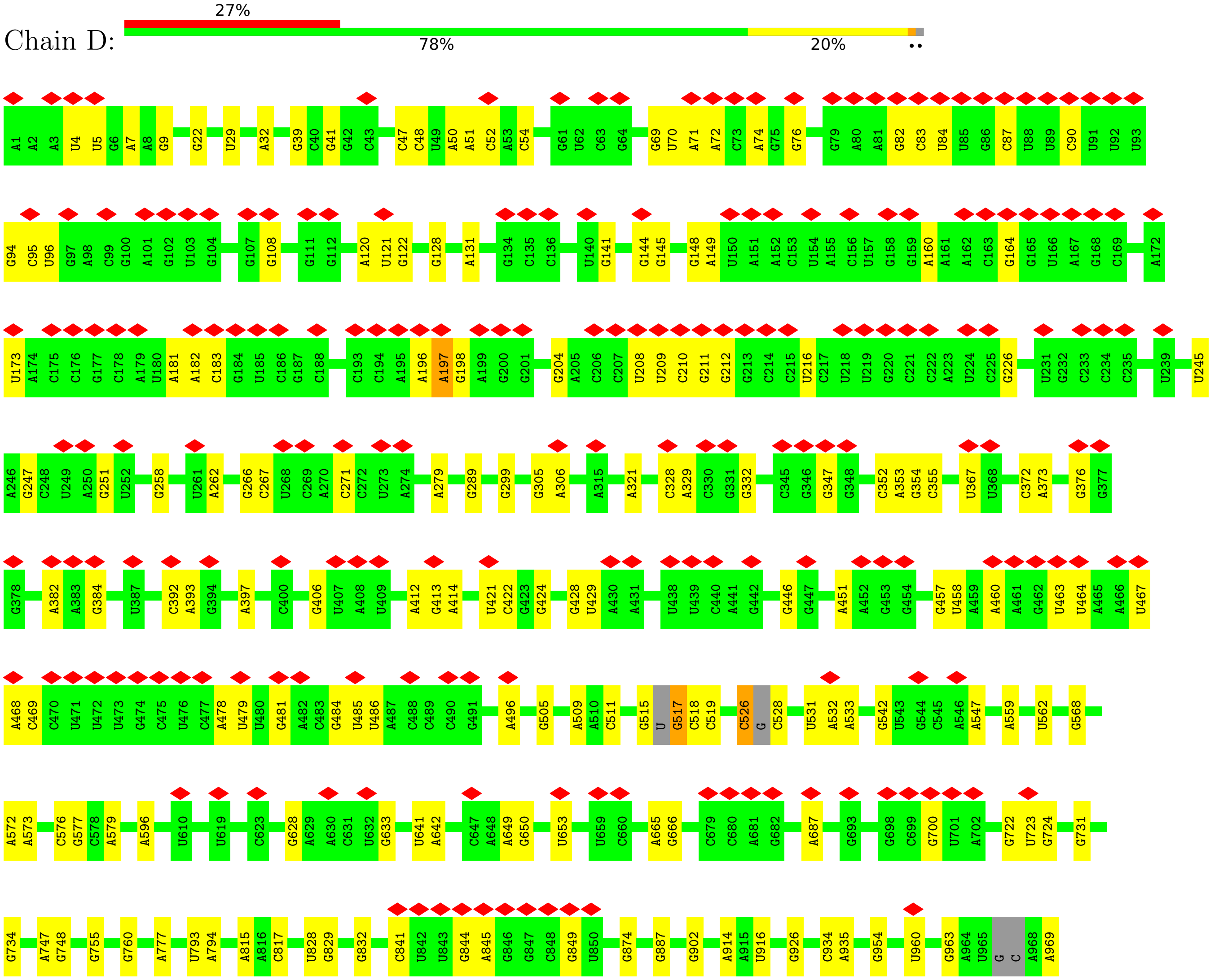
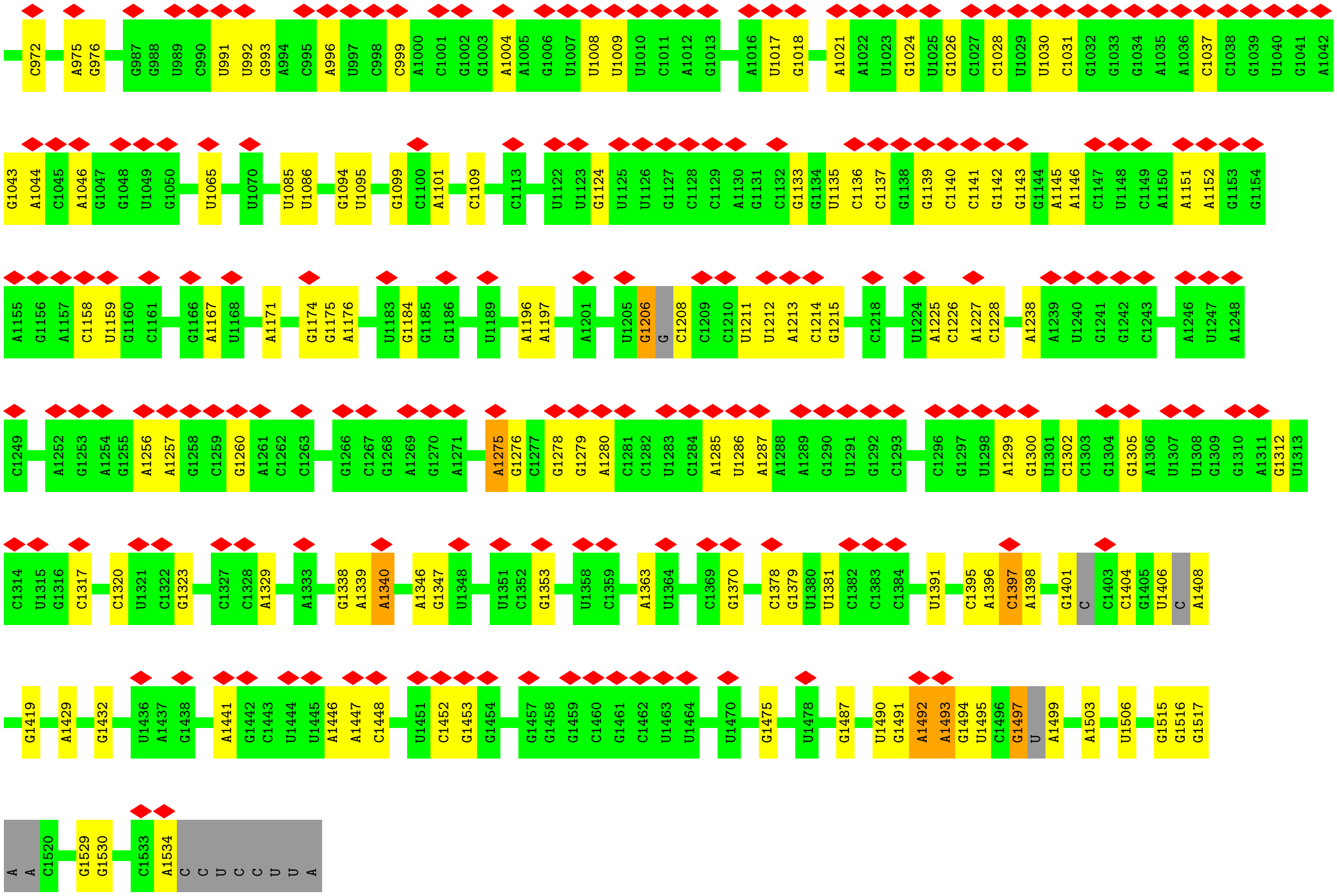


- Molecule 14: 30S ribosomal protein S18



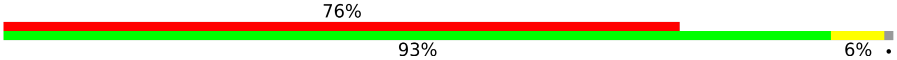
- Molecule 15: 16S rRNA

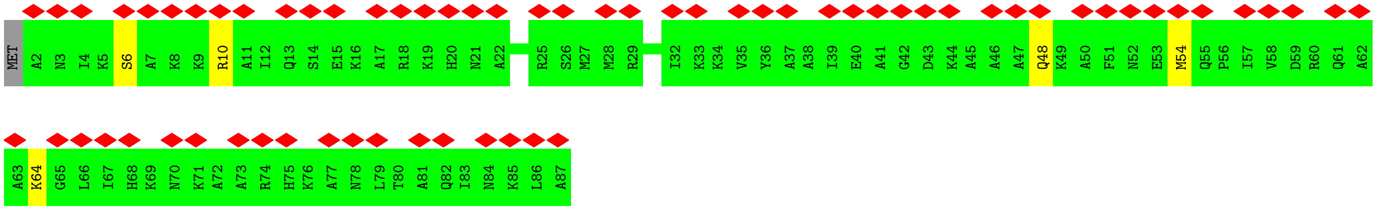




- Molecule 16: 30S ribosomal protein S20

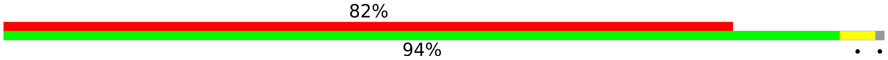
Chain E:

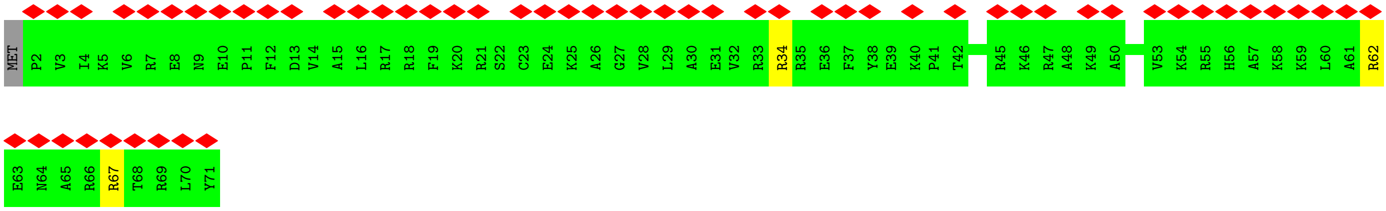




- Molecule 17: 30S ribosomal protein S21

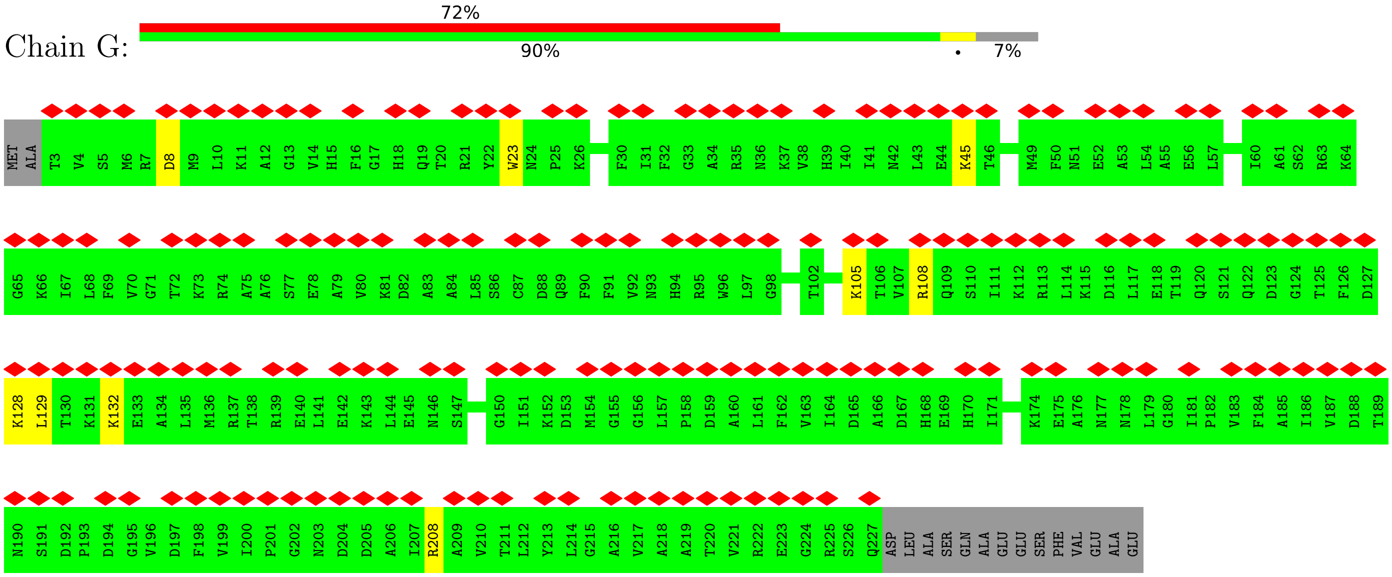
Chain F:





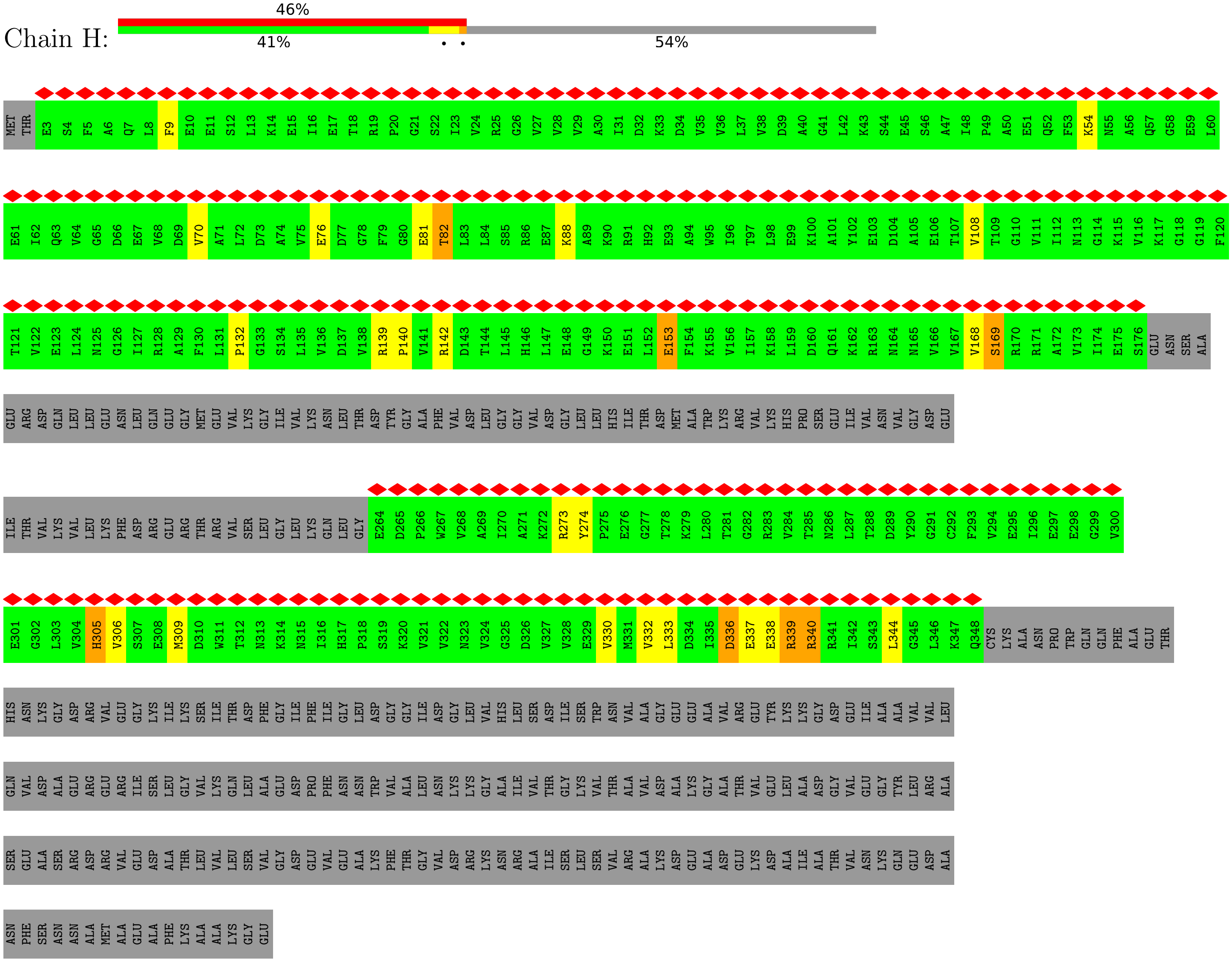
- Molecule 18: 30S ribosomal protein S2

Chain G:

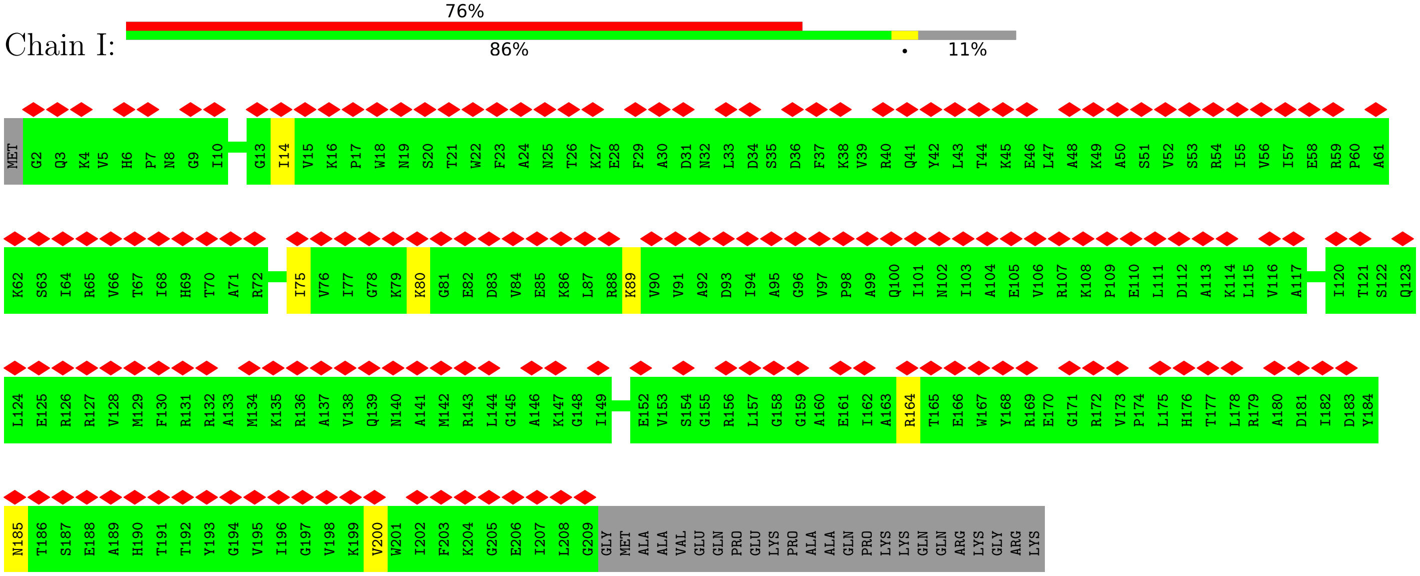


• Molecule 19: 30S ribosomal protein S1

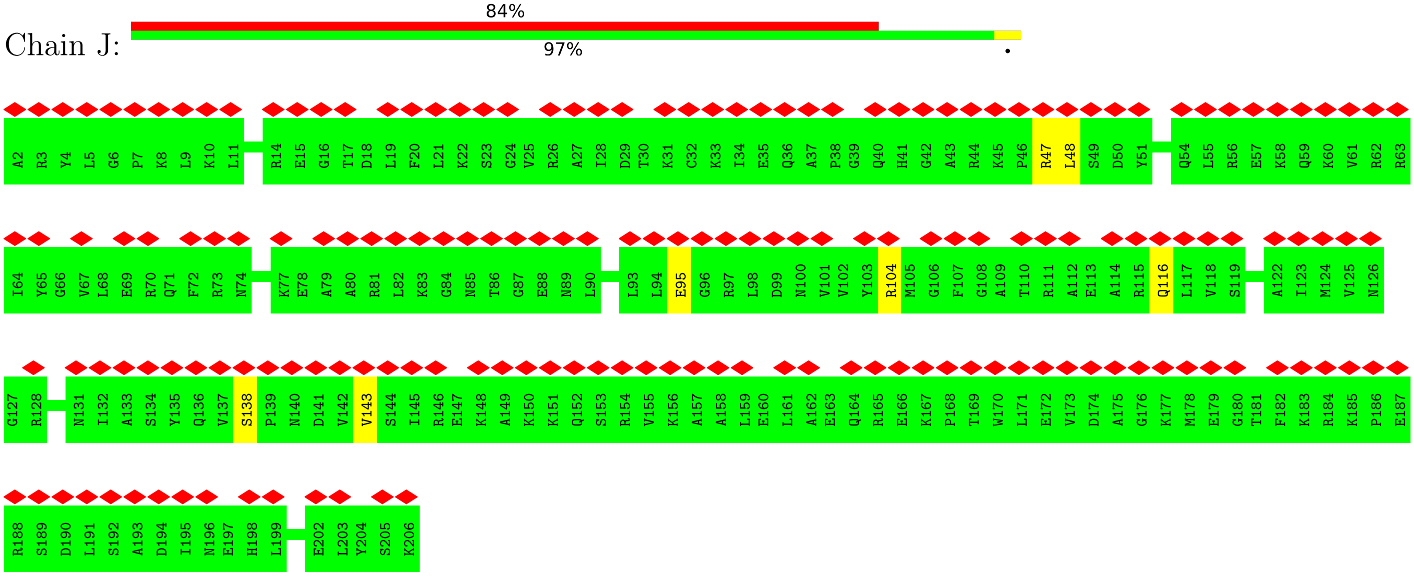
Chain H:



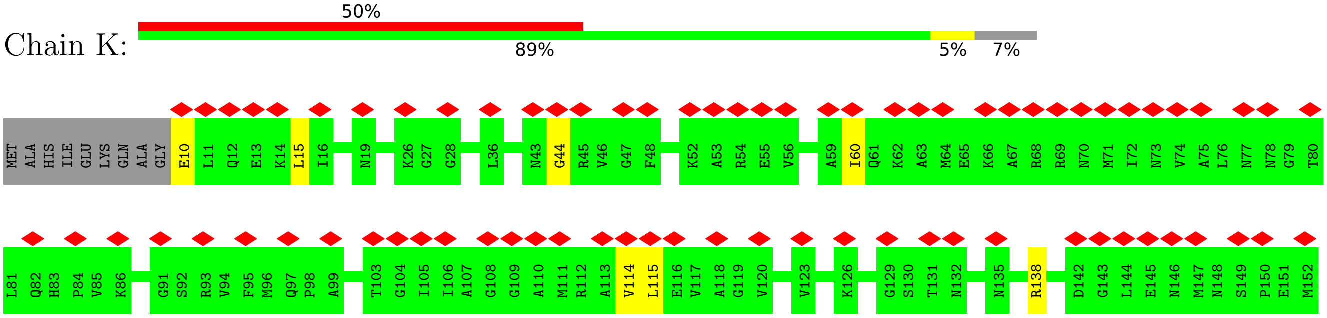
- Molecule 20: 30S ribosomal protein S3

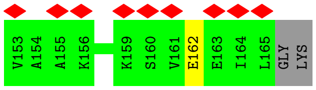


- Molecule 21: 30S ribosomal protein S4



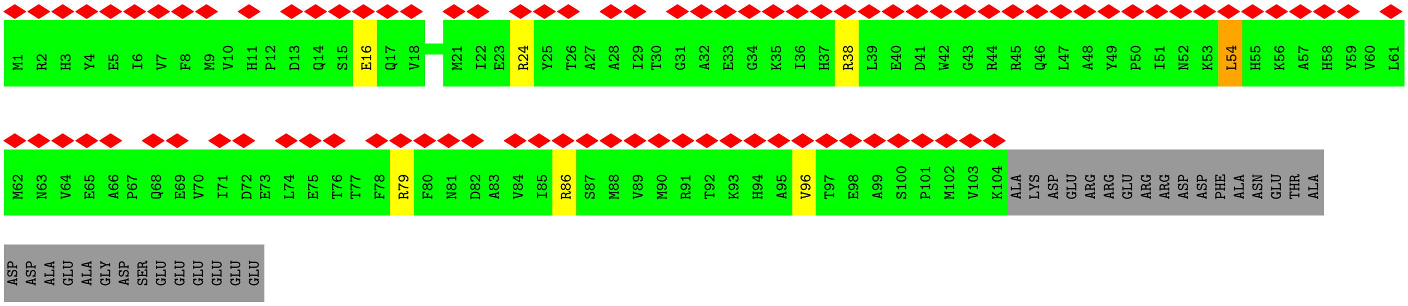
- Molecule 22: 30S ribosomal protein S5





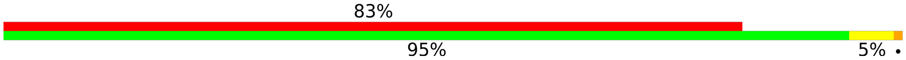
- Molecule 23: 30S ribosomal protein S6

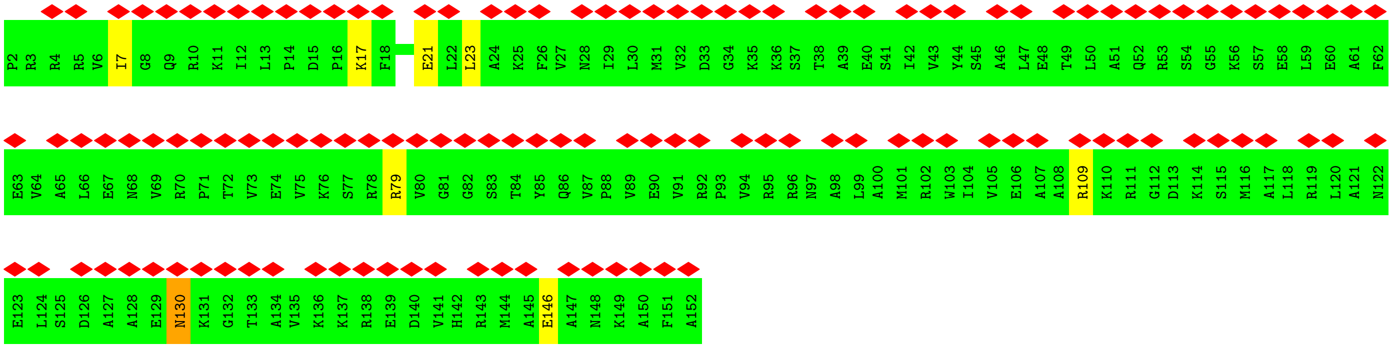
Chain L:



- Molecule 24: 30S ribosomal protein S7

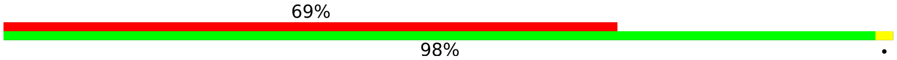
Chain M:

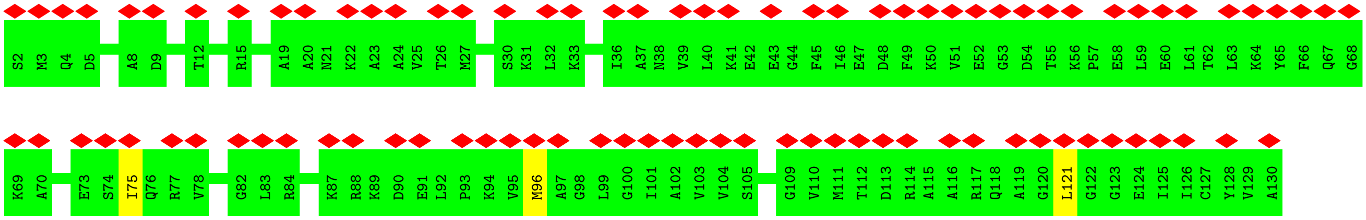




- Molecule 25: 30S ribosomal protein S8

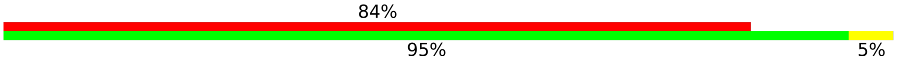
Chain N:

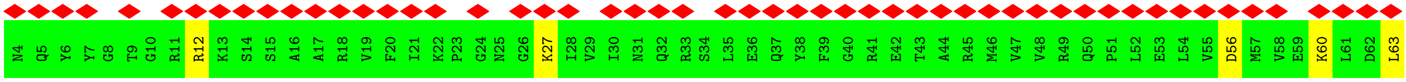


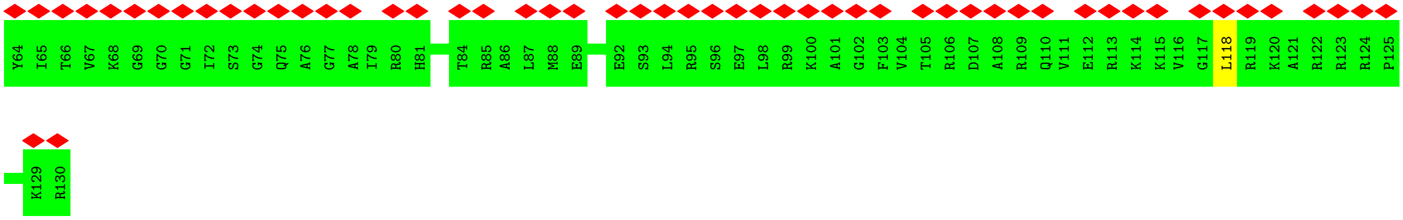


- Molecule 26: 30S ribosomal protein S9

Chain O:

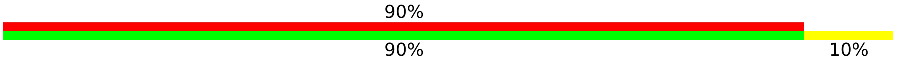


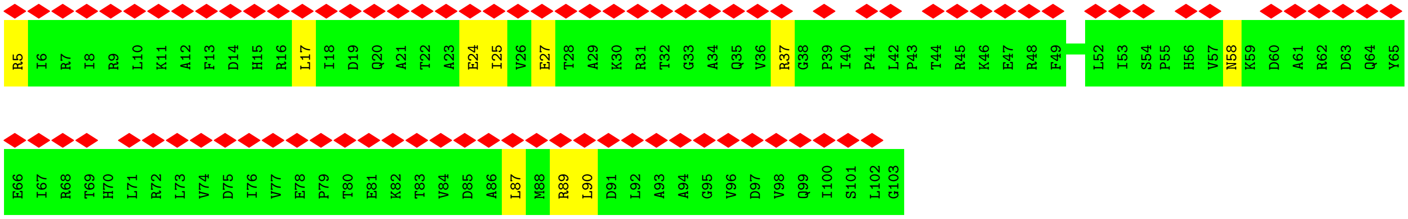




- Molecule 27: 30S ribosomal protein S10

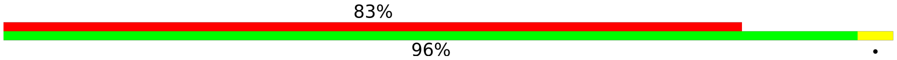
Chain P:

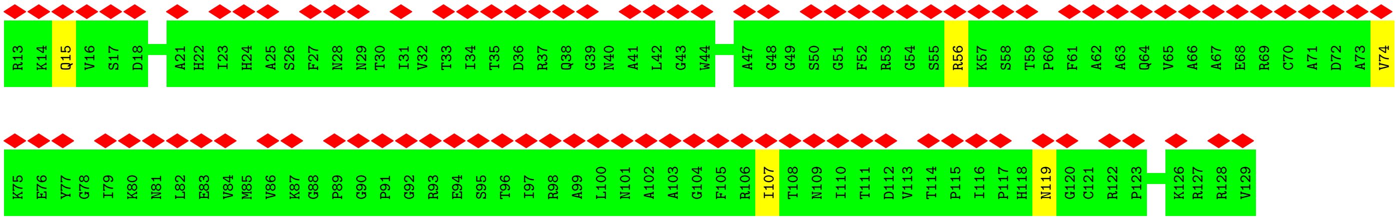




- Molecule 28: 30S ribosomal protein S11

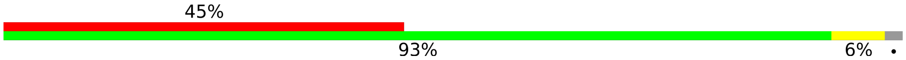
Chain Q:

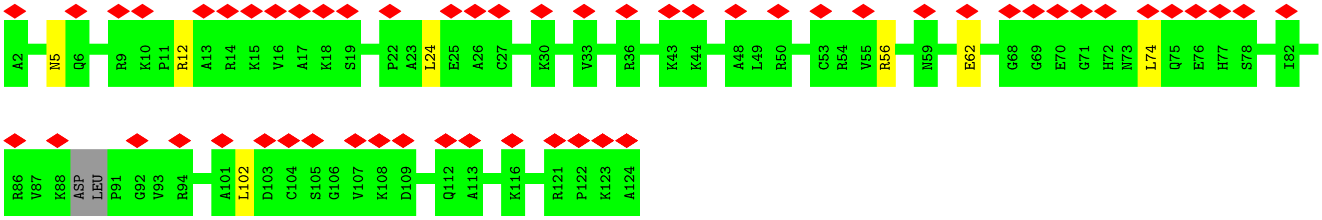




- Molecule 29: 30S ribosomal protein S12

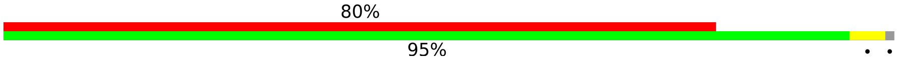
Chain R:

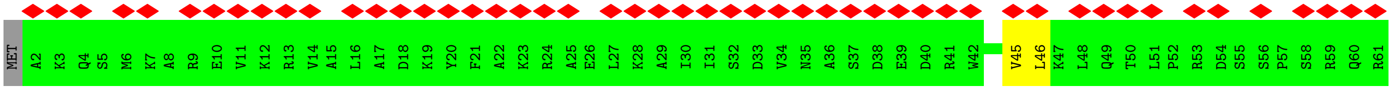


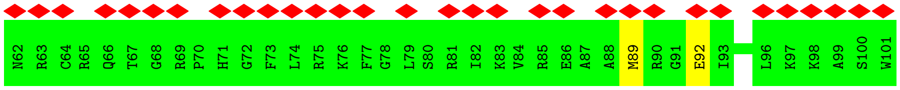


- Molecule 30: 30S ribosomal protein S14

Chain S:

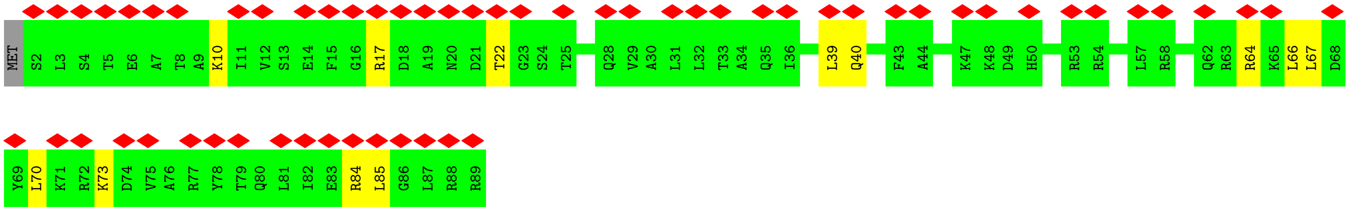






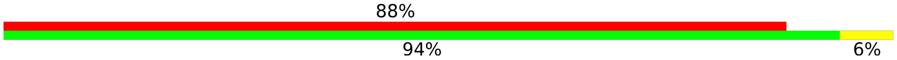
- Molecule 31: 30S ribosomal protein S15

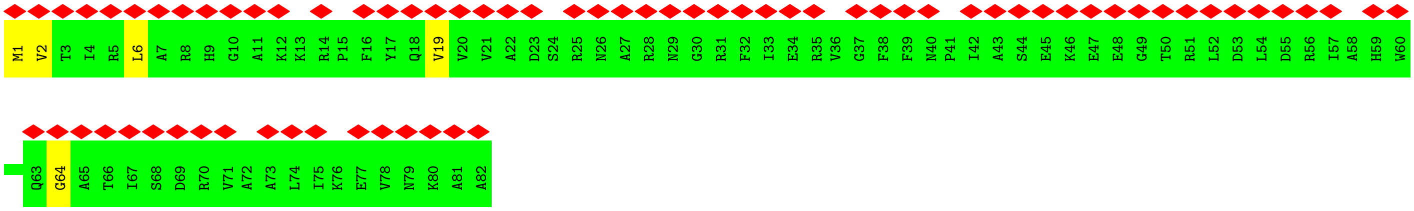
Chain T:



- Molecule 32: 30S ribosomal protein S16

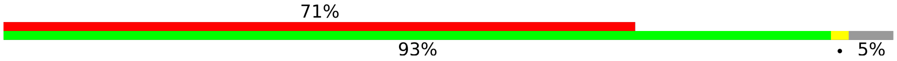
Chain U:

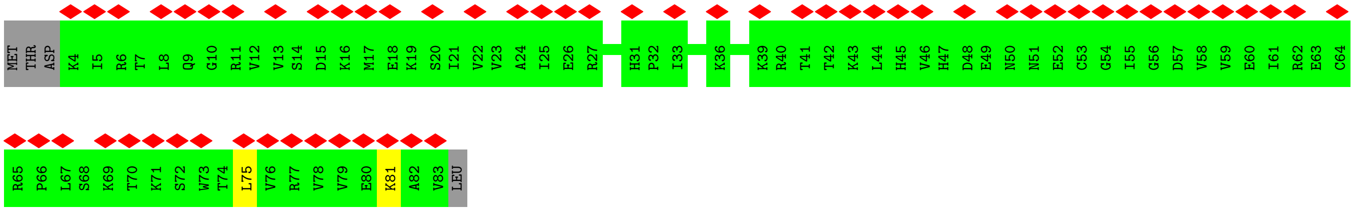




- Molecule 33: 30S ribosomal protein S17

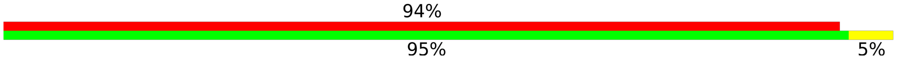
Chain V:

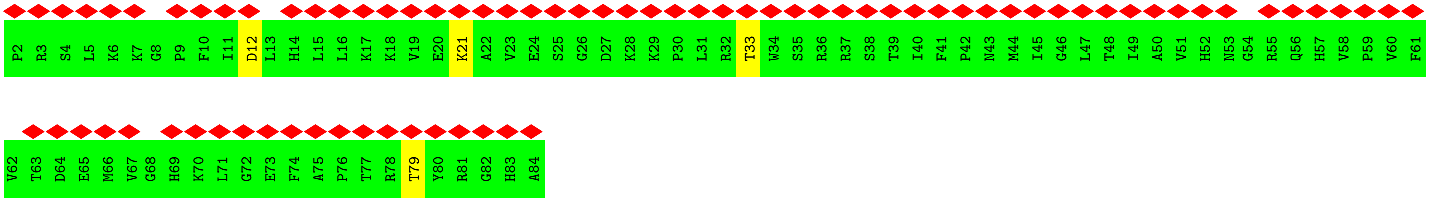




- Molecule 34: 30S ribosomal protein S19

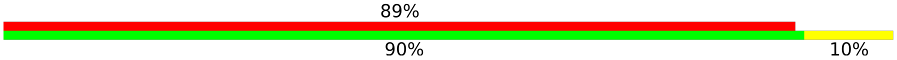
Chain W:

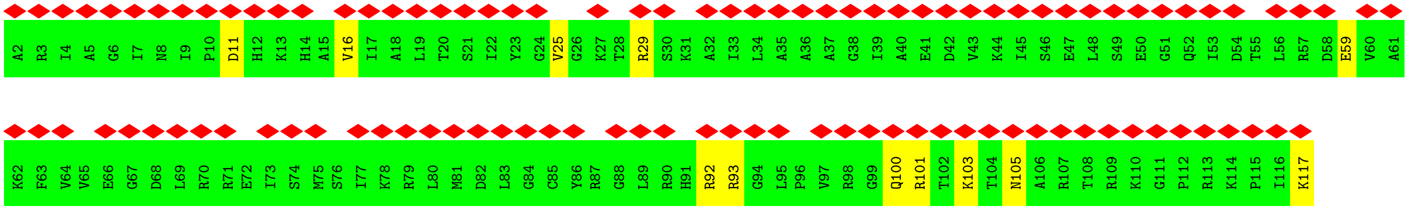




- Molecule 35: 30S ribosomal protein S13

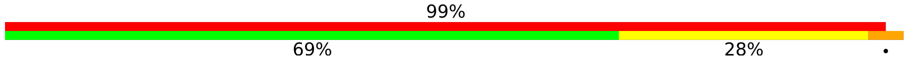
Chain X:

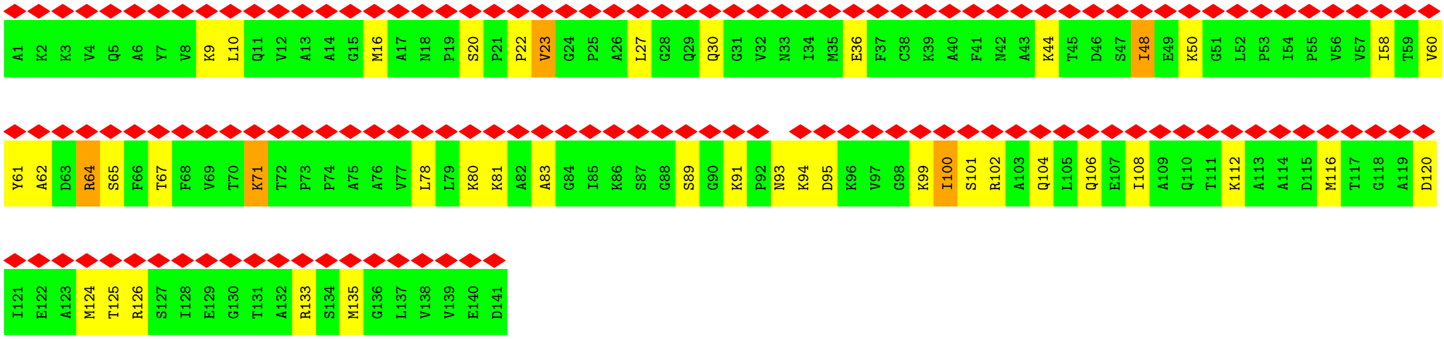




- Molecule 36: 50S ribosomal protein L11

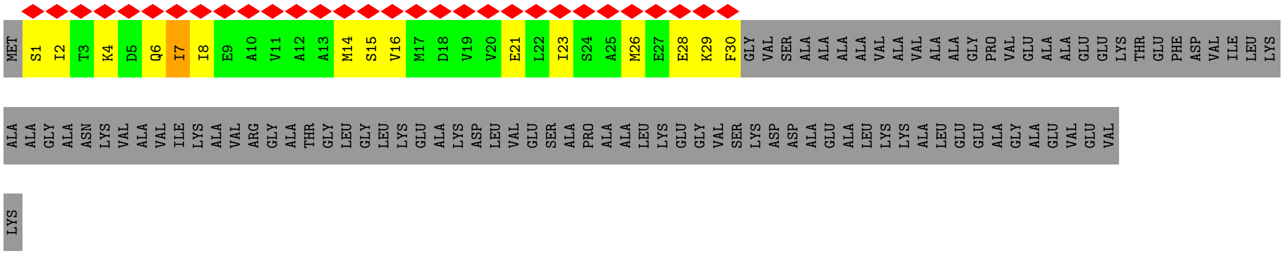
Chain Y:





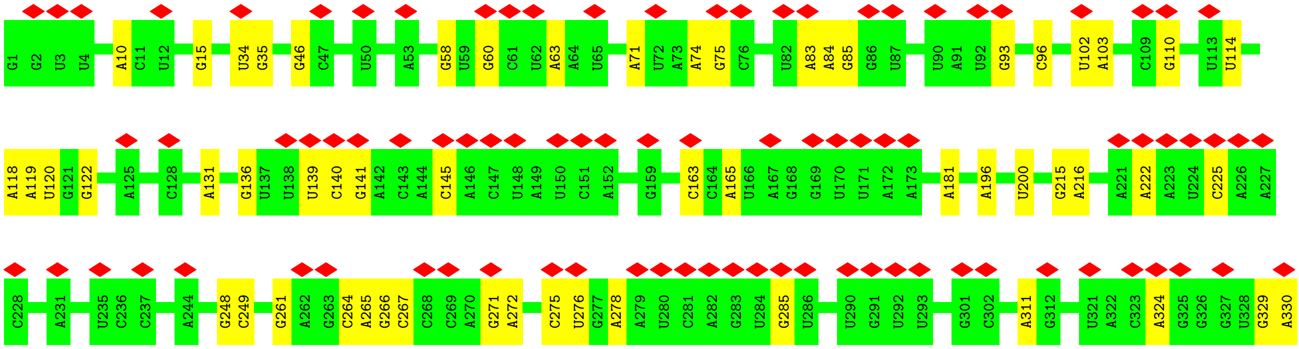
- Molecule 37: 50S ribosomal protein L7/L12

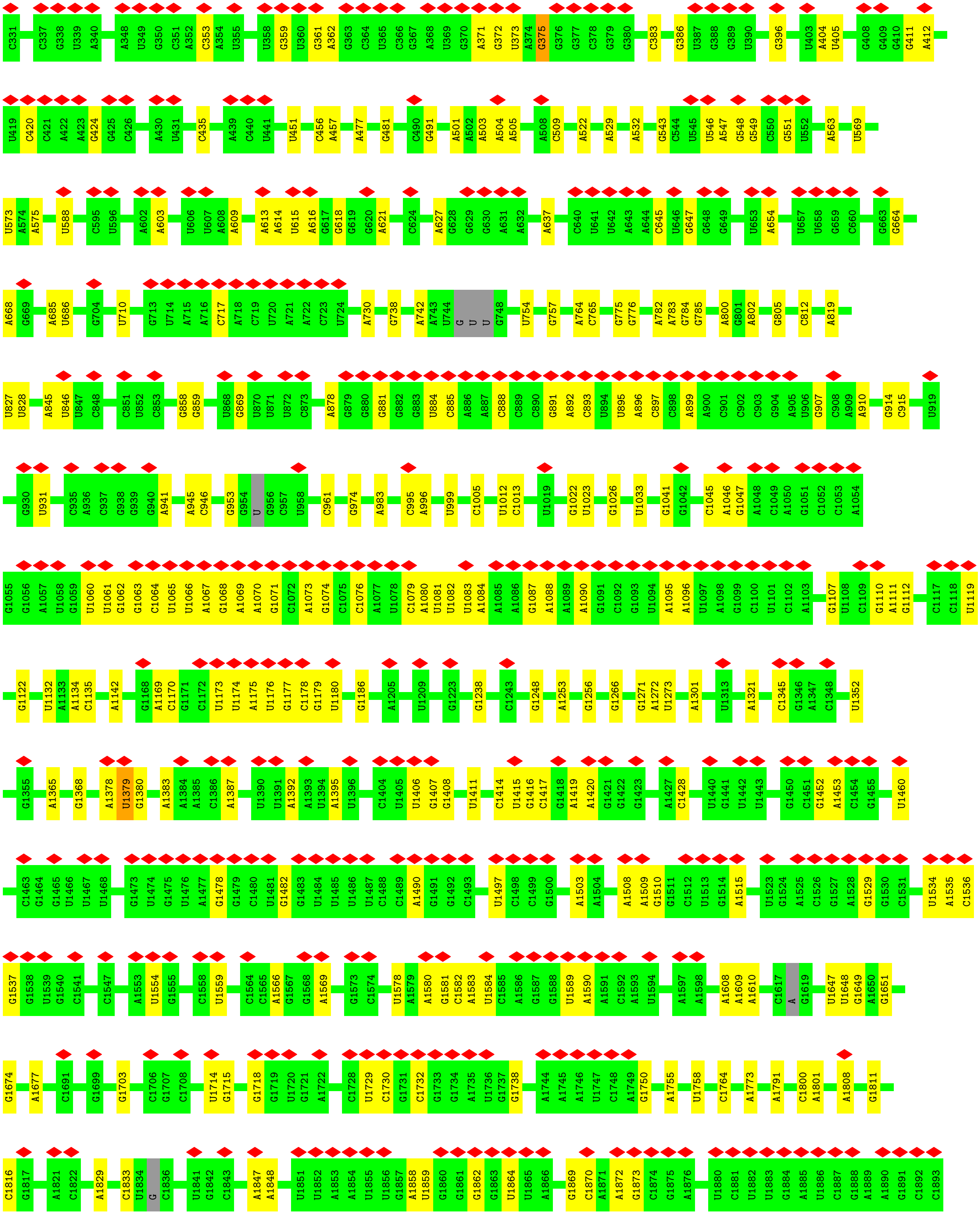
Chain Z:



- Molecule 38: 23S rRNA

Chain a:

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U573 A574 A575 U588 C595 U596 A602 A603 U606 U607 A608 A609 A613 A614 U615 A616 G617 G618 G619 G620 A621 C624 A627 G628 G629 G630 A631 A632 A637 C640 U641 U642 A643 A644 C645 U646 G647 G648 G649 U653 A654 U657 U658 G659 C660 G663 G664
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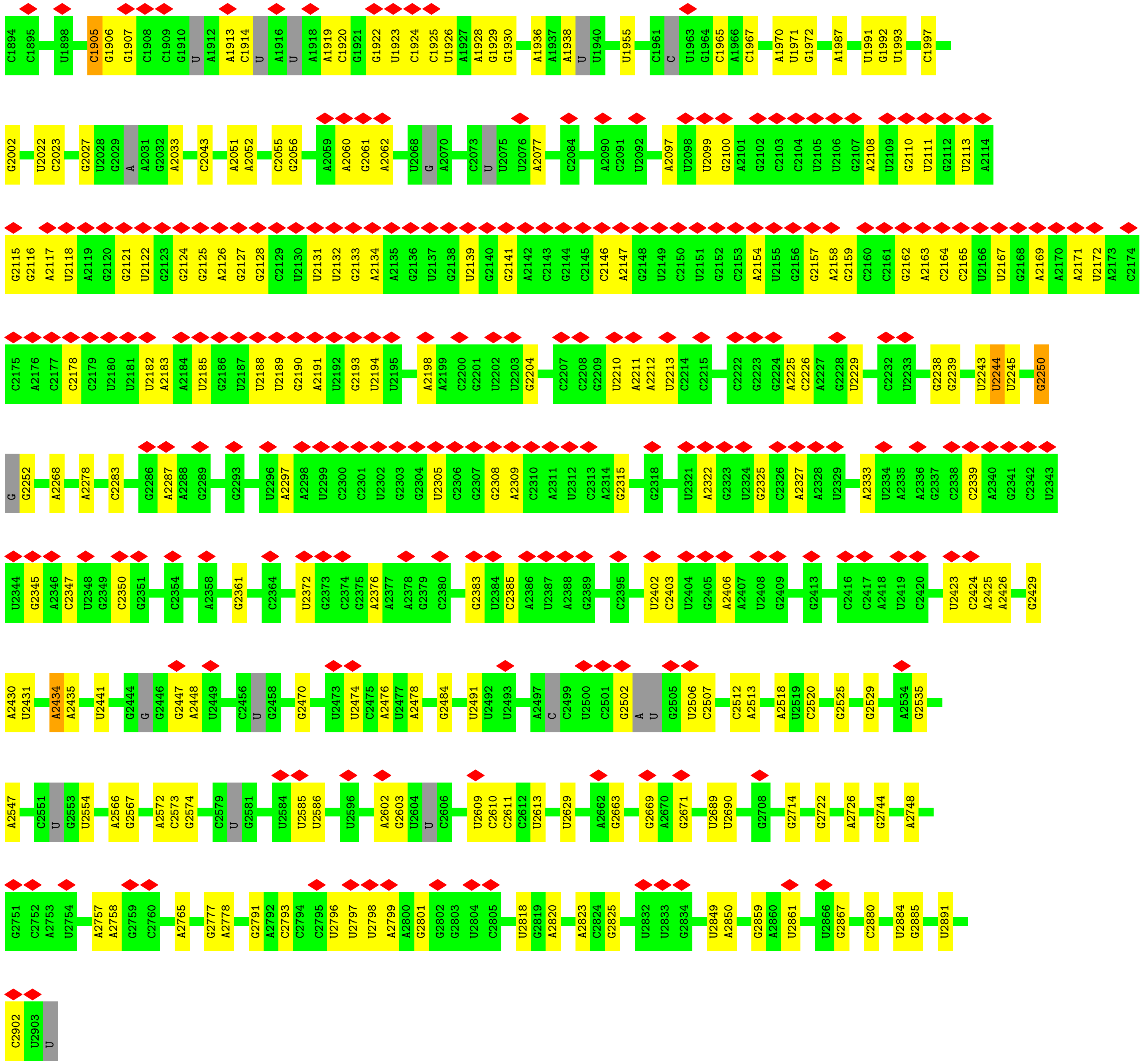
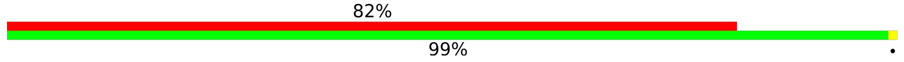
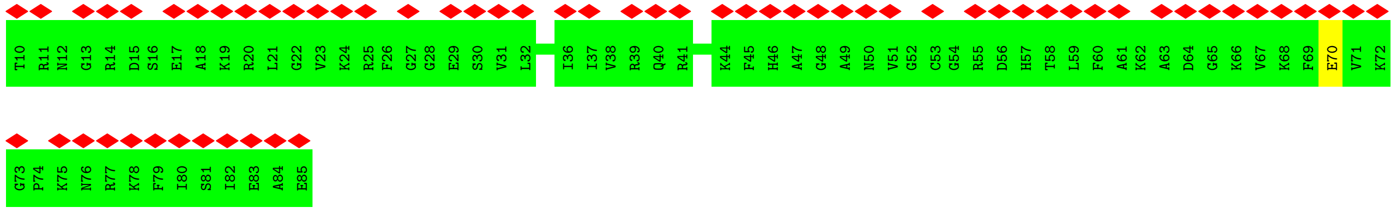
G1674 A1677 C1691 G1699 G1703 C1706 G1707 C1708 U1714 G1715 G1718 G1719 U1720 G1721 A1722 C1728 U1729 C1730 G1731 C1732 G1733 G1734 A1735 U1736 G1737 G1738 A1744 A1745 A1746 U1747 C1748 A1749 G1750 A1755 U1758 C1764 A1773 A1791 C1800 A1801 A1808 G1811
C1816 G1817 A1821 C1822 A1829 C1833 U1834 G C1836 U1841 G1842 C1843 A1847 A1848 U1851 U1852 A1853 A1854 U1855 U1856 G1857 A1858 U1859 G1860 G1861 G1862 G1863 U1864 U1865 A1866 G1869 C1870 A1871 A1872 G1873 C1874 G1875 A1876 U1880 C1881 U1882 U1883 G1884 A1885 U1886 C1887 G1888 A1889 A1890 G1891 C1892 C1893



- Molecule 39: 50S ribosomal protein L27

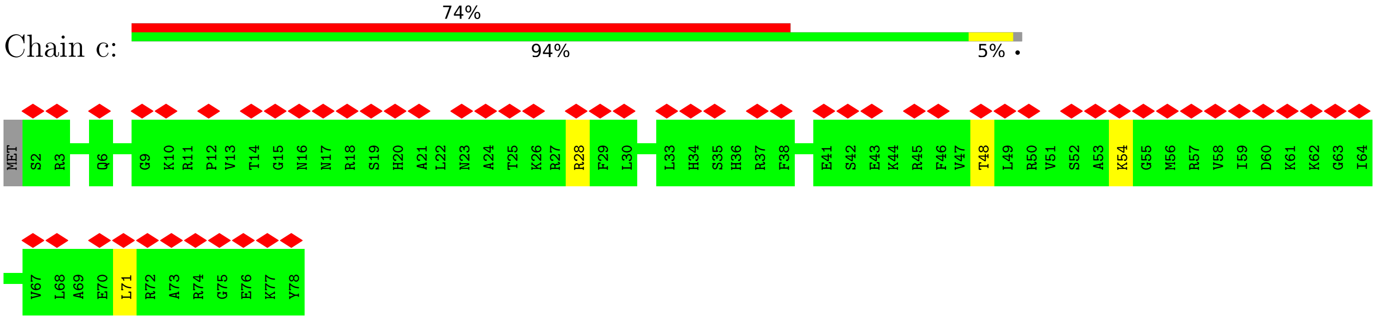
Chain b:





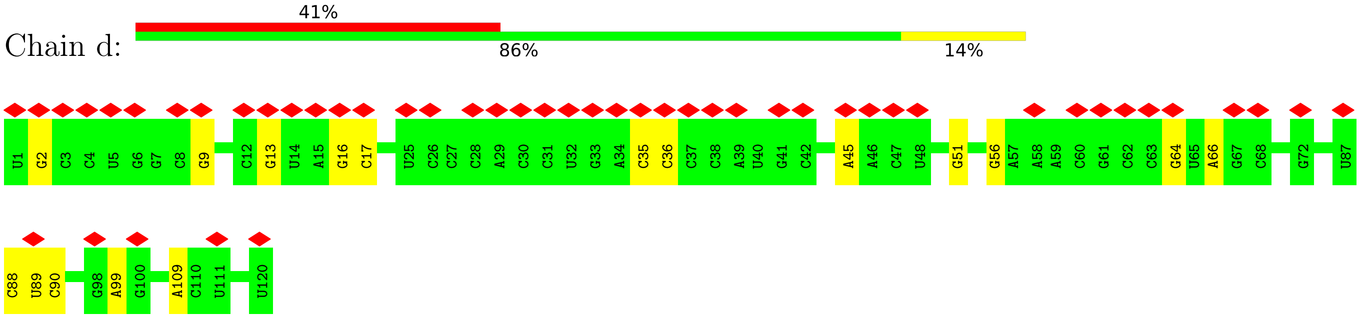
- Molecule 40: 50S ribosomal protein L28

Chain c:



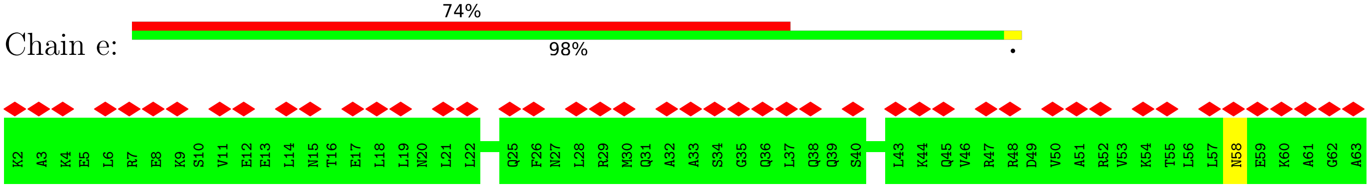
- Molecule 41: 5S rRNA

Chain d:



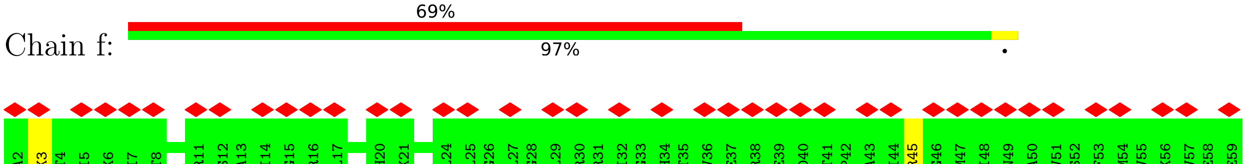
- Molecule 42: 50S ribosomal protein L29

Chain e:



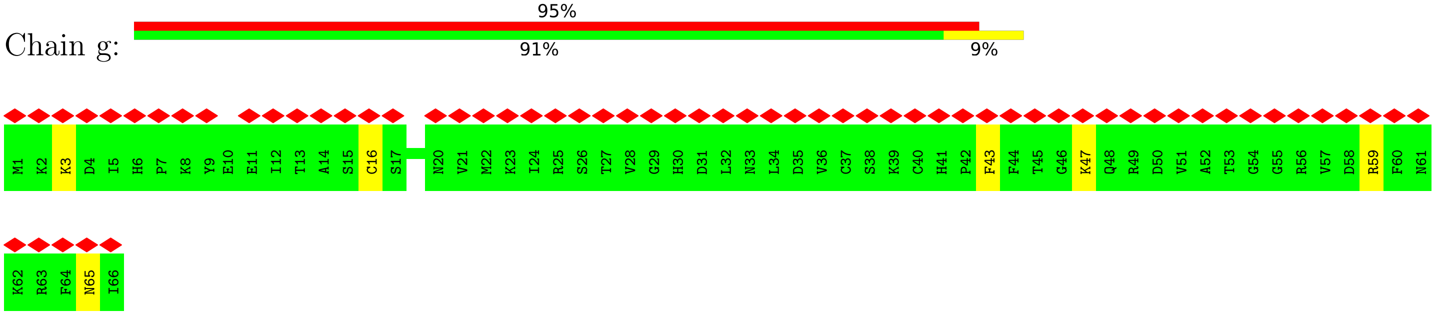
- Molecule 43: 50S ribosomal protein L30

Chain f:



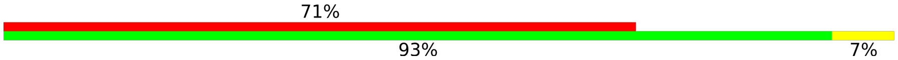
- Molecule 44: 50S ribosomal protein L31

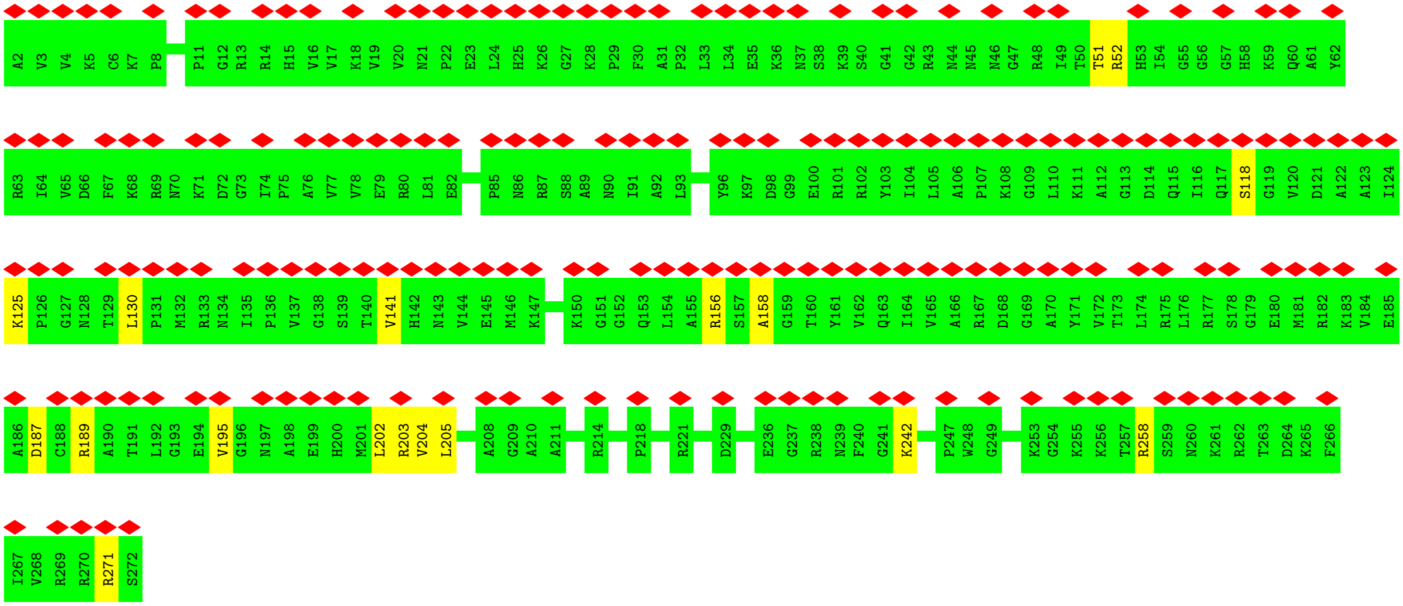
Chain g:



- Molecule 45: 50S ribosomal protein L2

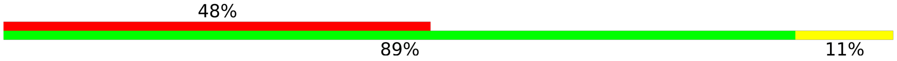
Chain h:

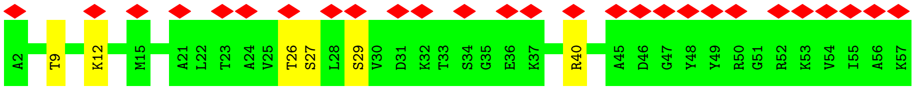




- Molecule 46: 50S ribosomal protein L32

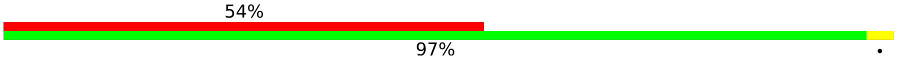
Chain i:

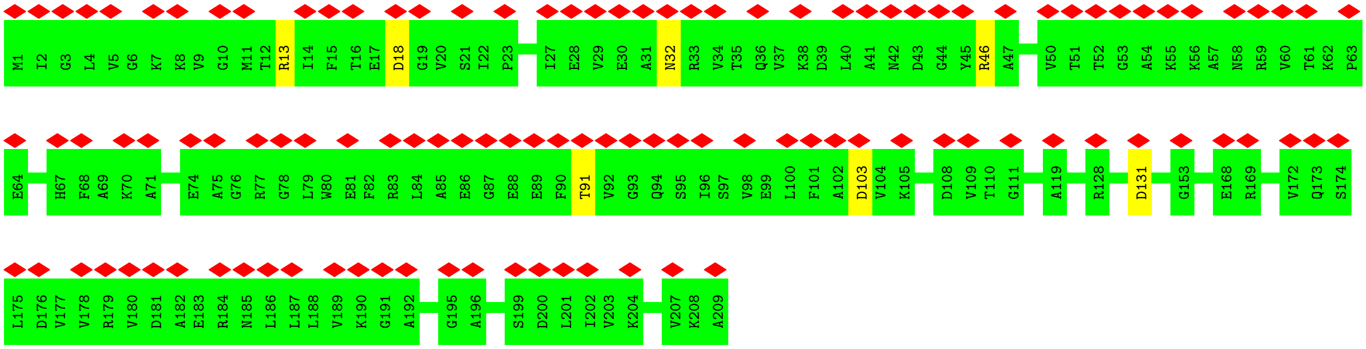




- Molecule 47: 50S ribosomal protein L3

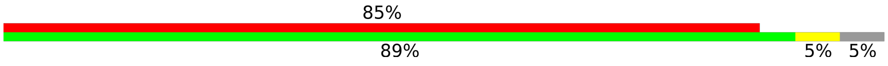
Chain j:

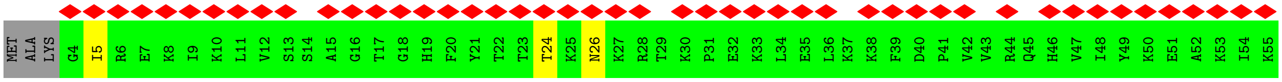




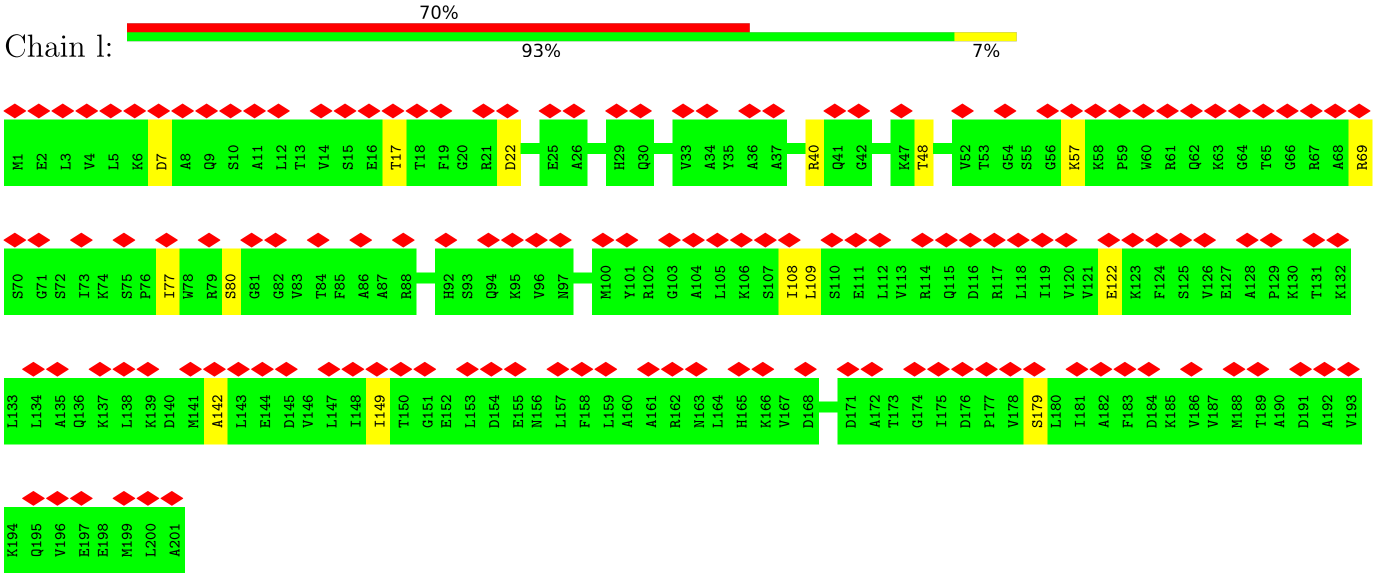
- Molecule 48: 50S ribosomal protein L33

Chain k:

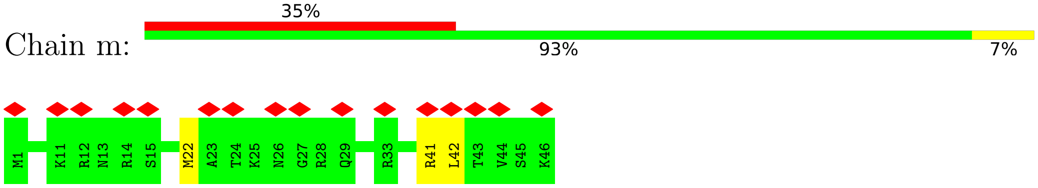




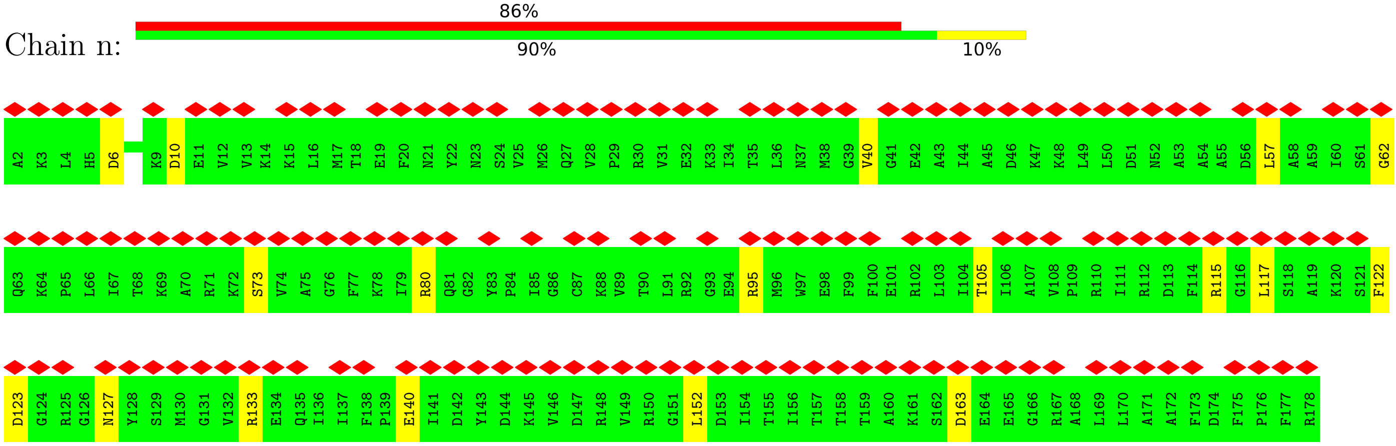
- Molecule 49: 50S ribosomal protein L4



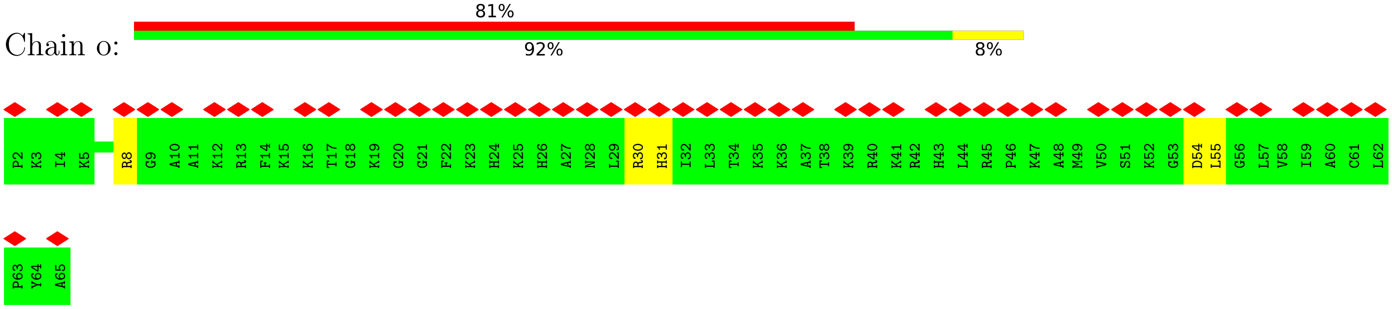
- Molecule 50: 50S ribosomal protein L34



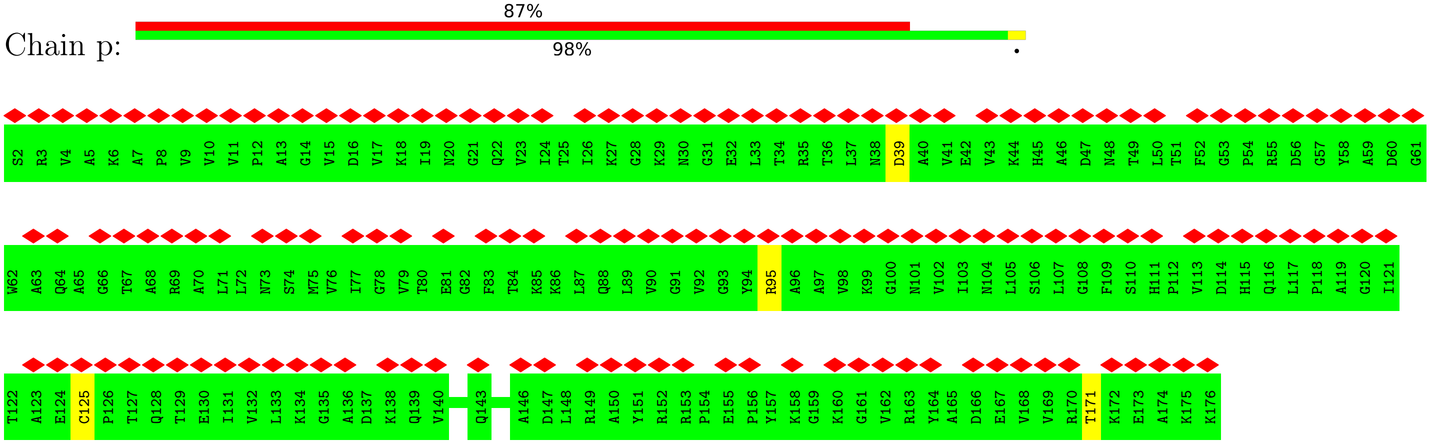
- Molecule 51: 50S ribosomal protein L5



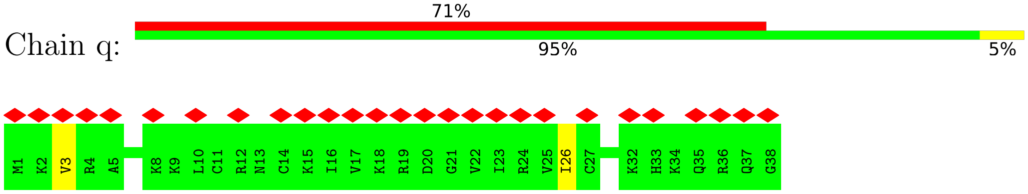
- Molecule 52: 50S ribosomal protein L35



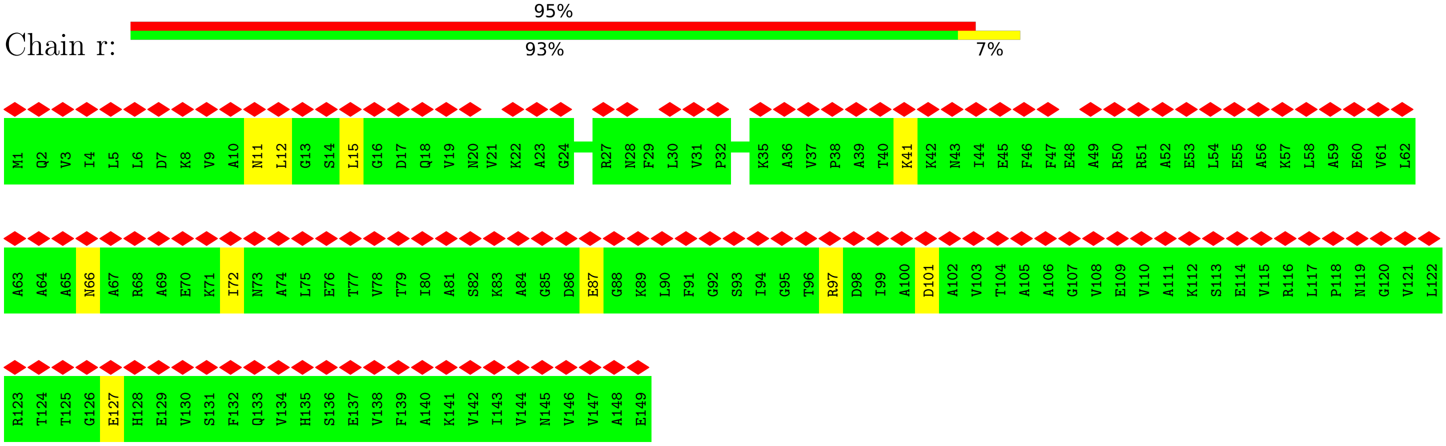
- Molecule 53: 50S ribosomal protein L6



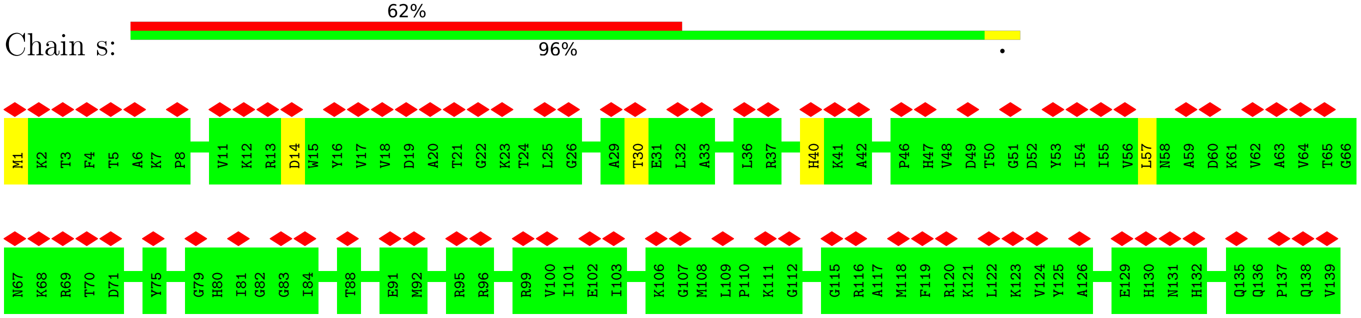
- Molecule 54: 50S ribosomal protein L36

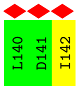


- Molecule 55: 50S ribosomal protein L9



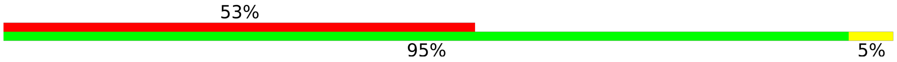
- Molecule 56: 50S ribosomal protein L13

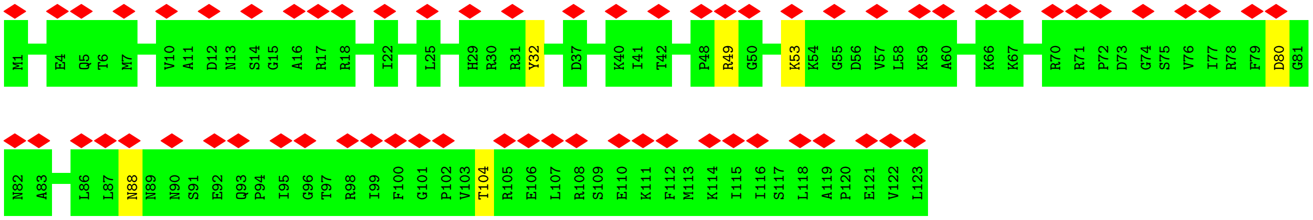




- Molecule 57: 50S ribosomal protein L14

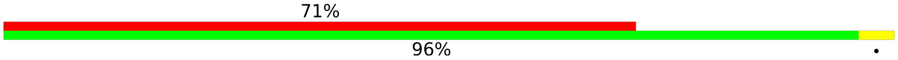
Chain t:

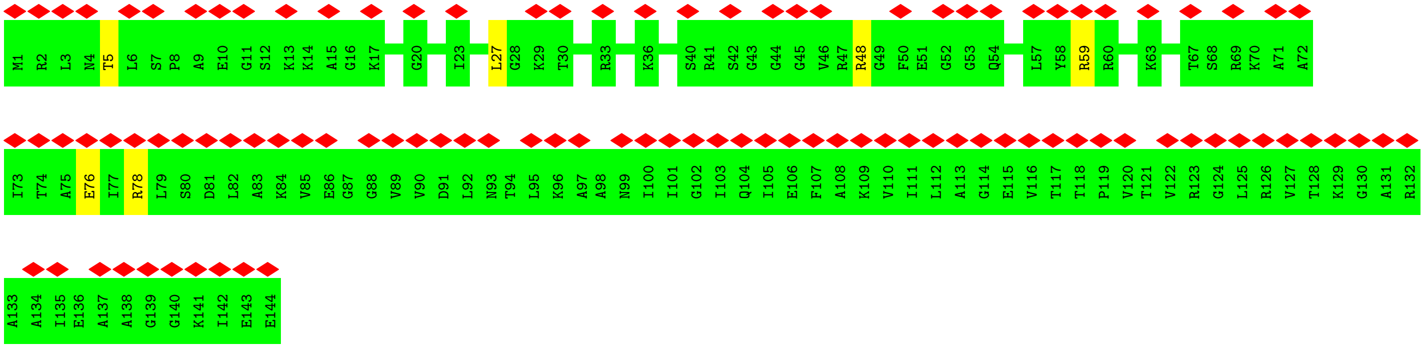




- Molecule 58: 50S ribosomal protein L15

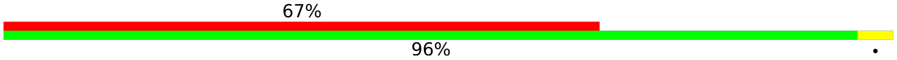
Chain u:

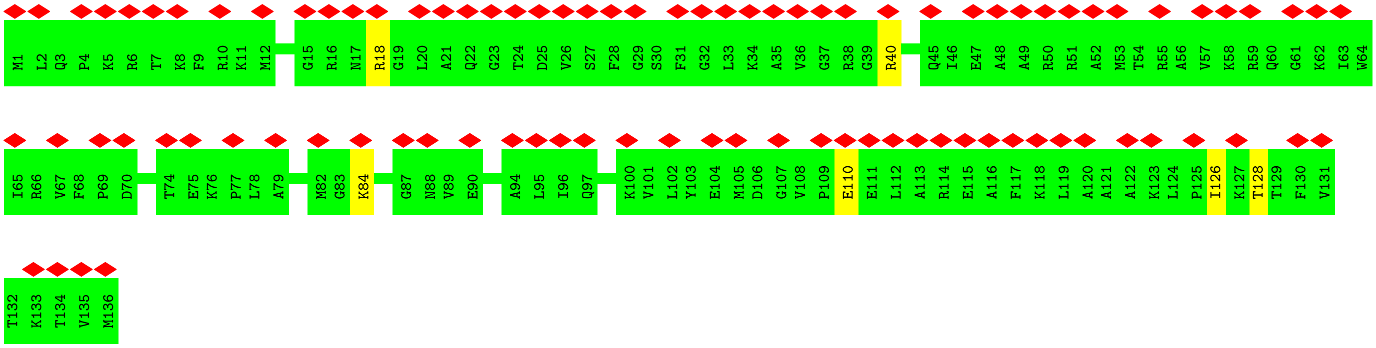




- Molecule 59: 50S ribosomal protein L16

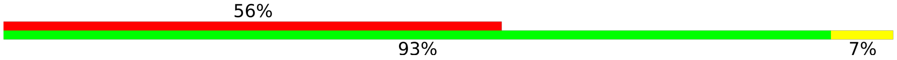
Chain v:

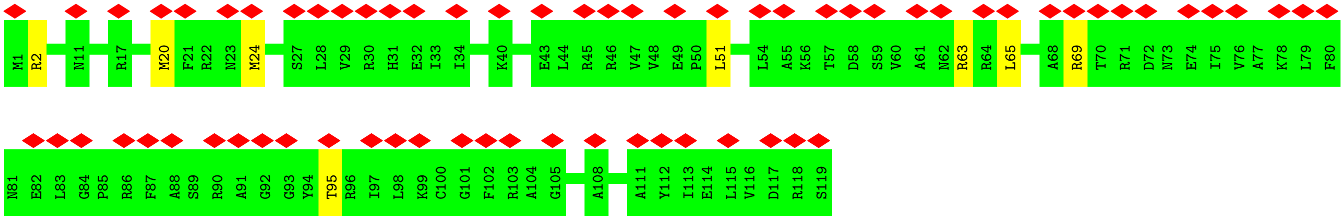




- Molecule 60: 50S ribosomal protein L17

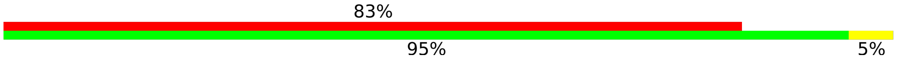
Chain w:

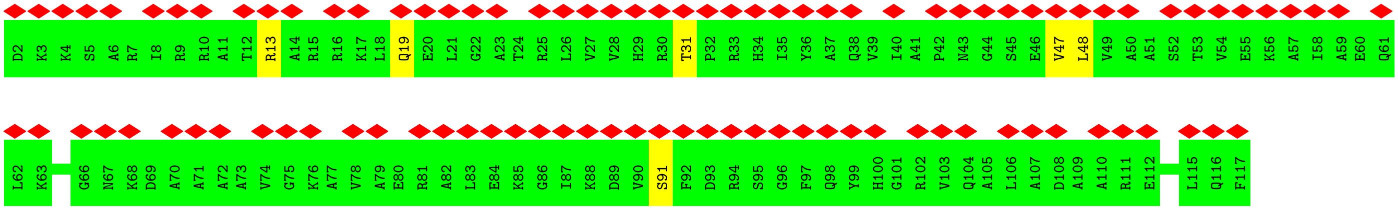




- Molecule 61: 50S ribosomal protein L18

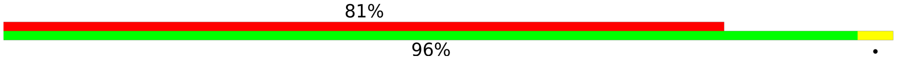
Chain x:

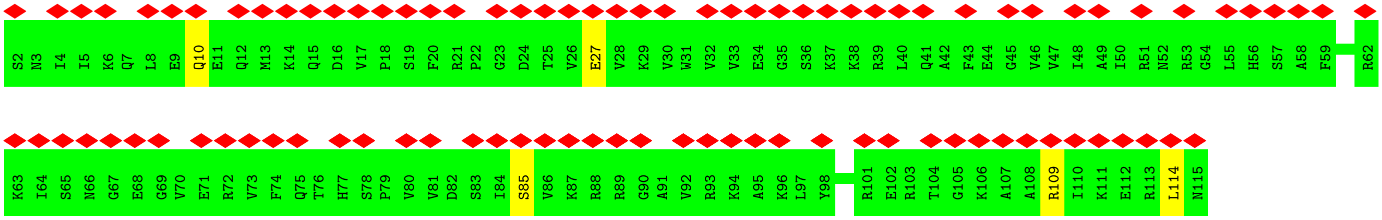




- Molecule 62: 50S ribosomal protein L19

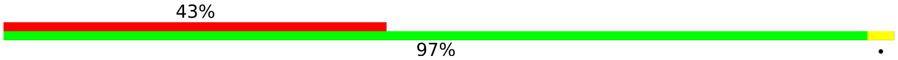
Chain y:

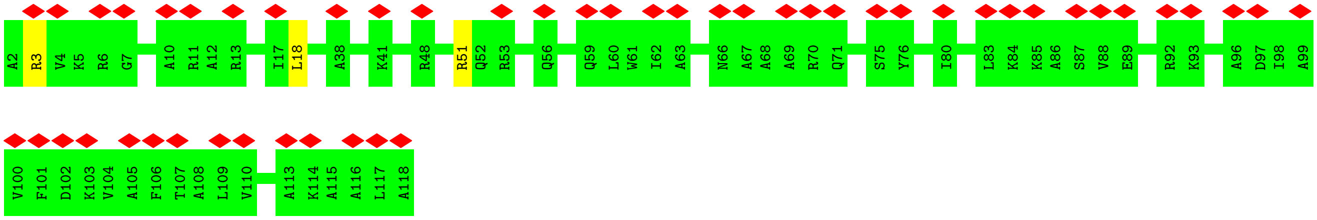




- Molecule 63: 50S ribosomal protein L20

Chain z:





4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	27650	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.067	Depositor
Minimum map value	-0.032	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.017	Depositor
Map size (Å)	532.48, 532.48, 532.48	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	0	0.38	0/829	0.67	0/1107
2	1	0.49	0/864	0.82	0/1156
3	2	0.41	0/752	0.71	0/1005
4	3	0.35	0/796	0.66	2/1062 (0.2%)
5	4	0.40	0/766	0.68	0/1025
6	5	1.13	6/528 (1.1%)	0.97	1/810 (0.1%)
7	6	1.11	4/603 (0.7%)	0.97	0/926
8	7	0.57	2/747 (0.3%)	0.88	3/1160 (0.3%)
9	9	0.79	2/1131 (0.2%)	0.64	1/1524 (0.1%)
10	A	0.38	0/1810	0.75	1/2821 (0.0%)
10	B	0.46	1/1810 (0.1%)	0.86	7/2821 (0.2%)
11	AA	0.58	2/10591 (0.0%)	0.75	15/14289 (0.1%)
12	AC	0.48	0/1808	0.62	1/2450 (0.0%)
12	AD	0.39	0/1789	0.57	0/2425
13	AE	0.52	4/10545 (0.0%)	0.66	5/14236 (0.0%)
14	C	0.48	0/553	0.83	0/743
15	D	0.34	10/36610 (0.0%)	0.74	30/57091 (0.1%)
16	E	0.57	0/675	0.85	0/895
17	F	0.56	0/597	0.87	0/792
18	G	0.49	0/1791	0.71	0/2413
19	H	0.54	1/1746 (0.1%)	1.03	13/2382 (0.5%)
20	I	0.43	0/1663	0.71	0/2241
21	J	0.47	0/1665	0.73	0/2227
22	K	0.45	0/1165	0.75	0/1568
23	L	0.43	0/867	0.75	1/1171 (0.1%)
24	M	0.50	0/1195	0.81	0/1602
25	N	0.41	0/989	0.69	0/1326
26	O	0.43	0/1034	0.75	0/1375
27	P	0.43	0/800	0.75	0/1082
28	Q	0.40	0/893	0.70	0/1205
29	R	0.35	0/952	0.74	0/1274
30	S	0.49	0/817	0.79	0/1088

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
31	T	0.53	0/722	0.86	0/964
32	U	0.44	0/659	0.78	0/884
33	V	0.34	0/657	0.62	0/881
34	W	0.38	0/680	0.62	0/915
35	X	0.49	0/909	0.86	0/1215
36	Y	0.67	0/1046	0.59	0/1410
37	Z	0.69	0/227	0.57	0/304
38	a	0.38	3/69247 (0.0%)	0.72	17/107985 (0.0%)
39	b	0.39	0/589	0.71	0/779
40	c	0.48	0/635	0.82	2/848 (0.2%)
41	d	0.29	0/2872	0.70	0/4478
42	e	0.53	0/502	0.83	0/667
43	f	0.45	0/452	0.78	0/605
44	g	0.43	0/531	0.68	0/709
45	h	0.39	0/2121	0.78	0/2852
46	i	0.40	0/450	0.79	0/599
47	j	0.44	0/1586	0.69	0/2134
48	k	0.35	0/433	0.64	0/576
49	l	0.46	0/1571	0.77	0/2113
50	m	0.53	0/380	0.99	0/498
51	n	0.49	0/1434	0.88	3/1926 (0.2%)
52	o	0.45	0/513	0.83	0/676
53	p	0.39	0/1333	0.67	0/1805
54	q	0.37	0/303	0.77	0/397
55	r	0.43	0/1122	0.69	0/1515
56	s	0.50	0/1152	0.75	0/1551
57	t	0.41	0/955	0.78	0/1279
58	u	0.40	0/1062	0.76	0/1413
59	v	0.47	0/1093	0.82	0/1460
60	w	0.52	0/964	0.87	0/1289
61	x	0.46	0/902	0.81	0/1209
62	y	0.41	0/929	0.73	1/1242 (0.1%)
63	z	0.60	0/960	0.91	0/1278
All	All	0.43	35/188372 (0.0%)	0.74	103/277748 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
10	A	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
10	B	0	2
11	AA	0	10
13	AE	0	5
19	H	0	3
35	X	0	1
All	All	0	23

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	9	130	PRO	N-CA	13.73	1.70	1.47
15	D	1516	G	O3'-P	-13.42	1.45	1.61
15	D	1339	A	O3'-P	10.59	1.73	1.61
11	AA	374	GLU	C-N	10.44	1.54	1.34
13	AE	88	CYS	CB-SG	-10.14	1.65	1.82
6	5	109	DT	O3'-P	8.71	1.71	1.61
15	D	145	G	O3'-P	8.43	1.71	1.61
15	D	196	A	O3'-P	8.31	1.71	1.61
7	6	10	DG	C1'-N9	-8.27	1.35	1.47
11	AA	850	ILE	N-CA	-8.19	1.29	1.46
15	D	1275	A	O3'-P	7.76	1.70	1.61
19	H	169	SER	N-CA	7.50	1.61	1.46
38	a	2434	A	O3'-P	7.47	1.70	1.61
15	D	1515	G	O3'-P	-7.28	1.52	1.61
6	5	121	DG	C1'-N9	-7.27	1.37	1.47
8	7	19	G	C1'-N9	-7.20	1.36	1.46
15	D	1395	C	O3'-P	7.17	1.69	1.61
8	7	-10	U	C1'-N1	6.97	1.59	1.48
15	D	1490	U	O3'-P	6.82	1.69	1.61
6	5	112	DG	C1'-N9	-6.74	1.37	1.47
15	D	1492	A	O3'-P	6.59	1.69	1.61
38	a	1905	C	O3'-P	6.59	1.69	1.61
38	a	2167	U	O3'-P	6.56	1.69	1.61
6	5	100	DA	C1'-N9	-6.45	1.38	1.47
7	6	21	DA	C1'-N9	-6.39	1.38	1.47
13	AE	93	THR	CA-C	6.23	1.69	1.52
9	9	129	LEU	C-N	6.11	1.45	1.34
6	5	116	DG	C1'-N9	-6.07	1.38	1.47
6	5	115	DA	C1'-N9	-6.00	1.38	1.47
13	AE	70	CYS	CA-CB	-5.79	1.41	1.53
7	6	28	DA	C1'-N9	-5.74	1.39	1.47
10	B	36	U	O3'-P	5.73	1.68	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	D	1397	C	O3'-P	5.72	1.68	1.61
7	6	24	DT	C1'-N1	5.36	1.56	1.49
13	AE	801	VAL	CB-CG2	-5.01	1.42	1.52

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	D	1516	G	P-O3'-C3'	-18.99	96.91	119.70
15	D	1516	G	O3'-P-O5'	13.81	130.24	104.00
11	AA	1250	SER	C-N-CA	11.14	149.56	121.70
38	a	2252	G	N9-C1'-C2'	-10.93	99.80	114.00
15	D	1401	G	N9-C1'-C2'	-10.68	100.12	114.00
51	n	73	SER	N-CA-CB	-10.60	94.61	110.50
15	D	1499	A	N9-C1'-C2'	-10.29	100.63	114.00
15	D	528	C	N1-C1'-C2'	-10.22	100.71	114.00
19	H	169	SER	N-CA-C	9.97	137.93	111.00
15	D	1339	A	P-O3'-C3'	9.86	131.54	119.70
10	B	29	G	N9-C1'-C2'	-9.75	101.28	112.00
10	B	28	C	P-O3'-C3'	9.64	131.26	119.70
13	AE	271	ARG	NE-CZ-NH2	-9.38	115.61	120.30
11	AA	375	PRO	CA-N-CD	-9.32	98.45	111.50
15	D	196	A	P-O3'-C3'	9.30	130.85	119.70
15	D	526	C	N1-C1'-C2'	-8.86	102.26	112.00
19	H	88	LYS	C-N-CA	8.73	143.53	121.70
38	a	2167	U	P-O3'-C3'	8.62	130.04	119.70
15	D	1208	C	N1-C1'-C2'	-8.56	102.58	112.00
15	D	1206	G	N9-C1'-C2'	-8.36	102.80	112.00
9	9	130	PRO	CA-N-CD	-8.25	99.95	111.50
38	a	2434	A	P-O3'-C3'	8.25	129.59	119.70
11	AA	995	ASP	O-C-N	-8.24	109.52	122.70
11	AA	376	PRO	N-CA-CB	-8.01	93.69	103.30
15	D	1406	U	N1-C1'-C2'	-7.77	103.46	112.00
15	D	1275	A	P-O3'-C3'	7.67	128.90	119.70
38	a	1905	C	P-O3'-C3'	7.65	128.88	119.70
15	D	1492	A	P-O3'-C3'	7.55	128.76	119.70
15	D	1490	U	P-O3'-C3'	7.55	128.76	119.70
19	H	305	HIS	N-CA-C	7.44	131.09	111.00
10	B	29	G	C3'-C2'-O2'	7.37	134.67	113.30
8	7	-11	A	OP2-P-O3'	7.22	121.09	105.20
15	D	1206	G	C4'-C3'-O3'	7.14	127.27	113.00
15	D	1493	A	C2'-C3'-O3'	7.13	125.18	109.50
10	B	35	A	P-O3'-C3'	7.10	128.22	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	a	2245	U	N1-C1'-C2'	-7.05	104.25	112.00
15	D	145	G	P-O3'-C3'	7.04	128.15	119.70
15	D	1516	G	OP1-P-O3'	-6.98	89.85	105.20
15	D	1395	C	P-O3'-C3'	6.94	128.03	119.70
11	AA	855	PRO	N-CA-CB	-6.88	95.04	102.60
8	7	-11	A	O3'-P-O5'	-6.79	91.11	104.00
51	n	73	SER	CB-CA-C	6.73	122.88	110.10
11	AA	995	ASP	CA-C-N	6.69	131.91	117.20
15	D	1515	G	O3'-P-O5'	-6.67	91.34	104.00
15	D	1401	G	C4'-C3'-O3'	6.64	126.27	113.00
38	a	2250	G	C4'-C3'-O3'	-6.61	95.53	109.40
38	a	2243	U	N1-C1'-C2'	-6.60	104.74	112.00
38	a	1379	U	C2'-C3'-O3'	6.54	124.16	113.70
15	D	1515	G	P-O3'-C3'	6.50	127.50	119.70
19	H	339	ARG	C-N-CA	6.46	137.84	121.70
11	AA	935	THR	CA-CB-OG1	-6.45	95.46	109.00
15	D	515	G	N9-C1'-C2'	-6.41	104.95	112.00
15	D	1497	G	N9-C1'-C2'	-6.40	104.96	112.00
15	D	1408	A	N9-C1'-C2'	-6.39	104.97	112.00
6	5	109	DT	P-O3'-C3'	6.39	127.36	119.70
10	B	34	C	P-O3'-C3'	6.36	127.34	119.70
12	AC	117	HIS	CB-CA-C	-6.21	97.97	110.40
11	AA	849	GLU	C-N-CA	6.09	136.93	121.70
11	AA	1004	ASP	CB-CA-C	6.00	122.40	110.40
19	H	140	PRO	N-CA-CB	5.97	110.47	103.30
11	AA	943	LYS	CA-C-O	-5.94	107.64	120.10
10	B	29	G	P-O3'-C3'	5.93	126.82	119.70
11	AA	727	VAL	N-CA-C	-5.91	95.03	111.00
19	H	330	VAL	N-CA-C	5.90	126.93	111.00
19	H	336	ASP	CB-CA-C	-5.90	98.61	110.40
11	AA	943	LYS	CA-C-N	5.87	130.11	117.20
38	a	754	U	N1-C1'-C2'	5.86	121.62	114.00
19	H	168	VAL	C-N-CA	5.82	136.25	121.70
19	H	132	PRO	N-CA-CB	5.81	110.28	103.30
13	AE	903	LEU	C-N-CA	5.73	136.02	121.70
15	D	517	G	C5'-C4'-C3'	5.71	125.14	116.00
19	H	344	LEU	CA-CB-CG	5.66	128.32	115.30
38	a	2244	U	C1'-C2'-O2'	-5.63	93.71	110.60
51	n	127	ASN	CB-CA-C	5.63	121.66	110.40
13	AE	363	LEU	CA-CB-CG	5.59	128.17	115.30
23	L	54	LEU	CA-CB-CG	5.57	128.11	115.30
38	a	783	A	C4'-C3'-O3'	5.47	123.94	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	AA	1233	LEU	CA-CB-CG	5.45	127.83	115.30
40	c	28	ARG	NE-CZ-NH2	-5.44	117.58	120.30
62	y	109	ARG	NE-CZ-NH2	5.38	122.99	120.30
15	D	1397	C	P-O3'-C3'	5.35	126.12	119.70
4	3	22	ARG	NE-CZ-NH1	5.33	122.97	120.30
15	D	1340	A	C5'-C4'-C3'	5.31	124.50	116.00
11	AA	728	ASP	N-CA-C	5.30	125.31	111.00
38	a	742	A	C8-N9-C1'	-5.26	118.24	127.70
38	a	404	A	C2'-C3'-O3'	5.21	122.04	113.70
15	D	1340	A	C5'-C4'-O4'	5.19	115.33	109.10
38	a	2244	U	C4'-C3'-O3'	5.16	123.33	113.00
19	H	169	SER	N-CA-CB	-5.16	102.76	110.50
8	7	-8	U	C2'-C3'-O3'	5.14	121.93	113.70
11	AA	817	LEU	CB-CG-CD2	-5.14	102.26	111.00
38	a	742	A	C4-N9-C1'	5.11	135.49	126.30
4	3	22	ARG	NE-CZ-NH2	-5.10	117.75	120.30
38	a	2252	G	C4'-C3'-O3'	5.10	123.19	113.00
10	B	48	C	N1-C1'-C2'	5.07	120.59	114.00
40	c	28	ARG	NE-CZ-NH1	5.06	122.83	120.30
15	D	197	A	C2'-C3'-O3'	5.06	121.80	113.70
10	A	48	C	N1-C1'-C2'	5.05	120.57	114.00
13	AE	73	GLY	N-CA-C	5.02	125.65	113.10
19	H	153	GLU	N-CA-C	-5.02	97.45	111.00
13	AE	807	LEU	CB-CG-CD2	-5.02	102.47	111.00
38	a	375	G	C2'-C3'-O3'	5.01	121.72	113.70
19	H	332	VAL	N-CA-C	5.01	124.53	111.00

There are no chirality outliers.

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	A	19	G	Sidechain
10	A	7	G	Sidechain
11	AA	1134	GLN	Peptide
11	AA	1157	GLN	Peptide
11	AA	1158	LYS	Peptide
11	AA	205	PRO	Peptide
11	AA	594	VAL	Peptide
11	AA	595	THR	Peptide
11	AA	596	ASP	Mainchain
11	AA	696	ASP	Peptide
11	AA	746	ALA	Peptide

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Mol	Chain	Res	Type	Group
11	AA	853	ASP	Mainchain
13	AE	1184	ASP	Peptide
13	AE	1326	GLN	Peptide
13	AE	313	GLY	Peptide
13	AE	416	ILE	Peptide
13	AE	804	ALA	Peptide
10	B	19	G	Sidechain
10	B	7	G	Sidechain
19	H	274	TYR	Peptide
19	H	81	GLU	Peptide
19	H	82	THR	Peptide
35	X	100	GLN	Mainchain

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	0	101/103 (98%)	97 (96%)	3 (3%)	1 (1%)	15	52
2	1	108/110 (98%)	104 (96%)	4 (4%)	0	100	100
3	2	92/100 (92%)	90 (98%)	2 (2%)	0	100	100
4	3	101/104 (97%)	96 (95%)	4 (4%)	1 (1%)	15	52
5	4	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
9	9	146/165 (88%)	95 (65%)	37 (25%)	14 (10%)	0	10
11	AA	1318/1342 (98%)	1150 (87%)	136 (10%)	32 (2%)	6	35
12	AC	228/329 (69%)	215 (94%)	11 (5%)	2 (1%)	17	54
12	AD	226/329 (69%)	212 (94%)	14 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	AE	1329/1407 (94%)	1200 (90%)	120 (9%)	9 (1%)	22	60
14	C	64/75 (85%)	63 (98%)	1 (2%)	0	100	100
16	E	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
17	F	68/71 (96%)	68 (100%)	0	0	100	100
18	G	223/241 (92%)	210 (94%)	13 (6%)	0	100	100
19	H	255/557 (46%)	188 (74%)	55 (22%)	12 (5%)	2	23
20	I	206/233 (88%)	197 (96%)	8 (4%)	1 (0%)	29	67
21	J	203/205 (99%)	198 (98%)	5 (2%)	0	100	100
22	K	154/167 (92%)	146 (95%)	7 (4%)	1 (1%)	25	63
23	L	102/135 (76%)	97 (95%)	4 (4%)	1 (1%)	15	52
24	M	149/151 (99%)	144 (97%)	4 (3%)	1 (1%)	22	60
25	N	127/129 (98%)	121 (95%)	5 (4%)	1 (1%)	19	58
26	O	125/127 (98%)	115 (92%)	9 (7%)	1 (1%)	19	58
27	P	97/99 (98%)	88 (91%)	8 (8%)	1 (1%)	15	52
28	Q	115/117 (98%)	104 (90%)	9 (8%)	2 (2%)	9	42
29	R	117/123 (95%)	116 (99%)	1 (1%)	0	100	100
30	S	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
31	T	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
32	U	80/82 (98%)	75 (94%)	4 (5%)	1 (1%)	12	47
33	V	78/84 (93%)	74 (95%)	4 (5%)	0	100	100
34	W	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
35	X	114/116 (98%)	107 (94%)	5 (4%)	2 (2%)	8	40
36	Y	139/141 (99%)	102 (73%)	25 (18%)	12 (9%)	1	12
37	Z	28/121 (23%)	19 (68%)	7 (25%)	2 (7%)	1	16
39	b	74/76 (97%)	69 (93%)	5 (7%)	0	100	100
40	c	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
42	e	60/62 (97%)	57 (95%)	3 (5%)	0	100	100
43	f	56/58 (97%)	53 (95%)	3 (5%)	0	100	100
44	g	64/66 (97%)	63 (98%)	1 (2%)	0	100	100
45	h	269/271 (99%)	259 (96%)	9 (3%)	1 (0%)	34	71
46	i	54/56 (96%)	51 (94%)	3 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	j	207/209 (99%)	198 (96%)	9 (4%)	0	100	100
48	k	50/55 (91%)	50 (100%)	0	0	100	100
49	l	199/201 (99%)	190 (96%)	8 (4%)	1 (0%)	29	67
50	m	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
51	n	175/177 (99%)	162 (93%)	11 (6%)	2 (1%)	14	50
52	o	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
53	p	173/175 (99%)	161 (93%)	12 (7%)	0	100	100
54	q	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
55	r	147/149 (99%)	136 (92%)	11 (8%)	0	100	100
56	s	140/142 (99%)	135 (96%)	5 (4%)	0	100	100
57	t	121/123 (98%)	111 (92%)	10 (8%)	0	100	100
58	u	142/144 (99%)	135 (95%)	7 (5%)	0	100	100
59	v	134/136 (98%)	129 (96%)	5 (4%)	0	100	100
60	w	117/119 (98%)	107 (92%)	10 (8%)	0	100	100
61	x	114/116 (98%)	108 (95%)	6 (5%)	0	100	100
62	y	112/114 (98%)	105 (94%)	7 (6%)	0	100	100
63	z	115/117 (98%)	110 (96%)	4 (4%)	1 (1%)	17	54
All	All	9274/10209 (91%)	8519 (92%)	653 (7%)	102 (1%)	18	50

All (102) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	9	88	HIS
11	AA	596	ASP
11	AA	853	ASP
11	AA	859	GLU
11	AA	862	LEU
11	AA	873	ILE
11	AA	937	ASP
11	AA	993	PRO
19	H	139	ARG
19	H	153	GLU
19	H	169	SER
19	H	306	VAL
19	H	340	ARG
26	O	56	ASP

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Mol	Chain	Res	Type
35	X	103	LYS
36	Y	48	ILE
9	9	33	VAL
9	9	119	PRO
11	AA	375	PRO
11	AA	856	ASN
11	AA	870	ILE
11	AA	940	GLU
11	AA	985	GLU
11	AA	1003	THR
11	AA	1158	LYS
13	AE	175	GLU
19	H	108	VAL
19	H	309	MET
19	H	333	LEU
36	Y	93	ASN
45	h	158	ALA
49	l	142	ALA
63	z	3	ARG
9	9	48	ALA
9	9	91	ALA
9	9	118	ILE
9	9	130	PRO
11	AA	376	PRO
11	AA	723	VAL
11	AA	728	ASP
11	AA	935	THR
11	AA	980	VAL
11	AA	1005	GLU
11	AA	1045	GLY
12	AC	164	ASP
12	AC	165	GLU
13	AE	51	PRO
13	AE	805	GLN
19	H	76	GLU
19	H	142	ARG
24	M	130	ASN
27	P	58	ASN
28	Q	119	ASN
36	Y	20	SER
36	Y	64	ARG
36	Y	106	GLN

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Mol	Chain	Res	Type
9	9	69	PHE
9	9	73	LYS
9	9	108	VAL
9	9	129	LEU
9	9	133	GLU
11	AA	850	ILE
11	AA	943	LYS
11	AA	995	ASP
13	AE	174	ASP
13	AE	193	ASP
19	H	82	THR
20	I	80	LYS
35	X	105	ASN
36	Y	83	ALA
37	Z	21	GLU
51	n	40	VAL
9	9	28	ALA
11	AA	917	SER
11	AA	991	LYS
11	AA	997	TRP
11	AA	1044	PRO
13	AE	91	GLU
19	H	70	VAL
36	Y	22	PRO
36	Y	71	LYS
36	Y	89	SER
37	Z	7	ILE
4	3	39	ILE
13	AE	49	PHE
13	AE	73	GLY
13	AE	904	ALA
36	Y	62	ALA
23	L	96	VAL
36	Y	23	VAL
36	Y	100	ILE
1	0	44	GLY
11	AA	697	LYS
11	AA	1159	VAL
11	AA	1317	PRO
22	K	44	GLY
28	Q	74	VAL
32	U	64	GLY

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Mol	Chain	Res	Type
9	9	54	VAL
51	n	62	GLY
11	AA	933	VAL
25	N	75	ILE

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	0	84/84 (100%)	78 (93%)	6 (7%)	14	42
2	1	93/93 (100%)	84 (90%)	9 (10%)	8	29
3	2	81/84 (96%)	76 (94%)	5 (6%)	18	46
4	3	84/85 (99%)	78 (93%)	6 (7%)	14	42
5	4	78/78 (100%)	74 (95%)	4 (5%)	24	52
9	9	112/123 (91%)	65 (58%)	47 (42%)	0	0
11	AA	1140/1157 (98%)	1039 (91%)	101 (9%)	9	34
12	AC	198/286 (69%)	182 (92%)	16 (8%)	11	38
12	AD	196/286 (68%)	194 (99%)	2 (1%)	76	85
13	AE	1120/1168 (96%)	1051 (94%)	69 (6%)	18	46
14	C	57/65 (88%)	55 (96%)	2 (4%)	36	61
16	E	65/66 (98%)	60 (92%)	5 (8%)	13	40
17	F	60/61 (98%)	57 (95%)	3 (5%)	24	52
18	G	187/199 (94%)	178 (95%)	9 (5%)	25	53
19	H	137/461 (30%)	128 (93%)	9 (7%)	16	44
20	I	171/190 (90%)	165 (96%)	6 (4%)	36	61
21	J	172/172 (100%)	165 (96%)	7 (4%)	30	57
22	K	119/126 (94%)	112 (94%)	7 (6%)	19	48
23	L	91/116 (78%)	85 (93%)	6 (7%)	16	44
24	M	124/124 (100%)	116 (94%)	8 (6%)	17	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	N	104/104 (100%)	102 (98%)	2 (2%)	57	75
26	O	105/105 (100%)	100 (95%)	5 (5%)	25	53
27	P	86/86 (100%)	77 (90%)	9 (10%)	7	27
28	Q	90/90 (100%)	87 (97%)	3 (3%)	38	62
29	R	101/103 (98%)	94 (93%)	7 (7%)	15	43
30	S	83/84 (99%)	79 (95%)	4 (5%)	25	53
31	T	76/77 (99%)	64 (84%)	12 (16%)	2	16
32	U	65/65 (100%)	61 (94%)	4 (6%)	18	46
33	V	74/78 (95%)	72 (97%)	2 (3%)	44	66
34	W	72/72 (100%)	68 (94%)	4 (6%)	21	49
35	X	94/94 (100%)	85 (90%)	9 (10%)	8	30
36	Y	109/109 (100%)	72 (66%)	37 (34%)	0	1
37	Z	26/85 (31%)	12 (46%)	14 (54%)	0	0
39	b	58/58 (100%)	57 (98%)	1 (2%)	60	78
40	c	67/68 (98%)	64 (96%)	3 (4%)	27	54
42	e	54/54 (100%)	53 (98%)	1 (2%)	57	75
43	f	48/48 (100%)	46 (96%)	2 (4%)	30	56
44	g	59/59 (100%)	53 (90%)	6 (10%)	7	28
45	h	216/216 (100%)	199 (92%)	17 (8%)	12	39
46	i	47/47 (100%)	41 (87%)	6 (13%)	4	21
47	j	164/164 (100%)	157 (96%)	7 (4%)	29	56
48	k	47/49 (96%)	44 (94%)	3 (6%)	17	45
49	l	165/165 (100%)	151 (92%)	14 (8%)	10	37
50	m	38/38 (100%)	35 (92%)	3 (8%)	12	39
51	n	148/148 (100%)	134 (90%)	14 (10%)	8	30
52	o	51/51 (100%)	46 (90%)	5 (10%)	8	29
53	p	136/136 (100%)	132 (97%)	4 (3%)	42	64
54	q	34/34 (100%)	32 (94%)	2 (6%)	19	48
55	r	114/114 (100%)	104 (91%)	10 (9%)	10	34
56	s	116/116 (100%)	110 (95%)	6 (5%)	23	51
57	t	104/104 (100%)	98 (94%)	6 (6%)	20	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
58	u	103/103 (100%)	97 (94%)	6 (6%)	20	48
59	v	109/109 (100%)	103 (94%)	6 (6%)	21	50
60	w	99/99 (100%)	91 (92%)	8 (8%)	11	38
61	x	86/86 (100%)	80 (93%)	6 (7%)	15	42
62	y	99/99 (100%)	95 (96%)	4 (4%)	31	57
63	z	89/89 (100%)	87 (98%)	2 (2%)	52	71
All	All	7705/8430 (91%)	7124 (92%)	581 (8%)	17	40

All (581) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	10	LYS
1	0	13	ARG
1	0	48	LYS
1	0	51	VAL
1	0	68	ARG
1	0	86	GLN
2	1	7	HIS
2	1	19	LEU
2	1	30	SER
2	1	41	LYS
2	1	69	LEU
2	1	97	LEU
2	1	107	VAL
2	1	109	ASP
2	1	110	ARG
3	2	1	MET
3	2	24	MET
3	2	37	ASP
3	2	59	ASN
3	2	93	LEU
4	3	52	LEU
4	3	68	SER
4	3	72	ILE
4	3	89	ASP
4	3	99	ASN
4	3	101	GLU
5	4	40	ILE
5	4	41	GLU
5	4	69	GLU

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Mol	Chain	Res	Type
5	4	71	LYS
9	9	1	MET
9	9	3	LEU
9	9	4	ASN
9	9	5	LEU
9	9	6	GLN
9	9	7	ASP
9	9	11	ILE
9	9	14	GLU
9	9	23	LEU
9	9	24	SER
9	9	27	VAL
9	9	30	SER
9	9	31	ARG
9	9	34	THR
9	9	36	ASP
9	9	37	LYS
9	9	39	THR
9	9	42	ARG
9	9	43	LYS
9	9	51	TYR
9	9	52	MET
9	9	56	ARG
9	9	57	ASN
9	9	61	ARG
9	9	62	ARG
9	9	69	PHE
9	9	70	GLU
9	9	71	CYS
9	9	72	LEU
9	9	81	LEU
9	9	86	MET
9	9	94	ARG
9	9	96	PHE
9	9	98	GLU
9	9	106	PHE
9	9	107	GLU
9	9	109	LYS
9	9	113	PHE
9	9	117	LEU
9	9	122	GLN
9	9	123	ILE

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Mol	Chain	Res	Type
9	9	125	ARG
9	9	133	GLU
9	9	134	GLU
9	9	138	ARG
9	9	142	THR
9	9	143	MET
11	AA	376	PRO
11	AA	723	VAL
11	AA	728	ASP
11	AA	731	ARG
11	AA	752	ASN
11	AA	817	LEU
11	AA	840	SER
11	AA	844	LYS
11	AA	845	LEU
11	AA	851	THR
11	AA	854	ILE
11	AA	855	PRO
11	AA	857	VAL
11	AA	862	LEU
11	AA	864	LYS
11	AA	865	LEU
11	AA	866	ASP
11	AA	867	GLU
11	AA	868	SER
11	AA	871	VAL
11	AA	873	ILE
11	AA	876	GLU
11	AA	884	VAL
11	AA	886	LYS
11	AA	890	LYS
11	AA	912	ASP
11	AA	913	VAL
11	AA	914	LYS
11	AA	918	LEU
11	AA	933	VAL
11	AA	936	ARG
11	AA	939	VAL
11	AA	941	LYS
11	AA	943	LYS
11	AA	944	ARG
11	AA	949	GLU

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Mol	Chain	Res	Type
11	AA	950	GLU
11	AA	951	MET
11	AA	952	GLN
11	AA	953	LEU
11	AA	954	LYS
11	AA	955	GLN
11	AA	957	LYS
11	AA	958	LYS
11	AA	959	ASP
11	AA	960	LEU
11	AA	962	GLU
11	AA	963	GLU
11	AA	964	LEU
11	AA	965	GLN
11	AA	967	LEU
11	AA	968	GLU
11	AA	971	LEU
11	AA	973	SER
11	AA	974	ARG
11	AA	979	LEU
11	AA	980	VAL
11	AA	985	GLU
11	AA	988	LYS
11	AA	989	LEU
11	AA	991	LYS
11	AA	992	LEU
11	AA	994	ARG
11	AA	995	ASP
11	AA	997	TRP
11	AA	998	LEU
11	AA	999	GLU
11	AA	1002	LEU
11	AA	1005	GLU
11	AA	1006	GLU
11	AA	1007	LYS
11	AA	1008	GLN
11	AA	1009	ASN
11	AA	1010	GLN
11	AA	1013	GLN
11	AA	1019	ASP
11	AA	1020	GLU
11	AA	1022	LYS

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Mol	Chain	Res	Type
11	AA	1023	HIS
11	AA	1024	GLU
11	AA	1025	PHE
11	AA	1026	GLU
11	AA	1027	LYS
11	AA	1029	LEU
11	AA	1032	LYS
11	AA	1034	ARG
11	AA	1035	LYS
11	AA	1038	GLN
11	AA	1041	ASP
11	AA	1042	LEU
11	AA	1046	VAL
11	AA	1047	LEU
11	AA	1048	LYS
11	AA	1151	LEU
11	AA	1159	VAL
11	AA	1250	SER
11	AA	1252	SER
11	AA	1253	LEU
11	AA	1254	VAL
11	AA	1256	GLN
11	AA	1259	LEU
12	AC	12	ARG
12	AC	62	ASP
12	AC	65	LEU
12	AC	72	GLU
12	AC	91	ARG
12	AC	134	THR
12	AC	158	ARG
12	AC	159	ILE
12	AC	160	HIS
12	AC	162	GLU
12	AC	163	GLU
12	AC	165	GLU
12	AC	166	ARG
12	AC	168	ILE
12	AC	170	ARG
12	AC	171	LEU
12	AD	12	ARG
12	AD	208	ASN
13	AE	40	LYS

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Mol	Chain	Res	Type
13	AE	42	GLU
13	AE	44	ILE
13	AE	46	TYR
13	AE	47	ARG
13	AE	49	PHE
13	AE	50	LYS
13	AE	52	GLU
13	AE	53	ARG
13	AE	54	ASP
13	AE	60	ARG
13	AE	67	ASP
13	AE	70	CYS
13	AE	72	CYS
13	AE	74	LYS
13	AE	76	LYS
13	AE	77	ARG
13	AE	78	LEU
13	AE	81	ARG
13	AE	87	LYS
13	AE	88	CYS
13	AE	91	GLU
13	AE	94	GLN
13	AE	95	THR
13	AE	99	ARG
13	AE	100	GLU
13	AE	117	LEU
13	AE	119	SER
13	AE	123	ARG
13	AE	132	LEU
13	AE	135	ILE
13	AE	142	GLU
13	AE	144	TYR
13	AE	145	VAL
13	AE	147	ILE
13	AE	152	THR
13	AE	154	LEU
13	AE	157	GLN
13	AE	159	ILE
13	AE	175	GLU
13	AE	180	MET
13	AE	190	LYS
13	AE	193	ASP

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Mol	Chain	Res	Type
13	AE	196	GLN
13	AE	210	SER
13	AE	215	LYS
13	AE	216	LYS
13	AE	222	LYS
13	AE	223	LEU
13	AE	227	PHE
13	AE	232	ASN
13	AE	233	LYS
13	AE	237	MET
13	AE	238	ILE
13	AE	239	LEU
13	AE	240	THR
13	AE	244	VAL
13	AE	271	ARG
13	AE	385	LEU
13	AE	386	GLU
13	AE	390	LEU
13	AE	393	THR
13	AE	394	ILE
13	AE	395	LYS
13	AE	514	THR
13	AE	709	ARG
13	AE	836	ARG
13	AE	1172	LYS
13	AE	1373	ARG
14	C	33	ILE
14	C	74	HIS
16	E	6	SER
16	E	10	ARG
16	E	48	GLN
16	E	54	MET
16	E	64	LYS
17	F	34	ARG
17	F	62	ARG
17	F	67	ARG
18	G	8	ASP
18	G	23	TRP
18	G	45	LYS
18	G	105	LYS
18	G	108	ARG
18	G	128	LYS

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Mol	Chain	Res	Type
18	G	129	LEU
18	G	132	LYS
18	G	208	ARG
19	H	9	PHE
19	H	54	LYS
19	H	273	ARG
19	H	305	HIS
19	H	336	ASP
19	H	337	GLU
19	H	338	GLU
19	H	339	ARG
19	H	340	ARG
20	I	14	ILE
20	I	75	ILE
20	I	89	LYS
20	I	164	ARG
20	I	185	ASN
20	I	200	VAL
21	J	47	ARG
21	J	48	LEU
21	J	95	GLU
21	J	104	ARG
21	J	116	GLN
21	J	138	SER
21	J	143	VAL
22	K	10	GLU
22	K	15	LEU
22	K	60	ILE
22	K	114	VAL
22	K	115	LEU
22	K	138	ARG
22	K	162	GLU
23	L	16	GLU
23	L	24	ARG
23	L	38	ARG
23	L	54	LEU
23	L	79	ARG
23	L	86	ARG
24	M	7	ILE
24	M	17	LYS
24	M	21	GLU
24	M	23	LEU

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Mol	Chain	Res	Type
24	M	79	ARG
24	M	109	ARG
24	M	130	ASN
24	M	146	GLU
25	N	96	MET
25	N	121	LEU
26	O	12	ARG
26	O	27	LYS
26	O	60	LYS
26	O	63	LEU
26	O	118	LEU
27	P	5	ARG
27	P	17	LEU
27	P	24	GLU
27	P	25	ILE
27	P	27	GLU
27	P	37	ARG
27	P	87	LEU
27	P	89	ARG
27	P	90	LEU
28	Q	15	GLN
28	Q	56	ARG
28	Q	107	ILE
29	R	5	ASN
29	R	12	ARG
29	R	24	LEU
29	R	56	ARG
29	R	62	GLU
29	R	74	LEU
29	R	102	LEU
30	S	45	VAL
30	S	46	LEU
30	S	89	MET
30	S	92	GLU
31	T	10	LYS
31	T	17	ARG
31	T	22	THR
31	T	39	LEU
31	T	40	GLN
31	T	64	ARG
31	T	66	LEU
31	T	67	LEU

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Mol	Chain	Res	Type
31	T	70	LEU
31	T	73	LYS
31	T	84	ARG
31	T	85	LEU
32	U	1	MET
32	U	2	VAL
32	U	6	LEU
32	U	19	VAL
33	V	75	LEU
33	V	81	LYS
34	W	12	ASP
34	W	21	LYS
34	W	33	THR
34	W	79	THR
35	X	11	ASP
35	X	16	VAL
35	X	25	VAL
35	X	29	ARG
35	X	59	GLU
35	X	92	ARG
35	X	93	ARG
35	X	101	ARG
35	X	117	LYS
36	Y	9	LYS
36	Y	10	LEU
36	Y	16	MET
36	Y	23	VAL
36	Y	27	LEU
36	Y	30	GLN
36	Y	36	GLU
36	Y	44	LYS
36	Y	48	ILE
36	Y	50	LYS
36	Y	58	ILE
36	Y	60	VAL
36	Y	61	TYR
36	Y	64	ARG
36	Y	65	SER
36	Y	67	THR
36	Y	71	LYS
36	Y	78	LEU
36	Y	80	LYS

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Mol	Chain	Res	Type
36	Y	81	LYS
36	Y	91	LYS
36	Y	94	LYS
36	Y	95	ASP
36	Y	99	LYS
36	Y	100	ILE
36	Y	101	SER
36	Y	102	ARG
36	Y	104	GLN
36	Y	108	ILE
36	Y	112	LYS
36	Y	116	MET
36	Y	120	ASP
36	Y	124	MET
36	Y	125	THR
36	Y	126	ARG
36	Y	133	ARG
36	Y	135	MET
37	Z	1	SER
37	Z	2	ILE
37	Z	4	LYS
37	Z	6	GLN
37	Z	7	ILE
37	Z	8	ILE
37	Z	14	MET
37	Z	15	SER
37	Z	16	VAL
37	Z	23	ILE
37	Z	26	MET
37	Z	28	GLU
37	Z	29	LYS
37	Z	30	PHE
39	b	70	GLU
40	c	48	THR
40	c	54	LYS
40	c	71	LEU
42	e	58	ASN
43	f	3	LYS
43	f	45	ARG
44	g	3	LYS
44	g	16	CYS
44	g	43	PHE

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Mol	Chain	Res	Type
44	g	47	LYS
44	g	59	ARG
44	g	65	ASN
45	h	51	THR
45	h	52	ARG
45	h	118	SER
45	h	125	LYS
45	h	130	LEU
45	h	141	VAL
45	h	156	ARG
45	h	187	ASP
45	h	189	ARG
45	h	195	VAL
45	h	202	LEU
45	h	203	ARG
45	h	204	VAL
45	h	205	LEU
45	h	242	LYS
45	h	258	ARG
45	h	271	ARG
46	i	9	THR
46	i	12	LYS
46	i	26	THR
46	i	27	SER
46	i	29	SER
46	i	40	ARG
47	j	13	ARG
47	j	18	ASP
47	j	32	ASN
47	j	46	ARG
47	j	91	THR
47	j	103	ASP
47	j	131	ASP
48	k	5	ILE
48	k	24	THR
48	k	26	ASN
49	l	7	ASP
49	l	17	THR
49	l	22	ASP
49	l	40	ARG
49	l	48	THR
49	l	57	LYS

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Mol	Chain	Res	Type
49	l	69	ARG
49	l	77	ILE
49	l	80	SER
49	l	108	ILE
49	l	109	LEU
49	l	122	GLU
49	l	149	ILE
49	l	179	SER
50	m	22	MET
50	m	41	ARG
50	m	42	LEU
51	n	6	ASP
51	n	10	ASP
51	n	57	LEU
51	n	80	ARG
51	n	95	ARG
51	n	105	THR
51	n	115	ARG
51	n	117	LEU
51	n	122	PHE
51	n	123	ASP
51	n	133	ARG
51	n	140	GLU
51	n	152	LEU
51	n	163	ASP
52	o	8	ARG
52	o	30	ARG
52	o	31	HIS
52	o	54	ASP
52	o	55	LEU
53	p	39	ASP
53	p	95	ARG
53	p	125	CYS
53	p	171	THR
54	q	3	VAL
54	q	26	ILE
55	r	11	ASN
55	r	12	LEU
55	r	15	LEU
55	r	41	LYS
55	r	66	ASN
55	r	72	ILE

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Mol	Chain	Res	Type
55	r	87	GLU
55	r	97	ARG
55	r	101	ASP
55	r	127	GLU
56	s	1	MET
56	s	14	ASP
56	s	30	THR
56	s	40	HIS
56	s	57	LEU
56	s	142	ILE
57	t	32	TYR
57	t	49	ARG
57	t	53	LYS
57	t	80	ASP
57	t	88	ASN
57	t	104	THR
58	u	5	THR
58	u	27	LEU
58	u	48	ARG
58	u	59	ARG
58	u	76	GLU
58	u	78	ARG
59	v	18	ARG
59	v	40	ARG
59	v	84	LYS
59	v	110	GLU
59	v	126	ILE
59	v	128	THR
60	w	2	ARG
60	w	20	MET
60	w	24	MET
60	w	51	LEU
60	w	63	ARG
60	w	65	LEU
60	w	69	ARG
60	w	95	THR
61	x	13	ARG
61	x	19	GLN
61	x	31	THR
61	x	47	VAL
61	x	48	LEU
61	x	91	SER

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Mol	Chain	Res	Type
62	y	10	GLN
62	y	27	GLU
62	y	85	SER
62	y	114	LEU
63	z	18	LEU
63	z	51	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
9	9	103	ASN
11	AA	1236	ASN
18	G	18	HIS
22	K	70	ASN
35	X	105	ASN
58	u	4	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	A	75/76 (98%)	29 (38%)	6 (8%)
10	B	75/76 (98%)	35 (46%)	6 (8%)
15	D	1515/1542 (98%)	288 (19%)	35 (2%)
38	a	2859/2904 (98%)	532 (18%)	0
41	d	119/120 (99%)	17 (14%)	0
8	7	31/32 (96%)	21 (67%)	3 (9%)
All	All	4674/4750 (98%)	922 (19%)	50 (1%)

All (922) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	7	-9	G
8	7	-8	U
8	7	-7	U
8	7	-5	U
8	7	-4	U
8	7	-3	U
8	7	-2	U
8	7	-1	U
8	7	0	U

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Mol	Chain	Res	Type
8	7	1	U
8	7	2	U
8	7	3	U
8	7	4	U
8	7	5	U
8	7	6	U
8	7	7	G
8	7	8	A
8	7	9	U
8	7	10	U
8	7	12	G
8	7	13	G
10	A	2	G
10	A	6	G
10	A	7	G
10	A	8	U
10	A	10	G
10	A	13	C
10	A	14	A
10	A	15	G
10	A	16	C
10	A	17	C
10	A	18	G
10	A	19	G
10	A	20	U
10	A	21	A
10	A	22	G
10	A	23	C
10	A	46	G
10	A	47	U
10	A	48	C
10	A	49	G
10	A	52	G
10	A	57	A
10	A	58	A
10	A	59	A
10	A	61	C
10	A	66	C
10	A	69	C
10	A	71	C
10	A	73	A
10	B	2	G

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Mol	Chain	Res	Type
10	B	6	G
10	B	7	G
10	B	8	U
10	B	10	G
10	B	13	C
10	B	14	A
10	B	15	G
10	B	16	C
10	B	17	C
10	B	18	G
10	B	19	G
10	B	20	U
10	B	21	A
10	B	22	G
10	B	23	C
10	B	30	G
10	B	31	G
10	B	32	C
10	B	36	U
10	B	37	A
10	B	38	A
10	B	46	G
10	B	47	U
10	B	48	C
10	B	49	G
10	B	52	G
10	B	57	A
10	B	58	A
10	B	59	A
10	B	61	C
10	B	66	C
10	B	69	C
10	B	71	C
10	B	73	A
15	D	4	U
15	D	5	U
15	D	9	G
15	D	22	G
15	D	29	U
15	D	32	A
15	D	39	G
15	D	41	G

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Mol	Chain	Res	Type
15	D	47	C
15	D	48	C
15	D	50	A
15	D	51	A
15	D	52	C
15	D	54	C
15	D	69	G
15	D	70	U
15	D	71	A
15	D	72	A
15	D	74	A
15	D	76	G
15	D	82	G
15	D	83	C
15	D	84	U
15	D	87	C
15	D	90	C
15	D	94	G
15	D	95	C
15	D	96	U
15	D	108	G
15	D	120	A
15	D	122	G
15	D	128	G
15	D	131	A
15	D	141	G
15	D	144	G
15	D	148	G
15	D	149	A
15	D	160	A
15	D	164	G
15	D	173	U
15	D	181	A
15	D	182	A
15	D	197	A
15	D	198	G
15	D	204	G
15	D	208	U
15	D	209	U
15	D	210	C
15	D	211	G
15	D	212	G

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Mol	Chain	Res	Type
15	D	216	U
15	D	226	G
15	D	245	U
15	D	247	G
15	D	251	G
15	D	258	G
15	D	262	A
15	D	266	G
15	D	267	C
15	D	271	C
15	D	279	A
15	D	289	G
15	D	299	G
15	D	306	A
15	D	321	A
15	D	328	C
15	D	329	A
15	D	332	G
15	D	347	G
15	D	352	C
15	D	353	A
15	D	354	G
15	D	355	C
15	D	367	U
15	D	372	C
15	D	373	A
15	D	376	G
15	D	382	A
15	D	384	G
15	D	392	C
15	D	393	A
15	D	397	A
15	D	406	G
15	D	412	A
15	D	413	G
15	D	414	A
15	D	421	U
15	D	422	C
15	D	424	G
15	D	429	U
15	D	446	G
15	D	451	A

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Mol	Chain	Res	Type
15	D	457	G
15	D	458	U
15	D	460	A
15	D	463	U
15	D	464	U
15	D	467	U
15	D	468	A
15	D	469	C
15	D	478	A
15	D	479	U
15	D	481	G
15	D	484	G
15	D	485	U
15	D	486	U
15	D	505	G
15	D	509	A
15	D	511	C
15	D	518	C
15	D	519	C
15	D	526	C
15	D	531	U
15	D	532	A
15	D	533	A
15	D	542	G
15	D	547	A
15	D	559	A
15	D	562	U
15	D	568	G
15	D	572	A
15	D	573	A
15	D	576	C
15	D	577	G
15	D	579	A
15	D	596	A
15	D	628	G
15	D	633	G
15	D	642	A
15	D	649	A
15	D	650	G
15	D	653	U
15	D	665	A
15	D	666	G

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Mol	Chain	Res	Type
15	D	687	A
15	D	700	G
15	D	723	U
15	D	724	G
15	D	731	G
15	D	734	G
15	D	747	A
15	D	748	G
15	D	755	G
15	D	760	G
15	D	777	A
15	D	793	U
15	D	794	A
15	D	815	A
15	D	817	C
15	D	828	U
15	D	829	G
15	D	832	G
15	D	841	C
15	D	844	G
15	D	845	A
15	D	849	G
15	D	874	G
15	D	887	G
15	D	902	G
15	D	914	A
15	D	916	U
15	D	926	G
15	D	934	C
15	D	935	A
15	D	954	G
15	D	960	U
15	D	963	G
15	D	969	A
15	D	972	C
15	D	975	A
15	D	976	G
15	D	991	U
15	D	992	U
15	D	993	G
15	D	996	A
15	D	999	C

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Mol	Chain	Res	Type
15	D	1004	A
15	D	1008	U
15	D	1009	U
15	D	1017	U
15	D	1018	G
15	D	1021	A
15	D	1024	G
15	D	1026	G
15	D	1028	C
15	D	1030	U
15	D	1031	C
15	D	1037	C
15	D	1043	G
15	D	1044	A
15	D	1046	A
15	D	1065	U
15	D	1085	U
15	D	1086	U
15	D	1094	G
15	D	1095	U
15	D	1099	G
15	D	1101	A
15	D	1124	G
15	D	1133	G
15	D	1135	U
15	D	1136	C
15	D	1137	C
15	D	1139	G
15	D	1140	C
15	D	1141	C
15	D	1142	G
15	D	1143	G
15	D	1145	A
15	D	1146	A
15	D	1151	A
15	D	1152	A
15	D	1158	C
15	D	1159	U
15	D	1167	A
15	D	1171	A
15	D	1174	G
15	D	1175	G

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Mol	Chain	Res	Type
15	D	1176	A
15	D	1184	G
15	D	1196	A
15	D	1197	A
15	D	1206	G
15	D	1211	U
15	D	1212	U
15	D	1213	A
15	D	1214	C
15	D	1215	G
15	D	1226	C
15	D	1227	A
15	D	1228	C
15	D	1238	A
15	D	1256	A
15	D	1257	A
15	D	1260	G
15	D	1275	A
15	D	1276	G
15	D	1278	G
15	D	1279	G
15	D	1280	A
15	D	1285	A
15	D	1286	U
15	D	1287	A
15	D	1299	A
15	D	1300	G
15	D	1302	C
15	D	1305	G
15	D	1312	G
15	D	1317	C
15	D	1320	C
15	D	1323	G
15	D	1329	A
15	D	1338	G
15	D	1340	A
15	D	1346	A
15	D	1347	G
15	D	1353	G
15	D	1363	A
15	D	1370	G
15	D	1378	C

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Mol	Chain	Res	Type
15	D	1379	G
15	D	1381	U
15	D	1391	U
15	D	1396	A
15	D	1397	C
15	D	1398	A
15	D	1404	C
15	D	1419	G
15	D	1429	A
15	D	1441	A
15	D	1446	A
15	D	1447	A
15	D	1448	C
15	D	1452	C
15	D	1453	G
15	D	1475	G
15	D	1487	G
15	D	1492	A
15	D	1493	A
15	D	1494	G
15	D	1495	U
15	D	1497	G
15	D	1503	A
15	D	1506	U
15	D	1517	G
15	D	1529	G
15	D	1530	G
15	D	1534	A
38	a	10	A
38	a	15	G
38	a	34	U
38	a	35	G
38	a	46	G
38	a	58	G
38	a	60	G
38	a	63	A
38	a	71	A
38	a	74	A
38	a	75	G
38	a	83	A
38	a	84	A
38	a	85	G

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Mol	Chain	Res	Type
38	a	93	G
38	a	96	C
38	a	102	U
38	a	103	A
38	a	110	G
38	a	114	U
38	a	118	A
38	a	119	A
38	a	120	U
38	a	122	G
38	a	131	A
38	a	136	G
38	a	139	U
38	a	140	C
38	a	141	G
38	a	145	C
38	a	163	C
38	a	165	A
38	a	181	A
38	a	196	A
38	a	200	U
38	a	215	G
38	a	216	A
38	a	222	A
38	a	225	C
38	a	248	G
38	a	249	C
38	a	261	G
38	a	264	C
38	a	265	A
38	a	266	G
38	a	267	C
38	a	271	G
38	a	272	A
38	a	275	C
38	a	276	U
38	a	278	A
38	a	285	G
38	a	311	A
38	a	324	A
38	a	329	G
38	a	330	A

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Mol	Chain	Res	Type
38	a	353	C
38	a	359	G
38	a	361	G
38	a	362	A
38	a	371	A
38	a	372	G
38	a	373	U
38	a	375	G
38	a	383	C
38	a	386	G
38	a	396	G
38	a	405	U
38	a	411	G
38	a	412	A
38	a	420	C
38	a	424	G
38	a	435	C
38	a	451	U
38	a	456	C
38	a	457	A
38	a	477	A
38	a	481	G
38	a	491	G
38	a	501	A
38	a	503	A
38	a	504	A
38	a	505	A
38	a	509	C
38	a	522	A
38	a	529	A
38	a	532	A
38	a	543	G
38	a	546	U
38	a	547	A
38	a	548	G
38	a	549	G
38	a	551	G
38	a	563	A
38	a	569	U
38	a	573	U
38	a	575	A
38	a	588	U

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Mol	Chain	Res	Type
38	a	603	A
38	a	609	A
38	a	613	A
38	a	614	A
38	a	615	U
38	a	616	A
38	a	618	G
38	a	621	A
38	a	627	A
38	a	637	A
38	a	645	C
38	a	647	G
38	a	654	A
38	a	664	G
38	a	668	A
38	a	685	A
38	a	686	U
38	a	710	U
38	a	717	C
38	a	730	A
38	a	738	G
38	a	757	G
38	a	764	A
38	a	765	C
38	a	775	G
38	a	776	G
38	a	782	A
38	a	784	G
38	a	785	G
38	a	800	A
38	a	802	A
38	a	805	G
38	a	812	C
38	a	819	A
38	a	827	U
38	a	828	U
38	a	845	A
38	a	846	U
38	a	858	G
38	a	859	G
38	a	869	G
38	a	878	A

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Mol	Chain	Res	Type
38	a	881	G
38	a	884	U
38	a	885	C
38	a	888	C
38	a	891	G
38	a	892	A
38	a	893	C
38	a	895	U
38	a	896	A
38	a	897	C
38	a	899	A
38	a	907	G
38	a	910	A
38	a	914	G
38	a	915	C
38	a	931	U
38	a	941	A
38	a	945	A
38	a	946	C
38	a	953	G
38	a	961	C
38	a	974	G
38	a	983	A
38	a	995	C
38	a	996	A
38	a	999	U
38	a	1005	C
38	a	1012	U
38	a	1013	C
38	a	1022	G
38	a	1023	U
38	a	1026	G
38	a	1033	U
38	a	1041	G
38	a	1045	C
38	a	1046	A
38	a	1047	G
38	a	1060	U
38	a	1061	U
38	a	1062	G
38	a	1063	G
38	a	1064	C

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Mol	Chain	Res	Type
38	a	1065	U
38	a	1066	U
38	a	1067	A
38	a	1068	G
38	a	1069	A
38	a	1070	A
38	a	1071	G
38	a	1073	A
38	a	1074	G
38	a	1076	C
38	a	1079	C
38	a	1080	A
38	a	1081	U
38	a	1082	U
38	a	1083	U
38	a	1084	A
38	a	1087	G
38	a	1088	A
38	a	1090	A
38	a	1095	A
38	a	1096	A
38	a	1107	G
38	a	1110	G
38	a	1111	A
38	a	1112	G
38	a	1119	U
38	a	1122	G
38	a	1132	U
38	a	1134	A
38	a	1135	C
38	a	1142	A
38	a	1169	A
38	a	1170	C
38	a	1173	U
38	a	1174	U
38	a	1175	A
38	a	1176	U
38	a	1177	G
38	a	1178	C
38	a	1179	G
38	a	1180	U
38	a	1186	G

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Mol	Chain	Res	Type
38	a	1238	G
38	a	1248	G
38	a	1253	A
38	a	1256	G
38	a	1266	G
38	a	1271	G
38	a	1272	A
38	a	1273	U
38	a	1301	A
38	a	1321	A
38	a	1345	C
38	a	1352	U
38	a	1365	A
38	a	1368	G
38	a	1378	A
38	a	1379	U
38	a	1380	G
38	a	1383	A
38	a	1387	A
38	a	1392	A
38	a	1395	A
38	a	1406	U
38	a	1407	G
38	a	1408	G
38	a	1411	U
38	a	1414	C
38	a	1415	U
38	a	1416	G
38	a	1417	C
38	a	1419	A
38	a	1420	A
38	a	1428	C
38	a	1452	G
38	a	1453	A
38	a	1460	U
38	a	1478	G
38	a	1482	G
38	a	1490	A
38	a	1497	U
38	a	1503	A
38	a	1508	A
38	a	1509	A

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Mol	Chain	Res	Type
38	a	1510	G
38	a	1515	A
38	a	1529	G
38	a	1534	U
38	a	1535	A
38	a	1536	C
38	a	1537	G
38	a	1554	U
38	a	1559	U
38	a	1566	A
38	a	1569	A
38	a	1578	U
38	a	1580	A
38	a	1581	G
38	a	1582	C
38	a	1583	A
38	a	1584	U
38	a	1589	U
38	a	1590	A
38	a	1608	A
38	a	1609	A
38	a	1610	A
38	a	1647	U
38	a	1648	U
38	a	1649	G
38	a	1651	G
38	a	1674	G
38	a	1677	A
38	a	1703	G
38	a	1714	U
38	a	1715	G
38	a	1718	G
38	a	1729	U
38	a	1730	C
38	a	1732	C
38	a	1738	G
38	a	1750	G
38	a	1755	A
38	a	1758	U
38	a	1764	C
38	a	1773	A
38	a	1791	A

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Mol	Chain	Res	Type
38	a	1800	C
38	a	1801	A
38	a	1808	A
38	a	1811	G
38	a	1816	C
38	a	1829	A
38	a	1833	C
38	a	1847	A
38	a	1848	A
38	a	1858	A
38	a	1859	U
38	a	1862	G
38	a	1864	U
38	a	1869	G
38	a	1870	C
38	a	1872	A
38	a	1873	G
38	a	1905	C
38	a	1906	G
38	a	1907	G
38	a	1913	A
38	a	1914	C
38	a	1919	A
38	a	1920	C
38	a	1922	G
38	a	1923	U
38	a	1924	C
38	a	1925	C
38	a	1926	U
38	a	1928	A
38	a	1929	G
38	a	1930	G
38	a	1936	A
38	a	1938	A
38	a	1955	U
38	a	1965	C
38	a	1967	C
38	a	1970	A
38	a	1971	U
38	a	1972	G
38	a	1987	A
38	a	1991	U

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Mol	Chain	Res	Type
38	a	1992	G
38	a	1993	U
38	a	1997	C
38	a	2002	G
38	a	2022	U
38	a	2023	C
38	a	2027	G
38	a	2033	A
38	a	2043	C
38	a	2051	A
38	a	2052	A
38	a	2055	C
38	a	2056	G
38	a	2060	A
38	a	2061	G
38	a	2062	A
38	a	2077	A
38	a	2097	A
38	a	2099	U
38	a	2100	G
38	a	2108	A
38	a	2110	G
38	a	2111	U
38	a	2113	U
38	a	2115	G
38	a	2116	G
38	a	2117	A
38	a	2118	U
38	a	2121	G
38	a	2122	U
38	a	2124	G
38	a	2125	G
38	a	2126	A
38	a	2127	G
38	a	2128	G
38	a	2131	U
38	a	2132	U
38	a	2133	G
38	a	2134	A
38	a	2139	U
38	a	2141	G
38	a	2146	C

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Mol	Chain	Res	Type
38	a	2147	A
38	a	2154	A
38	a	2157	G
38	a	2158	A
38	a	2159	G
38	a	2162	G
38	a	2163	A
38	a	2164	C
38	a	2165	C
38	a	2169	A
38	a	2171	A
38	a	2172	U
38	a	2178	C
38	a	2182	U
38	a	2183	A
38	a	2185	U
38	a	2188	U
38	a	2189	U
38	a	2190	G
38	a	2191	A
38	a	2193	G
38	a	2194	U
38	a	2198	A
38	a	2204	G
38	a	2210	U
38	a	2211	A
38	a	2212	A
38	a	2213	U
38	a	2225	A
38	a	2226	C
38	a	2229	U
38	a	2238	G
38	a	2239	G
38	a	2244	U
38	a	2250	G
38	a	2268	A
38	a	2278	A
38	a	2283	C
38	a	2287	A
38	a	2297	A
38	a	2305	U
38	a	2308	G

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Mol	Chain	Res	Type
38	a	2309	A
38	a	2315	G
38	a	2322	A
38	a	2325	G
38	a	2327	A
38	a	2333	A
38	a	2339	C
38	a	2345	G
38	a	2347	C
38	a	2350	C
38	a	2361	G
38	a	2372	U
38	a	2376	A
38	a	2383	G
38	a	2385	C
38	a	2402	U
38	a	2403	C
38	a	2406	A
38	a	2423	U
38	a	2424	C
38	a	2425	A
38	a	2426	A
38	a	2429	G
38	a	2430	A
38	a	2431	U
38	a	2434	A
38	a	2435	A
38	a	2441	U
38	a	2447	G
38	a	2448	A
38	a	2470	G
38	a	2474	U
38	a	2476	A
38	a	2478	A
38	a	2484	G
38	a	2491	U
38	a	2502	G
38	a	2506	U
38	a	2507	C
38	a	2512	C
38	a	2513	A
38	a	2518	A

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Mol	Chain	Res	Type
38	a	2520	C
38	a	2525	G
38	a	2529	G
38	a	2535	G
38	a	2547	A
38	a	2554	U
38	a	2566	A
38	a	2567	G
38	a	2572	A
38	a	2573	C
38	a	2574	G
38	a	2585	U
38	a	2586	U
38	a	2602	A
38	a	2603	G
38	a	2609	U
38	a	2610	C
38	a	2611	C
38	a	2613	U
38	a	2629	U
38	a	2663	G
38	a	2669	G
38	a	2671	G
38	a	2689	U
38	a	2690	U
38	a	2714	G
38	a	2722	G
38	a	2726	A
38	a	2744	G
38	a	2748	A
38	a	2757	A
38	a	2758	A
38	a	2765	A
38	a	2777	G
38	a	2778	A
38	a	2791	G
38	a	2793	C
38	a	2796	U
38	a	2797	U
38	a	2798	U
38	a	2799	A
38	a	2801	G

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Mol	Chain	Res	Type
38	a	2818	U
38	a	2820	A
38	a	2823	A
38	a	2825	G
38	a	2849	U
38	a	2850	A
38	a	2859	G
38	a	2861	U
38	a	2867	G
38	a	2880	C
38	a	2884	U
38	a	2885	G
38	a	2891	U
38	a	2902	C
41	d	2	G
41	d	9	G
41	d	13	G
41	d	16	G
41	d	17	C
41	d	35	C
41	d	36	C
41	d	45	A
41	d	51	G
41	d	56	G
41	d	64	G
41	d	66	A
41	d	88	C
41	d	89	U
41	d	90	C
41	d	99	A
41	d	109	A

All (50) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	7	-8	U
8	7	-5	U
8	7	-3	U
10	A	6	G
10	A	7	G
10	A	9	G
10	A	22	G

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Mol	Chain	Res	Type
10	A	60	U
10	A	70	G
10	B	6	G
10	B	7	G
10	B	9	G
10	B	22	G
10	B	37	A
10	B	60	U
15	D	7	A
15	D	70	U
15	D	121	U
15	D	181	A
15	D	183	C
15	D	197	A
15	D	209	U
15	D	305	G
15	D	328	C
15	D	428	G
15	D	496	A
15	D	517	G
15	D	531	U
15	D	532	A
15	D	562	U
15	D	641	U
15	D	722	G
15	D	793	U
15	D	991	U
15	D	992	U
15	D	1109	C
15	D	1145	A
15	D	1196	A
15	D	1211	U
15	D	1212	U
15	D	1213	A
15	D	1214	C
15	D	1225	A
15	D	1299	A
15	D	1396	A
15	D	1432	G
15	D	1447	A
15	D	1491	G
15	D	1492	A

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Mol	Chain	Res	Type
15	D	1493	A

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 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

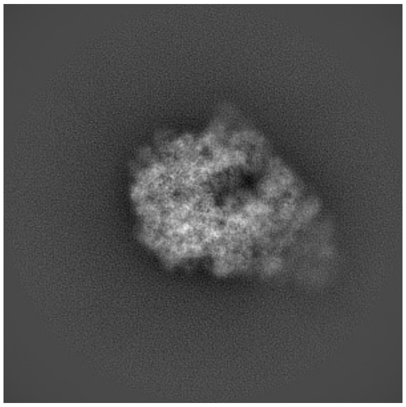
6 Map visualisation

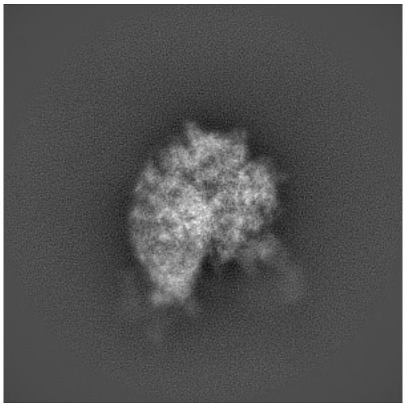
This section contains visualisations of the EMDB entry EMD-21494. These allow visual inspection of the internal detail of the map and identification of artifacts.

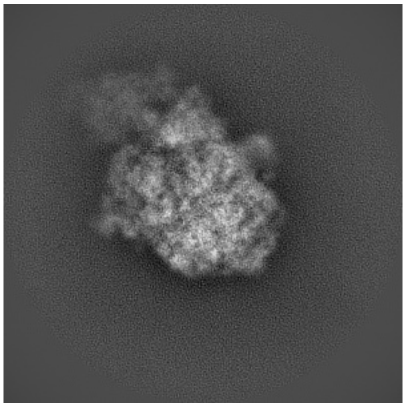
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

6.1.1 Primary map


X

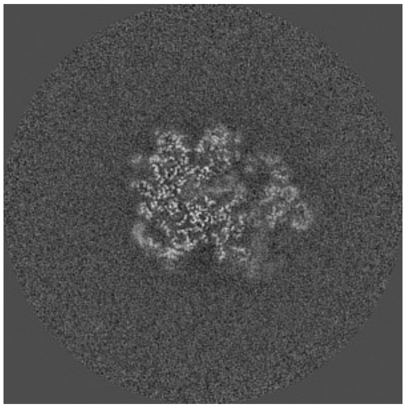

Y

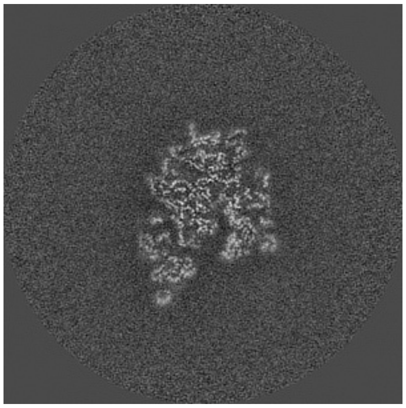

Z

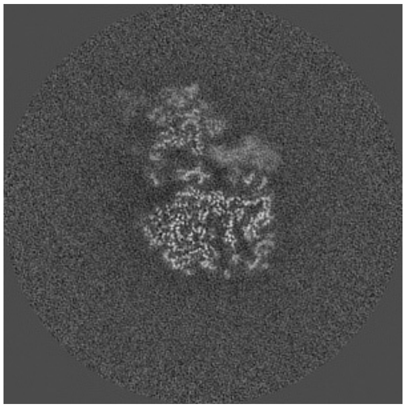
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map


X Index: 256

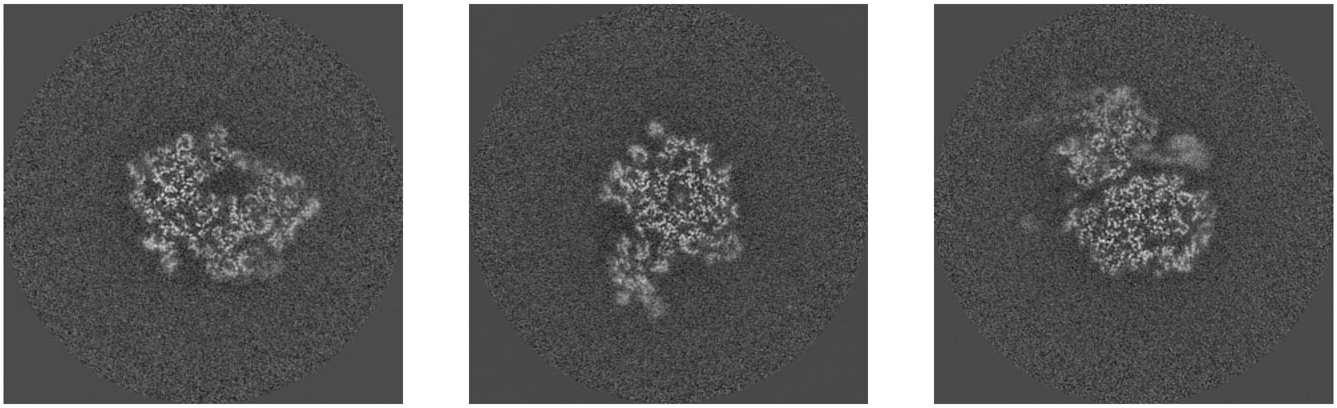

Y Index: 256


Z Index: 256

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

6.3 Largest variance slices ⓘ

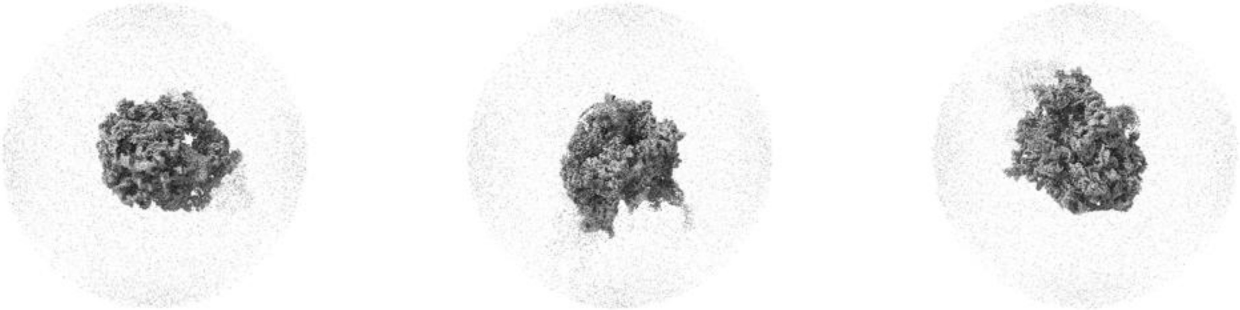
6.3.1 Primary map


X Index: 240 Y Index: 231 Z Index: 248

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

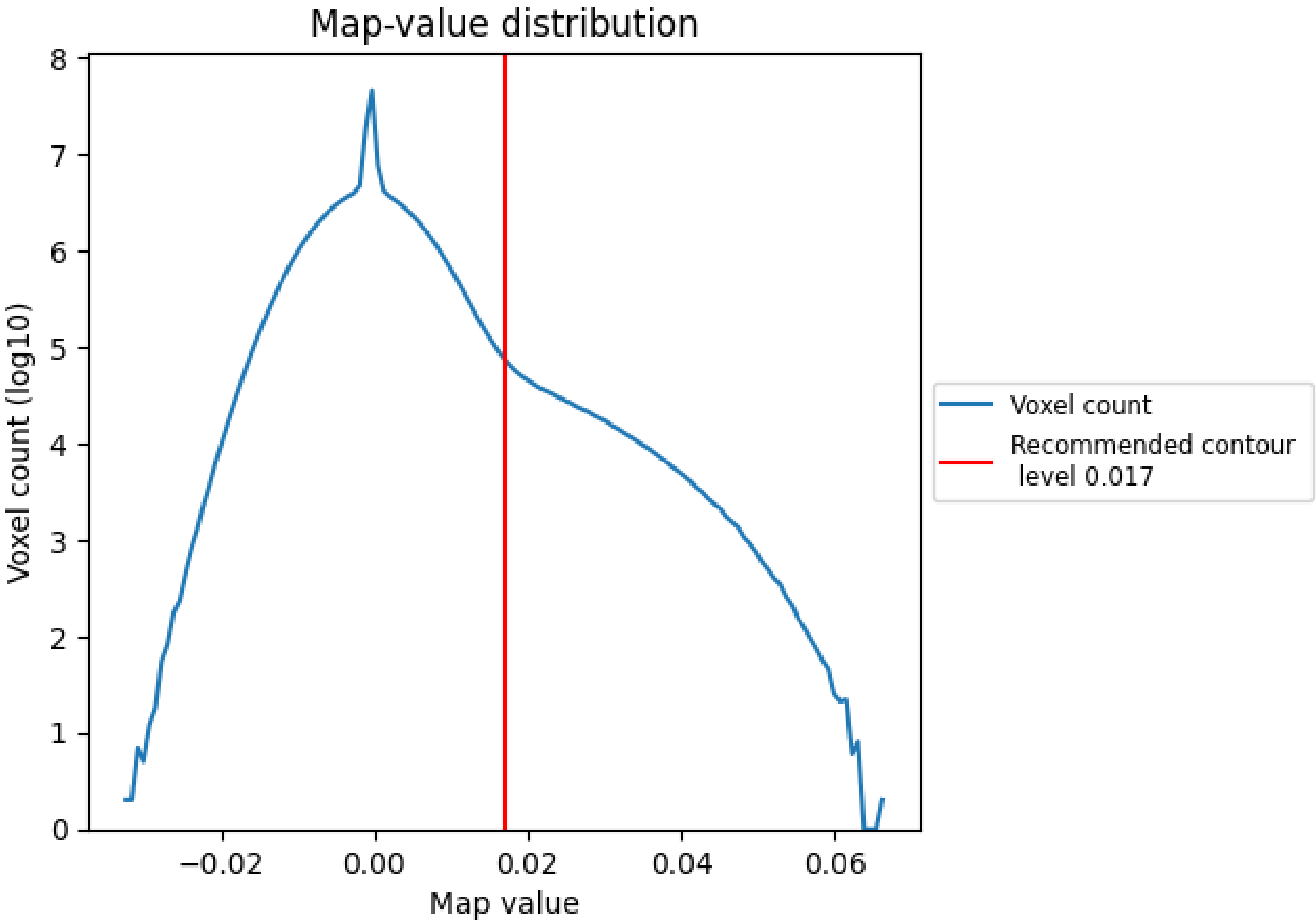
6.5 Mask visualisation ⓘ

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

7 Map analysis ⓘ

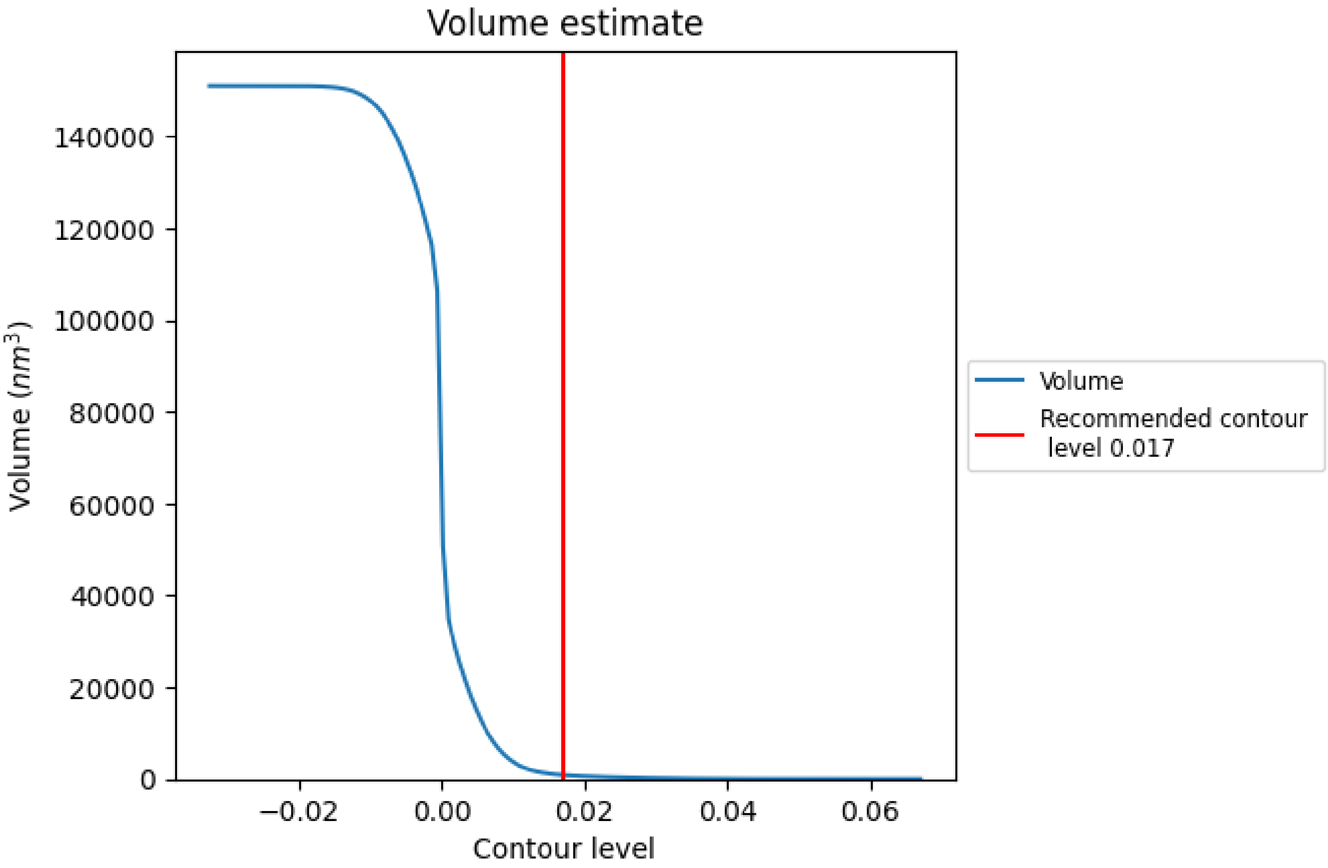
This section contains the results of statistical analysis of the map.

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.

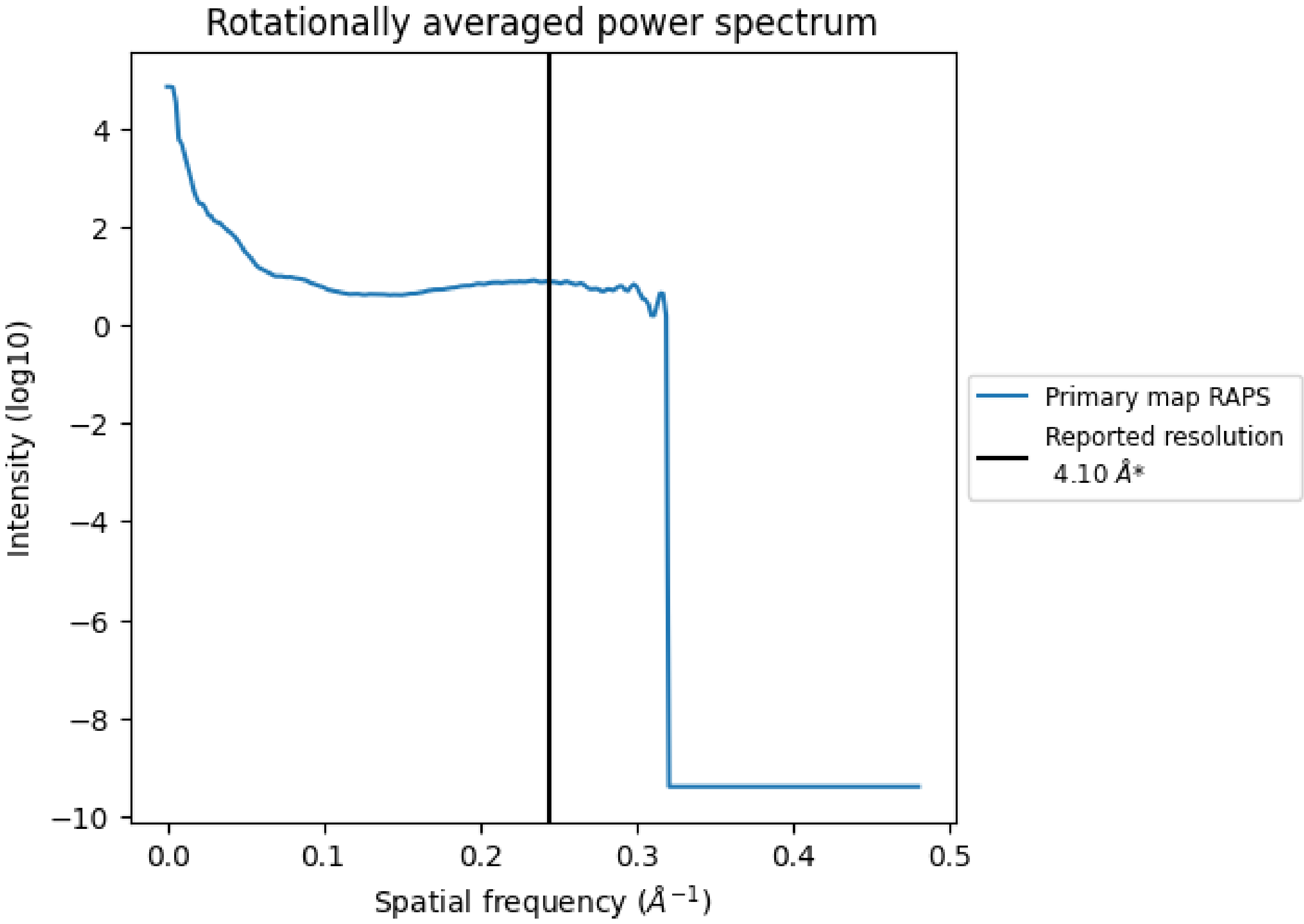
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 887 nm^3; this corresponds to an approximate mass of 801 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 0.244 $Å^{-1}$

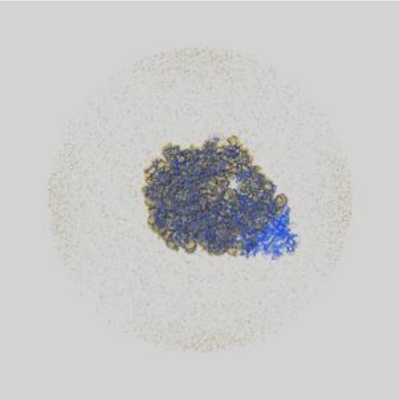
8 Fourier-Shell correlation ⓘ

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

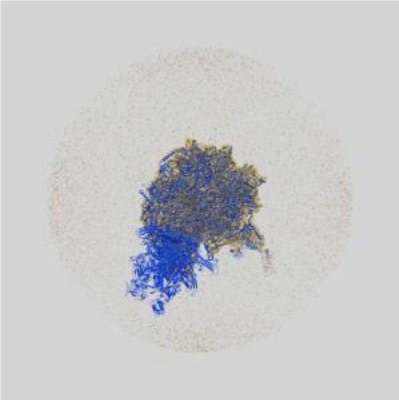
9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-21494 and PDB model 6VZJ. Per-residue inclusion information can be found in section 3 on page 16.

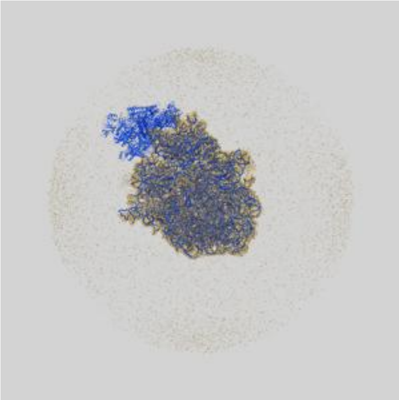
9.1 Map-model overlay ⓘ



X



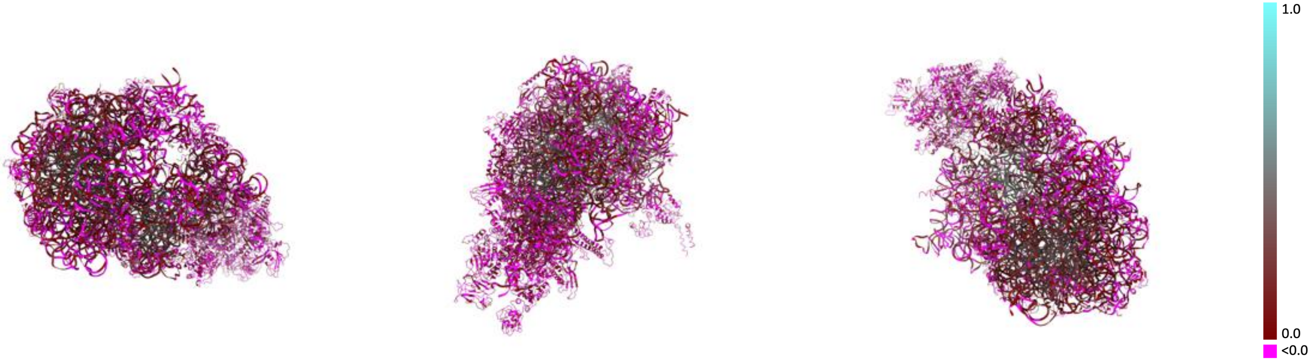
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.017 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

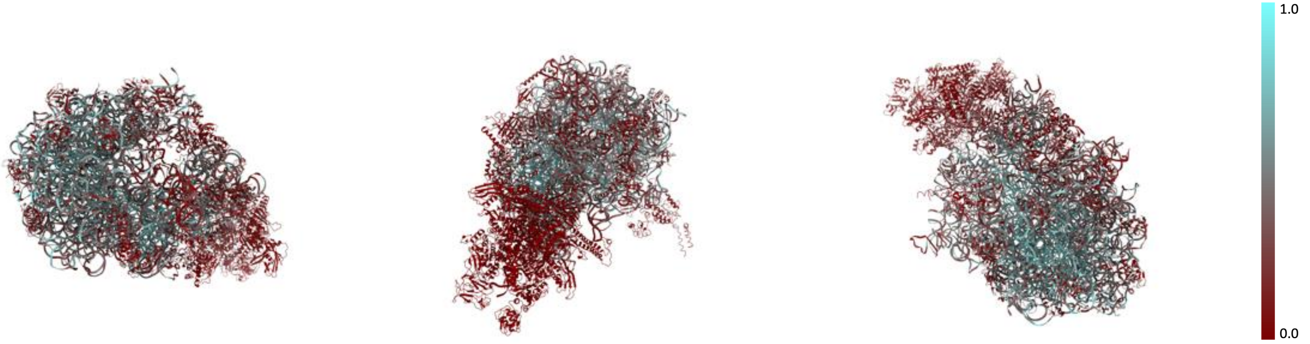
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

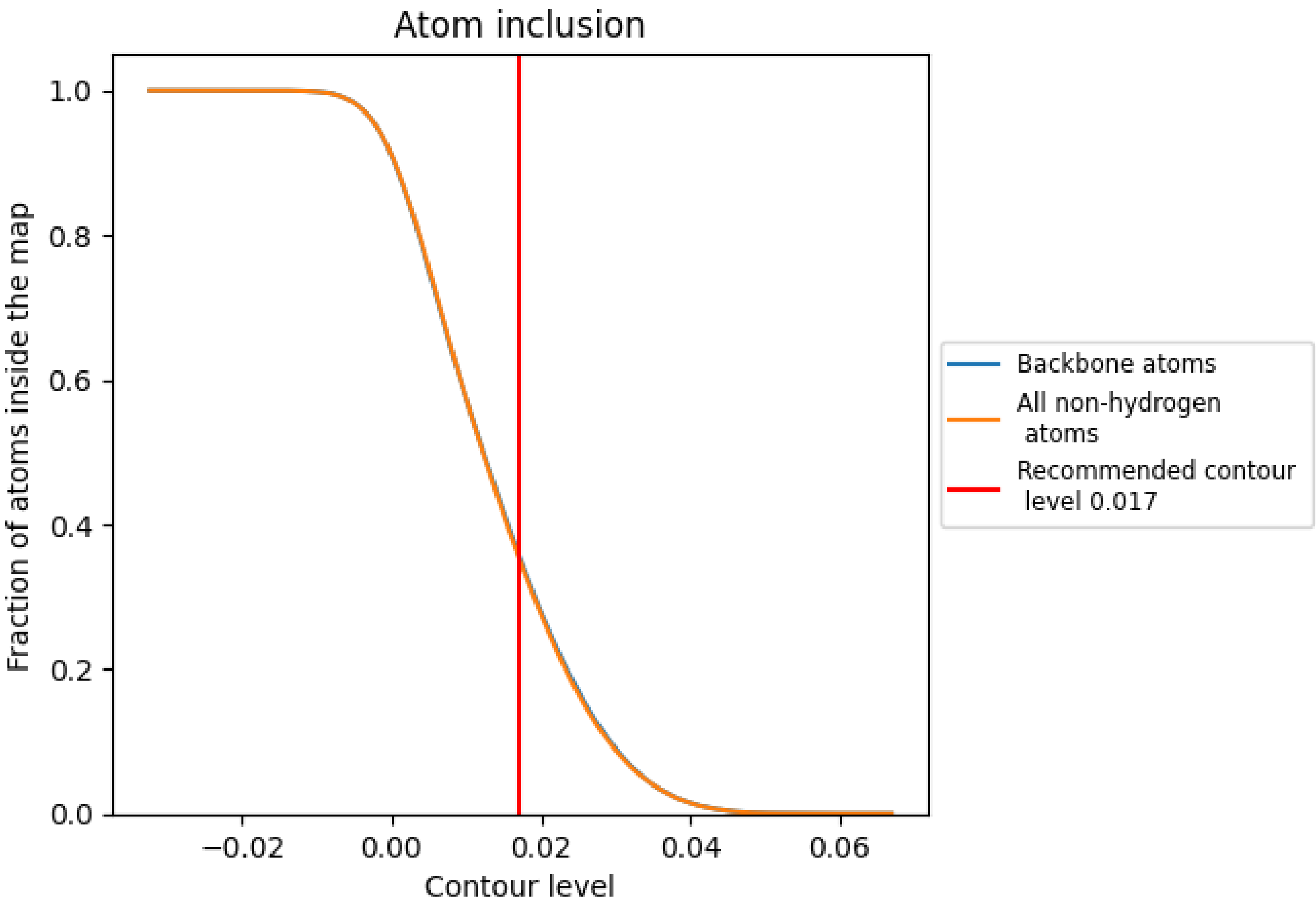
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.017).

9.4 Atom inclusion ⓘ



At the recommended contour level, 36% of all backbone atoms, 36% 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 (0.017) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3561	0.1230
0	0.3225	0.1140
1	0.4282	0.2450
2	0.2507	0.0600
3	0.2307	0.0170
4	0.2575	0.0510
5	0.0021	-0.0050
6	0.0055	0.0520
7	0.0134	0.0190
9	0.0695	0.0020
A	0.1765	0.0960
AA	0.0017	0.0230
AC	0.0017	0.0180
AD	0.0012	0.0130
AE	0.0022	0.0180
B	0.1265	0.0350
C	0.2409	0.0790
D	0.5257	0.1880
E	0.2125	0.0040
F	0.2200	0.1780
G	0.2308	0.1020
H	0.0082	0.0140
I	0.2082	0.1290
J	0.2270	0.1030
K	0.4115	0.2670
L	0.1620	0.0260
M	0.1897	0.1040
N	0.3250	0.1810
O	0.2002	0.0480
P	0.2026	0.0890
Q	0.2474	0.1310
R	0.4365	0.3000
S	0.2183	0.0610
T	0.3145	0.1390
U	0.1467	-0.0110

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Chain	Atom inclusion	Q-score
V	0.2769	0.1500
W	0.0912	0.0010
X	0.1417	-0.0100
Y	0.0440	-0.0160
Z	0.0132	-0.0140
a	0.5301	0.1630
b	0.2332	0.0450
c	0.2745	0.0890
d	0.4496	0.0400
e	0.2495	0.0100
f	0.3326	0.1300
g	0.0959	-0.0160
h	0.3070	0.1140
i	0.4579	0.2290
j	0.3758	0.1720
k	0.1794	-0.0210
l	0.2704	0.0700
m	0.4845	0.2710
n	0.1682	0.0010
o	0.2444	0.0650
p	0.1911	0.0070
q	0.3185	0.1040
r	0.0766	-0.0010
s	0.3691	0.1680
t	0.3702	0.2120
u	0.2881	0.0750
v	0.3426	0.1570
w	0.3976	0.1670
x	0.1889	-0.0690
y	0.2613	0.1010
z	0.4504	0.2090