Full wwPDB EM Validation Report (i)

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 (i) symbol.

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

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

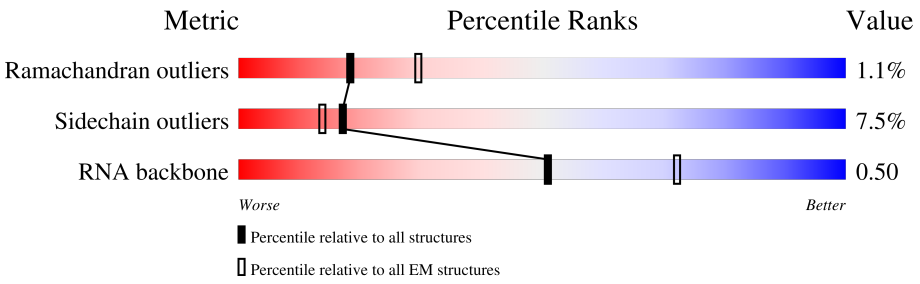
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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	65%; 93%; 7%
2	1	110	44%; 92%; 8%
3	2	100	78%; 89%; 5%; 6%
4	3	104	76%; 91%; 8%; •
5	4	94	77%; 96%; •
6	5	36	64%; 47%; 17%; 36%
7	6	36	75%; 64%; 11%; 25%
8	7	32	100%; 25%; 72%; •

Continued on next page...

Continued from previous page...

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%

Continued on next page...

Continued from previous page...

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%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
57	t	123	53% 95% 5%
58	u	144	71% 96% .
59	v	136	67% 96% .
60	w	119	56% 93% 7%
61	x	116	83% 95% 5%
62	y	114	81% 96% .
63	z	117	43% 97% .

2 Entry composition (i)

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
			Total	C	H	N	O	P		
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

Continued on next page...

Continued from previous page...

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
			Total	C	H	N	O	S		
46	i	56	903	269	459	94	80	1	0	0

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

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

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

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

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

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

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

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

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

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

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

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

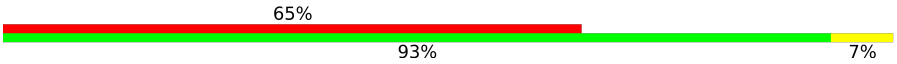
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
65	AE	2	2	2	0

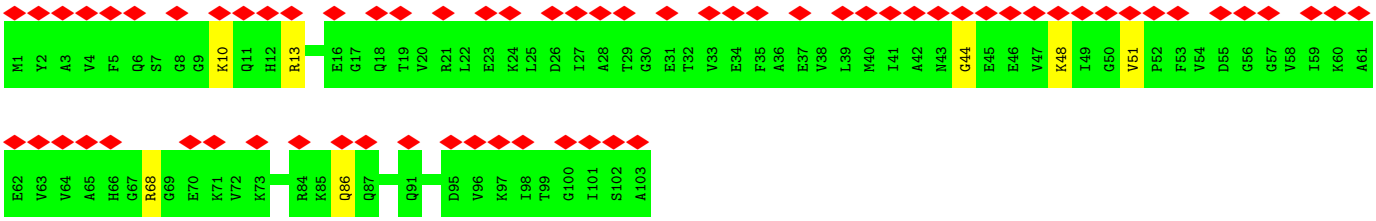
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 50S ribosomal protein L21

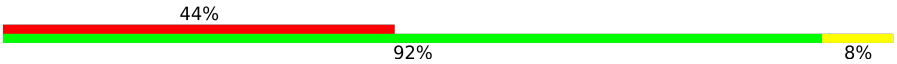
Chain 0:

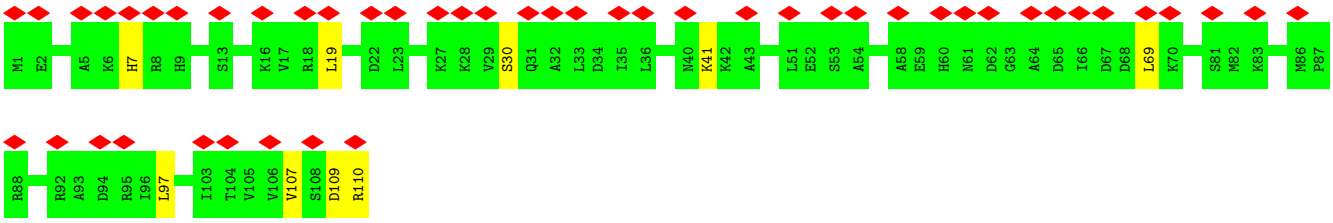




- Molecule 2: 50S ribosomal protein L22

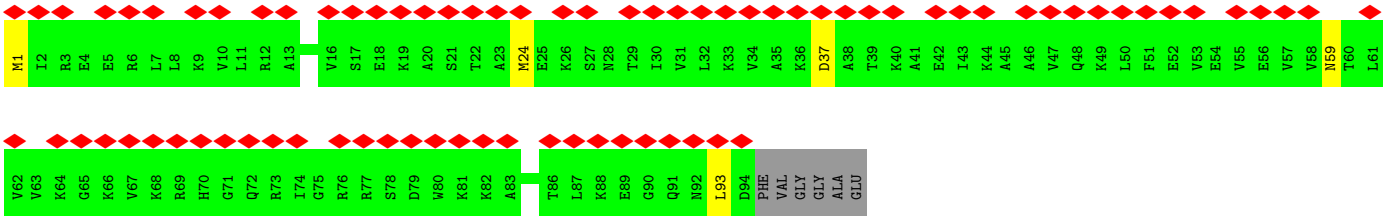
Chain 1:





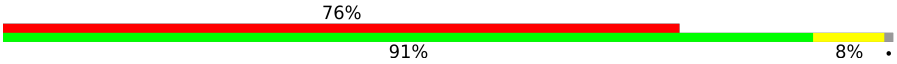
- Molecule 3: 50S ribosomal protein L23

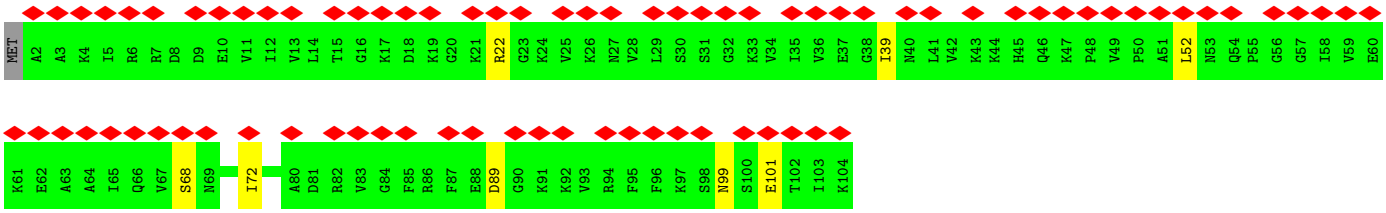
Chain 2:



- Molecule 4: 50S ribosomal protein L24

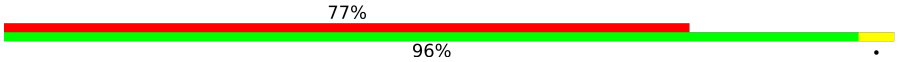
Chain 3:

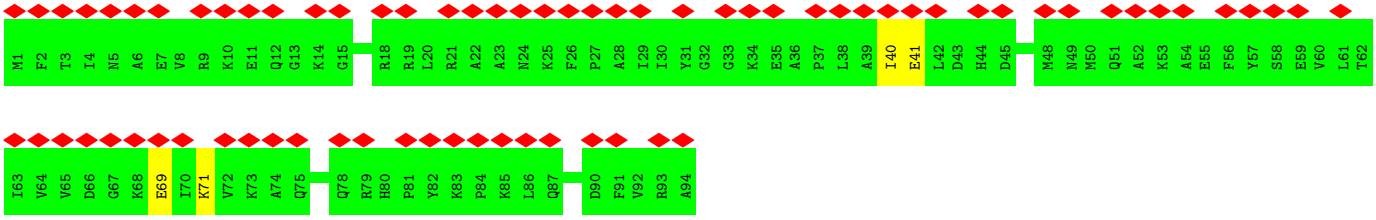




- Molecule 5: 50S ribosomal protein L25

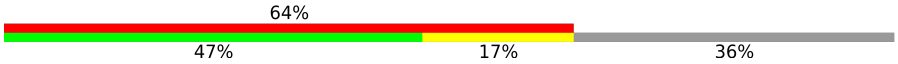
Chain 4:

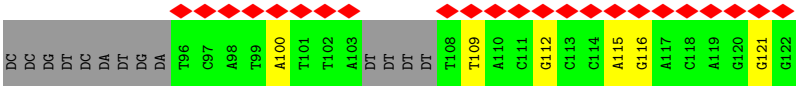




- Molecule 6: NT DNA

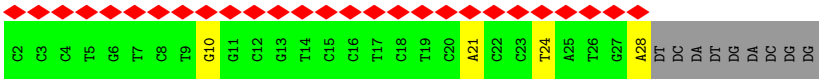
Chain 5:





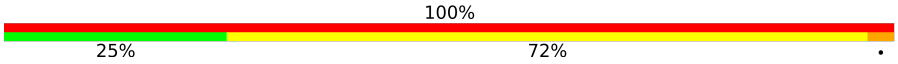
- Molecule 7: T DNA

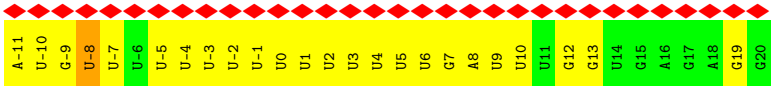
Chain 6:



- Molecule 8: mRNA with 27 nt long spacer

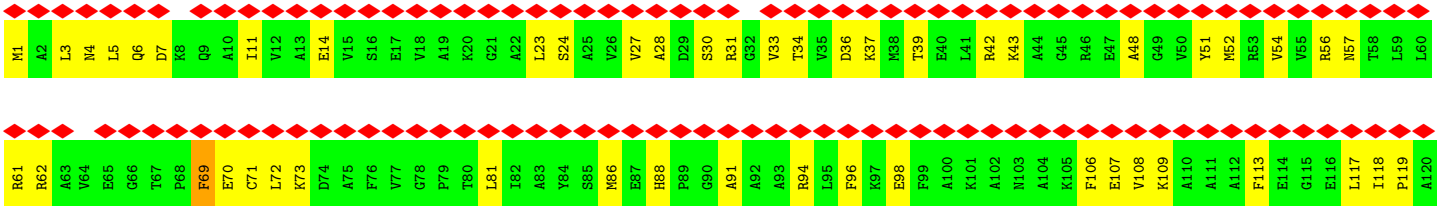
Chain 7:

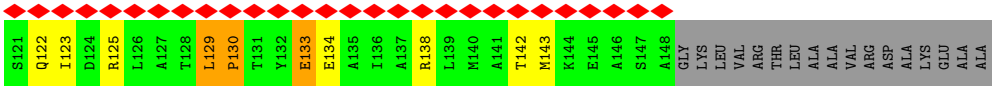




- Molecule 9: 50S ribosomal protein L10

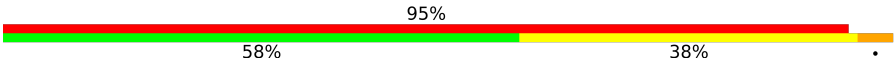
Chain 9:

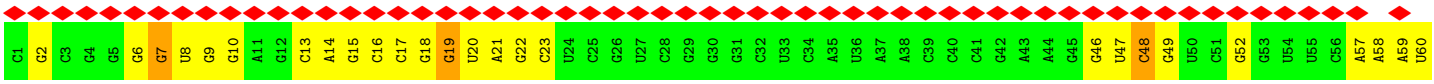


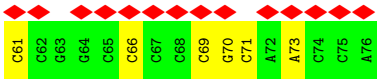


- Molecule 10: E-site and P-site tRNA (fMet)

Chain A:

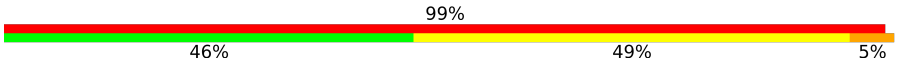


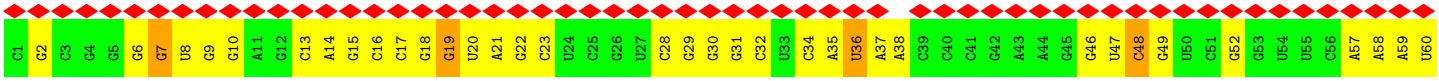


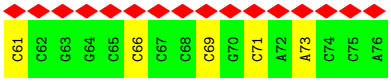


- Molecule 10: E-site and P-site tRNA (fMet)

Chain B:

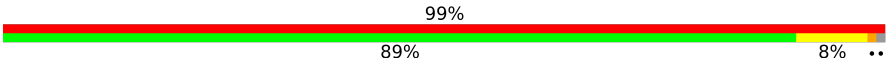


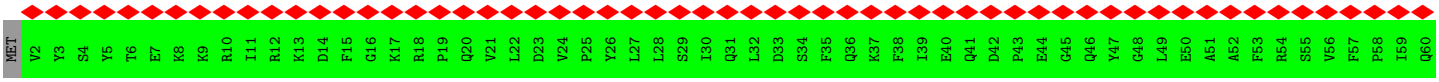


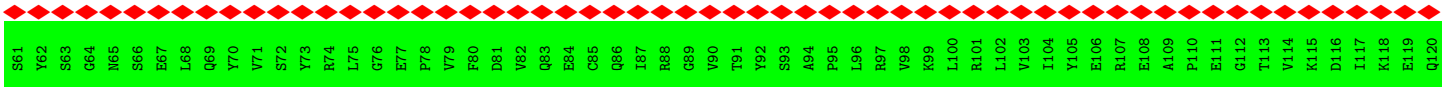


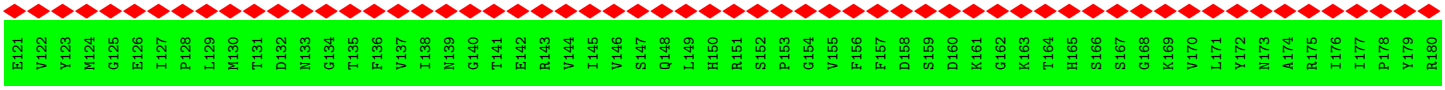
- Molecule 11: DNA-directed RNA polymerase subunit beta

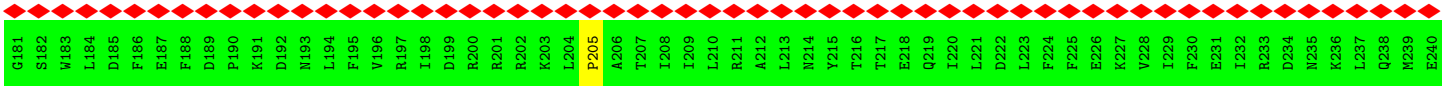
Chain AA:

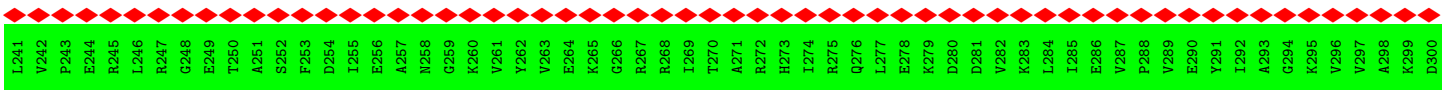


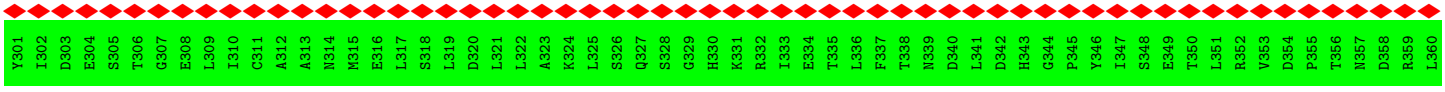












S361 A362 L363 V364 E365 I366 Y367 R368 M369 M370 R371 P372 G373 E374 P375 P376 T377 R378 E379 A380 A381 E382 S383 L384 F385 E386 N387 L388 F389 F390 S391 E392 D393 R394 Y395 D396 L397 S398 A399 V400 G401 R402 M403 K404 F405 N406 R407 S408 L409 L410 R411 E412 E413 I414 E415 G416 S417 G418 I419 L420

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 T748 D749 I750 V751 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

D781 V782 L783 A784 D785 G786 P787 S788 T789 D790 L791 G792 E793 L794 A795 L796 G797 Q798 N799 M800 R801 V802 A803 F804 M805 P806 W807 N808 G809 Y810 N811 F812 E813 D814 S815 I816 L817 V818 S819 E820 R821 V822 V823 Q824 E825 D826 R827 F828 T829 T830 I831 H832 I833 Q834 E835 L836 A837 C838 V839 S840

R841 D842 T843 K844 L845 G846 P847 E848 E849 I850 T851 A852 D853 I854 P855 N856 V857 G858 E859 A860 A861 L862 S863 K864 L865 D866 E867 S868 G869 I870 V871 Y872 I873 G874 A875 E876 V877 T878 G879 G880 D881 I882 L883 V884 G885 K886 V887 T888 P889 K890 G891 GLU THR GLN LEU THR PRO GLU GLU LYS

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

L1021 K1022 H1023 E1024 F1025 E1026 K1027 K1028 L1029 E1030 A1031 K1032 R1033 R1034 K1035 I1036 T1037 Q1038 G1039 D1040 D1041 L1042 A1043 P1044 G1045 V1046 L1047 K1048 I1049 V1050 K1051 V1052 Y1053 L1054 A1055 V1056 K1057 R1058 R1059 I1060 Q1061 P1062 G1063 D1064 K1065 M1066 A1067 G1068 R1069 H1070 G1071 N1072 K1073 G1074 V1075 I1076 S1077 K1078 I1079 N1080

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

L1141 R1142 E1143 F1144 I1145 Q1146 R1147 A1148 Y1149 D1150 L1151 G1152 A1153 D1154 V1155 R1156 Q1157 K1158 V1159 D1160 L1161 S1162 T1163 F1164 S1165 D1166 E1167 E1168 V1169 M1170 R1171 L1172 A1173 E1174 N1175 L1176 R1177 K1178 G1179 M1180 P1181 I1182 A1183 T1184 P1185 V1186 F1187 D1188 G1189 A1190 K1191 E1192 A1193 E1194 I1195 K1196 E1197 L1198 L1199 K1200

L1201 G1202 D1203 L1204 P1205 T1206 S1207 G1208 Q1209 I1210 R1211 L1212 Y1213 D1214 G1215 R1216 T1217 G1218 E1219 Q1220 F1221 E1222 R1223 P1224 V1225 T1226 V1227 G1228 Y1229 M1230 Y1231 M1232 L1233 K1234 L1235 N1236 H1237 L1238 V1239 D1240 D1241 K1242 M1243 H1244 A1245 R1246 S1247 T1248 G1249 S1250 Y1251 S1252 L1253 V1254 T1255 Q1256 Q1257 P1258 L1259 G1260

G1261 K1262 A1263 Q1264 F1265 G1266 G1267 Q1268 R1269 F1270 G1271 E1272 M1273 E1274 V1275 W1276 A1277 L1278 E1279 A1280 Y1281 G1282 A1283 A1284 Y1285 T1286 L1287 Q1288 E1289 M1290 L1291 T1292 V1293 K1294 S1295 D1296 D1297 V1298 N1299 G1300 R1301 T1302 K1303 M1304 Y1305 K1306 N1307 I1308 V1309 D1310 G1311 N1312 H1313 Q1314 M1315 E1316 P1317 G1318 M1319 P1320

E1321 S1322 F1323 N1324 V1325 L1326 L1327 K1328 E1329 I1330 R1331 S1332 L1333 G1334 I1335 N1336 I1337 E1338 L1339 E1340 D1341 E1342

- Molecule 12: DNA-directed RNA polymerase subunit alpha

Chain AC: 70% 64% 5% 30%

MET GLN GLY SER VAL T6 E7 F8 L9 K10 P11 R12 L13 V14 D15 I16 E17 Q18 V19 S20 S21 T22 H23 A24 K25 V26 T27 L28 E29 P30 L31 E32 R33 G34 F35 G36 H37 T38 L39 G40 N41 A42 L43 R44 R45 I46 L47 L48 S49 S50 M51 P52 G53 C54 A55 V56 T57 E58 V59 E60

I61 D62 G63 V64 L65 H66 E67 Y68 S69 T70 K71 E72 G73 V74 Q75 E76 D77 I78 L79 E80 I81 L82 L83 N84 L85 K86 G87 L88 A89 V90 R91 V92 Q93 G94 K95 D96 E97 V98 I99 L100 T101 L102 N103 K104 S105 G106 I107 G108 P109 V110 T111 A112 A113 D114 I115 T116 H117 D118 G119 D120

V121 E122 I123 V124 K125 P126 Q127 H128 V129 I130 C131 H132 L133 T134 D135 E136 N137 A138 S139 I140 S141 M142 R143 I144 K145 V146 Q147 R148 G149 R150 G151 Y152 V153 P154 A155 S156 T157 R158 I159 H160 S161 E162 E163 D164 E165 R166 P167 I168 G169 R170 L171 L172 V173 D174 A175 C176 Y177 S178 P179 V180

E181 R182 I183 A184 Y185 N186 V187 E188 A189 A190 R191 V192 E193 Q194 R195 T196 D197 L198 D199 K200 L201 V202 I203 E204 M205 E206 T207 N208 G209 T210 I211 D212 P213 E214 E215 A216 I217 R218 R219 A220 A221 T222 I223 L224 A225 E226 Q227 L228 E229 A230 F231 V232 D233 L234 R235 ASP VAL ARG GLN PRO

GLU VAL LYS GLU GLU LYS PRO GLU PHE ASP PRO ILE LEU LEU ARG PRO VAL ASP ASP LEU GLU LEU THR VAL ARG SER ALA ASN CYS LEU LYS ALA GLU ALA ILE HIS TYR ILE GLY ASP LEU VAL GLN ARG THR GLU VAL GLU LEU LEU LYS THR PRO ASN LEU GLY LYS LYS SER LEU

THR GLU ILE LYS ASP VAL LEU ALA SER ARG GLY LEU SER LEU GLY MET ARG LEU GLU ASN TRP PRO PRO ALA SER ILE ALA ASP GLU

- Molecule 12: DNA-directed RNA polymerase subunit alpha

Chain AD: 69% 69% 31%

MET GLN GLY SER VAL T6 E7 F8 L9 K10 P11 R12 L13 V14 D15 I16 E17 Q18 V19 S20 S21 T22 H23 A24 K25 V26 T27 L28 E29 P30 L31 E32 R33 G34 F35 G36 H37 T38 L39 G40 N41 A42 L43 R44 R45 I46 L47 L48 S49 S50 M51 P52 G53 C54 A55 V56 T57 E58 V59 E60

I61 D62 G63 V64 L65 H66 E67 Y68 S69 T70 K71 E72 G73 V74 Q75 E76 D77 I78 L79 E80 I81 L82 L83 N84 L85 K86 G87 L88 A89 V90 R91 V92 Q93 G94 K95 D96 E97 V98 I99 L100 T101 L102 N103 K104 S105 G106 I107 G108 P109 V110 T111 A112 A113 D114 I115 T116 H117 D118 G119 D120

V121 E122 I123 V124 K125 P126 Q127 H128 V129 I130 C131 H132 L133 T134 D135 E136 N137 A138 S139 I140 S141 M142 R143 I144 K145 V146 Q147 R148 G149 R150 G151 Y152 V153 P154 A155 S156 T157 R158 I159 H160 S161 E162 E163 D164 E165 R166 P167 I168 G169 R170 L171 L172 V173 D174 A175 C176 Y177 S178 P179 V180

E181 R182 I183 A184 Y185 N186 V187 E188 A189 A190 R191 V192 E193 Q194 R195 T196 D197 L198 D199 K200 L201 V202 I203 E204 M205 E206 T207 N208 G209 T210 I211 D212 P213 E214 E215 A216 I217 R218 R219 A220 A221 T222 I223 L224 A225 E226 Q227 L228 E229 A230 F231 V232 D233 LEU ARG ASP VAL ARG GLN PRO

GLU VAL LYS GLU GLU LYS PRO GLU PHE ASP PRO ILE LEU LEU ARG PRO VAL ASP ASP LEU GLU LEU THR VAL ARG SER ALA ASN CYS LEU LYS ALA GLU ALA ILE HIS TYR ILE GLY ASP LEU VAL GLN ARG THR GLU VAL GLU LEU LEU LYS THR PRO ASN LEU GLY LYS LYS SER LEU

THR GLU ILE LYS ASP VAL LEU ALA SER ARG GLY LEU SER LEU GLY MET ARG LEU GLU ASN TRP PRO PRO ALA SER ILE ALA ASP GLU

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

Chain AE: 95% 89% 5% • 5%

MET LYS ASP LEU LEU LYS PHE LEU LYS ALA GLN THR LYS THR GLU E16 F17 D18 A19 I20 K21 I22 A23 L24 A25 S26 P27 D28 M29 I30 R31 S32 W33 S34 F35 G36 E37 V38 K39 K40 P41 E42 T43 I44 N45 Y46 R47 T48 F49 K50 P51 E52 R53 D54 G55 L56 F57 C58 A59 R60

I61 F62 G63 P64 V65 K66 D67 Y68 E69 C70 L71 C72 G73 K74 Y75 K76 R77 L78 K79 H80 R81 G82 V83 I84 C85 E86 K87 C88 G89 V90 E91 V92 T93 Q94 T95 K96 V97 R98 R99 E100 R101 M102 G103 H104 I105 E106 L107 A108 S109 P110 T111 A112 H113 I114 W115 F116 L117 K118 S119 L120

P121 S122 R123 I124 G125 L126 L127 L128 D129 M130 P131 L132 R133 D134 I135 E136 R137 V138 L139 Y140 F141 E142 S143 Y144 V145 V146 I147 E148 G149 G150 M151 T152 N153 L154 E155 R156 Q157 Q158 I159 L160 T161 E162 E163 Q164 Y165 L166 D167 A168 L169 E170 E171 F172 G173 D174 E175 F176 D177 A178 K179 M180

G181 A182 E183 A184 I185 Q186 A187 L188 L189 K190 S191 M192 D193 L194 E195 Q196 E197 C198 E199 Q200 L201 R202 E203 E204 L205 N206 E207 T208 N209 S210 E211 T212 K213 R214 K215 K216 L217 T218 K219 R220 I221 K222 L223 L224 E225 A226 F227 V228 Q229 S230 G231 N232 K233 P234 E235 W236 M237 I238 L239 T240

V241 L242 P243 V244 L245 P246 P247 D248 L249 R250 P251 L252 V253 P254 L255 D256 G257 G258 R259 F260 A261 T262 S263 D264 L265 N266 D267 L268 Y269 R270 R271 V272 I273 N274 R275 N276 N277 R278 L279 K280 R281 L282 L283 D284 L285 A286 A287 P288 D289 I290 I291 V292 R293 N294 E295 K296 R297 M298 L299 Q300

E301 A302 V303 D304 A305 L306 L307 D308 N309 G310 R311 R312 G313 R314 A315 I316 T317 G318 S319 N320 K321 R322 P323 L324 K325 S326 L327 A328 D329 M330 I331 K332 G333 K334 Q335 G336 R337 F338 R339 Q340 N341 L342 L343 G344 K345 R346 V347 D348 Y349 S350 G351 R352 S353 V354 I355 T356 V357 G358 P359 Y360

L361 R362 L363 H364 Q365 C366 G367 L368 P369 K370 K371 M372 A373 L374 E375 L376 F377 K378 P379 F380 I381 Y382 G383 K384 L385 E386 L387 R388 G389 L390 A391 T392 T393 I394 K395 A396 A397 K398 K399 M400 V401 E402 R403 E404 E405 A406 A407 V408 H409 D410 I411 L412 D413 E414 V415 I416 R417 E418 H419 P420

V421 L422 L423 N424 R425 A426 P427 T428 L429 H430 R431 L432 G433 I434 Q435 A436 F437 E438 P439 V440 L441 I442 E443 G444 K445 A446 I447 Q448 L449 H450 P451 L452 V453 C454 A455 A456 Y457 N458 A459 D460 F461 D462 G463 D464 Q465 M466 A467 V468 H469 V470 P471 L472 T473 L474 E475 A476 Q477 L478 E479 A480

R481 A482 L483 M484 M485 S486 T487 N488 M489 I490 L491 S492 P493 A494 N495 G496 E497 P498 I499 I500 V501 P502 S503 Q504 D505 V506 V507 L508 G509 L510 Y511 Y512 M513 T514 R515 D516 C517 V518 N519 A520 K521 G522 E523 G524 M525 V526 L527 T528 G529 P530 K531 E532 A533 E534 R535 L536 Y537 R538 S539 G540

L541 A542 S543 L544 H545 A546 R547 V548 K549 V550 R551 I552 T553 E554 Y555 E556 K557 D558 A559 N560 G561 E562 L563 V564 A565 K566 T567 S568 L569 K570 D571 T572 T573 V574 G575 R576 A577 I578 L579 W580 M581 I582 V583 P584 K585 G586 L587 P588 Y589 S590 I591 V592 N593 Q594 A595 L596 G597 K598 K599 A600

I601 S602 K603 M604 L605 N606 T607 G608 Y609 R610 I611 L612 G613 L614 K615 P616 T617 V618 I619 F620 A621 D622 Q623 I624 M625 Y626 T627 G628 F629 A630 Y631 A632 A633 R634 S635 G636 A637 S638 V639 G640 I641 D642 D643 M644 V645 I646 P647 E648 K649 K650 H651 E652 I653 I654 S655 E656 A657 E658 A659 E660

V661 A662 E663 I664 Q665 E666 Q667 F668 Q669 S670 G671 L672 V673 T674 A675 G676 E677 R678 Y679 N680 K681 V682 I683 D684 I685 W686 A687 A688 A689 N690 D691 R692 V693 S694 K695 A696 M697 M698 D699 N700 L701 Q702 T703 E704 T705 V706 I707 M708 R709 D710 G711 Q712 E713 E714 K715 Q716 V717 S718 F719 N720

S721 I722 Y723 M724 M725 A726 D727 S728 G729 A730 R731 G732 S733 A734 A735 Q736 I737 R738 Q739 L740 A741 G742 M743 R744 G745 L746 M747 A748 K749 P750 D751 G752 S753 I754 I755 E756 T757 P758 I759 T760 A761 N762 F763 R764 E765 G766 L767 N768 V769 L770 Q771 Y772 F773 I774 S775 T776 H777 G778 A779 R780

K781 G782 L783 A784 D785 T786 A787 L788 K789 T790 A791 N792 S793 G794 Y795 L796 T797 R798 R799 L800 V801 D802 V803 A804 Q805 D806 L807 V808 V809 T810 E811 D812 D813 C814 G815 T816 H817 E818 G819 I820 M821 M822 T823 P824 V825 I826 E827 G828 G829 D830 V831 K832 E833 P834 L835 R836 D837 R838 V839 L840

G841 R842 V843 T844 A845 E846 D847 V848 L849 K850 P851 G852 T853 A854 D855 I856 L857 V858 P859 R860 N861 T862 L863 L864 H865 E866 Q867 W868 C869 D870 L871 L872 E873 E874 N875 S876 V877 D878 A879 V880 K881 V882 R883 S884 V885 V886 S887 C888 D889 T890 D891 F892 G893 V894 C895 A896 H897 C898 Y899 G900

R901 D902 L903 A904 R905 G906 H907 I908 I909 N910 K911 G912 E913 A914 I915 G916 V917 I918 A919 A920 Q921 S922 I923 G924 E925 P926 G927 T928 Q929 L930 T931 R932 R933 THR PHE HIS ILE GLY GLY ALA ALA SER ARG ALA ALA ALA GLU S948 S949 I950 Q951 V952 K953 N954 K955 G956 S957 I958 K959 L960

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

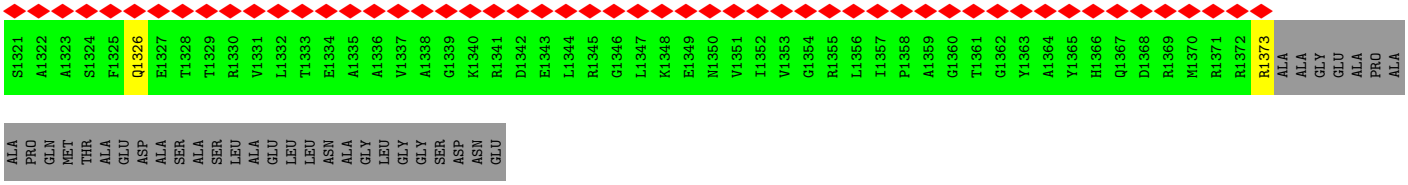
D1021 P1022 H1023 T1024 M1025 P1026 V1027 I1028 T1029 E1030 V1031 S1032 G1033 F1034 V1035 R1036 F1037 T1038 D1039 M1040 I1041 D1042 G1043 Q1044 T1045 I1046 T1047 R1048 Q1049 T1050 D1051 E1052 L1053 T1054 G1055 L1056 S1057 S1058 L1059 V1060 V1061 L1062 D1063 S1064 A1065 E1066 R1067 T1068 A1069 G1070 G1071 K1072 D1073 L1074 R1075 P1076 A1077 L1078 K1079 I1080

V1081 D1082 A1083 Q1084 G1085 N1086 D1087 V1088 L1089 I1090 P1091 G1092 T1093 D1094 M1095 P1096 A1097 Q1098 Y1099 F1100 L1101 P1102 G1103 K1104 A1105 I1106 V1107 Q1108 L1109 E1110 D1111 G1112 V1113 Q1114 I1115 S1116 S1117 G1118 D1119 T1120 L1121 A1122 R1123 I1124 P1125 Q1126 GLU SER GLY GLY THR LYS ASP ILE THR G1136 G1137 L1138 P1139 R1140

V1141 A1142 D1143 L1144 F1145 E1146 A1147 R1148 R1149 P1150 K1151 E1152 P1153 A1154 I1155 L1156 A1157 E1158 I1159 S1160 G1161 I1162 V1163 S1164 F1165 G1166 K1167 E1168 T1169 K1170 G1171 K1172 R1173 R1174 L1175 V1176 I1177 T1178 P1179 V1180 D1181 G1182 S1183 D1184 P1185 Y1186 E1187 E1188 M1189 I1190 P1191 K1192 W1193 R1194 Q1195 L1196 N1197 V1198 F1199 E1200

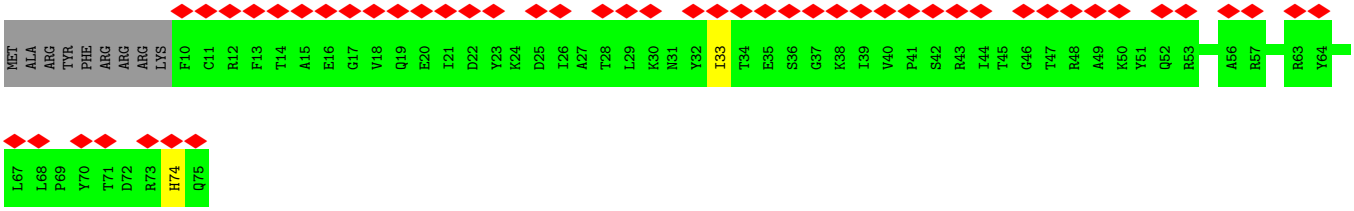
G1201 E1202 R1203 V1204 E1205 R1206 G1207 D1208 V1209 I1210 S1211 D1212 G1213 P1214 E1215 A1216 P1217 H1218 D1219 I1220 L1221 R1222 L1223 R1224 G1225 V1226 H1227 A1228 V1229 T1230 R1231 Y1232 I1233 V1234 N1235 E1236 V1237 Q1238 D1239 V1240 Y1241 R1242 L1243 Q1244 G1245 V1246 K1247 I1248 N1249 D1250 K1251 H1252 I1253 E1254 V1255 I1256 V1257 R1258 Q1259 M1260

L1261 R1262 K1263 A1264 T1265 I1266 V1267 N1268 A1269 G1270 S1271 S1272 D1273 F1274 L1275 E1276 G1277 E1278 Q1279 V1280 E1281 Y1282 S1283 R1284 V1285 K1286 I1287 A1288 N1289 R1290 E1291 L1292 E1293 A1294 N1295 G1296 K1297 V1298 G1299 A1300 T1301 Y1302 S1303 R1304 D1305 L1306 L1307 G1308 I1309 T1310 K1311 A1312 S1313 L1314 A1315 T1316 E1317 S1318 F1319 I1320



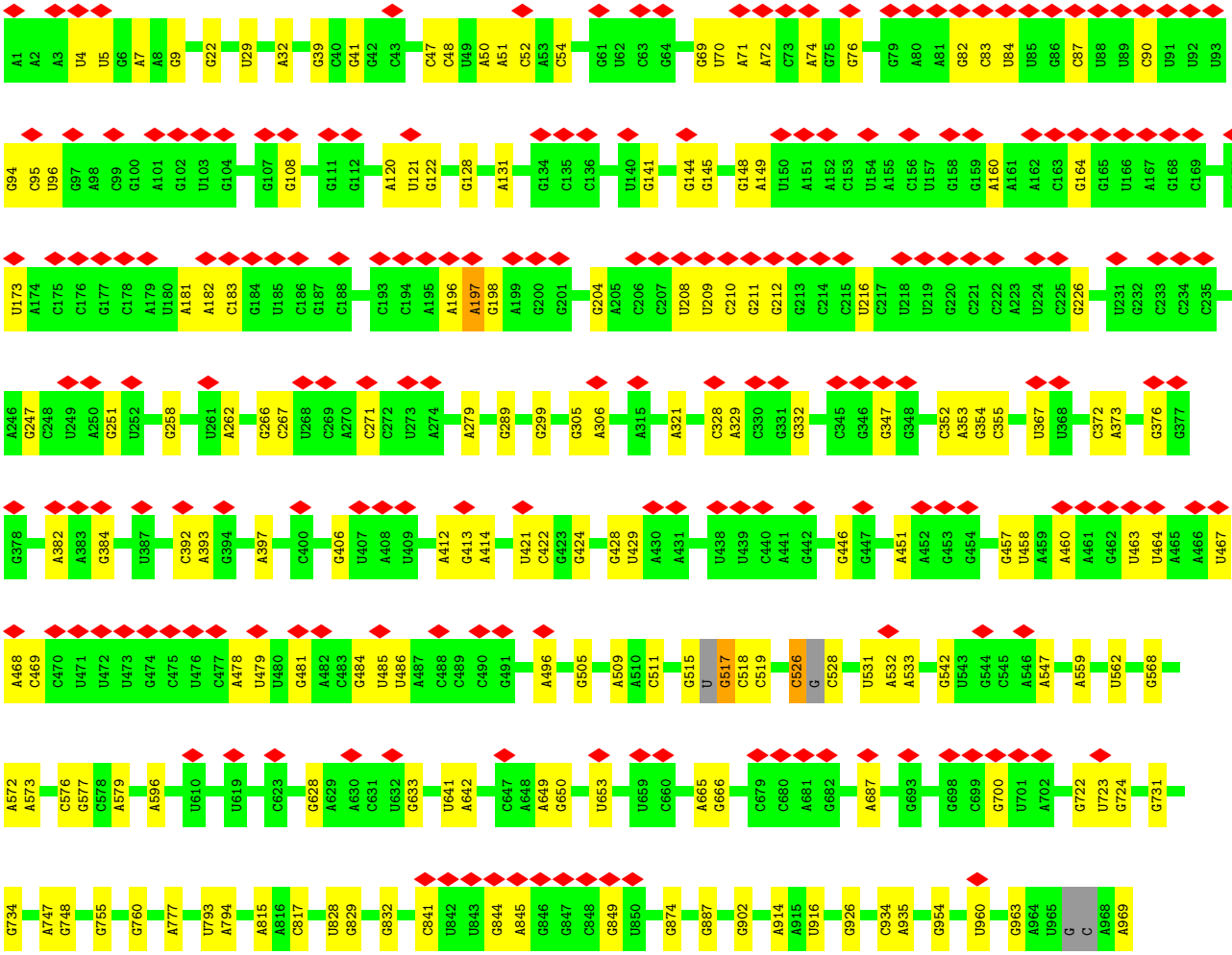
• Molecule 14: 30S ribosomal protein S18

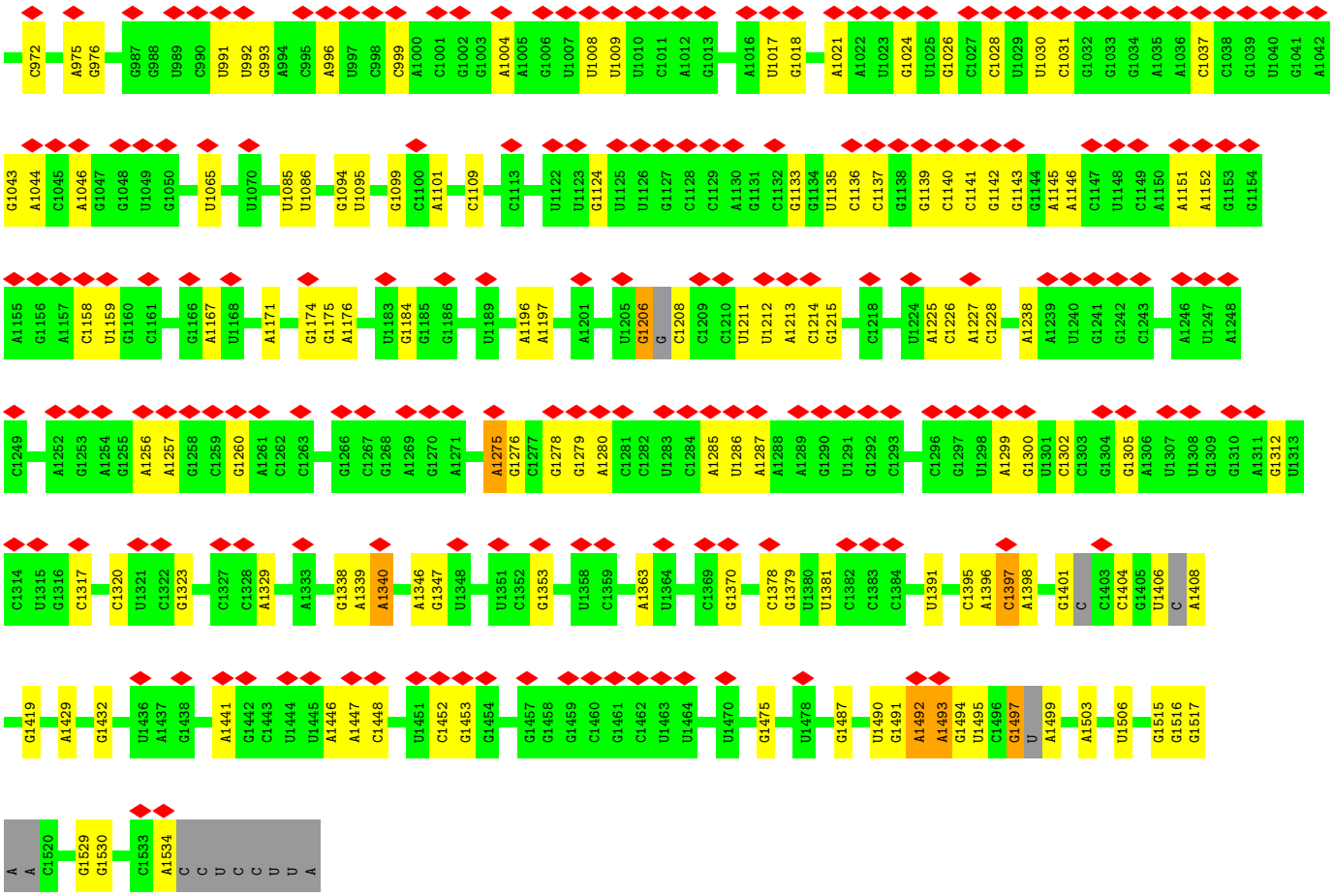
Chain C:



• Molecule 15: 16S rRNA

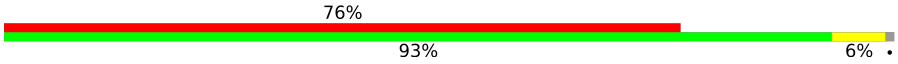
Chain D:

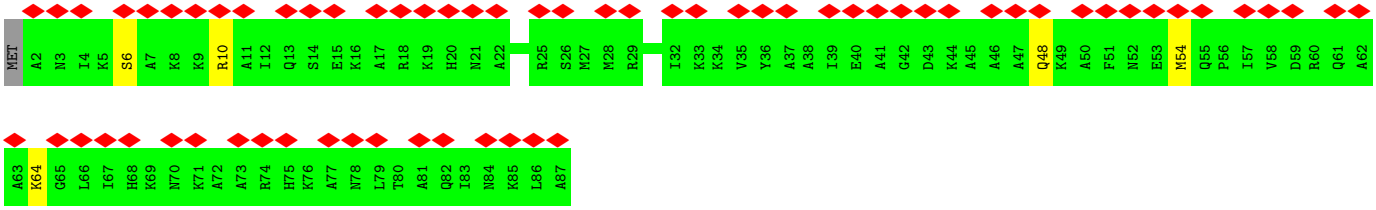




- Molecule 16: 30S ribosomal protein S20

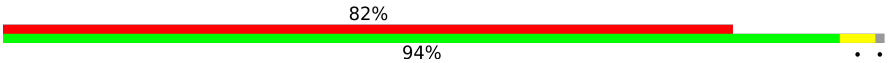
Chain E:

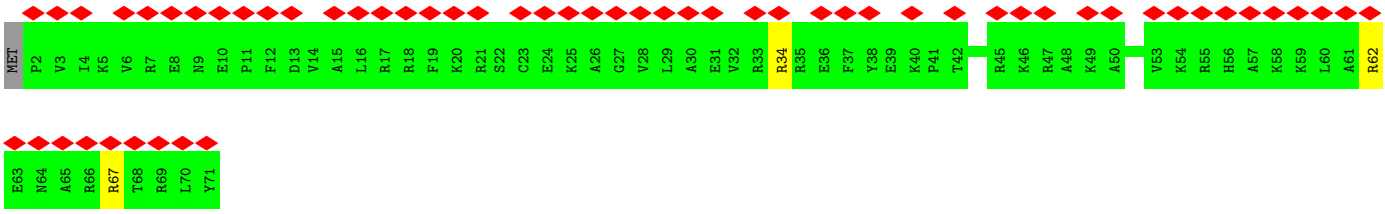




- Molecule 17: 30S ribosomal protein S21

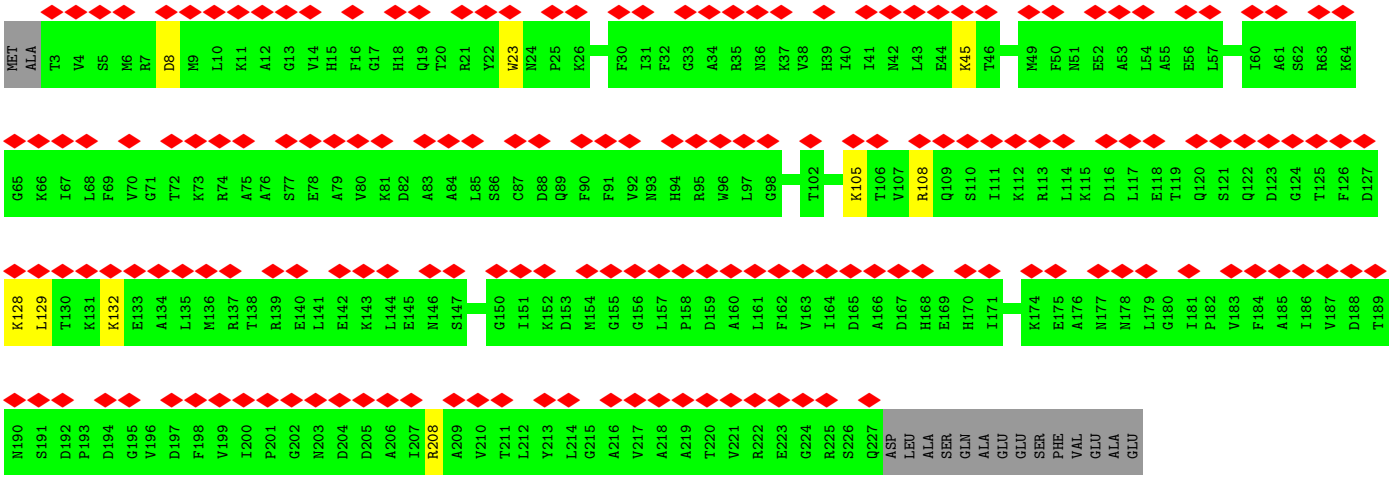
Chain F:





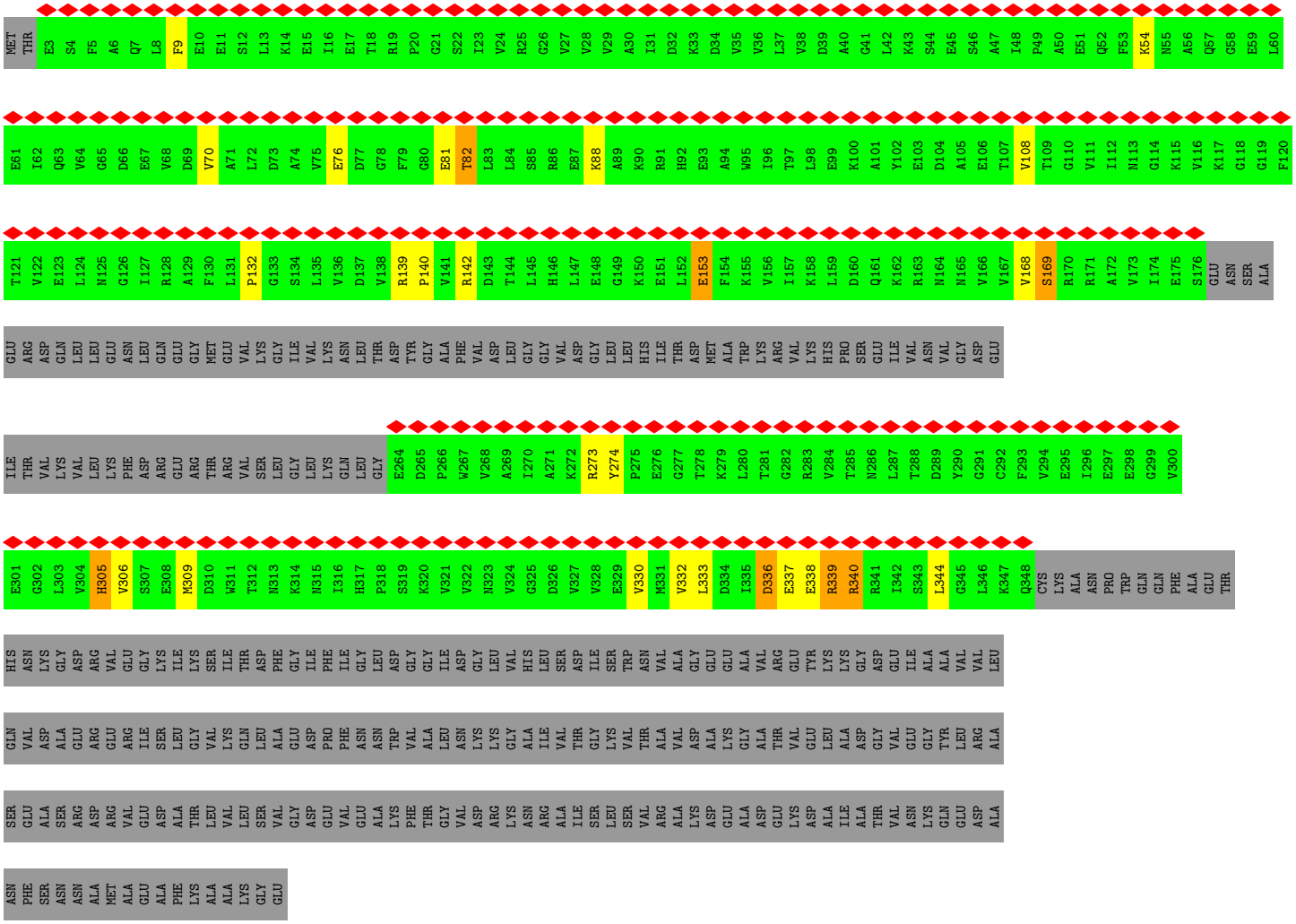
- Molecule 18: 30S ribosomal protein S2

Chain G:



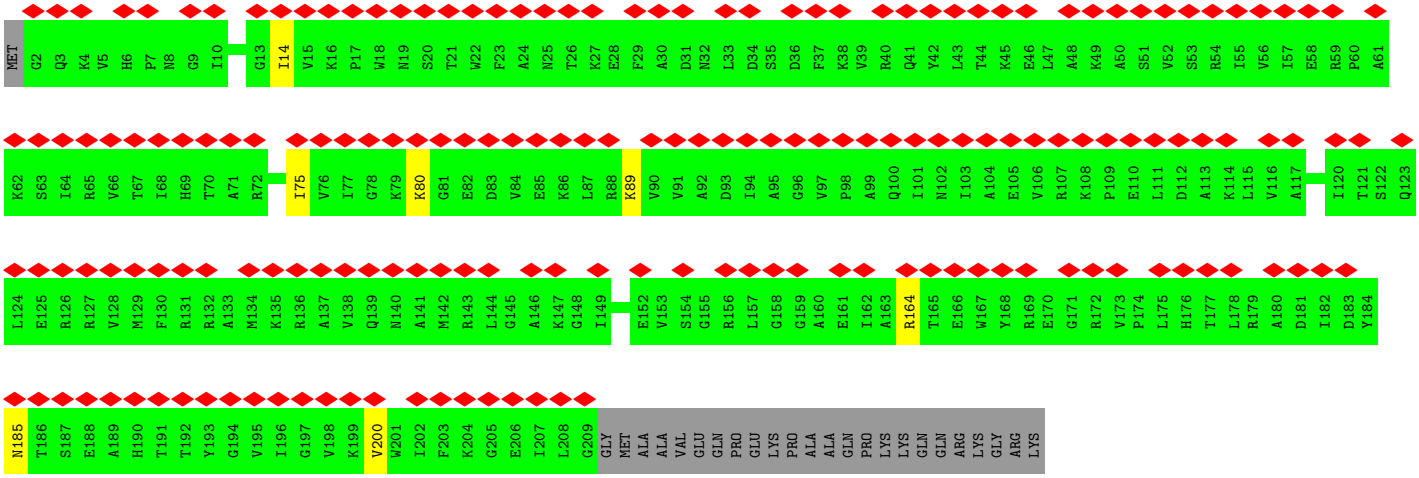
- Molecule 19: 30S ribosomal protein S1

Chain H:



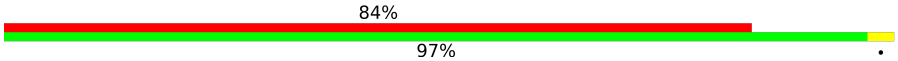
- Molecule 20: 30S ribosomal protein S3

Chain I:



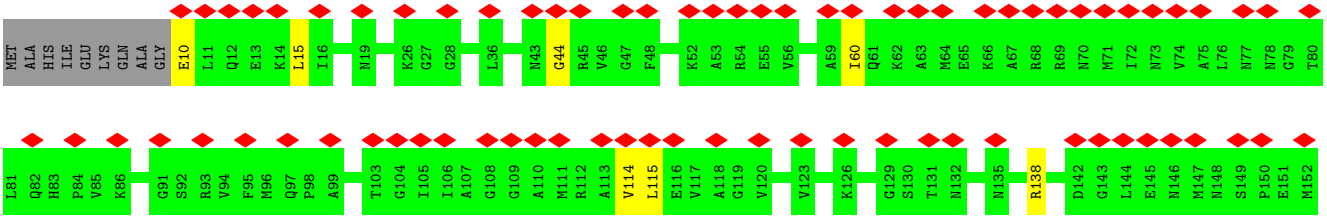
- Molecule 21: 30S ribosomal protein S4

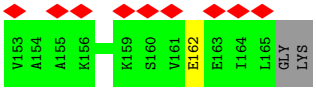
Chain J:



- Molecule 22: 30S ribosomal protein S5

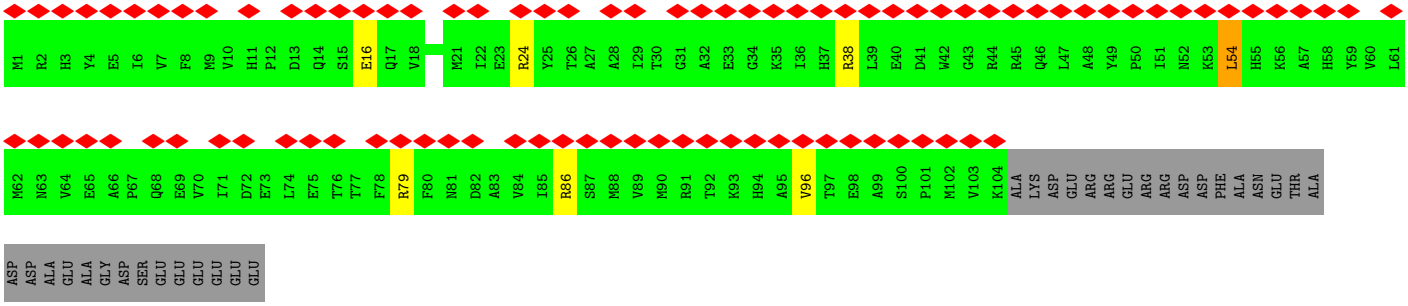
Chain K:





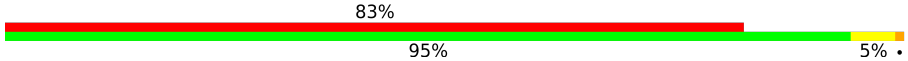
• Molecule 23: 30S ribosomal protein S6

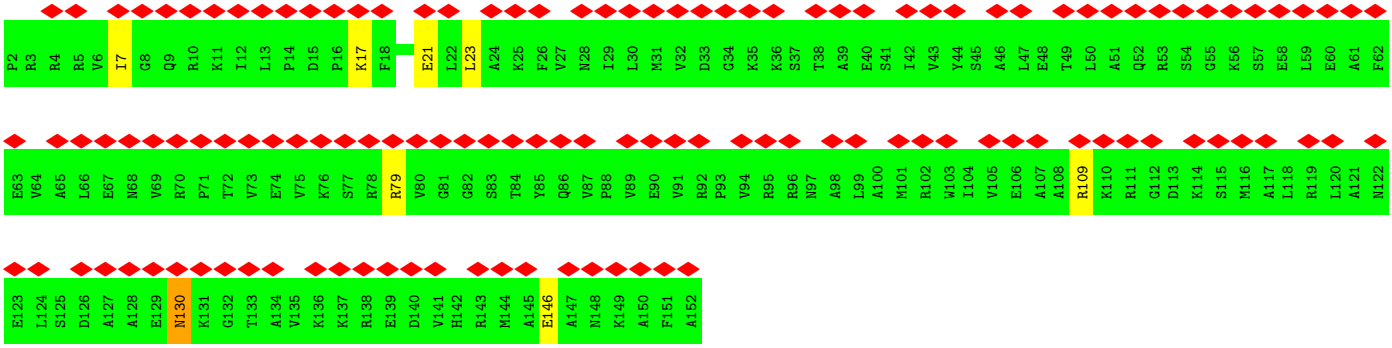
Chain L:



• Molecule 24: 30S ribosomal protein S7

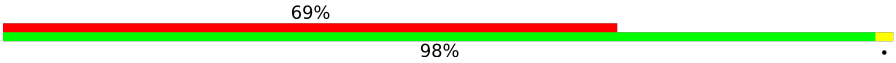
Chain M:

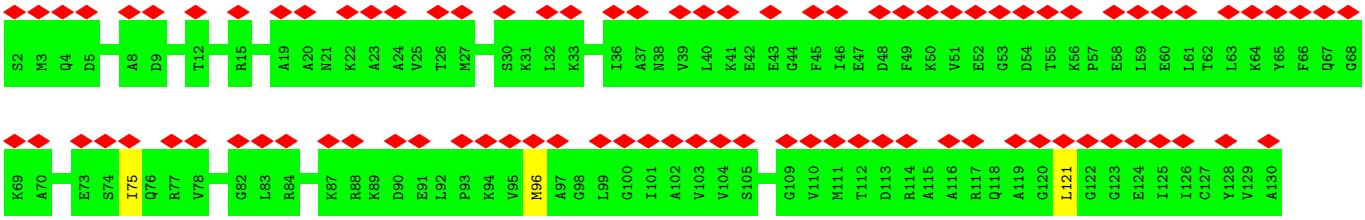




• Molecule 25: 30S ribosomal protein S8

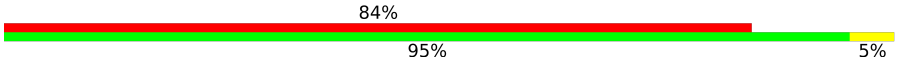
Chain N:

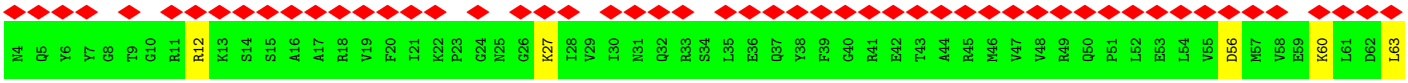


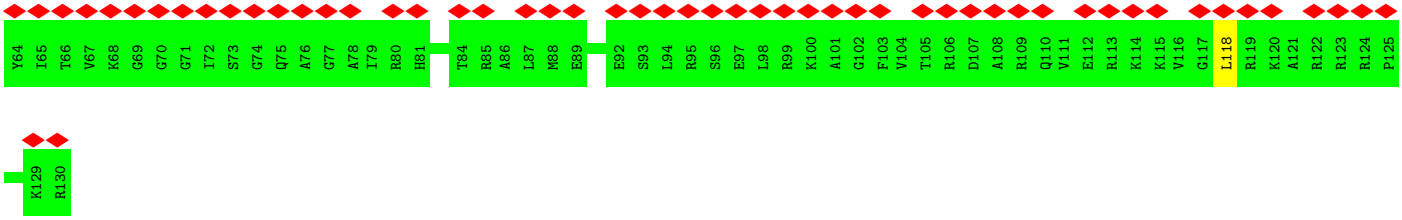


• Molecule 26: 30S ribosomal protein S9

Chain O:

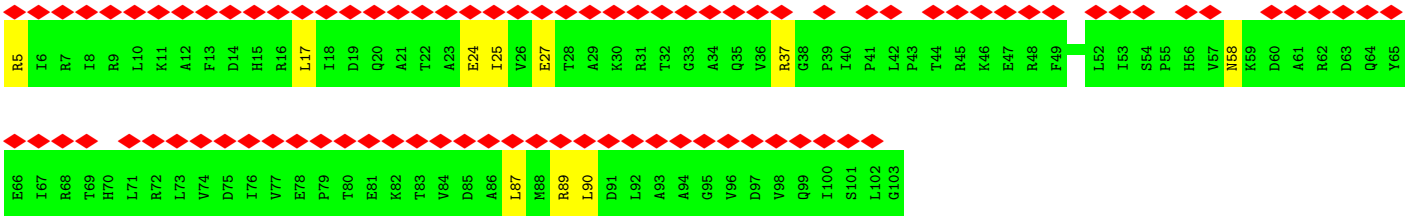






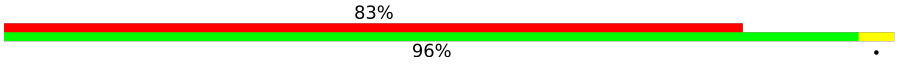
- Molecule 27: 30S ribosomal protein S10

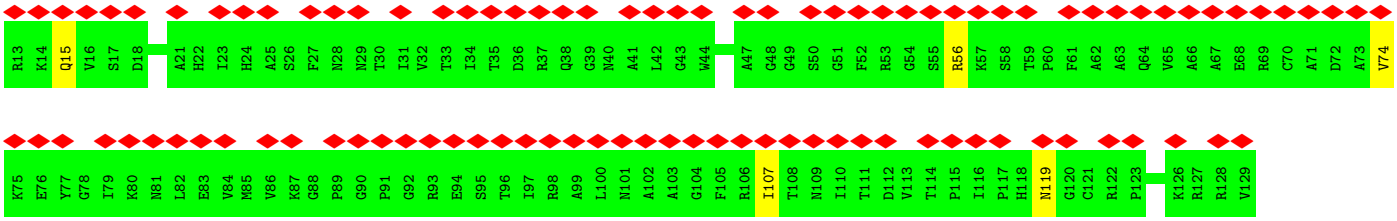
Chain P:



- Molecule 28: 30S ribosomal protein S11

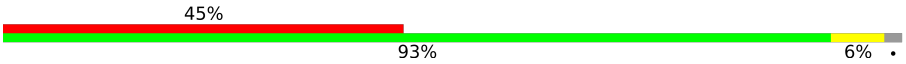
Chain Q:

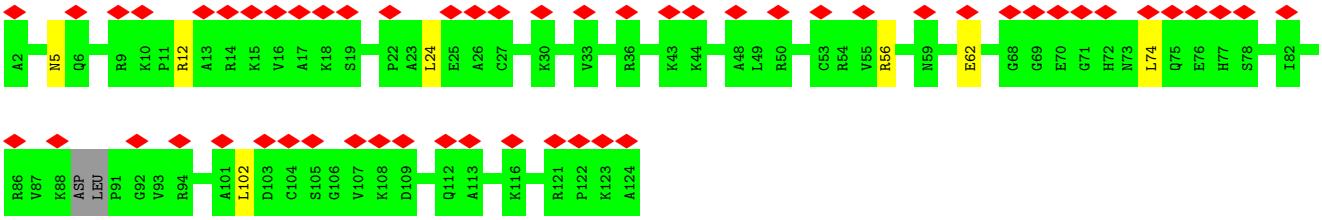




- Molecule 29: 30S ribosomal protein S12

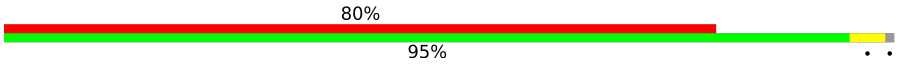
Chain R:

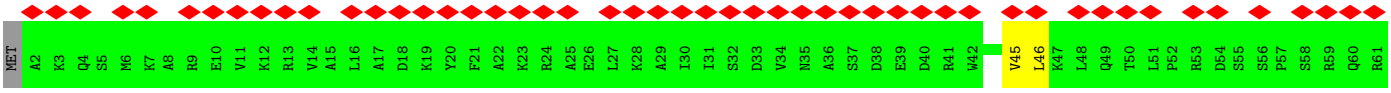


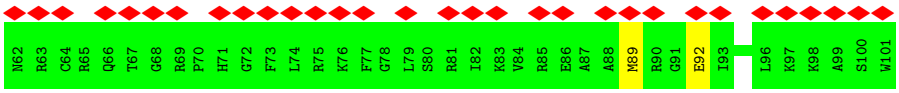


- Molecule 30: 30S ribosomal protein S14

Chain S:

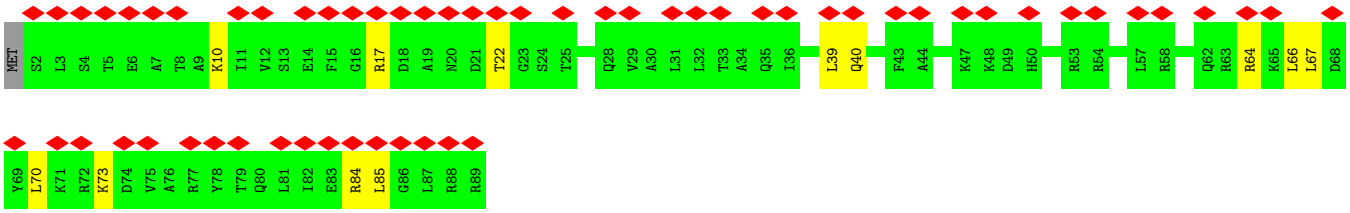






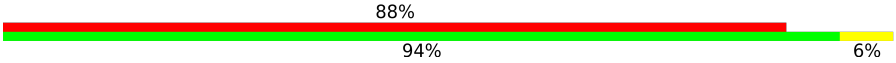
- Molecule 31: 30S ribosomal protein S15

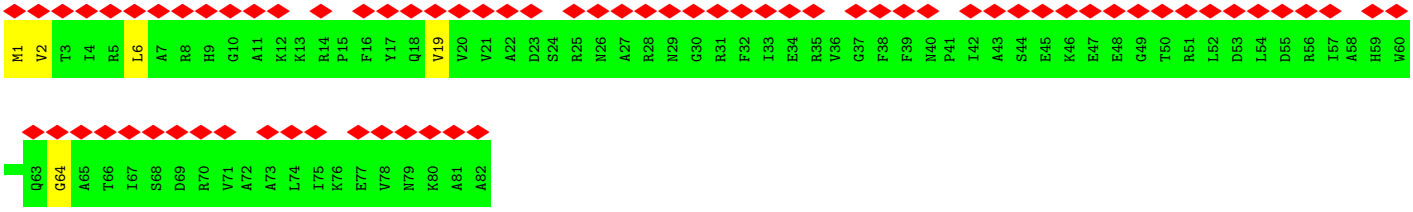
Chain T:



- Molecule 32: 30S ribosomal protein S16

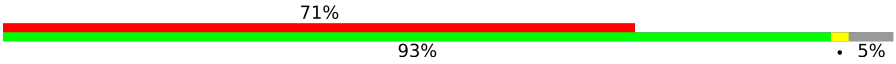
Chain U:

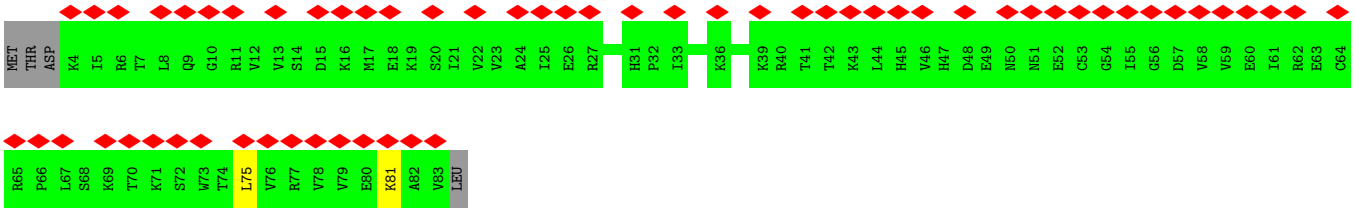




- Molecule 33: 30S ribosomal protein S17

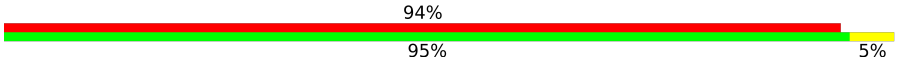
Chain V:

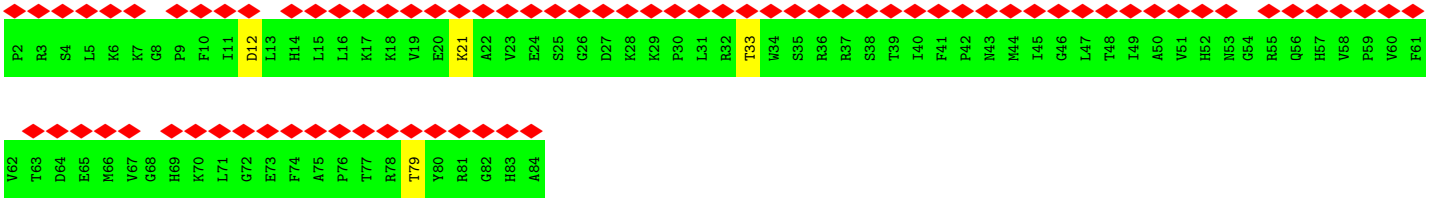




- Molecule 34: 30S ribosomal protein S19

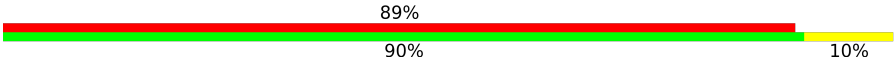
Chain W:

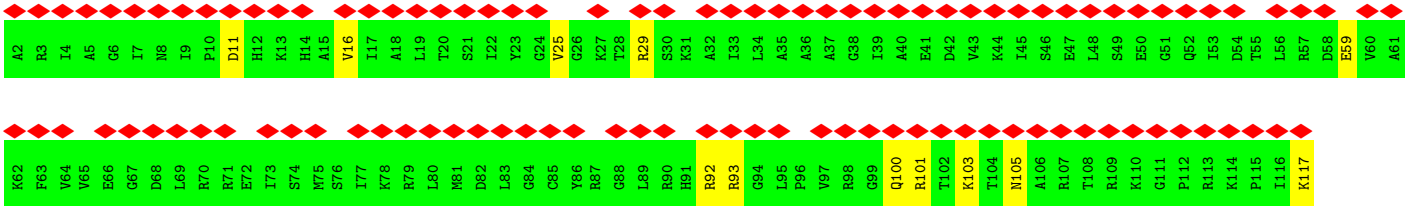




- Molecule 35: 30S ribosomal protein S13

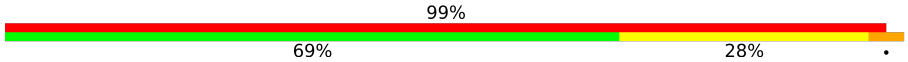
Chain X:

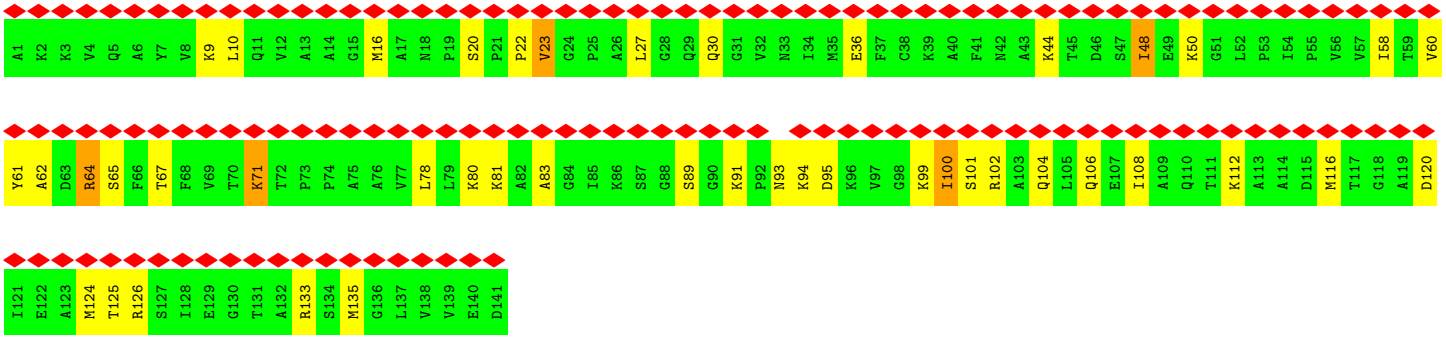




- Molecule 36: 50S ribosomal protein L11

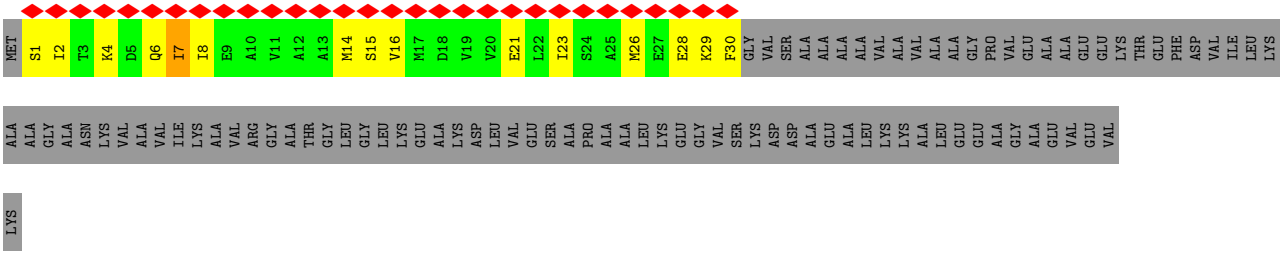
Chain Y:





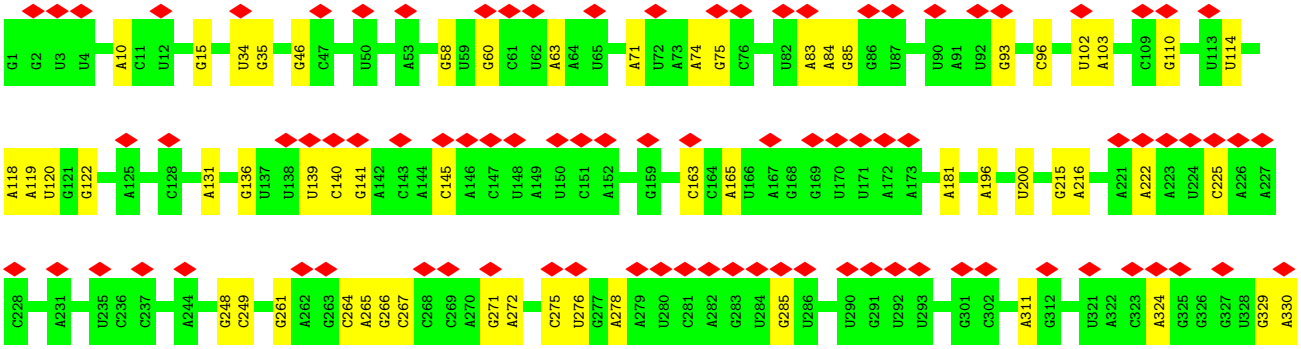
- Molecule 37: 50S ribosomal protein L7/L12

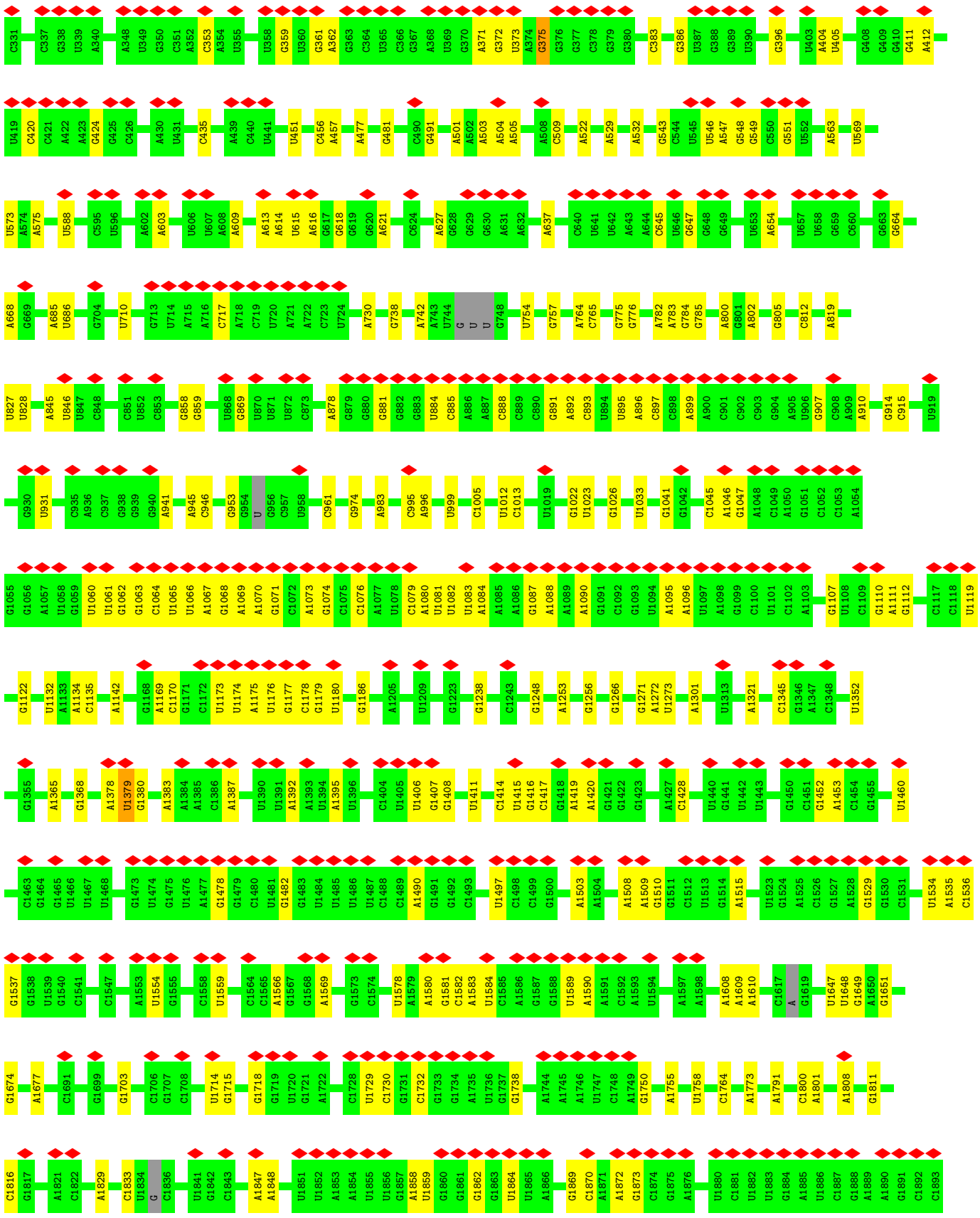
Chain Z:

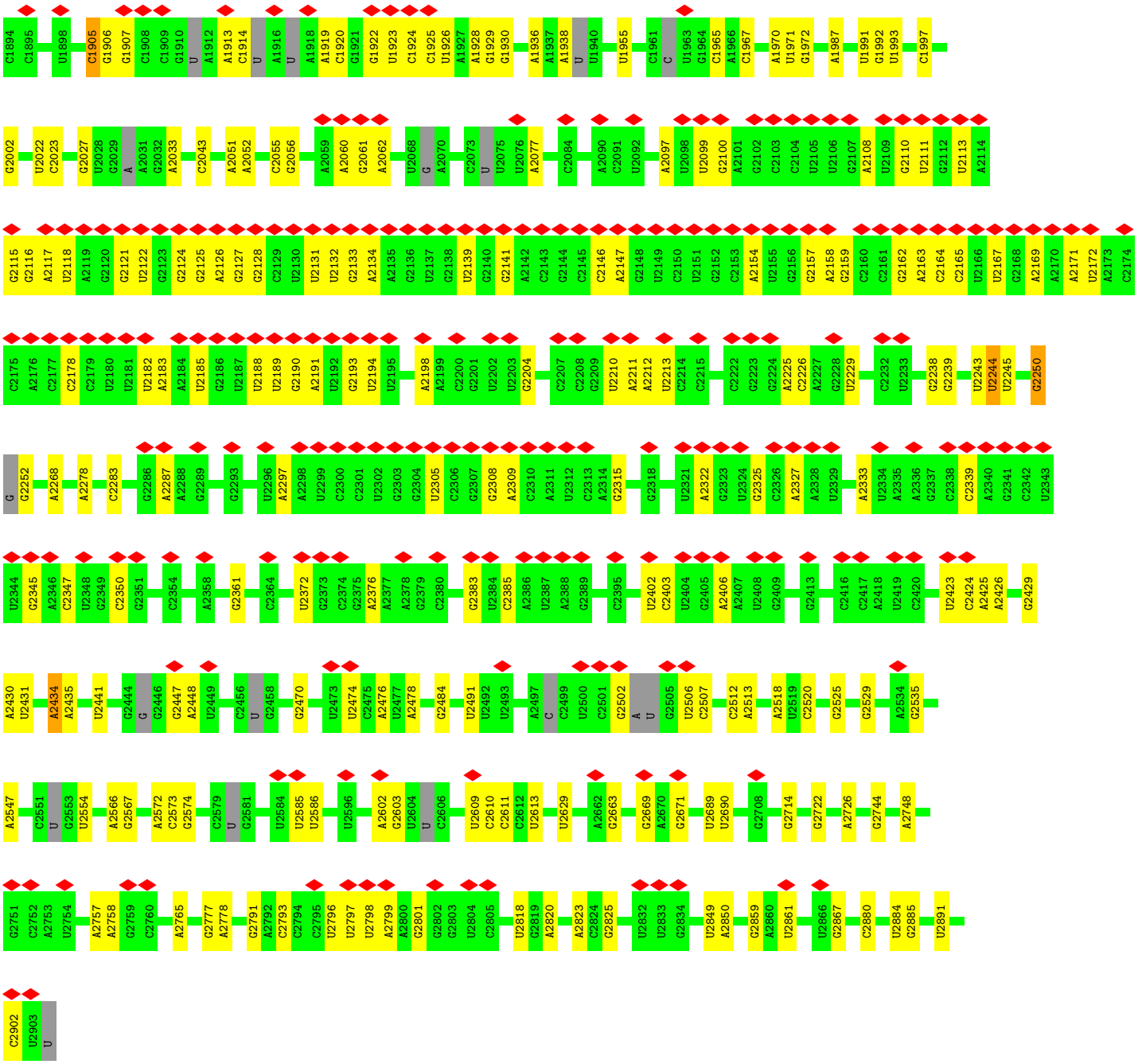


- Molecule 38: 23S rRNA

Chain a:

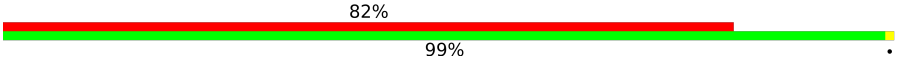


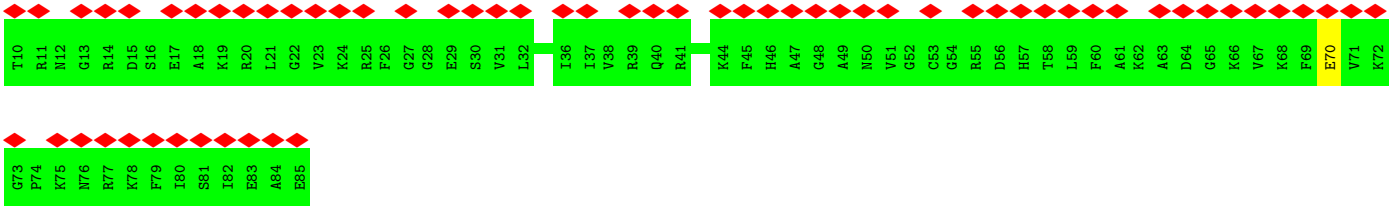

C331 C337 G338 U339 A340 A348 U349 G350 C351 A352 C353 A354 U355 U358 G359 U360 G361 A362 G363 C364 U365 C366 G367 A368 U369 G370 A371 G372 U373 A374 G375 G376 G377 C378 G379 G380 C383 G386 U387 G388 G389 U390 G396 U403 A404 U405 G408 G409 G410 G411 A412
U419 C420 C421 A422 A423 G424 G425 C426 A430 U431 C435 A439 C440 U441 U451 C456 A457 A477 G481 C490 G491 A501 A502 A503 A504 A505 A508 C509 A522 A529 A532 G543 C544 U545 U546 A547 G548 G549 C550 G551 U552 A563 U569
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
A668 G669 A685 U686 G704 U710 G713 U714 A715 A716 C717 A718 C719 U720 A721 A722 C723 U724 A730 G738 A742 A743 U744 G U U G748 U754 G757 A764 C765 G775 G776 A782 A783 G784 G785 A800 G801 A802 G805 C812 A819
U827 U828 A845 U846 U847 C848 C851 U852 C853 G858 G859 U868 G869 U870 U871 U872 C873 A878 G879 G880 G881 G882 G883 U884 C885 A886 A887 C888 C889 C890 G891 A892 C893 U894 U895 A896 C897 C898 A899 A900 C901 C902 C903 G904 A905 U906 G907 C908 A909 A910 G914 C915 U919
G930 U931 C935 A936 C937 G938 G939 G940 A941 A945 C946 G953 G954 U G956 C957 U958 C961 G974 A983 C995 A996 U999 C1005 U1012 C1013 U1019 G1022 U1023 G1026 U1033 G1041 G1042 C1045 A1046 G1047 A1048 C1049 A1050 G1051 C1052 C1053 A1054
G1055 G1056 A1057 U1058 G1059 U1060 U1061 G1062 G1063 C1064 U1065 U1066 A1067 G1068 A1069 A1070 G1071 C1072 A1073 G1074 C1075 C1076 A1077 U1078 C1079 A1080 U1081 U1082 U1083 A1084 A1085 A1086 G1087 A1088 A1089 A1090 G1091 C1092 G1093 U1094 A1095 A1096 U1097 A1098 G1099 C1100 U1101 C1102 A1103 G1107 U1108 C1109 G1110 A1111 G1112 C1117 C1118 U1119
G1122 U1132 A1133 A1134 C1135 A1142 G1168 A1169 C1170 G1171 C1172 U1173 U1174 A1175 U1176 G1177 C1178 G1179 U1180 G1186 A1205 U1209 G1223 G1238 C1243 G1248 A1253 G1256 G1266 G1271 A1272 U1273 A1301 U1313 A1321 C1345 G1346 A1347 C1348 U1352
C1355 A1365 G1368 A1378 U1379 G1380 A1383 A1384 A1385 C1386 A1387 U1390 U1391 A1392 A1393 U1394 A1395 U1396 C1404 U1405 U1406 G1407 G1408 U1411 C1414 U1415 G1416 C1417 G1418 A1419 A1420 G1421 G1422 G1423 A1427 C1428 U1440 G1441 U1442 U1443 G1450 C1451 G1452 A1453 C1454 G1455 U1460
C1463 G1464 G1465 U1466 U1467 U1468 G1473 U1474 G1475 U1476 A1477 G1478 G1479 C1480 U1481 G1482 G1483 U1484 U1485 U1486 U1487 C1488 C1489 A1490 G1491 G1492 C1493 U1497 C1498 C1499 G1500 A1503 A1504 A1508 A1509 G1510 G1511 C1512 U1513 G1514 A1515 U1523 G1524 A1525 C1526 G1527 A1528 G1529 G1530 C1531 U1534 A1535 C1536
G1537 G1538 U1539 G1540 C1541 C1547 A1553 U1554 G1555 C1558 U1559 C1564 C1565 A1566 G1567 G1568 A1569 G1573 C1574 U1578 A1579 A1580 G1581 C1582 A1583 U1584 C1585 A1586 G1587 G1588 U1589 A1590 A1591 C1592 A1593 U1594 A1597 A1598 A1608 A1609 A1610 C1617 A G1619 U1647 U1648 G1649 A1650 G1651
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 C1863 U1864 U1865 A1866 G1869 C1870 A1871 A1872 G1873 C1874 G1875 A1876 U1880 C1881 U1882 U1883 G1884 A1885 U1886 C1887 G1888 A1889 A1890 C1891 C1892 C1893



- Molecule 39: 50S ribosomal protein L27

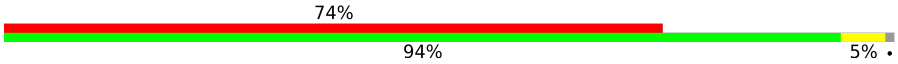
Chain b:

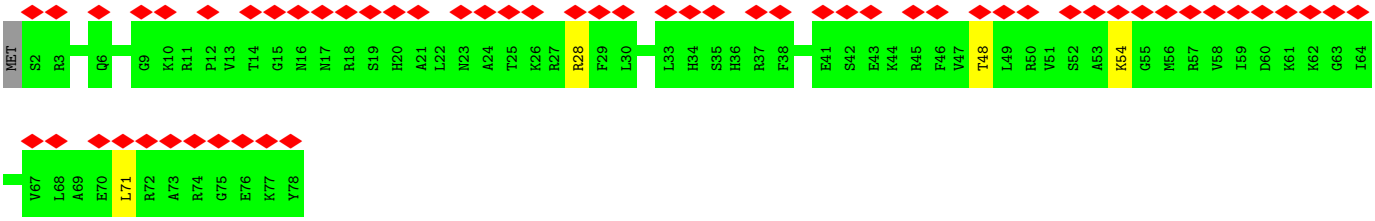




- Molecule 40: 50S ribosomal protein L28

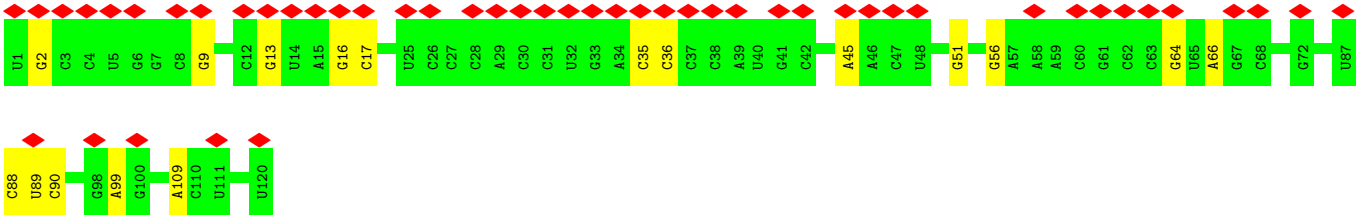
Chain c:





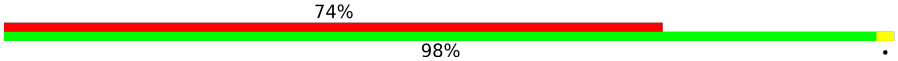
- Molecule 41: 5S rRNA

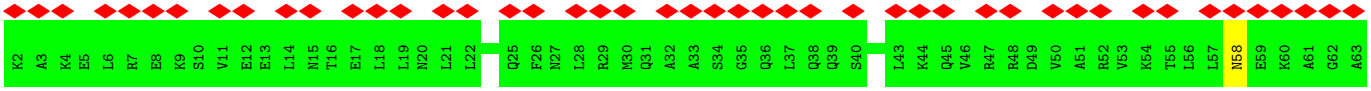
Chain d:



- Molecule 42: 50S ribosomal protein L29

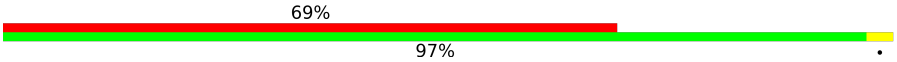
Chain e:

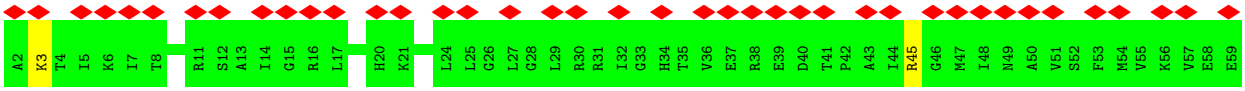




- Molecule 43: 50S ribosomal protein L30

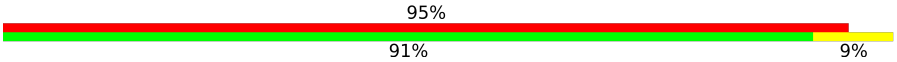
Chain f:

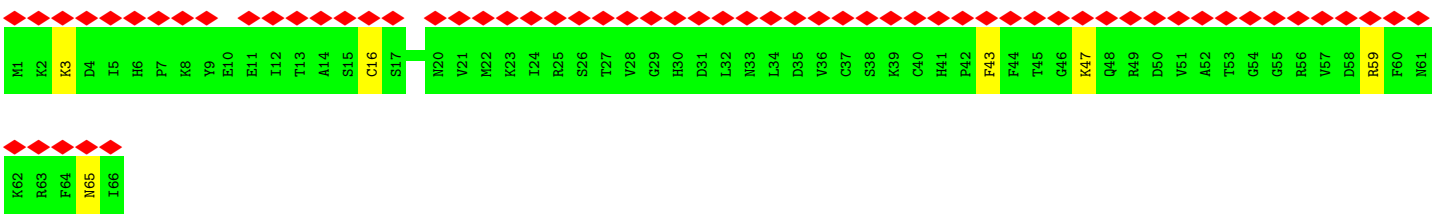




- Molecule 44: 50S ribosomal protein L31

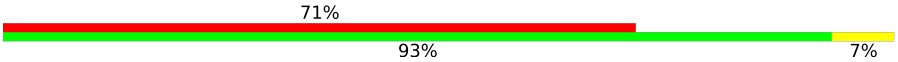
Chain g:

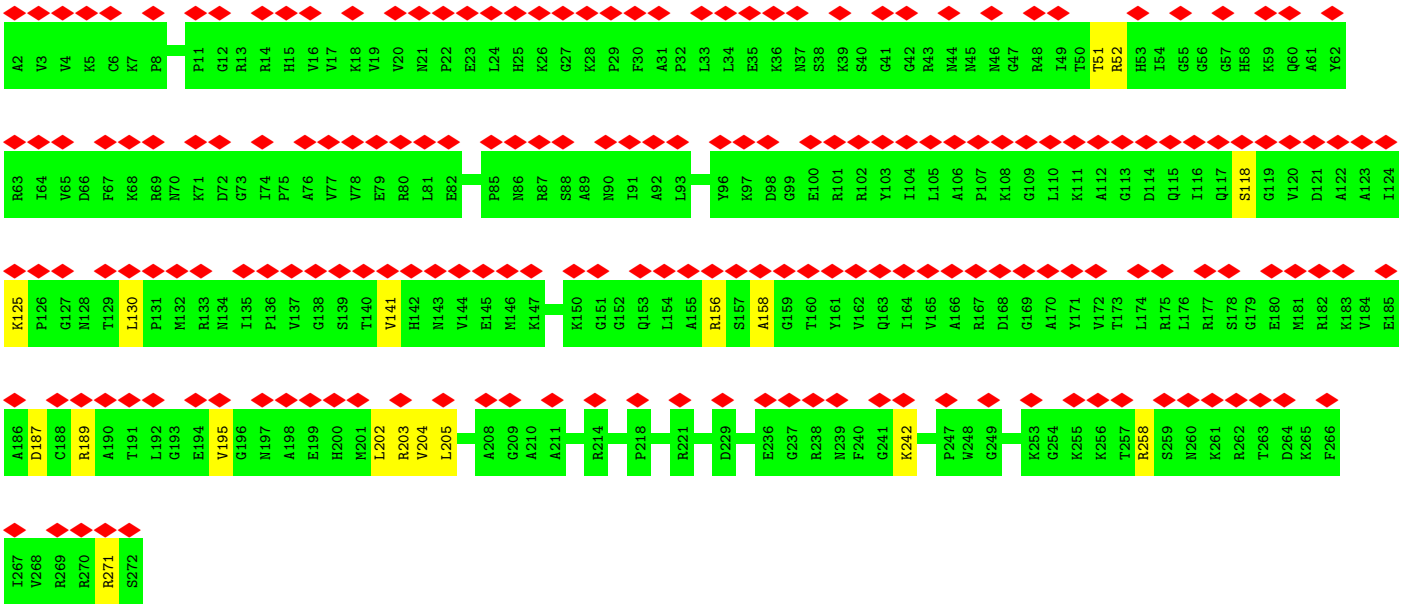




- Molecule 45: 50S ribosomal protein L2

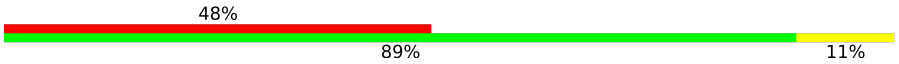
Chain h:

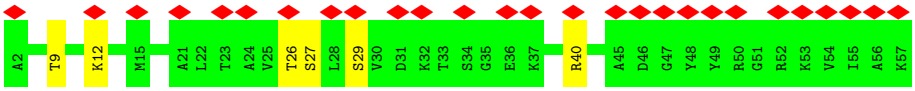




- Molecule 46: 50S ribosomal protein L32

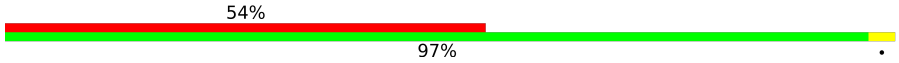
Chain i:

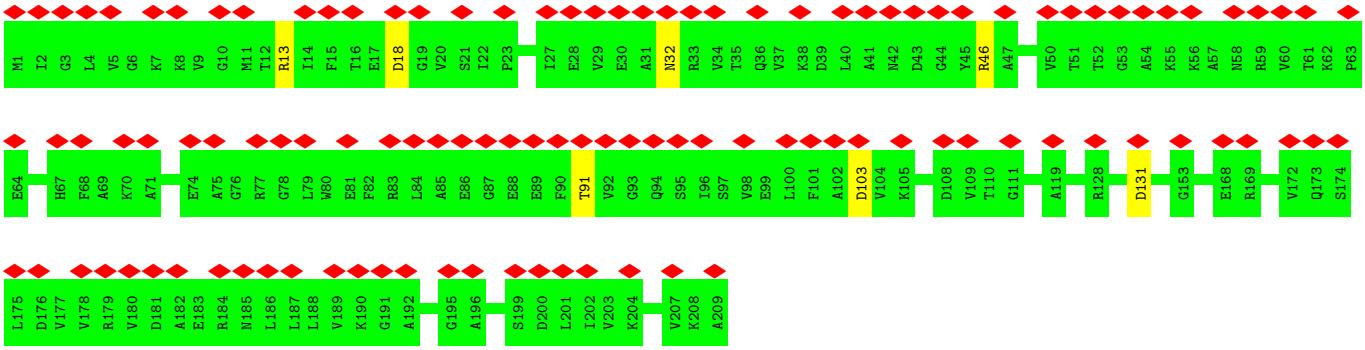




- Molecule 47: 50S ribosomal protein L3

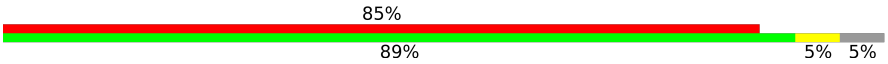
Chain j:

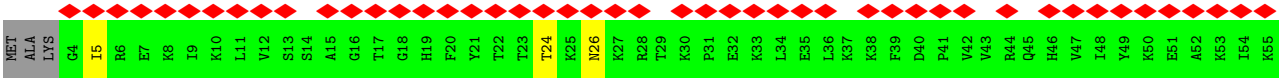




- Molecule 48: 50S ribosomal protein L33

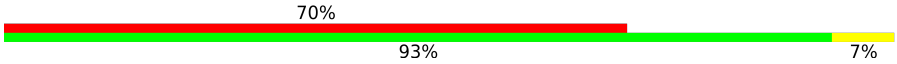
Chain k:

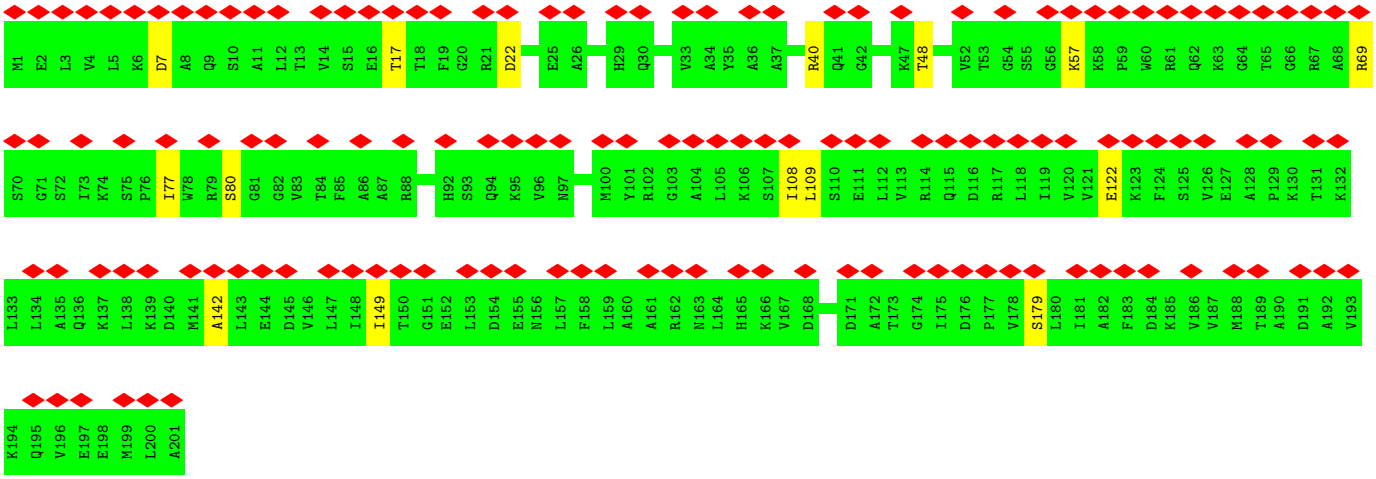




- Molecule 49: 50S ribosomal protein L4

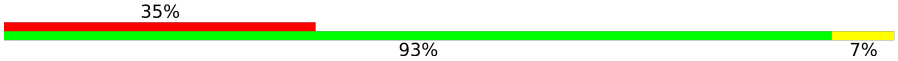
Chain l:

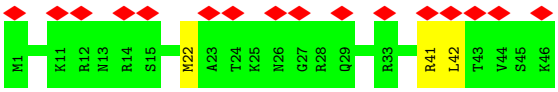




- Molecule 50: 50S ribosomal protein L34

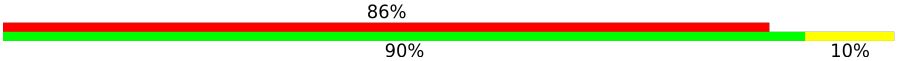
Chain m:

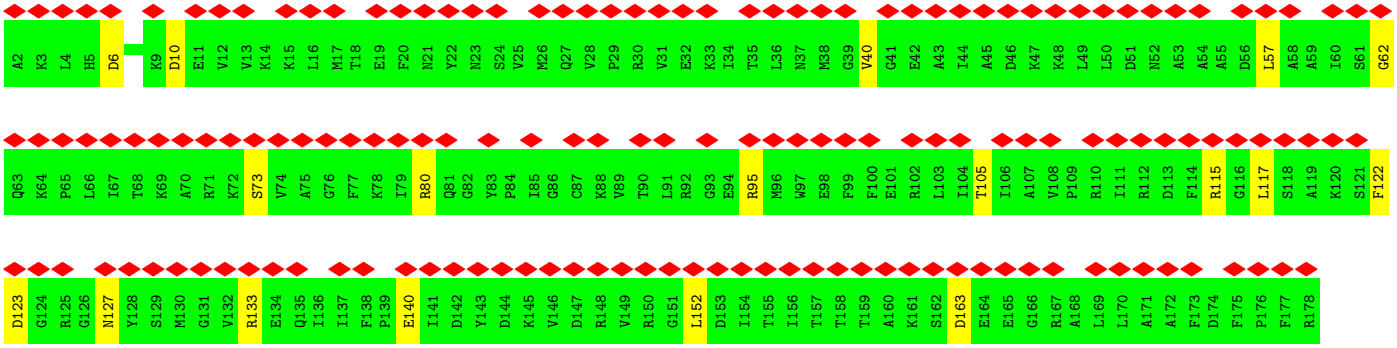




- Molecule 51: 50S ribosomal protein L5

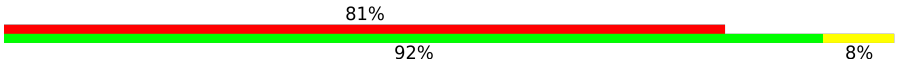
Chain n:





- Molecule 52: 50S ribosomal protein L35

Chain o:



- Molecule 53: 50S ribosomal protein L6

Chain p: 87% 98%

S2 R3 V4 A5 K6 A7 P8 V9 V10 V11 P12 A13 G14 V15 D16 V17 K18 I19 N20 G21 Q22 V23 I24 T25 I26 K27 G28 K29 M30 G31 E32 L33 T34 R35 T36 L37 N38 D39 A40 V41 E42 V43 K44 H45 A46 D47 N48 T49 L50 T51 F52 G53 P54 R55 D56 G57 Y58 A59 D60 G61

W62 A63 Q64 A65 G66 T67 A68 R69 A70 L71 L72 N73 S74 M75 V76 I77 G78 V79 T80 E81 G82 F83 T84 K85 K86 L87 Q88 L89 V90 G91 V92 G93 Y94 R95 A96 A97 V98 K99 G100 N101 V102 I103 N104 L105 S106 L107 G108 F109 S110 H111 P112 V113 D114 H115 Q116 L117 P118 A119 G120 I121

T122 A123 E124 C125 P126 T127 Q128 T129 E130 I131 V132 L133 K134 G135 A136 D137 K138 Q139 V140 Q143 A146 D147 L148 R149 A150 Y151 R152 R153 P154 E155 P156 Y157 K158 G159 K160 G161 V162 R163 Y164 A165 D166 E167 V168 V169 R170 T171 K172 E173 A174 K175 K176

- Molecule 54: 50S ribosomal protein L36

Chain q: 71% 95% 5%

M1 K2 V3 R4 A5 K8 K9 L10 C11 R12 N13 C14 K15 I16 V17 K18 R19 D20 G21 V22 I23 R24 V25 I26 C27 K32 H33 K34 Q35 R36 Q37 G38

- Molecule 55: 50S ribosomal protein L9

Chain r: 95% 93% 7%

M1 Q2 V3 I4 L5 L6 D7 K8 V9 A10 N11 L12 G13 S14 L15 G16 D17 Q18 V19 N20 V21 K22 A23 G24 R27 N28 F29 L30 V31 P32 K35 A36 V37 P38 A39 T40 K41 K42 N43 I44 E45 F46 F47 E48 A49 R50 R51 A52 E53 L54 E55 A56 K57 L58 A59 E60 V61 L62

A63 A64 A65 N66 A67 R68 A69 E70 K71 I72 N73 A74 L75 E76 T77 V78 T79 I80 A81 S82 K83 A84 G85 D86 E87 G88 K89 L90 F91 G92 S93 I94 G95 T96 R97 D98 I99 A100 D101 A102 V103 T104 A105 A106 G107 V108 E109 V110 A111 K112 S113 E114 V115 R116 L117 P118 N119 G120 V121 L122

R123 T124 T125 G126 E127 H128 E129 V130 S131 F132 Q133 V134 H135 S136 E137 V138 F139 A140 K141 V142 I143 V144 N145 V146 V147 A148 E149

- Molecule 56: 50S ribosomal protein L13

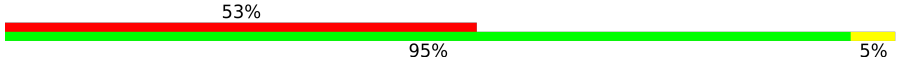
Chain s: 62% 96%

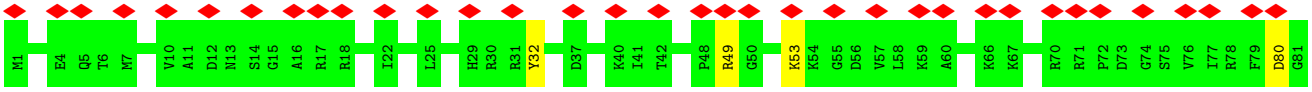
M1 K2 T3 F4 T5 A6 K7 P8 V11 K12 R13 D14 W15 Y16 V17 V18 D19 A20 T21 G22 K23 T24 L25 G26 A29 T30 E31 L32 A33 L36 R37 H40 K41 A42 P46 H47 V48 D49 T50 G51 D52 Y53 I54 I55 V56 L57 N58 A59 D60 K61 V62 A63 V64 T65 G66

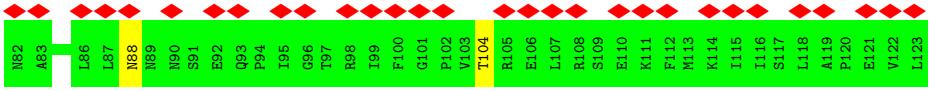
M67 K68 R69 T70 D71 Y75 G79 H80 I81 G82 G83 I84 T88 E91 M92 R95 R96 R99 V100 I101 E102 I103 K106 G107 M108 L109 P110 K111 G112 G115 R116 A117 M118 F119 R120 K121 L122 K123 V124 Y125 A126 E129 H130 N131 H132 Q135 Q136 P137 Q138 V139

• Molecule 57: 50S ribosomal protein L14

Chain t:

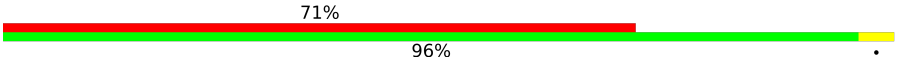


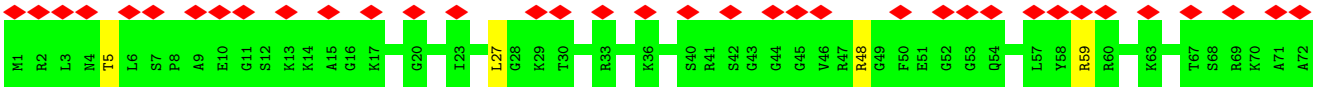


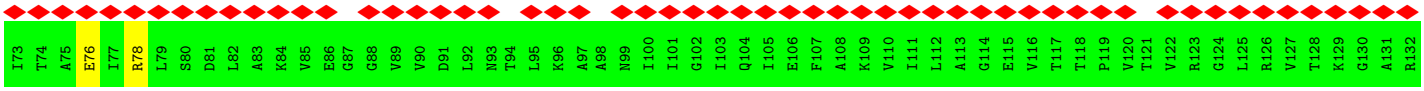


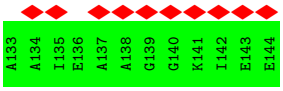
• Molecule 58: 50S ribosomal protein L15

Chain u:



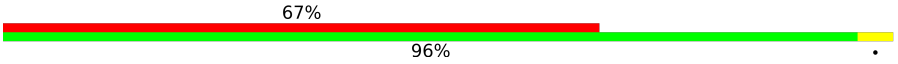


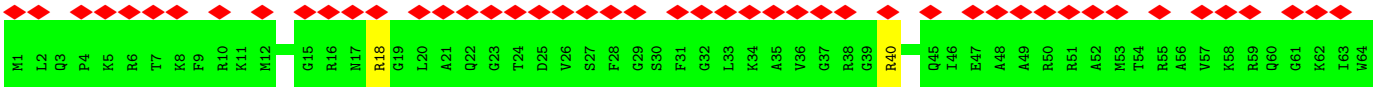


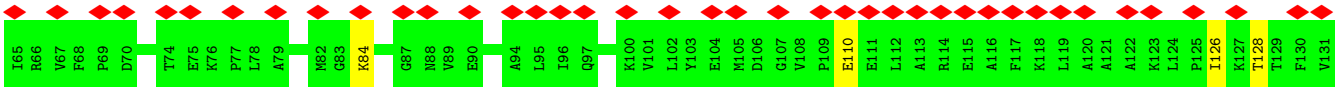


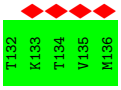
• Molecule 59: 50S ribosomal protein L16

Chain v:



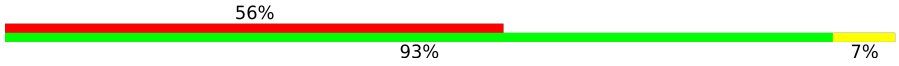


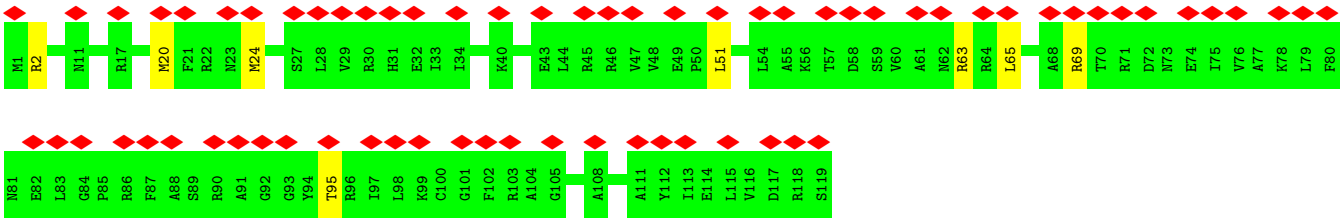




• Molecule 60: 50S ribosomal protein L17

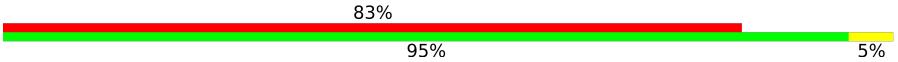
Chain w:

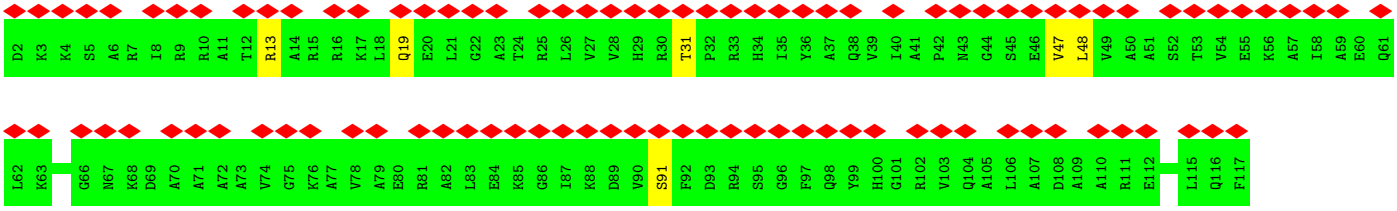




- Molecule 61: 50S ribosomal protein L18

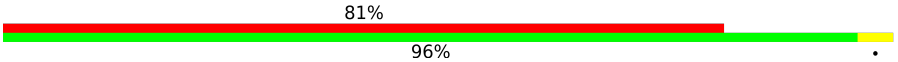
Chain x:

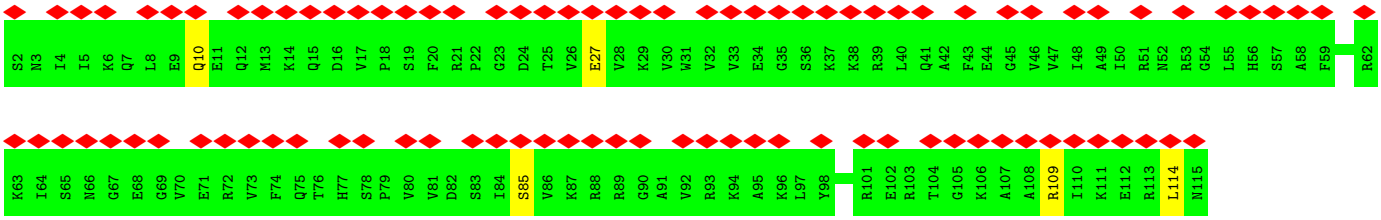




- Molecule 62: 50S ribosomal protein L19

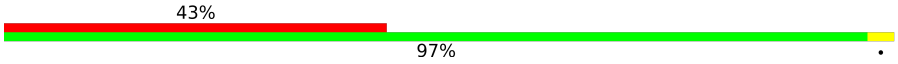
Chain y:

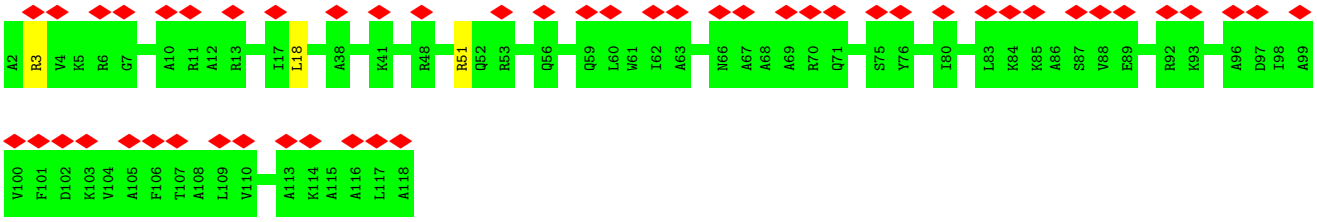




- Molecule 63: 50S ribosomal protein L20

Chain z:





4 Experimental information (i)

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 ($e^-/Å^2$)	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 (i)

5.1 Standard geometry (i)

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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 (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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 (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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 (i)

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	D	1493	A

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

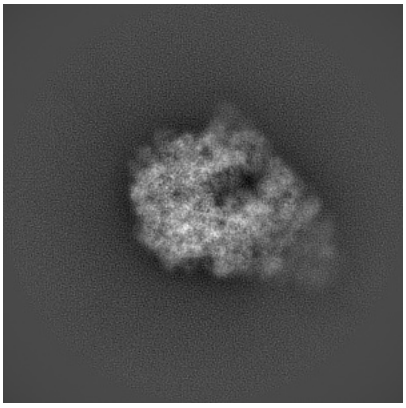
6 Map visualisation (i)

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

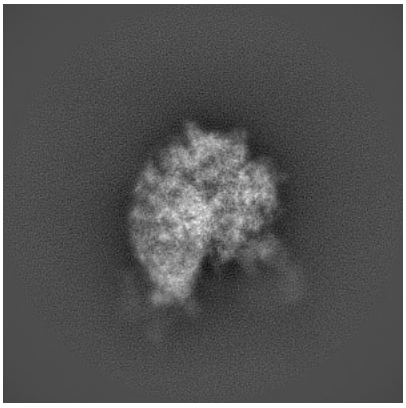
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

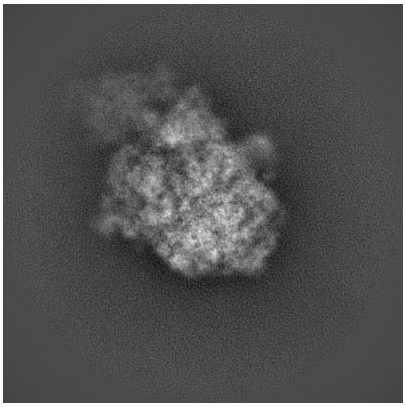
6.1.1 Primary map



X



Y

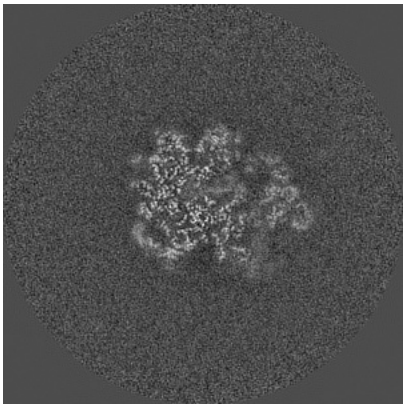


Z

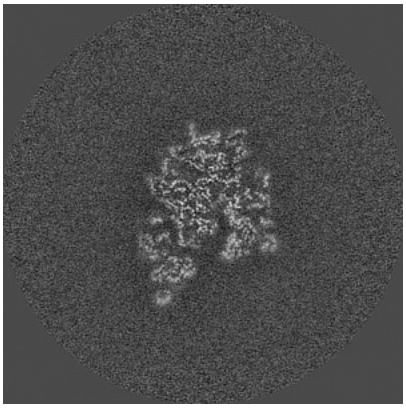
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

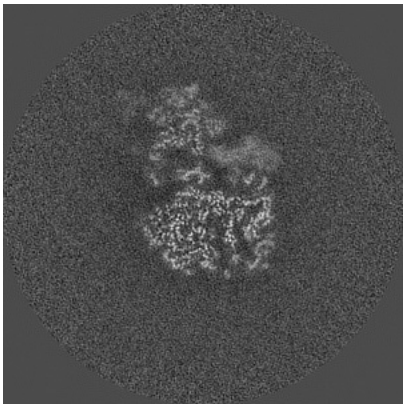
6.2.1 Primary map



X Index: 256



Y Index: 256

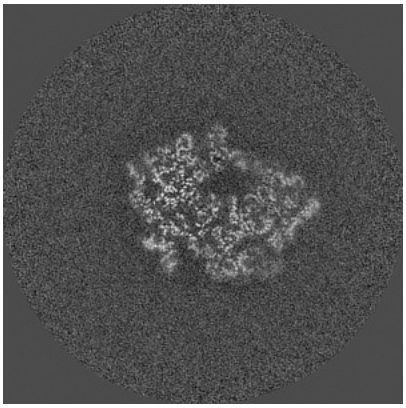


Z Index: 256

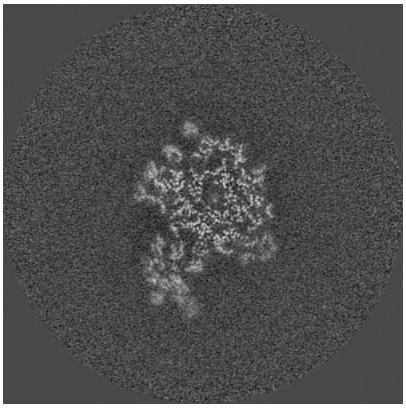
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

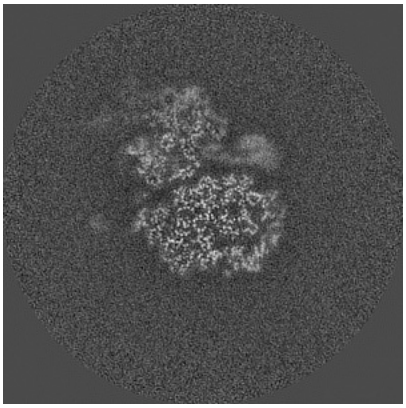
6.3.1 Primary map



X Index: 240



Y Index: 231

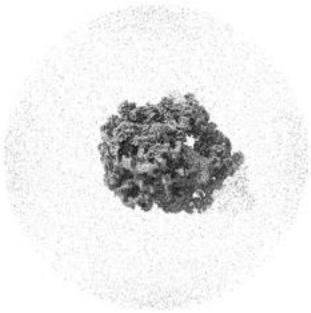


Z Index: 248

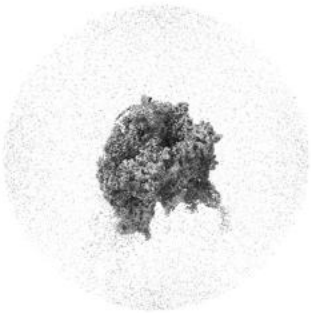
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

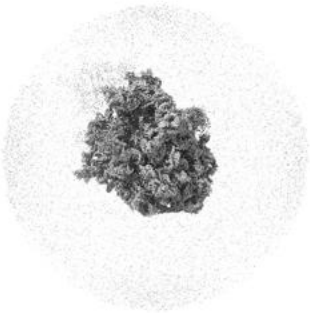
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.017. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

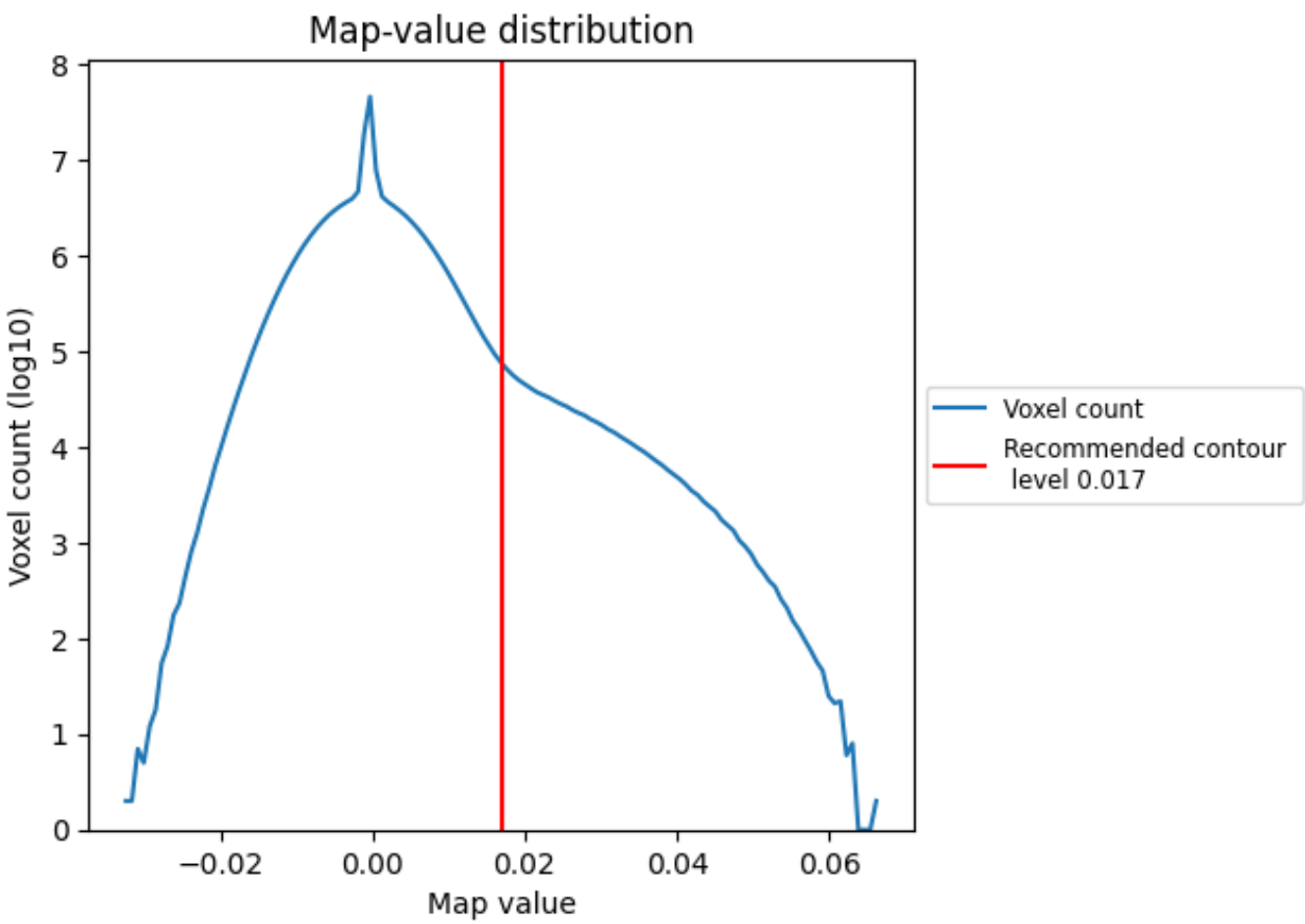
6.5 Mask visualisation (i)

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

7 Map analysis (i)

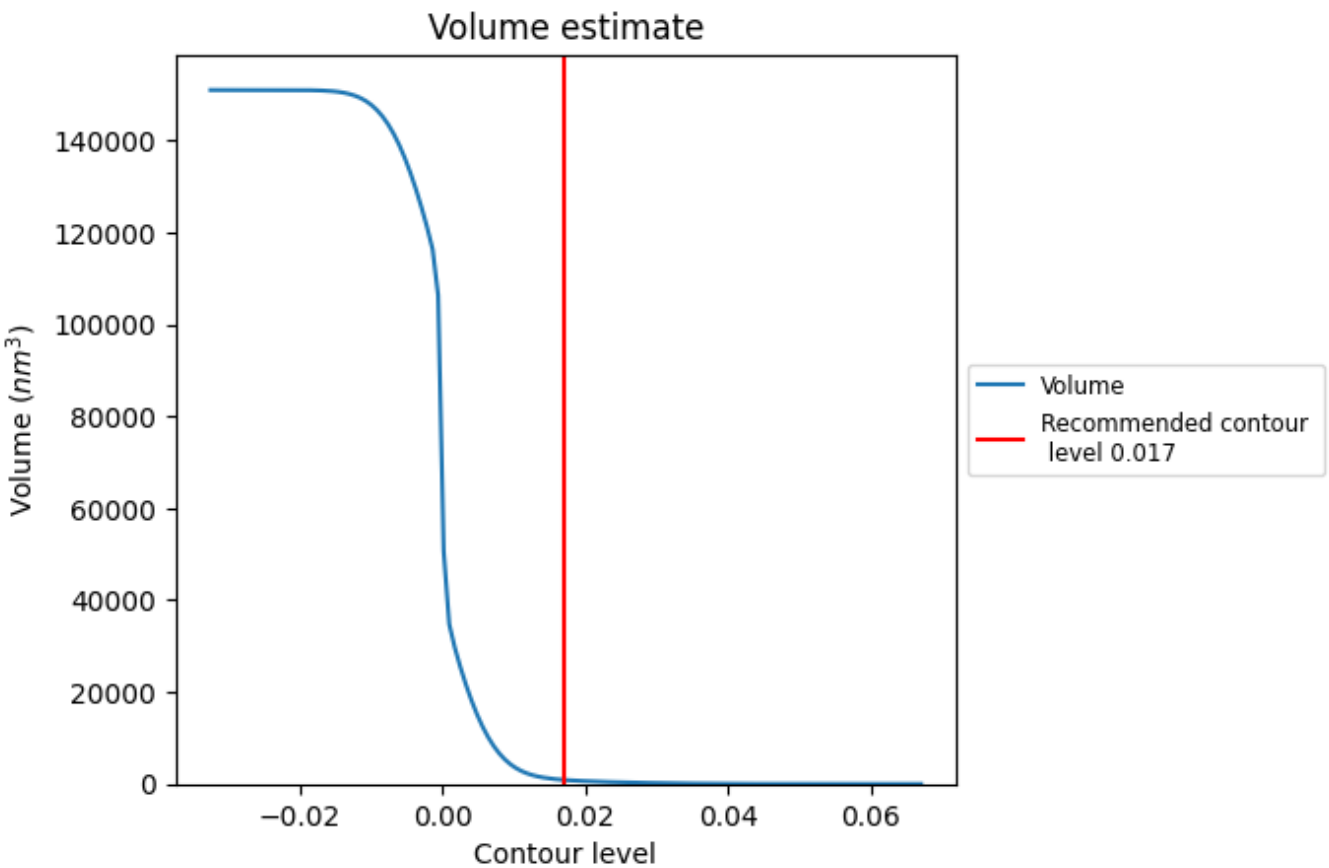
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

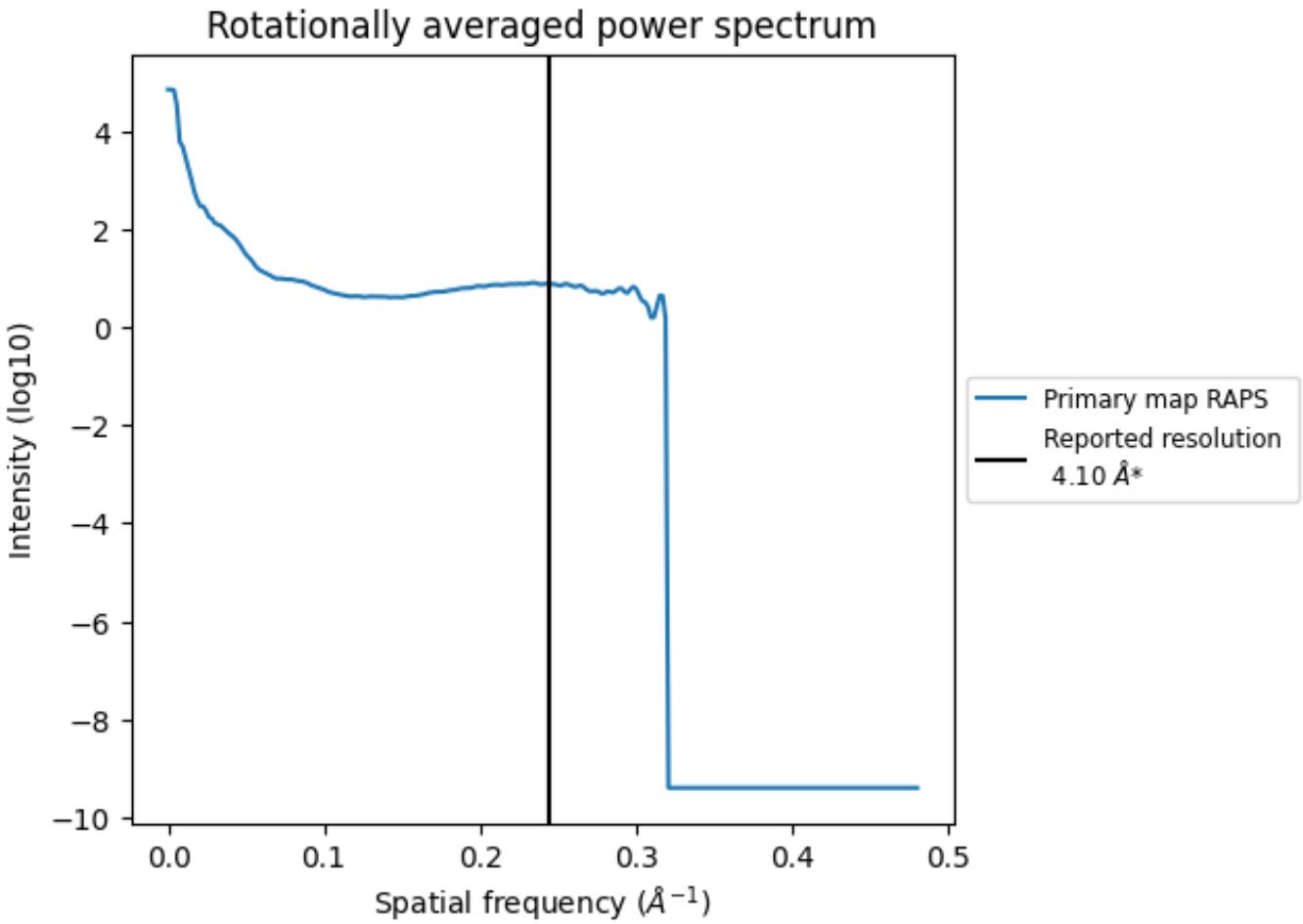
7.2 Volume estimate (i)



The volume at the recommended contour level is 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 (i)



*Reported resolution corresponds to spatial frequency of 0.244 Å^{-1}

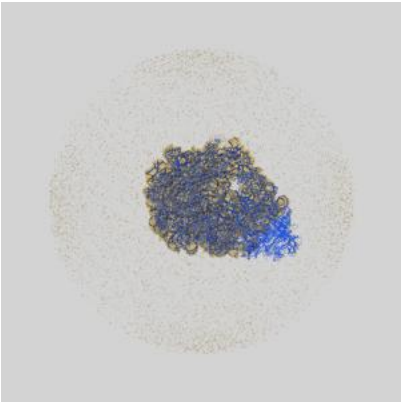
8 Fourier-Shell correlation (i)

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

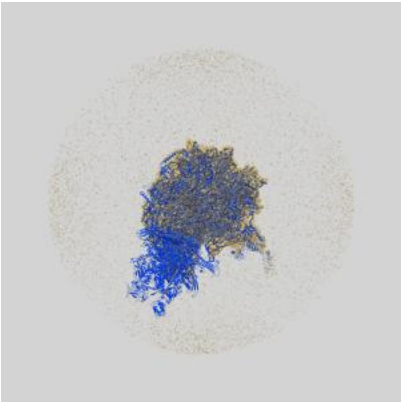
9 Map-model fit (i)

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

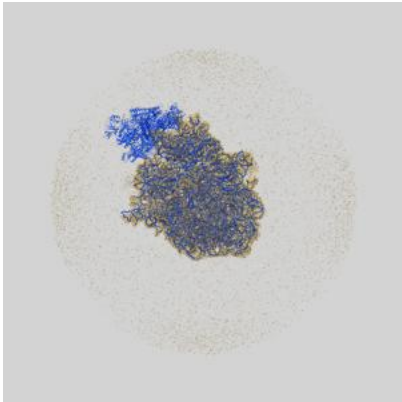
9.1 Map-model overlay (i)



X



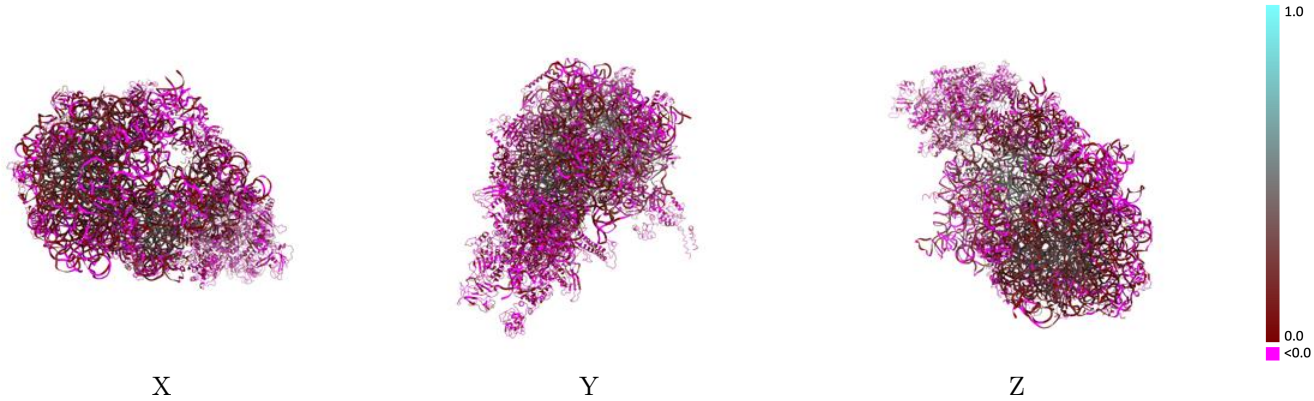
Y



Z

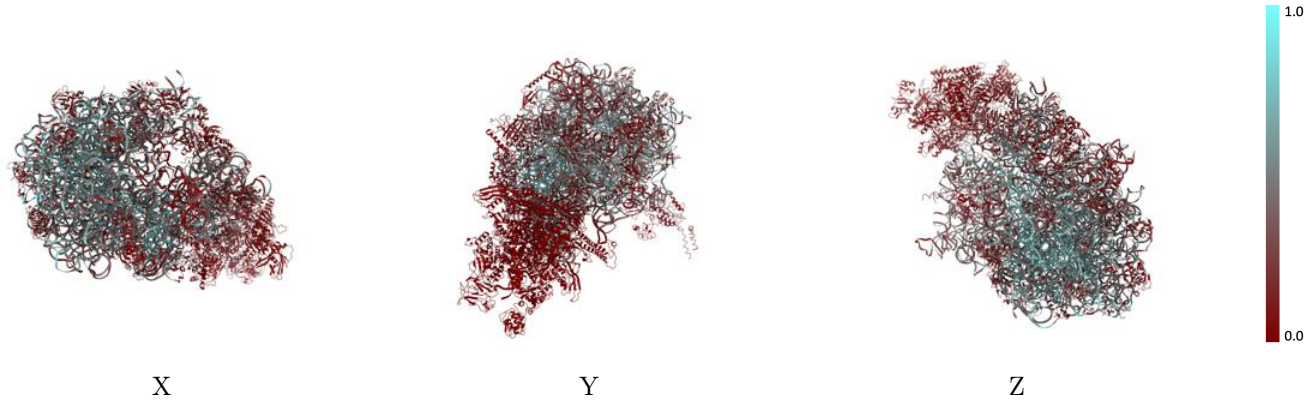
The images above show the 3D surface view of the map at the recommended contour level 0.017 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



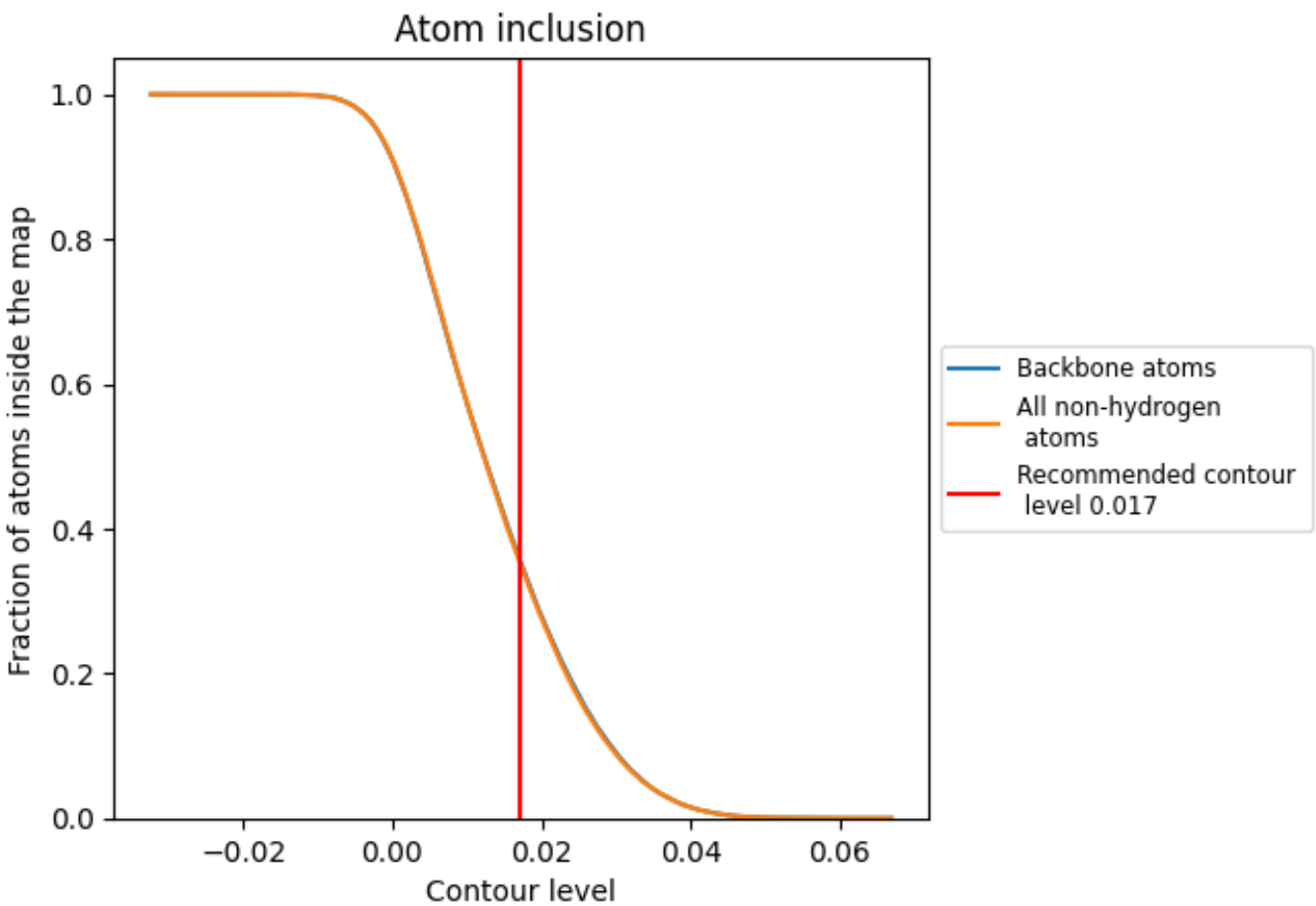
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (i)



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 (i)

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

Continued on next page...

Continued from previous page...

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