



wwPDB EM Validation Summary Report ⓘ

Nov 9, 2024 – 07:48 PM EST

PDB ID : 6X6T
EMDB ID : EMD-22082
Title : Cryo-EM structure of an Escherichia coli coupled transcription-translati
on complex B1 (TTC-B1) containing an mRNA with a 24 nt long spacer,
transcription factors NusA and NusG, and fMet-tRNAs at P-site and E-site
Authors : Molodtsov, V.; Ebright, R.H.; Wang, C.; Su, M.
Deposited on : 2020-05-29
Resolution : 3.20 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

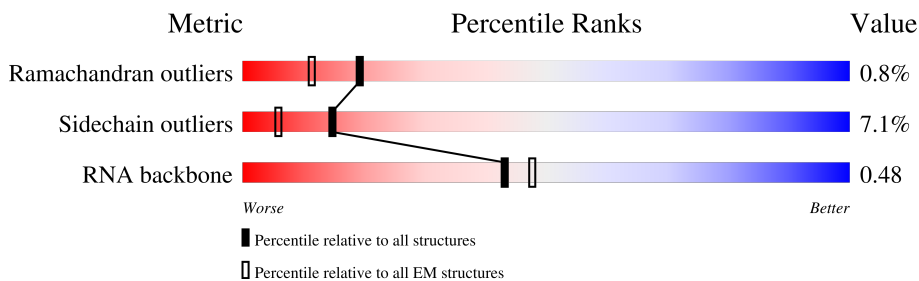
EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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 $\leq 5\%$. 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	68% (Upper red bar) 96% (Red) 96% (Orange) 96% (Yellow) 96% (Green)
2	1	110	79% (Upper red bar) 92% (Red) 92% (Orange) 92% (Yellow) 92% (Green) 8% (Grey)
3	2	100	63% (Upper red bar) 90% (Red) 90% (Orange) 90% (Yellow) 90% (Green) 6% (Grey)
4	3	104	48% (Upper red bar) 93% (Red) 93% (Orange) 93% (Yellow) 93% (Green) 6% (Grey)
5	4	94	59% (Upper red bar) 97% (Red) 97% (Orange) 97% (Yellow) 97% (Green)
6	5	36	64% (Upper red bar) 47% (Red) 17% (Orange) 36% (Yellow) 36% (Green)
7	6	36	75% (Upper red bar) 64% (Red) 11% (Orange) 25% (Yellow) 25% (Green)
8	7	41	71% (Upper red bar) 24% (Red) 41% (Orange) 15% (Yellow) 20% (Green)

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Mol	Chain	Length	Quality of chain
9	9	165	75% 67% 22% 10%
10	A	76	45% 46% 47% 7%
10	B	76	50% 38% 49% 13%
11	AA	1342	100% 99%
12	AB	181	77% 67% 18% 10%
13	AC	329	91% 90% 9%
13	AD	329	91% 91% 9%
14	AE	1407	95% 89% 5% 5%
15	AF	91	90% 90% 10%
16	AG	495	74% 69% 27%
17	C	75	40% 84% 12%
18	D	1542	27% 78% 21%
19	E	87	75% 95%
20	F	71	59% 94%
21	G	241	39% 88% 5% 7%
22	H	557	45% 42% 54%
23	I	233	33% 85% 11%
24	J	206	52% 97%
25	K	167	58% 87% 7% 7%
26	L	135	52% 69% 8% 23%
27	M	179	18% 79% 5% 16%
28	N	130	63% 97%
29	O	130	30% 92% 5%
30	P	103	45% 84% 12%
31	Q	129	29% 88% 9%

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Mol	Chain	Length	Quality of chain
32	R	124	70% 91% 6%
33	S	101	45% 94% 5%
34	T	89	66% 83% 16%
35	U	82	66% 94% 6%
36	V	84	49% 90% 5% 5%
37	W	92	55% 86% 10%
38	X	118	59% 86% 12%
39	Y	142	97% 84% 15%
40	Z	121	25% 17% 7% 75%
41	a	2904	47% 78% 20%
42	b	85	62% 89% 11%
43	c	78	58% 95% ..
44	d	120	37% 85% 15%
45	e	63	59% 98% .
46	f	59	63% 93% 5% .
47	g	70	73% 87% 7% 6%
48	h	273	66% 94% 5% .
49	i	57	67% 88% 11% .
50	j	209	66% 95% 5%
51	k	55	62% 91% 5%
52	l	201	69% 95% 5%
53	m	46	65% 93% 7%
54	n	179	68% 91% 8% .
55	o	65	63% 92% 5% ..
56	p	177	76% 95% ..

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Mol	Chain	Length	Quality of chain
57	q	38	<p>79% 95% 5%</p>
58	r	149	<p>72% 94% 6%</p>
59	s	142	<p>71% 96% •</p>
60	t	123	<p>67% 93% 7%</p>
61	u	144	<p>62% 95% 5%</p>
62	v	136	<p>72% 97% •</p>
63	w	127	<p>59% 89% 5% 6%</p>
64	x	117	<p>60% 95% • •</p>
65	y	115	<p>62% 96% • •</p>
66	z	118	<p>63% 96% • •</p>

2 Entry composition [i](#)

There are 68 unique types of molecules in this entry. The entry contains 291628 atoms, of which 109913 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 24 nt long spacer.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
8	7	33	784	307	97	96	251	33	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	AA	1340	10567	6631	1841	2052	43	0	0

- Molecule 12 is a protein called Transcription termination/antitermination protein NusG.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
12	AB	162	1283	816	1	222	237	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	AC	301	2094	1296	379	413	6	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	AD	299	2078	1287	378	407	6	0	0

- Molecule 14 is a protein called DNA-directed RNA polymerase subunit beta'.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AE	1384	VAL	MET	conflict	UNP A0A4S1NBU2

- Molecule 15 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	AF	82	650	396	122	131	1	0	0

- Molecule 16 is a protein called Transcription termination/antitermination protein NusA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	AG	495	3852	2396	669	774	13	0	0

- Molecule 17 is a protein called 30S ribosomal protein S18.

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

- Molecule 18 is a RNA chain called 16S rRNA.

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

- Molecule 19 is a protein called 30S ribosomal protein S20.

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

- Molecule 20 is a protein called 30S ribosomal protein S21.

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

- Molecule 21 is a protein called 30S ribosomal protein S2.

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

- Molecule 22 is a protein called 30S ribosomal protein S1.

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

- Molecule 23 is a protein called 30S ribosomal protein S3.

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

- Molecule 24 is a protein called 30S ribosomal protein S4.

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

- Molecule 25 is a protein called 30S ribosomal protein S5.

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

- Molecule 26 is a protein called 30S ribosomal protein S6.

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

- Molecule 27 is a protein called 30S ribosomal protein S7.

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

- Molecule 28 is a protein called 30S ribosomal protein S8.

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

- Molecule 29 is a protein called 30S ribosomal protein S9.

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

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

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

- Molecule 31 is a protein called 30S ribosomal protein S11.

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

- Molecule 32 is a protein called 30S ribosomal protein S12.

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

- Molecule 33 is a protein called 30S ribosomal protein S14.

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

- Molecule 34 is a protein called 30S ribosomal protein S15.

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

- Molecule 35 is a protein called 30S ribosomal protein S16.

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

- Molecule 36 is a protein called 30S ribosomal protein S17.

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

- Molecule 37 is a protein called 30S ribosomal protein S19.

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

- Molecule 38 is a protein called 30S ribosomal protein S13.

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

- Molecule 39 is a protein called 50S ribosomal protein L11.

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

- Molecule 40 is a protein called 50S ribosomal protein L7/L12.

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

- Molecule 41 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
41	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 42 is a protein called 50S ribosomal protein L27.

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

- Molecule 43 is a protein called 50S ribosomal protein L28.

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

- Molecule 44 is a RNA chain called 5S rRNA.

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

- Molecule 45 is a protein called 50S ribosomal protein L29.

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

- Molecule 46 is a protein called 50S ribosomal protein L30.

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

- Molecule 47 is a protein called 50S ribosomal protein L31.

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

- Molecule 48 is a protein called 50S ribosomal protein L2.

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

- Molecule 49 is a protein called 50S ribosomal protein L32.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L33.

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

- Molecule 52 is a protein called 50S ribosomal protein L4.

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

- Molecule 53 is a protein called 50S ribosomal protein L34.

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

- Molecule 54 is a protein called 50S ribosomal protein L5.

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

- Molecule 55 is a protein called 50S ribosomal protein L35.

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

- Molecule 56 is a protein called 50S ribosomal protein L6.

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

- Molecule 57 is a protein called 50S ribosomal protein L36.

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

- Molecule 58 is a protein called 50S ribosomal protein L9.

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

- Molecule 59 is a protein called 50S ribosomal protein L13.

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

- Molecule 60 is a protein called 50S ribosomal protein L14.

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

- Molecule 61 is a protein called 50S ribosomal protein L15.

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

- Molecule 62 is a protein called 50S ribosomal protein L16.

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

- Molecule 63 is a protein called 50S ribosomal protein L17.

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

- Molecule 64 is a protein called 50S ribosomal protein L18.

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

- Molecule 65 is a protein called 50S ribosomal protein L19.

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

- Molecule 66 is a protein called 50S ribosomal protein L20.

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

- Molecule 67 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
67	7	1	Total	Mg	0
			1	1	

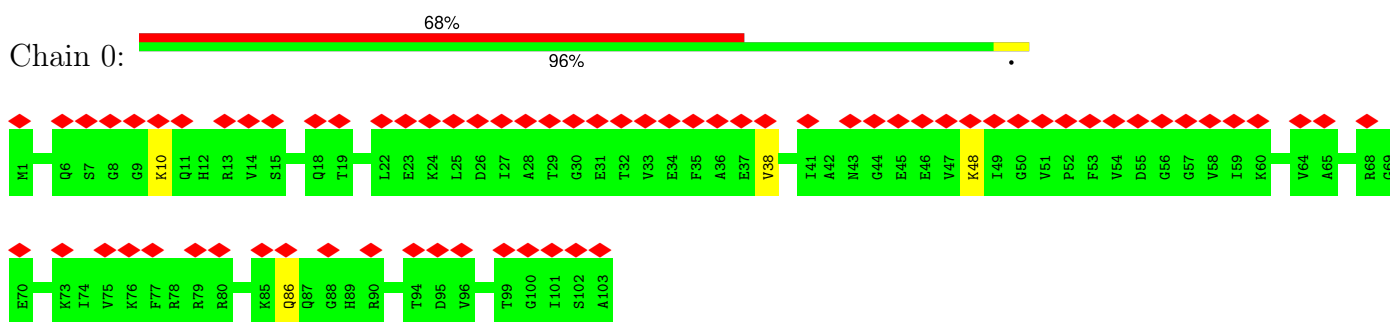
- Molecule 68 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
68	AA	2	Total	Zn	0
			2	2	

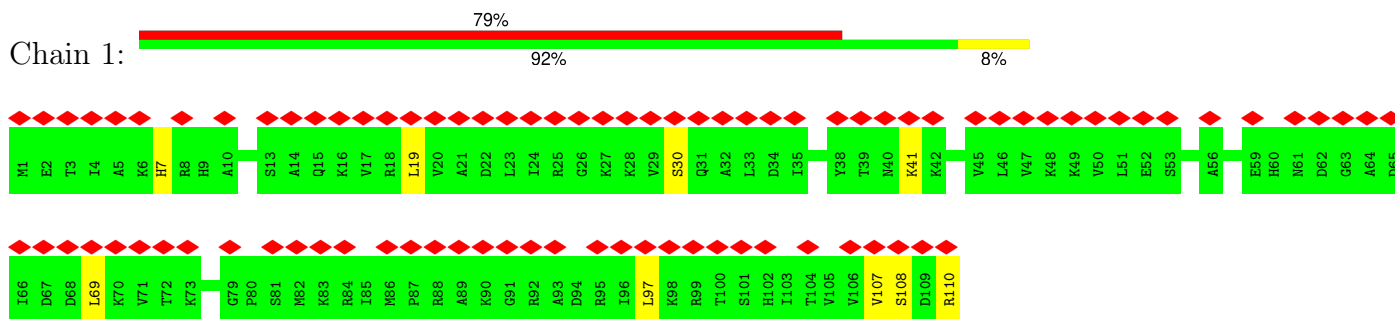
3 Residue-property plots [i](#)

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.

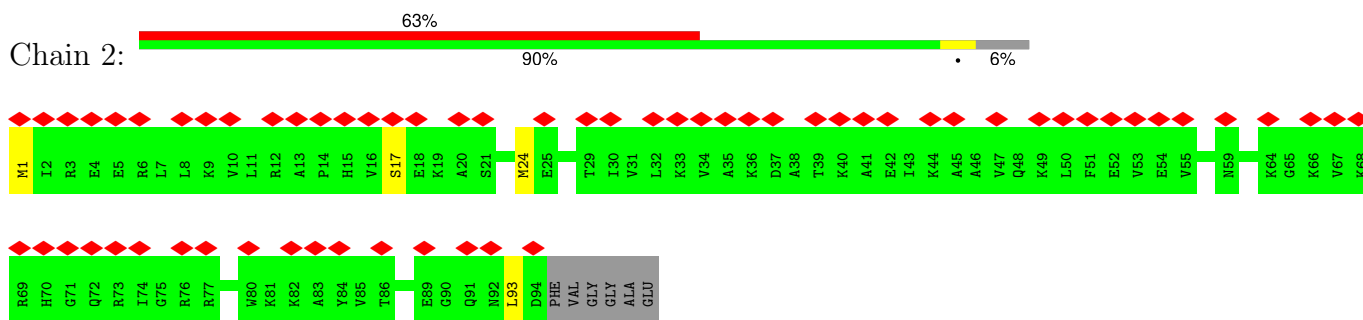
- Molecule 1: 50S ribosomal protein L21



- Molecule 2: 50S ribosomal protein L22

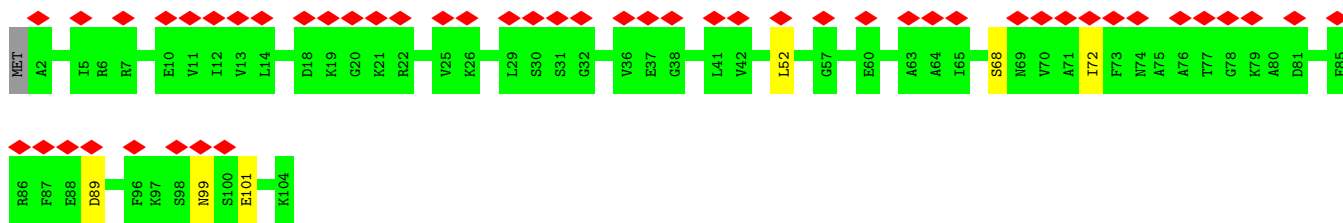


- Molecule 3: 50S ribosomal protein L23

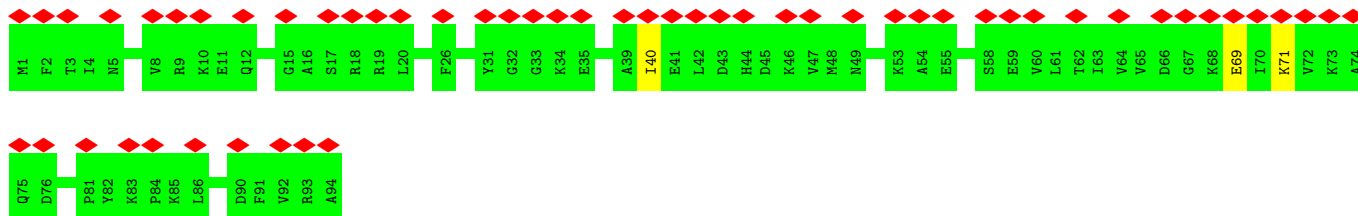


- Molecule 4: 50S ribosomal protein L24

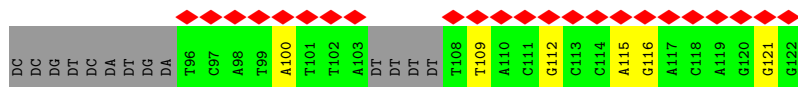




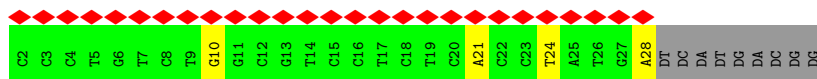
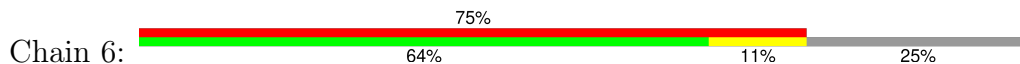
• Molecule 5: 50S ribosomal protein L25



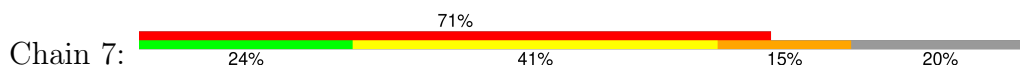
• Molecule 6: NT DNA



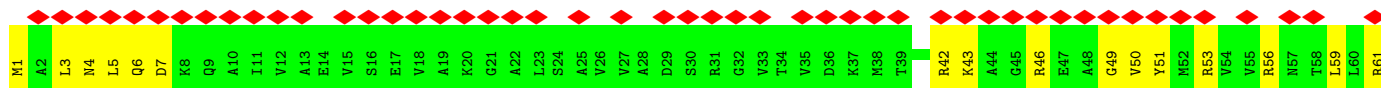
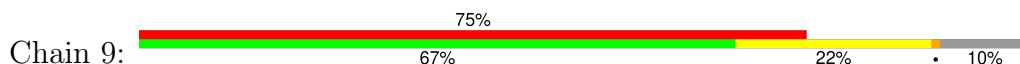
• Molecule 7: T DNA

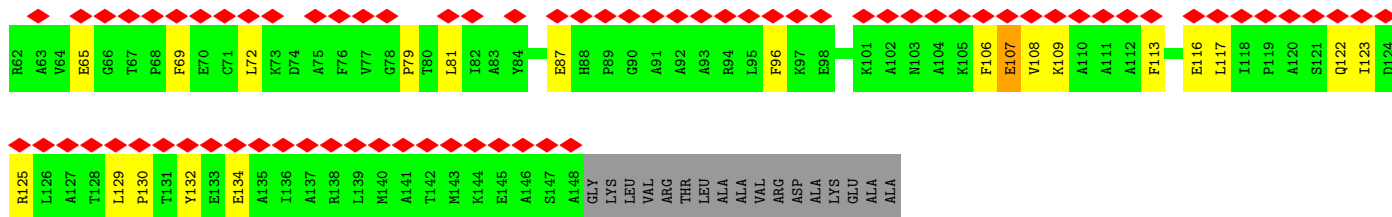


• Molecule 8: mRNA with 24 nt long spacer

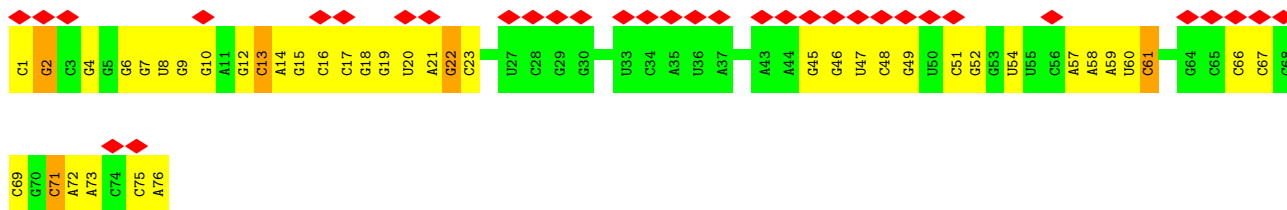


• Molecule 9: 50S ribosomal protein L10

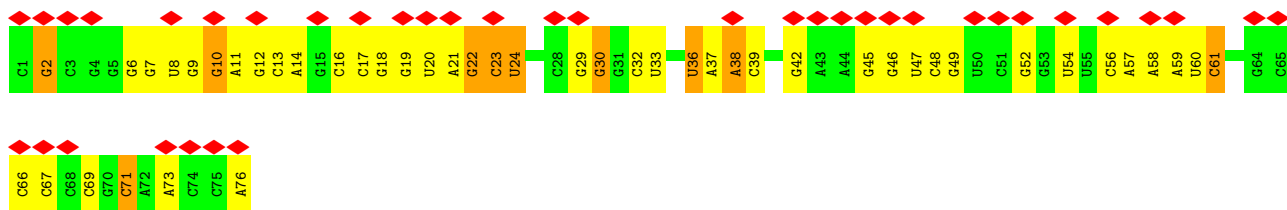
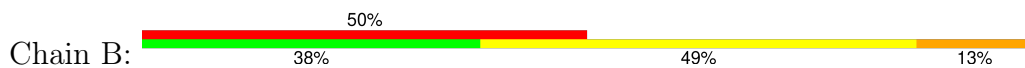




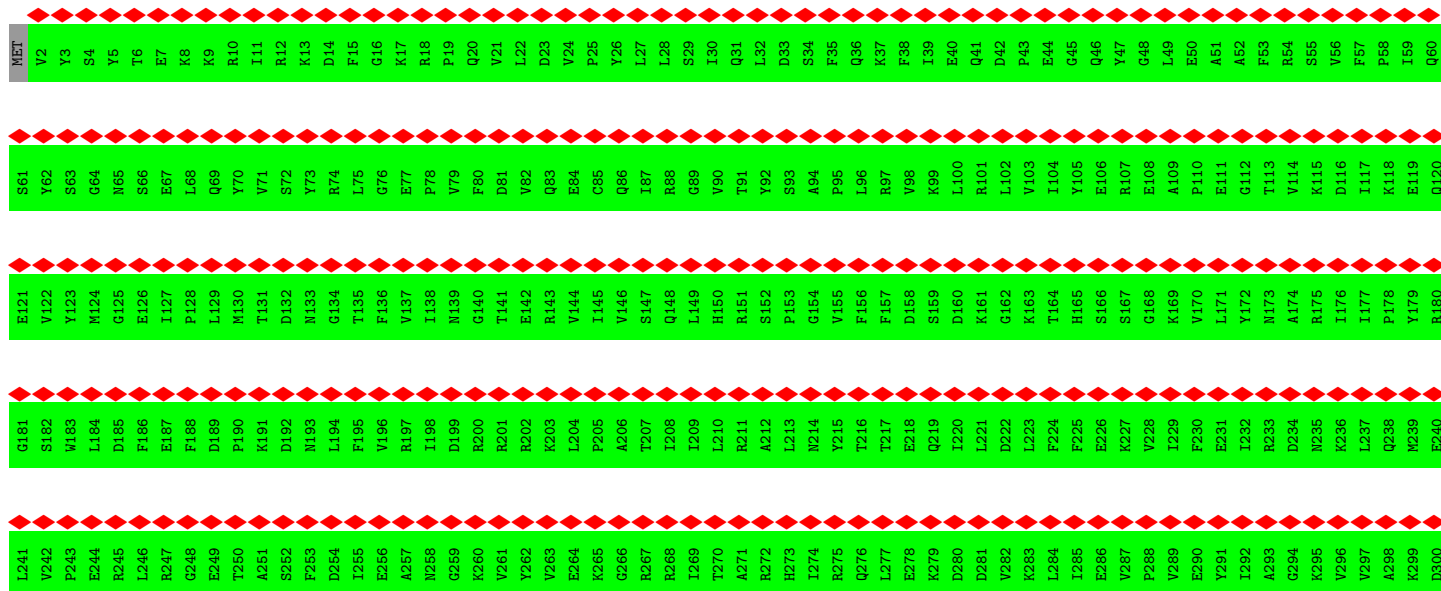
• Molecule 10: E-site and P-site tRNA (fMet)



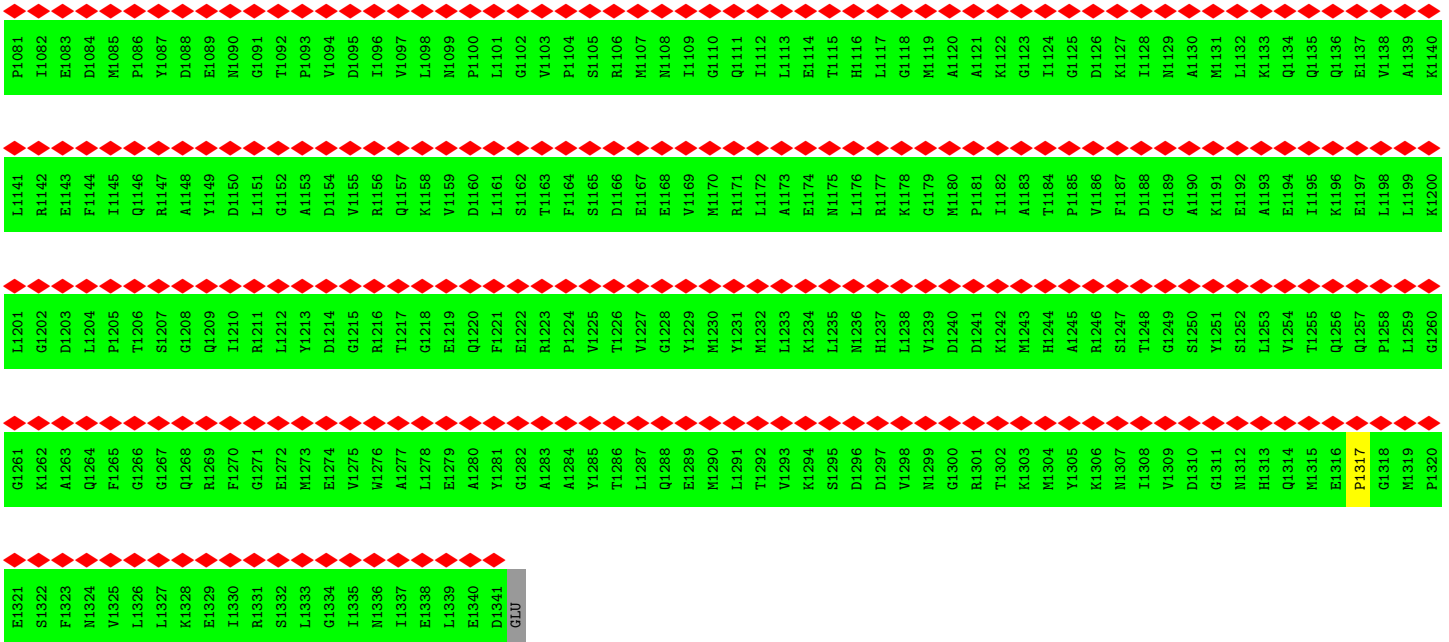
• Molecule 10: E-site and P-site tRNA (fMet)



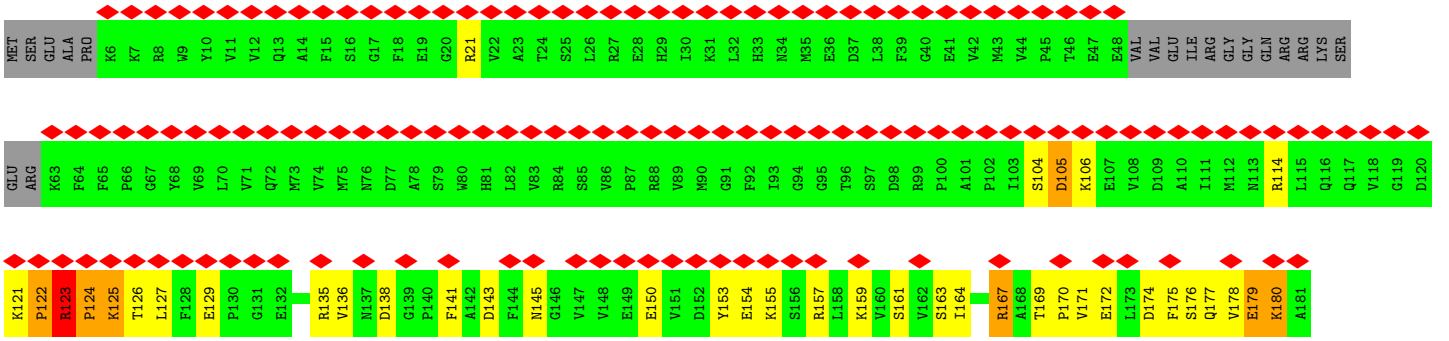
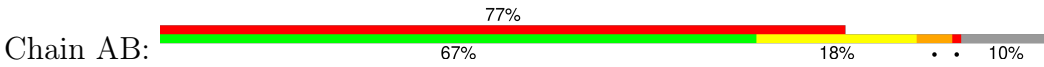
• Molecule 11: DNA-directed RNA polymerase subunit beta



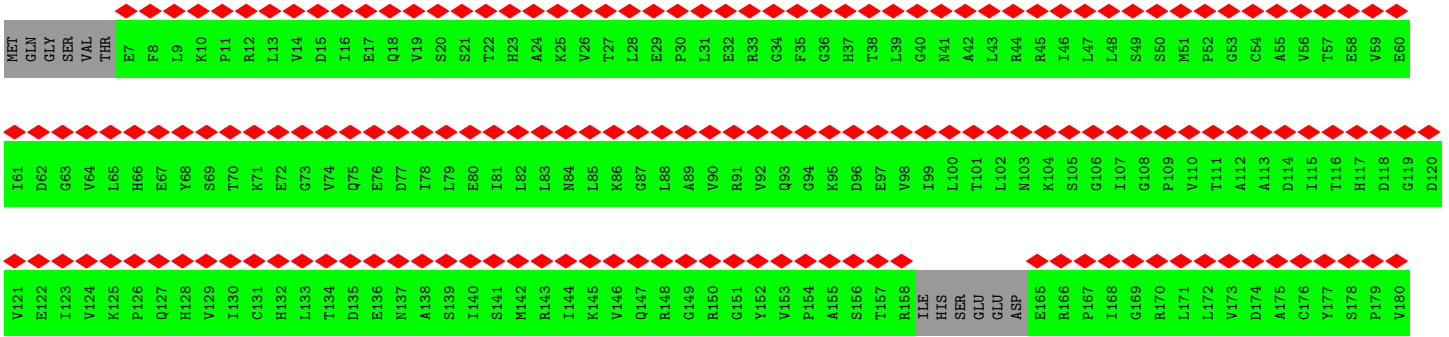
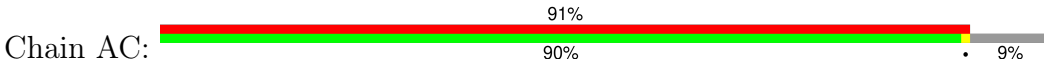
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H1023	E963	T843	L783	V723	V663	I603	A543	D483	D423	L363	D303
E1024	L964	K844	A784	V724	G664	H604	G544	L484	D424	V364	E304
F1025	Q965	L845	D785	V725	A665	Y605	F545	D485	I425	E365	S305
E1026	F966	G846	G786	Q726	S666	L606	E546	T486	I426	I366	T306
K1027	L967	P847	P787	V727	L667	S607	V547	L487	D427	Y367	G307
K1028	E968	E848	S788	D728	1668	A608	R548	M488	V428	R368	E308
L1029	A969	E849	T789	A729	P669	I609	D549	P489	M429	M369	L309
E1030	G970	T850	D790	S730	F670	E610	V550	Q490	K430	M370	I310
A1031	L971	T851	L791	R731	L671	E611	H551	D491	K431	R371	C311
K1032	F972	A852	G792	I732	E672	G612	P552	M492	L432	P372	A312
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R1034	R974	L854	L794	I734	D674	Y614	H554	M494	D434	E374	N314
K1035	I975	P855	A795	K735	D675	V615	Y555	A495	I435	P375	M315
I1036	R976	N856	L796	V736	A676	I616	G556	K496	R436	P376	E316
T1037	A977	V857	G797	M737	N677	A617	R557	P497	R437	T377	L317
Q1038	V978	G858	Q798	E738	R678	Q618	V558	I498	G438	R378	S318
G1039	L979	E859	M799	D739	A679	A619	C559	S499	K439	E379	L319
D1040	V980	A860	H800	E740	L680	N620	P560	A500	G440	A380	D320
D1041	A981	A861	R801	M741	M681	S621	I561	A501	E441	A381	L321
L1042	N922	L862	V802	Y742	G682	N622	E562	V502	D442	E382	L322
A1043	G923	S863	A803	P743	A683	L623	T563	K503	D443	S383	A323
P1044	V924	K864	F804	G744	N684	D624	P564	E504	D444	L384	K324
E985	S925	L865	M805	E745	M685	E625	E565	F505	I445	F385	L325
G1046	G926	D866	P806	A746	Q686	E626	G566	F506	D446	E386	S326
L1047	T927	E867	M807	G747	R687	G627	P567	F507	H447	N387	Q327
K1048	V928	S868	N808	I748	Q688	H628	N568	S508	L448	L388	S328
L989	I929	G869	G809	D749	A689	F629	I569	S509	G449	F389	G329
V1050	D930	T870	Y810	I750	V690	V630	G570	Q510	N450	F390	H330
K1051	V931	H871	M811	Y751	P691	E631	L571	L511	R451	S391	K331
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Y1053	R933	L873	E813	L753	L693	L633	N573	Q513	I453	D393	I333
L1054	F934	G874	D814	T754	R694	V634	S574	F514	R454	R394	E334
A1055	T935	A875	S815	K755	A695	T635	L575	S455	S455	Y395	T335
V1056	R936	E876	I816	Y756	D696	G636	S576	D516	V456	D396	L336
K1057	D937	V877	L817	T757	K697	R637	V577	Q517	G457	L397	F337
L998	G938	T878	V818	R758	P698	S638	V578	N518	E458	S398	T338
R1059	V939	G879	S819	S759	L699	K639	A579	N519	M459	A399	N339
I1060	E940	G880	E820	N760	V700	G640	Q580	P520	A460	V400	D340
Q1061	D941	D881	R821	Q761	G701	E641	T581	L521	E461	G401	L341
L1002	D942	I882	V822	T762	T702	S642	N582	S522	R402	R402	D342
G1063	K943	L883	R823	T763	G703	S643	E583	E523	Q463	M403	H343
D1064	R944	H884	Q824	C764	M704	L644	Y584	I524	F464	K404	G344
E1005	A945	G885	E825	I765	E705	F645	G585	T525	R465	F405	P345
M1066	L946	K886	D826	N766	R706	S646	G586	H526	V466	M406	P346
A1067	E947	V887	R827	Q767	A707	R647	L587	K527	G467	R407	I347
Q1068	I948	T888	F828	M768	V708	D648	E588	R528	L468	S408	S348
R1069	E949	P889	T829	P769	A709	Q649	T589	R529	V469	L409	E349
H1070	Q950	K890	T830	C770	V710	V650	P590	I530	R470	L409	T350
G1071	L951	G891	L831	V771	D711	D651	Y591	S531	V471	R411	L351
K1072	Q952	E892	H832	S772	S712	Y652	R592	A532	E472	E412	R352
I1073	L953	T893	L833	L773	G713	M653	K593	L533	R473	E413	V353
G1074	K954	D894	Q834	G774	V714	D654	Y594	G534	A474	I414	D354
V1075	Q955	L895	E835	E775	T715	V655	T595	P535	V475	E415	P355
I1076	A956	T896	L836	P776	A716	S656	D596	G536	K476	G416	T356
S1077	K957	P897	A837	V777	V717	T657	G597	G537	E477	S417	N357
K1078	I958	E898	C838	E778	A718	Q658	V598	L538	R478	G418	R358
I1079	D959	E899	V839	R779	K719	Q659	V599	T539	L479	I419	R359
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• Molecule 12: Transcription termination/antitermination protein NusG

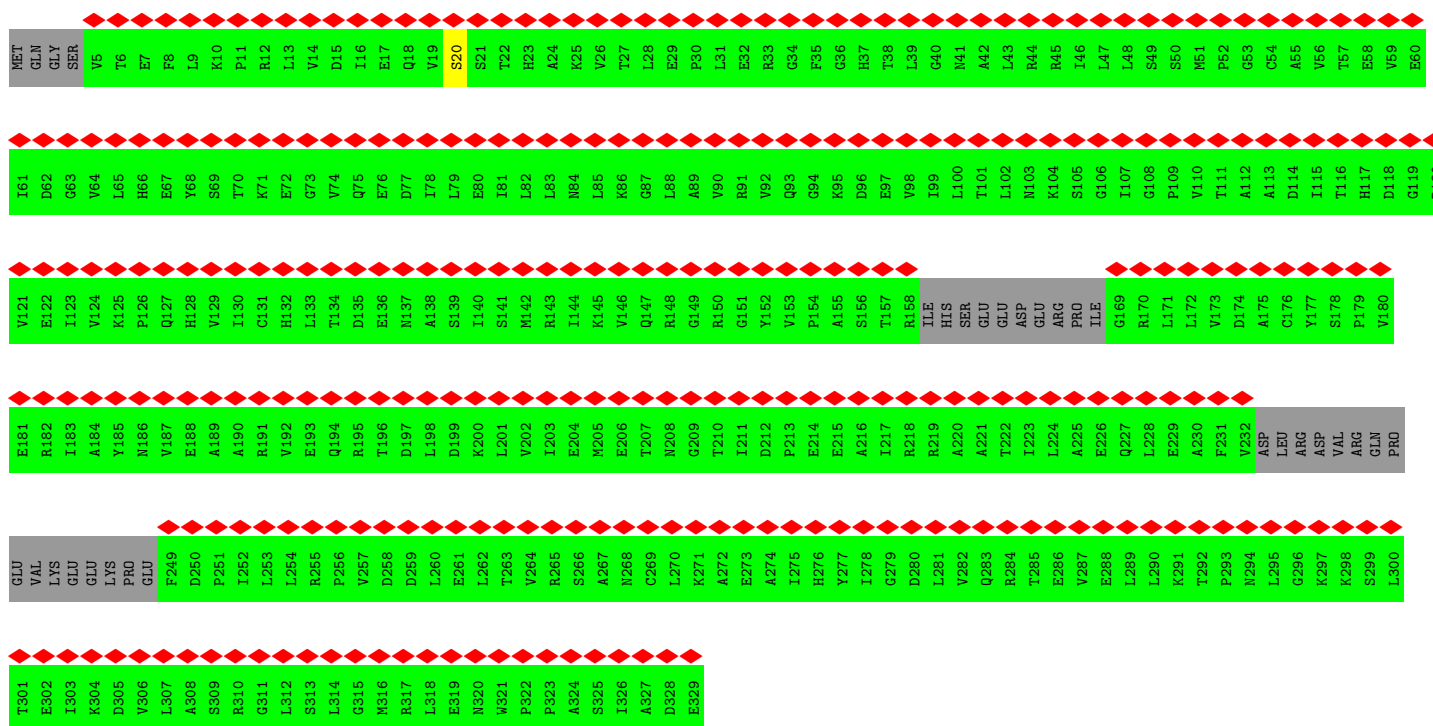


• Molecule 13: DNA-directed RNA polymerase subunit alpha

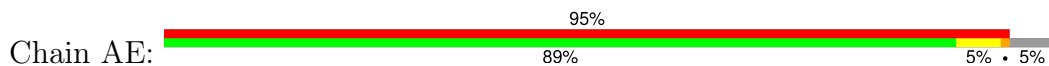




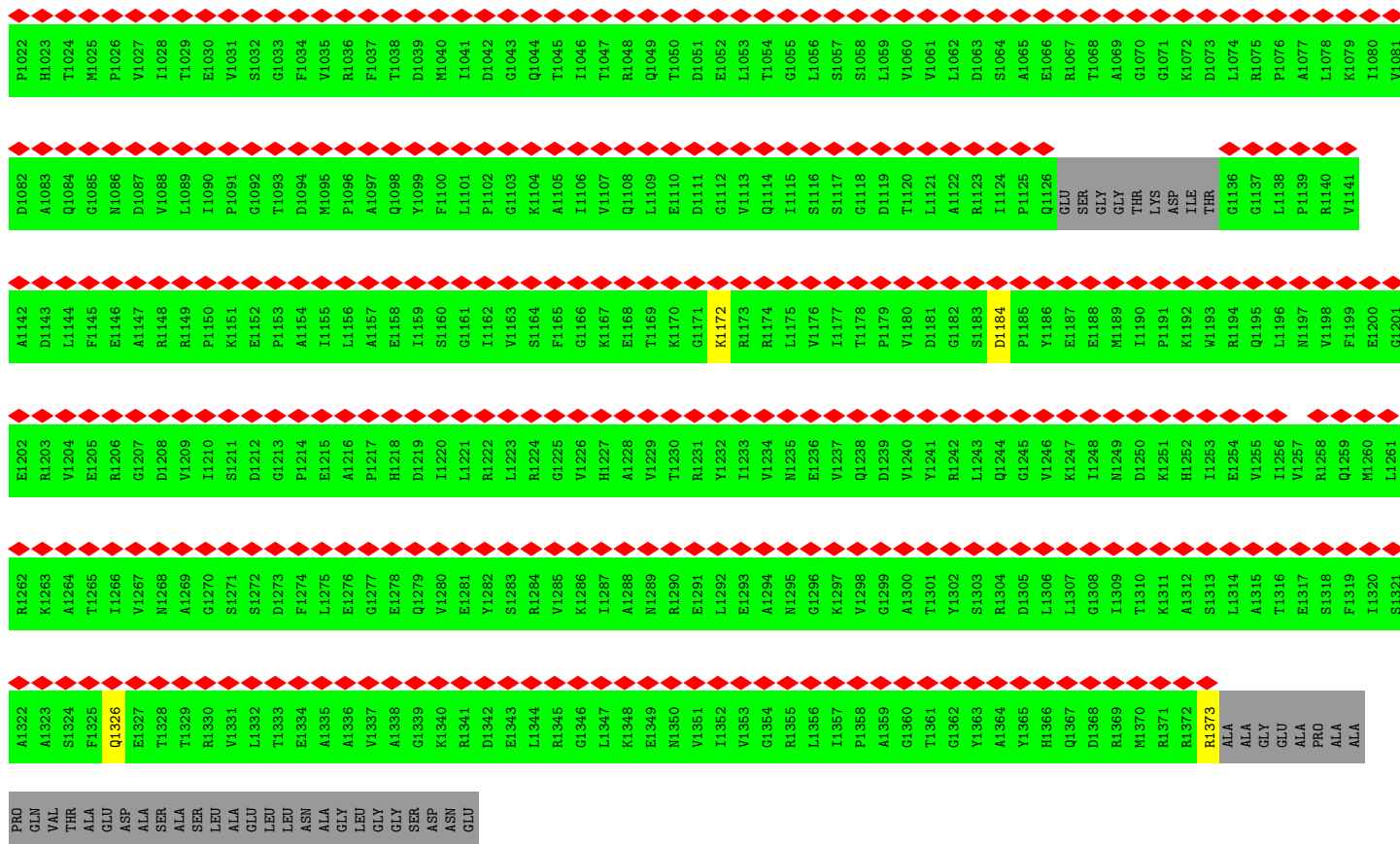
• Molecule 13: DNA-directed RNA polymerase subunit alpha



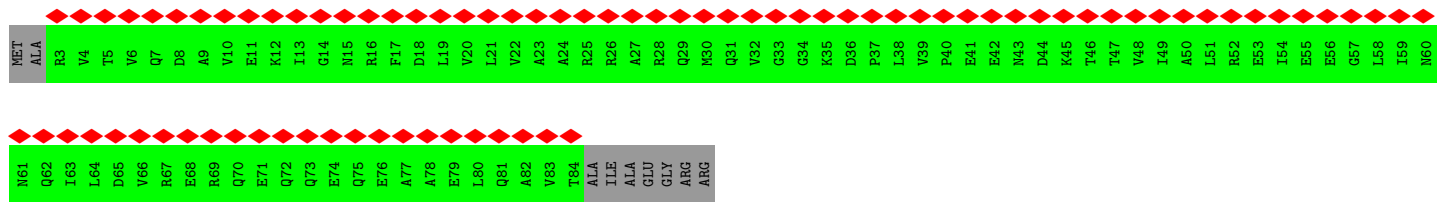
• Molecule 14: DNA-directed RNA polymerase subunit beta



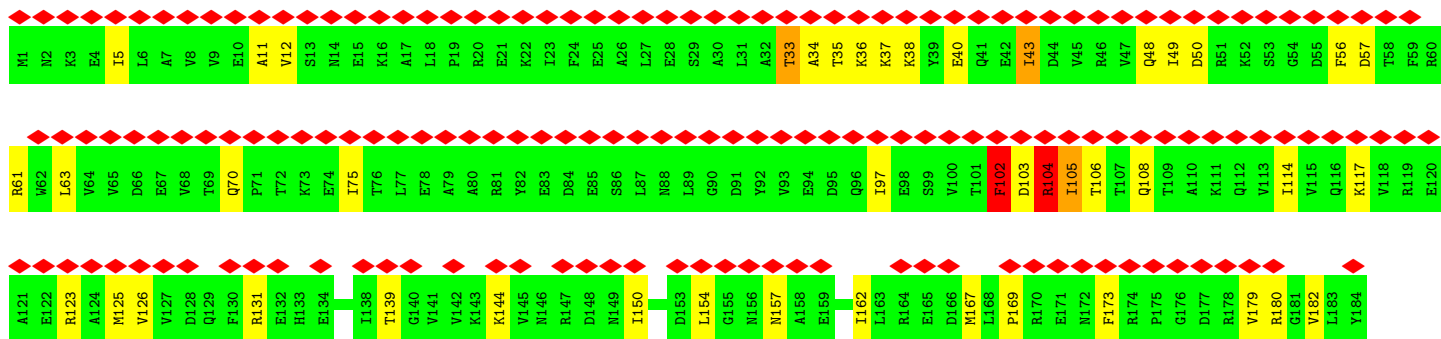
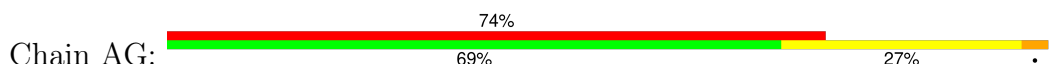
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L242	P243	V244	L245	P246	P247	D248	L249	R250	P251	L252	V253	P254	L255	D256	G257	G258	R259	F260	A261	T262	S263	D264	L265	N266	D267	L268	Y269	R270	R271	V272	I273	K274	N275	N276	N277	R278	L279	K280	R281	L282	L283	D284	L285	A286	A287	P288	D289	I290	G291	V292	R293	N294	E295	W296	R297	M298	L299	Q300	E301	
A302	V303	D304	A305	L306	L307	D308	N309	K310	G311	R312	G313	R314	A315	L316	T317	G318	S319	N320	K321	R322	S323	L324	K325	S326	L327	R328	A328	D329	M330	I331	K332	G333	K334	Q335	G336	R337	F338	R339	Q340	N341	L342	L343	G344	K345	R346	R347	D348	Y349	S350	G351	R352	S353	V354	E355	T356	R357	G358	L359	Y360	L361
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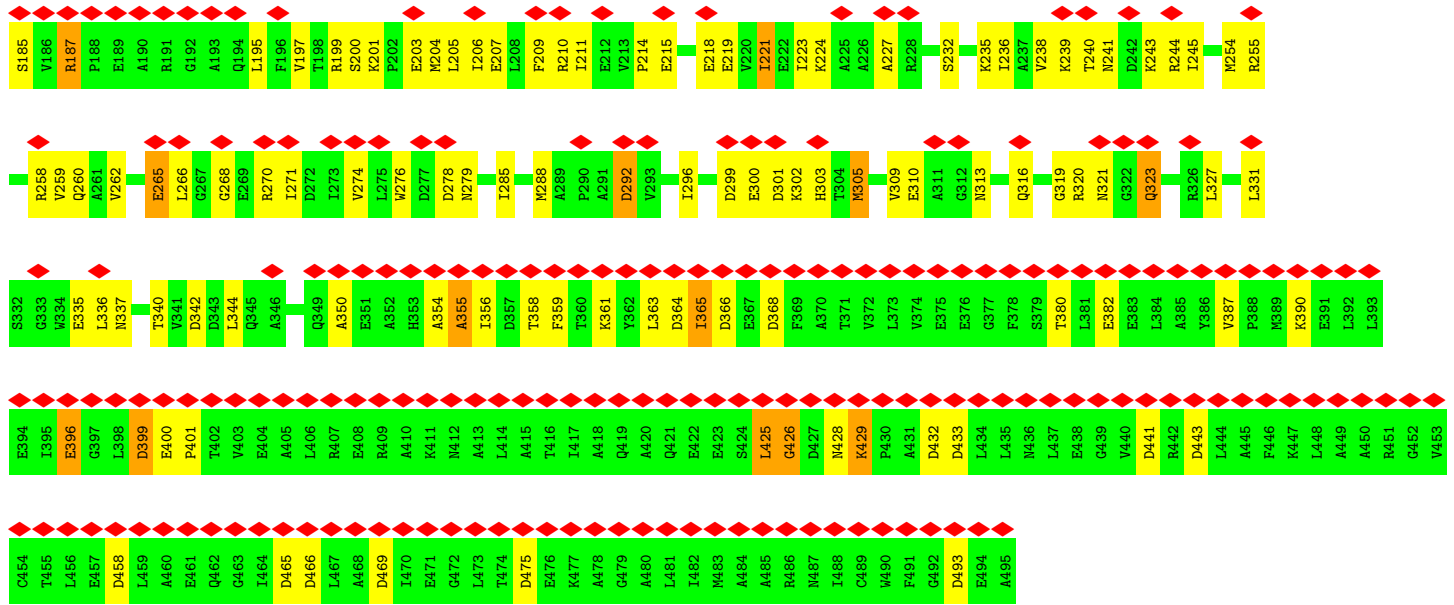


• Molecule 15: DNA-directed RNA polymerase subunit omega

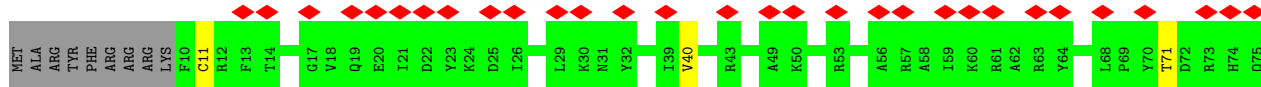
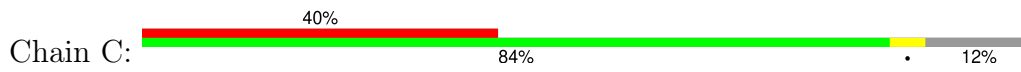


• Molecule 16: Transcription termination/antitermination protein NusA

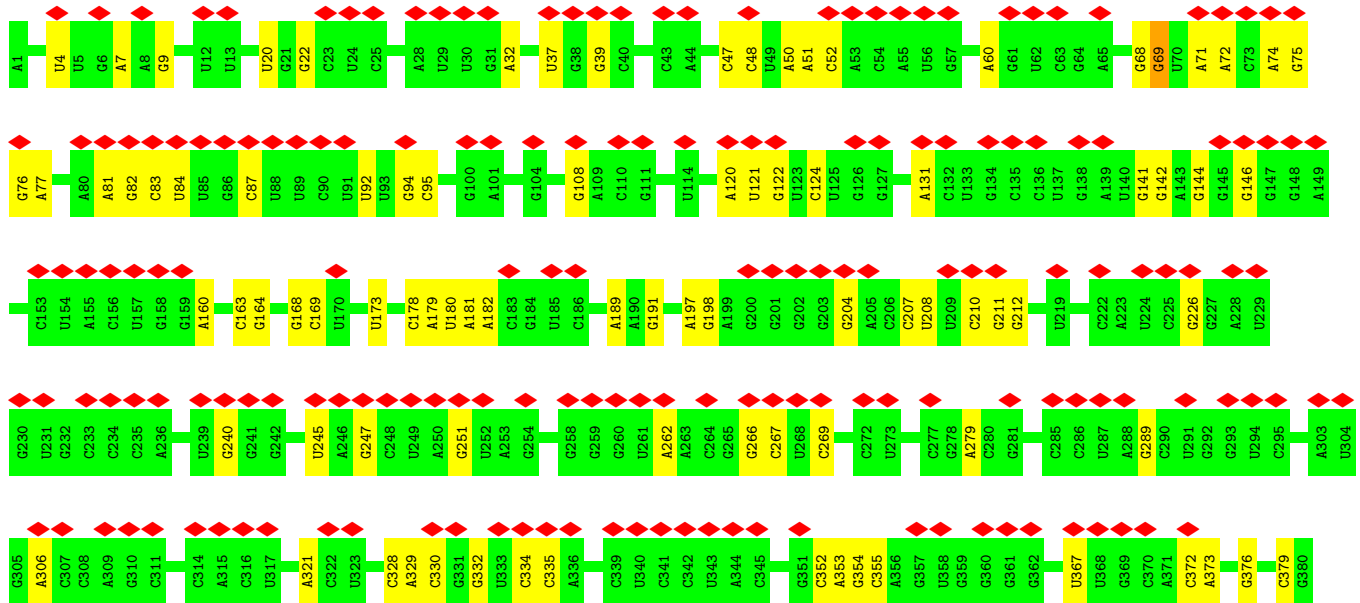
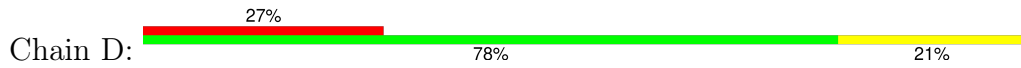


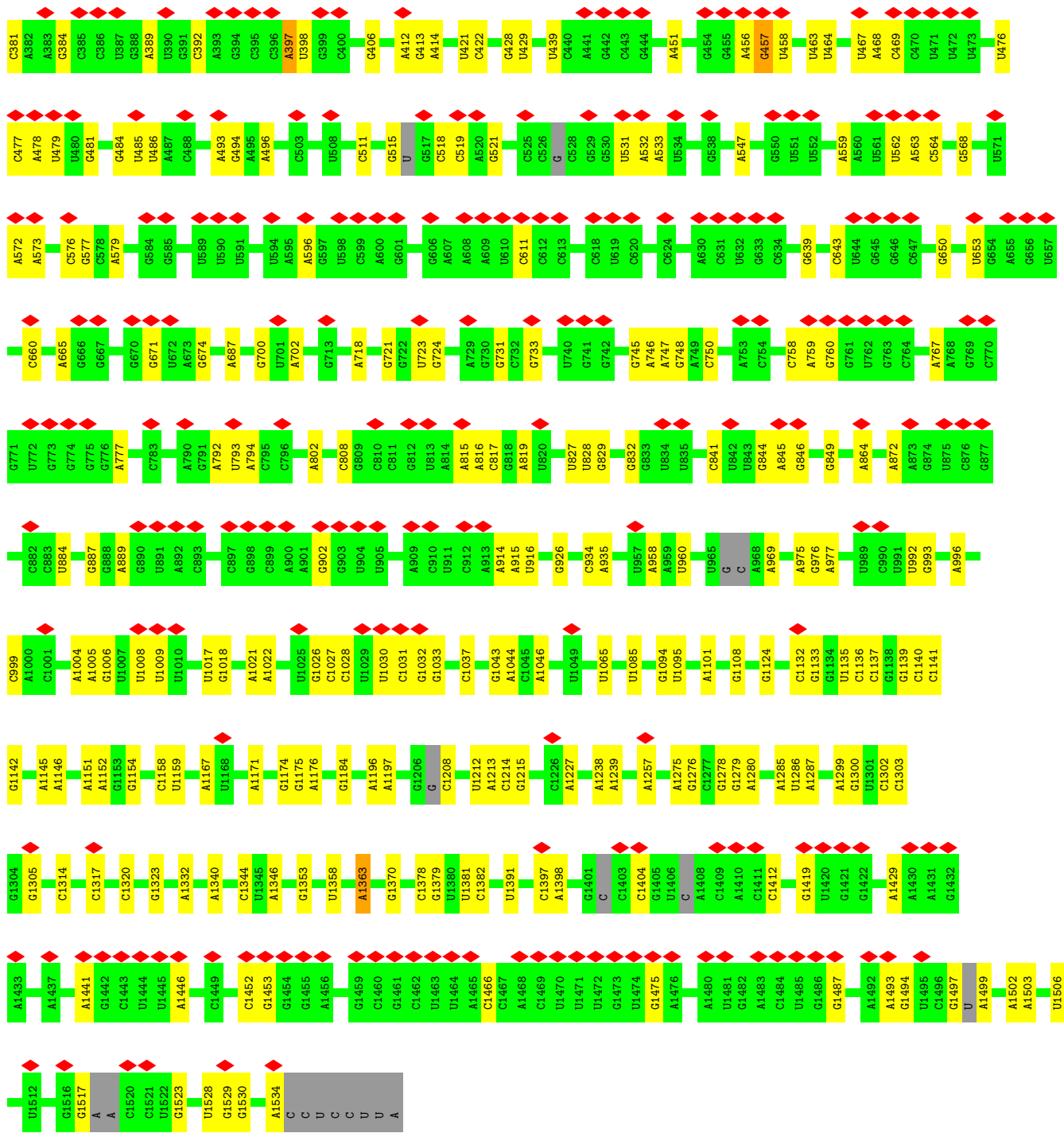


• Molecule 17: 30S ribosomal protein S18

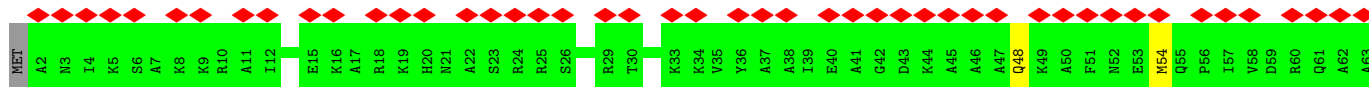
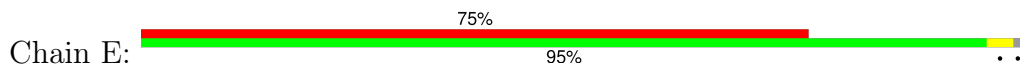


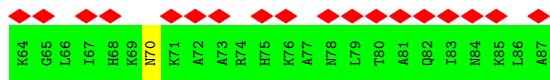
• Molecule 18: 16S rRNA



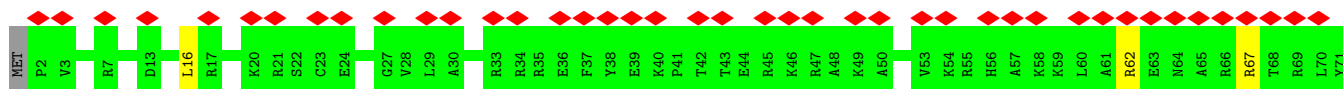


• Molecule 19: 30S ribosomal protein S20

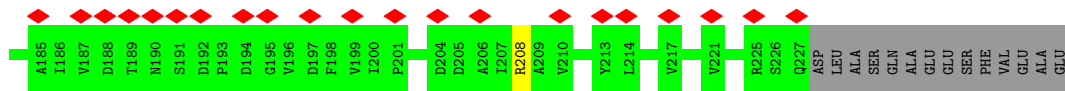
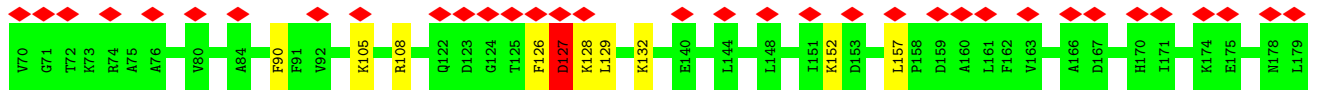
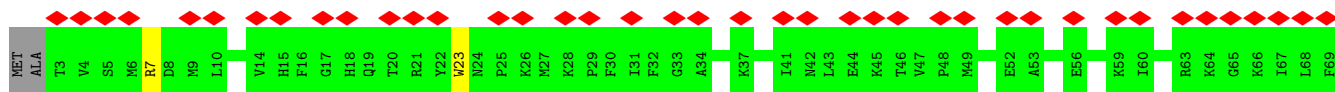
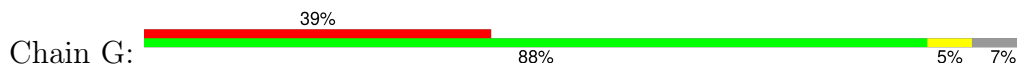




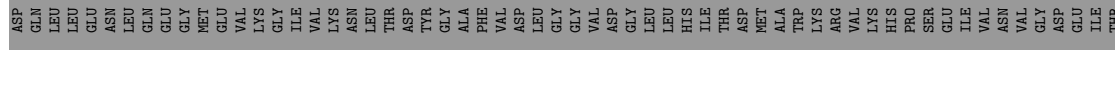
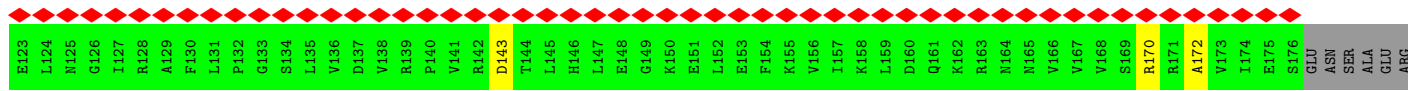
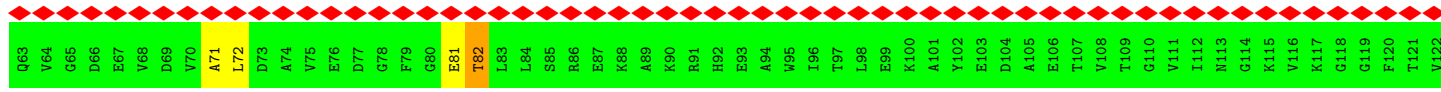
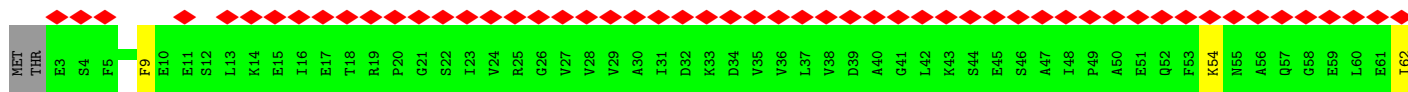
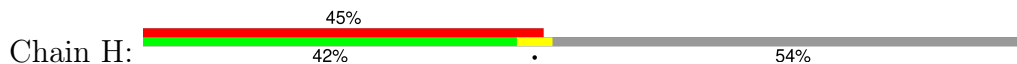
• Molecule 20: 30S ribosomal protein S21

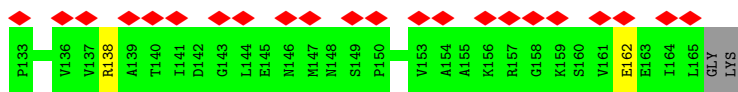


• Molecule 21: 30S ribosomal protein S2

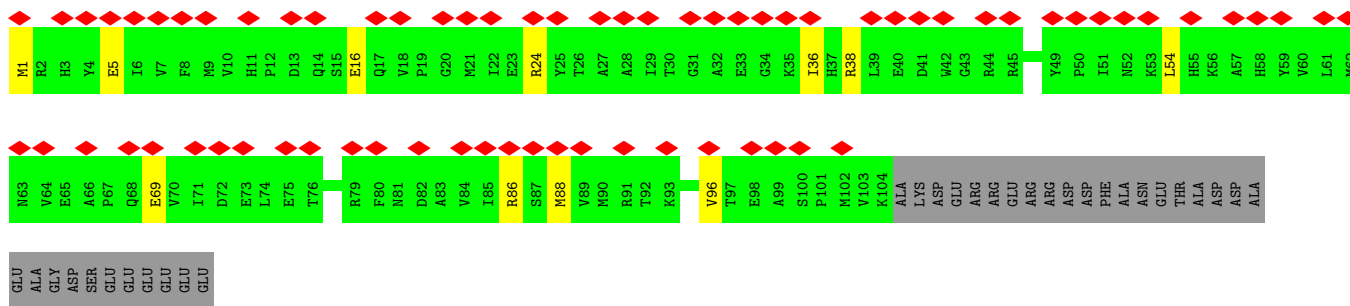


• Molecule 22: 30S ribosomal protein S1

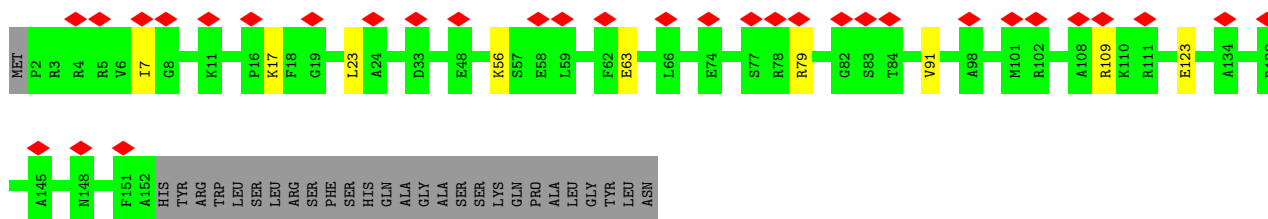
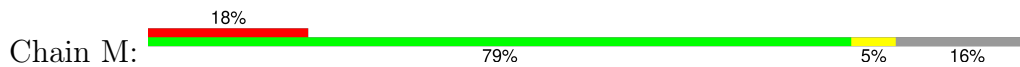




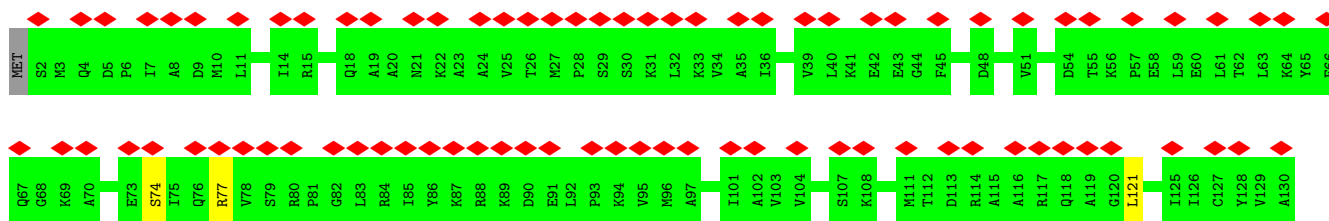
• Molecule 26: 30S ribosomal protein S6



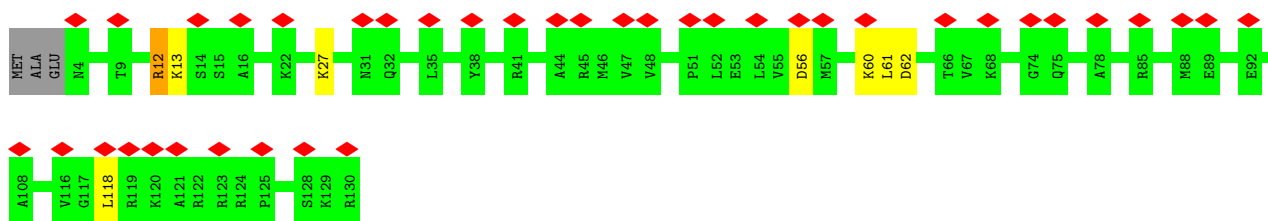
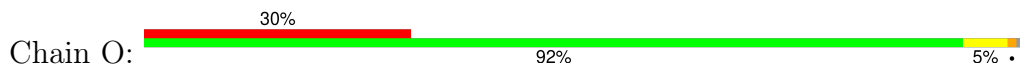
• Molecule 27: 30S ribosomal protein S7



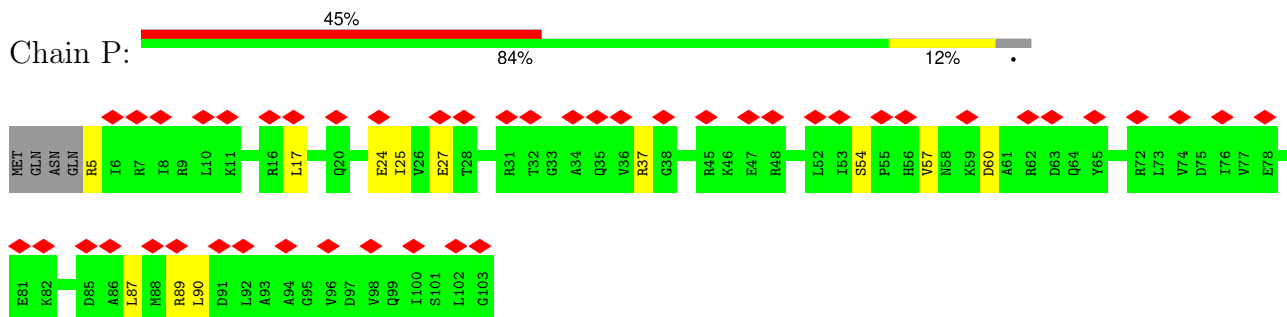
• Molecule 28: 30S ribosomal protein S8



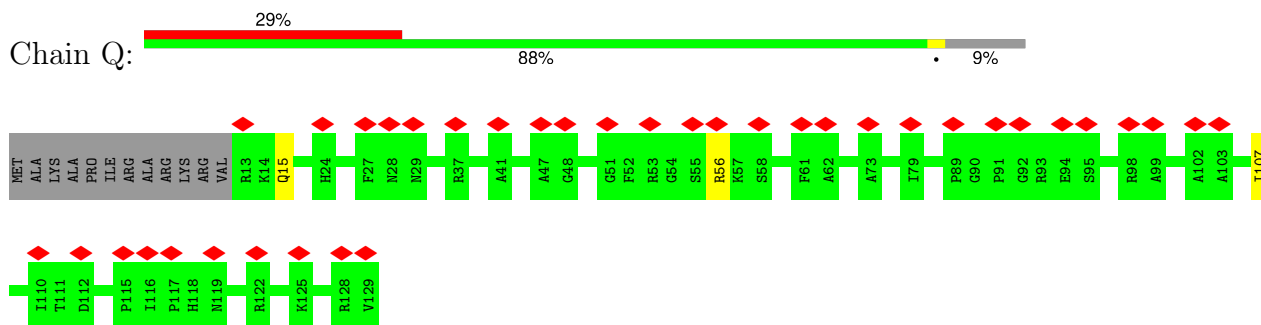
• Molecule 29: 30S ribosomal protein S9



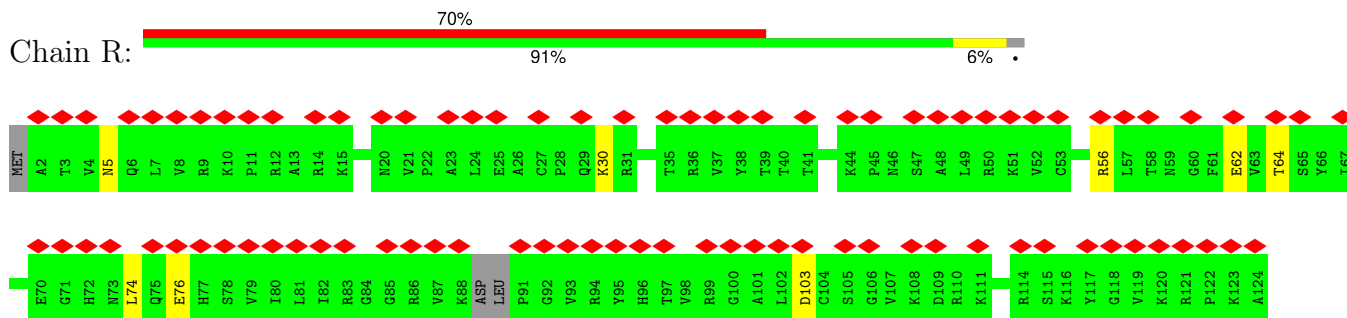
• Molecule 30: 30S ribosomal protein S10



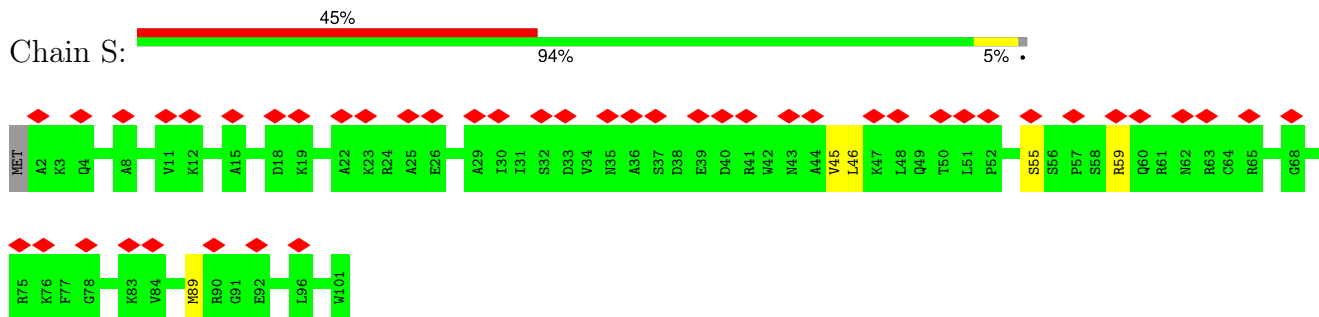
• Molecule 31: 30S ribosomal protein S11



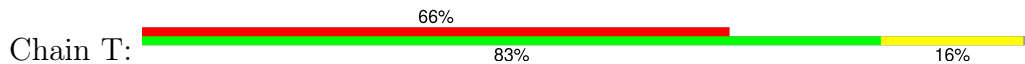
• Molecule 32: 30S ribosomal protein S12

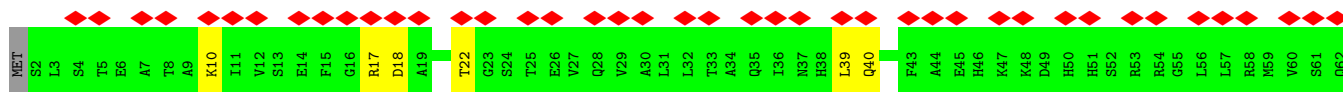


• Molecule 33: 30S ribosomal protein S14

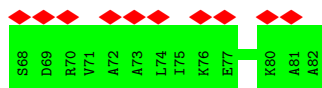


• Molecule 34: 30S ribosomal protein S15

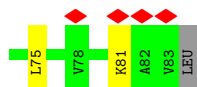
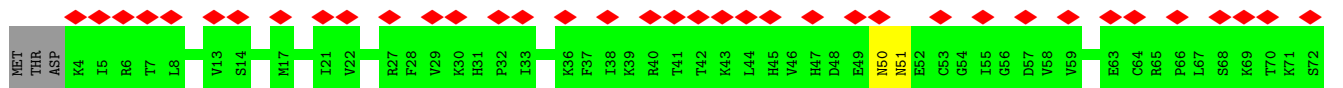




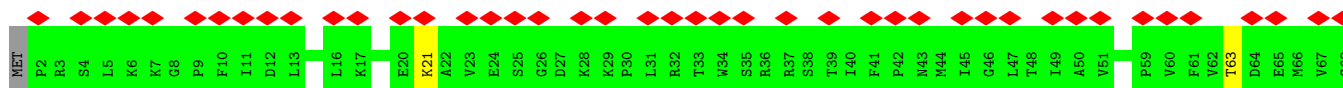
• Molecule 35: 30S ribosomal protein S16



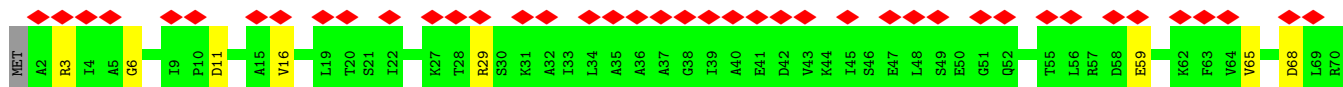
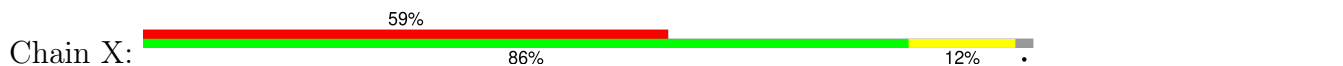
• Molecule 36: 30S ribosomal protein S17

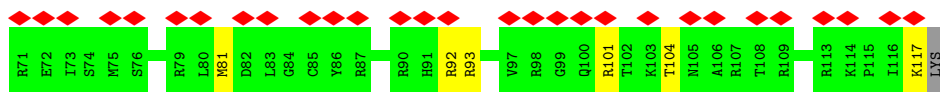


• Molecule 37: 30S ribosomal protein S19

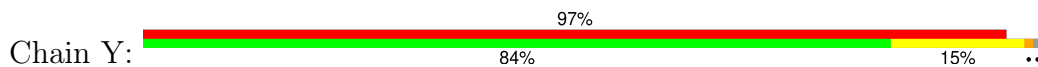


• Molecule 38: 30S ribosomal protein S13

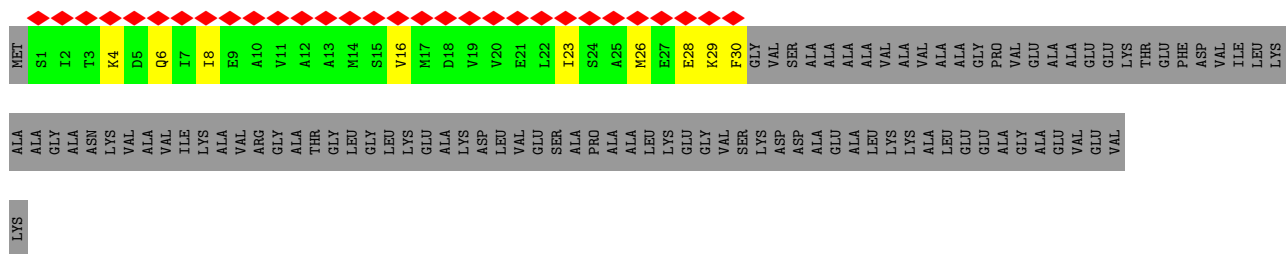




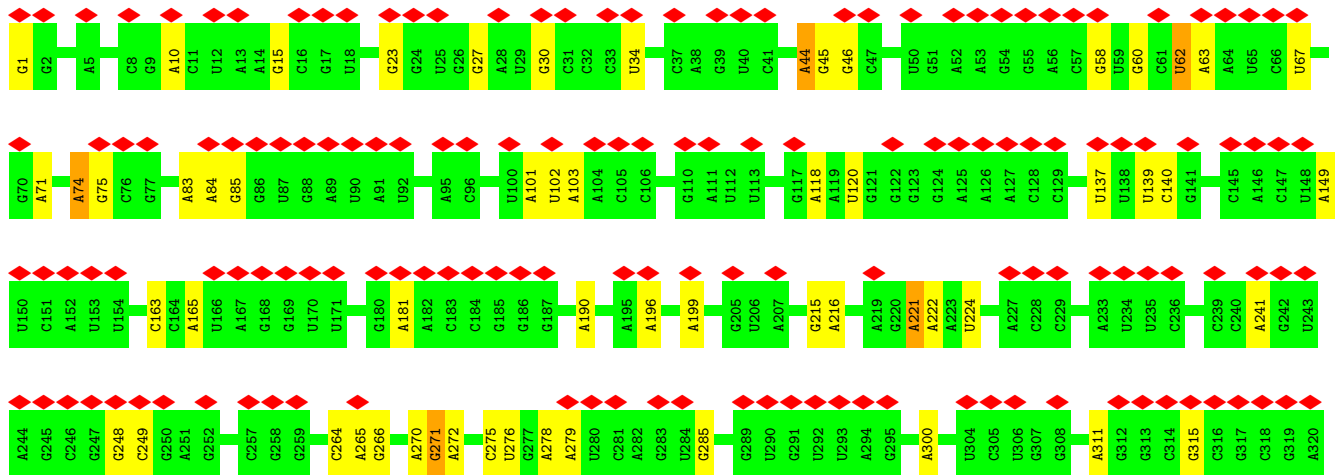
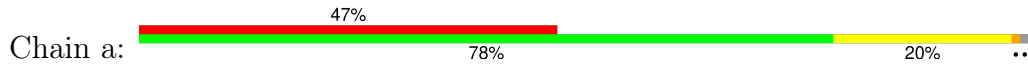
- Molecule 39: 50S ribosomal protein L11

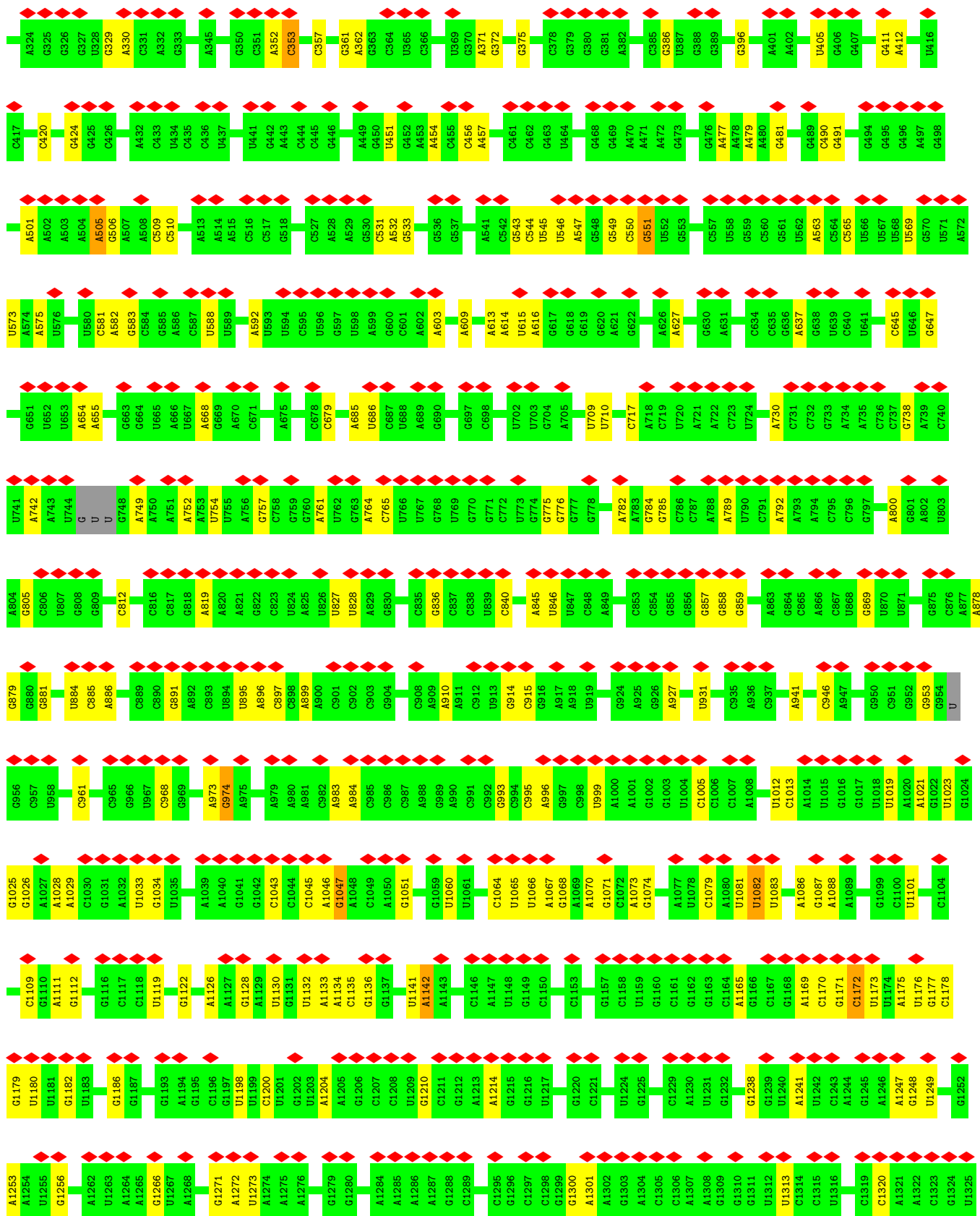


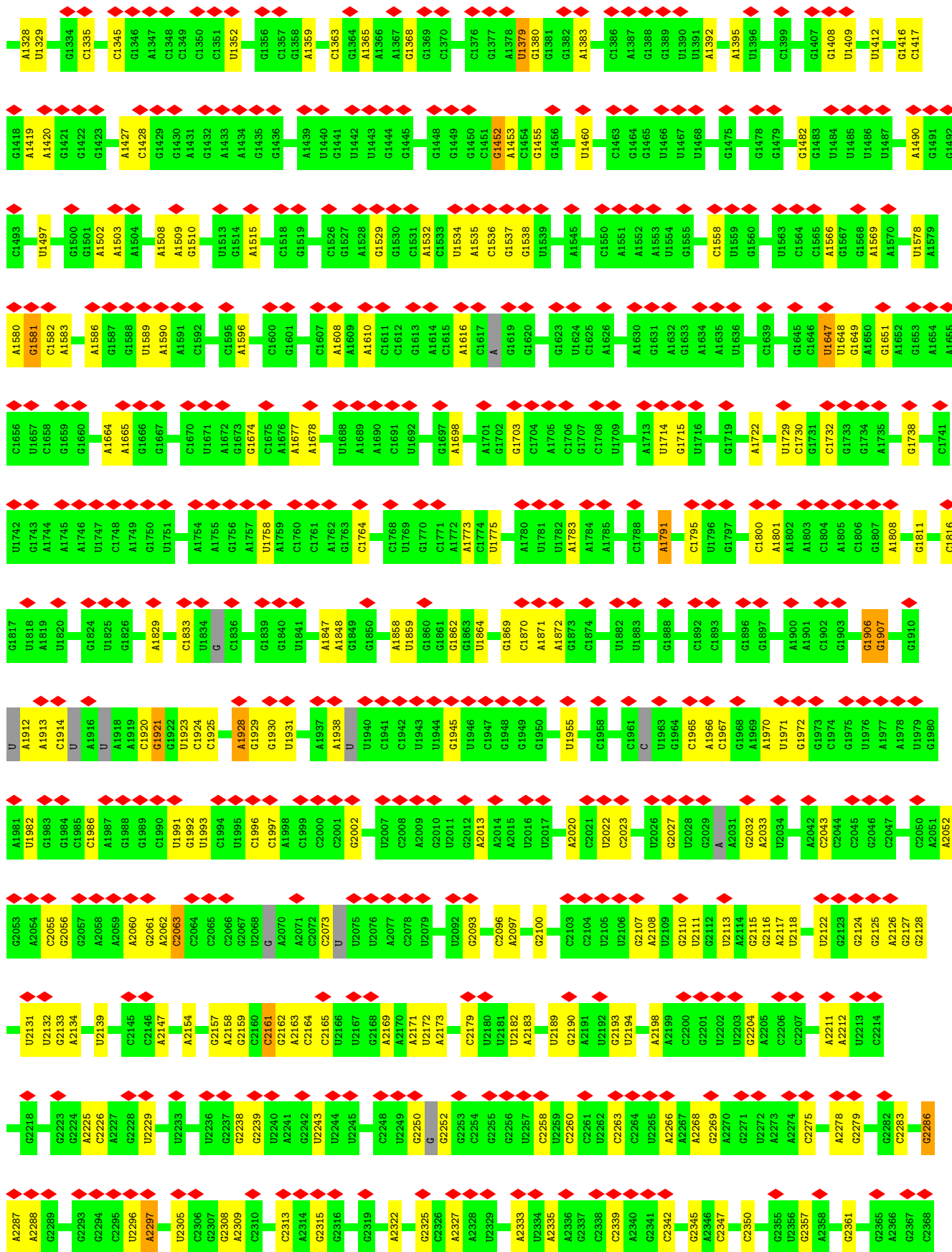
- Molecule 40: 50S ribosomal protein L7/L12

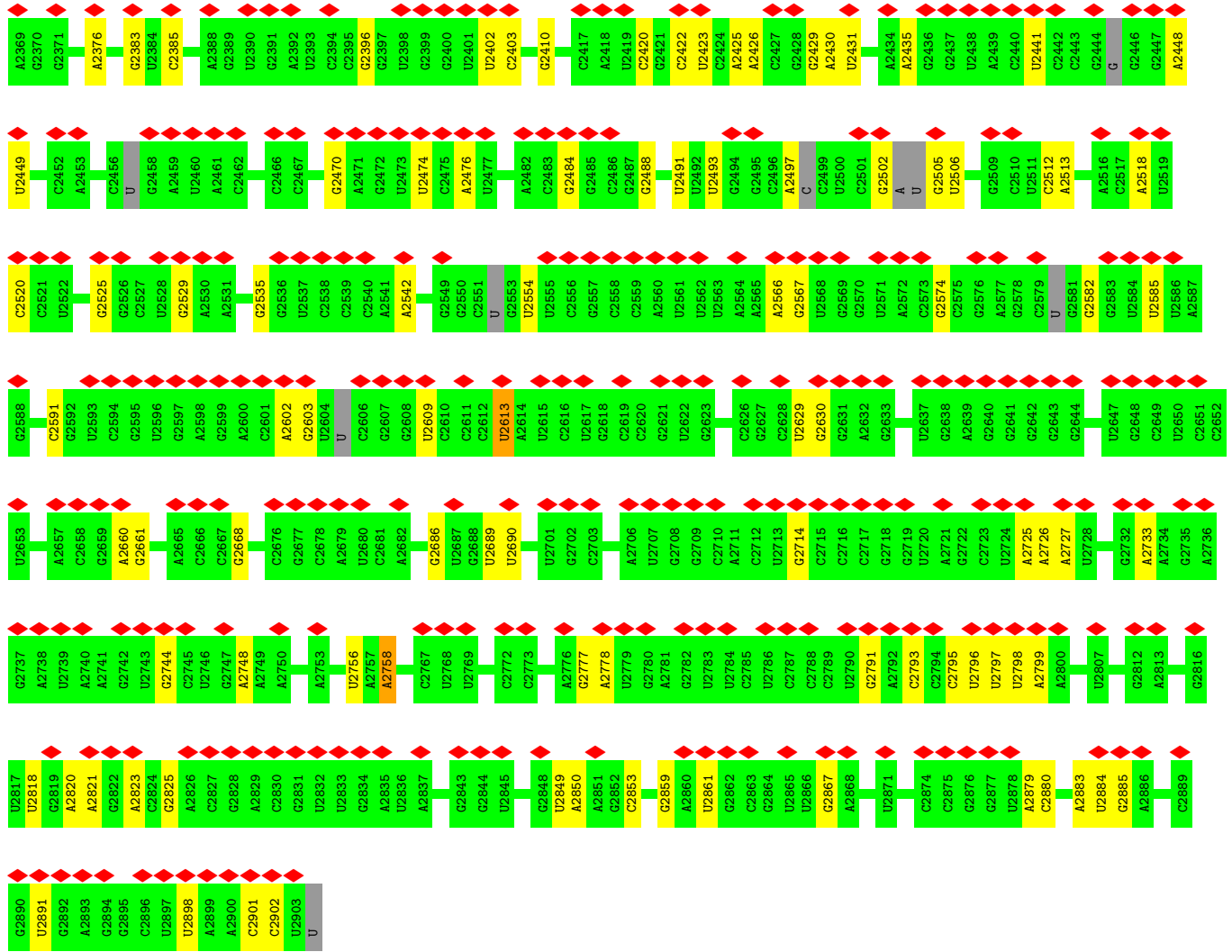


- Molecule 41: 23S rRNA

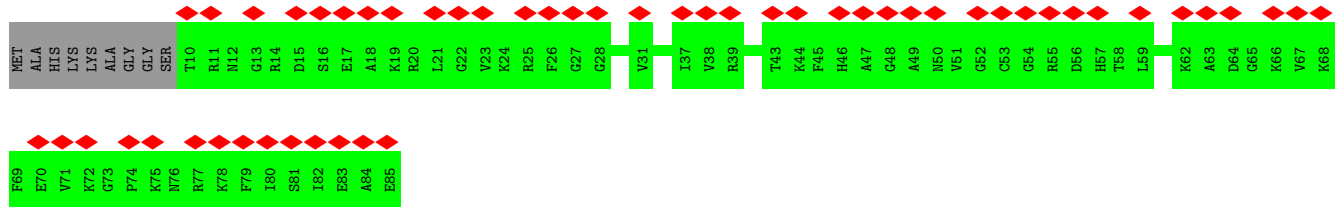
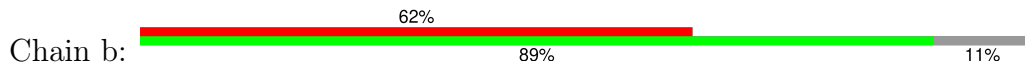




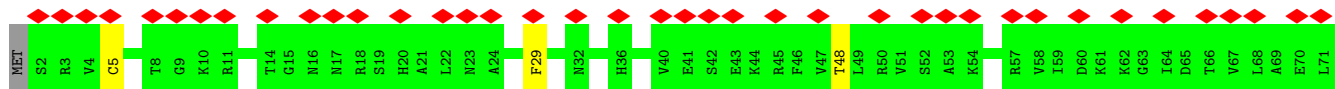


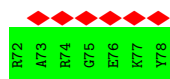


• Molecule 42: 50S ribosomal protein L27

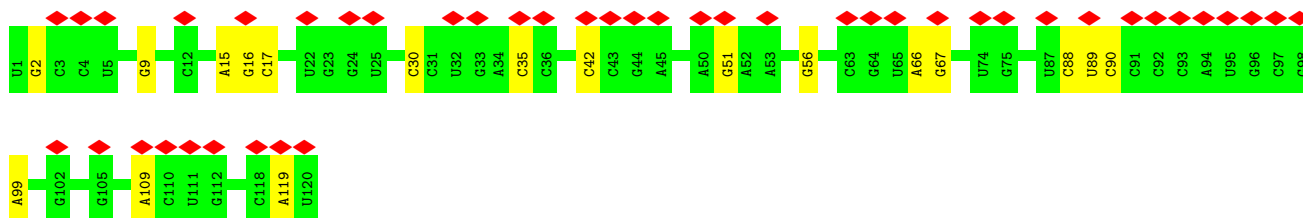
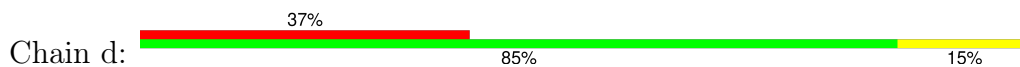


• Molecule 43: 50S ribosomal protein L28

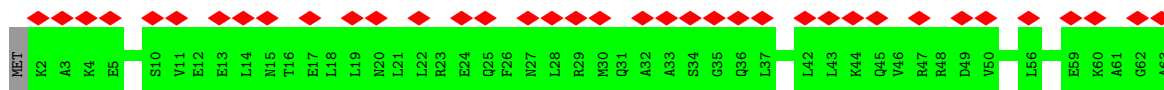




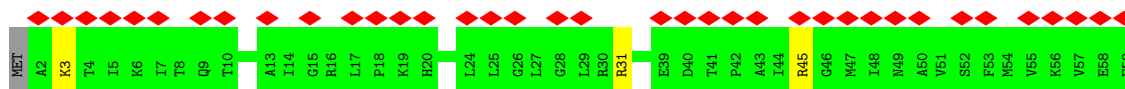
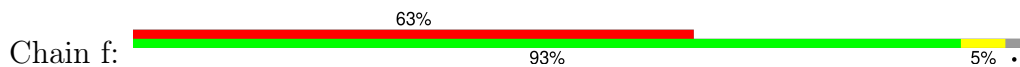
- Molecule 44: 5S rRNA



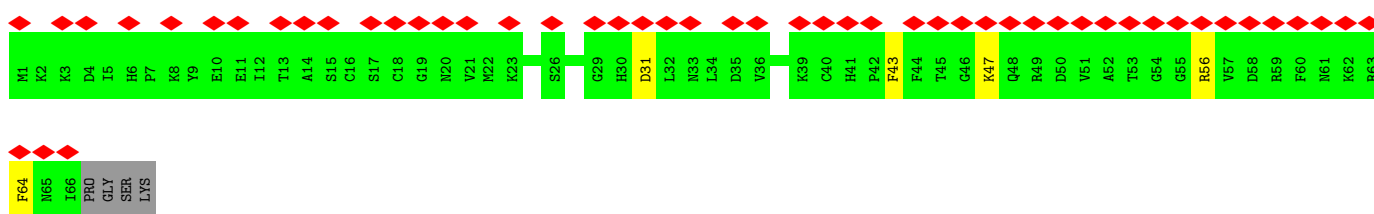
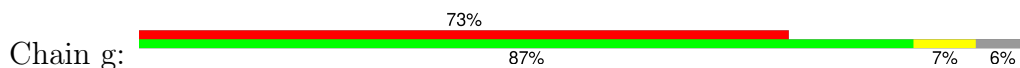
- Molecule 45: 50S ribosomal protein L29



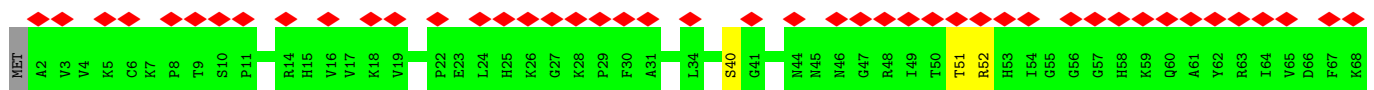
- Molecule 46: 50S ribosomal protein L30

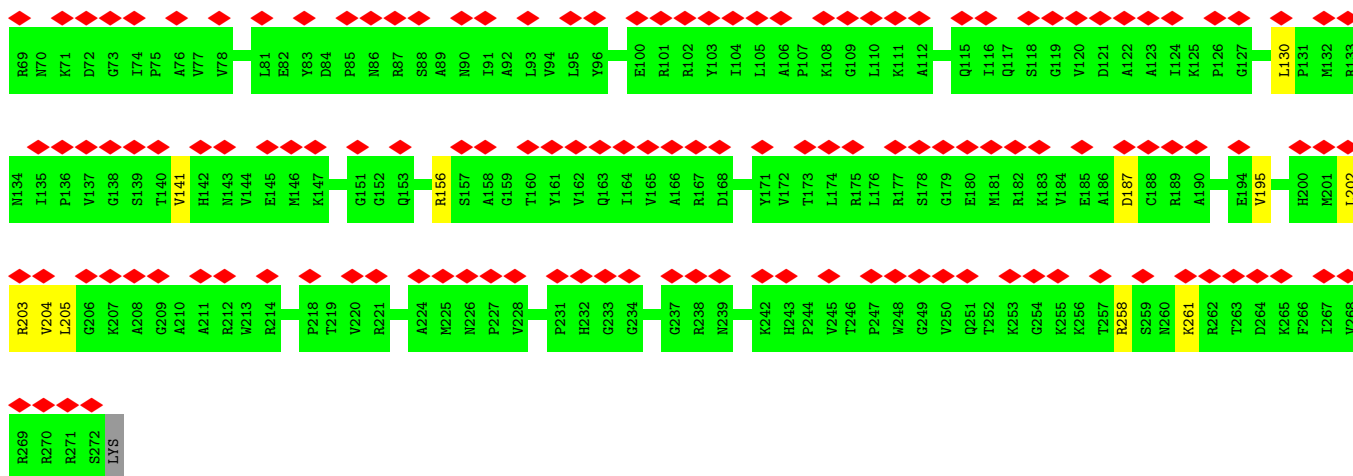


- Molecule 47: 50S ribosomal protein L31

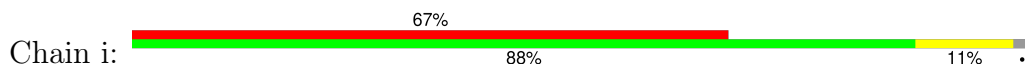


- Molecule 48: 50S ribosomal protein L2

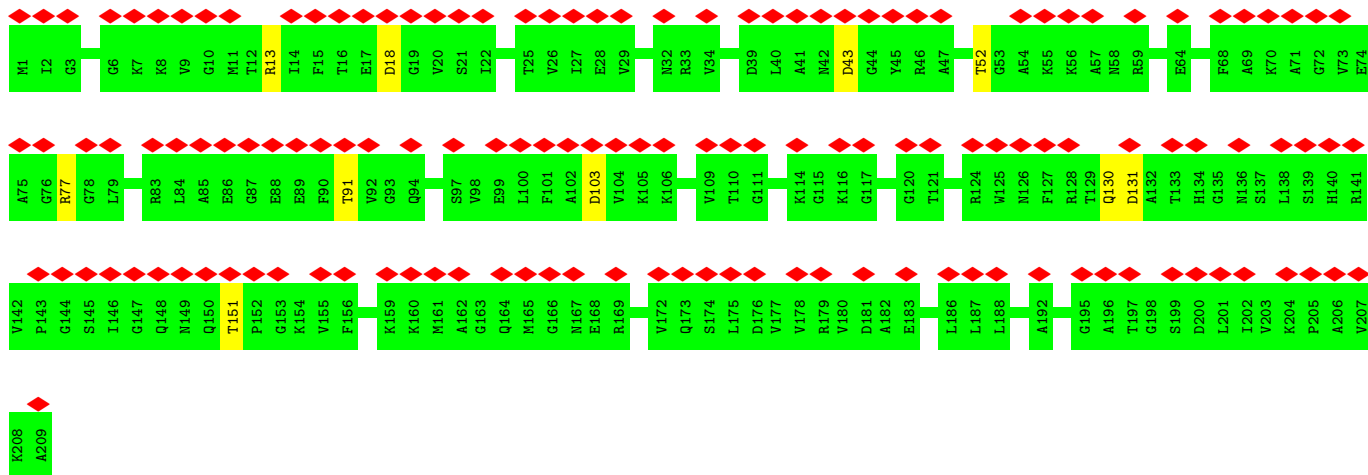
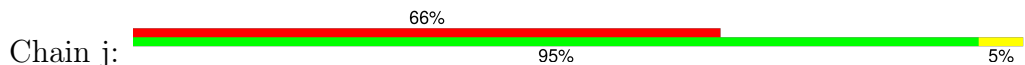




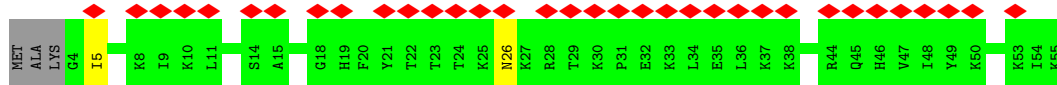
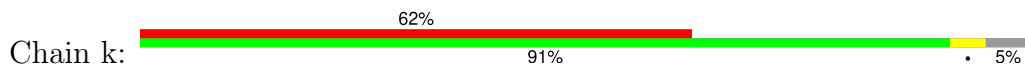
• Molecule 49: 50S ribosomal protein L32



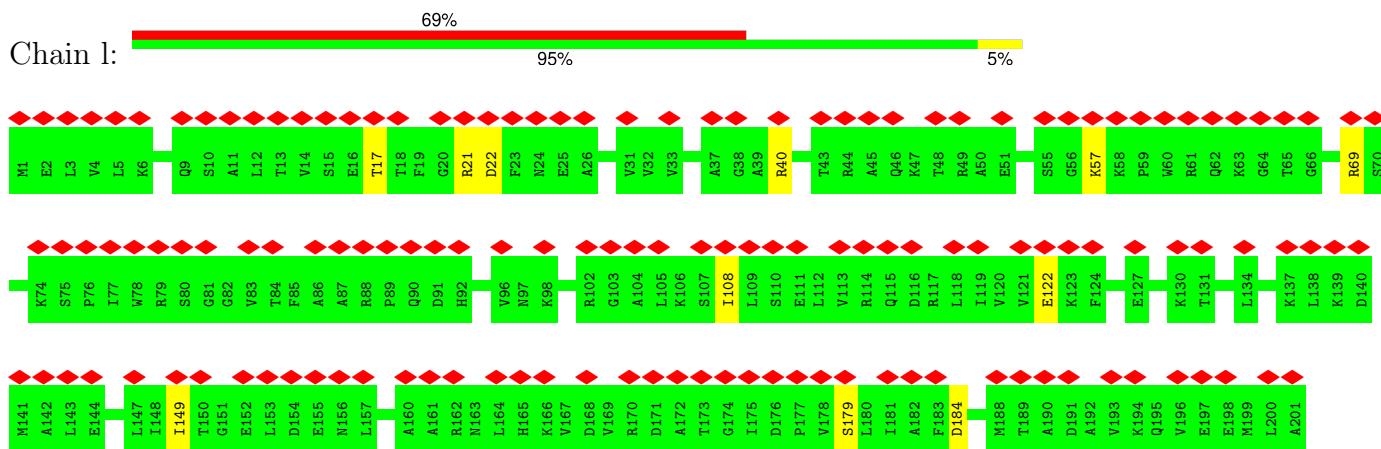
• Molecule 50: 50S ribosomal protein L3



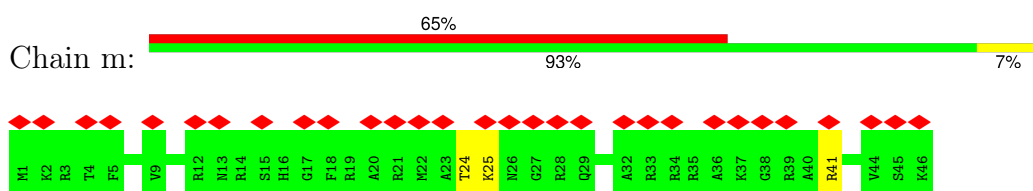
• Molecule 51: 50S ribosomal protein L33



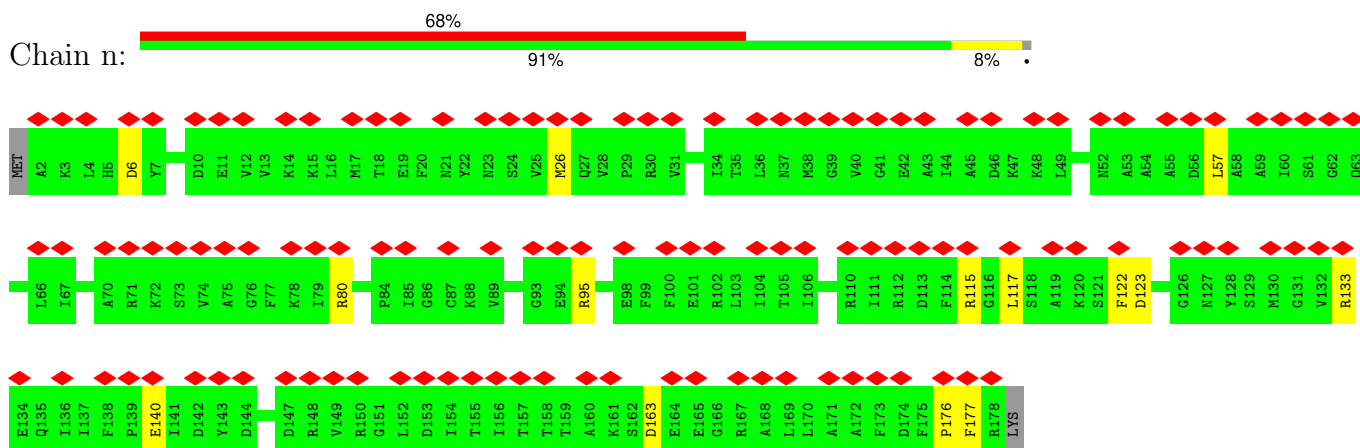
• Molecule 52: 50S ribosomal protein L4



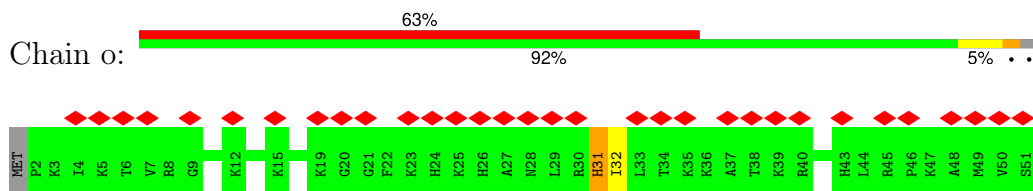
• Molecule 53: 50S ribosomal protein L34



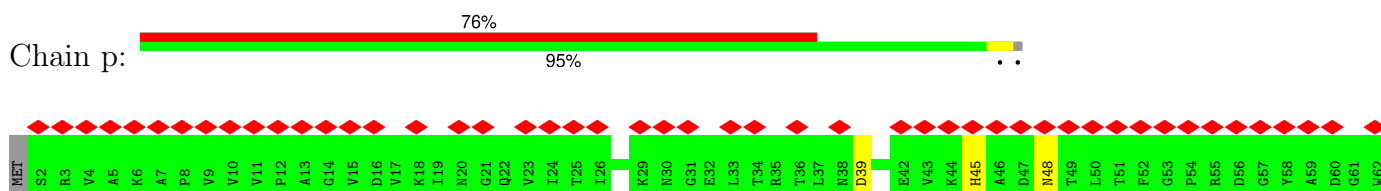
• Molecule 54: 50S ribosomal protein L5

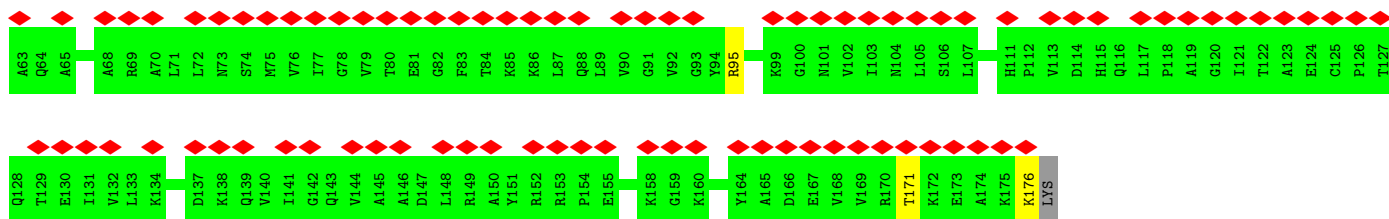


• Molecule 55: 50S ribosomal protein L35

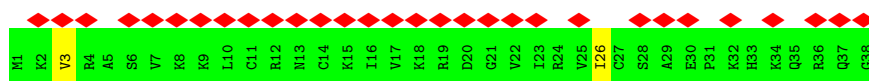
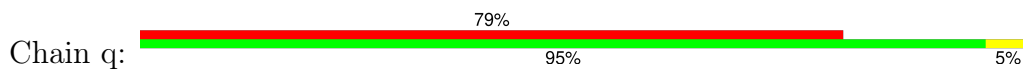


• Molecule 56: 50S ribosomal protein L6

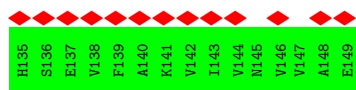
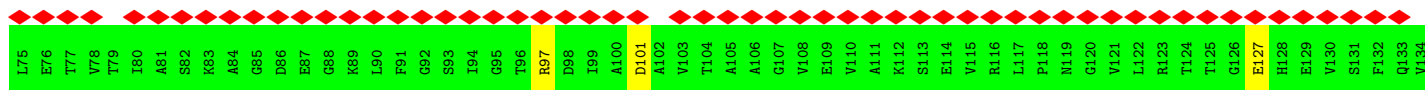
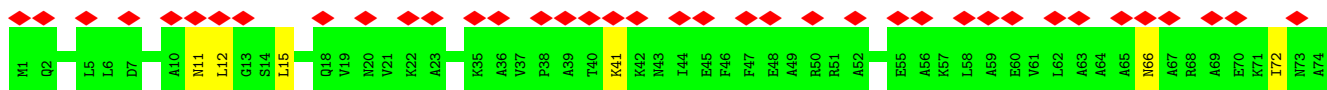
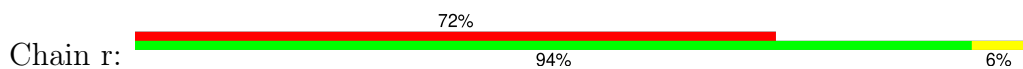




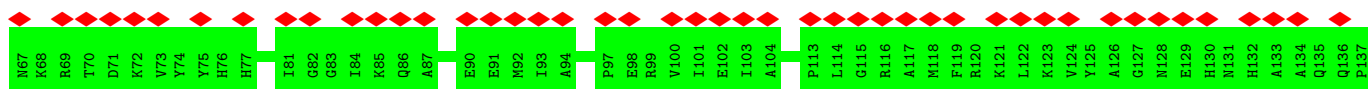
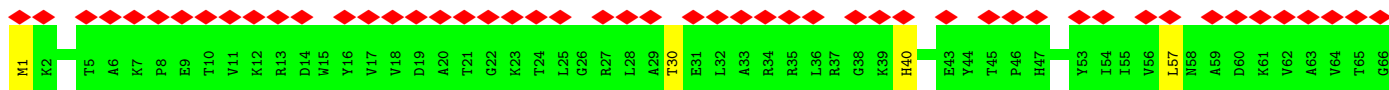
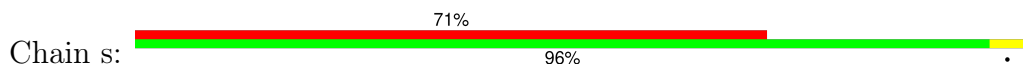
• Molecule 57: 50S ribosomal protein L36



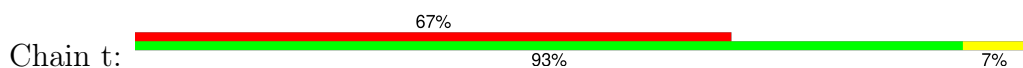
• Molecule 58: 50S ribosomal protein L9

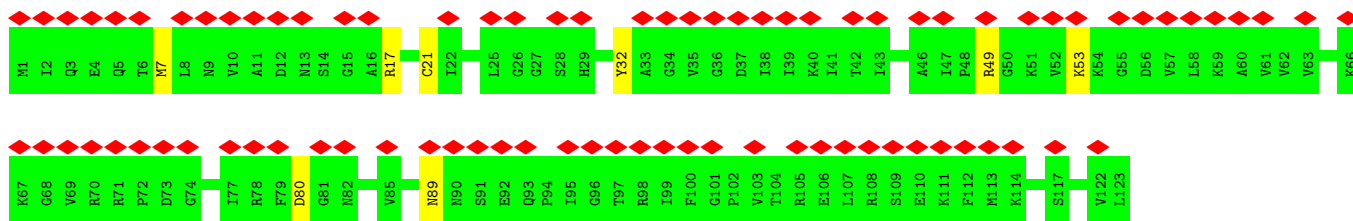


• Molecule 59: 50S ribosomal protein L13

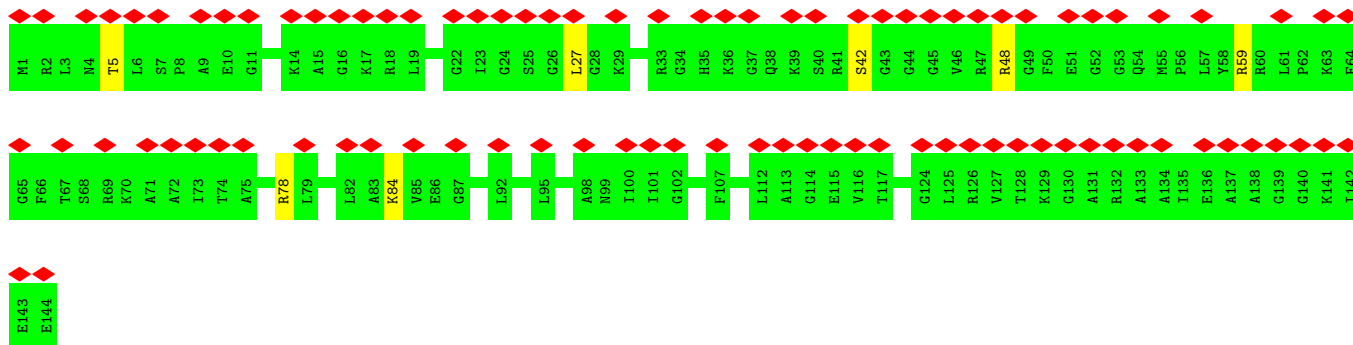


• Molecule 60: 50S ribosomal protein L14

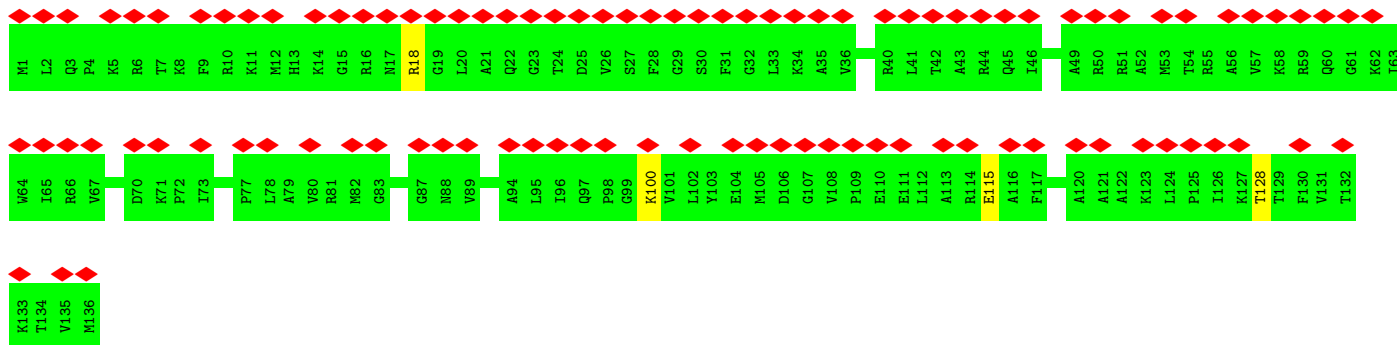




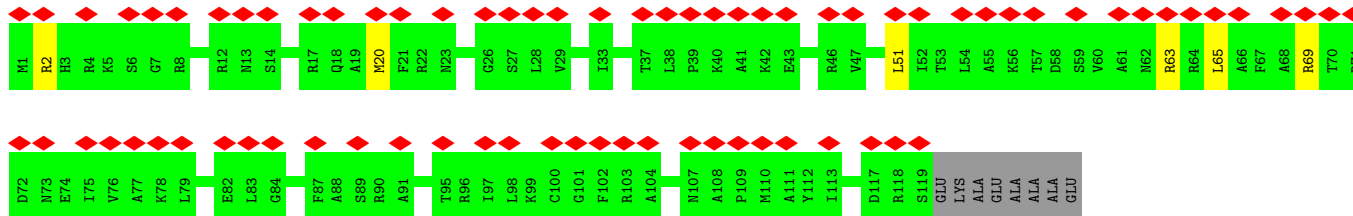
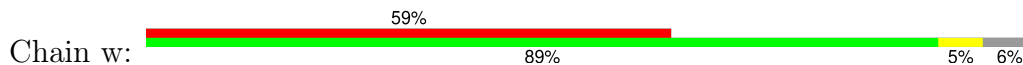
• Molecule 61: 50S ribosomal protein L15



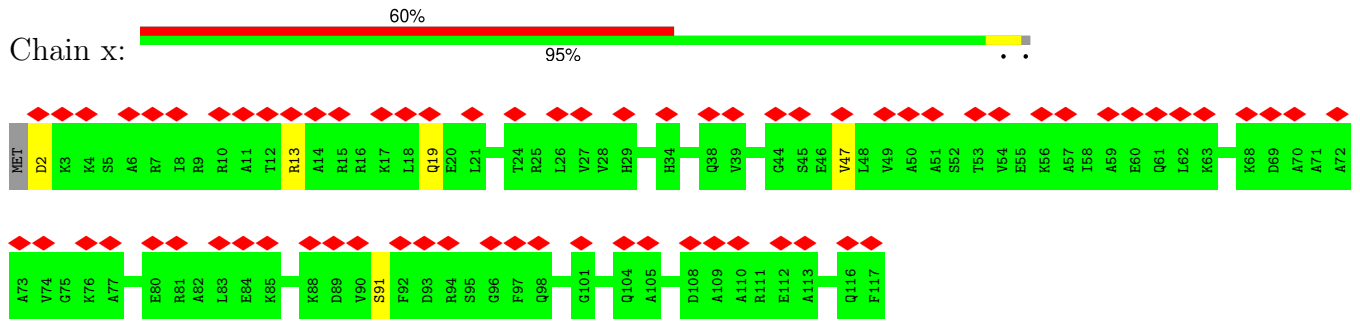
• Molecule 62: 50S ribosomal protein L16



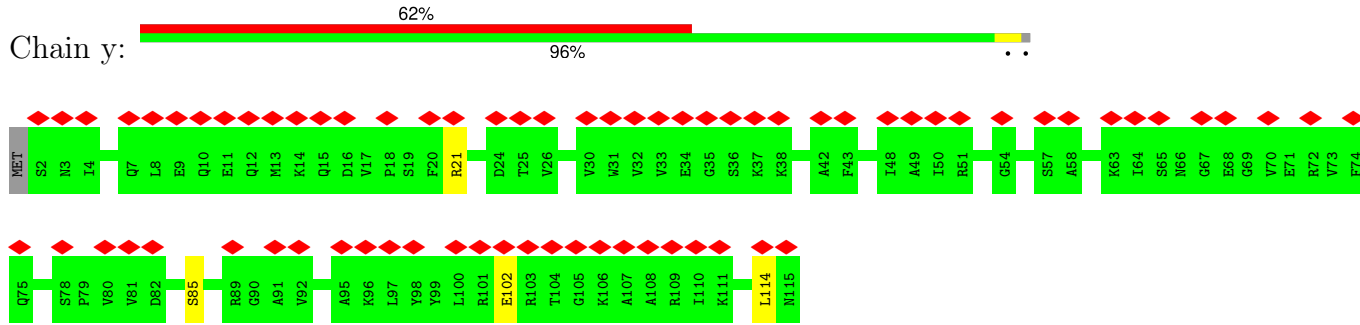
• Molecule 63: 50S ribosomal protein L17



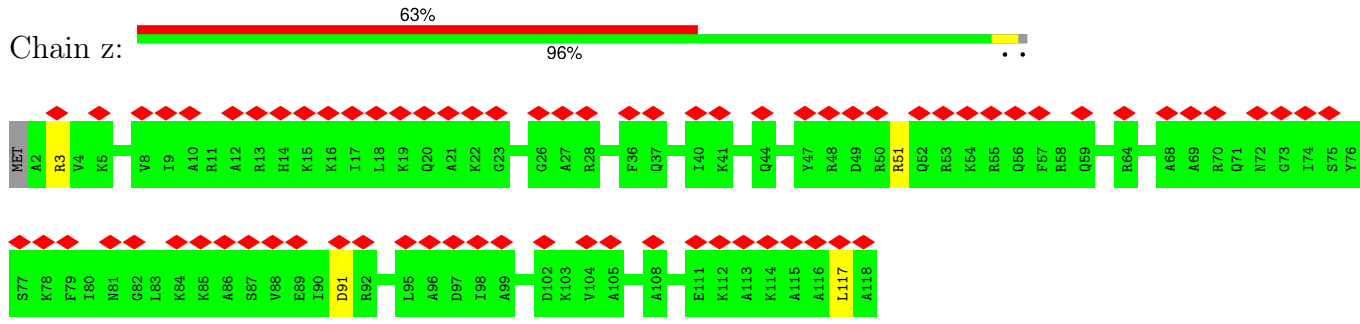
• Molecule 64: 50S ribosomal protein L18



• Molecule 65: 50S ribosomal protein L19



• Molecule 66: 50S ribosomal protein L20



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	38957	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	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	0.065	Depositor
Minimum map value	-0.026	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.014	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: ZN, MG

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	0.61	0/829	0.54	0/1107
2	1	0.59	0/864	0.55	0/1156
3	2	0.55	0/752	0.52	0/1005
4	3	0.53	0/796	0.53	0/1062
5	4	0.51	0/766	0.49	0/1025
6	5	1.13	6/528 (1.1%)	0.97	1/810 (0.1%)
7	6	1.11	4/603 (0.7%)	0.96	0/926
8	7	0.72	1/761 (0.1%)	1.80	23/1178 (2.0%)
9	9	0.35	0/1131	0.60	0/1524
10	A	0.71	2/1810 (0.1%)	1.25	18/2821 (0.6%)
10	B	0.95	1/1810 (0.1%)	1.50	25/2821 (0.9%)
11	AA	0.44	1/10736 (0.0%)	0.61	2/14487 (0.0%)
12	AB	0.68	2/1310 (0.2%)	0.67	2/1766 (0.1%)
13	AC	0.38	0/2113	0.58	0/2877
13	AD	0.34	0/2096	0.59	0/2854
14	AE	0.52	4/10545 (0.0%)	0.66	6/14236 (0.0%)
15	AF	0.33	0/652	0.57	0/879
16	AG	0.64	1/3897 (0.0%)	0.89	30/5273 (0.6%)
17	C	0.61	1/553 (0.2%)	0.62	0/743
18	D	1.35	22/36610 (0.1%)	1.18	99/57091 (0.2%)
19	E	0.46	0/675	0.46	0/895
20	F	0.50	0/597	0.47	0/792
21	G	0.58	1/1791 (0.1%)	0.57	1/2413 (0.0%)
22	H	0.31	0/1746	0.58	0/2382
23	I	0.53	0/1663	0.51	0/2241
24	J	0.53	0/1665	0.49	0/2227
25	K	0.60	0/1165	0.57	0/1568
26	L	0.54	0/867	0.49	0/1171
27	M	0.47	0/1195	0.53	0/1602
28	N	0.57	0/989	0.51	0/1326
29	O	0.51	0/1034	0.53	0/1375
30	P	0.46	0/800	0.54	0/1082

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	Q	0.52	0/893	0.50	0/1205
32	R	0.60	0/952	0.55	0/1274
33	S	0.53	0/817	0.50	0/1088
34	T	0.52	0/722	0.51	0/964
35	U	0.54	0/659	0.52	0/884
36	V	0.55	0/657	0.51	0/881
37	W	0.47	0/680	0.51	0/915
38	X	0.45	0/909	0.51	0/1215
39	Y	0.51	2/1046 (0.2%)	0.62	0/1410
40	Z	0.24	0/227	0.40	0/304
41	a	1.45	45/69247 (0.1%)	1.12	140/107985 (0.1%)
42	b	0.59	0/589	0.51	0/779
43	c	0.57	0/635	0.55	0/848
44	d	1.23	0/2872	1.00	0/4478
45	e	0.48	0/502	0.50	0/667
46	f	0.52	0/452	0.51	0/605
47	g	0.39	0/531	0.52	0/709
48	h	0.64	0/2121	0.54	0/2852
49	i	0.57	0/450	0.55	0/599
50	j	0.63	0/1586	0.55	0/2134
51	k	0.60	0/433	0.54	0/576
52	l	0.54	0/1571	0.52	0/2113
53	m	0.63	0/380	0.54	0/498
54	n	0.47	0/1434	0.52	0/1926
55	o	0.58	0/513	0.55	0/676
56	p	0.49	0/1333	0.52	0/1805
57	q	0.58	0/303	0.55	0/397
58	r	0.40	0/1122	0.50	0/1515
59	s	0.64	0/1152	0.51	0/1551
60	t	0.63	0/955	0.52	0/1279
61	u	0.55	0/1062	0.56	0/1413
62	v	0.60	0/1093	0.53	0/1460
63	w	0.60	0/964	0.52	0/1289
64	x	0.49	0/902	0.49	0/1209
65	y	0.63	0/929	0.52	0/1242
66	z	0.68	0/960	0.50	0/1278
All	All	1.12	93/195002 (0.0%)	0.97	347/286738 (0.1%)

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
9	9	0	3
13	AC	0	3
13	AD	0	1
14	AE	0	5
16	AG	0	7
21	G	0	2
22	H	0	5
29	O	0	1
54	n	0	1
55	o	0	1
All	All	0	29

The worst 5 of 93 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	AB	124	PRO	N-CA	13.13	1.69	1.47
21	G	157	LEU	C-N	10.81	1.54	1.34
14	AE	88	CYS	CB-SG	-10.21	1.64	1.82
41	a	74	A	C6-N1	-9.21	1.29	1.35
16	AG	429	LYS	C-N	8.82	1.51	1.34

The worst 5 of 347 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	D	37	U	C5-C4-O4	35.68	147.31	125.90
18	D	884	U	C5-C4-O4	35.09	146.95	125.90
41	a	1019	U	C5-C4-O4	34.63	146.68	125.90
18	D	827	U	C5-C4-O4	34.07	146.34	125.90
41	a	1141	U	C5-C4-O4	33.77	146.16	125.90

There are no chirality outliers.

5 of 29 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	9	107	GLU	Peptide
9	9	117	LEU	Peptide
9	9	49	GLY	Peptide
13	AC	192	VAL	Peptide
13	AC	319	GLU	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	101/103 (98%)	92 (91%)	9 (9%)	0	100	100
2	1	108/110 (98%)	104 (96%)	4 (4%)	0	100	100
3	2	92/100 (92%)	89 (97%)	3 (3%)	0	100	100
4	3	101/104 (97%)	97 (96%)	4 (4%)	0	100	100
5	4	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
9	9	146/165 (88%)	107 (73%)	37 (25%)	2 (1%)	9	40
11	AA	1338/1342 (100%)	1206 (90%)	126 (9%)	6 (0%)	30	64
12	AB	158/181 (87%)	119 (75%)	26 (16%)	13 (8%)	1	4
13	AC	295/329 (90%)	274 (93%)	19 (6%)	2 (1%)	19	54
13	AD	293/329 (89%)	269 (92%)	24 (8%)	0	100	100
14	AE	1329/1407 (94%)	1199 (90%)	121 (9%)	9 (1%)	19	54
15	AF	80/91 (88%)	77 (96%)	3 (4%)	0	100	100
16	AG	493/495 (100%)	377 (76%)	85 (17%)	31 (6%)	1	8
17	C	64/75 (85%)	61 (95%)	3 (5%)	0	100	100
19	E	84/87 (97%)	82 (98%)	2 (2%)	0	100	100
20	F	68/71 (96%)	67 (98%)	1 (2%)	0	100	100
21	G	223/241 (92%)	209 (94%)	13 (6%)	1 (0%)	30	64
22	H	255/557 (46%)	201 (79%)	45 (18%)	9 (4%)	3	20
23	I	206/233 (88%)	200 (97%)	6 (3%)	0	100	100
24	J	203/206 (98%)	199 (98%)	4 (2%)	0	100	100
25	K	154/167 (92%)	146 (95%)	6 (4%)	2 (1%)	10	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	L	102/135 (76%)	97 (95%)	4 (4%)	1 (1%)	13	47
27	M	149/179 (83%)	139 (93%)	9 (6%)	1 (1%)	19	54
28	N	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
29	O	125/130 (96%)	118 (94%)	6 (5%)	1 (1%)	16	51
30	P	97/103 (94%)	88 (91%)	8 (8%)	1 (1%)	13	47
31	Q	115/129 (89%)	105 (91%)	10 (9%)	0	100	100
32	R	117/124 (94%)	112 (96%)	4 (3%)	1 (1%)	14	49
33	S	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
34	T	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
35	U	80/82 (98%)	77 (96%)	3 (4%)	0	100	100
36	V	78/84 (93%)	74 (95%)	4 (5%)	0	100	100
37	W	81/92 (88%)	78 (96%)	3 (4%)	0	100	100
38	X	114/118 (97%)	104 (91%)	8 (7%)	2 (2%)	7	35
39	Y	139/142 (98%)	113 (81%)	25 (18%)	1 (1%)	19	54
40	Z	28/121 (23%)	24 (86%)	4 (14%)	0	100	100
42	b	74/85 (87%)	70 (95%)	4 (5%)	0	100	100
43	c	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
45	e	60/63 (95%)	59 (98%)	1 (2%)	0	100	100
46	f	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
47	g	64/70 (91%)	62 (97%)	2 (3%)	0	100	100
48	h	269/273 (98%)	254 (94%)	15 (6%)	0	100	100
49	i	54/57 (95%)	48 (89%)	6 (11%)	0	100	100
50	j	207/209 (99%)	198 (96%)	9 (4%)	0	100	100
51	k	50/55 (91%)	49 (98%)	1 (2%)	0	100	100
52	l	199/201 (99%)	192 (96%)	7 (4%)	0	100	100
53	m	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
54	n	175/179 (98%)	168 (96%)	6 (3%)	1 (1%)	22	57
55	o	62/65 (95%)	56 (90%)	5 (8%)	1 (2%)	8	37
56	p	173/177 (98%)	165 (95%)	7 (4%)	1 (1%)	22	57
57	q	36/38 (95%)	36 (100%)	0	0	100	100
58	r	147/149 (99%)	137 (93%)	10 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
59	s	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
60	t	121/123 (98%)	114 (94%)	7 (6%)	0	100	100
61	u	142/144 (99%)	133 (94%)	9 (6%)	0	100	100
62	v	134/136 (98%)	126 (94%)	8 (6%)	0	100	100
63	w	117/127 (92%)	111 (95%)	6 (5%)	0	100	100
64	x	114/117 (97%)	113 (99%)	1 (1%)	0	100	100
65	y	112/115 (97%)	109 (97%)	3 (3%)	0	100	100
66	z	115/118 (98%)	110 (96%)	5 (4%)	0	100	100
All	All	10159/11072 (92%)	9310 (92%)	763 (8%)	86 (1%)	19	51

5 of 86 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	9	79	PRO
11	AA	888	THR
12	AB	121	LYS
12	AB	122	PRO
12	AB	123	ARG

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%)	80 (95%)	4 (5%)	21	55
2	1	93/93 (100%)	84 (90%)	9 (10%)	6	27
3	2	81/84 (96%)	77 (95%)	4 (5%)	21	54
4	3	84/85 (99%)	78 (93%)	6 (7%)	12	42
5	4	78/78 (100%)	75 (96%)	3 (4%)	28	60
9	9	112/123 (91%)	79 (70%)	33 (30%)	0	1
11	AA	1155/1157 (100%)	1142 (99%)	13 (1%)	70	86
12	AB	138/158 (87%)	105 (76%)	33 (24%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	AC	186/286 (65%)	186 (100%)	0	100	100
13	AD	185/286 (65%)	185 (100%)	0	100	100
14	AE	1120/1168 (96%)	1051 (94%)	69 (6%)	15	47
15	AF	70/75 (93%)	70 (100%)	0	100	100
16	AG	409/409 (100%)	296 (72%)	113 (28%)	0	1
17	C	57/65 (88%)	55 (96%)	2 (4%)	31	63
19	E	65/66 (98%)	62 (95%)	3 (5%)	23	56
20	F	60/61 (98%)	57 (95%)	3 (5%)	20	54
21	G	187/199 (94%)	177 (95%)	10 (5%)	19	52
22	H	137/461 (30%)	125 (91%)	12 (9%)	8	32
23	I	171/190 (90%)	162 (95%)	9 (5%)	19	52
24	J	172/173 (99%)	166 (96%)	6 (4%)	31	63
25	K	119/126 (94%)	110 (92%)	9 (8%)	11	39
26	L	91/116 (78%)	81 (89%)	10 (11%)	5	23
27	M	124/147 (84%)	116 (94%)	8 (6%)	14	45
28	N	104/105 (99%)	101 (97%)	3 (3%)	37	67
29	O	105/107 (98%)	98 (93%)	7 (7%)	13	44
30	P	86/90 (96%)	75 (87%)	11 (13%)	3	17
31	Q	90/99 (91%)	87 (97%)	3 (3%)	33	64
32	R	101/104 (97%)	94 (93%)	7 (7%)	13	43
33	S	83/84 (99%)	78 (94%)	5 (6%)	16	48
34	T	76/77 (99%)	62 (82%)	14 (18%)	1	7
35	U	65/65 (100%)	60 (92%)	5 (8%)	10	39
36	V	74/78 (95%)	70 (95%)	4 (5%)	18	51
37	W	72/79 (91%)	68 (94%)	4 (6%)	17	50
38	X	94/96 (98%)	82 (87%)	12 (13%)	3	17
39	Y	109/110 (99%)	89 (82%)	20 (18%)	1	7
40	Z	26/85 (31%)	17 (65%)	9 (35%)	0	0
42	b	58/63 (92%)	58 (100%)	0	100	100
43	c	67/68 (98%)	64 (96%)	3 (4%)	23	56
45	e	54/55 (98%)	54 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	f	48/49 (98%)	45 (94%)	3 (6%)	15	46
47	g	59/62 (95%)	54 (92%)	5 (8%)	8	34
48	h	216/218 (99%)	202 (94%)	14 (6%)	14	45
49	i	47/48 (98%)	41 (87%)	6 (13%)	3	17
50	j	164/164 (100%)	154 (94%)	10 (6%)	15	47
51	k	47/49 (96%)	45 (96%)	2 (4%)	25	57
52	l	165/165 (100%)	154 (93%)	11 (7%)	13	44
53	m	38/38 (100%)	35 (92%)	3 (8%)	10	38
54	n	148/150 (99%)	136 (92%)	12 (8%)	9	36
55	o	51/52 (98%)	48 (94%)	3 (6%)	16	48
56	p	136/138 (99%)	131 (96%)	5 (4%)	29	62
57	q	34/34 (100%)	32 (94%)	2 (6%)	16	48
58	r	114/114 (100%)	105 (92%)	9 (8%)	10	38
59	s	116/116 (100%)	111 (96%)	5 (4%)	25	57
60	t	104/104 (100%)	96 (92%)	8 (8%)	10	39
61	u	103/103 (100%)	96 (93%)	7 (7%)	13	43
62	v	109/109 (100%)	105 (96%)	4 (4%)	29	62
63	w	99/103 (96%)	93 (94%)	6 (6%)	15	47
64	x	86/87 (99%)	81 (94%)	5 (6%)	17	49
65	y	99/100 (99%)	95 (96%)	4 (4%)	27	59
66	z	89/90 (99%)	85 (96%)	4 (4%)	23	56
All	All	8314/9148 (91%)	7720 (93%)	594 (7%)	15	42

5 of 594 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
43	c	5	CYS
62	v	115	GLU
48	h	52	ARG
40	Z	30	PHE
54	n	6	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
21	G	18	HIS
27	M	148	ASN
21	G	39	HIS
26	L	63	ASN
31	Q	15	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	A	76/76 (100%)	33 (43%)	10 (13%)
10	B	75/76 (98%)	41 (54%)	8 (10%)
18	D	1513/1542 (98%)	282 (18%)	8 (0%)
41	a	2859/2904 (98%)	534 (18%)	0
44	d	119/120 (99%)	18 (15%)	0
8	7	32/41 (78%)	19 (59%)	4 (12%)
All	All	4674/4759 (98%)	927 (19%)	30 (0%)

5 of 927 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	7	-19	U
8	7	-17	U
8	7	-16	U
8	7	-15	U
8	7	-14	U

5 of 30 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
10	B	6	G
18	D	1145	A
10	B	21	A
18	D	1493	A
18	D	428	G

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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.

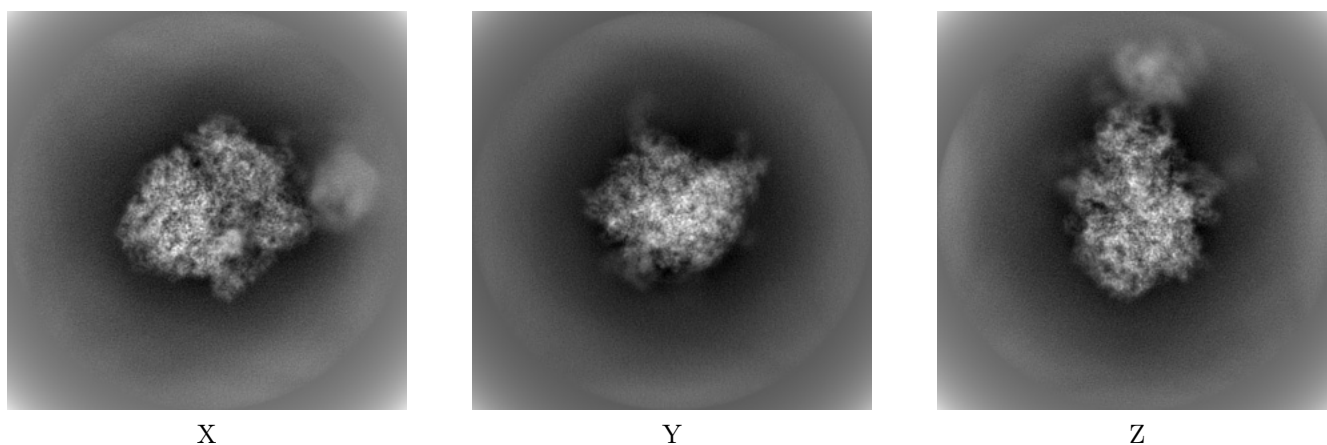
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22082. 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](#)

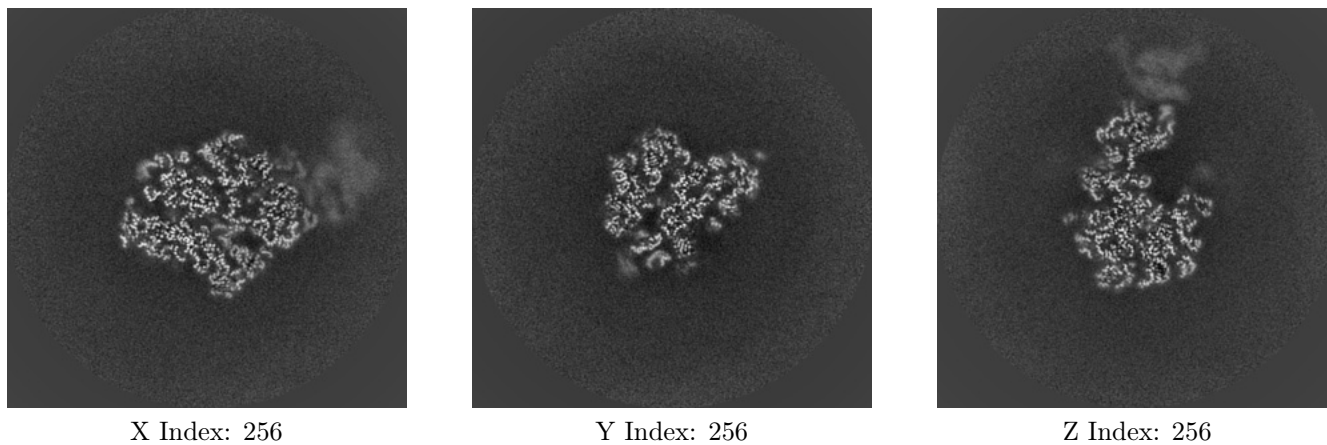
6.1.1 Primary map



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

6.2 Central slices [i](#)

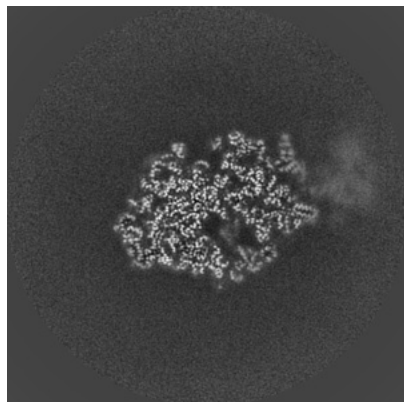
6.2.1 Primary map



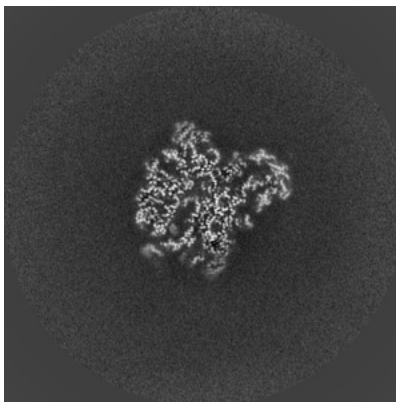
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

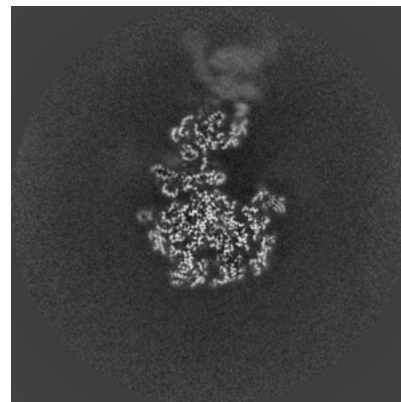
6.3.1 Primary map



X Index: 242



Y Index: 250

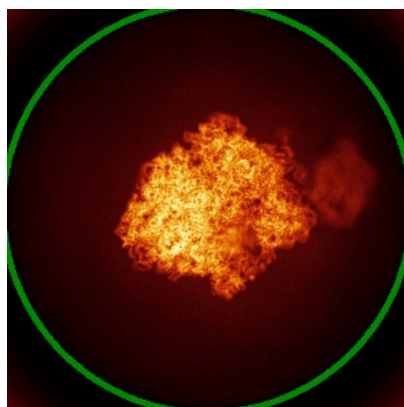


Z Index: 259

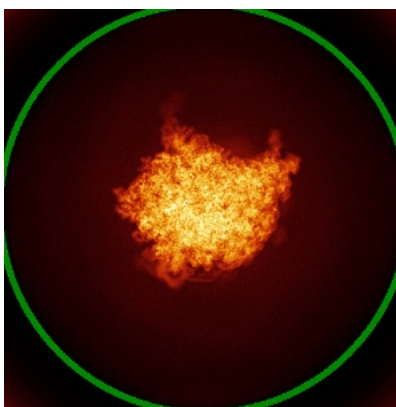
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

6.4.1 Primary map



X



Y

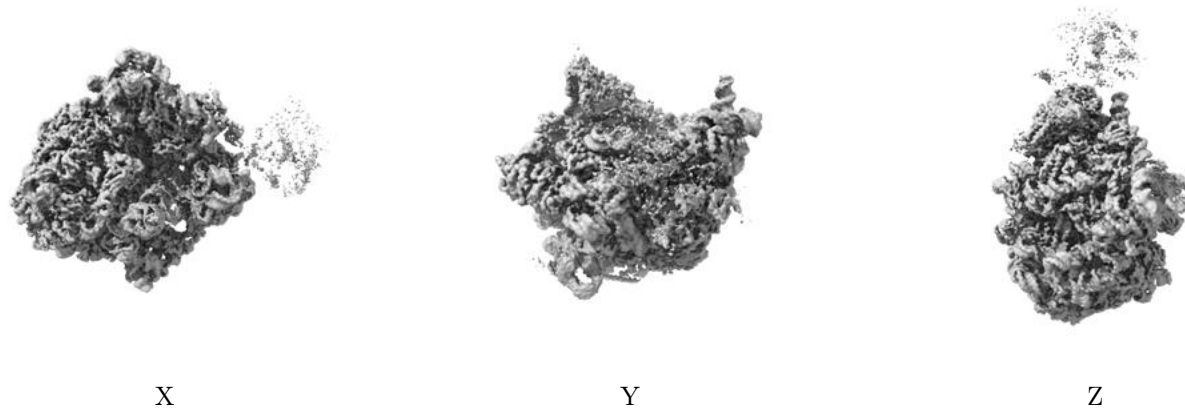


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.014. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

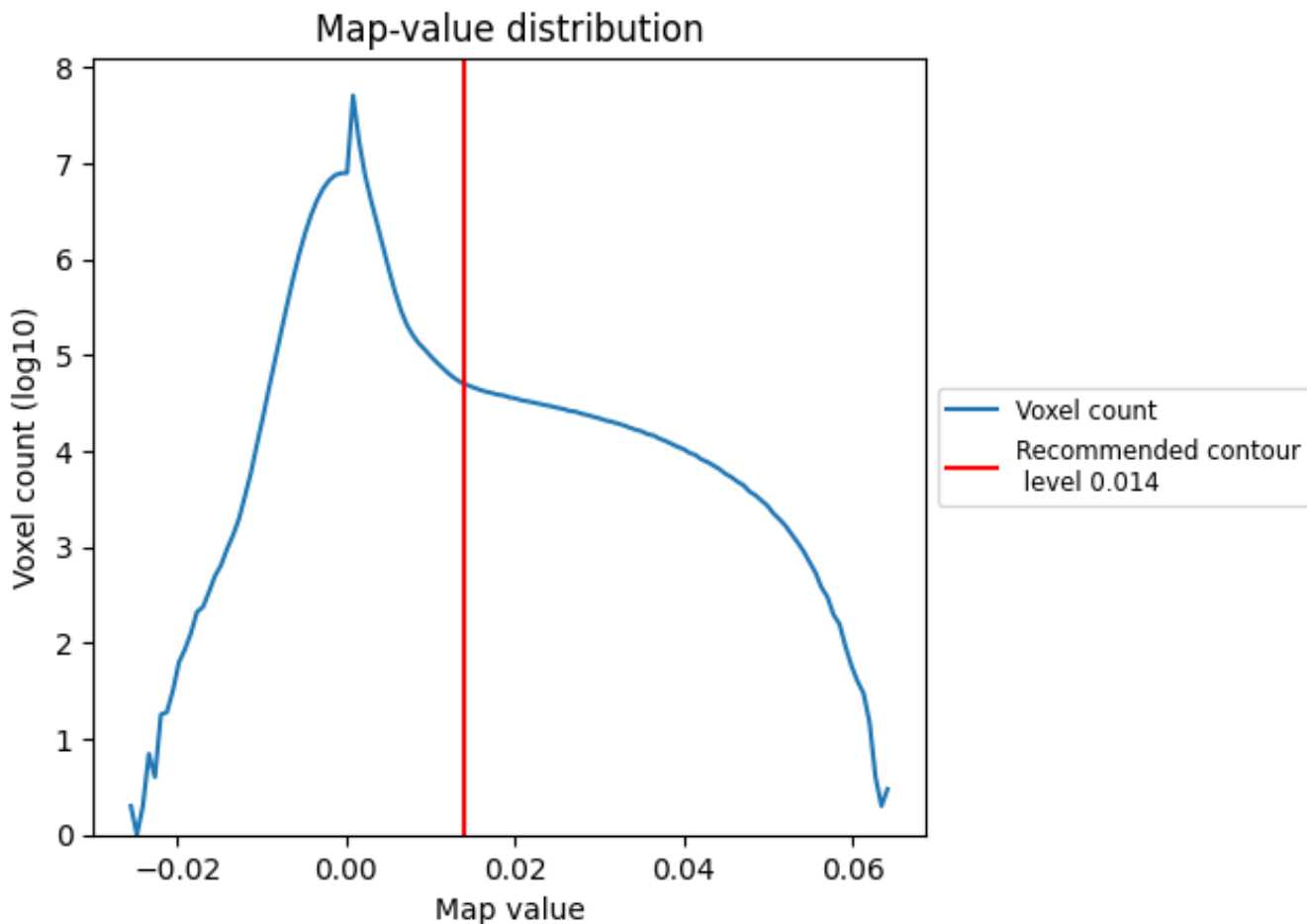
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

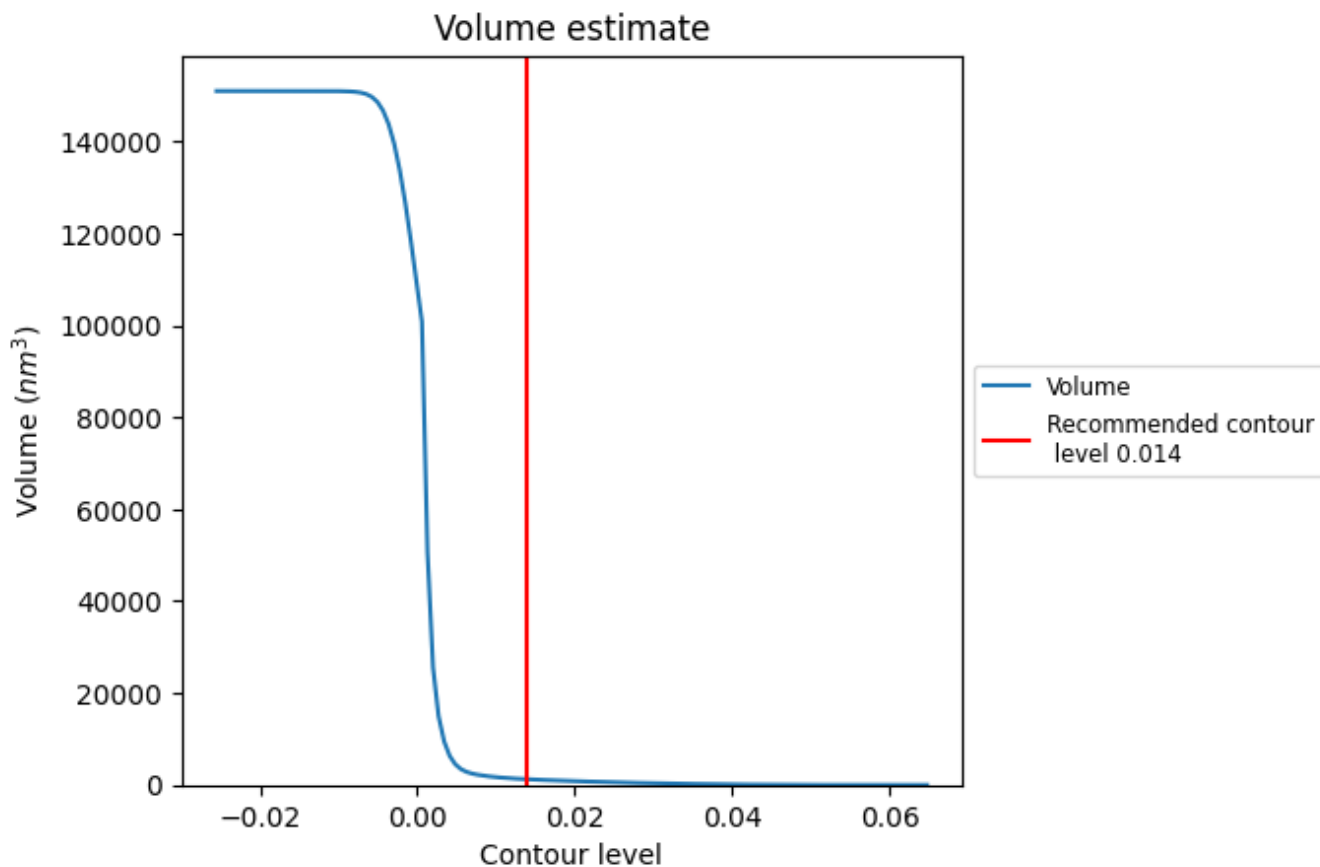
This section contains the results of statistical analysis of the map.

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.

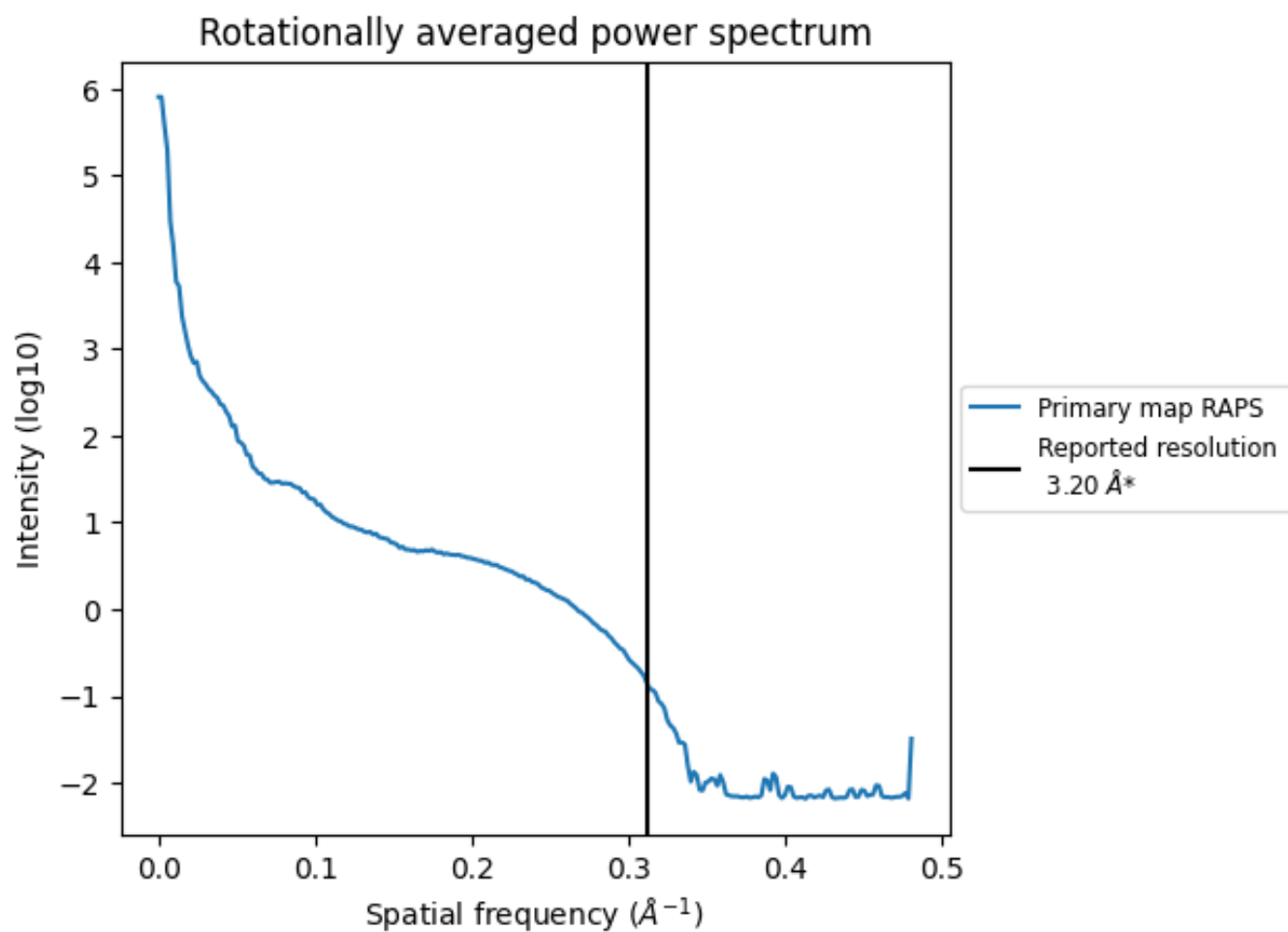
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1238 nm³; this corresponds to an approximate mass of 1118 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 0.312 Å⁻¹

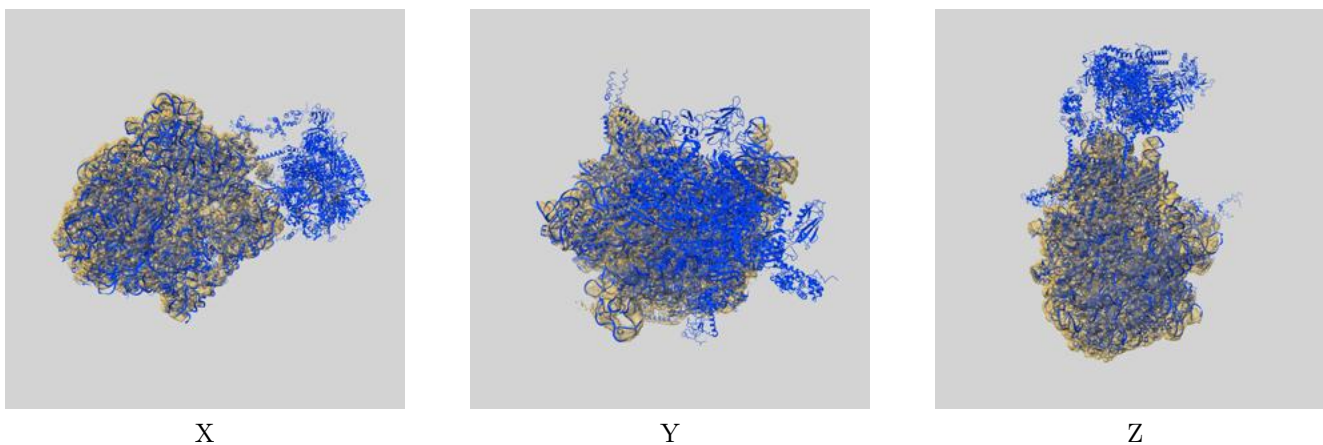
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

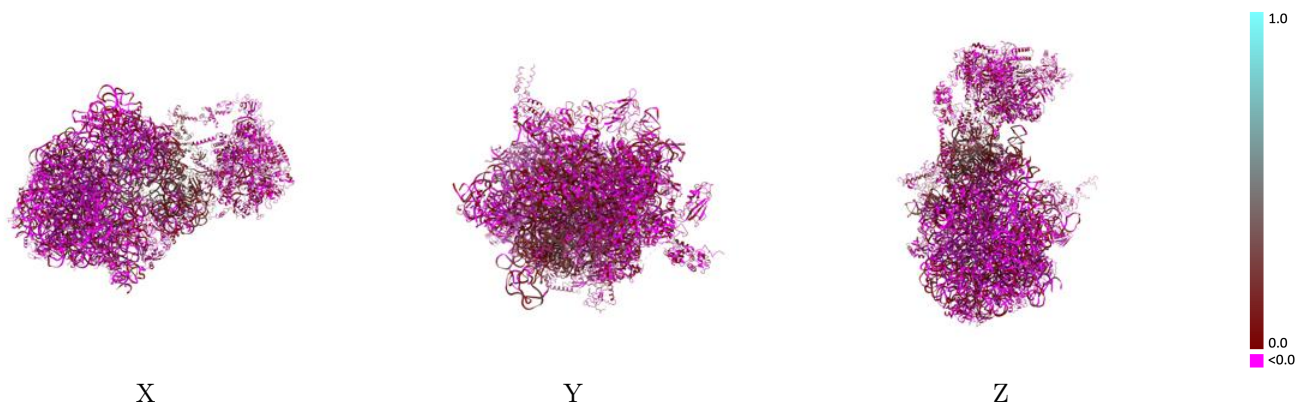
This section contains information regarding the fit between EMDB map EMD-22082 and PDB model 6X6T. Per-residue inclusion information can be found in section 3 on page 17.

9.1 Map-model overlay [i](#)



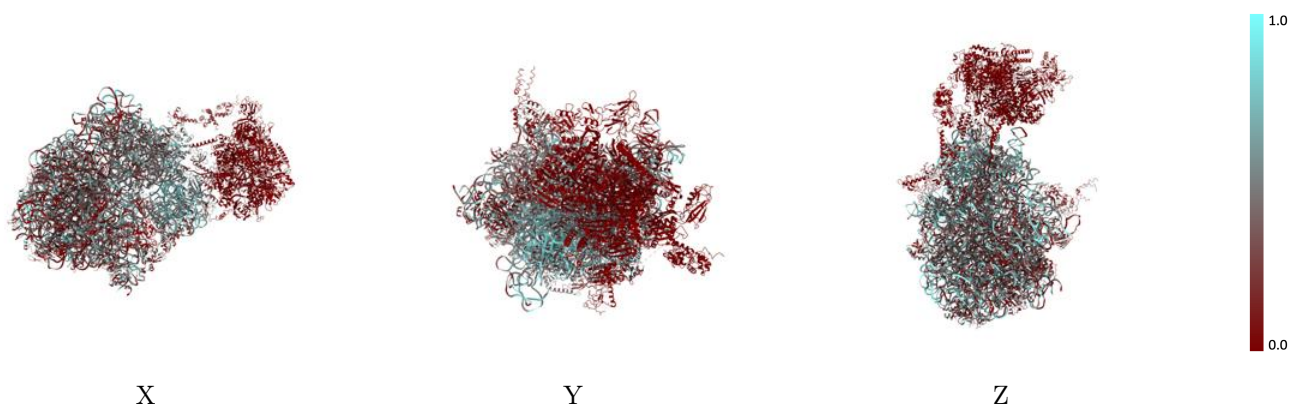
The images above show the 3D surface view of the map at the recommended contour level 0.014 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



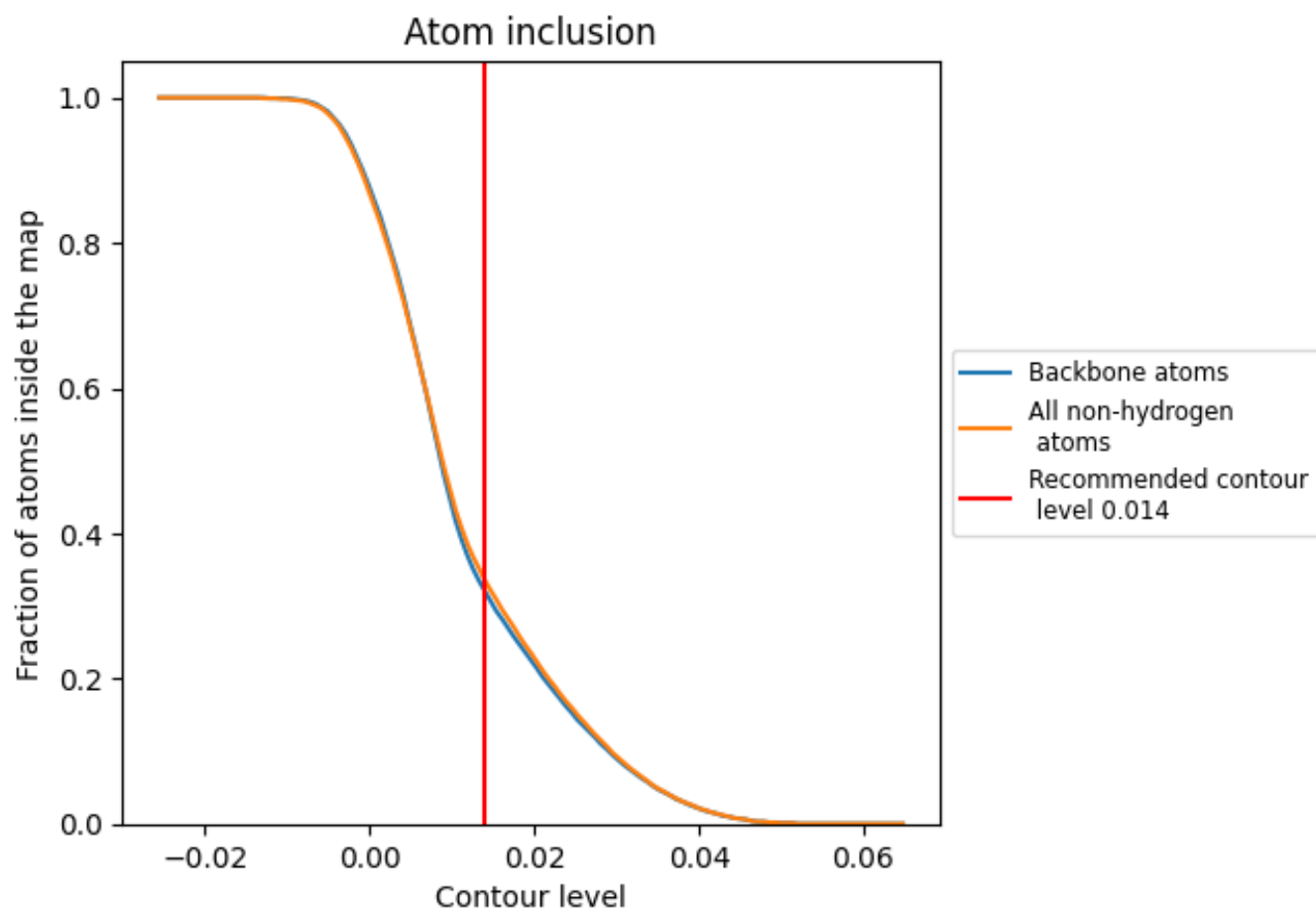
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.014).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 32% of all backbone atoms, 34% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.014) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3360	 0.0150
0	 0.2720	 -0.0410
1	 0.2300	 -0.0340
2	 0.2890	 0.0050
3	 0.4240	 0.0080
4	 0.3270	 0.0250
5	 0.0250	 0.0380
6	 0.0760	 0.0390
7	 0.1340	 0.0770
9	 0.1540	 0.0020
A	 0.4380	 0.0920
AA	 0.0070	 0.0250
AB	 0.1210	 0.1110
AC	 0.0010	 0.0090
AD	 0.0010	 0.0120
AE	 0.0030	 0.0160
AF	 0.0000	 0.0220
AG	 0.1970	 0.1380
B	 0.4330	 0.0350
C	 0.4020	 0.0440
D	 0.5580	 0.0510
E	 0.2630	 -0.0470
F	 0.3720	 0.1300
G	 0.4710	 0.1440
H	 0.0300	 0.0480
I	 0.5160	 0.2070
J	 0.4130	 0.0240
K	 0.3480	 0.0120
L	 0.3170	 -0.0540
M	 0.5520	 0.2370
N	 0.2880	 -0.0650
O	 0.5360	 0.1620
P	 0.4380	 0.1200
Q	 0.5270	 0.1840
R	 0.2590	 -0.0640



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Chain	Atom inclusion	Q-score
S	█ 0.4380	█ 0.1180
T	█ 0.3040	█ -0.0380
U	█ 0.3090	█ -0.0520
V	█ 0.3730	█ -0.0230
W	█ 0.3460	█ -0.0050
X	█ 0.3550	█ 0.0100
Y	█ 0.0340	█ -0.0050
Z	█ 0.0000	█ 0.0130
a	█ 0.4330	█ -0.0200
b	█ 0.2620	█ -0.0670
c	█ 0.3560	█ -0.0570
d	█ 0.4860	█ -0.0050
e	█ 0.3520	█ -0.0330
f	█ 0.2960	█ 0.0030
g	█ 0.2430	█ 0.0390
h	█ 0.2920	█ -0.0770
i	█ 0.3530	█ -0.0260
j	█ 0.2900	█ -0.0160
k	█ 0.3090	█ -0.0500
l	█ 0.2990	█ -0.0110
m	█ 0.3380	█ -0.0130
n	█ 0.2830	█ -0.0430
o	█ 0.3180	█ -0.0230
p	█ 0.2090	█ -0.0260
q	█ 0.2330	█ -0.0190
r	█ 0.2470	█ 0.0160
s	█ 0.2660	█ -0.0210
t	█ 0.2770	█ 0.0020
u	█ 0.3100	█ -0.0260
v	█ 0.2800	█ -0.0150
w	█ 0.3380	█ -0.0330
x	█ 0.3560	█ -0.0420
y	█ 0.3130	█ -0.0130
z	█ 0.3030	█ -0.0140