wwPDB EM Validation Summary Report (i)

Nov 13, 2022 – 03:10 PM EST

PDB ID	:	6X7F
EMDB ID	:	EMD-22084
Title	:	Cryo-EM structure of an Escherichia coli coupled transcription-translation complex B2 (TTC-B2) 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	:	3.50 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 (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:

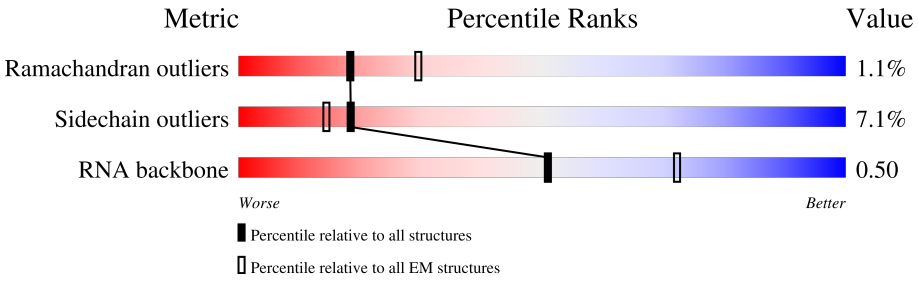
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 3.50 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	42% 93% 7%
2	1	110	41% 93% 7%
3	2	100	36% 89% 5% 6%
4	3	104	39% 91% 8%
5	4	94	24% 96%
6	5	36	28% 47% 17% 36%
7	6	36	14% 64% 11% 25%
8	7	41	37% 29% 46% 5% 20%

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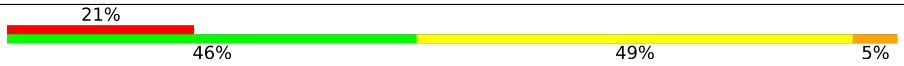
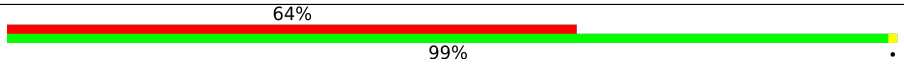
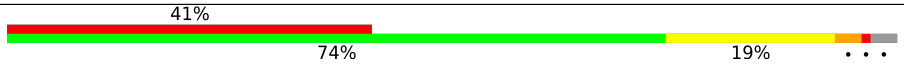
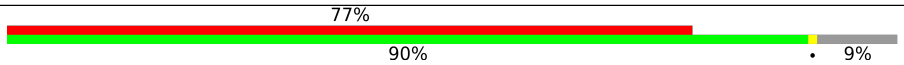
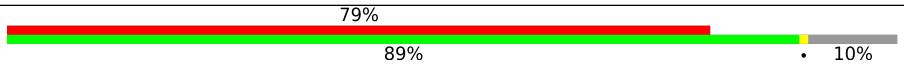
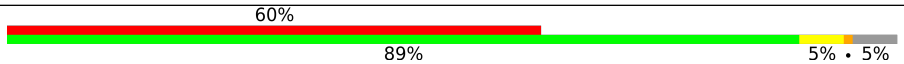
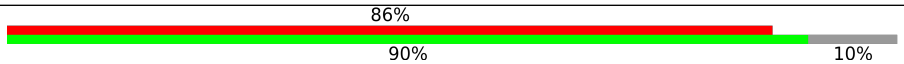
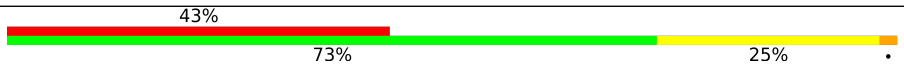
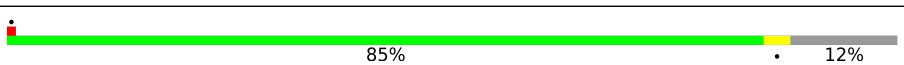
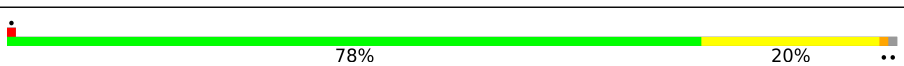
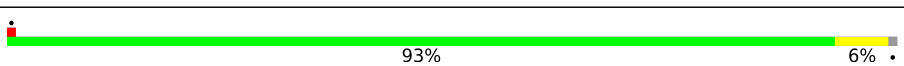
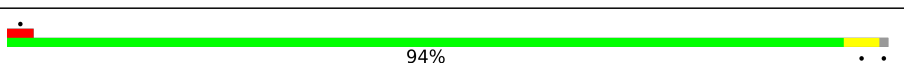
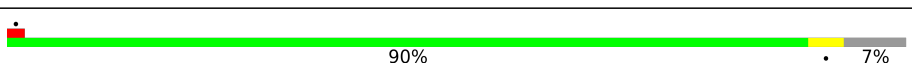
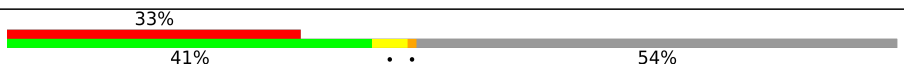
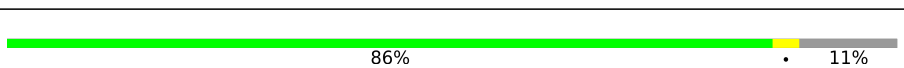
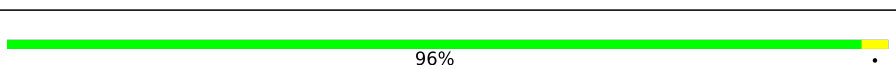
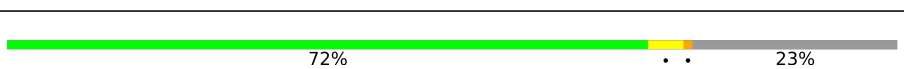
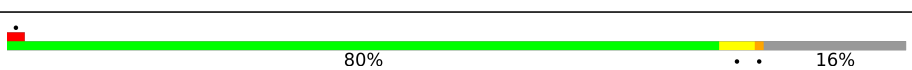
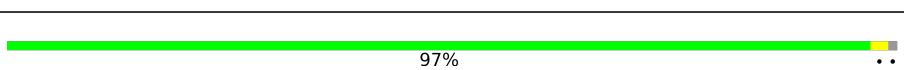
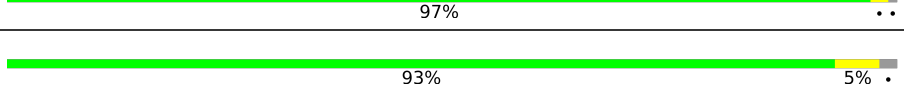
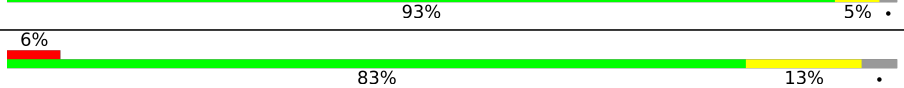
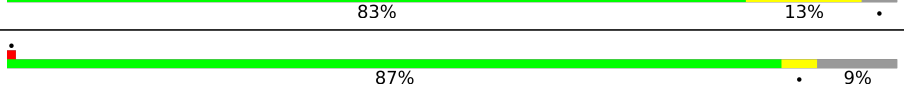
Mol	Chain	Length	Quality of chain
9	9	165	
10	A	76	
10	B	76	
11	AA	1342	
12	AB	181	
13	AC	329	
13	AD	329	
14	AE	1407	
15	AF	91	
16	AG	495	
17	C	75	
18	D	1542	
19	E	87	
20	F	71	
21	G	241	
22	H	557	
23	I	233	
24	J	206	
25	K	167	
26	L	135	
27	M	179	
28	N	130	
29	O	130	
30	P	103	
31	Q	129	

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Mol	Chain	Length	Quality of chain
32	R	124	92% 6%
33	S	101	95%
34	T	89	85% 13%
35	U	82	93% 7%
36	V	84	93% 5%
37	W	92	30% 86% 10%
38	X	118	35% 88% 10%
39	Y	142	54% 68% 27%
40	Z	121	19% 12% 12% 75%
41	a	2904	8% 81% 18%
42	b	85	28% 88% 11%
43	c	78	47% 94% 5%
44	d	120	86% 14%
45	e	63	35% 97%
46	f	59	34% 95%
47	g	70	26% 86% 9% 6%
48	h	273	38% 93% 7%
49	i	57	54% 88% 11%
50	j	209	46% 97%
51	k	55	24% 89% 5% 5%
52	l	201	46% 93% 7%
53	m	46	54% 93% 7%
54	n	179	18% 89% 10%
55	o	65	51% 91% 8%
56	p	177	22% 97%

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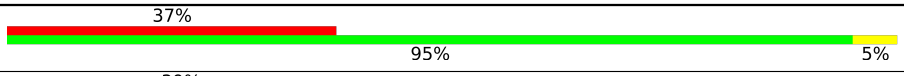
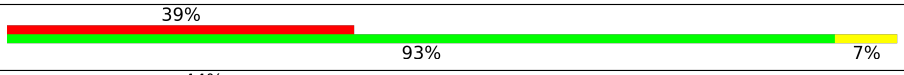
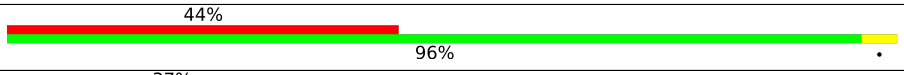
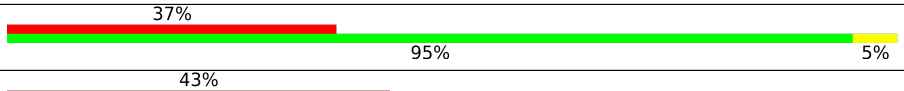
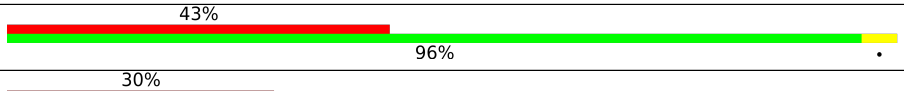
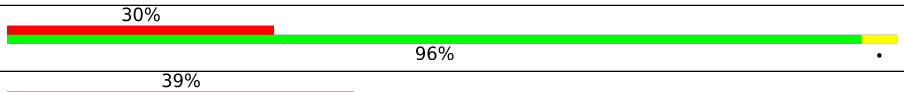
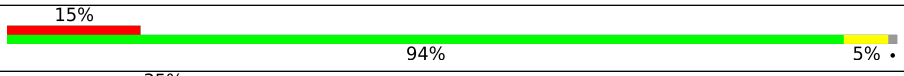
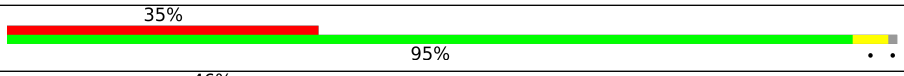
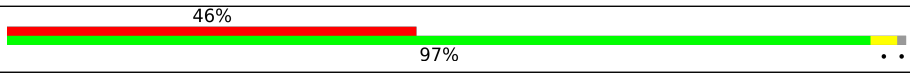
Mol	Chain	Length	Quality of chain
57	q	38	
58	r	149	
59	s	142	
60	t	123	
61	u	144	
62	v	136	
63	w	127	
64	x	117	
65	y	115	
66	z	118	

2 Entry composition (i)

There are 68 unique types of molecules in this entry. The entry contains 291738 atoms, of which 109912 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
1	0	103	Total	C	H	N	O	S	0	0
			1655	516	839	153	145	2		

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

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

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

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

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

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

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

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

- Molecule 6 is a DNA chain called NT DNA.

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

- Molecule 7 is a DNA chain called T DNA.

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

- Molecule 8 is a RNA chain called mRNA with 24 nt long spacer.

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	U	deletion	GB 1848954948
B	?	-	U	deletion	GB 1848954948

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AB	175	Total	C	N	O	S	0	0
			1403	889	250	257	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AC	301	Total	C	N	O	S	0	0
			2094	1296	379	413	6		
13	AD	297	Total	C	N	O	S	0	0
			2068	1281	376	405	6		

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

- 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
26	L	104	Total	C	H	N	O	S	0	0
			1694	536	846	153	152	7		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 42 is a protein called 50S ribosomal protein L27.

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

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

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

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

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

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

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

- 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
53	m	46	Total	C	H	N	O	S	0	0
			795	228	418	90	57	2		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

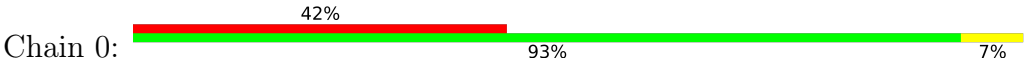
Mol	Chain	Residues	Atoms		AltConf
68	AE	2	Total 2	Zn 2	0

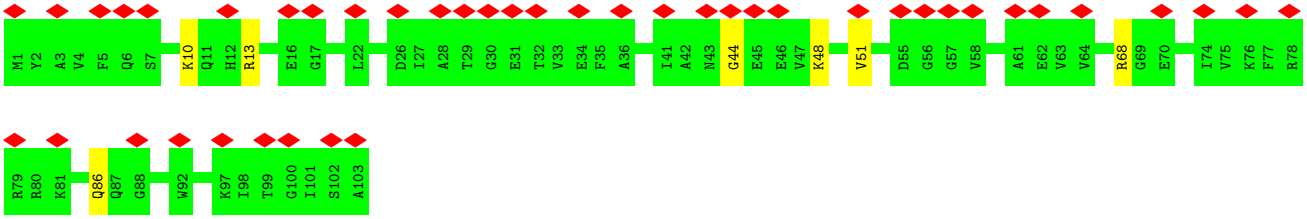
3 Residue-property plots (i)

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

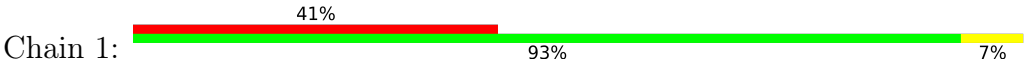
Chain 0:

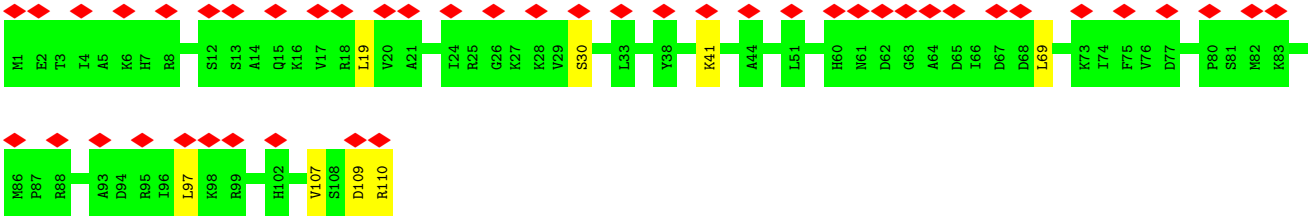




• Molecule 2: 50S ribosomal protein L22

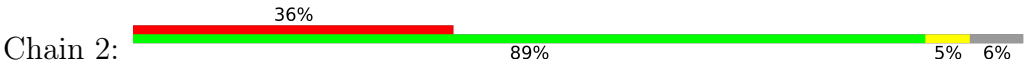
Chain 1:

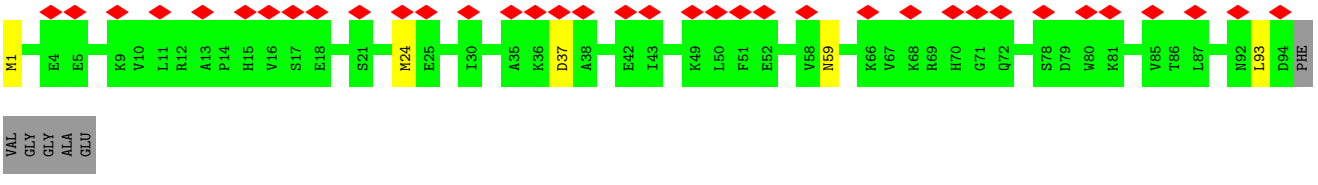




• Molecule 3: 50S ribosomal protein L23

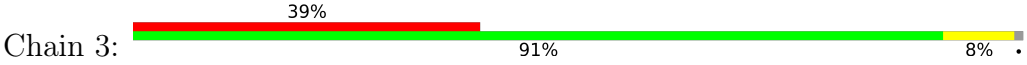
Chain 2:

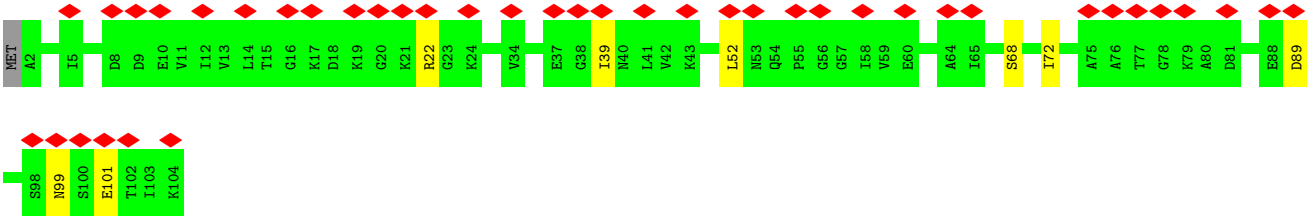




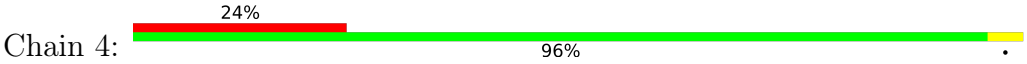
• Molecule 4: 50S ribosomal protein L24

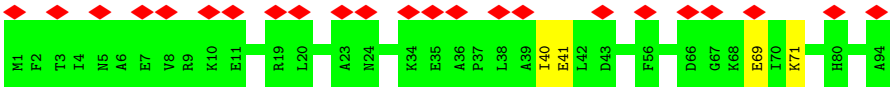
Chain 3:



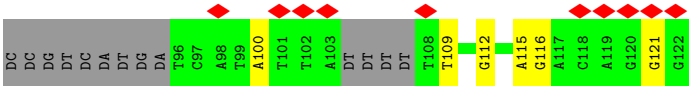


• Molecule 5: 50S ribosomal protein L25

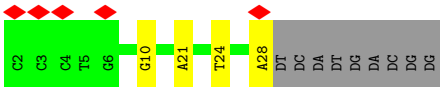




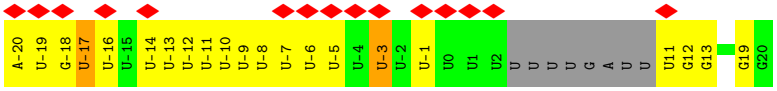
• Molecule 6: NT DNA



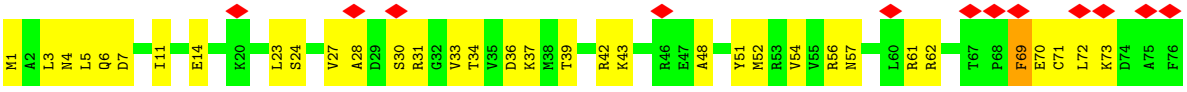
• Molecule 7: T DNA

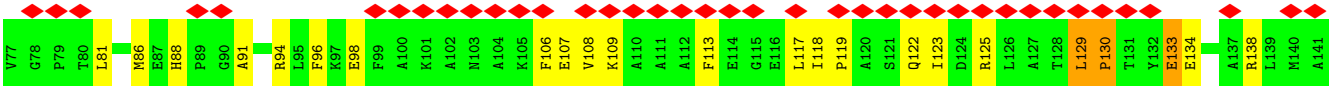


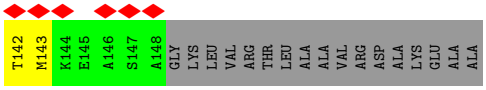
• Molecule 8: mRNA with 24 nt long spacer



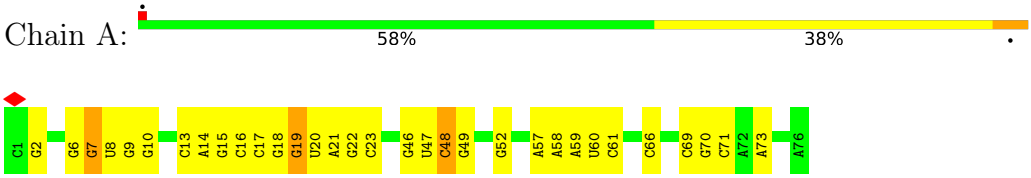
• Molecule 9: 50S ribosomal protein L10



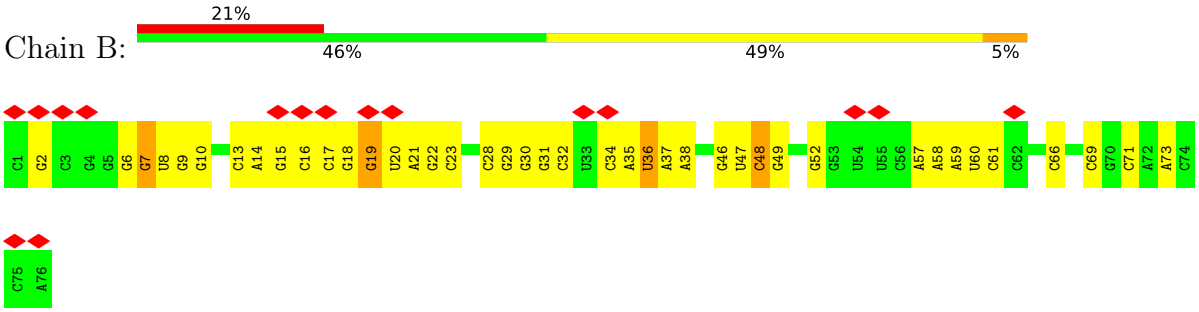




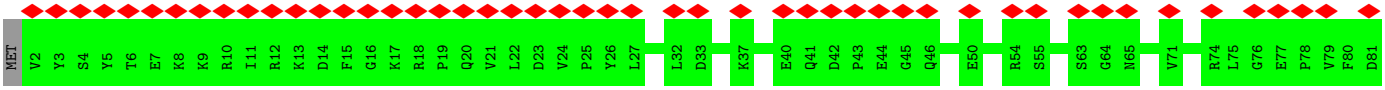
• Molecule 10: E-site and P-site tRNA (fMet)

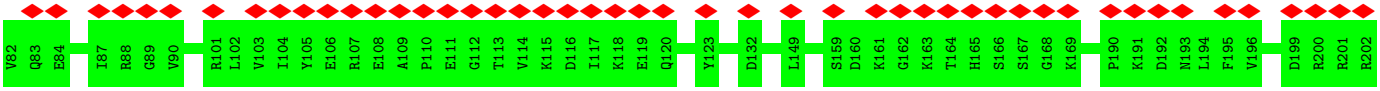


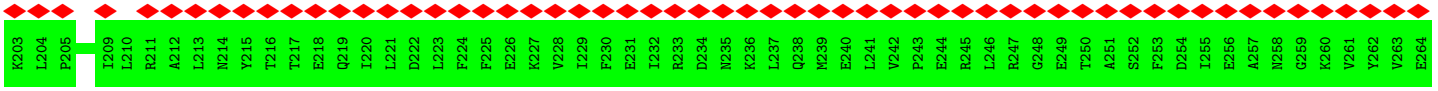
• Molecule 10: E-site and P-site tRNA (fMet)

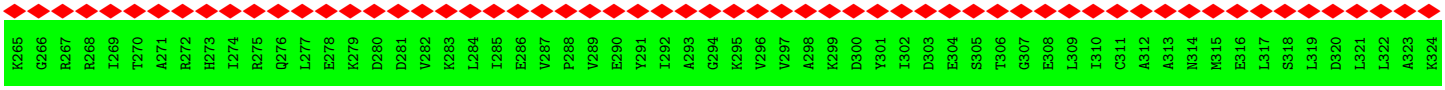


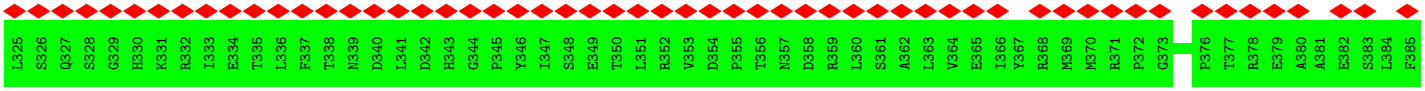
• Molecule 11: DNA-directed RNA polymerase subunit beta

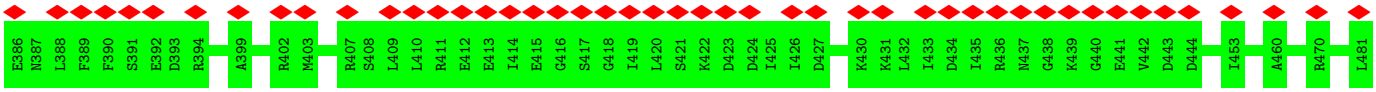


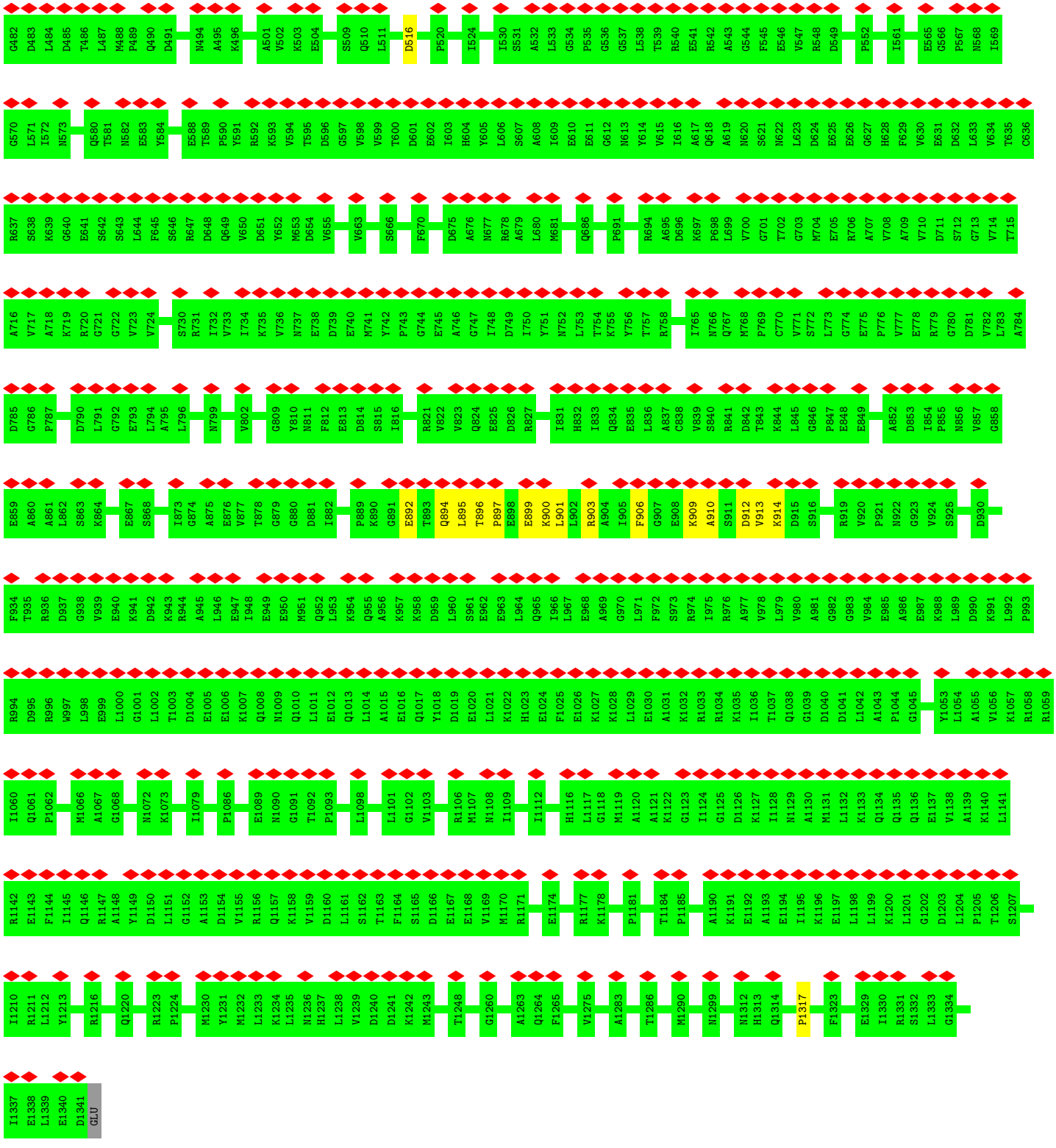






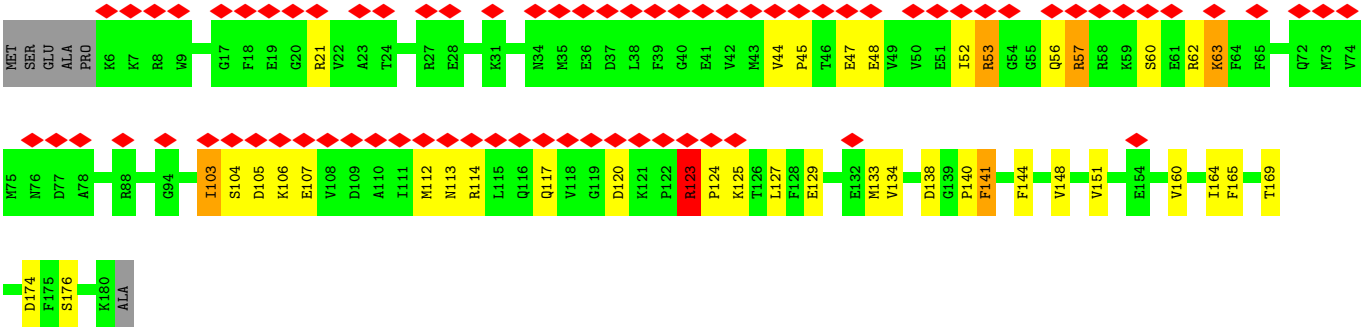






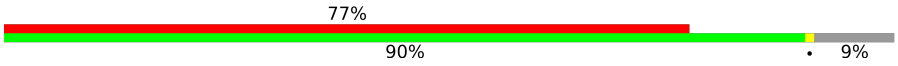
• Molecule 12: Transcription termination/antitermination protein NusG

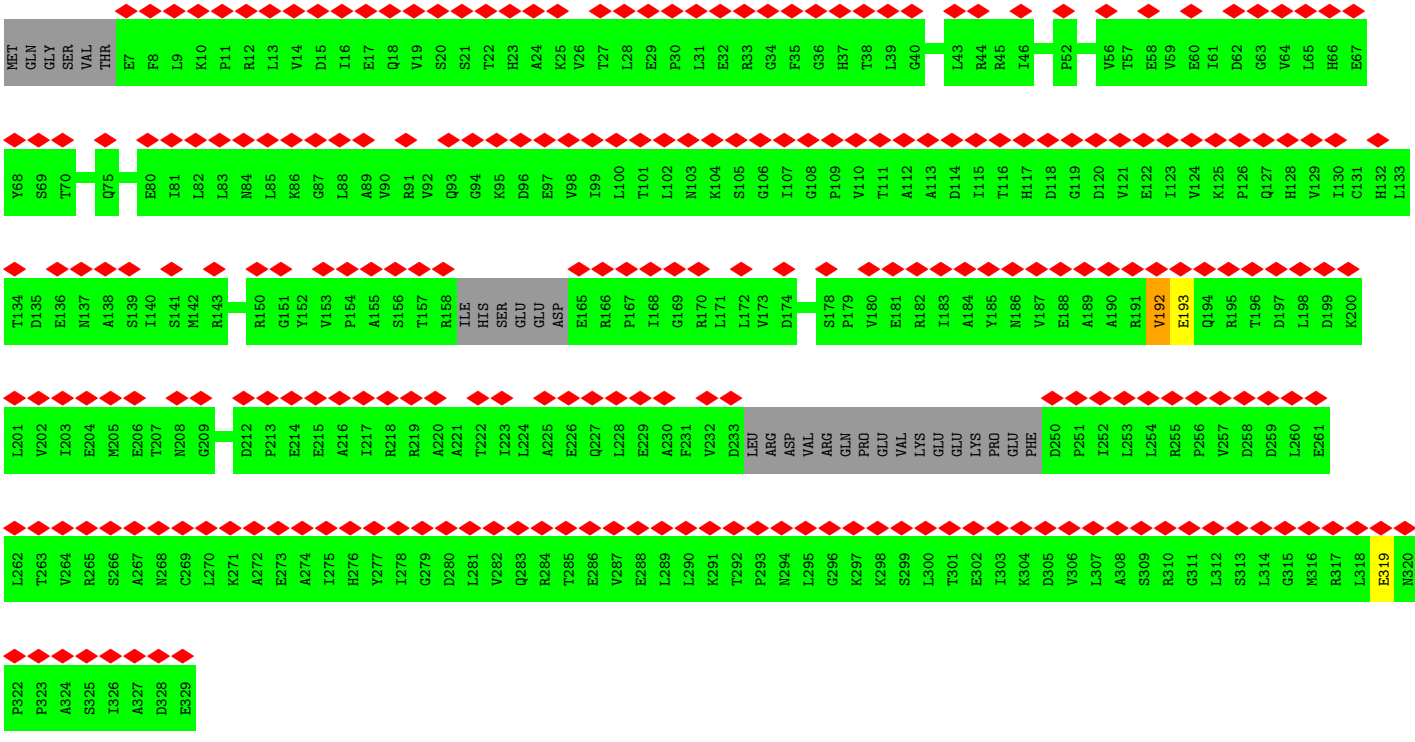
Chain AB:



• Molecule 13: DNA-directed RNA polymerase subunit alpha

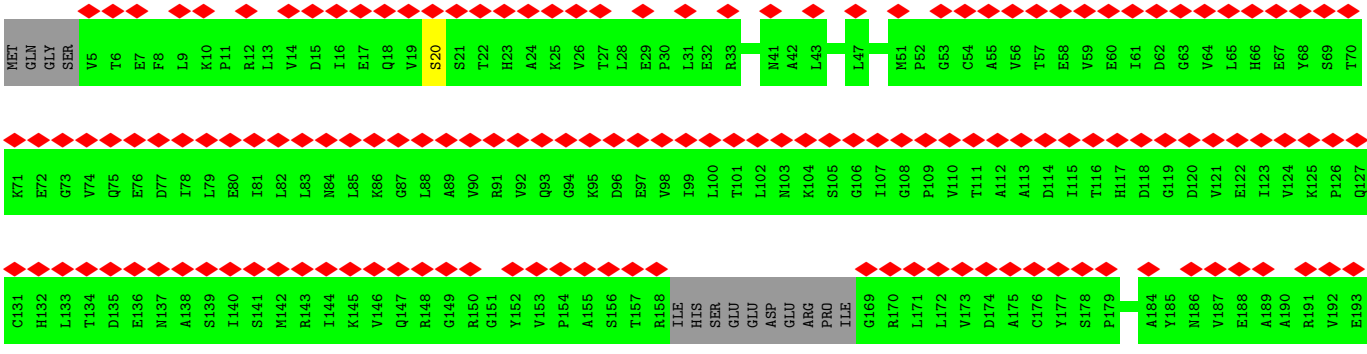
Chain AC:

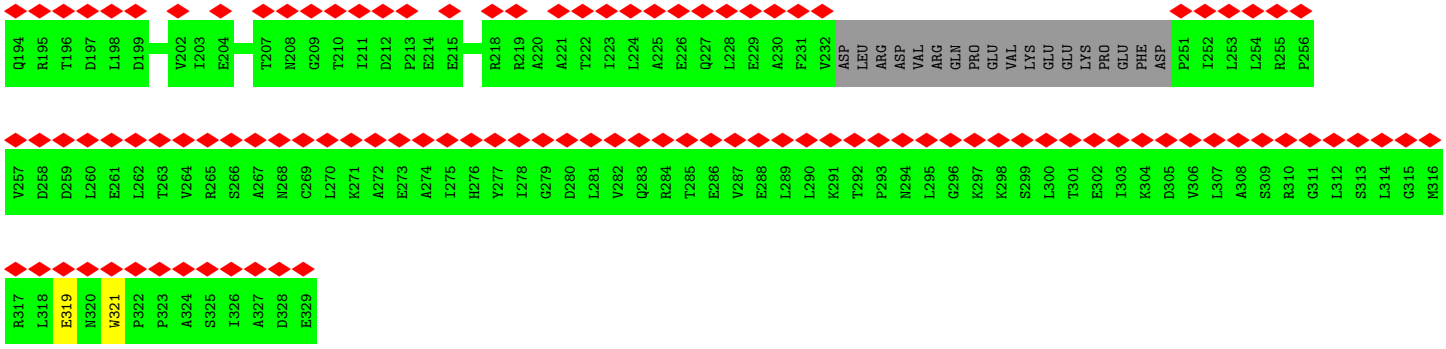




• Molecule 13: DNA-directed RNA polymerase subunit alpha

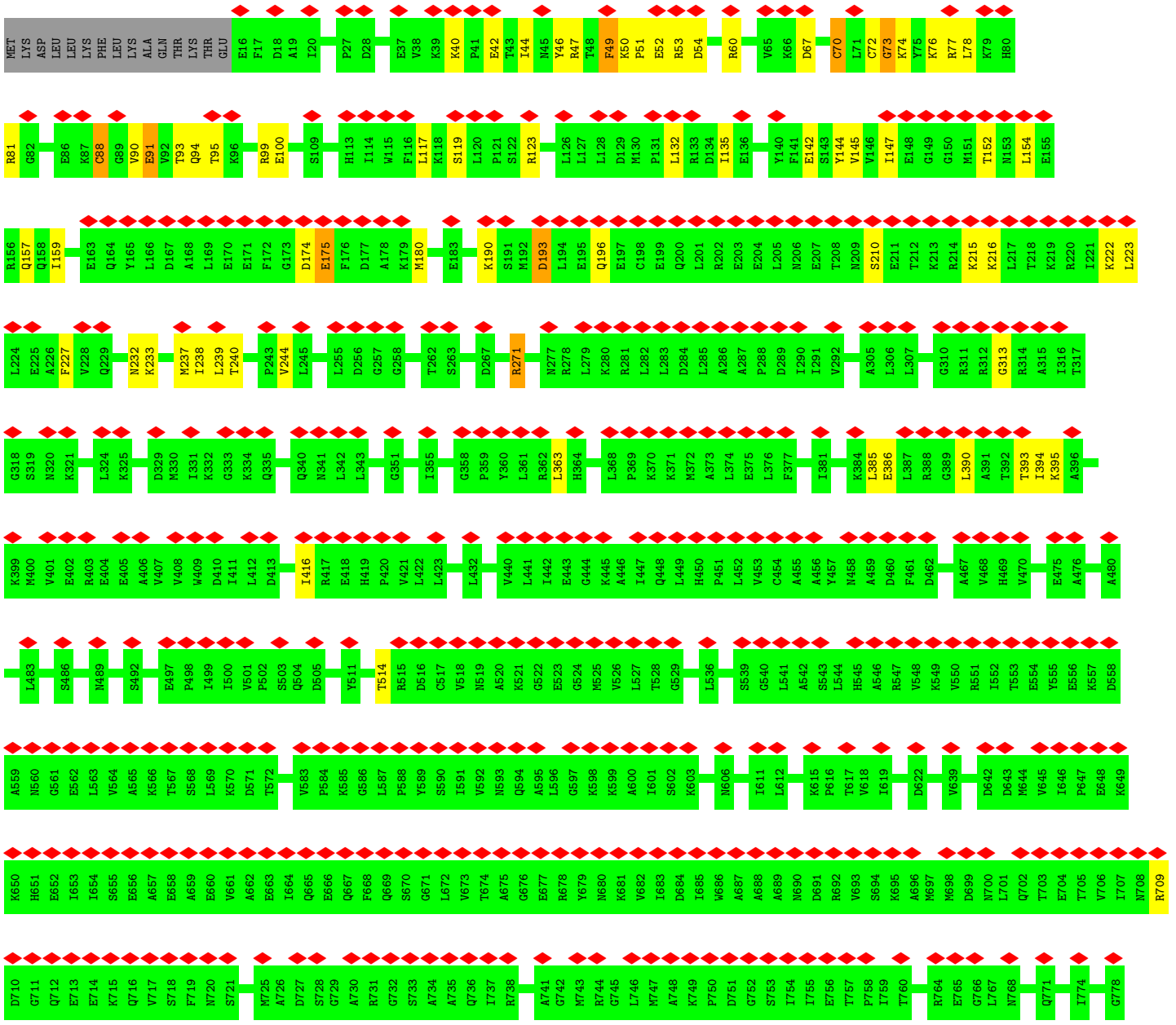
Chain AD:

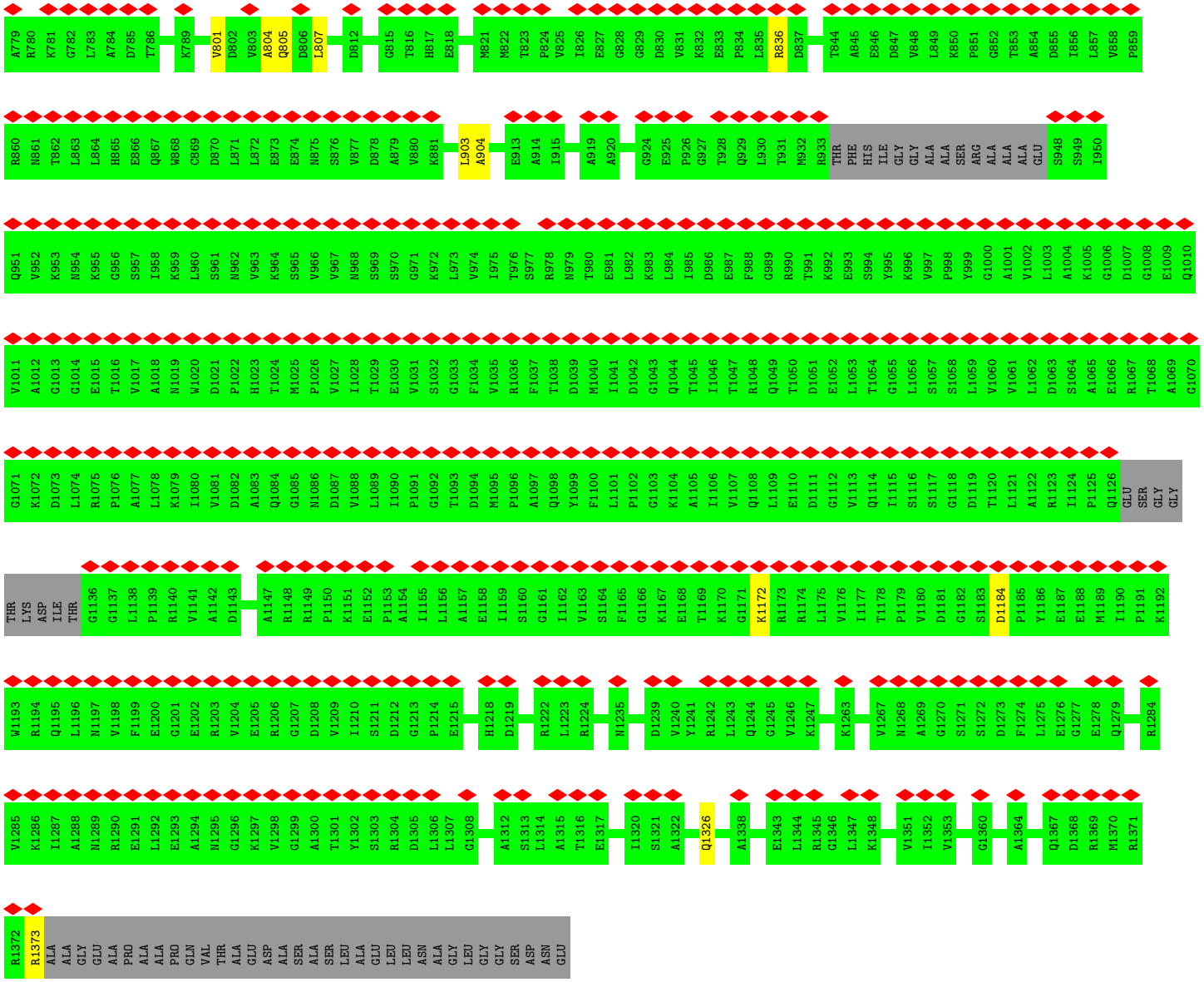




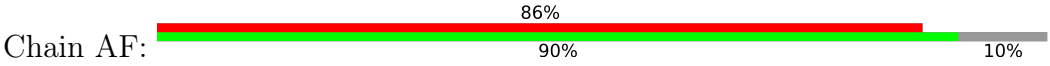
• Molecule 14: DNA-directed RNA polymerase subunit beta'

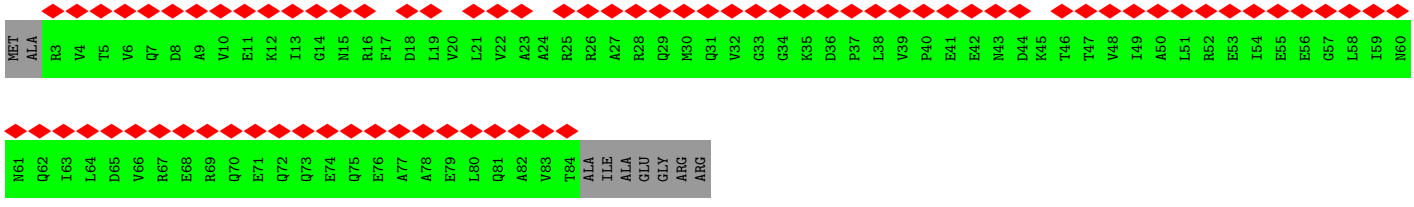
Chain AE:



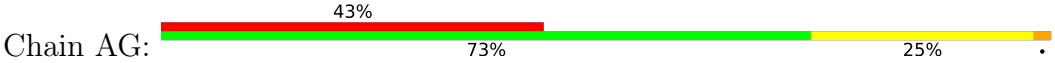


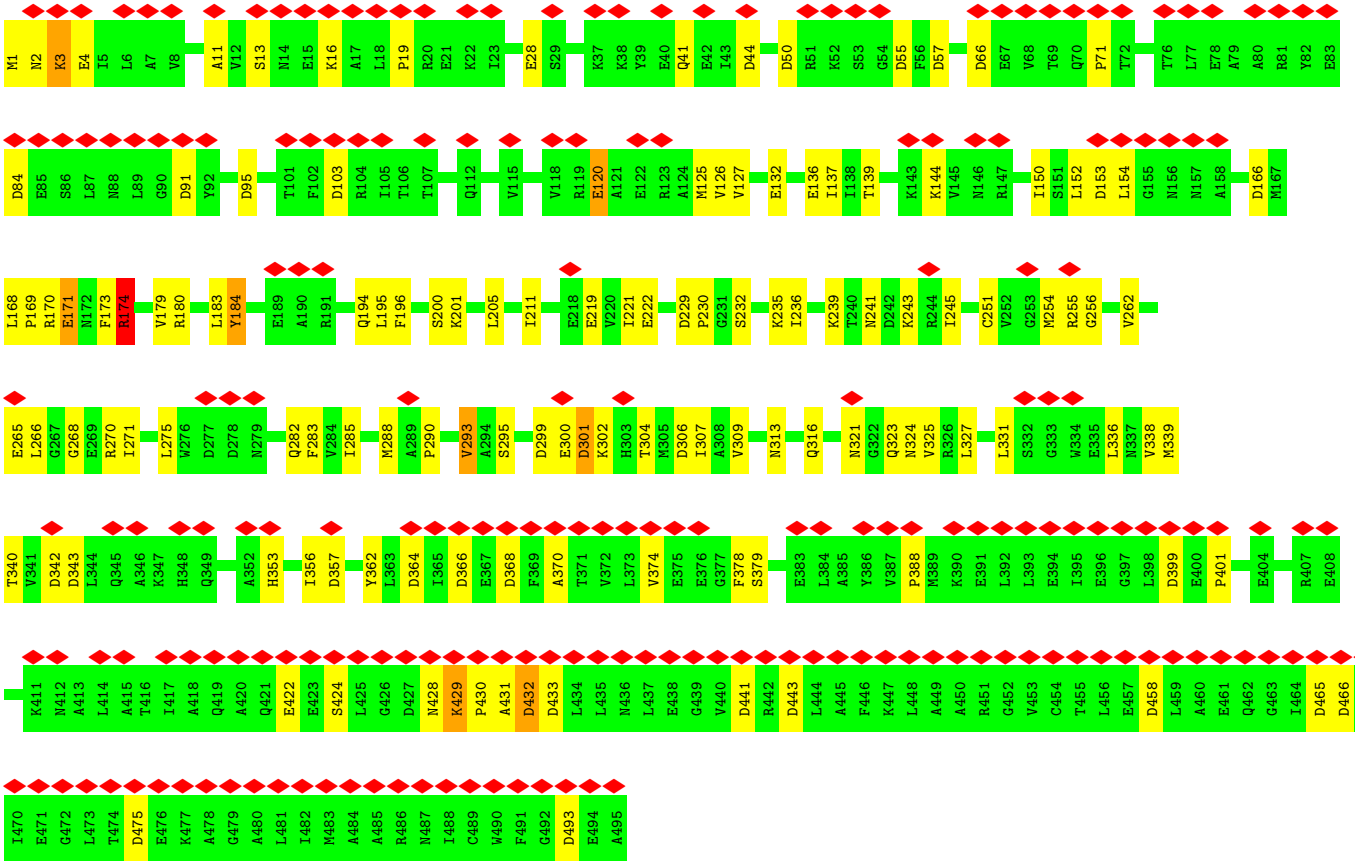
• Molecule 15: DNA-directed RNA polymerase subunit omega





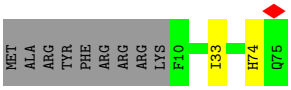
• Molecule 16: Transcription termination/antitermination protein NusA





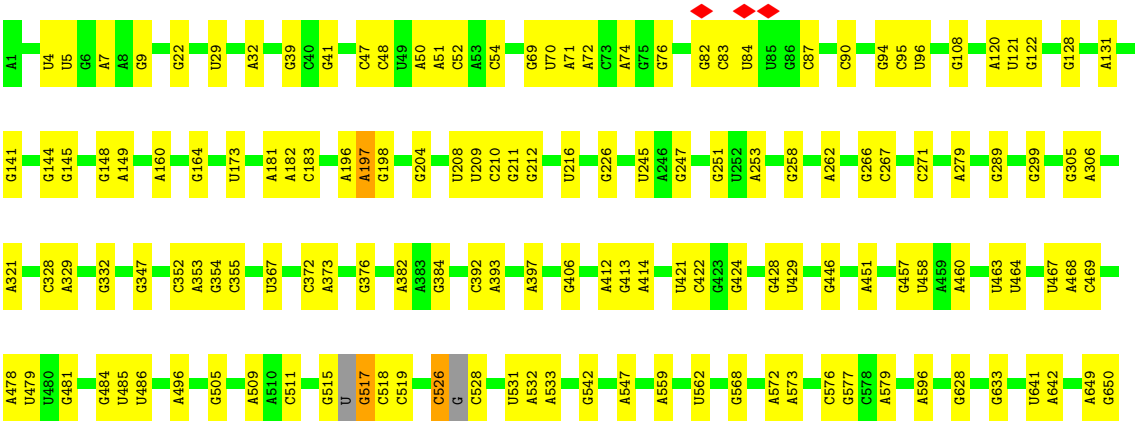
• Molecule 17: 30S ribosomal protein S18

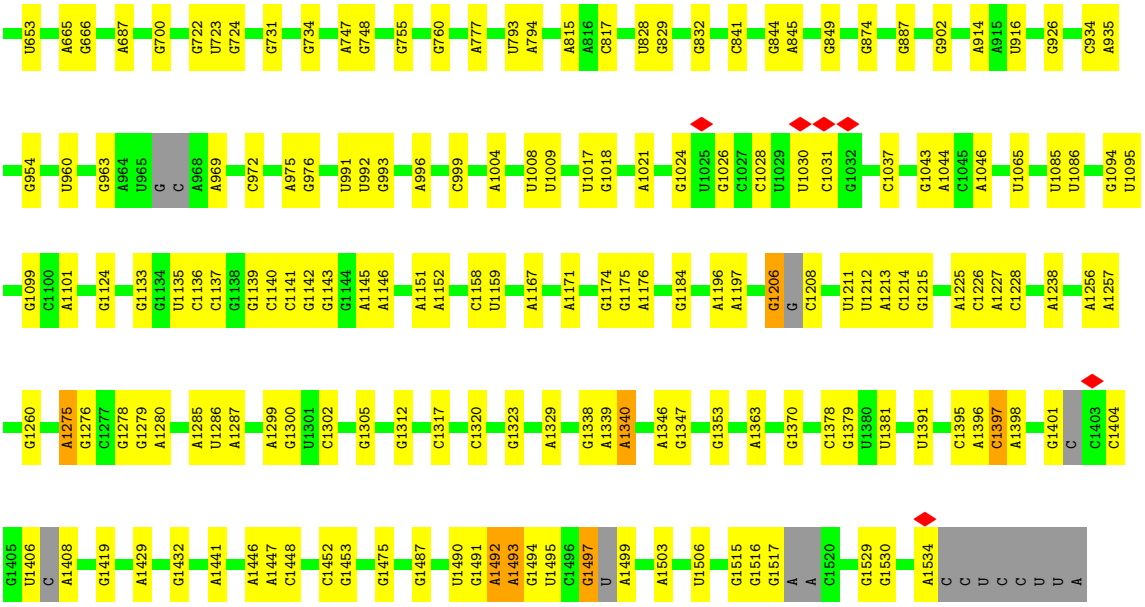
Chain C:



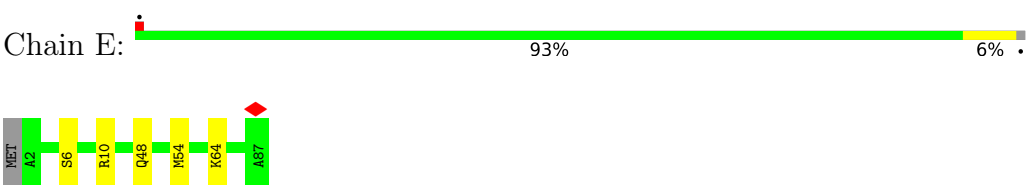
• Molecule 18: 16S rRNA

Chain D:

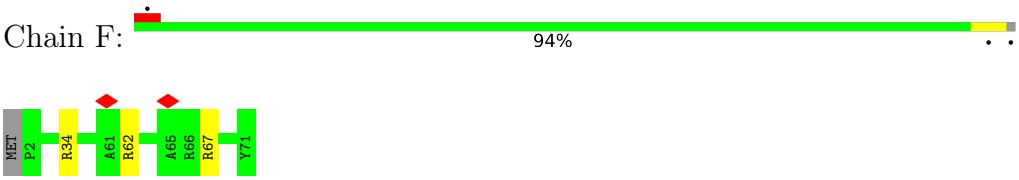




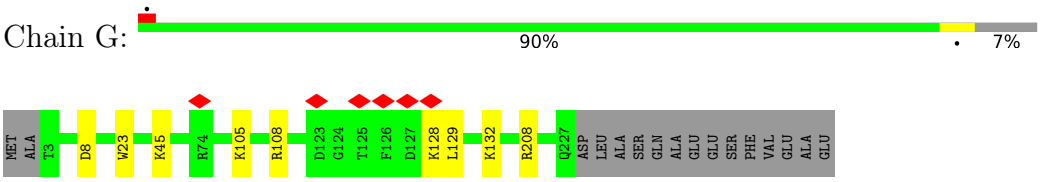
• Molecule 19: 30S ribosomal protein S20



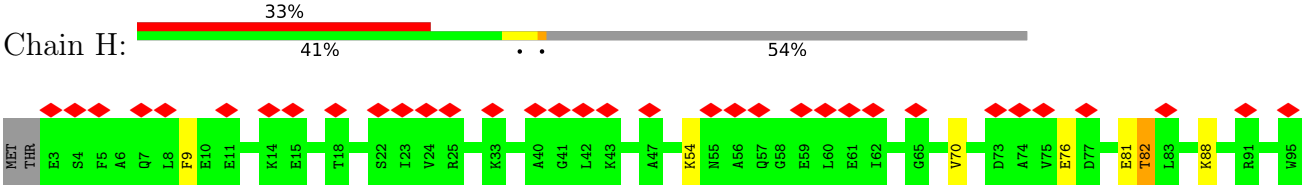
• Molecule 20: 30S ribosomal protein S21

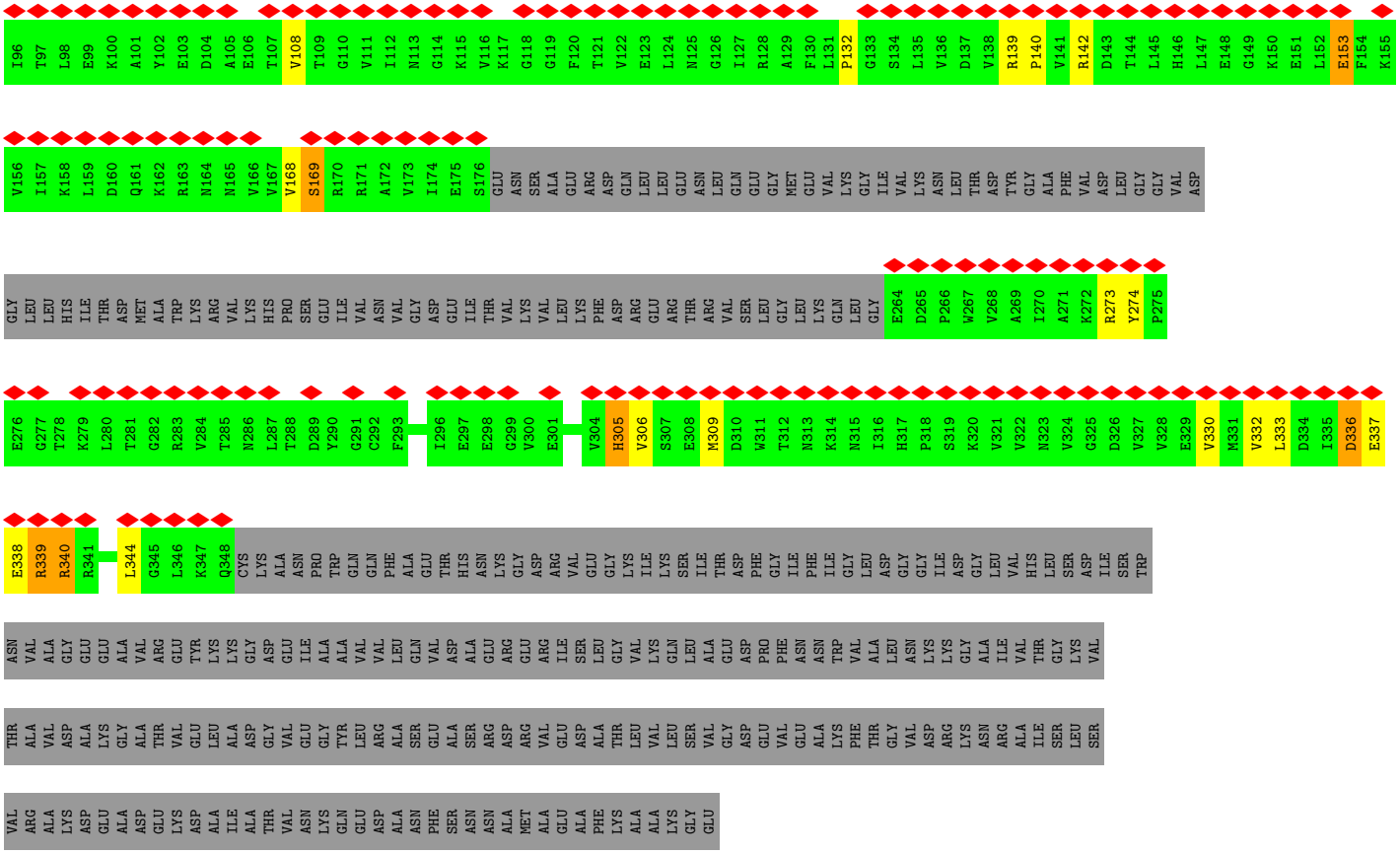


• Molecule 21: 30S ribosomal protein S2



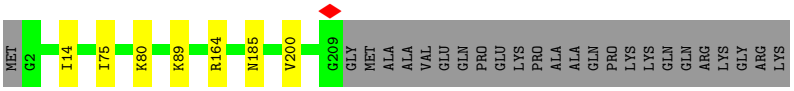
• Molecule 22: 30S ribosomal protein S1





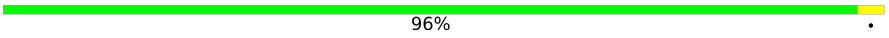
• Molecule 23: 30S ribosomal protein S3

Chain I:



• Molecule 24: 30S ribosomal protein S4

Chain J:

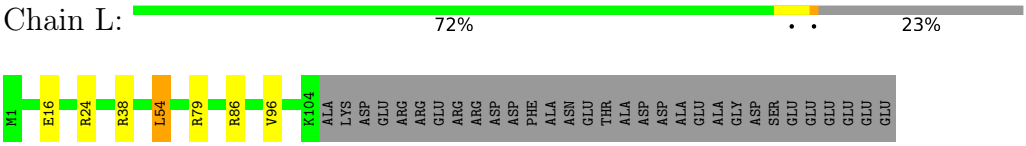


• Molecule 25: 30S ribosomal protein S5

Chain K:

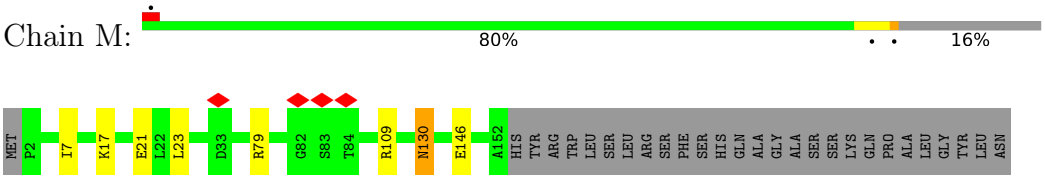
• Molecule 26: 30S ribosomal protein S6

Chain L:



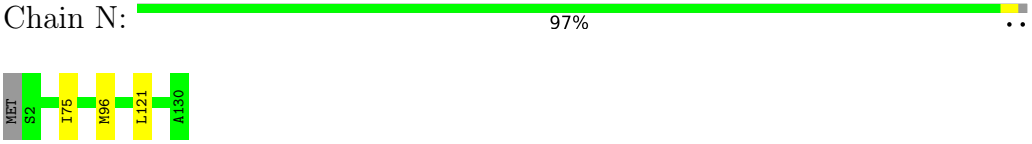
• Molecule 27: 30S ribosomal protein S7

Chain M:



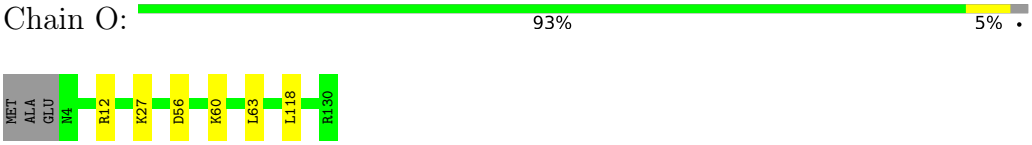
• Molecule 28: 30S ribosomal protein S8

Chain N:



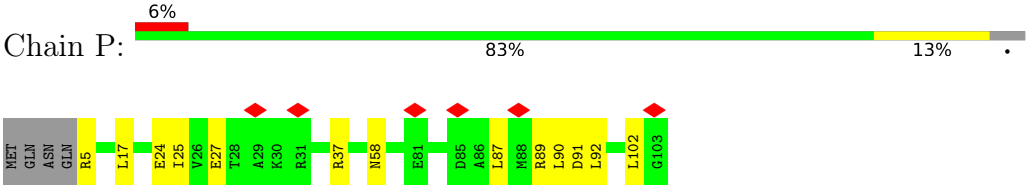
• Molecule 29: 30S ribosomal protein S9

Chain O:



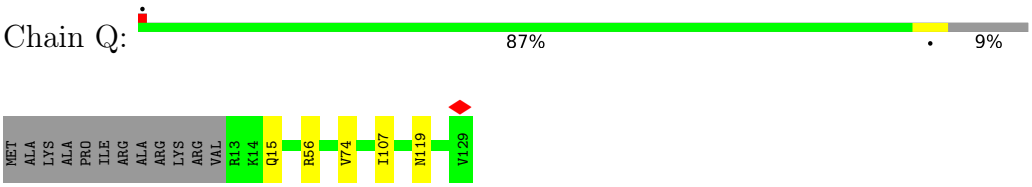
• Molecule 30: 30S ribosomal protein S10

Chain P:



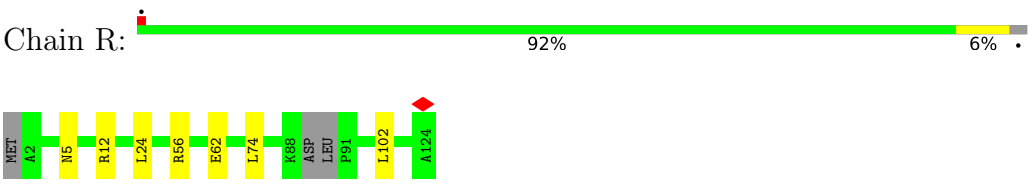
• Molecule 31: 30S ribosomal protein S11

Chain Q:



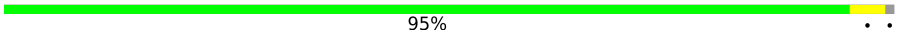
• Molecule 32: 30S ribosomal protein S12

Chain R:



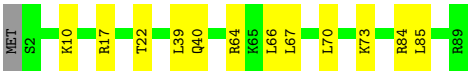
• Molecule 33: 30S ribosomal protein S14

Chain S:



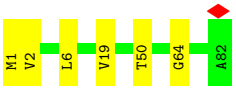
• Molecule 34: 30S ribosomal protein S15

Chain T:



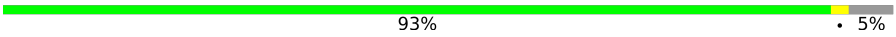
• Molecule 35: 30S ribosomal protein S16

Chain U:



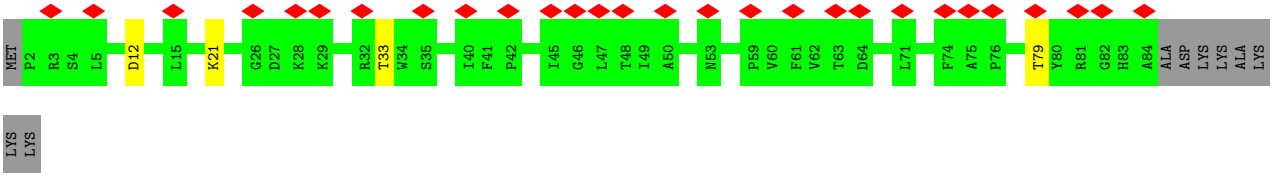
• Molecule 36: 30S ribosomal protein S17

Chain V:



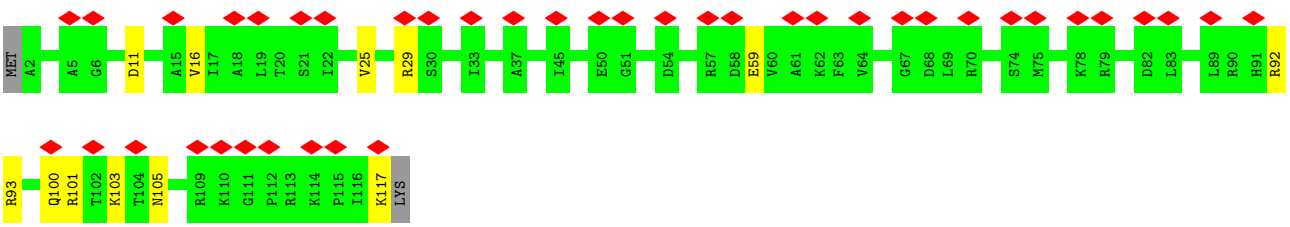
• Molecule 37: 30S ribosomal protein S19

Chain W:



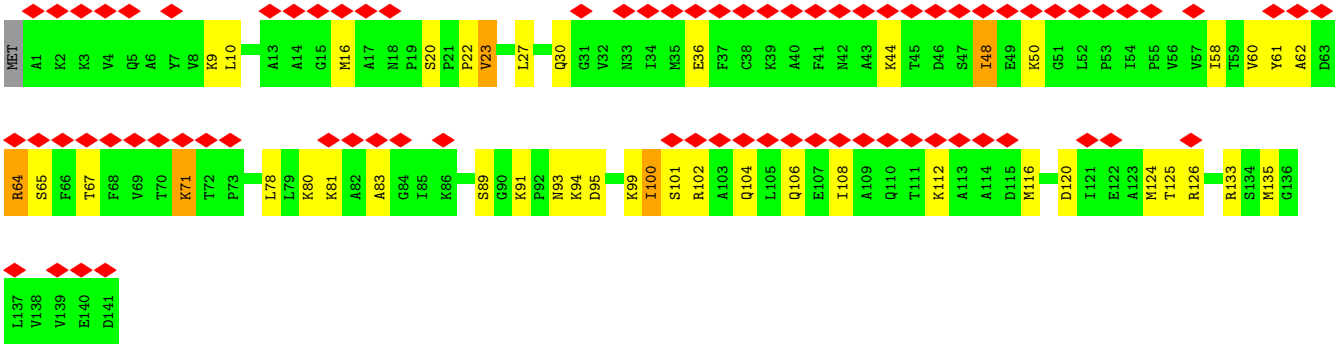
• Molecule 38: 30S ribosomal protein S13

Chain X:



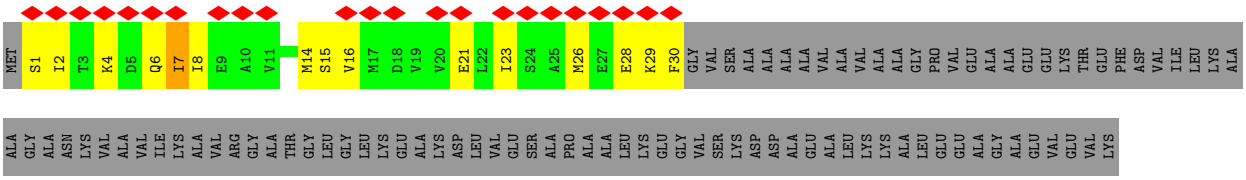
• Molecule 39: 50S ribosomal protein L11

Chain Y:



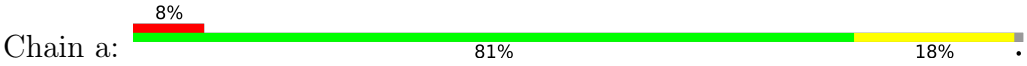
• Molecule 40: 50S ribosomal protein L7/L12

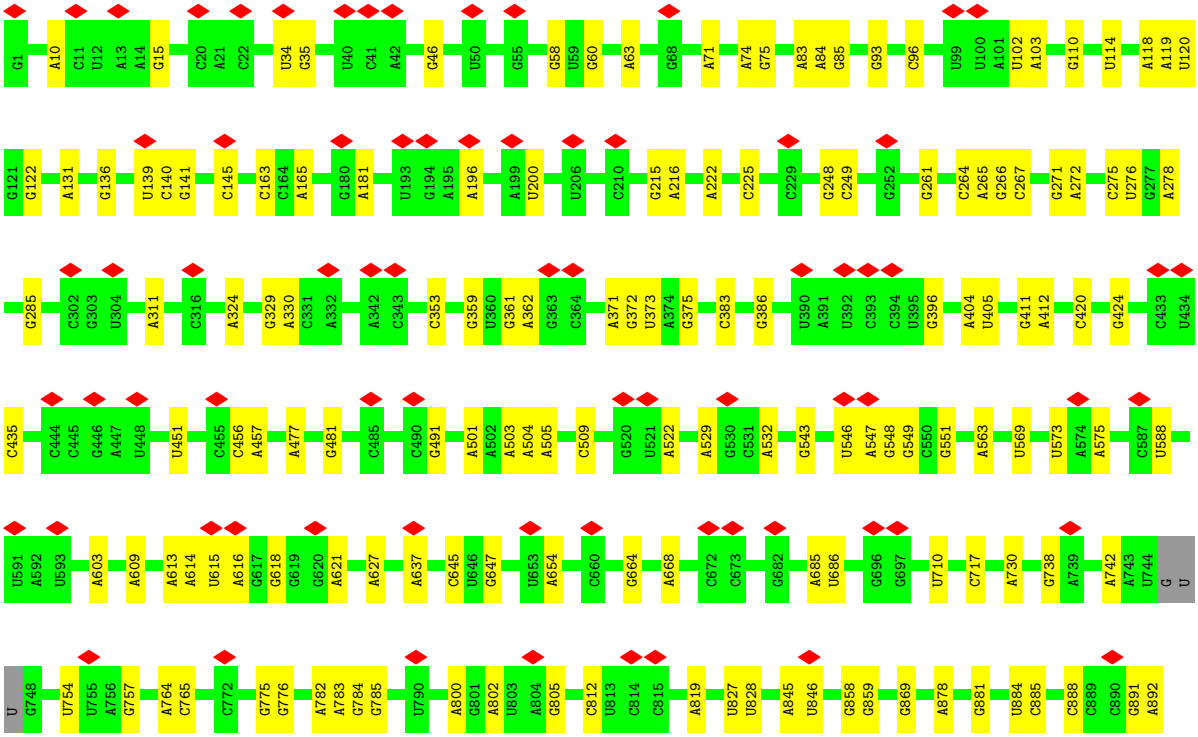
Chain Z:

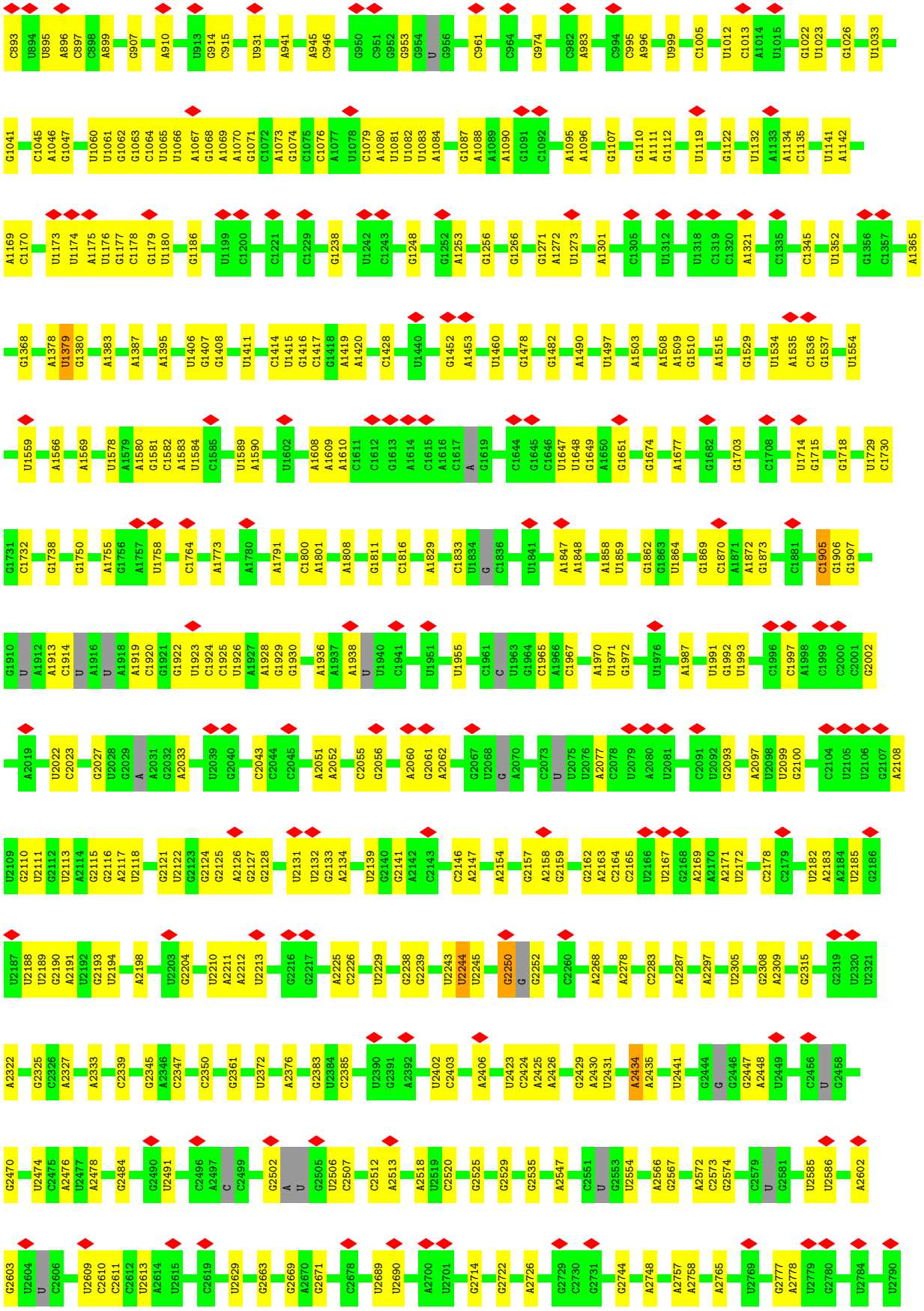


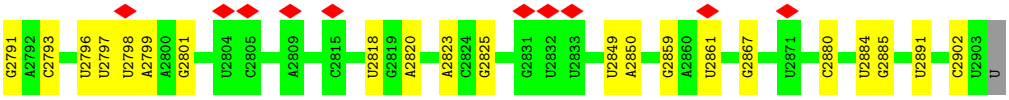
• Molecule 41: 23S rRNA

Chain a:



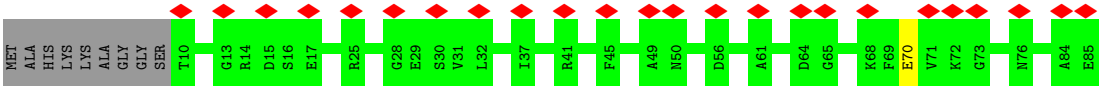






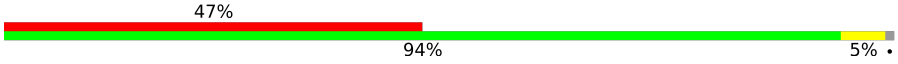
• Molecule 42: 50S ribosomal protein L27

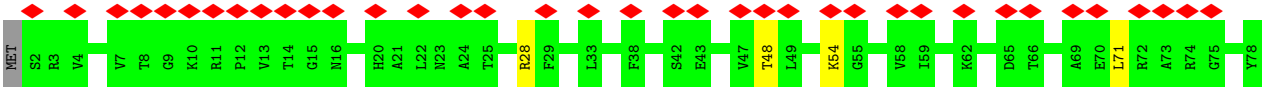
Chain b:



• Molecule 43: 50S ribosomal protein L28

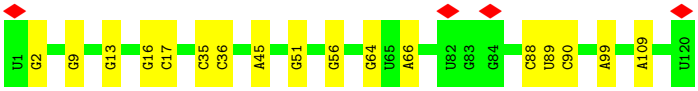
Chain c:





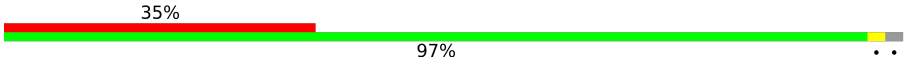
• Molecule 44: 5S rRNA

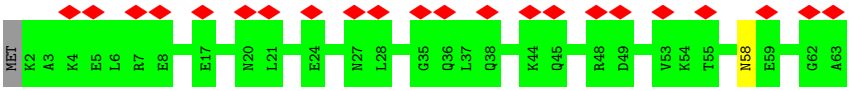
Chain d:



• Molecule 45: 50S ribosomal protein L29

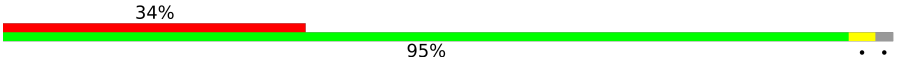
Chain e:

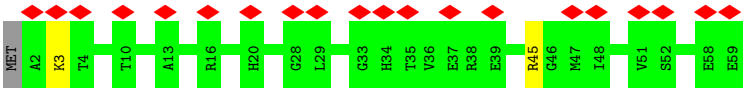




• Molecule 46: 50S ribosomal protein L30

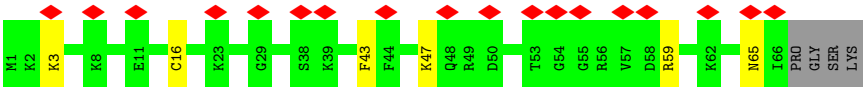
Chain f:





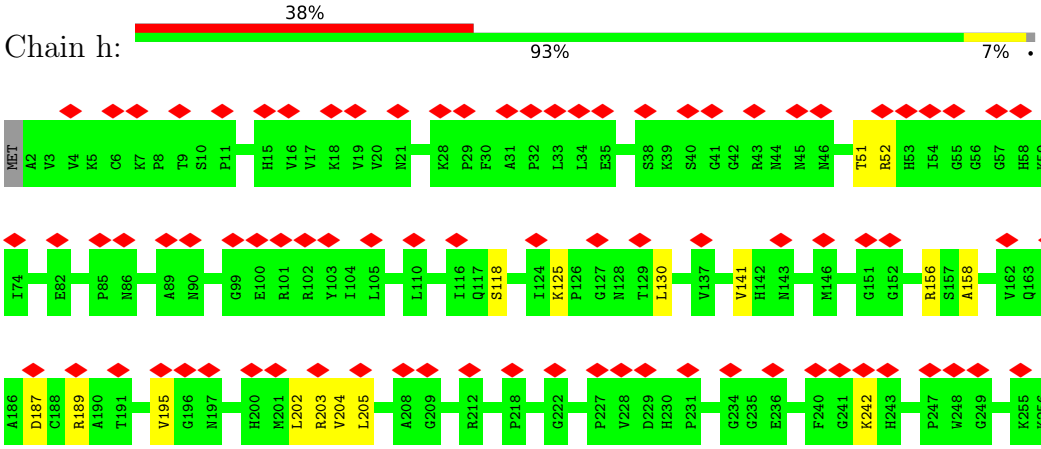
• Molecule 47: 50S ribosomal protein L31

Chain g:



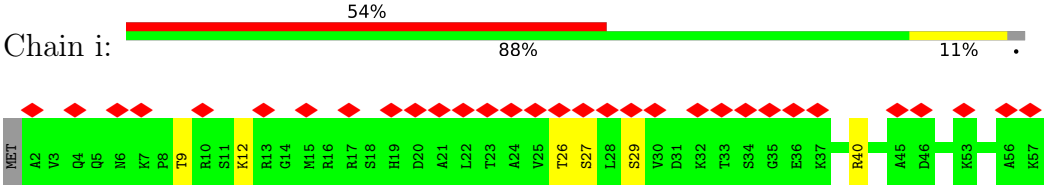
• Molecule 48: 50S ribosomal protein L2

Chain h:



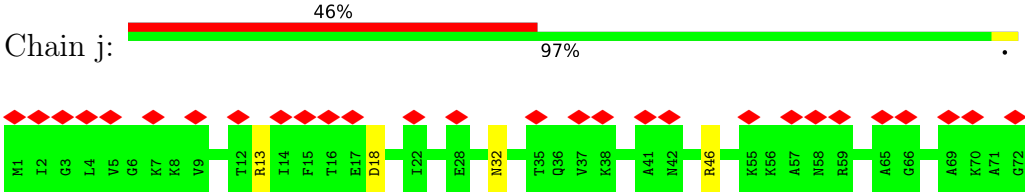
• Molecule 49: 50S ribosomal protein L32

Chain i:



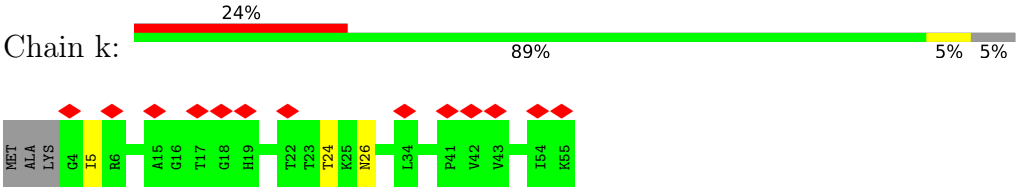
• Molecule 50: 50S ribosomal protein L3

Chain j:



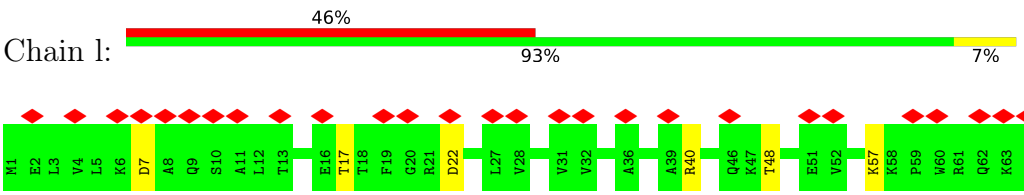
• Molecule 51: 50S ribosomal protein L33

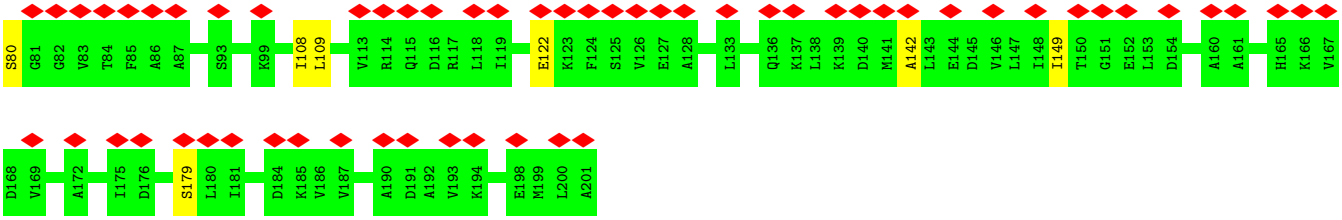
Chain k:



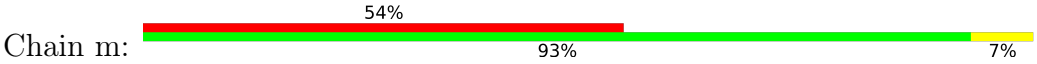
• Molecule 52: 50S ribosomal protein L4

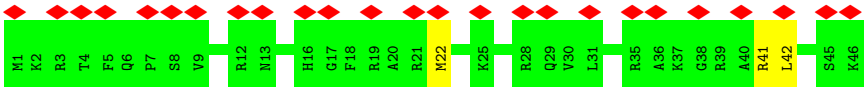
Chain l:



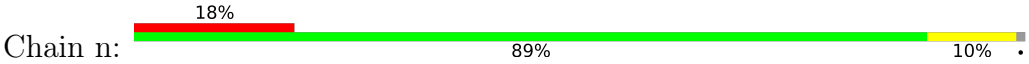


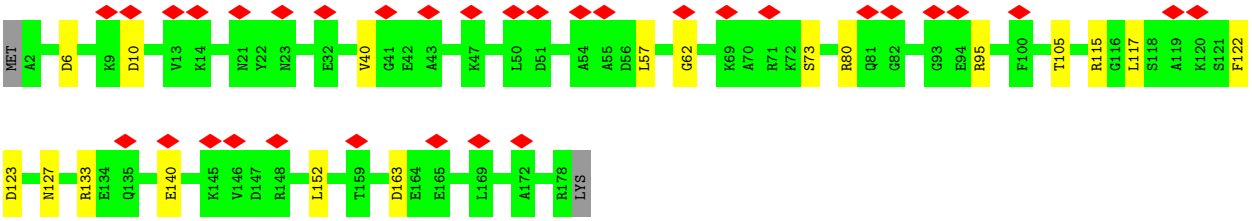
• Molecule 53: 50S ribosomal protein L34



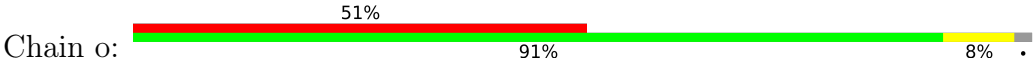


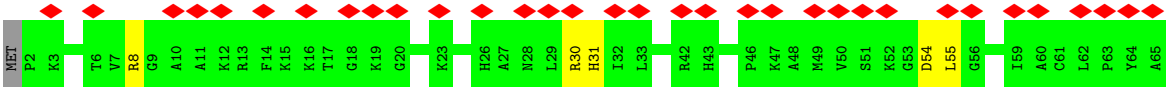
• Molecule 54: 50S ribosomal protein L5



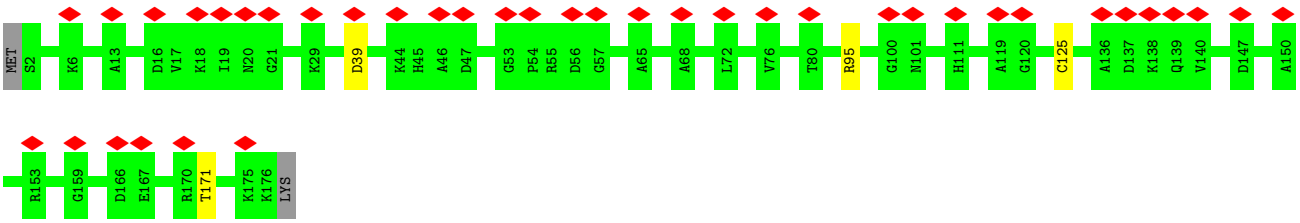


• Molecule 55: 50S ribosomal protein L35

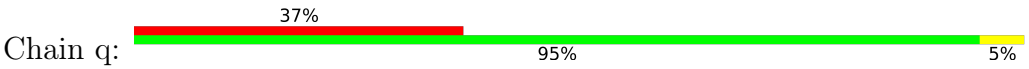


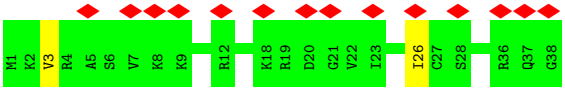


• Molecule 56: 50S ribosomal protein L6



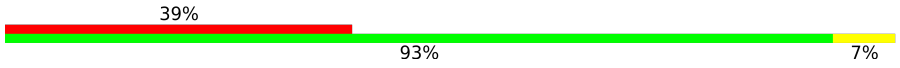
• Molecule 57: 50S ribosomal protein L36

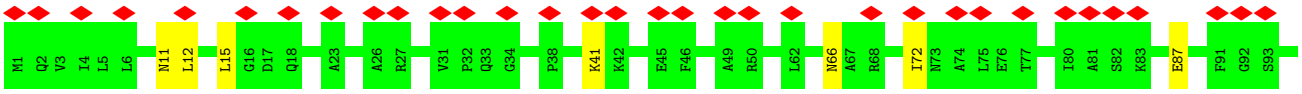


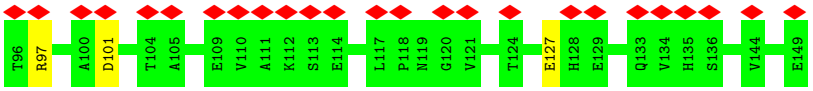


• Molecule 58: 50S ribosomal protein L9

Chain r:

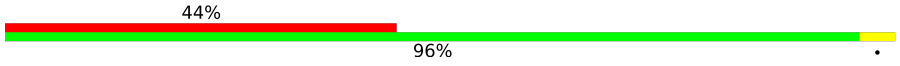


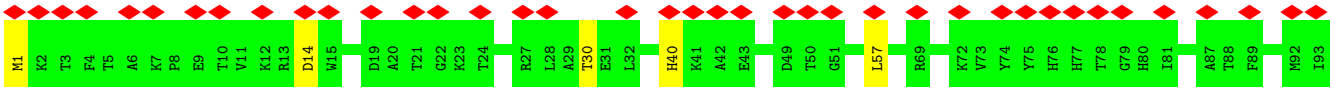


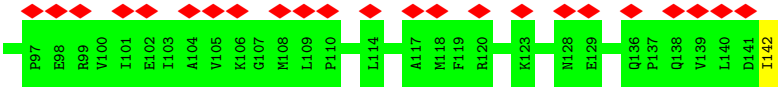


• Molecule 59: 50S ribosomal protein L13

Chain s:

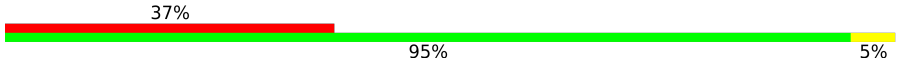


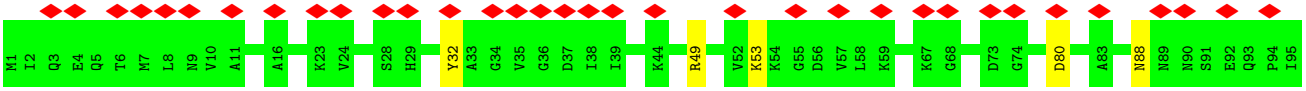


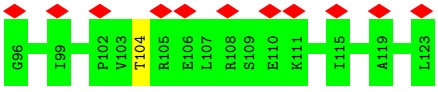


• Molecule 60: 50S ribosomal protein L14

Chain t:

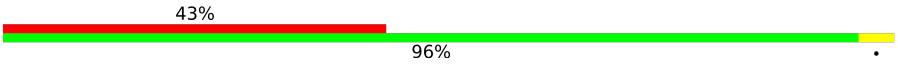


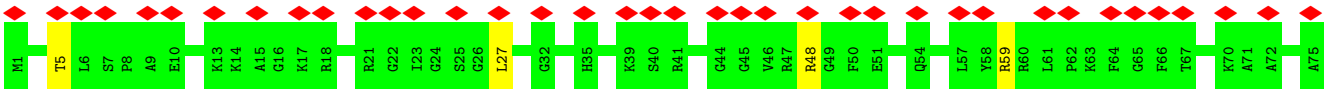


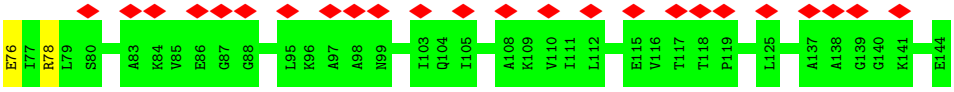


• Molecule 61: 50S ribosomal protein L15

Chain u:

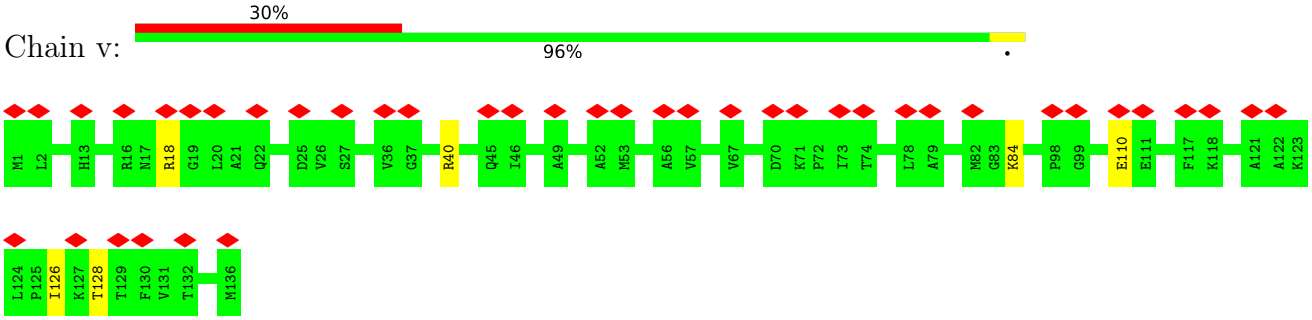






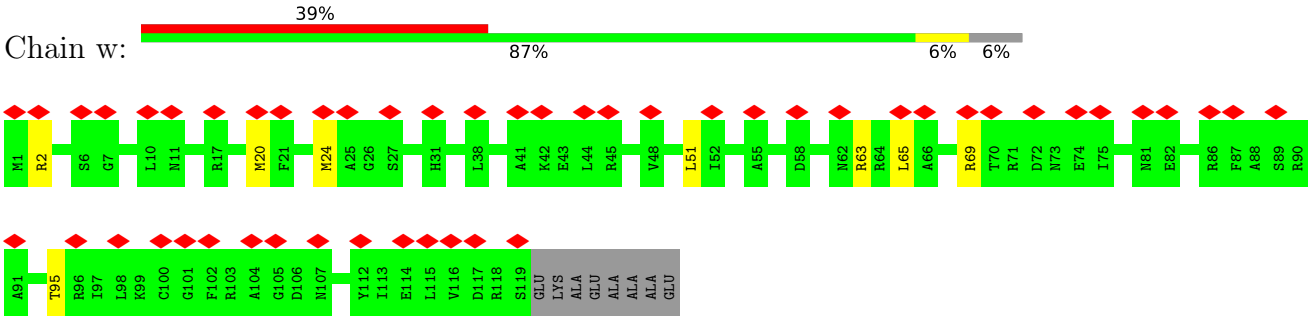
• Molecule 62: 50S ribosomal protein L16

Chain v:



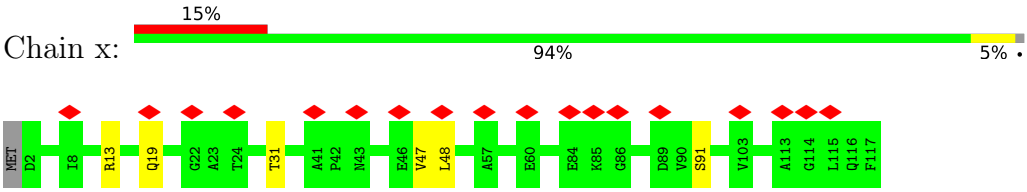
• Molecule 63: 50S ribosomal protein L17

Chain w:



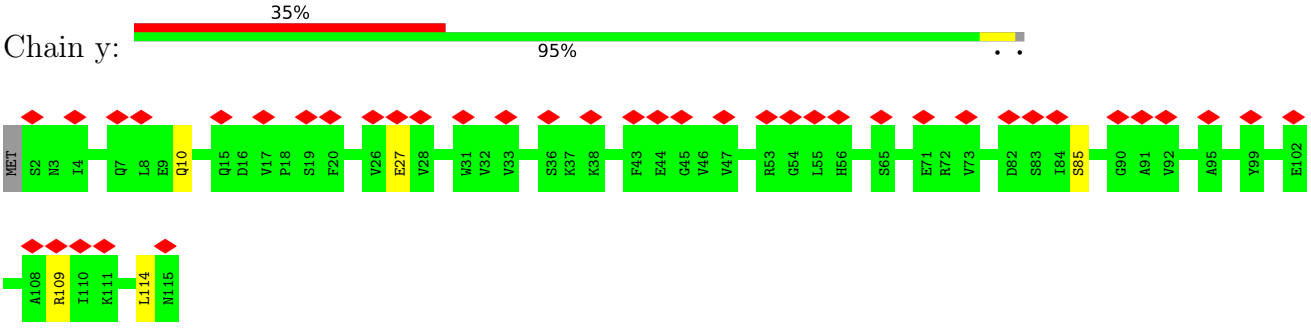
• Molecule 64: 50S ribosomal protein L18

Chain x:



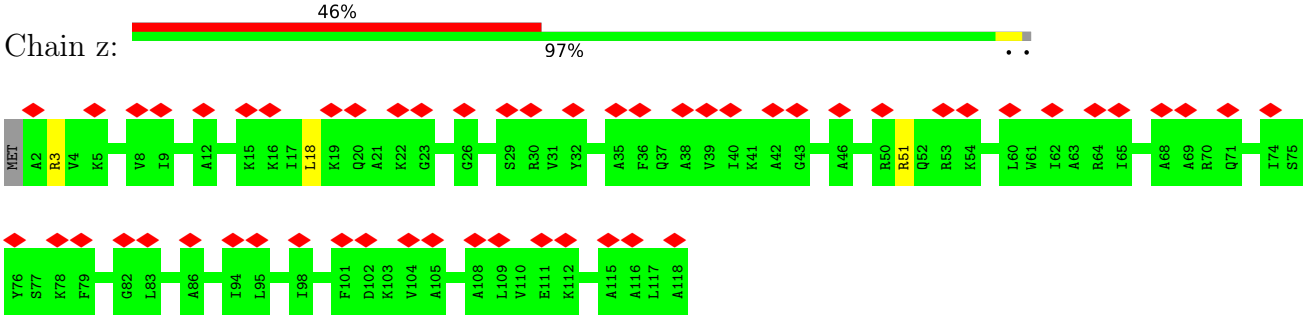
• Molecule 65: 50S ribosomal protein L19

Chain y:



• Molecule 66: 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	45450	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	0.061	Depositor
Minimum map value	-0.027	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.00868	Depositor
Map size (Å)	532.48, 532.48, 532.48	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	0	0.38	0/829	0.67	0/1107
2	1	0.48	0/864	0.82	0/1156
3	2	0.41	0/752	0.70	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	0.61	3/761 (0.4%)	0.92	3/1178 (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	0.43	0/10736	0.61	3/14487 (0.0%)
12	AB	0.75	3/1433 (0.2%)	0.64	1/1930 (0.1%)
13	AC	0.38	0/2113	0.58	0/2877
13	AD	0.34	0/2086	0.59	0/2840
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	0.58	1/3897 (0.0%)	0.77	35/5273 (0.7%)
17	C	0.48	0/553	0.83	0/743
18	D	0.34	10/36610 (0.0%)	0.73	30/57091 (0.1%)
19	E	0.57	0/675	0.85	0/895
20	F	0.56	0/597	0.87	0/792
21	G	0.48	0/1791	0.71	0/2413
22	H	0.54	1/1746 (0.1%)	1.03	13/2382 (0.5%)
23	I	0.43	0/1663	0.71	0/2241
24	J	0.47	0/1665	0.73	0/2227
25	K	0.45	0/1165	0.76	0/1568
26	L	0.43	0/867	0.76	1/1171 (0.1%)
27	M	0.50	0/1195	0.81	0/1602
28	N	0.41	0/989	0.69	0/1326
29	O	0.43	0/1034	0.75	0/1375
30	P	0.45	0/800	0.76	0/1082

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
31	Q	0.40	0/893	0.70	0/1205
32	R	0.35	0/952	0.74	0/1274
33	S	0.49	0/817	0.79	0/1088
34	T	0.53	0/722	0.86	0/964
35	U	0.44	0/659	0.79	0/884
36	V	0.34	0/657	0.61	0/881
37	W	0.38	0/680	0.62	0/915
38	X	0.49	0/909	0.87	0/1215
39	Y	0.67	0/1046	0.58	0/1410
40	Z	0.69	0/227	0.57	0/304
41	a	0.38	3/69247 (0.0%)	0.72	18/107985 (0.0%)
42	b	0.39	0/589	0.71	0/779
43	c	0.48	0/635	0.81	2/848 (0.2%)
44	d	0.29	0/2872	0.69	0/4478
45	e	0.54	0/502	0.82	0/667
46	f	0.45	0/452	0.78	0/605
47	g	0.43	0/531	0.68	0/709
48	h	0.39	0/2121	0.78	0/2852
49	i	0.40	0/450	0.79	0/599
50	j	0.44	0/1586	0.69	0/2134
51	k	0.35	0/433	0.65	0/576
52	l	0.46	0/1571	0.77	0/2113
53	m	0.53	0/380	0.99	0/498
54	n	0.49	0/1434	0.88	3/1926 (0.2%)
55	o	0.45	0/513	0.83	0/676
56	p	0.39	0/1333	0.67	0/1805
57	q	0.37	0/303	0.77	0/397
58	r	0.43	0/1122	0.69	0/1515
59	s	0.50	0/1152	0.75	0/1551
60	t	0.41	0/955	0.78	0/1279
61	u	0.40	0/1062	0.76	0/1413
62	v	0.46	0/1093	0.81	0/1460
63	w	0.52	0/964	0.87	0/1289
64	x	0.46	0/902	0.81	0/1209
65	y	0.41	0/929	0.72	1/1242 (0.1%)
66	z	0.60	0/960	0.92	0/1278
All	All	0.42	38/195115 (0.0%)	0.73	128/286888 (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
10	B	0	2
11	AA	0	2
12	AB	0	1
13	AC	0	3
13	AD	0	3
14	AE	0	5
16	AG	0	5
22	H	0	3
38	X	0	1
All	All	0	27

The worst 5 of 38 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	9	130	PRO	N-CA	13.75	1.70	1.47
12	AB	45	PRO	N-CA	13.69	1.70	1.47
18	D	1516	G	O3'-P	-13.39	1.45	1.61
18	D	1339	A	O3'-P	10.55	1.73	1.61
14	AE	88	CYS	CB-SG	-10.19	1.65	1.82

The worst 5 of 128 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	D	1516	G	P-O3'-C3'	-19.01	96.89	119.70
18	D	1516	G	O3'-P-O5'	13.79	130.20	104.00
41	a	2252	G	N9-C1'-C2'	-10.97	99.73	114.00
18	D	1401	G	N9-C1'-C2'	-10.70	100.09	114.00
54	n	73	SER	N-CA-CB	-10.62	94.58	110.50

There are no chirality outliers.

5 of 27 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	A	19	G	Sidechain
10	A	7	G	Sidechain
11	AA	900	LYS	Mainchain
11	AA	910	ALA	Peptide
12	AB	104	SER	Mainchain

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	0	101/103 (98%)	97 (96%)	3 (3%)	1 (1%)	15 54
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 54
5	4	92/94 (98%)	91 (99%)	1 (1%)	0	100 100
9	9	146/165 (88%)	95 (65%)	37 (25%)	14 (10%)	0 8
11	AA	1338/1342 (100%)	1215 (91%)	120 (9%)	3 (0%)	47 81
12	AB	173/181 (96%)	136 (79%)	26 (15%)	11 (6%)	1 14
13	AC	295/329 (90%)	274 (93%)	19 (6%)	2 (1%)	22 61
13	AD	291/329 (88%)	268 (92%)	23 (8%)	0	100 100
14	AE	1329/1407 (94%)	1199 (90%)	121 (9%)	9 (1%)	22 61
15	AF	80/91 (88%)	77 (96%)	3 (4%)	0	100 100
16	AG	493/495 (100%)	413 (84%)	56 (11%)	24 (5%)	2 19
17	C	64/75 (85%)	63 (98%)	1 (2%)	0	100 100
19	E	84/87 (97%)	83 (99%)	1 (1%)	0	100 100
20	F	68/71 (96%)	68 (100%)	0	0	100 100
21	G	223/241 (92%)	210 (94%)	13 (6%)	0	100 100
22	H	255/557 (46%)	188 (74%)	55 (22%)	12 (5%)	2 20
23	I	206/233 (88%)	196 (95%)	9 (4%)	1 (0%)	29 68
24	J	203/206 (98%)	198 (98%)	5 (2%)	0	100 100
25	K	154/167 (92%)	146 (95%)	7 (4%)	1 (1%)	25 64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
26	L	102/135 (76%)	97 (95%)	4 (4%)	1 (1%)	15 54
27	M	149/179 (83%)	144 (97%)	4 (3%)	1 (1%)	22 61
28	N	127/130 (98%)	121 (95%)	5 (4%)	1 (1%)	19 58
29	O	125/130 (96%)	115 (92%)	9 (7%)	1 (1%)	19 58
30	P	97/103 (94%)	87 (90%)	8 (8%)	2 (2%)	7 38
31	Q	115/129 (89%)	104 (90%)	9 (8%)	2 (2%)	9 42
32	R	117/124 (94%)	116 (99%)	1 (1%)	0	100 100
33	S	98/101 (97%)	96 (98%)	2 (2%)	0	100 100
34	T	86/89 (97%)	82 (95%)	4 (5%)	0	100 100
35	U	80/82 (98%)	75 (94%)	4 (5%)	1 (1%)	12 48
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%)	107 (94%)	5 (4%)	2 (2%)	8 41
39	Y	139/142 (98%)	102 (73%)	25 (18%)	12 (9%)	1 9
40	Z	28/121 (23%)	19 (68%)	7 (25%)	2 (7%)	1 12
42	b	74/85 (87%)	69 (93%)	5 (7%)	0	100 100
43	c	75/78 (96%)	72 (96%)	3 (4%)	0	100 100
45	e	60/63 (95%)	57 (95%)	3 (5%)	0	100 100
46	f	56/59 (95%)	53 (95%)	3 (5%)	0	100 100
47	g	64/70 (91%)	63 (98%)	1 (2%)	0	100 100
48	h	269/273 (98%)	259 (96%)	9 (3%)	1 (0%)	34 72
49	i	54/57 (95%)	51 (94%)	3 (6%)	0	100 100
50	j	207/209 (99%)	198 (96%)	9 (4%)	0	100 100
51	k	50/55 (91%)	50 (100%)	0	0	100 100
52	l	199/201 (99%)	190 (96%)	8 (4%)	1 (0%)	29 68
53	m	44/46 (96%)	43 (98%)	1 (2%)	0	100 100
54	n	175/179 (98%)	162 (93%)	11 (6%)	2 (1%)	14 52
55	o	62/65 (95%)	59 (95%)	3 (5%)	0	100 100
56	p	173/177 (98%)	161 (93%)	12 (7%)	0	100 100
57	q	36/38 (95%)	35 (97%)	1 (3%)	0	100 100
58	r	147/149 (99%)	136 (92%)	11 (8%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
59	s	140/142 (99%)	135 (96%)	5 (4%)	0	100	100
60	t	121/123 (98%)	111 (92%)	10 (8%)	0	100	100
61	u	142/144 (99%)	135 (95%)	7 (5%)	0	100	100
62	v	134/136 (98%)	129 (96%)	5 (4%)	0	100	100
63	w	117/127 (92%)	108 (92%)	9 (8%)	0	100	100
64	x	114/117 (97%)	108 (95%)	6 (5%)	0	100	100
65	y	112/115 (97%)	105 (94%)	7 (6%)	0	100	100
66	z	115/118 (98%)	110 (96%)	4 (4%)	1 (1%)	17	56
All	All	10172/11072 (92%)	9323 (92%)	740 (7%)	109 (1%)	18	52

5 of 109 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	9	88	HIS
11	AA	913	VAL
12	AB	60	SER
12	AB	123	ARG
16	AG	3	LYS

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	46
2	1	93/93 (100%)	85 (91%)	8 (9%)	10	38
3	2	81/84 (96%)	76 (94%)	5 (6%)	18	51
4	3	84/85 (99%)	78 (93%)	6 (7%)	14	46
5	4	78/78 (100%)	74 (95%)	4 (5%)	24	57
9	9	112/123 (91%)	65 (58%)	47 (42%)	0	0
11	AA	1155/1157 (100%)	1145 (99%)	10 (1%)	78	90
12	AB	154/158 (98%)	121 (79%)	33 (21%)	1	5

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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%)	1052 (94%)	68 (6%)	18 51
15	AF	70/75 (93%)	70 (100%)	0	100 100
16	AG	409/409 (100%)	327 (80%)	82 (20%)	1 7
17	C	57/65 (88%)	55 (96%)	2 (4%)	36 67
19	E	65/66 (98%)	60 (92%)	5 (8%)	13 42
20	F	60/61 (98%)	57 (95%)	3 (5%)	24 58
21	G	187/199 (94%)	178 (95%)	9 (5%)	25 60
22	H	137/461 (30%)	128 (93%)	9 (7%)	16 49
23	I	171/190 (90%)	165 (96%)	6 (4%)	36 67
24	J	172/173 (99%)	165 (96%)	7 (4%)	30 63
25	K	119/126 (94%)	112 (94%)	7 (6%)	19 53
26	L	91/116 (78%)	85 (93%)	6 (7%)	16 49
27	M	124/147 (84%)	116 (94%)	8 (6%)	17 50
28	N	104/105 (99%)	102 (98%)	2 (2%)	57 80
29	O	105/107 (98%)	100 (95%)	5 (5%)	25 60
30	P	86/90 (96%)	75 (87%)	11 (13%)	4 22
31	Q	90/99 (91%)	87 (97%)	3 (3%)	38 68
32	R	101/104 (97%)	94 (93%)	7 (7%)	15 47
33	S	83/84 (99%)	79 (95%)	4 (5%)	25 60
34	T	76/77 (99%)	64 (84%)	12 (16%)	2 15
35	U	65/65 (100%)	60 (92%)	5 (8%)	13 42
36	V	74/78 (95%)	72 (97%)	2 (3%)	44 73
37	W	72/79 (91%)	68 (94%)	4 (6%)	21 54
38	X	94/96 (98%)	85 (90%)	9 (10%)	8 34
39	Y	109/110 (99%)	72 (66%)	37 (34%)	0 1
40	Z	26/85 (31%)	12 (46%)	14 (54%)	0 0
42	b	58/63 (92%)	57 (98%)	1 (2%)	60 82
43	c	67/68 (98%)	64 (96%)	3 (4%)	27 61
45	e	54/55 (98%)	53 (98%)	1 (2%)	57 80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
46	f	48/49 (98%)	46 (96%)	2 (4%)	30 63
47	g	59/62 (95%)	53 (90%)	6 (10%)	7 32
48	h	216/218 (99%)	199 (92%)	17 (8%)	12 41
49	i	47/48 (98%)	41 (87%)	6 (13%)	4 22
50	j	164/164 (100%)	157 (96%)	7 (4%)	29 62
51	k	47/49 (96%)	44 (94%)	3 (6%)	17 50
52	l	165/165 (100%)	151 (92%)	14 (8%)	10 39
53	m	38/38 (100%)	35 (92%)	3 (8%)	12 41
54	n	148/150 (99%)	134 (90%)	14 (10%)	8 34
55	o	51/52 (98%)	46 (90%)	5 (10%)	8 33
56	p	136/138 (99%)	132 (97%)	4 (3%)	42 71
57	q	34/34 (100%)	32 (94%)	2 (6%)	19 53
58	r	114/114 (100%)	104 (91%)	10 (9%)	10 38
59	s	116/116 (100%)	110 (95%)	6 (5%)	23 56
60	t	104/104 (100%)	98 (94%)	6 (6%)	20 53
61	u	103/103 (100%)	97 (94%)	6 (6%)	20 53
62	v	109/109 (100%)	103 (94%)	6 (6%)	21 54
63	w	99/103 (96%)	91 (92%)	8 (8%)	11 41
64	x	86/87 (99%)	80 (93%)	6 (7%)	15 46
65	y	99/100 (99%)	95 (96%)	4 (4%)	31 64
66	z	89/90 (99%)	87 (98%)	2 (2%)	52 78
All	All	8330/9148 (91%)	7742 (93%)	588 (7%)	18 46

5 of 588 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
48	h	130	LEU
63	w	65	LEU
49	i	9	THR
48	h	125	LYS
54	n	140	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
13	AD	66	HIS
14	AE	294	ASN
16	AG	428	ASN
13	AD	227	GLN
15	AF	31	GLN

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%)
18	D	1514/1542 (98%)	289 (19%)	34 (2%)
41	a	2859/2904 (98%)	532 (18%)	0
44	d	119/120 (99%)	17 (14%)	0
8	7	32/41 (78%)	17 (53%)	4 (12%)
All	All	4674/4759 (98%)	919 (19%)	50 (1%)

5 of 919 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	7	-18	G
8	7	-17	U
8	7	-16	U
8	7	-14	U
8	7	-13	U

5 of 50 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
18	D	531	U
18	D	992	U
18	D	1493	A
18	D	532	A
18	D	722	G

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 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.

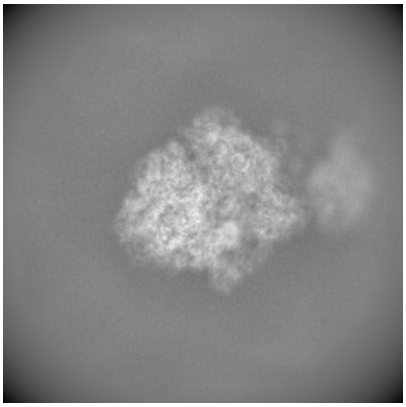
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-22084. These allow visual inspection of the internal detail of the map and identification of artifacts.

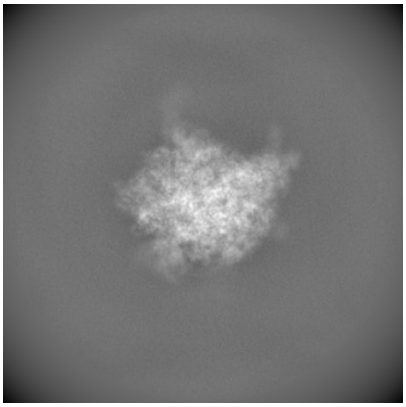
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

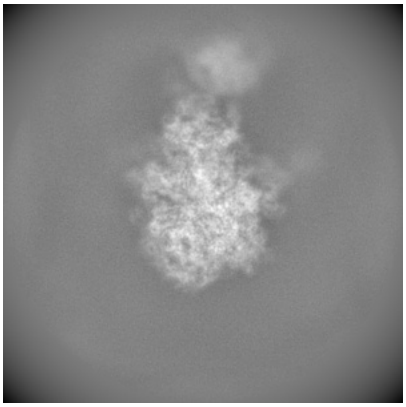
6.1.1 Primary map



X



Y

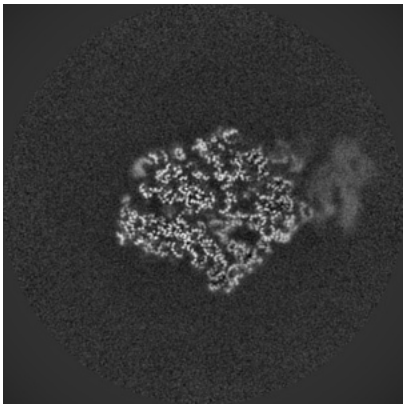


Z

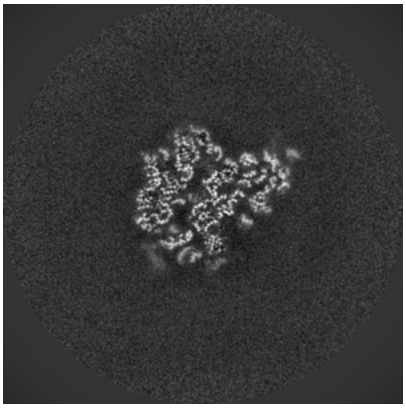
The images above show the map projected in three orthogonal directions.

6.2 Central slices

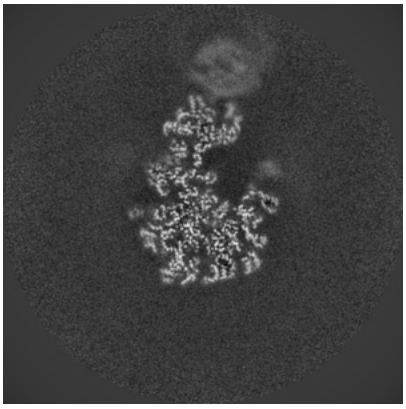
6.2.1 Primary map



X Index: 256



Y Index: 256

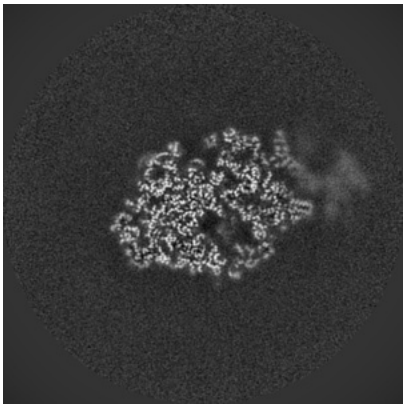


Z Index: 256

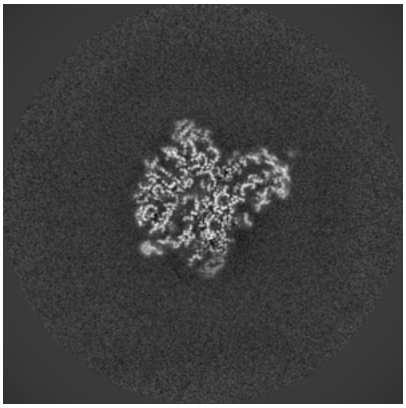
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

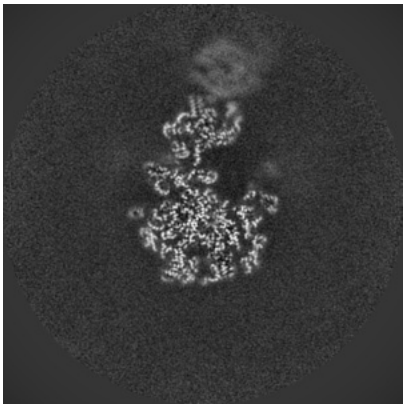
6.3.1 Primary map



X Index: 242



Y Index: 250



Z Index: 258

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 0.00868. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

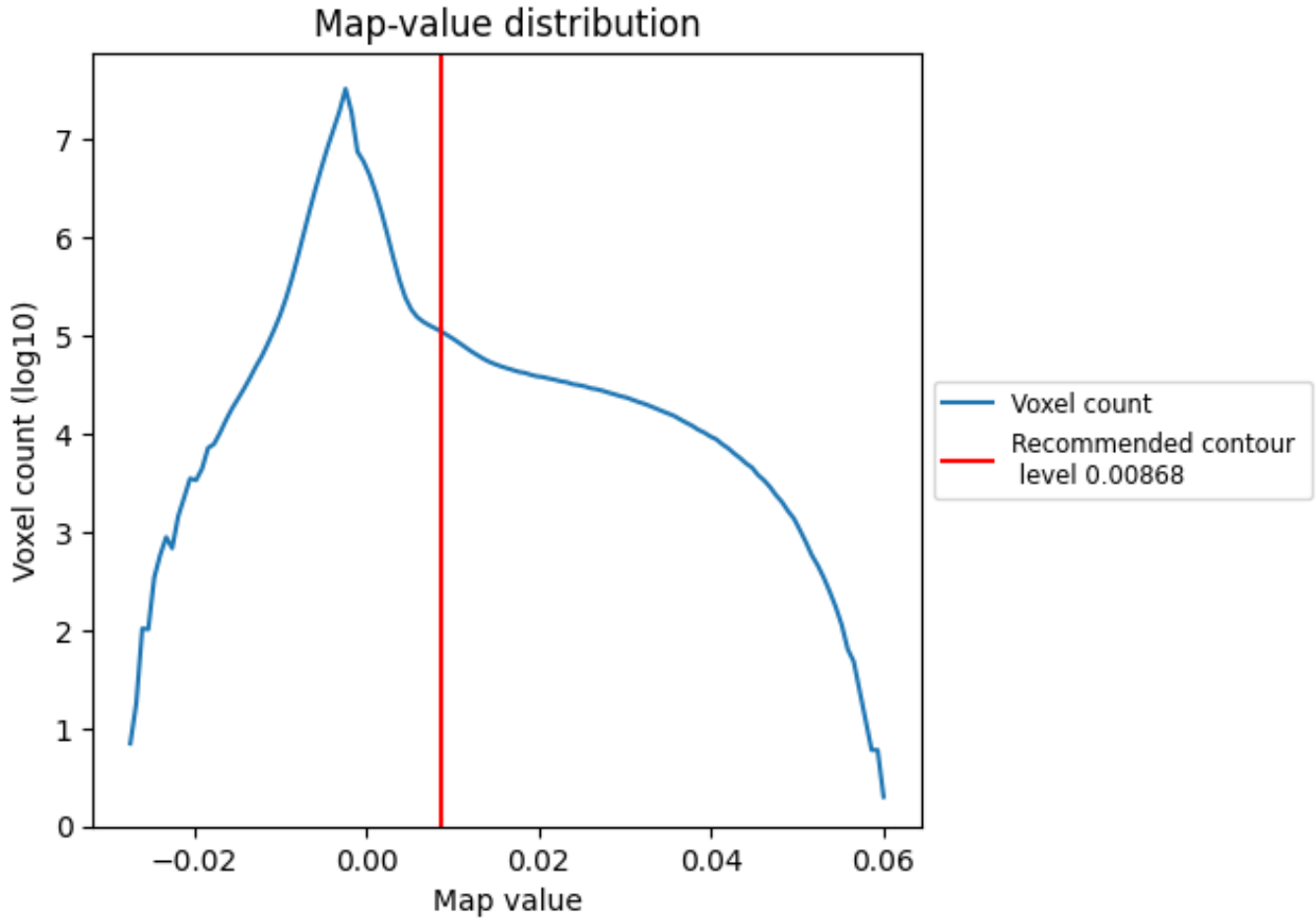
6.5 Mask visualisation (i)

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

7 Map analysis

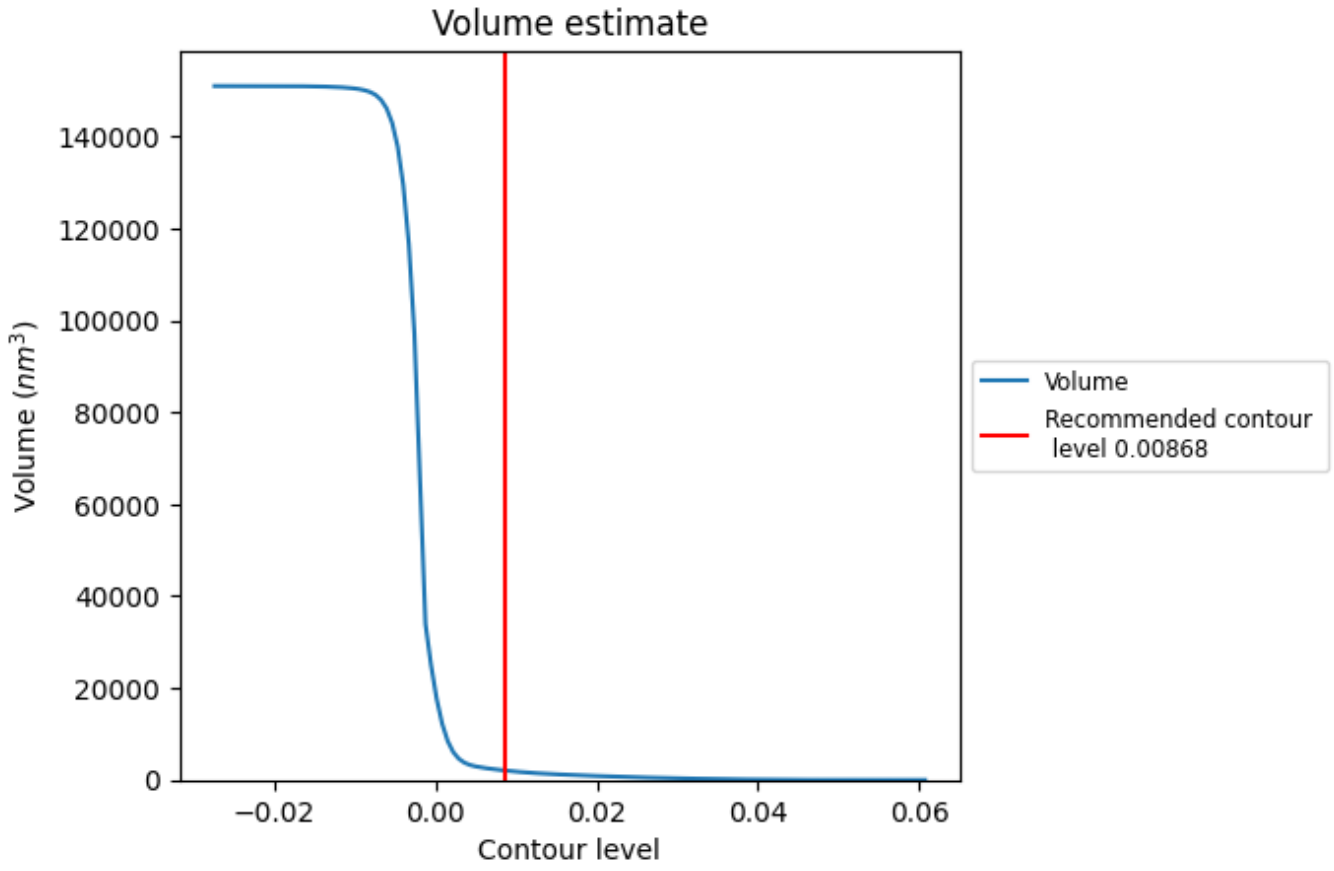
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

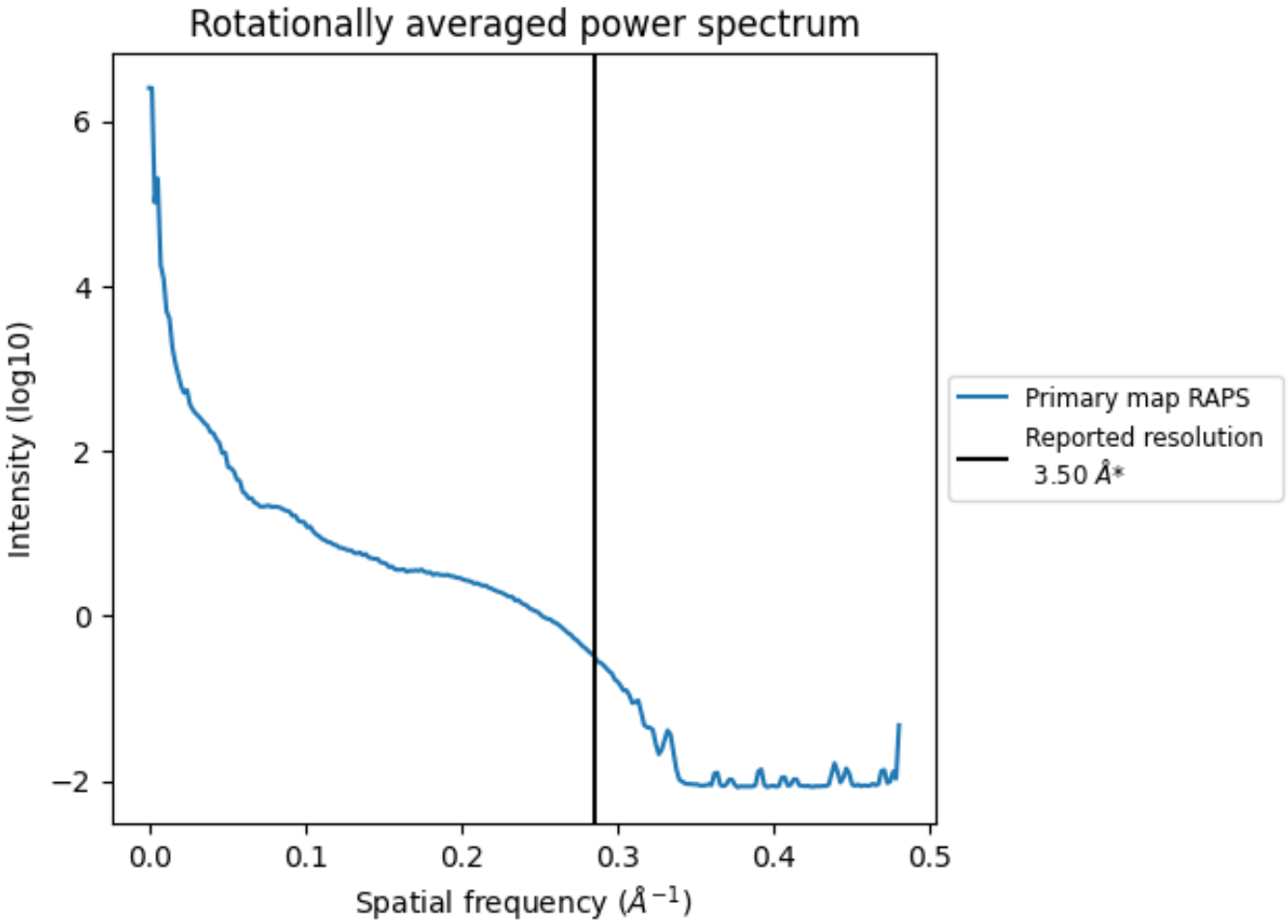
7.2 Volume estimate (i)



The volume at the recommended contour level is 2046 nm^3; this corresponds to an approximate mass of 1848 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 0.286 Å^{-1}

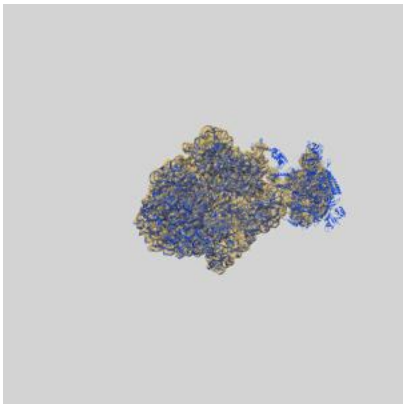
8 Fourier-Shell correlation

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

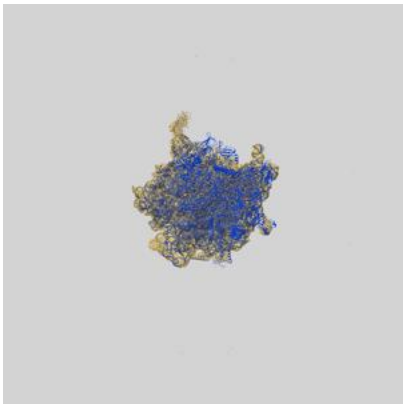
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-22084 and PDB model 6X7F. Per-residue inclusion information can be found in section 3 on page 17.

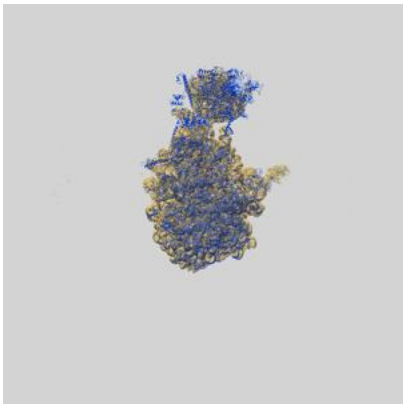
9.1 Map-model overlay



X



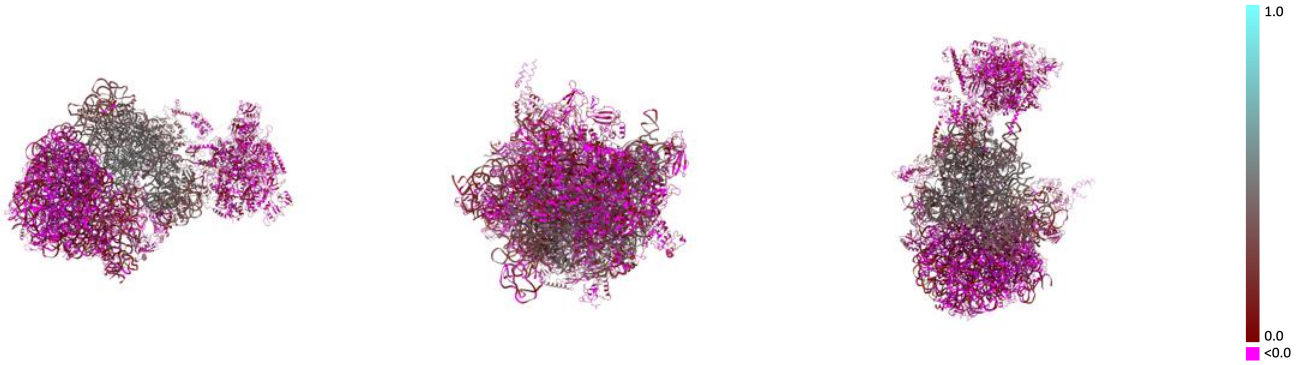
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.00868 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

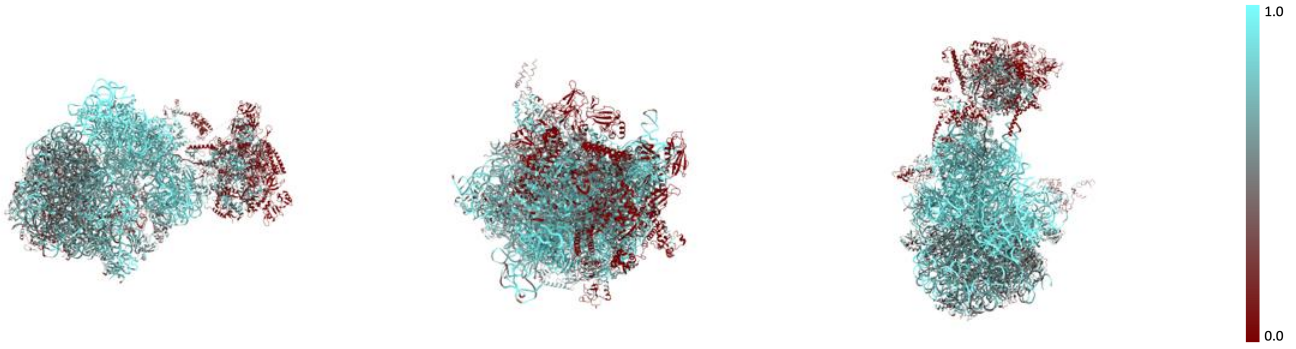
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

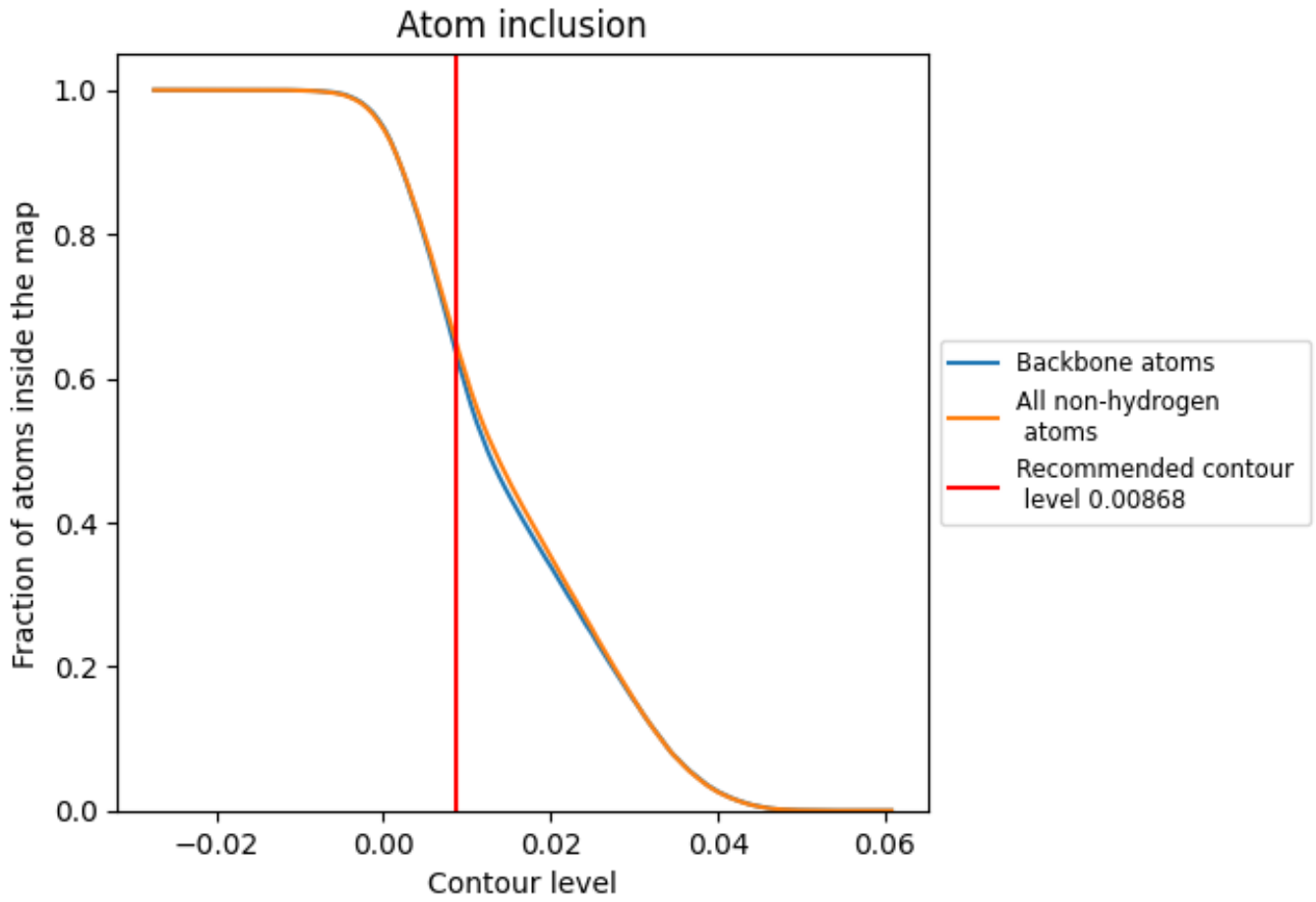
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.00868).

9.4 Atom inclusion (i)



At the recommended contour level, 64% of all backbone atoms, 65% 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 (0.00868) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6496	0.1190
0	0.5194	-0.0330
1	0.4904	-0.0410
2	0.5137	-0.0410
3	0.5219	-0.0190
4	0.5921	0.0360
5	0.4301	0.0620
6	0.6531	0.0800
7	0.5269	0.0730
9	0.5649	0.0760
A	0.8241	0.1510
AA	0.3147	0.0280
AB	0.4635	0.1140
AC	0.1883	0.0250
AD	0.1426	0.0260
AE	0.3141	0.0260
AF	0.0836	0.0270
AG	0.4770	0.1020
B	0.6852	0.1050
C	0.8241	0.3760
D	0.9803	0.3900
E	0.8609	0.3190
F	0.7746	0.3290
G	0.8288	0.3410
H	0.2739	0.0500
I	0.8346	0.3790
J	0.8560	0.3850
K	0.8673	0.4210
L	0.8307	0.3460
M	0.8033	0.3120
N	0.8719	0.4070
O	0.8509	0.3080
P	0.7673	0.2900
Q	0.8605	0.3980
R	0.8464	0.4390

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Chain	Atom inclusion	Q-score
S	0.8643	0.3540
T	0.8652	0.3730
U	0.8868	0.3690
V	0.8623	0.3850
W	0.5549	0.0330
X	0.5806	0.0270
Y	0.3894	0.0680
Z	0.1938	-0.0110
a	0.7048	0.0100
b	0.5883	0.0210
c	0.4293	-0.0450
d	0.8151	0.0780
e	0.5481	0.0140
f	0.5367	-0.0350
g	0.5910	0.0400
h	0.4970	-0.0400
i	0.4416	-0.0600
j	0.4785	-0.0620
k	0.5670	-0.0250
l	0.4908	-0.0190
m	0.4056	-0.0810
n	0.6489	0.0580
o	0.4440	-0.0410
p	0.6107	0.0660
q	0.5582	-0.0130
r	0.4854	0.0680
s	0.4873	-0.0500
t	0.4843	-0.0350
u	0.4766	-0.0250
v	0.5624	0.0130
w	0.4918	-0.0820
x	0.6512	0.0400
y	0.5169	-0.0200
z	0.4835	-0.0540