



wwPDB EM Validation Summary Report ⓘ

Nov 3, 2024 – 03:46 AM EST

PDB ID : 6XIJ
EMDB ID : EMD-22193
Title : Escherichia coli transcription-translation complex A (TTC-A) containing an
24 nt long mRNA spacer, NusG, and fMet-tRNAs at E-site and P-site
Authors : Molodtsov, V.; Wang, C.; Su, M.; Ebright, R.H.
Deposited on : 2020-06-20
Resolution : 8.00 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:

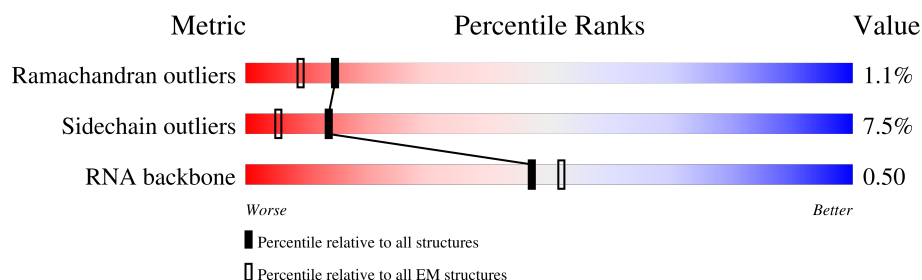
EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) :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

1 Overall quality at a glance

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

The reported resolution of this entry is 8.00 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	<div> <div>36%</div> <div>93%</div> <div>7%</div> </div>
2	1	110	<div> <div>36%</div> <div>93%</div> <div>7%</div> </div>
3	2	100	<div> <div>41%</div> <div>89%</div> <div>5%</div> <div>6%</div> </div>
4	3	104	<div> <div>30%</div> <div>91%</div> <div>8%</div> </div>
5	4	94	<div> <div>33%</div> <div>96%</div> </div>
6	5	36	<div> <div>58%</div> <div>47%</div> <div>17%</div> <div>36%</div> </div>
7	6	36	<div> <div>69%</div> <div>64%</div> <div>11%</div> <div>25%</div> </div>
8	7	33	<div> <div>42%</div> <div>24%</div> <div>39%</div> <div>33%</div> </div>

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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	C	75	
16	D	1542	
17	E	87	
18	F	71	
19	G	241	
20	H	557	
21	I	233	
22	J	206	
23	K	167	
24	L	135	
25	M	179	
26	N	130	
27	O	130	
28	P	103	
29	Q	129	
30	R	124	
31	S	101	

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Mol	Chain	Length	Quality of chain
32	T	89	
33	U	82	
34	V	84	
35	W	92	
36	X	118	
37	Y	142	
38	Z	121	
39	a	2904	
40	b	85	
41	c	78	
42	d	120	
43	e	63	
44	f	59	
45	g	70	
46	h	273	
47	i	57	
48	j	209	
49	k	55	
50	l	201	
51	m	46	
52	n	179	
53	o	65	
54	p	177	
55	q	38	
56	r	149	

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Mol	Chain	Length	Quality of chain
57	s	142	<div> <div>44%</div> <div>96%</div> <div>.</div> </div>
58	t	123	<div> <div>73%</div> <div>95%</div> <div>5%</div> </div>
59	u	144	<div> <div>46%</div> <div>96%</div> <div>.</div> </div>
60	v	136	<div> <div>46%</div> <div>96%</div> <div>.</div> </div>
61	w	127	<div> <div>24%</div> <div>87%</div> <div>6%</div> <div>6%</div> </div>
62	x	117	<div> <div>43%</div> <div>94%</div> <div>5%</div> <div>.</div> </div>
63	y	115	<div> <div>66%</div> <div>95%</div> <div>.</div> <div>.</div> </div>
64	z	118	<div> <div>30%</div> <div>96%</div> <div>.</div> <div>.</div> </div>

2 Entry composition

There are 66 unique types of molecules in this entry. The entry contains 300463 atoms, of which 124723 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	22	Total	C	H	N	O	P	0	0
			564	208	97	74	163	22		

- 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		

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

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
12	AB	98	Total	C	H	N	O	S	0	0
			1573	505	783	139	140	6		

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

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

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Mol	Chain	Residues	Atoms						AltConf	Trace
13	AD	228	Total	C	H	N	O	S	0	0
			3556	1100	1789	312	349	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	conflict	UNP A0A4S1NBU2

- Molecule 15 is a protein called 30S ribosomal protein S18.

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

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

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

- Molecule 17 is a protein called 30S ribosomal protein S20.

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

- Molecule 18 is a protein called 30S ribosomal protein S21.

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

- Molecule 19 is a protein called 30S ribosomal protein S2.

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

- Molecule 20 is a protein called 30S ribosomal protein S1.

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

- Molecule 21 is a protein called 30S ribosomal protein S3.

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

- Molecule 22 is a protein called 30S ribosomal protein S4.

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

- Molecule 23 is a protein called 30S ribosomal protein S5.

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

- Molecule 24 is a protein called 30S ribosomal protein S6.

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

- Molecule 25 is a protein called 30S ribosomal protein S7.

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

- Molecule 26 is a protein called 30S ribosomal protein S8.

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

- Molecule 27 is a protein called 30S ribosomal protein S9.

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

- Molecule 28 is a protein called 30S ribosomal protein S10.

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

- Molecule 29 is a protein called 30S ribosomal protein S11.

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

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

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

- Molecule 31 is a protein called 30S ribosomal protein S14.

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

- Molecule 32 is a protein called 30S ribosomal protein S15.

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

- Molecule 33 is a protein called 30S ribosomal protein S16.

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

- Molecule 34 is a protein called 30S ribosomal protein S17.

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

- Molecule 35 is a protein called 30S ribosomal protein S19.

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

- Molecule 36 is a protein called 30S ribosomal protein S13.

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

- Molecule 37 is a protein called 50S ribosomal protein L11.

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

- Molecule 38 is a protein called 50S ribosomal protein L7/L12.

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

- Molecule 39 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
39	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	conflict	GB 937521852

- Molecule 40 is a protein called 50S ribosomal protein L27.

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

- Molecule 41 is a protein called 50S ribosomal protein L28.

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

- Molecule 42 is a RNA chain called 5S rRNA.

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

- Molecule 43 is a protein called 50S ribosomal protein L29.

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

- Molecule 44 is a protein called 50S ribosomal protein L30.

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

- Molecule 45 is a protein called 50S ribosomal protein L31.

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

- Molecule 46 is a protein called 50S ribosomal protein L2.

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

- Molecule 47 is a protein called 50S ribosomal protein L32.

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

- Molecule 48 is a protein called 50S ribosomal protein L3.

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

- Molecule 49 is a protein called 50S ribosomal protein L33.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L34.

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

- Molecule 52 is a protein called 50S ribosomal protein L5.

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

- Molecule 53 is a protein called 50S ribosomal protein L35.

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

- Molecule 54 is a protein called 50S ribosomal protein L6.

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

- Molecule 55 is a protein called 50S ribosomal protein L36.

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

- Molecule 56 is a protein called 50S ribosomal protein L9.

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

- Molecule 57 is a protein called 50S ribosomal protein L13.

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

- Molecule 58 is a protein called 50S ribosomal protein L14.

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

- Molecule 59 is a protein called 50S ribosomal protein L15.

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

- Molecule 60 is a protein called 50S ribosomal protein L16.

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

- Molecule 61 is a protein called 50S ribosomal protein L17.

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

- Molecule 62 is a protein called 50S ribosomal protein L18.

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

- Molecule 63 is a protein called 50S ribosomal protein L19.

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

- Molecule 64 is a protein called 50S ribosomal protein L20.

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

- Molecule 65 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

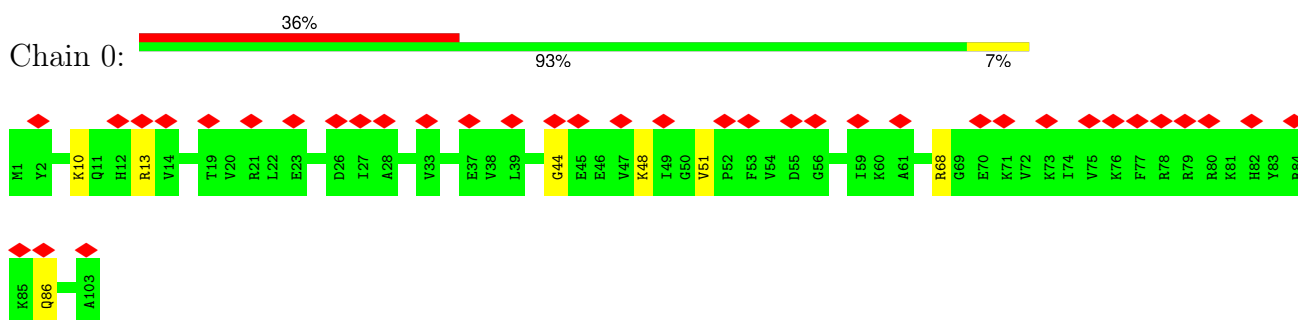
- Molecule 66 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

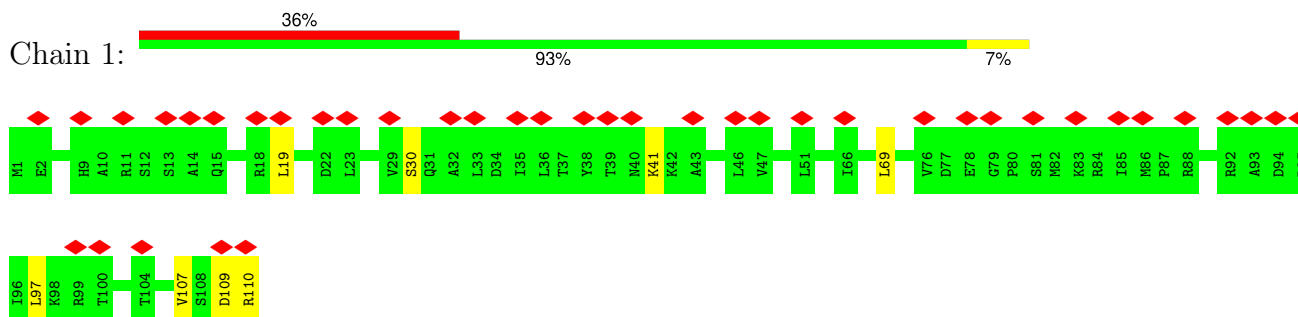
3 Residue-property plots [i](#)

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.

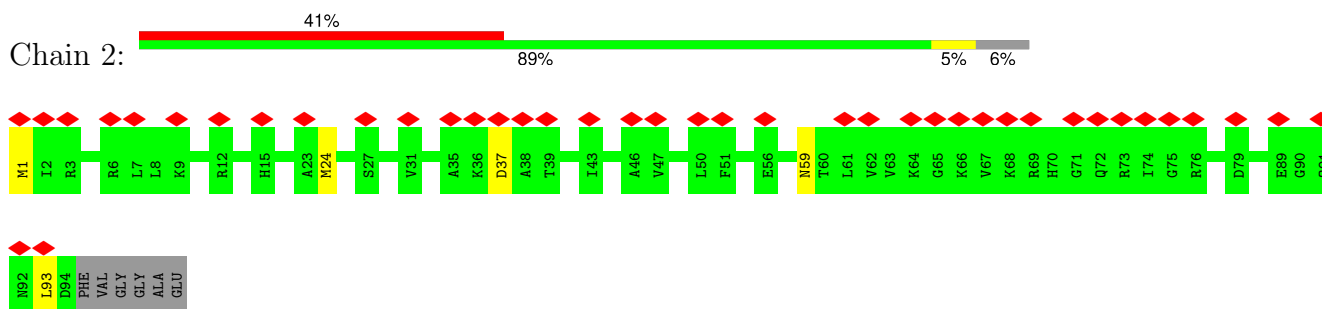
- Molecule 1: 50S ribosomal protein L21



- Molecule 2: 50S ribosomal protein L22



- Molecule 3: 50S ribosomal protein L23

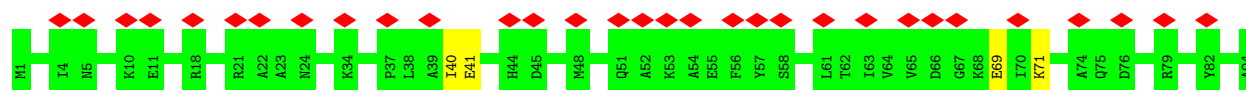


- Molecule 4: 50S ribosomal protein L24

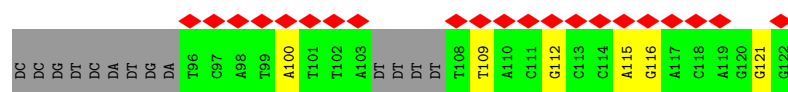




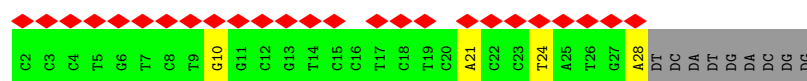
- Molecule 5: 50S ribosomal protein L25



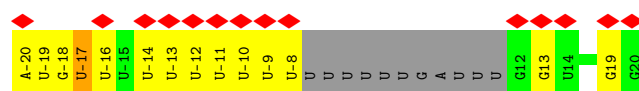
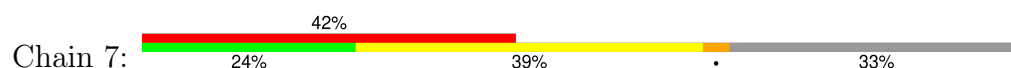
- Molecule 6: NT DNA



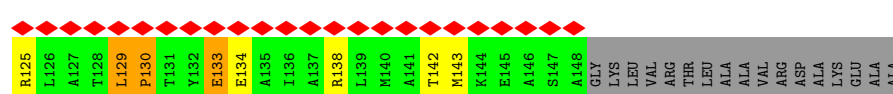
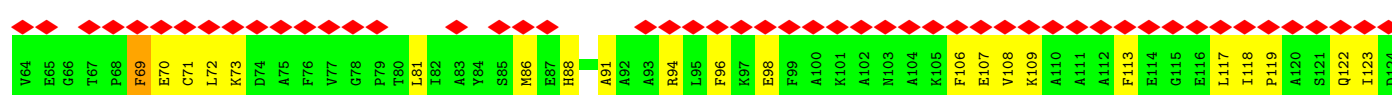
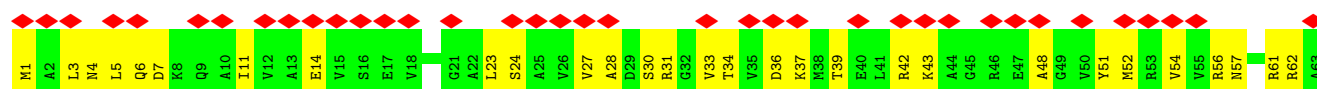
- Molecule 7: T DNA



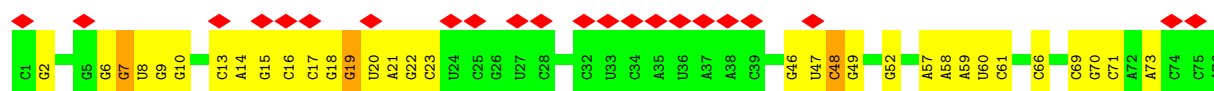
- Molecule 8: mRNA with 24 nt long spacer



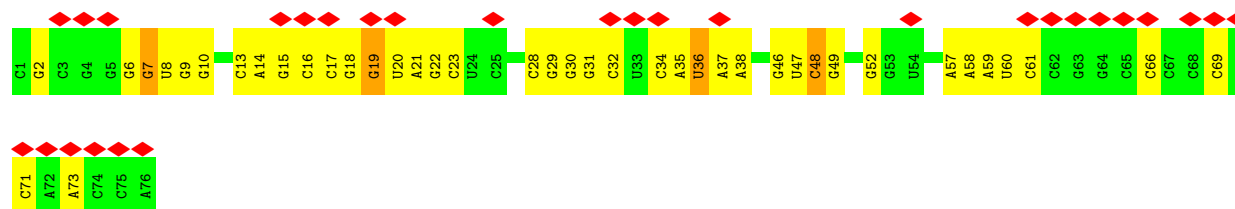
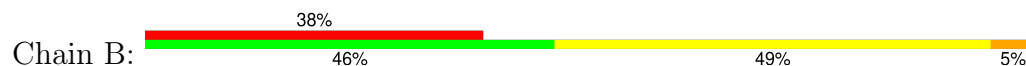
- Molecule 9: 50S ribosomal protein L10



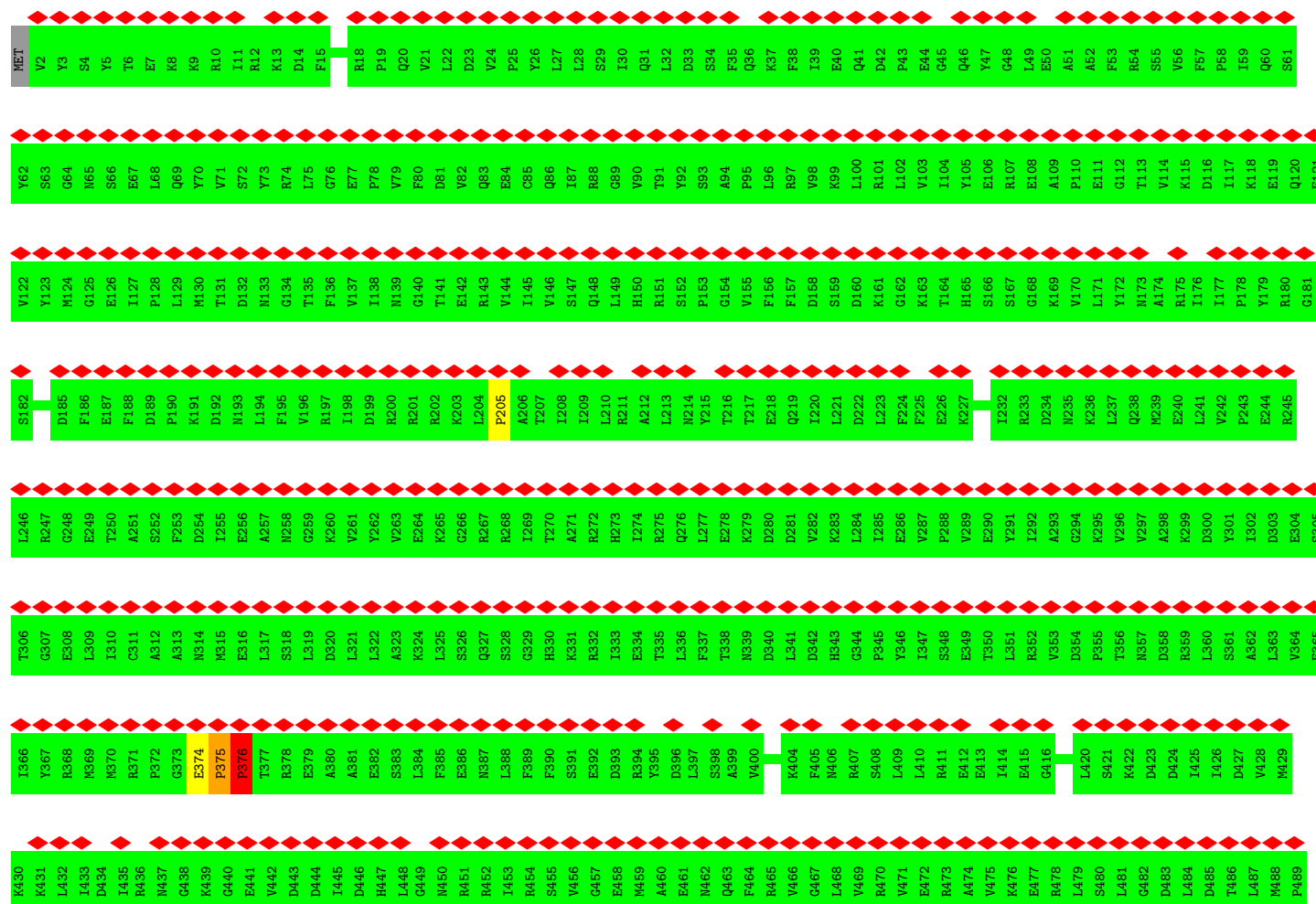
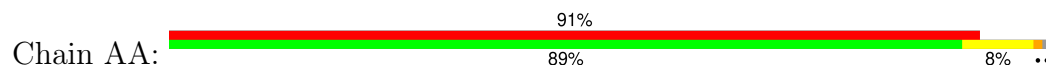
- Molecule 10: E-site and P-site tRNA (fMet)



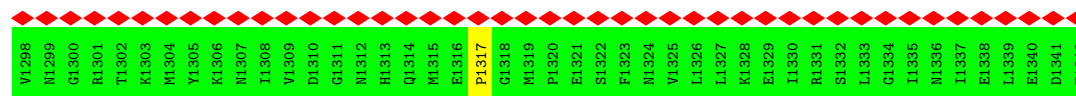
• Molecule 10: E-site and P-site tRNA (fMet)



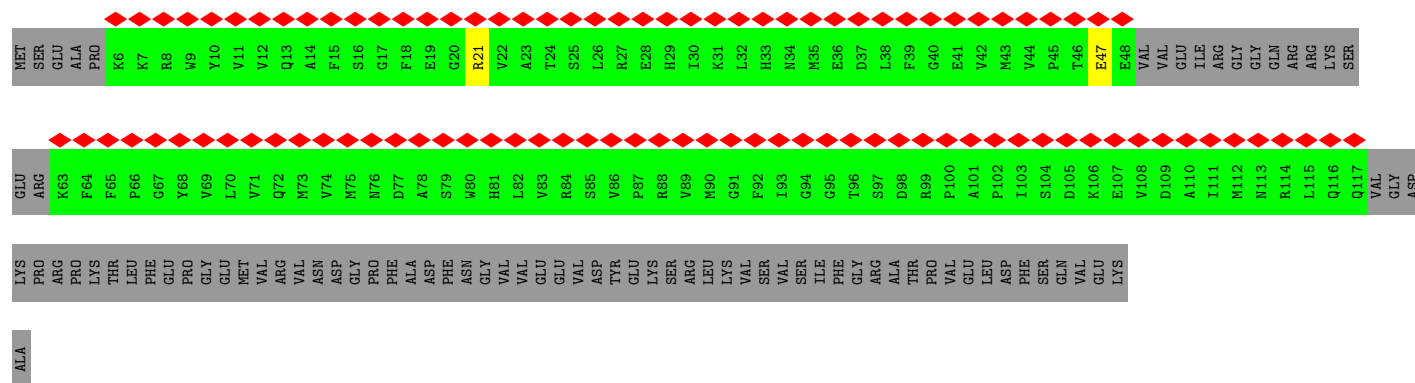
• Molecule 11: DNA-directed RNA polymerase subunit beta



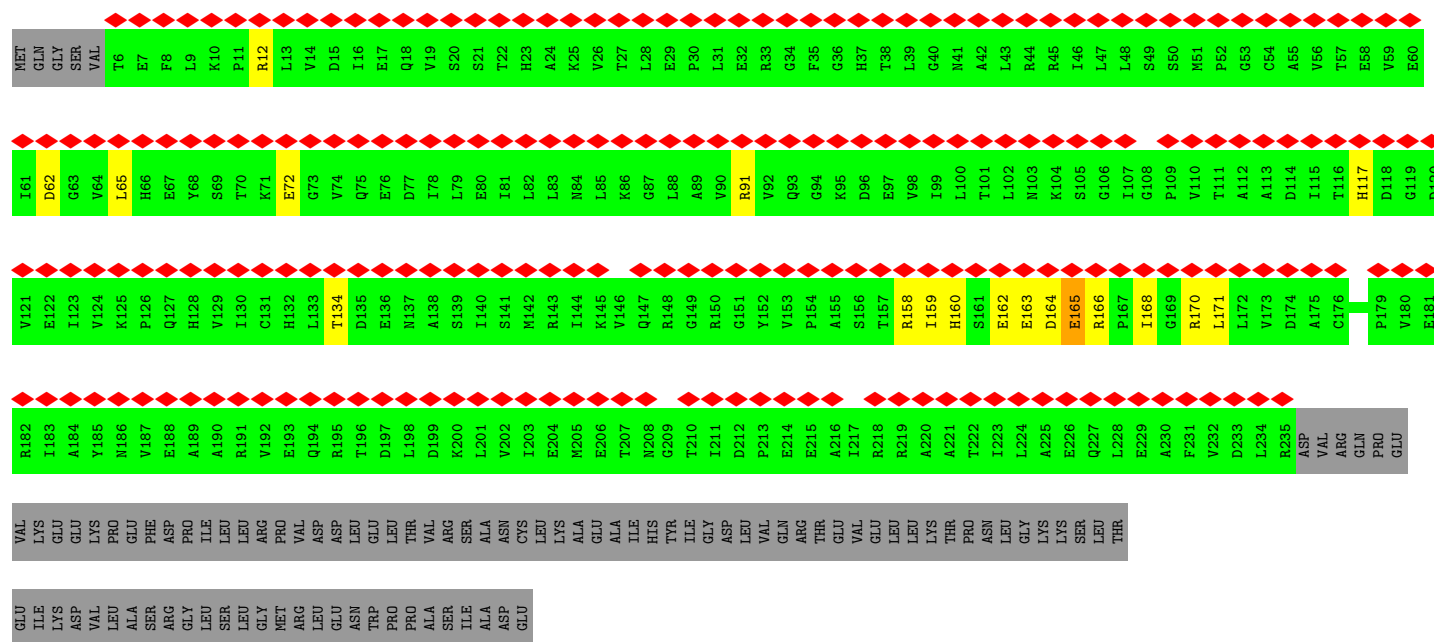
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D1241	M1180	M1119	R1059	E999	V939	G879	S819	S759	P698	V630	H551	D491
D1241	P1181	A1120	I1060	L1000	E940	G880	E820	T760	L999	E631	T553	I493
M1243	A1183	A1121	Q1061	L1001	K941	D881	R821	Q761	V700	D632	H564	N494
H1244	T1184	G1123	P1062	L1002	D942	I882	V822	T763	G701	L633	G555	A495
A1245	P1185	I1124	G1063	T1003	K943	L883	V823	C764	G703	V634	G566	K496
R1246	V1186	G1125	D1064	D1004	R944	V884	Q824	T765	N704	C636	R567	P497
S1247	F1187	D1126	K1065	E1005	A945	G885	E825	N766	E705	R637	V568	I498
T1248	F1187	K1127	M1066	E1006	L946	K886	D826	Q767	R706	S638	I561	S499
D1248	D1188	I1128	A1067	E947	I948	T888	F828	T768	A707	K639	E562	A501
G1249	G1189	M1129	G1068	Q1008	E948	P889	T829	P769	V708	G640	T563	V502
S1250	A1190	A1130	R1069	N1009	E949	P889	T829	C770	A709	S641	P564	K503
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S1252	E1192	L1011	G1071	L1011	M951	G891	H831	S772	S712	S643	G566	F505
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V1254	E1194	Q1013	K1073	L953	T992	G1013	L833	G774	V714	F645	N568	G507
T1255	I1195	L1014	G1074	L1014	K954	L953	Q834	E775	T715	S646	I569	S508
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K1257	E1197	Q1136	T1076	A1016	Q956	P980	L836	V777	V717	D648	L571	Q510
P1258	L1198	E1137	S1077	E1017	A957	G1017	A837	E778	A718	Q649	N573	L511
L1259	K1199	V1138	K1078	Y1018	K958	L953	C938	R779	K719		G562	L511
G1260	K1200	L1141	I1079	D1019	D959	L953	V839	E780	K720	D654	V663	L511
T1261	L1201	R1142	N1080	E1020	L960	ARG	S840	G780	R720	V655	G664	P520
K1262	G1202	E1143	P1081	L1021	S961	ALA	R841	D781	G721	S656	T581	N520
A1263	D1203	F1144	I1082	K1022	E962	PHE	D842	V782	G722	S656		L521
Q1264	L1204	E1083	E1083	E1023	E963	PHE	T843	L783	V723	L667		E522
F1265	P1205	Q1146	D1084	E1024	L964	GLY	K844	G784	V724	Q658		I524
G1266	T1206	R1147	M1085	F1025	Q965	GLU	L845	D785	Q725	S662		D516
T1267	S1207	A1148	P1086	E1026	I966	L953	G846	G786	Y726	V663		N518
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F1270	I1210	L1151	E1089	L1029	A969	V913	E949	T789	S730	G666	G585	E522
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M1273	E1213	V1155	P1093	K1032	S973	S916	A852	E793	V733			
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V1275	G1215	Q1157	D1095	K1035	L975	R919	P855	A795	V736	A676	D596	K527
T1276	R1216	K1158	T1096	L1036	R976	V920	N856	L796	N737	N677	D601	I530
A1277	T1217	V1159	I1096	T1037	A977	P921	V857	Q797	E738	I603	E602	S531
L1278	G1218	D1160	V1097	Q1038	V978	N922	G858	Q798	D739	A679	H604	A532
E1279	E1219	L1161	L1098	M1099	L979	G923	E859	N900	E740	L680	Y605	G534
Q1280	Q1220	S1162	P1100	N1099	V980	V924	A860	R801	M741	M681		G534
Y1281	F1221	T1163	P1100	D1040	A981	S925	A861	V802	P743	A683	A608	P535
E1282	E1222	F1164	L1101	D1041	G982	G926	L862	A803	G744	N684	E610	G536
A1283	P1223	S1165	G1102	L1042	V984	T927	S963	F804	E745	M685		G537
A1284	T1224	D1166	V1103	A1043	G983	V928	K864	N805	A746	Q686	A619	L538
L1285	V1225	E1167	P1104	P1044	E985	I929	L865	P806	G747	R687	N620	R540
T1286	T1226	E1168	S1105	G1045	A986	D930	E867	N807	I748	Q688	S621	R540
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Q1288	G1228	M1170	M1107	L1047	E987	Q932	S868	G809	D749	V690	L623	R542
E1289	Y1229	R1171	N1108	K1048	K988	V933	G869	Y810	I750	P691	G624	G544
M1290	M1230	L1172	I1109	I1049	L989	V933	I370	N811	T751	T692	E625	F545
Y1291	Y1231	A1173	G1110	V1050	K991	F934	V871	F812	N752	L693	G627	E546
T1292	M1232	E1174	Q1111	K1051	T935	T935	E872	E513	L753	R694		V547
V1293	L1233	L1112	I1112	V1052	L992	R936	I873	D814	T754	A695		R548
K1294	K1234	M1175	L1113	Y1053	P993		E874	S815	K755			D549
L1295	N1235	L1176	E1114	Y1053	R994		A875					
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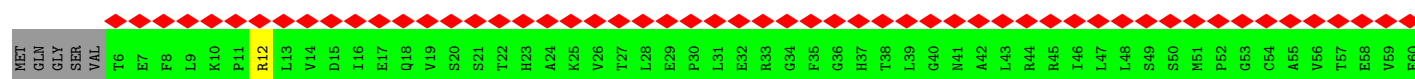
• Molecule 12: Transcription termination/antitermination protein NusG

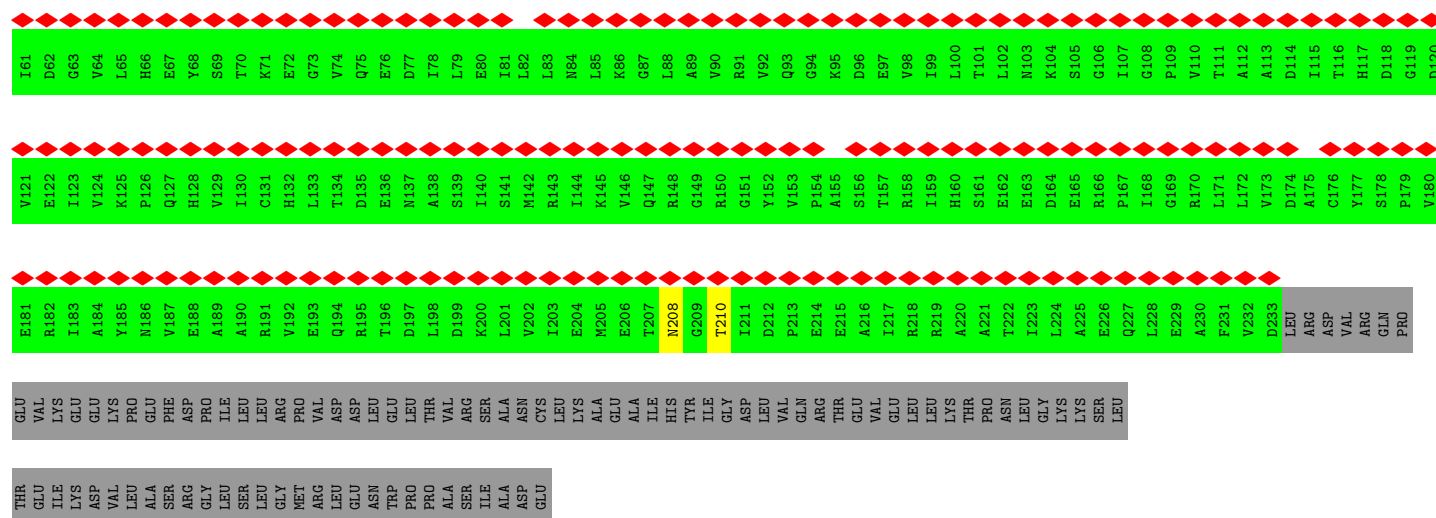


• Molecule 13: DNA-directed RNA polymerase subunit alpha

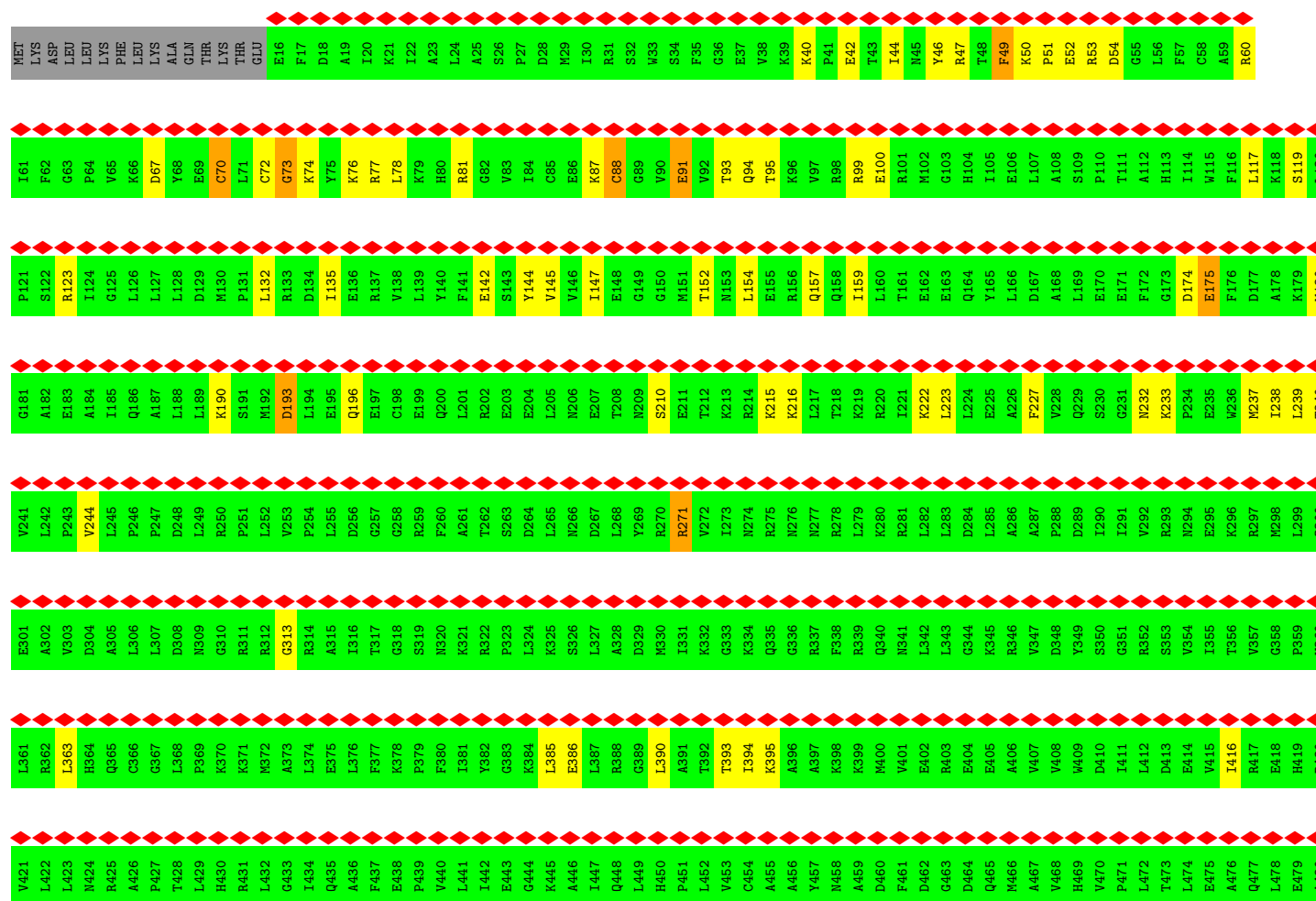
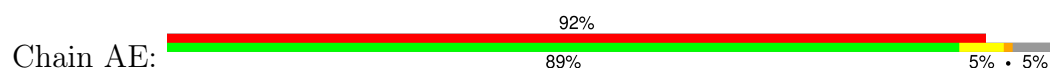


• Molecule 13: DNA-directed RNA polymerase subunit alpha

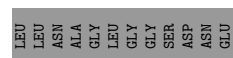
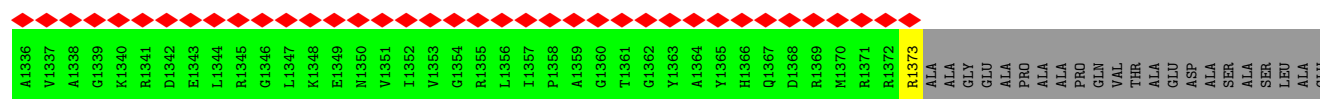
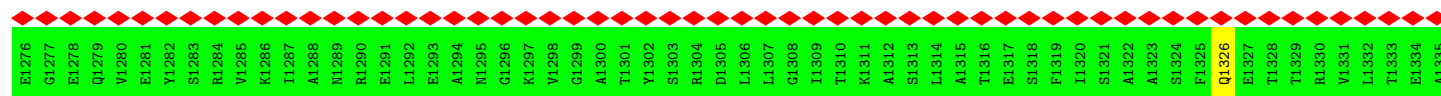




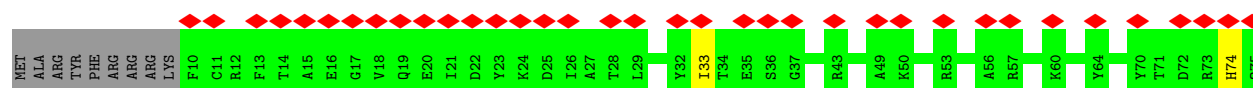
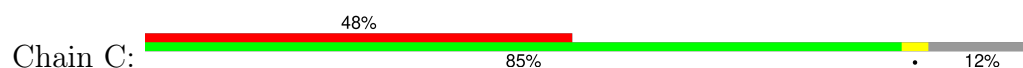
• Molecule 14: DNA-directed RNA polymerase subunit beta'



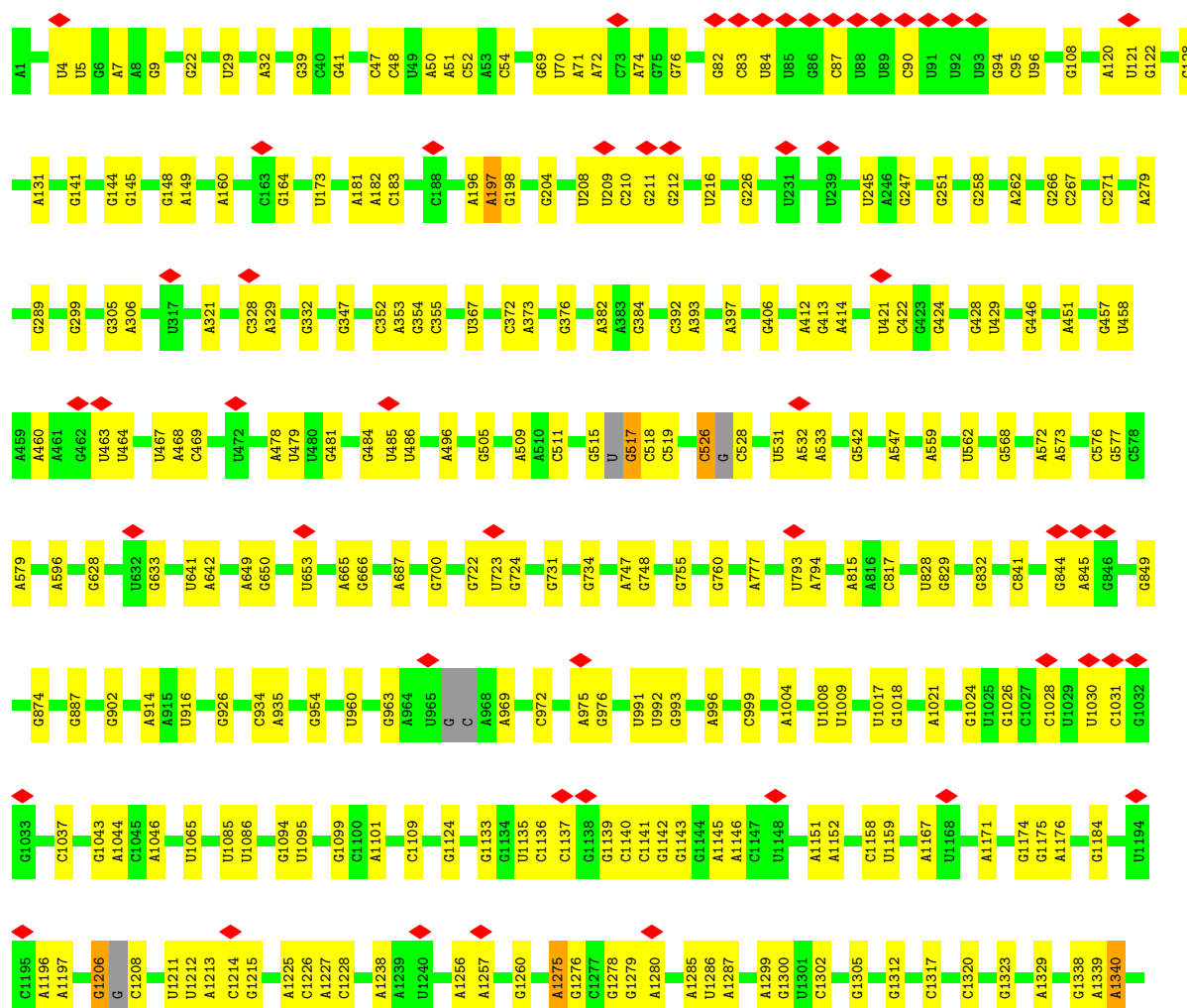
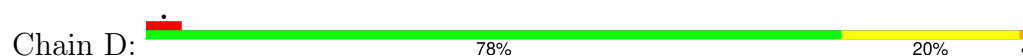
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L483	S543	K603	E666	A730	G794	D855	V917	S977	T1038	Q1098	E1158	H1218
M484	L544	M604	Q667	R731	Y795	T856	T918	R978	D1039	Y1099	I1159	D1219
M485	H545	L605	F668	G732	L796	L857	A919	R979	M1040	F1100	S1160	I1220
S486	A546	M606	Q669	S733	T797	V858	A920	T980	I1041	L1101	G1161	L1221
T487	R547	T607	Q670	A734	R798	P859	Q921	E981	D1042	P1102	I1162	R1222
N488	V548	C608	G671	A735	R799	R860	S922	L982	G1043	G1103	V1163	L1223
N489	K549	Y609	G672	A736	L800	T861	I923	K983	Q1044	K1104	S1164	R1224
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L491	R551	I611	V673	R738	D802	L863	E925	I985	I1046	I1106	G1166	V1226
S492	I552	G613	T674	Q739	A904	L864	P926	E986	T1047	V1107	K1167	H1227
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A494	E554	L614	G676	A741	D806	E866	T928	F988	Q1049	L1109	T1169	V1229
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P498	E497	V618	K681	M747	E811	D870	M933	E993	T1054	Q1114	R1173	I1233
I499	I499	I619	V682	A748	D812	L871	T933	E994	G1055	I1115	L1175	V1234
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V501	G561	A621	D684	T745	D814	E873	HIS	K996	T1057	S1117	I1177	V1237
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S503	L563	I624	M686	G752	G815	M875	GLY	Y998	L1059	D1119	P1179	D1239
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L510	K570	A630	V693	F763	T623	S884	S948	G1006	E1066	GLU	E1187	V1246
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Y512	T572	A633	K695		V825	V886	Q951	G1008	T1068	GLY	M1189	I1248
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R515	D516	G636	Q702	M768	G628	T890	D891	A1012	G1072	ASP	K1192	H1252
D517	R576	A577	V706	V769	G629	F892	F892	G1013	D1073	THR	W1193	E1254
C517	A578	S637	I707	Q771	D830	G893	G956	G1014	L1074	G1136	R1194	E1254
V518	I578	A638	I708	Y772	V831	V894	S957	G1015	R1075	G1137	Q1195	V1255
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G522	I582	D642	G711	T776	L835		S961		K1079	V1141	F1199	Q1259
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V526	G586	I646	E714	A779	V839		P902	H1023	A1083	F1145	R1203	K1263
L527	L587	P647	E715	R780	L840		L904	T1024	Q1084	A1146	V1204	A1264
T528	P588	Q649	K715	K781	L841		R905	M1025	G1085	A1147	E1205	T1265
G529	Y589	K650	V717	G782	G841		G906	P1026	M1086	V1027	R1148	I1266
P530	H651	E532	S718	A784	R642		H907	V1028	D1087	I1028	R1149	V1267
K531	I591	E533	F719	I785	V643		T908	T1029	V1088	E1030	P1150	N1268
E532	V592	E532	D720	T786	E946		I909	T1029	L1089	E1030	K1151	A1269
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E534	Q594	I654	I722	L788	V848		K911	I1032	G1092	P1091	P1153	S1271
R535	A595	A657	Y723	K789	L849		T912	S1032	T1093	G1092	A1154	D1272
L536	L596	E558	M724	T790	K950		E913	F1034	D1094	M1095	P1214	F1274
Y537	G597	A659	M725		P851		A914	V1035				L1275
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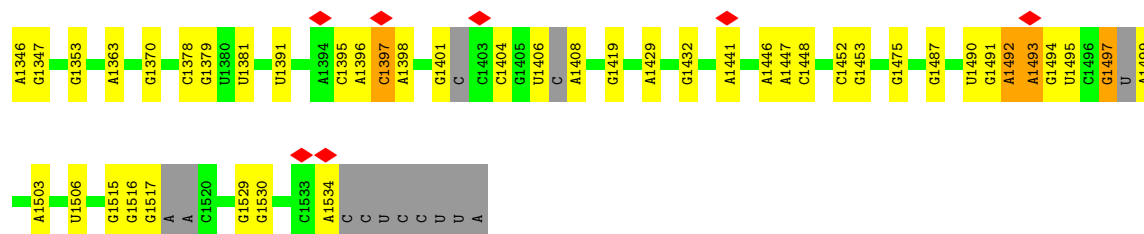


• Molecule 15: 30S ribosomal protein S18

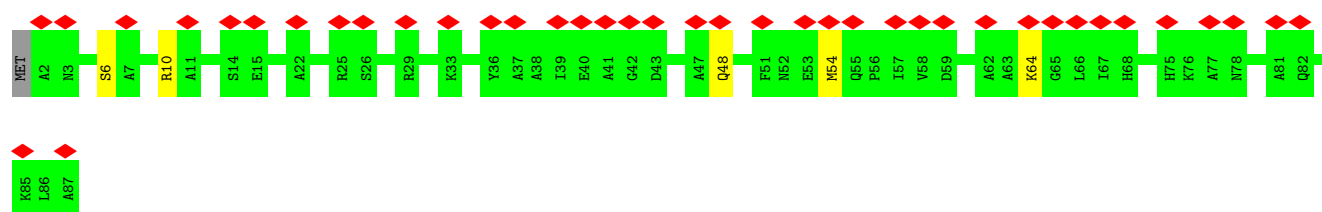
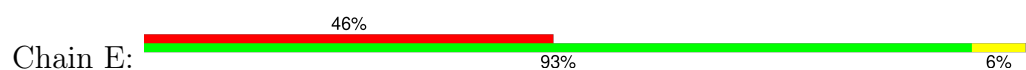


• Molecule 16: 16S rRNA





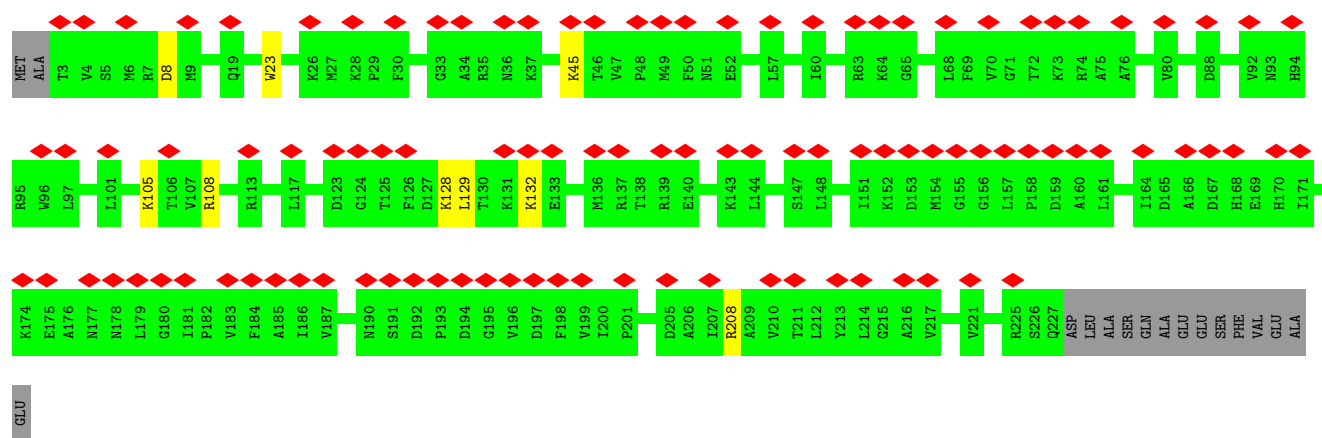
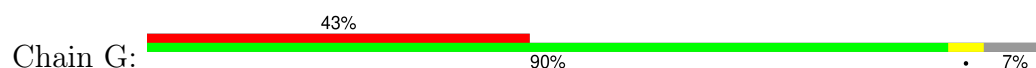
• Molecule 17: 30S ribosomal protein S20



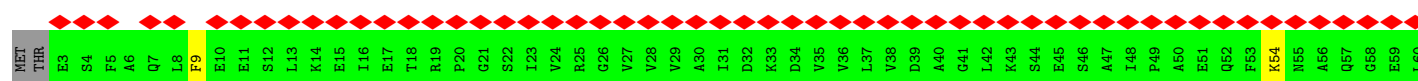
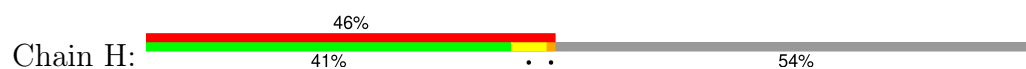
• Molecule 18: 30S ribosomal protein S21

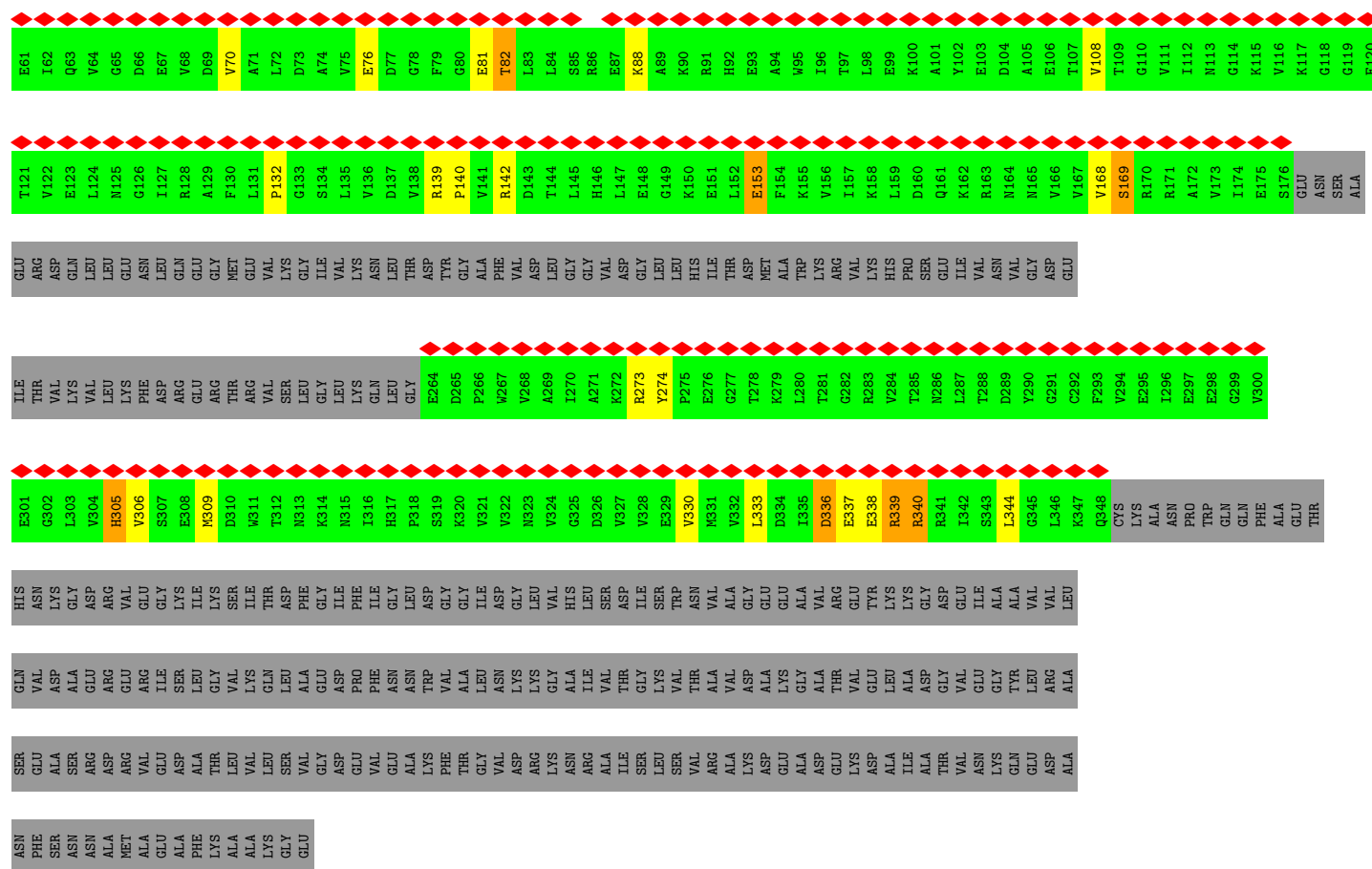


• Molecule 19: 30S ribosomal protein S2

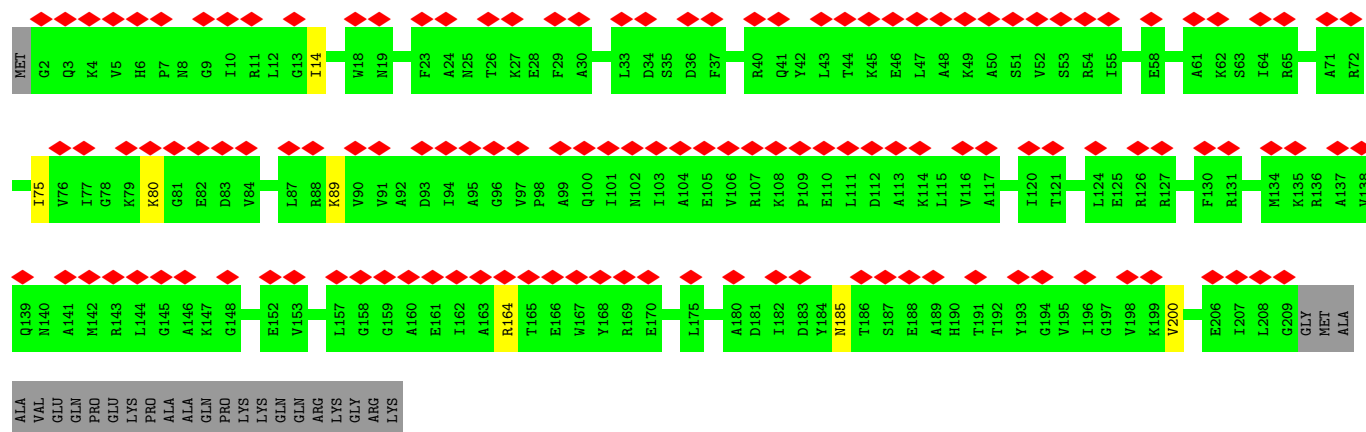
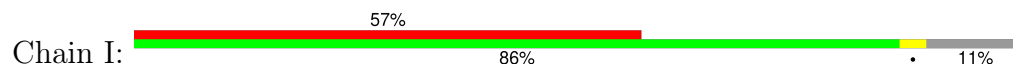


• Molecule 20: 30S ribosomal protein S1



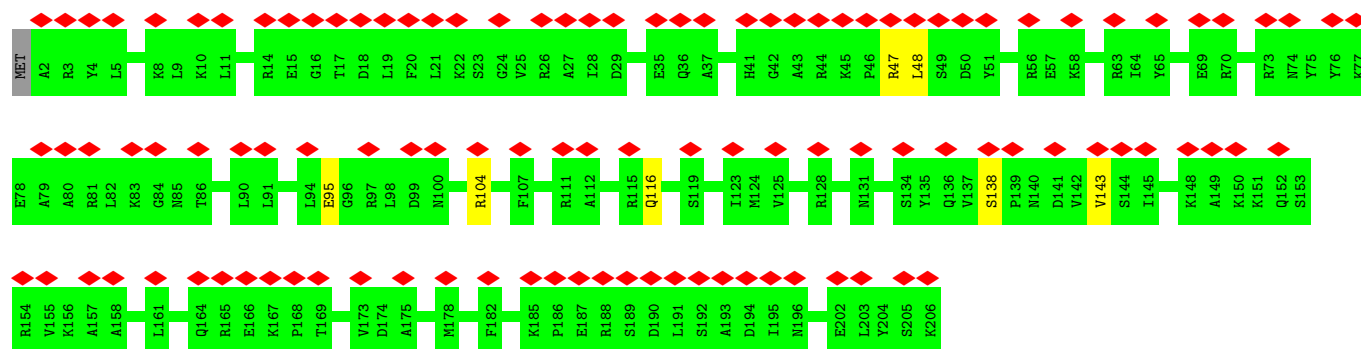


• Molecule 21: 30S ribosomal protein S3

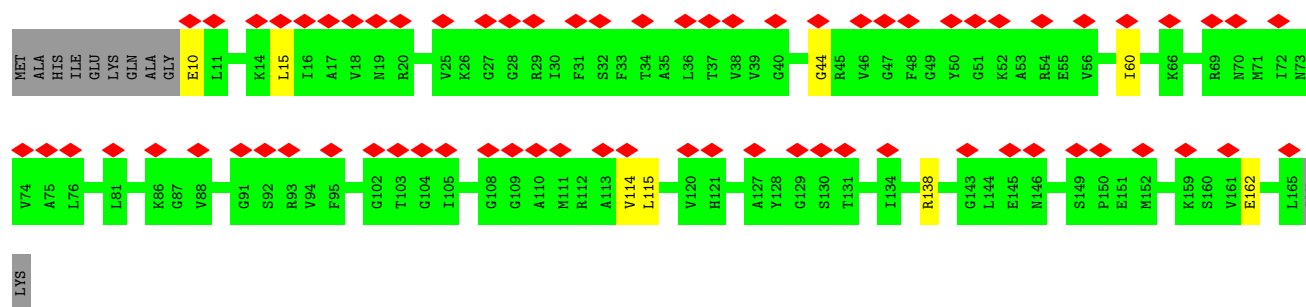
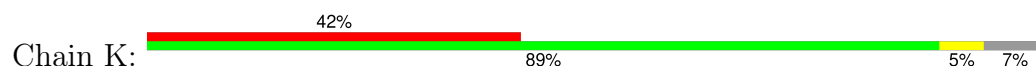


• Molecule 22: 30S ribosomal protein S4

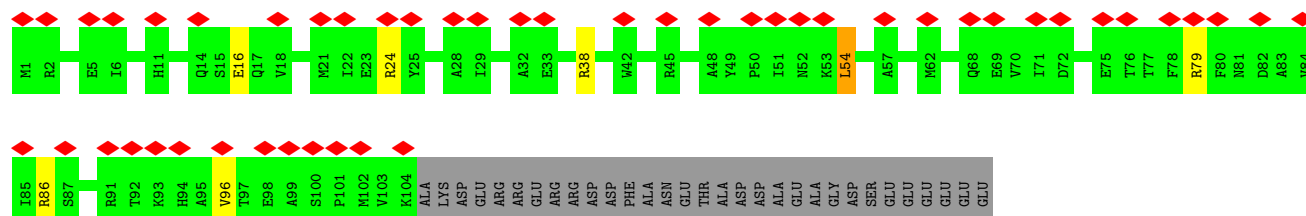




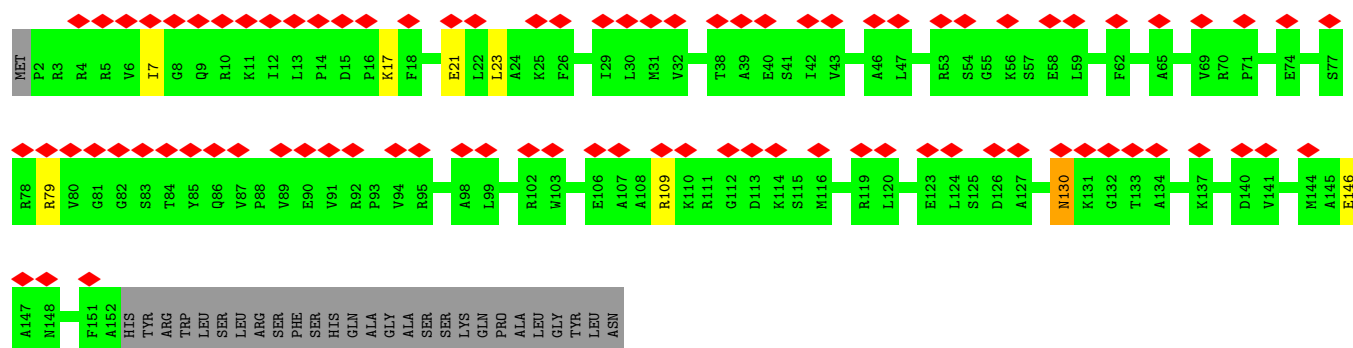
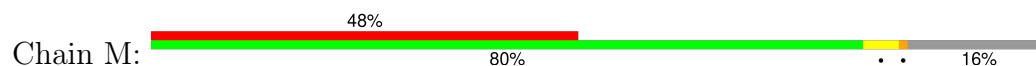
- Molecule 23: 30S ribosomal protein S5



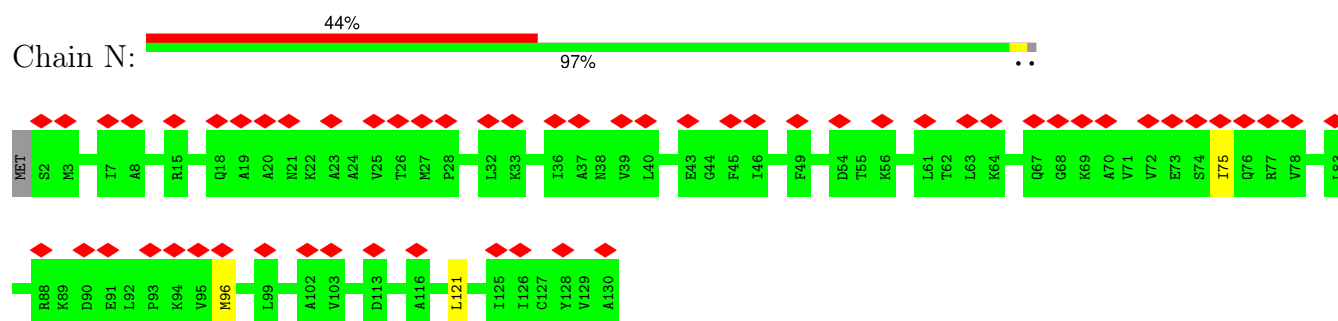
- Molecule 24: 30S ribosomal protein S6



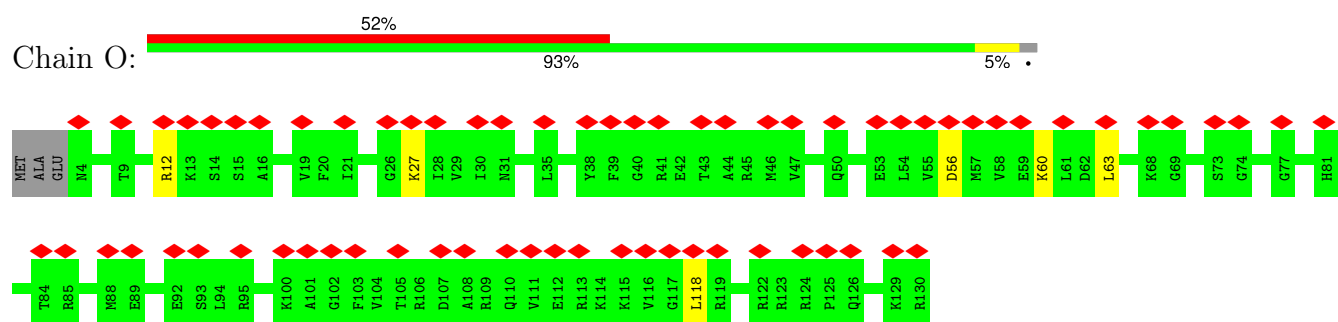
- Molecule 25: 30S ribosomal protein S7



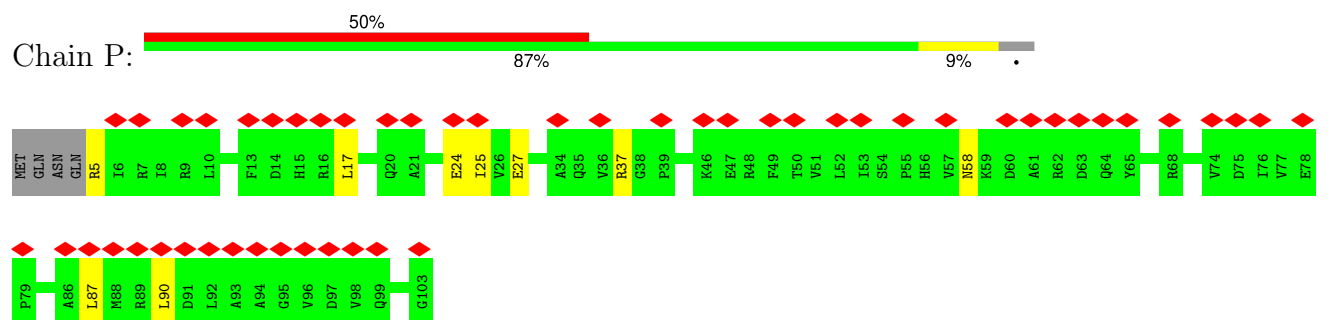
- Molecule 26: 30S ribosomal protein S8



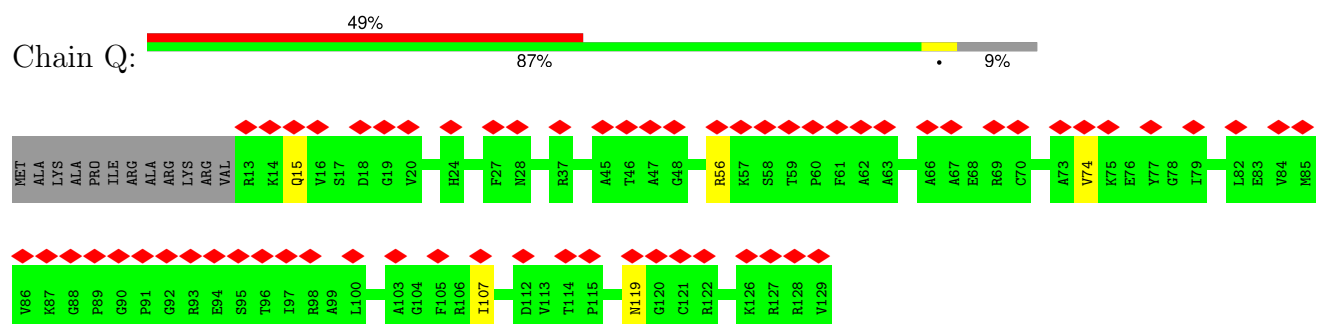
- Molecule 27: 30S ribosomal protein S9



- Molecule 28: 30S ribosomal protein S10

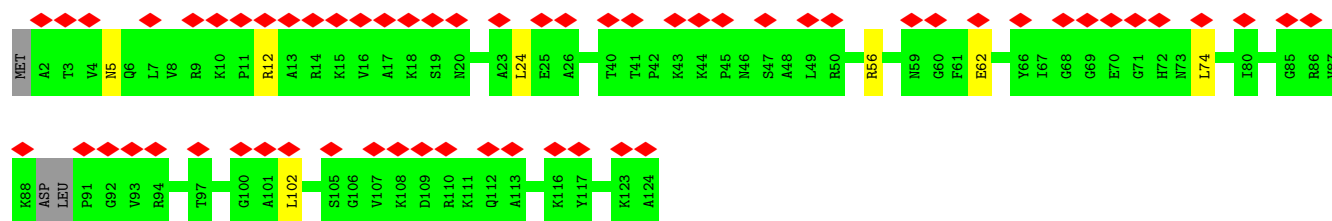


- Molecule 29: 30S ribosomal protein S11

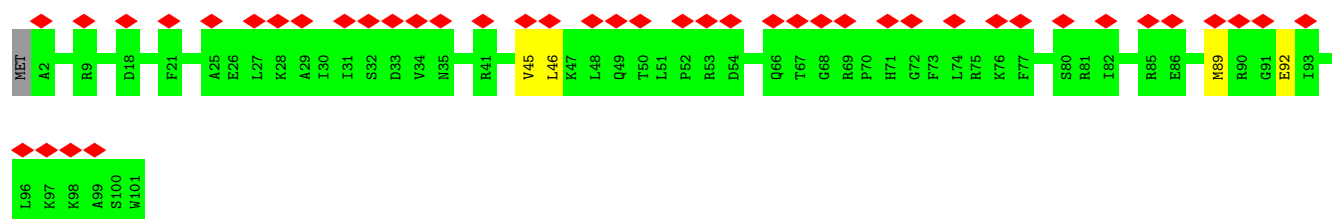
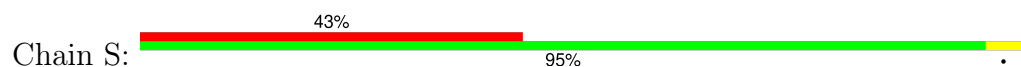


- Molecule 30: 30S ribosomal protein S12

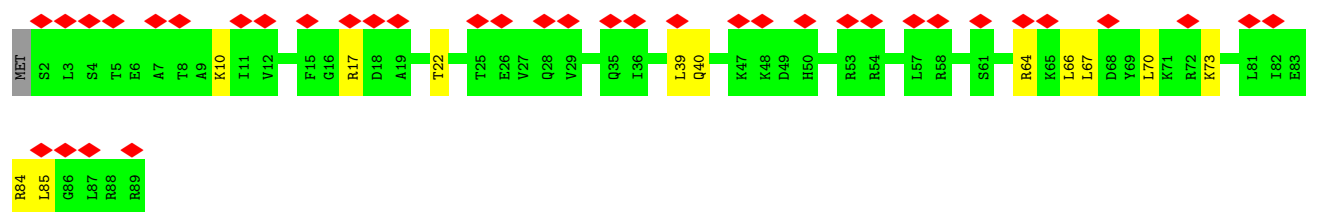
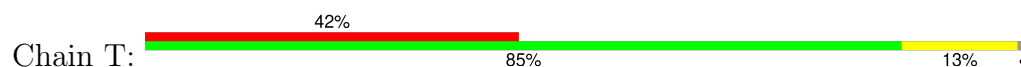




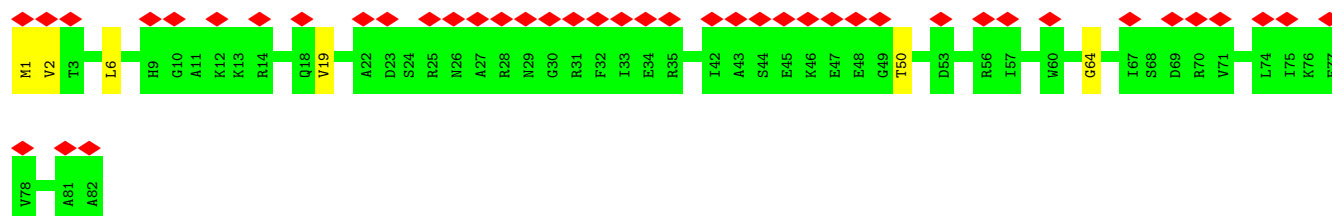
• Molecule 31: 30S ribosomal protein S14



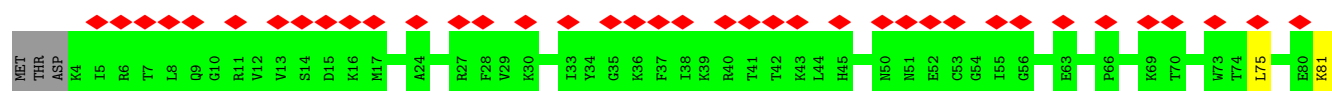
• Molecule 32: 30S ribosomal protein S15



• Molecule 33: 30S ribosomal protein S16



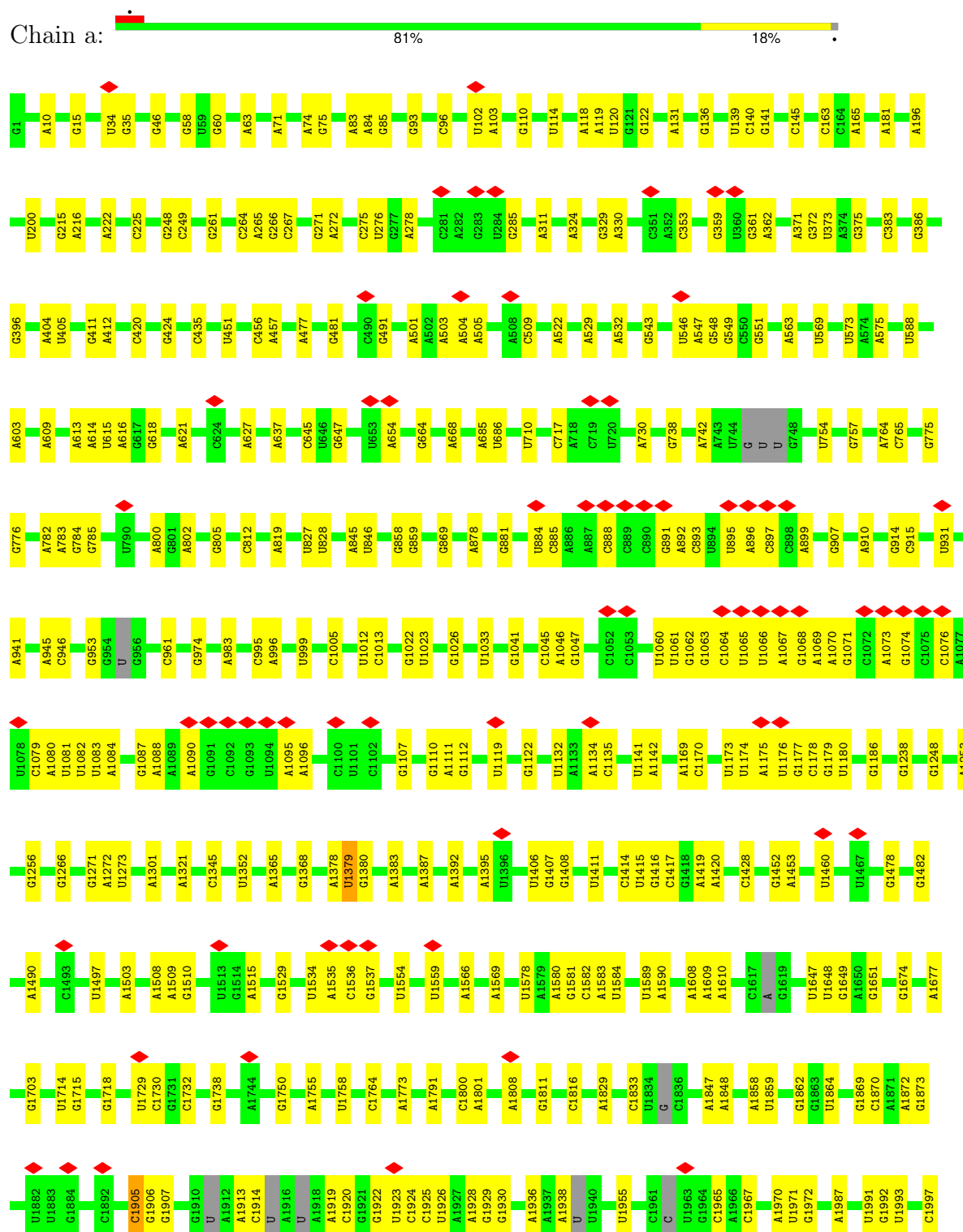
• Molecule 34: 30S ribosomal protein S17

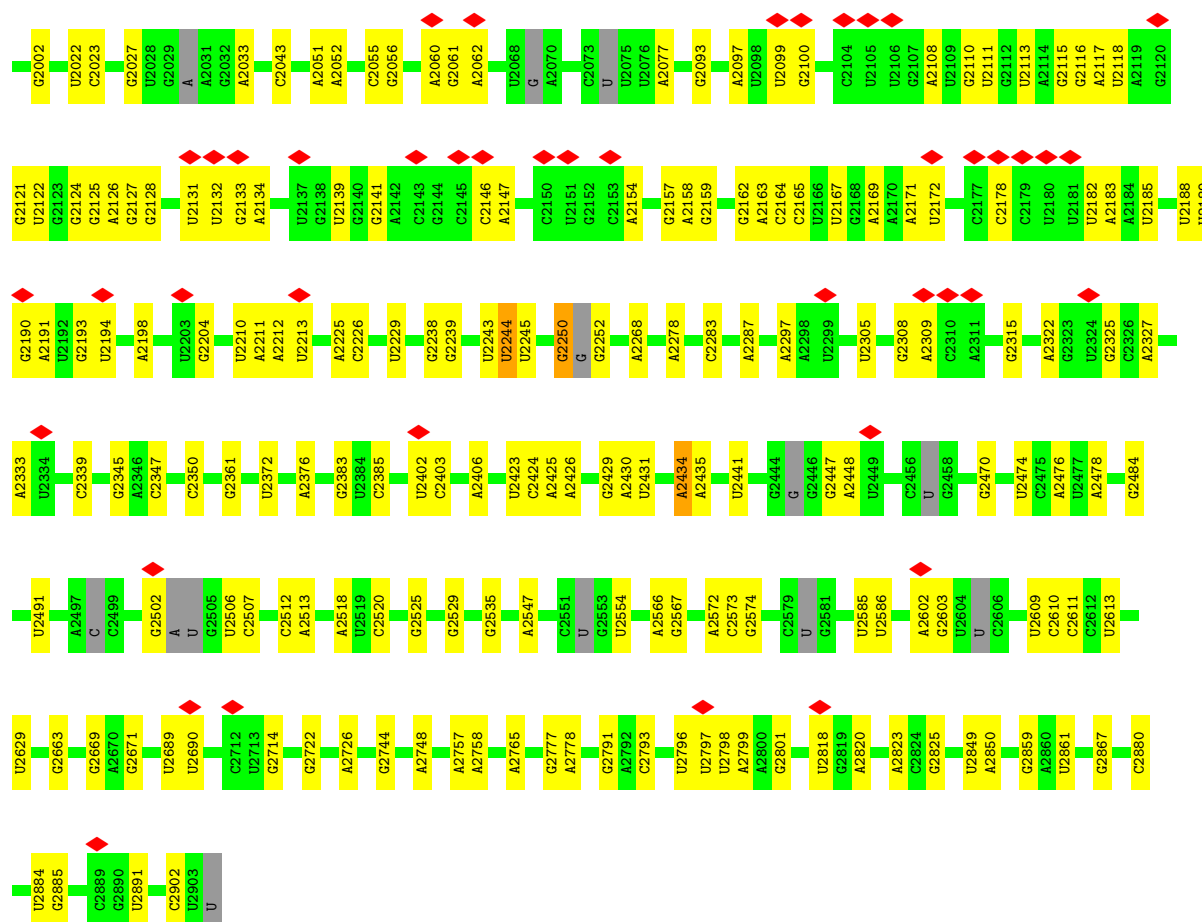


LYS

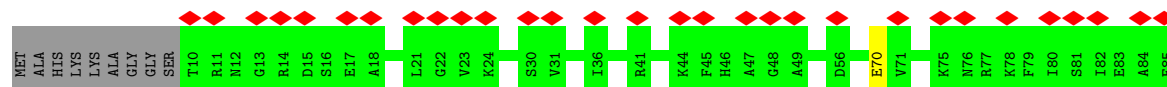
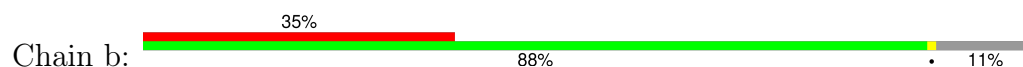
• Molecule 39: 23S rRNA

Chain a:

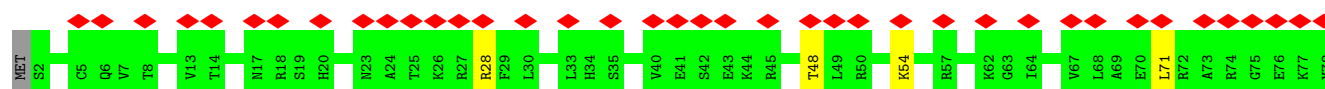




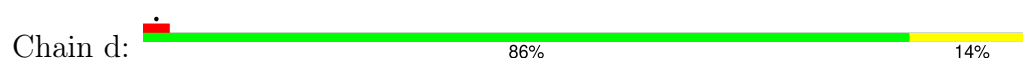
- Molecule 40: 50S ribosomal protein L27



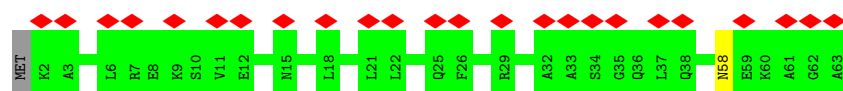
- Molecule 41: 50S ribosomal protein L28



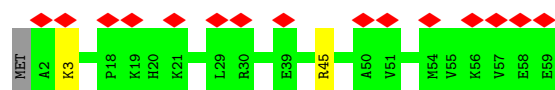
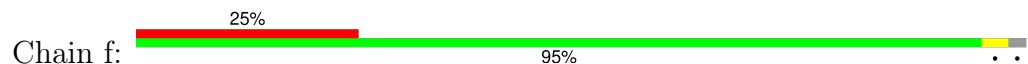
- Molecule 42: 5S rRNA



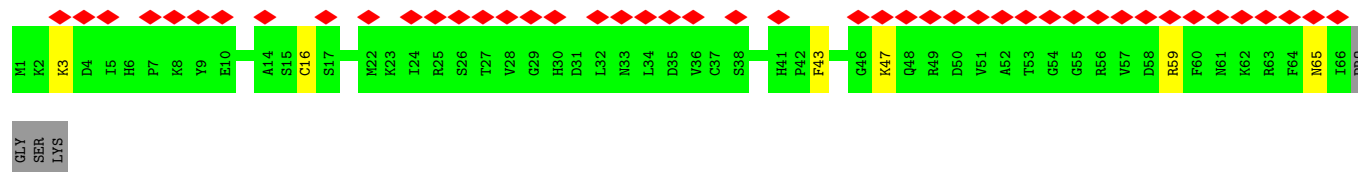
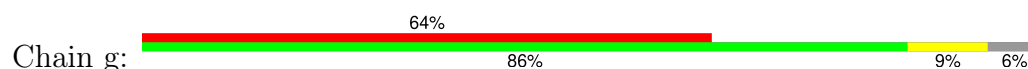
- Molecule 43: 50S ribosomal protein L29



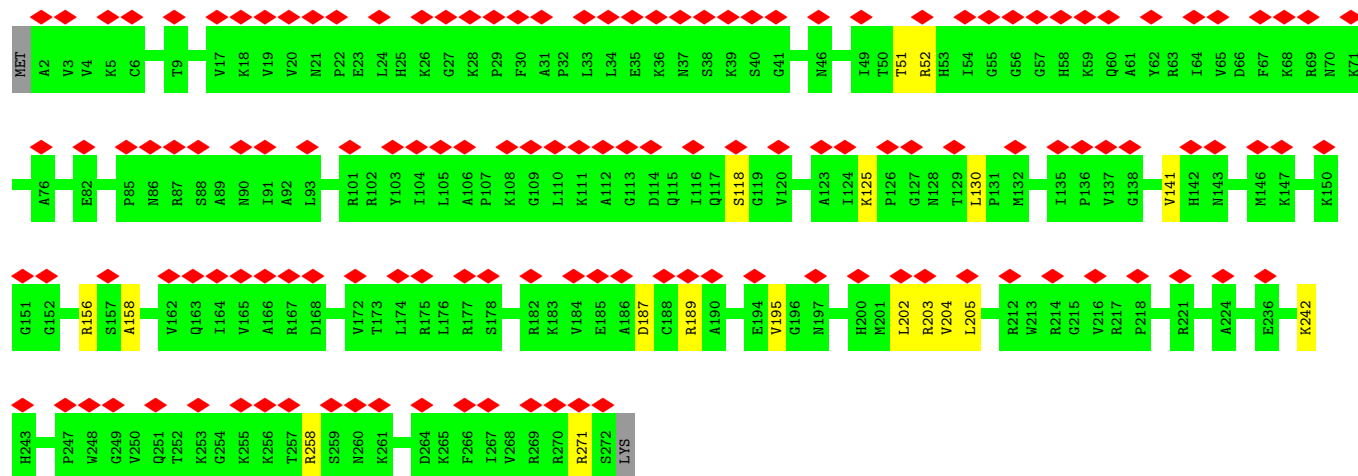
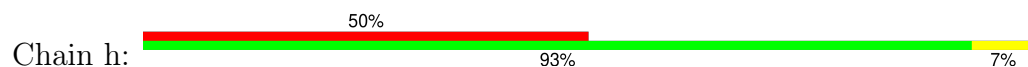
- Molecule 44: 50S ribosomal protein L30



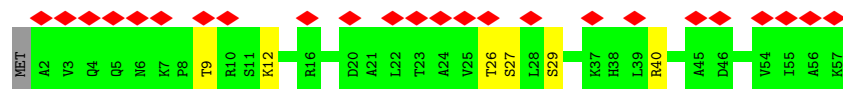
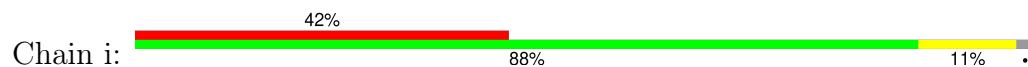
- Molecule 45: 50S ribosomal protein L31



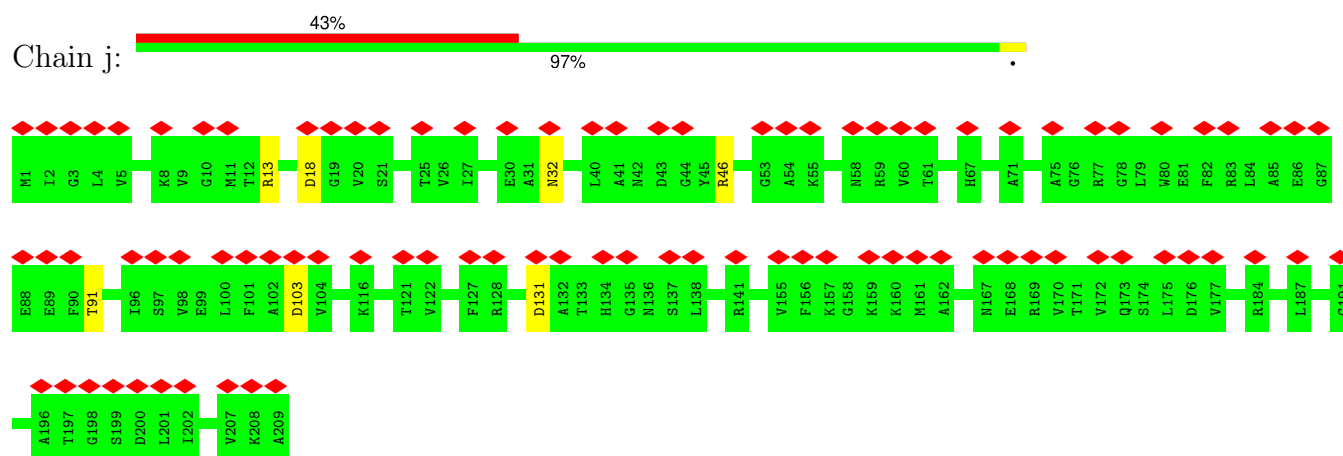
- Molecule 46: 50S ribosomal protein L2



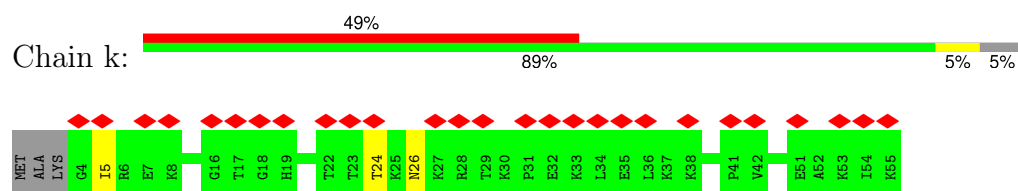
- Molecule 47: 50S ribosomal protein L32



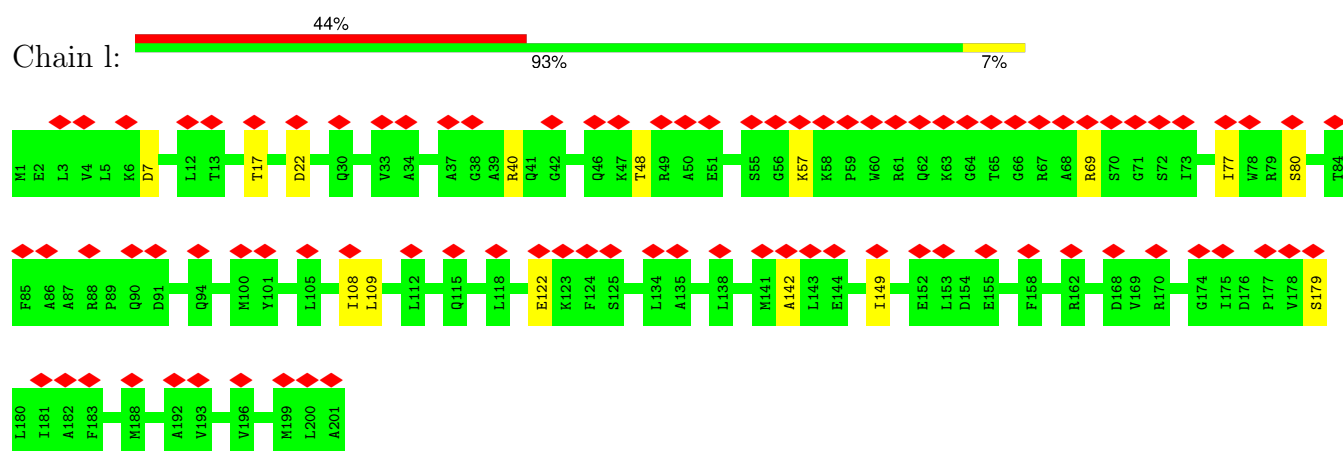
- Molecule 48: 50S ribosomal protein L3



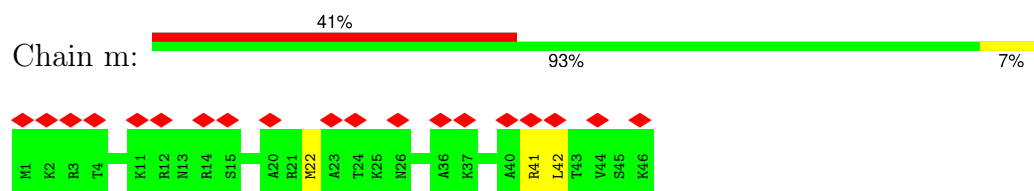
- Molecule 49: 50S ribosomal protein L33



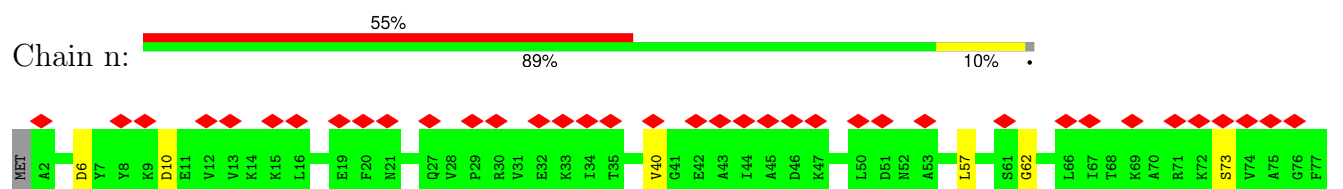
- Molecule 50: 50S ribosomal protein L4

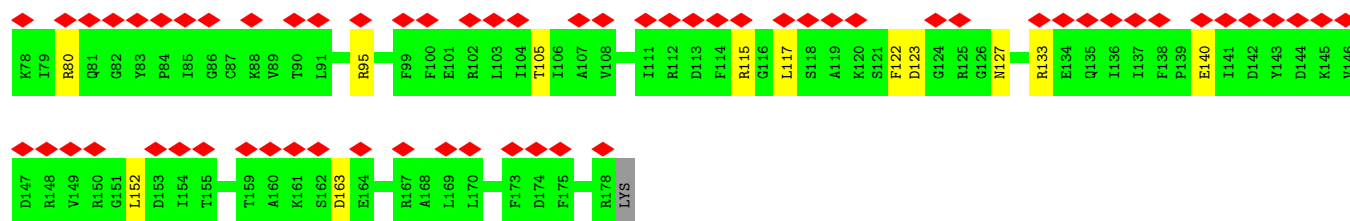


- Molecule 51: 50S ribosomal protein L34

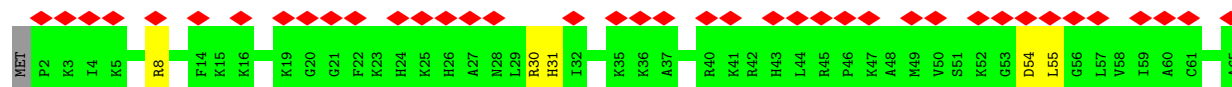
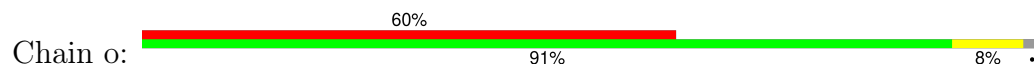


- Molecule 52: 50S ribosomal protein L5

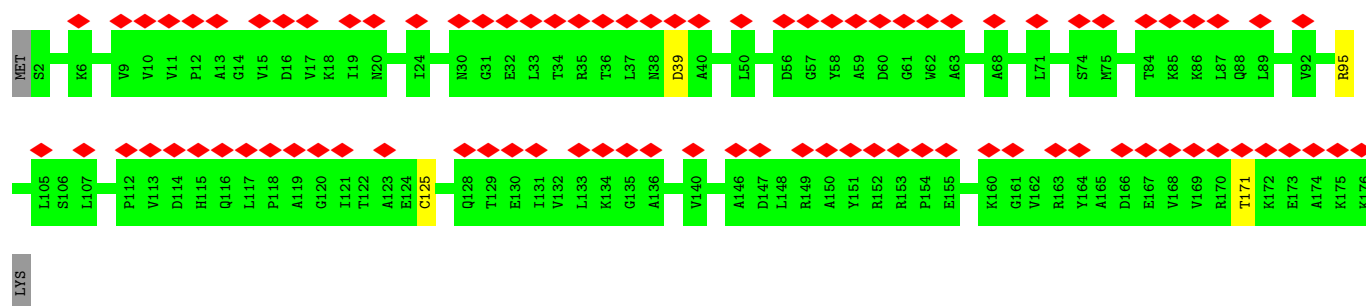




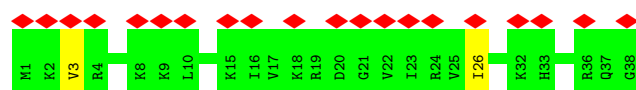
• Molecule 53: 50S ribosomal protein L35



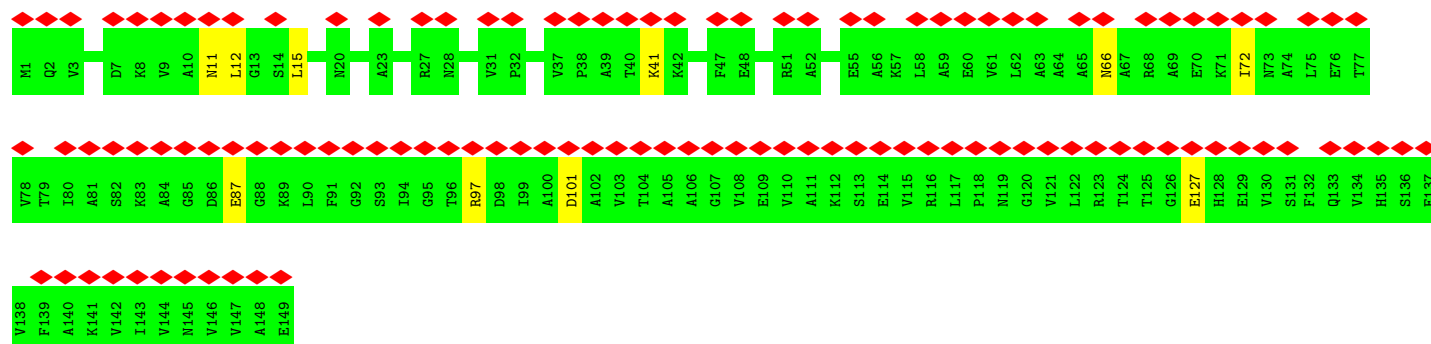
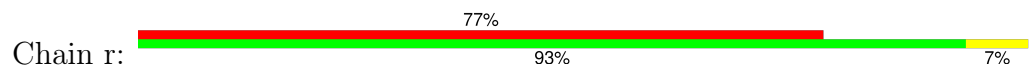
• Molecule 54: 50S ribosomal protein L6



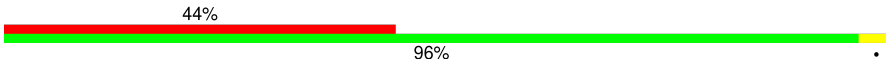
• Molecule 55: 50S ribosomal protein L36

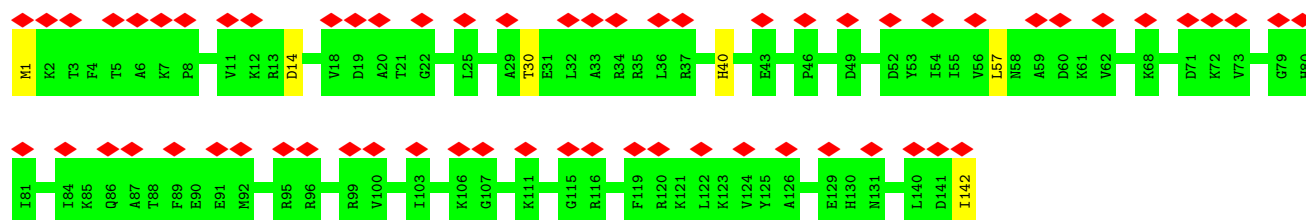


• Molecule 56: 50S ribosomal protein L9



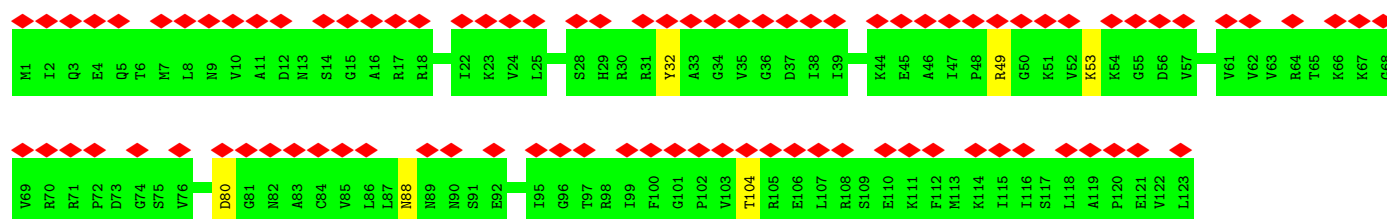
- Molecule 57: 50S ribosomal protein L13

Chain s: 



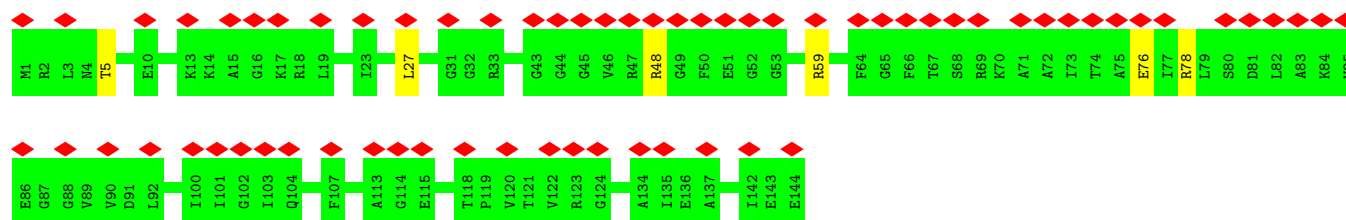
- Molecule 58: 50S ribosomal protein L14

Chain t: 



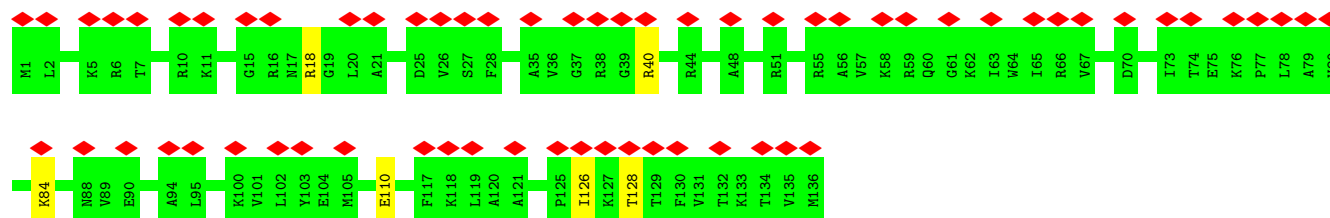
- Molecule 59: 50S ribosomal protein L15

Chain u: 




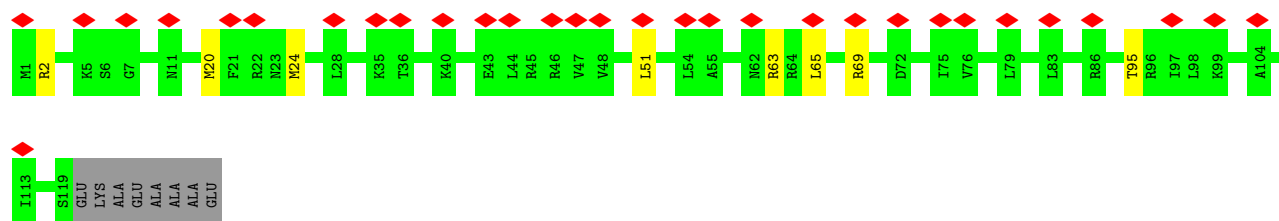
- Molecule 60: 50S ribosomal protein L16

Chain v: 



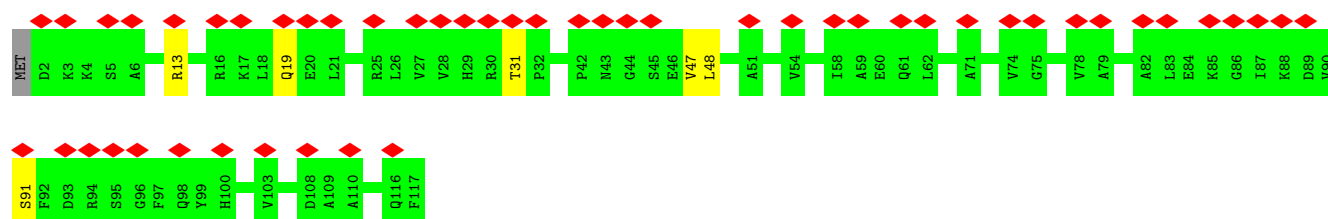
- Molecule 61: 50S ribosomal protein L17

Chain w: 



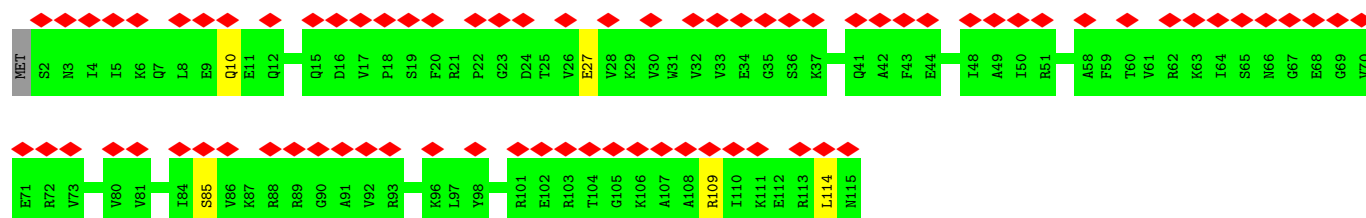
- Molecule 62: 50S ribosomal protein L18

Chain x: 43% 94% 5%



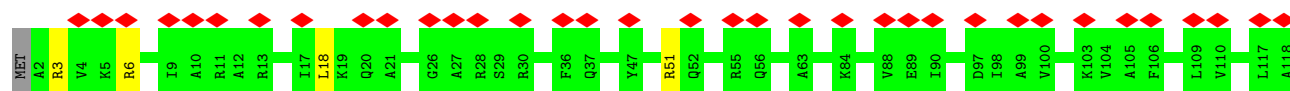
- Molecule 63: 50S ribosomal protein L19

Chain y: 66% 95%



- Molecule 64: 50S ribosomal protein L20

Chain z: 30% 96%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	4000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	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	0.029	Depositor
Minimum map value	-0.014	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.009	Depositor
Map size (\AA)	532.48, 532.48, 532.48	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.04, 1.04, 1.04	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	0	0.38	0/829	0.67	0/1107
2	1	0.49	0/864	0.82	0/1156
3	2	0.42	0/752	0.71	0/1005
4	3	0.35	0/796	0.67	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	1.12	4/603 (0.7%)	0.97	0/926
8	7	0.67	2/519 (0.4%)	0.99	3/804 (0.4%)
9	9	0.79	2/1131 (0.2%)	0.64	1/1524 (0.1%)
10	A	0.39	0/1810	0.75	1/2821 (0.0%)
10	B	0.46	1/1810 (0.1%)	0.86	7/2821 (0.2%)
11	AA	0.59	2/10591 (0.0%)	0.75	15/14289 (0.1%)
12	AB	0.43	0/808	0.60	0/1088
13	AC	0.48	0/1808	0.62	1/2450 (0.0%)
13	AD	0.39	0/1789	0.56	0/2425
14	AE	0.52	3/10545 (0.0%)	0.66	5/14236 (0.0%)
15	C	0.48	0/553	0.83	0/743
16	D	0.34	10/36610 (0.0%)	0.74	30/57091 (0.1%)
17	E	0.57	0/675	0.86	0/895
18	F	0.56	0/597	0.87	0/792
19	G	0.49	0/1791	0.71	0/2413
20	H	0.54	1/1746 (0.1%)	1.03	12/2382 (0.5%)
21	I	0.44	0/1663	0.71	0/2241
22	J	0.47	0/1665	0.73	0/2227
23	K	0.45	0/1165	0.75	0/1568
24	L	0.43	0/867	0.75	1/1171 (0.1%)
25	M	0.50	0/1195	0.81	0/1602
26	N	0.41	0/989	0.69	0/1326
27	O	0.43	0/1034	0.75	0/1375
28	P	0.43	0/800	0.75	0/1082
29	Q	0.40	0/893	0.70	0/1205
30	R	0.36	0/952	0.74	0/1274

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	S	0.49	0/817	0.78	0/1088
32	T	0.53	0/722	0.86	0/964
33	U	0.44	0/659	0.78	0/884
34	V	0.34	0/657	0.61	0/881
35	W	0.38	0/680	0.62	0/915
36	X	0.49	0/909	0.87	0/1215
37	Y	0.67	0/1046	0.58	0/1410
38	Z	0.69	0/227	0.57	0/304
39	a	0.38	3/69247 (0.0%)	0.72	18/107985 (0.0%)
40	b	0.39	0/589	0.70	0/779
41	c	0.48	0/635	0.81	1/848 (0.1%)
42	d	0.29	0/2872	0.69	0/4478
43	e	0.54	0/502	0.83	0/667
44	f	0.45	0/452	0.78	0/605
45	g	0.43	0/531	0.68	0/709
46	h	0.39	0/2121	0.78	0/2852
47	i	0.40	0/450	0.79	0/599
48	j	0.44	0/1586	0.69	0/2134
49	k	0.35	0/433	0.65	0/576
50	l	0.46	0/1571	0.77	0/2113
51	m	0.53	0/380	0.99	0/498
52	n	0.49	0/1434	0.88	3/1926 (0.2%)
53	o	0.46	0/513	0.83	0/676
54	p	0.39	0/1333	0.67	0/1805
55	q	0.37	0/303	0.77	0/397
56	r	0.43	0/1122	0.69	0/1515
57	s	0.50	0/1152	0.75	0/1551
58	t	0.41	0/955	0.78	0/1279
59	u	0.40	0/1062	0.76	0/1413
60	v	0.47	0/1093	0.82	0/1460
61	w	0.52	0/964	0.87	0/1289
62	x	0.46	0/902	0.81	0/1209
63	y	0.41	0/929	0.73	1/1242 (0.1%)
64	z	0.60	0/960	0.91	1/1278 (0.1%)
All	All	0.43	34/188952 (0.0%)	0.74	103/278480 (0.0%)

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

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

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
10	B	0	2
11	AA	0	10
14	AE	0	5
20	H	0	3
36	X	0	1
All	All	0	23

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	9	130	PRO	N-CA	13.73	1.70	1.47
16	D	1516	G	O3'-P	-13.37	1.45	1.61
16	D	1339	A	O3'-P	10.52	1.73	1.61
11	AA	374	GLU	C-N	10.46	1.54	1.34
14	AE	88	CYS	CB-SG	-10.17	1.65	1.82

The worst 5 of 103 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	D	1516	G	P-O3'-C3'	-19.03	96.86	119.70
16	D	1516	G	O3'-P-O5'	13.79	130.21	104.00
11	AA	1250	SER	C-N-CA	11.14	149.55	121.70
39	a	2252	G	N9-C1'-C2'	-10.95	99.76	114.00
16	D	1401	G	N9-C1'-C2'	-10.70	100.09	114.00

There are no chirality outliers.

5 of 23 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	A	19	G	Sidechain
10	A	7	G	Sidechain
11	AA	205	PRO	Peptide
11	AA	594	VAL	Peptide
11	AA	595	THR	Peptide

5.2 Too-close contacts

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	101/103 (98%)	97 (96%)	3 (3%)	1 (1%)	13	49
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%)	13	49
5	4	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
9	9	146/165 (88%)	95 (65%)	37 (25%)	14 (10%)	0	7
11	AA	1318/1342 (98%)	1149 (87%)	137 (10%)	32 (2%)	5	27
12	AB	94/181 (52%)	88 (94%)	6 (6%)	0	100	100
13	AC	228/329 (69%)	215 (94%)	11 (5%)	2 (1%)	14	52
13	AD	226/329 (69%)	213 (94%)	12 (5%)	1 (0%)	30	68
14	AE	1329/1407 (94%)	1200 (90%)	120 (9%)	9 (1%)	19	57
15	C	64/75 (85%)	63 (98%)	1 (2%)	0	100	100
17	E	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
18	F	68/71 (96%)	68 (100%)	0	0	100	100
19	G	223/241 (92%)	210 (94%)	13 (6%)	0	100	100
20	H	255/557 (46%)	188 (74%)	55 (22%)	12 (5%)	2	16
21	I	206/233 (88%)	196 (95%)	9 (4%)	1 (0%)	25	64
22	J	203/206 (98%)	198 (98%)	5 (2%)	0	100	100
23	K	154/167 (92%)	146 (95%)	7 (4%)	1 (1%)	22	60
24	L	102/135 (76%)	97 (95%)	4 (4%)	1 (1%)	13	49
25	M	149/179 (83%)	144 (97%)	4 (3%)	1 (1%)	19	57
26	N	127/130 (98%)	121 (95%)	5 (4%)	1 (1%)	16	55
27	O	125/130 (96%)	115 (92%)	9 (7%)	1 (1%)	16	55
28	P	97/103 (94%)	88 (91%)	8 (8%)	1 (1%)	13	49
29	Q	115/129 (89%)	104 (90%)	9 (8%)	2 (2%)	7	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	R	117/124 (94%)	116 (99%)	1 (1%)	0	100	100
31	S	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
32	T	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
33	U	80/82 (98%)	75 (94%)	4 (5%)	1 (1%)	10	43
34	V	78/84 (93%)	74 (95%)	4 (5%)	0	100	100
35	W	81/92 (88%)	78 (96%)	3 (4%)	0	100	100
36	X	114/118 (97%)	107 (94%)	5 (4%)	2 (2%)	7	35
37	Y	139/142 (98%)	102 (73%)	25 (18%)	12 (9%)	0	9
38	Z	28/121 (23%)	19 (68%)	7 (25%)	2 (7%)	1	11
40	b	74/85 (87%)	69 (93%)	5 (7%)	0	100	100
41	c	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
43	e	60/63 (95%)	57 (95%)	3 (5%)	0	100	100
44	f	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
45	g	64/70 (91%)	63 (98%)	1 (2%)	0	100	100
46	h	269/273 (98%)	259 (96%)	9 (3%)	1 (0%)	30	68
47	i	54/57 (95%)	51 (94%)	3 (6%)	0	100	100
48	j	207/209 (99%)	198 (96%)	9 (4%)	0	100	100
49	k	50/55 (91%)	50 (100%)	0	0	100	100
50	l	199/201 (99%)	190 (96%)	8 (4%)	1 (0%)	25	64
51	m	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
52	n	175/179 (98%)	162 (93%)	11 (6%)	2 (1%)	12	47
53	o	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
54	p	173/177 (98%)	161 (93%)	12 (7%)	0	100	100
55	q	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
56	r	147/149 (99%)	136 (92%)	11 (8%)	0	100	100
57	s	140/142 (99%)	135 (96%)	5 (4%)	0	100	100
58	t	121/123 (98%)	111 (92%)	10 (8%)	0	100	100
59	u	142/144 (99%)	135 (95%)	7 (5%)	0	100	100
60	v	134/136 (98%)	129 (96%)	5 (4%)	0	100	100
61	w	117/127 (92%)	107 (92%)	10 (8%)	0	100	100
62	x	114/117 (97%)	108 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
63	y	112/115 (97%)	105 (94%)	7 (6%)	0	100	100
64	z	115/118 (98%)	110 (96%)	4 (4%)	1 (1%)	14	52
All	All	9368/10486 (89%)	8607 (92%)	658 (7%)	103 (1%)	15	47

5 of 103 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	9	88	HIS
11	AA	596	ASP
11	AA	853	ASP
11	AA	859	GLU
11	AA	862	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	84/84 (100%)	78 (93%)	6 (7%)	12	32
2	1	93/93 (100%)	85 (91%)	8 (9%)	8	26
3	2	81/84 (96%)	76 (94%)	5 (6%)	15	36
4	3	84/85 (99%)	78 (93%)	6 (7%)	12	32
5	4	78/78 (100%)	74 (95%)	4 (5%)	20	41
9	9	112/123 (91%)	65 (58%)	47 (42%)	0	0
11	AA	1140/1157 (98%)	1039 (91%)	101 (9%)	8	25
12	AB	86/158 (54%)	84 (98%)	2 (2%)	45	64
13	AC	198/286 (69%)	182 (92%)	16 (8%)	9	28
13	AD	196/286 (68%)	194 (99%)	2 (1%)	73	82
14	AE	1120/1168 (96%)	1051 (94%)	69 (6%)	15	36
15	C	57/65 (88%)	55 (96%)	2 (4%)	31	51
17	E	65/66 (98%)	60 (92%)	5 (8%)	10	30
18	F	60/61 (98%)	57 (95%)	3 (5%)	20	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	G	187/199 (94%)	178 (95%)	9 (5%)	21	43
20	H	137/461 (30%)	128 (93%)	9 (7%)	14	34
21	I	171/190 (90%)	165 (96%)	6 (4%)	31	51
22	J	172/173 (99%)	165 (96%)	7 (4%)	26	47
23	K	119/126 (94%)	112 (94%)	7 (6%)	16	37
24	L	91/116 (78%)	85 (93%)	6 (7%)	14	34
25	M	124/147 (84%)	116 (94%)	8 (6%)	14	35
26	N	104/105 (99%)	102 (98%)	2 (2%)	52	69
27	O	105/107 (98%)	100 (95%)	5 (5%)	21	43
28	P	86/90 (96%)	78 (91%)	8 (9%)	7	23
29	Q	90/99 (91%)	87 (97%)	3 (3%)	33	52
30	R	101/104 (97%)	94 (93%)	7 (7%)	13	33
31	S	83/84 (99%)	79 (95%)	4 (5%)	21	43
32	T	76/77 (99%)	64 (84%)	12 (16%)	2	10
33	U	65/65 (100%)	60 (92%)	5 (8%)	10	30
34	V	74/78 (95%)	72 (97%)	2 (3%)	40	58
35	W	72/79 (91%)	68 (94%)	4 (6%)	17	38
36	X	94/96 (98%)	85 (90%)	9 (10%)	7	22
37	Y	109/110 (99%)	72 (66%)	37 (34%)	0	1
38	Z	26/85 (31%)	12 (46%)	14 (54%)	0	0
40	b	58/63 (92%)	57 (98%)	1 (2%)	56	72
41	c	67/68 (98%)	64 (96%)	3 (4%)	23	45
43	e	54/55 (98%)	53 (98%)	1 (2%)	52	69
44	f	48/49 (98%)	46 (96%)	2 (4%)	25	46
45	g	59/62 (95%)	53 (90%)	6 (10%)	6	20
46	h	216/218 (99%)	199 (92%)	17 (8%)	10	29
47	i	47/48 (98%)	41 (87%)	6 (13%)	3	14
48	j	164/164 (100%)	157 (96%)	7 (4%)	25	46
49	k	47/49 (96%)	44 (94%)	3 (6%)	14	35
50	l	165/165 (100%)	151 (92%)	14 (8%)	8	27
51	m	38/38 (100%)	35 (92%)	3 (8%)	10	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	n	148/150 (99%)	134 (90%)	14 (10%)	7	22
53	o	51/52 (98%)	46 (90%)	5 (10%)	6	21
54	p	136/138 (99%)	132 (97%)	4 (3%)	37	56
55	q	34/34 (100%)	32 (94%)	2 (6%)	16	37
56	r	114/114 (100%)	104 (91%)	10 (9%)	8	25
57	s	116/116 (100%)	110 (95%)	6 (5%)	19	40
58	t	104/104 (100%)	98 (94%)	6 (6%)	17	38
59	u	103/103 (100%)	97 (94%)	6 (6%)	17	38
60	v	109/109 (100%)	103 (94%)	6 (6%)	18	39
61	w	99/103 (96%)	91 (92%)	8 (8%)	9	28
62	x	86/87 (99%)	80 (93%)	6 (7%)	12	32
63	y	99/100 (99%)	95 (96%)	4 (4%)	27	47
64	z	89/90 (99%)	87 (98%)	2 (2%)	47	65
All	All	7791/8664 (90%)	7209 (92%)	582 (8%)	14	31

5 of 582 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
46	h	202	LEU
62	x	47	VAL
48	j	13	ARG
46	h	195	VAL
53	o	54	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
23	K	70	ASN
32	T	40	GLN
36	X	105	ASN
11	AA	1236	ASN
9	9	103	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	A	75/76 (98%)	29 (38%)	6 (8%)
10	B	75/76 (98%)	35 (46%)	6 (8%)
16	D	1515/1542 (98%)	288 (19%)	35 (2%)
39	a	2859/2904 (98%)	533 (18%)	0
42	d	119/120 (99%)	17 (14%)	0
8	7	20/33 (60%)	11 (55%)	3 (15%)
All	All	4663/4751 (98%)	913 (19%)	50 (1%)

5 of 913 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
16	D	532	A
16	D	1109	C
16	D	1493	A
16	D	562	U
16	D	793	U

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.

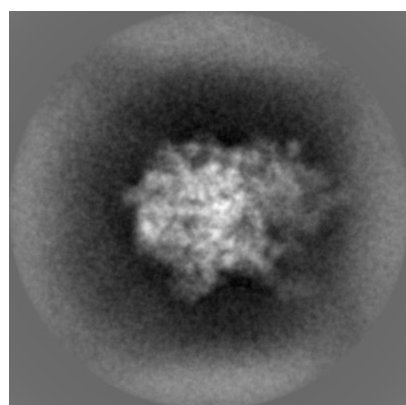
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22193. These allow visual inspection of the internal detail of the map and identification of artifacts.

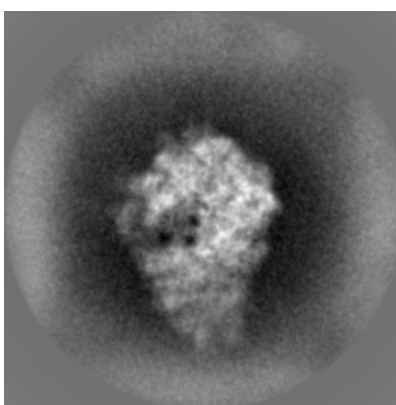
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

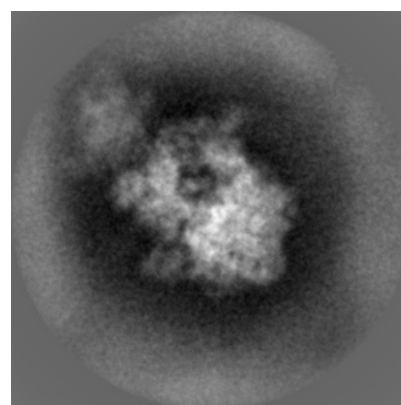
6.1.1 Primary map



X



Y

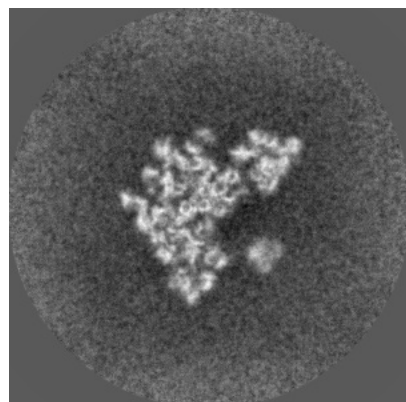


Z

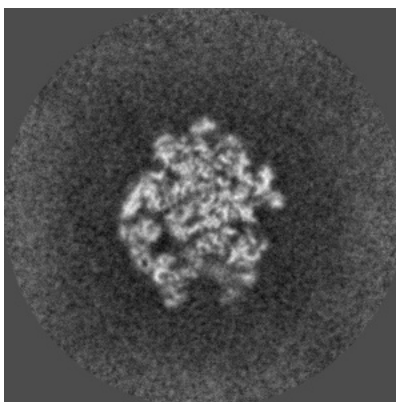
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

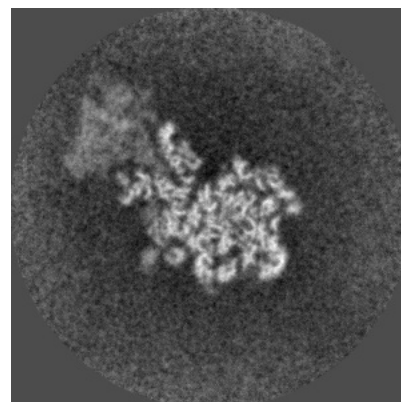
6.2.1 Primary map



X Index: 256



Y Index: 256

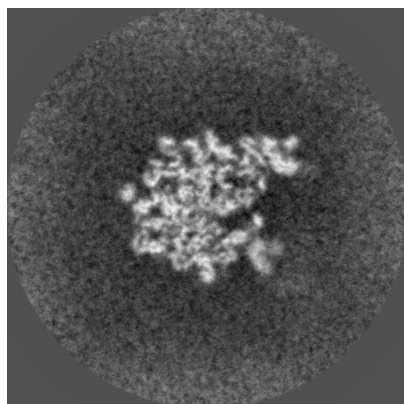


Z Index: 256

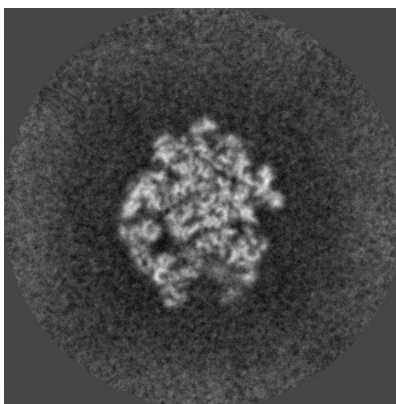
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

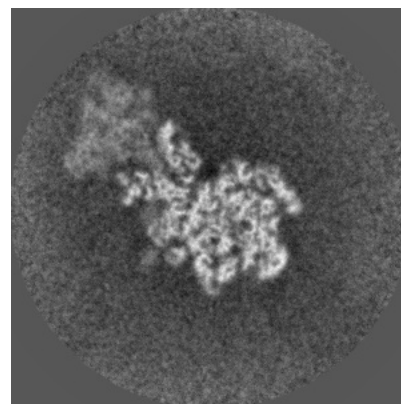
6.3.1 Primary map



X Index: 272



Y Index: 257

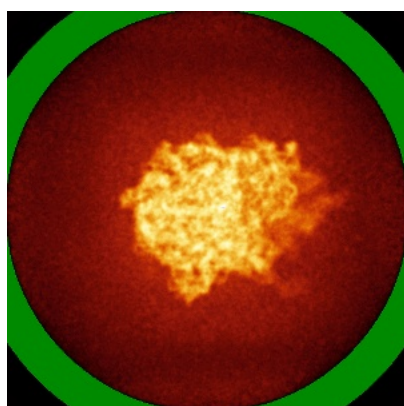


Z Index: 258

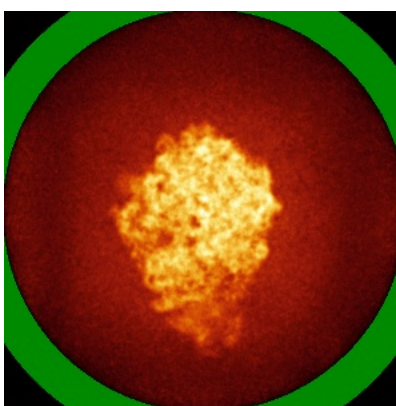
The images above show the largest variance slices of the map in three orthogonal directions.

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

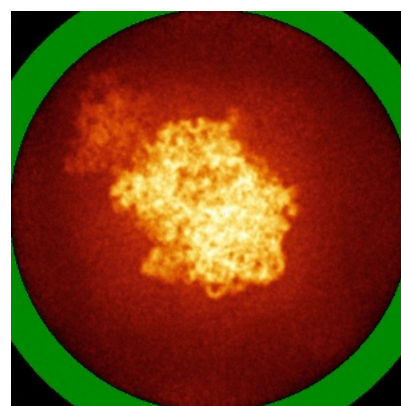
6.4.1 Primary map



X



Y

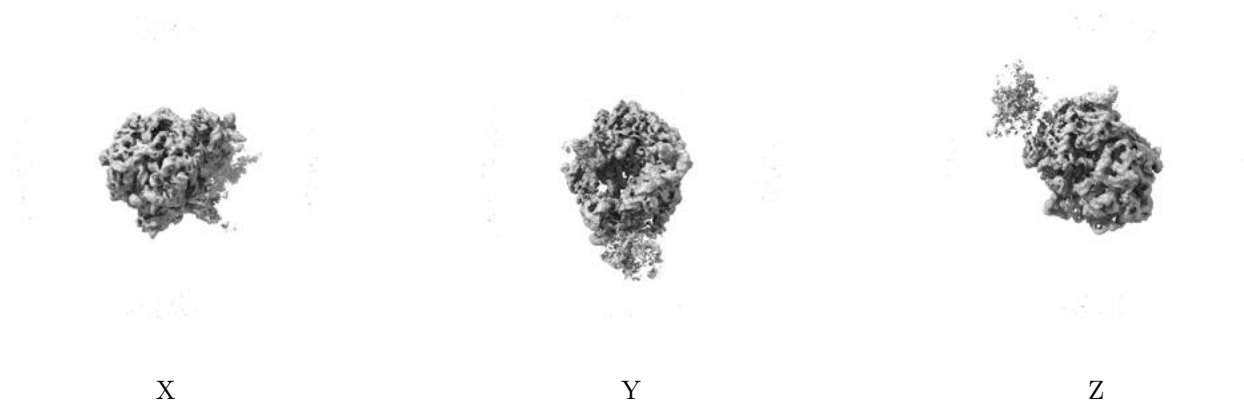


Z

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

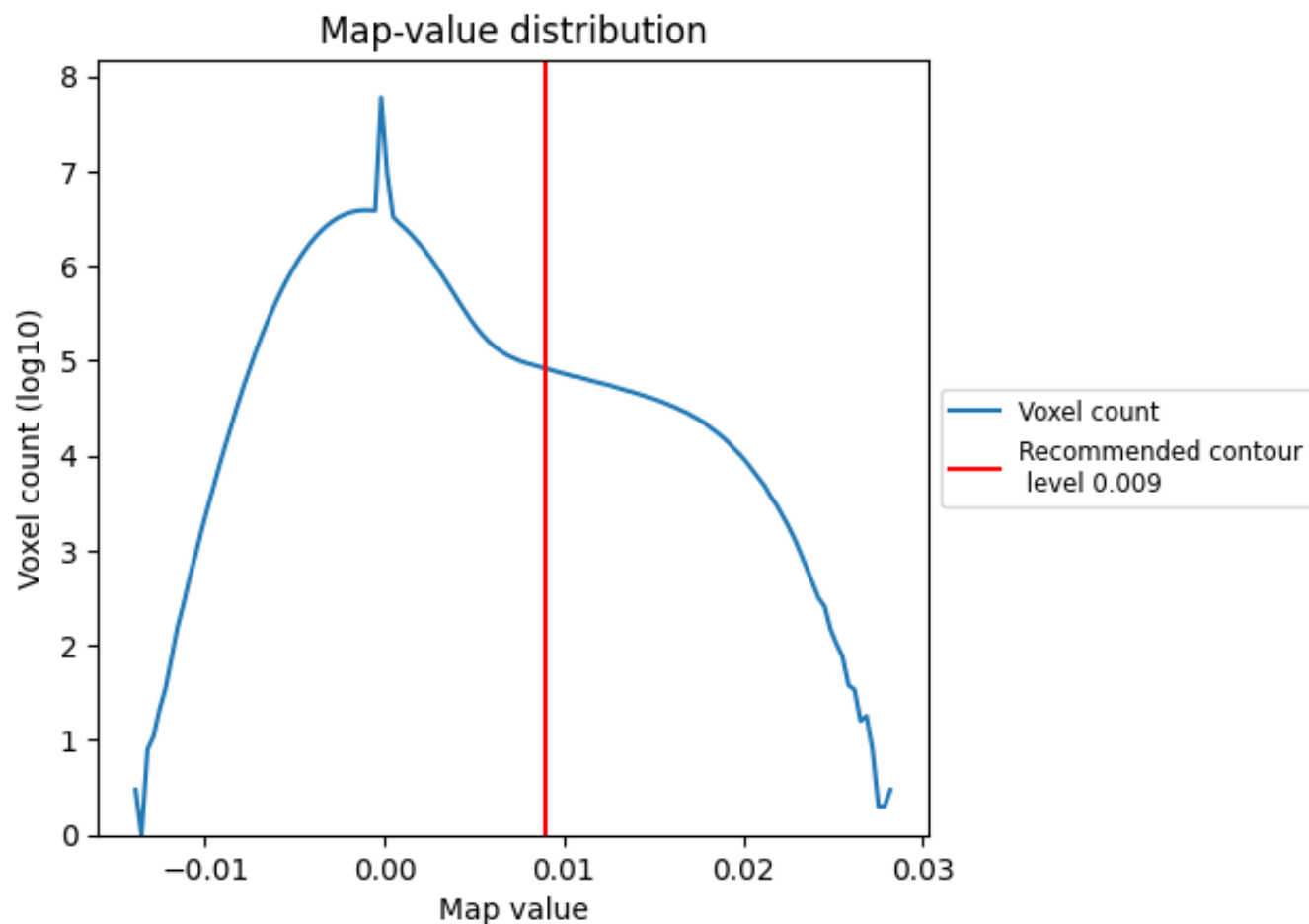
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

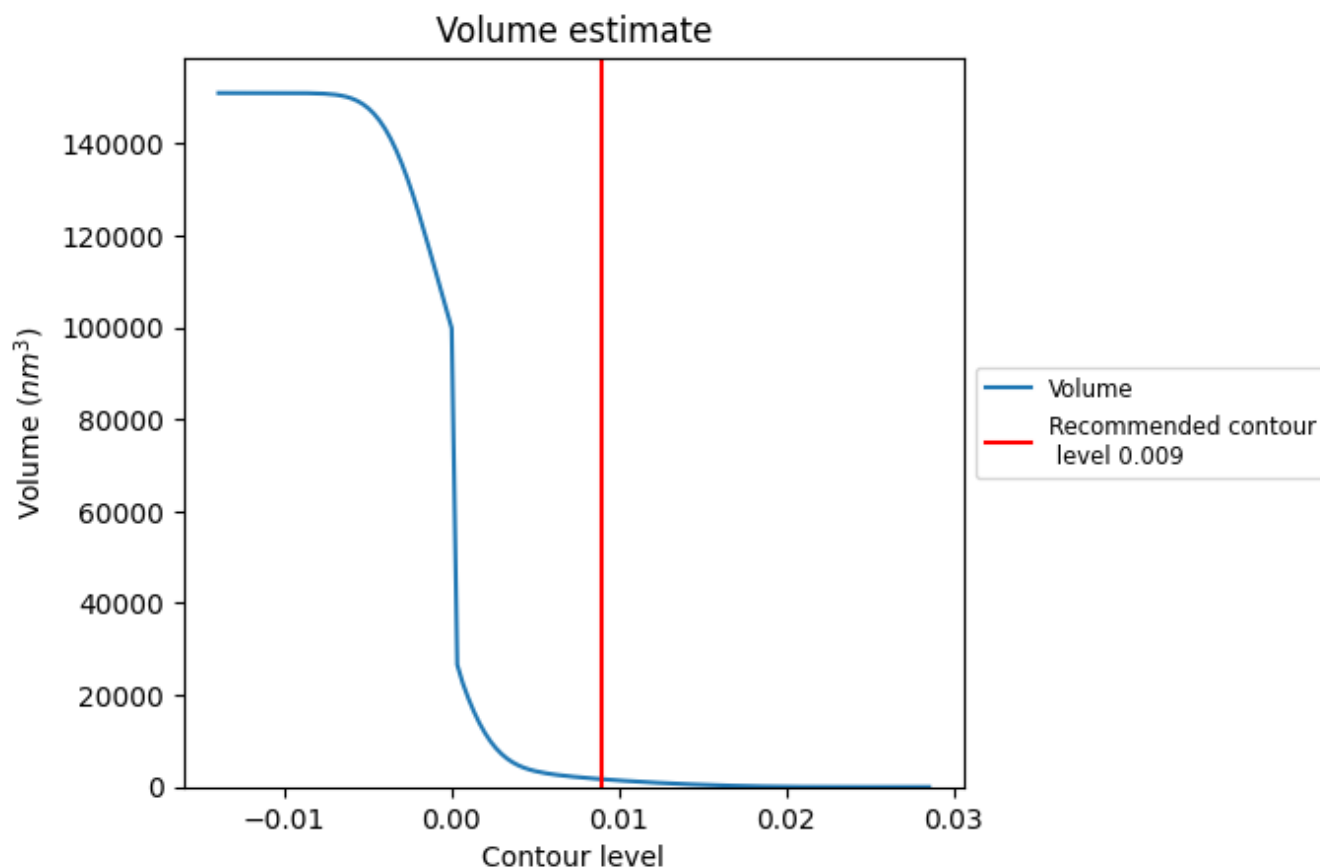
This section contains the results of statistical analysis of the map.

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.

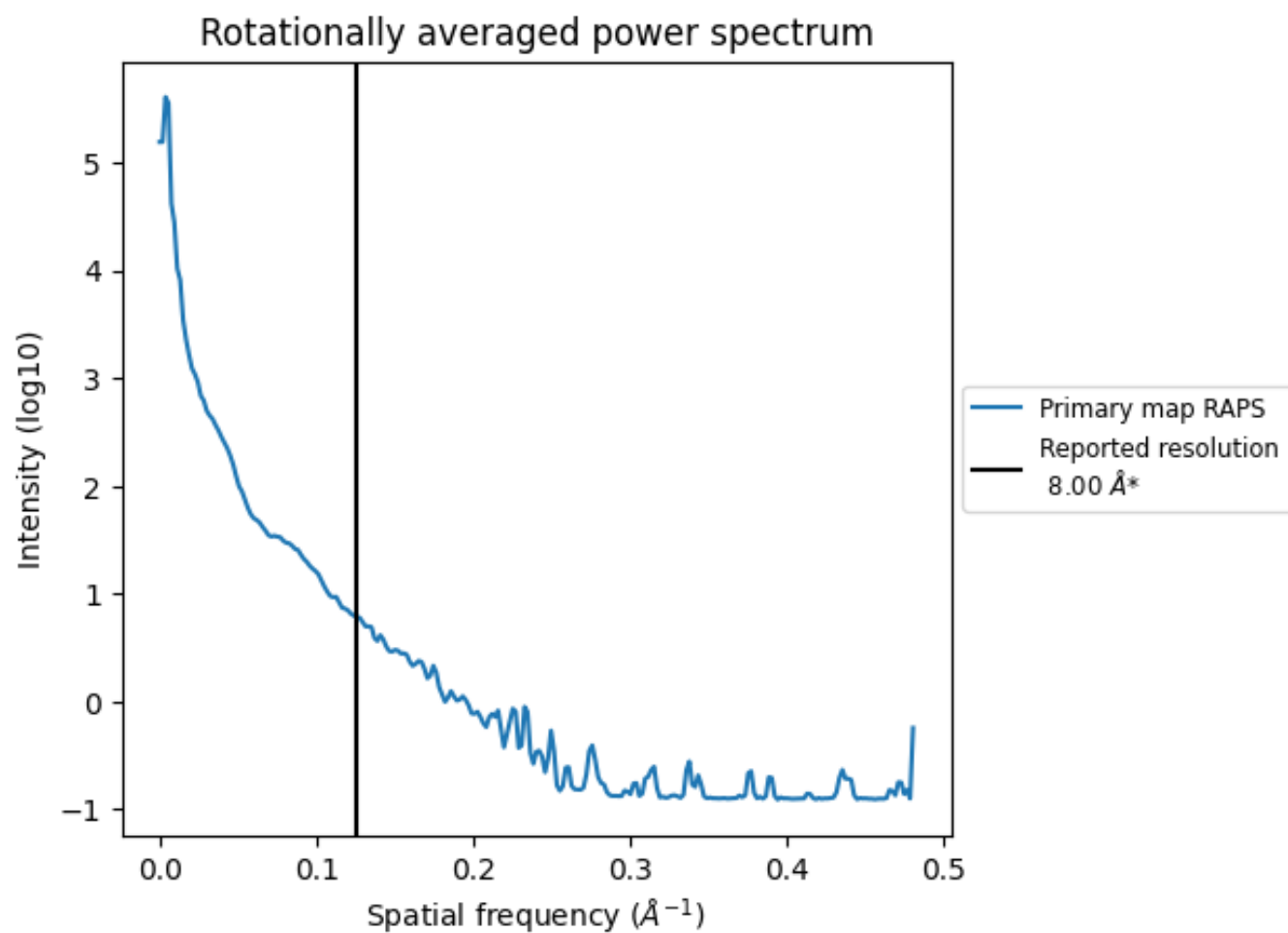
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1692 nm^3 ; this corresponds to an approximate mass of 1529 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.125 Å⁻¹

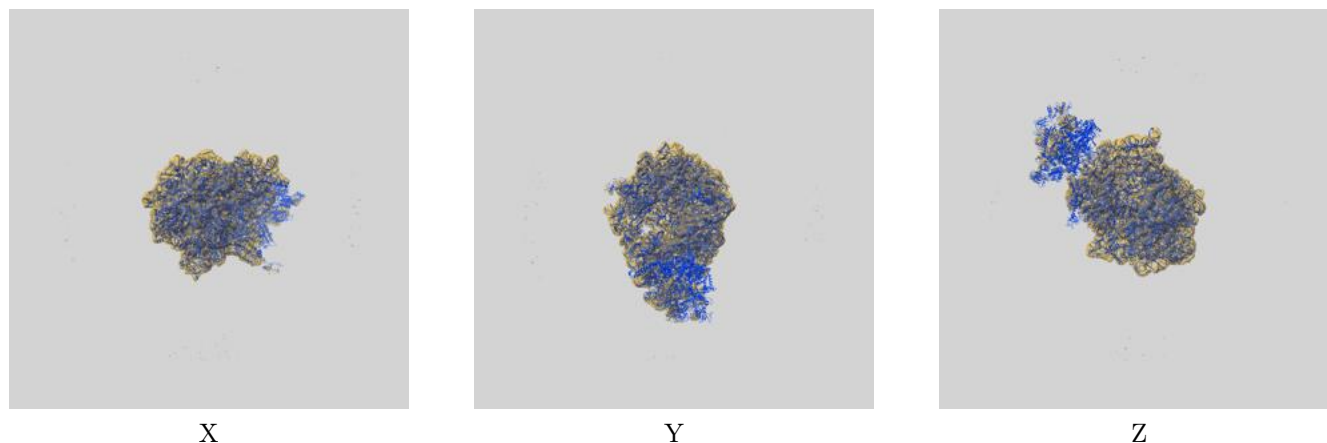
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

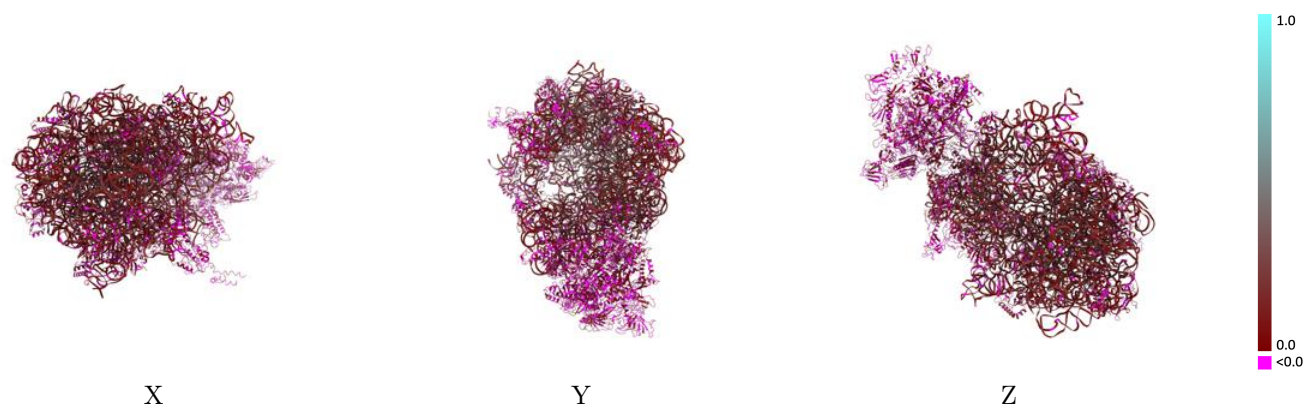
This section contains information regarding the fit between EMDB map EMD-22193 and PDB model 6XIJ. Per-residue inclusion information can be found in section 3 on page 16.

9.1 Map-model overlay [i](#)



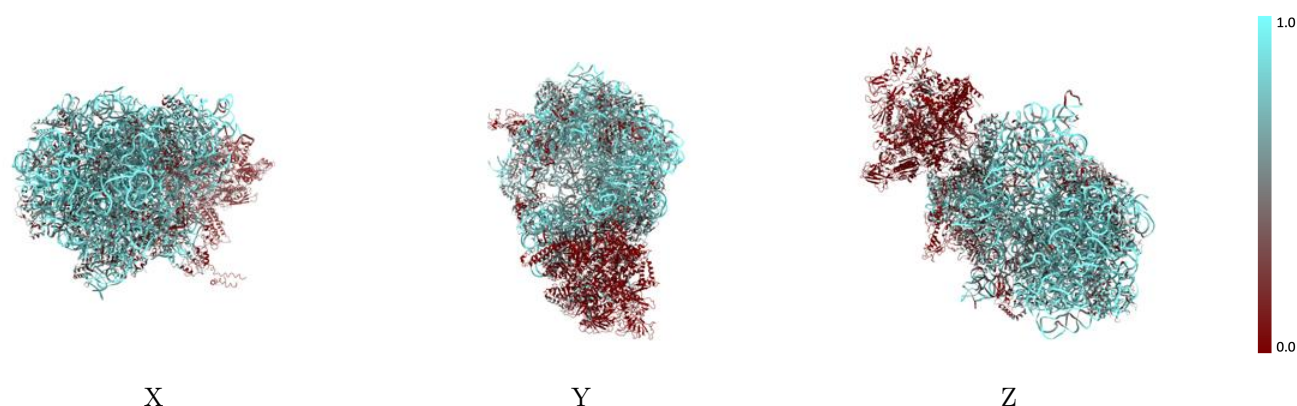
The images above show the 3D surface view of the map at the recommended contour level 0.009 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



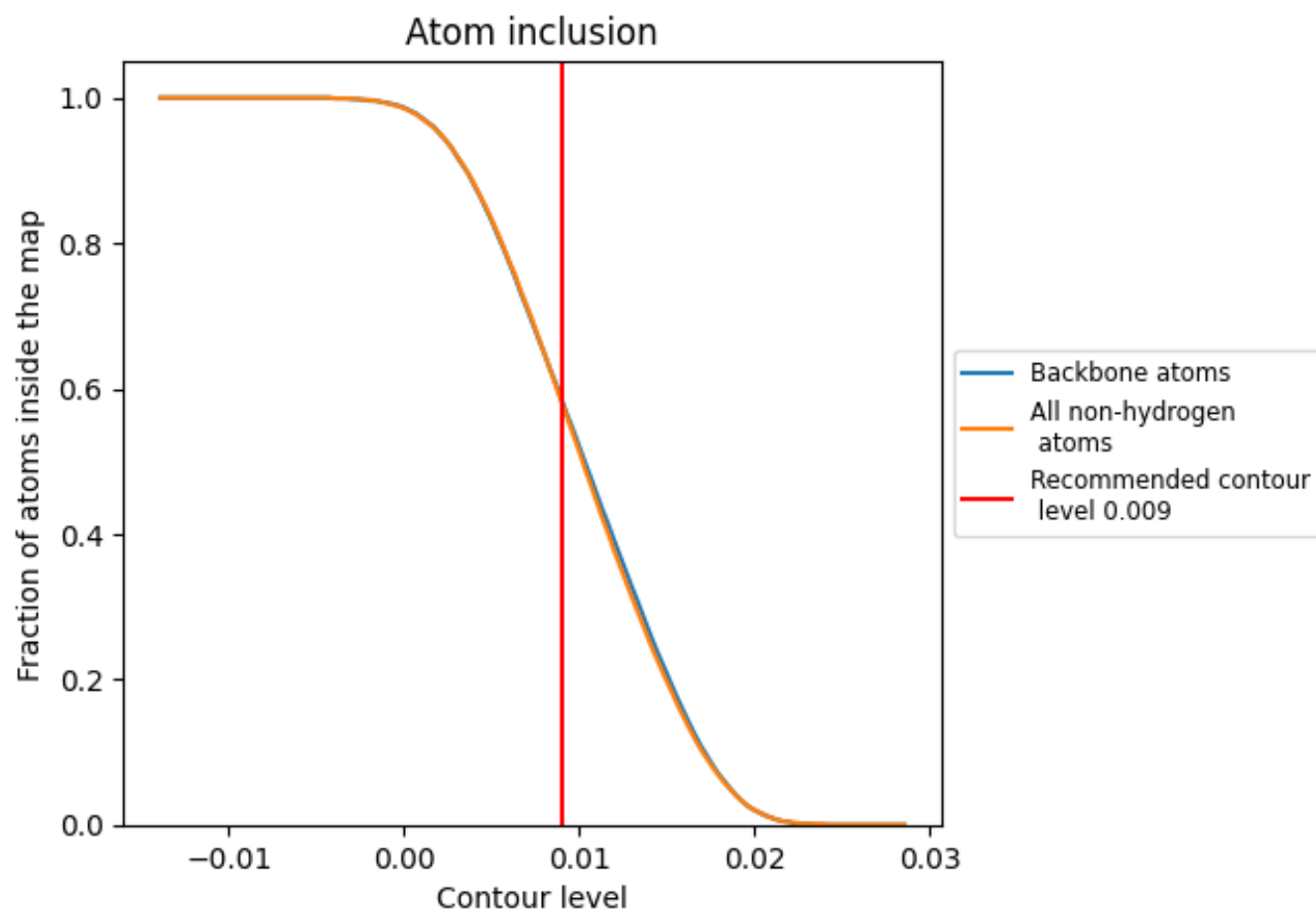
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.009).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 58% of all backbone atoms, 58% 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 (0.009) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5810	 0.1280
0	 0.5510	 0.1000
1	 0.5060	 0.1330
2	 0.4400	 0.0890
3	 0.5790	 0.0730
4	 0.5800	 0.1160
5	 0.1210	 0.0280
6	 0.1400	 0.1000
7	 0.2590	 0.0880
9	 0.2290	 0.0370
A	 0.5560	 0.1330
AA	 0.0860	 0.0410
AB	 0.0000	 0.0390
AC	 0.0320	 0.0410
AD	 0.0160	 0.0600
AE	 0.0400	 0.0400
B	 0.5320	 0.0790
C	 0.3500	 0.1010
D	 0.8240	 0.1720
E	 0.4850	 0.0870
F	 0.2930	 0.1420
G	 0.4350	 0.1050
H	 0.0090	 0.0250
I	 0.3280	 0.1090
J	 0.3930	 0.1010
K	 0.4500	 0.1640
L	 0.4100	 0.1070
M	 0.3790	 0.1060
N	 0.4760	 0.1400
O	 0.4550	 0.0520
P	 0.3900	 0.0860
Q	 0.3750	 0.1120
R	 0.3970	 0.1660
S	 0.4830	 0.0840
T	 0.4620	 0.1180



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Chain	Atom inclusion	Q-score
U	 0.4160	 0.0850
V	 0.4050	 0.1160
W	 0.3310	 0.0430
X	 0.3330	 0.0750
Y	 0.1480	 0.0260
Z	 0.0440	 -0.0080
a	 0.8350	 0.1690
b	 0.4810	 0.0860
c	 0.4340	 0.1150
d	 0.8100	 0.1230
e	 0.5730	 0.0600
f	 0.5640	 0.1240
g	 0.2740	 0.0540
h	 0.4110	 0.1200
i	 0.5370	 0.1230
j	 0.4830	 0.0970
k	 0.4040	 0.0760
l	 0.4730	 0.1080
m	 0.4960	 0.1650
n	 0.3960	 0.0630
o	 0.3320	 0.0950
p	 0.3920	 0.0600
q	 0.3730	 0.0550
r	 0.2230	 0.0860
s	 0.4820	 0.1030
t	 0.2540	 0.1020
u	 0.4560	 0.1060
v	 0.4300	 0.1080
w	 0.5850	 0.0980
x	 0.5050	 0.0500
y	 0.3040	 0.0980
z	 0.5670	 0.1230