



wwPDB EM Validation Summary Report ⓘ

Mar 29, 2026 – 09:51 PM UTC

PDB ID : 6XIJ / pdb_00006xij
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:

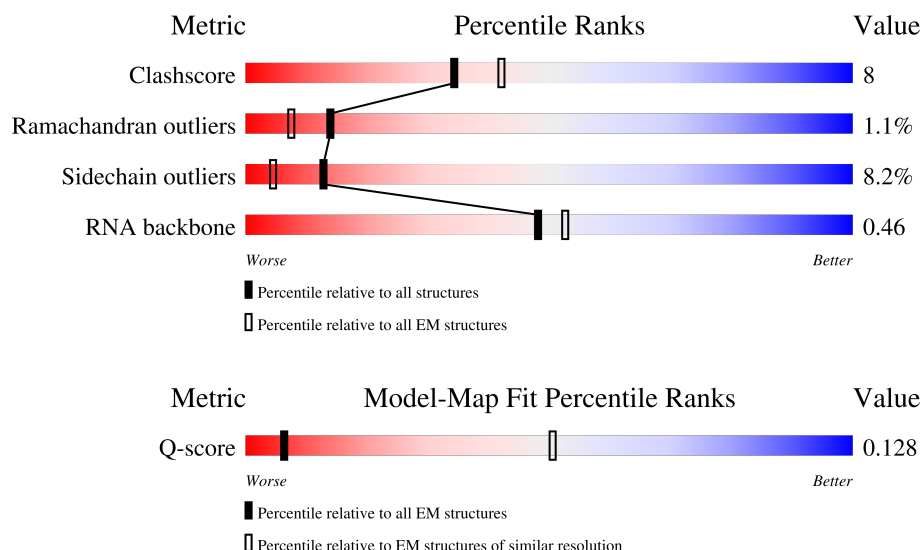
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	361 (7.50 - 8.50)

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	36% 84% 15% .
2	1	110	36% 75% 25%
3	2	100	41% 84% 8% 6%

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Mol	Chain	Length	Quality of chain
4	3	104	
5	4	94	
6	5	36	
7	6	36	
8	7	33	
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	

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Mol	Chain	Length	Quality of chain
27	O	130	
28	P	103	
29	Q	129	
30	R	124	
31	S	101	
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	

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Mol	Chain	Length	Quality of chain
52	n	179	
53	o	65	
54	p	177	
55	q	38	
56	r	149	
57	s	142	
58	t	123	
59	u	144	
60	v	136	
61	w	127	
62	x	117	
63	y	115	
64	z	118	

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 (CCD ID: MG) (formula: Mg).

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

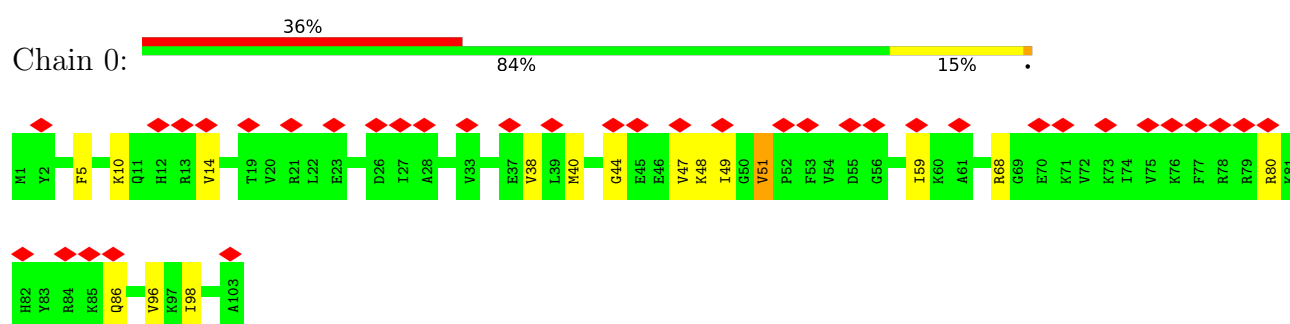
- Molecule 66 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

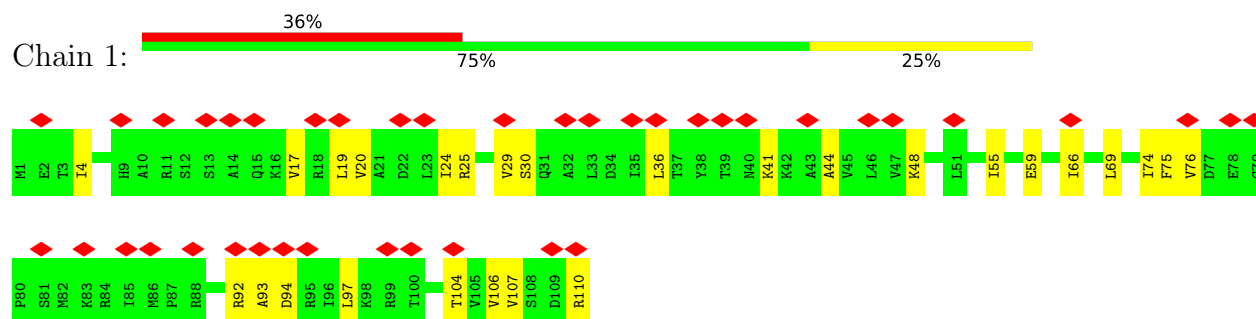
3 Residue-property plots [i](#)

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.

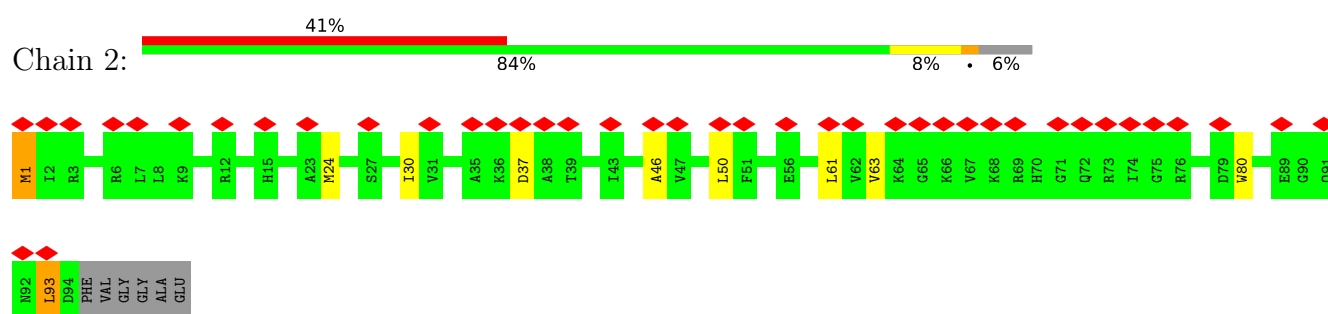
- Molecule 1: 50S ribosomal protein L21



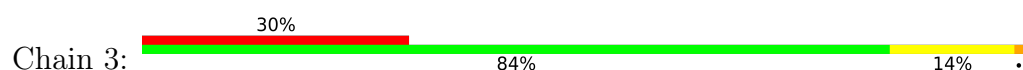
- Molecule 2: 50S ribosomal protein L22

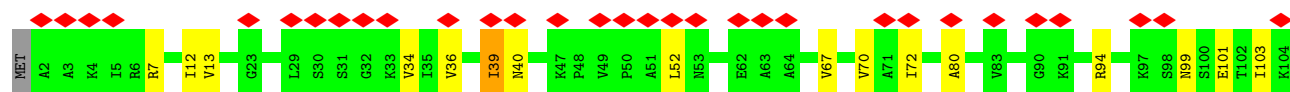


- Molecule 3: 50S ribosomal protein L23

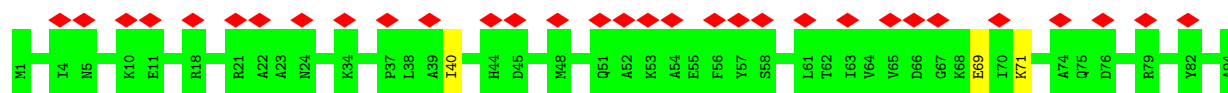


- Molecule 4: 50S ribosomal protein L24

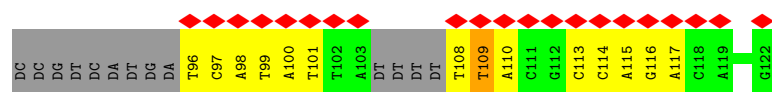
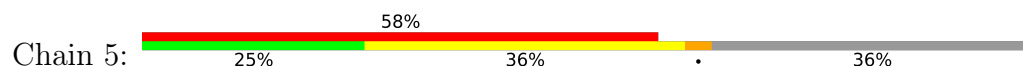




- Molecule 5: 50S ribosomal protein L25



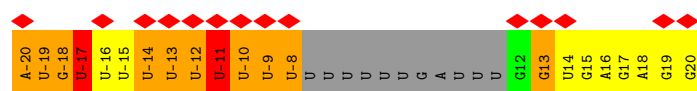
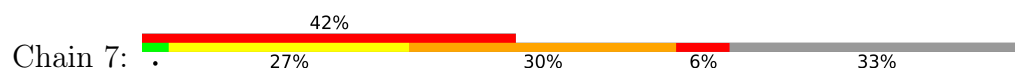
- Molecule 6: NT DNA



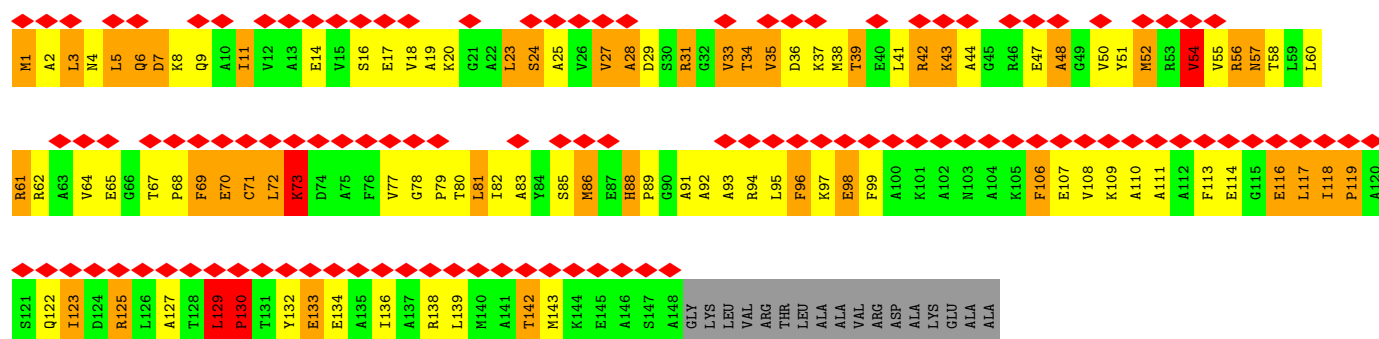
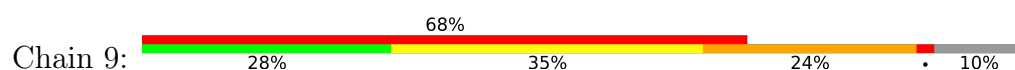
- Molecule 7: T DNA



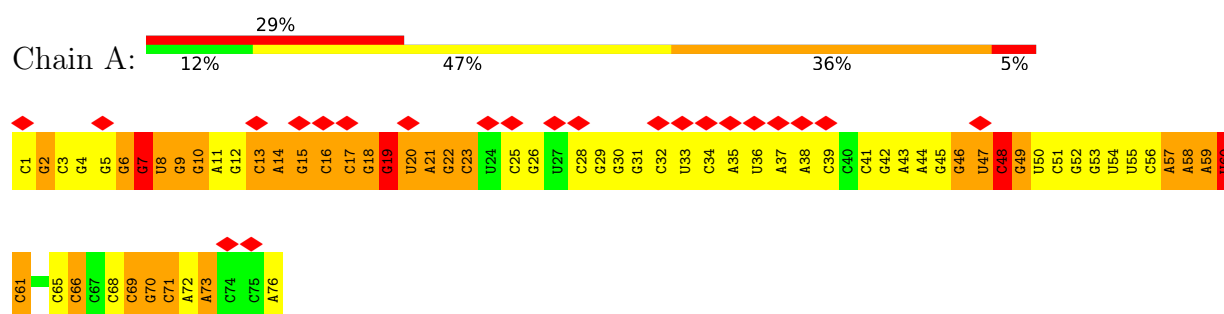
- Molecule 8: mRNA with 24 nt long spacer



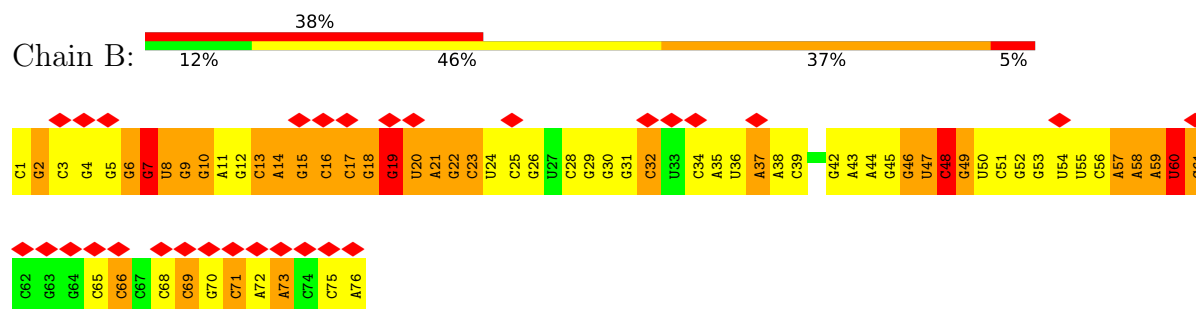
- Molecule 9: 50S ribosomal protein L10



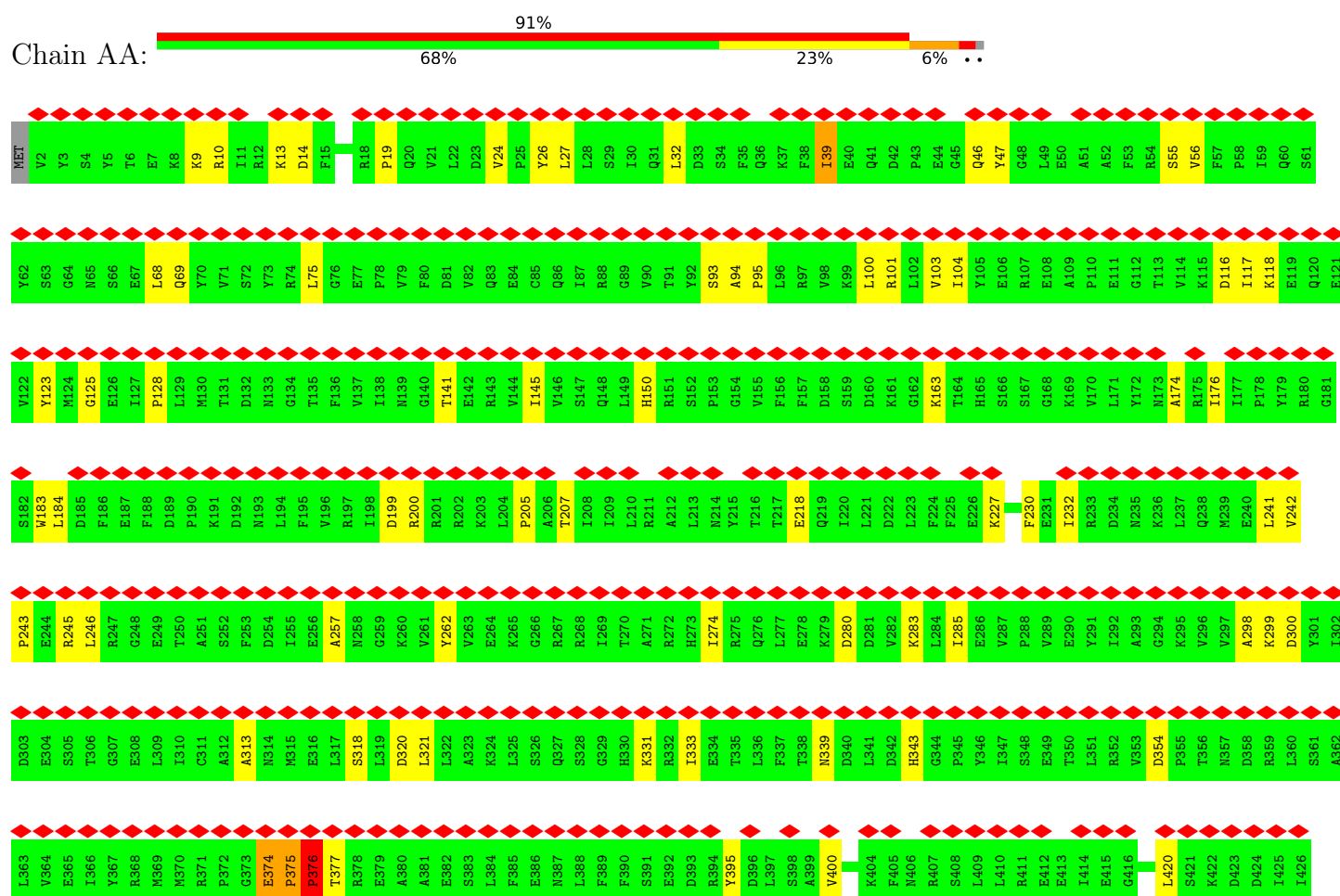
- Molecule 10: E-site and P-site tRNA (fMet)



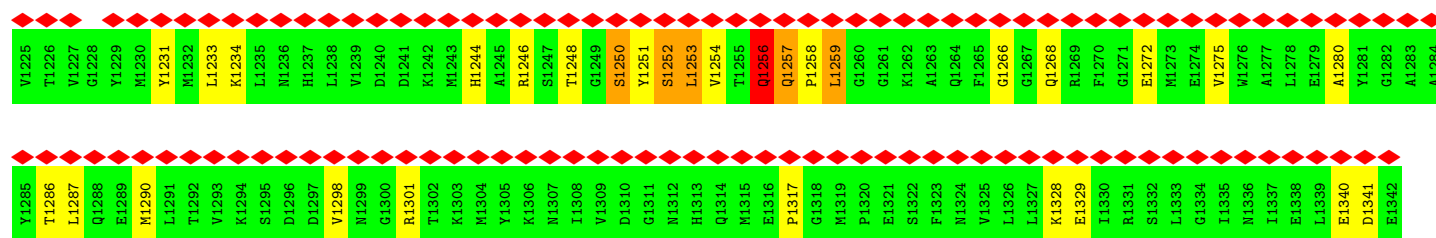
• Molecule 10: E-site and P-site tRNA (fMet)



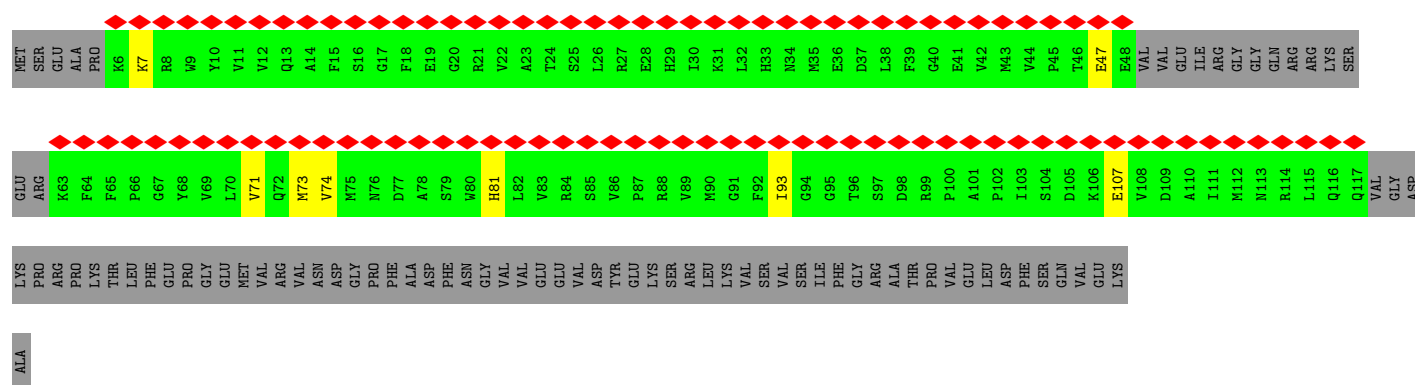
• Molecule 11: DNA-directed RNA polymerase subunit beta



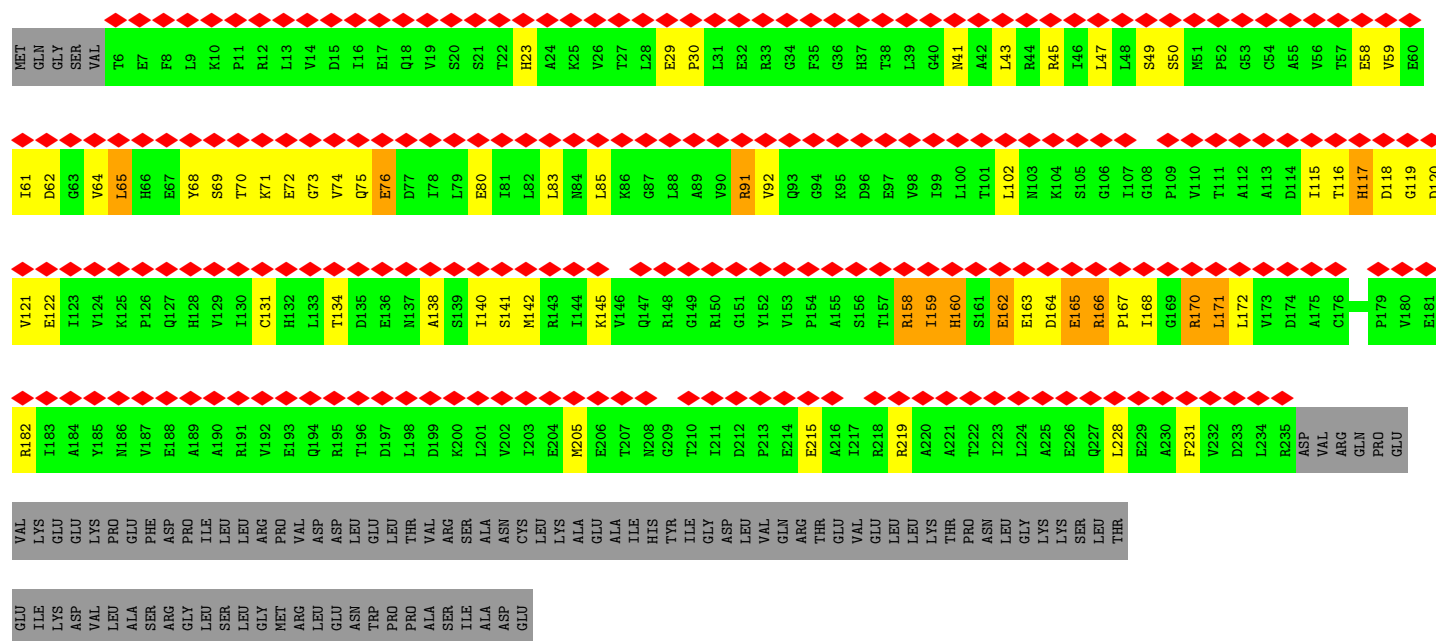
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E1167	V1046	A886	G926	P806	A746	M885	A619	D549	P489	M429
E1168	L1047	E887	T927	M807	G747	Q686	M620	V550	Q490	K430
V1169	K1048	K888	V928	N808	T748	R687	S621	H551	D491	K431
M1170	I1109	L889	V929	G809	D749	Q688	M622	P552	M492	L432
R1171	G1110	D990	D930	H810	T750	A689	L623	T553	I493	I433
L1172	K1051	K991	V931	N811	T751	V690	D624	H554	N494	D434
A1173	V1052	L992	Q932	F812	N752	P691	E625	Y555	A495	I435
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G1179	R1058	L998	Q938	V818	Y758	K697	D632	I562	A501	V441
M1180	R1059	E999	V939	S819	T759	P698	L633	T563	V502	V442
P1181	I1060	L1000	E940	E820	N760	L699	V634	P564	K503	D443
I1182	Q1061	G1001	R941	R821	Q761	T701	T635	E565	E504	D444
A1183	P1062	L1002	D942	V822	N762	T702	C636	G566	F505	I445
T1184	G1063	T1003	X943	V623	T763	G703	R637	P567	F506	I446
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V1186	K1065	E1005	A945	E825	T765	E705	K639	N568	L448	L448
D1126	M1066	L946	L946	D826	N766	E706	G640	I569	S508	G449
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A1130	Q1070	R890	E950	T630	C770	A709	L644	S574	Q513	I453
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L1132	M1072	THR	R953	H832	T772	G713	S646	S576	M515	S455
K1133	K1073	GLN	L954	T633	L773	V714	R647	V577	D516	V456
Q1134	G1074	LEU	K954	Q834	G774	T715	D648	Y578	Q517	G457
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V1138	K1078	LYS	K958	C838	E778	A719	S656	Y584	L521	E461
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L1201	M1080	LEU	L960	S840	G780	G721	Q659	F586	E523	Q463
G1202	P1081	ARG	S961	R841	D781	G722	Q659	L587	I524	F464
D1203	I1082	ALA	T962	D842	L782	V723	V661	E588	T525	R465
L1204	E1083	PHE	E963	T843	A784	V724	S662	K593	V526	V466
P1205	D1084	GLY	L964	K944	D785	Q725	V663	V594	K527	G467
T1206	F1025	LYS	Q965	L845	T786	T726	G664	T595	R528	L468
S1207	E1026	ALA	L966	G846	G787	V727	A665	D596	R529	V469
G1208	K1027	S911	L967	P847	F788	D728	S666	D601	I530	R470
Q1209	E1028	D912	E968	E848	T789	A729	L667	E602	S531	V471
I1210	L1029	V913	A969	E849	T790	S730	I668	I603	A532	E472
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L1212	A1031	D915	L971	T851	G792	I732	D674	Y605	G534	A474
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V1159	T1037	P921	A977	V857	G797	E738	A679	E611	E541	S480
D1160	V1097	N922	V978	G858	Q798	D739	L680	G811	G542	L481
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S1162	G1039	V960	V960	A860	M600	T741	G682		G544	L484
T1163	P1100	A981	G982	A861	R601	Y742			E545	D485
F1164	L1101	G982	G983	L862	V602	P743				T486
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• Molecule 12: Transcription termination/antitermination protein NusG



• Molecule 13: DNA-directed RNA polymerase subunit alpha

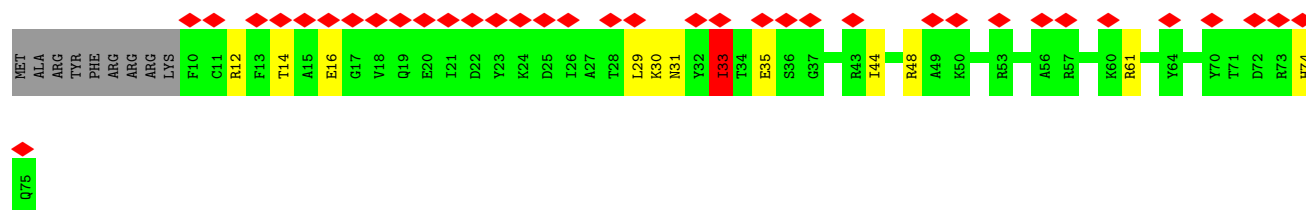
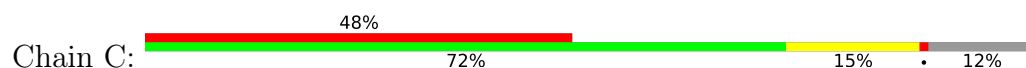


• Molecule 13: DNA-directed RNA polymerase subunit alpha

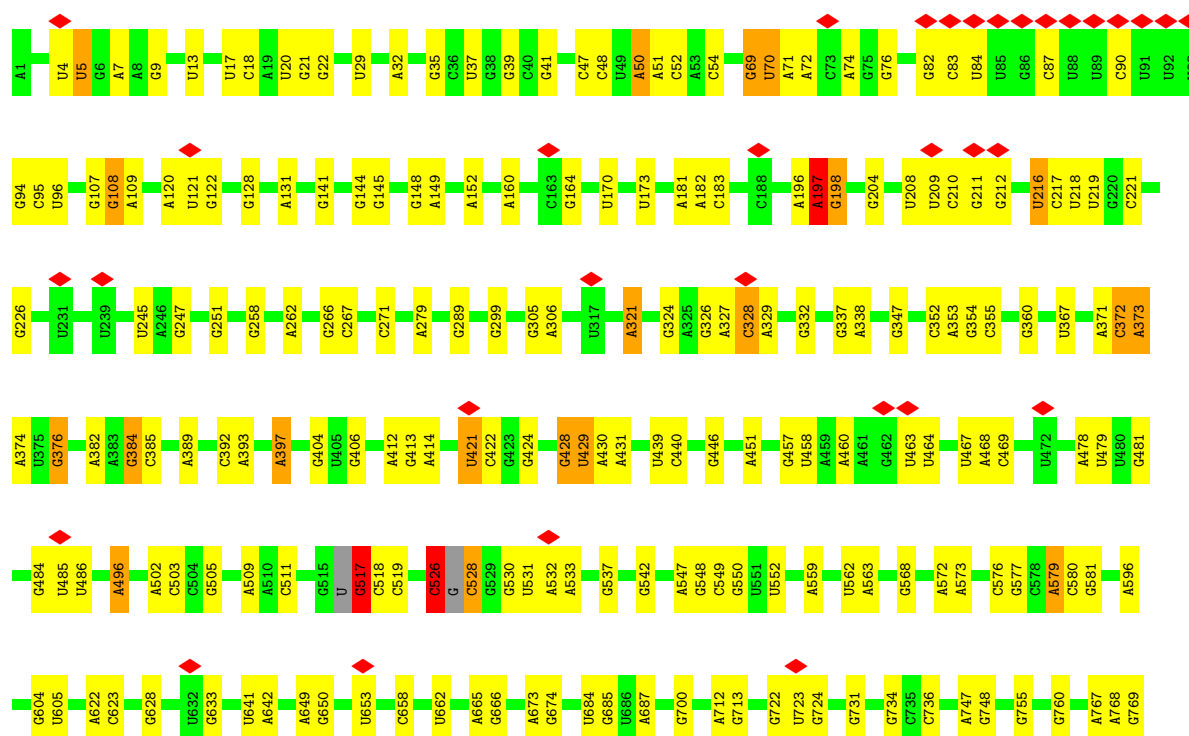


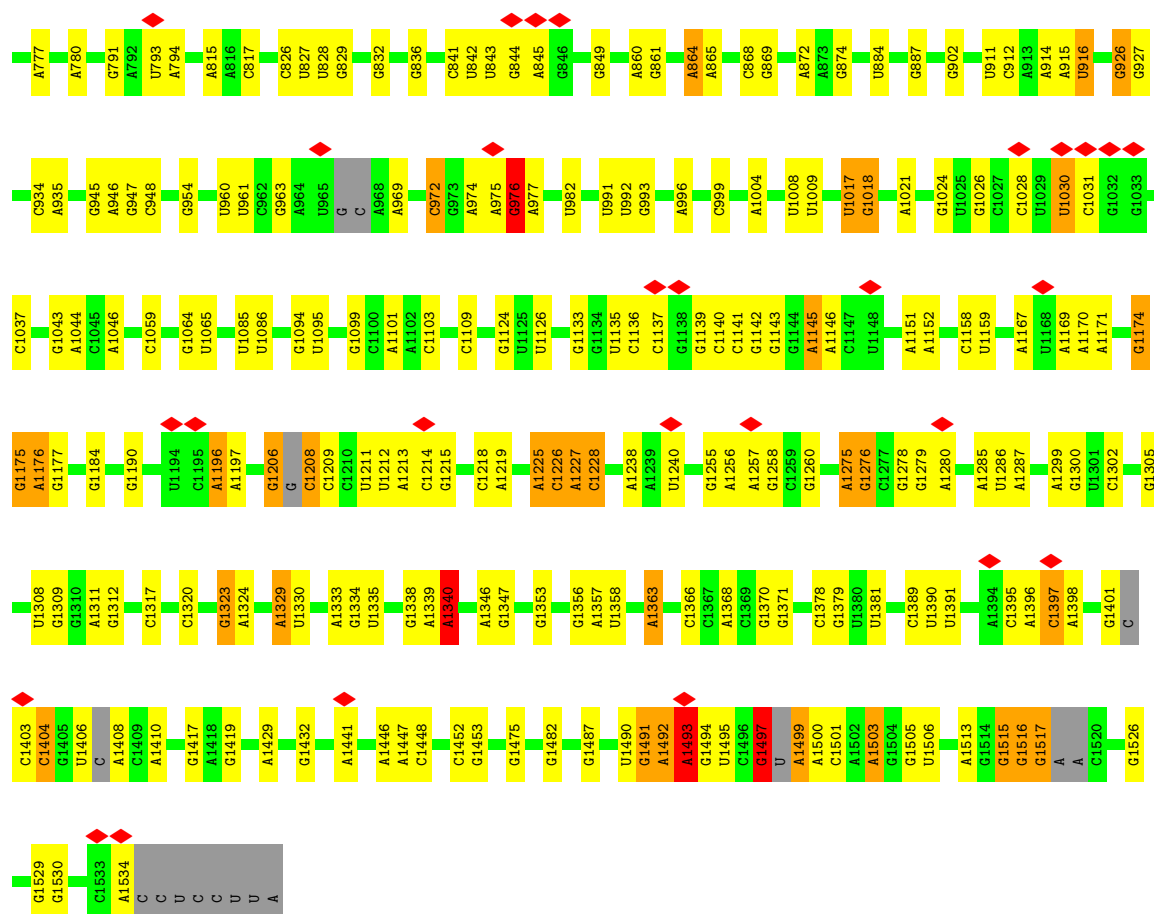
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G1033	F1034	V1035	R1036	F1037	T1038	D1039	M1040	T1041	L1042	G1043	Q1044	T1045	I1046	T1047	R1048	G1049	T1050	D1051	E1052	L1053	T1054	G1055	L1056	S1057	S1058	L1059	V1060	V1061	L1062	D1063	S1064	A1065	E1066	R1067	T1068	A1069	G1070	G1071	K1072	D1073	L1074	R1075	P1076	A1077	L1078	K1079	I1080	D1082	A1083	Q1084	G1085	N1086	D1087	V1088	L1089	P1091	G1092						
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- Molecule 15: 30S ribosomal protein S18

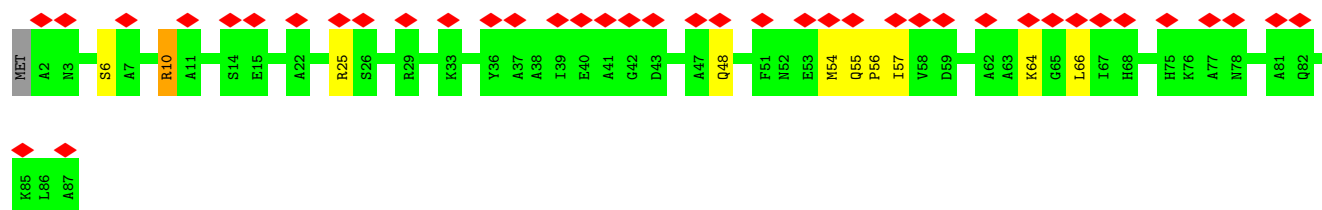
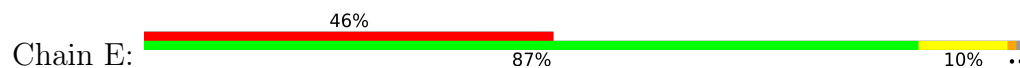


- Molecule 16: 16S rRNA

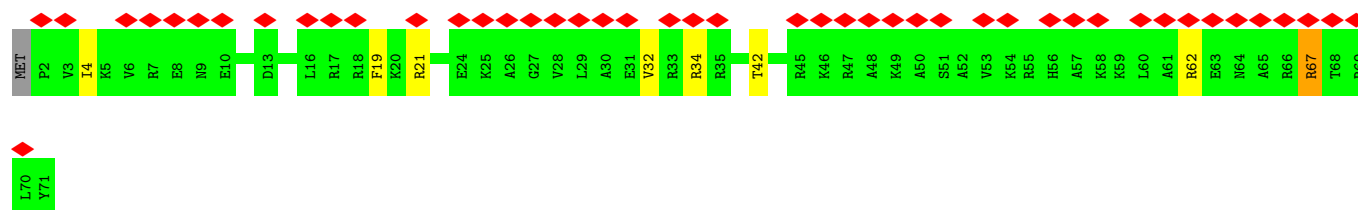
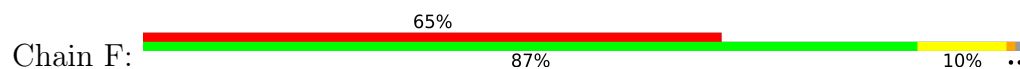




• Molecule 17: 30S ribosomal protein S20

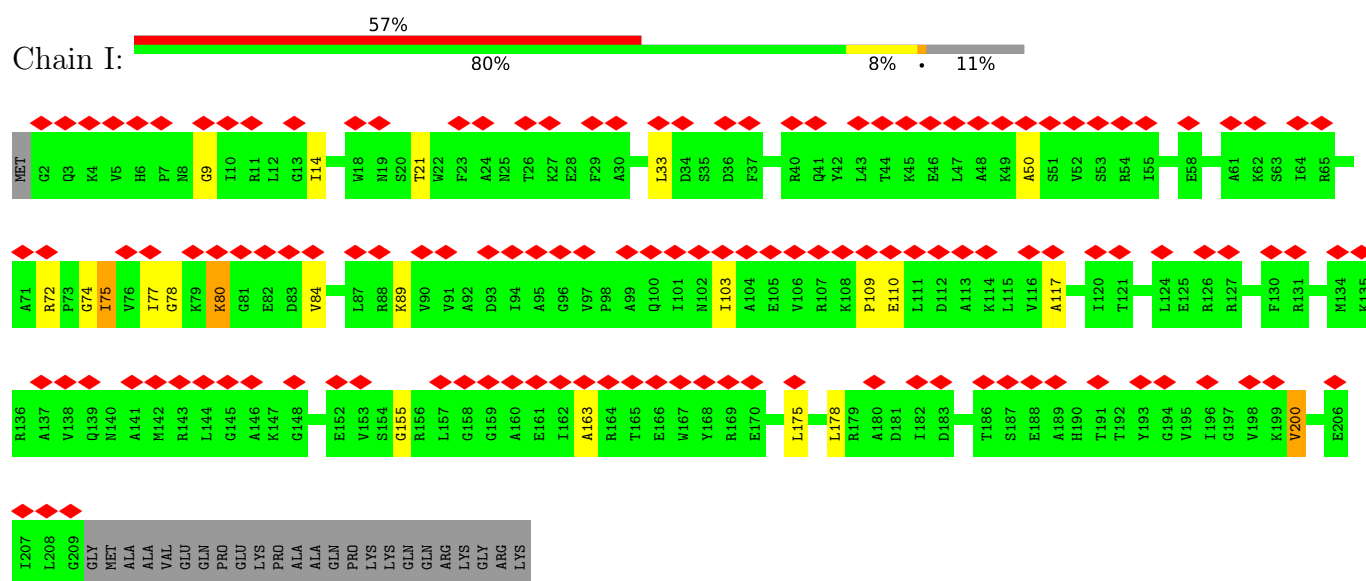


• Molecule 18: 30S ribosomal protein S21

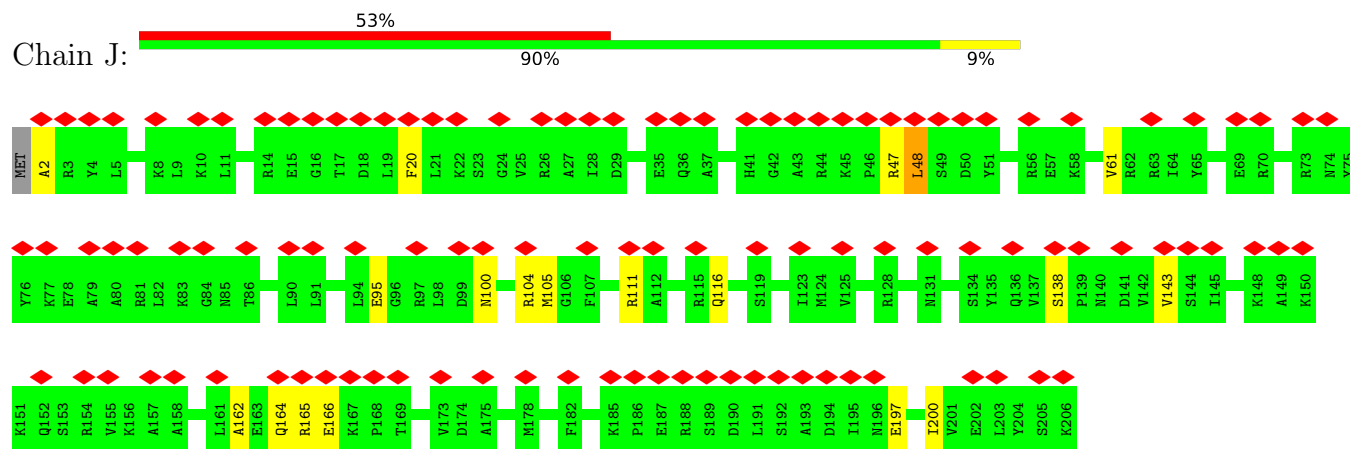


• Molecule 19: 30S ribosomal protein S2

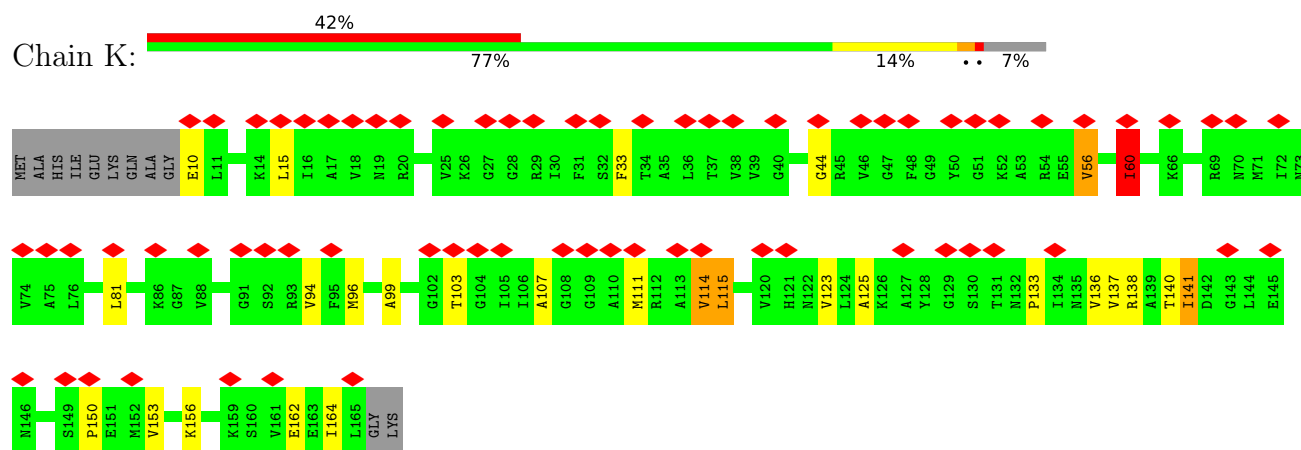




- Molecule 22: 30S ribosomal protein S4

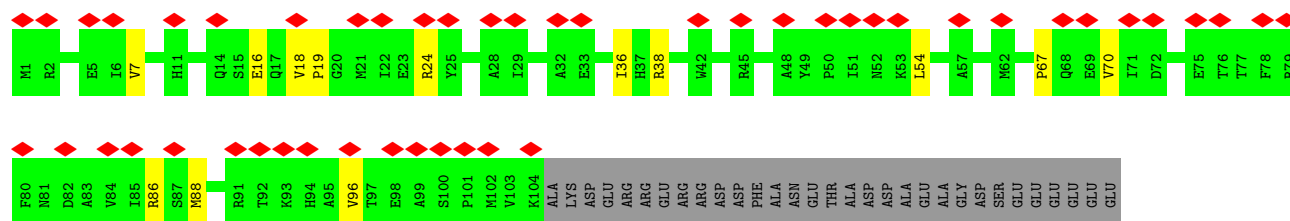


- Molecule 23: 30S ribosomal protein S5

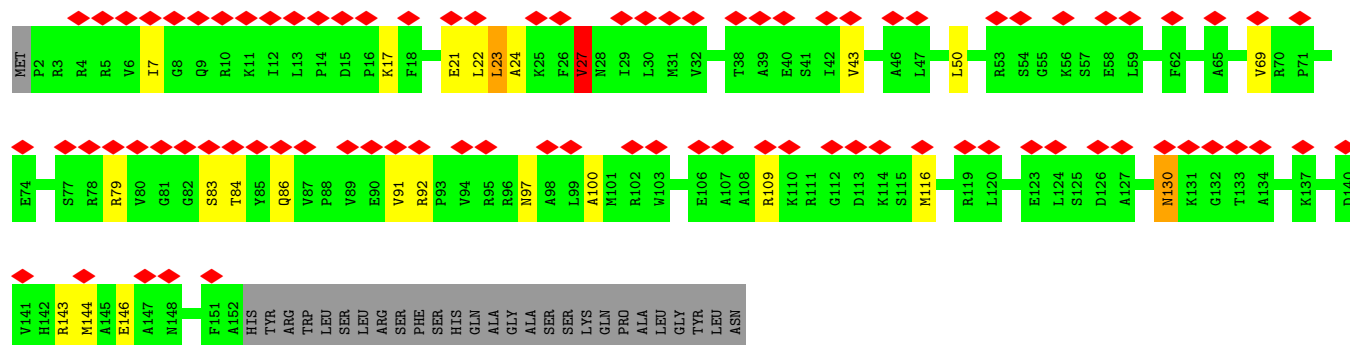


- Molecule 24: 30S ribosomal protein S6

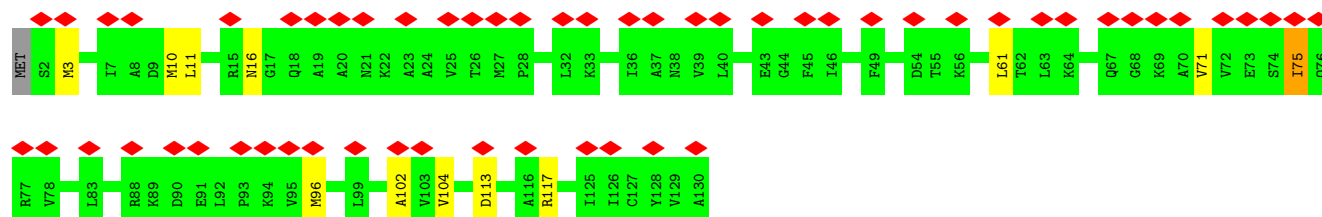
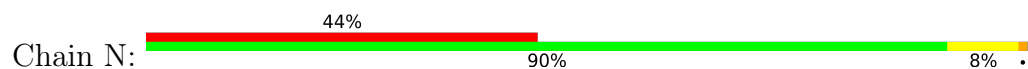




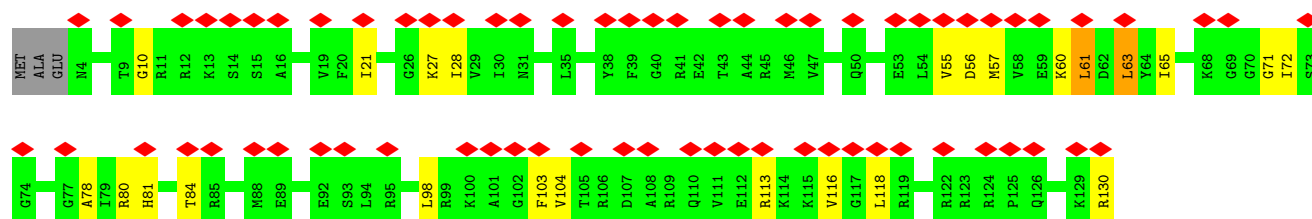
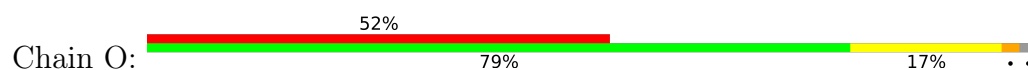
• Molecule 25: 30S ribosomal protein S7



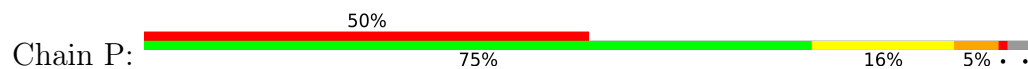
• Molecule 26: 30S ribosomal protein S8

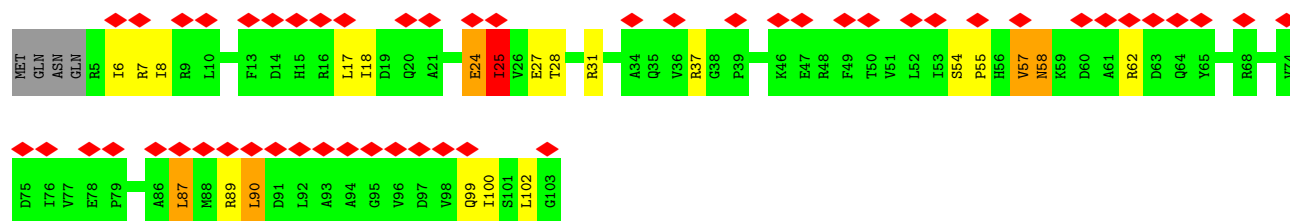


• Molecule 27: 30S ribosomal protein S9

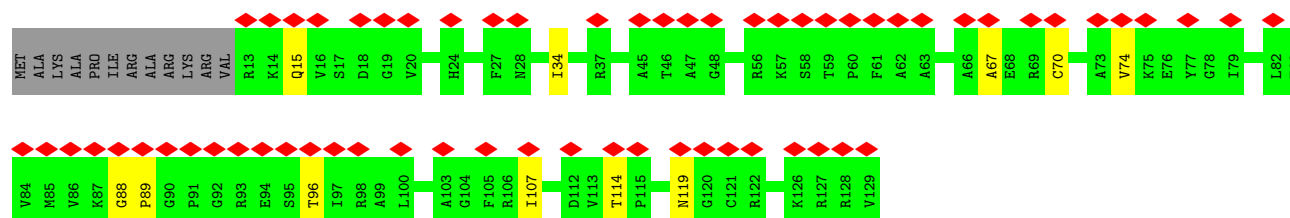
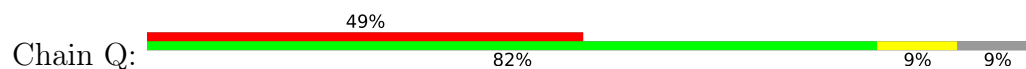


• Molecule 28: 30S ribosomal protein S10

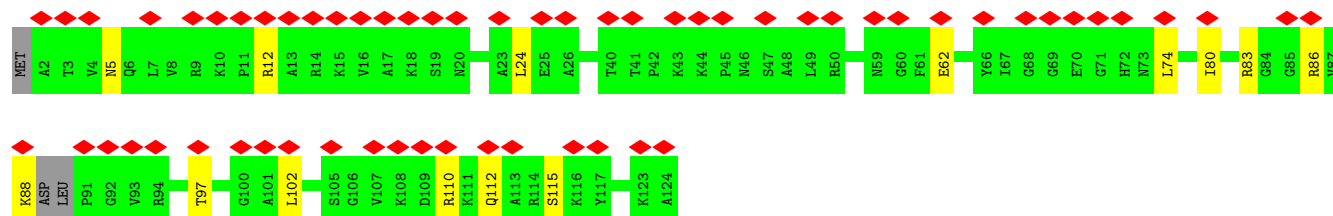
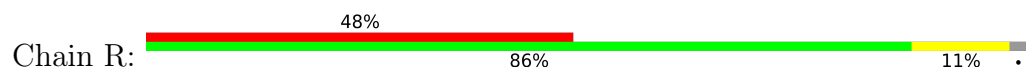




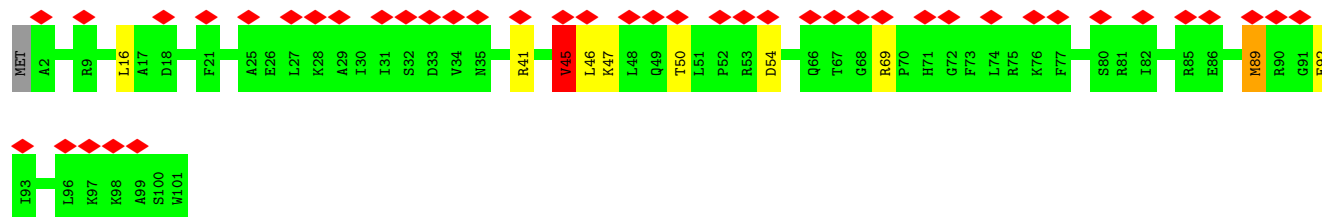
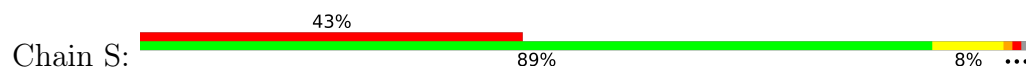
- Molecule 29: 30S ribosomal protein S11



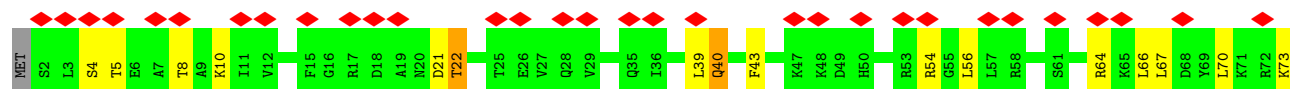
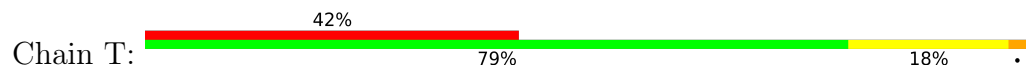
- Molecule 30: 30S ribosomal protein S12

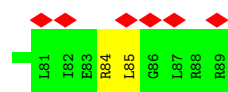


- Molecule 31: 30S ribosomal protein S14

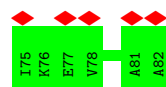
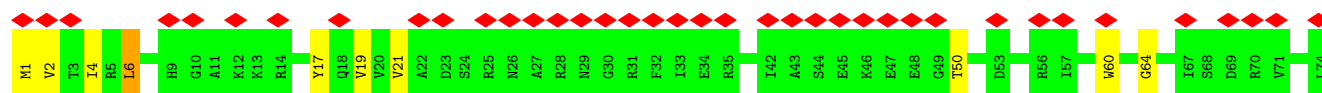
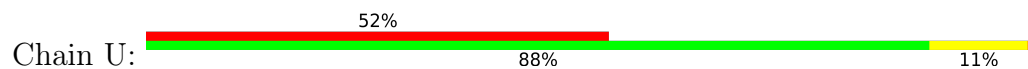


- Molecule 32: 30S ribosomal protein S15

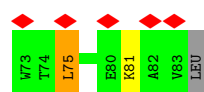
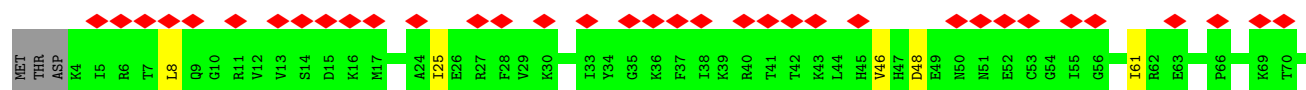
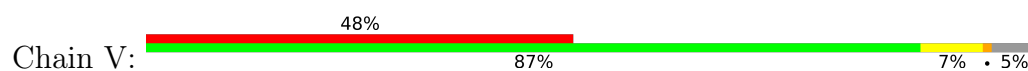




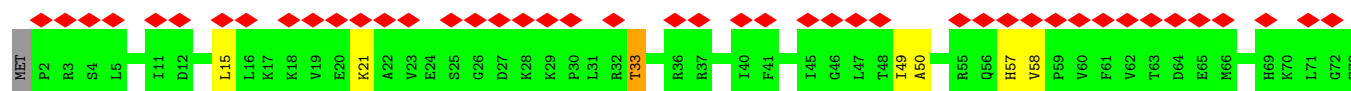
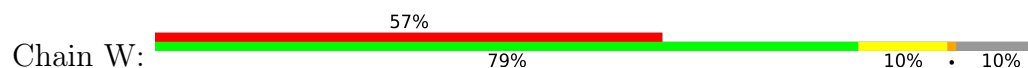
- Molecule 33: 30S ribosomal protein S16



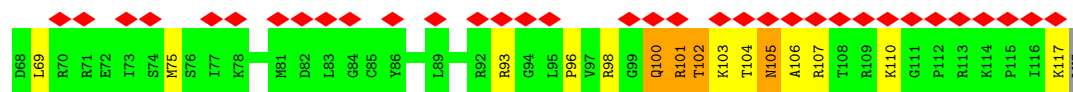
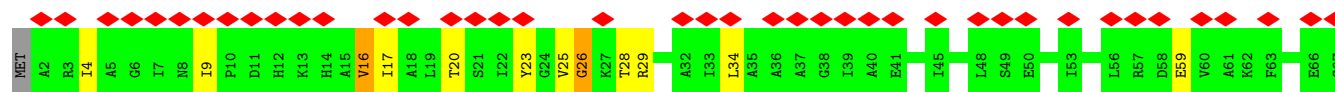
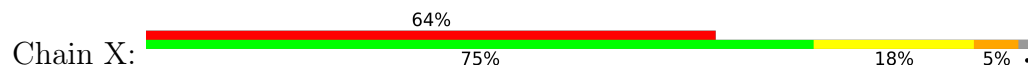
- Molecule 34: 30S ribosomal protein S17



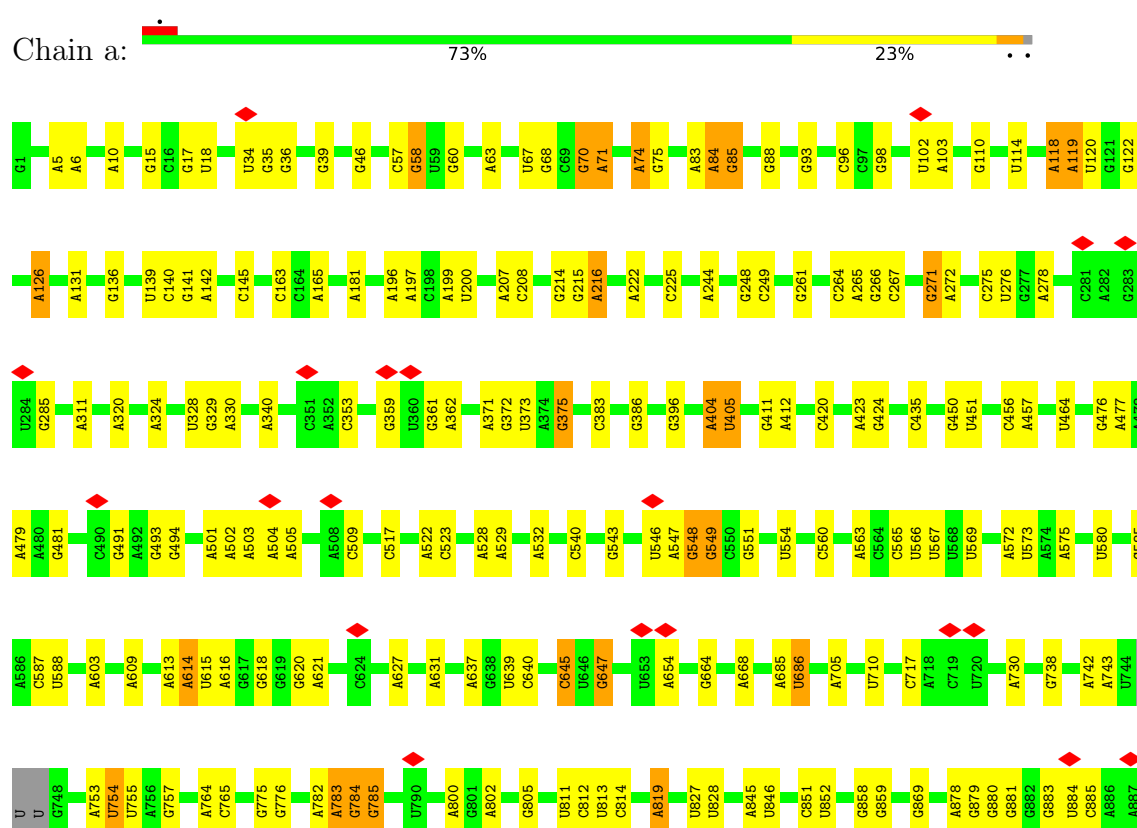
- Molecule 35: 30S ribosomal protein S19

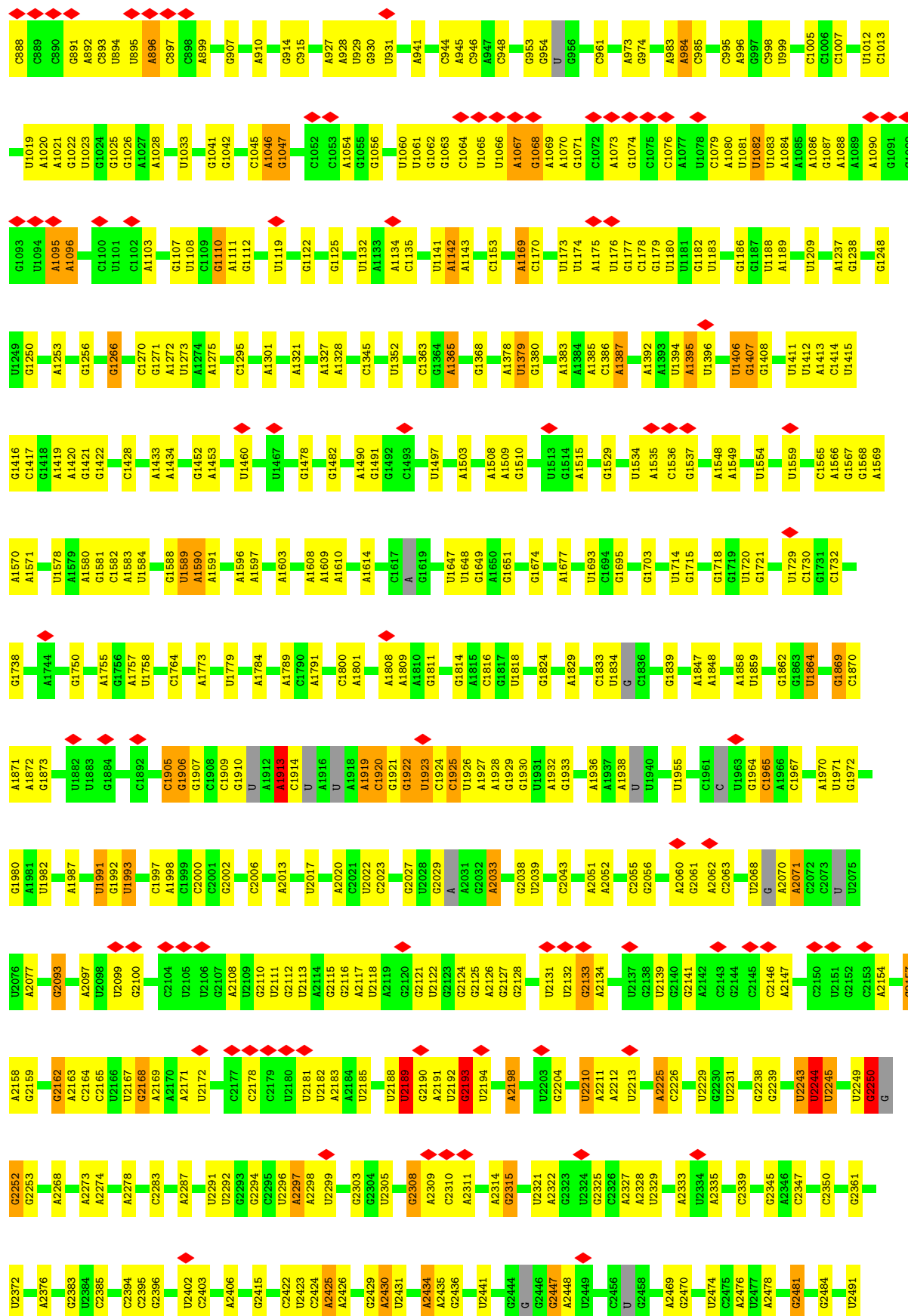


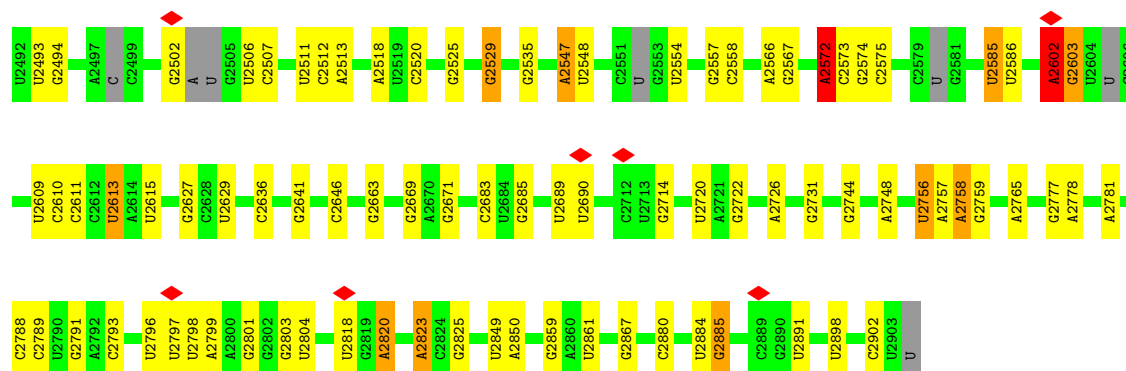
- Molecule 36: 30S ribosomal protein S13



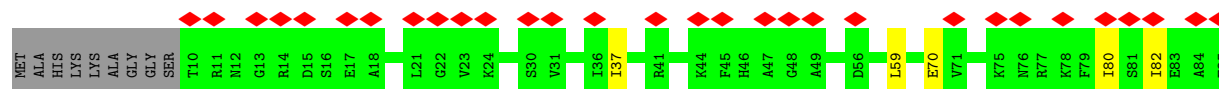
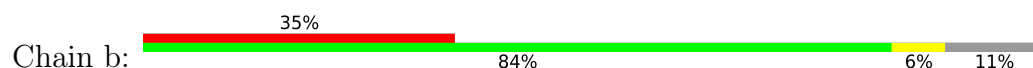
- Molecule 37: 50S ribosomal protein L11



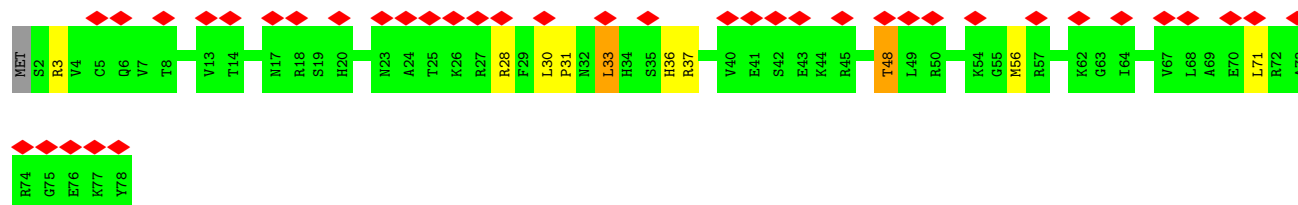
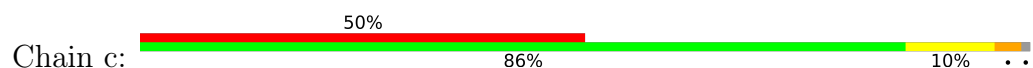




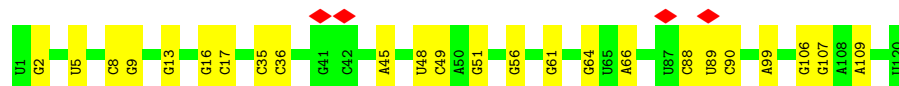
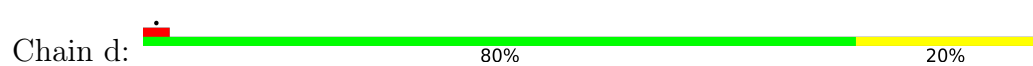
- Molecule 40: 50S ribosomal protein L27



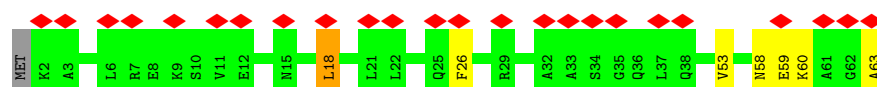
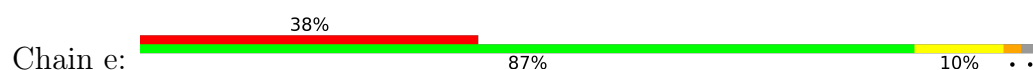
- Molecule 41: 50S ribosomal protein L28



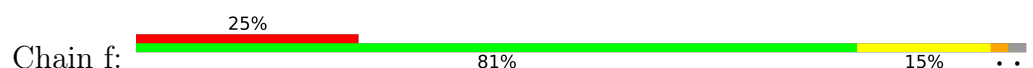
- Molecule 42: 5S rRNA

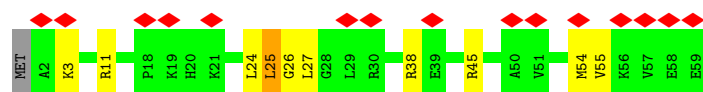


- Molecule 43: 50S ribosomal protein L29



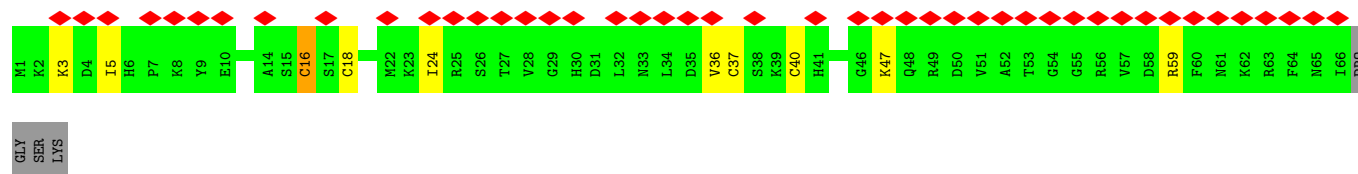
- Molecule 44: 50S ribosomal protein L30





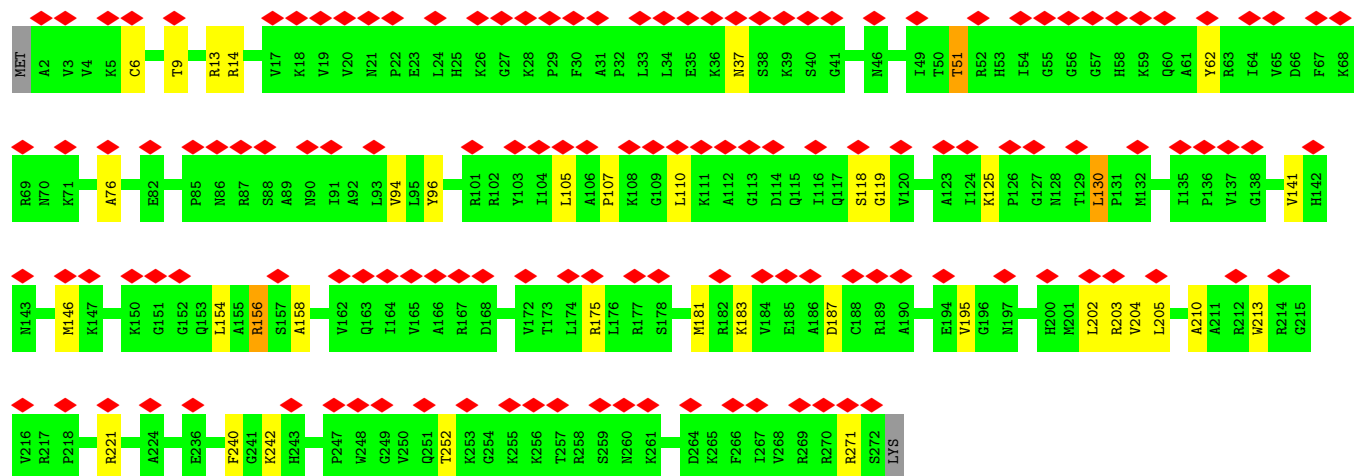
- Molecule 45: 50S ribosomal protein L31

Chain g:



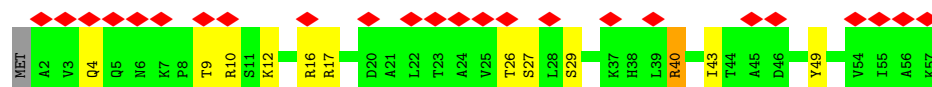
- Molecule 46: 50S ribosomal protein L2

Chain h:



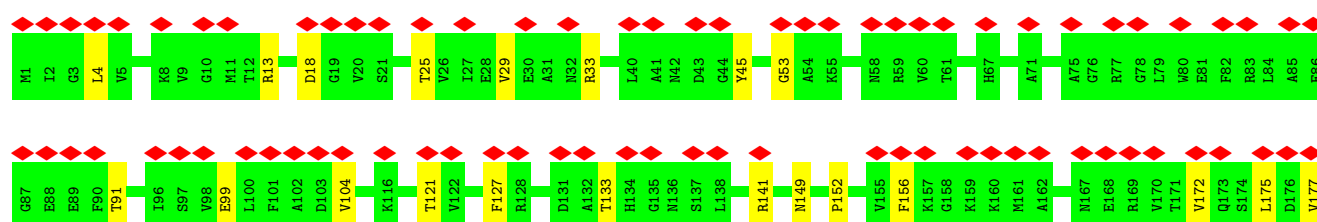
- Molecule 47: 50S ribosomal protein L32

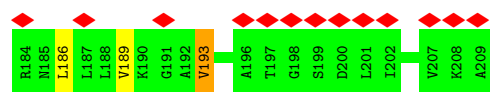
Chain i:



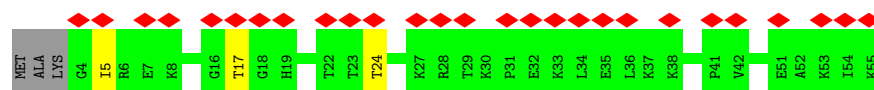
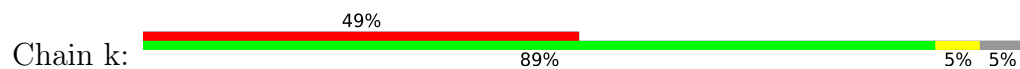
- Molecule 48: 50S ribosomal protein L3

Chain j:

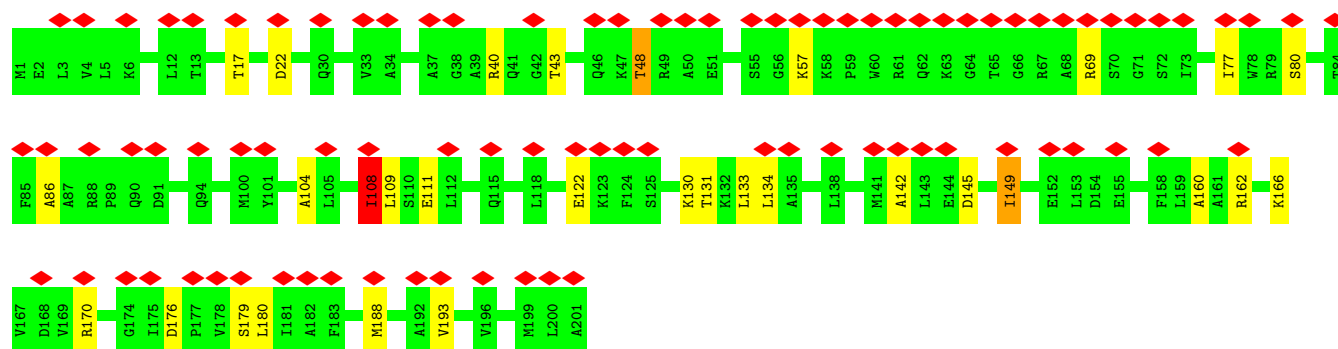
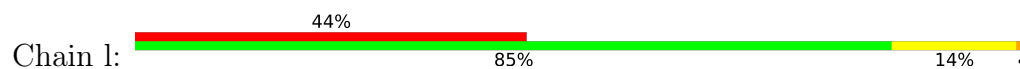




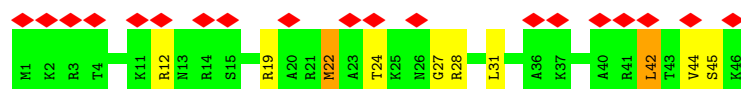
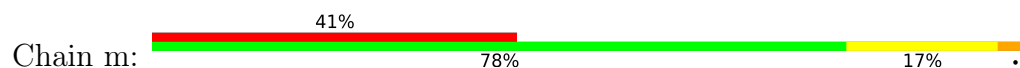
- Molecule 49: 50S ribosomal protein L33



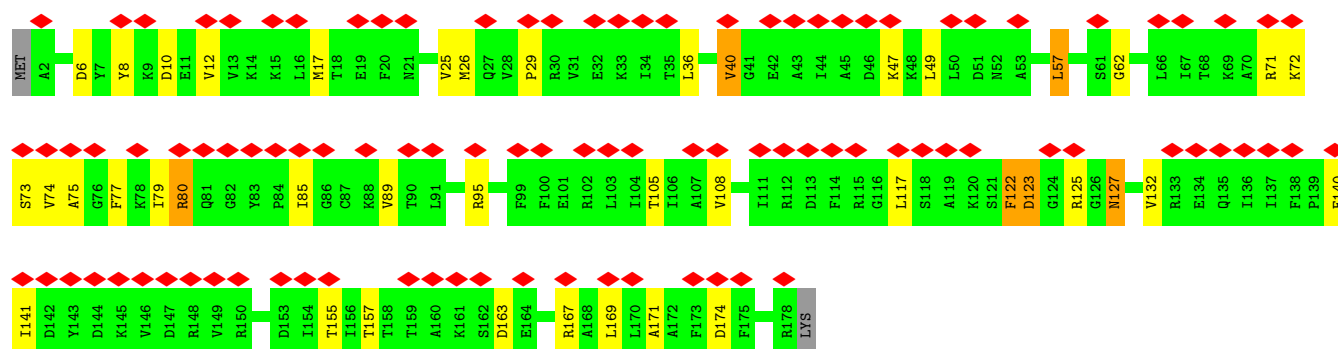
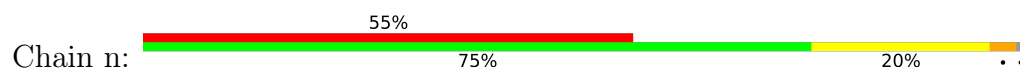
- Molecule 50: 50S ribosomal protein L4



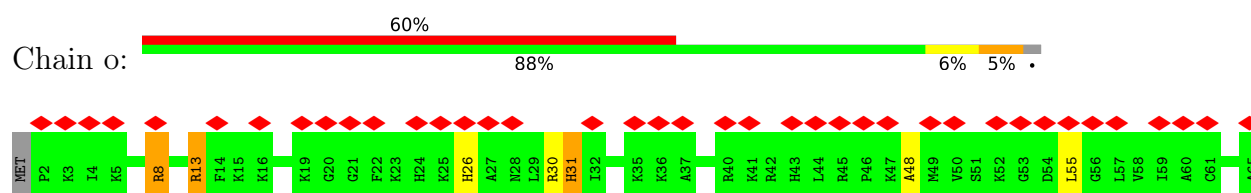
- Molecule 51: 50S ribosomal protein L34



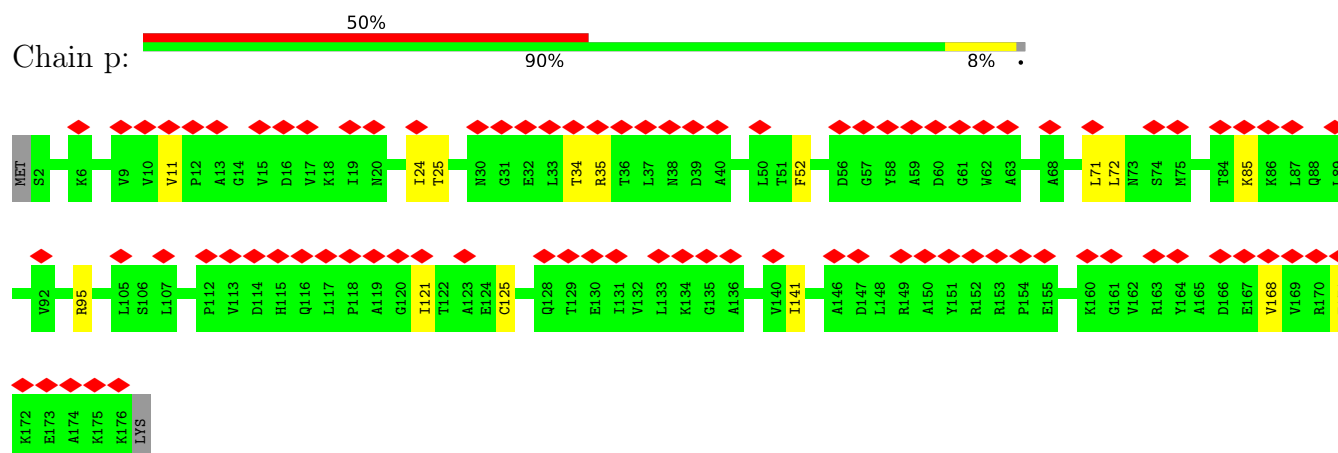
- Molecule 52: 50S ribosomal protein L5



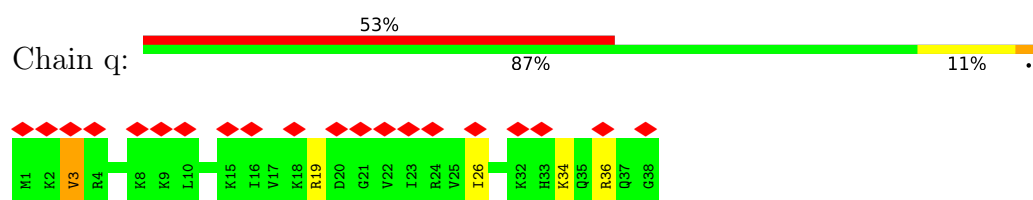
- Molecule 53: 50S ribosomal protein L35



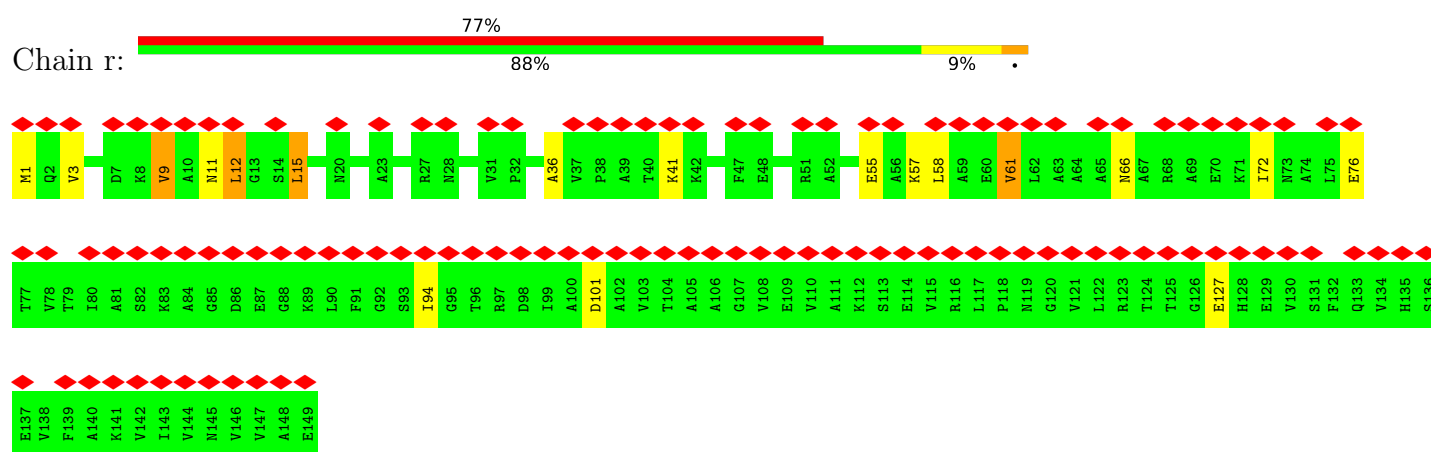
• Molecule 54: 50S ribosomal protein L6



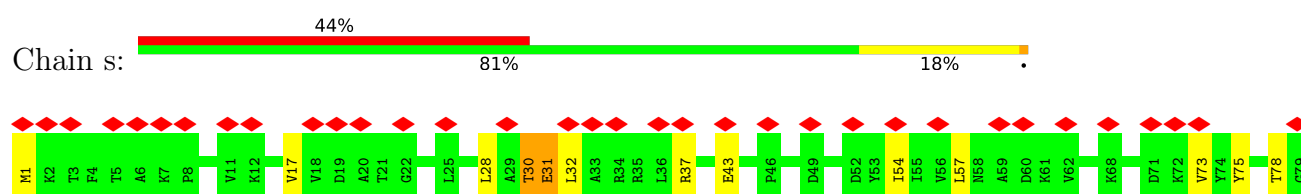
• Molecule 55: 50S ribosomal protein L36

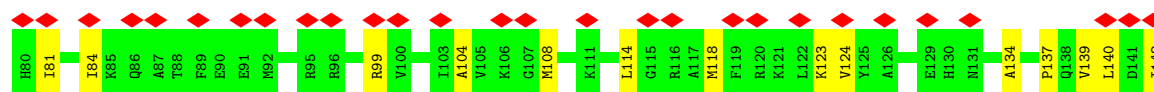


• Molecule 56: 50S ribosomal protein L9

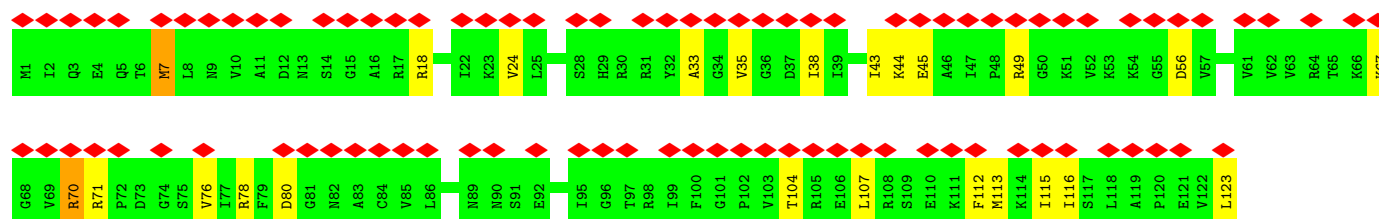
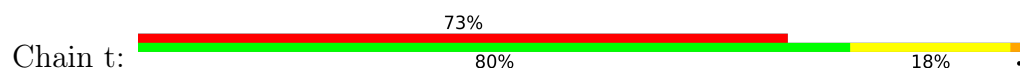


• Molecule 57: 50S ribosomal protein L13

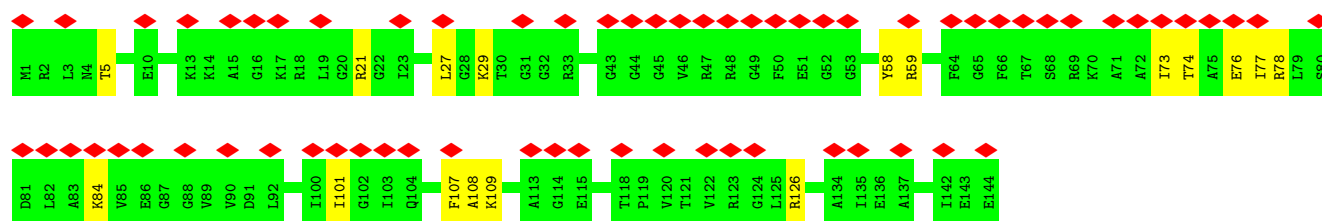
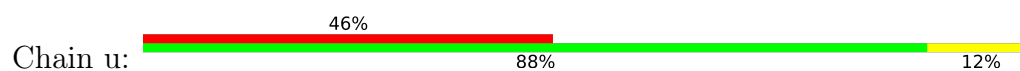




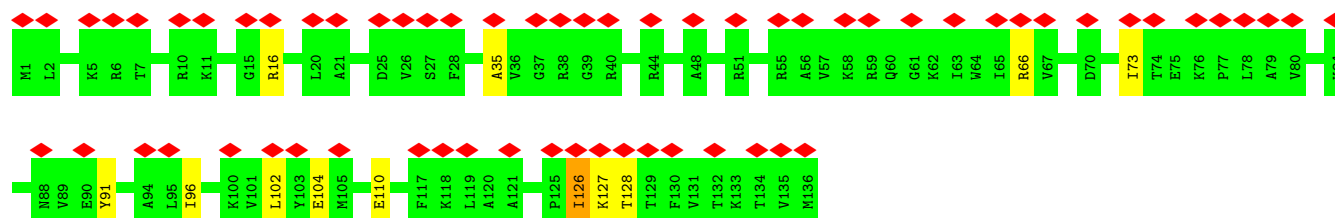
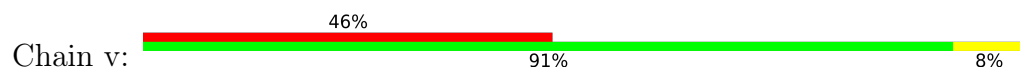
- Molecule 58: 50S ribosomal protein L14



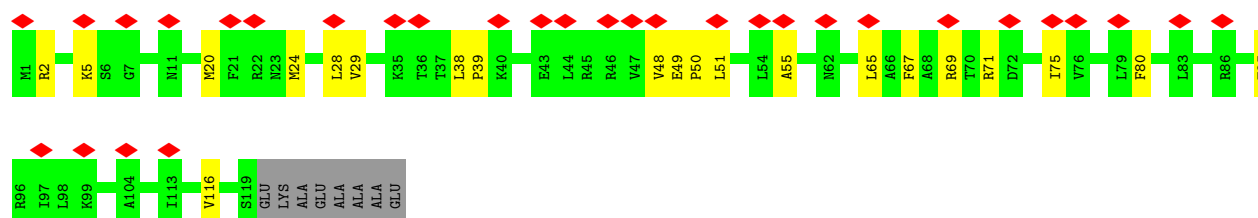
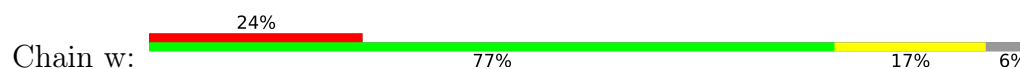
- Molecule 59: 50S ribosomal protein L15



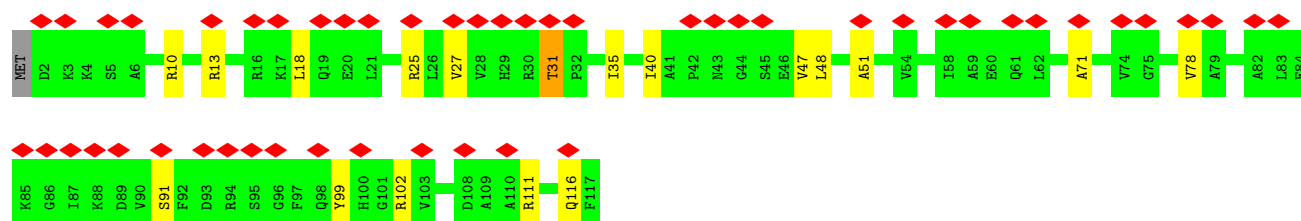
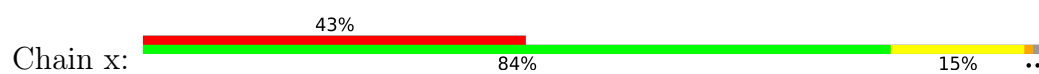
- Molecule 60: 50S ribosomal protein L16



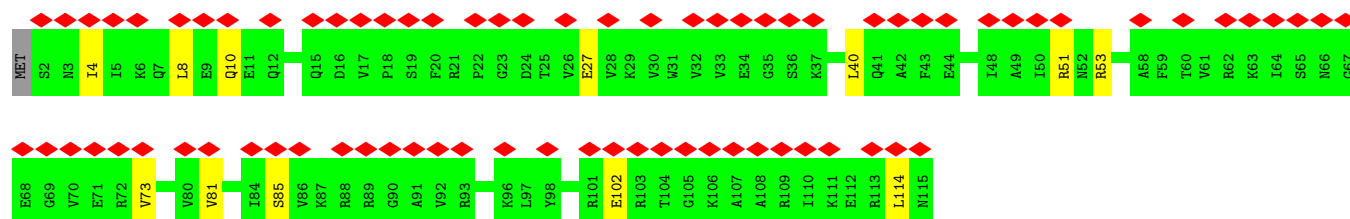
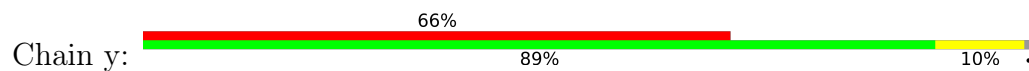
- Molecule 61: 50S ribosomal protein L17



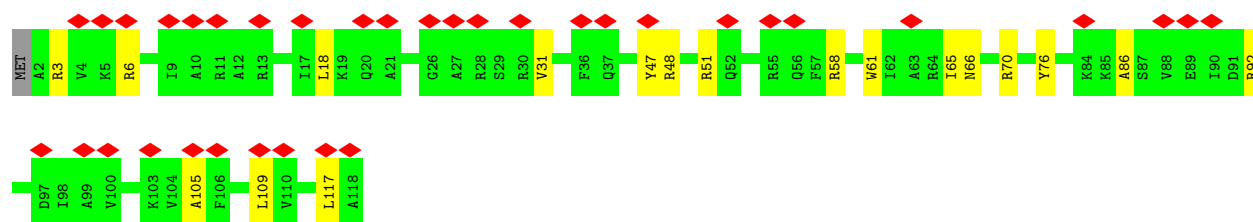
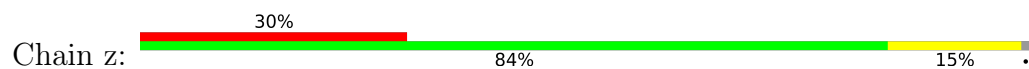
- Molecule 62: 50S ribosomal protein L18



• Molecule 63: 50S ribosomal protein L19



• Molecule 64: 50S ribosomal protein L20



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	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 (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: ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	0	0.49	0/829	0.74	0/1107
2	1	0.67	0/864	1.08	0/1156
3	2	0.54	0/752	0.89	0/1005
4	3	0.47	0/796	0.77	0/1062
5	4	0.52	0/766	0.88	0/1025
6	5	0.63	1/528 (0.2%)	0.55	0/810
7	6	0.55	1/603 (0.2%)	0.56	0/926
8	7	0.64	2/519 (0.4%)	0.92	3/804 (0.4%)
9	9	1.15	3/1131 (0.3%)	1.30	3/1524 (0.2%)
10	A	0.36	0/1810	0.72	3/2821 (0.1%)
10	B	0.43	0/1810	0.87	9/2821 (0.3%)
11	AA	0.67	13/10591 (0.1%)	0.96	54/14289 (0.4%)
12	AB	0.43	1/808 (0.1%)	0.70	2/1088 (0.2%)
13	AC	0.60	4/1808 (0.2%)	0.73	9/2450 (0.4%)
13	AD	0.39	0/1789	0.55	0/2425
14	AE	0.54	8/10545 (0.1%)	0.74	23/14236 (0.2%)
15	C	0.66	0/553	1.14	2/743 (0.3%)
16	D	0.40	9/36610 (0.0%)	0.75	39/57091 (0.1%)
17	E	0.76	0/675	1.32	0/895
18	F	0.71	0/597	1.20	0/792
19	G	0.65	0/1791	1.08	1/2413 (0.0%)
20	H	0.76	4/1746 (0.2%)	1.58	34/2382 (1.4%)
21	I	0.58	0/1663	0.98	0/2241
22	J	0.63	0/1665	1.08	0/2227
23	K	0.64	1/1165 (0.1%)	1.06	2/1568 (0.1%)
24	L	0.58	0/867	0.94	0/1171
25	M	0.68	0/1195	1.19	3/1602 (0.2%)
26	N	0.55	0/989	0.91	0/1326
27	O	0.58	0/1034	1.02	1/1375 (0.1%)
28	P	0.60	0/800	1.10	4/1082 (0.4%)
29	Q	0.55	0/893	0.91	0/1205
30	R	0.49	0/952	0.81	0/1274

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	S	0.64	0/817	1.11	1/1088 (0.1%)
32	T	0.69	0/722	1.21	0/964
33	U	0.58	0/659	0.99	0/884
34	V	0.46	0/657	0.73	0/881
35	W	0.51	0/680	0.83	0/915
36	X	0.67	0/909	1.21	3/1215 (0.2%)
37	Y	1.03	0/1046	1.08	0/1410
38	Z	1.02	0/227	1.12	0/304
39	a	0.40	3/69247 (0.0%)	0.75	58/107985 (0.1%)
40	b	0.51	0/589	0.76	0/779
41	c	0.63	0/635	0.97	0/848
42	d	0.37	0/2872	0.69	0/4478
43	e	0.70	0/502	1.19	0/667
44	f	0.62	0/452	1.02	0/605
45	g	0.55	0/531	0.99	1/709 (0.1%)
46	h	0.54	0/2121	0.85	0/2852
47	i	0.52	0/450	0.94	0/599
48	j	0.59	0/1586	0.87	0/2134
49	k	0.46	0/433	0.80	0/576
50	l	0.61	0/1571	1.03	1/2113 (0.0%)
51	m	0.68	0/380	1.22	0/498
52	n	0.62	0/1434	1.18	10/1926 (0.5%)
53	o	0.64	0/513	1.10	1/676 (0.1%)
54	p	0.58	0/1333	0.89	0/1805
55	q	0.50	0/303	0.88	0/397
56	r	0.63	0/1122	0.97	1/1515 (0.1%)
57	s	0.68	0/1152	1.02	2/1551 (0.1%)
58	t	0.57	0/955	0.88	0/1279
59	u	0.55	0/1062	0.96	1/1413 (0.1%)
60	v	0.59	0/1093	0.97	0/1460
61	w	0.67	0/964	1.13	0/1289
62	x	0.61	0/902	1.09	0/1209
63	y	0.52	0/929	0.79	0/1242
64	z	0.80	0/960	1.25	0/1278
All	All	0.50	50/188952 (0.0%)	0.84	271/278480 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
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 50 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	9	130	PRO	N-CA	18.18	1.70	1.47
11	AA	374	GLU	C-N	17.59	1.54	1.33
11	AA	850	ILE	N-CA	-13.13	1.29	1.46
14	AE	93	THR	CA-C	12.21	1.69	1.52
20	H	169	SER	N-CA	11.79	1.61	1.46

The worst 5 of 271 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	D	1516	G	O3'-P-O5'	17.47	130.21	104.00
11	AA	727	VAL	N-CA-C	-17.17	95.11	110.74
20	H	88	LYS	CA-C-N	16.93	143.57	120.38
20	H	88	LYS	C-N-CA	16.93	143.57	120.38
10	B	29	G	C3'-C2'-O2'	15.95	134.63	110.70

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

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	816	839	839	8	0
2	1	857	922	922	14	0
3	2	746	811	811	7	0
4	3	788	844	844	10	0
5	4	753	780	780	0	0
6	5	472	260	261	23	0
7	6	542	305	306	24	0
8	7	467	97	231	80	0
9	9	1117	0	1153	169	0
10	A	1620	826	826	173	0
10	B	1620	813	827	140	0
11	AA	10425	10426	10428	376	0
12	AB	790	783	783	7	0
13	AC	1786	1813	1813	82	0
13	AD	1767	1789	1789	47	0
14	AE	10388	10612	10611	373	0
15	C	544	559	560	23	0
16	D	32703	16423	16459	224	0
17	E	669	719	719	4	0
18	F	589	629	629	8	0
19	G	1760	1785	1785	46	0
20	H	1730	1454	1454	208	0
21	I	1636	1710	1710	37	0
22	J	1643	1707	1707	30	0
23	K	1152	1196	1196	21	0
24	L	848	846	846	3	0
25	M	1181	1235	1235	33	0
26	N	979	1031	1031	6	0
27	O	1022	1070	1070	13	0
28	P	790	831	831	36	0
29	Q	877	887	887	4	0
30	R	939	1001	1001	8	0
31	S	805	844	844	5	0
32	T	714	734	734	8	0
33	U	649	666	666	3	0
34	V	648	691	691	4	0
35	W	663	688	688	3	0
36	X	900	964	964	57	0
37	Y	1032	0	1088	83	0
38	Z	227	0	237	20	0
39	a	61841	31077	31123	295	0
40	b	582	599	599	3	0
41	c	625	652	652	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	d	2569	1301	1301	4	0
43	e	501	531	531	4	0
44	f	448	488	488	7	0
45	g	522	520	520	10	0
46	h	2082	2154	2154	18	0
47	i	444	459	458	6	0
48	j	1565	1617	1616	13	0
49	k	426	464	464	0	0
50	l	1552	1619	1619	13	0
51	m	377	418	418	10	0
52	n	1410	1443	1444	27	0
53	o	504	572	572	4	0
54	p	1313	1358	1358	7	0
55	q	302	343	343	2	0
56	r	1111	1148	1148	6	0
57	s	1129	1162	1162	14	0
58	t	946	1023	1023	12	0
59	u	1053	1129	1129	8	0
60	v	1074	1157	1157	5	0
61	w	951	994	994	8	0
62	x	892	923	923	9	0
63	y	917	962	962	4	0
64	z	947	1020	1019	12	0
65	AE	1	0	0	0	0
66	AE	2	0	0	0	0
All	All	175740	124723	127433	2428	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 2428 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:H:131:LEU:CB	20:H:167:VAL:CA	1.78	1.59
15:C:12:ARG:HG3	20:H:264:GLU:CB	1.30	1.57
20:H:131:LEU:CB	20:H:167:VAL:HA	1.03	1.48
11:AA:1026:GLU:HG3	16:D:1030:U:C2	1.54	1.42
9:9:130:PRO:N	9:9:130:PRO:CA	1.70	1.40

There are no symmetry-related clashes.

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%)	12	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%)	12	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%)	4	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	51
13	AD	226/329 (69%)	213 (94%)	12 (5%)	1 (0%)	30	67
14	AE	1329/1407 (94%)	1200 (90%)	120 (9%)	9 (1%)	18	56
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%)	24	63
22	J	203/206 (98%)	198 (98%)	5 (2%)	0	100	100
23	K	154/167 (92%)	146 (95%)	7 (4%)	1 (1%)	21	59
24	L	102/135 (76%)	97 (95%)	4 (4%)	1 (1%)	12	49
25	M	149/179 (83%)	144 (97%)	4 (3%)	1 (1%)	18	56
26	N	127/130 (98%)	121 (95%)	5 (4%)	1 (1%)	16	54
27	O	125/130 (96%)	115 (92%)	9 (7%)	1 (1%)	16	54
28	P	97/103 (94%)	88 (91%)	8 (8%)	1 (1%)	12	49
29	Q	115/129 (89%)	104 (90%)	9 (8%)	2 (2%)	7	36

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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%)	9	42
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%)	6	34
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	67
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%)	24	63
51	m	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
52	n	175/179 (98%)	162 (93%)	11 (6%)	2 (1%)	11	46
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	51
All	All	9368/10486 (89%)	8607 (92%)	658 (7%)	103 (1%)	14	46

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%)	76 (90%)	8 (10%)	8	25
2	1	93/93 (100%)	86 (92%)	7 (8%)	12	33
3	2	81/84 (96%)	77 (95%)	4 (5%)	22	43
4	3	84/85 (99%)	79 (94%)	5 (6%)	17	39
5	4	78/78 (100%)	75 (96%)	3 (4%)	29	50
9	9	112/123 (91%)	63 (56%)	49 (44%)	0	0
11	AA	1140/1157 (98%)	1027 (90%)	113 (10%)	7	24
12	AB	86/158 (54%)	85 (99%)	1 (1%)	63	75
13	AC	198/286 (69%)	183 (92%)	15 (8%)	12	33
13	AD	196/286 (68%)	193 (98%)	3 (2%)	57	72
14	AE	1120/1168 (96%)	1046 (93%)	74 (7%)	15	37
15	C	57/65 (88%)	55 (96%)	2 (4%)	32	53
17	E	65/66 (98%)	61 (94%)	4 (6%)	16	38
18	F	60/61 (98%)	57 (95%)	3 (5%)	22	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	G	187/199 (94%)	174 (93%)	13 (7%)	14	35
20	H	137/461 (30%)	124 (90%)	13 (10%)	8	25
21	I	171/190 (90%)	163 (95%)	8 (5%)	23	45
22	J	172/173 (99%)	164 (95%)	8 (5%)	23	45
23	K	119/126 (94%)	111 (93%)	8 (7%)	15	36
24	L	91/116 (78%)	84 (92%)	7 (8%)	12	32
25	M	124/147 (84%)	113 (91%)	11 (9%)	9	28
26	N	104/105 (99%)	101 (97%)	3 (3%)	37	58
27	O	105/107 (98%)	99 (94%)	6 (6%)	18	40
28	P	86/90 (96%)	77 (90%)	9 (10%)	6	21
29	Q	90/99 (91%)	88 (98%)	2 (2%)	45	64
30	R	101/104 (97%)	95 (94%)	6 (6%)	18	39
31	S	83/84 (99%)	79 (95%)	4 (5%)	23	44
32	T	76/77 (99%)	65 (86%)	11 (14%)	3	13
33	U	65/65 (100%)	60 (92%)	5 (8%)	12	32
34	V	74/78 (95%)	71 (96%)	3 (4%)	27	49
35	W	72/79 (91%)	66 (92%)	6 (8%)	10	30
36	X	94/96 (98%)	87 (93%)	7 (7%)	13	33
37	Y	109/110 (99%)	69 (63%)	40 (37%)	0	1
38	Z	26/85 (31%)	10 (38%)	16 (62%)	0	0
40	b	58/63 (92%)	57 (98%)	1 (2%)	53	69
41	c	67/68 (98%)	64 (96%)	3 (4%)	24	46
43	e	54/55 (98%)	51 (94%)	3 (6%)	19	40
44	f	48/49 (98%)	43 (90%)	5 (10%)	7	22
45	g	59/62 (95%)	54 (92%)	5 (8%)	10	29
46	h	216/218 (99%)	199 (92%)	17 (8%)	11	32
47	i	47/48 (98%)	41 (87%)	6 (13%)	4	15
48	j	164/164 (100%)	156 (95%)	8 (5%)	22	43
49	k	47/49 (96%)	44 (94%)	3 (6%)	16	37
50	l	165/165 (100%)	151 (92%)	14 (8%)	10	29
51	m	38/38 (100%)	36 (95%)	2 (5%)	20	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	n	148/150 (99%)	130 (88%)	18 (12%)	5	17
53	o	51/52 (98%)	47 (92%)	4 (8%)	11	32
54	p	136/138 (99%)	130 (96%)	6 (4%)	25	47
55	q	34/34 (100%)	31 (91%)	3 (9%)	9	28
56	r	114/114 (100%)	102 (90%)	12 (10%)	6	21
57	s	116/116 (100%)	106 (91%)	10 (9%)	10	29
58	t	104/104 (100%)	97 (93%)	7 (7%)	15	36
59	u	103/103 (100%)	96 (93%)	7 (7%)	14	36
60	v	109/109 (100%)	105 (96%)	4 (4%)	30	51
61	w	99/103 (96%)	91 (92%)	8 (8%)	11	31
62	x	86/87 (99%)	80 (93%)	6 (7%)	14	35
63	y	99/100 (99%)	91 (92%)	8 (8%)	11	31
64	z	89/90 (99%)	85 (96%)	4 (4%)	24	46
All	All	7791/8664 (90%)	7150 (92%)	641 (8%)	13	31

5 of 641 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
38	Z	3	THR
55	q	26	ILE
38	Z	30	PHE
38	Z	2	ILE
48	j	99	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 66 such sidechains are listed below:

Mol	Chain	Res	Type
53	o	28	ASN
55	q	35	GLN
63	y	115	ASN
14	AE	1238	GLN
14	AE	1195	GLN

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%)	289 (19%)	35 (2%)
39	a	2859/2904 (98%)	542 (18%)	0
42	d	119/120 (99%)	17 (14%)	0
8	7	20/33 (60%)	11 (55%)	3 (15%)
All	All	4663/4751 (98%)	923 (19%)	50 (1%)

5 of 923 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

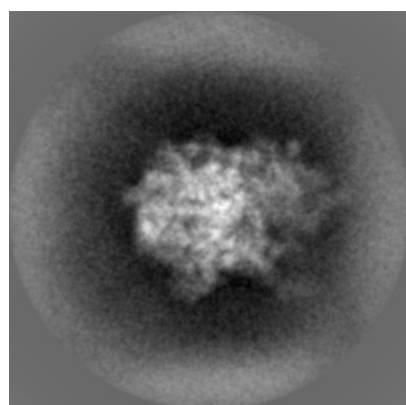
6 Map visualisation [i](#)

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.

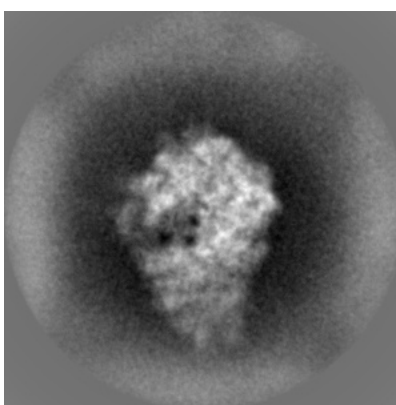
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

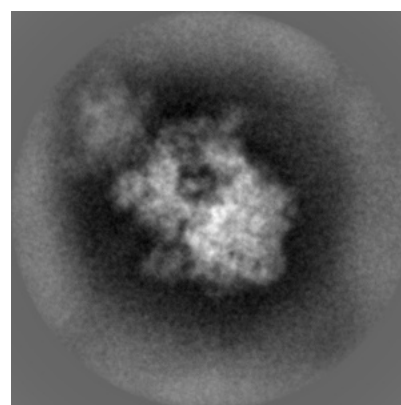
6.1.1 Primary map



X



Y

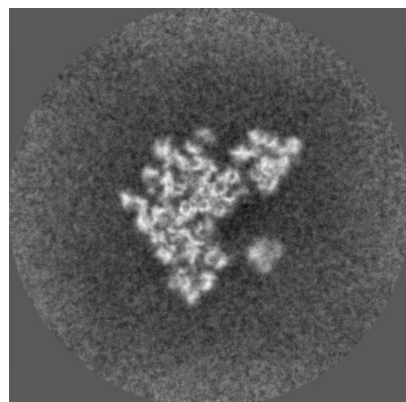


Z

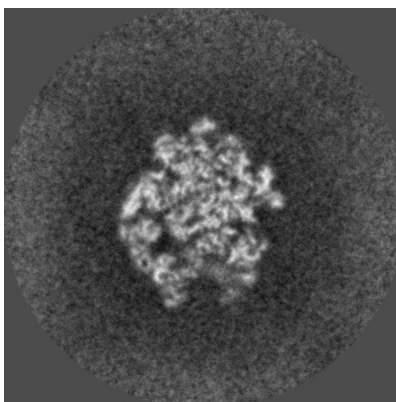
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

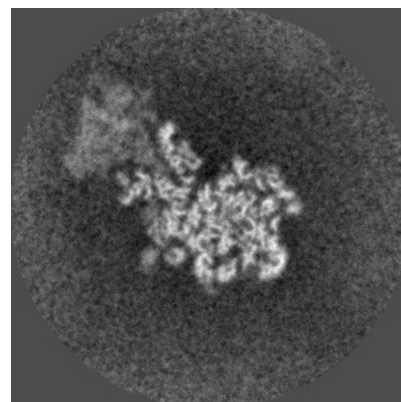
6.2.1 Primary map



X Index: 256



Y Index: 256

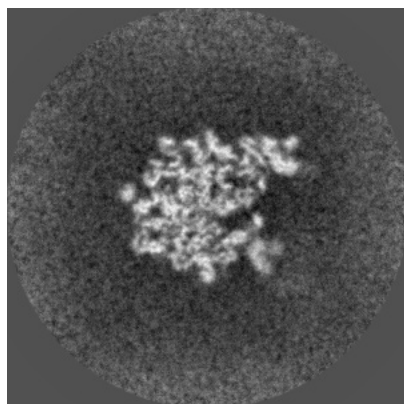


Z Index: 256

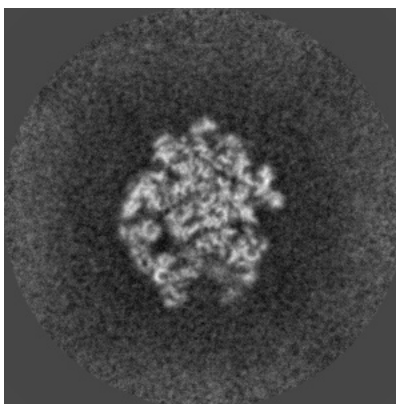
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

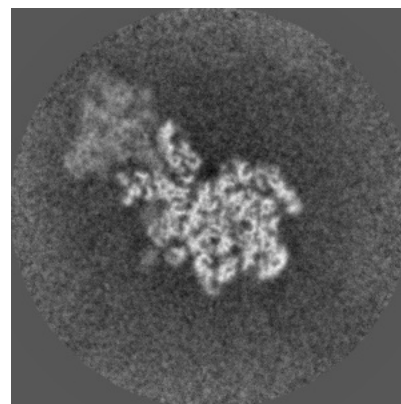
6.3.1 Primary map



X Index: 272



Y Index: 257

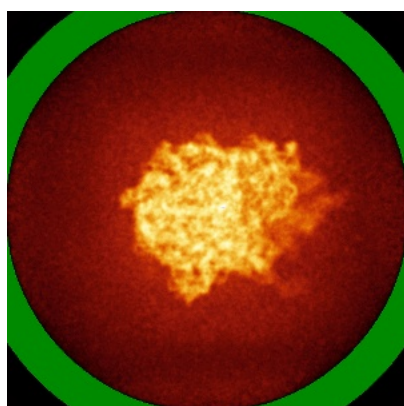


Z Index: 258

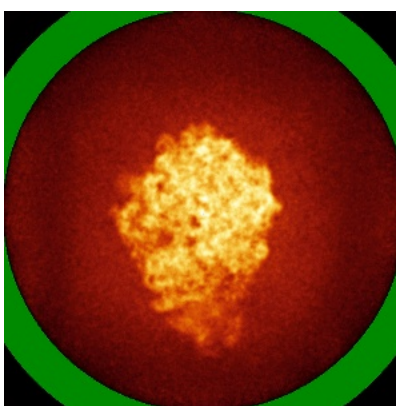
The images above show the largest variance slices of the map in three orthogonal directions.

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

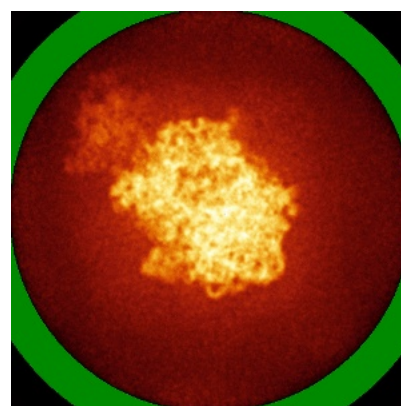
6.4.1 Primary map



X



Y

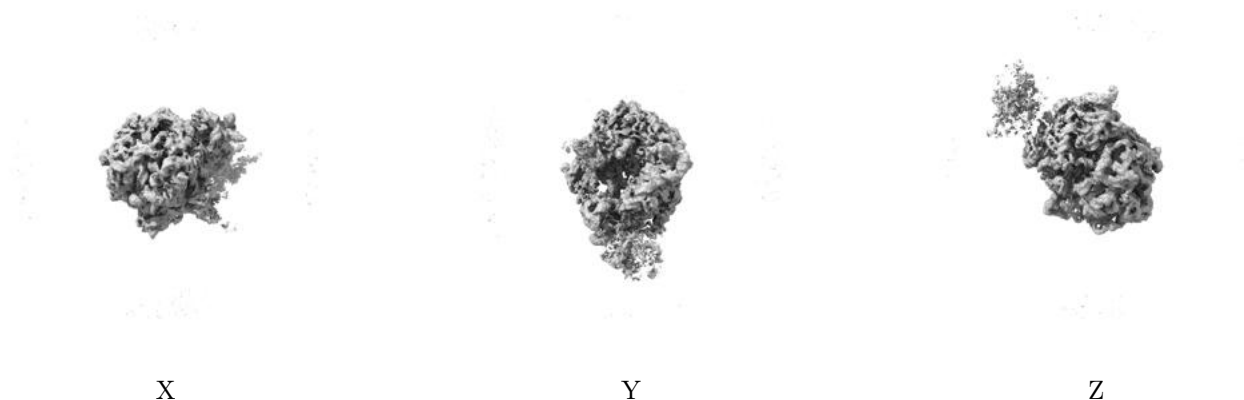


Z

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.

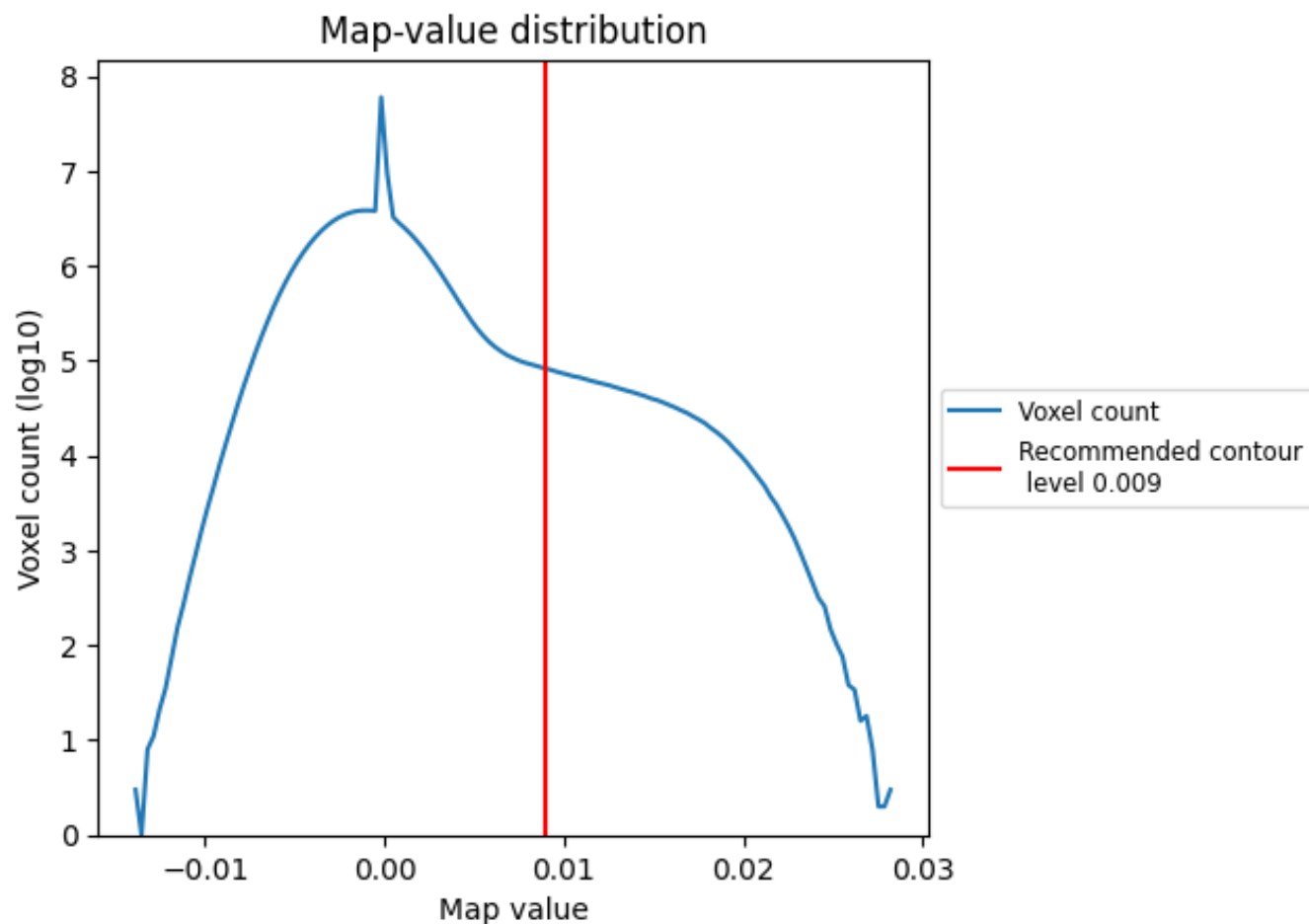
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

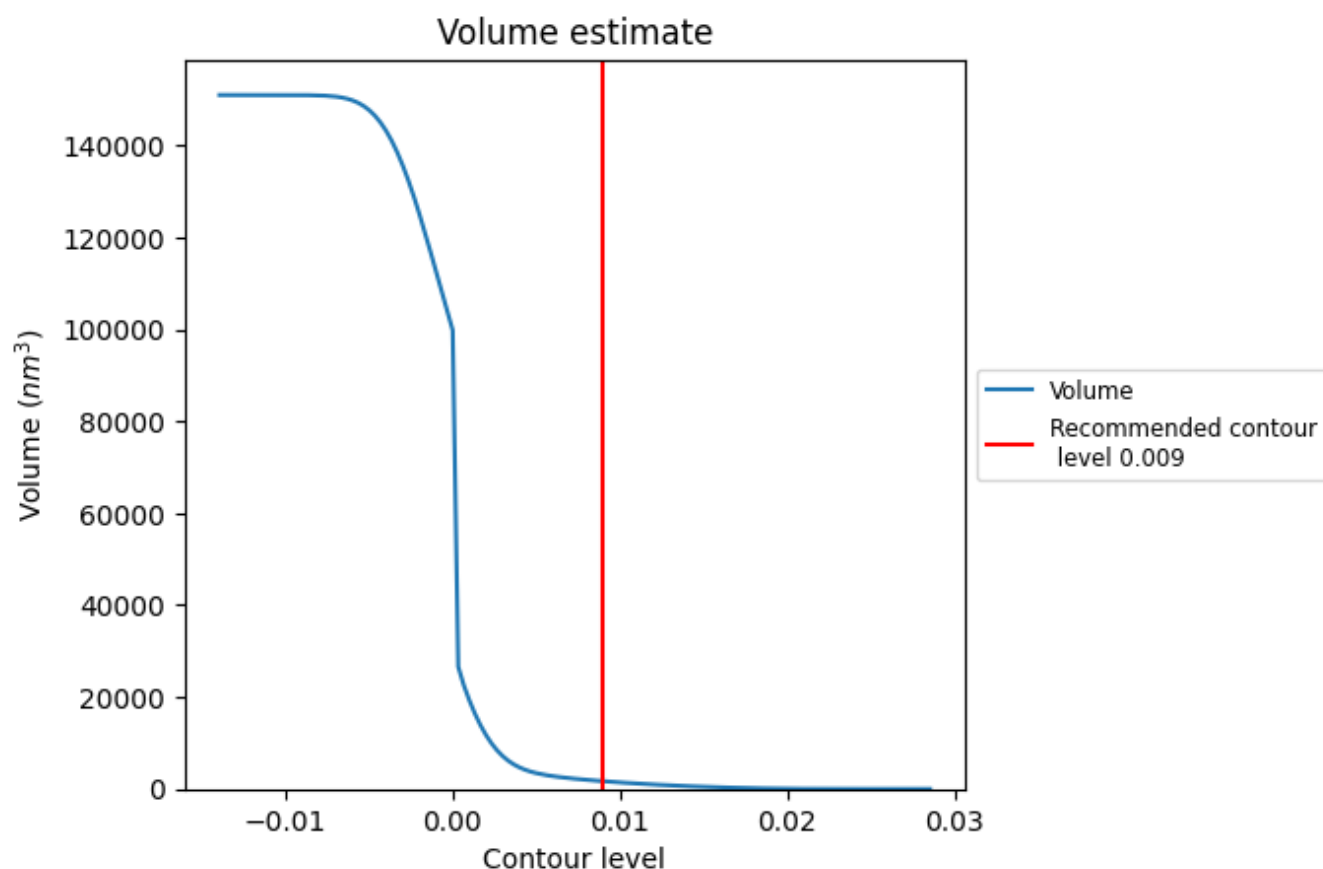
This section contains the results of statistical analysis of the map.

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.

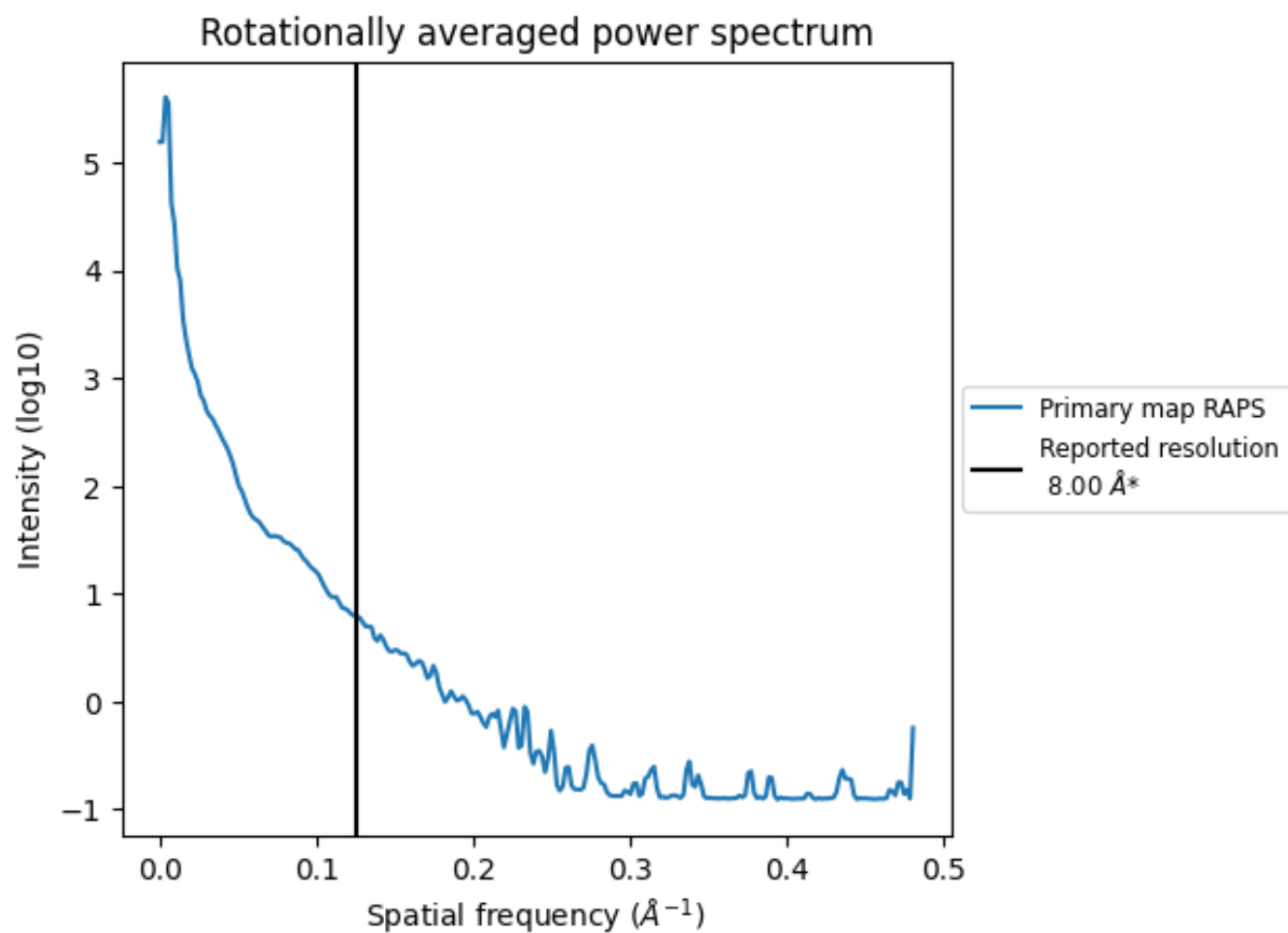
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1692 nm³; 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

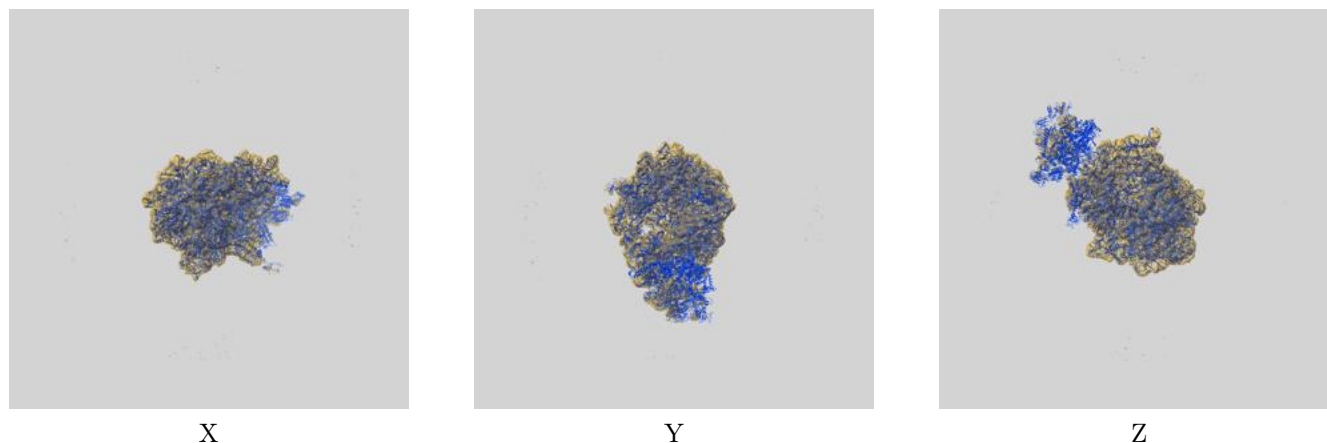
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

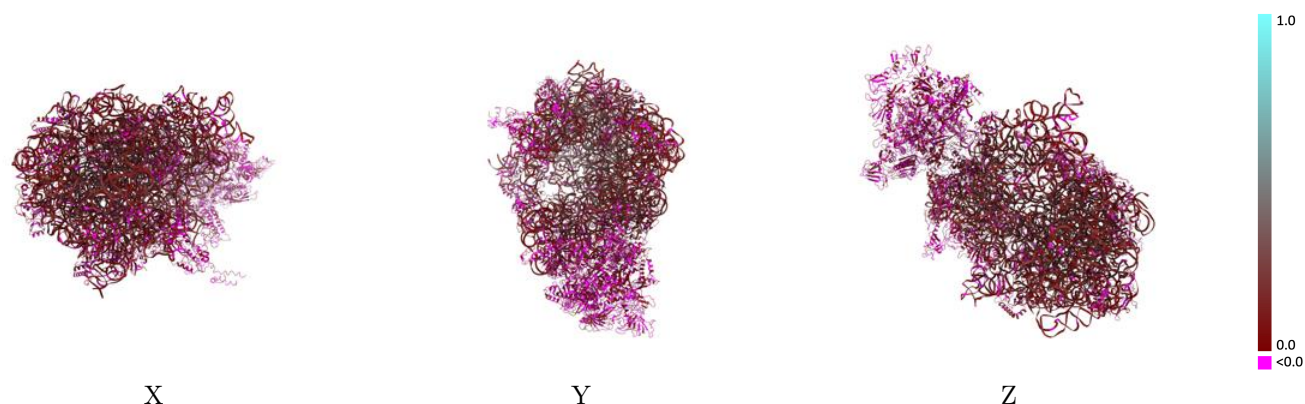
This section contains information regarding the fit between EMDB map EMD-22193 and PDB model 6XIJ. Per-residue inclusion information can be found in section 3 on page 16.

9.1 Map-model overlay [i](#)



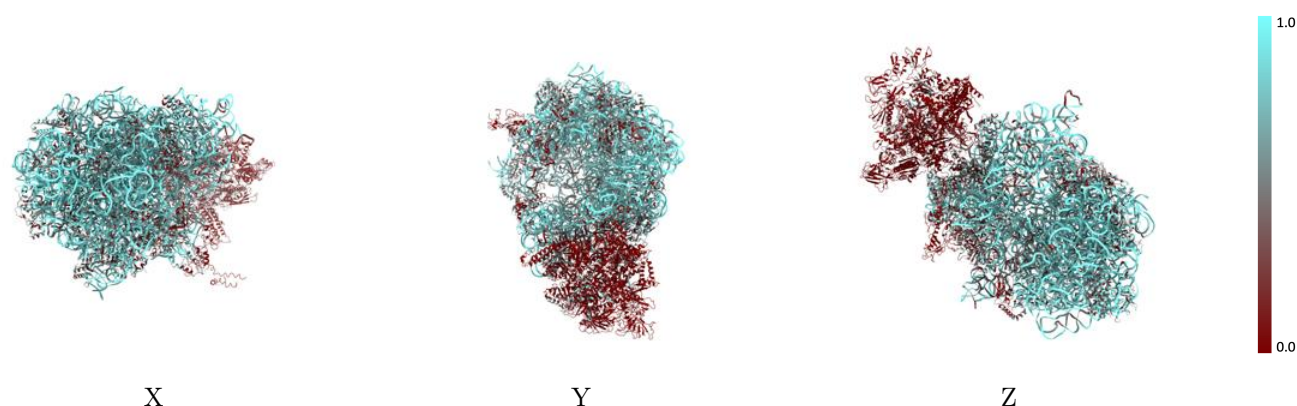
The images above show the 3D surface view of the map at the recommended contour level 0.009 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



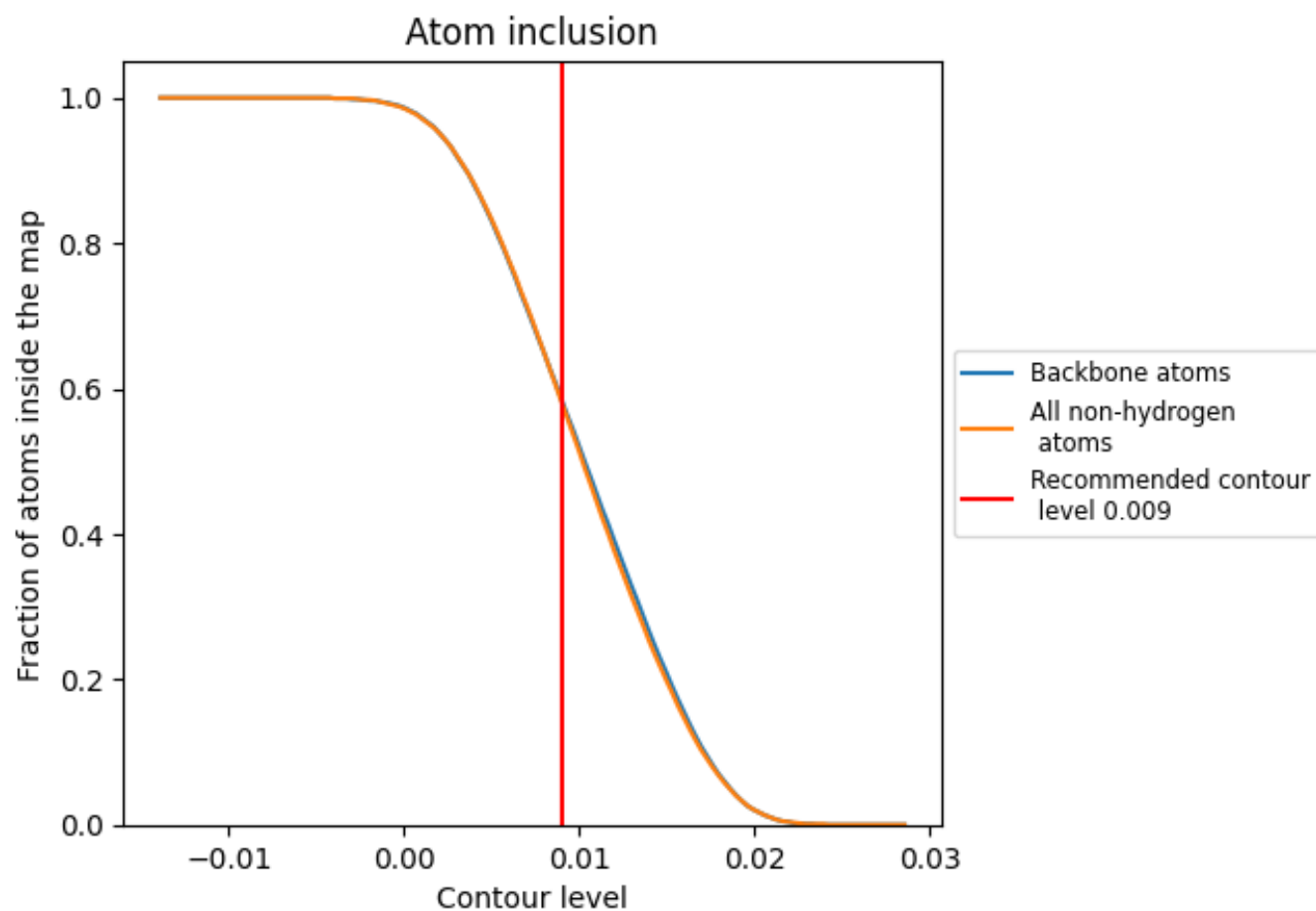
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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