



wwPDB EM Validation Summary Report ⓘ

Mar 27, 2026 – 12:19 PM UTC

PDB ID : 6R7Q / pdb_00006r7q
EMDB ID : EMD-4745
Title : Structure of XBP1u-paused ribosome nascent chain complex with Sec61.
Authors : Shanmuganathan, V.; Cheng, J.; Braunger, K.; Berninghausen, O.; Beatrix, B.; Beckmann, R.
Deposited on : 2019-03-29
Resolution : 3.90 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

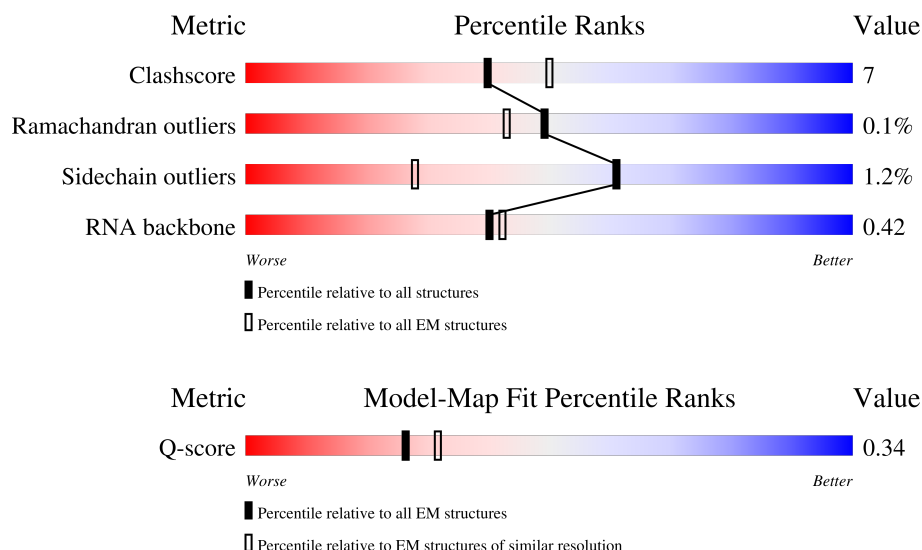
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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	8855 (3.40 - 4.40)

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	AA	55	65% 85% 15%
2	BB	189	61% 79% 19% .
3	CC	206	38% 81% 19%

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Mol	Chain	Length	Quality of chain
4	DD	185	
5	EE	151	
6	FF	62	
7	GG	100	
8	HH	83	
9	II	144	
10	JJ	83	
11	KK	132	
12	LL	101	
13	MM	136	
14	0	68	
15	1	24	
16	2	75	
17	3	75	
18	4	6	
19	5	3544	
20	6	313	
21	7	120	
22	8	151	
23	9	55	
24	NN	124	
25	OO	75	
26	PP	141	
27	QQ	149	
28	RR	117	

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Mol	Chain	Length	Quality of chain
29	A	248	
30	B	394	
31	C	362	
32	D	293	
33	E	251	
34	F	225	
35	G	240	
36	H	190	
37	I	213	
38	J	170	
39	K	1698	
40	L	210	
41	M	138	
42	N	203	
43	O	199	
44	P	153	
45	Q	187	
46	R	180	
47	S	176	
48	T	159	
49	U	99	
50	V	131	
51	W	121	
52	X	118	
53	Y	134	

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Mol	Chain	Length	Quality of chain
54	Z	135	
55	SS	96	
56	a	147	
57	b	116	
58	c	98	
59	d	107	
60	e	128	
61	f	109	
62	g	114	
63	h	122	
64	i	102	
65	j	86	
66	k	69	
67	l	50	
68	m	52	
69	n	25	
70	o	104	
71	p	91	
72	q	217	
73	r	124	
74	s	196	
75	t	153	
76	u	213	
77	v	221	
78	w	228	

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Mol	Chain	Length	Quality of chain
79	x	262	
80	y	191	
81	z	237	
82	TT	129	
83	UU	142	
84	VV	141	
85	WW	120	
86	XX	461	
87	YY	62	
88	ZZ	29	

2 Entry composition

There are 90 unique types of molecules in this entry. The entry contains 219898 atoms, of which 0 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 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	55	Total	C	N	O	S	0	0
			443	274	97	71	1		

- Molecule 2 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	BB	185	Total	C	N	O	S	0	0
			1488	952	271	264	1		

- Molecule 3 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	CC	206	Total	C	N	O	S	0	0
			1686	1058	332	291	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CC	47	ARG	GLY	conflict	UNP G1TJW1

- Molecule 4 is a protein called Ribosomal protein S9 (Predicted).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	DD	185	Total	C	N	O	S	0	0
			1525	969	306	248	2		

- Molecule 5 is a protein called Ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	EE	143	Total	C	N	O	S	0	0
			1175	749	222	198	6		

- Molecule 6 is a protein called Ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	FF	62	Total	C	N	O	S	0	0
			488	297	97	92	2		

- Molecule 7 is a protein called uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	GG	100	Total	C	N	O	S	0	0
			795	498	152	141	4		

- Molecule 8 is a protein called eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	HH	83	Total	C	N	O	S	0	0
			636	393	117	121	5		

- Molecule 9 is a protein called uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	II	144	Total	C	N	O	S	0	0
			1190	746	241	202	1		

- Molecule 10 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	JJ	83	Total	C	N	O	S	0	0
			651	408	121	115	7		

- Molecule 11 is a protein called eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	KK	132	Total	C	N	O	S	0	0
			1068	670	199	195	4		

- Molecule 12 is a protein called eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LL	101	Total	C	N	O	S	0	0
			814	507	170	132	5		

- Molecule 13 is a protein called uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	MM	136	Total	C	N	O	S	0	0
			1016	621	199	190	6		

- Molecule 14 is a protein called eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	0	68	Total	C	N	O	S	0	0
			555	351	103	94	7		

- Molecule 15 is a protein called X-box-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	1	24	Total	C	N	O	S	0	0
			204	137	35	30	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	255	ALA	SER	conflict	UNP P17861

- Molecule 16 is a RNA chain called P-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	2	75	Total	C	N	O	P	0	0
			1594	713	285	522	74		

- Molecule 17 is a RNA chain called E-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	3	75	Total	C	N	O	P	0	0
			1597	714	287	522	74		

- Molecule 18 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	4	6	Total	C	N	O	P	0	0
			127	57	21	43	6		

- Molecule 19 is a RNA chain called 28S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	5	3543	Total	C	N	O	P	0	0
			75972	33833	13910	24686	3543		

- Molecule 20 is a protein called ribosomal protein RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	6	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

- Molecule 21 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	7	120	Total	C	N	O	P	0	0
			2558	1141	456	842	119		

- Molecule 22 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	8	151	Total	C	N	O	P	0	0
			3208	1432	564	1062	150		

- Molecule 23 is a protein called uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	9	55	Total	C	N	O	S	0	0
			459	286	94	74	5		

- Molecule 24 is a protein called eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	NN	124	Total	C	N	O	S	0	0
			1011	640	198	168	5		

- Molecule 25 is a protein called ribosomal protein eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	OO	75	Total	C	N	O	S	0	0
			598	382	111	104	1		

- Molecule 26 is a protein called eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	PP	141	Total	C	N	O	S	0	0
			1097	688	211	195	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
PP	119	GLY	TRP	conflict	UNP G1TN62

- Molecule 27 is a protein called ribosomal protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	QQ	149	Total	C	N	O	S	0	0
			1202	770	228	203	1		

- Molecule 28 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	RR	117	Total	C	N	O	S	0	0
			908	570	161	169	8		

- Molecule 29 is a protein called uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	A	248	Total	C	N	O	S	0	0
			1898	1189	389	314	6		

- Molecule 30 is a protein called uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	B	394	Total	C	N	O	S	0	0
			3172	2020	597	542	13		

- Molecule 31 is a protein called uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	C	362	Total	C	N	O	S	0	0
			2883	1812	577	480	14		

- Molecule 32 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	D	293	Total	C	N	O	S	0	0
			2391	1512	438	427	14		

- Molecule 33 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	E	216	Total	C	N	O	S	0	0
			1729	1115	329	282	3		

- Molecule 34 is a protein called uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	F	225	Total	C	N	O	S	0	0
			1875	1205	358	303	9		

- Molecule 35 is a protein called eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	G	233	Total	C	N	O	S	0	0
			1879	1199	361	315	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	244	GLY	CYS	conflict	UNP G1STW0

- Molecule 36 is a protein called uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	H	190	Total	C	N	O	S	0	0
			1516	954	284	272	6		

- Molecule 37 is a protein called Ribosomal protein L10 (Predicted).

Mol	Chain	Residues	Atoms					AltConf	Trace
37	I	205	Total	C	N	O	S	0	0
			1664	1056	321	274	13		

- Molecule 38 is a protein called Ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	J	170	Total	C	N	O	S	0	0
			1362	861	254	241	6		

- Molecule 39 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	K	1698	Total	C	N	O	P	0	0
			36249	16180	6508	11864	1697		

- Molecule 40 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	L	210	Total	C	N	O	S	0	0
			1702	1065	354	279	4		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	47	ALA	-	insertion	UNP G1TPV0
L	48	PRO	-	insertion	UNP G1TPV0
L	49	ARG	-	insertion	UNP G1TPV0
L	50	PRO	-	insertion	UNP G1TPV0
L	51	ALA	-	insertion	UNP G1TPV0
L	52	ALA	-	insertion	UNP G1TPV0
L	53	GLY	-	insertion	UNP G1TPV0
L	54	PRO	-	insertion	UNP G1TPV0
L	55	ILE	-	insertion	UNP G1TPV0

- Molecule 41 is a protein called Ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	M	138	Total	C	N	O	S	0	0
			1137	727	221	182	7		

- Molecule 42 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	N	203	Total	C	N	O	S	0	0
			1701	1072	359	266	4		

- Molecule 43 is a protein called uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	O	199	Total	C	N	O	S	0	0
			1630	1051	319	255	5		

- Molecule 44 is a protein called uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	P	153	Total	C	N	O	S	0	0
			1242	777	241	215	9		

- Molecule 45 is a protein called eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Q	187	Total	C	N	O	S	0	0
			1515	946	315	250	4		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	6	ARG	LEU	conflict	UNP G1TX70
Q	14	ARG	TRP	conflict	UNP G1TX70
Q	23	ILE	MET	conflict	UNP G1TX70
Q	24	TYR	CYS	conflict	UNP G1TX70
Q	38	ARG	HIS	conflict	UNP G1TX70
Q	57	ASN	LYS	conflict	UNP G1TX70
Q	66	MET	VAL	conflict	UNP G1TX70
Q	74	GLY	ASP	conflict	UNP G1TX70
Q	75	ARG	PRO	conflict	UNP G1TX70
Q	86	VAL	ILE	conflict	UNP G1TX70
Q	110	ARG	HIS	conflict	UNP G1TX70
Q	117	GLY	GLU	conflict	UNP G1TX70
Q	124	ASP	HIS	conflict	UNP G1TX70
Q	150	ARG	GLN	conflict	UNP G1TX70
Q	172	ARG	GLY	conflict	UNP G1TX70
Q	184	ARG	TRP	conflict	UNP G1TX70

- Molecule 46 is a protein called eL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	R	180	Total	C	N	O	S	0	0
			1508	933	328	238	9		

- Molecule 47 is a protein called eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	S	176	Total	C	N	O	S	0	0
			1462	930	285	236	11		

- Molecule 48 is a protein called eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	T	159	Total	C	N	O	S	0	0
			1298	823	252	217	6		

- Molecule 49 is a protein called eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	U	99	Total	C	N	O	S	0	0
			809	519	141	147	2		

- Molecule 50 is a protein called eL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	V	131	Total	C	N	O	S	0	0
			979	618	184	172	5		

- Molecule 51 is a protein called Ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	W	106	Total	C	N	O	S	0	0
			860	538	174	144	4		

- Molecule 52 is a protein called uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	X	118	Total	C	N	O	S	0	0
			967	618	181	167	1		

- Molecule 53 is a protein called Ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	Y	134	Total	C	N	O	S	0	0
			1115	700	226	186	3		

- Molecule 54 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	Z	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

- Molecule 55 is a protein called eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	SS	96	Total	C	N	O	S	0	0
			810	530	143	131	6		

- Molecule 56 is a protein called uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	a	147	Total	C	N	O	S	0	0
			1162	734	239	185	4		

- Molecule 57 is a protein called eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	b	104	Total	C	N	O	S	0	0
			848	527	189	129	3		

- Molecule 58 is a protein called eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	c	98	Total	C	N	O	S	0	0
			761	481	134	140	6		

- Molecule 59 is a protein called eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	d	107	Total	C	N	O	S	0	0
			888	560	171	155	2		

- Molecule 60 is a protein called eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	e	128	Total	C	N	O	S	0	0
			1053	667	216	165	5		

- Molecule 61 is a protein called eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	f	109	Total	C	N	O	S	0	0
			876	555	174	143	4		

- Molecule 62 is a protein called eL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	g	114	Total	C	N	O	S	0	0
			906	566	187	147	6		

- Molecule 63 is a protein called uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	h	122	Total	C	N	O	S	0	0
			1013	640	204	168	1		

- Molecule 64 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	i	102	Total	C	N	O	S	0	0
			830	520	176	129	5		

- Molecule 65 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	j	86	Total	C	N	O	S	0	0
			705	434	155	111	5		

- Molecule 66 is a protein called eL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	k	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

- Molecule 67 is a protein called eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	l	50	Total	C	N	O	S	0	0
			447	286	96	64	1		

- Molecule 68 is a protein called eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	m	52	Total	C	N	O	S	0	0
			429	266	90	67	6		

- Molecule 69 is a protein called 60s ribosomal protein l41.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	n	25	Total	C	N	O	S	0	0
			239	145	64	27	3		

- Molecule 70 is a protein called eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	o	104	Total	C	N	O	S	0	0
			851	533	174	138	6		

- Molecule 71 is a protein called ribosomal protein eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	p	91	Total	C	N	O	S	0	0
			708	445	136	120	7		

- Molecule 72 is a protein called uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	q	217	Total	C	N	O	S	0	0
			1710	1086	300	316	8		

- Molecule 73 is a protein called eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	r	124	Total	C	N	O	S	0	0
			994	616	205	167	6		

- Molecule 74 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	s	196	Total	C	N	O	S	0	0
			1507	959	263	276	9		

- Molecule 75 is a protein called uL11.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	t	153	Total	C	N	O	S	0	0
			1160	722	218	217	3		

- Molecule 76 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	u	213	Total	C	N	O	S	0	0
			1729	1098	309	308	14		

- Molecule 77 is a protein called uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	v	221	Total	C	N	O	S	0	0
			1716	1111	295	301	9		

- Molecule 78 is a protein called Ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	w	228	Total	C	N	O	S	0	0
			1768	1126	318	316	8		

- Molecule 79 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	x	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
x	25	GLY	SER	conflict	UNP G1TK17
x	51	ARG	LYS	conflict	UNP G1TK17
x	78	THR	ALA	conflict	UNP G1TK17
x	156	VAL	MET	conflict	UNP G1TK17

- Molecule 80 is a protein called Ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	y	185	Total	C	N	O	S	0	0
			1471	921	277	266	7		

- Molecule 81 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	z	237	Total	C	N	O	S	0	0
			1923	1200	387	329	7		

- Molecule 82 is a protein called Ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	TT	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 83 is a protein called Ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	UU	142	Total	C	N	O	S	0	0
			1128	717	213	195	3		

- Molecule 84 is a protein called Ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	VV	141	Total	C	N	O	S	0	0
			1098	693	219	183	3		

- Molecule 85 is a protein called uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	WW	120	Total	C	N	O	S	0	0
			997	635	187	168	7		

- Molecule 86 is a protein called Protein transport protein Sec61 subunit alpha isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	XX	426	Total	C	N	O	S	0	0
			3313	2181	535	576	21		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
XX	145	SER	THR	conflict	UNP P38377

- Molecule 87 is a protein called Protein transport protein Sec61 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	YY	62	Total	C	N	O	S	0	0
			494	326	86	79	3		

- Molecule 88 is a protein called Protein transport protein Sec61 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
88	ZZ	29	Total	C	N	O	S	0	0
			229	157	36	34	2		

- Molecule 89 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
89	LL	1	Total	Zn	0
			1	1	
89	g	1	Total	Zn	0
			1	1	
89	j	1	Total	Zn	0
			1	1	
89	m	1	Total	Zn	0
			1	1	
89	o	1	Total	Zn	0
			1	1	
89	p	1	Total	Zn	0
			1	1	

- Molecule 90 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
90	5	201	Total	Mg	0
			201	201	
90	7	7	Total	Mg	0
			7	7	
90	8	4	Total	Mg	0
			4	4	
90	B	1	Total	Mg	0
			1	1	
90	K	78	Total	Mg	0
			78	78	
90	P	2	Total	Mg	0
			2	2	
90	V	1	Total	Mg	0
			1	1	

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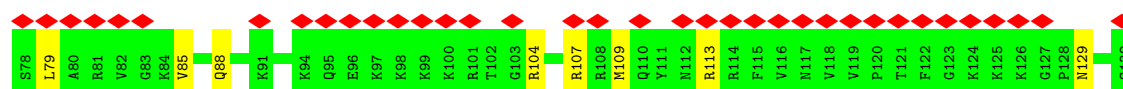
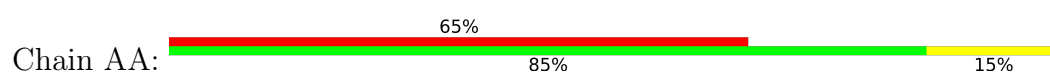
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
90	a	1	Total 1	Mg 1	0
90	e	1	Total 1	Mg 1	0
90	g	1	Total 1	Mg 1	0
90	j	1	Total 1	Mg 1	0
90	y	1	Total 1	Mg 1	0

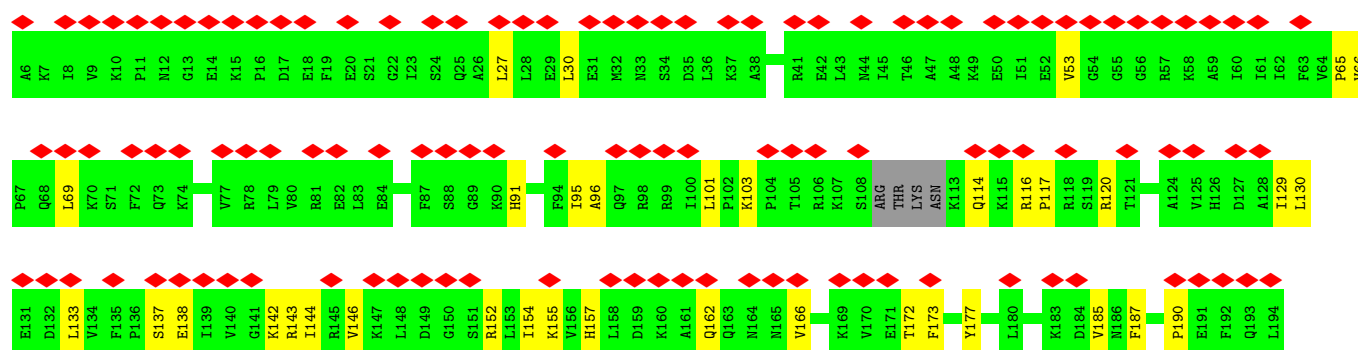
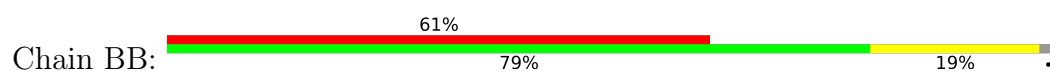
3 Residue-property plots

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.

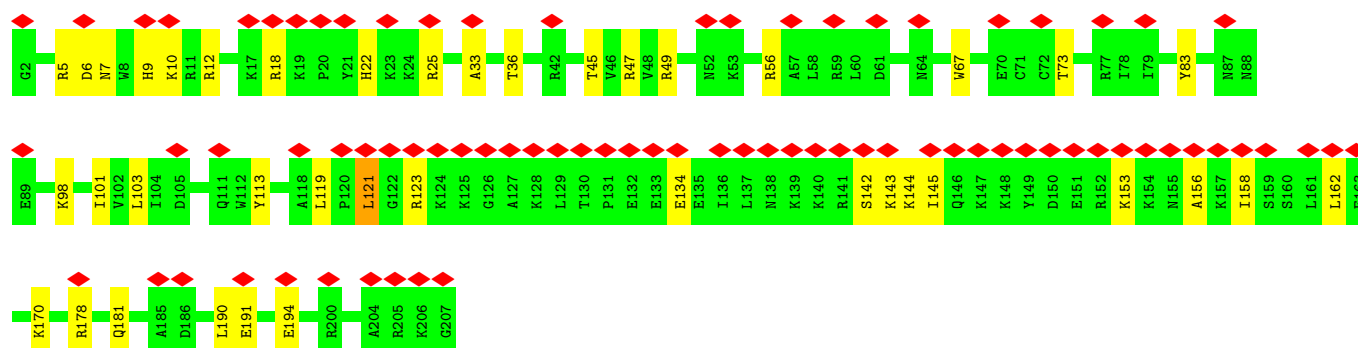
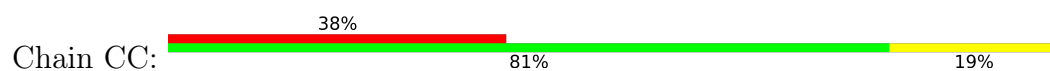
• Molecule 1: 40S ribosomal protein S30



• Molecule 2: 40S ribosomal protein S7

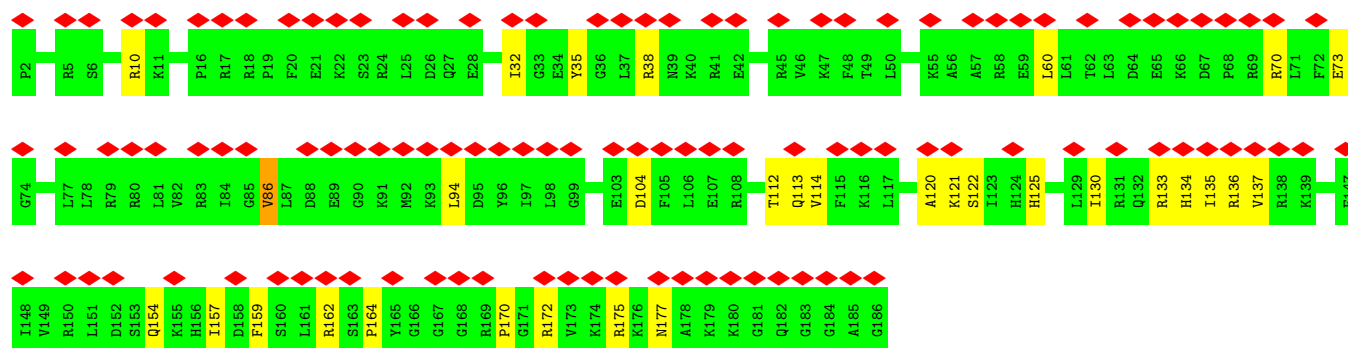


• Molecule 3: 40S ribosomal protein S8



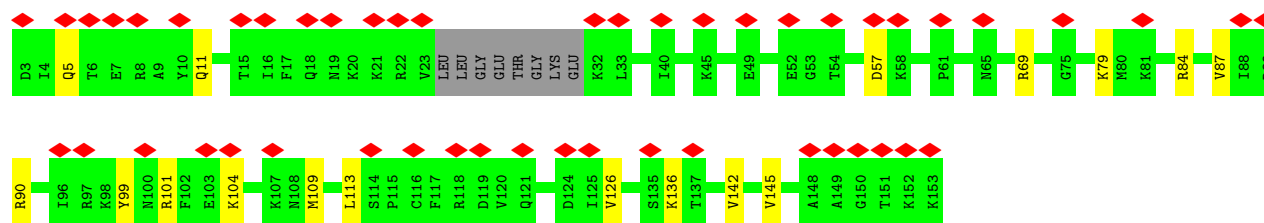
- Molecule 4: Ribosomal protein S9 (Predicted)

Chain DD: 



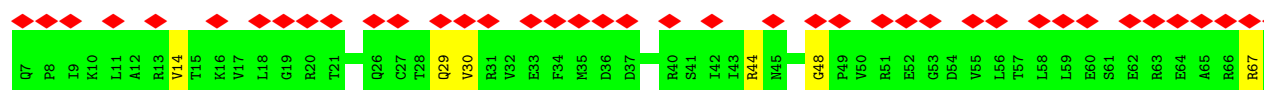
- Molecule 5: Ribosomal protein S11

Chain EE: 



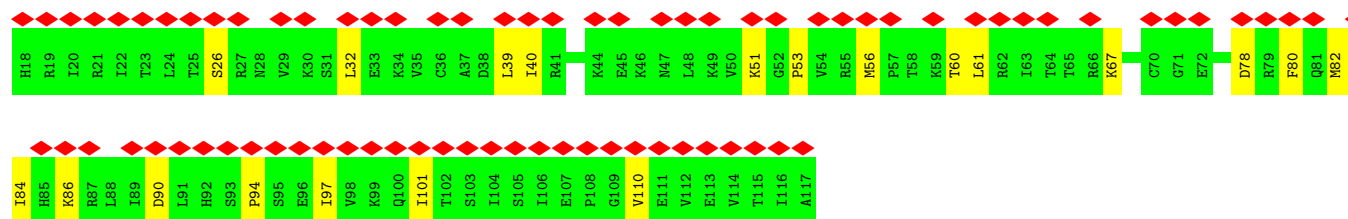
- Molecule 6: Ribosomal protein S28

Chain FF: 



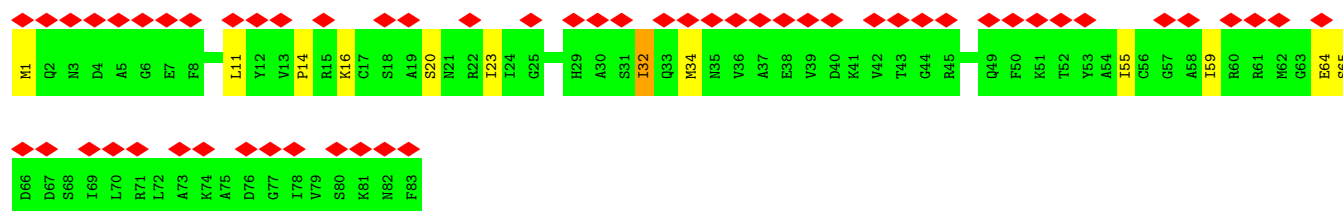
- Molecule 7: uS10

Chain GG: 

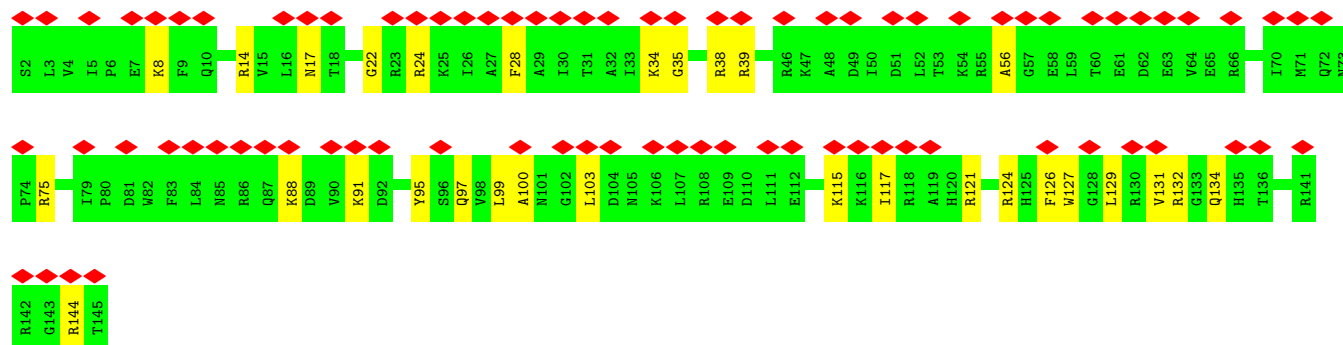
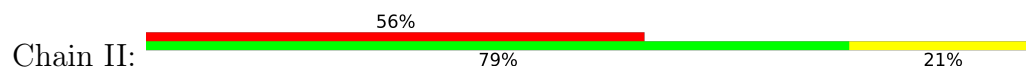


- Molecule 8: eS21

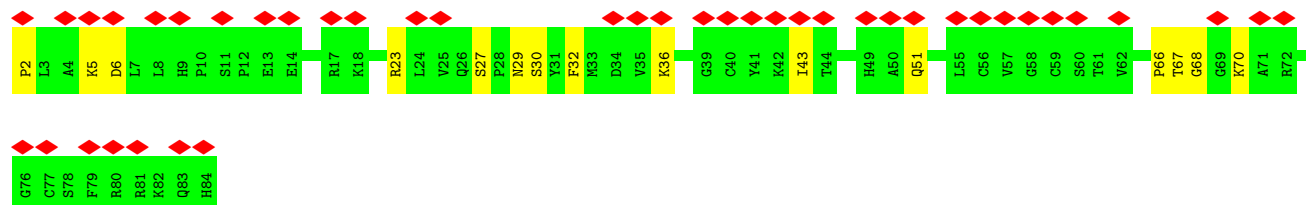
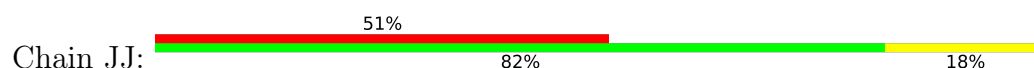
Chain HH: 



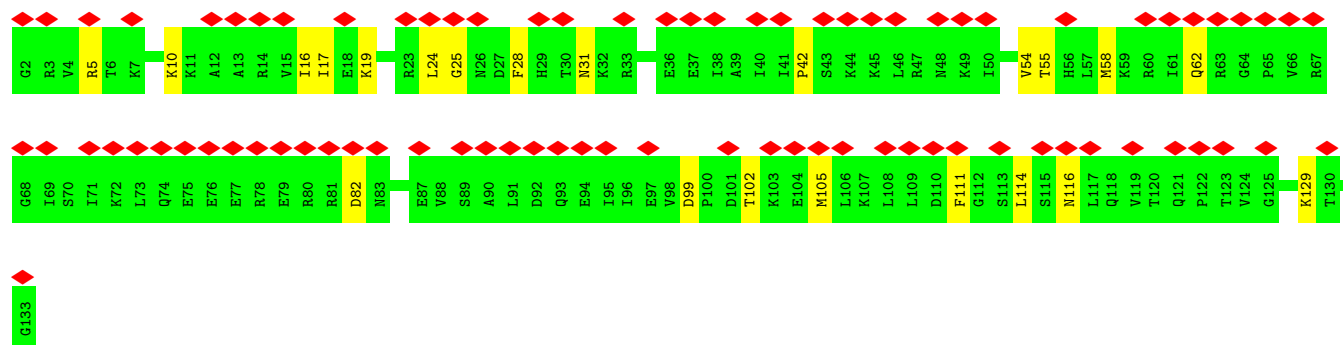
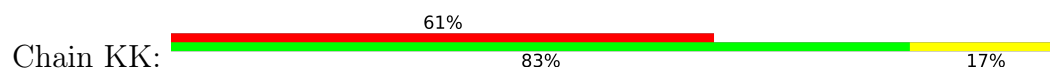
• Molecule 9: uS13



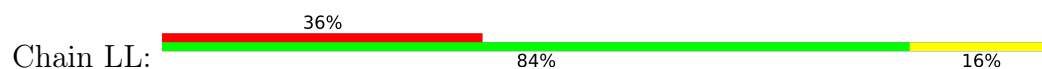
• Molecule 10: 40S ribosomal protein S27

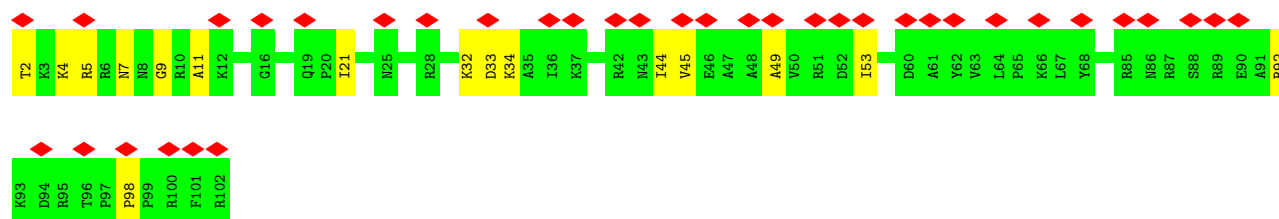


• Molecule 11: eS17

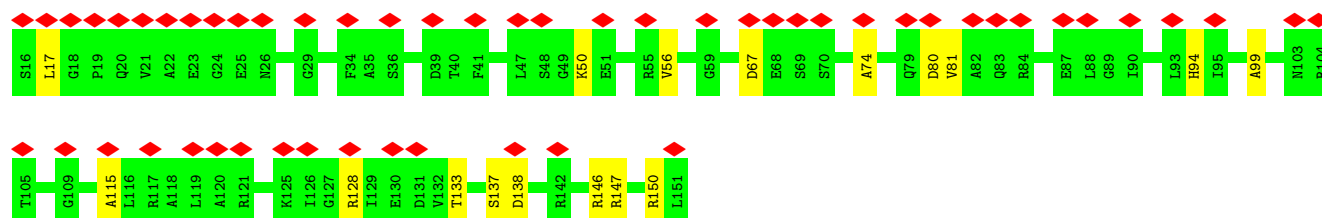
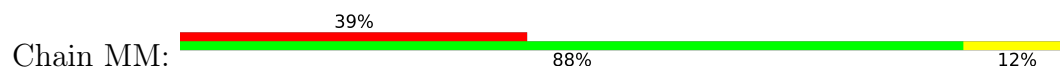


• Molecule 12: eS26

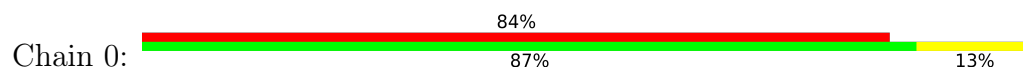




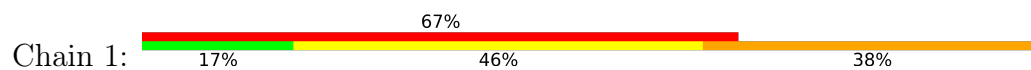
- Molecule 13: uS11



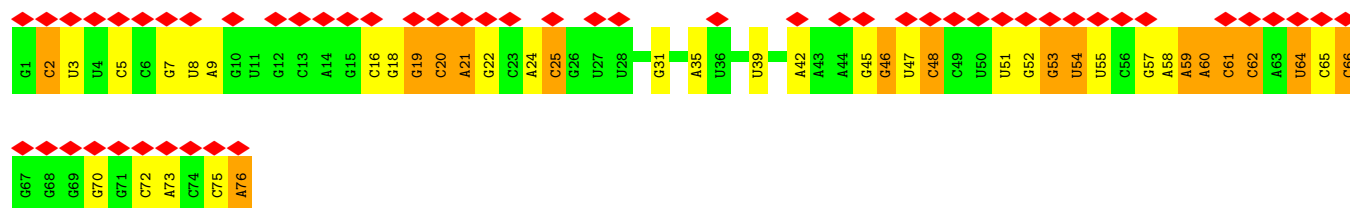
- Molecule 14: eS31



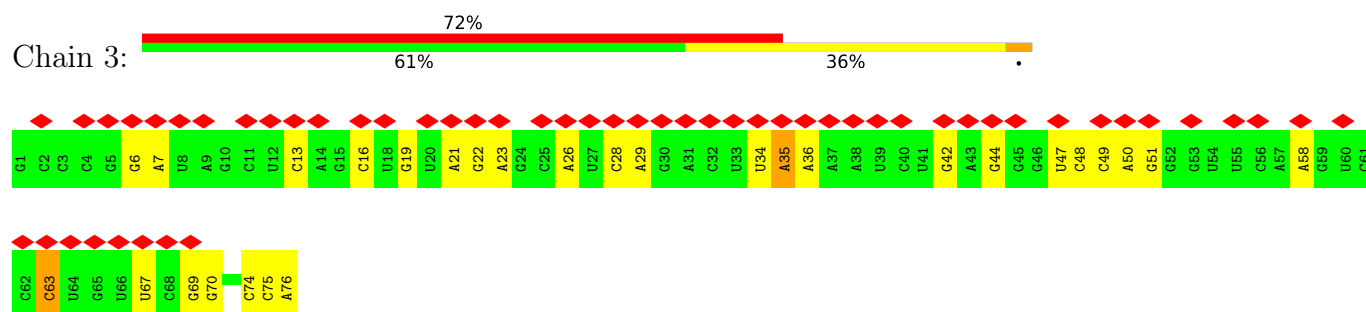
- Molecule 15: X-box-binding protein 1



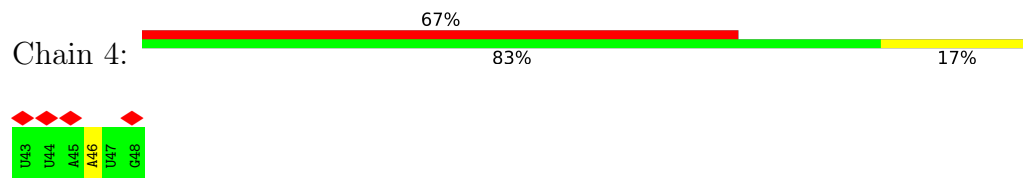
- Molecule 16: P-tRNA



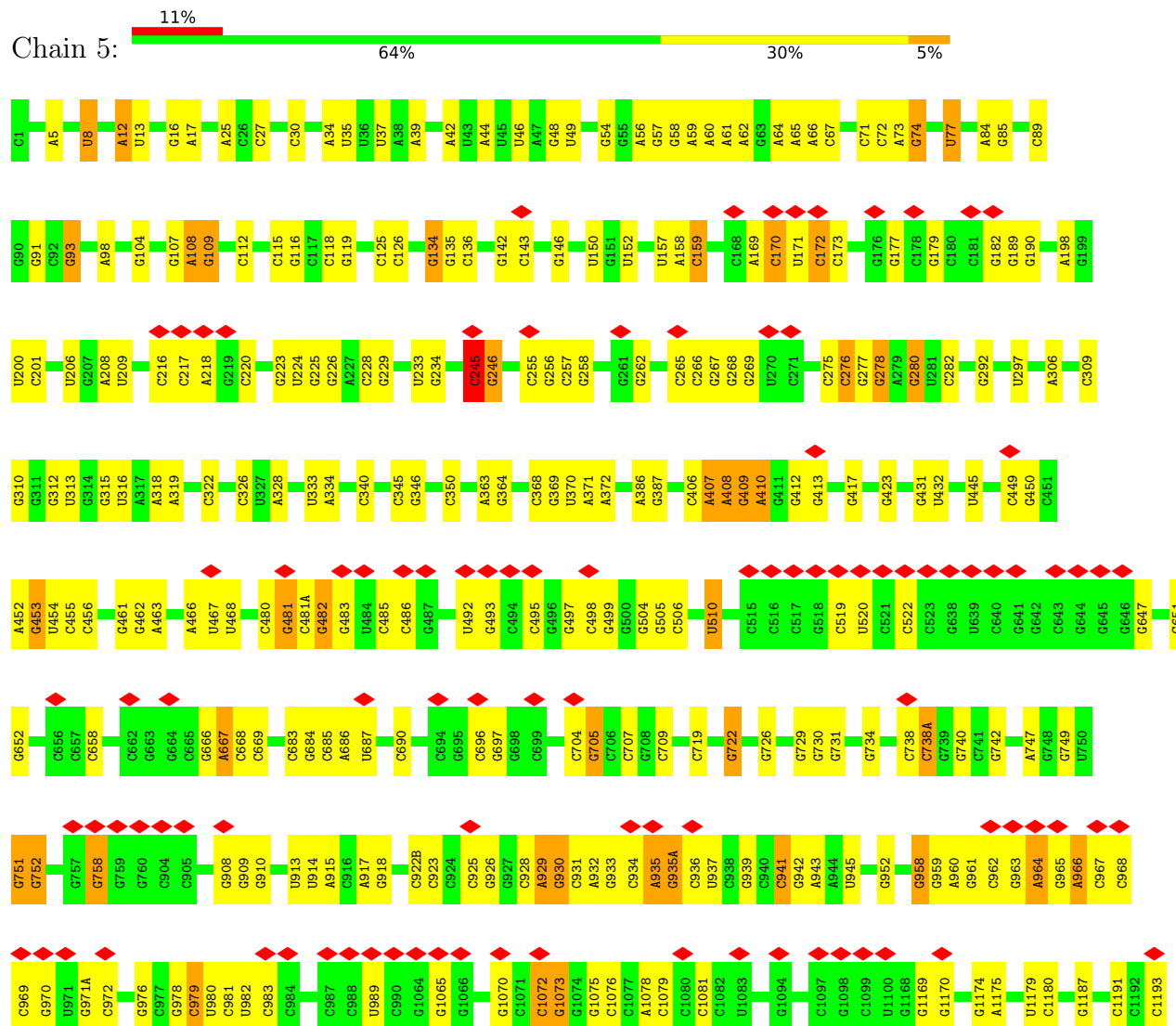
- Molecule 17: E-tRNA

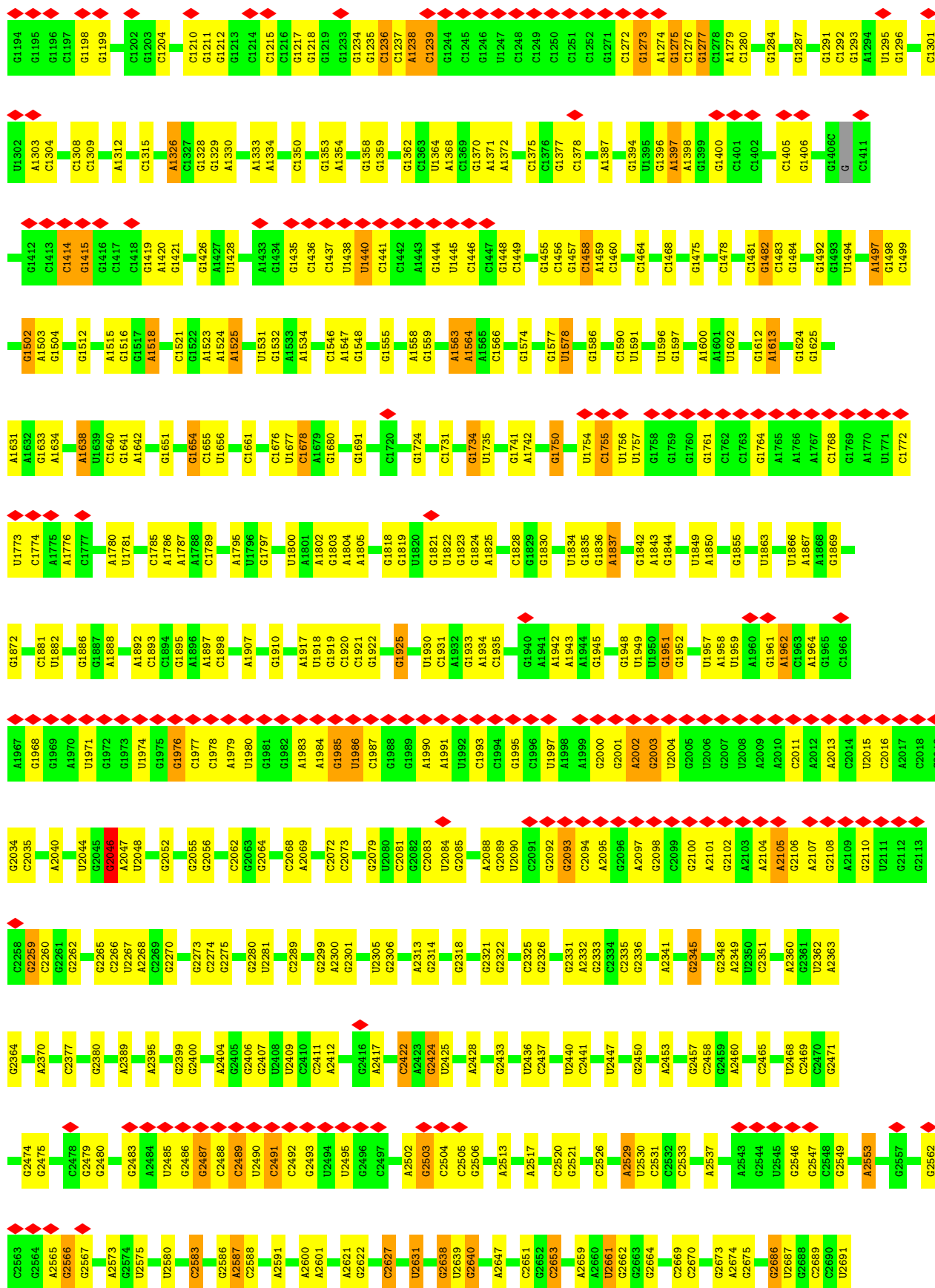


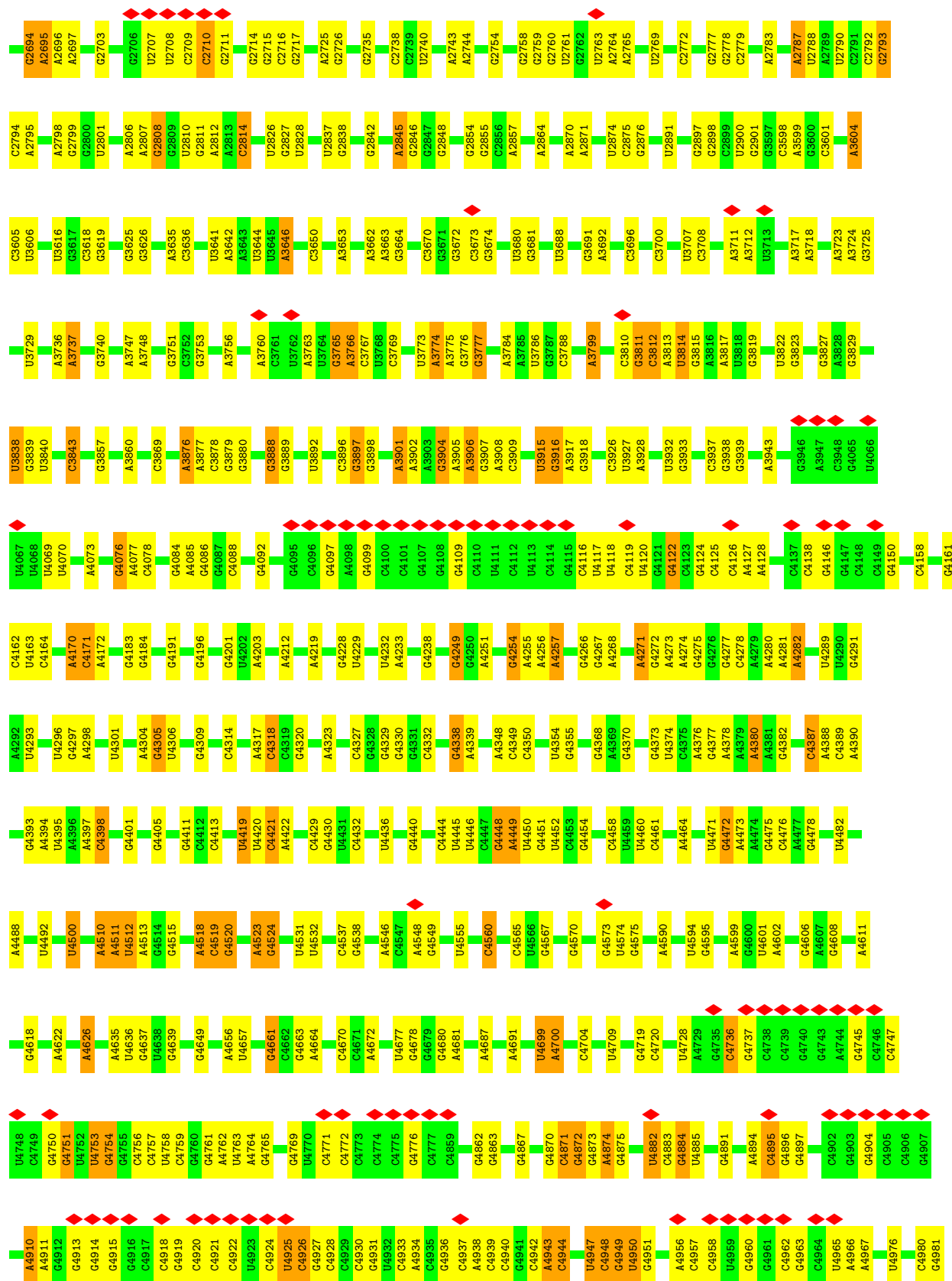
- Molecule 18: messenger RNA



- Molecule 19: 28S ribosomal RNA

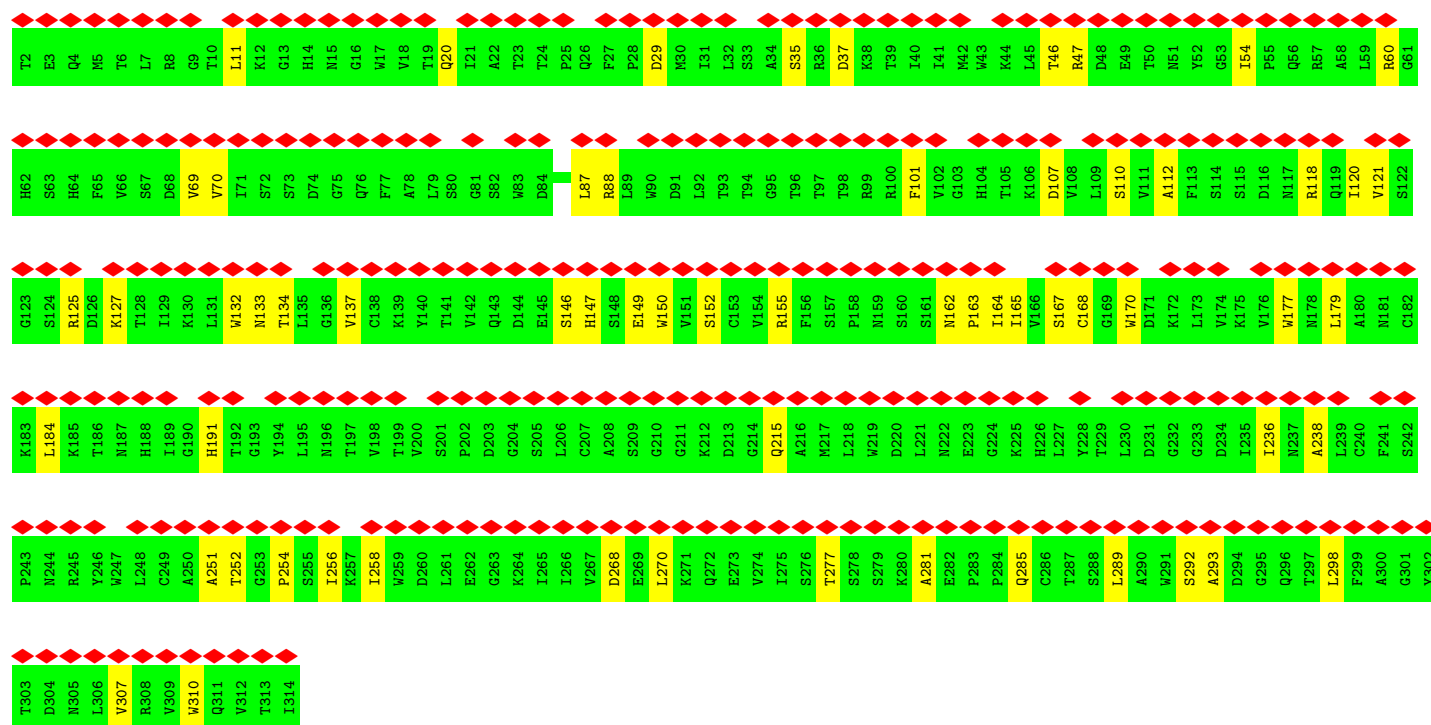
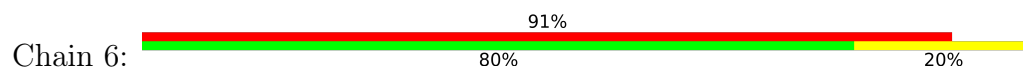




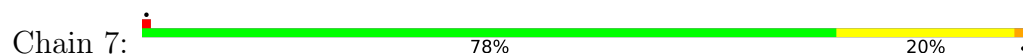




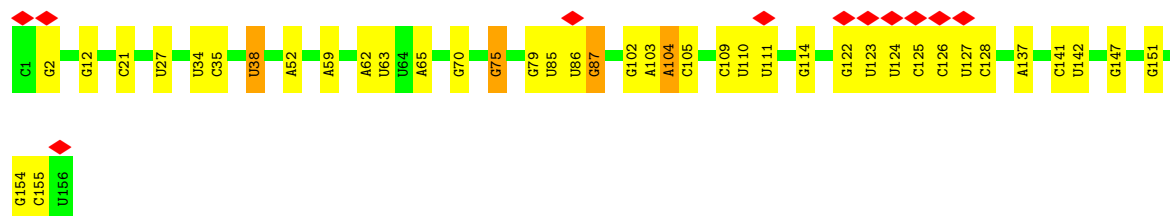
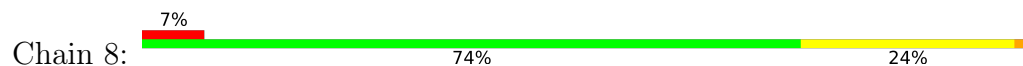
• Molecule 20: ribosomal protein RACK1



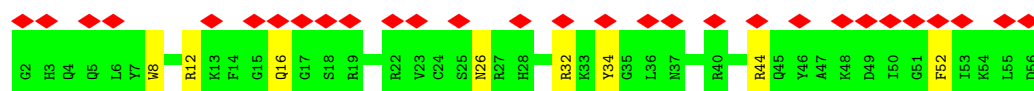
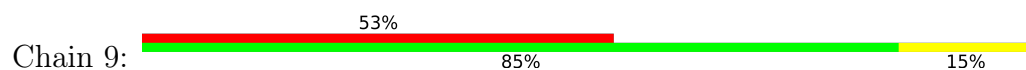
• Molecule 21: 5S ribosomal RNA



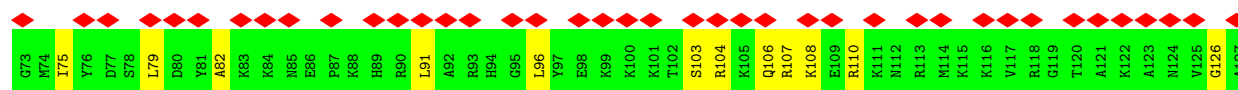
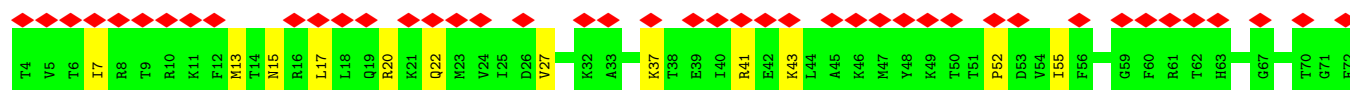
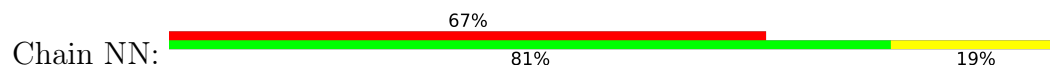
• Molecule 22: 5.8S ribosomal RNA



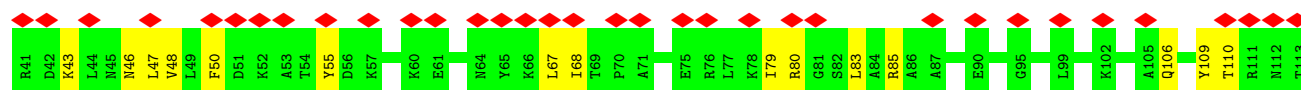
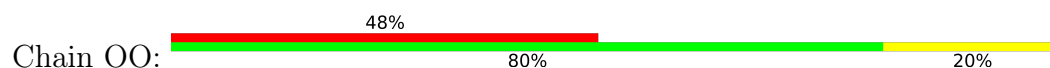
• Molecule 23: uS14



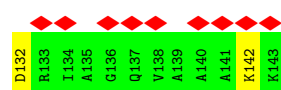
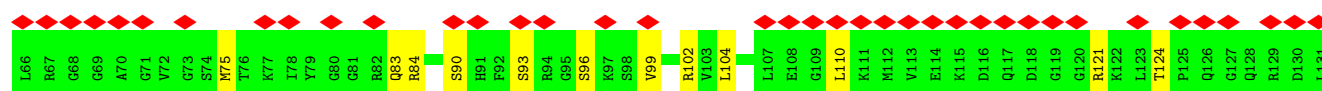
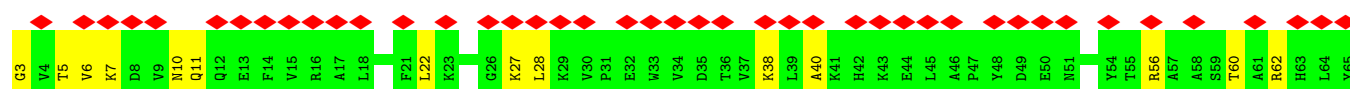
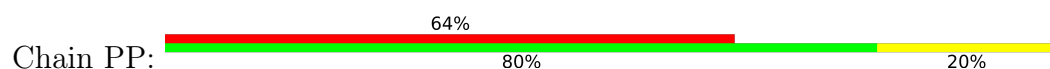
• Molecule 24: eS24



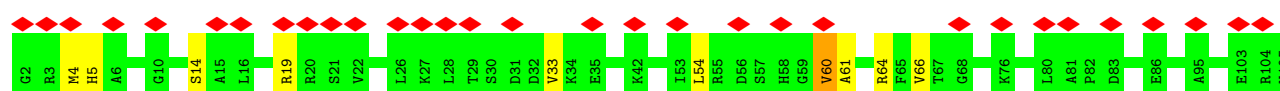
• Molecule 25: ribosomal protein eS25

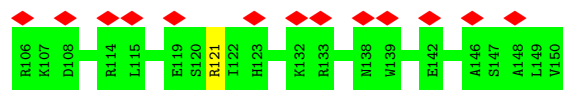


• Molecule 26: eS19

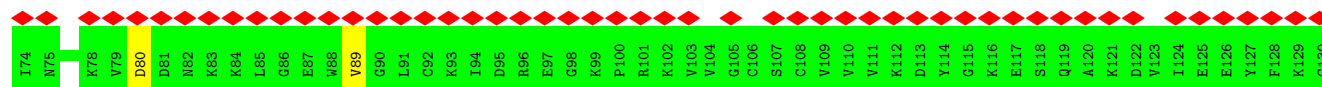
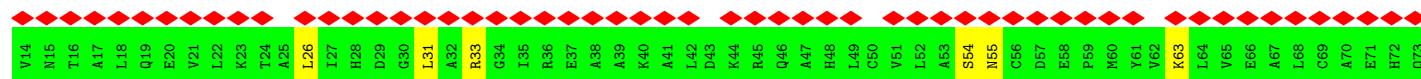


• Molecule 27: ribosomal protein uS15

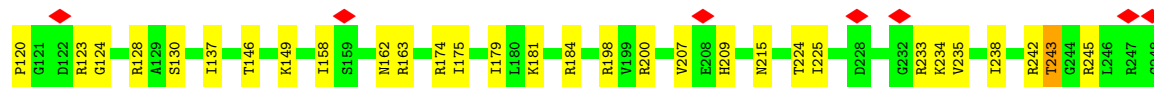
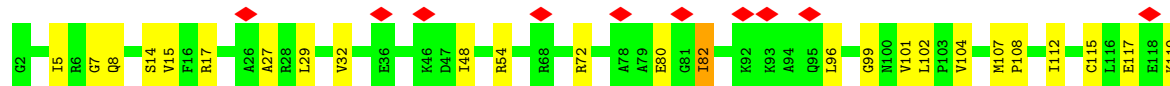
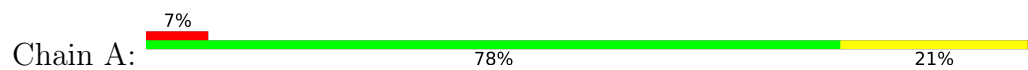




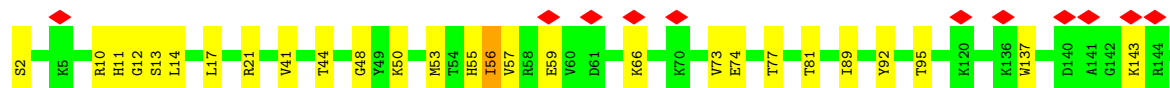
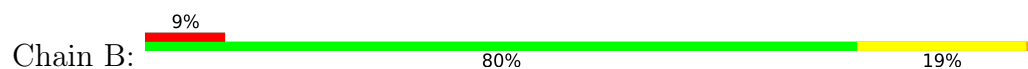
- Molecule 28: 40S ribosomal protein S12



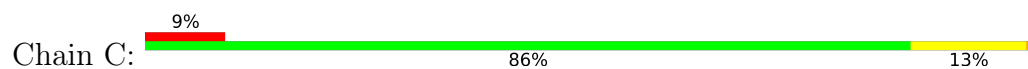
- Molecule 29: uL2

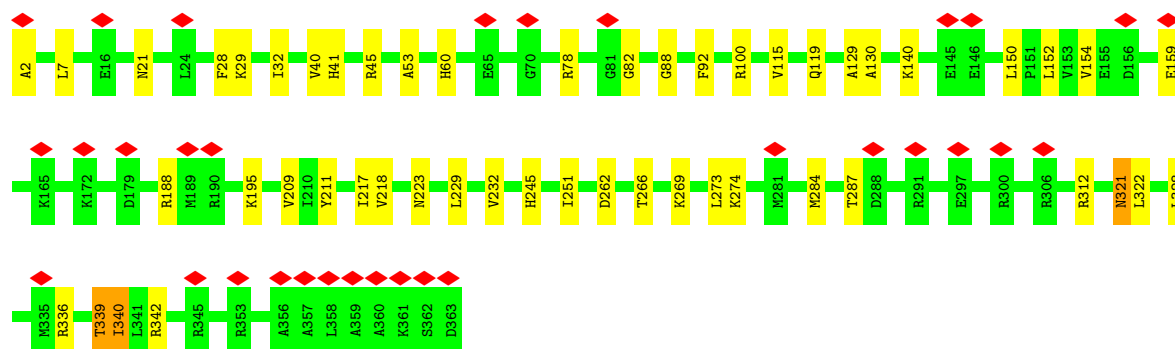


- Molecule 30: uL3

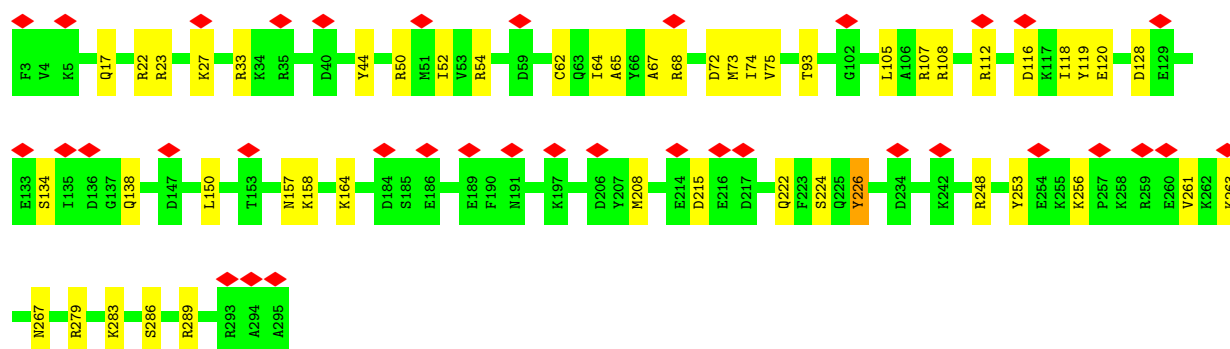
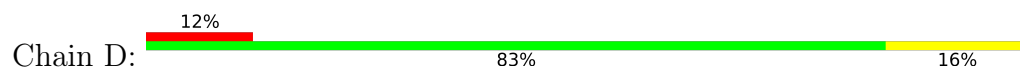


- Molecule 31: uL4

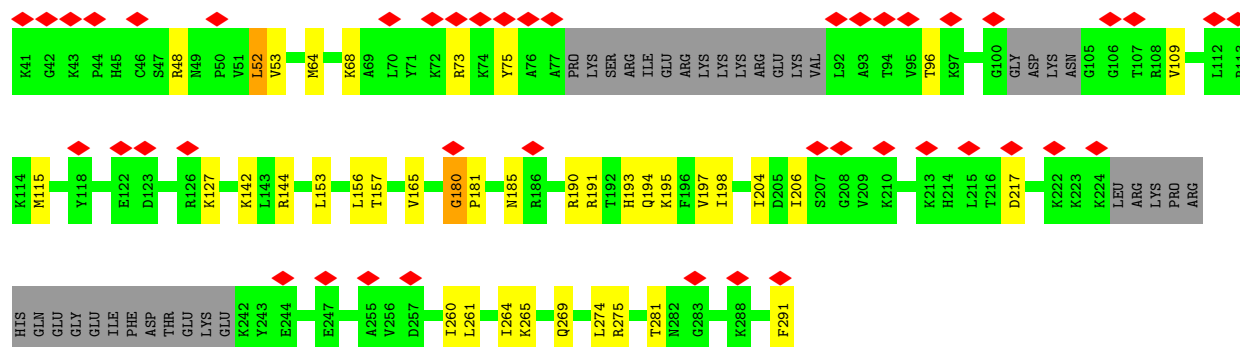




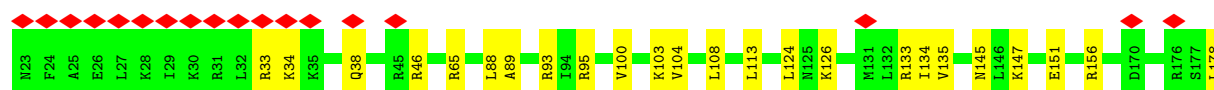
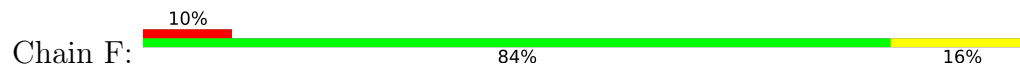
• Molecule 32: 60S ribosomal protein L5

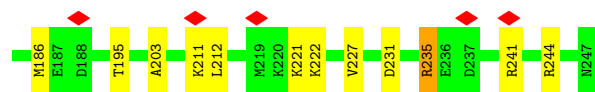


• Molecule 33: 60S ribosomal protein L6

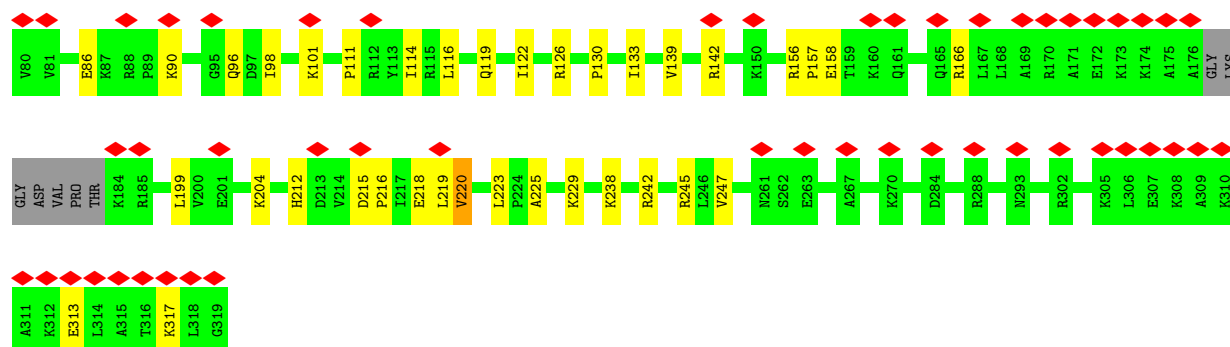
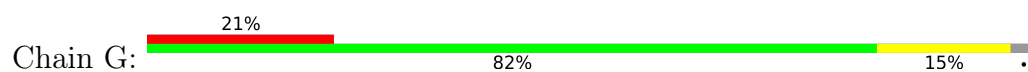


• Molecule 34: uL30

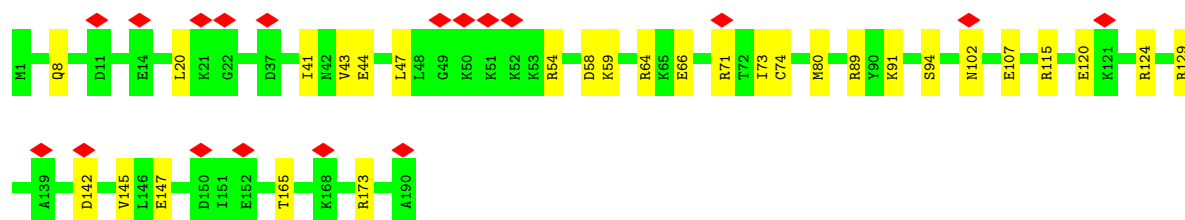
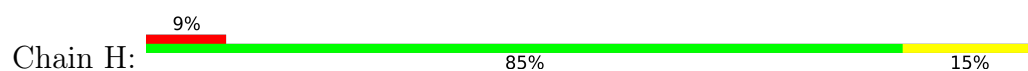




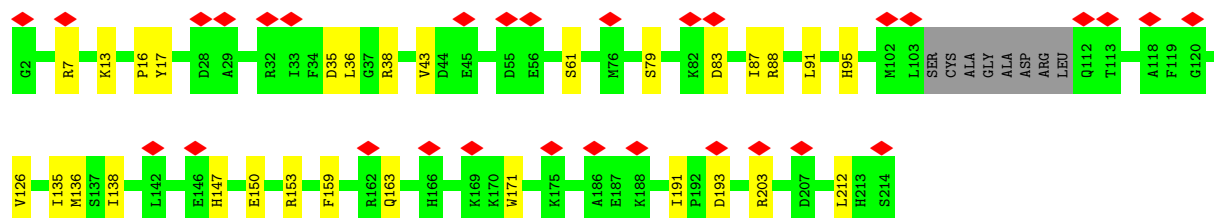
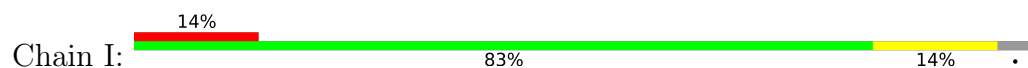
- Molecule 35: eL8



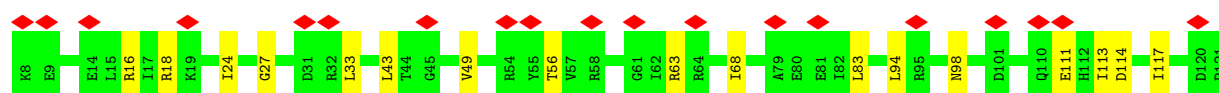
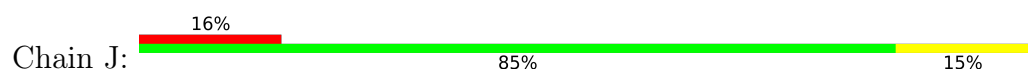
- Molecule 36: uL6

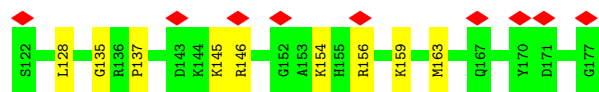


- Molecule 37: Ribosomal protein L10 (Predicted)

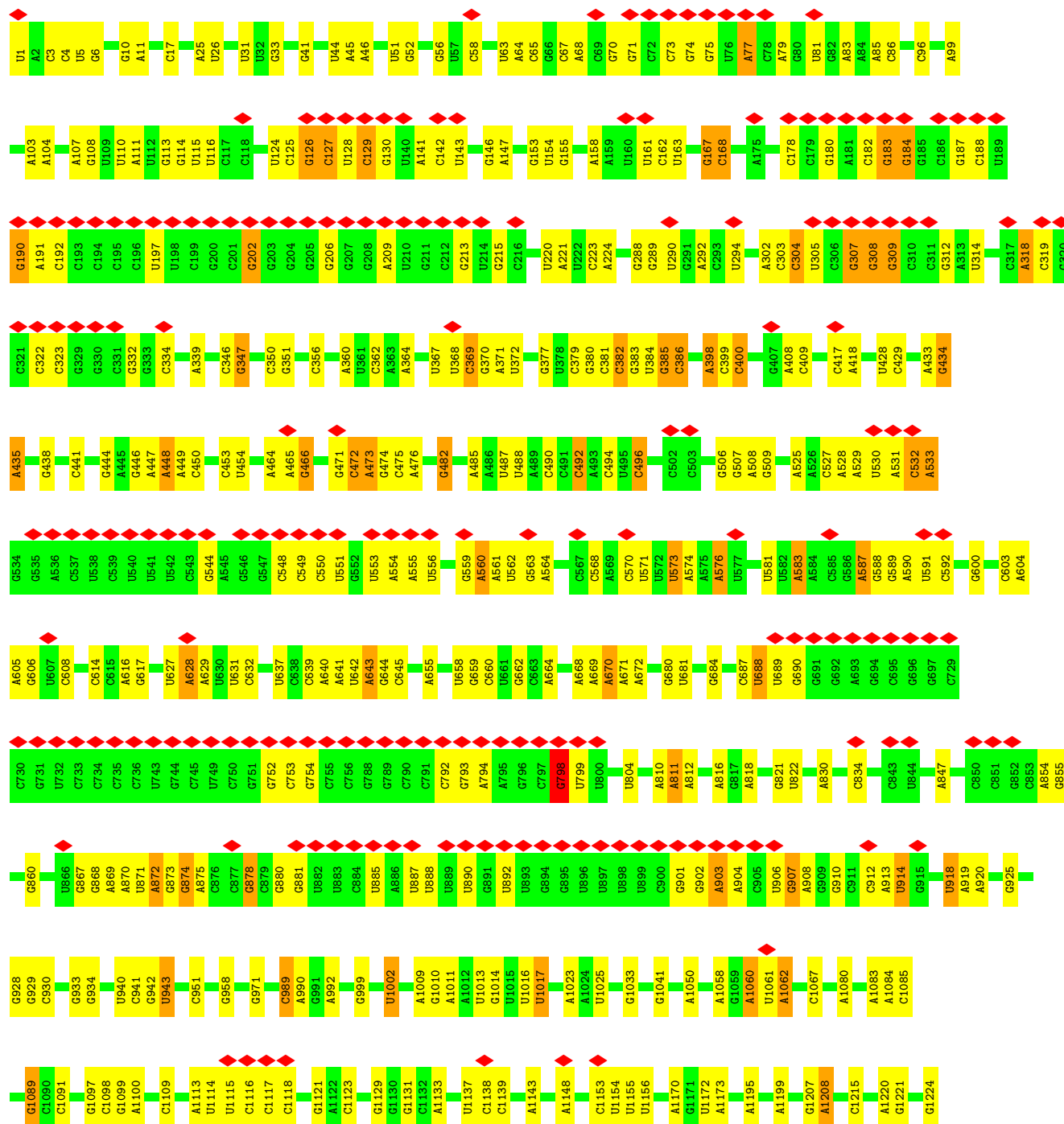


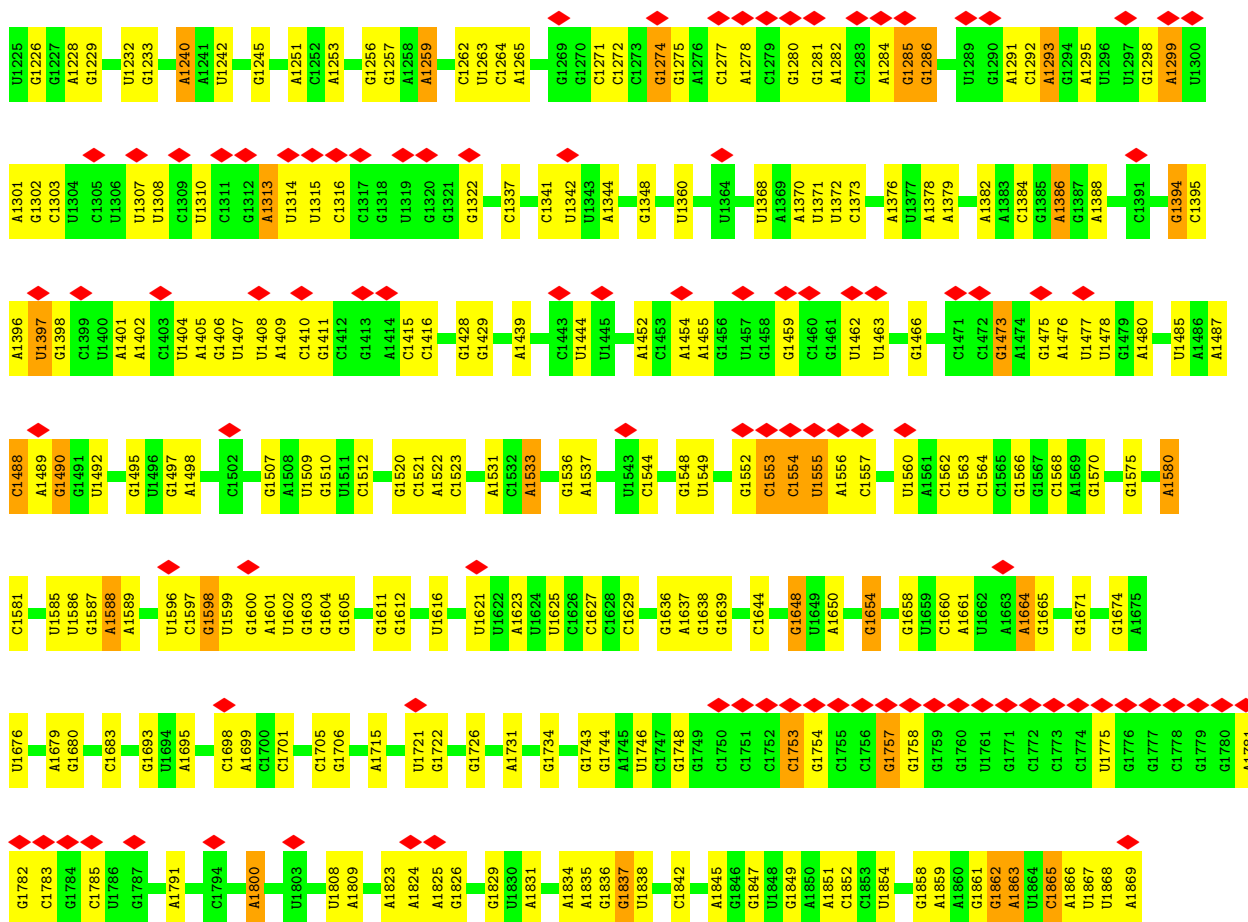
- Molecule 38: Ribosomal protein L11



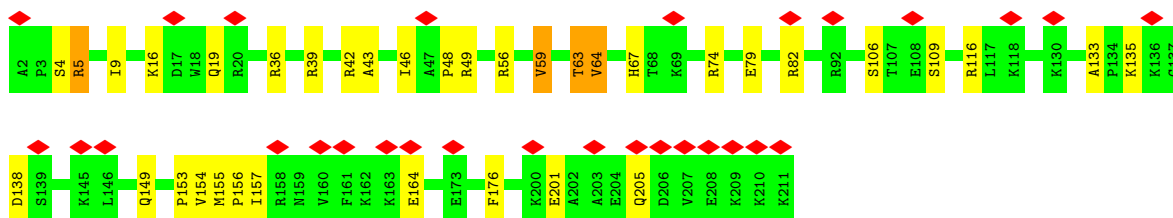
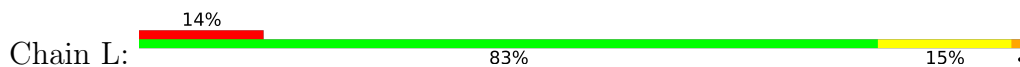


• Molecule 39: 18S ribosomal RNA

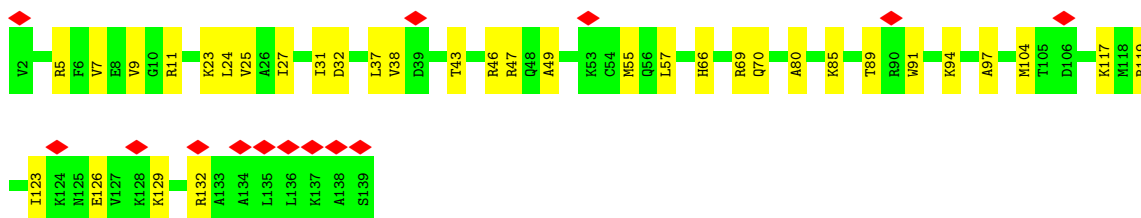
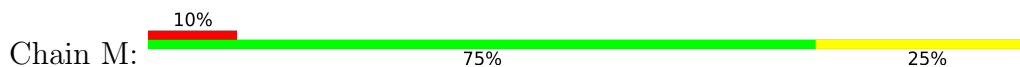




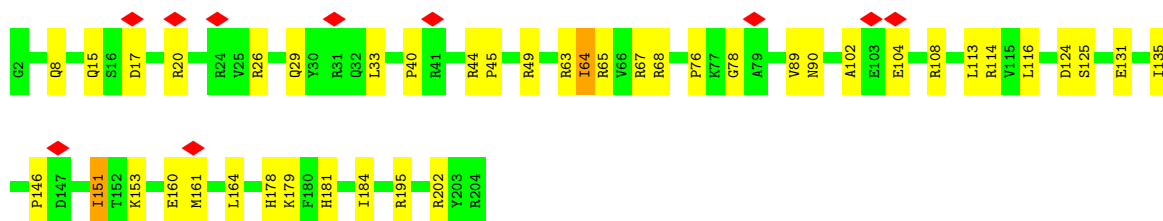
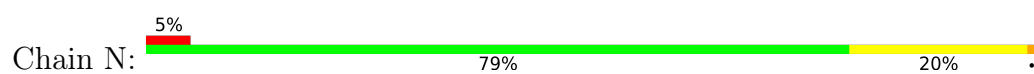
• Molecule 40: 60S ribosomal protein L13



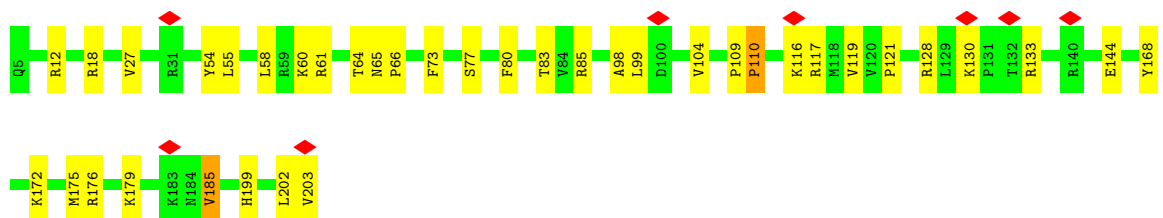
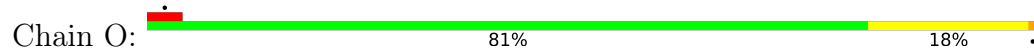
• Molecule 41: Ribosomal protein L14



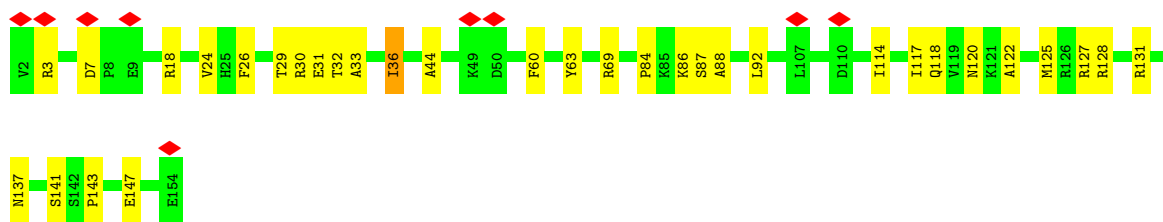
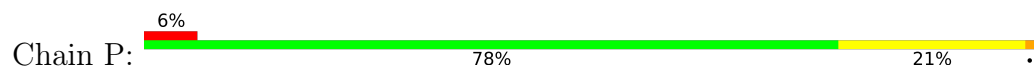
• Molecule 42: Ribosomal protein L15



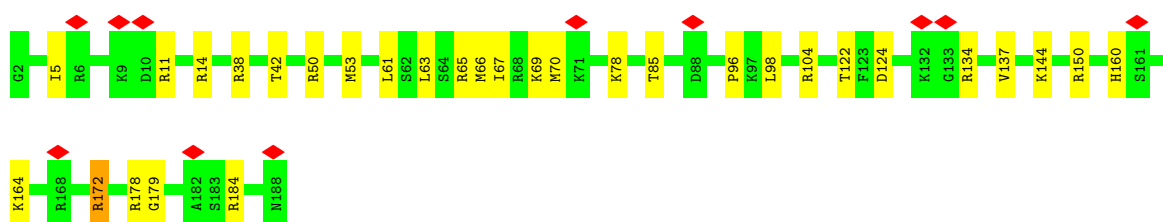
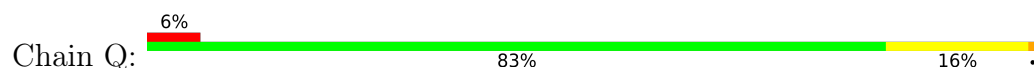
• Molecule 43: uL13



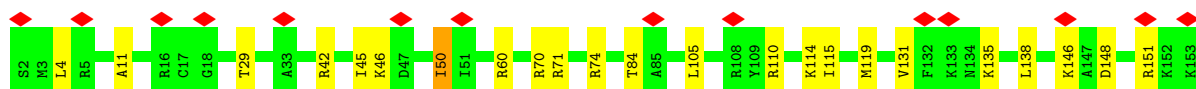
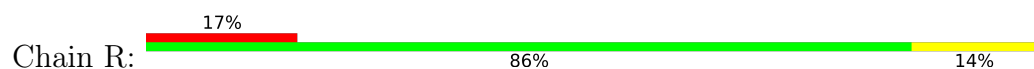
• Molecule 44: uL22

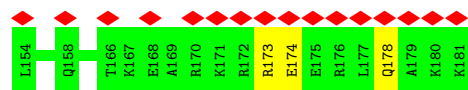


• Molecule 45: eL18

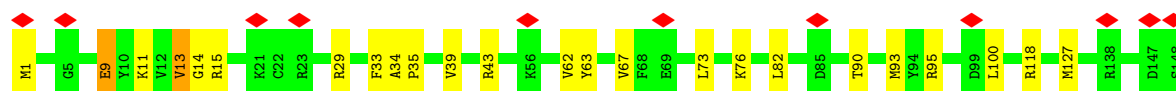
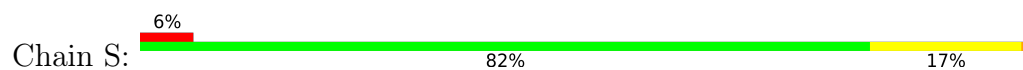


• Molecule 46: eL19

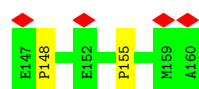
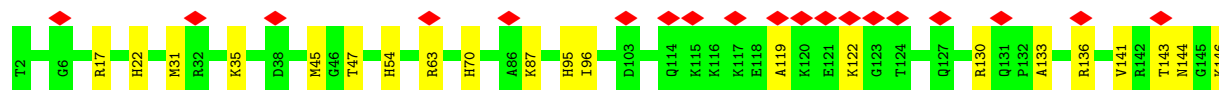
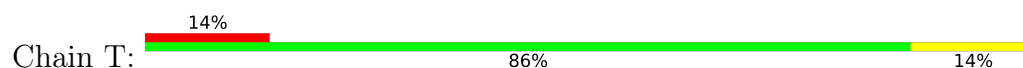




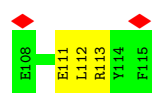
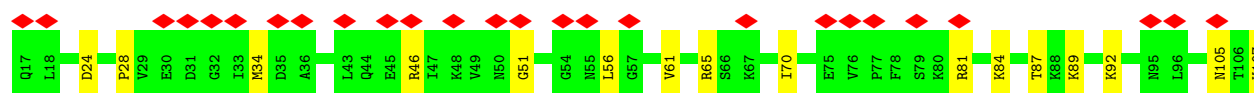
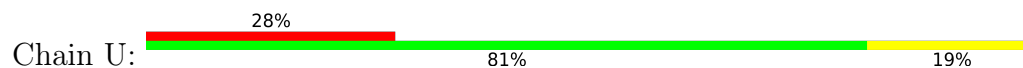
• Molecule 47: eL20



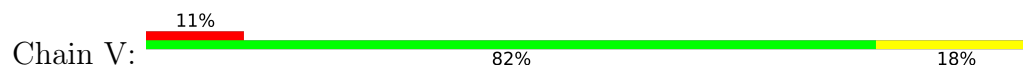
• Molecule 48: eL21



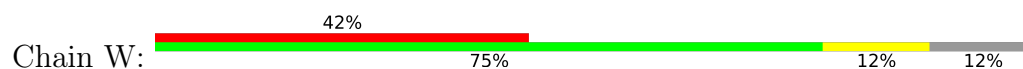
• Molecule 49: eL22

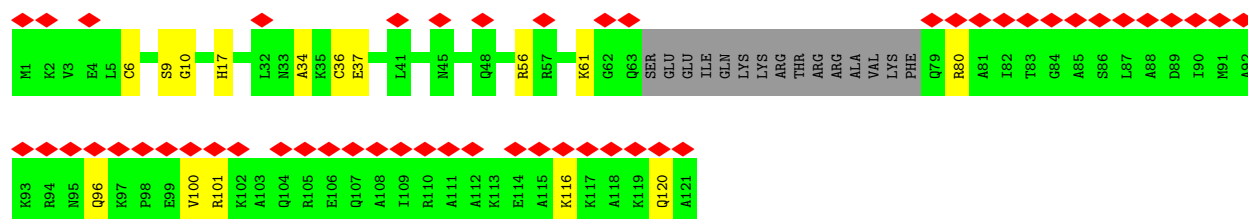


• Molecule 50: eL14

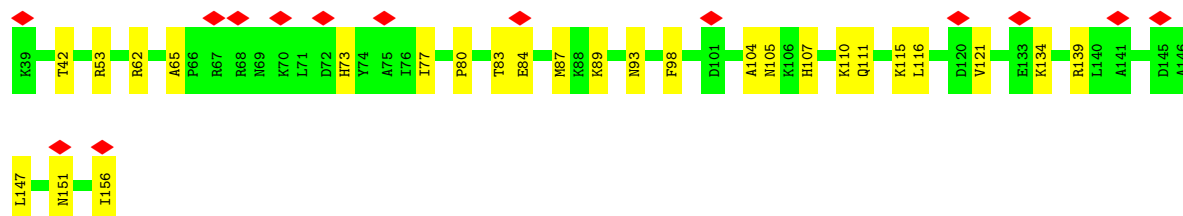
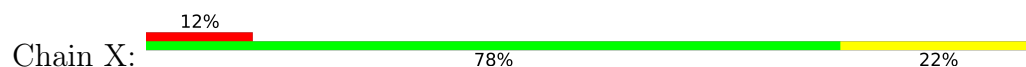


• Molecule 51: Ribosomal protein L24

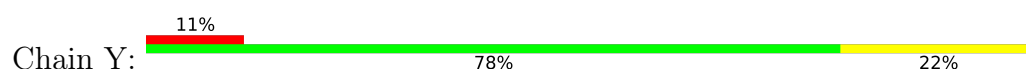




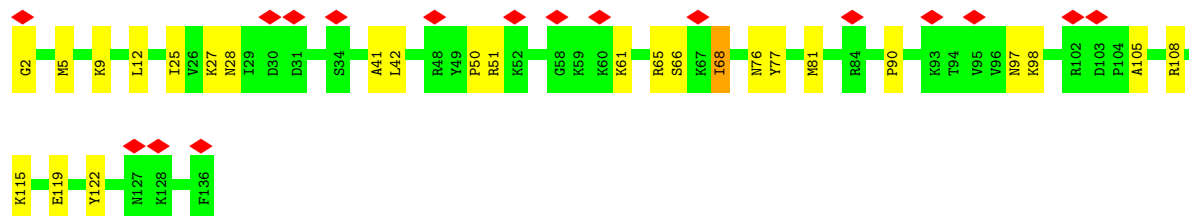
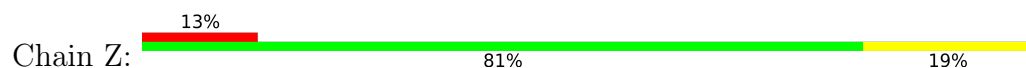
• Molecule 52: uL23



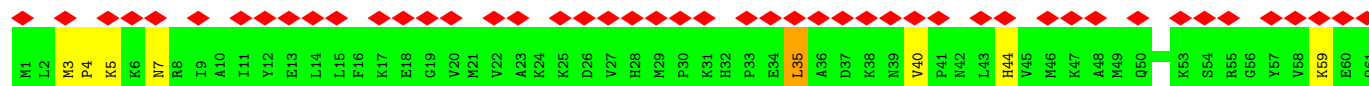
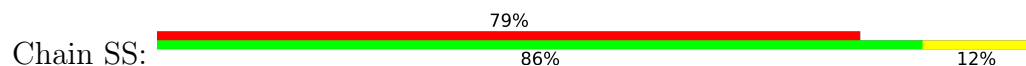
• Molecule 53: Ribosomal protein L26

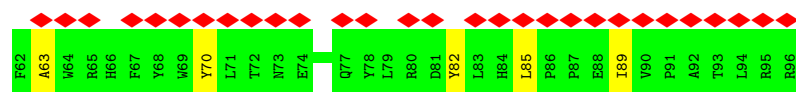


• Molecule 54: 60S ribosomal protein L27

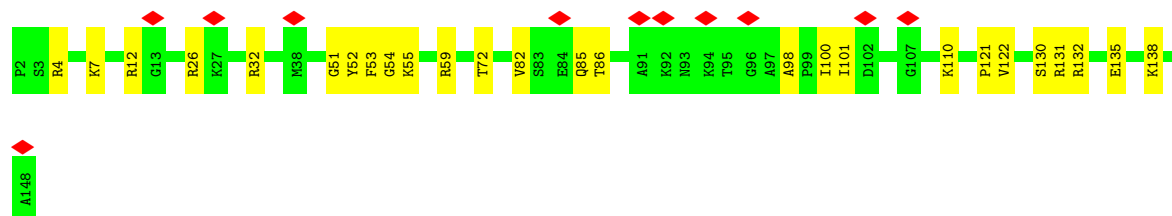
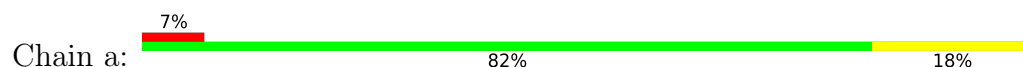


• Molecule 55: eS10

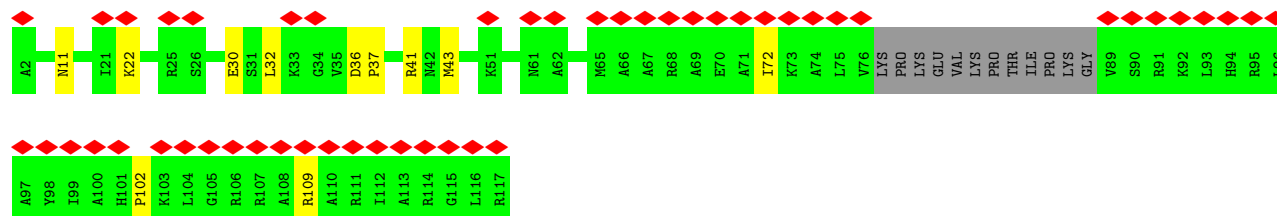
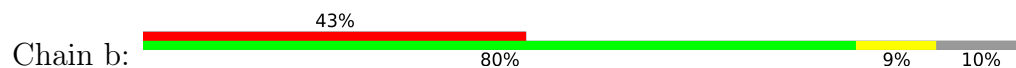




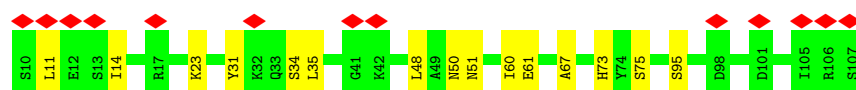
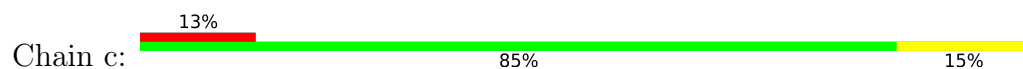
• Molecule 56: uL15



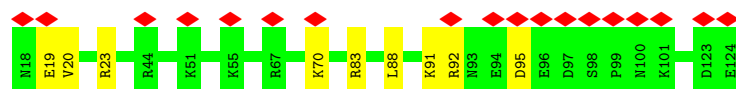
• Molecule 57: eL29



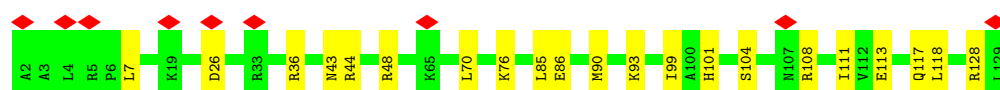
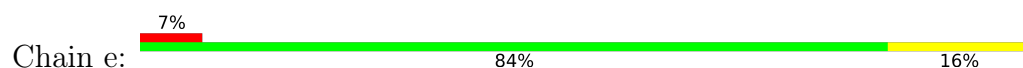
• Molecule 58: eL30



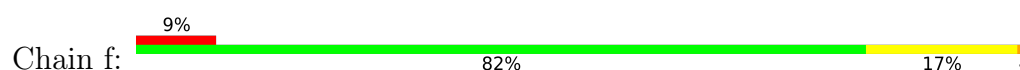
• Molecule 59: eL31



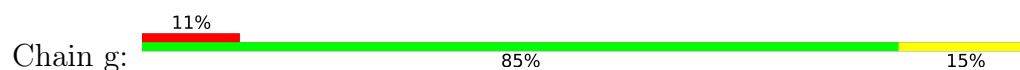
• Molecule 60: eL32



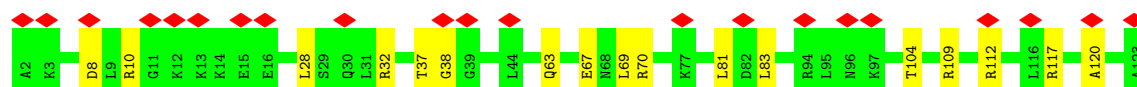
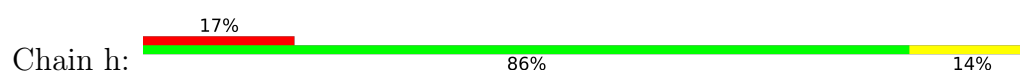
• Molecule 61: eL33



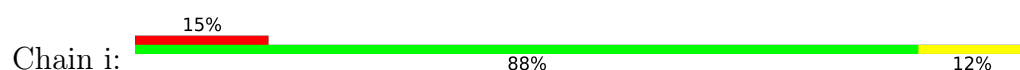
- Molecule 62: eL34



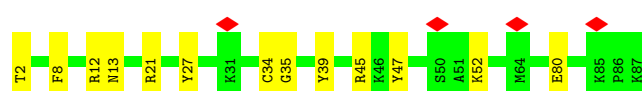
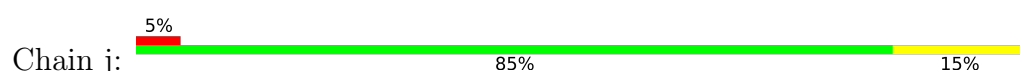
- Molecule 63: uL29



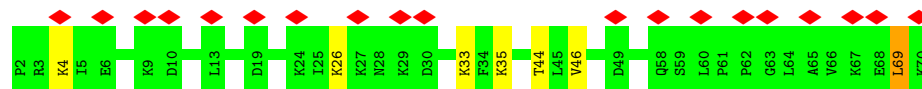
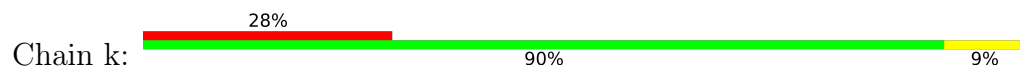
- Molecule 64: 60S ribosomal protein L36



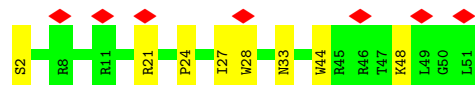
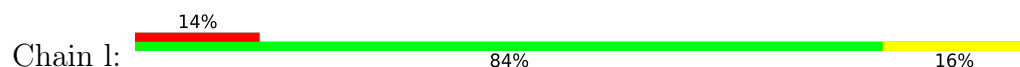
- Molecule 65: Ribosomal protein L37



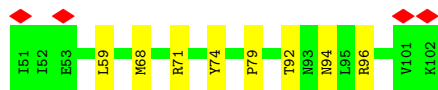
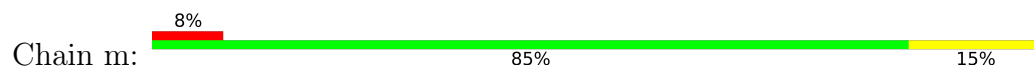
- Molecule 66: eL38



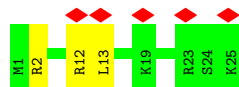
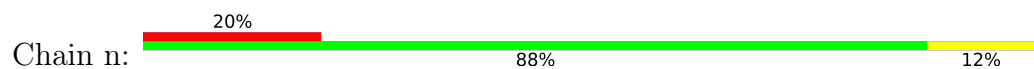
- Molecule 67: eL39



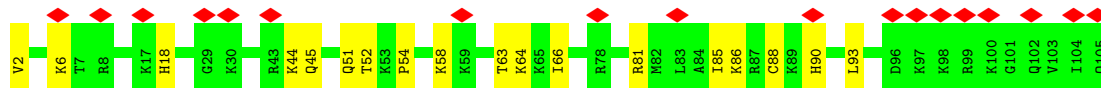
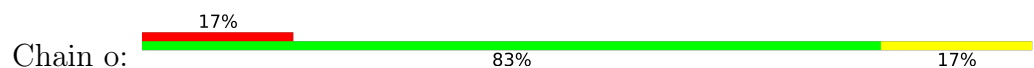
- Molecule 68: eL40



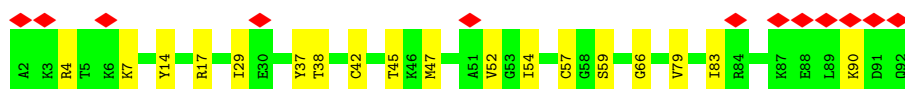
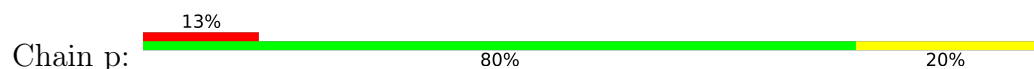
- Molecule 69: 60s ribosomal protein l41



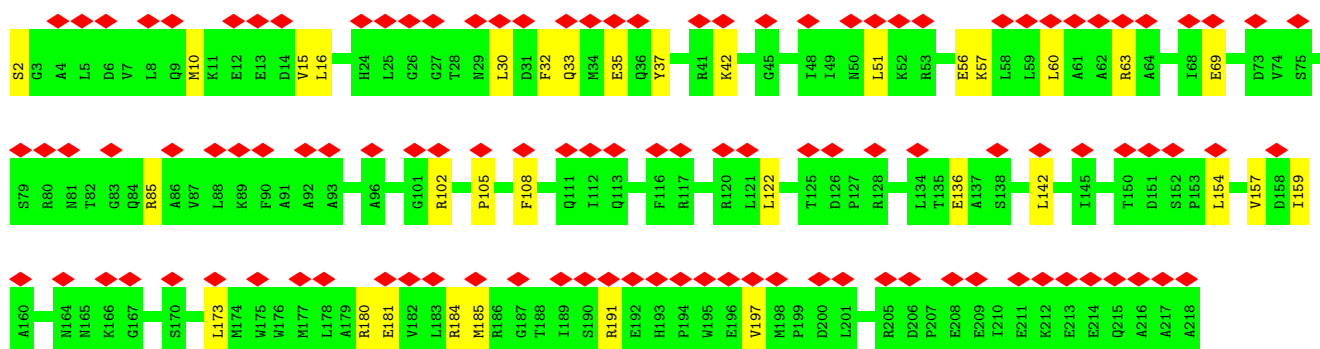
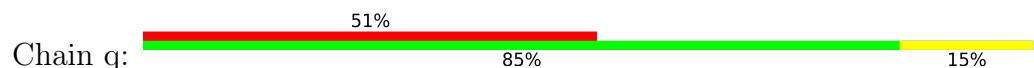
- Molecule 70: eL42



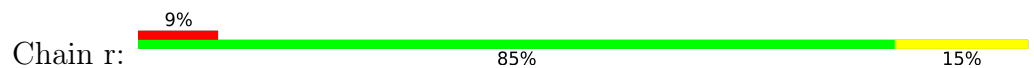
- Molecule 71: ribosomal protein eL43

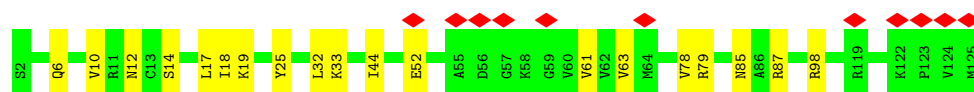


- Molecule 72: uS2

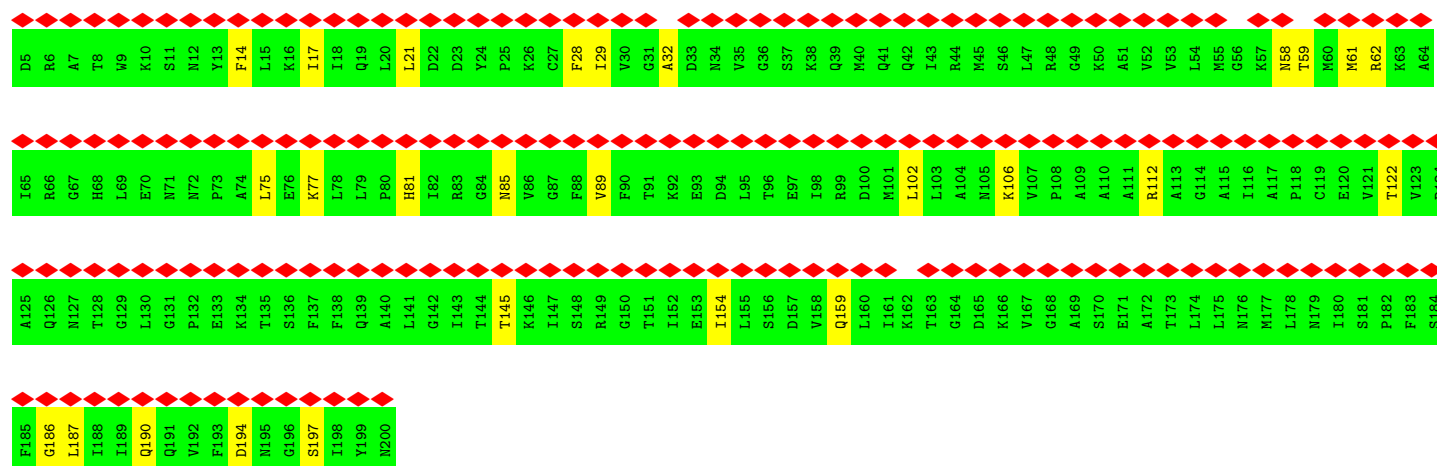
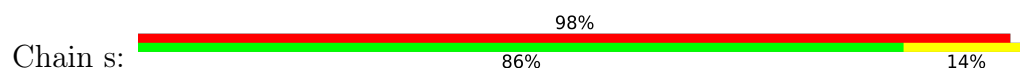


- Molecule 73: eL28

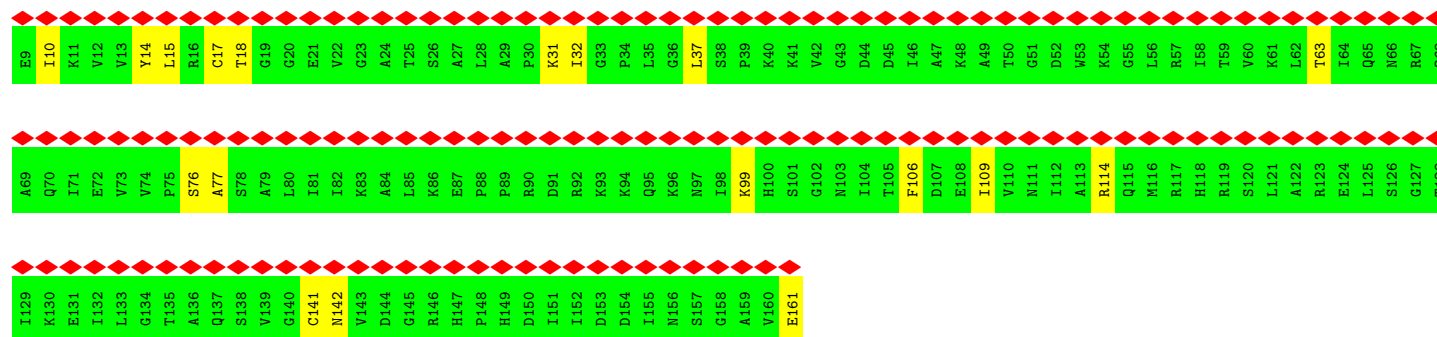
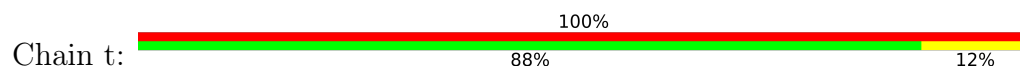




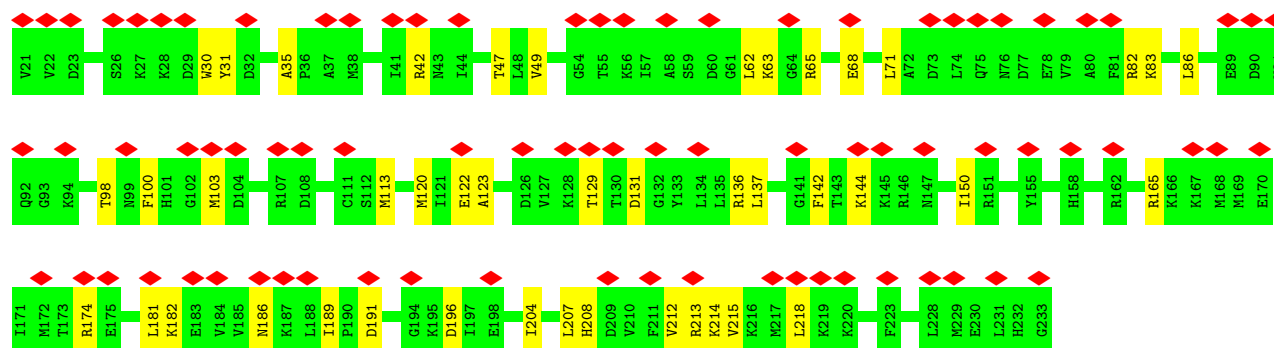
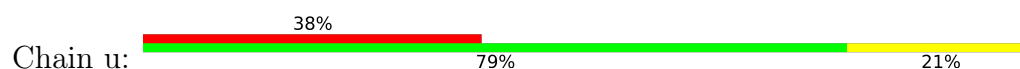
• Molecule 74: 60S acidic ribosomal protein P0



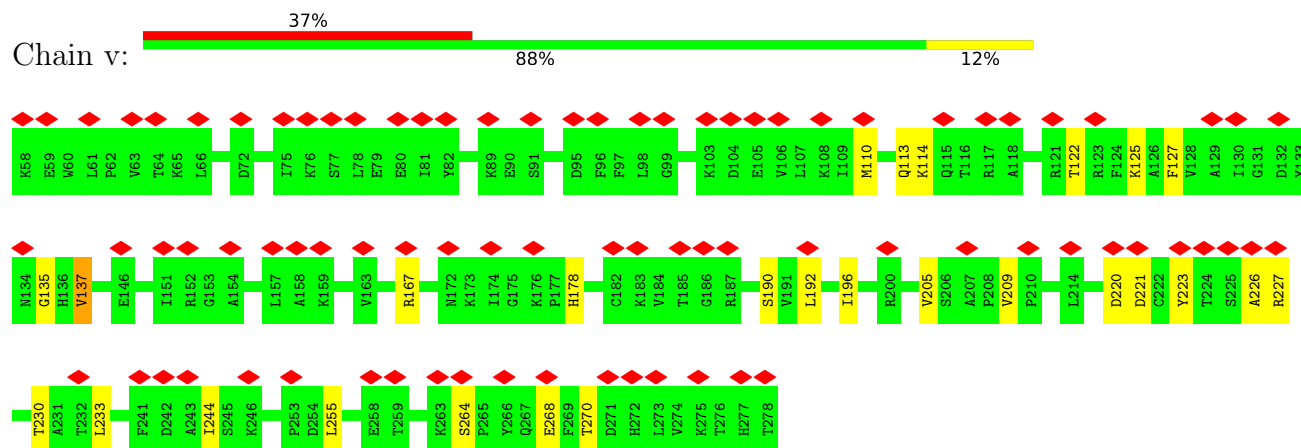
• Molecule 75: uL11



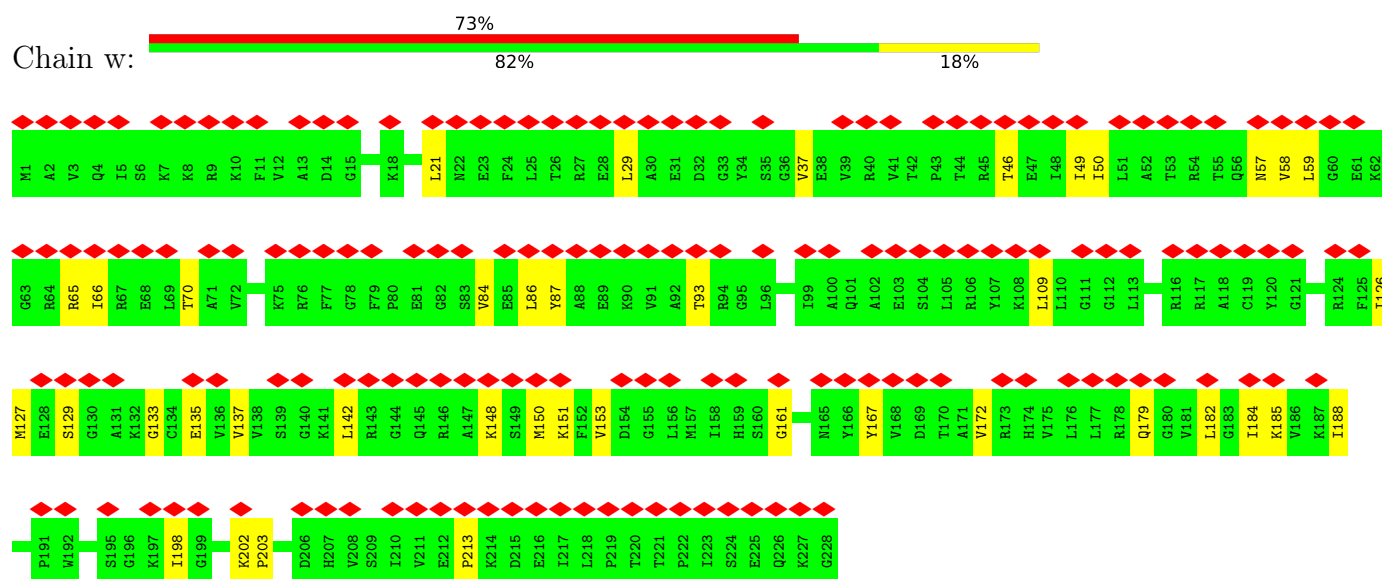
• Molecule 76: 40S ribosomal protein S3a



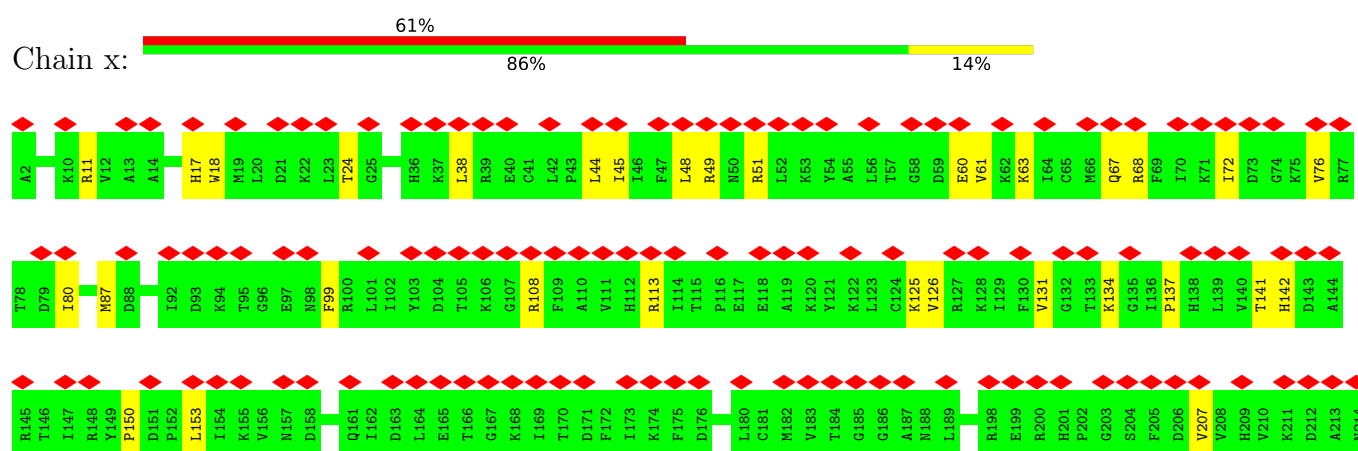
- Molecule 77: uS5

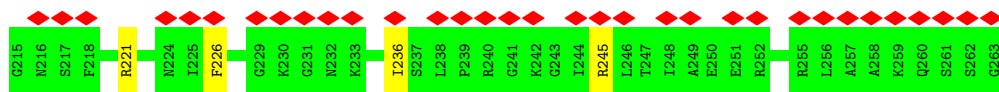


- Molecule 78: Ribosomal protein S3

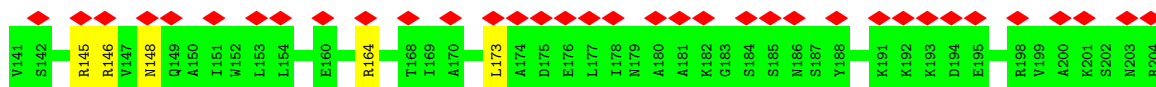
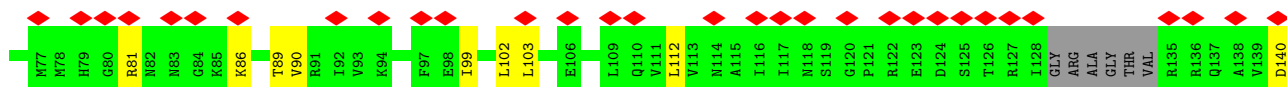
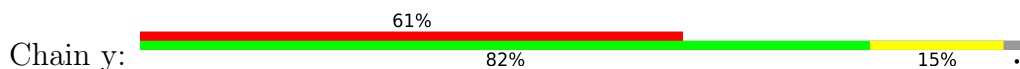


- Molecule 79: 40S ribosomal protein S4

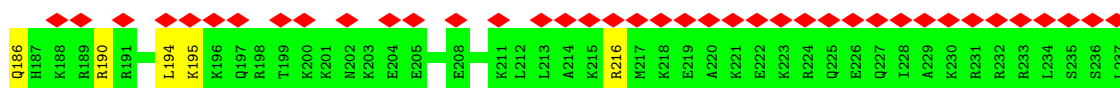
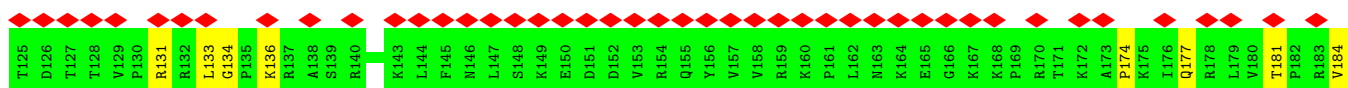
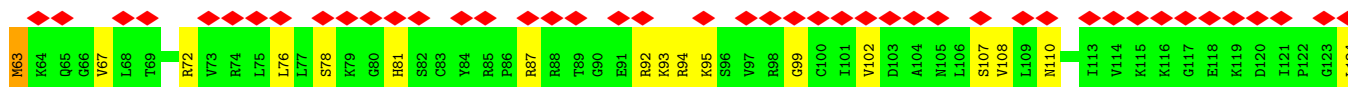
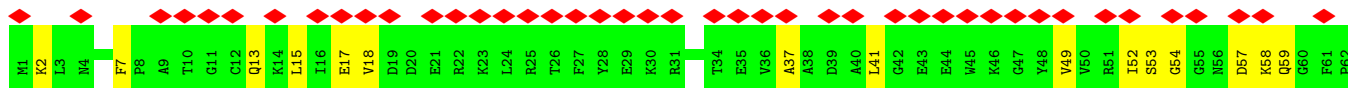
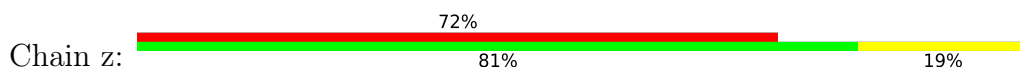




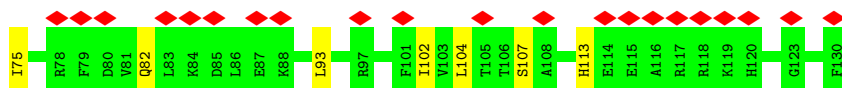
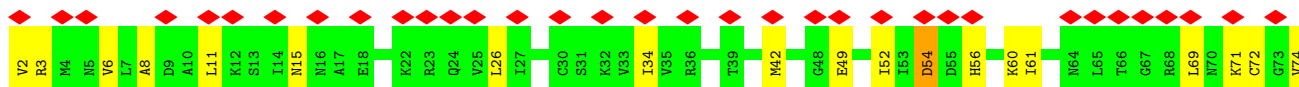
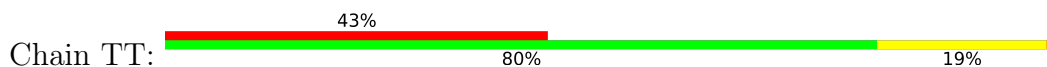
• Molecule 80: Ribosomal protein S5



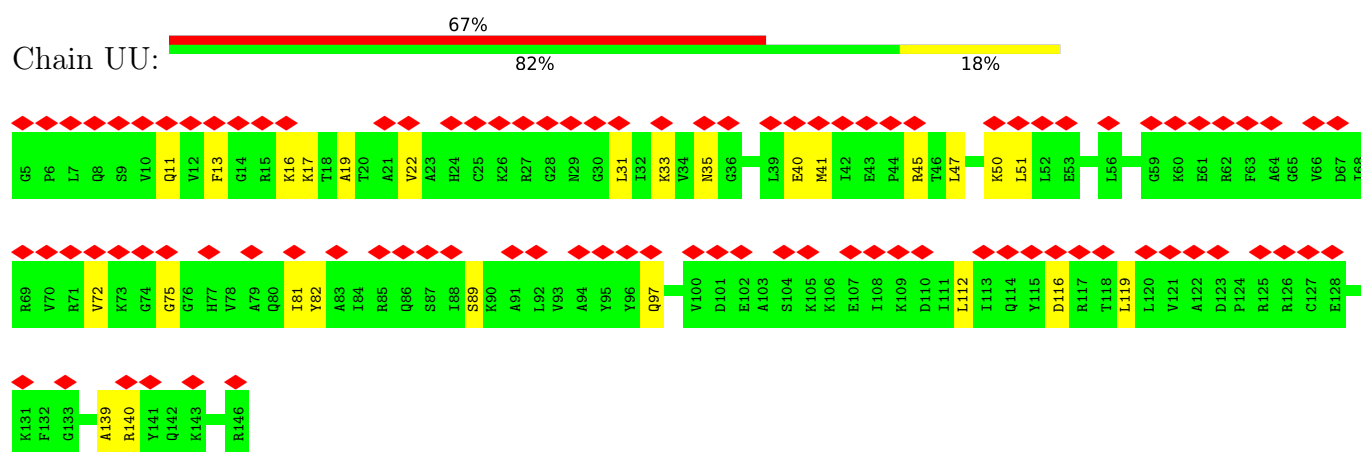
• Molecule 81: 40S ribosomal protein S6



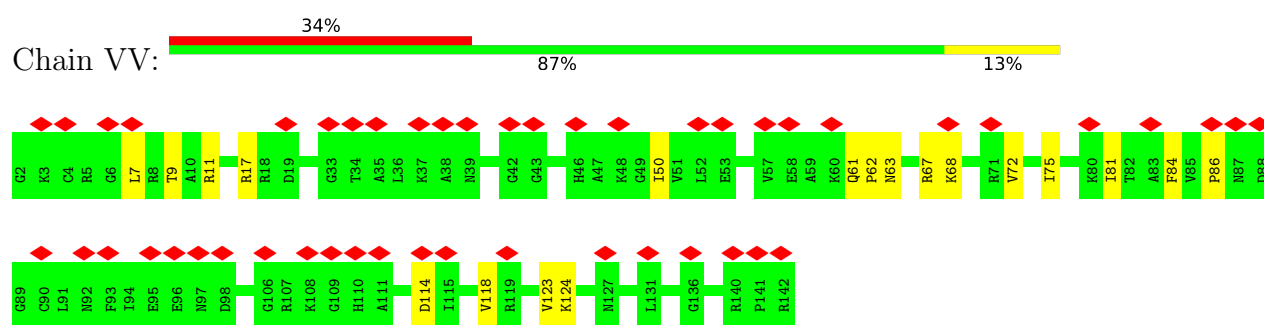
• Molecule 82: Ribosomal protein S15a



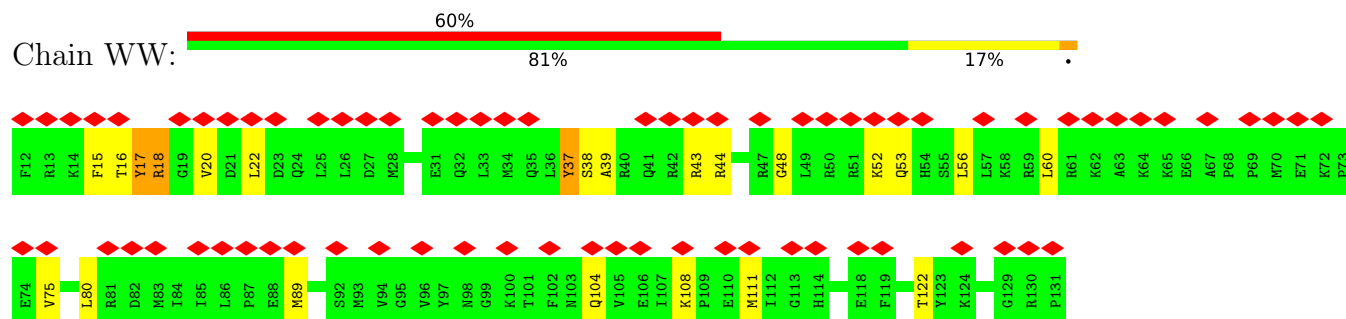
• Molecule 83: Ribosomal protein S16



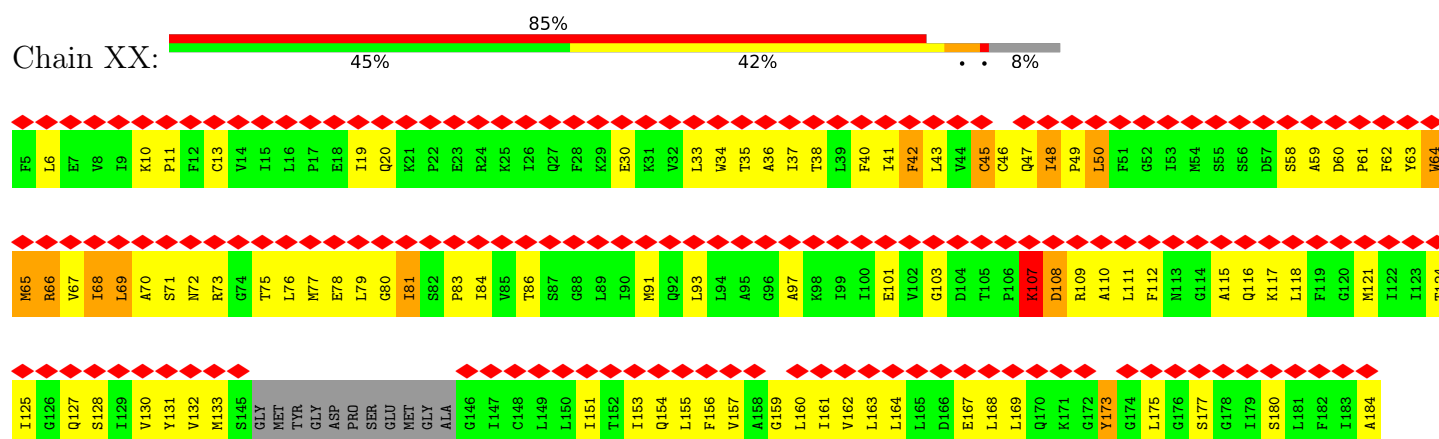
• Molecule 84: Ribosomal protein S23

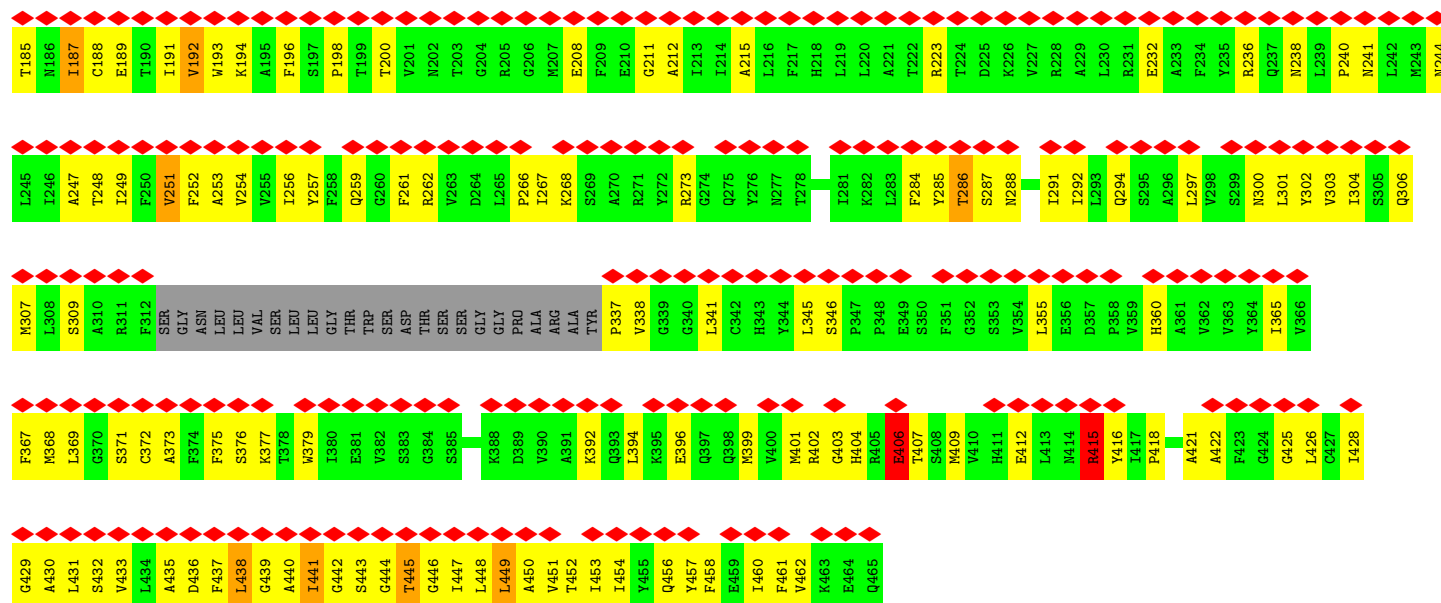


• Molecule 85: uS19

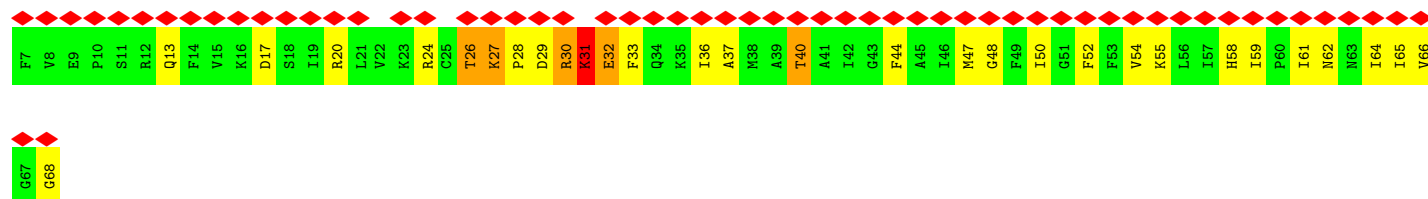


• Molecule 86: Protein transport protein Sec61 subunit alpha isoform 1

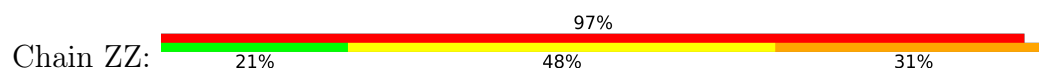




- Molecule 87: Protein transport protein Sec61 subunit gamma



- Molecule 88: Protein transport protein Sec61 subunit beta



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	12749	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	28	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.460	Depositor
Minimum map value	-0.305	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.08	Depositor
Map size ($\text{\AA}$)	429.264, 429.264, 429.264	wwPDB
Map dimensions	396, 396, 396	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.084, 1.084, 1.084	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	AA	0.27	0/447	0.57	0/587
2	BB	0.29	0/1510	0.69	3/2022 (0.1%)
3	CC	0.38	0/1715	0.71	0/2287
4	DD	0.32	0/1550	0.64	1/2069 (0.0%)
5	EE	0.40	0/1195	0.66	0/1597
6	FF	0.30	0/490	0.61	0/656
7	GG	0.30	0/805	0.65	0/1081
8	HH	0.31	0/643	0.61	0/860
9	II	0.32	0/1208	0.69	0/1618
10	JJ	0.32	0/665	0.66	0/891
11	KK	0.26	0/1082	0.58	0/1452
12	LL	0.38	0/828	0.71	0/1109
13	MM	0.41	0/1029	0.72	0/1380
14	0	0.23	0/567	0.60	0/753
15	1	0.63	0/216	1.14	1/298 (0.3%)
16	2	0.47	2/1780 (0.1%)	0.62	0/2770
17	3	0.26	0/1783	0.43	0/2773
18	4	0.35	0/141	0.49	0/217
19	5	0.51	0/84978	0.54	12/132528 (0.0%)
20	6	0.24	0/2493	0.57	0/3394
21	7	0.49	0/2858	0.45	0/4455
22	8	0.51	0/3581	0.48	0/5577
23	9	0.31	0/470	0.62	0/623
24	NN	0.26	0/1028	0.62	0/1366
25	OO	0.29	0/604	0.59	0/810
26	PP	0.28	0/1115	0.64	0/1493
27	QQ	0.36	0/1226	0.59	0/1649
28	RR	0.25	0/918	0.64	0/1233
29	A	0.57	0/1936	0.84	1/2596 (0.0%)
30	B	0.53	0/3240	0.77	0/4339
31	C	0.52	0/2937	0.76	1/3946 (0.0%)
32	D	0.45	0/2437	0.71	0/3264

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	E	0.44	0/1762	0.73	0/2362
34	F	0.51	0/1911	0.72	0/2549
35	G	0.45	0/1910	0.71	0/2569
36	H	0.47	0/1535	0.75	2/2063 (0.1%)
37	I	0.48	0/1702	0.65	0/2272
38	J	0.42	0/1385	0.76	0/1852
39	K	0.36	0/40531	0.49	4/63162 (0.0%)
40	L	0.48	0/1733	0.73	0/2316
41	M	0.46	0/1158	0.76	0/1547
42	N	0.58	0/1746	0.77	0/2338
43	O	0.53	0/1662	0.75	2/2222 (0.1%)
44	P	0.53	0/1268	0.78	1/1700 (0.1%)
45	Q	0.55	0/1539	0.80	0/2054
46	R	0.47	0/1524	0.72	1/2013 (0.0%)
47	S	0.53	0/1501	0.72	0/2012
48	T	0.56	1/1326 (0.1%)	0.74	0/1770
49	U	0.36	0/823	0.64	0/1104
50	V	0.53	0/993	0.78	0/1332
51	W	0.43	0/873	0.63	0/1158
52	X	0.44	0/984	0.72	0/1323
53	Y	0.48	0/1132	0.69	0/1504
54	Z	0.46	0/1130	0.74	0/1507
55	SS	0.26	0/834	0.68	2/1125 (0.2%)
56	a	0.56	0/1191	0.79	0/1590
57	b	0.39	0/861	0.67	0/1138
58	c	0.43	0/771	0.66	0/1034
59	d	0.51	0/903	0.76	0/1216
60	e	0.54	0/1071	0.77	2/1429 (0.1%)
61	f	0.57	0/895	0.78	0/1198
62	g	0.49	0/916	0.77	0/1220
63	h	0.44	0/1021	0.65	0/1348
64	i	0.43	0/841	0.69	0/1112
65	j	0.53	0/720	0.78	0/952
66	k	0.39	0/575	0.61	0/761
67	l	0.49	0/459	0.71	0/608
68	m	0.51	0/435	0.67	0/575
69	n	0.53	0/240	0.83	0/305
70	o	0.49	0/864	0.70	0/1140
71	p	0.49	0/718	0.76	0/953
72	q	0.37	1/1747 (0.1%)	0.71	2/2374 (0.1%)
73	r	0.52	0/1010	0.78	0/1354
74	s	0.24	0/1530	0.56	0/2064
75	t	0.25	0/1174	0.66	0/1582

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	u	0.35	0/1756	0.64	0/2350
77	v	0.35	0/1753	0.68	1/2369 (0.0%)
78	w	0.28	0/1796	0.64	0/2417
79	x	0.32	0/2118	0.62	0/2849
80	y	0.31	0/1492	0.69	1/2005 (0.0%)
81	z	0.29	0/1946	0.62	0/2590
82	TT	0.37	0/1051	0.68	0/1406
83	UU	0.31	0/1146	0.66	0/1534
84	VV	0.37	0/1116	0.69	0/1490
85	WW	0.31	0/1017	0.67	0/1358
86	XX	0.91	1/3379 (0.0%)	1.01	12/4572 (0.3%)
87	YY	0.45	0/504	0.90	0/673
88	ZZ	0.52	0/236	1.50	5/321 (1.6%)
All	All	0.46	5/235689 (0.0%)	0.60	54/345434 (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
8	HH	0	1
9	II	0	1
30	B	0	1
31	C	0	1
33	E	0	1
34	F	0	1
35	G	0	1
40	L	0	1
41	M	0	1
42	N	0	3
47	S	0	1
57	b	0	1
59	d	0	1
72	q	0	1
73	r	0	1
82	TT	0	1
84	VV	0	1
85	WW	0	2
86	XX	0	3
87	YY	0	1
All	All	0	25

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	XX	107	LYS	C-N	43.40	1.94	1.33
16	2	7	G	C1'-N9	-7.04	1.36	1.47
48	T	130	ARG	C-N	-5.97	1.25	1.33
72	q	197	VAL	C-N	-5.82	1.22	1.33
16	2	66	C	C1'-N1	5.73	1.57	1.48

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	XX	107	LYS	O-C-N	-18.30	98.25	122.59
31	C	340	ILE	N-CA-C	-11.70	102.37	111.62
88	ZZ	69	GLY	CA-C-N	11.44	134.14	119.84
88	ZZ	69	GLY	C-N-CA	11.44	134.14	119.84
72	q	197	VAL	CA-C-N	11.30	135.81	120.67

There are no chirality outliers.

5 of 25 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	B	257	TRP	Peptide
31	C	339	THR	Peptide
33	E	180	GLY	Peptide
8	HH	32	ILE	Peptide
9	II	99	LEU	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	AA	443	0	492	6	0
2	BB	1488	0	1582	21	0
3	CC	1686	0	1772	29	0
4	DD	1525	0	1640	22	0
5	EE	1175	0	1249	10	0
6	FF	488	0	514	4	0
7	GG	795	0	862	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	HH	636	0	637	8	0
9	II	1190	0	1249	21	0
10	JJ	651	0	672	11	0
11	KK	1068	0	1121	17	0
12	LL	814	0	864	13	0
13	MM	1016	0	1039	14	0
14	0	555	0	567	8	0
15	1	204	0	193	76	0
16	2	1594	0	811	78	0
17	3	1597	0	813	9	0
18	4	127	0	64	0	0
19	5	75972	0	38379	523	0
20	6	2436	0	2393	37	0
21	7	2558	0	1296	16	0
22	8	3208	0	1629	15	0
23	9	459	0	452	9	0
24	NN	1011	0	1083	18	0
25	OO	598	0	656	14	0
26	PP	1097	0	1132	22	0
27	QQ	1202	0	1289	8	0
28	RR	908	0	939	5	0
29	A	1898	0	1993	37	0
30	B	3172	0	3310	50	0
31	C	2883	0	3053	31	0
32	D	2391	0	2424	35	0
33	E	1729	0	1887	28	0
34	F	1875	0	1995	28	0
35	G	1879	0	2027	26	0
36	H	1516	0	1597	18	0
37	I	1664	0	1712	20	0
38	J	1362	0	1399	16	0
39	K	36249	0	18308	265	0
40	L	1702	0	1820	25	0
41	M	1137	0	1211	25	0
42	N	1701	0	1749	30	0
43	O	1630	0	1778	26	0
44	P	1242	0	1274	23	0
45	Q	1515	0	1634	26	0
46	R	1508	0	1664	17	0
47	S	1462	0	1508	29	0
48	T	1298	0	1366	21	0
49	U	809	0	833	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	V	979	0	1039	13	0
51	W	860	0	903	10	0
52	X	967	0	1038	48	0
53	Y	1115	0	1205	19	0
54	Z	1107	0	1182	15	0
55	SS	810	0	836	6	0
56	a	1162	0	1209	26	0
57	b	848	0	920	10	0
58	c	761	0	794	9	0
59	d	888	0	930	6	0
60	e	1053	0	1147	15	0
61	f	876	0	912	15	0
62	g	906	0	998	12	0
63	h	1013	0	1147	21	0
64	i	830	0	916	8	0
65	j	705	0	737	12	0
66	k	569	0	637	4	0
67	l	447	0	480	27	0
68	m	429	0	465	5	0
69	n	239	0	289	2	0
70	o	851	0	920	12	0
71	p	708	0	756	12	0
72	q	1710	0	1708	22	0
73	r	994	0	1051	12	0
74	s	1507	0	1564	14	0
75	t	1160	0	1218	11	0
76	u	1729	0	1803	26	0
77	v	1716	0	1806	18	0
78	w	1768	0	1866	25	0
79	x	2076	0	2177	25	0
80	y	1471	0	1522	21	0
81	z	1923	0	2089	36	0
82	TT	1034	0	1080	18	0
83	UU	1128	0	1195	19	0
84	VV	1098	0	1167	11	0
85	WW	997	0	1045	17	0
86	XX	3313	0	3425	735	0
87	YY	494	0	527	194	0
88	ZZ	229	0	245	128	0
89	LL	1	0	0	0	0
89	g	1	0	0	0	0
89	j	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
89	m	1	0	0	0	0
89	o	1	0	0	0	0
89	p	1	0	0	0	0
90	5	201	0	0	0	0
90	7	7	0	0	0	0
90	8	4	0	0	0	0
90	B	1	0	0	0	0
90	K	78	0	0	0	0
90	P	2	0	0	0	0
90	V	1	0	0	0	0
90	a	1	0	0	0	0
90	e	1	0	0	0	0
90	g	1	0	0	0	0
90	j	1	0	0	0	0
90	y	1	0	0	0	0
All	All	219898	0	164879	2665	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 7.

The worst 5 of 2665 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)
86:XX:66:ARG:HH22	86:XX:70:ALA:CA	1.06	1.67
86:XX:19:ILE:HG21	88:ZZ:70:PRO:CD	1.22	1.64
86:XX:19:ILE:CG2	88:ZZ:70:PRO:HD3	1.23	1.59
16:2:48:C:C4	16:2:59:A:C8	1.86	1.57
86:XX:188:CYS:HA	87:YY:44:PHE:CE1	1.35	1.57

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AA	53/55 (96%)	51 (96%)	2 (4%)	0	100	100
2	BB	181/189 (96%)	174 (96%)	7 (4%)	0	100	100
3	CC	204/206 (99%)	194 (95%)	10 (5%)	0	100	100
4	DD	183/185 (99%)	179 (98%)	4 (2%)	0	100	100
5	EE	139/151 (92%)	132 (95%)	7 (5%)	0	100	100
6	FF	60/62 (97%)	57 (95%)	3 (5%)	0	100	100
7	GG	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
8	HH	81/83 (98%)	76 (94%)	5 (6%)	0	100	100
9	II	142/144 (99%)	135 (95%)	7 (5%)	0	100	100
10	JJ	81/83 (98%)	77 (95%)	4 (5%)	0	100	100
11	KK	130/132 (98%)	123 (95%)	7 (5%)	0	100	100
12	LL	99/101 (98%)	91 (92%)	8 (8%)	0	100	100
13	MM	134/136 (98%)	126 (94%)	8 (6%)	0	100	100
14	0	66/68 (97%)	61 (92%)	5 (8%)	0	100	100
15	1	22/24 (92%)	13 (59%)	7 (32%)	2 (9%)	0	9
20	6	311/313 (99%)	283 (91%)	28 (9%)	0	100	100
23	9	53/55 (96%)	51 (96%)	2 (4%)	0	100	100
24	NN	122/124 (98%)	119 (98%)	3 (2%)	0	100	100
25	OO	73/75 (97%)	70 (96%)	3 (4%)	0	100	100
26	PP	139/141 (99%)	130 (94%)	9 (6%)	0	100	100
27	QQ	147/149 (99%)	145 (99%)	2 (1%)	0	100	100
28	RR	115/117 (98%)	104 (90%)	11 (10%)	0	100	100
29	A	246/248 (99%)	231 (94%)	15 (6%)	0	100	100
30	B	392/394 (100%)	368 (94%)	24 (6%)	0	100	100
31	C	360/362 (99%)	341 (95%)	19 (5%)	0	100	100
32	D	291/293 (99%)	281 (97%)	10 (3%)	0	100	100
33	E	208/251 (83%)	195 (94%)	13 (6%)	0	100	100
34	F	223/225 (99%)	214 (96%)	9 (4%)	0	100	100
35	G	229/240 (95%)	222 (97%)	7 (3%)	0	100	100
36	H	188/190 (99%)	178 (95%)	10 (5%)	0	100	100
37	I	201/213 (94%)	191 (95%)	10 (5%)	0	100	100
38	J	168/170 (99%)	162 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	L	208/210 (99%)	198 (95%)	7 (3%)	3 (1%)	9	38
41	M	136/138 (99%)	130 (96%)	6 (4%)	0	100	100
42	N	201/203 (99%)	189 (94%)	12 (6%)	0	100	100
43	O	197/199 (99%)	191 (97%)	6 (3%)	0	100	100
44	P	151/153 (99%)	145 (96%)	6 (4%)	0	100	100
45	Q	185/187 (99%)	177 (96%)	8 (4%)	0	100	100
46	R	178/180 (99%)	175 (98%)	3 (2%)	0	100	100
47	S	174/176 (99%)	165 (95%)	9 (5%)	0	100	100
48	T	157/159 (99%)	147 (94%)	10 (6%)	0	100	100
49	U	97/99 (98%)	91 (94%)	6 (6%)	0	100	100
50	V	129/131 (98%)	123 (95%)	6 (5%)	0	100	100
51	W	102/121 (84%)	98 (96%)	4 (4%)	0	100	100
52	X	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
53	Y	132/134 (98%)	129 (98%)	3 (2%)	0	100	100
54	Z	133/135 (98%)	128 (96%)	4 (3%)	1 (1%)	16	50
55	SS	94/96 (98%)	88 (94%)	6 (6%)	0	100	100
56	a	145/147 (99%)	139 (96%)	6 (4%)	0	100	100
57	b	100/116 (86%)	96 (96%)	4 (4%)	0	100	100
58	c	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
59	d	105/107 (98%)	97 (92%)	8 (8%)	0	100	100
60	e	126/128 (98%)	122 (97%)	4 (3%)	0	100	100
61	f	107/109 (98%)	102 (95%)	5 (5%)	0	100	100
62	g	112/114 (98%)	110 (98%)	2 (2%)	0	100	100
63	h	120/122 (98%)	117 (98%)	3 (2%)	0	100	100
64	i	100/102 (98%)	97 (97%)	3 (3%)	0	100	100
65	j	84/86 (98%)	82 (98%)	2 (2%)	0	100	100
66	k	67/69 (97%)	66 (98%)	1 (2%)	0	100	100
67	l	48/50 (96%)	45 (94%)	3 (6%)	0	100	100
68	m	50/52 (96%)	49 (98%)	1 (2%)	0	100	100
69	n	23/25 (92%)	23 (100%)	0	0	100	100
70	o	102/104 (98%)	97 (95%)	5 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
71	p	89/91 (98%)	86 (97%)	3 (3%)	0	100	100
72	q	215/217 (99%)	202 (94%)	13 (6%)	0	100	100
73	r	122/124 (98%)	113 (93%)	9 (7%)	0	100	100
74	s	194/196 (99%)	181 (93%)	13 (7%)	0	100	100
75	t	151/153 (99%)	135 (89%)	16 (11%)	0	100	100
76	u	211/213 (99%)	202 (96%)	9 (4%)	0	100	100
77	v	219/221 (99%)	213 (97%)	6 (3%)	0	100	100
78	w	226/228 (99%)	218 (96%)	8 (4%)	0	100	100
79	x	260/262 (99%)	249 (96%)	11 (4%)	0	100	100
80	y	181/191 (95%)	169 (93%)	12 (7%)	0	100	100
81	z	235/237 (99%)	228 (97%)	7 (3%)	0	100	100
82	TT	127/129 (98%)	119 (94%)	8 (6%)	0	100	100
83	UU	140/142 (99%)	133 (95%)	7 (5%)	0	100	100
84	VV	139/141 (99%)	132 (95%)	5 (4%)	2 (1%)	9	38
85	WW	118/120 (98%)	111 (94%)	6 (5%)	1 (1%)	16	50
86	XX	412/461 (89%)	363 (88%)	45 (11%)	4 (1%)	12	45
87	YY	60/62 (97%)	50 (83%)	8 (13%)	2 (3%)	3	24
88	ZZ	27/29 (93%)	25 (93%)	1 (4%)	1 (4%)	2	22
All	All	12040/12364 (97%)	11420 (95%)	604 (5%)	16 (0%)	49	80

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	1	249	TRP
86	XX	107	LYS
86	XX	108	ASP
86	XX	445	THR
40	L	64	VAL

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	AA	46/46 (100%)	46 (100%)	0	100	100
2	BB	165/169 (98%)	165 (100%)	0	100	100
3	CC	178/178 (100%)	176 (99%)	2 (1%)	65	74
4	DD	161/161 (100%)	161 (100%)	0	100	100
5	EE	130/136 (96%)	130 (100%)	0	100	100
6	FF	55/55 (100%)	55 (100%)	0	100	100
7	GG	92/92 (100%)	92 (100%)	0	100	100
8	HH	67/67 (100%)	66 (98%)	1 (2%)	57	70
9	II	125/125 (100%)	124 (99%)	1 (1%)	73	77
10	JJ	75/75 (100%)	75 (100%)	0	100	100
11	KK	119/119 (100%)	119 (100%)	0	100	100
12	LL	88/88 (100%)	88 (100%)	0	100	100
13	MM	106/106 (100%)	106 (100%)	0	100	100
14	0	61/61 (100%)	61 (100%)	0	100	100
15	1	22/22 (100%)	14 (64%)	8 (36%)	0	1
20	6	272/272 (100%)	272 (100%)	0	100	100
23	9	48/48 (100%)	48 (100%)	0	100	100
24	NN	107/107 (100%)	106 (99%)	1 (1%)	70	75
25	OO	66/66 (100%)	66 (100%)	0	100	100
26	PP	111/111 (100%)	110 (99%)	1 (1%)	70	75
27	QQ	130/130 (100%)	129 (99%)	1 (1%)	73	77
28	RR	99/99 (100%)	99 (100%)	0	100	100
29	A	190/190 (100%)	185 (97%)	5 (3%)	40	60
30	B	342/342 (100%)	336 (98%)	6 (2%)	51	67
31	C	302/302 (100%)	296 (98%)	6 (2%)	48	65
32	D	247/247 (100%)	246 (100%)	1 (0%)	84	83
33	E	190/223 (85%)	189 (100%)	1 (0%)	81	82
34	F	196/196 (100%)	193 (98%)	3 (2%)	57	70
35	G	200/205 (98%)	199 (100%)	1 (0%)	81	82
36	H	169/169 (100%)	169 (100%)	0	100	100
37	I	175/180 (97%)	175 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	J	143/143 (100%)	140 (98%)	3 (2%)	47	65
40	L	175/175 (100%)	172 (98%)	3 (2%)	53	68
41	M	117/117 (100%)	115 (98%)	2 (2%)	53	68
42	N	171/171 (100%)	168 (98%)	3 (2%)	51	67
43	O	171/171 (100%)	171 (100%)	0	100	100
44	P	134/134 (100%)	133 (99%)	1 (1%)	76	78
45	Q	164/164 (100%)	162 (99%)	2 (1%)	63	72
46	R	159/159 (100%)	158 (99%)	1 (1%)	78	80
47	S	157/157 (100%)	153 (98%)	4 (2%)	42	62
48	T	139/139 (100%)	137 (99%)	2 (1%)	59	71
49	U	89/89 (100%)	89 (100%)	0	100	100
50	V	101/101 (100%)	99 (98%)	2 (2%)	48	65
51	W	86/100 (86%)	86 (100%)	0	100	100
52	X	106/106 (100%)	105 (99%)	1 (1%)	70	75
53	Y	124/124 (100%)	121 (98%)	3 (2%)	43	63
54	Z	117/117 (100%)	116 (99%)	1 (1%)	70	75
55	SS	87/87 (100%)	86 (99%)	1 (1%)	65	74
56	a	119/119 (100%)	118 (99%)	1 (1%)	73	77
57	b	84/95 (88%)	83 (99%)	1 (1%)	63	72
58	c	84/84 (100%)	84 (100%)	0	100	100
59	d	98/98 (100%)	98 (100%)	0	100	100
60	e	114/114 (100%)	114 (100%)	0	100	100
61	f	88/88 (100%)	86 (98%)	2 (2%)	44	63
62	g	98/98 (100%)	94 (96%)	4 (4%)	27	51
63	h	109/109 (100%)	109 (100%)	0	100	100
64	i	86/86 (100%)	85 (99%)	1 (1%)	63	72
65	j	73/73 (100%)	73 (100%)	0	100	100
66	k	64/64 (100%)	63 (98%)	1 (2%)	55	69
67	l	47/47 (100%)	47 (100%)	0	100	100
68	m	48/48 (100%)	47 (98%)	1 (2%)	47	65
69	n	24/24 (100%)	23 (96%)	1 (4%)	26	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
70	o	92/92 (100%)	92 (100%)	0	100	100
71	p	74/74 (100%)	71 (96%)	3 (4%)	27	51
72	q	180/181 (99%)	179 (99%)	1 (1%)	78	80
73	r	108/108 (100%)	106 (98%)	2 (2%)	50	66
74	s	164/164 (100%)	164 (100%)	0	100	100
75	t	126/126 (100%)	125 (99%)	1 (1%)	73	77
76	u	194/194 (100%)	192 (99%)	2 (1%)	68	75
77	v	187/187 (100%)	185 (99%)	2 (1%)	65	74
78	w	190/190 (100%)	190 (100%)	0	100	100
79	x	224/224 (100%)	224 (100%)	0	100	100
80	y	158/161 (98%)	157 (99%)	1 (1%)	78	80
81	z	207/207 (100%)	206 (100%)	1 (0%)	81	82
82	TT	112/112 (100%)	111 (99%)	1 (1%)	70	75
83	UU	117/117 (100%)	117 (100%)	0	100	100
84	VV	113/113 (100%)	112 (99%)	1 (1%)	70	75
85	WW	109/109 (100%)	109 (100%)	0	100	100
86	XX	360/387 (93%)	344 (96%)	16 (4%)	25	49
87	YY	53/53 (100%)	45 (85%)	8 (15%)	3	16
88	ZZ	26/26 (100%)	20 (77%)	6 (23%)	1	5
All	All	10504/10613 (99%)	10380 (99%)	124 (1%)	61	72

5 of 124 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
48	T	96	ILE
87	YY	26	THR
62	g	5	LEU
86	XX	462	VAL
88	ZZ	73	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 179 such sidechains are listed below:

Mol	Chain	Res	Type
57	b	6	ASN

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Mol	Chain	Res	Type
78	w	22	ASN
59	d	30	HIS
71	p	33	GLN
80	y	79	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
16	2	73/75 (97%)	26 (35%)	2 (2%)
17	3	72/75 (96%)	16 (22%)	0
18	4	5/6 (83%)	1 (20%)	0
19	5	3519/3544 (99%)	843 (23%)	73 (2%)
21	7	119/120 (99%)	14 (11%)	0
22	8	149/151 (98%)	26 (17%)	1 (0%)
39	K	1686/1698 (99%)	397 (23%)	25 (1%)
All	All	5623/5669 (99%)	1323 (23%)	101 (1%)

5 of 1323 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
16	2	2	C
16	2	5	C
16	2	8	U
16	2	9	A
16	2	16	C

5 of 101 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
19	5	3765	G
19	5	4884	G
39	K	1664	A
19	5	3888	G
19	5	4354	U

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

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 305 ligands modelled in this entry, 305 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
19	5	24
39	K	11
86	XX	6
17	3	2
22	8	1
16	2	1

The worst 5 of 45 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	2113:G	O3'	2258:C	P	41.14
1	5	1252:C	O3'	1271:G	P	36.47
1	5	1219:G	O3'	1233:G	P	20.39
1	K	697:G	O3'	729:C	P	18.51
1	5	3948:C	O3'	4065:G	P	18.39

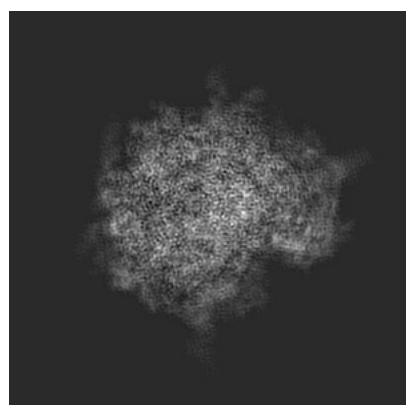
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4745. These allow visual inspection of the internal detail of the map and identification of artifacts.

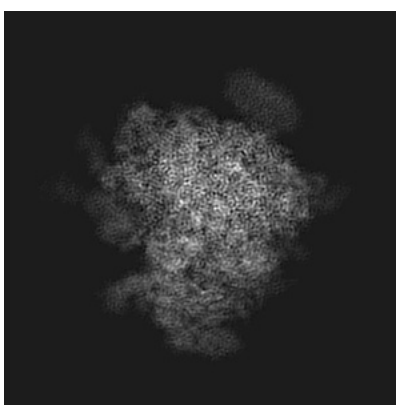
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

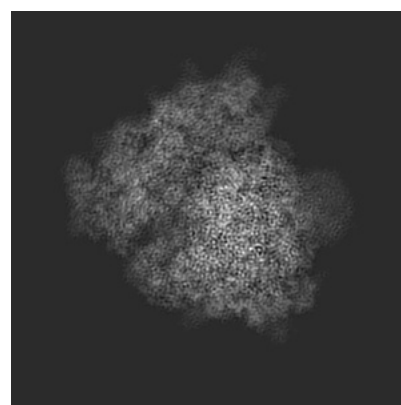
6.1.1 Primary map



X



Y

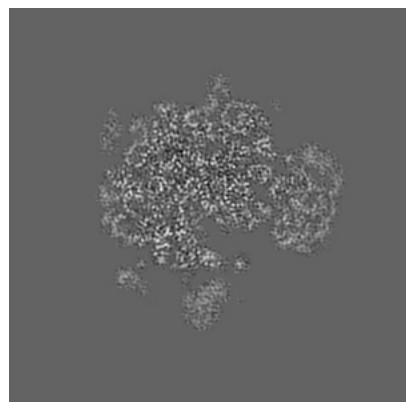


Z

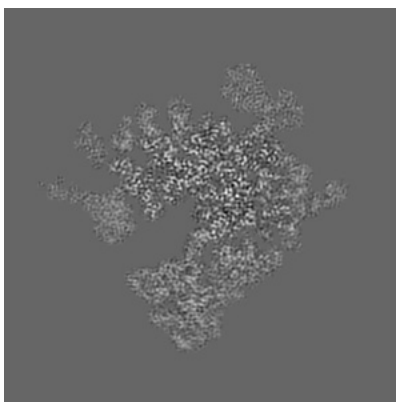
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

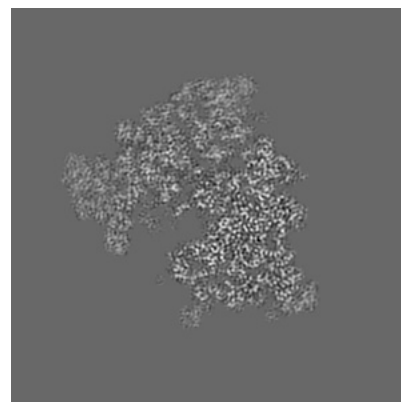
6.2.1 Primary map



X Index: 198



Y Index: 198

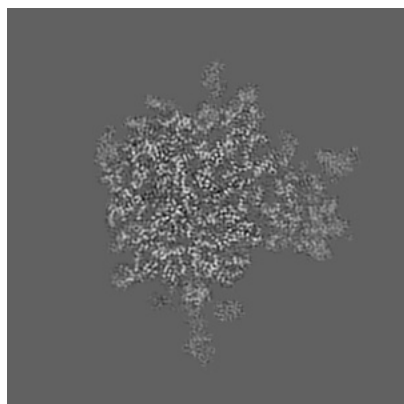


Z Index: 198

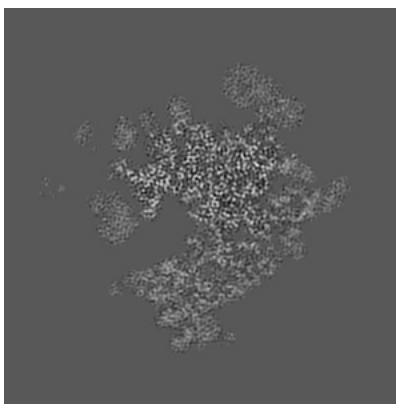
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

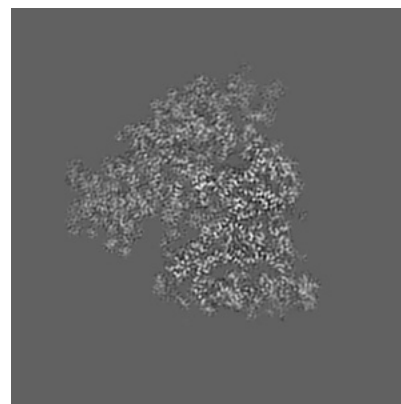
6.3.1 Primary map



X Index: 215



Y Index: 204

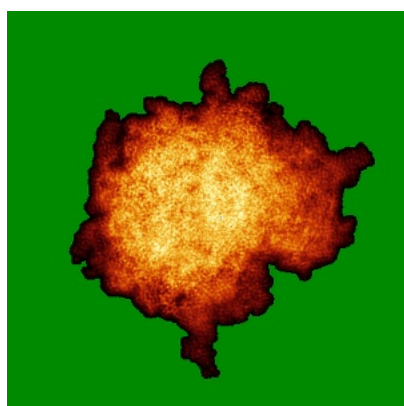


Z Index: 191

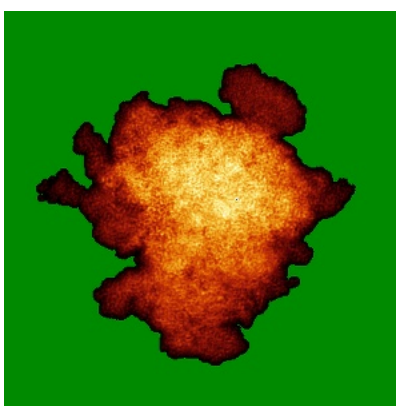
The images above show the largest variance slices of the map in three orthogonal directions.

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

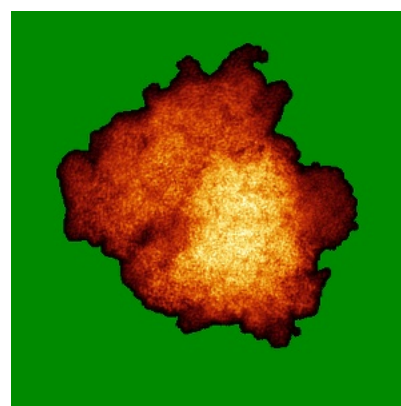
6.4.1 Primary map



X



Y

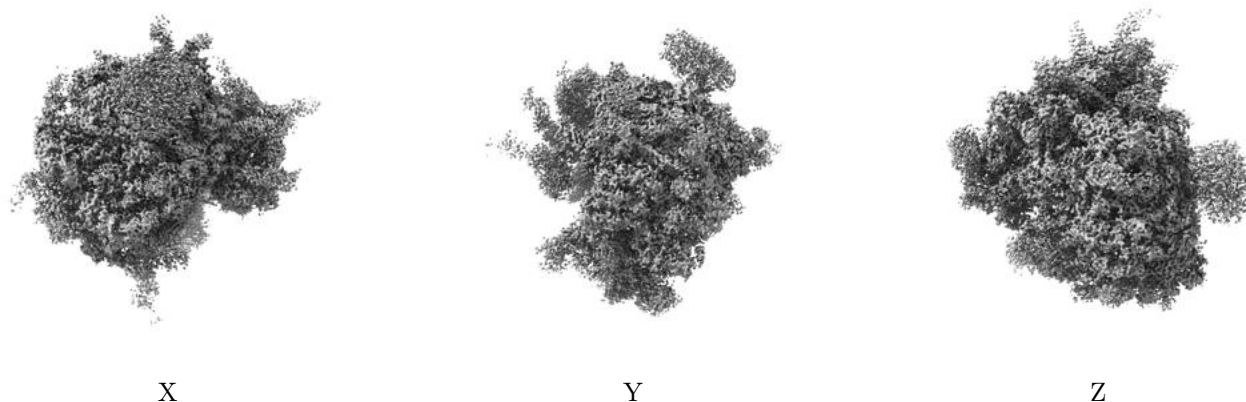


Z

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

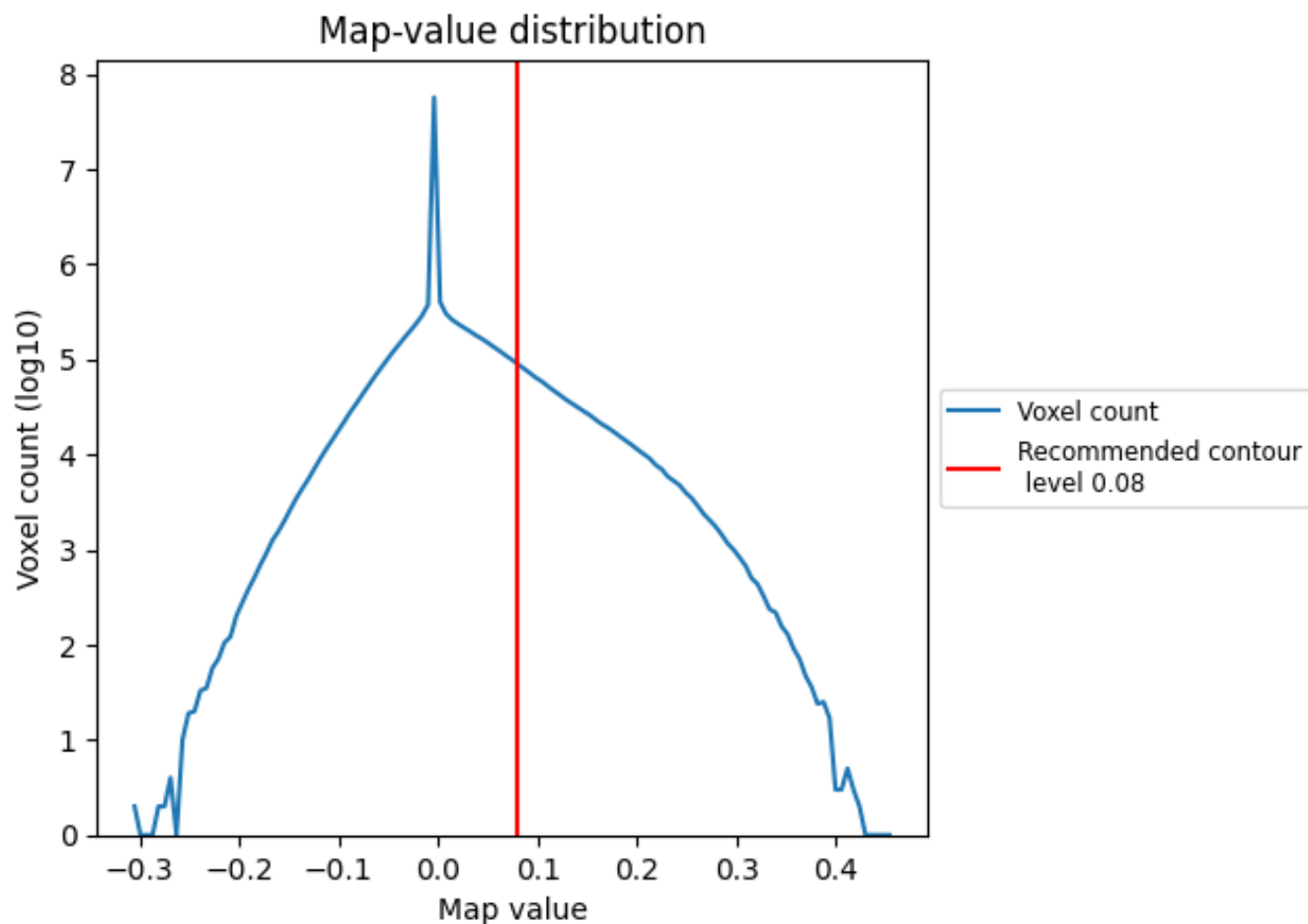
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

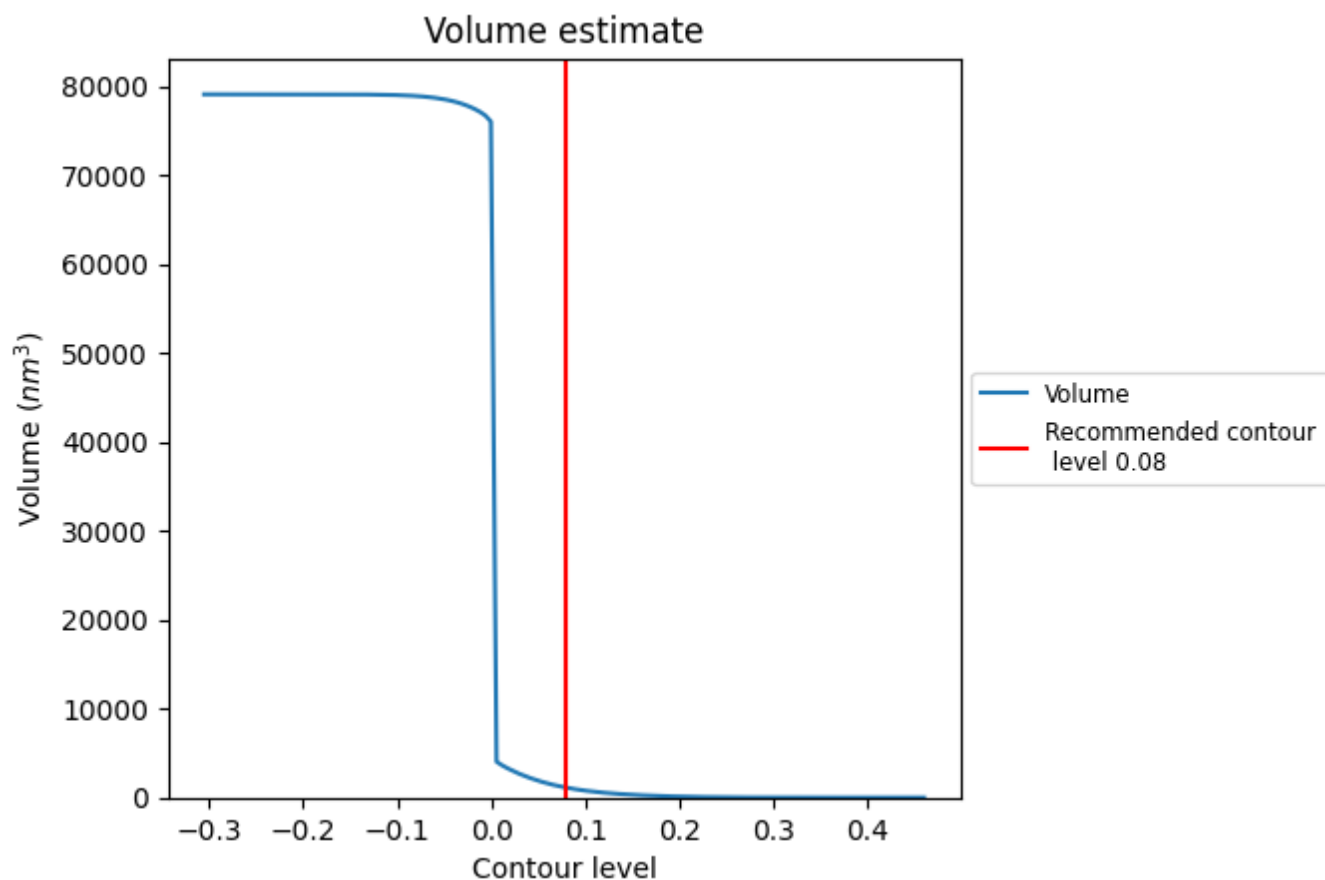
This section contains the results of statistical analysis of the map.

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.

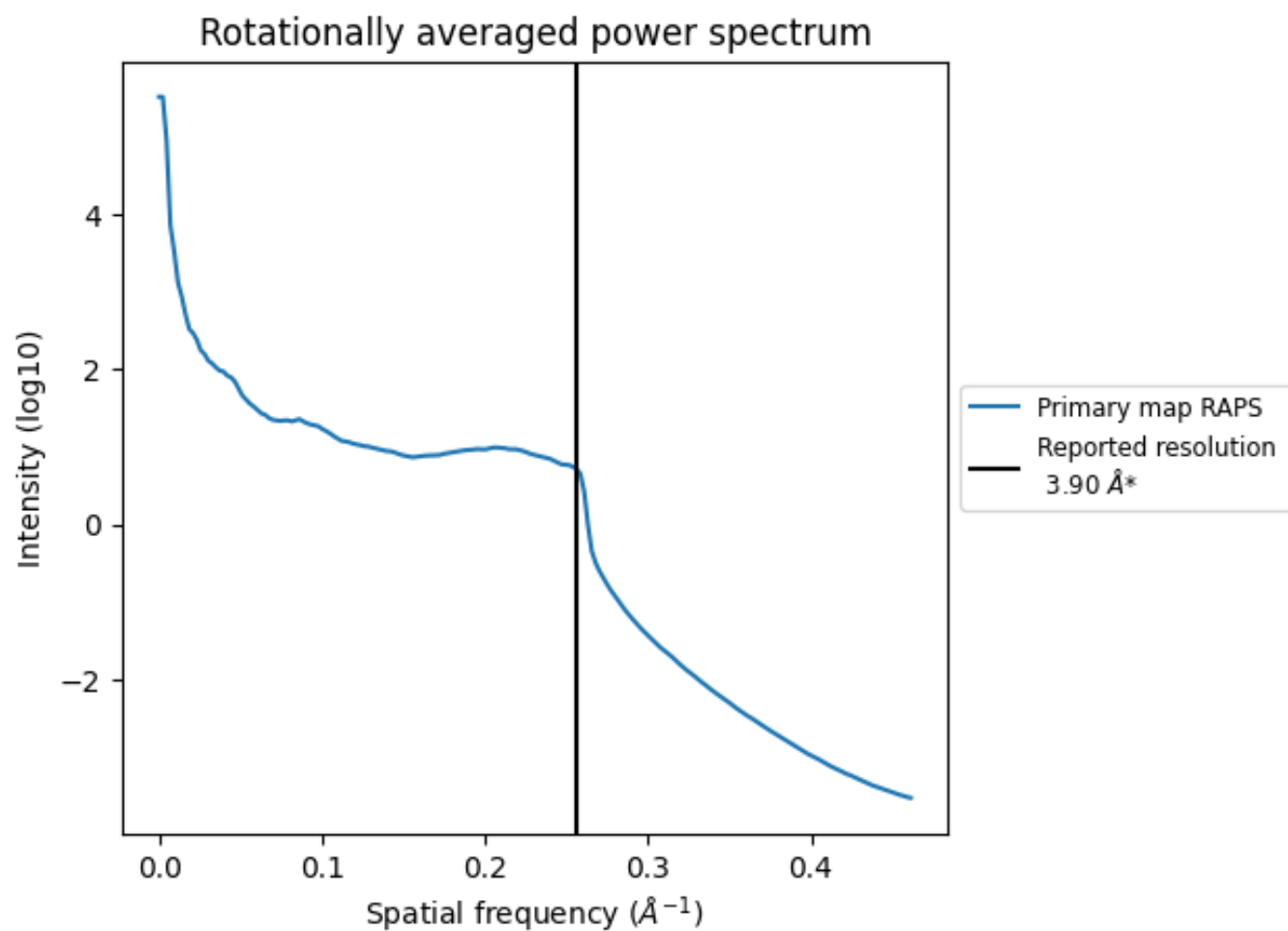
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 11111 nm³; this corresponds to an approximate mass of 1003 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 ⓘ

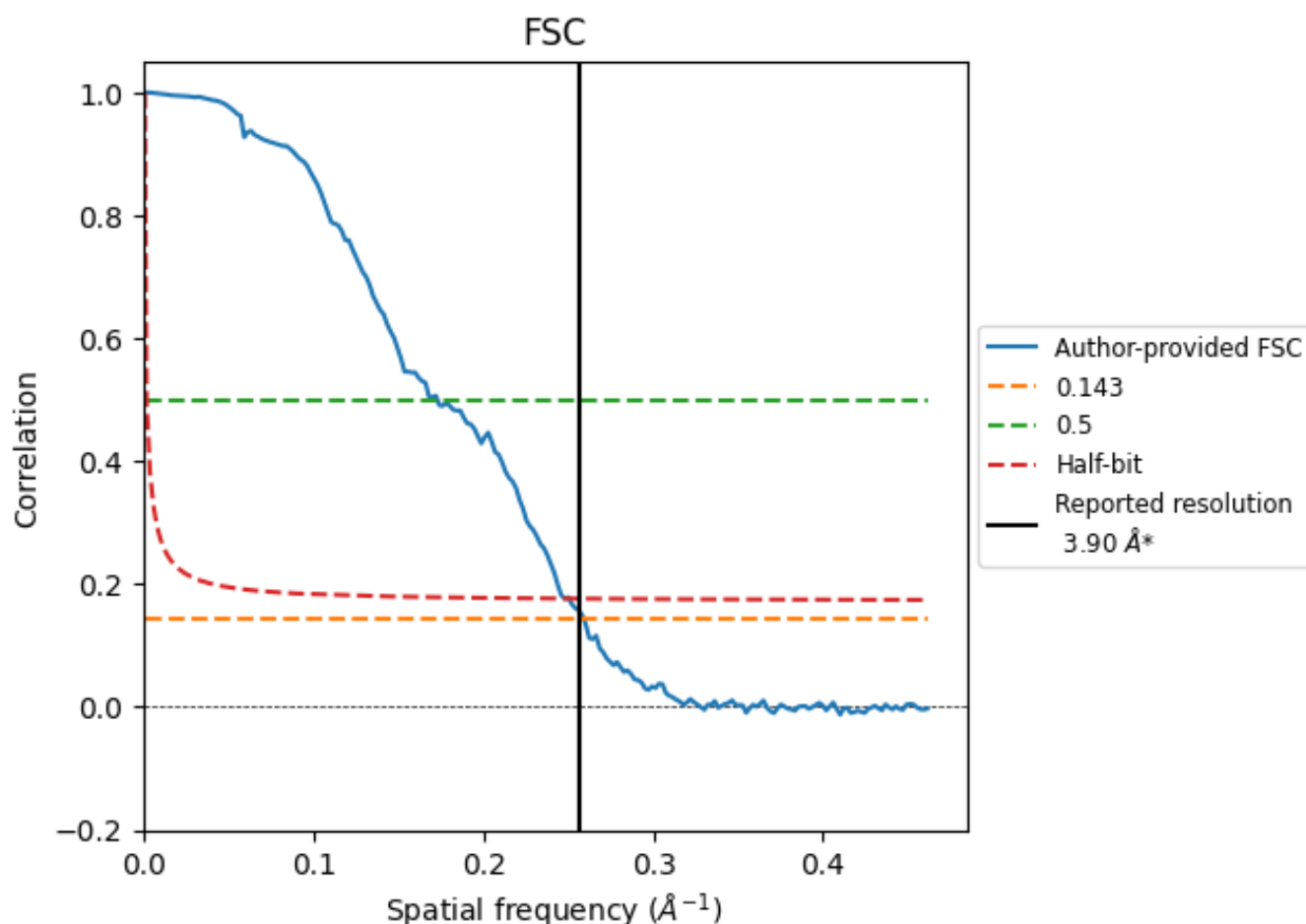


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

8.2 Resolution estimates [i](#)

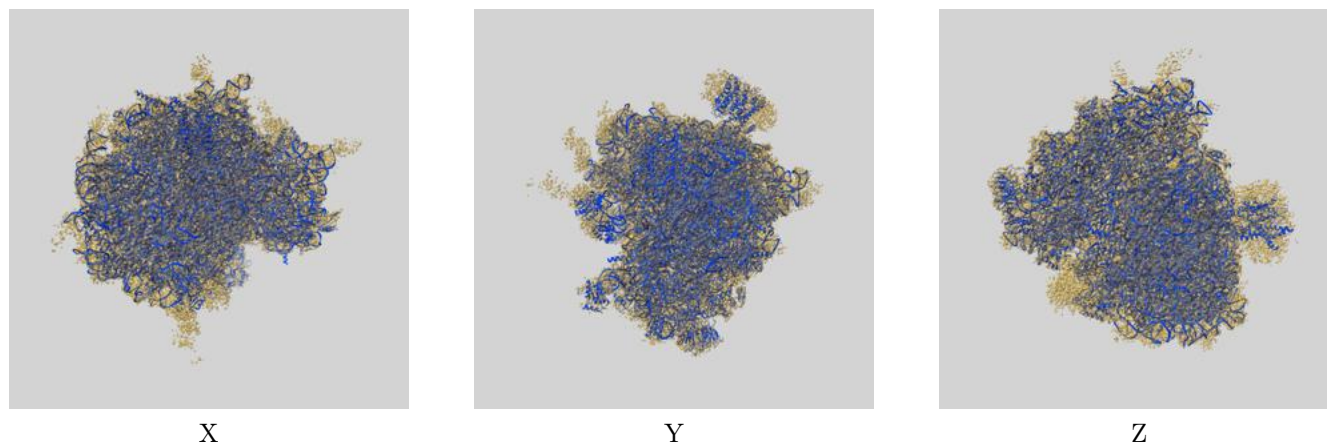
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.86	5.78	4.03
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

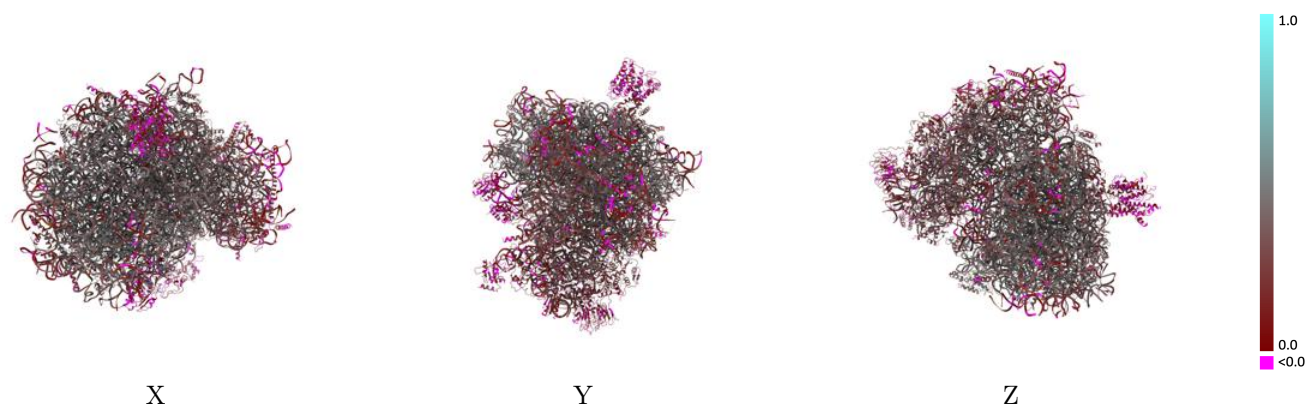
This section contains information regarding the fit between EMDB map EMD-4745 and PDB model 6R7Q. Per-residue inclusion information can be found in [section 3](#) on [page 23](#).

9.1 Map-model overlay [i](#)



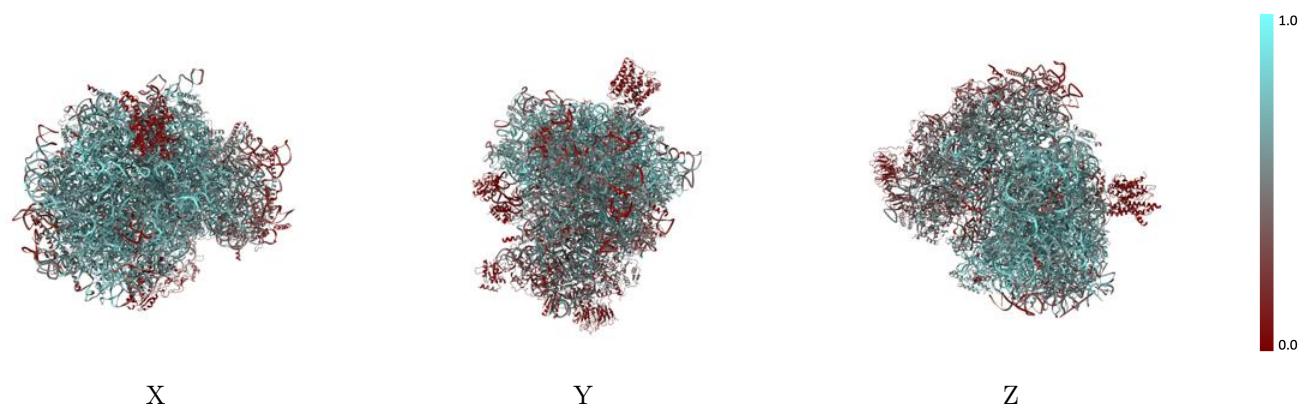
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



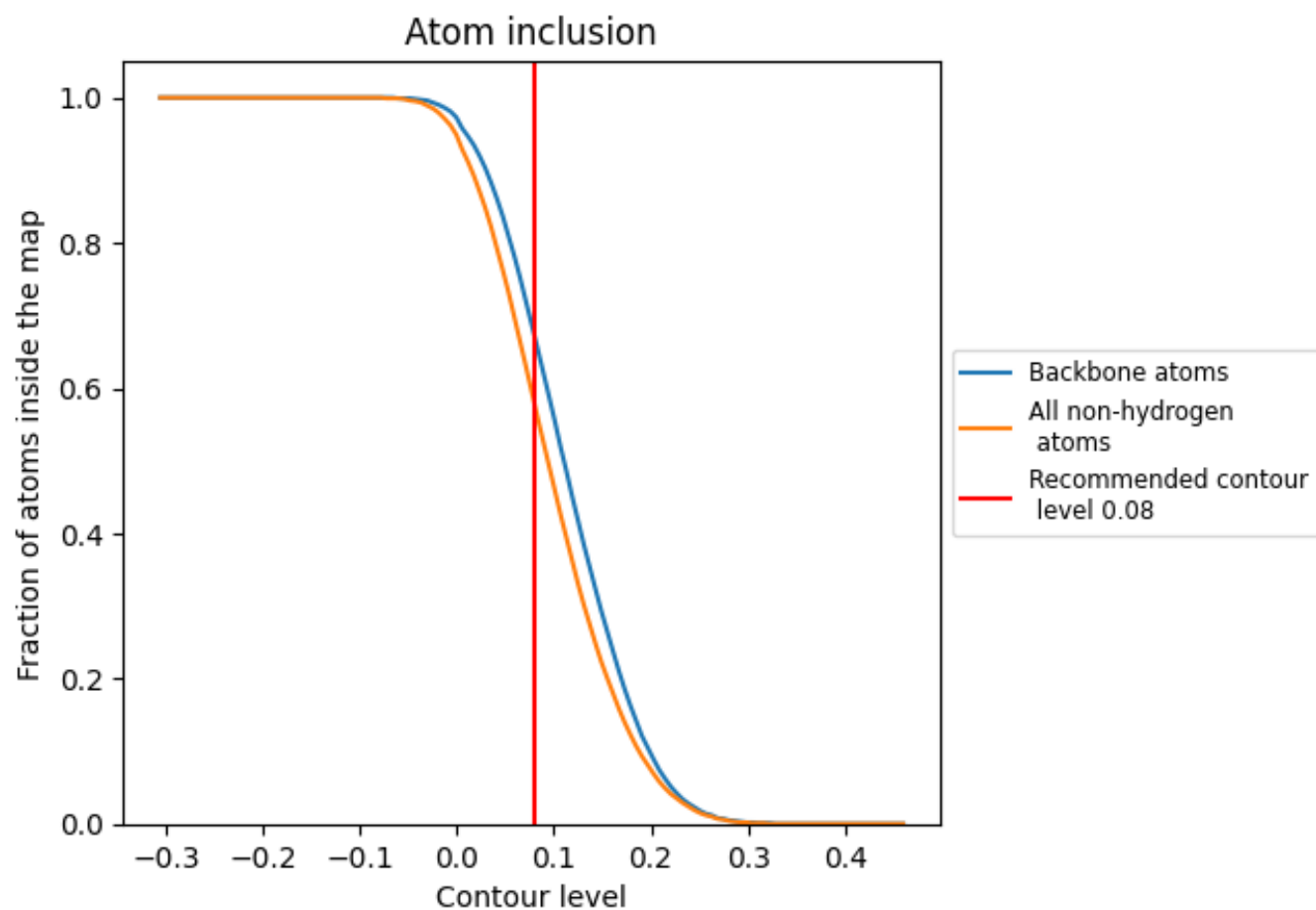
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.08).

9.4 Atom inclusion ⓘ



At the recommended contour level, 67% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5780	 0.3400
0	 0.1760	 0.1040
1	 0.3220	 0.4330
2	 0.3340	 0.2960
3	 0.2930	 0.1640
4	 0.3390	 0.2880
5	 0.7010	 0.3720
6	 0.1490	 0.1330
7	 0.7970	 0.4190
8	 0.7300	 0.3840
9	 0.4150	 0.3180
A	 0.6390	 0.4340
AA	 0.3070	 0.2330
B	 0.6480	 0.4220
BB	 0.3580	 0.2450
C	 0.6450	 0.4320
CC	 0.4470	 0.3300
D	 0.6060	 0.3800
DD	 0.3710	 0.2580
E	 0.5530	 0.3860
EE	 0.4820	 0.3610
F	 0.6040	 0.4130
FF	 0.3190	 0.2800
G	 0.5440	 0.3470
GG	 0.2530	 0.1790
H	 0.6130	 0.3950
HH	 0.3600	 0.2930
I	 0.6100	 0.4150
II	 0.3970	 0.2740
J	 0.5930	 0.3740
JJ	 0.4290	 0.2860
K	 0.5880	 0.3130
KK	 0.3390	 0.2560
L	 0.6090	 0.3820
LL	 0.4810	 0.3380



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Chain	Atom inclusion	Q-score
M	 0.6370	 0.4130
MM	 0.4770	 0.3470
N	 0.6800	 0.4340
NN	 0.3210	 0.2400
O	 0.6620	 0.4220
OO	 0.3960	 0.2500
P	 0.6480	 0.4360
PP	 0.3480	 0.2300
Q	 0.6360	 0.4320
QQ	 0.5050	 0.3570
R	 0.5840	 0.3650
RR	 0.1330	 0.0970
S	 0.6580	 0.4410
SS	 0.2850	 0.2010
T	 0.5990	 0.4100
TT	 0.4430	 0.3440
U	 0.5250	 0.3240
UU	 0.3310	 0.2460
V	 0.6280	 0.4260
VV	 0.4710	 0.3640
W	 0.4080	 0.2810
WW	 0.3440	 0.2270
X	 0.6120	 0.3900
XX	 0.1230	 0.0920
Y	 0.6210	 0.3910
YY	 0.1230	 0.1000
Z	 0.6040	 0.3780
ZZ	 0.0490	 0.0370
a	 0.6620	 0.4470
b	 0.4240	 0.3220
c	 0.5600	 0.3640
d	 0.5950	 0.3920
e	 0.6320	 0.4420
f	 0.6640	 0.4550
g	 0.6020	 0.4040
h	 0.6090	 0.3760
i	 0.5970	 0.3500
j	 0.6650	 0.4390
k	 0.5280	 0.3480
l	 0.5860	 0.4060
m	 0.6370	 0.4030
n	 0.5960	 0.3640

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Chain	Atom inclusion	Q-score
o	 0.5990	 0.4160
p	 0.6010	 0.4010
q	 0.4050	 0.2870
r	 0.6250	 0.4290
s	 0.0600	 0.0260
t	 0.0160	 0.0130
u	 0.4530	 0.3290
v	 0.4510	 0.3160
w	 0.2850	 0.2200
x	 0.3640	 0.2840
y	 0.3610	 0.2740
z	 0.3060	 0.2220