



## wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 10:35 AM UTC

PDB ID : 5IT7 / pdb\_00005it7  
EMDB ID : EMD-8123  
Title : Structure of the Kluyveromyces lactis 80S ribosome in complex with the cricket paralysis virus IRES and eEF2  
Authors : Murray, J.; Savva, C.G.; Shin, B.S.; Dever, T.E.; Ramakrishnan, V.; Fernandez, I.S.  
Deposited on : 2016-03-16  
Resolution : 3.60 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](mailto: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:

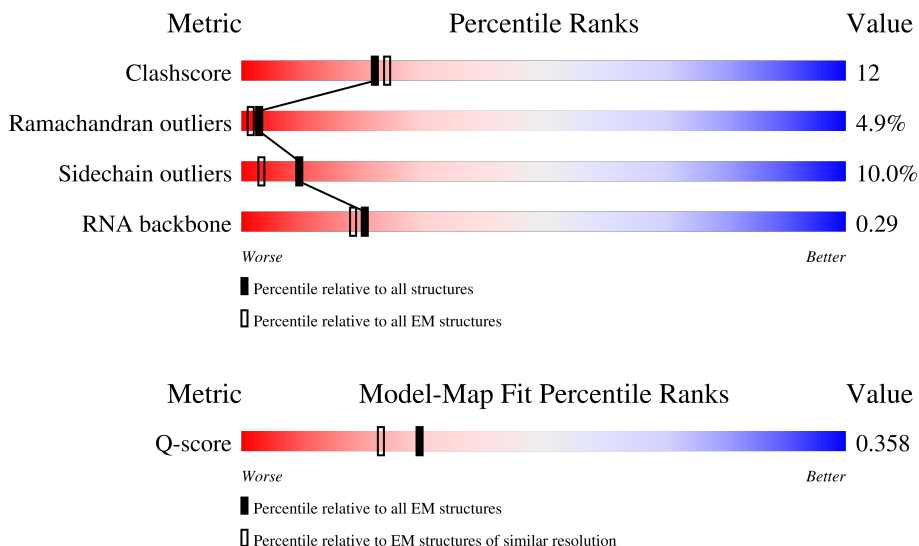
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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 3.60 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	12797 ( 3.10 - 4.10 )

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  $\geq 3$ , 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	5	3270	
2	7	121	
3	8	157	




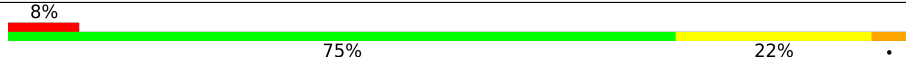
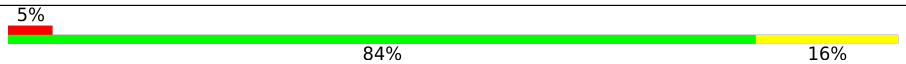

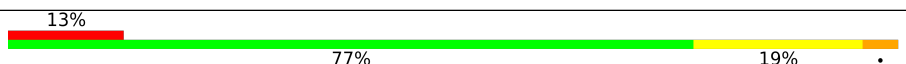
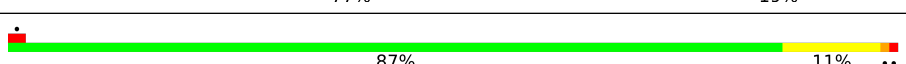
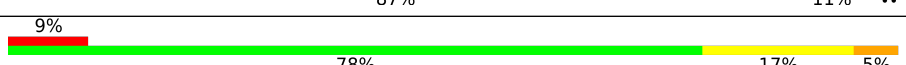
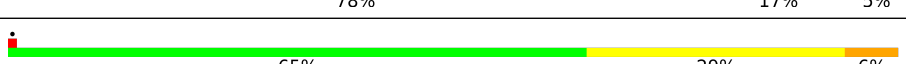
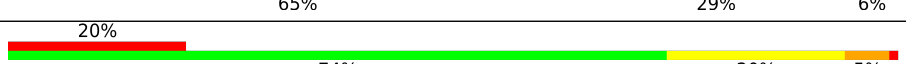
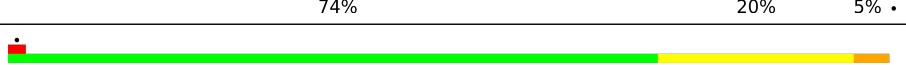







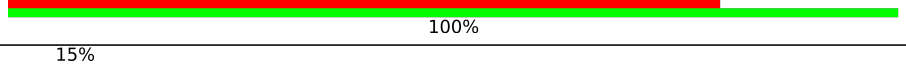
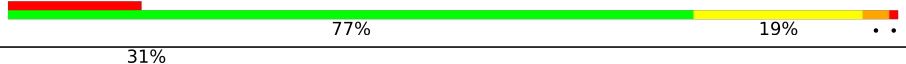


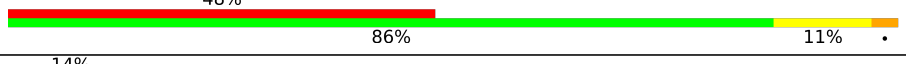

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	AA	249	65% 27% 6%
5	BB	384	65% 27% 8%
6	CC	360	66% 26% 8%
7	DD	295	8% 77% 21%
8	EE	170	9% 74% 14% 5% 5%
9	FF	222	73% 20% 7%
10	GG	233	7% 79% 18%
11	HH	191	6% 77% 21%
12	II	216	75% 19%
13	JJ	168	12% 80% 17%
14	LL	197	11% 79% 15% 6%
15	MM	136	5% 79% 18%
16	NN	202	73% 23%
17	OO	198	9% 46% 39% 6%
18	PP	180	9% 73% 22% 6%
19	QQ	184	77% 19%
20	RR	188	13% 80% 16%
21	SS	169	78% 21%
22	TT	158	70% 26%
23	UU	100	15% 92% 8%
24	VV	132	7% 68% 26% 6%
25	WW	62	5% 92% 8%
26	XX	121	7% 81% 17%
27	YY	125	78% 18%
28	ZZ	134	7% 71% 24% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	aa	147	
30	bb	57	
31	cc	97	
32	dd	106	
33	ee	122	
34	ff	105	
35	gg	121	
36	hh	116	
37	ii	98	
38	jj	85	
39	kk	76	
40	ll	49	
41	mm	51	
42	nn	25	
43	oo	101	
44	pp	87	
45	qq	217	
46	rr	195	
47	KK	147	
48	A	206	
49	B	214	
50	C	217	
51	D	223	
52	E	260	
53	F	206	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
54	G	226	47% 85% 13%
55	H	184	27% 80% 18%
56	I	200	30% 75% 18% 6%
57	J	182	14% 73% 22% 5%
58	K	96	63% 82% 16%
59	L	155	24% 74% 22%
60	M	122	93% 90% 9%
61	N	150	16% 85% 14%
62	O	127	20% 82% 13% 5%
63	P	123	64% 80% 13% 5%
64	Q	141	48% 79% 19%
65	R	129	46% 82% 15%
66	S	145	71% 84% 14%
67	T	143	48% 87% 13%
68	U	106	58% 87% 12%
69	V	87	11% 78% 21%
70	W	129	67% 26% 8%
71	X	145	9% 72% 19% 8%
72	Y	134	28% 81% 18%
73	Z	70	53% 89% 11%
74	a	100	19% 57% 31% 6% 6%
75	b	82	28% 85% 13%
76	c	63	52% 94% 6%
77	d	53	23% 89% 9%
78	e	55	38% 87% 13%

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
79	f	69	
80	g	324	
81	2	1798	
82	4	190	
83	1	827	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
85	ZN	jj	100	-	-	X	-

## 2 Entry composition

There are 87 unique types of molecules in this entry. The entry contains 215768 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 DNA/RNA hybrid called 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	5	3270	69896	31222	12579	22825	3270	0	0

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	7	121	2579	1152	461	845	121	0	0

- Molecule 3 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	8	157	3326	1488	573	1108	157	0	0

- Molecule 4 is a protein called KLLA0D16027p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	AA	249	1892	1176	385	330	1	0	0

- Molecule 5 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	BB	384	3064	1946	580	533	5	0	0

- Molecule 6 is a protein called KLLA0B07139p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	CC	359	2731	1715	522	491	3	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CC	3	ARG	ILE	conflict	UNP Q6CW41

- Molecule 7 is a protein called KLLA0D06941p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	DD	295	2384	1510	417	456	1	0	0

- Molecule 8 is a protein called KLLA0B04686p.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	EE	161	1300	834	243	223	0	0

- Molecule 9 is a protein called KLLA0D03410p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	FF	222	1774	1138	319	316	1	0	0

- Molecule 10 is a protein called KLLA0E00573p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	GG	233	1817	1160	324	330	3	0	0

- Molecule 11 is a protein called KLLA0F04499p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	HH	191	1528	965	277	284	2	0	0

- Molecule 12 is a protein called KLLA0D05643p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	II	207	1690	1074	319	292	5	0	0

- Molecule 13 is a protein called KLLA0F08261p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	JJ	168	1349	845	255	245	4	0	0

- Molecule 14 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	LL	197	1581	988	317	276		0	0

- Molecule 15 is a protein called KLLA0B13409p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	MM	136	1045	666	196	183		0	0

- Molecule 16 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	NN	202	1709	1069	359	280	1	0	0

- Molecule 17 is a protein called KLLA0F04675p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	OO	198	1571	1013	290	267	1	196	0

- Molecule 18 is a protein called KLLA0A06336p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	PP	180	1432	885	287	260		0	0

- Molecule 19 is a protein called KLLA0A07227p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	QQ	184	1444	911	290	243		0	0

- Molecule 20 is a protein called KLLA0E12453p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	RR	188	1522	933	328	259	2	0	0

- Molecule 21 is a protein called 60S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	SS	169	1416	916	259	238	3	0	0

- Molecule 22 is a protein called KLLA0E23651p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	TT	158	1262	797	240	220	5	0	0

- Molecule 23 is a protein called KLLA0D05181p.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
23	UU	100	807	524	131	152	0	0

- Molecule 24 is a protein called KLLA0E06997p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	VV	132	976	612	182	174	8	0	0

- Molecule 25 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
25	WW	62	515	330	103	82	0	0

- Molecule 26 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	XX	121	964	620	169	174	1	0	0

- Molecule 27 is a protein called KLLA0B05742p.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	YY	125	Total	C	N	O	0	0
			992	622	189	181		

- Molecule 28 is a protein called KLLA0E03455p.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	ZZ	134	Total	C	N	O	0	0
			1089	708	199	182		

- Molecule 29 is a protein called RPL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	aa	147	Total	C	N	O	S	0	0
			1156	740	225	189	2		

- Molecule 30 is a protein called KLLA0D16071p.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	bb	57	Total	C	N	O	0	0
			458	287	99	72		

- Molecule 31 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	cc	97	Total	C	N	O	S	0	0
			740	477	125	137	1		

- Molecule 32 is a protein called KLLA0B02937p.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	dd	106	Total	C	N	O	S	0	0
			869	553	167	147	2		

- Molecule 33 is a protein called KLLA0E06843p.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	ee	122	Total	C	N	O	S	0	0
			980	618	198	162	2		

- Molecule 34 is a protein called KLLA0D07405p.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	ff	105	Total	C	N	O	S	0	0
			837	531	161	144	1		

- Molecule 35 is a protein called KLLA0C08371p.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	gg	121	Total	C	N	O	S	0	0
			951	591	192	167	1		

- Molecule 36 is a protein called KLLA0F05247p.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	hh	116	Total	C	N	O	0	0
			961	608	187	166		

- Molecule 37 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	ii	98	Total	C	N	O	S	0	0
			766	479	155	131	1		

- Molecule 38 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	jj	85	Total	C	N	O	S	0	0
			675	410	148	111	6		

- Molecule 39 is a protein called KLLA0C18216p.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	kk	76	Total	C	N	O	0	0
			619	398	114	107		

- Molecule 40 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	ll	49	Total	C	N	O	S	0	0
			428	266	96	64	2		

- Molecule 41 is a protein called Ubiquitin fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	mm	51	Total	C	N	O	S	0	0
			410	254	85	66	5		

- Molecule 42 is a protein called 60S ribosomal protein L41-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	nn	25	Total	C	N	O	S	0	0
			233	142	63	27	1		

- Molecule 43 is a protein called 60S ribosomal protein L44.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	oo	101	Total	C	N	O	S	0	0
			814	509	163	136	6		

- Molecule 44 is a protein called KLLA0E05941p.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	pp	87	Total	C	N	O	S	0	0
			660	404	133	117	6		

- Molecule 45 is a protein called Ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	qq	217	Total	C	N	O	S	0	0
			1721	1100	300	312	9		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
qq	11	GLU	ASP	conflict	UNP Q6CWR9
qq	12	HIS	ASN	conflict	UNP Q6CWR9
qq	152	ARG	LYS	conflict	UNP Q6CWR9

- Molecule 46 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	rr	195	Total	C	N	O	S	0	0
			1508	968	258	278	4		

- Molecule 47 is a protein called uL11.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	KK	147	Total	C	N	O	0	0
			735	441	147	147		

- Molecule 48 is a protein called 40S ribosomal protein S0.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	A	206	Total	C	N	O	S	0	0
			1616	1035	285	294	2		

- Molecule 49 is a protein called 40S ribosomal protein S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	B	214	Total	C	N	O	S	0	0
			1722	1089	313	317	3		

- Molecule 50 is a protein called KLLA0F09812p.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	C	217	Total	C	N	O	S	0	0
			1629	1041	287	297	4		

- Molecule 51 is a protein called KLLA0D08305p.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	D	223	Total	C	N	O	S	0	0
			1744	1108	313	318	5		

- Molecule 52 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	E	260	Total	C	N	O	S	0	0
			2078	1322	393	359	4		

- Molecule 53 is a protein called KLLA0D10659p.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	F	206	Total	C	N	O	S	0	0
			1609	1008	298	300	3		

- Molecule 54 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	G	226	1812	1134	348	326	4	0	0

- Molecule 55 is a protein called KLLA0C13519p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	H	184	1483	950	270	263		0	0

- Molecule 56 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	I	188	1493	926	301	265	1	0	0

- Molecule 57 is a protein called KLLA0E23673p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	J	182	1471	929	287	254	1	0	0

- Molecule 58 is a protein called KLLA0B08173p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
58	K	96	809	533	129	146	1	0	0

- Molecule 59 is a protein called KLLA0A10483p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
59	L	155	1248	798	237	210	3	0	0

- Molecule 60 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
60	M	122	922	575	167	180	0	0

- Molecule 61 is a protein called KLLA0F18040p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
61	N	150	1187	756	223	206	2	0	0

- Molecule 62 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
62	O	127	942	578	188	173	3	0	0

- Molecule 63 is a protein called KLLA0F07843p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
63	P	123	980	628	179	168	5	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	130	ALA	-	expression tag	UNP Q6CKV4

- Molecule 64 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
64	Q	141	1105	709	204	192	0	0

- Molecule 65 is a protein called KLLA0B01474p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
65	R	129	1031	641	193	194	3	0	0

- Molecule 66 is a protein called KLLA0B01562p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
66	S	145	1193	741	240	210	2	0	0

- Molecule 67 is a protein called KLLA0A07194p.

Mol	Chain	Residues	Atoms				AltConf	Trace
67	T	143	Total	C	N	O	0	0
			1110	693	210	207		

- Molecule 68 is a protein called KLLA0F25542p.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	U	106	Total	C	N	O	S	0	0
			845	540	152	152	1		

- Molecule 69 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	V	87	Total	C	N	O	S	0	0
			687	424	126	135	2		

- Molecule 70 is a protein called 40S ribosomal protein S22.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	W	129	Total	C	N	O	S	0	0
			1021	651	187	180	3		

- Molecule 71 is a protein called RPS23.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	X	145	Total	C	N	O	S	0	0
			1127	713	219	192	3		

- Molecule 72 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms				AltConf	Trace
72	Y	134	Total	C	N	O	0	0
			1061	665	207	189		

- Molecule 73 is a protein called KLLA0B06182p.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	Z	70	Total	C	N	O	S	0	0
			558	355	104	98	1		

- Molecule 74 is a protein called KLLA0D05115p.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	a	100	Total	C	N	O	S	0	0
			798	491	170	131	6		

- Molecule 75 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	b	82	Total	C	N	O	S	0	0
			617	384	113	114	6		

- Molecule 76 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	c	63	Total	C	N	O	S	0	0
			494	305	98	90	1		

- Molecule 77 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	d	53	Total	C	N	O	S	0	0
			446	280	89	76	1		

- Molecule 78 is a protein called KLLA0C04809p.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	e	55	Total	C	N	O	S	0	0
			443	276	90	76	1		

- Molecule 79 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	f	69	Total	C	N	O	S	0	0
			549	352	102	91	4		

- Molecule 80 is a protein called KLLA0E12277p.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	g	318	Total	C	N	O	S	0	0
			2466	1561	430	470	5		

- Molecule 81 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
81	2	1780	37797	16892	6658	12467	1780	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	676	G	U	conflict	GB 49642208
2	678	U	G	conflict	GB 49642208

- Molecule 82 is DNA/RNA hybrid called cricket paralysis virus IRES.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
82	4	190	3950	1768	667	1325	190	0	0

- Molecule 83 is a protein called Eft2p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
83	1	827	6421	4070	1106	1216	29	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	310	GLU	ASP	conflict	UNP W7R097

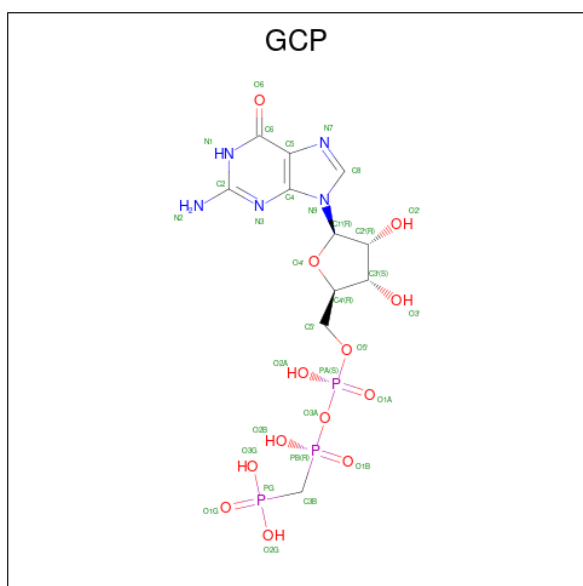
- Molecule 84 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
84	5	2	Total 2	Mg 2	0
84	N	1	Total 1	Mg 1	0
84	a	1	Total 1	Mg 1	0
84	f	1	Total 1	Mg 1	0
84	2	74	Total 74	Mg 74	0
84	1	1	Total 1	Mg 1	0

- Molecule 85 is ZINC ION (CCD ID: ZN) (formula: Zn).

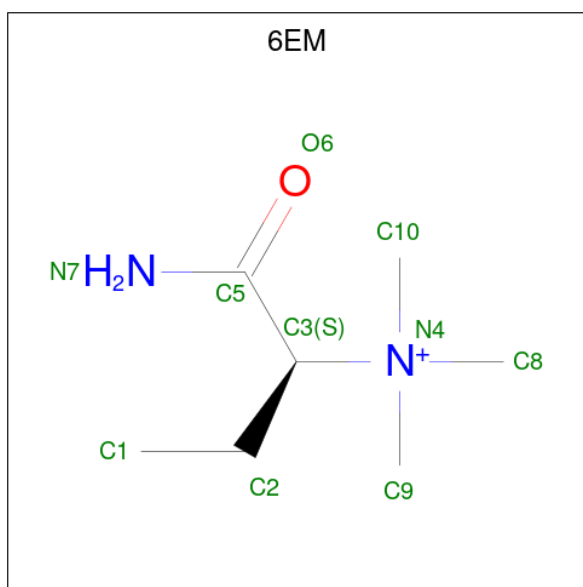
Mol	Chain	Residues	Atoms		AltConf
85	jj	1	Total	Zn	0
			1	1	
85	mm	1	Total	Zn	0
			1	1	
85	oo	1	Total	Zn	0
			1	1	
85	a	1	Total	Zn	0
			1	1	
85	b	1	Total	Zn	0
			1	1	
85	f	1	Total	Zn	0
			1	1	

- Molecule 86 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: GCP) (formula: C<sub>11</sub>H<sub>18</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					AltConf
86	1	1	Total	C	N	O	P	0
			32	11	5	13	3	

- Molecule 87 is (2S)-1-amino-N,N,N-trimethyl-1-oxobutan-2-aminium (CCD ID: 6EM) (formula: C<sub>7</sub>H<sub>17</sub>N<sub>2</sub>O).

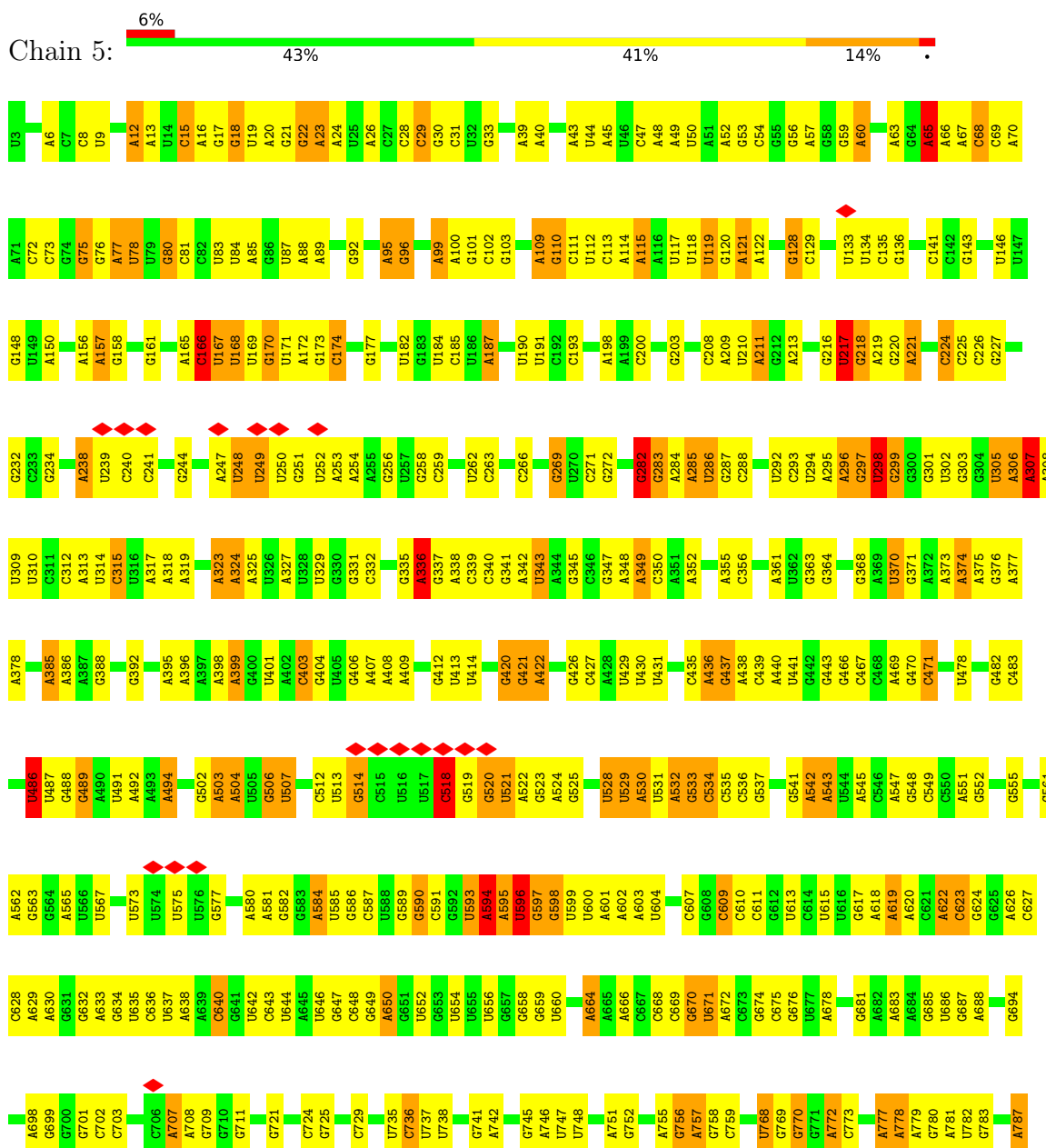


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
87	1	1	10	7	2	1	0

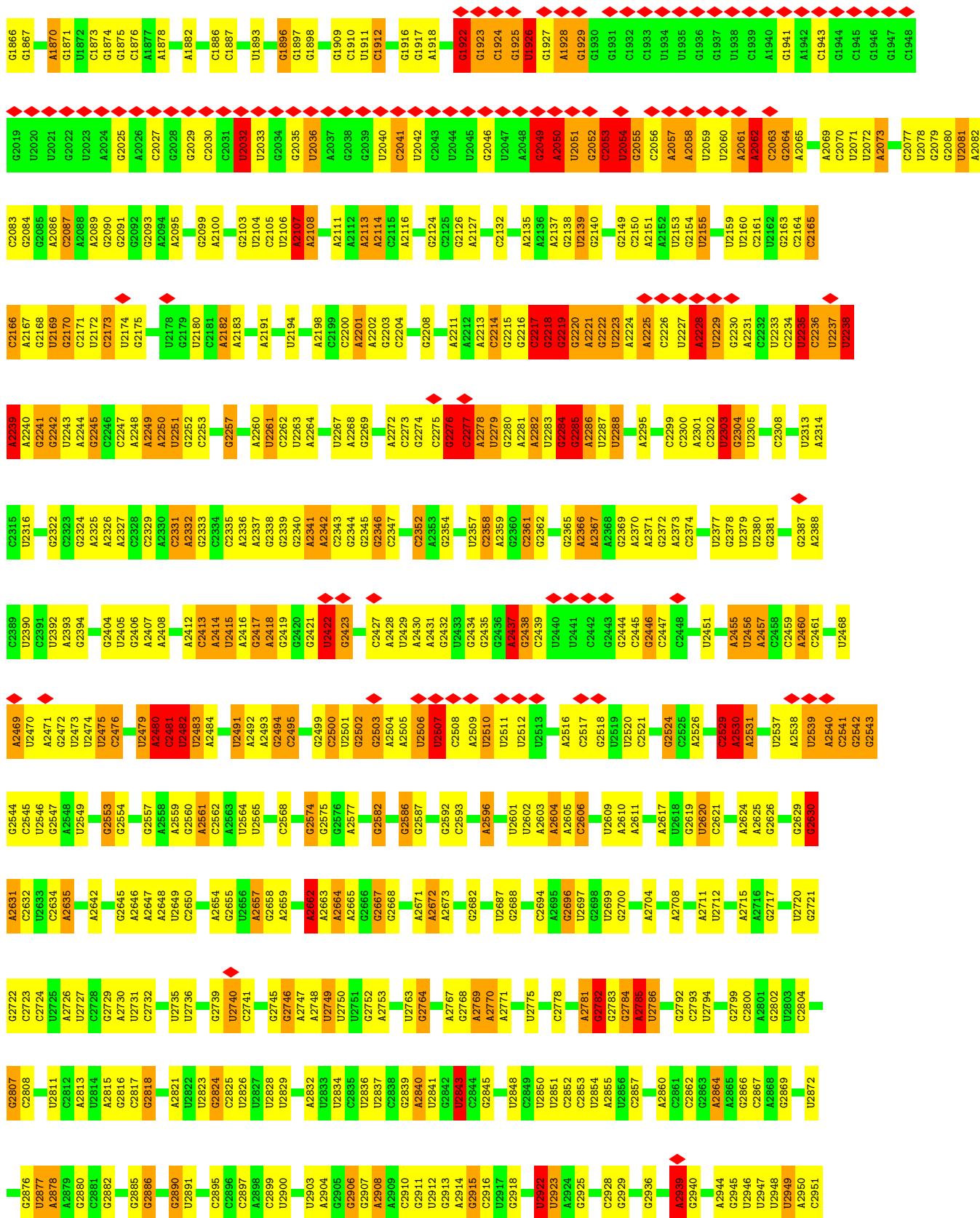
### 3 Residue-property plots

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.

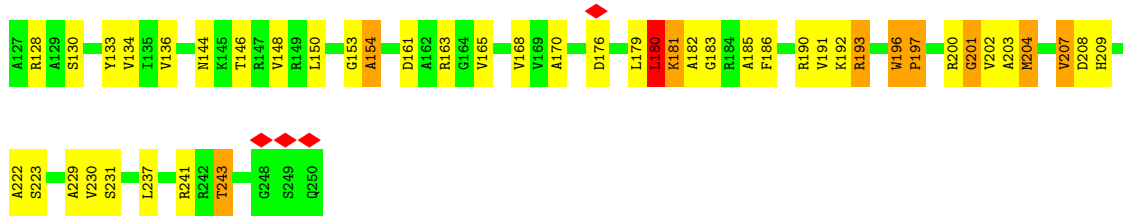
#### • Molecule 1: 25S ribosomal RNA



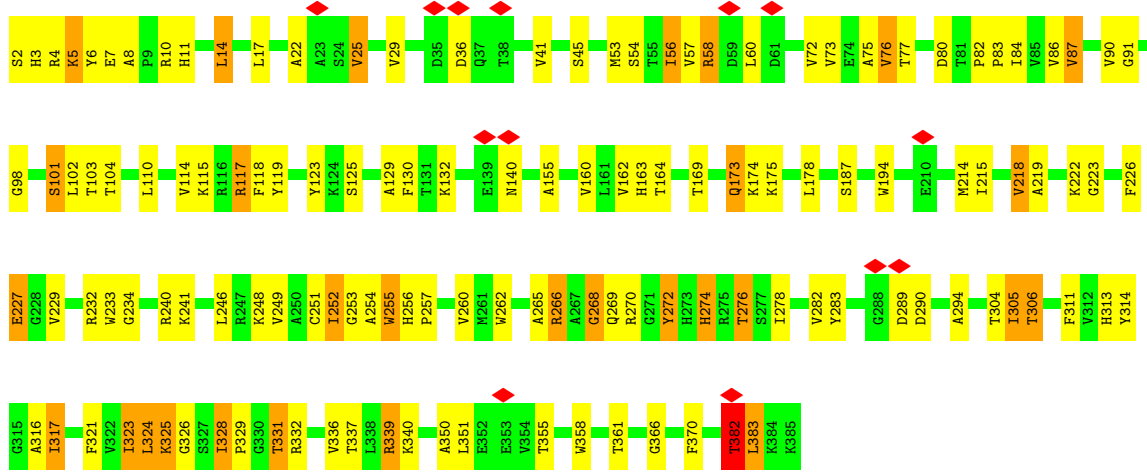




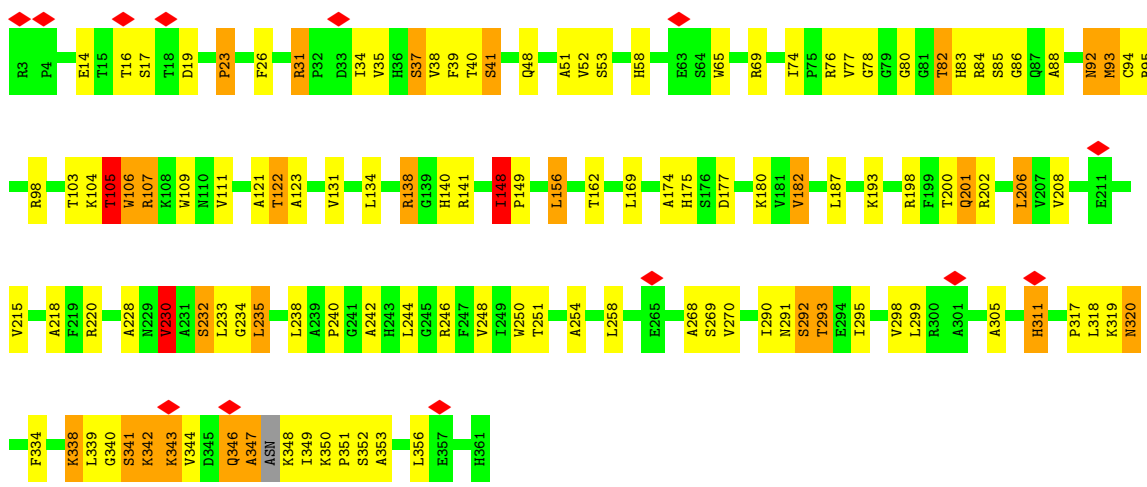




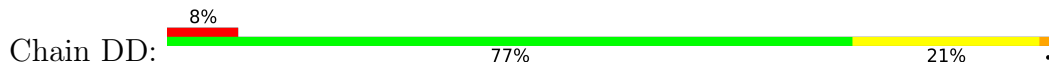
• Molecule 5: 60S ribosomal protein L3

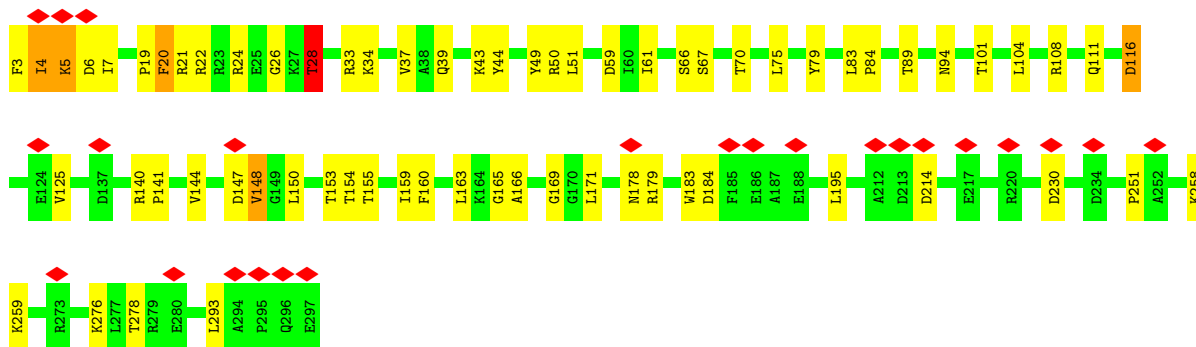


• Molecule 6: KLLA0B07139p

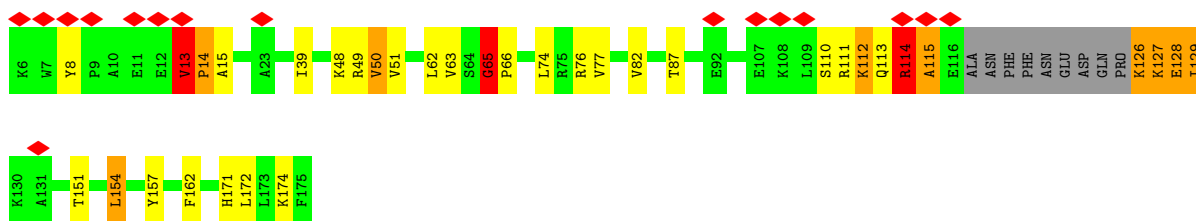
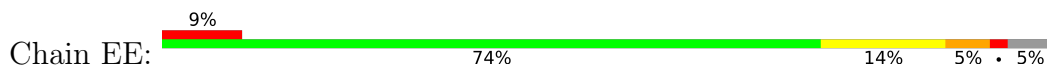


• Molecule 7: KLLA0D06941p

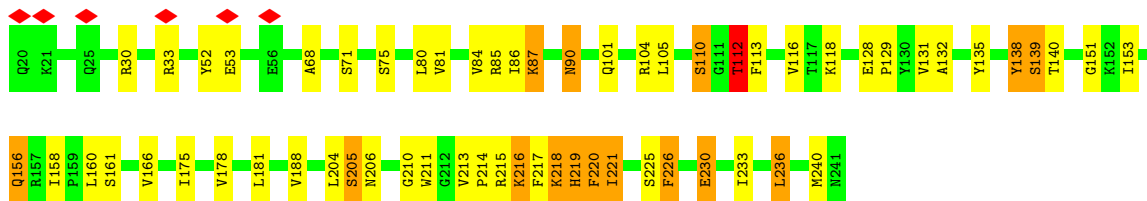
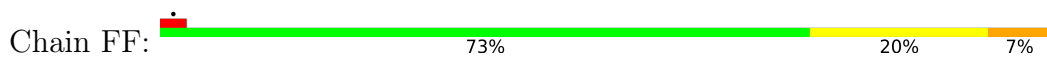




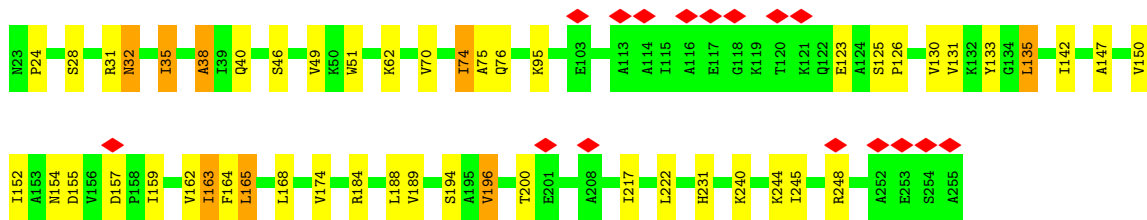
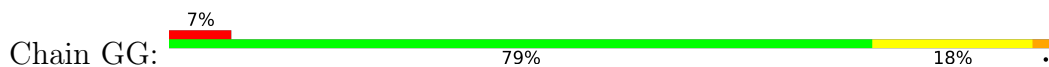
• Molecule 8: KLLA0B04686p



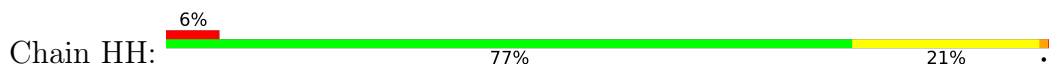
• Molecule 9: KLLA0D03410p

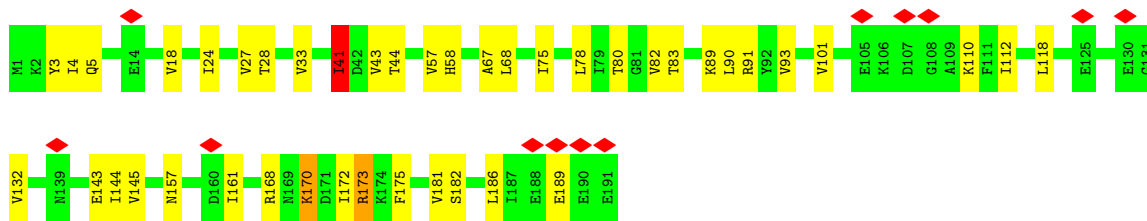


• Molecule 10: KLLA0E00573p

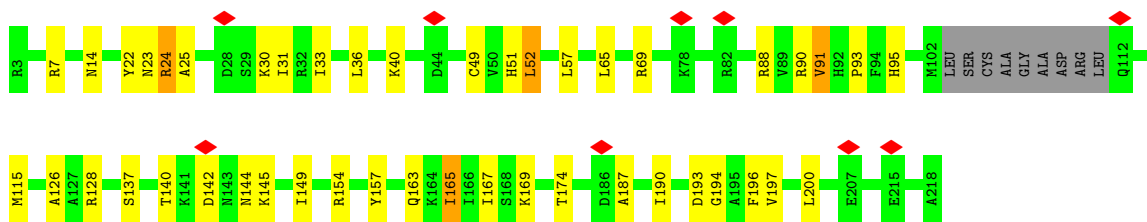
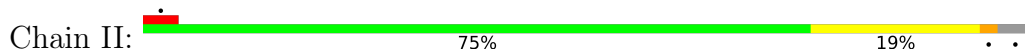


• Molecule 11: KLLA0F04499p

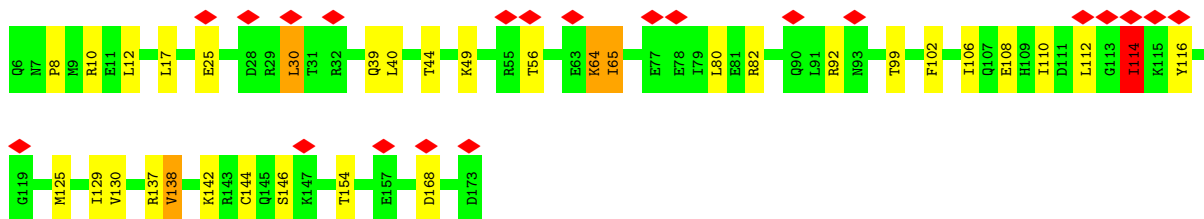
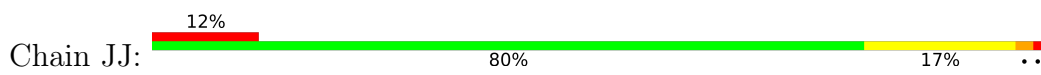




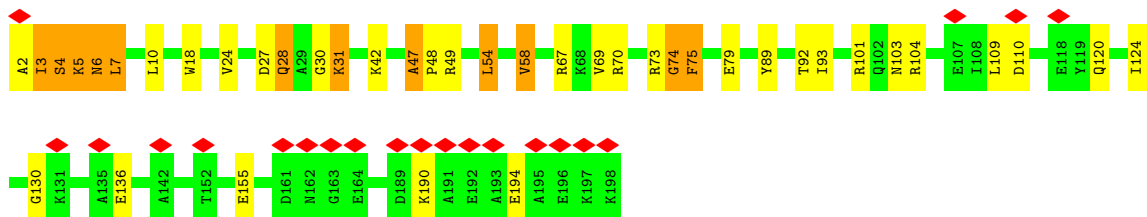
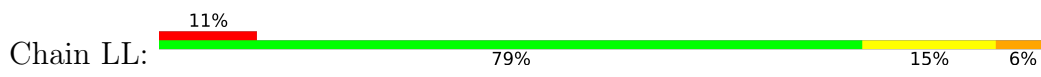
• Molecule 12: KLLA0D05643p



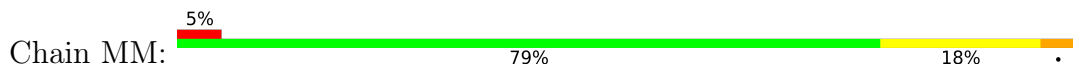
• Molecule 13: KLLA0F08261p



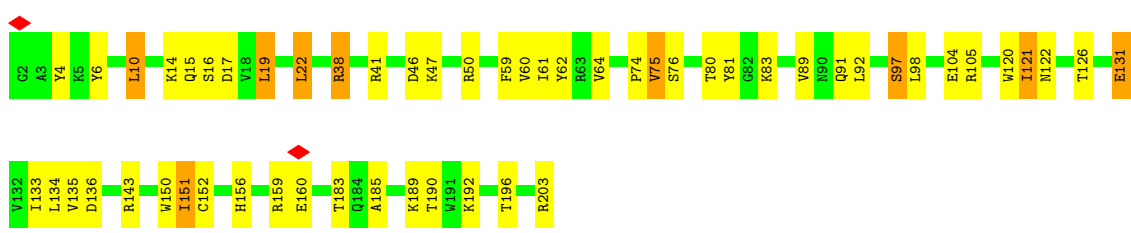
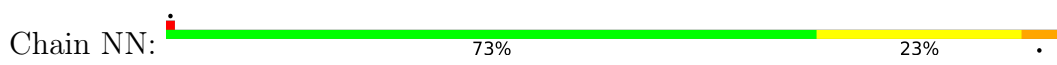
• Molecule 14: 60S ribosomal protein L13



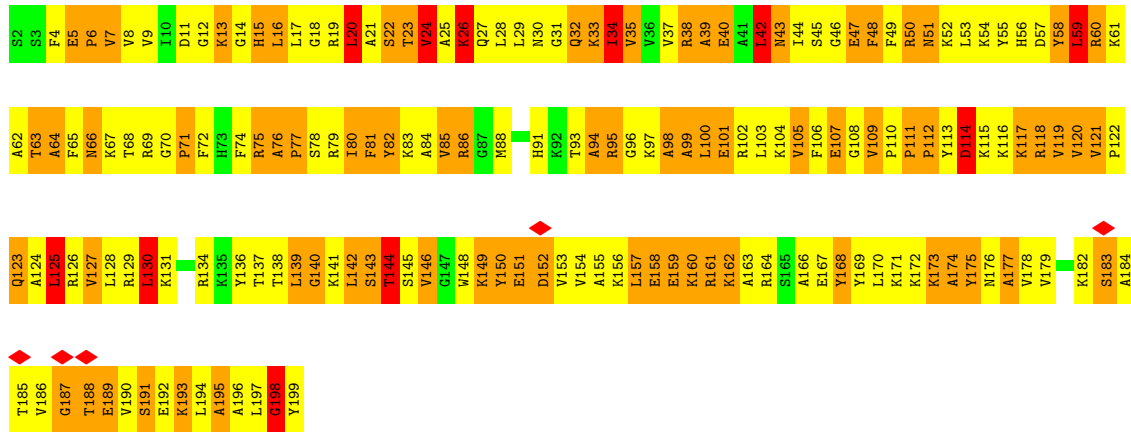
• Molecule 15: KLLA0B13409p



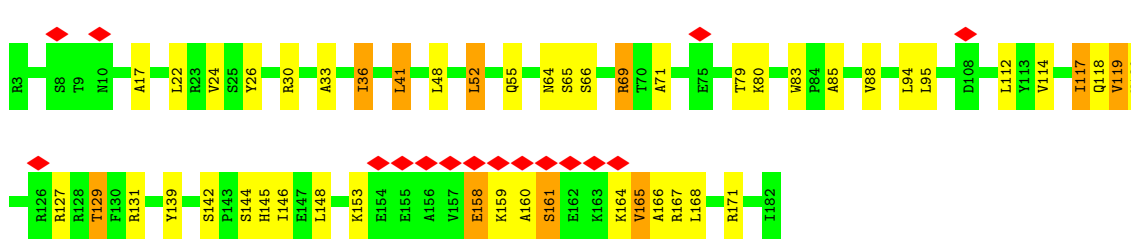
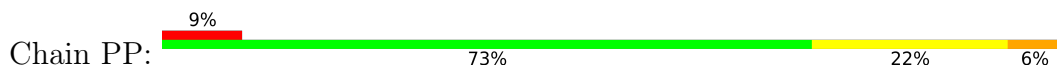
• Molecule 16: Ribosomal protein L15



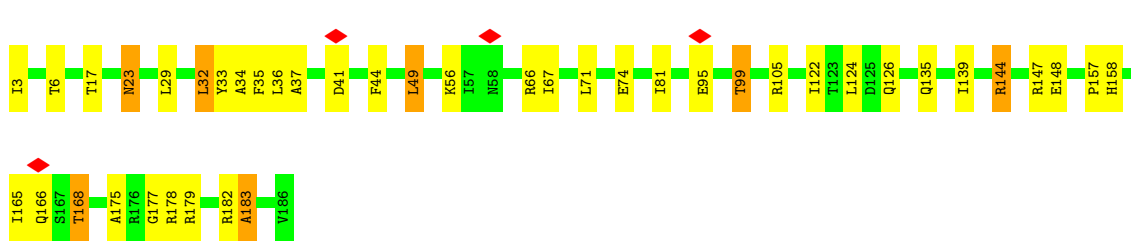
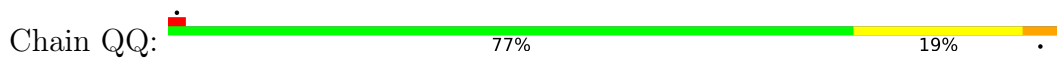
• Molecule 17: KLLA0F04675p



• Molecule 18: KLLA0A06336p



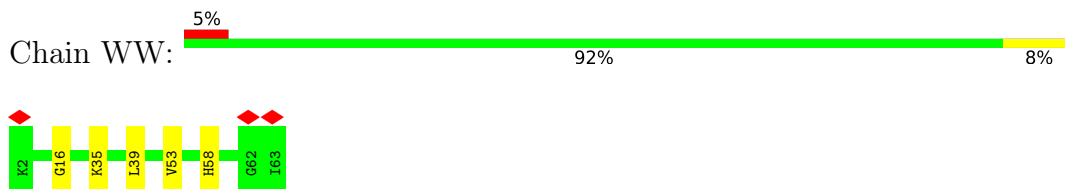
• Molecule 19: KLLA0A07227p



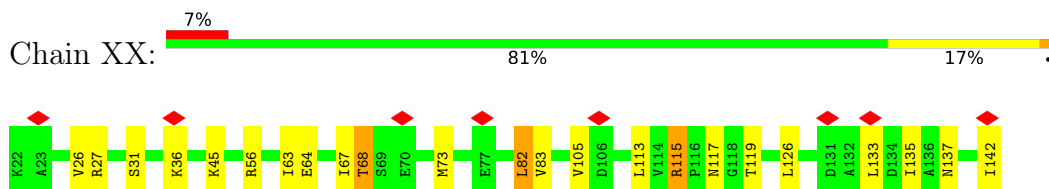
• Molecule 20: KLLA0E12453p



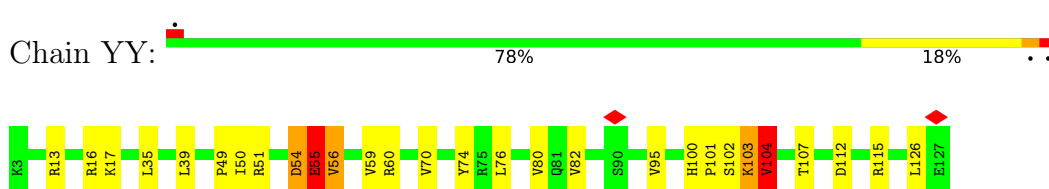
• Molecule 25: 60S ribosomal protein L24



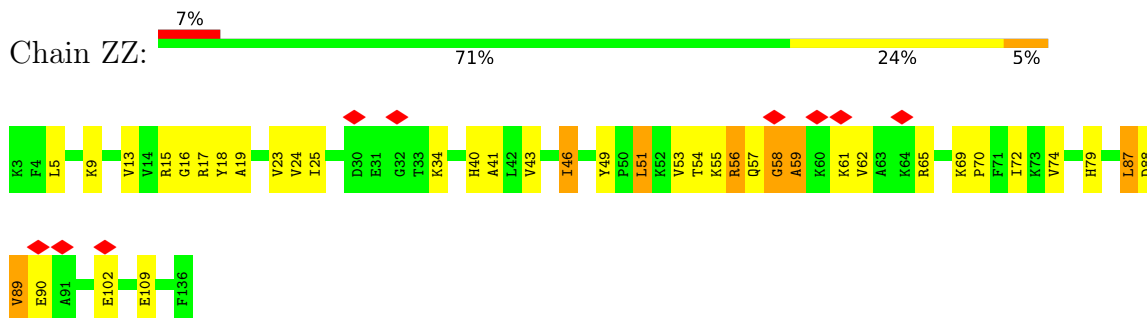
• Molecule 26: 60S ribosomal protein L25



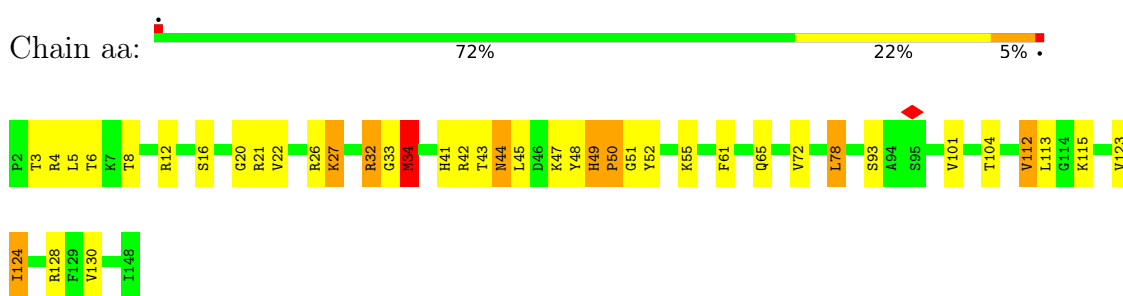
• Molecule 27: KLLA0B05742p



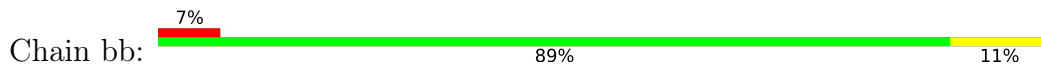
• Molecule 28: KLLA0E03455p



• Molecule 29: RPL28

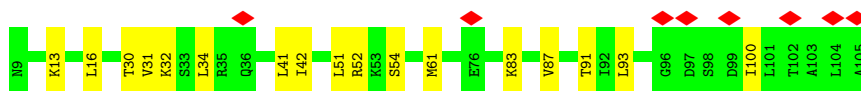
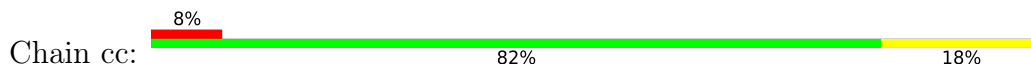


• Molecule 30: KLLA0D16071p

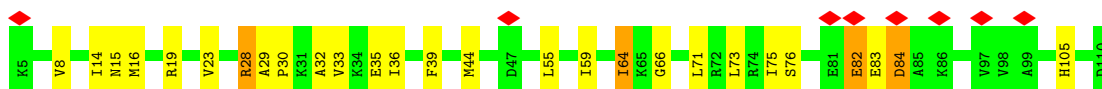
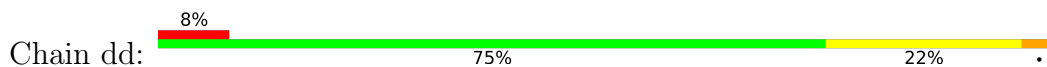




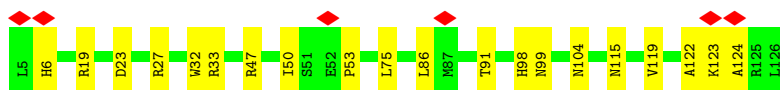
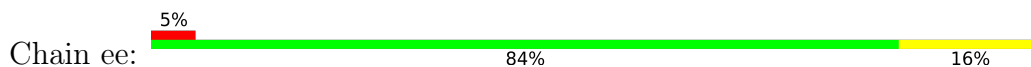
- Molecule 31: 60S ribosomal protein L30



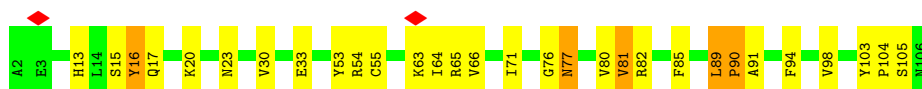
- Molecule 32: KLLA0B02937p



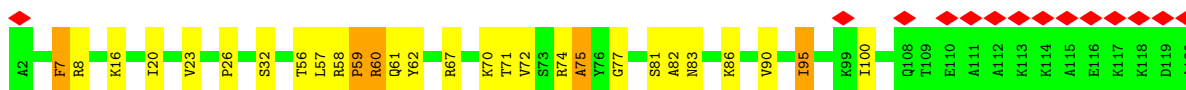
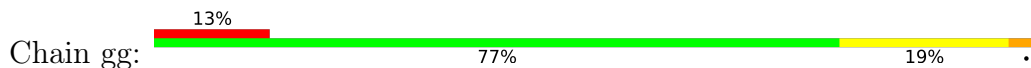
- Molecule 33: KLLA0E06843p



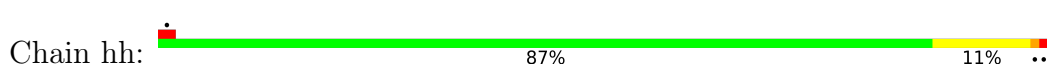
- Molecule 34: KLLA0D07405p

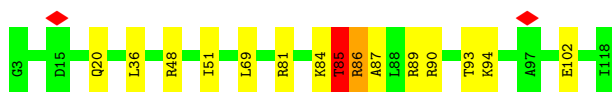


- Molecule 35: KLLA0C08371p

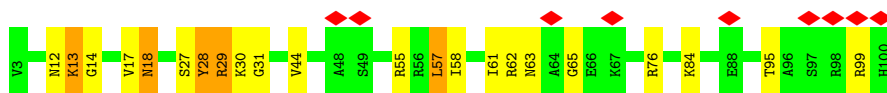
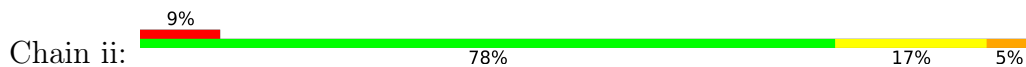


- Molecule 36: KLLA0F05247p

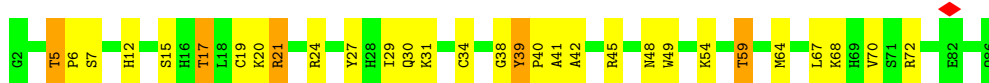




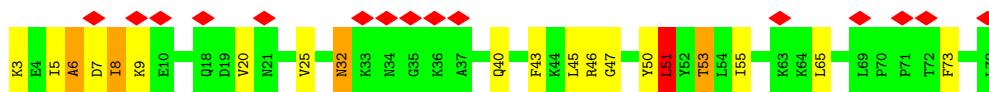
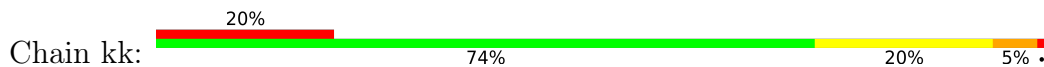
- Molecule 37: 60S ribosomal protein L36



- Molecule 38: Ribosomal protein L37



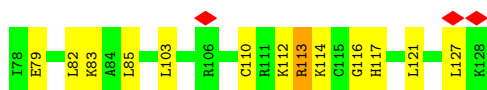
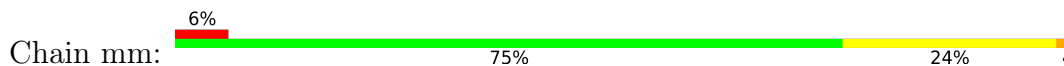
- Molecule 39: KLLA0C18216p



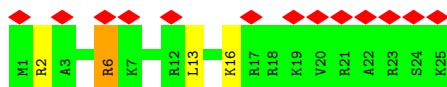
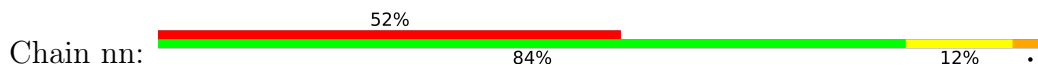
- Molecule 40: 60S ribosomal protein L39



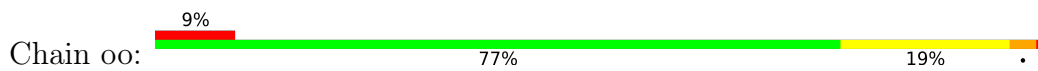
- Molecule 41: Ubiquitin fusion protein



- Molecule 42: 60S ribosomal protein L41-A



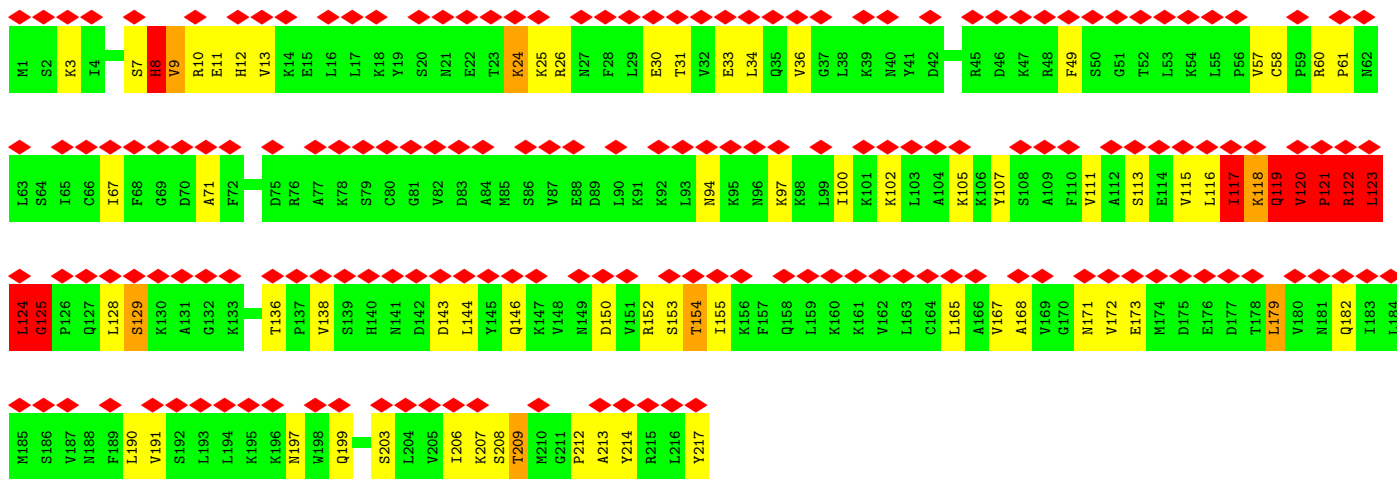
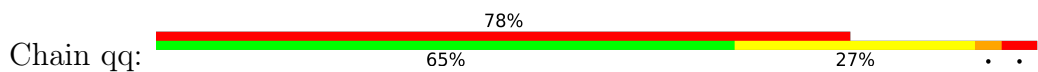
- Molecule 43: 60S ribosomal protein L44



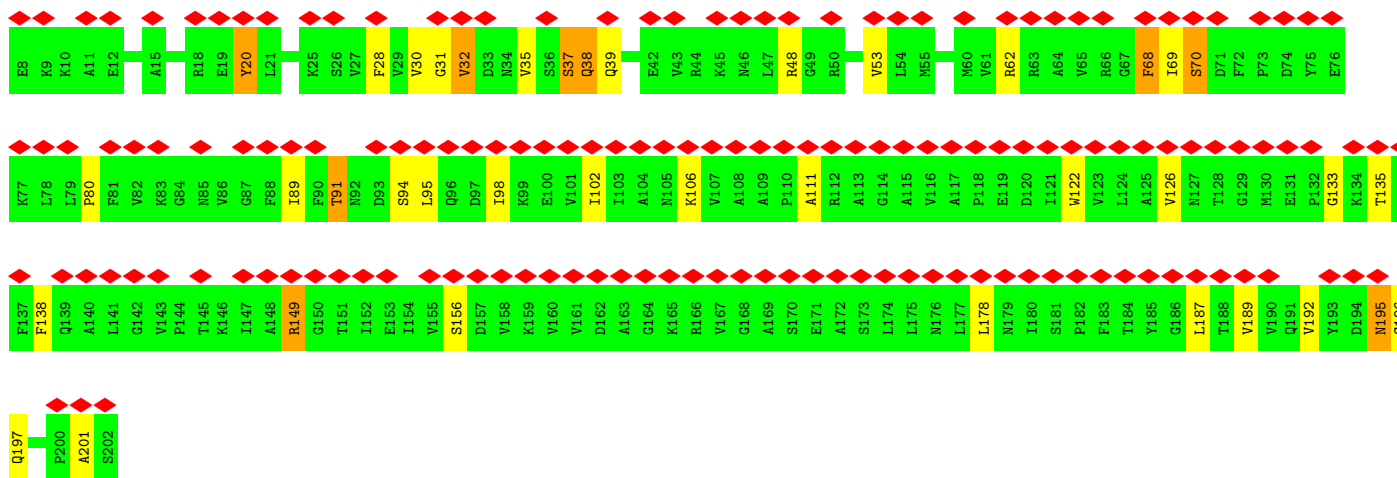
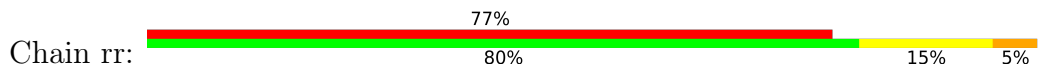
• Molecule 44: KLLA0E05941p



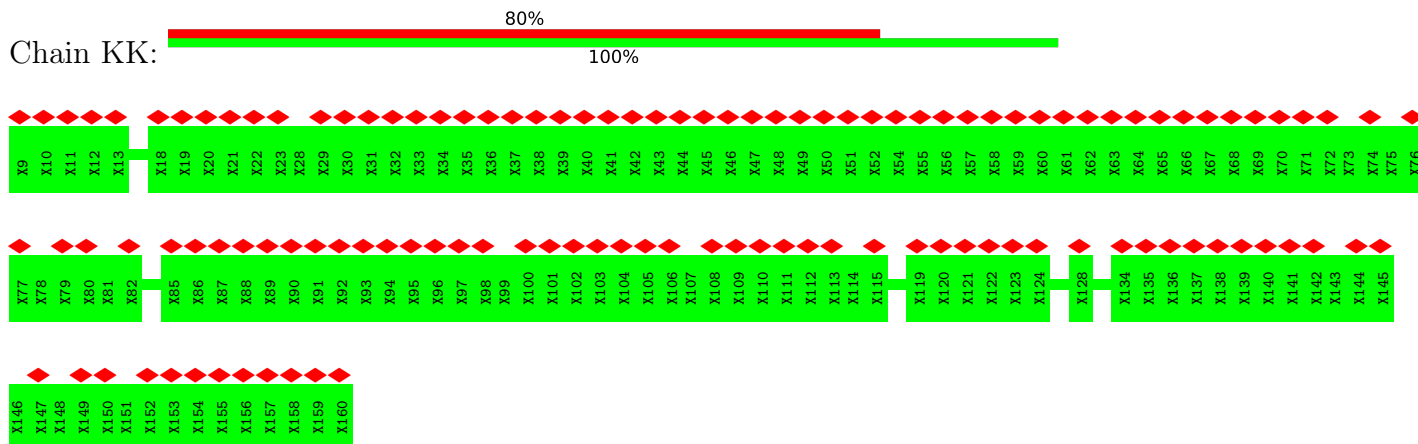
• Molecule 45: Ribosomal protein



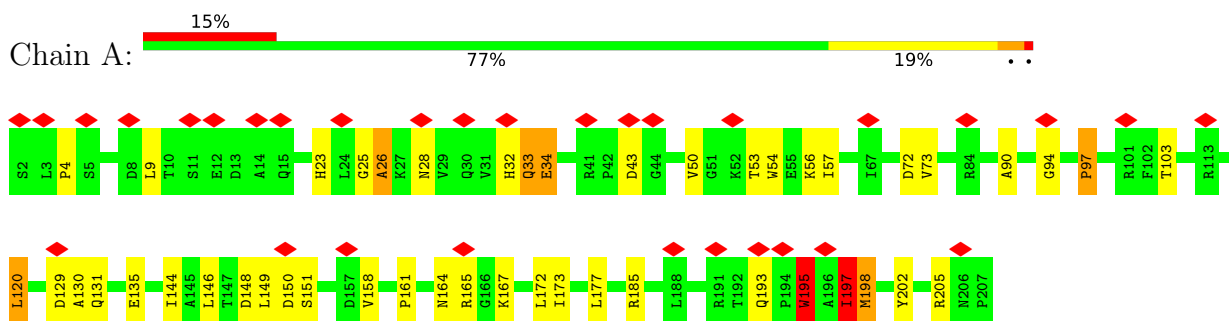
• Molecule 46: 60S acidic ribosomal protein P0



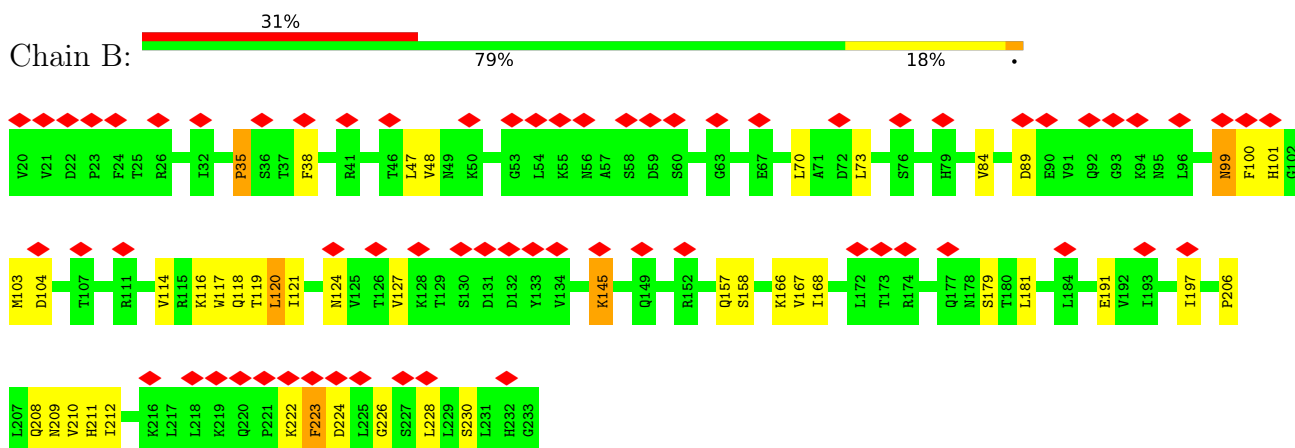
• Molecule 47: uL11



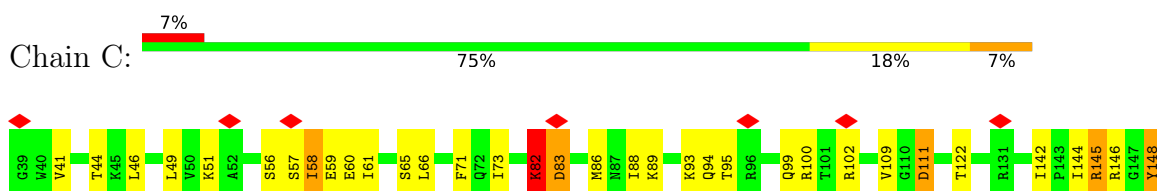
• Molecule 48: 40S ribosomal protein S0

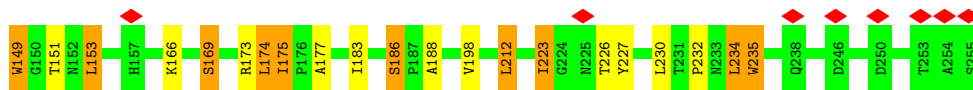


• Molecule 49: 40S ribosomal protein S1

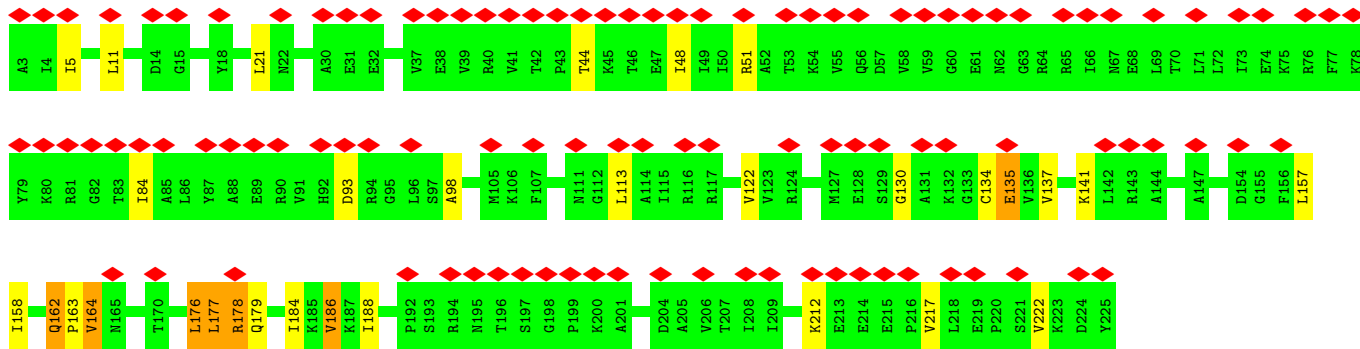
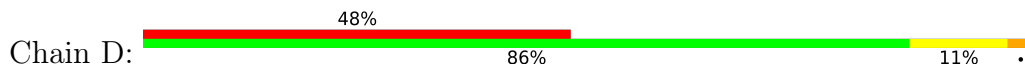


• Molecule 50: KLLA0F09812p

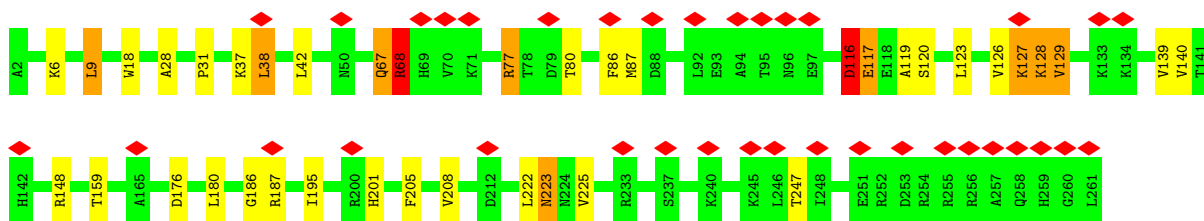
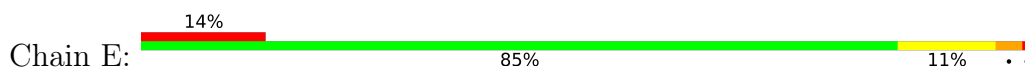




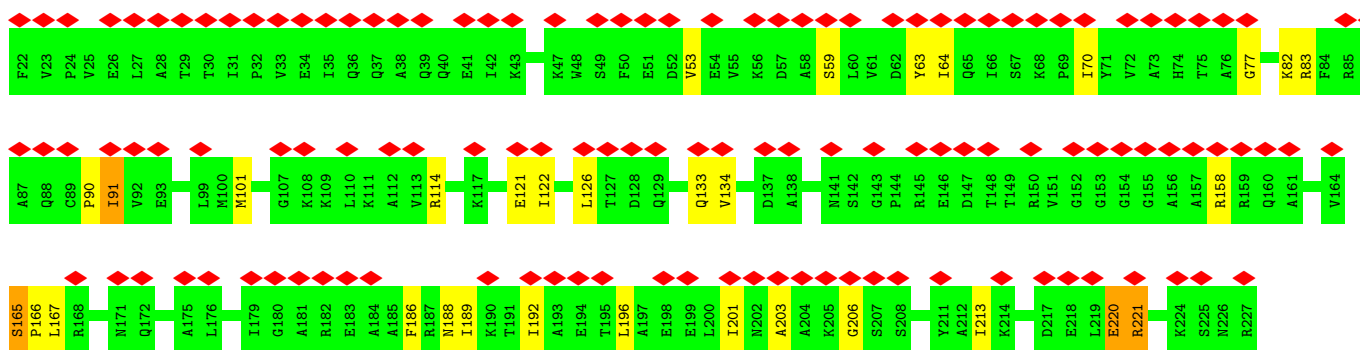
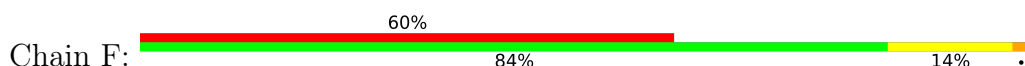
• Molecule 51: KLLA0D08305p



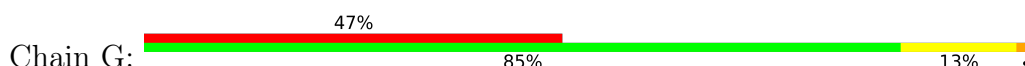
• Molecule 52: 40S ribosomal protein S4

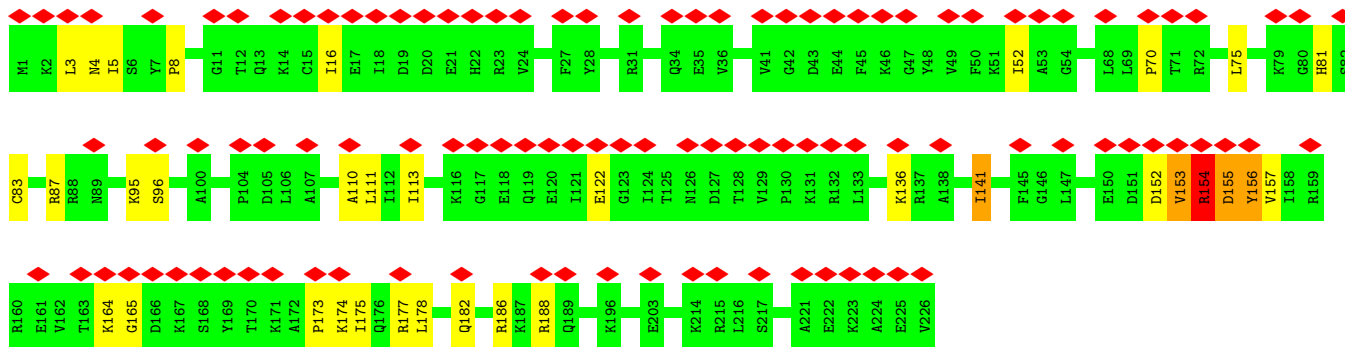


• Molecule 53: KLLA0D10659p

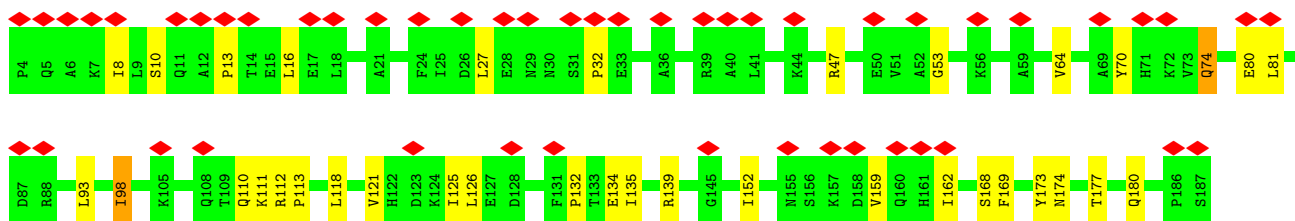
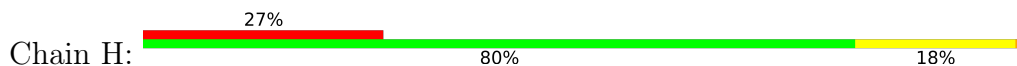


• Molecule 54: 40S ribosomal protein S6

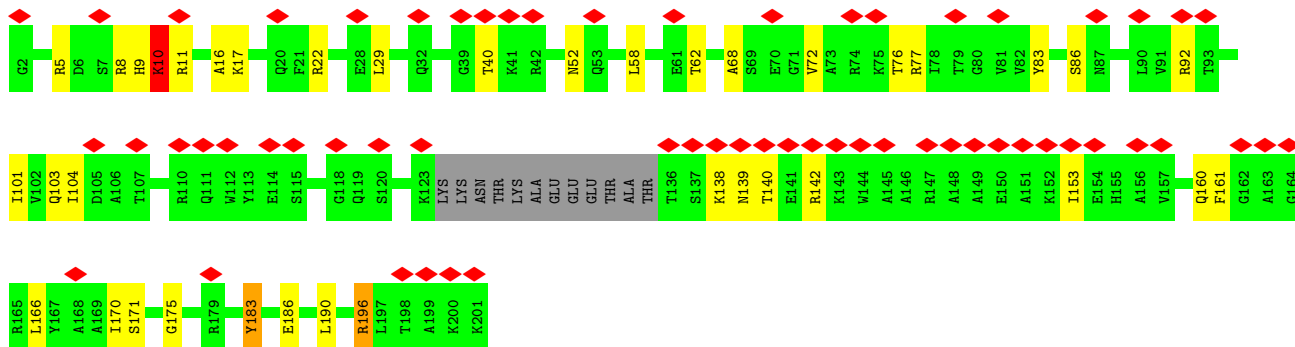
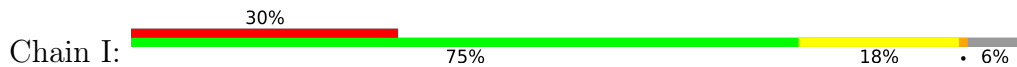




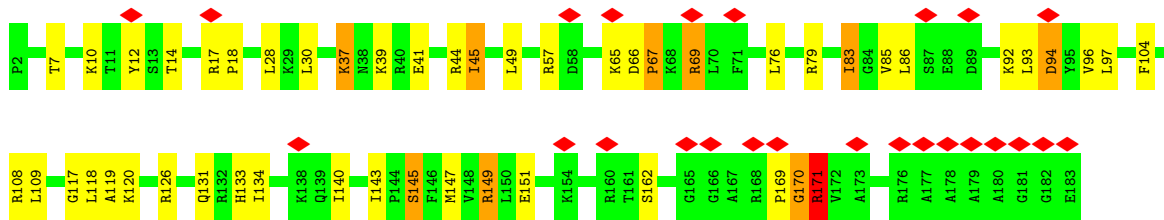
• Molecule 55: KLLA0C13519p



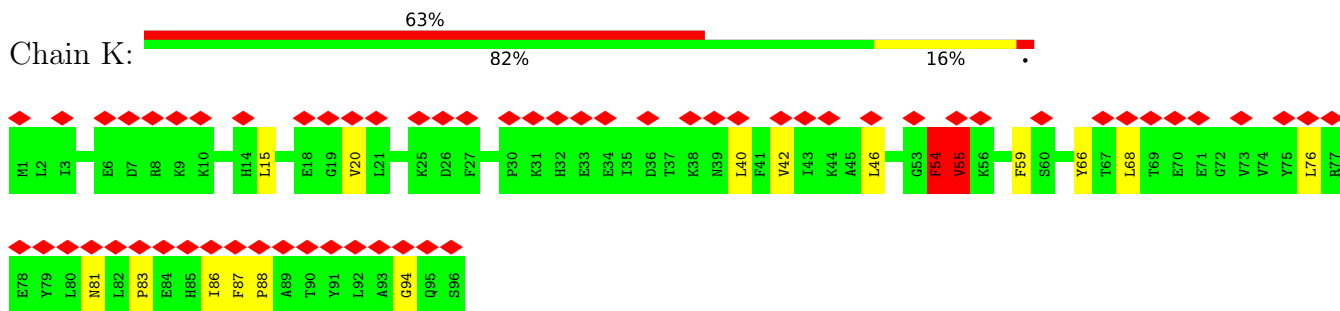
• Molecule 56: 40S ribosomal protein S8



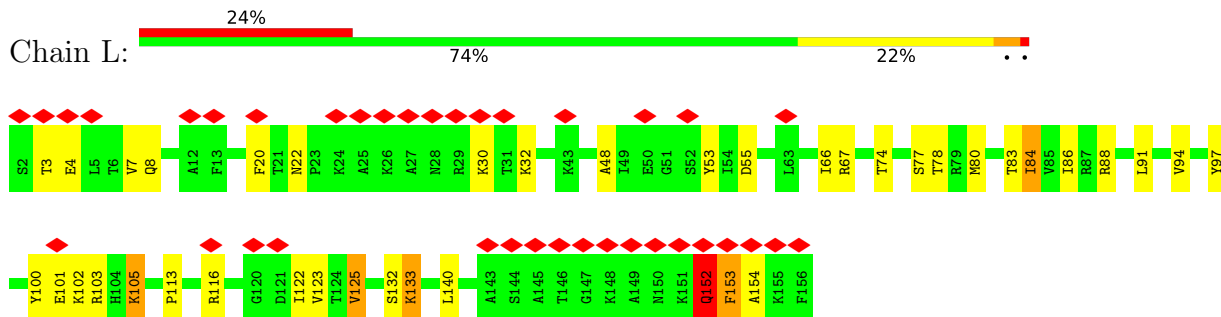
• Molecule 57: KLLA0E23673p



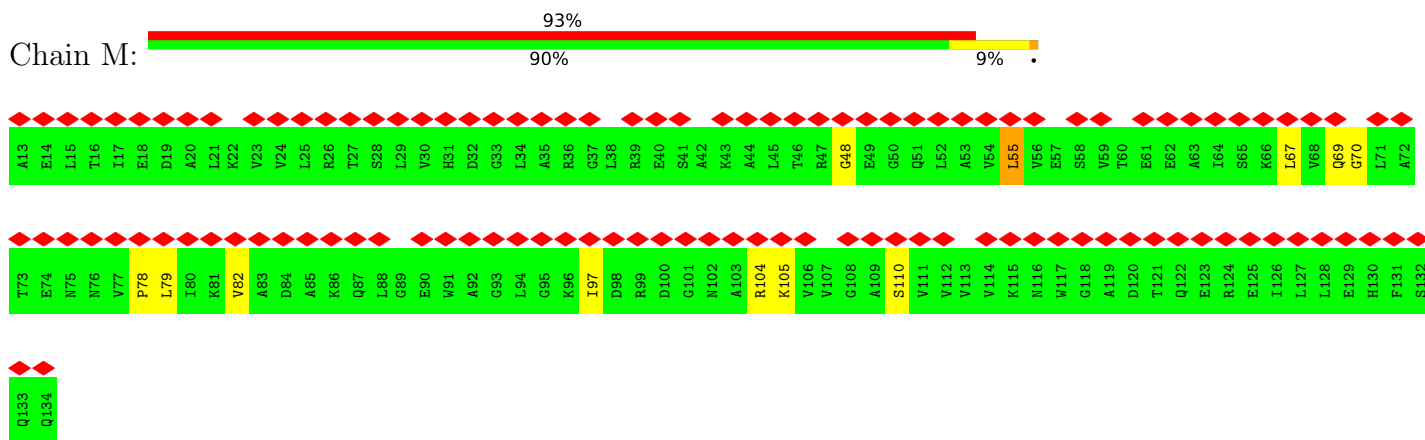
• Molecule 58: KLLA0B08173p



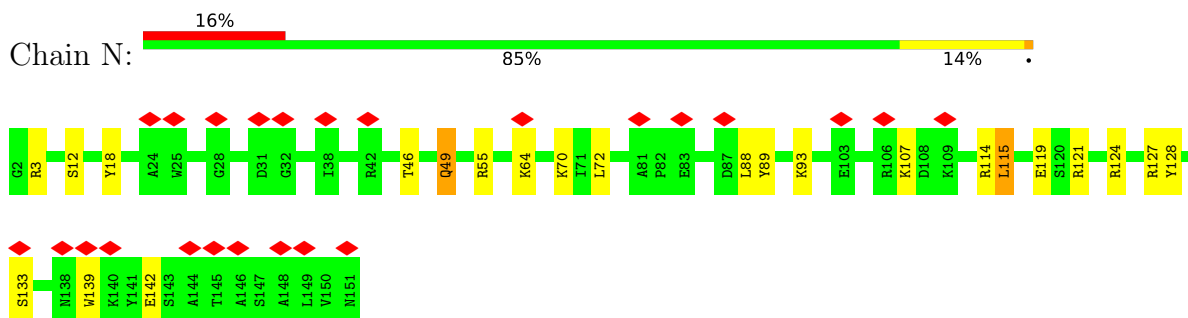
• Molecule 59: KLLA0A10483p



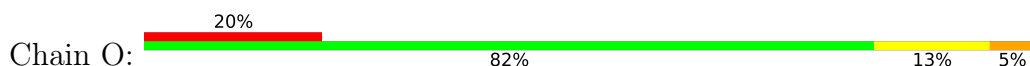
• Molecule 60: 40S ribosomal protein S12

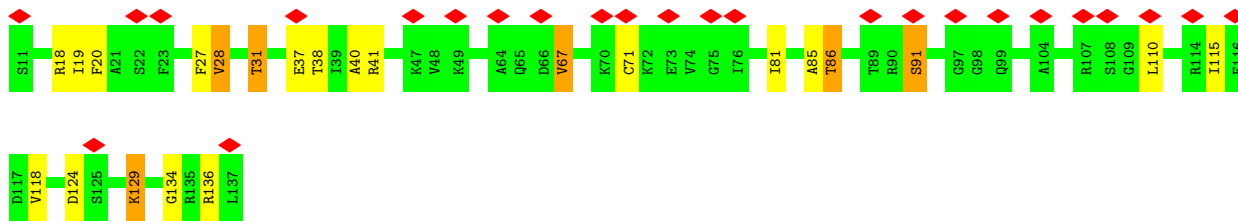


• Molecule 61: KLLA0F18040p

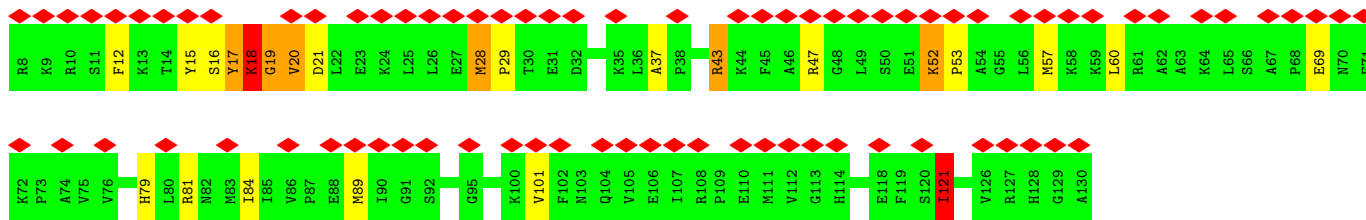
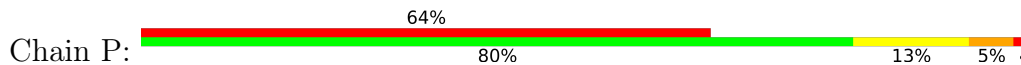


• Molecule 62: 40S ribosomal protein S14

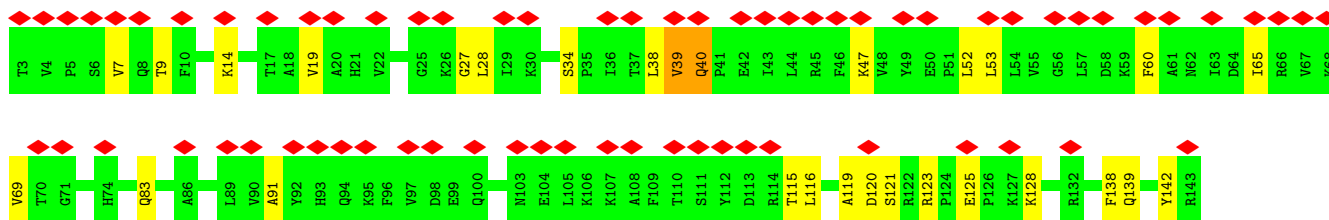
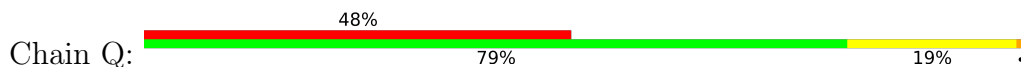




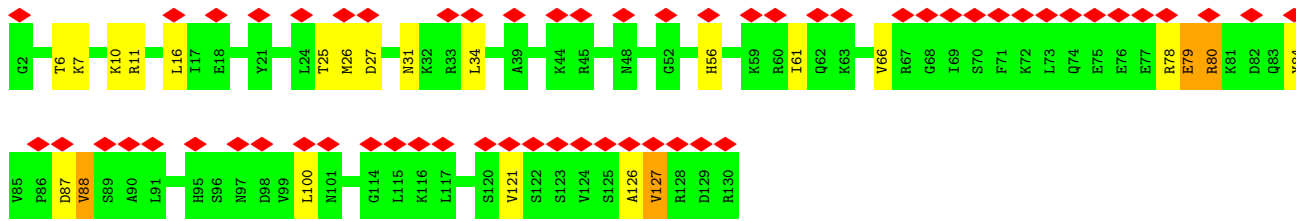
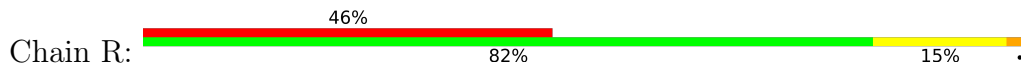
• Molecule 63: KLLA0F07843p



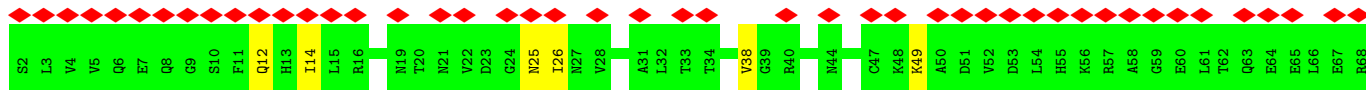
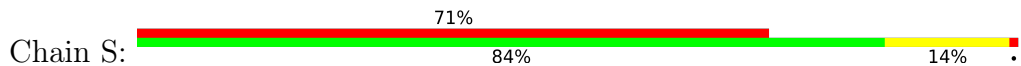
• Molecule 64: 40S ribosomal protein S16

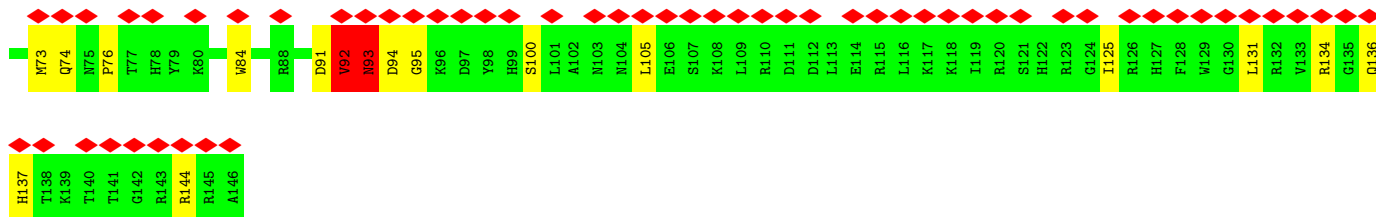


• Molecule 65: KLLA0B01474p

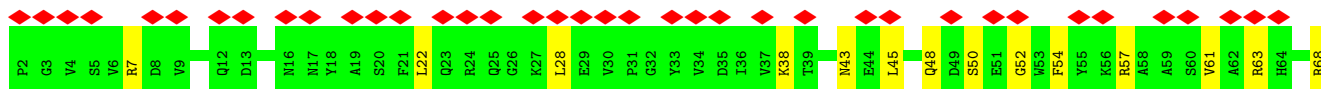
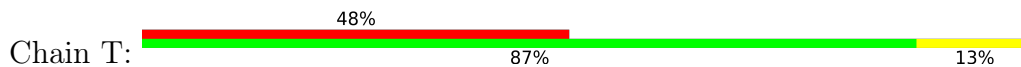


• Molecule 66: KLLA0B01562p

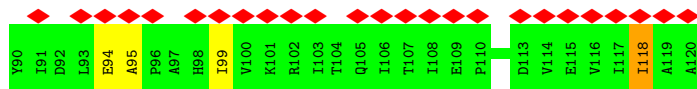
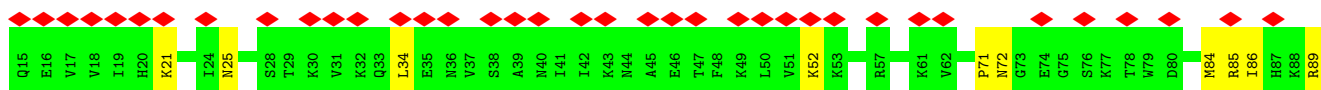
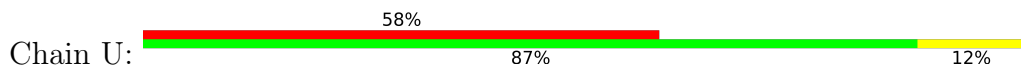




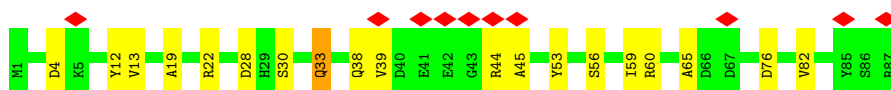
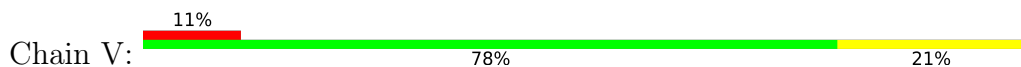
• Molecule 67: KLLA0A07194p



• Molecule 68: KLLA0F25542p



• Molecule 69: 40S ribosomal protein S21

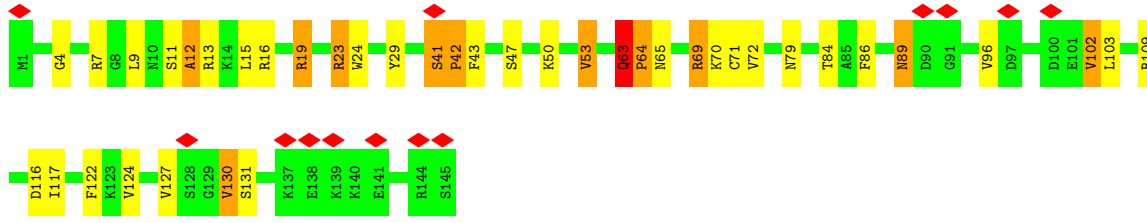


• Molecule 70: 40S ribosomal protein S22

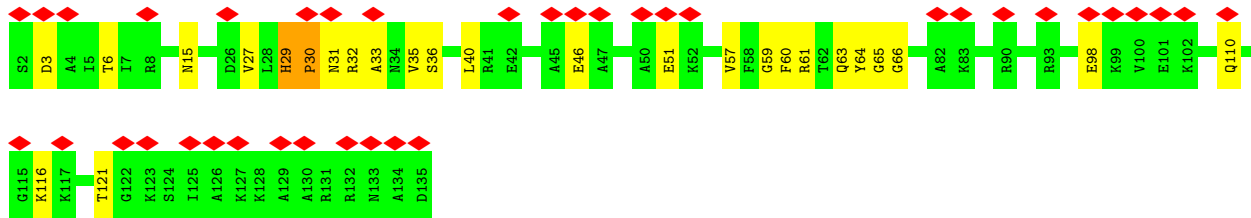
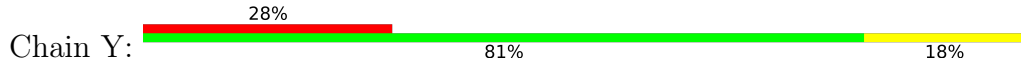


• Molecule 71: RPS23

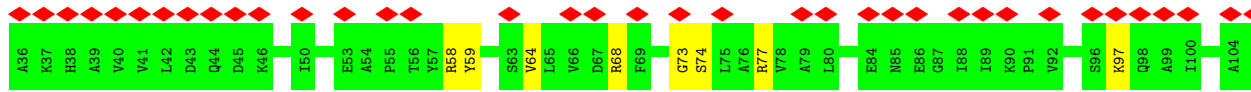
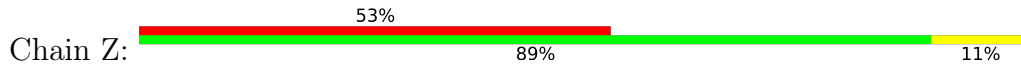




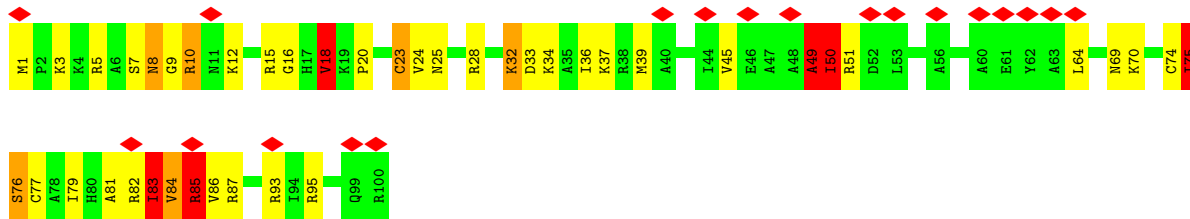
• Molecule 72: 40S ribosomal protein S24



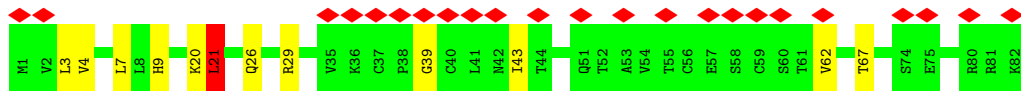
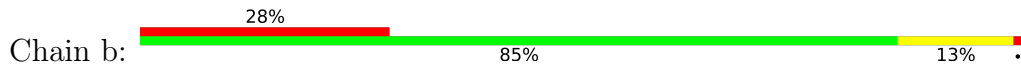
• Molecule 73: KLLA0B06182p



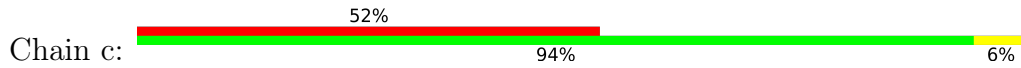
• Molecule 74: KLLA0D05115p

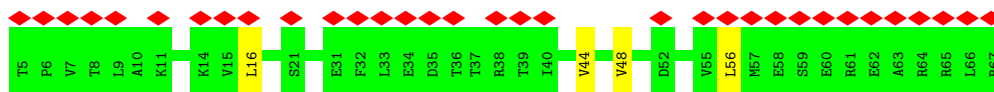


• Molecule 75: 40S ribosomal protein S27

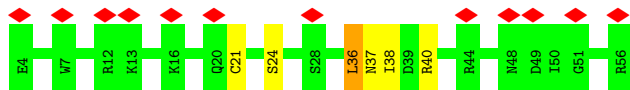
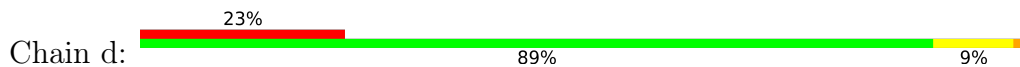


• Molecule 76: 40S ribosomal protein S28

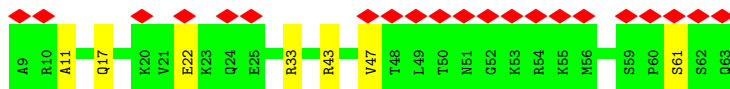
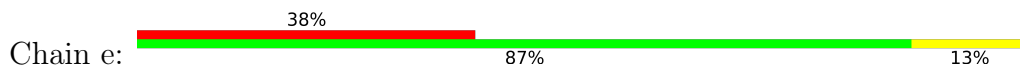




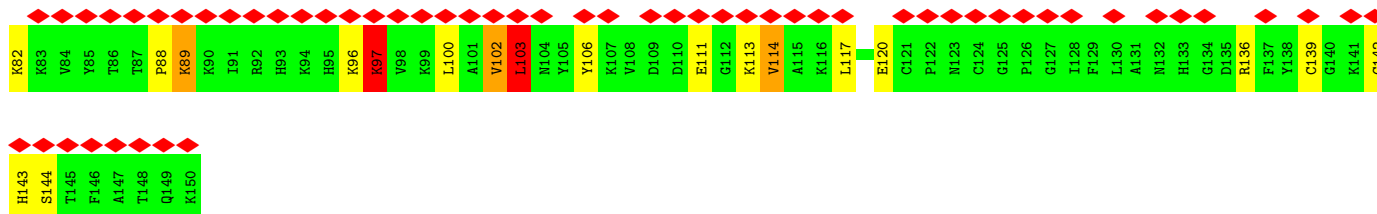
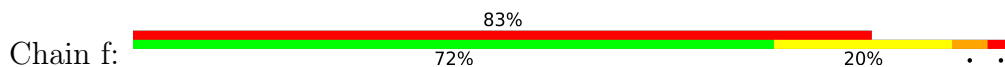
• Molecule 77: 40S ribosomal protein S29



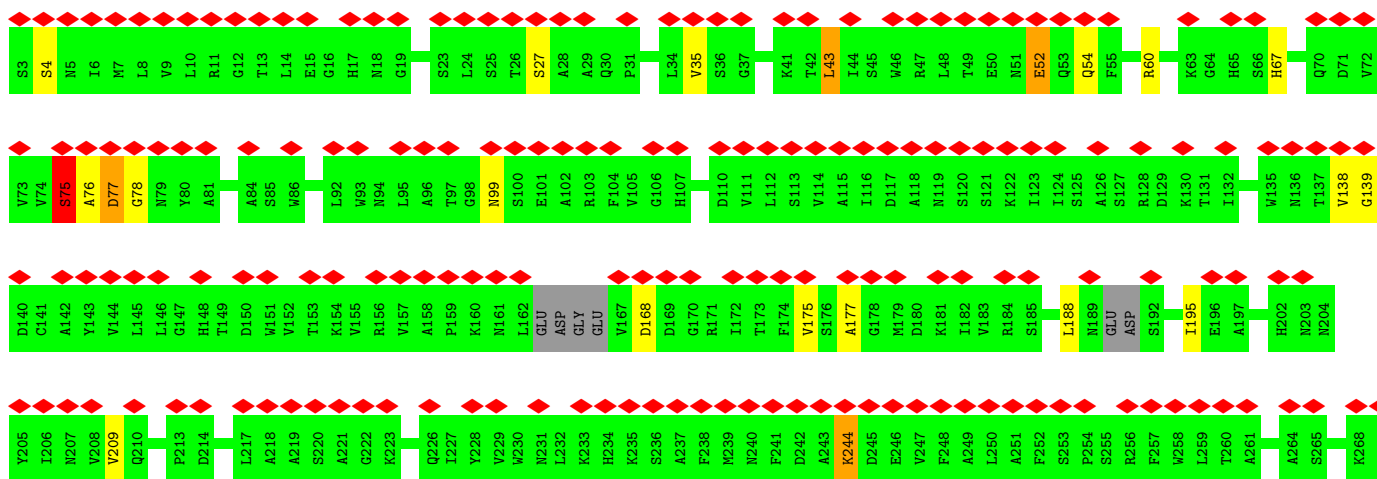
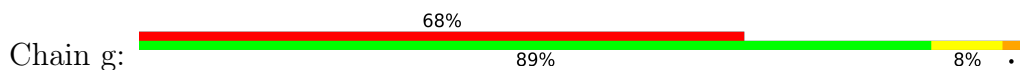
• Molecule 78: KLLA0C04809p

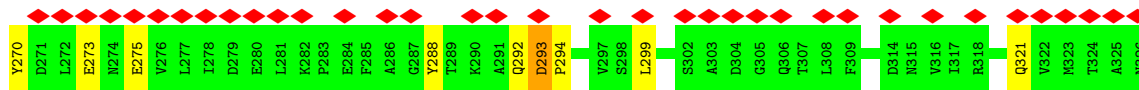


• Molecule 79: Ubiquitin-40S ribosomal protein S27a

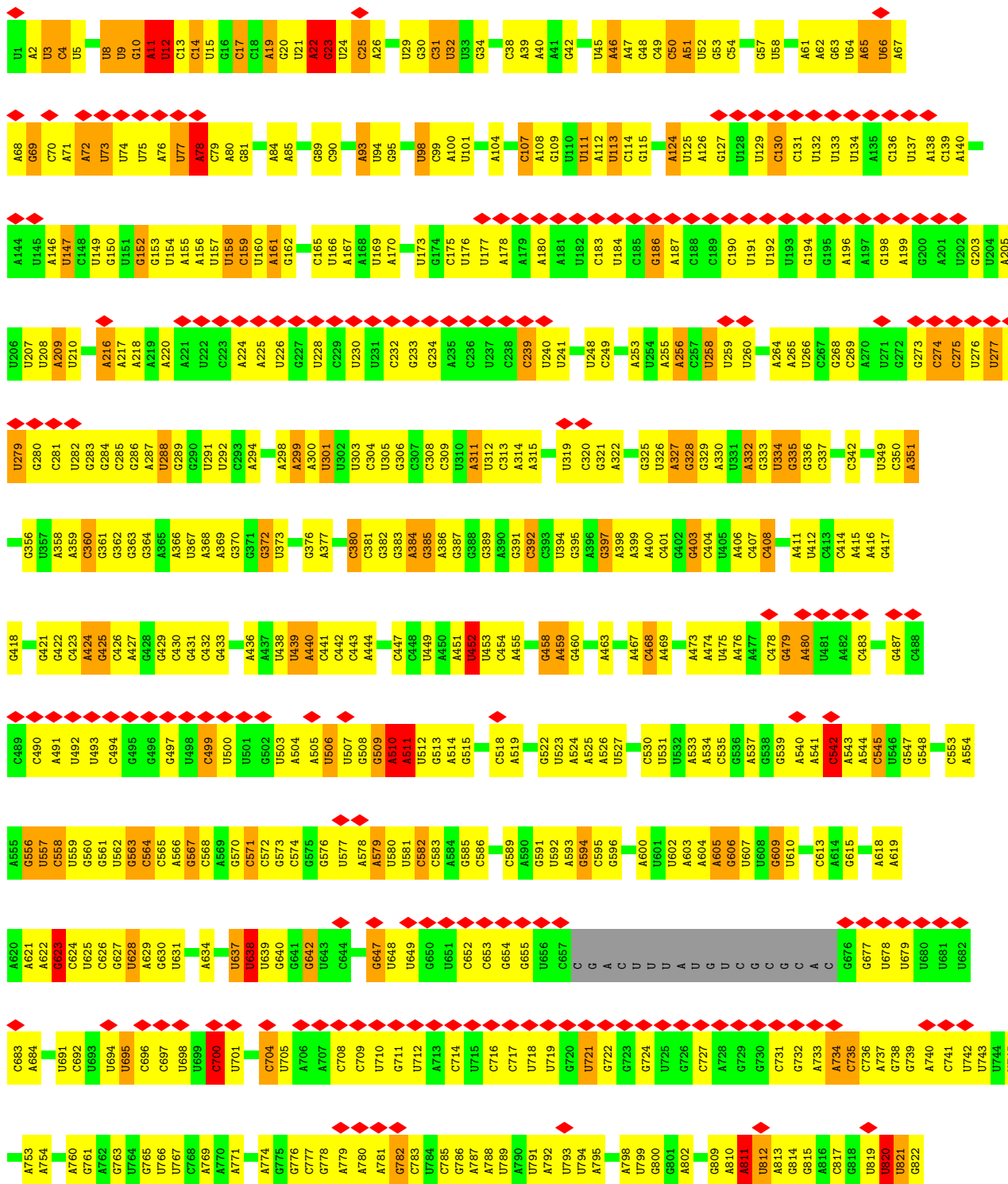


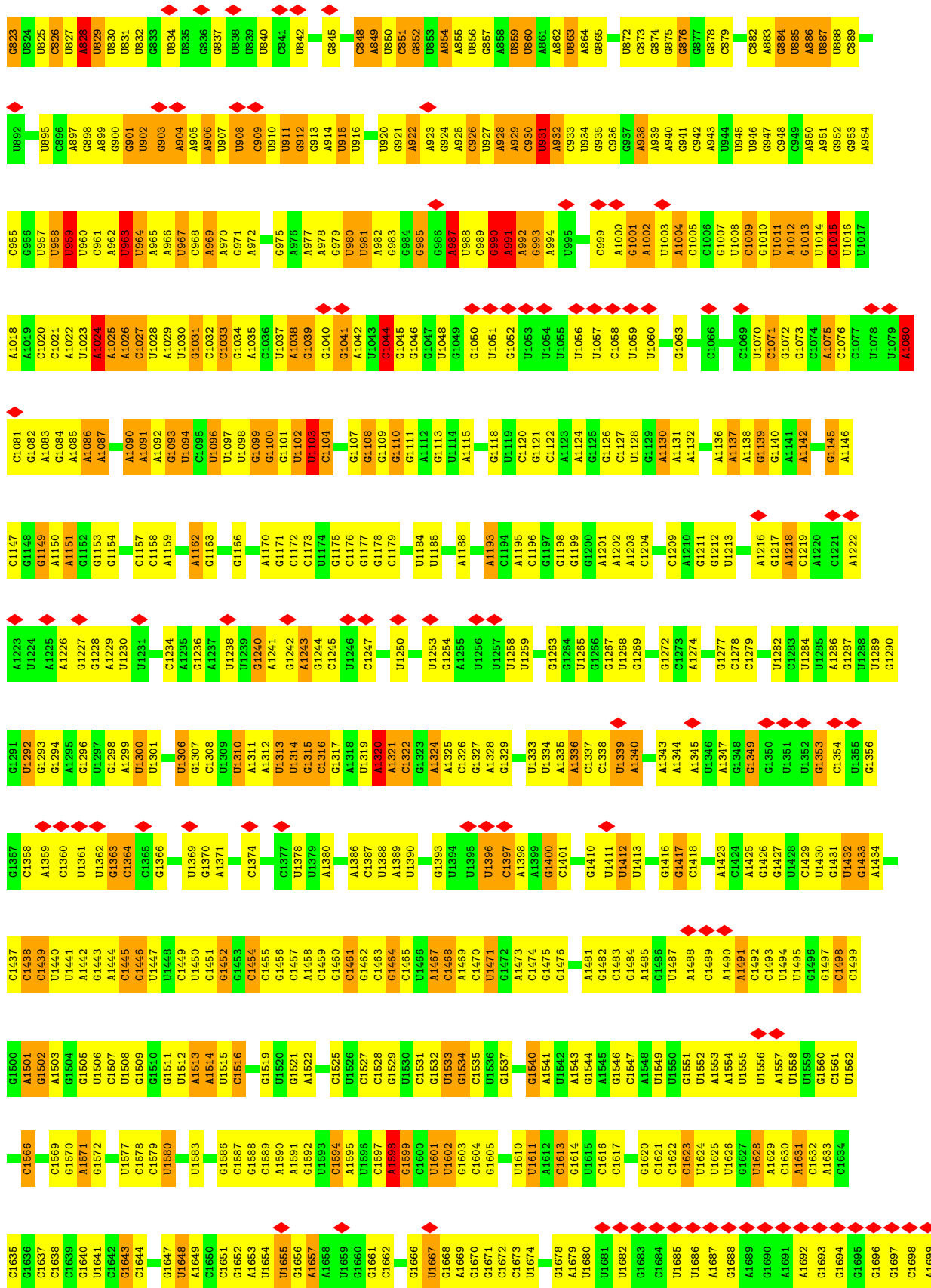
• Molecule 80: KLLA0E12277p

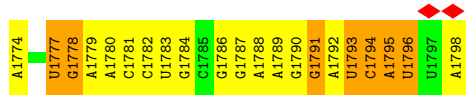
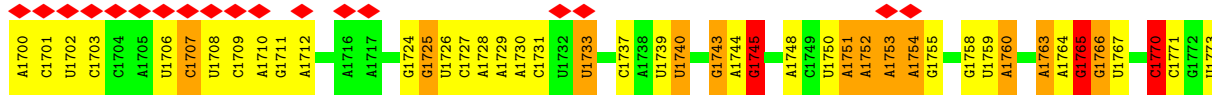




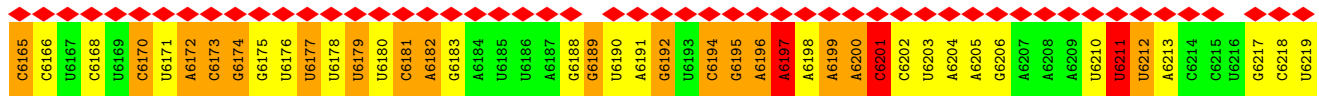
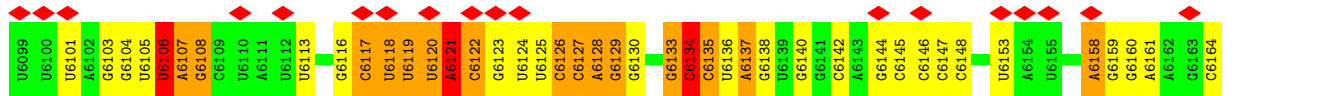
• Molecule 81: 18S ribosomal RNA



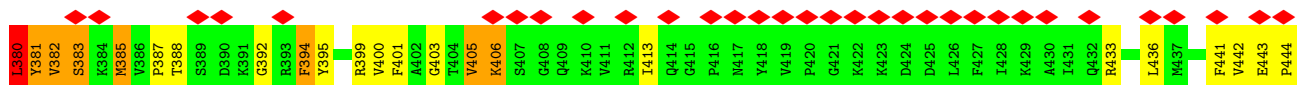
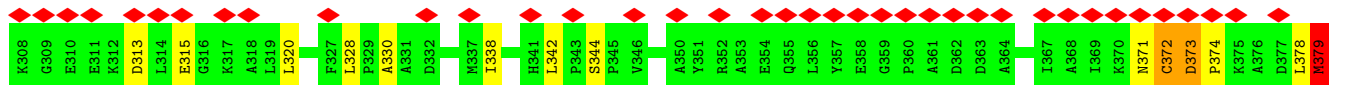
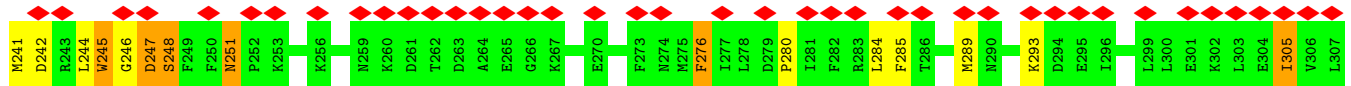
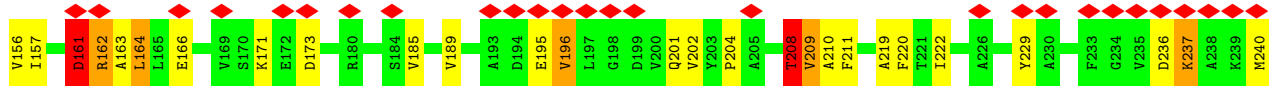
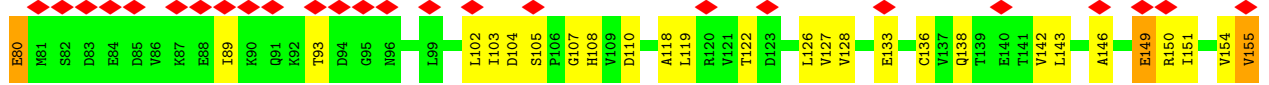
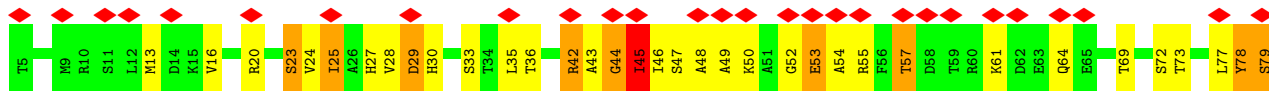
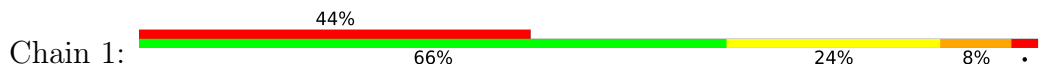


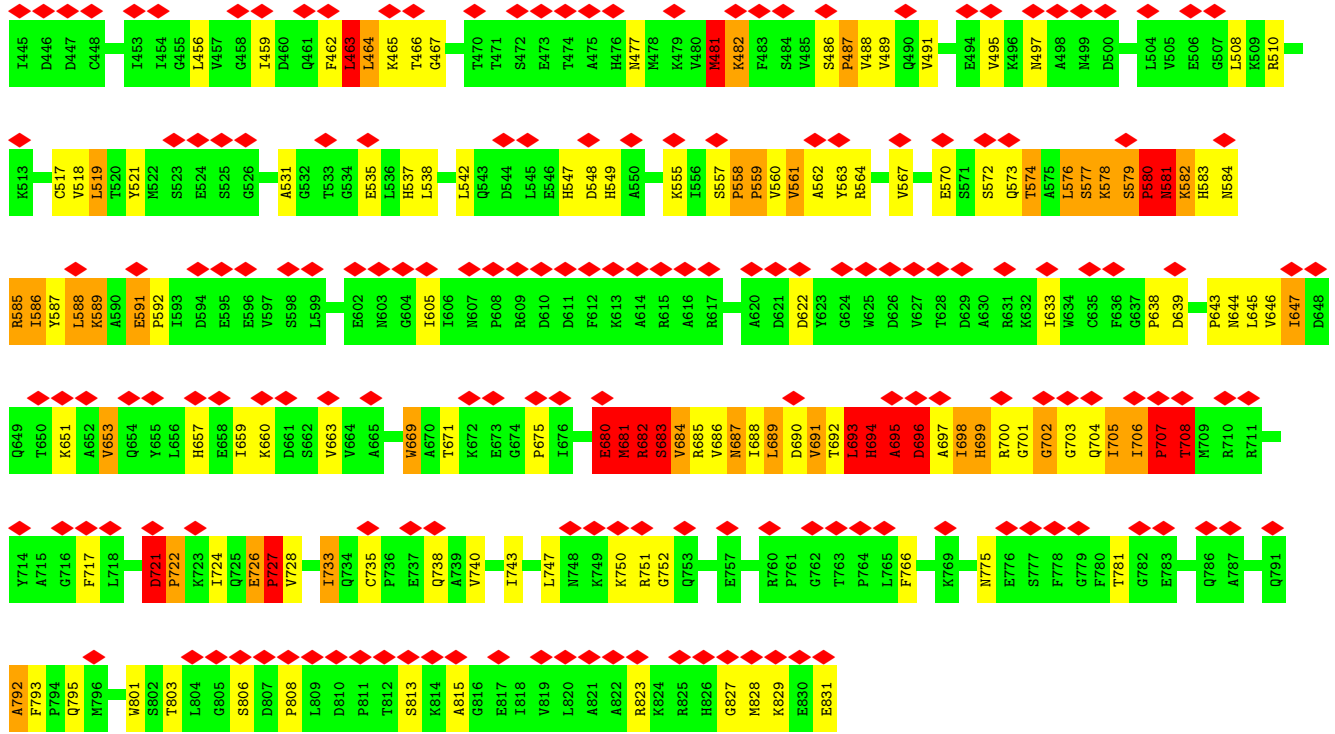


• Molecule 82: cricket paralysis virus IRES



• Molecule 83: Eft2p





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	37844	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	30	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	0.793	Depositor
Minimum map value	-0.578	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.044	Depositor
Recommended contour level	0.1	Depositor
Map size ( $\text{\AA}$ )	428.80002, 428.80002, 428.80002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.34, 1.34, 1.34	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: GCP, 6EM, 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	5	0.49	4/78233 (0.0%)	0.94	323/121966 (0.3%)
2	7	0.44	0/2883	0.80	0/4491
3	8	0.47	0/3714	0.90	8/5781 (0.1%)
4	AA	0.85	0/1926	1.01	2/2588 (0.1%)
5	BB	0.81	1/3136 (0.0%)	1.01	4/4225 (0.1%)
6	CC	0.73	0/2780	1.06	7/3760 (0.2%)
7	DD	0.58	0/2436	0.85	2/3292 (0.1%)
8	EE	0.59	0/1322	1.00	5/1776 (0.3%)
9	FF	0.74	1/1810 (0.1%)	1.00	3/2440 (0.1%)
10	GG	0.60	0/1846	0.97	3/2486 (0.1%)
11	HH	0.58	0/1547	0.89	1/2083 (0.0%)
12	II	0.64	0/1725	0.86	0/2310
13	JJ	0.55	0/1370	0.84	0/1835
14	LL	0.65	0/1607	0.97	2/2156 (0.1%)
15	MM	0.61	0/1060	0.95	0/1430
16	NN	0.87	0/1746	0.99	3/2339 (0.1%)
17	OO	0.98	0/1602	1.14	13/2151 (0.6%)
18	PP	0.80	0/1455	0.94	0/1952
19	QQ	0.64	0/1469	0.94	0/1970
20	RR	0.66	0/1539	0.92	0/2047
21	SS	0.65	0/1452	0.88	1/1956 (0.1%)
22	TT	0.69	0/1286	0.92	1/1722 (0.1%)
23	UU	0.50	0/824	0.79	0/1113
24	VV	0.78	0/991	1.01	0/1331
25	WW	0.65	0/528	0.82	1/703 (0.1%)
26	XX	0.65	0/979	0.90	0/1320
27	YY	0.60	0/1003	0.95	1/1339 (0.1%)
28	ZZ	0.63	0/1114	0.99	1/1493 (0.1%)
29	aa	0.78	0/1186	1.02	3/1590 (0.2%)
30	bb	0.58	0/468	0.86	0/621
31	cc	0.61	0/748	0.84	0/1005
32	dd	0.63	0/885	0.82	0/1186

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	ee	0.75	0/998	0.90	0/1332
34	ff	0.89	1/855 (0.1%)	1.06	4/1150 (0.3%)
35	gg	0.71	0/961	0.98	1/1281 (0.1%)
36	hh	0.55	0/970	0.88	0/1291
37	ii	0.59	0/773	0.94	0/1029
38	jj	0.99	0/690	1.05	3/913 (0.3%)
39	kk	0.66	1/626 (0.2%)	1.06	0/835
40	ll	0.74	0/435	0.89	0/577
41	mm	0.65	0/416	0.84	0/552
42	nn	0.57	0/234	0.81	0/300
43	oo	0.60	0/825	0.97	3/1086 (0.3%)
44	pp	0.80	0/667	1.10	2/891 (0.2%)
45	qq	0.98	15/1748 (0.9%)	1.11	16/2350 (0.7%)
46	rr	0.61	0/1535	0.90	0/2077
48	A	0.56	0/1656	0.92	1/2264 (0.0%)
49	B	0.57	0/1747	0.87	1/2353 (0.0%)
50	C	0.61	0/1659	1.03	8/2252 (0.4%)
51	D	0.53	0/1769	0.81	0/2378
52	E	0.57	0/2122	0.93	6/2861 (0.2%)
53	F	0.55	0/1628	0.92	4/2198 (0.2%)
54	G	0.71	3/1835 (0.2%)	0.91	8/2451 (0.3%)
55	H	0.52	0/1507	0.85	0/2028
56	I	0.58	0/1519	0.89	2/2033 (0.1%)
57	J	0.73	3/1495 (0.2%)	0.99	7/2001 (0.3%)
58	K	0.55	0/831	0.89	3/1123 (0.3%)
59	L	0.58	0/1276	0.93	3/1718 (0.2%)
60	M	0.61	0/929	0.82	0/1255
61	N	0.56	0/1210	0.92	0/1628
62	O	0.61	0/953	0.94	1/1279 (0.1%)
63	P	0.75	4/1000 (0.4%)	0.97	6/1343 (0.4%)
64	Q	0.56	0/1125	0.84	0/1510
65	R	0.55	0/1042	0.96	1/1399 (0.1%)
66	S	0.66	2/1212 (0.2%)	0.89	2/1629 (0.1%)
67	T	0.53	0/1129	0.85	0/1520
68	U	0.56	0/857	0.81	0/1158
69	V	0.54	0/696	0.81	0/938
70	W	0.67	0/1039	0.99	2/1399 (0.1%)
71	X	0.64	0/1145	0.95	2/1526 (0.1%)
72	Y	0.53	0/1075	0.87	2/1433 (0.1%)
73	Z	0.60	0/567	0.81	0/762
74	a	0.70	0/810	1.08	5/1084 (0.5%)
75	b	0.51	0/627	0.78	0/847
76	c	0.55	0/496	0.73	0/666

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
77	d	0.47	0/457	0.74	0/607
78	e	0.49	0/450	0.74	0/599
79	f	0.66	0/562	0.84	1/751 (0.1%)
80	g	0.53	0/2521	0.72	0/3431
81	2	0.44	3/42269 (0.0%)	0.87	101/65862 (0.2%)
82	4	0.43	1/4407 (0.0%)	0.89	13/6849 (0.2%)
83	1	0.61	1/6540 (0.0%)	1.12	43/8853 (0.5%)
All	All	0.56	40/230565 (0.0%)	0.93	635/338109 (0.2%)

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
1	5	0	6
4	AA	0	2
5	BB	0	1
6	CC	0	3
7	DD	0	1
8	EE	0	3
9	FF	0	2
14	LL	0	1
21	SS	0	1
27	YY	0	1
28	ZZ	0	1
29	aa	0	1
34	ff	0	1
35	gg	0	2
44	pp	0	3
45	qq	0	3
46	rr	0	1
48	A	0	2
49	B	0	1
50	C	0	3
51	D	0	1
52	E	0	3
53	F	0	1
58	K	0	1
59	L	0	1
62	O	0	1
63	P	0	1

*Continued on next page...*

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
64	Q	0	1
65	R	0	2
69	V	0	1
70	W	0	2
71	X	0	1
74	a	0	4
79	f	0	2
80	g	0	1
83	1	0	16
All	All	0	78

The worst 5 of 40 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	2219	G	O3'-P	-13.33	1.41	1.61
54	G	154	ARG	CA-C	12.64	1.69	1.52
57	J	170	GLY	CA-C	12.54	1.69	1.51
45	qq	123	LEU	N-CA	12.52	1.62	1.46
45	qq	119	GLN	CA-C	12.18	1.69	1.52

The worst 5 of 635 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	1	581	ASN	N-CA-CB	20.18	144.59	110.49
1	5	2218	G	C1'-C2'-O2'	14.74	133.92	111.80
83	1	580	PRO	N-CA-C	12.78	138.81	112.47
82	4	6121	A	C4'-C3'-O3'	12.42	131.63	113.00
81	2	931	U	C2'-C3'-O3'	-12.10	91.35	109.50

There are no chirality outliers.

5 of 78 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	5	1178	G	Sidechain
1	5	2049	G	Sidechain
1	5	2218	G	Sidechain
1	5	2219	G	Sidechain
1	5	2285	G	Sidechain

## 5.2 Too-close contacts [i](#)

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	5	69896	0	35118	1432	0
2	7	2579	0	1304	23	0
3	8	3326	0	1680	71	0
4	AA	1892	0	1954	56	0
5	BB	3064	0	3140	83	0
6	CC	2731	0	2842	90	0
7	DD	2384	0	2337	26	0
8	EE	1300	0	1393	26	0
9	FF	1774	0	1832	32	0
10	GG	1817	0	1927	33	0
11	HH	1528	0	1596	22	0
12	II	1690	0	1729	20	0
13	JJ	1349	0	1382	9	0
14	LL	1581	0	1661	48	0
15	MM	1045	0	1126	11	0
16	NN	1709	0	1763	23	0
17	OO	1571	0	1663	427	0
18	PP	1432	0	1465	26	0
19	QQ	1444	0	1541	26	0
20	RR	1522	0	1624	24	0
21	SS	1416	0	1461	17	0
22	TT	1262	0	1309	20	0
23	UU	807	0	821	5	0
24	VV	976	0	1021	31	0
25	WW	515	0	532	2	0
26	XX	964	0	1031	10	0
27	YY	992	0	1070	14	0
28	ZZ	1089	0	1150	24	0
29	aa	1156	0	1206	42	0
30	bb	458	0	486	2	0
31	cc	740	0	792	7	0
32	dd	869	0	920	12	0
33	ee	980	0	1048	9	0
34	ff	837	0	861	23	0
35	gg	951	0	1036	14	0
36	hh	961	0	1062	11	0
37	ii	766	0	840	12	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	jj	675	0	679	19	0
39	kk	619	0	675	22	0
40	ll	428	0	464	9	0
41	mm	410	0	446	8	0
42	nn	233	0	284	1	0
43	oo	814	0	875	9	0
44	pp	660	0	690	24	0
45	qq	1721	0	1820	188	0
46	rr	1508	0	1542	12	0
47	KK	735	0	177	0	0
48	A	1616	0	1636	21	0
49	B	1722	0	1793	17	0
50	C	1629	0	1710	19	0
51	D	1744	0	1826	9	0
52	E	2078	0	2157	9	0
53	F	1609	0	1679	7	0
54	G	1812	0	1911	35	0
55	H	1483	0	1579	8	0
56	I	1493	0	1515	13	0
57	J	1471	0	1553	36	0
58	K	809	0	810	6	0
59	L	1248	0	1311	19	0
60	M	922	0	953	2	0
61	N	1187	0	1251	8	0
62	O	942	0	979	9	0
63	P	980	0	1029	14	0
64	Q	1105	0	1170	9	0
65	R	1031	0	1082	7	0
66	S	1193	0	1217	11	0
67	T	1110	0	1124	7	0
68	U	845	0	913	3	0
69	V	687	0	682	7	0
70	W	1021	0	1056	20	0
71	X	1127	0	1210	23	0
72	Y	1061	0	1111	7	0
73	Z	558	0	585	2	0
74	a	798	0	854	34	0
75	b	617	0	643	2	0
76	c	494	0	534	2	0
77	d	446	0	436	2	0
78	e	443	0	481	1	0
79	f	549	0	564	3	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
80	g	2466	0	2406	7	0
81	2	37797	0	19015	705	0
82	4	3950	0	1982	200	0
83	1	6421	0	6490	463	0
84	1	1	0	0	0	0
84	2	74	0	0	0	0
84	5	2	0	0	0	0
84	N	1	0	0	0	0
84	a	1	0	0	0	0
84	f	1	0	0	0	0
85	a	1	0	0	0	0
85	b	1	0	0	0	0
85	f	1	0	0	0	0
85	jj	1	0	0	2	0
85	mm	1	0	0	0	0
85	oo	1	0	0	0	0
86	1	32	0	14	1	0
87	1	10	0	0	2	0
All	All	215768	0	160636	4281	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 12.

The worst 5 of 4281 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)
81:2:884:G:H2'	81:2:885:U:C1'	1.20	1.64
83:1:698:ILE:HG22	83:1:699:HIS:CD2	1.33	1.58
1:5:2217:C:C3'	1:5:2218:G:H5'	1.16	1.57
83:1:576:LEU:HD21	83:1:587:TYR:CD1	1.36	1.57
14:LL:3:ILE:CD1	29:aa:34:MET:HE3	1.29	1.56

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	
4	AA	247/249 (99%)	198 (80%)	35 (14%)	14 (6%)	1	13
5	BB	382/384 (100%)	311 (81%)	52 (14%)	19 (5%)	1	16
6	CC	357/360 (99%)	273 (76%)	57 (16%)	27 (8%)	1	9
7	DD	293/295 (99%)	254 (87%)	27 (9%)	12 (4%)	2	19
8	EE	157/170 (92%)	127 (81%)	22 (14%)	8 (5%)	1	15
9	FF	220/222 (99%)	182 (83%)	25 (11%)	13 (6%)	1	13
10	GG	231/233 (99%)	198 (86%)	25 (11%)	8 (4%)	3	23
11	HH	189/191 (99%)	168 (89%)	19 (10%)	2 (1%)	11	43
12	II	203/216 (94%)	179 (88%)	20 (10%)	4 (2%)	6	32
13	JJ	166/168 (99%)	136 (82%)	20 (12%)	10 (6%)	1	13
14	LL	195/197 (99%)	170 (87%)	17 (9%)	8 (4%)	2	19
15	MM	134/136 (98%)	124 (92%)	5 (4%)	5 (4%)	2	21
16	NN	200/202 (99%)	172 (86%)	25 (12%)	3 (2%)	8	37
17	OO	196/198 (99%)	88 (45%)	40 (20%)	68 (35%)	0	0
18	PP	178/180 (99%)	152 (85%)	19 (11%)	7 (4%)	2	20
19	QQ	182/184 (99%)	155 (85%)	23 (13%)	4 (2%)	5	30
20	RR	186/188 (99%)	155 (83%)	25 (13%)	6 (3%)	3	24
21	SS	167/169 (99%)	144 (86%)	18 (11%)	5 (3%)	3	25
22	TT	156/158 (99%)	126 (81%)	22 (14%)	8 (5%)	1	15
23	UU	98/100 (98%)	86 (88%)	12 (12%)	0	100	100
24	VV	130/132 (98%)	115 (88%)	10 (8%)	5 (4%)	2	21
25	WW	60/62 (97%)	53 (88%)	7 (12%)	0	100	100
26	XX	119/121 (98%)	107 (90%)	11 (9%)	1 (1%)	16	49
27	YY	123/125 (98%)	104 (85%)	16 (13%)	3 (2%)	4	29
28	ZZ	132/134 (98%)	107 (81%)	17 (13%)	8 (6%)	1	13
29	aa	145/147 (99%)	121 (83%)	17 (12%)	7 (5%)	2	16
30	bb	55/57 (96%)	48 (87%)	5 (9%)	2 (4%)	2	22
31	cc	95/97 (98%)	83 (87%)	12 (13%)	0	100	100
32	dd	104/106 (98%)	90 (86%)	9 (9%)	5 (5%)	2	16
33	ee	120/122 (98%)	104 (87%)	15 (12%)	1 (1%)	16	49

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	ff	103/105 (98%)	94 (91%)	8 (8%)	1 (1%)	12	45
35	gg	119/121 (98%)	102 (86%)	9 (8%)	8 (7%)	1	11
36	hh	114/116 (98%)	100 (88%)	11 (10%)	3 (3%)	4	27
37	ii	96/98 (98%)	75 (78%)	16 (17%)	5 (5%)	1	15
38	jj	83/85 (98%)	66 (80%)	16 (19%)	1 (1%)	10	41
39	kk	74/76 (97%)	55 (74%)	16 (22%)	3 (4%)	2	19
40	ll	47/49 (96%)	38 (81%)	7 (15%)	2 (4%)	2	18
41	mm	49/51 (96%)	41 (84%)	7 (14%)	1 (2%)	6	32
42	nn	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
43	oo	99/101 (98%)	74 (75%)	21 (21%)	4 (4%)	2	20
44	pp	85/87 (98%)	62 (73%)	14 (16%)	9 (11%)	0	5
45	qq	215/217 (99%)	166 (77%)	33 (15%)	16 (7%)	1	9
46	rr	193/195 (99%)	147 (76%)	30 (16%)	16 (8%)	0	8
48	A	204/206 (99%)	160 (78%)	31 (15%)	13 (6%)	1	12
49	B	212/214 (99%)	162 (76%)	43 (20%)	7 (3%)	3	24
50	C	215/217 (99%)	170 (79%)	34 (16%)	11 (5%)	1	15
51	D	221/223 (99%)	190 (86%)	24 (11%)	7 (3%)	3	24
52	E	258/260 (99%)	220 (85%)	26 (10%)	12 (5%)	2	17
53	F	204/206 (99%)	168 (82%)	29 (14%)	7 (3%)	3	23
54	G	224/226 (99%)	188 (84%)	28 (12%)	8 (4%)	2	22
55	H	182/184 (99%)	149 (82%)	21 (12%)	12 (7%)	1	12
56	I	184/200 (92%)	148 (80%)	29 (16%)	7 (4%)	2	21
57	J	180/182 (99%)	151 (84%)	19 (11%)	10 (6%)	1	14
58	K	94/96 (98%)	78 (83%)	12 (13%)	4 (4%)	2	18
59	L	153/155 (99%)	122 (80%)	24 (16%)	7 (5%)	2	17
60	M	120/122 (98%)	94 (78%)	22 (18%)	4 (3%)	3	24
61	N	148/150 (99%)	129 (87%)	17 (12%)	2 (1%)	9	38
62	O	125/127 (98%)	104 (83%)	18 (14%)	3 (2%)	4	29
63	P	121/123 (98%)	98 (81%)	16 (13%)	7 (6%)	1	13
64	Q	139/141 (99%)	120 (86%)	12 (9%)	7 (5%)	1	16
65	R	127/129 (98%)	99 (78%)	23 (18%)	5 (4%)	2	20

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
66	S	143/145 (99%)	117 (82%)	21 (15%)	5 (4%)	3	23
67	T	141/143 (99%)	126 (89%)	13 (9%)	2 (1%)	9	38
68	U	104/106 (98%)	92 (88%)	9 (9%)	3 (3%)	3	26
69	V	85/87 (98%)	66 (78%)	14 (16%)	5 (6%)	1	13
70	W	127/129 (98%)	104 (82%)	18 (14%)	5 (4%)	2	20
71	X	143/145 (99%)	112 (78%)	20 (14%)	11 (8%)	1	9
72	Y	132/134 (98%)	111 (84%)	13 (10%)	8 (6%)	1	13
73	Z	68/70 (97%)	57 (84%)	8 (12%)	3 (4%)	2	18
74	a	98/100 (98%)	68 (69%)	13 (13%)	17 (17%)	0	1
75	b	80/82 (98%)	61 (76%)	15 (19%)	4 (5%)	1	16
76	c	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
77	d	51/53 (96%)	40 (78%)	11 (22%)	0	100	100
78	e	53/55 (96%)	46 (87%)	4 (8%)	3 (6%)	1	13
79	f	67/69 (97%)	49 (73%)	12 (18%)	6 (9%)	0	6
80	g	312/324 (96%)	251 (80%)	50 (16%)	11 (4%)	3	23
83	1	825/827 (100%)	654 (79%)	120 (14%)	51 (6%)	1	12
All	All	12121/12322 (98%)	9932 (82%)	1590 (13%)	599 (5%)	3	16

5 of 599 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	AA	10	LYS
4	AA	34	TYR
4	AA	92	LYS
4	AA	181	LYS
4	AA	197	PRO

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	AA	190/190 (100%)	170 (90%)	20 (10%)	6	29
5	BB	323/323 (100%)	276 (85%)	47 (15%)	3	18
6	CC	288/291 (99%)	252 (88%)	36 (12%)	4	22
7	DD	243/243 (100%)	221 (91%)	22 (9%)	9	33
8	EE	139/147 (95%)	126 (91%)	13 (9%)	8	32
9	FF	188/188 (100%)	167 (89%)	21 (11%)	6	27
10	GG	192/194 (99%)	174 (91%)	18 (9%)	8	32
11	HH	173/173 (100%)	155 (90%)	18 (10%)	7	29
12	II	177/185 (96%)	157 (89%)	20 (11%)	5	26
13	JJ	144/144 (100%)	128 (89%)	16 (11%)	6	27
14	LL	162/162 (100%)	147 (91%)	15 (9%)	8	32
15	MM	109/109 (100%)	93 (85%)	16 (15%)	3	17
16	NN	175/175 (100%)	152 (87%)	23 (13%)	4	21
17	OO	163/163 (100%)	131 (80%)	32 (20%)	1	8
18	PP	148/148 (100%)	127 (86%)	21 (14%)	3	19
19	QQ	150/150 (100%)	137 (91%)	13 (9%)	9	34
20	RR	152/152 (100%)	145 (95%)	7 (5%)	24	51
21	SS	154/154 (100%)	144 (94%)	10 (6%)	15	43
22	TT	135/135 (100%)	116 (86%)	19 (14%)	3	19
23	UU	90/90 (100%)	89 (99%)	1 (1%)	65	74
24	VV	101/101 (100%)	89 (88%)	12 (12%)	5	24
25	WW	54/54 (100%)	51 (94%)	3 (6%)	19	47
26	XX	106/106 (100%)	92 (87%)	14 (13%)	4	21
27	YY	111/111 (100%)	99 (89%)	12 (11%)	6	28
28	ZZ	115/115 (100%)	105 (91%)	10 (9%)	9	34
29	aa	117/117 (100%)	106 (91%)	11 (9%)	8	32
30	bb	45/45 (100%)	44 (98%)	1 (2%)	45	65
31	cc	79/79 (100%)	72 (91%)	7 (9%)	9	33
32	dd	95/95 (100%)	88 (93%)	7 (7%)	13	39
33	ee	106/106 (100%)	98 (92%)	8 (8%)	12	39
34	ff	90/90 (100%)	82 (91%)	8 (9%)	9	33
35	gg	102/102 (100%)	97 (95%)	5 (5%)	22	49

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	hh	104/104 (100%)	99 (95%)	5 (5%)	23	50
37	ii	79/79 (100%)	73 (92%)	6 (8%)	12	39
38	jj	69/69 (100%)	62 (90%)	7 (10%)	7	30
39	kk	68/68 (100%)	61 (90%)	7 (10%)	7	30
40	ll	44/44 (100%)	40 (91%)	4 (9%)	9	33
41	mm	46/46 (100%)	43 (94%)	3 (6%)	15	43
42	nn	23/23 (100%)	19 (83%)	4 (17%)	2	12
43	oo	86/86 (100%)	76 (88%)	10 (12%)	5	25
44	pp	69/69 (100%)	57 (83%)	12 (17%)	2	12
45	qq	198/198 (100%)	181 (91%)	17 (9%)	10	34
46	rr	162/162 (100%)	149 (92%)	13 (8%)	11	37
48	A	174/174 (100%)	162 (93%)	12 (7%)	14	41
49	B	196/196 (100%)	177 (90%)	19 (10%)	8	31
50	C	176/176 (100%)	149 (85%)	27 (15%)	3	16
51	D	185/185 (100%)	168 (91%)	17 (9%)	8	33
52	E	223/223 (100%)	202 (91%)	21 (9%)	8	32
53	F	174/174 (100%)	161 (92%)	13 (8%)	12	39
54	G	192/192 (100%)	181 (94%)	11 (6%)	18	46
55	H	164/164 (100%)	150 (92%)	14 (8%)	10	35
56	I	148/158 (94%)	133 (90%)	15 (10%)	7	30
57	J	153/153 (100%)	137 (90%)	16 (10%)	6	29
58	K	88/88 (100%)	81 (92%)	7 (8%)	11	37
59	L	136/136 (100%)	126 (93%)	10 (7%)	13	39
60	M	97/97 (100%)	91 (94%)	6 (6%)	16	44
61	N	127/127 (100%)	114 (90%)	13 (10%)	7	30
62	O	96/96 (100%)	88 (92%)	8 (8%)	10	35
63	P	105/105 (100%)	95 (90%)	10 (10%)	8	32
64	Q	117/117 (100%)	108 (92%)	9 (8%)	12	38
65	R	117/117 (100%)	110 (94%)	7 (6%)	17	45
66	S	128/128 (100%)	115 (90%)	13 (10%)	7	30
67	T	117/117 (100%)	112 (96%)	5 (4%)	26	52

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
68	U	96/96 (100%)	89 (93%)	7 (7%)	13	40
69	V	73/73 (100%)	68 (93%)	5 (7%)	14	42
70	W	110/110 (100%)	92 (84%)	18 (16%)	2	14
71	X	120/120 (100%)	108 (90%)	12 (10%)	7	30
72	Y	108/108 (100%)	98 (91%)	10 (9%)	8	32
73	Z	60/60 (100%)	57 (95%)	3 (5%)	22	49
74	a	85/85 (100%)	66 (78%)	19 (22%)	1	6
75	b	72/72 (100%)	66 (92%)	6 (8%)	10	35
76	c	55/55 (100%)	53 (96%)	2 (4%)	31	56
77	d	46/46 (100%)	43 (94%)	3 (6%)	15	43
78	e	49/49 (100%)	46 (94%)	3 (6%)	17	45
79	f	58/60 (97%)	46 (79%)	12 (21%)	1	7
80	g	265/270 (98%)	248 (94%)	17 (6%)	16	43
83	1	700/702 (100%)	610 (87%)	90 (13%)	4	22
All	All	10374/10414 (100%)	9340 (90%)	1034 (10%)	9	30

5 of 1034 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
79	f	139	CYS
83	1	61	LYS
79	f	136	ARG
24	VV	33	ASN
22	TT	88	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 176 such sidechains are listed below:

Mol	Chain	Res	Type
53	F	172	GLN
67	T	91	HIS
54	G	65	GLN
61	N	49	GLN
71	X	22	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	5	3263/3270 (99%)	1000 (30%)	198 (6%)
2	7	120/121 (99%)	22 (18%)	4 (3%)
3	8	156/157 (99%)	42 (26%)	6 (3%)
81	2	1778/1798 (98%)	798 (44%)	127 (7%)
82	4	183/190 (96%)	90 (49%)	24 (13%)
All	All	5500/5536 (99%)	1952 (35%)	359 (6%)

5 of 1952 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	5	6	A
1	5	15	C
1	5	18	G
1	5	21	G
1	5	22	G

5 of 359 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
81	2	277	U
81	2	963	U
81	2	399	A
81	2	700	C
81	2	1107	G

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 88 ligands modelled in this entry, 86 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	6EM	1	903	83	8,9,9	0.94	1 (12%)	7,13,13	1.77	1 (14%)
86	GCP	1	902	84	32,34,34	1.78	7 (21%)	49,54,54	1.81	9 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	6EM	1	903	83	-	5/12/12/12	-
86	GCP	1	902	84	-	2/19/38/38	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	1	902	GCP	PG-O1G	5.97	1.62	1.50
86	1	902	GCP	PG-O3G	-3.33	1.47	1.55
86	1	902	GCP	PG-O2G	3.07	1.61	1.55
86	1	902	GCP	C5-C4	2.99	1.47	1.38
86	1	902	GCP	C6-N1	-2.39	1.34	1.38

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	1	902	GCP	C5-C4-N3	-5.48	119.67	128.39
86	1	902	GCP	C2-N3-C4	4.96	120.84	112.30
87	1	903	6EM	C9-N4-C3	4.01	120.13	110.52
86	1	902	GCP	PB-O3A-PA	-3.84	119.83	132.37
86	1	902	GCP	N9-C4-N3	3.75	133.46	125.95

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
86	1	902	GCP	C5'-O5'-PA-O1A
87	1	903	6EM	C1-C2-C3-C5
87	1	903	6EM	C1-C2-C3-N4
87	1	903	6EM	C2-C3-N4-C9

*Continued on next page...*

Continued from previous page...

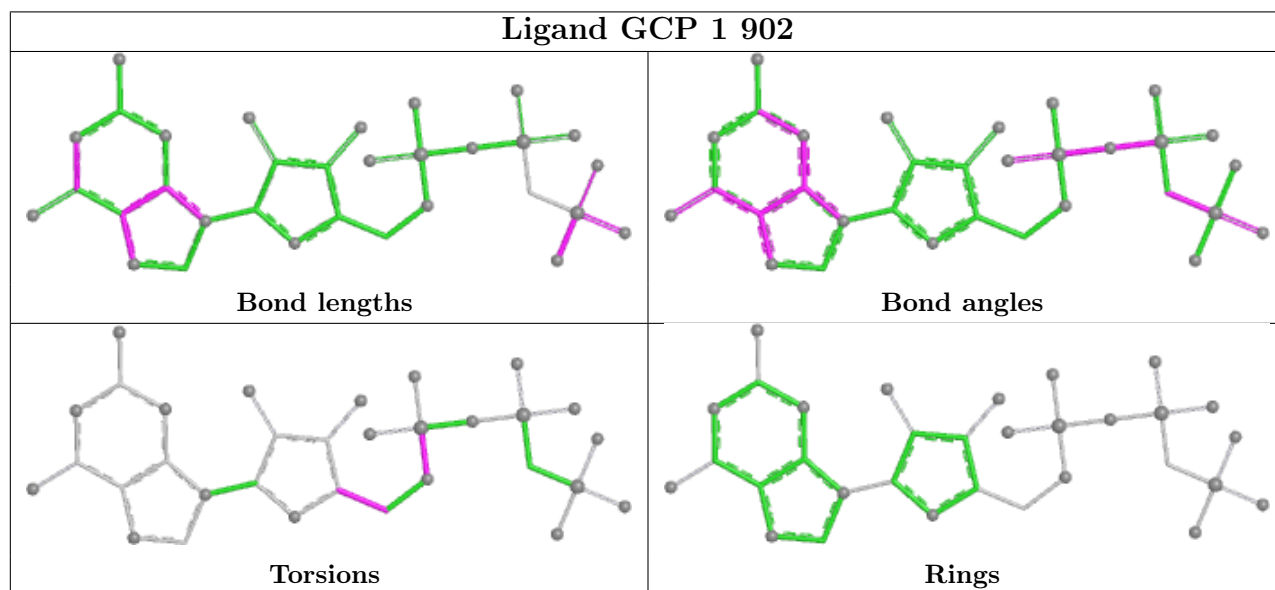
Mol	Chain	Res	Type	Atoms
87	1	903	6EM	C2-C3-N4-C10

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	1	903	6EM	2	0
86	1	902	GCP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	5	2
47	KK	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	443:G	O3'	466:G	P	31.65
1	5	1948:C	O3'	2019:G	P	17.88
1	KK	23:UNK	C	28:UNK	N	3.41
1	KK	52:UNK	C	54:UNK	N	3.29

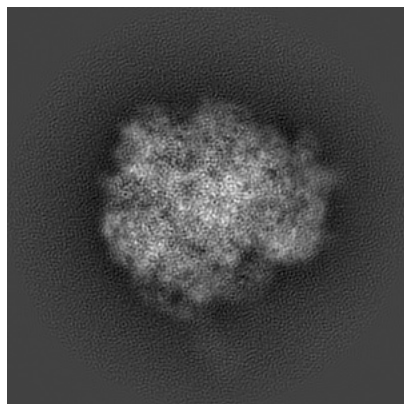
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8123. These allow visual inspection of the internal detail of the map and identification of artifacts.

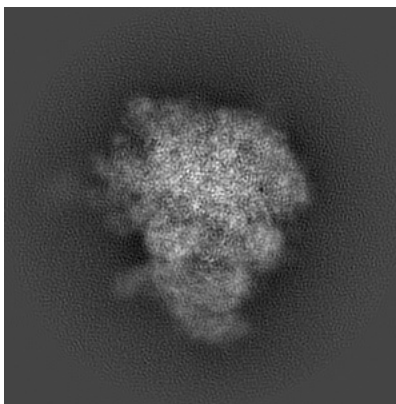
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

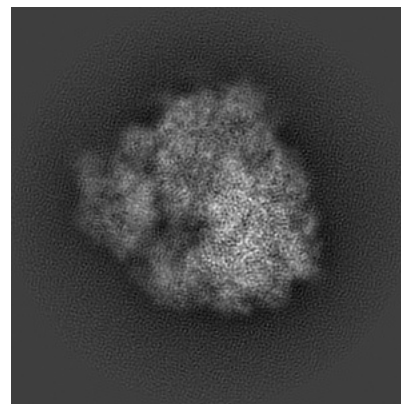
#### 6.1.1 Primary map



X

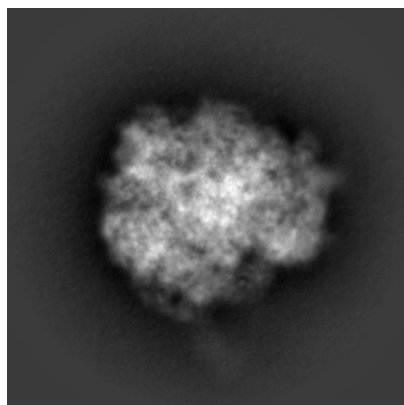


Y

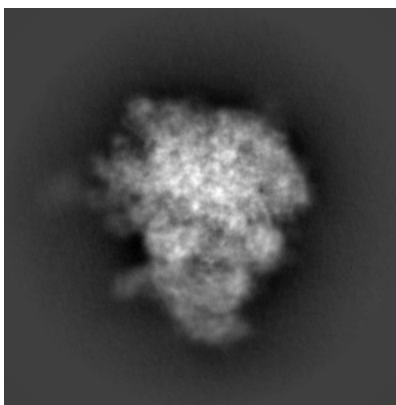


Z

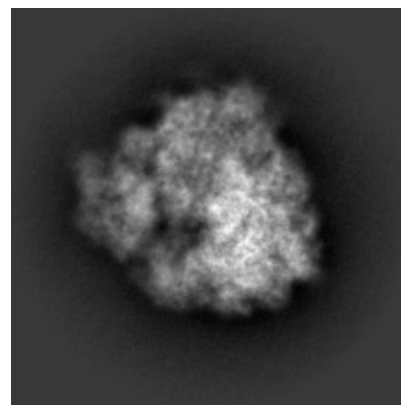
#### 6.1.2 Raw map



X



Y

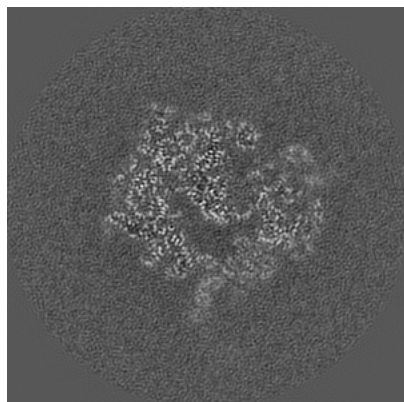


Z

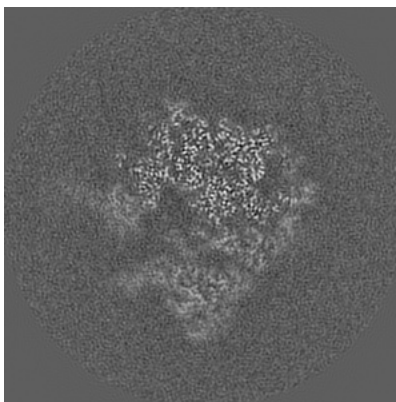
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

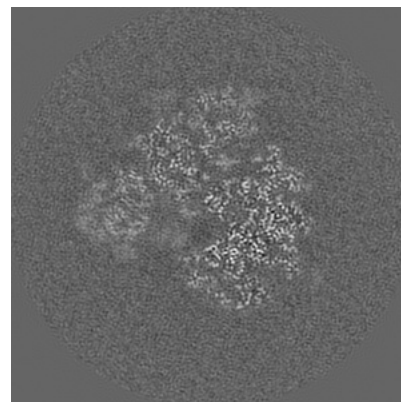
### 6.2.1 Primary map



X Index: 160

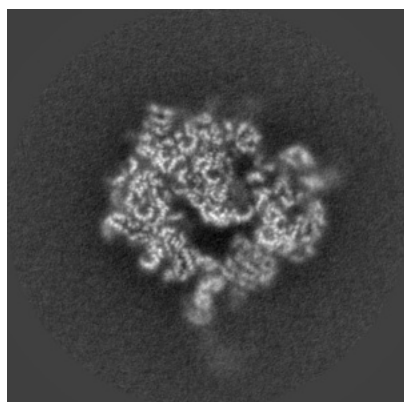


Y Index: 160

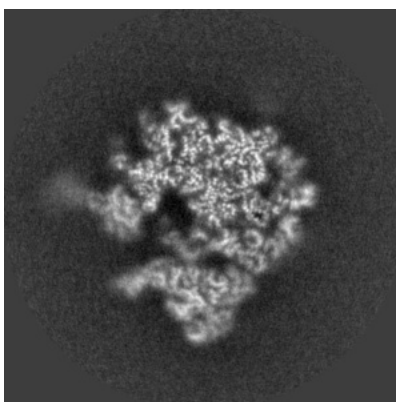


Z Index: 160

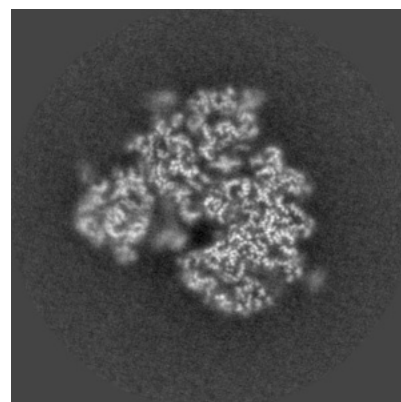
### 6.2.2 Raw map



X Index: 160



Y Index: 160

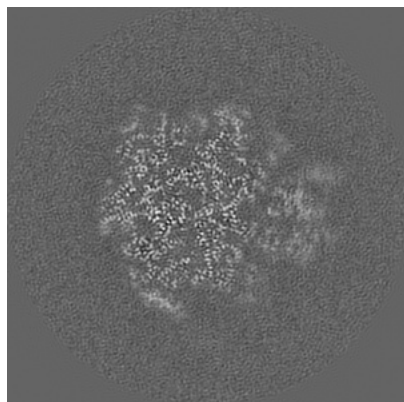


Z Index: 160

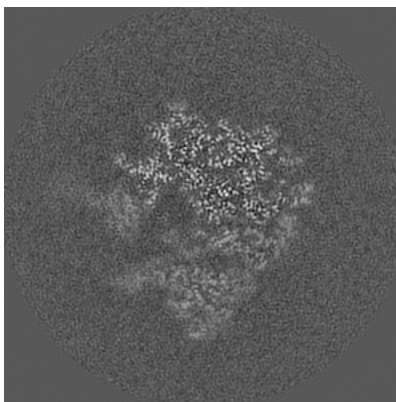
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

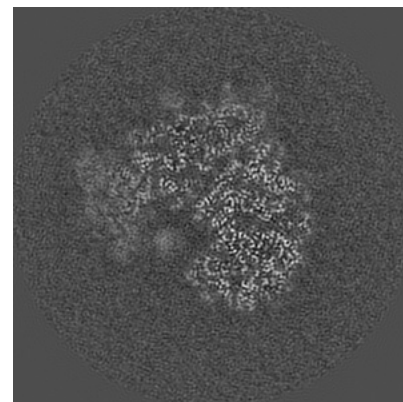
### 6.3.1 Primary map



X Index: 186

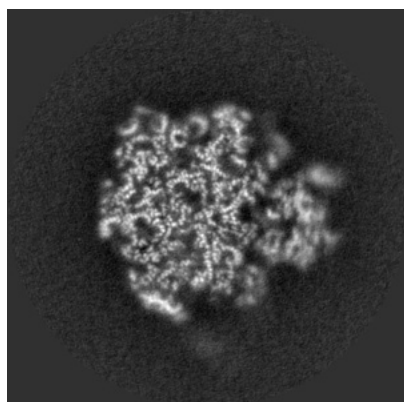


Y Index: 161

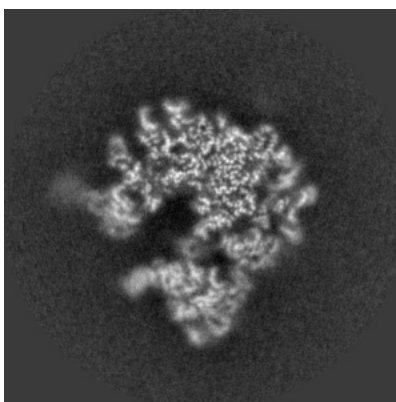


Z Index: 170

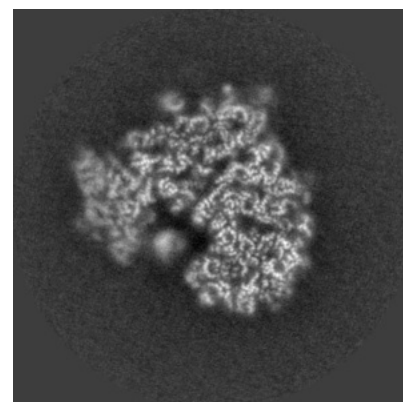
### 6.3.2 Raw map



X Index: 186



Y Index: 156

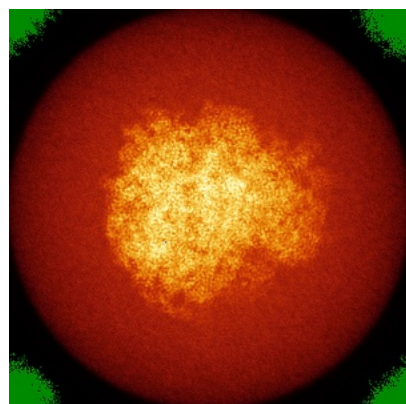


Z Index: 170

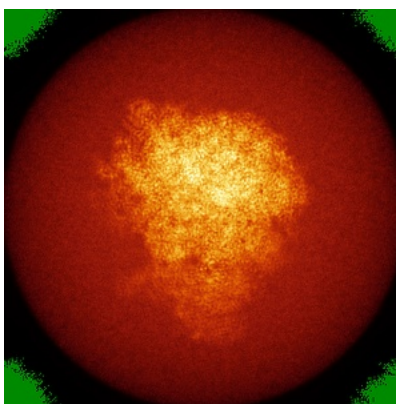
The images above show the largest variance slices of the map in three orthogonal directions.

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

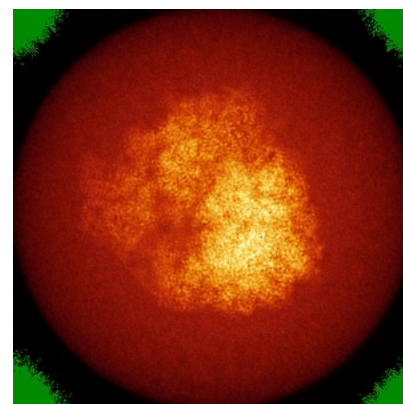
### 6.4.1 Primary map



X

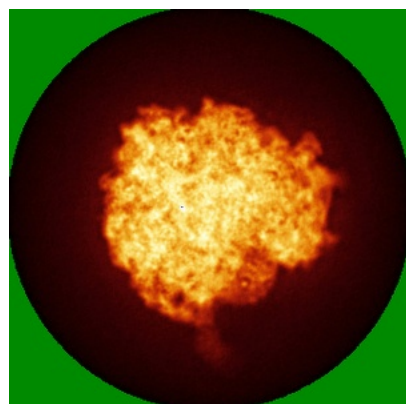


Y

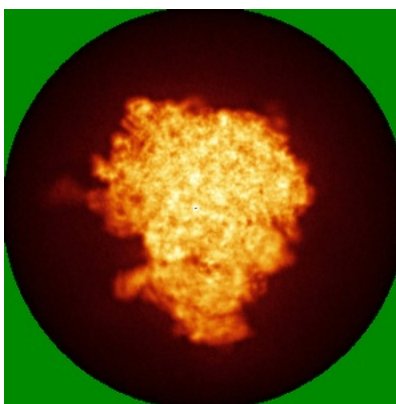


Z

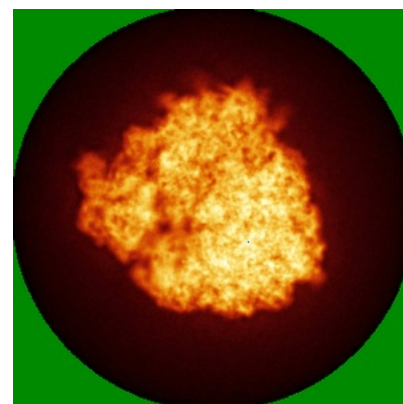
### 6.4.2 Raw map



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](#)

This section was not generated.

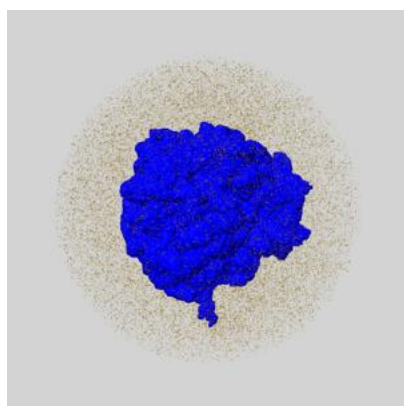
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

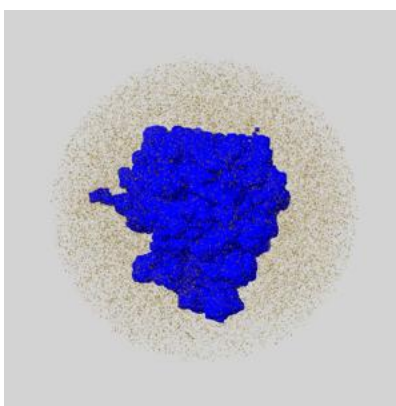
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

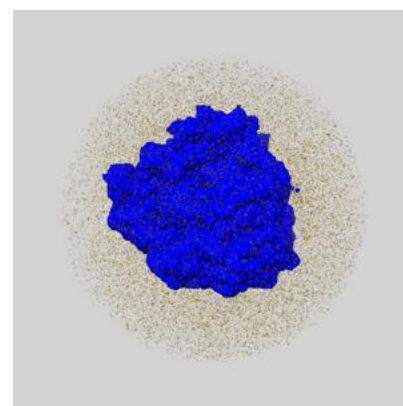
### 6.6.1 emd\_8123\_msk\_1.map [i](#)



X



Y

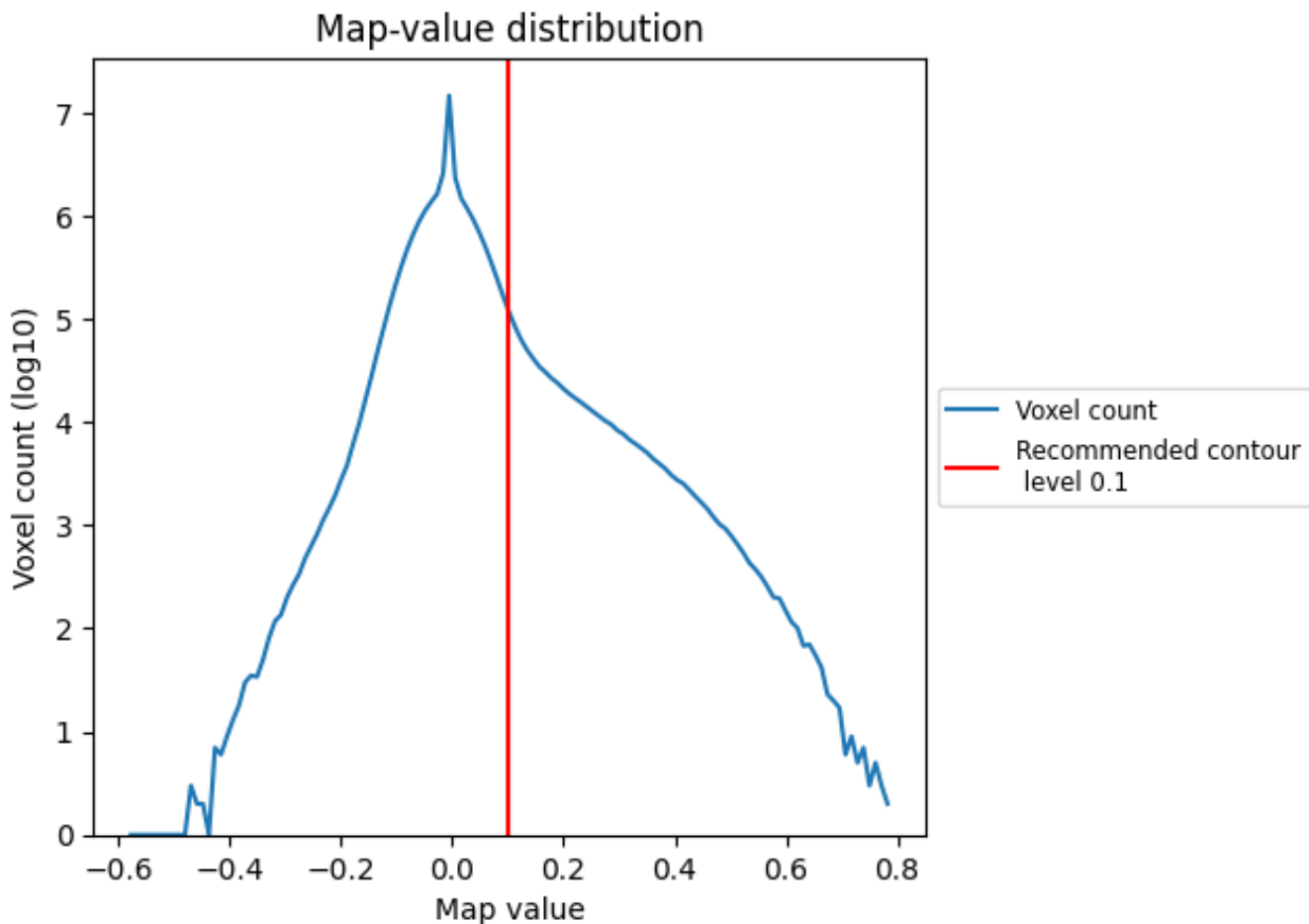


Z

## 7 Map analysis [i](#)

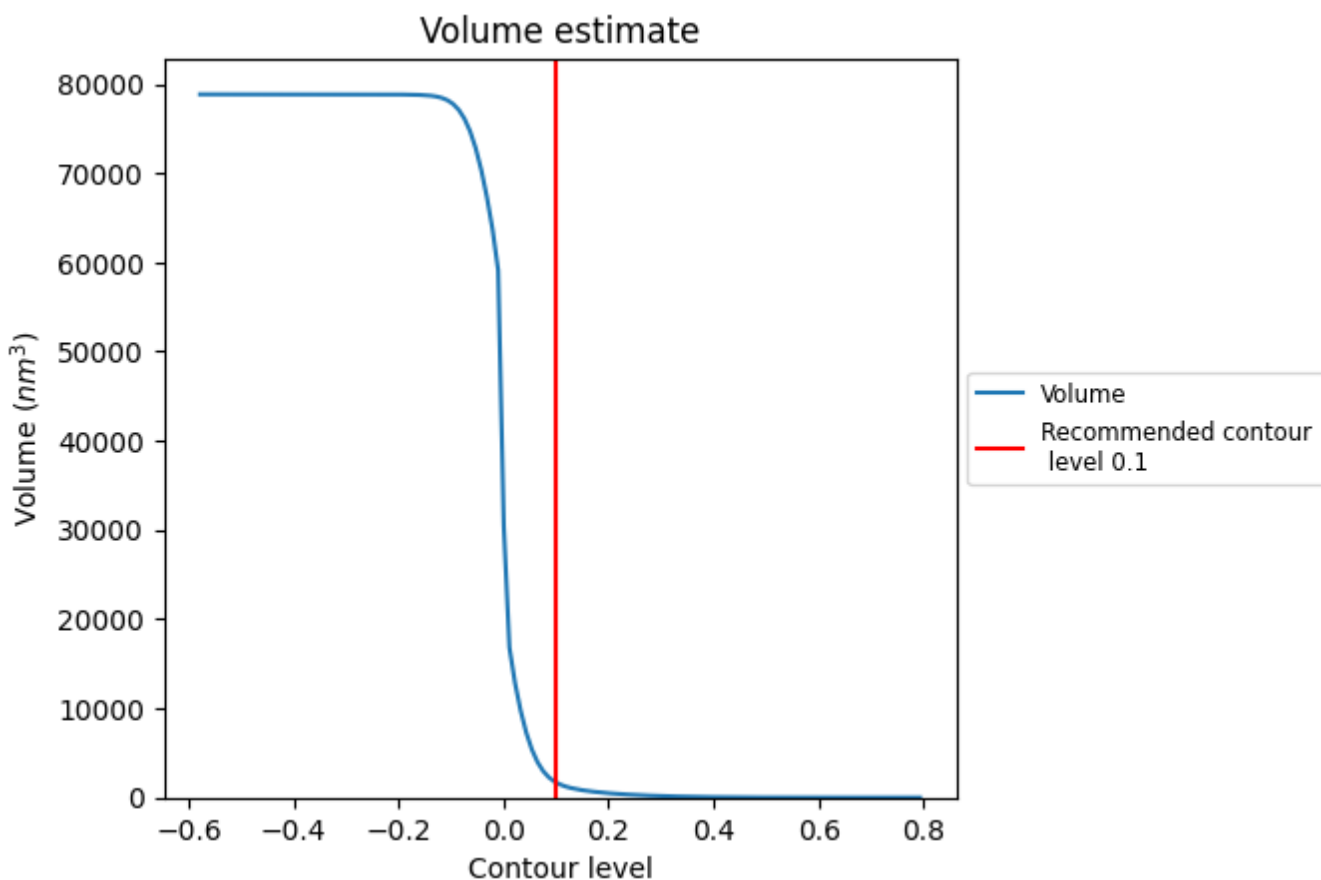
This section contains the results of statistical analysis of the map.

### 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.

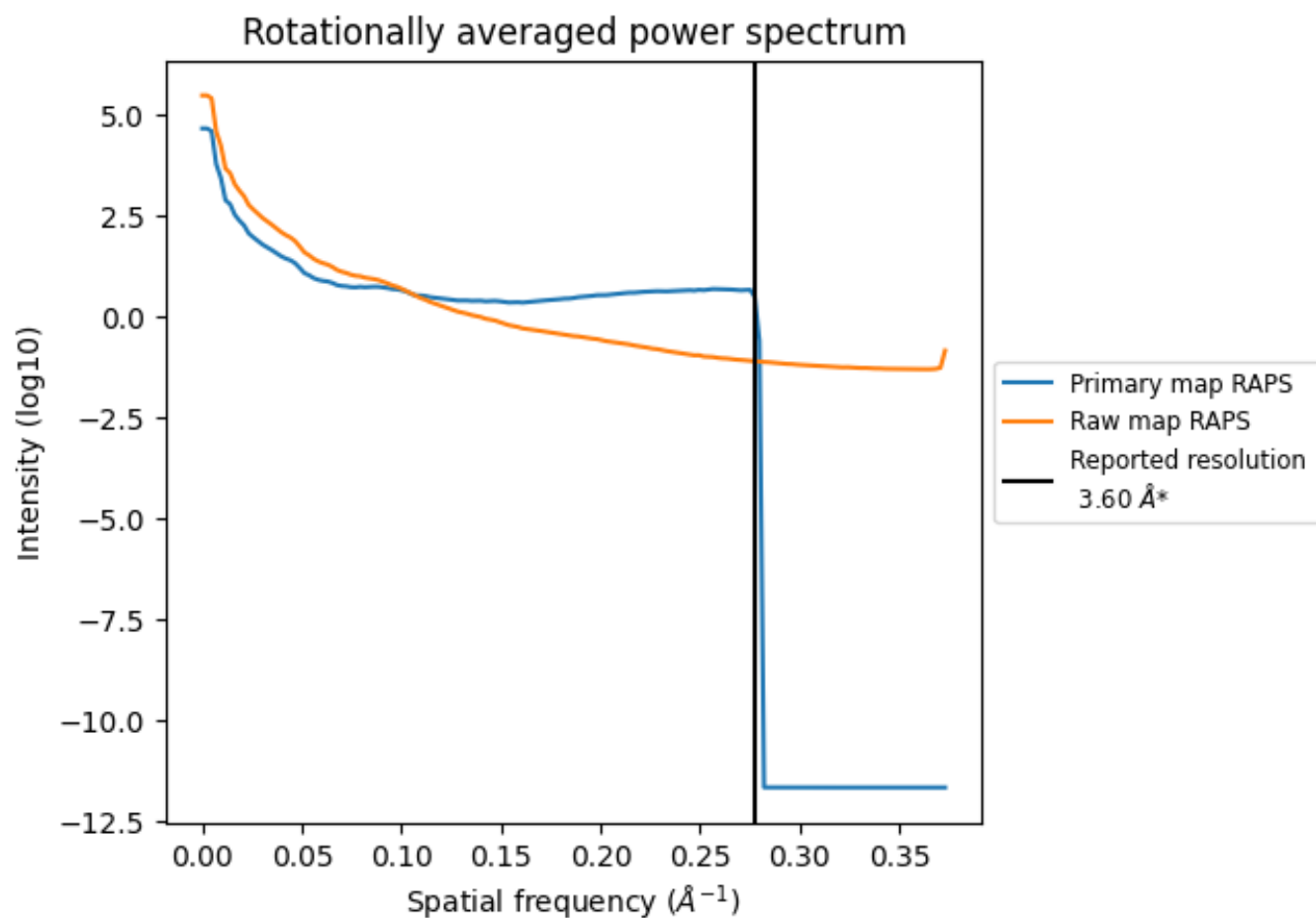
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1706 nm<sup>3</sup>; this corresponds to an approximate mass of 1541 kDa.

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

### 7.3 Rotationally averaged power spectrum i

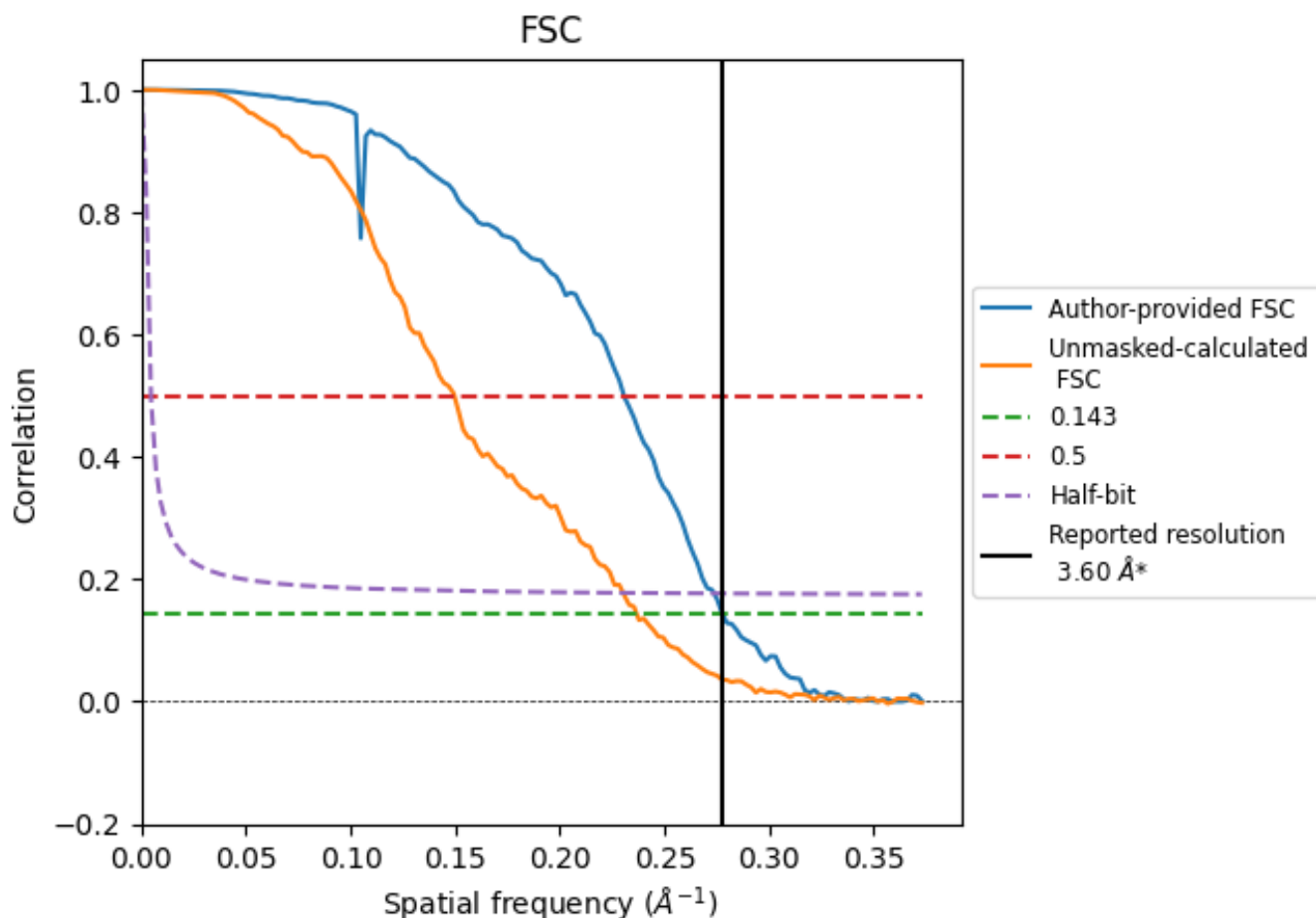


\*Reported resolution corresponds to spatial frequency of 0.278 Å<sup>-1</sup>

## 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 0.278 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

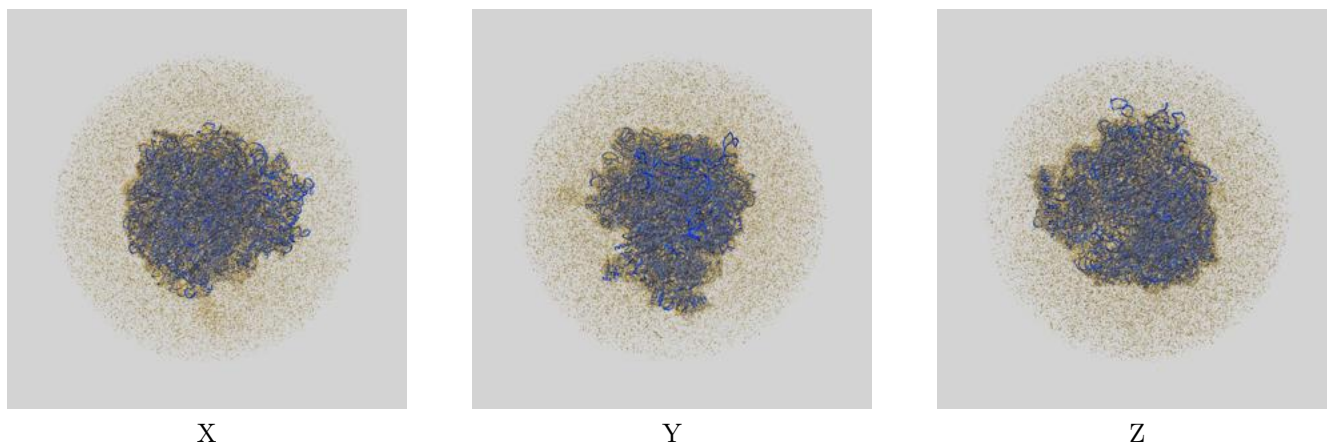
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.60	4.33	3.65
Unmasked-calculated*	4.22	6.69	4.34

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.22 differs from the reported value 3.6 by more than 10 %

## 9 Map-model fit [i](#)

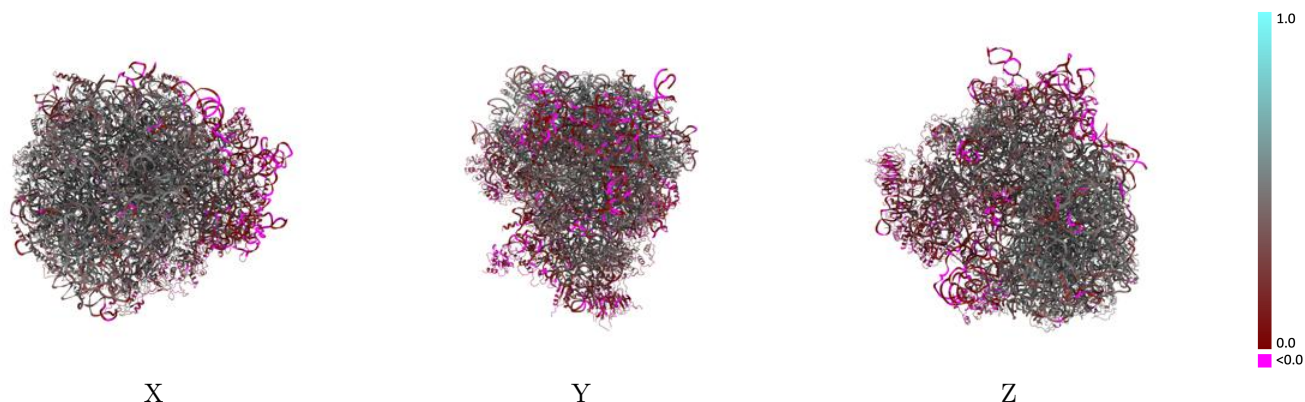
This section contains information regarding the fit between EMDB map EMD-8123 and PDB model 5IT7. Per-residue inclusion information can be found in section 3 on page 22.

### 9.1 Map-model overlay [i](#)



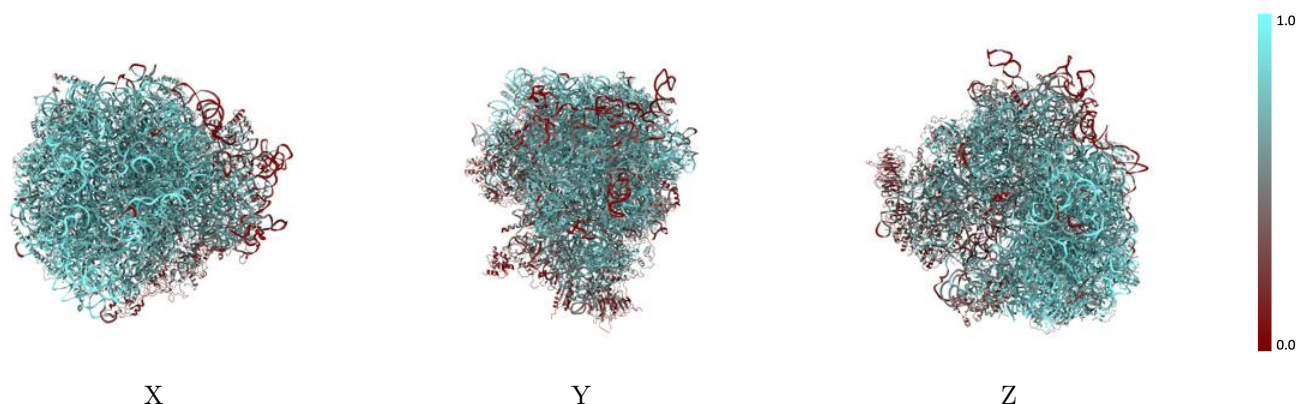
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



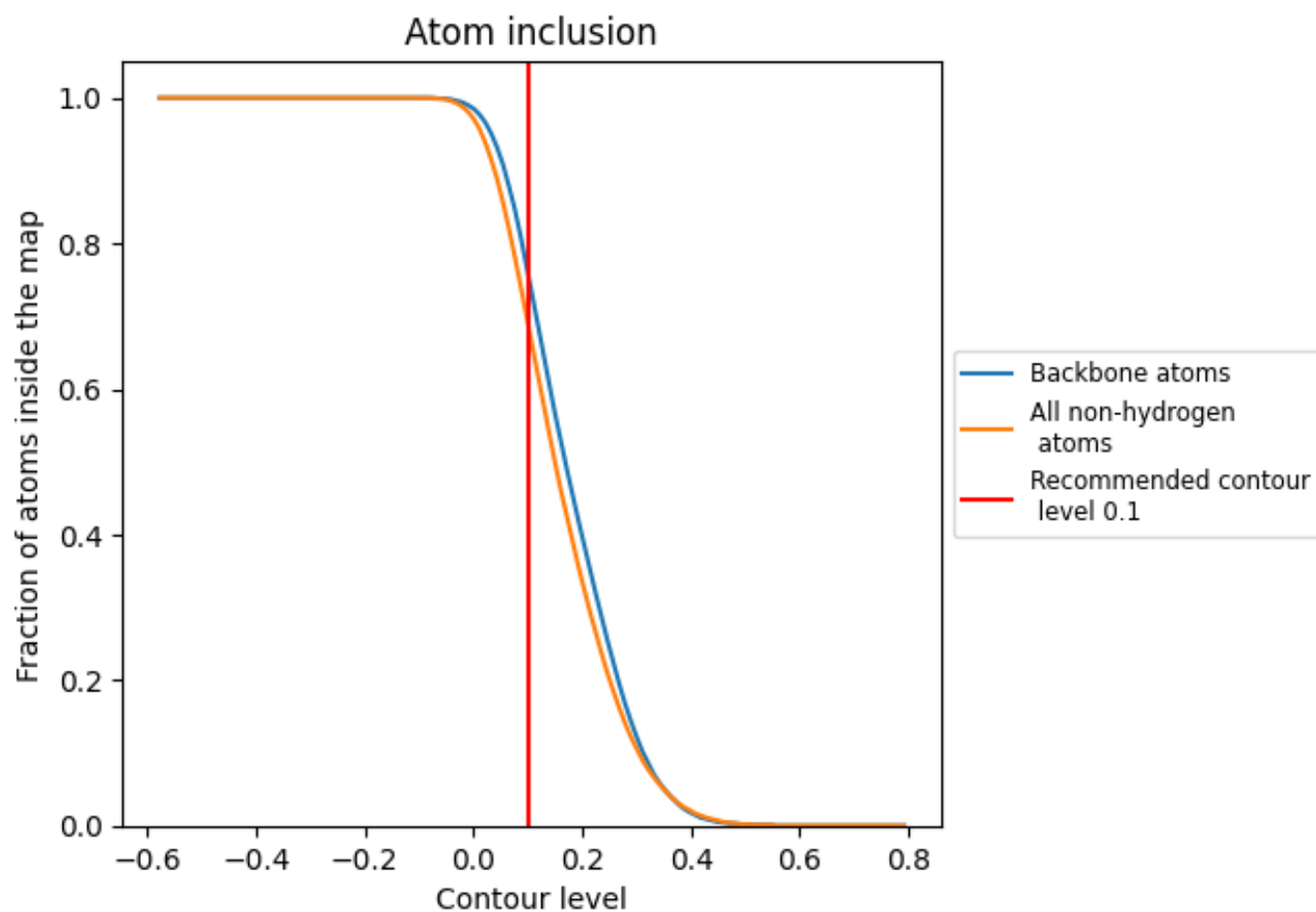
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 69% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6910	 0.3580
1	 0.4520	 0.2850
2	 0.6800	 0.2900
4	 0.3600	 0.0710
5	 0.8270	 0.4120
7	 0.8960	 0.4420
8	 0.8690	 0.4390
A	 0.6400	 0.3480
AA	 0.7470	 0.4820
B	 0.5230	 0.2830
BB	 0.7560	 0.4680
C	 0.6910	 0.4200
CC	 0.7430	 0.4550
D	 0.4110	 0.2220
DD	 0.7010	 0.3970
E	 0.6260	 0.3710
EE	 0.6990	 0.4020
F	 0.3470	 0.1690
FF	 0.7720	 0.4590
G	 0.4090	 0.1840
GG	 0.7030	 0.4140
H	 0.5610	 0.3020
HH	 0.7040	 0.4410
I	 0.5320	 0.2880
II	 0.7340	 0.4630
J	 0.6510	 0.3720
JJ	 0.6440	 0.3630
K	 0.3530	 0.1400
KK	 0.2490	 0.1270
L	 0.5780	 0.3540
LL	 0.7180	 0.4290
M	 0.1130	 0.0080
MM	 0.7500	 0.4410
N	 0.6220	 0.3860
NN	 0.7890	 0.4960

















*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
O	0.6040	0.3550
OO	0.8110	0.4960
P	0.3270	0.1460
PP	0.7390	0.4480
Q	0.4310	0.2100
QQ	0.7650	0.4760
R	0.4390	0.2200
RR	0.6780	0.4030
S	0.2840	0.1310
SS	0.7620	0.4760
T	0.4330	0.2070
TT	0.7540	0.4660
U	0.3340	0.1720
UU	0.6300	0.3760
V	0.6430	0.3730
VV	0.7080	0.4670
W	0.7480	0.4740
WW	0.7360	0.4570
X	0.6540	0.4420
XX	0.7180	0.4540
Y	0.5470	0.2820
YY	0.7320	0.4410
Z	0.3720	0.1310
ZZ	0.7240	0.4020
a	0.6300	0.3730
aa	0.7680	0.4700
b	0.5410	0.3040
bb	0.7240	0.4260
c	0.3630	0.1930
cc	0.6840	0.4300
d	0.5290	0.2700
dd	0.7240	0.4480
e	0.4870	0.3020
ee	0.7520	0.4740
f	0.1720	0.0460
ff	0.7790	0.5020
g	0.2980	0.1230
gg	0.6760	0.4270
hh	0.7320	0.4360
ii	0.6860	0.3910
jj	0.8250	0.5040
kk	0.6110	0.3480

*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
ll	 0.7790	 0.4820
mm	 0.7200	 0.4660
nn	 0.4530	 0.3530
oo	 0.6930	 0.4360
pp	 0.7070	 0.4600
qq	 0.2450	 0.0580
rr	 0.2680	 0.2120