



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 01:54 PM UTC

PDB ID : 5LZT / pdb_00005lzt
EMDB ID : EMD-4131
Title : Structure of the mammalian ribosomal termination complex with eRF1 and eRF3.
Authors : Shao, S.; Murray, J.; Brown, A.; Taunton, J.; Ramakrishnan, V.; Hegde, R.S.
Deposited on : 2016-10-02
Resolution : 3.65 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

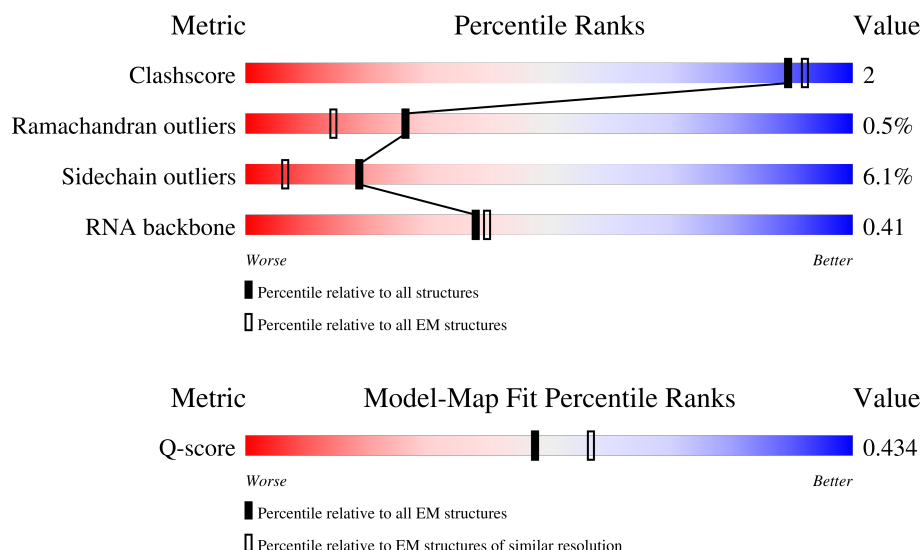
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

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

The reported resolution of this entry is 3.65 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.



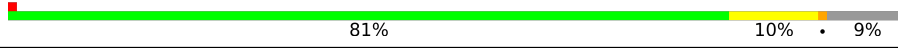
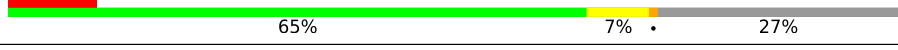
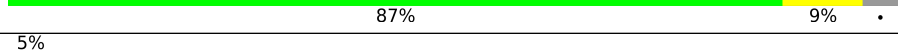
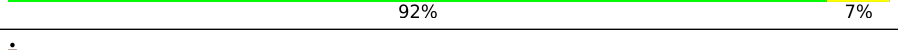
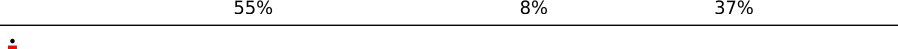
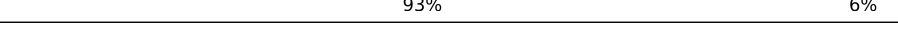
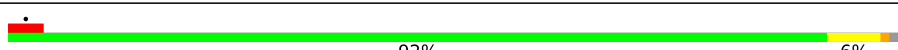
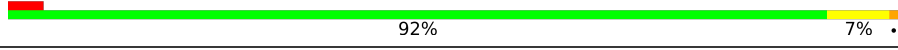
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11564 (3.15 - 4.15)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	257	
2	B	403	
3	C	425	

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Mol	Chain	Length	Quality of chain
4	D	297	
5	E	291	
6	F	247	
7	G	319	
8	H	192	
9	I	214	
10	J	178	
11	L	211	
12	M	218	
13	N	204	
14	O	203	
15	P	184	
16	Q	188	
17	R	196	
18	S	176	
19	T	160	
20	U	128	
21	V	140	
22	W	157	
23	X	156	
24	Y	145	
25	Z	136	
26	a	148	
27	b	245	
28	c	115	

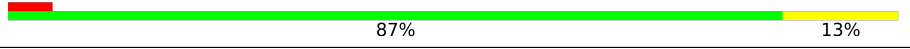
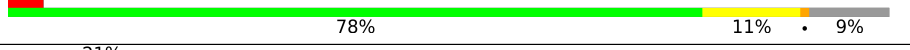
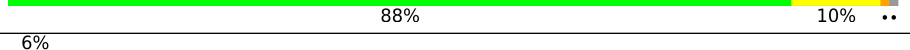
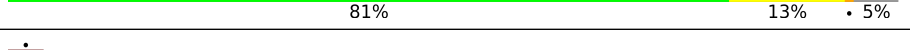
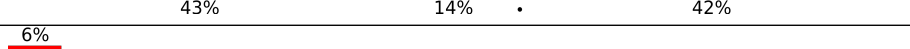
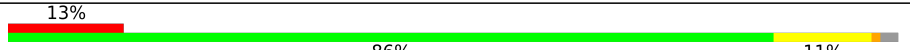
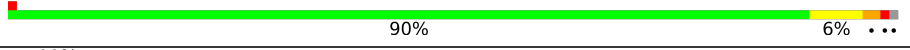
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Mol	Chain	Length	Quality of chain
29	d	125	
30	e	135	
31	f	110	
32	g	117	
33	h	123	
34	i	105	
35	j	97	
36	k	70	
37	l	51	
38	m	102	
39	n	25	
40	o	106	
41	p	92	
42	r	137	
43	s	318	
44	t	165	
45	1	15	
46	2	76	
47	3	75	
48	5	3543	
49	7	120	
50	8	156	
51	9	1869	
52	AA	295	
53	BB	264	

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Mol	Chain	Length	Quality of chain
54	CC	293	
55	DD	243	
56	EE	263	
57	FF	204	
58	GG	249	
59	HH	194	
60	II	208	
61	JJ	194	
62	KK	165	
63	LL	158	
64	MM	132	
65	NN	151	
66	OO	168	
67	PP	145	
68	QQ	146	
69	RR	135	
70	SS	152	
71	TT	145	
72	UU	119	
73	VV	83	
74	WW	130	
75	XX	143	
76	YY	130	
77	ZZ	125	
78	aa	115	

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Mol	Chain	Length	Quality of chain
79	bb	84	
80	cc	69	
81	dd	56	
82	ee	133	
83	ff	156	
84	gg	317	
85	hh	15	
86	ii	459	
87	jj	637	

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
89	ZN	p	100	-	-	X	-

2 Entry composition [i](#)

There are 90 unique types of molecules in this entry. The entry contains 222683 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called uL2.

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

- Molecule 2 is a protein called uL3.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	GLN	initiating methionine	UNP G1TL06

- Molecule 3 is a protein called uL4.

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

- Molecule 4 is a protein called uL18.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1	MET	LYS	initiating methionine	UNP G1SYJ6

- Molecule 5 is a protein called eL6.

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

- Molecule 6 is a protein called uL30.

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

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	61	ARG	GLY	conflict	UNP G1TUB1
F	93	ARG	GLY	conflict	UNP G1TUB1
F	131	MET	VAL	conflict	UNP G1TUB1
F	153	ILE	VAL	conflict	UNP G1TUB1

- Molecule 7 is a protein called eL8.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 8 is a protein called uL6.

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

- Molecule 9 is a protein called uL16.

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

- Molecule 10 is a protein called uL5.

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

- Molecule 11 is a protein called eL13.

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

- Molecule 12 is a protein called eL14.

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

- Molecule 13 is a protein called eL15.

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

- Molecule 14 is a protein called uL13.

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

- Molecule 15 is a protein called uL22.

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

- Molecule 16 is a protein called eL18.

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

- Molecule 17 is a protein called eL19.

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

- Molecule 18 is a protein called eL20.

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

- Molecule 19 is a protein called eL21.

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

- Molecule 20 is a protein called eL22.

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

- Molecule 21 is a protein called uL14.

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

- Molecule 22 is a protein called eL24.

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

- Molecule 23 is a protein called uL23.

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

- Molecule 24 is a protein called uL24.

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

- Molecule 25 is a protein called eL27.

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

- Molecule 26 is a protein called uL15.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	1	MET	GLN	conflict	UNP G1SNY0

- Molecule 27 is a protein called eL29.

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

- Molecule 28 is a protein called eL30.

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

- Molecule 29 is a protein called eL31.

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

- Molecule 30 is a protein called eL32.

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

- Molecule 31 is a protein called eL33.

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

- Molecule 32 is a protein called eL34.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
g	117	LYS	-	insertion	UNP G1U945

- Molecule 33 is a protein called uL29.

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

- Molecule 34 is a protein called eL36.

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

- Molecule 35 is a protein called eL37.

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

- Molecule 36 is a protein called eL38.

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

- Molecule 37 is a protein called eL39.

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

- Molecule 38 is a protein called eL40.

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

- Molecule 39 is a protein called eL41.

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

- Molecule 40 is a protein called eL42.

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

- Molecule 41 is a protein called eL43.

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

- Molecule 42 is a protein called eL28.

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

- Molecule 43 is a protein called uL10.

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

- Molecule 44 is a protein called uL11.

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

- Molecule 45 is a protein called Nascent chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	1	15	Total	C	N	O	S	0	0
			125	82	20	22	1		

- Molecule 46 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	2	76	Total	C	N	O	P	0	0
			1616	723	291	527	75		

- Molecule 47 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	3	75	Total	C	N	O	P	0	0
			1593	712	281	526	74		

- Molecule 48 is a RNA chain called 28S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	5	3543	Total	C	N	O	P	0	0
			75972	33833	13910	24686	3543		

- Molecule 49 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	7	120	Total	C	N	O	P	0	0
			2558	1141	456	842	119		

- Molecule 50 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	8	151	Total	C	N	O	P	0	0
			3208	1432	564	1062	150		

- Molecule 51 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	9	1698	Total	C	N	O	P	0	0
			36249	16180	6508	11864	1697		

- Molecule 52 is a protein called uS2.

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

- Molecule 53 is a protein called eS1.

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

- Molecule 54 is a protein called uS5.

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

- Molecule 55 is a protein called uS3.

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

- Molecule 56 is a protein called eS4.

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

- Molecule 57 is a protein called uS7.

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

- Molecule 58 is a protein called eS6.

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

- Molecule 59 is a protein called eS7.

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

- Molecule 60 is a protein called eS8.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 61 is a protein called uS4.

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

- Molecule 62 is a protein called eS10.

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

- Molecule 63 is a protein called uS17.

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

- Molecule 64 is a protein called eS12.

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

- Molecule 65 is a protein called uS15.

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

- Molecule 66 is a protein called uS11.

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

- Molecule 67 is a protein called uS19.

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

- Molecule 68 is a protein called uS9.

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

- Molecule 69 is a protein called eS17.

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

- Molecule 70 is a protein called uS13.

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

- Molecule 71 is a protein called eS19.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 72 is a protein called uS10.

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

- Molecule 73 is a protein called eS21.

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

- Molecule 74 is a protein called uS8.

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

- Molecule 75 is a protein called uS12.

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

- Molecule 76 is a protein called eS24.

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

- Molecule 77 is a protein called eS25.

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

- Molecule 78 is a protein called eS26.

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

- Molecule 79 is a protein called eS27.

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

- Molecule 80 is a protein called eS28.

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

- Molecule 81 is a protein called uS14.

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

- Molecule 82 is a protein called eS30.

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

- Molecule 83 is a protein called eS31.

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

- Molecule 84 is a protein called RACK1.

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

- Molecule 85 is a RNA chain called mRNA (UGA stop codon).

Mol	Chain	Residues	Atoms					AltConf	Trace
85	hh	15	Total	C	N	O	P	0	0
			317	142	54	106	15		

- Molecule 86 is a protein called eRF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	ii	419	Total	C	N	O	S	0	0
			3307	2104	562	629	12		

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
ii	-21	MET	-	initiating methionine	UNP P62495
ii	-20	ARG	-	expression tag	UNP P62495
ii	-19	GLY	-	expression tag	UNP P62495
ii	-18	SER	-	expression tag	UNP P62495
ii	-17	HIS	-	expression tag	UNP P62495
ii	-16	HIS	-	expression tag	UNP P62495
ii	-15	HIS	-	expression tag	UNP P62495
ii	-14	HIS	-	expression tag	UNP P62495
ii	-13	HIS	-	expression tag	UNP P62495
ii	-12	HIS	-	expression tag	UNP P62495
ii	-11	GLY	-	expression tag	UNP P62495
ii	-10	MET	-	expression tag	UNP P62495
ii	-9	ALA	-	expression tag	UNP P62495
ii	-8	SER	-	expression tag	UNP P62495
ii	-7	GLU	-	expression tag	UNP P62495
ii	-6	ASN	-	expression tag	UNP P62495
ii	-5	LEU	-	expression tag	UNP P62495
ii	-4	TYR	-	expression tag	UNP P62495
ii	-3	PHE	-	expression tag	UNP P62495

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Chain	Residue	Modelled	Actual	Comment	Reference
ii	-2	GLN	-	expression tag	UNP P62495
ii	-1	GLY	-	expression tag	UNP P62495
ii	0	SER	-	expression tag	UNP P62495

- Molecule 87 is a protein called eRF3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	jj	428	Total	C	N	O	S	0	0
			3368	2144	580	623	21		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
jj	100	ALA	VAL	conflict	UNP P15170

- Molecule 88 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
88	A	1	Total	Mg	0
			1	1	
88	B	1	Total	Mg	0
			1	1	
88	I	1	Total	Mg	0
			1	1	
88	P	3	Total	Mg	0
			3	3	
88	Q	1	Total	Mg	0
			1	1	
88	V	1	Total	Mg	0
			1	1	
88	a	1	Total	Mg	0
			1	1	
88	g	1	Total	Mg	0
			1	1	
88	j	1	Total	Mg	0
			1	1	
88	5	185	Total	Mg	0
			185	185	
88	7	5	Total	Mg	0
			5	5	
88	8	8	Total	Mg	0
			8	8	

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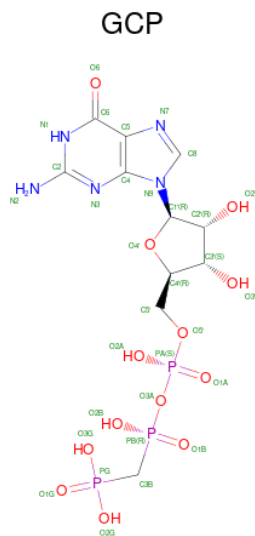
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Mol	Chain	Residues	Atoms		AltConf
88	9	71	Total 71	Mg 71	0
88	hh	1	Total 1	Mg 1	0
88	jj	1	Total 1	Mg 1	0

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

Mol	Chain	Residues	Atoms		AltConf
89	g	1	Total 1	Zn 1	0
89	j	1	Total 1	Zn 1	0
89	m	1	Total 1	Zn 1	0
89	o	1	Total 1	Zn 1	0
89	p	1	Total 1	Zn 1	0
89	aa	1	Total 1	Zn 1	0
89	dd	1	Total 1	Zn 1	0
89	ff	1	Total 1	Zn 1	0

- Molecule 90 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: GCP) (formula: C₁₁H₁₈N₅O₁₃P₃).



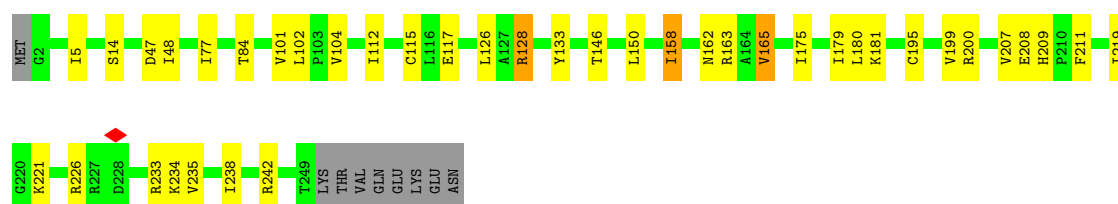
Mol	Chain	Residues	Atoms					AltConf
90	jj	1	Total	C	N	O	P	0
			32	11	5	13	3	

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.

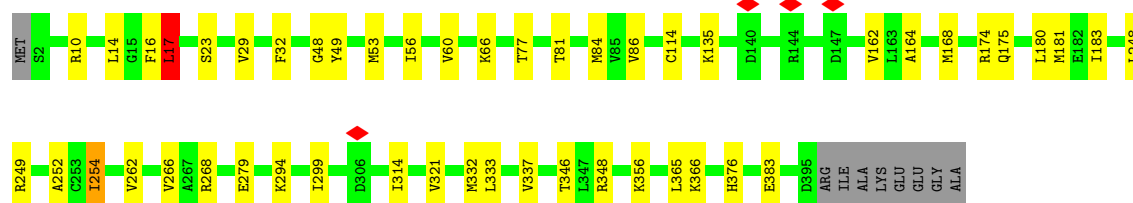
• Molecule 1: uL2

Chain A: 



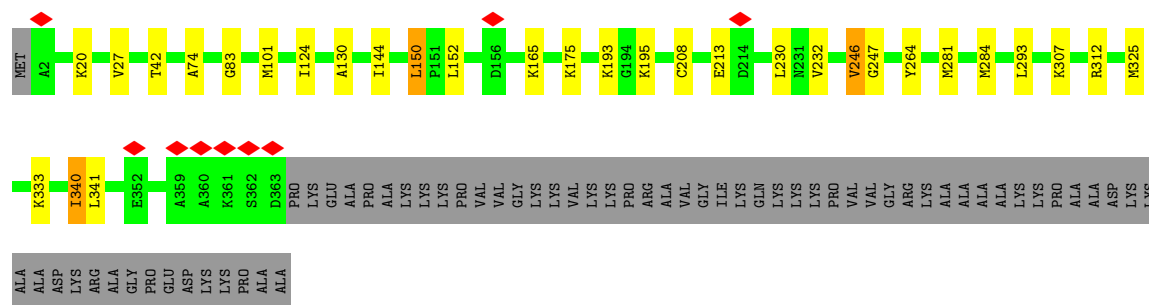
• Molecule 2: uL3

Chain B: 



• Molecule 3: uL4

Chain C: 



• Molecule 4: uL18

Top 1000 variants (from top to bottom): MET, GLY, G, A, Y16, R22, R23, T28, R33, V37, R50, V53, T56, I60, T64, A65, Y66, D72, M73, R89, A98, L103, L104, L105, A106, L109, K117, E120, E124, V125, E129, G140, R152, T153, T154, V159, V170.

Bottom 1000 variants (from bottom to top): E196, Q202, Y219, Q225, Y226, I227, D234, E238, R248, K258, R259, K262, K263, K264, A294, A295, GLU, SER.

[illegible]

Amino Acid Type	Count
MET	1
GLU	1
GLY	1
ALA	1
GLU	1
GLU	1
LYS	1
LYS	1
VAL	1
PRO	1
ALA	1
VAL	1
PRO	1
GLU	1
THR	1
LEU	1
LYS	1
LYS	1
LYS	1
ARG	1
ARG	1
N23	1
F24	1
A25	1
E26	1
Q38	1
L41	1
R46	1
R65	1
T66	1
E67	1
R75	1
L88	1
A89	1
F90	1
Y91	1
I92	1
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I94	1
R95	1
V100	1
L124	1
I129	1
I134	1
E151	1
Y154	1

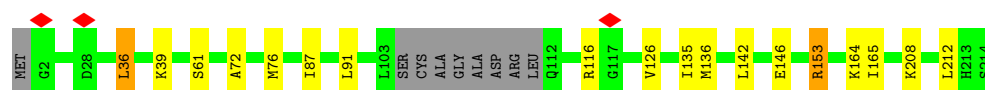
Met	SER	SER	SER	TYR	ARG	LEU	GLY	TYR	CYS	MET	LYS	GLU	GLU	ARG	HIS	ASN	LEU	VAL	CYS	LEU	TRP	GLN	SER	SER	PRO	GLY	ILE	LEU	ASN	SER	LYS	CYS	LEU	TRP	PRO	PHE	THR	ASN	ILE	HIS	LEU	LEU	VAL	GLY	ALA	LEU	PRO	ARG	GLU	GLY	ALA	GLY	GLY	ALA	TRP	GLY	GLY	ARG				
	SER	GLU	GLN	LEU	PRO	THR	CYS	SER	THR	THR	HIS	HIS	ASP	PHE	THR	TRP	ASP	LYS	V80			I93		P130	P131		M134		V139		R142		Q151		L158	A169	R170	A171	E172	K173	K174	A175	A176		GLY	LYS	GLY	ASP	VAL	ALA	PRO	THR	K184		L189		E201	M202	K203	K204		L210

Chain H:  87% 11% ..



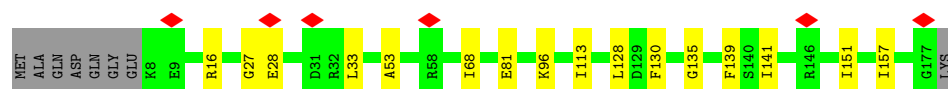
- Molecule 9: uL16

Chain I:  87% 7% . .

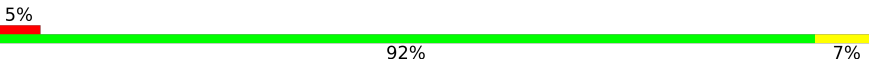


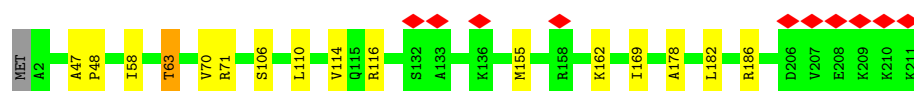
- Molecule 10: uL5

Chain J:  87% 9% .



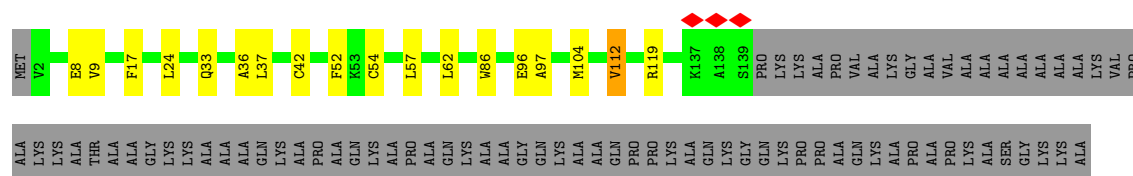
- Molecule 11: eL13

Chain L:  92% 7% 5%

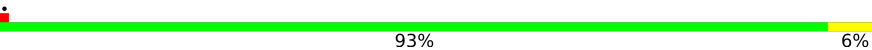


- Molecule 12: eL14

Chain M:  55% 8% 37%



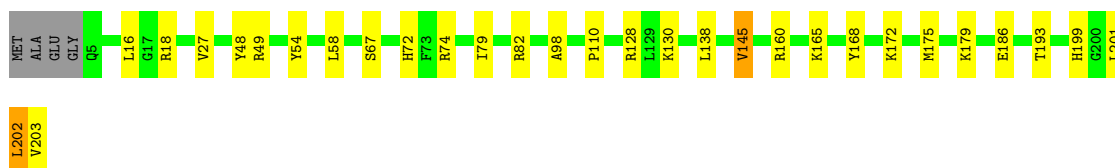
- Molecule 13: eL15

Chain N:  93% 6%

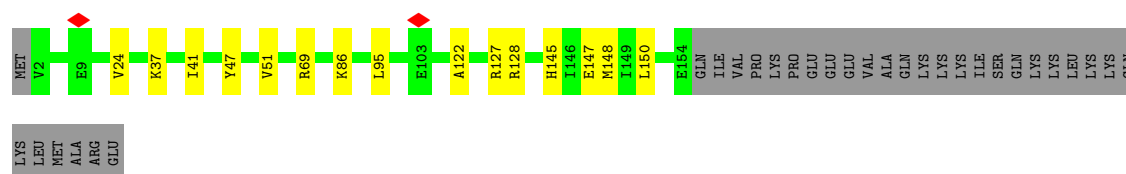
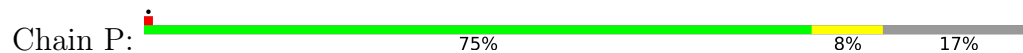


- Molecule 14: uL13

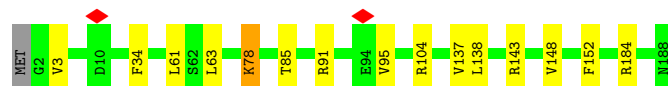
Chain O:  83% 14% ..



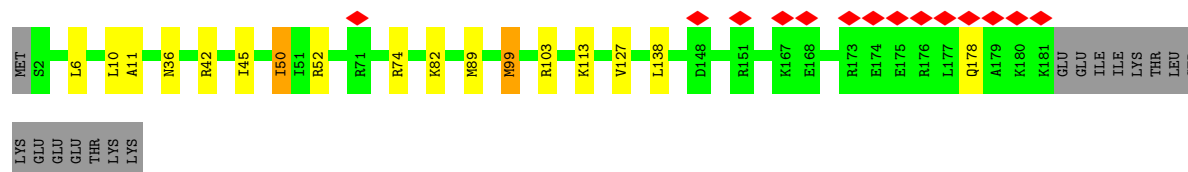
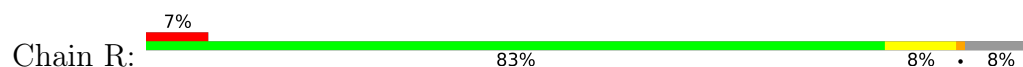
• Molecule 15: uL22



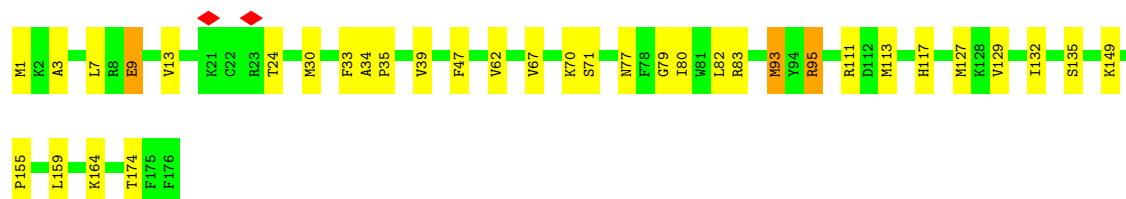
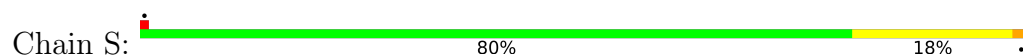
• Molecule 16: eL18



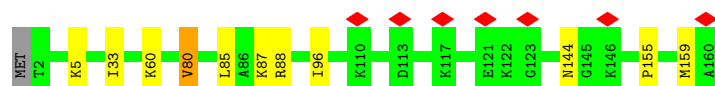
• Molecule 17: eL19



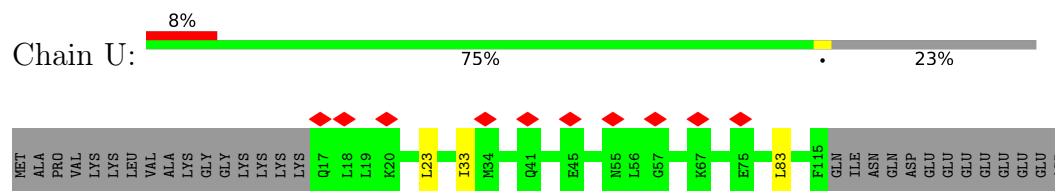
• Molecule 18: eL20



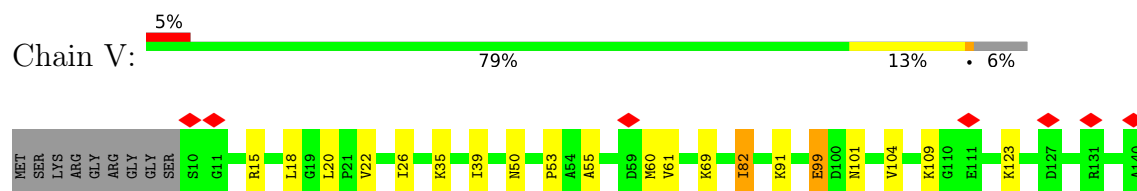
• Molecule 19: eL21



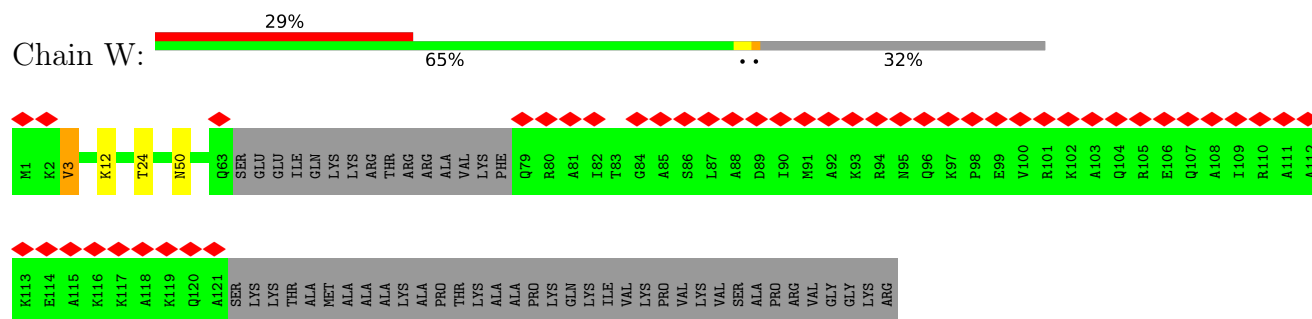
- Molecule 20: eL22



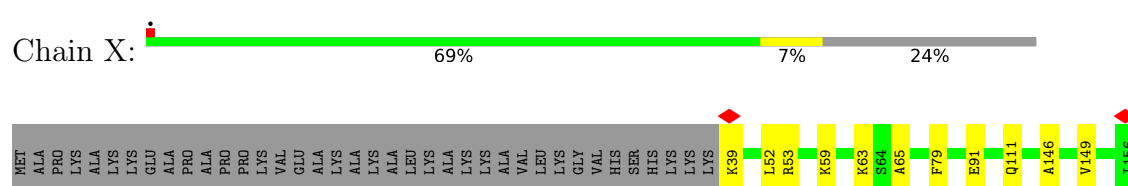
- Molecule 21: uL14



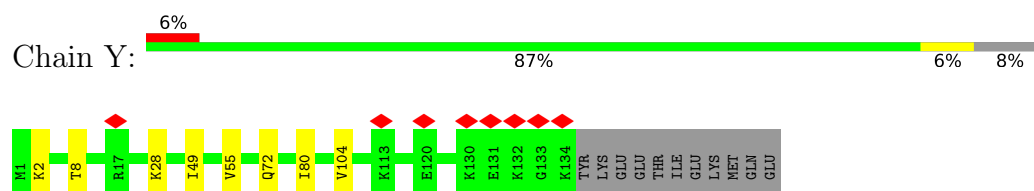
- Molecule 22: eL24



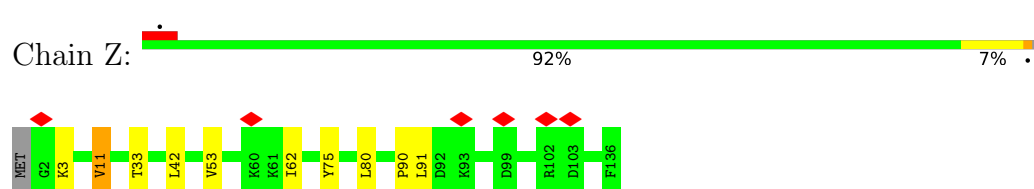
- Molecule 23: uL23



- Molecule 24: uL24

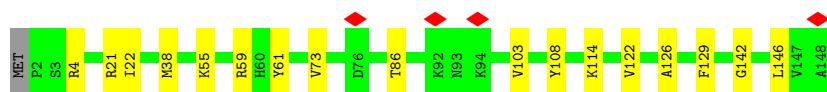


- Molecule 25: eL27



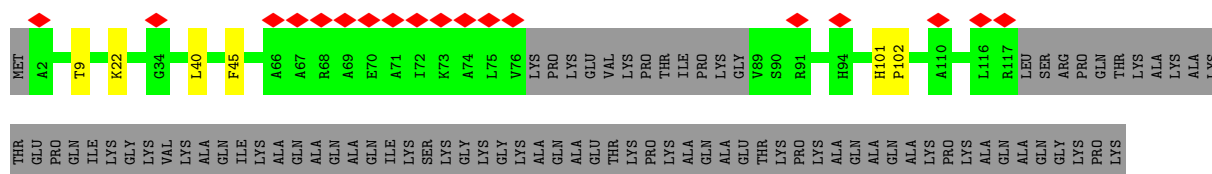
- Molecule 26: uL15

Chain a:  88% 11% .



• Molecule 27: eL29

Chain b:  7% 40% 58% .



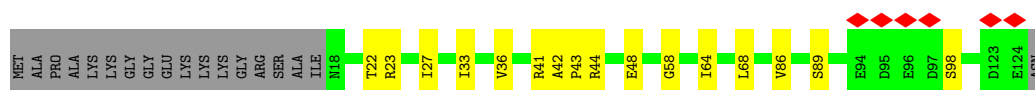
• Molecule 28: eL30

Chain c:  7% 83% 15% .



• Molecule 29: eL31

Chain d:  5% 73% 13% 14% .



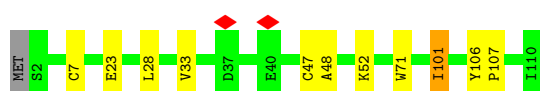
• Molecule 30: eL32

Chain e:  83% 12% 5% .

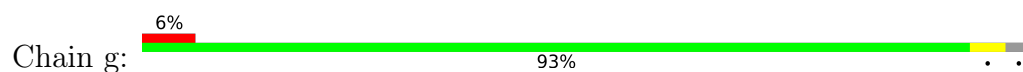


• Molecule 31: eL33

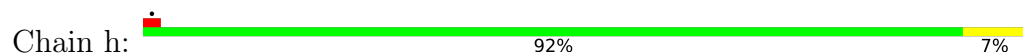
Chain f:  89% 9% ..



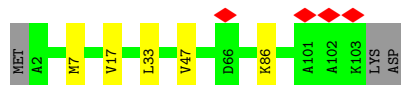
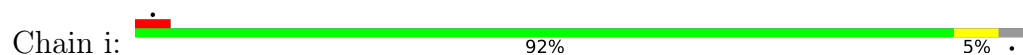
• Molecule 32: eL34



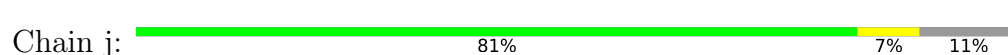
- Molecule 33: uL29



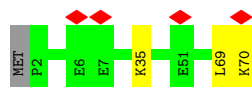
- Molecule 34: eL36



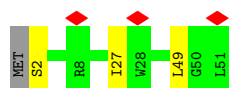
- Molecule 35: eL37



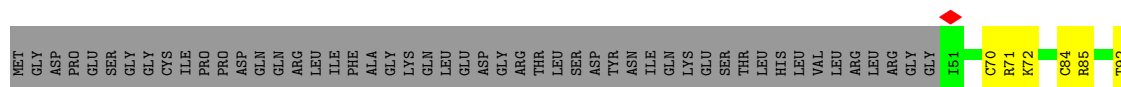
- Molecule 36: eL38



- Molecule 37: eL39

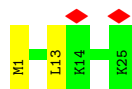


- Molecule 38: eL40

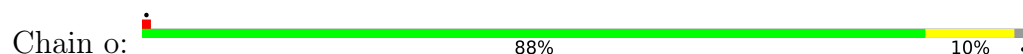




• Molecule 39: eL41



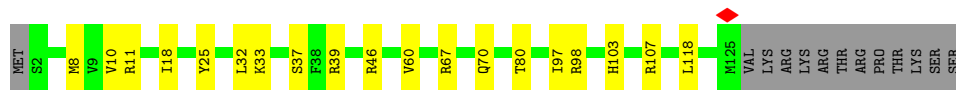
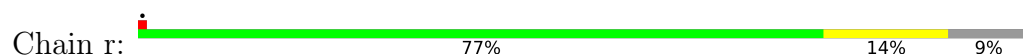
• Molecule 40: eL42



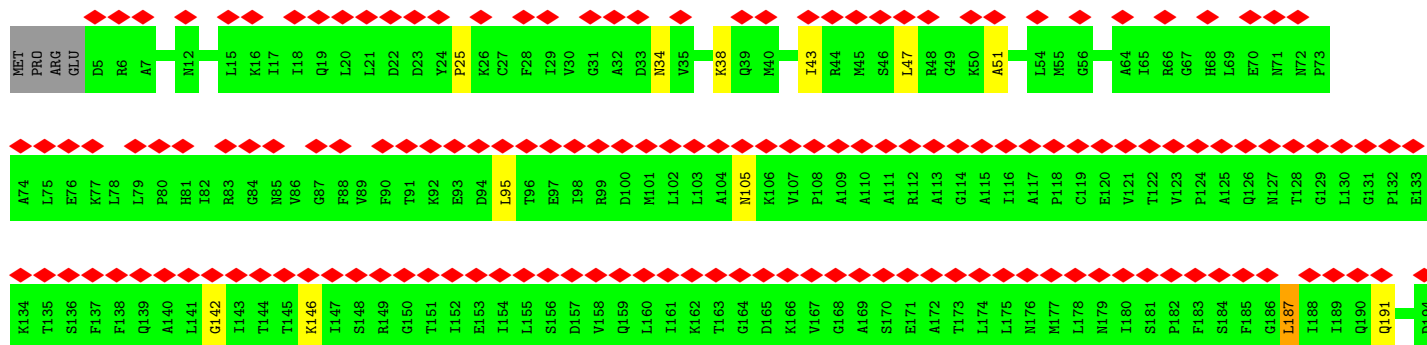
• Molecule 41: eL43

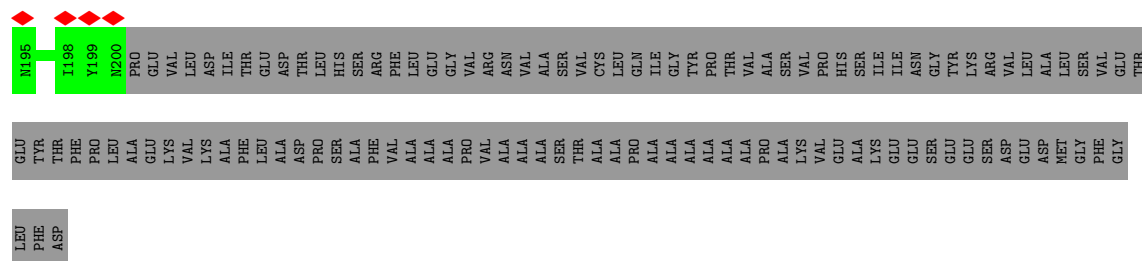


• Molecule 42: eL28

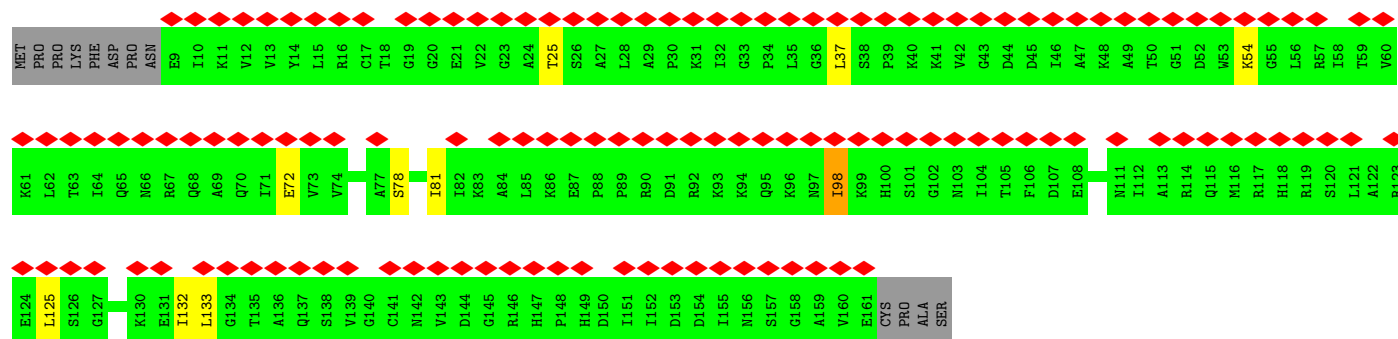
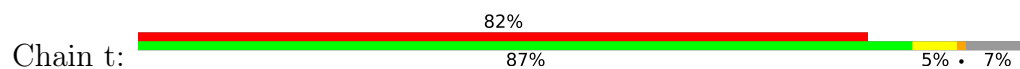


• Molecule 43: uL10

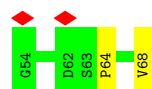
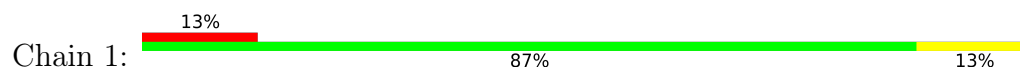




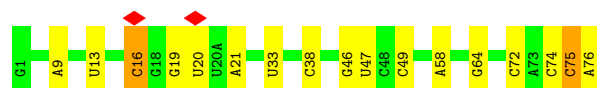
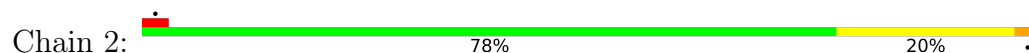
• Molecule 44: uL11



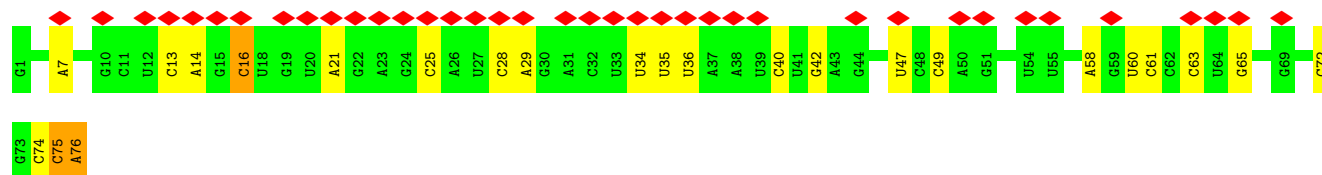
• Molecule 45: Nascent chain



• Molecule 46: P-site tRNA

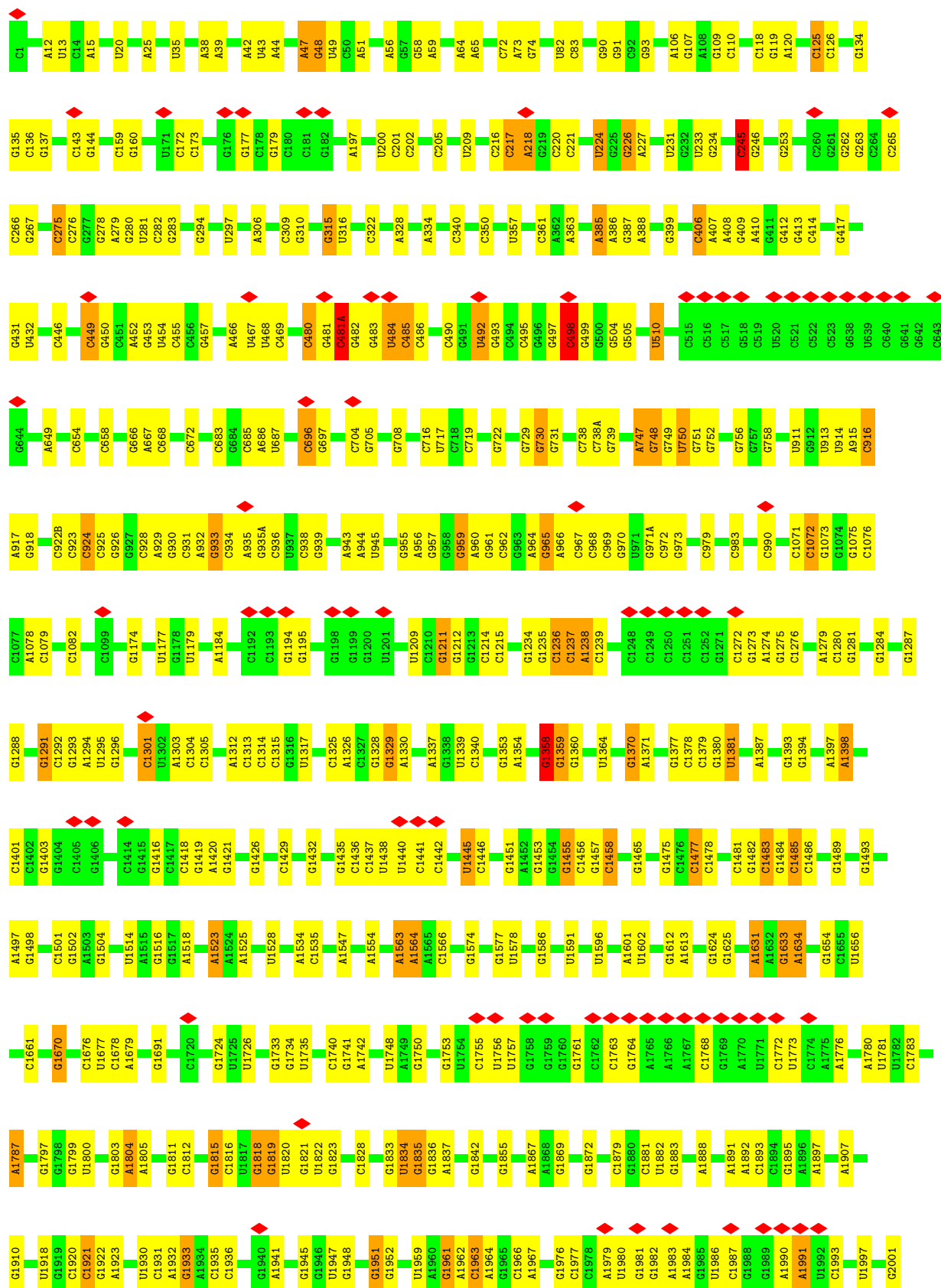


• Molecule 47: E-site tRNA

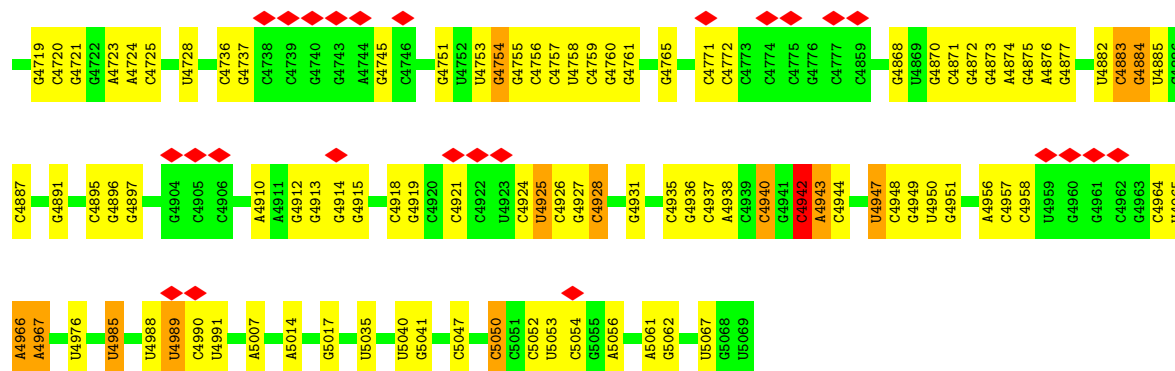


• Molecule 48: 28S ribosomal RNA

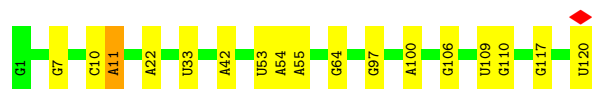
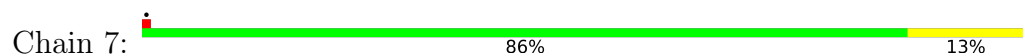




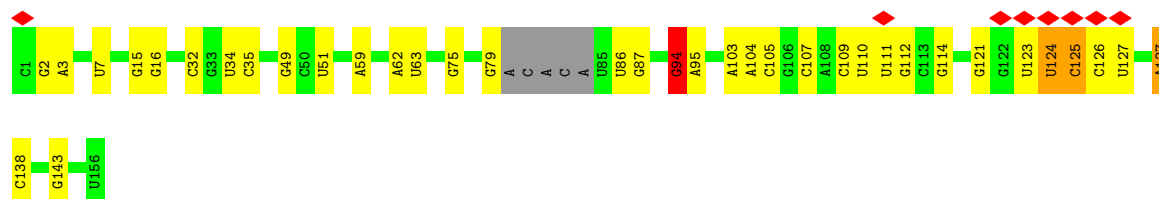
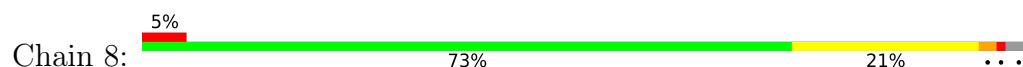
U4530	U4531	A4548	G4549	C4560	G4567	G4570	A4571	G4572	G4573	U4574	G4575	G4578	U4579	U4580	A4584	U4585	G4586	A4590	G4618	A4626	U4627	U4636	G4637	U4638	G4639	A4656	U4657	G4661	C4667	C4670	A4671	A4672	U4677	G4678	A4687	G4694	U4699	A4700	A4701	U4709										
U4395	C4398	G4401	A4415	U4419	U4420	C4421	A4422	U4423	G4429	U4501	A4504	G4505	U4506	C4514	A4517	C4518	C4519	G4526	U4529	U4530	A4531	A4536	U4547	U4548	U4549	U4550	A4553	U4557	A4558	A4559	A4564	A4565	A4566	A4567	A4568	A4569	A4570	A4571	A4572	A4573	A4574									
A4271	G4272	A4273	A4280	A4281	G4291	A4292	U4293	G4297	U4301	A4304	G4305	U4306	C4314	A4317	C4318	C4319	G4326	G4329	G4330	G4331	C4335	A4336	A4339	U4340	C4349	C4350	U4354	G4355	G4373	A4376	G4377	A4378	A4379	A4380	C4387	A4388	C4389	A4390	G4391	G4392	C4393	A4394								
G4150	C4158	C4162	U4163	C4164	U4165	G4166	G4167	U4168	U4169	A4170	C4171	G4183	U4184	U4190	G4191	A4203	U4210	G4211	A4212	A4213	U4218	A4219	A4220	C4221	G4225	U4229	U4232	A4233	C4241	G4249	G4250	A4251	G4254	A4255	A4256	A4257	C4258	U4259	U4260	C4261	U4265	G4266	G4267	A4268						
U3927	A3928	G3929	A3943	G3946	A3947	G3948	G4065	U4066	U4067	U4068	U4069	U4070	U4071	U4075	G4076	G4084	A4085	G4086	G4087	C4088	C4096	G4097	A4098	G4099	C4100	U4101	G4107	G4108	U4109	U4110	U4111	C4112	U4113	C4116	U4117	U4118	U4119	U4120	G4121	C4122	C4123	U4124	C4125	C4126	A4127	G4136	C4137	C4138	G4146	G4147
U3786	U3798	A3799	U3800	U3801	G3809	C3810	G3811	C3812	C3813	U3814	U3817	U3818	G3819	U3822	U3831	U3838	G3839	U3840	U3851	G3859	A3867	G3873	A3876	A3877	C3878	G3879	C3888	G3889	U3892	G3897	A3901	G3904	A3905	U3906	G3907	U3914	U3915	G3916	A3917	C3918	G3919									
A3653	A3656	A3662	G3671	G3672	C3673	G3674	U3690	G3691	A3692	C3696	G3697	C3698	G3710	A3711	A3712	G3722	A3723	A3724	G3725	U3729	A3733	G3740	A3747	A3748	G3749	G3750	G3753	A3756	A3759	A3760	G3765	A3766	U3773	A3774	A3775	G3776	G3777	U3778	A3783	A3784	A3785									
C2794	A2795	G2796	C2797	A2798	A2806	A2807	G2808	C2814	U2826	G2827	U2828	U2829	A2835	A2836	U2837	U2839	G2842	A2845	G2855	A2864	C2875	G2876	G2884	U2891	G2896	G2897	C3598	A3599	G3603	A3604	C3605	G3615	U3616	G3617	C3620	G3625	G3626	A3635	U3644											
G2673	A2676	G2681	G2686	U2687	G2688	C2689	G2693	G2694	A2696	U2707	U2708	C2709	G2710	G2711	G2712	G2713	G2714	G2715	C2716	C2719	G2720	G2721	A2725	G2726	C2738	C2739	U2740	U2741	G2742	A2743	A2744	G2754	A2755	G2760	U2761	U2762	U2763	A2764	U2769	C2772	A2787	U2788	A2789	U2790						
G2503	C2504	C2505	G2506	A2513	G2521	U2530	A2537	G2544	U2545	G2546	C2547	U2554	G2555	C2561	G2562	C2563	G2564	A2565	G2566	C2571	U2575	C2583	G2586	A2587	A2601	G2618	G2619	G2620	A2623	C2627	G2638	U2639	G2640	A2647	U2661	G2662	C2663	C2669	C2670											
U2397	U2398	G2399	G2402	G2406	U2407	U2408	U2409	G2416	A2417	A2422	U2423	U2424	U2425	U2426	G2427	A2428	A2429	G2433	G2439	U2440	C2441	G2450	C2458	G2459	U2467	U2468	C2469	C2470	G2471	G2474	G2475	G2479	G2483	A2484	U2485	G2486	G2487	C2488	C2489	U2490	C2491	G2492	G2493	U2494	U2495	A2502				
G2106	A2107	G2108	A2109	G2110	G2113	G2158	G2159	G2261	G2262	G2265	C2266	U2267	A2268	C2269	G2270	G2275	G2278	A2279	G2288	C2289	A2300	G2301	A2313	G2314	G2322	G2331	U2332	G2333	C2340	G2343	A2347	G2348	C2349	U2350	C2351	G2357	G2364	A2367	G2370	A2371	A2395	A2396								
A2002	G2003	U2004	G2005	U2006	G2007	U2008	C2011	U2015	G2024	A2025	A2026	C2031	U2032	U2044	G2045	G2046	A2047	U2048	G2052	G2055	G2056	A2057	C2062	A2063	G2064	C2068	A2069	U2070	U2084	G2085	C2088	G2089	U2090	C2091	G2092	G2093	C2094	A2095	U2097	C2098	C2099	G2100	A2101	G2102	A2103	A2105				



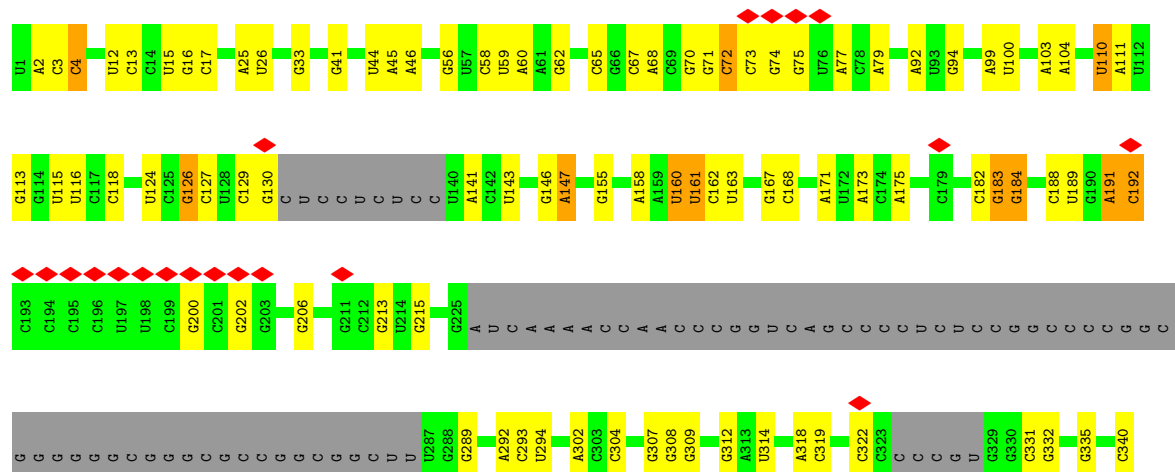
• Molecule 49: 5S ribosomal RNA



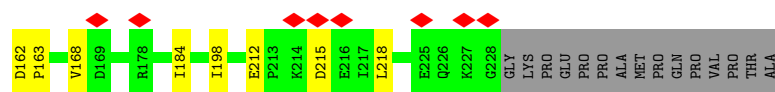
• Molecule 50: 5.8S ribosomal RNA



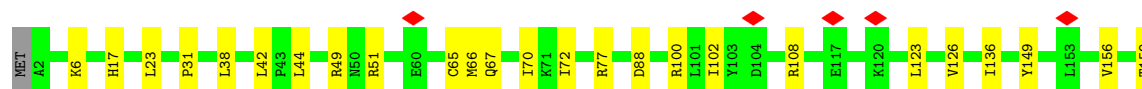
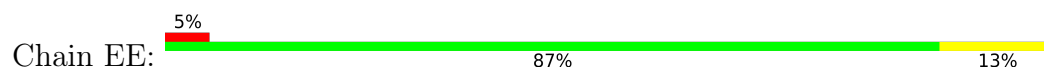
• Molecule 51: 18S ribosomal RNA



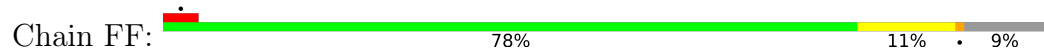




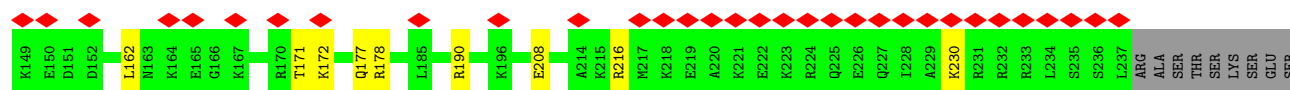
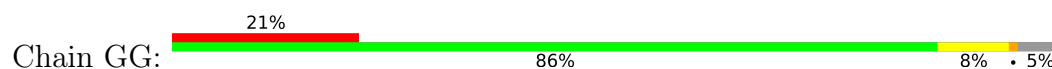
• Molecule 56: eS4



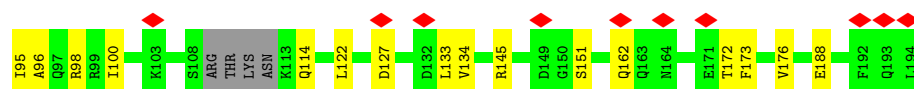
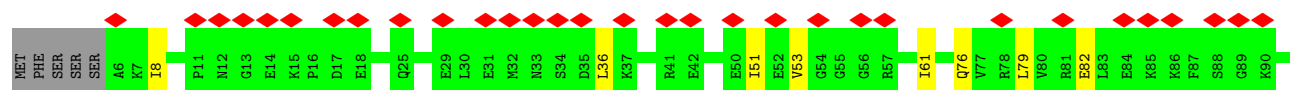
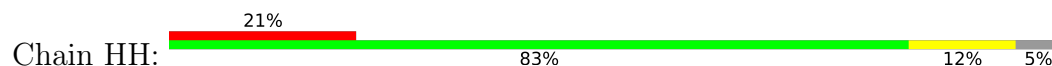
• Molecule 57: uS7



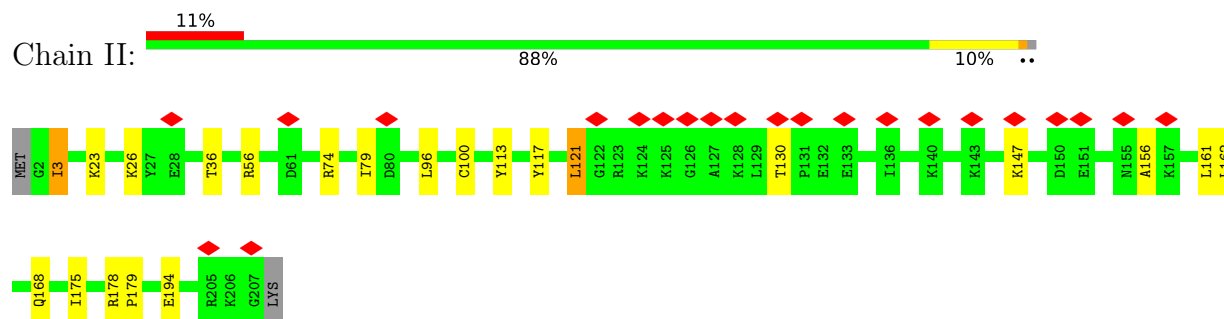
• Molecule 58: eS6



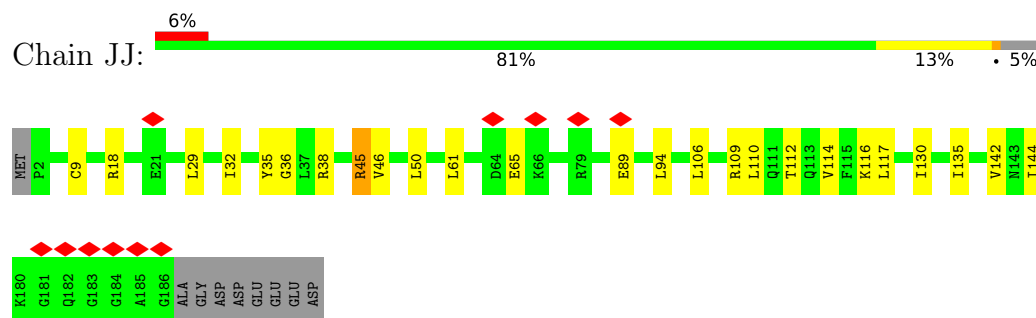
• Molecule 59: eS7



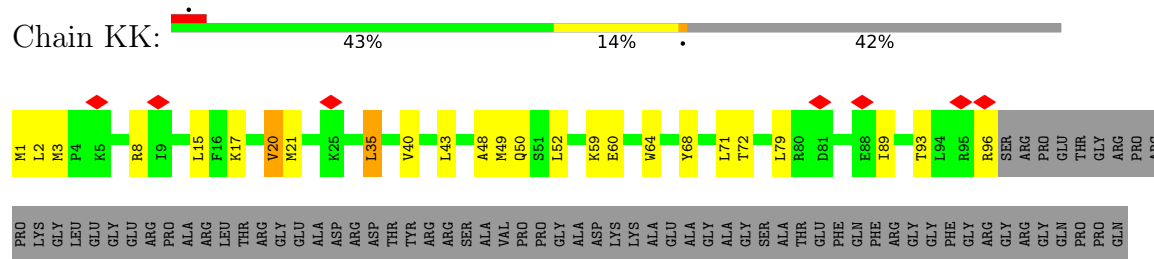
- Molecule 60: eS8



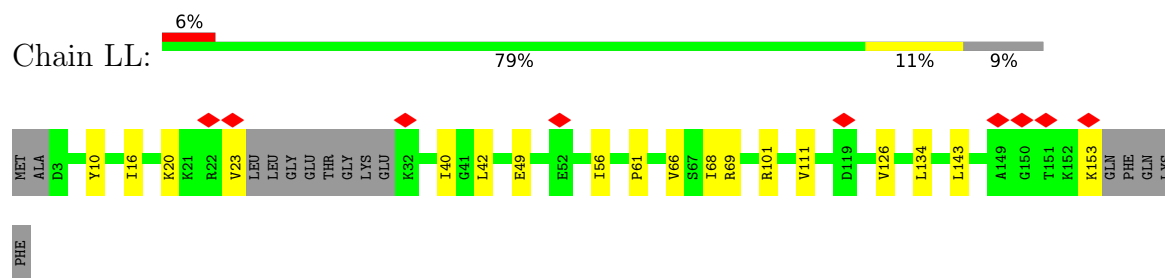
- Molecule 61: uS4



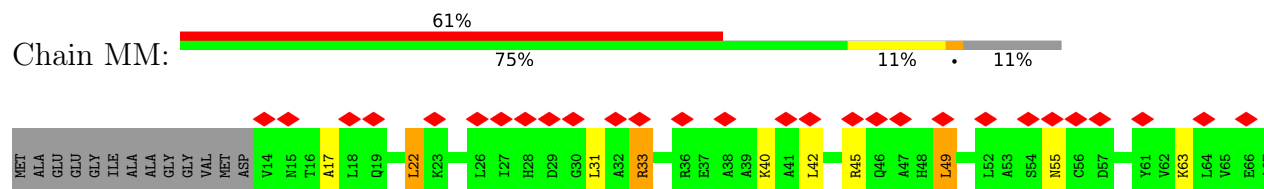
- Molecule 62: eS10

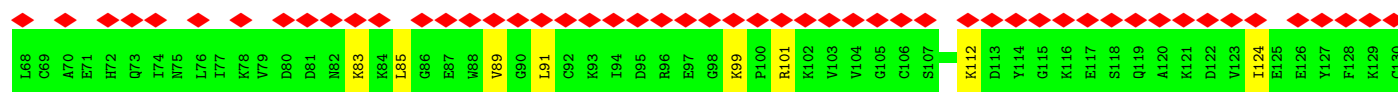


- Molecule 63: uS17



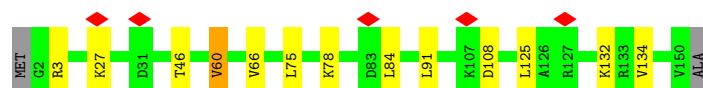
- Molecule 64: eS12



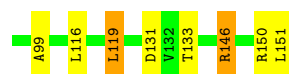
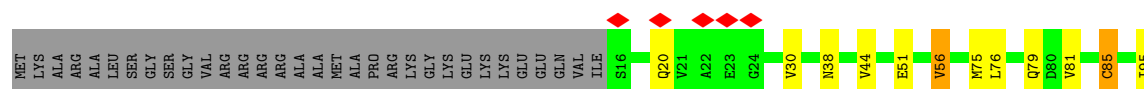


LYS
LYS

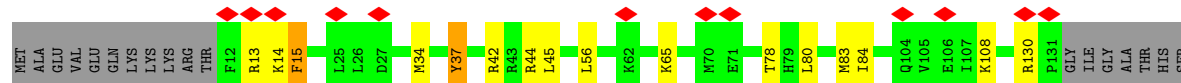
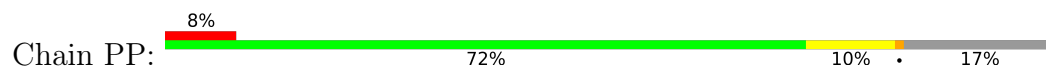
• Molecule 65: uS15



• Molecule 66: uS11

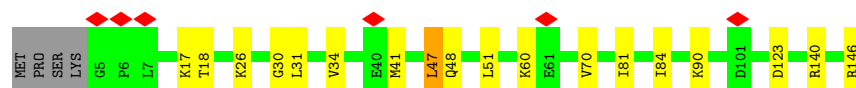
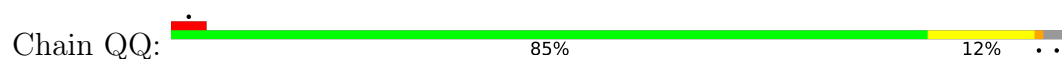


• Molecule 67: uS19

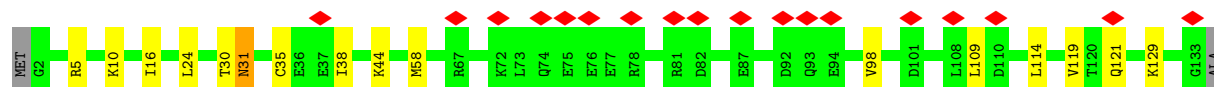
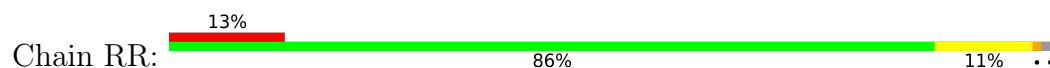


SER
ARG
PHE
ILE
PRO
LEU
LYS

• Molecule 68: uS9



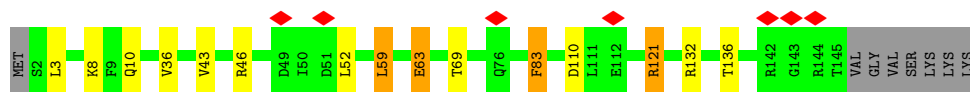
• Molecule 69: eS17



VAL

● Molecule 70: uS13

Chain SS:  5% 85% 7% 5%



● Molecule 71: eS19

Chain TT:  87% 9% ..

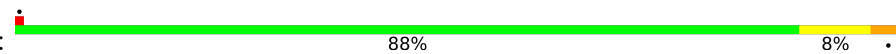


● Molecule 72: uS10

Chain UU:  9% 74% 9% 16%



● Molecule 73: eS21

Chain VV:  88% 8% .



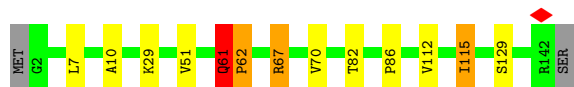
● Molecule 74: uS8

Chain WW:  83% 16% .



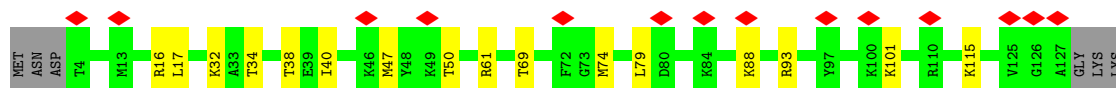
● Molecule 75: uS12

Chain XX:  90% 6% ...

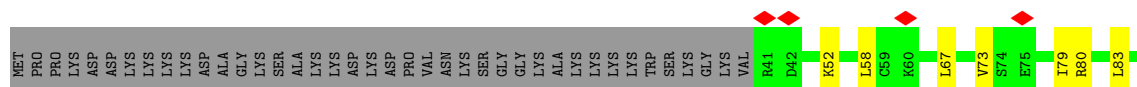


● Molecule 76: eS24

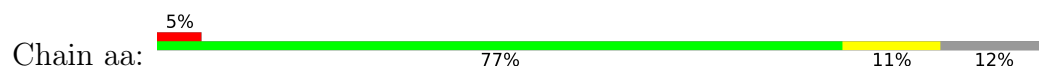
Chain YY:  11% 83% 12% 5%



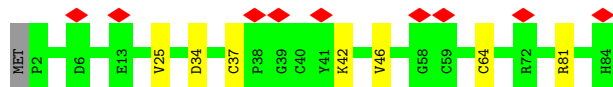
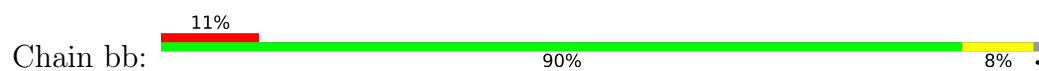
• Molecule 77: eS25



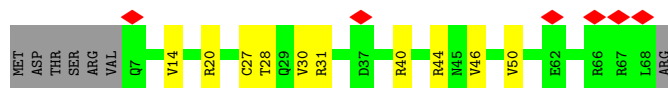
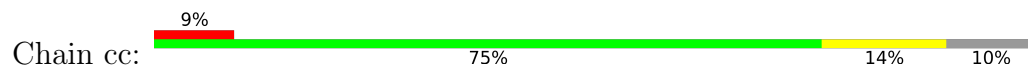
• Molecule 78: eS26



• Molecule 79: eS27



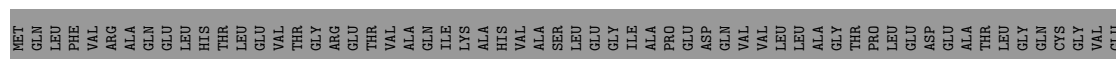
• Molecule 80: eS28

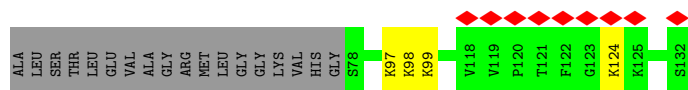


• Molecule 81: uS14

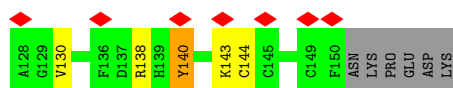
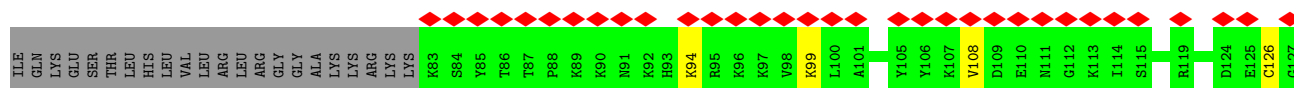
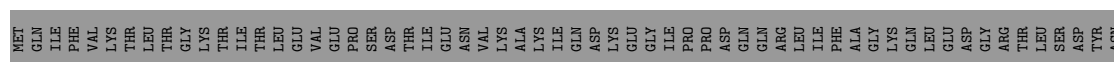
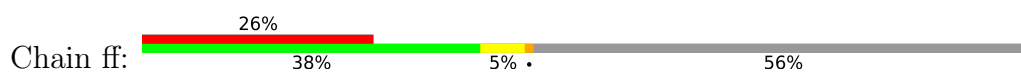


• Molecule 82: eS30

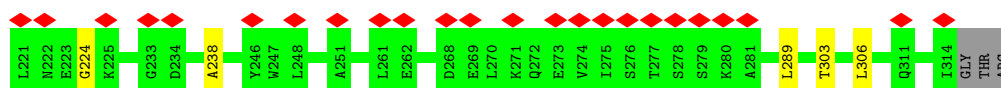




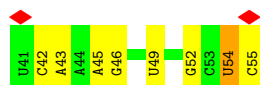
• Molecule 83: eS31



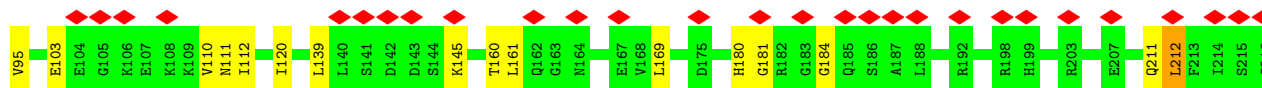
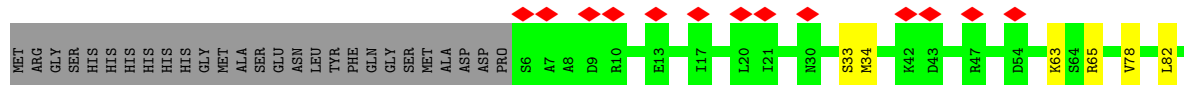
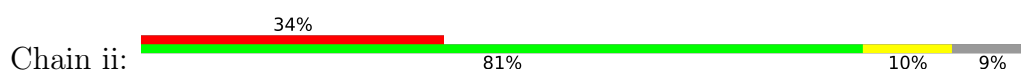
• Molecule 84: RACK1

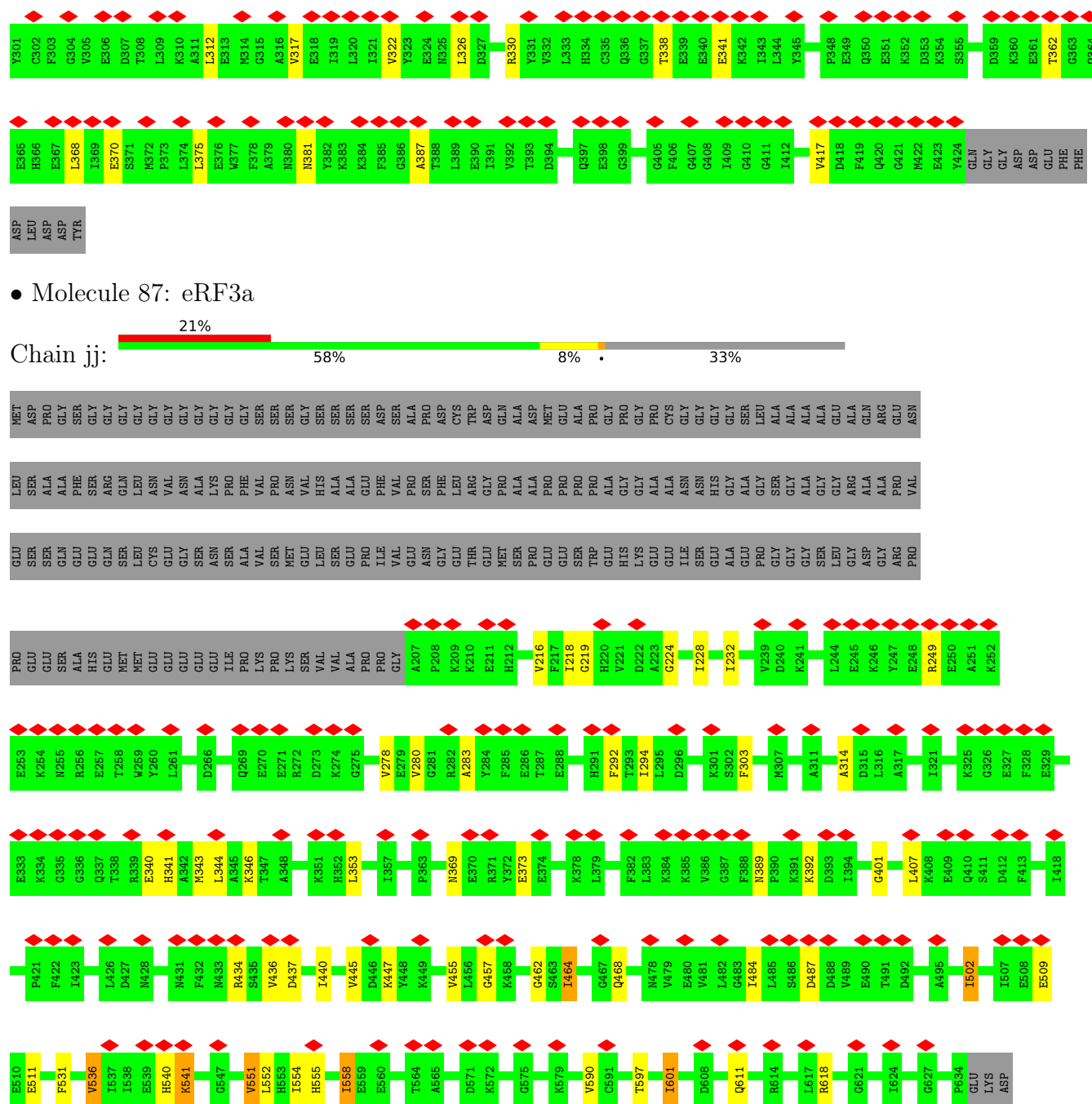


• Molecule 85: mRNA (UGA stop codon)



• Molecule 86: eRF1





• Molecule 87: eRF3a



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	61752	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	104478	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.800	Depositor
Minimum map value	-0.493	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	562.8, 562.8, 562.8	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3399999, 1.3399999, 1.3399999	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: ZN, GCP, 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	A	0.47	0/1936	0.78	0/2596
2	B	0.44	0/3240	0.76	0/4339
3	C	0.46	0/2937	0.79	2/3946 (0.1%)
4	D	0.45	0/2437	0.80	1/3264 (0.0%)
5	E	0.47	0/1762	0.78	1/2362 (0.0%)
6	F	0.48	0/1911	0.81	0/2549
7	G	0.48	0/1910	0.82	2/2569 (0.1%)
8	H	0.41	0/1535	0.69	0/2063
9	I	0.42	0/1702	0.74	0/2272
10	J	0.44	0/1385	0.75	0/1852
11	L	0.48	0/1733	0.81	0/2316
12	M	0.46	0/1158	0.82	0/1547
13	N	0.46	0/1746	0.78	0/2338
14	O	0.46	0/1662	0.83	1/2222 (0.0%)
15	P	0.48	0/1268	0.81	1/1700 (0.1%)
16	Q	0.46	0/1539	0.80	0/2054
17	R	0.47	0/1524	0.80	0/2013
18	S	0.48	0/1501	0.82	2/2012 (0.1%)
19	T	0.45	0/1326	0.72	0/1770
20	U	0.46	0/823	0.71	0/1104
21	V	0.45	0/993	0.77	0/1332
22	W	0.47	0/873	0.78	1/1158 (0.1%)
23	X	0.45	0/984	0.74	0/1323
24	Y	0.44	0/1132	0.77	0/1504
25	Z	0.46	0/1130	0.75	0/1507
26	a	0.43	0/1191	0.80	1/1590 (0.1%)
27	b	0.45	0/861	0.80	0/1138
28	c	0.45	0/771	0.78	0/1034
29	d	0.47	0/903	0.75	0/1216
30	e	0.45	0/1071	0.79	0/1429
31	f	0.47	0/895	0.77	0/1198
32	g	0.45	0/916	0.76	0/1220

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	h	0.43	0/1021	0.81	0/1348
34	i	0.45	0/841	0.77	0/1112
35	j	0.47	0/720	0.81	0/952
36	k	0.44	0/575	0.72	0/761
37	l	0.46	0/459	0.78	0/608
38	m	0.46	0/435	0.78	0/575
39	n	0.41	0/240	0.83	0/305
40	o	0.44	0/864	0.71	0/1140
41	p	0.44	0/718	0.81	0/953
42	r	0.49	0/1010	0.86	1/1354 (0.1%)
43	s	0.54	0/1530	0.74	0/2064
44	t	0.57	0/1174	0.82	0/1582
45	1	0.51	0/129	0.86	0/173
46	2	0.35	0/1805	0.69	0/2809
47	3	0.37	0/1777	0.68	0/2763
48	5	0.37	0/84973	0.73	78/132508 (0.1%)
49	7	0.37	0/2858	0.71	0/4455
50	8	0.37	0/3581	0.71	2/5577 (0.0%)
51	9	0.37	1/40524 (0.0%)	0.73	30/63134 (0.0%)
52	AA	0.47	0/1747	0.80	0/2374
53	BB	0.43	0/1756	0.80	0/2350
54	CC	0.47	0/1753	0.83	0/2369
55	DD	0.50	0/1796	0.79	0/2417
56	EE	0.49	0/2118	0.78	1/2849 (0.0%)
57	FF	0.47	0/1492	0.87	0/2005
58	GG	0.51	0/1946	0.83	2/2590 (0.1%)
59	HH	0.51	0/1510	0.80	0/2022
60	II	0.47	0/1715	0.77	0/2287
61	JJ	0.45	0/1550	0.85	0/2069
62	KK	0.49	0/834	0.83	0/1125
63	LL	0.46	0/1195	0.76	0/1597
64	MM	0.53	0/918	0.87	0/1233
65	NN	0.46	0/1226	0.85	0/1649
66	OO	0.48	0/1029	0.93	1/1380 (0.1%)
67	PP	0.49	0/1017	0.83	0/1358
68	QQ	0.47	0/1146	0.76	0/1534
69	RR	0.48	0/1082	0.80	0/1452
70	SS	0.48	0/1208	0.82	0/1618
71	TT	0.49	0/1115	0.87	0/1493
72	UU	0.47	0/805	0.83	1/1081 (0.1%)
73	VV	0.49	0/643	0.83	1/860 (0.1%)
74	WW	0.46	0/1051	0.79	0/1406
75	XX	0.42	0/1116	0.79	0/1490

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	YY	0.47	0/1028	0.77	0/1366
77	ZZ	0.48	0/604	0.81	0/810
78	aa	0.48	0/828	0.85	0/1109
79	bb	0.47	0/665	0.72	0/891
80	cc	0.46	0/490	0.76	0/656
81	dd	0.47	0/470	0.74	0/623
82	ee	0.46	0/447	0.85	0/587
83	ff	0.50	0/567	0.74	0/753
84	gg	0.46	0/2493	0.69	0/3394
85	hh	0.39	0/353	0.78	0/547
86	ii	0.50	0/3361	0.83	0/4519
87	jj	0.52	0/3435	0.78	0/4633
All	All	0.42	1/238498 (0.0%)	0.76	129/349206 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
74	WW	0	1
75	XX	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	9	583	A	C1'-N9	-5.03	1.40	1.48

The worst 5 of 129 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	9	1835	A	C2'-C3'-O3'	12.62	128.43	109.50
48	5	2068	C	C4'-C3'-O3'	9.74	124.01	109.40
48	5	385	A	C4'-C3'-O3'	9.52	123.68	109.40
48	5	1818	G	C2'-C3'-O3'	9.31	123.47	109.50
48	5	2046	G	C2'-C3'-O3'	9.29	123.43	109.50

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	16	PHE	Peptide
74	WW	27	ILE	Peptide
75	XX	61	GLN	Peptide

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	A	1898	0	1993	20	0
2	B	3172	0	3310	23	0
3	C	2883	0	3053	9	0
4	D	2391	0	2424	14	0
5	E	1729	0	1887	11	0
6	F	1875	0	1995	12	0
7	G	1879	0	2027	11	0
8	H	1516	0	1597	10	0
9	I	1664	0	1712	5	0
10	J	1362	0	1399	7	0
11	L	1702	0	1820	11	0
12	M	1137	0	1211	9	0
13	N	1701	0	1749	4	0
14	O	1630	0	1778	15	0
15	P	1242	0	1274	5	0
16	Q	1515	0	1634	6	0
17	R	1508	0	1664	5	0
18	S	1462	0	1508	16	0
19	T	1298	0	1366	5	0
20	U	809	0	833	1	0
21	V	979	0	1039	7	0
22	W	860	0	903	3	0
23	X	967	0	1040	3	0
24	Y	1115	0	1205	1	0
25	Z	1107	0	1182	4	0
26	a	1162	0	1209	11	0
27	b	848	0	920	1	0
28	c	761	0	794	0	0
29	d	888	0	930	9	0
30	e	1053	0	1147	5	0
31	f	876	0	912	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	g	906	0	999	0	0
33	h	1013	0	1147	4	0
34	i	830	0	916	3	0
35	j	705	0	737	2	0
36	k	569	0	637	1	0
37	l	447	0	480	1	0
38	m	429	0	465	2	0
39	n	239	0	289	0	0
40	o	851	0	920	5	0
41	p	708	0	758	6	0
42	r	994	0	1051	7	0
43	s	1507	0	1564	3	0
44	t	1160	0	1218	3	0
45	1	125	0	117	1	0
46	2	1616	0	824	5	0
47	3	1593	0	811	5	0
48	5	75972	0	38393	146	0
49	7	2558	0	1296	2	0
50	8	3208	0	1629	5	0
51	9	36249	0	18316	104	0
52	AA	1710	0	1708	12	0
53	BB	1729	0	1803	15	0
54	CC	1716	0	1806	10	0
55	DD	1768	0	1866	8	0
56	EE	2076	0	2177	8	0
57	FF	1471	0	1522	12	0
58	GG	1923	0	2089	9	0
59	HH	1488	0	1582	5	0
60	II	1686	0	1772	6	0
61	JJ	1525	0	1640	12	0
62	KK	810	0	836	9	0
63	LL	1175	0	1249	4	0
64	MM	908	0	939	8	0
65	NN	1202	0	1289	2	0
66	OO	1016	0	1039	9	0
67	PP	997	0	1045	6	0
68	QQ	1128	0	1195	8	0
69	RR	1068	0	1121	5	0
70	SS	1190	0	1249	3	0
71	TT	1097	0	1132	5	0
72	UU	795	0	862	4	0
73	VV	636	0	637	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
74	WW	1034	0	1080	9	0
75	XX	1098	0	1167	4	0
76	YY	1011	0	1083	1	0
77	ZZ	598	0	656	6	0
78	aa	814	0	864	4	0
79	bb	651	0	672	2	0
80	cc	488	0	514	6	0
81	dd	459	0	449	2	0
82	ee	443	0	492	0	0
83	ff	555	0	566	5	0
84	gg	2436	0	2393	7	0
85	hh	317	0	161	1	0
86	ii	3307	0	3346	16	0
87	jj	3368	0	3422	26	0
88	5	185	0	0	0	0
88	7	5	0	0	0	0
88	8	8	0	0	0	0
88	9	71	0	0	0	0
88	A	1	0	0	0	0
88	B	1	0	0	0	0
88	I	1	0	0	0	0
88	P	3	0	0	0	0
88	Q	1	0	0	0	0
88	V	1	0	0	0	0
88	a	1	0	0	0	0
88	g	1	0	0	0	0
88	hh	1	0	0	0	0
88	j	1	0	0	0	0
88	jj	1	0	0	0	0
89	aa	1	0	0	0	0
89	dd	1	0	0	0	0
89	ff	1	0	0	1	0
89	g	1	0	0	0	0
89	j	1	0	0	0	0
89	m	1	0	0	0	0
89	o	1	0	0	0	0
89	p	1	0	0	2	0
90	jj	32	0	14	0	0
All	All	222683	0	167519	689	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 2.

The worst 5 of 689 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)
87:jj:346:LYS:CD	87:jj:389:ASN:OD1	1.65	1.41
83:ff:144:CYS:SG	89:ff:200:ZN:ZN	1.24	1.26
48:5:2367:A:N1	48:5:2788:U:O4	1.66	1.25
51:9:1137:U:O4	51:9:1148:A:N1	1.68	1.23
87:jj:346:LYS:HD3	87:jj:389:ASN:OD1	1.01	1.18

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	246/257 (96%)	218 (89%)	26 (11%)	2 (1%)	16	45
2	B	392/403 (97%)	360 (92%)	29 (7%)	3 (1%)	16	45
3	C	360/425 (85%)	337 (94%)	21 (6%)	2 (1%)	21	51
4	D	291/297 (98%)	275 (94%)	15 (5%)	1 (0%)	36	64
5	E	208/291 (72%)	191 (92%)	17 (8%)	0	100	100
6	F	223/247 (90%)	212 (95%)	10 (4%)	1 (0%)	30	58
7	G	229/319 (72%)	216 (94%)	11 (5%)	2 (1%)	14	43
8	H	188/192 (98%)	178 (95%)	10 (5%)	0	100	100
9	I	201/214 (94%)	185 (92%)	16 (8%)	0	100	100
10	J	168/178 (94%)	161 (96%)	7 (4%)	0	100	100
11	L	208/211 (99%)	196 (94%)	11 (5%)	1 (0%)	24	55
12	M	136/218 (62%)	123 (90%)	12 (9%)	1 (1%)	18	48
13	N	201/204 (98%)	187 (93%)	13 (6%)	1 (0%)	24	55
14	O	197/203 (97%)	188 (95%)	8 (4%)	1 (0%)	24	55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	P	151/184 (82%)	142 (94%)	9 (6%)	0	100	100
16	Q	185/188 (98%)	173 (94%)	12 (6%)	0	100	100
17	R	178/196 (91%)	173 (97%)	5 (3%)	0	100	100
18	S	174/176 (99%)	159 (91%)	14 (8%)	1 (1%)	21	51
19	T	157/160 (98%)	147 (94%)	10 (6%)	0	100	100
20	U	97/128 (76%)	87 (90%)	10 (10%)	0	100	100
21	V	129/140 (92%)	120 (93%)	9 (7%)	0	100	100
22	W	102/157 (65%)	97 (95%)	4 (4%)	1 (1%)	12	41
23	X	116/156 (74%)	107 (92%)	9 (8%)	0	100	100
24	Y	132/145 (91%)	122 (92%)	10 (8%)	0	100	100
25	Z	133/136 (98%)	126 (95%)	5 (4%)	2 (2%)	8	33
26	a	145/148 (98%)	131 (90%)	14 (10%)	0	100	100
27	b	100/245 (41%)	94 (94%)	5 (5%)	1 (1%)	12	41
28	c	96/115 (84%)	93 (97%)	3 (3%)	0	100	100
29	d	105/125 (84%)	89 (85%)	15 (14%)	1 (1%)	12	41
30	e	126/135 (93%)	120 (95%)	6 (5%)	0	100	100
31	f	107/110 (97%)	97 (91%)	8 (8%)	2 (2%)	6	30
32	g	112/117 (96%)	105 (94%)	7 (6%)	0	100	100
33	h	120/123 (98%)	118 (98%)	2 (2%)	0	100	100
34	i	100/105 (95%)	94 (94%)	5 (5%)	1 (1%)	12	41
35	j	84/97 (87%)	78 (93%)	6 (7%)	0	100	100
36	k	67/70 (96%)	65 (97%)	2 (3%)	0	100	100
37	l	48/51 (94%)	44 (92%)	4 (8%)	0	100	100
38	m	50/102 (49%)	47 (94%)	3 (6%)	0	100	100
39	n	23/25 (92%)	23 (100%)	0	0	100	100
40	o	102/106 (96%)	98 (96%)	4 (4%)	0	100	100
41	p	89/92 (97%)	83 (93%)	5 (6%)	1 (1%)	11	39
42	r	122/137 (89%)	112 (92%)	9 (7%)	1 (1%)	16	45
43	s	194/318 (61%)	176 (91%)	16 (8%)	2 (1%)	12	41
44	t	151/165 (92%)	135 (89%)	14 (9%)	2 (1%)	9	36
45	l	13/15 (87%)	10 (77%)	2 (15%)	1 (8%)	1	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	AA	215/295 (73%)	203 (94%)	11 (5%)	1 (0%)	24	55
53	BB	211/264 (80%)	198 (94%)	12 (6%)	1 (0%)	24	55
54	CC	219/293 (75%)	206 (94%)	13 (6%)	0	100	100
55	DD	226/243 (93%)	213 (94%)	12 (5%)	1 (0%)	30	58
56	EE	260/263 (99%)	246 (95%)	14 (5%)	0	100	100
57	FF	181/204 (89%)	170 (94%)	9 (5%)	2 (1%)	11	39
58	GG	235/249 (94%)	224 (95%)	11 (5%)	0	100	100
59	HH	181/194 (93%)	171 (94%)	10 (6%)	0	100	100
60	II	204/208 (98%)	192 (94%)	11 (5%)	1 (0%)	24	55
61	JJ	183/194 (94%)	177 (97%)	6 (3%)	0	100	100
62	KK	94/165 (57%)	89 (95%)	4 (4%)	1 (1%)	11	39
63	LL	139/158 (88%)	130 (94%)	9 (6%)	0	100	100
64	MM	115/132 (87%)	103 (90%)	12 (10%)	0	100	100
65	NN	147/151 (97%)	142 (97%)	4 (3%)	1 (1%)	18	48
66	OO	134/168 (80%)	123 (92%)	9 (7%)	2 (2%)	8	33
67	PP	118/145 (81%)	105 (89%)	12 (10%)	1 (1%)	16	45
68	QQ	140/146 (96%)	132 (94%)	7 (5%)	1 (1%)	18	48
69	RR	130/135 (96%)	120 (92%)	10 (8%)	0	100	100
70	SS	142/152 (93%)	135 (95%)	7 (5%)	0	100	100
71	TT	139/145 (96%)	130 (94%)	8 (6%)	1 (1%)	18	48
72	UU	98/119 (82%)	91 (93%)	7 (7%)	0	100	100
73	VV	81/83 (98%)	79 (98%)	2 (2%)	0	100	100
74	WW	127/130 (98%)	120 (94%)	5 (4%)	2 (2%)	7	32
75	XX	139/143 (97%)	128 (92%)	8 (6%)	3 (2%)	5	27
76	YY	122/130 (94%)	115 (94%)	7 (6%)	0	100	100
77	ZZ	73/125 (58%)	70 (96%)	3 (4%)	0	100	100
78	aa	99/115 (86%)	93 (94%)	4 (4%)	2 (2%)	6	29
79	bb	81/84 (96%)	75 (93%)	6 (7%)	0	100	100
80	cc	60/69 (87%)	58 (97%)	2 (3%)	0	100	100
81	dd	53/56 (95%)	48 (91%)	5 (9%)	0	100	100
82	ee	53/133 (40%)	51 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
83	ff	66/156 (42%)	59 (89%)	7 (11%)	0	100	100
84	gg	311/317 (98%)	285 (92%)	24 (8%)	2 (1%)	21	51
86	ii	417/459 (91%)	387 (93%)	24 (6%)	6 (1%)	9	34
87	jj	426/637 (67%)	371 (87%)	50 (12%)	5 (1%)	10	38
All	All	12375/14486 (85%)	11531 (93%)	780 (6%)	64 (0%)	26	55

5 of 64 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
75	XX	62	PRO
86	ii	258	TYR
86	ii	272	THR
87	jj	224	GLY
87	jj	280	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	190/199 (96%)	176 (93%)	14 (7%)	13	37
2	B	342/348 (98%)	324 (95%)	18 (5%)	20	45
3	C	302/347 (87%)	285 (94%)	17 (6%)	19	44
4	D	247/250 (99%)	235 (95%)	12 (5%)	22	47
5	E	190/251 (76%)	178 (94%)	12 (6%)	16	41
6	F	196/215 (91%)	185 (94%)	11 (6%)	19	44
7	G	200/272 (74%)	190 (95%)	10 (5%)	22	46
8	H	169/171 (99%)	158 (94%)	11 (6%)	15	40
9	I	175/181 (97%)	165 (94%)	10 (6%)	18	43
10	J	143/149 (96%)	137 (96%)	6 (4%)	26	49
11	L	175/176 (99%)	172 (98%)	3 (2%)	53	65
12	M	117/161 (73%)	110 (94%)	7 (6%)	17	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	N	171/172 (99%)	165 (96%)	6 (4%)	32	53
14	O	171/173 (99%)	160 (94%)	11 (6%)	16	41
15	P	134/163 (82%)	129 (96%)	5 (4%)	30	52
16	Q	164/165 (99%)	156 (95%)	8 (5%)	22	47
17	R	159/175 (91%)	147 (92%)	12 (8%)	12	37
18	S	157/157 (100%)	143 (91%)	14 (9%)	9	31
19	T	139/140 (99%)	131 (94%)	8 (6%)	18	43
20	U	89/114 (78%)	88 (99%)	1 (1%)	65	71
21	V	101/107 (94%)	91 (90%)	10 (10%)	7	29
22	W	86/126 (68%)	86 (100%)	0	100	100
23	X	106/134 (79%)	99 (93%)	7 (7%)	15	40
24	Y	124/135 (92%)	118 (95%)	6 (5%)	23	47
25	Z	117/118 (99%)	113 (97%)	4 (3%)	32	53
26	a	119/120 (99%)	117 (98%)	2 (2%)	53	65
27	b	84/184 (46%)	80 (95%)	4 (5%)	23	47
28	c	84/98 (86%)	81 (96%)	3 (4%)	31	53
29	d	98/110 (89%)	95 (97%)	3 (3%)	35	55
30	e	114/121 (94%)	104 (91%)	10 (9%)	9	31
31	f	88/89 (99%)	82 (93%)	6 (7%)	14	40
32	g	98/100 (98%)	93 (95%)	5 (5%)	21	46
33	h	109/110 (99%)	106 (97%)	3 (3%)	38	57
34	i	86/89 (97%)	84 (98%)	2 (2%)	44	61
35	j	73/80 (91%)	70 (96%)	3 (4%)	27	50
36	k	64/65 (98%)	62 (97%)	2 (3%)	35	55
37	l	47/48 (98%)	45 (96%)	2 (4%)	26	49
38	m	48/90 (53%)	45 (94%)	3 (6%)	16	41
39	n	24/24 (100%)	22 (92%)	2 (8%)	10	33
40	o	92/94 (98%)	87 (95%)	5 (5%)	20	45
41	p	74/75 (99%)	72 (97%)	2 (3%)	39	57
42	r	108/121 (89%)	100 (93%)	8 (7%)	13	37
43	s	164/258 (64%)	158 (96%)	6 (4%)	30	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	t	126/137 (92%)	121 (96%)	5 (4%)	28	50
45	1	13/13 (100%)	13 (100%)	0	100	100
52	AA	180/245 (74%)	166 (92%)	14 (8%)	11	36
53	BB	194/231 (84%)	177 (91%)	17 (9%)	9	31
54	CC	187/225 (83%)	177 (95%)	10 (5%)	20	45
55	DD	190/202 (94%)	172 (90%)	18 (10%)	8	30
56	EE	224/225 (100%)	205 (92%)	19 (8%)	10	32
57	FF	158/170 (93%)	147 (93%)	11 (7%)	14	39
58	GG	207/218 (95%)	195 (94%)	12 (6%)	18	43
59	HH	165/174 (95%)	150 (91%)	15 (9%)	9	31
60	II	178/180 (99%)	164 (92%)	14 (8%)	11	35
61	JJ	161/168 (96%)	148 (92%)	13 (8%)	11	34
62	KK	87/136 (64%)	73 (84%)	14 (16%)	2	13
63	LL	130/142 (92%)	118 (91%)	12 (9%)	8	30
64	MM	99/108 (92%)	86 (87%)	13 (13%)	4	19
65	NN	130/131 (99%)	121 (93%)	9 (7%)	14	39
66	OO	106/130 (82%)	96 (91%)	10 (9%)	8	30
67	PP	109/130 (84%)	100 (92%)	9 (8%)	10	33
68	QQ	117/121 (97%)	108 (92%)	9 (8%)	12	36
69	RR	119/121 (98%)	109 (92%)	10 (8%)	10	33
70	SS	125/132 (95%)	111 (89%)	14 (11%)	6	24
71	TT	111/115 (96%)	104 (94%)	7 (6%)	16	41
72	UU	92/107 (86%)	87 (95%)	5 (5%)	20	45
73	VV	67/67 (100%)	62 (92%)	5 (8%)	12	37
74	WW	112/113 (99%)	106 (95%)	6 (5%)	20	45
75	XX	113/115 (98%)	106 (94%)	7 (6%)	16	41
76	YY	107/112 (96%)	93 (87%)	14 (13%)	4	19
77	ZZ	66/103 (64%)	62 (94%)	4 (6%)	17	42
78	aa	88/98 (90%)	80 (91%)	8 (9%)	9	31
79	bb	75/76 (99%)	71 (95%)	4 (5%)	20	45
80	cc	55/62 (89%)	50 (91%)	5 (9%)	9	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
81	dd	48/49 (98%)	45 (94%)	3 (6%)	16	41
82	ee	46/106 (43%)	42 (91%)	4 (9%)	9	32
83	ff	61/140 (44%)	57 (93%)	4 (7%)	15	40
84	gg	272/275 (99%)	264 (97%)	8 (3%)	37	56
86	ii	361/394 (92%)	344 (95%)	17 (5%)	23	47
87	jj	372/520 (72%)	352 (95%)	20 (5%)	20	45
All	All	10789/12266 (88%)	10126 (94%)	663 (6%)	19	42

5 of 663 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
63	LL	69	ARG
76	YY	17	LEU
64	MM	83	LYS
63	LL	56	ILE
69	RR	35	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 151 such sidechains are listed below:

Mol	Chain	Res	Type
68	QQ	8	GLN
87	jj	313	GLN
70	SS	73	ASN
78	aa	86	ASN
87	jj	611	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
46	2	74/76 (97%)	13 (17%)	0
47	3	72/75 (96%)	24 (33%)	2 (2%)
48	5	3519/3543 (99%)	893 (25%)	169 (4%)
49	7	119/120 (99%)	14 (11%)	2 (1%)
50	8	149/156 (95%)	32 (21%)	6 (4%)
51	9	1682/1869 (89%)	431 (25%)	71 (4%)
85	hh	14/15 (93%)	8 (57%)	0
All	All	5629/5854 (96%)	1415 (25%)	250 (4%)

5 of 1415 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
46	2	9	A
46	2	13	U
46	2	16	C
46	2	19	G
46	2	20	U

5 of 250 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
48	5	2490	U
51	9	1215	C
48	5	4232	U
51	9	1137	U
51	9	1535	U

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 291 ligands modelled in this entry, 290 are monoatomic - leaving 1 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	$\# Z > 2$
90	GCP	jj	700	88	32,34,34	1.74	7 (21%)	49,54,54	1.82	8 (16%)

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
90	GCP	jj	700	88	-	6/19/38/38	0/3/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
90	jj	700	GCP	PG-O1G	5.58	1.61	1.50
90	jj	700	GCP	C5-C4	3.20	1.47	1.38
90	jj	700	GCP	PG-O2G	2.96	1.61	1.55
90	jj	700	GCP	PG-O3G	-2.96	1.48	1.55
90	jj	700	GCP	PB-O3A	2.16	1.60	1.58

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
90	jj	700	GCP	C5-C4-N3	-6.00	118.84	128.39
90	jj	700	GCP	C2-N3-C4	5.23	121.32	112.30
90	jj	700	GCP	N9-C4-N3	4.57	135.08	125.95
90	jj	700	GCP	PB-O3A-PA	-3.63	120.51	132.37
90	jj	700	GCP	C6-C5-N7	3.55	136.75	130.29

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

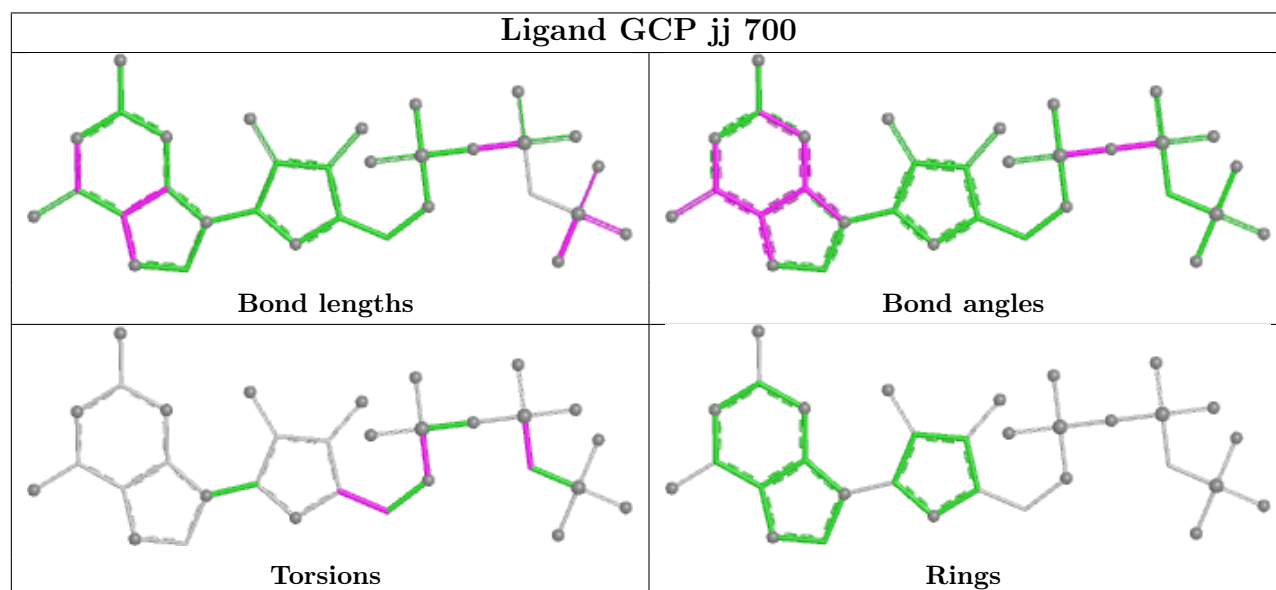
Mol	Chain	Res	Type	Atoms
90	jj	700	GCP	PG-C3B-PB-O1B
90	jj	700	GCP	PG-C3B-PB-O2B
90	jj	700	GCP	PG-C3B-PB-O3A
90	jj	700	GCP	C5'-O5'-PA-O3A
90	jj	700	GCP	C5'-O5'-PA-O1A

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
48	5	30
51	9	7
47	3	2
46	2	1

The worst 5 of 40 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	2113:G	O3'	2258:C	P	41.06
1	5	1252:C	O3'	1271:G	P	35.64
1	5	1219:G	O3'	1233:G	P	22.79
1	5	3948:C	O3'	4065:G	P	19.75

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	1406(C):G	O3'	1411:C	P	18.65

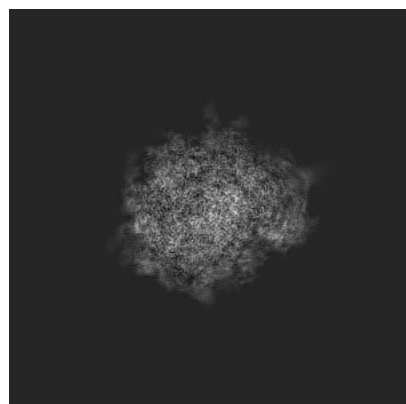
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4131. These allow visual inspection of the internal detail of the map and identification of artifacts.

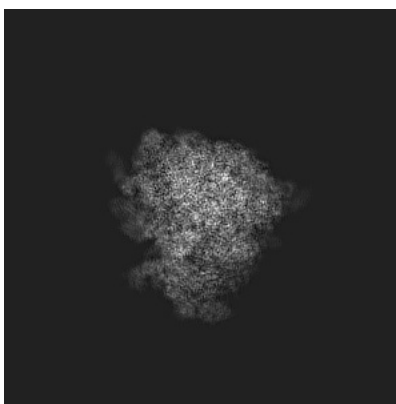
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

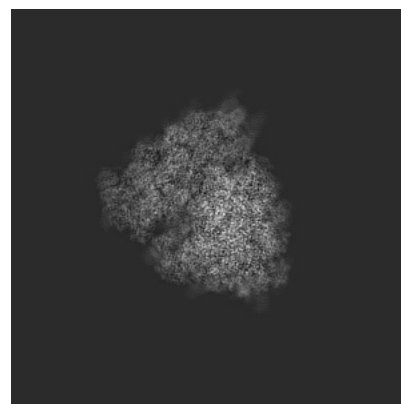
6.1.1 Primary map



X

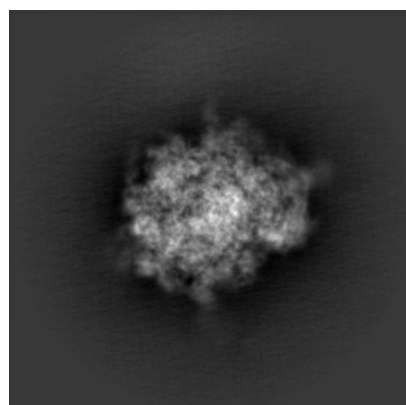


Y

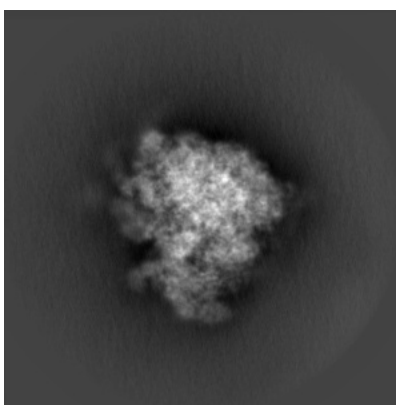


Z

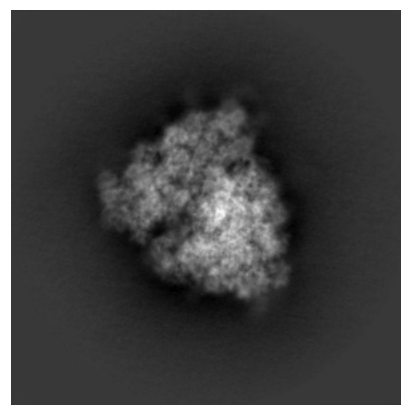
6.1.2 Raw map



X



Y

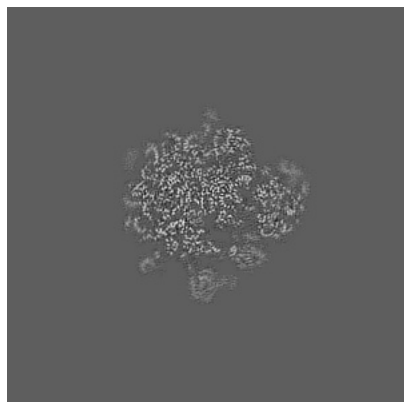


Z

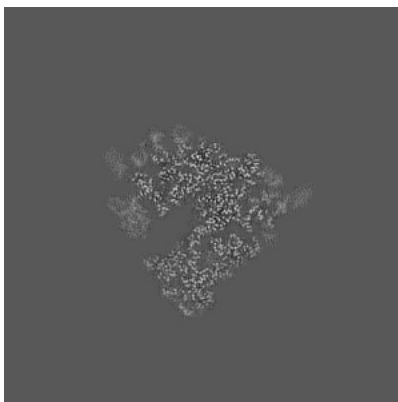
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

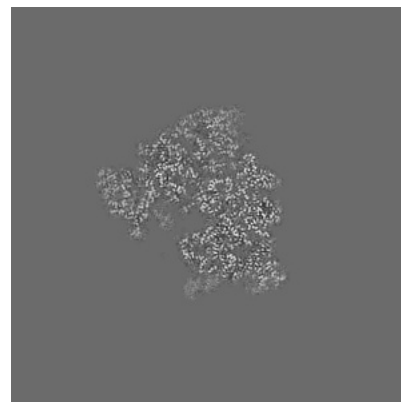
6.2.1 Primary map



X Index: 210

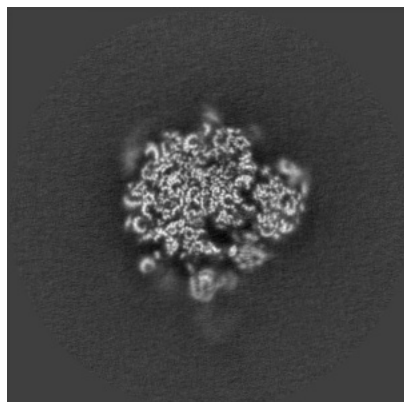


Y Index: 210

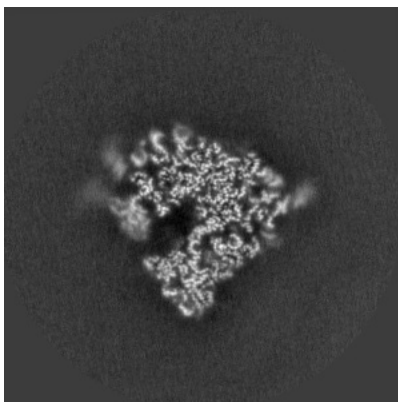


Z Index: 210

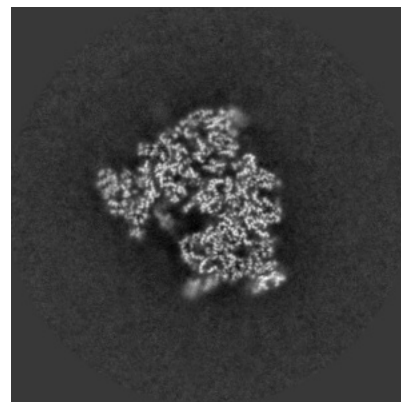
6.2.2 Raw map



X Index: 210



Y Index: 210

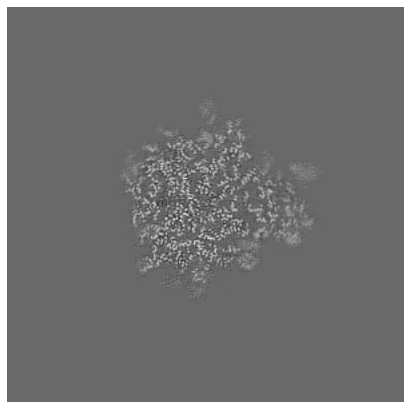


Z Index: 210

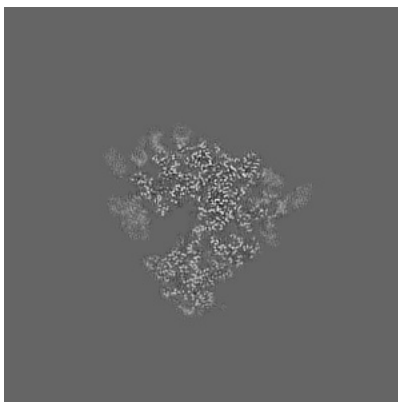
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

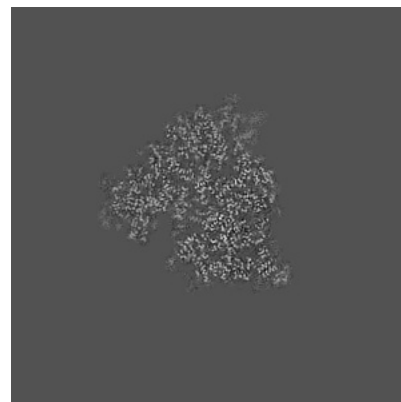
6.3.1 Primary map



X Index: 222

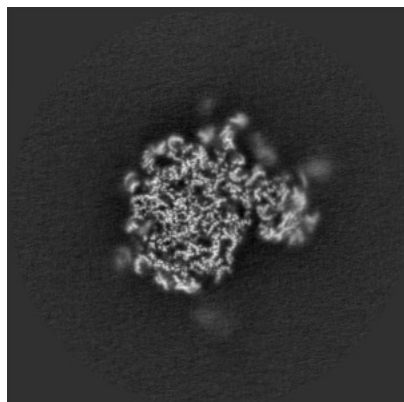


Y Index: 211

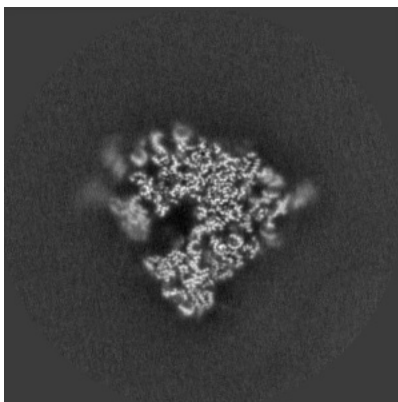


Z Index: 202

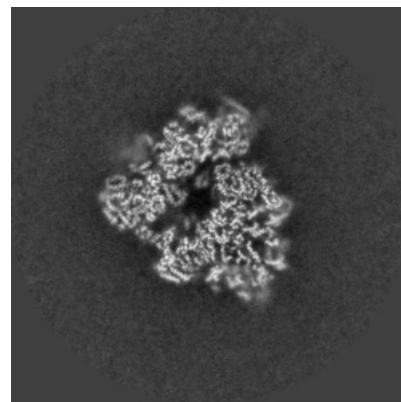
6.3.2 Raw map



X Index: 233



Y Index: 211

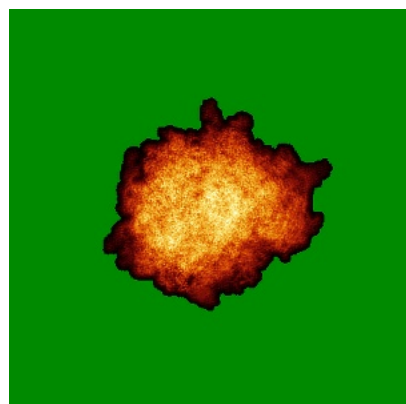


Z Index: 186

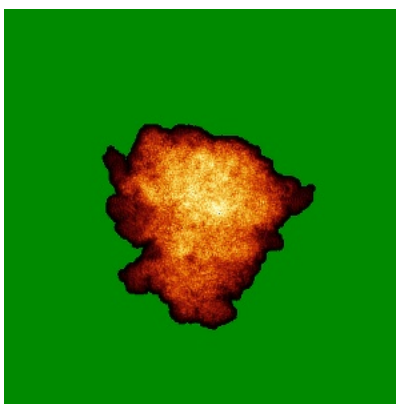
The images above show the largest variance slices of the map in three orthogonal directions.

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

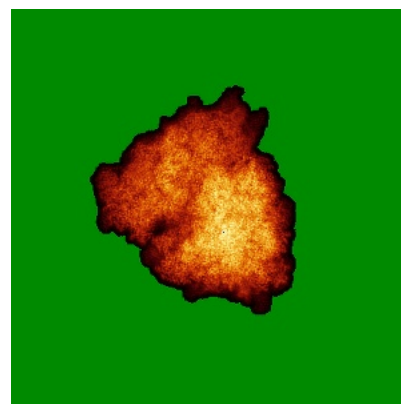
6.4.1 Primary map



X

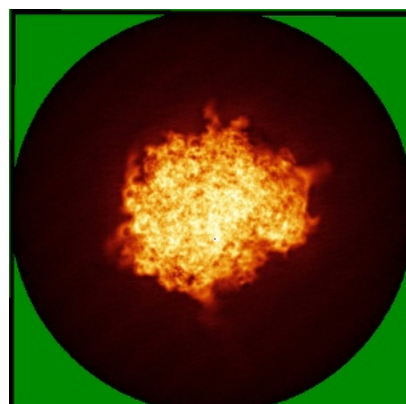


Y

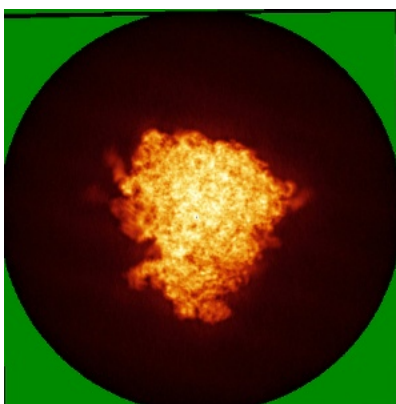


Z

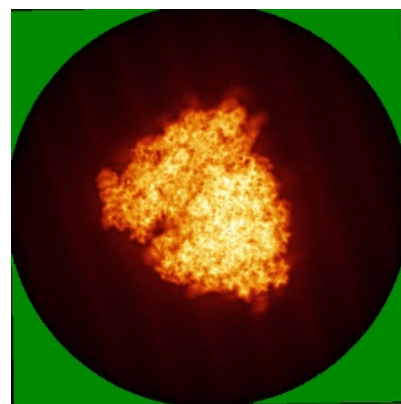
6.4.2 Raw map



X



Y

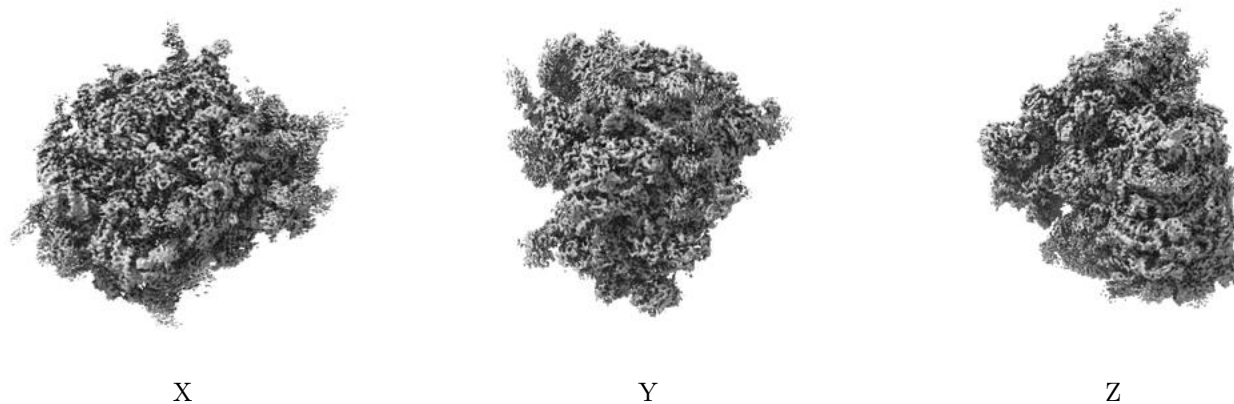


Z

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](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

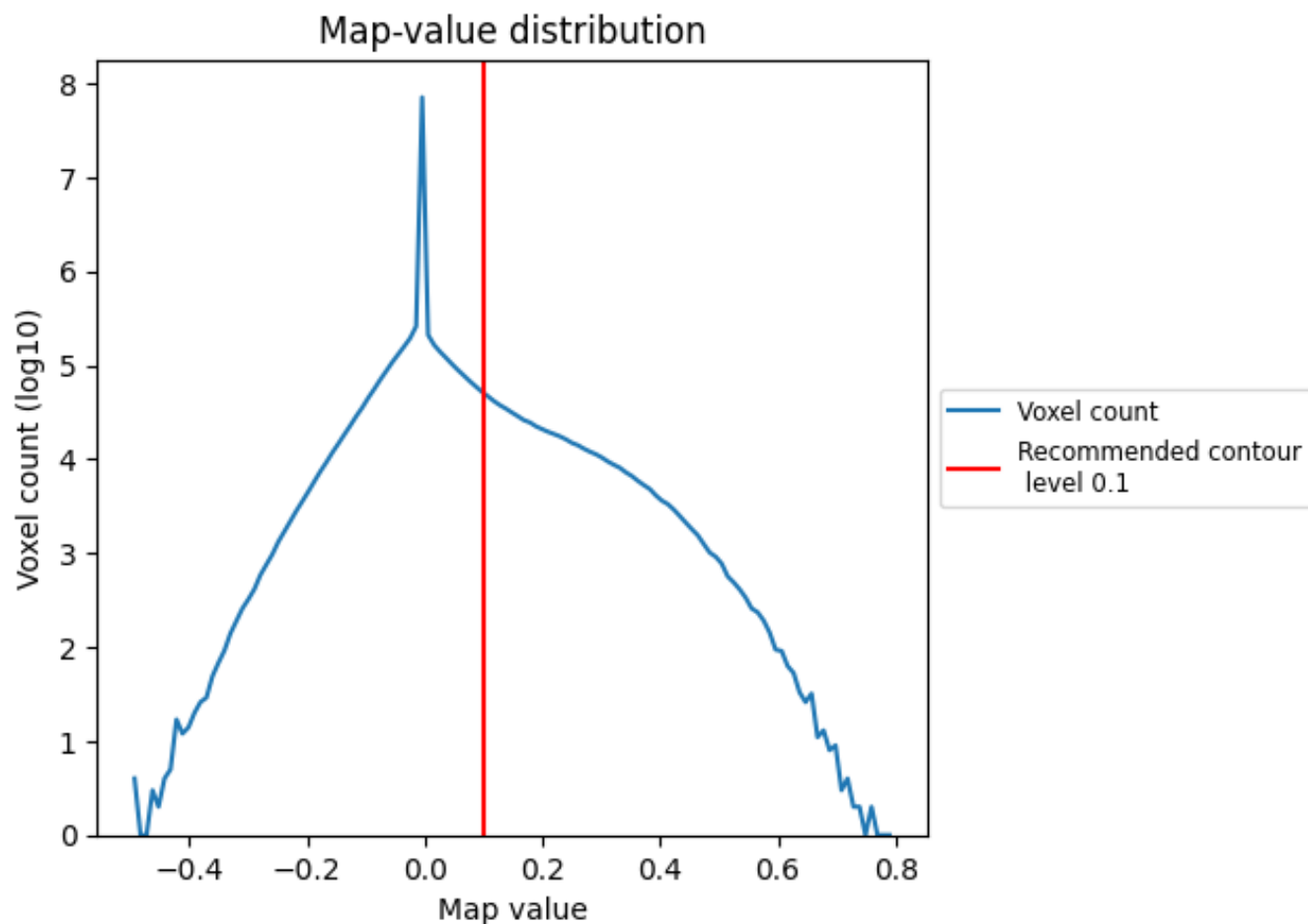
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

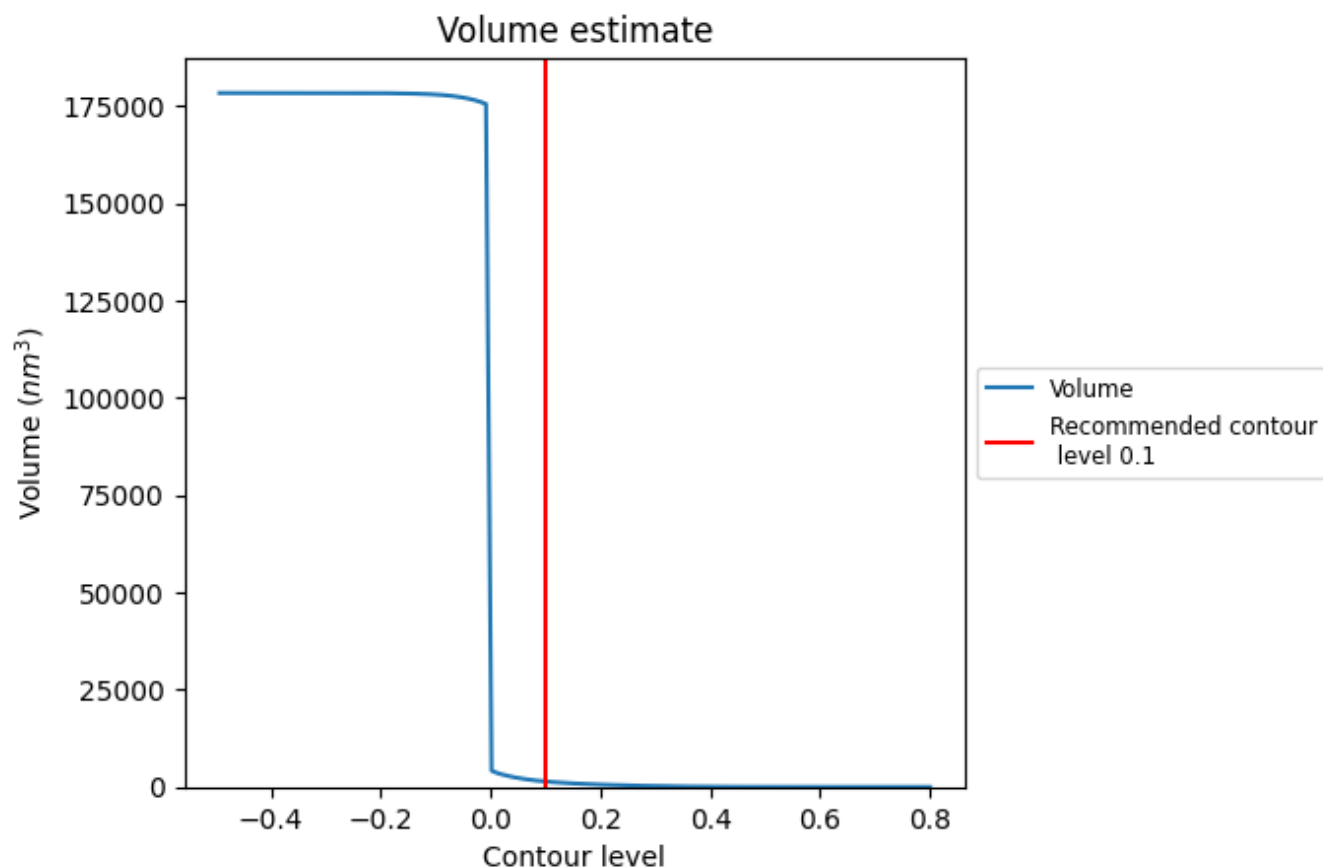
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

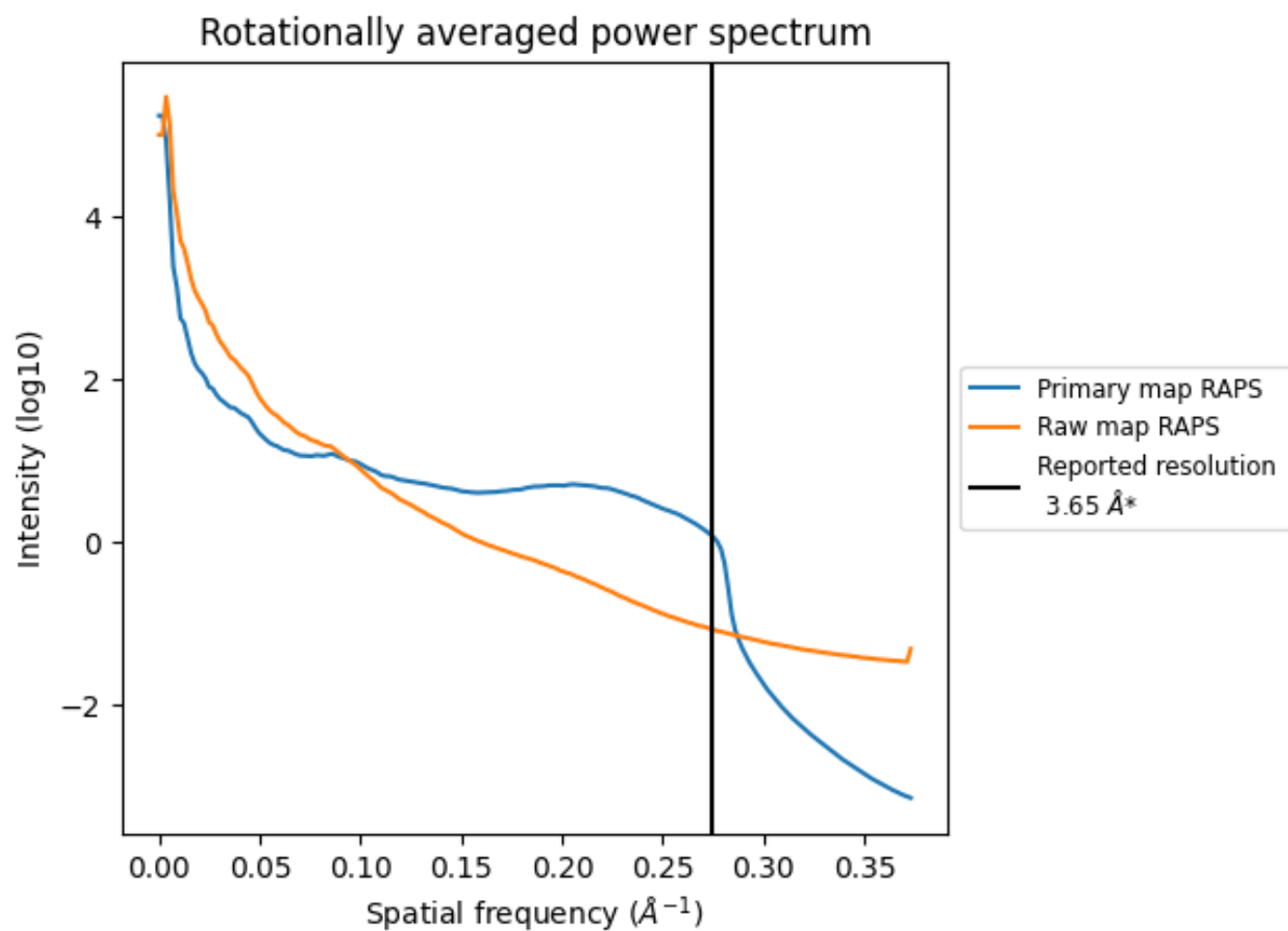
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1409 nm^3 ; this corresponds to an approximate mass of 1273 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

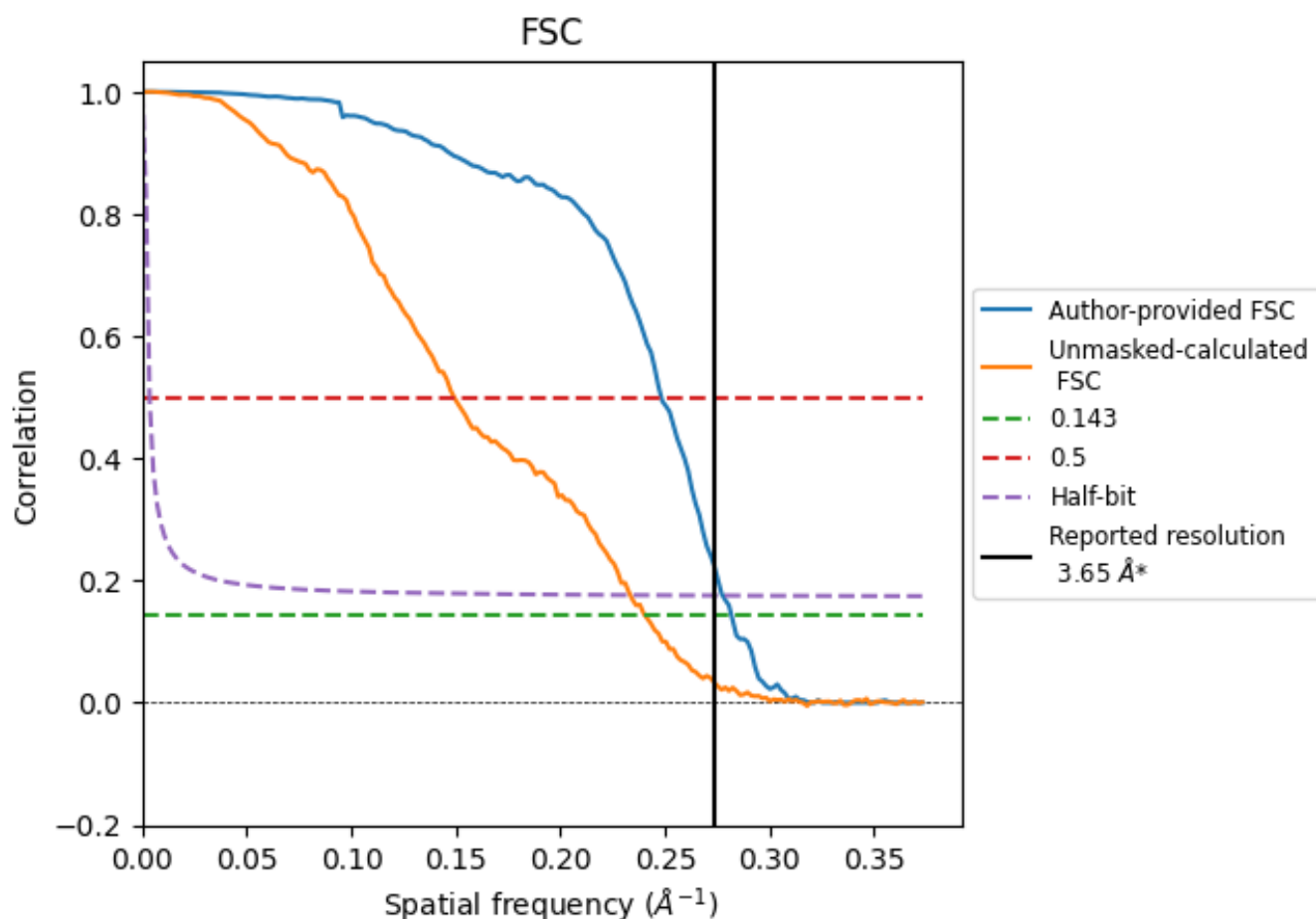


*Reported resolution corresponds to spatial frequency of $0.274 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.274 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

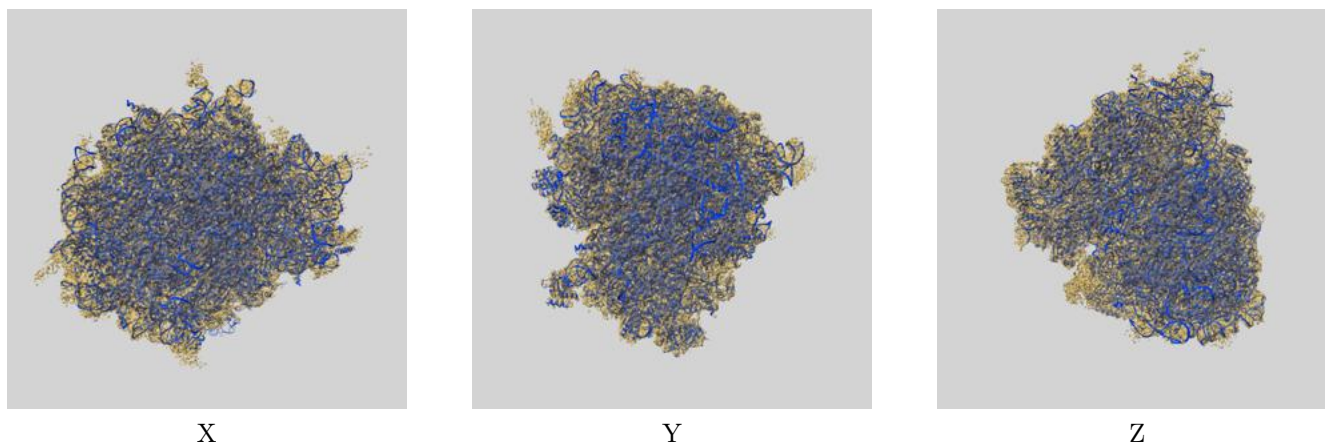
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.65	-	-
Author-provided FSC curve	3.55	4.03	3.60
Unmasked-calculated*	4.16	6.71	4.28

*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 4.16 differs from the reported value 3.65 by more than 10 %

9 Map-model fit [i](#)

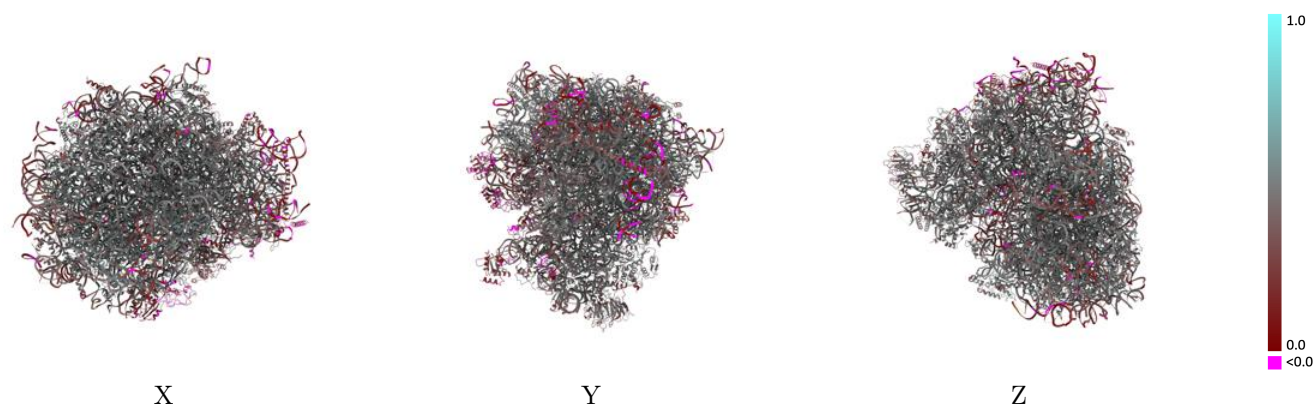
This section contains information regarding the fit between EMDB map EMD-4131 and PDB model 5LZT. Per-residue inclusion information can be found in [section 3](#) on [page 24](#).

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](#)

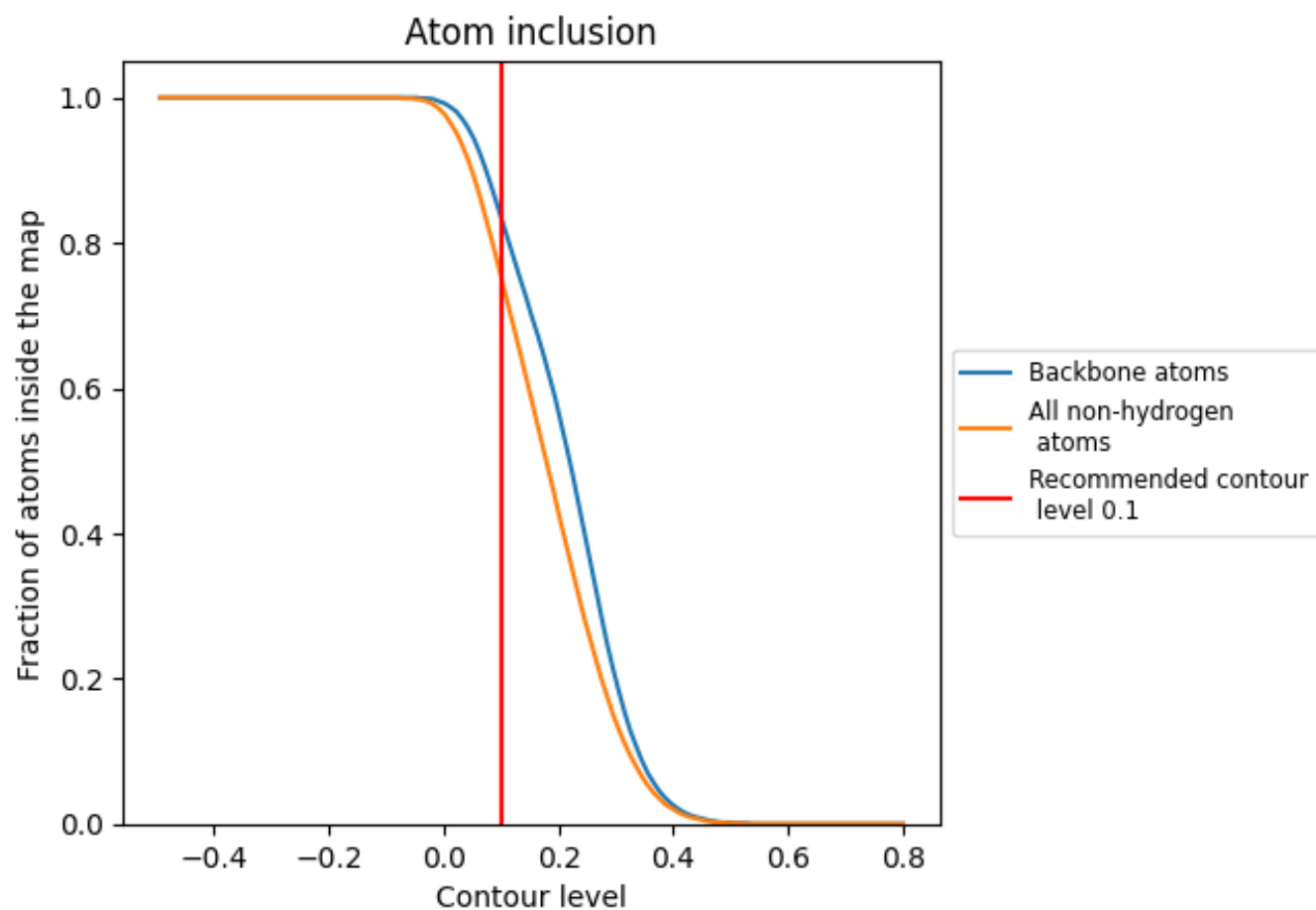


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 75% 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	 0.7540	 0.4340
1	 0.5870	 0.4450
2	 0.8010	 0.4240
3	 0.3870	 0.2490
5	 0.8250	 0.4360
7	 0.8970	 0.4710
8	 0.8440	 0.4440
9	 0.8020	 0.4180
A	 0.7740	 0.5010
AA	 0.6790	 0.4470
B	 0.7740	 0.4950
BB	 0.6940	 0.4600
C	 0.7680	 0.4960
CC	 0.7050	 0.4700
D	 0.7590	 0.4590
DD	 0.6270	 0.4280
E	 0.7780	 0.4740
EE	 0.7000	 0.4420
F	 0.7800	 0.4950
FF	 0.6900	 0.4530
G	 0.6600	 0.4150
GG	 0.5670	 0.3460
H	 0.7340	 0.4830
HH	 0.5440	 0.3770
I	 0.7350	 0.4830
II	 0.6720	 0.4350
J	 0.7210	 0.4550
JJ	 0.7220	 0.4450
KK	 0.6900	 0.4260
L	 0.7310	 0.4700
LL	 0.7130	 0.4710
M	 0.7750	 0.4910
MM	 0.2950	 0.1990
N	 0.7890	 0.5040
NN	 0.7080	 0.4680



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Chain	Atom inclusion	Q-score
O	 0.7680	 0.4900
OO	 0.7260	 0.4750
P	 0.7890	 0.5070
PP	 0.6530	 0.4130
Q	 0.7550	 0.4990
QQ	 0.7160	 0.4610
R	 0.7040	 0.4490
RR	 0.6170	 0.4240
S	 0.8000	 0.5060
SS	 0.7120	 0.4390
T	 0.7410	 0.4810
TT	 0.7170	 0.4410
U	 0.6710	 0.4040
UU	 0.6270	 0.4200
V	 0.7260	 0.4940
VV	 0.7110	 0.4640
W	 0.4900	 0.3390
WW	 0.7280	 0.4950
X	 0.7180	 0.4680
XX	 0.7110	 0.4900
Y	 0.7430	 0.4720
YY	 0.6440	 0.4110
Z	 0.7610	 0.4560
ZZ	 0.6550	 0.4160
a	 0.7870	 0.4970
aa	 0.7240	 0.4650
b	 0.6470	 0.4110
bb	 0.6590	 0.4280
c	 0.7140	 0.4630
cc	 0.6320	 0.4530
d	 0.7360	 0.4790
dd	 0.7380	 0.4740
e	 0.7640	 0.4960
ee	 0.6380	 0.4120
f	 0.8040	 0.5170
ff	 0.3600	 0.2610
g	 0.7060	 0.4670
gg	 0.6080	 0.3930
h	 0.7170	 0.4600
hh	 0.7140	 0.3910
i	 0.7120	 0.4560
ii	 0.4620	 0.3240

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Chain	Atom inclusion	Q-score
j	 0.7880	 0.4990
jj	 0.5020	 0.3280
k	 0.6660	 0.4320
l	 0.7260	 0.4840
m	 0.7620	 0.4750
n	 0.6650	 0.4660
o	 0.7410	 0.4870
p	 0.7500	 0.4860
r	 0.8120	 0.5060
s	 0.2030	 0.1760
t	 0.1480	 0.1400