wwPDB EM Validation Summary Report (i)

Nov 3, 2024 – 06:31 am GMT

PDB ID	:	5LZT
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 (i) 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 (1)) were used in the production of this report:

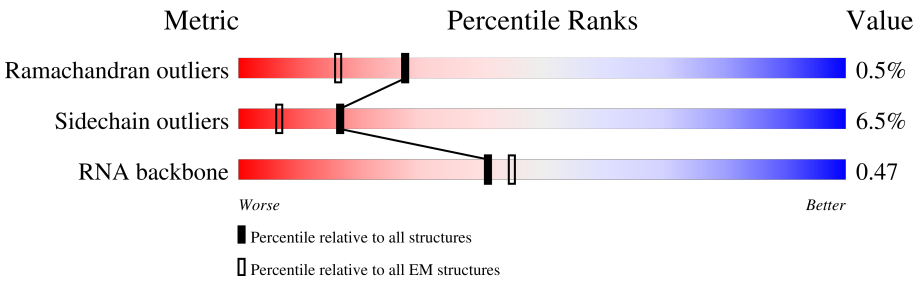
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (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)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	91% 5% •
2	B	403	• 93% 5% •
3	C	425	• 81% • 15%
4	D	297	• 94% • •
5	E	291	• 70% • 26%
6	F	247	• 86% 5% 9%
7	G	319	10% 69% • 27%
8	H	192	• 93% 6% •

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Mol	Chain	Length	Quality of chain
9	I	214	92%
10	J	178	92%
11	L	211	5% 96%
12	M	218	59% 5% 37%
13	N	204	95%
14	O	203	92% 6%
15	P	184	79% 17%
16	Q	188	95%
17	R	196	7% 86% 6% 8%
18	S	176	93% 7%
19	T	160	93% 6%
20	U	128	8% 75% 23%
21	V	140	5% 88% 6% 6%
22	W	157	29% 66% 32%
23	X	156	72% 24%
24	Y	145	6% 88% 5% 8%
25	Z	136	96%
26	a	148	97%
27	b	245	7% 41% 58%
28	c	115	7% 83% 15%
29	d	125	5% 79% 6% 14%
30	e	135	88% 7% 5%
31	f	110	92% 7%
32	g	117	6% 93%
33	h	123	94% 5%

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Mol	Chain	Length	Quality of chain
34	i	105	95%
35	j	97	84% 5% 11%
36	k	70	6% 96%
37	l	51	6% 96%
38	m	102	48% 49%
39	n	25	8% 92% 8%
40	o	106	92% 6%
41	p	92	97%
42	r	137	85% 5% 9%
43	s	318	49% 59% 38%
44	t	165	82% 88% 7%
45	1	15	13% 93% 7%
46	2	76	83% 17%
47	3	75	51% 69% 31%
48	5	3543	5% 74% 26%
49	7	120	87% 13%
50	8	156	5% 76% 21%
51	9	1869	6% 67% 23% 9%
52	AA	295	6% 69% 26%
53	BB	264	73% 7% 19%
54	CC	293	71% 25%
55	DD	243	9% 87% 7% 6%
56	EE	263	5% 91% 8%
57	FF	204	83% 8% 9%
58	GG	249	21% 89% 6% 5%

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Mol	Chain	Length	Quality of chain
59	HH	194	21% 89% 7% 5%
60	II	208	11% 91% 8%
61	JJ	194	6% 88% 8% 5%
62	KK	165	50% 8% 42%
63	LL	158	6% 84% 6% 9%
64	MM	132	61% 78% 11% 11%
65	NN	151	90% 9%
66	OO	168	71% 10% 19%
67	PP	145	8% 74% 8% 17%
68	QQ	146	92% 5%
69	RR	135	13% 91% 7%
70	SS	152	5% 86% 9% 5%
71	TT	145	91% 6%
72	UU	119	9% 79% 5% 16%
73	VV	83	95% 5%
74	WW	130	90% 9%
75	XX	143	92% 6%
76	YY	130	11% 83% 12% 5%
77	ZZ	125	6% 57% 40%
78	aa	115	5% 81% 6% 12%
79	bb	84	11% 90% 8%
80	cc	69	9% 83% 7% 10%
81	dd	56	5% 96%
82	ee	133	7% 38% 59%
83	ff	156	26% 40% 56%

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Mol	Chain	Length	Quality of chain
84	gg	317	15% 95%
85	hh	15	13% 47% 53%
86	ii	459	34% 85% 6% 9%
87	jj	637	21% 64% 33%

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
			Total	C	N	O	S		
1	A	248	1898	1189	389	314	6	0	0

- Molecule 2 is a protein called uL3.

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

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
			Total	C	N	O	S		
3	C	362	2883	1812	577	480	14	0	0

- Molecule 4 is a protein called uL18.

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

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
			Total	C	N	O	S		
5	E	216	1729	1115	329	282	3	0	0

- Molecule 6 is a protein called uL30.

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

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
			Total	C	N	O	S		
7	G	233	1879	1199	361	315	4	0	0

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
			Total	C	N	O	S		
8	H	190	1516	954	284	272	6	0	0

- Molecule 9 is a protein called uL16.

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

- Molecule 10 is a protein called uL5.

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

- Molecule 11 is a protein called eL13.

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

- Molecule 12 is a protein called eL14.

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

- Molecule 13 is a protein called eL15.

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

- Molecule 14 is a protein called uL13.

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

- Molecule 15 is a protein called uL22.

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

- Molecule 16 is a protein called eL18.

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

- Molecule 17 is a protein called eL19.

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

- Molecule 18 is a protein called eL20.

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

- Molecule 19 is a protein called eL21.

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

- Molecule 20 is a protein called eL22.

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

- Molecule 21 is a protein called uL14.

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

- Molecule 22 is a protein called eL24.

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

- Molecule 23 is a protein called uL23.

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

- Molecule 24 is a protein called uL24.

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

- Molecule 25 is a protein called eL27.

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

- Molecule 26 is a protein called uL15.

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

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
			Total	C	N	O	S		
27	b	104	848	527	189	129	3	0	0

- Molecule 28 is a protein called eL30.

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

- Molecule 29 is a protein called eL31.

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

- Molecule 30 is a protein called eL32.

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

- Molecule 31 is a protein called eL33.

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

- Molecule 32 is a protein called eL34.

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

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
			Total	C	N	O	S		
33	h	122	1013	640	204	168	1	0	0

- Molecule 34 is a protein called eL36.

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

- Molecule 35 is a protein called eL37.

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

- Molecule 36 is a protein called eL38.

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

- Molecule 37 is a protein called eL39.

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

- Molecule 38 is a protein called eL40.

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

- Molecule 39 is a protein called eL41.

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

- Molecule 40 is a protein called eL42.

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

- Molecule 41 is a protein called eL43.

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

- Molecule 42 is a protein called eL28.

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

- Molecule 43 is a protein called uL10.

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

- Molecule 44 is a protein called uL11.

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

- Molecule 45 is a protein called Nascent chain.

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 52 is a protein called uS2.

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

- Molecule 53 is a protein called eS1.

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

- Molecule 54 is a protein called uS5.

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

- Molecule 55 is a protein called uS3.

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

- Molecule 56 is a protein called eS4.

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

- Molecule 57 is a protein called uS7.

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

- Molecule 58 is a protein called eS6.

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

- Molecule 59 is a protein called eS7.

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

- Molecule 60 is a protein called eS8.

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

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
			Total	C	N	O	S		
61	JJ	185	1525	969	306	248	2	0	0

- Molecule 62 is a protein called eS10.

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

- Molecule 63 is a protein called uS17.

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

- Molecule 64 is a protein called eS12.

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

- Molecule 65 is a protein called uS15.

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

- Molecule 66 is a protein called uS11.

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

- Molecule 67 is a protein called uS19.

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

- Molecule 68 is a protein called uS9.

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

- Molecule 69 is a protein called eS17.

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

- Molecule 70 is a protein called uS13.

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

- Molecule 71 is a protein called eS19.

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

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
			Total	C	N	O	S		
72	UU	100	795	498	152	141	4	0	0

- Molecule 73 is a protein called eS21.

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

- Molecule 74 is a protein called uS8.

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

- Molecule 75 is a protein called uS12.

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

- Molecule 76 is a protein called eS24.

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

- Molecule 77 is a protein called eS25.

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

- Molecule 78 is a protein called eS26.

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

- Molecule 79 is a protein called eS27.

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

- Molecule 80 is a protein called eS28.

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

- Molecule 81 is a protein called uS14.

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

- Molecule 82 is a protein called eS30.

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

- Molecule 83 is a protein called eS31.

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

- Molecule 84 is a protein called RACK1.

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

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

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

- Molecule 86 is a protein called eRF1.

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

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
			Total	C	N	O	S		
87	jj	428	3368	2144	580	623	21	0	0

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 (three-letter code: MG) (formula: Mg).

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

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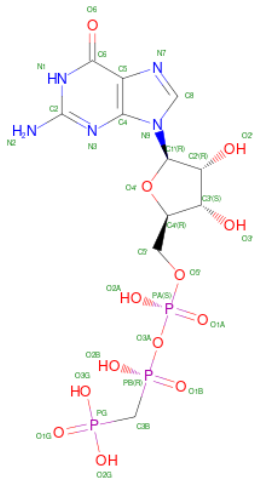
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
88	9	71	71	71	0
			Total	Mg	
88	hh	1	1	1	0
			Total	Mg	
88	jj	1	1	1	0

- Molecule 89 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 90 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).

GCP



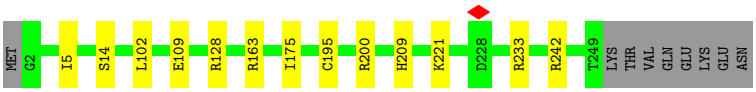
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
90	jj	1	32	11	5	13	3	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

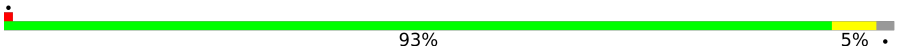
- Molecule 1: uL2

Chain A:



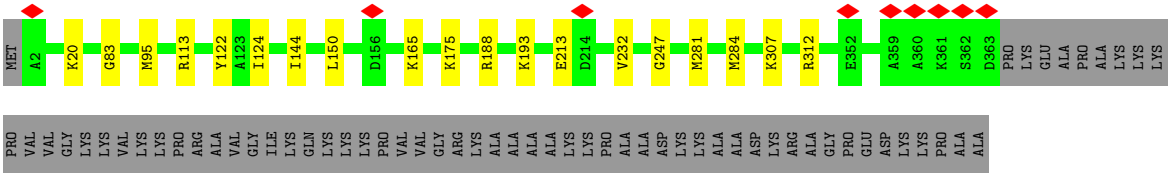
- Molecule 2: uL3

Chain B:



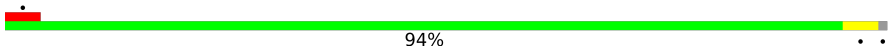
- Molecule 3: uL4

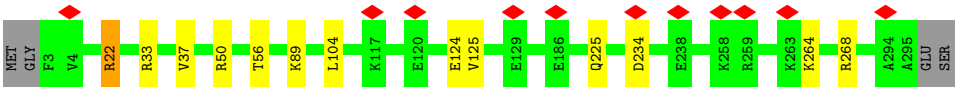
Chain C:



- Molecule 4: uL18

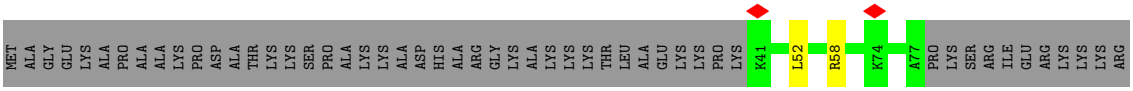
Chain D:





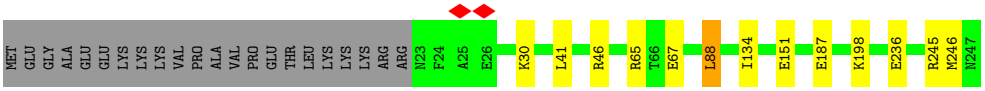
- Molecule 5: eL6

Chain E:



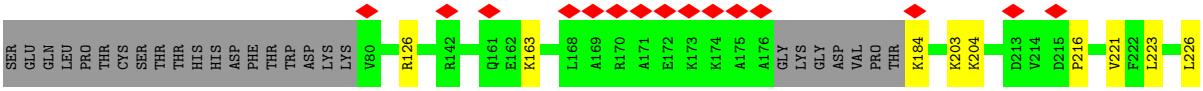
- Molecule 6: uL30

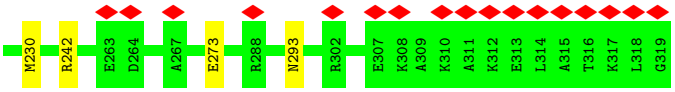
Chain F:



- Molecule 7: eL8

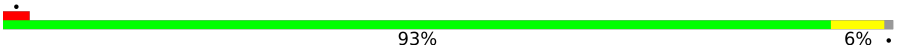
Chain G:

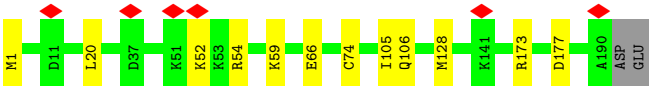




- Molecule 8: uL6

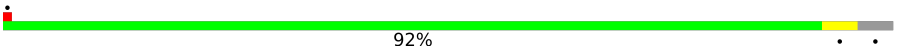
Chain H:

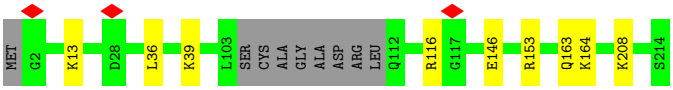




- Molecule 9: uL16

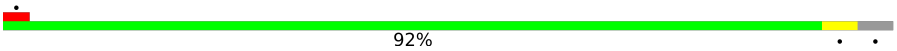
Chain I:

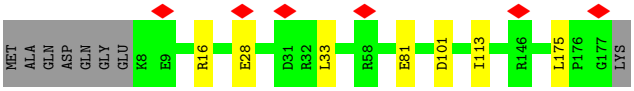




- Molecule 10: uL5

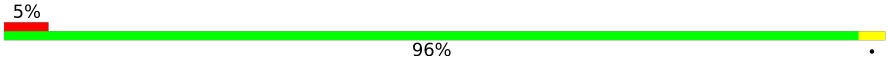
Chain J:

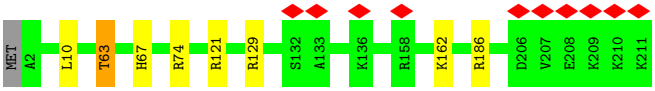




- Molecule 11: eL13

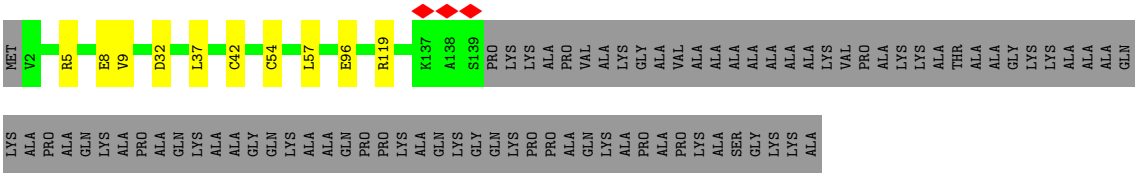
Chain L:





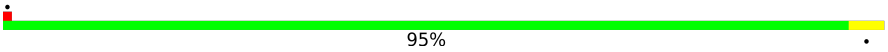
- Molecule 12: eL14

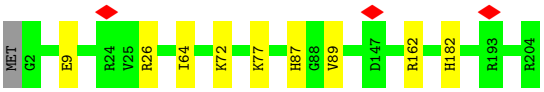
Chain M:



- Molecule 13: eL15

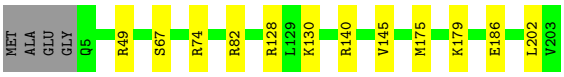
Chain N:





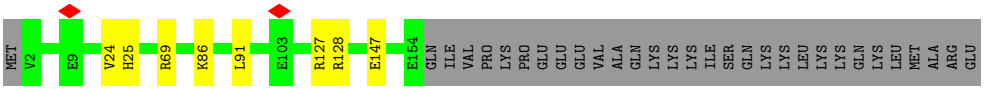
- Molecule 14: uL13

Chain O:



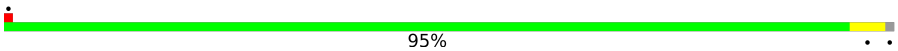
- Molecule 15: uL22

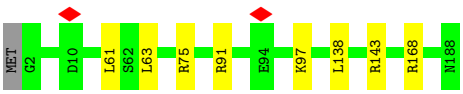
Chain P:



- Molecule 16: eL18

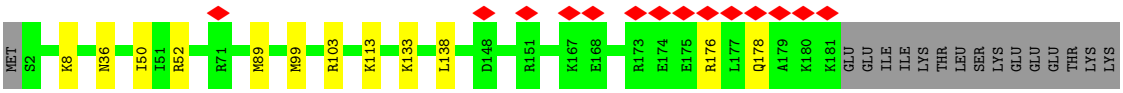
Chain Q:





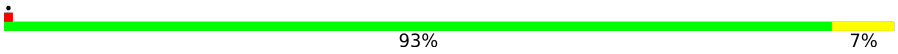
- Molecule 17: eL19

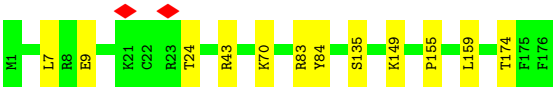
Chain R:



- Molecule 18: eL20

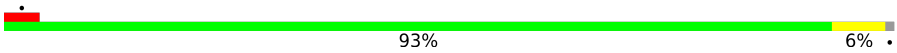
Chain S:

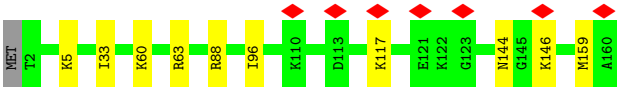




- Molecule 19: eL21

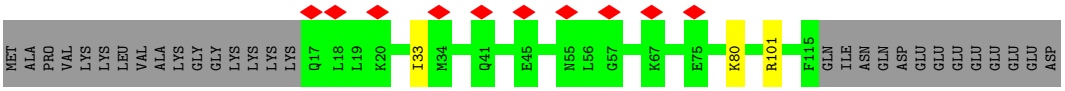
Chain T:





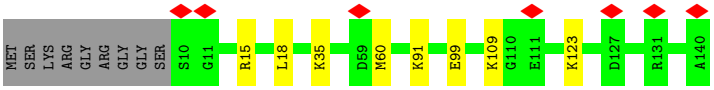
- Molecule 20: eL22

Chain U:



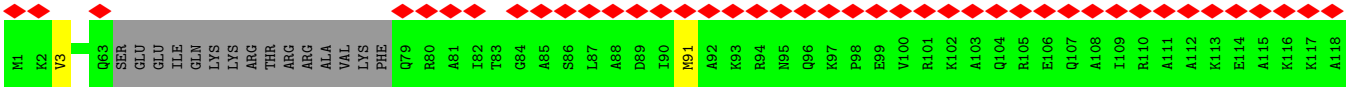
- Molecule 21: uL14

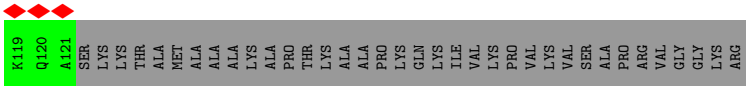
Chain V:



- Molecule 22: eL24

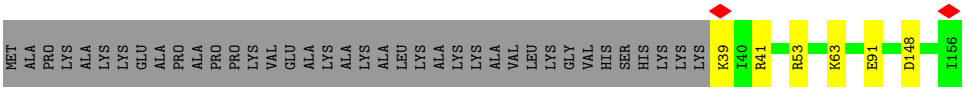
Chain W:





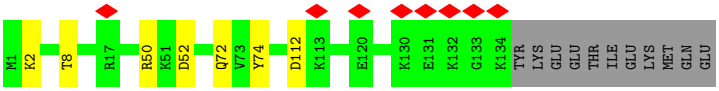
- Molecule 23: uL23

Chain X:



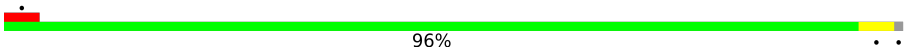
• Molecule 24: uL24

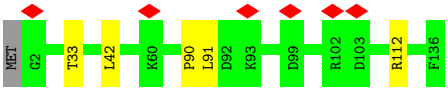
Chain Y:



• Molecule 25: eL27

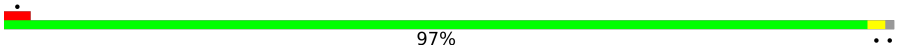
Chain Z:

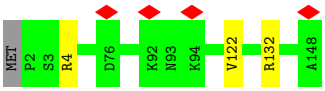




• Molecule 26: uL15

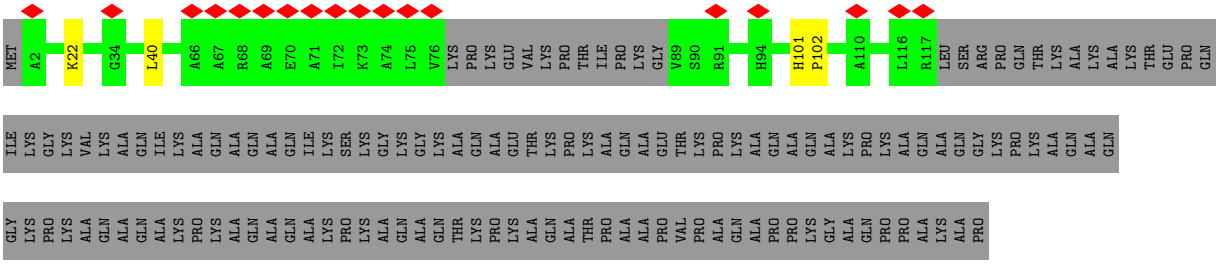
Chain a:





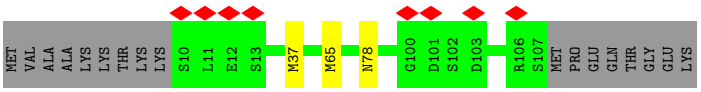
• Molecule 27: eL29

Chain b:



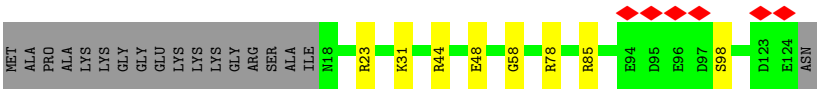
• Molecule 28: eL30

Chain c:



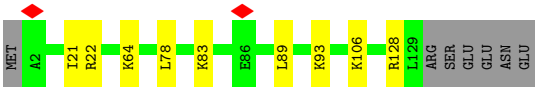
• Molecule 29: eL31

Chain d:



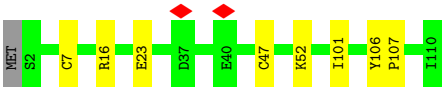
- Molecule 30: eL32

Chain e:



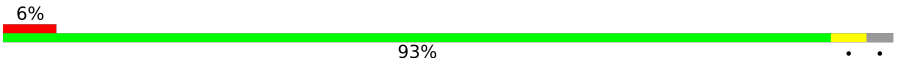
- Molecule 31: eL33

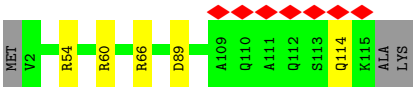
Chain f:



- Molecule 32: eL34

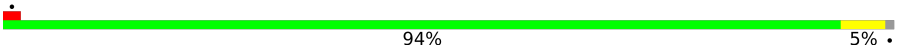
Chain g:





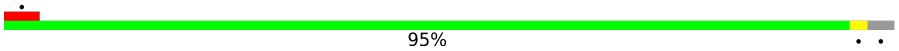
- Molecule 33: uL29

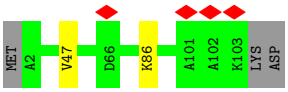
Chain h:



- Molecule 34: eL36

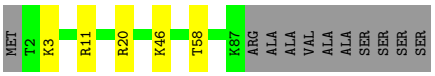
Chain i:





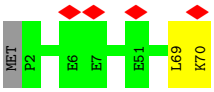
- Molecule 35: eL37

Chain j:



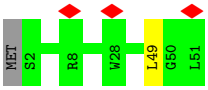
- Molecule 36: eL38

Chain k: 6% 96%



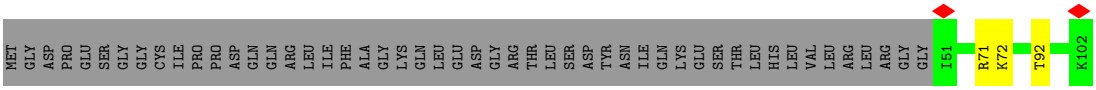
• Molecule 37: eL39

Chain l: 6% 96%



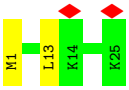
• Molecule 38: eL40

Chain m: 48% 49%



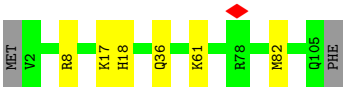
• Molecule 39: eL41

Chain n: 8% 92% 8%



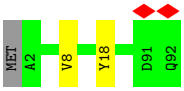
• Molecule 40: eL42

Chain o: 92% 6%



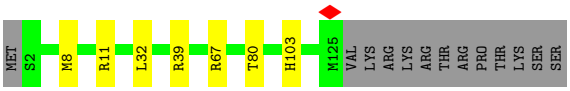
• Molecule 41: eL43

Chain p: 97%



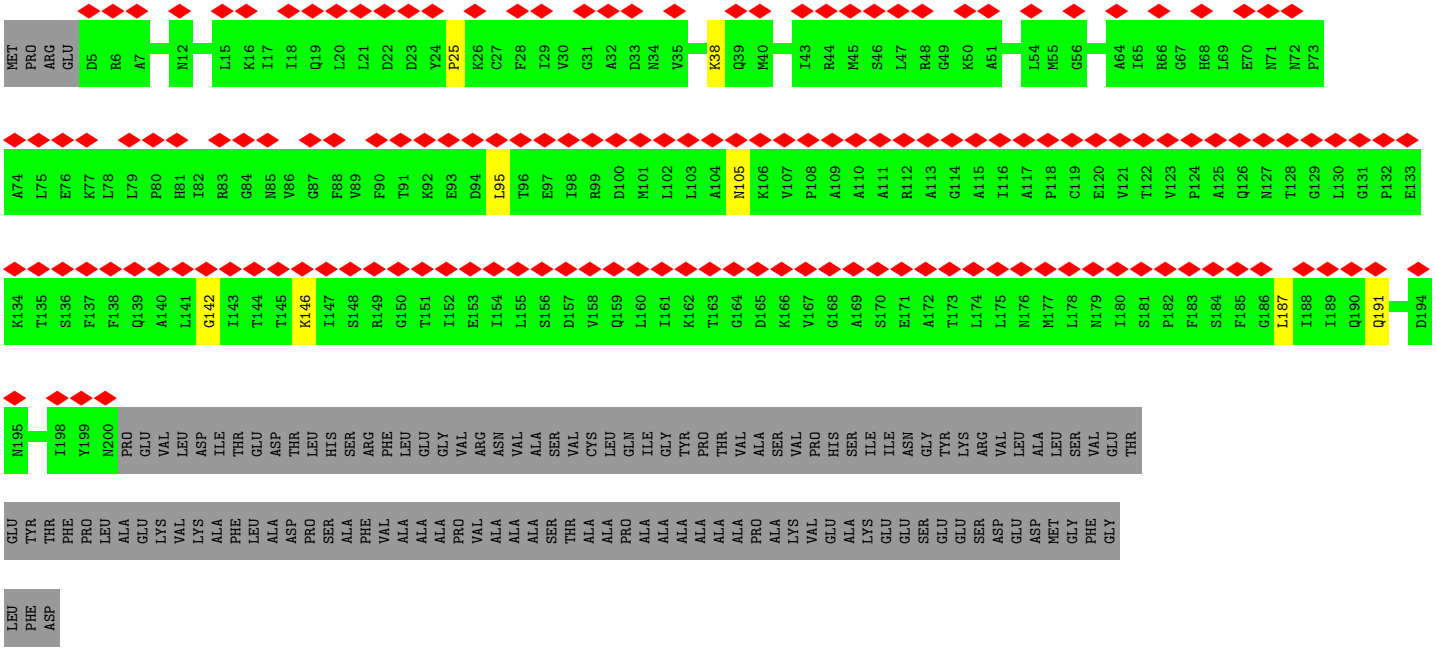
• Molecule 42: eL28

Chain r: 85% 5% 9%



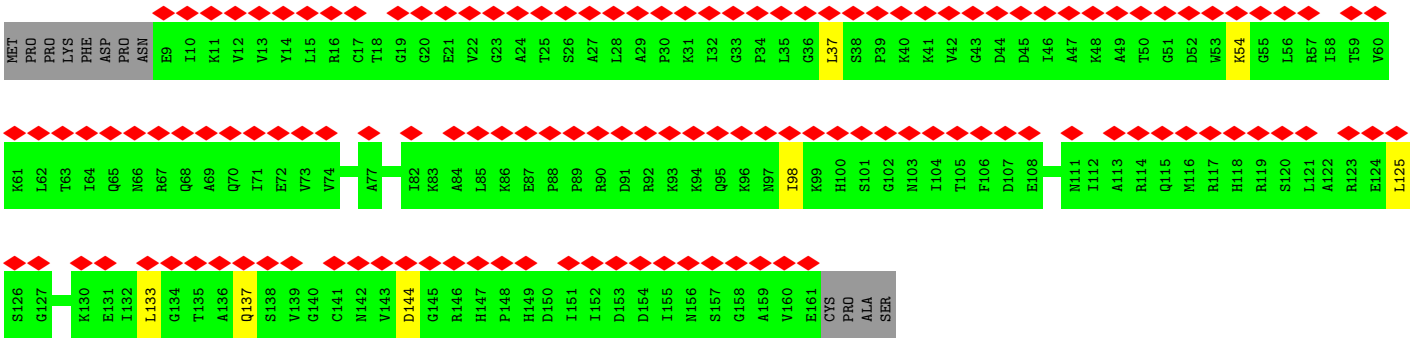
- Molecule 43: uL10

Chain s:



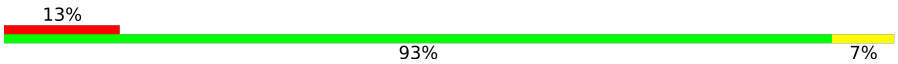
- Molecule 44: uL11

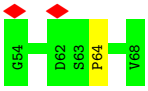
Chain t:



- Molecule 45: Nascent chain

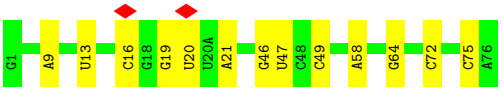
Chain 1:





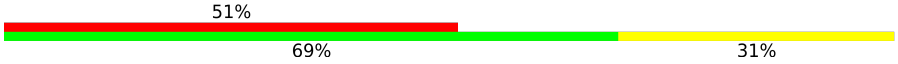
- Molecule 46: P-site tRNA

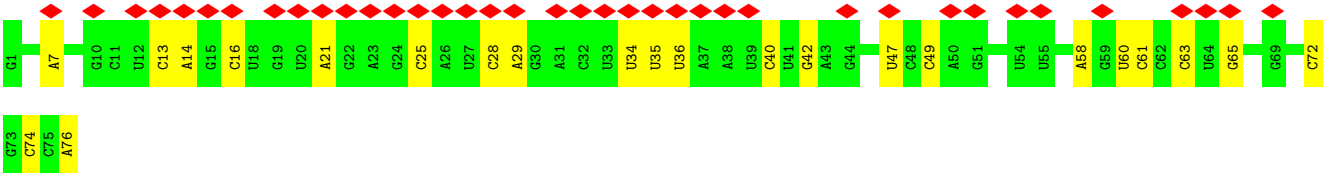
Chain 2:



- Molecule 47: E-site tRNA

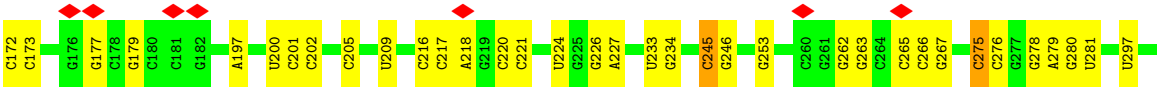
Chain 3:

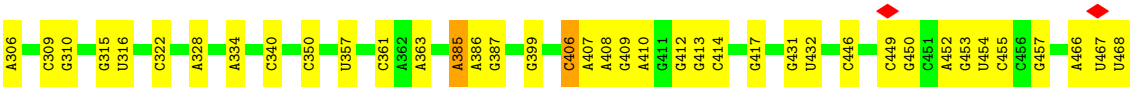


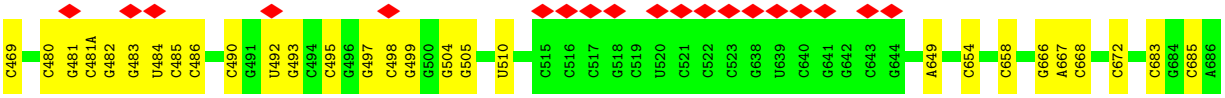


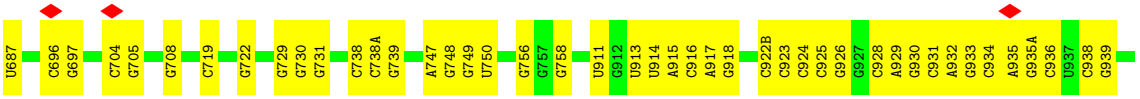
- Molecule 48: 28S ribosomal RNA

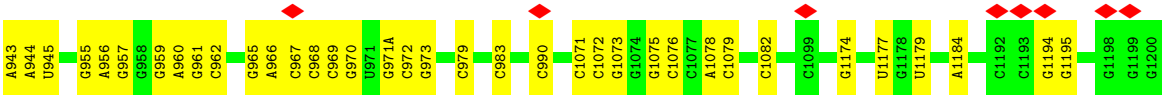
Chain 5:

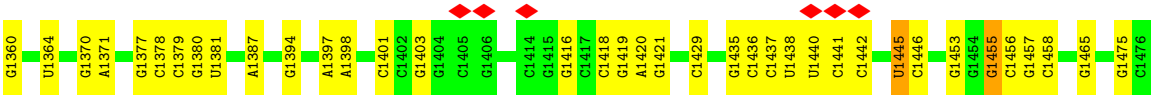


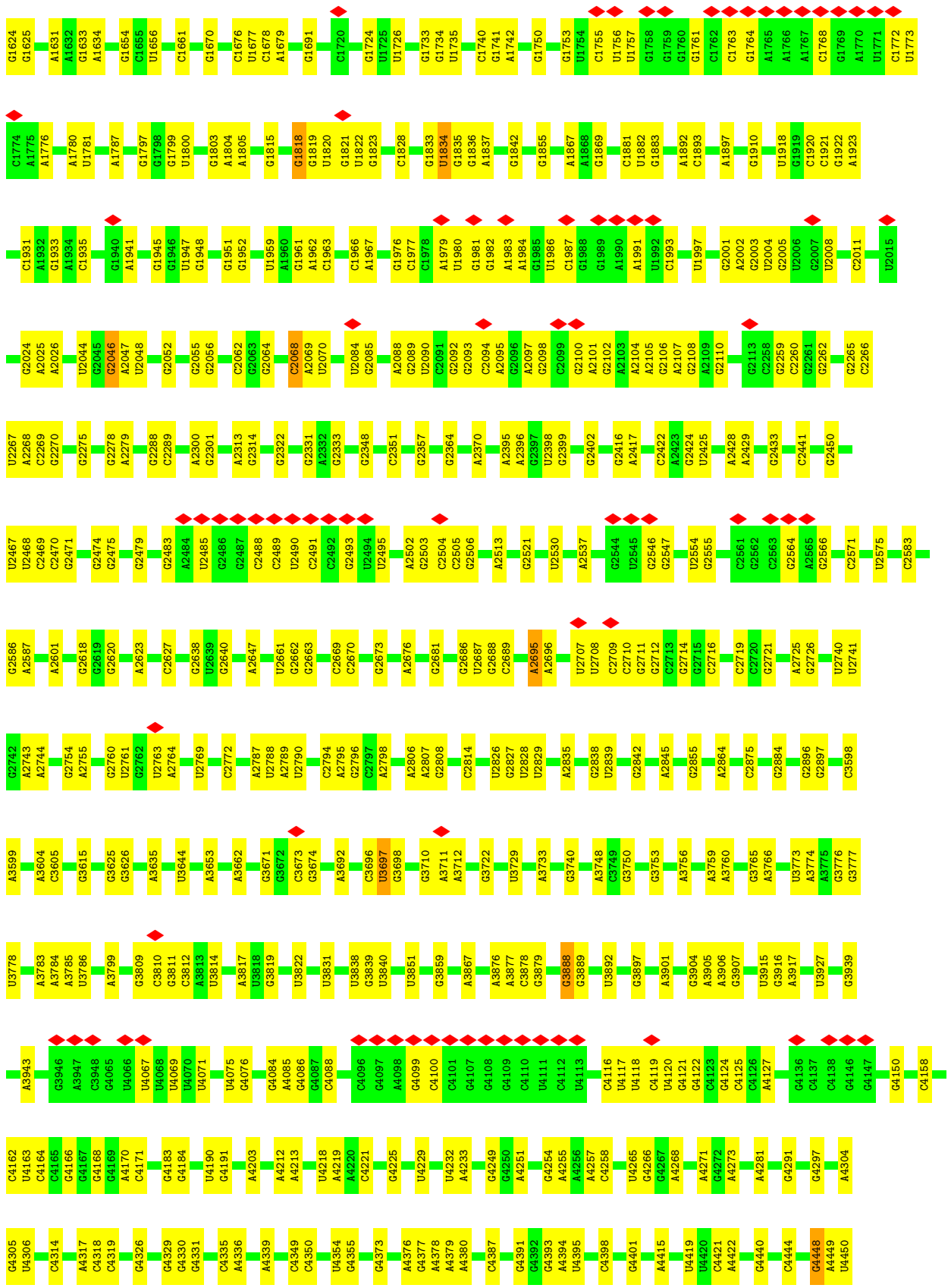


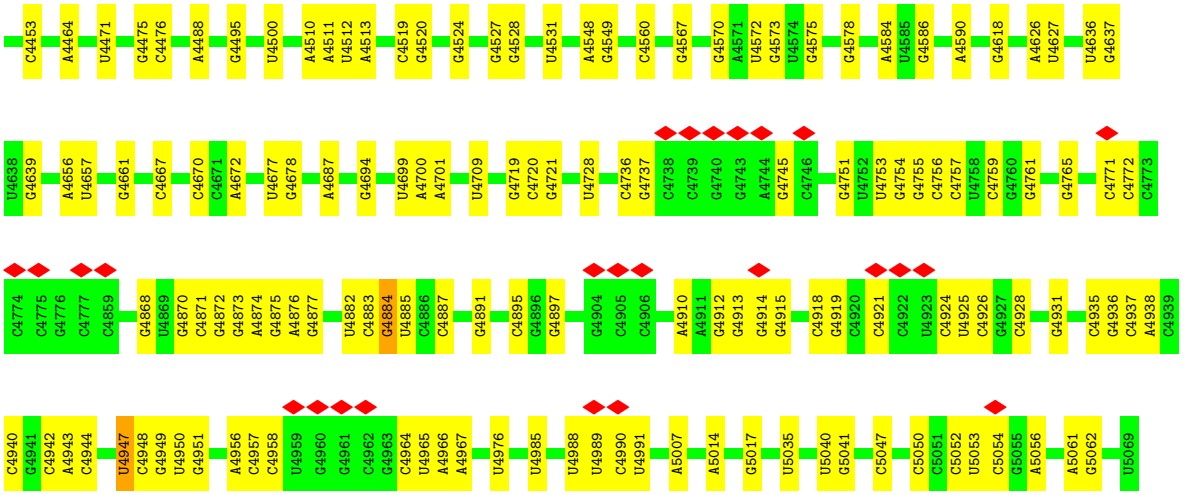









G1624 G1625 A1631 A1632 G1633 A1634 G1654 C1655 U1656 C1661 G1670 C1676 U1677 C1678 A1679 G1691 C1720 G1724 U1725 U1726 G1733 G1734 U1735 C1740 G1741 A1742 G1750 G1753 U1754 C1755 U1756 U1757 G1758 G1759 G1760 G1761 C1762 C1763 G1764 A1765 A1766 A1767 C1768 G1769 A1770 U1771 C1772 U1773
C1774 A1775 A1776 A1780 U1781 A1787 G1797 G1798 G1799 U1800 G1803 A1804 A1805 G1815 G1818 G1819 U1820 G1821 U1822 G1823 C1828 G1833 U1834 G1835 G1836 A1837 G1842 G1855 A1867 A1868 G1869 C1881 U1882 G1883 A1892 C1893 A1897 G1910 U1918 G1919 C1920 C1921 G1922 A1923
C1931 A1932 G1933 A1934 C1935 G1940 A1941 G1945 G1946 U1947 G1948 G1951 G1952 U1959 A1960 G1961 A1962 C1963 C1966 A1967 G1976 C1977 C1978 A1979 U1980 G1981 G1982 A1983 A1984 G1985 U1986 C1987 G1988 G1989 A1990 A1991 U1992 C1993 U1997 G2001 A2002 G2003 U2004 G2005 U2006 G2007 U2008 C2011 U2015
G2024 A2025 A2026 U2044 G2045 G2046 A2047 U2048 G2052 G2055 G2056 C2062 G2063 G2064 C2068 A2069 U2070 U2084 G2085 A2088 G2089 U2090 C2091 G2092 G2093 C2094 A2095 G2096 A2097 G2098 C2099 G2100 A2101 G2102 A2103 A2104 A2105 G2106 A2107 G2108 A2109 G2110 G2113 C2258 G2259 C2260 G2261 G2262 G2265 C2266
U2267 A2268 C2269 G2270 G2275 G2278 A2279 G2288 C2289 A2300 G2301 A2313 G2314 G2322 G2331 A2332 G2333 G2348 C2351 G2357 G2364 A2370 A2395 A2396 G2397 U2398 G2399 G2402 G2416 A2417 C2422 A2423 G2424 U2425 A2428 A2429 G2433 C2441 G2450
U2467 U2468 C2469 C2470 G2471 G2474 G2475 G2479 G2483 A2484 U2485 G2486 G2487 C2488 C2489 U2490 C2491 C2492 G2493 U2494 U2495 A2502 G2503 C2504 C2505 G2506 A2513 G2521 U2530 A2537 G2544 U2545 G2546 G2547 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 G2663 C2669 C2670 G2673 A2676 G2681 C2686 U2687 G2688 C2689 A2695 A2696 U2707 U2708 C2709 C2710 G2711 G2712 C2713 G2714 G2715 C2716 C2719 C2720 G2721 A2725 G2726 U2740 U2741
G2742 A2743 A2744 G2754 A2755 G2760 U2761 G2762 U2763 A2764 U2769 C2772 A2787 U2788 A2789 U2790 C2794 A2795 G2796 C2797 A2798 A2806 A2807 G2808 C2814 U2826 G2827 U2828 U2829 A2835 G2838 U2839 G2842 A2845 G2855 A2864 C2875 G2884 G2896 G2897 C3598
A3599 A3604 C3605 G3615 G3625 G3626 A3635 U3644 A3653 A3662 G3671 G3672 C3673 G3674 A3692 C3696 U3697 G3698 G3710 A3711 A3712 G3722 U3729 A3733 G3740 A3748 C3749 G3750 G3753 A3756 A3759 A3760 G3765 A3766 U3773 A3774 A3775 G3776 G3777
U3778 A3783 A3784 A3785 U3786 A3799 G3809 C3810 G3811 C3812 A3813 U3814 A3817 U3818 G3819 U3822 U3831 U3838 G3839 U3840 U3851 G3859 A3867 A3876 A3877 C3878 G3879 G3888 G3889 U3892 G3897 A3901 G3904 A3905 A3906 G3907 U3915 G3916 A3917 U3927 G3939
A3943 G3946 A3947 C3948 G4065 U4066 U4067 U4068 U4069 U4070 U4071 U4075 G4076 G4084 A4085 G4086 G4087 C4088 C4096 G4097 A4098 G4099 C4100 C4101 G4107 G4108 G4109 C4110 U4111 C4112 U4113 C4116 U4117 U4118 C4119 U4120 G4121 G4122 C4123 G4124 C4125 C4126 A4127 G4136 C4137 C4138 G4146 G4147 G4150 C4158
C4162 U4163 C4164 C4165 G4166 G4167 G4168 G4169 A4170 C4171 G4183 G4184 U4190 G4191 A4203 A4212 A4213 U4218 A4219 A4220 C4221 G4225 U4229 U4232 A4233 G4249 G4250 A4251 G4254 A4255 A4256 A4257 C4258 U4265 G4266 G4267 A4268 A4271 G4272 A4273 A4281 G4291 G4297 A4304
G4305 U4306 C4314 A4317 C4318 C4319 G4326 G4329 G4330 G4331 C4335 A4336 A4339 C4349 C4350 U4354 G4355 G4373 A4376 G4377 A4378 A4379 A4380 C4387 G4391 G4392 G4393 A4394 U4395 C4398 G4401 A4415 U4419 U4420 C4421 A4422 G4440 C4444 G4448 A4449 U4450

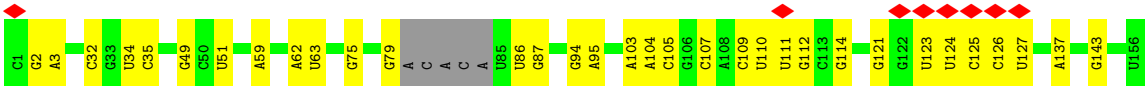


- Molecule 49: 5S ribosomal RNA

Chain 7:

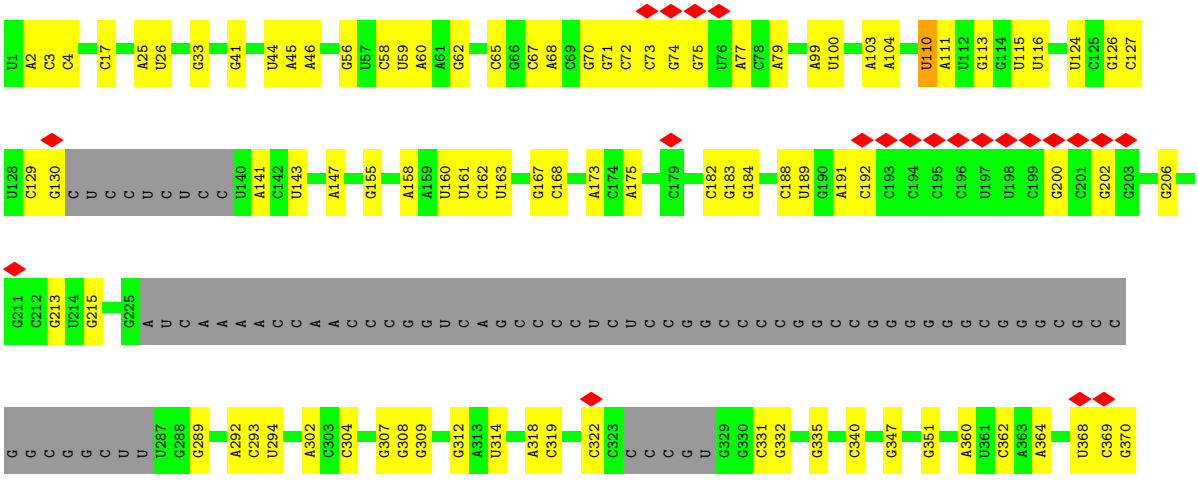
- Molecule 50: 5.8S ribosomal RNA

Chain 8:



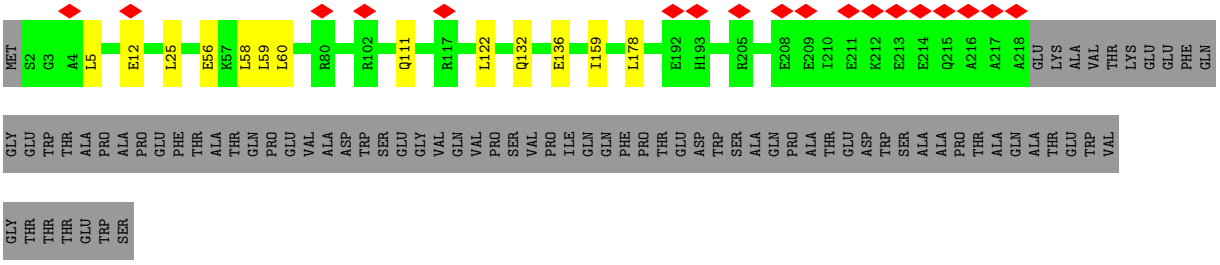
- Molecule 51: 18S ribosomal RNA

Chain 9:



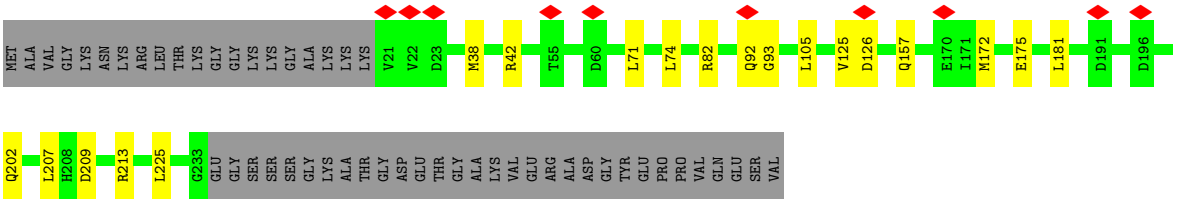
- Molecule 52: uS2

Chain AA:



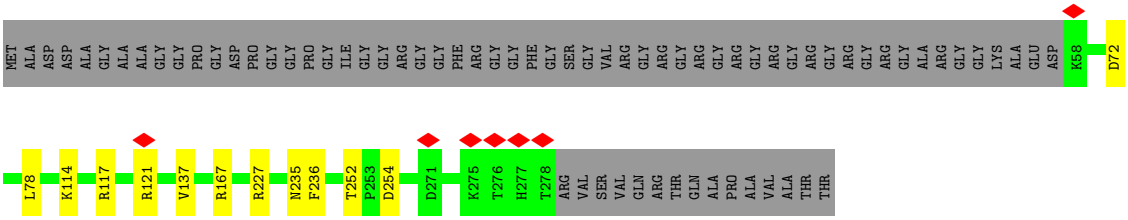
- Molecule 53: eS1

Chain BB:



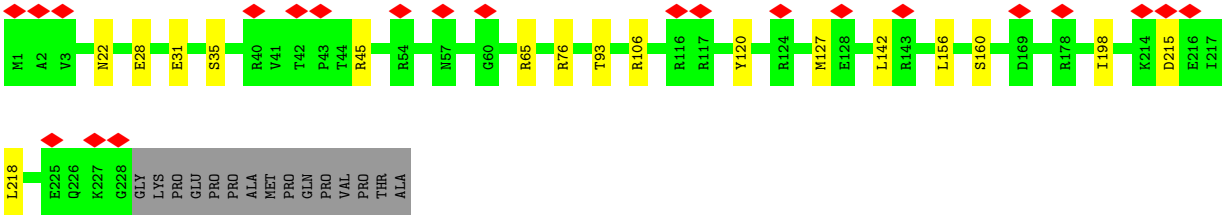
- Molecule 54: uS5

Chain CC:



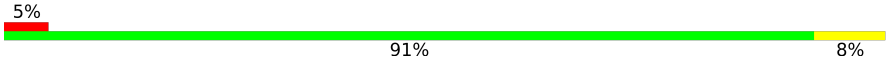
- Molecule 55: uS3

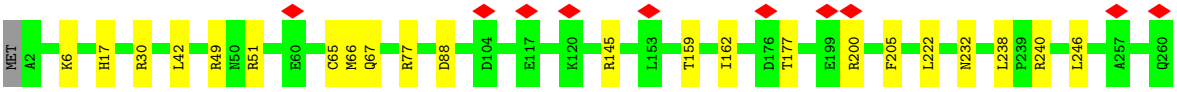
Chain DD:



- Molecule 56: eS4

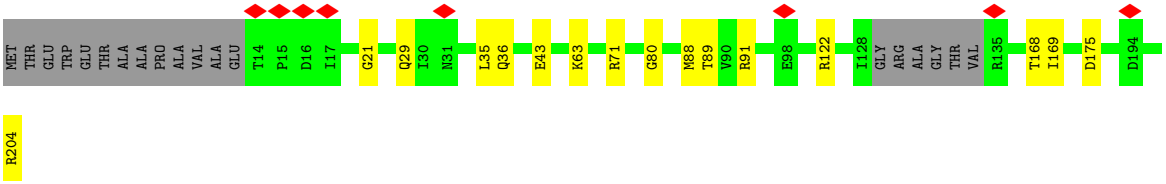
Chain EE:





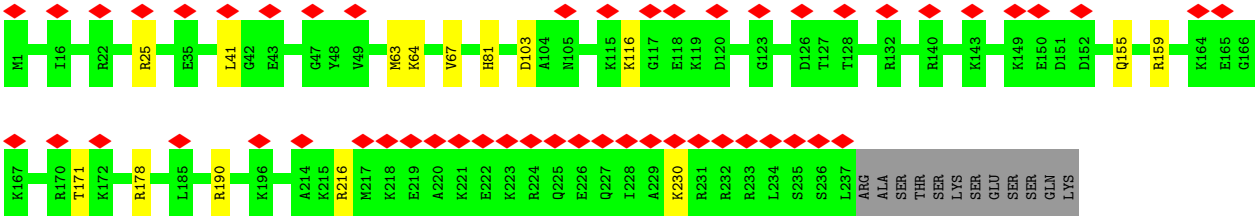
• Molecule 57: uS7

Chain FF:



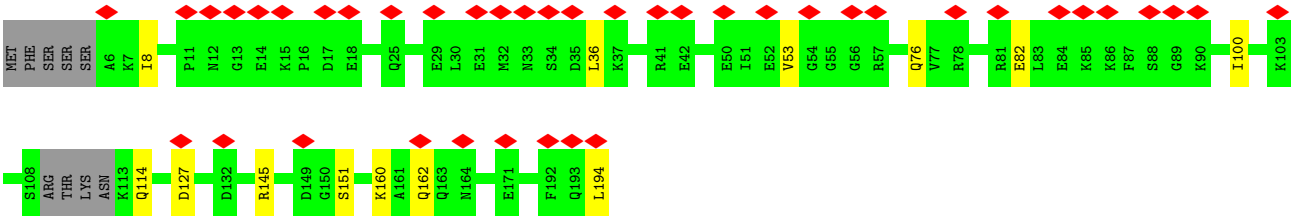
• Molecule 58: eS6

Chain GG:



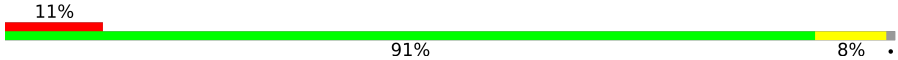
• Molecule 59: eS7

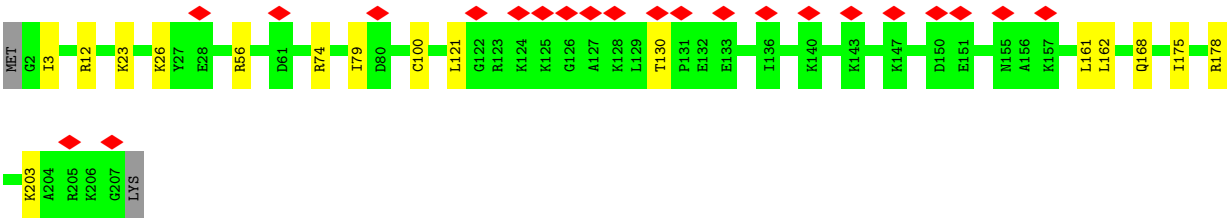
Chain HH:



• Molecule 60: eS8

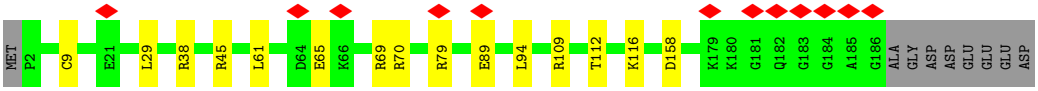
Chain II:





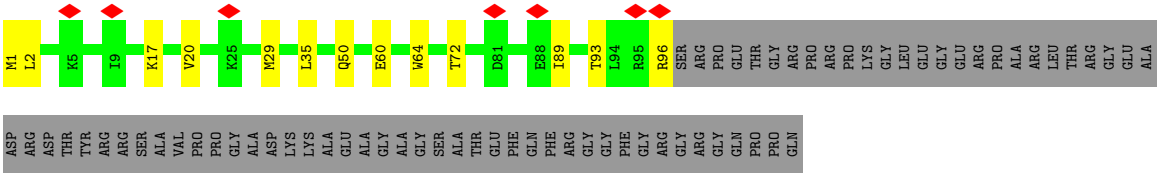
• Molecule 61: uS4

Chain JJ:



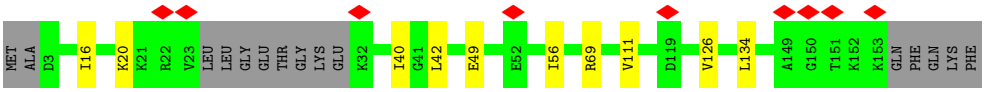
- Molecule 62: eS10

Chain KK:



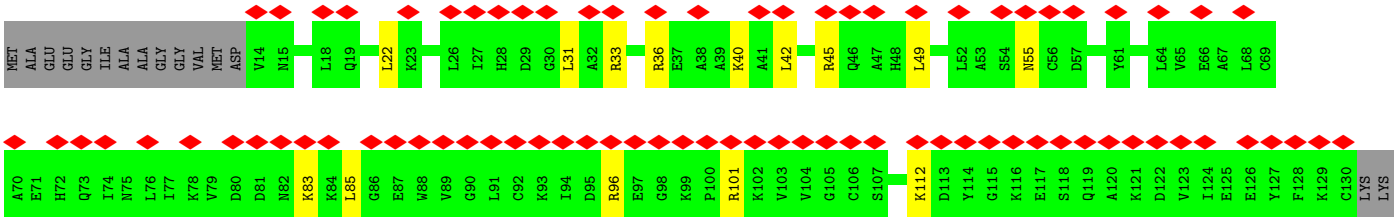
- Molecule 63: uS17

Chain LL:



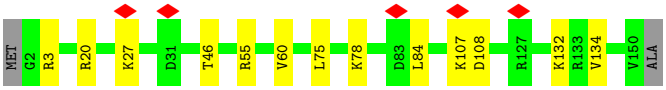
- Molecule 64: eS12

Chain MM:



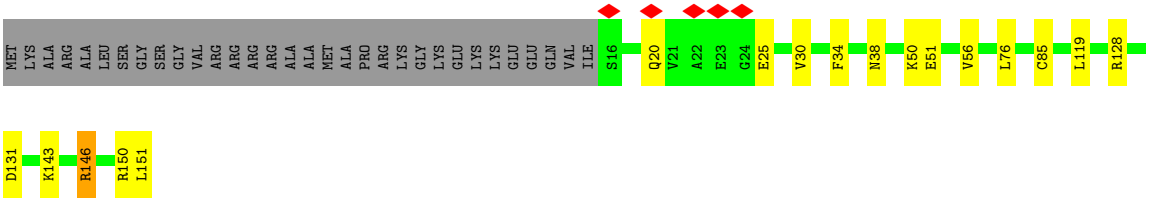
- Molecule 65: uS15

Chain NN:



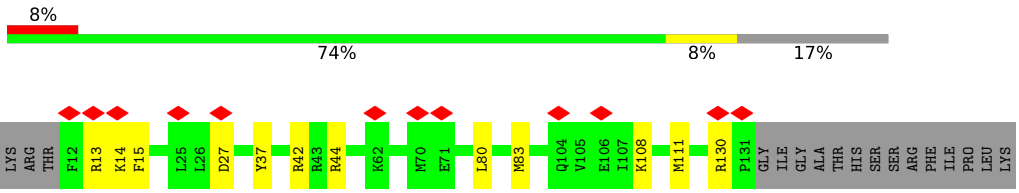
- Molecule 66: uS11

Chain OO:



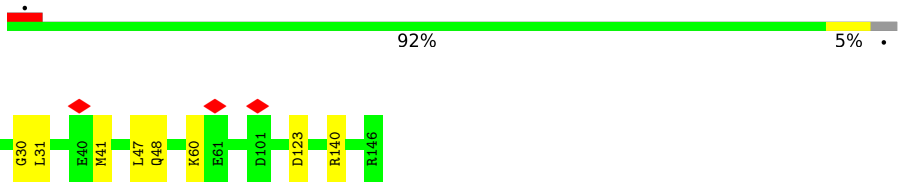
- Molecule 67: uS19

Chain PP:



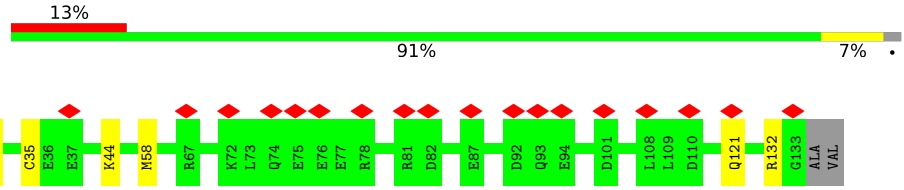
- Molecule 68: uS9

Chain QQ:



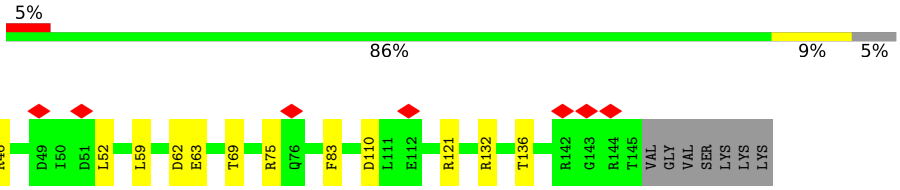
- Molecule 69: eS17

Chain RR:



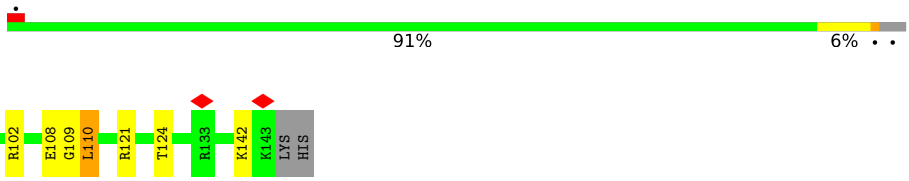
- Molecule 70: uS13

Chain SS:



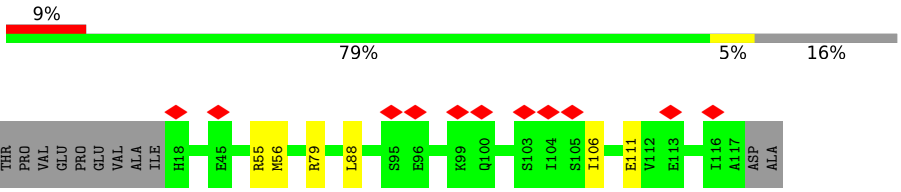
- Molecule 71: eS19

Chain TT:



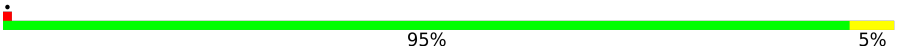
- Molecule 72: uS10

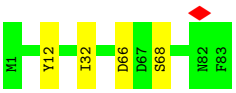
Chain UU:



- Molecule 73: eS21

Chain VV:



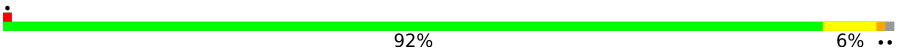


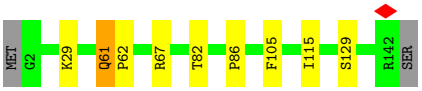
- Molecule 74: uS8

Chain WW:

- Molecule 75: uS12

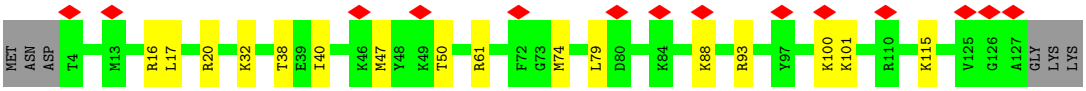
Chain XX:





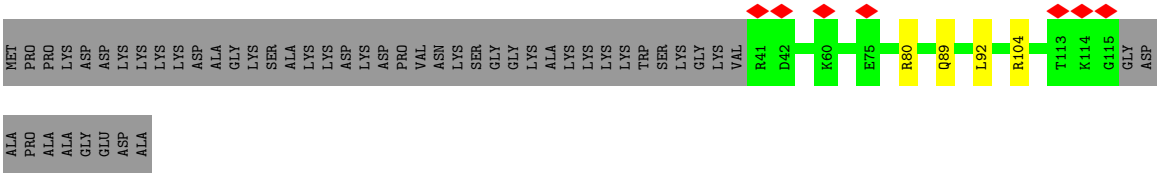
- Molecule 76: eS24

Chain YY:



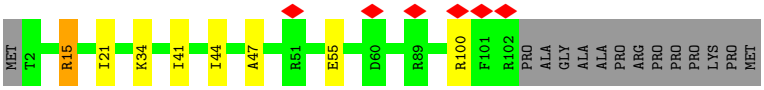
- Molecule 77: eS25

Chain ZZ:



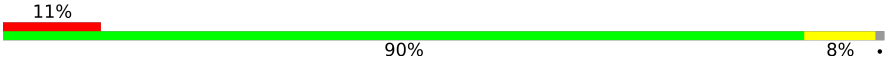
- Molecule 78: eS26

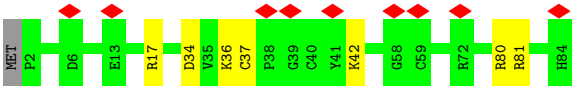
Chain aa:



- Molecule 79: eS27

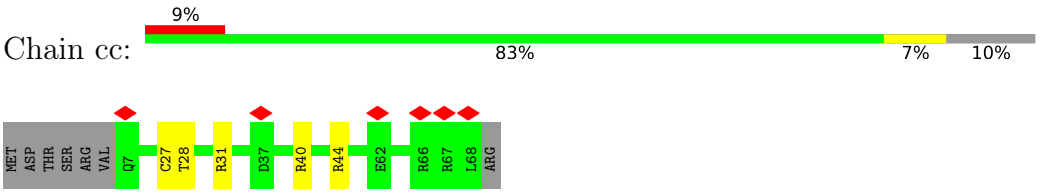
Chain bb:





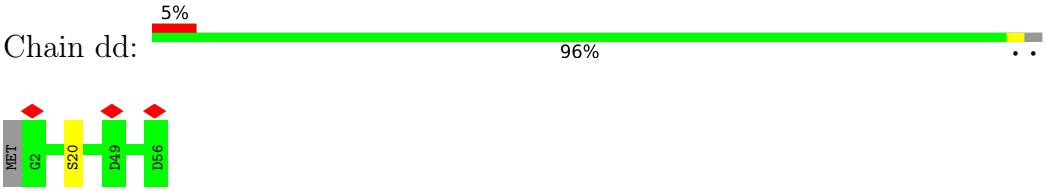
- Molecule 80: eS28

Chain cc:



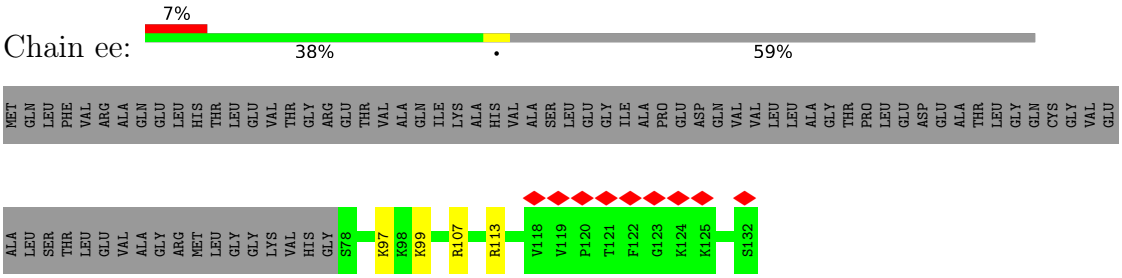
- Molecule 81: uS14

Chain dd:



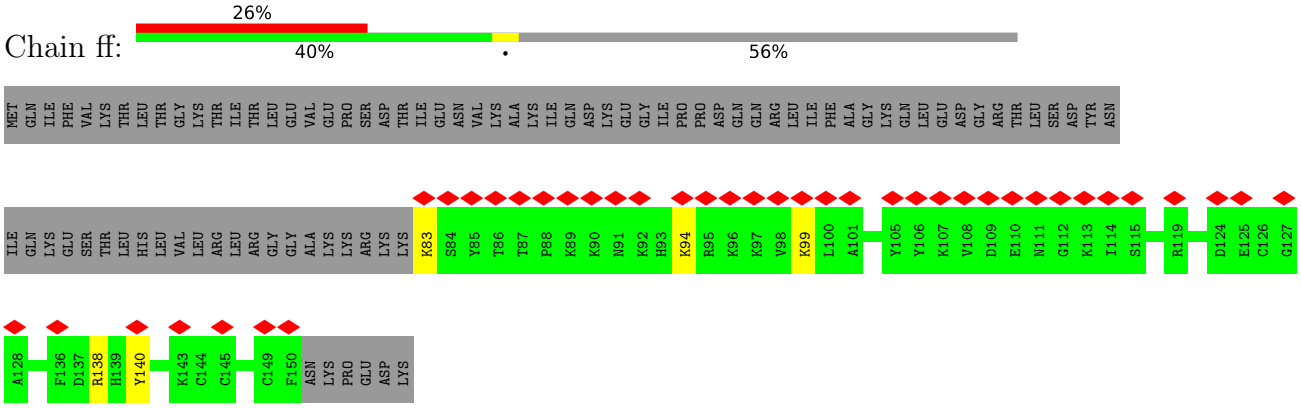
- Molecule 82: eS30

Chain ee:



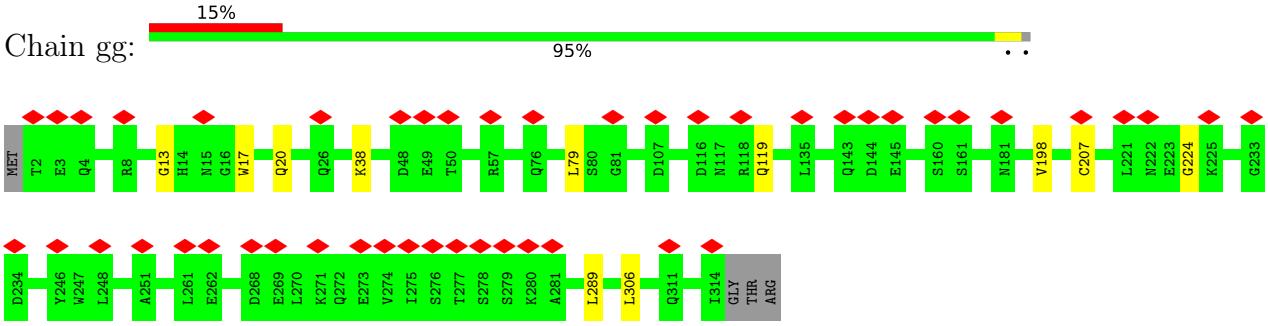
- Molecule 83: eS31

Chain ff:



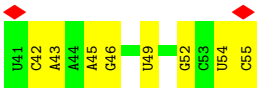
- Molecule 84: RACK1

Chain gg:



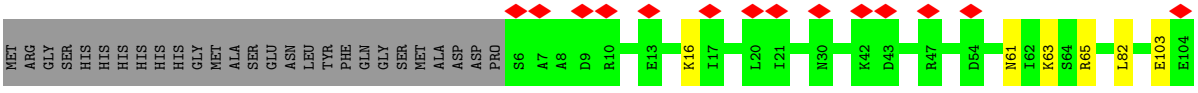
- Molecule 85: mRNA (UGA stop codon)

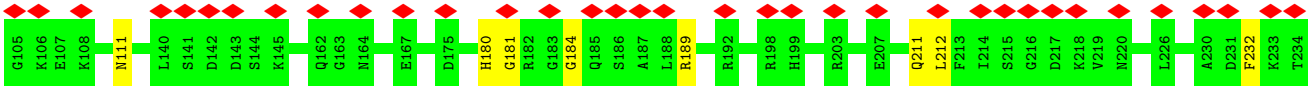
Chain hh:

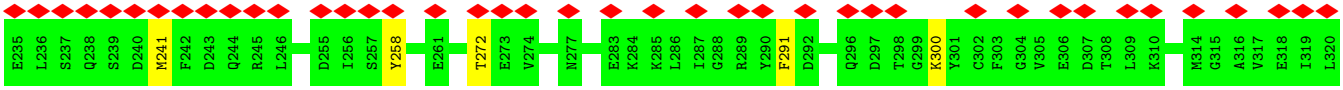


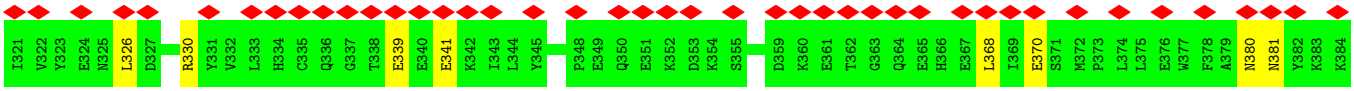
• Molecule 86: eRF1

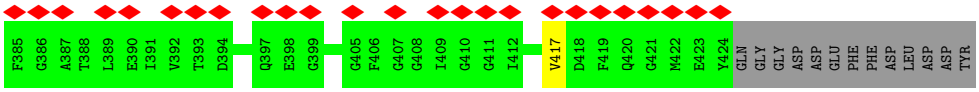
Chain ii:





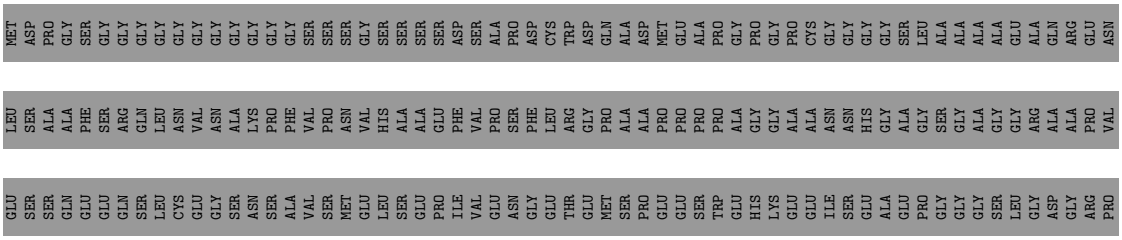


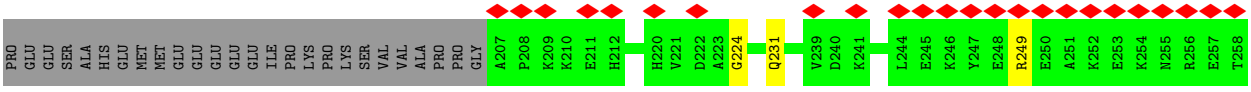


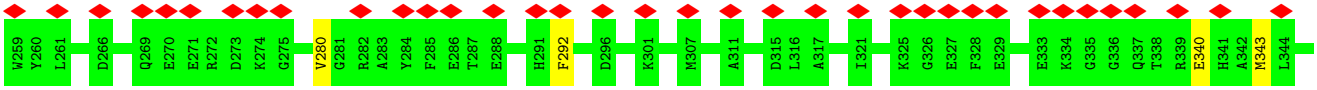


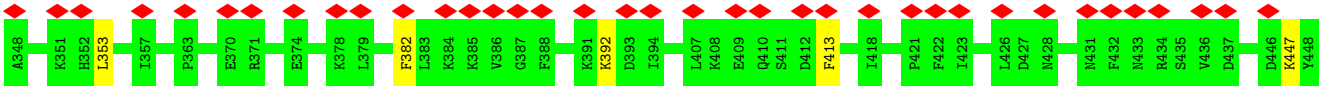
• Molecule 87: eRF3a

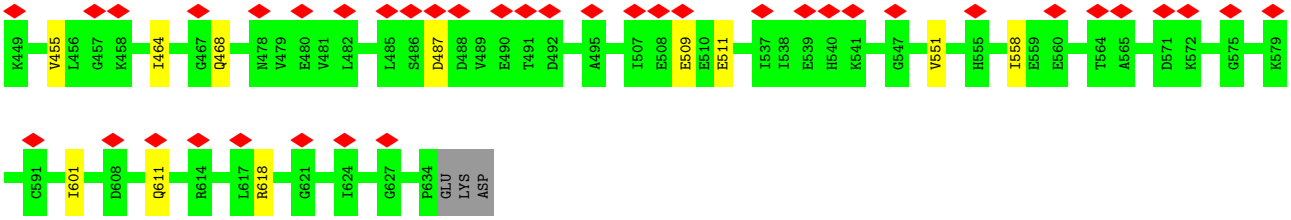
Chain jj:










K449
V455
L456
G457
K458
I464
G467
Q468
N478
V479
E480
V481
L482
L485
S486
D487
D488
V489
E490
T491
D492
A495
I507
E508
E509
E510
E511
I537
I538
E539
H540
K541
G547
V551
H555
I558
E559
E560
T564
A565
D571
K572
G575
K579

C591
I601
D608
Q611
R614
I617
R618
G621
I624
G627
F634
GLU
LYS
ASP

4 Experimental information (i)

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 ($e^-/Å^2$)	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	0.34	0/1936	0.69	0/2596
2	B	0.33	0/3240	0.64	0/4339
3	C	0.33	0/2937	0.66	0/3946
4	D	0.34	0/2437	0.61	3/3264 (0.1%)
5	E	0.33	0/1762	0.63	0/2362
6	F	0.36	0/1911	0.66	1/2549 (0.0%)
7	G	0.33	0/1910	0.62	0/2569
8	H	0.31	0/1535	0.60	0/2063
9	I	0.33	0/1702	0.60	0/2272
10	J	0.33	0/1385	0.61	0/1852
11	L	0.34	0/1733	0.67	0/2316
12	M	0.35	0/1158	0.65	0/1547
13	N	0.35	0/1746	0.67	0/2338
14	O	0.34	0/1662	0.66	0/2222
15	P	0.36	0/1268	0.64	0/1700
16	Q	0.35	0/1539	0.72	0/2054
17	R	0.34	0/1524	0.67	0/2013
18	S	0.37	0/1501	0.68	0/2012
19	T	0.33	0/1326	0.60	0/1770
20	U	0.35	0/823	0.55	0/1104
21	V	0.34	0/993	0.62	0/1332
22	W	0.34	0/873	0.56	0/1158
23	X	0.33	0/984	0.60	0/1323
24	Y	0.33	0/1132	0.62	0/1504
25	Z	0.34	0/1130	0.61	0/1507
26	a	0.32	0/1191	0.61	0/1590
27	b	0.34	0/861	0.58	0/1138
28	c	0.32	0/771	0.54	0/1034
29	d	0.34	0/903	0.66	0/1216
30	e	0.34	0/1071	0.66	0/1429
31	f	0.36	0/895	0.69	0/1198
32	g	0.33	0/916	0.67	0/1220

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	h	0.32	0/1021	0.61	0/1348
34	i	0.34	0/841	0.60	0/1112
35	j	0.36	0/720	0.72	0/952
36	k	0.32	0/575	0.55	0/761
37	l	0.35	0/459	0.63	0/608
38	m	0.34	0/435	0.61	0/575
39	n	0.34	0/240	0.67	0/305
40	o	0.34	0/864	0.61	0/1140
41	p	0.32	0/718	0.62	0/953
42	r	0.35	0/1010	0.69	0/1354
43	s	0.36	0/1530	0.50	0/2064
44	t	0.36	0/1174	0.52	0/1582
45	1	0.41	0/129	0.61	0/173
46	2	0.22	0/1805	0.67	0/2809
47	3	0.21	0/1777	0.66	0/2763
48	5	0.27	0/84973	0.68	22/132508 (0.0%)
49	7	0.26	0/2858	0.67	0/4455
50	8	0.28	0/3581	0.67	0/5577
51	9	0.25	0/40524	0.69	10/63134 (0.0%)
52	AA	0.33	0/1747	0.60	0/2374
53	BB	0.33	0/1756	0.63	0/2350
54	CC	0.34	0/1753	0.62	0/2369
55	DD	0.35	0/1796	0.61	0/2417
56	EE	0.34	0/2118	0.64	0/2849
57	FF	0.33	0/1492	0.61	0/2005
58	GG	0.35	0/1946	0.67	0/2590
59	HH	0.35	0/1510	0.59	0/2022
60	II	0.34	0/1715	0.63	0/2287
61	JJ	0.33	0/1550	0.68	0/2069
62	KK	0.34	0/834	0.59	0/1125
63	LL	0.35	0/1195	0.66	0/1597
64	MM	0.36	0/918	0.61	0/1233
65	NN	0.33	0/1226	0.62	0/1649
66	OO	0.34	0/1029	0.78	1/1380 (0.1%)
67	PP	0.34	0/1017	0.64	0/1358
68	QQ	0.32	0/1146	0.61	0/1534
69	RR	0.33	0/1082	0.60	0/1452
70	SS	0.34	0/1208	0.68	0/1618
71	TT	0.36	0/1115	0.63	1/1493 (0.1%)
72	UU	0.34	0/805	0.65	0/1081
73	VV	0.36	0/643	0.67	0/860
74	WW	0.34	0/1051	0.69	0/1406
75	XX	0.32	0/1116	0.64	0/1490

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
76	YY	0.35	0/1028	0.61	0/1366
77	ZZ	0.33	0/604	0.59	0/810
78	aa	0.35	0/828	0.74	0/1109
79	bb	0.33	0/665	0.59	0/891
80	cc	0.33	0/490	0.65	0/656
81	dd	0.37	0/470	0.62	0/623
82	ee	0.35	0/447	0.70	0/587
83	ff	0.36	0/567	0.56	0/753
84	gg	0.32	0/2493	0.55	0/3394
85	hh	0.31	0/353	0.77	0/547
86	ii	0.35	0/3361	0.54	0/4519
87	jj	0.35	0/3435	0.55	0/4633
All	All	0.30	0/238498	0.66	38/349206 (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

There are no bond length outliers.

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	9	1835	A	C2'-C3'-O3'	8.60	128.43	109.50
4	D	22	ARG	NE-CZ-NH1	8.45	124.52	120.30
51	9	1394	G	C2'-C3'-O3'	7.70	126.44	109.50
48	5	406	C	C2'-C3'-O3'	7.30	125.56	109.50
48	5	1477	C	C2'-C3'-O3'	6.95	124.81	113.70

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

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Mol	Chain	Res	Type	Group
75	XX	61	GLN	Peptide

5.2 Too-close contacts (i)

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

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	48
2	B	392/403 (97%)	360 (92%)	29 (7%)	3 (1%)	16	48
3	C	360/425 (85%)	337 (94%)	21 (6%)	2 (1%)	22	54
4	D	291/297 (98%)	275 (94%)	15 (5%)	1 (0%)	37	67
5	E	208/291 (72%)	191 (92%)	17 (8%)	0	100	100
6	F	223/247 (90%)	212 (95%)	10 (4%)	1 (0%)	30	62
7	G	229/319 (72%)	216 (94%)	11 (5%)	2 (1%)	14	46
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%)	25	57
12	M	136/218 (62%)	123 (90%)	12 (9%)	1 (1%)	19	51
13	N	201/204 (98%)	187 (93%)	13 (6%)	1 (0%)	25	57
14	O	197/203 (97%)	188 (95%)	8 (4%)	1 (0%)	25	57
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	S	174/176 (99%)	159 (91%)	14 (8%)	1 (1%)	22	54
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%)	13	44
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	36
26	a	145/148 (98%)	131 (90%)	14 (10%)	0	100	100
27	b	100/245 (41%)	94 (94%)	5 (5%)	1 (1%)	13	44
28	c	96/115 (84%)	93 (97%)	3 (3%)	0	100	100
29	d	105/125 (84%)	89 (85%)	15 (14%)	1 (1%)	13	44
30	e	126/135 (93%)	120 (95%)	6 (5%)	0	100	100
31	f	107/110 (97%)	97 (91%)	8 (8%)	2 (2%)	6	33
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%)	13	44
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%)	12	42
42	r	122/137 (89%)	112 (92%)	9 (7%)	1 (1%)	16	48
43	s	194/318 (61%)	176 (91%)	16 (8%)	2 (1%)	13	44
44	t	151/165 (92%)	135 (89%)	14 (9%)	2 (1%)	10	39
45	1	13/15 (87%)	10 (77%)	2 (15%)	1 (8%)	1	9
52	AA	215/295 (73%)	203 (94%)	11 (5%)	1 (0%)	25	57
53	BB	211/264 (80%)	198 (94%)	12 (6%)	1 (0%)	25	57
54	CC	219/293 (75%)	206 (94%)	13 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	DD	226/243 (93%)	213 (94%)	12 (5%)	1 (0%)	30	62
56	EE	260/263 (99%)	246 (95%)	14 (5%)	0	100	100
57	FF	181/204 (89%)	170 (94%)	9 (5%)	2 (1%)	12	42
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%)	25	57
61	JJ	183/194 (94%)	177 (97%)	6 (3%)	0	100	100
62	KK	94/165 (57%)	89 (95%)	4 (4%)	1 (1%)	12	42
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%)	19	51
66	OO	134/168 (80%)	123 (92%)	9 (7%)	2 (2%)	8	36
67	PP	118/145 (81%)	105 (89%)	12 (10%)	1 (1%)	16	48
68	QQ	140/146 (96%)	132 (94%)	7 (5%)	1 (1%)	19	51
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%)	19	51
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%)	8	35
75	XX	139/143 (97%)	128 (92%)	8 (6%)	3 (2%)	5	30
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	32
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
83	ff	66/156 (42%)	59 (89%)	7 (11%)	0	100	100
84	gg	311/317 (98%)	285 (92%)	24 (8%)	2 (1%)	22	54
86	ii	417/459 (91%)	387 (93%)	24 (6%)	6 (1%)	9	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
87	jj	426/637 (67%)	371 (87%)	50 (12%)	5 (1%)	11	40
All	All	12375/14486 (85%)	11531 (93%)	780 (6%)	64 (0%)	27	57

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 (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	
1	A	190/199 (96%)	179 (94%)	11 (6%)	17	43
2	B	342/348 (98%)	325 (95%)	17 (5%)	20	46
3	C	302/347 (87%)	285 (94%)	17 (6%)	17	44
4	D	247/250 (99%)	235 (95%)	12 (5%)	21	46
5	E	190/251 (76%)	177 (93%)	13 (7%)	13	38
6	F	196/215 (91%)	184 (94%)	12 (6%)	15	42
7	G	200/272 (74%)	189 (94%)	11 (6%)	18	44
8	H	169/171 (99%)	157 (93%)	12 (7%)	12	37
9	I	175/181 (97%)	166 (95%)	9 (5%)	20	46
10	J	143/149 (96%)	136 (95%)	7 (5%)	21	46
11	L	175/176 (99%)	167 (95%)	8 (5%)	23	48
12	M	117/161 (73%)	108 (92%)	9 (8%)	10	35
13	N	171/172 (99%)	163 (95%)	8 (5%)	22	47
14	O	171/173 (99%)	160 (94%)	11 (6%)	14	40
15	P	134/163 (82%)	126 (94%)	8 (6%)	16	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	Q	164/165 (99%)	156 (95%)	8 (5%)	21	46
17	R	159/175 (91%)	147 (92%)	12 (8%)	11	35
18	S	157/157 (100%)	146 (93%)	11 (7%)	12	37
19	T	139/140 (99%)	129 (93%)	10 (7%)	12	36
20	U	89/114 (78%)	86 (97%)	3 (3%)	32	55
21	V	101/107 (94%)	93 (92%)	8 (8%)	10	34
22	W	86/126 (68%)	85 (99%)	1 (1%)	67	79
23	X	106/134 (79%)	100 (94%)	6 (6%)	17	43
24	Y	124/135 (92%)	117 (94%)	7 (6%)	17	44
25	Z	117/118 (99%)	114 (97%)	3 (3%)	41	60
26	a	119/120 (99%)	116 (98%)	3 (2%)	42	61
27	b	84/184 (46%)	81 (96%)	3 (4%)	30	54
28	c	84/98 (86%)	81 (96%)	3 (4%)	30	54
29	d	98/110 (89%)	91 (93%)	7 (7%)	12	37
30	e	114/121 (94%)	105 (92%)	9 (8%)	10	34
31	f	88/89 (99%)	82 (93%)	6 (7%)	13	38
32	g	98/100 (98%)	93 (95%)	5 (5%)	20	46
33	h	109/110 (99%)	103 (94%)	6 (6%)	18	44
34	i	86/89 (97%)	85 (99%)	1 (1%)	67	79
35	j	73/80 (91%)	68 (93%)	5 (7%)	13	38
36	k	64/65 (98%)	62 (97%)	2 (3%)	35	57
37	l	47/48 (98%)	46 (98%)	1 (2%)	48	67
38	m	48/90 (53%)	45 (94%)	3 (6%)	15	41
39	n	24/24 (100%)	22 (92%)	2 (8%)	9	32
40	o	92/94 (98%)	86 (94%)	6 (6%)	14	39
41	p	74/75 (99%)	73 (99%)	1 (1%)	62	77
42	r	108/121 (89%)	102 (94%)	6 (6%)	17	44
43	s	164/258 (64%)	158 (96%)	6 (4%)	29	53
44	t	126/137 (92%)	121 (96%)	5 (4%)	27	51
45	1	13/13 (100%)	13 (100%)	0	100	100
52	AA	180/245 (74%)	168 (93%)	12 (7%)	13	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	BB	194/231 (84%)	176 (91%)	18 (9%)	7	28
54	CC	187/225 (83%)	175 (94%)	12 (6%)	14	40
55	DD	190/202 (94%)	174 (92%)	16 (8%)	9	32
56	EE	224/225 (100%)	202 (90%)	22 (10%)	6	26
57	FF	158/170 (93%)	144 (91%)	14 (9%)	8	30
58	GG	207/218 (95%)	192 (93%)	15 (7%)	12	36
59	HH	165/174 (95%)	152 (92%)	13 (8%)	10	34
60	II	178/180 (99%)	163 (92%)	15 (8%)	9	32
61	JJ	161/168 (96%)	146 (91%)	15 (9%)	7	28
62	KK	87/136 (64%)	75 (86%)	12 (14%)	3	16
63	LL	130/142 (92%)	120 (92%)	10 (8%)	10	35
64	MM	99/108 (92%)	85 (86%)	14 (14%)	3	15
65	NN	130/131 (99%)	118 (91%)	12 (9%)	7	29
66	OO	106/130 (82%)	91 (86%)	15 (14%)	2	15
67	PP	109/130 (84%)	98 (90%)	11 (10%)	6	25
68	QQ	117/121 (97%)	110 (94%)	7 (6%)	16	42
69	RR	119/121 (98%)	110 (92%)	9 (8%)	11	35
70	SS	125/132 (95%)	111 (89%)	14 (11%)	5	22
71	TT	111/115 (96%)	103 (93%)	8 (7%)	12	36
72	UU	92/107 (86%)	86 (94%)	6 (6%)	14	39
73	VV	67/67 (100%)	63 (94%)	4 (6%)	16	42
74	WW	112/113 (99%)	103 (92%)	9 (8%)	10	34
75	XX	113/115 (98%)	107 (95%)	6 (5%)	19	45
76	YY	107/112 (96%)	91 (85%)	16 (15%)	2	14
77	ZZ	66/103 (64%)	62 (94%)	4 (6%)	15	42
78	aa	88/98 (90%)	81 (92%)	7 (8%)	10	34
79	bb	75/76 (99%)	68 (91%)	7 (9%)	7	28
80	cc	55/62 (89%)	50 (91%)	5 (9%)	7	29
81	dd	48/49 (98%)	47 (98%)	1 (2%)	48	67
82	ee	46/106 (43%)	42 (91%)	4 (9%)	8	31
83	ff	61/140 (44%)	56 (92%)	5 (8%)	9	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
84	gg	272/275 (99%)	263 (97%)	9 (3%)	33	56
86	ii	361/394 (92%)	339 (94%)	22 (6%)	15	42
87	jj	372/520 (72%)	354 (95%)	18 (5%)	21	47
All	All	10789/12266 (88%)	10088 (94%)	701 (6%)	17	39

5 of 701 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
61	JJ	112	THR
71	TT	108	GLU
62	KK	93	THR
61	JJ	109	ARG
66	OO	76	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
80	cc	26	GLN
87	jj	499	ASN
86	ii	67	ASN
87	jj	214	ASN
87	jj	555	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
46	2	74/76 (97%)	13 (17%)	0
47	3	72/75 (96%)	22 (30%)	2 (2%)
48	5	3514/3543 (99%)	876 (24%)	169 (4%)
49	7	119/120 (99%)	14 (11%)	2 (1%)
50	8	149/156 (95%)	32 (21%)	6 (4%)
51	9	1679/1869 (89%)	422 (25%)	71 (4%)
85	hh	14/15 (93%)	8 (57%)	0
All	All	5621/5854 (96%)	1387 (24%)	250 (4%)

5 of 1387 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
46	2	9	A

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Mol	Chain	Res	Type
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	27,34,34	1.85	7 (25%)	34,54,54	1.96	8 (23%)

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	-	6/15/38/38	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	5.39	1.61	1.50
90	jj	700	GCP	C5-C6	4.50	1.49	1.41
90	jj	700	GCP	PG-O2G	2.91	1.61	1.54
90	jj	700	GCP	PG-O3G	-2.87	1.48	1.54
90	jj	700	GCP	C5-C4	2.49	1.47	1.40

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
90	jj	700	GCP	C2-N3-C4	5.22	121.32	115.36
90	jj	700	GCP	C4-C5-C6	-4.43	116.56	120.80
90	jj	700	GCP	PB-O3A-PA	-3.80	120.51	132.56
90	jj	700	GCP	C2-N1-C6	3.77	121.92	115.93
90	jj	700	GCP	N3-C2-N1	-3.57	122.47	127.22

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

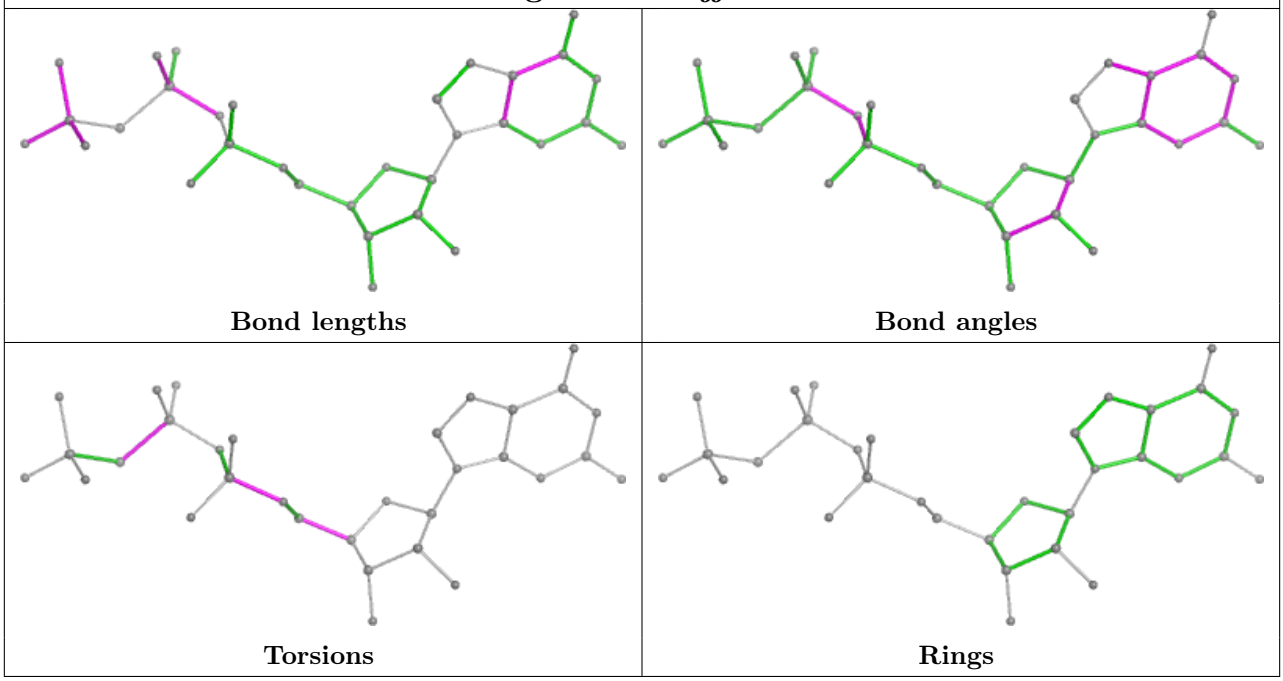
There are no ring outliers.

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 then 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.

Ligand GCP jj 700



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

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	3948:C	O3'	4065:G	P	19.75
1	5	1406(C):G	O3'	1411:C	P	18.65

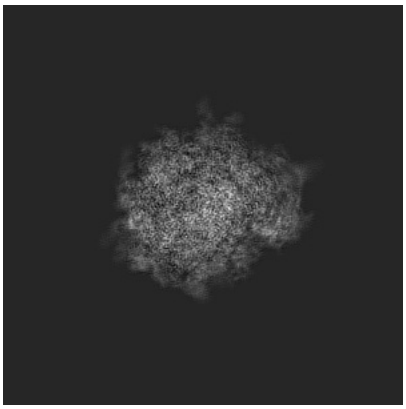
6 Map visualisation (i)

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.

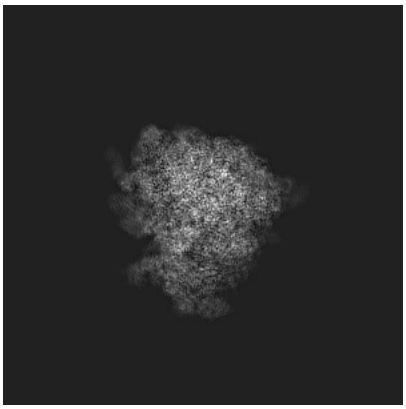
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

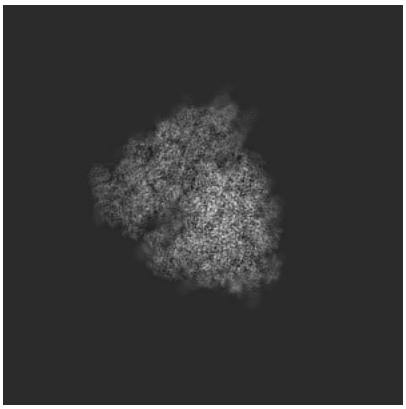
6.1.1 Primary map



X

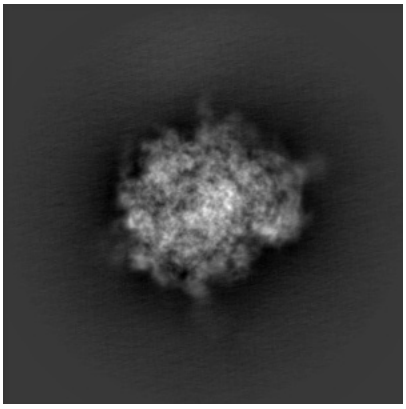


Y

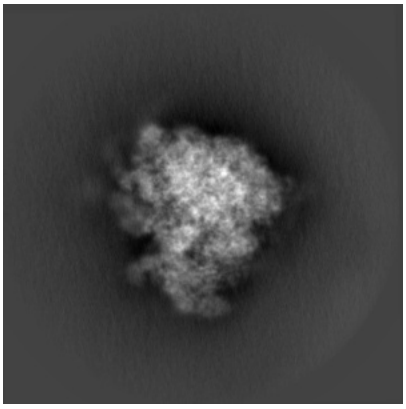


Z

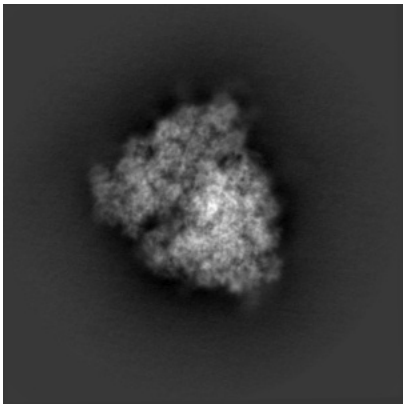
6.1.2 Raw map



X



Y

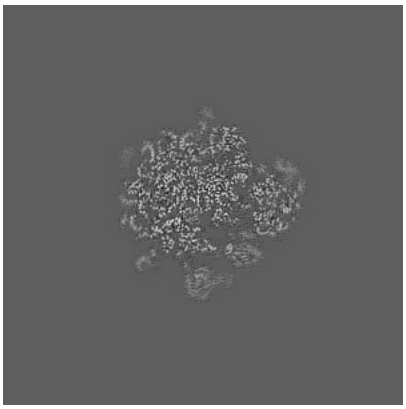


Z

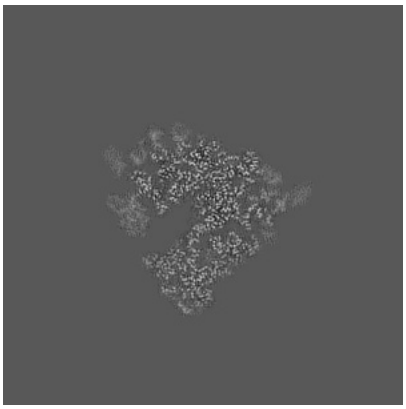
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

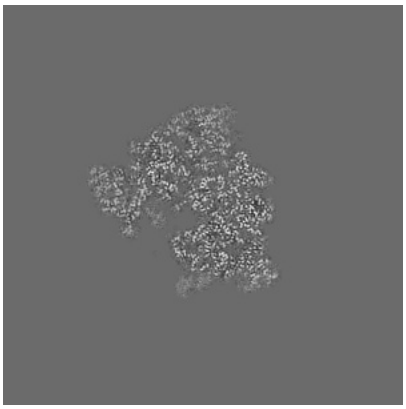
6.2.1 Primary map



X Index: 210

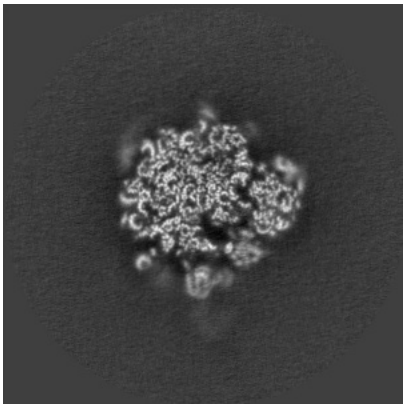


Y Index: 210

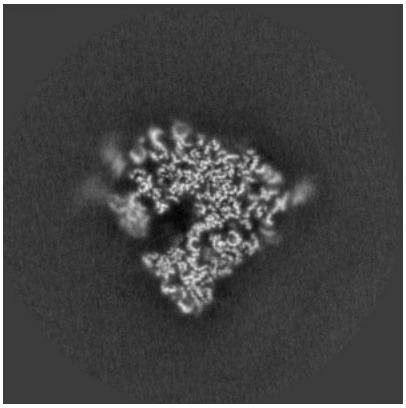


Z Index: 210

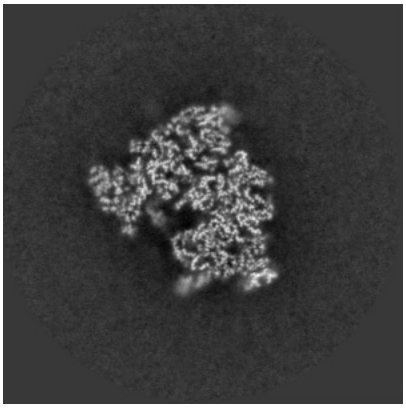
6.2.2 Raw map



X Index: 210



Y Index: 210

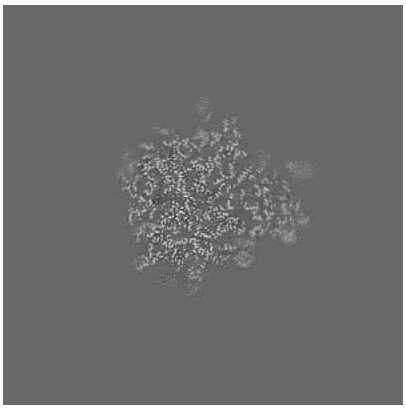


Z Index: 210

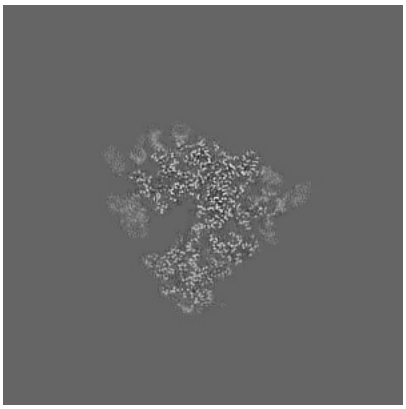
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

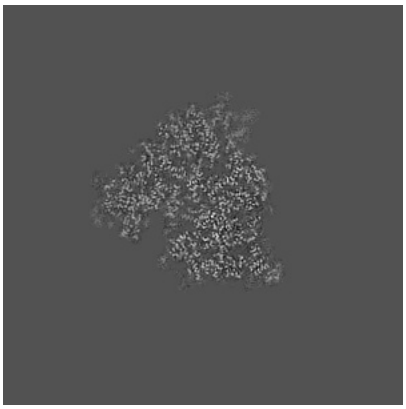
6.3.1 Primary map



X Index: 222

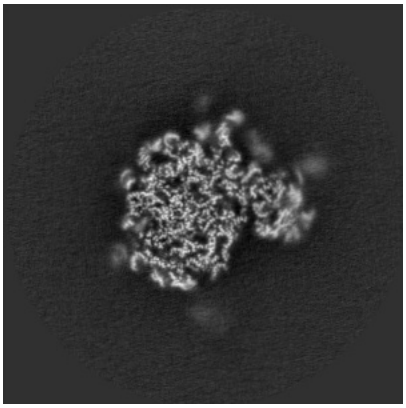


Y Index: 211

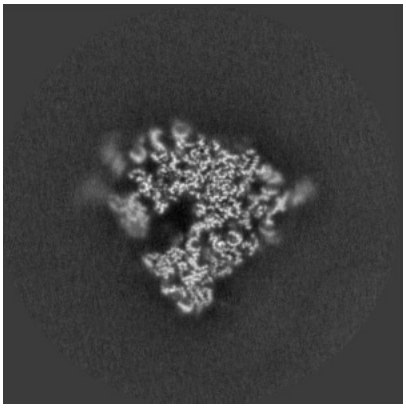


Z Index: 202

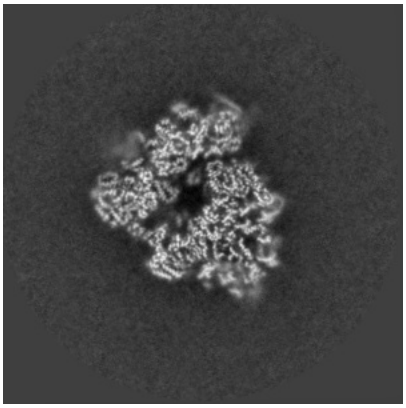
6.3.2 Raw map



X Index: 233



Y Index: 211

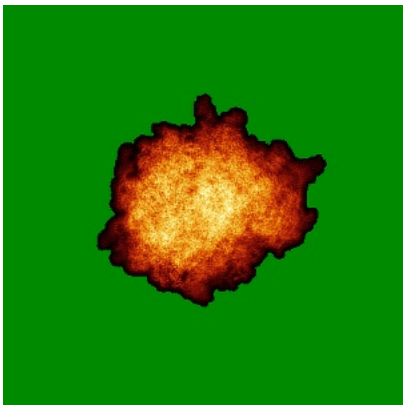


Z Index: 186

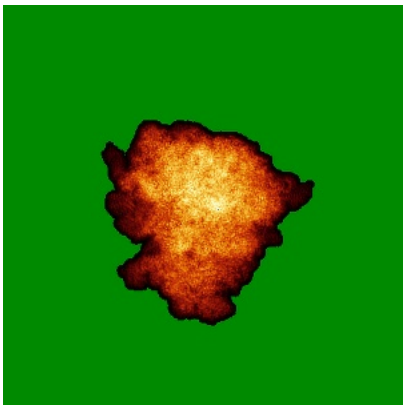
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

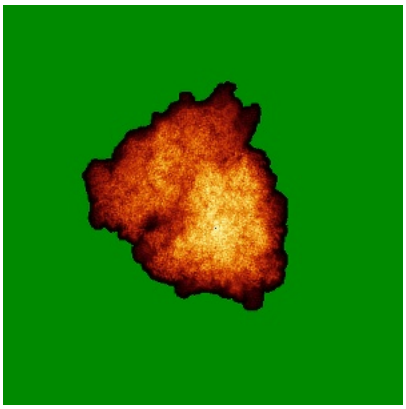
6.4.1 Primary map



X

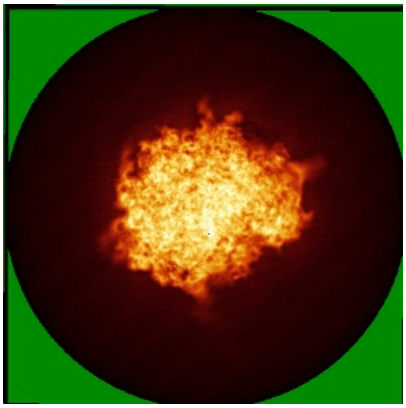


Y

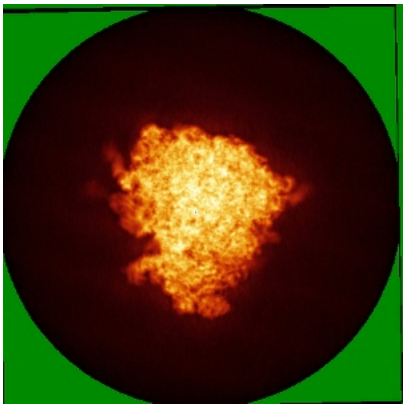


Z

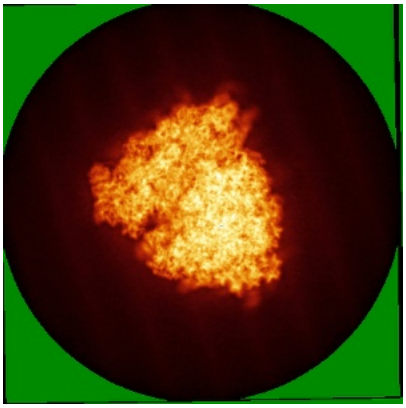
6.4.2 Raw map



X



Y

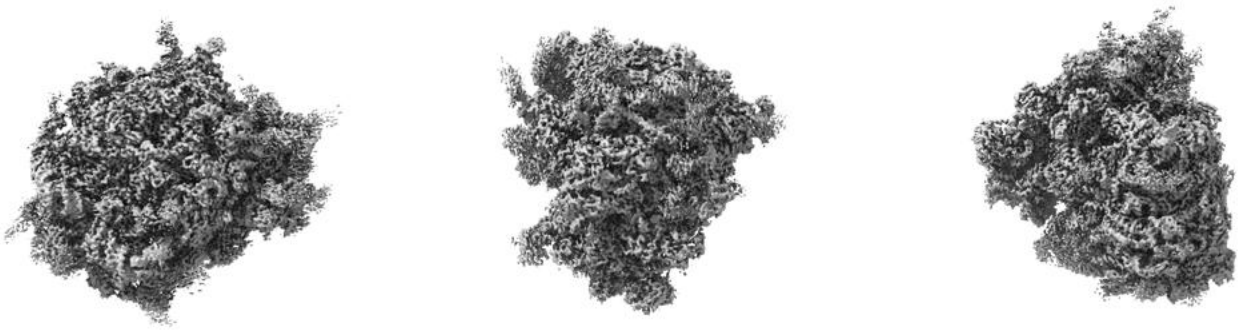


Z

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



X Y Z

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

X Y Z

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.

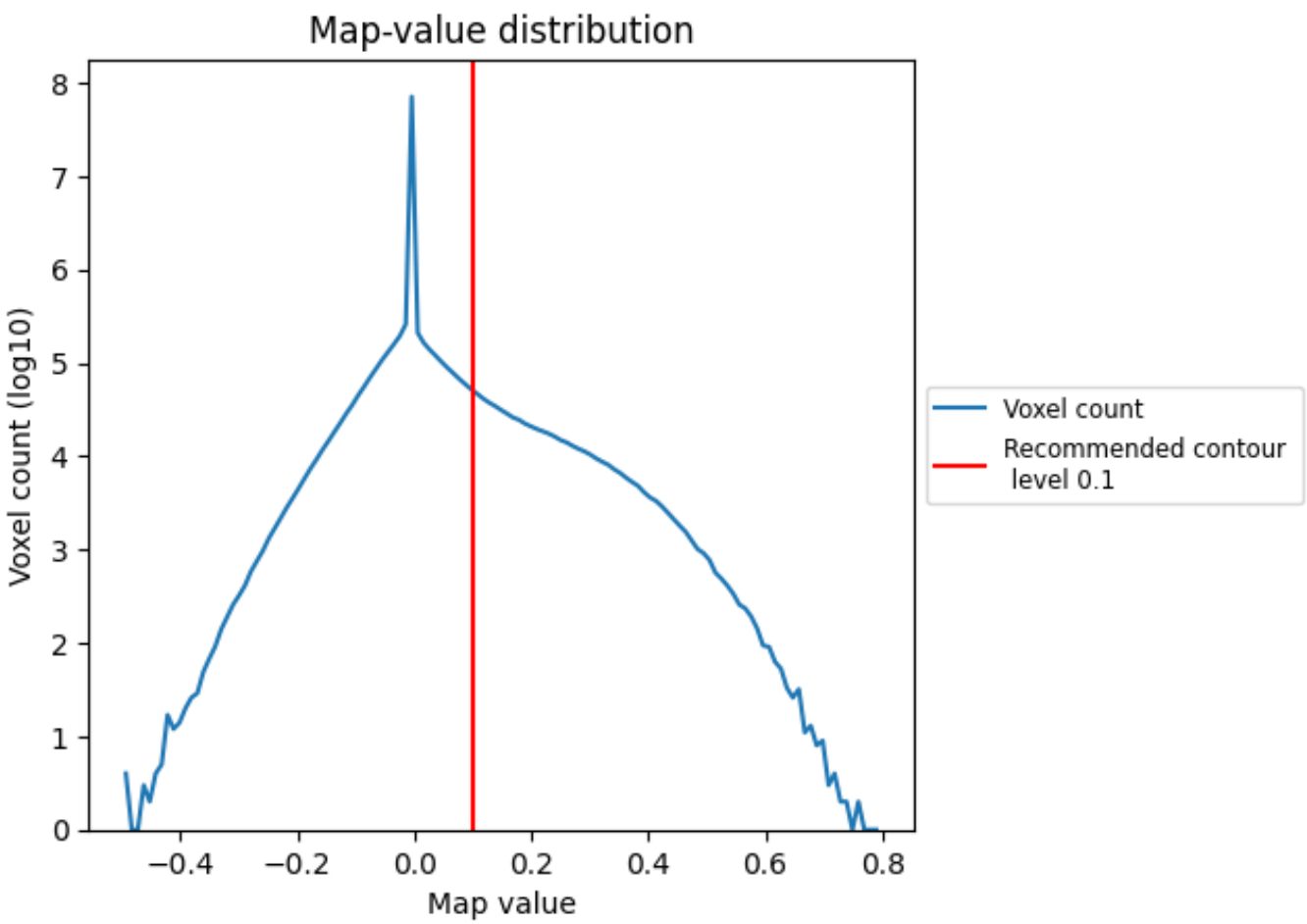
6.6 Mask visualisation (i)

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

7 Map analysis (i)

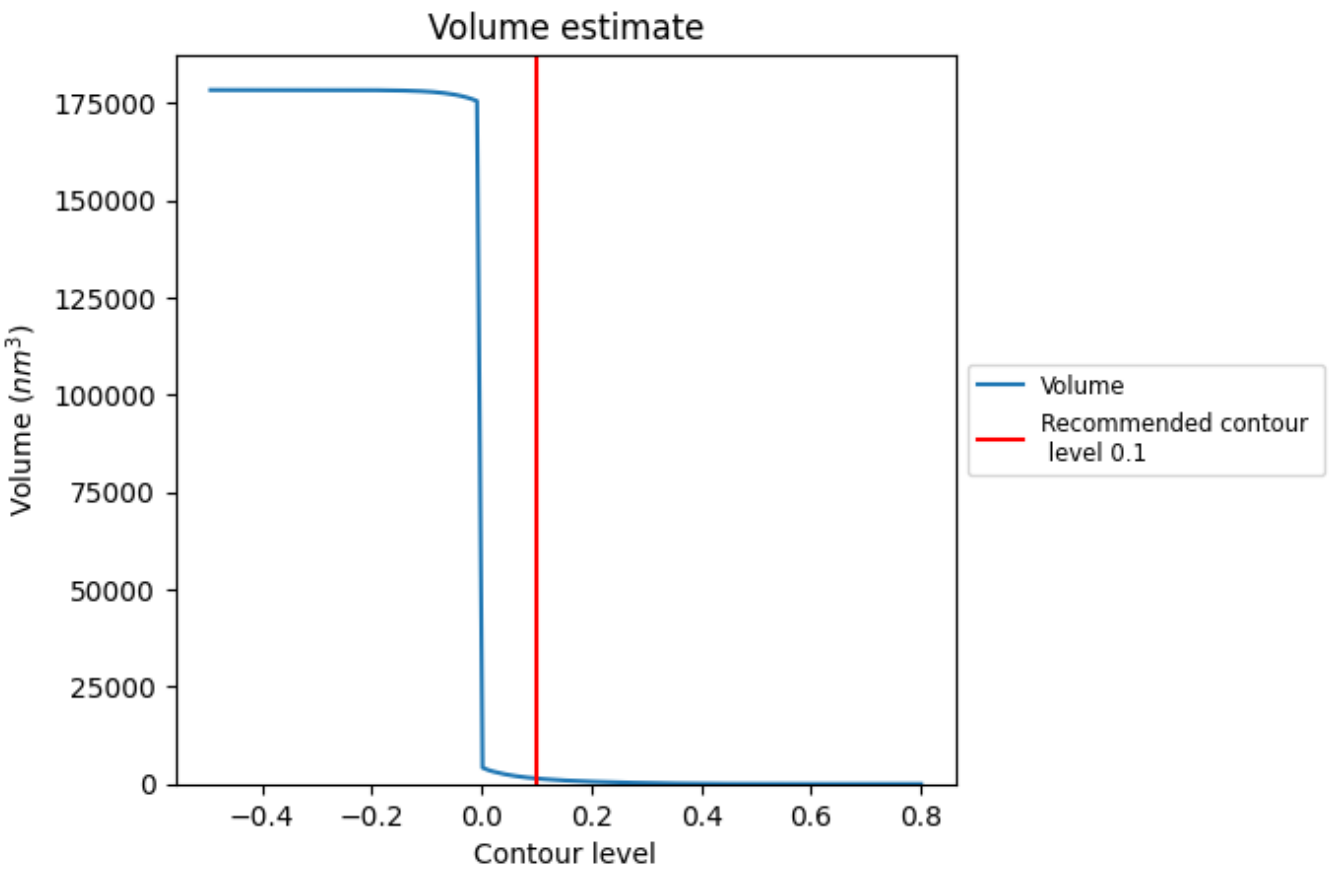
This section contains the results of statistical analysis of the map.

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.

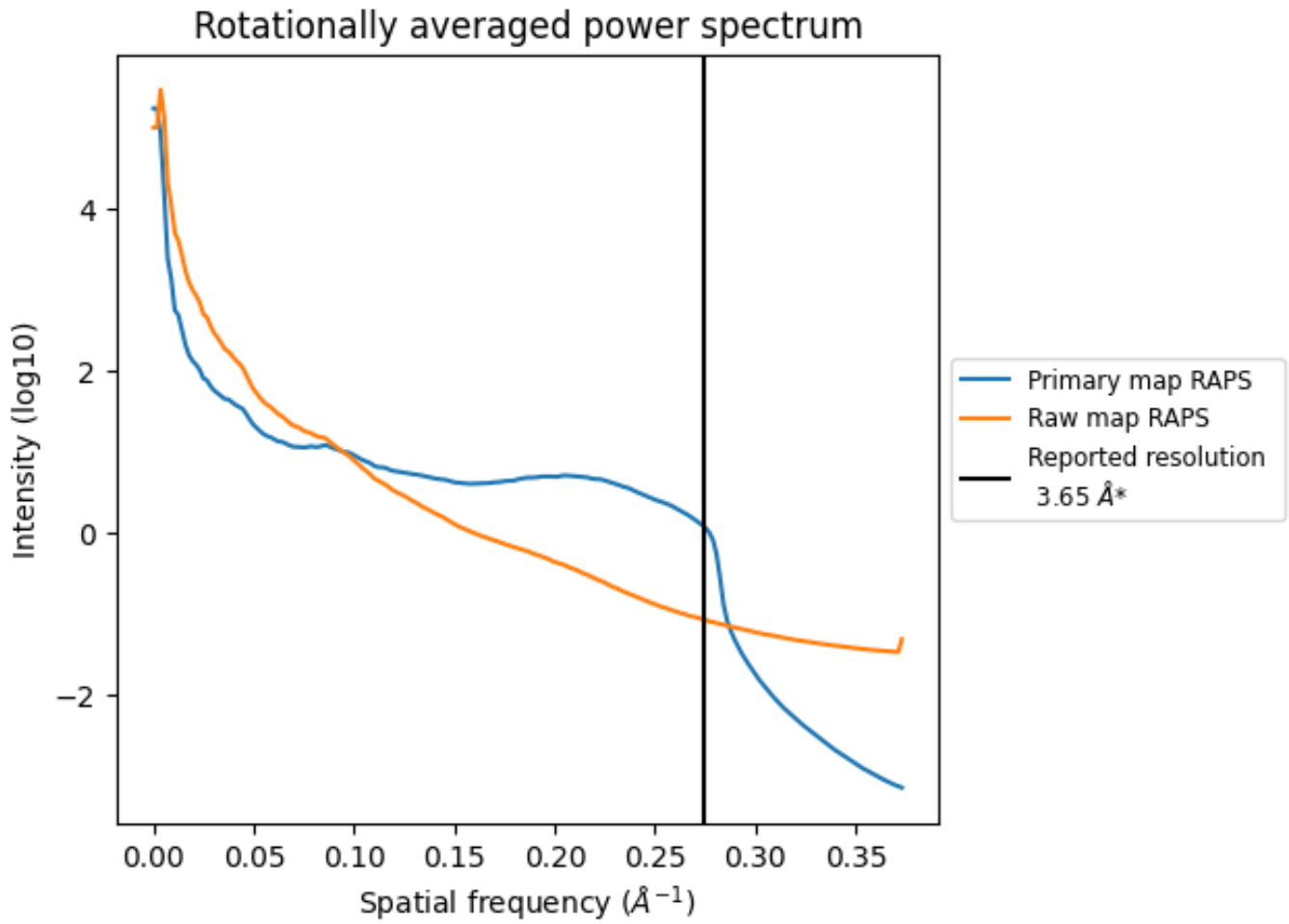
7.2 Volume estimate (i)



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 (i)

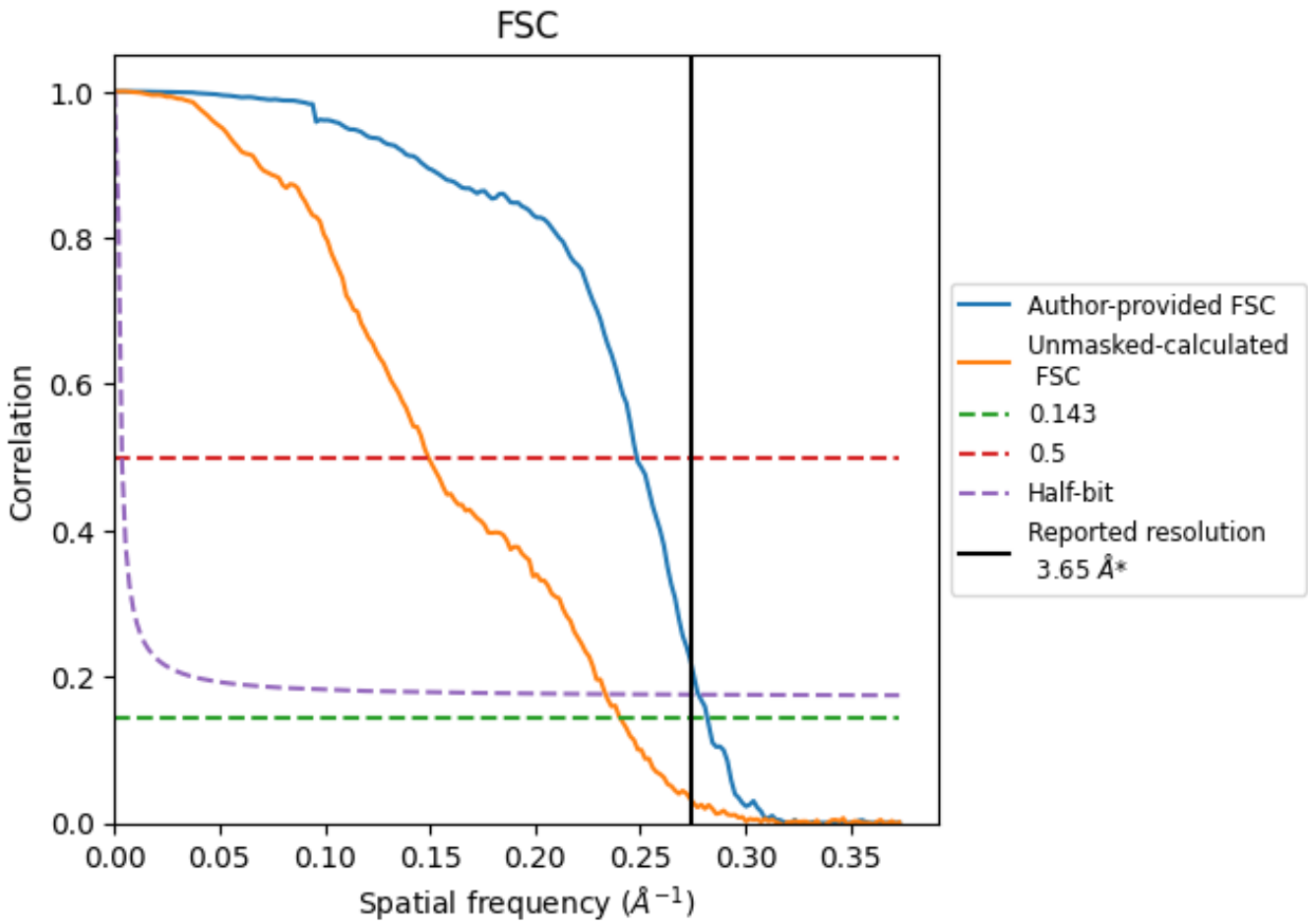


*Reported resolution corresponds to spatial frequency of 0.274 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.274 Å^{-1}

8.2 Resolution estimates (i)

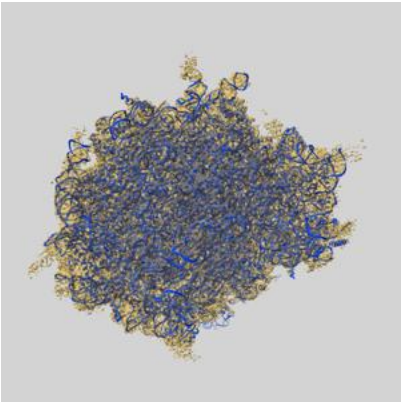
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.65	-	-
Author-provided FSC curve	3.55	4.03	3.60
Unmasked-calculated*	4.16	6.71	4.28

*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 %

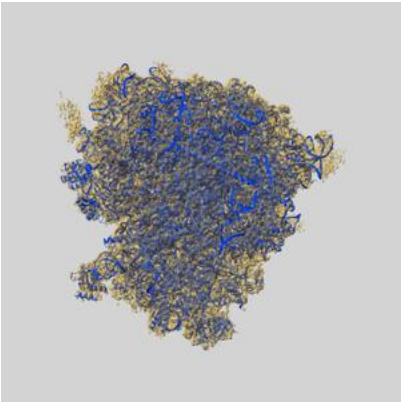
9 Map-model fit (i)

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.

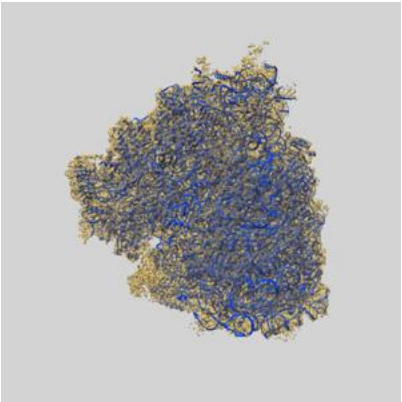
9.1 Map-model overlay (i)



X



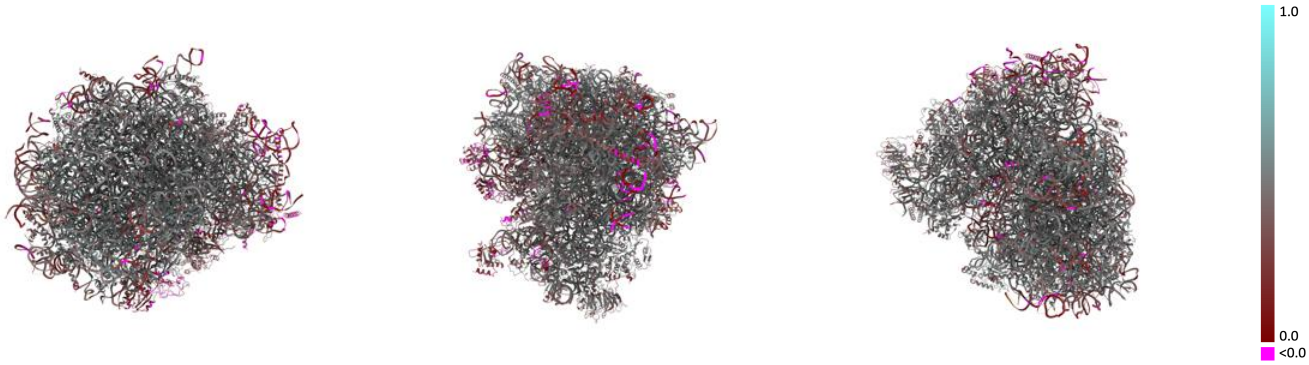
Y



Z

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.

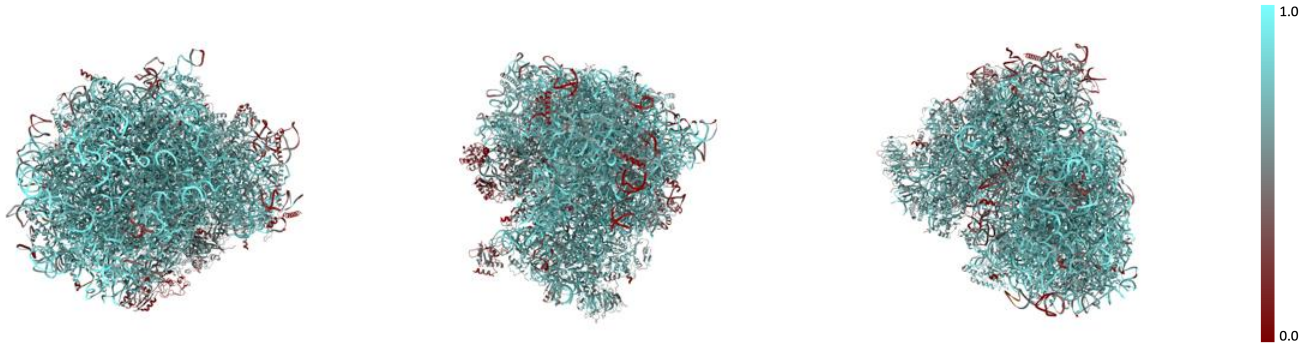
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

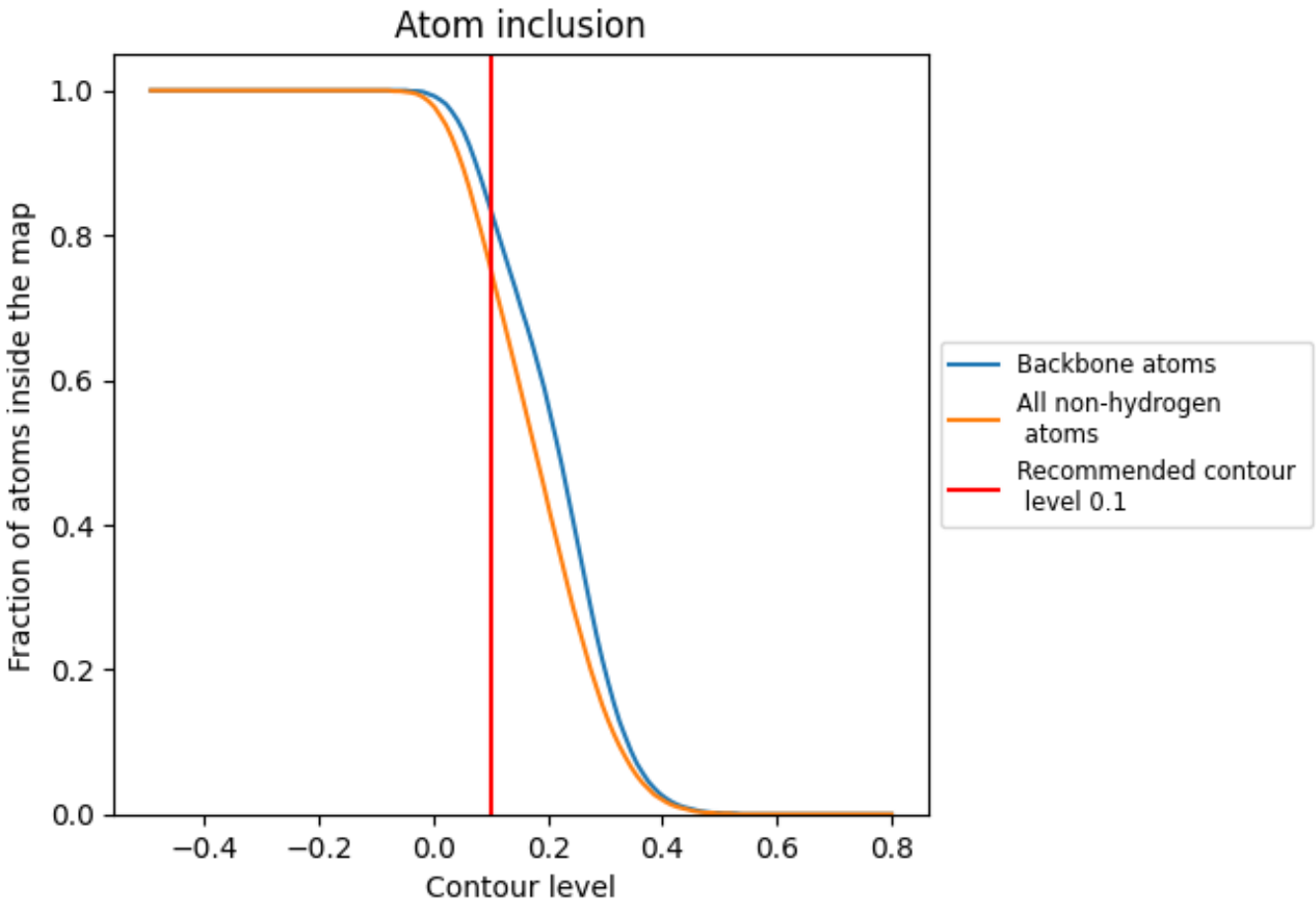
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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, 84% of all backbone atoms, 75% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

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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Continued from previous page...

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