wwPDB EM Validation Summary Report (i)

Nov 20, 2022 – 10:45 AM EST

PDB ID	:	3JAG
EMDB ID	:	EMD-3038
Title	:	Structure of a mammalian ribosomal termination complex with ABCE1, eRF1(AAQ), and the UAA stop codon
Authors	:	Brown, A.; Shao, S.; Murray, J.; Hegde, R.S.; Ramakrishnan, V.
Deposited on	:	2015-06-10
Resolution	:	3.65 Å(reported)
Based on initial models	:	3J7P, 1DT9, 3BK7, 3J92, 4V51

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:

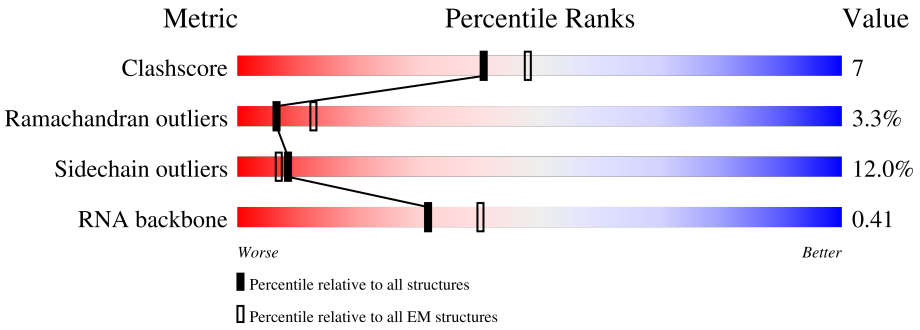
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	244	80% 16% ·
2	B	394	81% 17% ·
3	C	362	· 73% 24% ·
4	D	292	· 83% 16% ·
5	E	248	10% 67% 24% · 5%
6	F	225	· 80% 17% ·
7	G	241	10% 78% 21% ·

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Mol	Chain	Length	Quality of chain
8	H	190	82% 16%
9	I	213	70% 20% 5%
10	J	169	81% 18%
11	L	210	74% 23%
12	M	138	73% 25%
13	N	203	80% 19%
14	O	199	79% 17%
15	P	153	87% 12%
16	Q	187	82% 17%
17	R	180	76% 21%
18	S	175	75% 22%
19	T	159	79% 20%
20	U	99	83% 15%
21	V	131	82% 17%
22	W	63	89% 10%
23	X	119	85% 14%
24	Y	134	81% 16%
25	Z	135	78% 21%
26	a	147	88% 12%
27	b	75	11% 92% 8%
28	c	94	88% 12%
29	d	107	5% 83% 15%
30	e	128	84% 16%
31	f	109	83% 16%
32	g	114	5% 88% 12%

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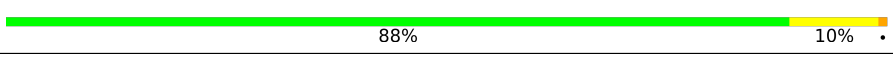
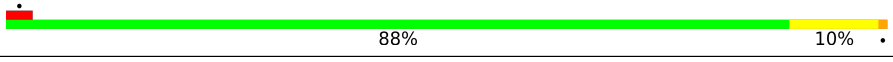
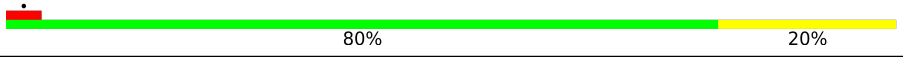
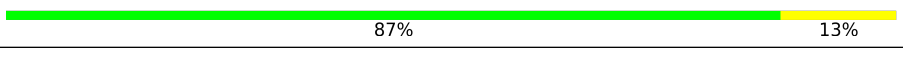
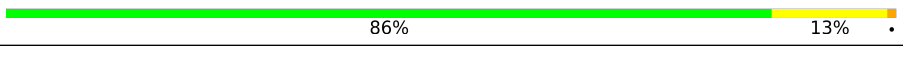
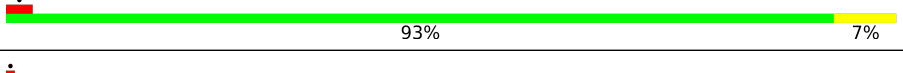
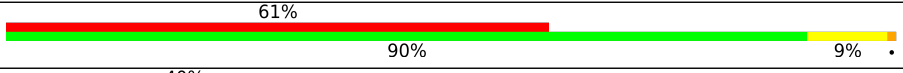
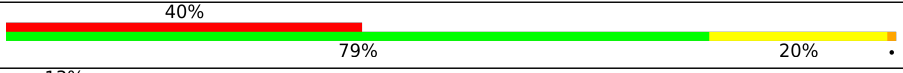
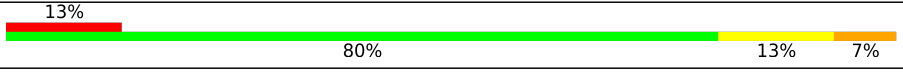
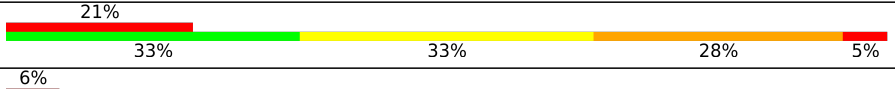
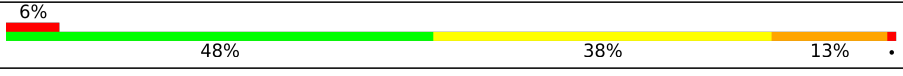
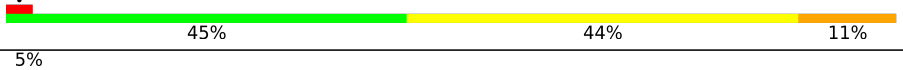
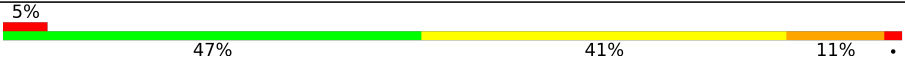
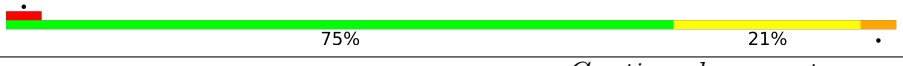
Mol	Chain	Length	Quality of chain
33	h	122	
34	i	102	
35	j	86	
36	k	69	
37	l	50	
38	m	52	
39	n	23	
40	o	104	
41	p	91	
42	r	125	
43	s	198	
44	t	163	
45	1	15	
46	2	76	
47	3	75	
48	5	3662	
49	7	120	
50	8	156	
51	9	1719	
52	AA	208	
53	BB	213	
54	CC	218	
55	DD	227	
56	EE	262	
57	FF	191	

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Mol	Chain	Length	Quality of chain
58	GG	237	8% 75% 24%
59	HH	189	11% 78% 18%
60	II	206	7% 74% 24%
61	JJ	185	78% 17%
62	KK	98	9% 68% 30%
63	LL	152	10% 80% 17%
64	MM	124	45% 77% 22%
65	NN	150	79% 19%
66	OO	136	67% 24% 7%
67	PP	127	10% 77% 20%
68	QQ	141	84% 12%
69	RR	129	7% 80% 16%
70	SS	137	78% 18%
71	TT	141	82% 13% 5%
72	UU	104	9% 83% 14%
73	VV	83	80% 18%
74	WW	129	82% 16%
75	XX	141	77% 21%
76	YY	126	6% 75% 22%
77	ZZ	75	5% 84% 16%
78	aa	98	82% 18%
79	bb	83	6% 81% 18%
80	cc	61	5% 85% 15%
81	dd	53	81% 19%
82	ee	57	18% 84% 16%

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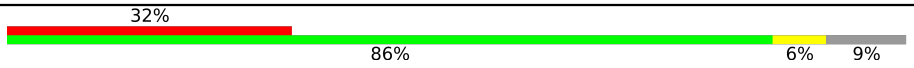
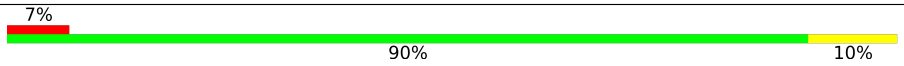
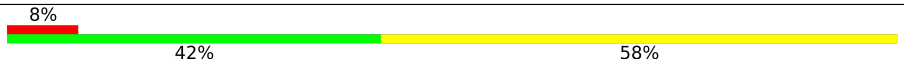
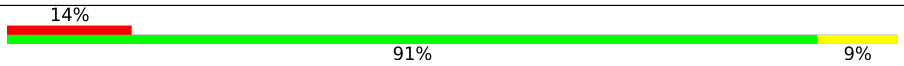
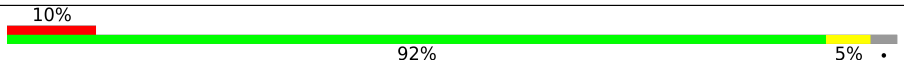
Mol	Chain	Length	Quality of chain
83	ff	69	
84	gg	313	
85	hh	12	
86	ii	416	
87	jj	594	

2 Entry composition (i)

There are 91 unique types of molecules in this entry. The entry contains 226469 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	244	1868	1171	382	309	6	0	0

- Molecule 2 is a protein called uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	394	3148	2007	591	537	13	0	0

- 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

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	361	LYS	-	EXPRESSION TAG	UNP G1SVW5
C	362	SER	-	EXPRESSION TAG	UNP G1SVW5
C	363	ASP	-	EXPRESSION TAG	UNP G1SVW5

- Molecule 4 is a protein called uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	292	2386	1509	437	426	14	0	0

- Molecule 5 is a protein called eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	236	1898	1215	362	318	3	0	0

- Molecule 6 is a protein called uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	225	Total	C	N	O	S	0	0
			1870	1202	358	301	9		

- Molecule 7 is a protein called eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	241	Total	C	N	O	S	0	0
			1934	1233	371	326	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	191	GLY	CYS	CONFLICT	UNP G1STW0

- Molecule 8 is a protein called uL6.

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

- Molecule 9 is a protein called uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	204	Total	C	N	O	S	0	0
			1655	1051	319	272	13		

- Molecule 10 is a protein called uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	169	Total	C	N	O	S	0	0
			1353	855	252	240	6		

- Molecule 11 is a protein called eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	210	Total	C	N	O	S	0	0
			1703	1065	354	280	4		

- Molecule 12 is a protein called eL14.

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

- Molecule 13 is a protein called eL15.

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

- Molecule 14 is a protein called uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	199	Total	C	N	O	S	0	0
			1638	1056	321	256	5		

- Molecule 15 is a protein called uL22.

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

- Molecule 16 is a protein called eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	187	Total	C	N	O	S	0	0
			1506	941	311	249	5		

- Molecule 17 is a protein called eL19.

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

- Molecule 18 is a protein called eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	175	Total	C	N	O	S	0	0
			1454	925	284	235	10		

- Molecule 19 is a protein called eL21.

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

- Molecule 20 is a protein called eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	99	Total	C	N	O	S	0	0
			808	518	141	147	2		

- Molecule 21 is a protein called uL14.

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

- Molecule 22 is a protein called eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	63	Total	C	N	O	S	0	0
			528	337	103	85	3		

- Molecule 23 is a protein called uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	119	Total	C	N	O	S	0	0
			976	624	183	168	1		

- Molecule 24 is a protein called uL24.

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

- Molecule 25 is a protein called eL27.

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

- Molecule 26 is a protein called uL15.

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

- Molecule 27 is a protein called eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	75	Total	C	N	O	S	0	0
			609	378	130	98	3		

- Molecule 28 is a protein called eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	c	94	Total	C	N	O	S	0	0
			732	465	130	131	6		

- Molecule 29 is a protein called eL31.

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

- Molecule 30 is a protein called eL32.

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

- Molecule 31 is a protein called eL33.

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

- Molecule 32 is a protein called eL34.

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

- Molecule 33 is a protein called uL29.

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

- Molecule 34 is a protein called eL36.

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

- Molecule 35 is a protein called eL37.

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

- Molecule 36 is a protein called eL38.

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

- Molecule 37 is a protein called eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	l	50	Total	C	N	O	S	0	0
			444	281	98	64	1		

- Molecule 38 is a protein called eL40.

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

- Molecule 39 is a protein called eL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	23	Total	C	N	O	S	0	0
			222	134	61	25	2		

- Molecule 40 is a protein called eL42.

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

- Molecule 41 is a protein called eL43.

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

- Molecule 42 is a protein called eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	r	125	Total	C	N	O	S	0	0
			1001	621	206	168	6		

- Molecule 43 is a protein called uL10.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	s	198	Total	C	N	O	S	0	0
			1523	969	265	280	9		

- Molecule 44 is a protein called uL11.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	t	163	Total	C	N	O	S	0	0
			1238	773	230	230	5		

- Molecule 45 is a protein called peptide.

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

- Molecule 46 is a RNA chain called tRNA(Val).

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

- Molecule 47 is a RNA chain called tRNA(Lys).

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
48	5	3662	Total	C	N	O	P	0	0
			78486	34947	14363	25515	3661		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	8	156	Total	C	N	O	P	0	0
			3314	1480	585	1094	155		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
51	9	1719	Total	C	N	O	P	0	0
			36680	16371	6586	12005	1718		

- Molecule 52 is a protein called uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	AA	208	Total	C	N	O	S	0	0
			1642	1045	289	300	8		

- Molecule 53 is a protein called eS1.

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

- Molecule 54 is a protein called uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	CC	218	Total	C	N	O	S	0	0
			1694	1103	287	297	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CC	194	ARG	HIS	CONFLICT	UNP G1TUT9

- Molecule 55 is a protein called uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	DD	227	Total	C	N	O	S	0	0
			1764	1124	317	315	8		

- Molecule 56 is a protein called eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	EE	262	Total	C	N	O	S	0	0
			2073	1323	384	357	9		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
EE	25	GLY	SER	CONFLICT	UNP G1TK17

- Molecule 57 is a protein called uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	FF	191	Total	C	N	O	S	0	0
			1509	943	286	273	7		

- Molecule 58 is a protein called eS6.

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

- Molecule 59 is a protein called eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	HH	189	Total	C	N	O	S	0	0
			1521	969	280	271	1		

- Molecule 60 is a protein called eS8.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 61 is a protein called uS4.

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

- Molecule 62 is a protein called eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	KK	98	Total	C	N	O	S	0	0
			827	539	148	134	6		

- Molecule 63 is a protein called uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	LL	152	Total	C	N	O	S	0	0
			1238	788	232	212	6		

- Molecule 64 is a protein called eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	MM	124	Total	C	N	O	S	0	0
			958	600	170	179	9		

- Molecule 65 is a protein called uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	NN	150	Total	C	N	O	S	0	0
			1208	773	229	205	1		

- Molecule 66 is a protein called uS11.

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

- Molecule 67 is a protein called uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	PP	127	Total	C	N	O	S	0	0
			1060	673	201	179	7		

- Molecule 68 is a protein called uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	QQ	141	Total	C	N	O	S	0	0
			1124	715	212	194	3		

- Molecule 69 is a protein called eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	RR	129	Total	C	N	O	S	0	0
			1047	658	193	191	5		

- Molecule 70 is a protein called uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	SS	137	Total	C	N	O	S	0	0
			1139	714	231	193	1		

- Molecule 71 is a protein called eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	TT	141	Total	C	N	O	S	0	0
			1102	692	212	195	3		

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 72 is a protein called uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	UU	104	Total	C	N	O	S	0	0
			821	514	155	148	4		

- Molecule 73 is a protein called eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	VV	83	Total	C	N	O	S	0	0
			636	394	118	119	5		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
VV	3	ASN	SER	CONFLICT	UNP G1TM82
VV	4	ASP	ASN	CONFLICT	UNP G1TM82
VV	50	PHE	SER	CONFLICT	UNP G1TM82
VV	75	ALA	SER	CONFLICT	UNP G1TM82

- Molecule 74 is a protein called uS8.

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

- Molecule 75 is a protein called uS12.

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

- Molecule 76 is a protein called eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	YY	126	Total	C	N	O	S	0	0
			1023	646	200	172	5		

- Molecule 77 is a protein called eS25.

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

- Molecule 78 is a protein called eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	aa	98	Total	C	N	O	S	0	0
			781	486	161	129	5		

- Molecule 79 is a protein called eS27.

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

- Molecule 80 is a protein called eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	cc	61	Total	C	N	O	S	0	0
			475	290	92	91	2		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
cc	18	ILE	LEU	CONFLICT	UNP G1TIB4
cc	20	LYS	ARG	CONFLICT	UNP G1TIB4
cc	40	HIS	ARG	CONFLICT	UNP G1TIB4
cc	42	THR	ILE	CONFLICT	UNP G1TIB4

- Molecule 81 is a protein called uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	dd	53	Total	C	N	O	S	0	0
			445	278	90	72	5		

- Molecule 82 is a protein called eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	ee	57	Total	C	N	O	S	0	0
			457	282	101	73	1		

- Molecule 83 is a protein called eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	ff	63	Total	C	N	O	S	0	0
			527	336	99	86	6		

- Molecule 84 is a protein called RACK1.

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

- Molecule 85 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	hh	12	Total	C	N	O	P	0	0
			256	115	46	83	12		

- Molecule 86 is a protein called eRF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	ii	416	Total	C	N	O	S	0	0
			3280	2087	559	623	11		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
ii	183	ALA	GLY	ENGINEERED MUTATION	UNP P62495
ii	184	ALA	GLY	ENGINEERED MUTATION	UNP P62495

- Molecule 87 is a protein called ABCE1.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	jj	577	Total	C	N	O	S	0	0
			4551	2910	780	830	31		

- Molecule 88 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
88	C	1	Total	Mg	0
			1	1	
88	I	1	Total	Mg	0
			1	1	
88	P	1	Total	Mg	0
			1	1	
88	Q	1	Total	Mg	0
			1	1	
88	V	1	Total	Mg	0
			1	1	
88	g	1	Total	Mg	0
			1	1	

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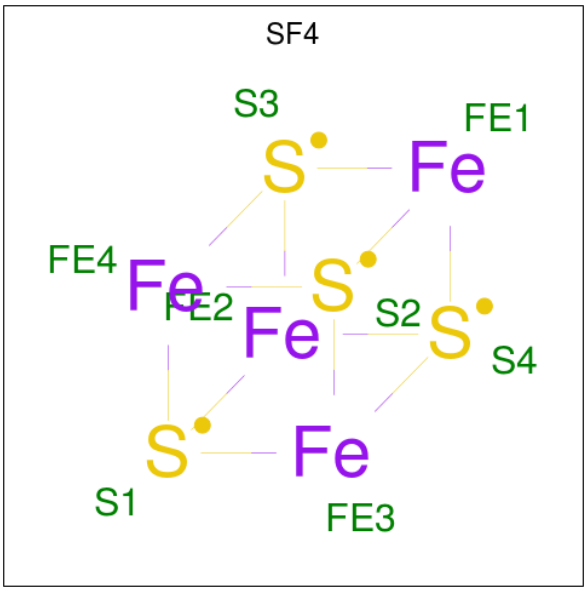
Mol	Chain	Residues	Atoms	AltConf
88	5	146	Total Mg 146 146	0
88	7	5	Total Mg 5 5	0
88	8	2	Total Mg 2 2	0
88	9	35	Total Mg 35 35	0
88	hh	1	Total Mg 1 1	0

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

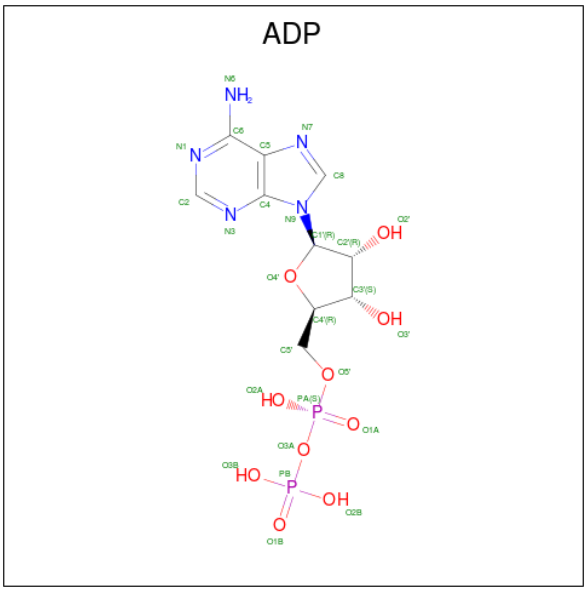
Mol	Chain	Residues	Atoms	AltConf
89	g	1	Total Zn 1 1	0
89	j	1	Total Zn 1 1	0
89	m	1	Total Zn 1 1	0
89	o	1	Total Zn 1 1	0
89	p	1	Total Zn 1 1	0
89	aa	1	Total Zn 1 1	0
89	dd	1	Total Zn 1 1	0
89	ff	1	Total Zn 1 1	0

- Molecule 90 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
90	jj	1	Total	Fe	S	0
			16	8	8	
90	jj	1	Total	Fe	S	0
			16	8	8	

- Molecule 91 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
91	jj	1	Total	C	N	O	P	0
			54	20	10	20	4	

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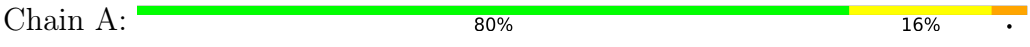
Mol	Chain	Residues	Atoms					AltConf
91	jj	1	Total	C	N	O	P	0
			54	20	10	20	4	

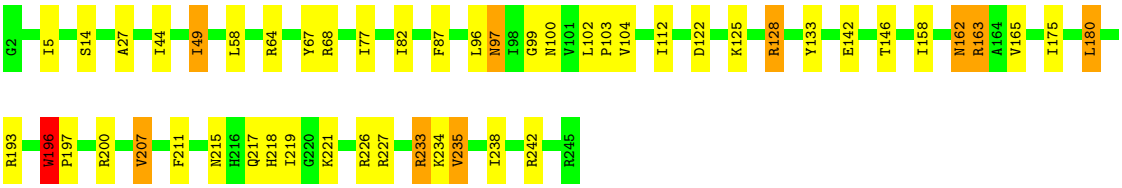
3 Residue-property plots (i)

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

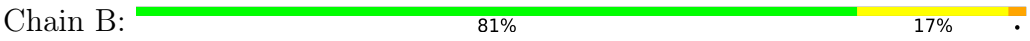
Chain A:

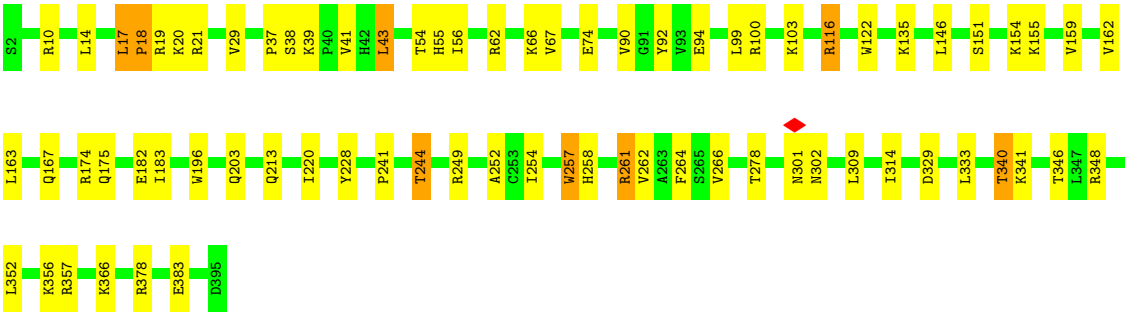




- Molecule 2: uL3

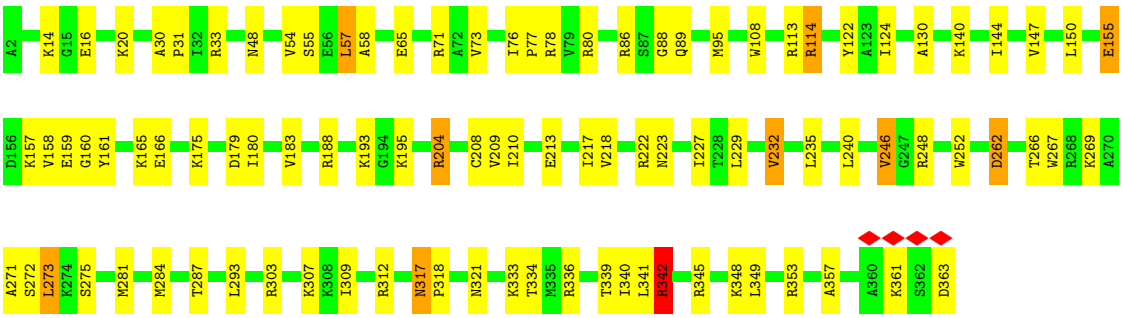
Chain B:





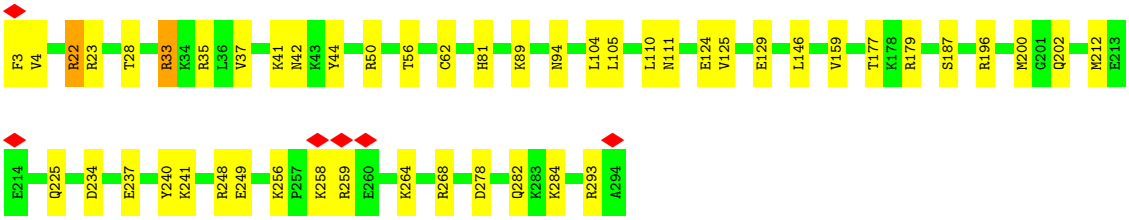
- Molecule 3: uL4

Chain C:



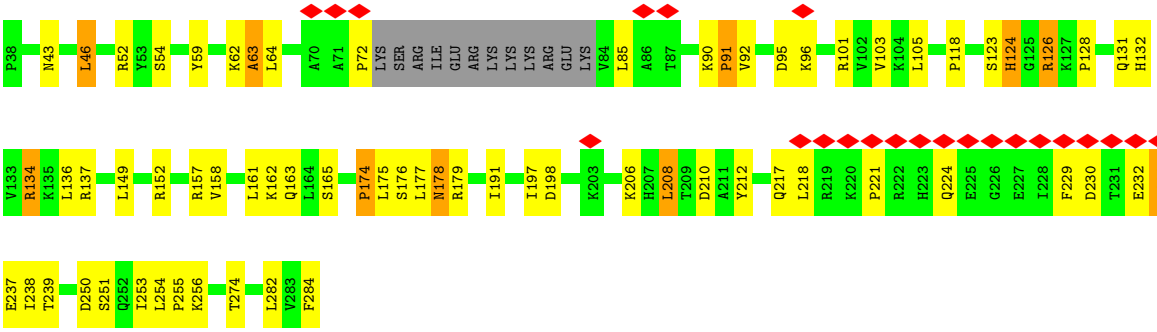
• Molecule 4: uL18

Chain D:



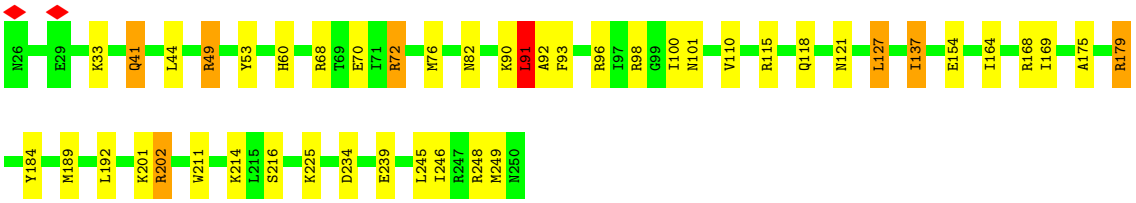
• Molecule 5: eL6

Chain E:



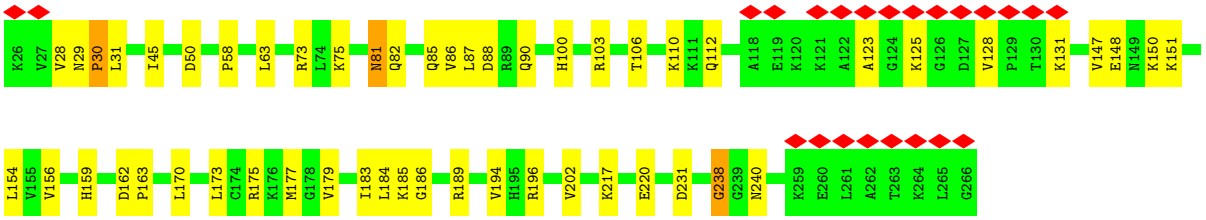
• Molecule 6: uL30

Chain F:



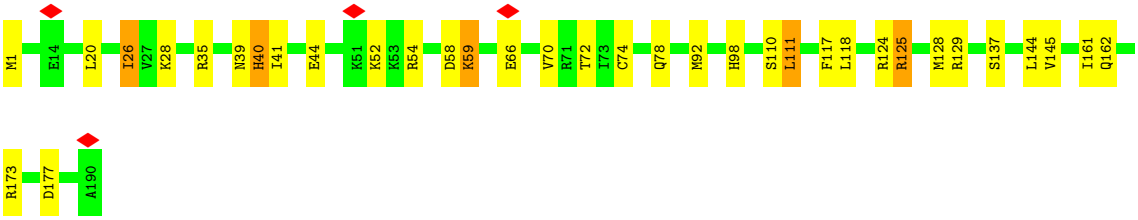
• Molecule 7: eL8

Chain G:



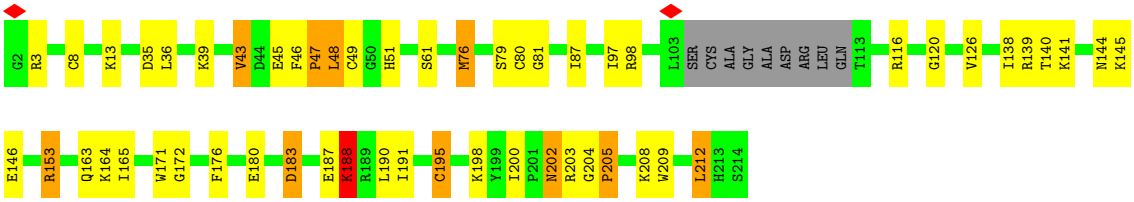
• Molecule 8: uL6

Chain H:



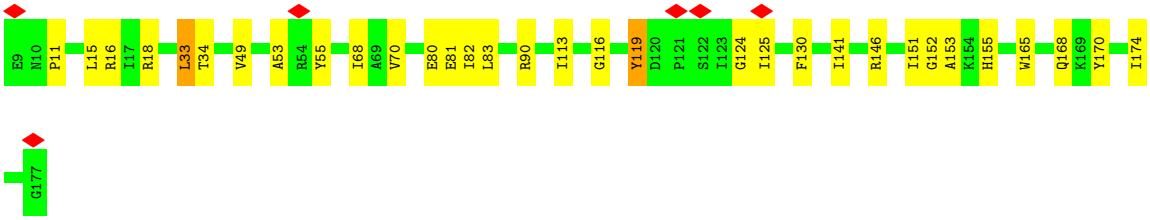
• Molecule 9: uL16

Chain I:



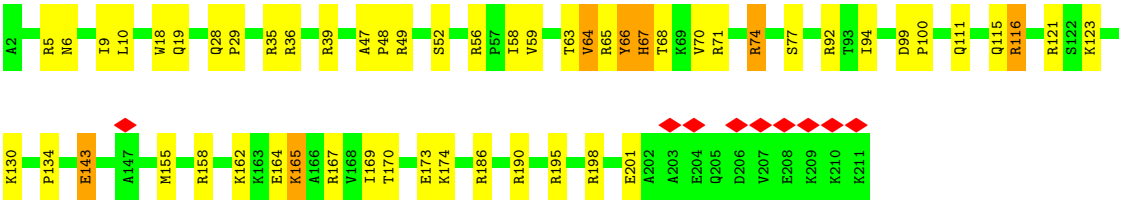
• Molecule 10: uL5

Chain J:



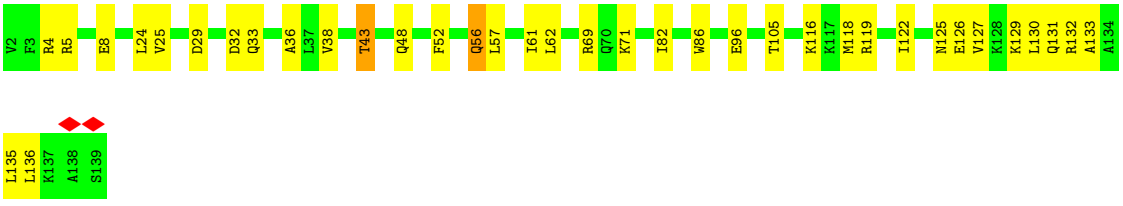
• Molecule 11: eL13

Chain L:



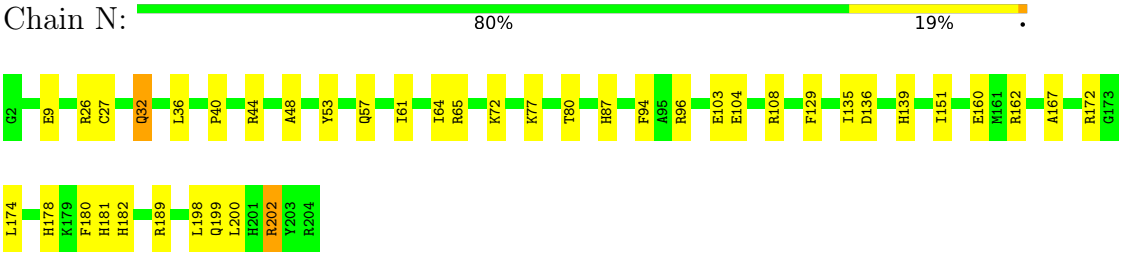
• Molecule 12: eL14

Chain M:



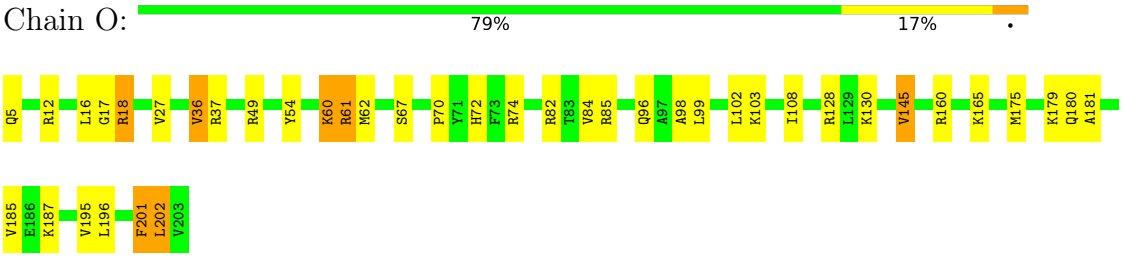
• Molecule 13: eL15

Chain N:



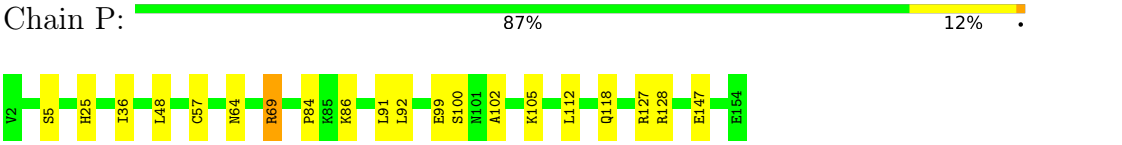
• Molecule 14: uL13

Chain O:



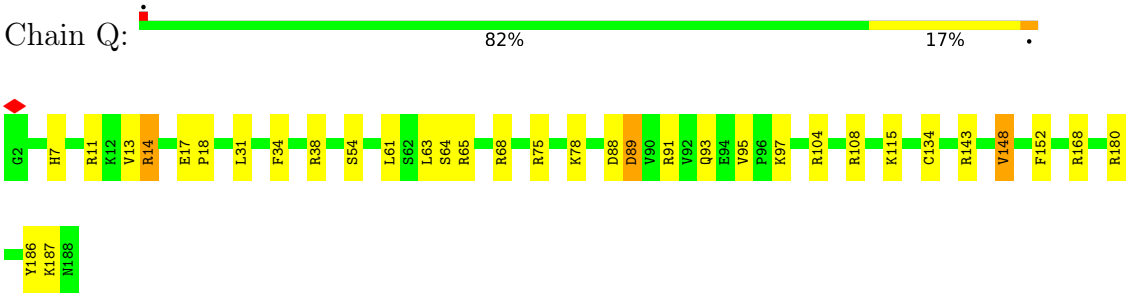
• Molecule 15: uL22

Chain P:



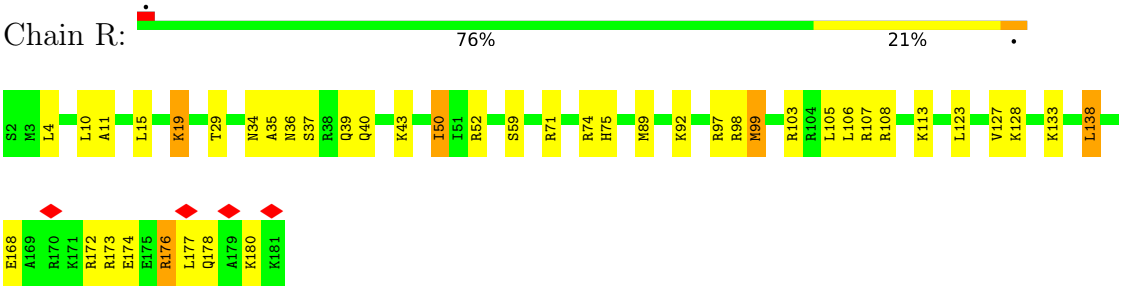
• Molecule 16: eL18

Chain Q:



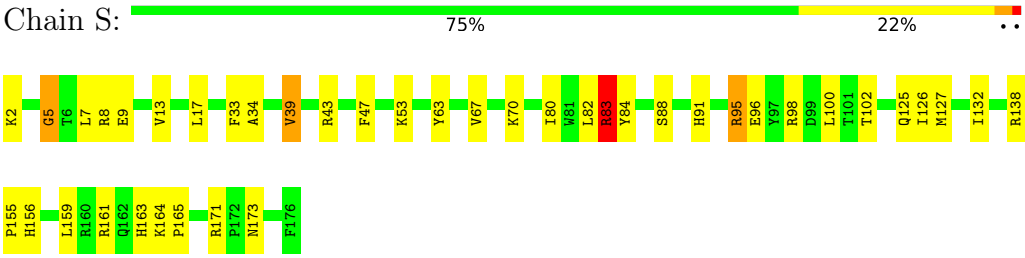
• Molecule 17: eL19

Chain R:



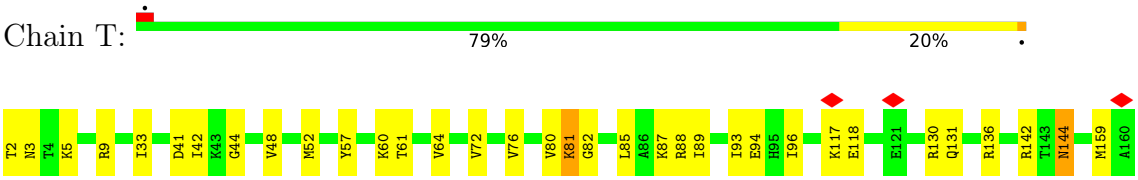
• Molecule 18: eL20

Chain S:



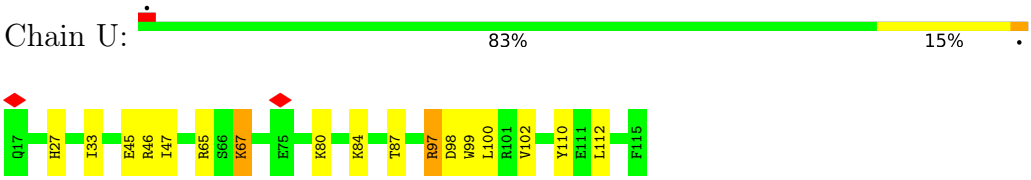
• Molecule 19: eL21

Chain T:



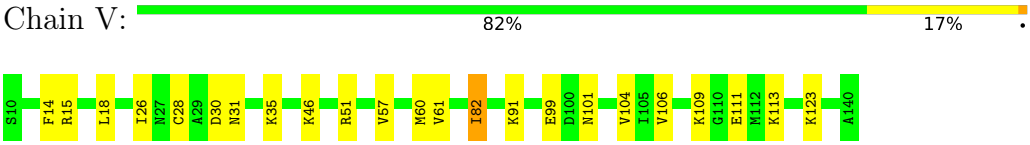
• Molecule 20: eL22

Chain U:



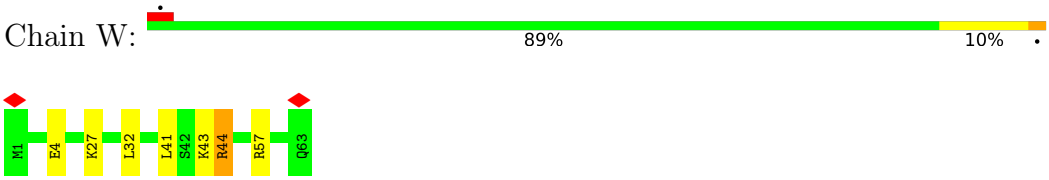
• Molecule 21: uL14

Chain V:



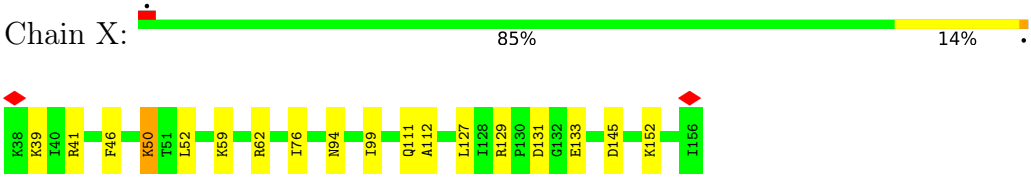
• Molecule 22: eL24

Chain W:



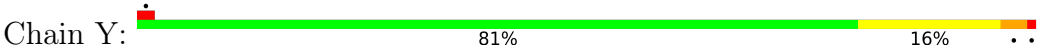
• Molecule 23: uL23

Chain X:



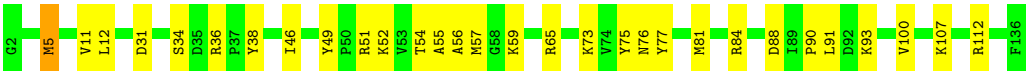
• Molecule 24: uL24

Chain Y:



• Molecule 25: eL27

Chain Z:

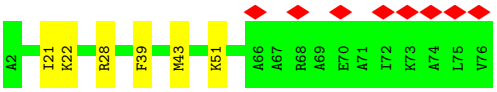


• Molecule 26: uL15

Chain a:

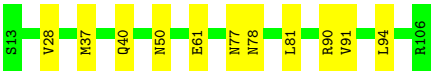
• Molecule 27: eL29

Chain b:



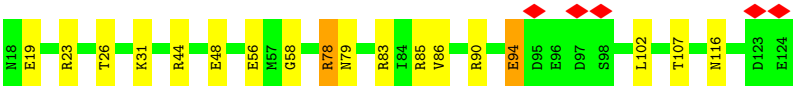
• Molecule 28: eL30

Chain c:



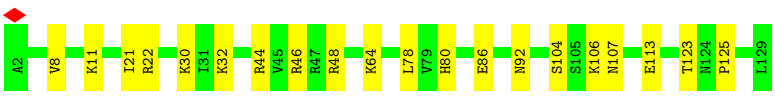
• Molecule 29: eL31

Chain d:



• Molecule 30: eL32

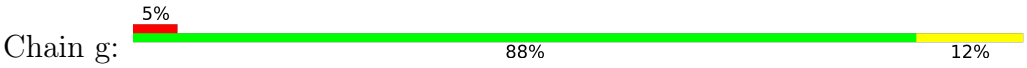
Chain e:

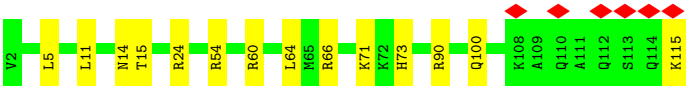


• Molecule 31: eL33

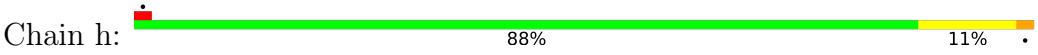
Chain f:

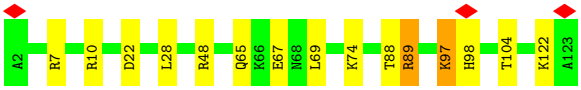
• Molecule 32: eL34



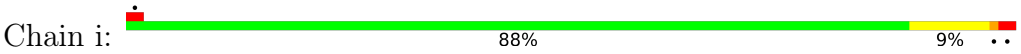


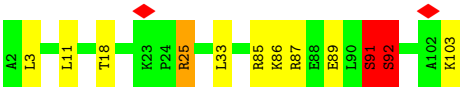
• Molecule 33: uL29



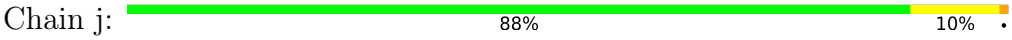


• Molecule 34: eL36

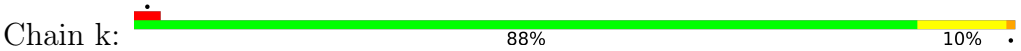


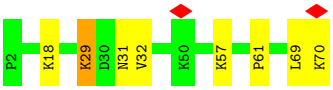


• Molecule 35: eL37

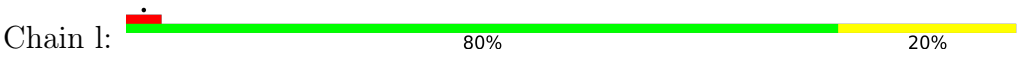


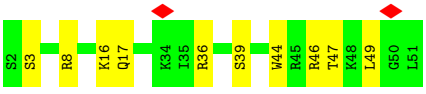
• Molecule 36: eL38



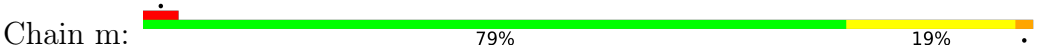


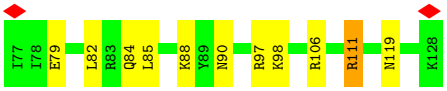
• Molecule 37: eL39





• Molecule 38: eL40



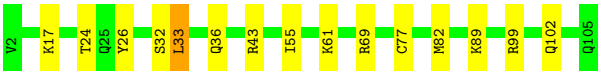


• Molecule 39: eL41

Chain n:

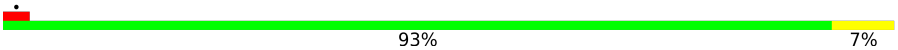
• Molecule 40: eL42

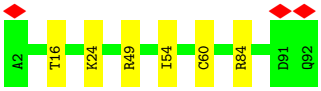
Chain o:



• Molecule 41: eL43

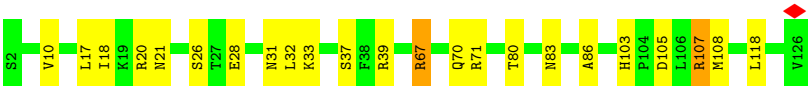
Chain p:





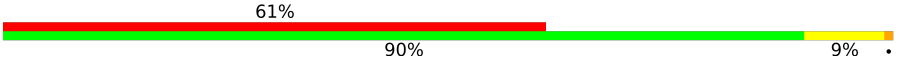
• Molecule 42: eL28

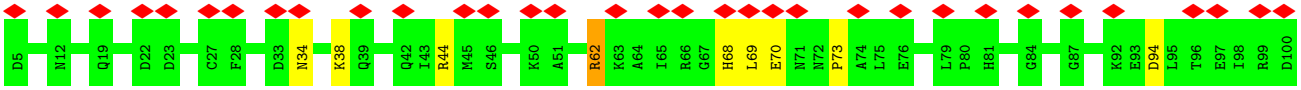
Chain r:

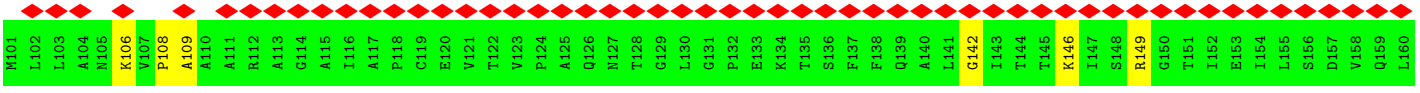


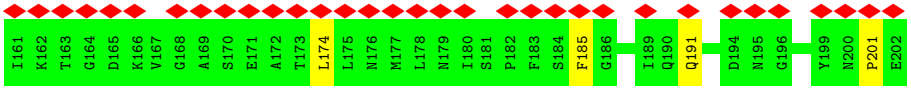
• Molecule 43: uL10

Chain s:



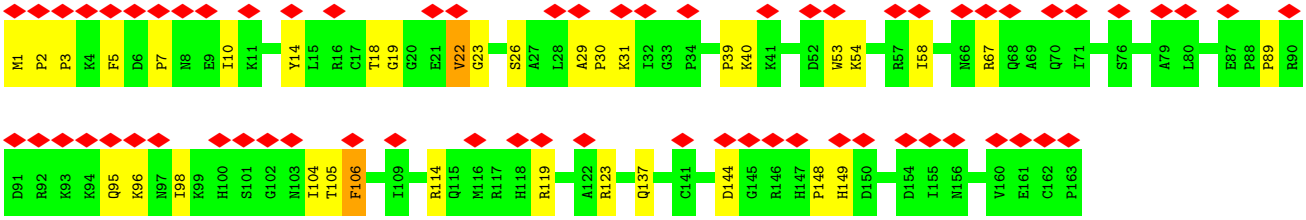




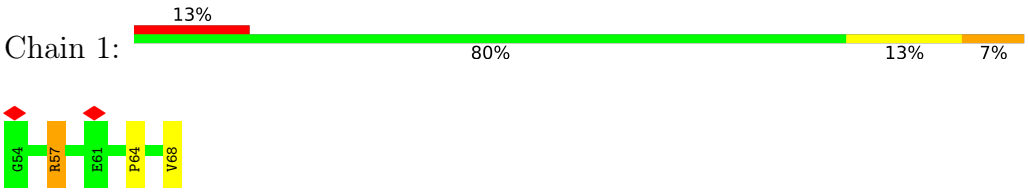


• Molecule 44: uL11

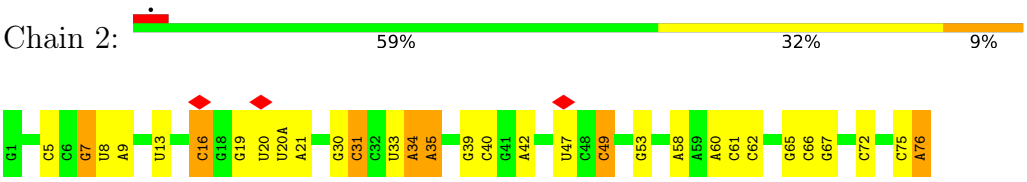
Chain t:



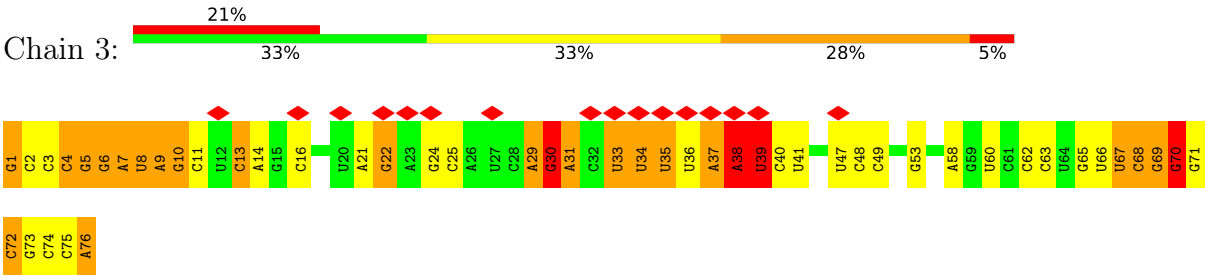
• Molecule 45: peptide



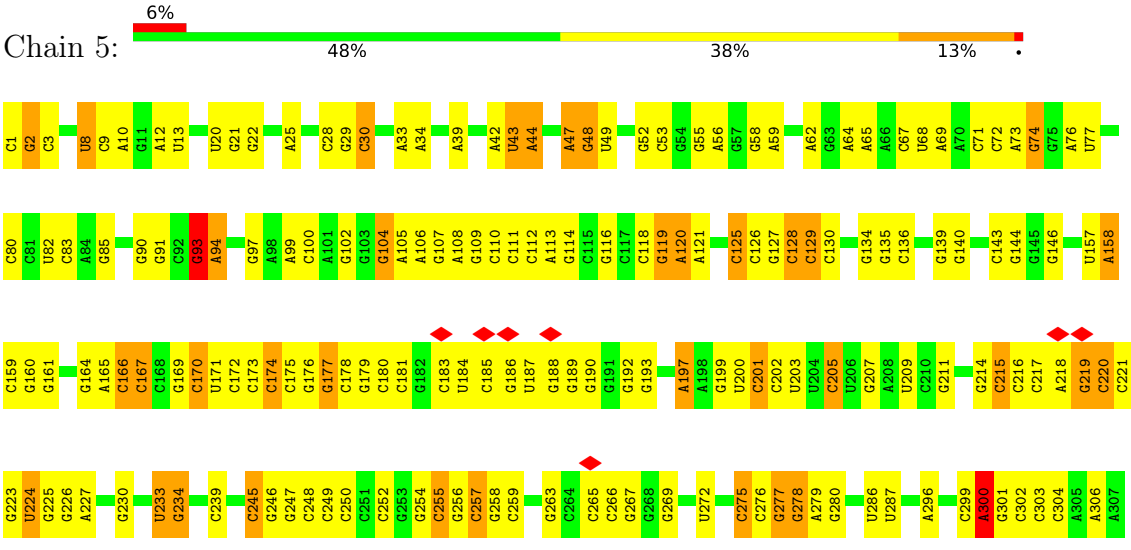
• Molecule 46: tRNA(Val)

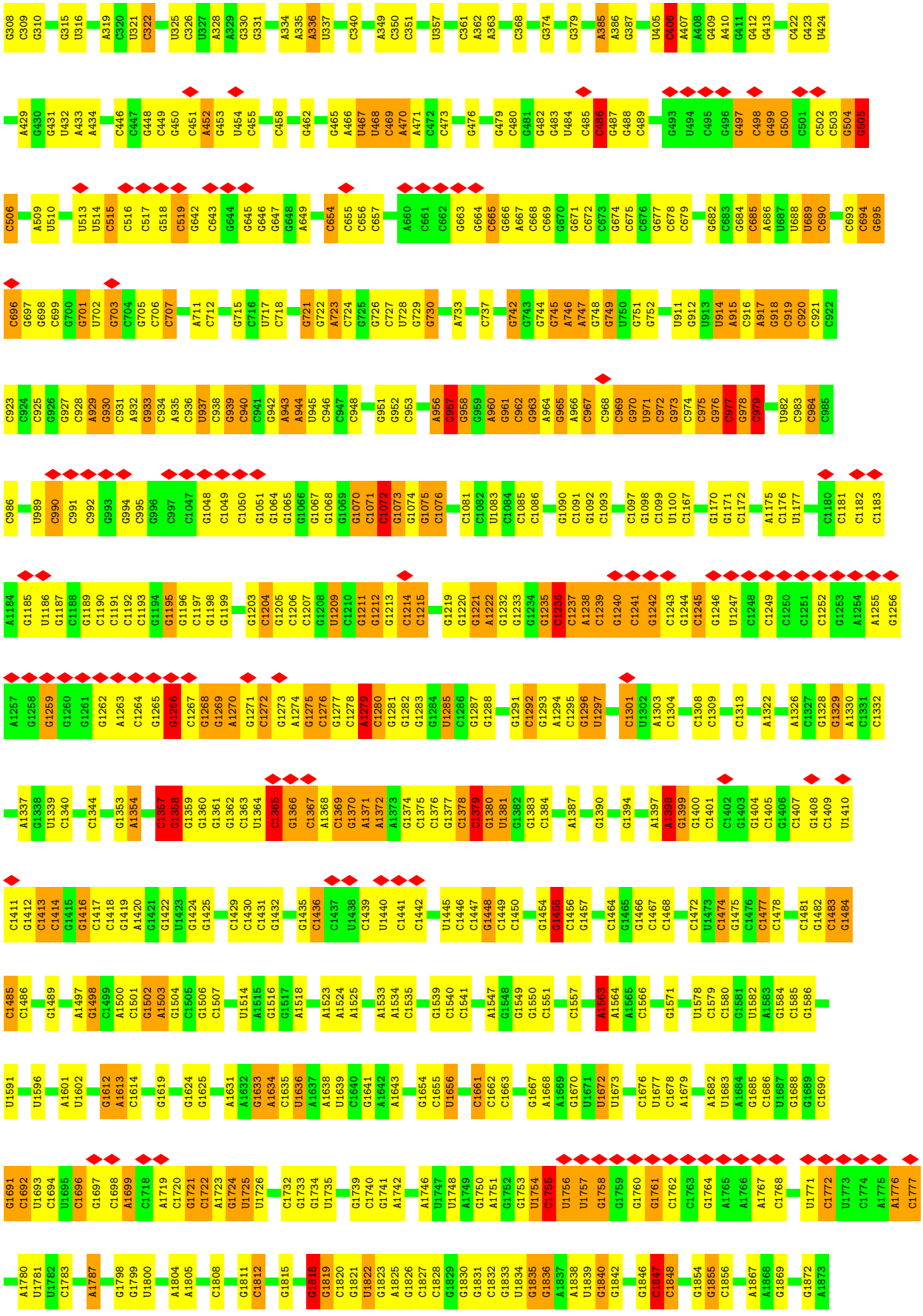


• Molecule 47: tRNA(Lys)



• Molecule 48: 28S ribosomal RNA

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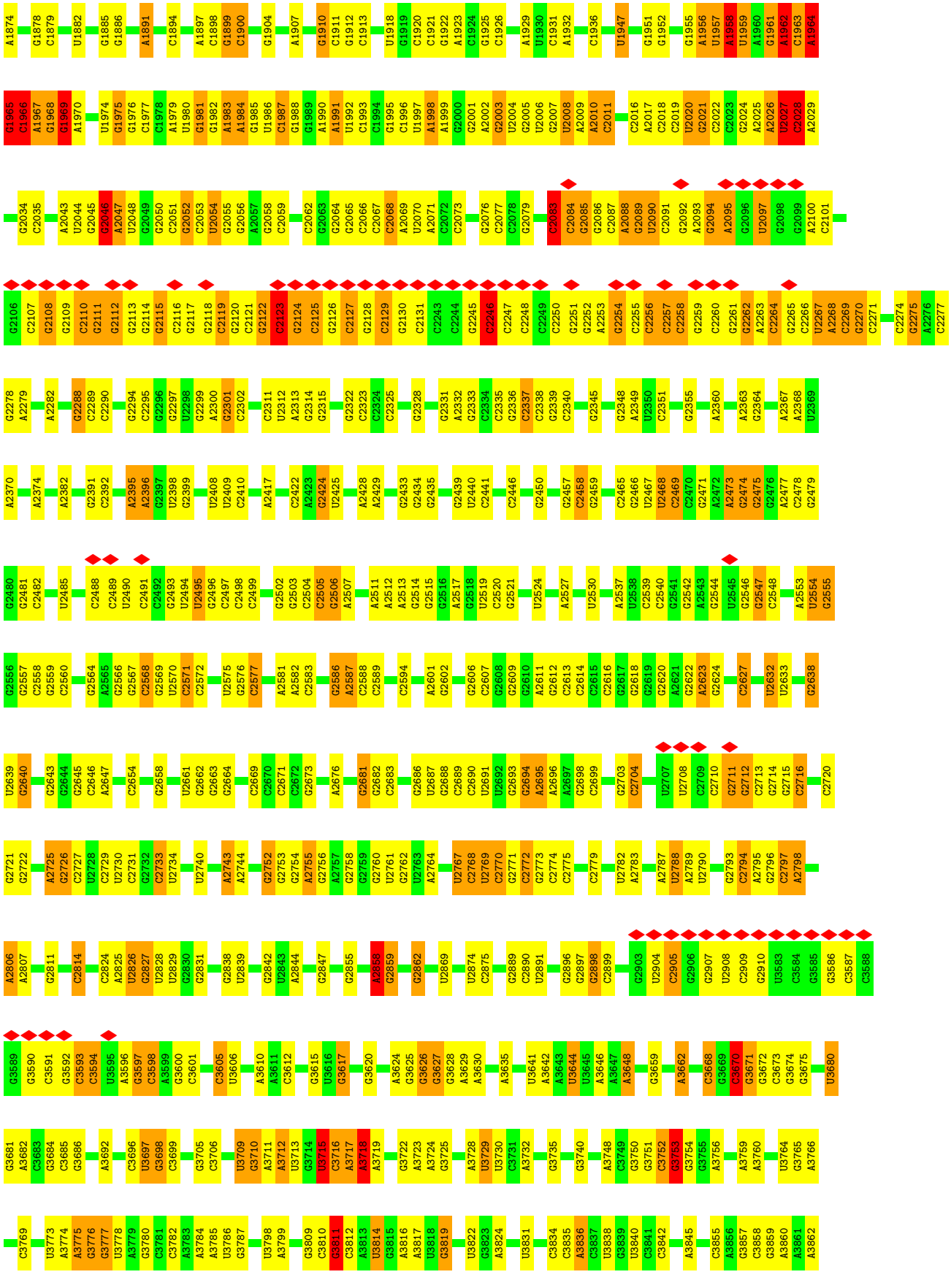
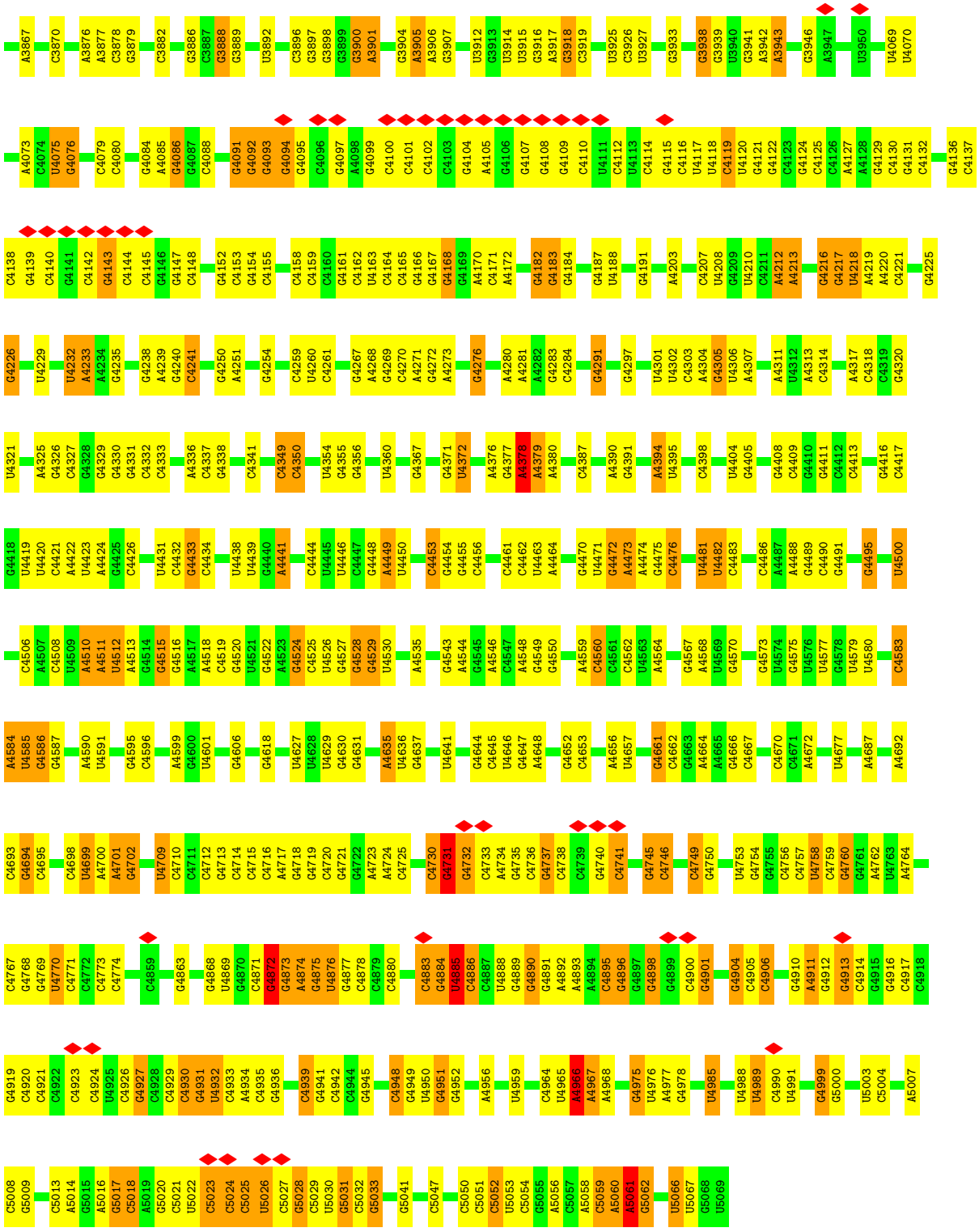
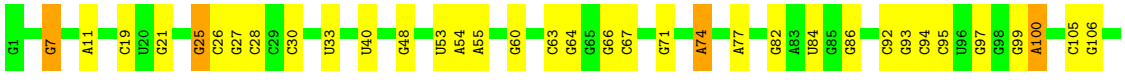
A429 G430 G431 U432 A433 A434 C446 C447 G448 C449 G450 C451 A452 G453 U454 C455 C458 G462 G465 A466 U467 U468 C469 A470 A471 C472 C473 G476 G479 C480 G481 G482 G483 U484 C485 C486 G487 G488 C489 G493 U494 C495 G496 G497 C498 G499 G500 C501 C502 C503 G504 G505
C506 A509 U510 U513 U514 C515 C516 C517 G518 C519 G642 C643 G644 G645 G646 G647 G648 A649 C654 C655 C656 C657 A660 C661 C662 G663 G664 C665 G666 A667 C668 C669 G670 G671 C672 C673 G674 C675 C676 G677 C678 C679 G682 C683 G684 C685 A686 U687 U688 U689 G690 C693 G694 G695
C696 G697 G698 C699 G700 G701 U702 G703 C704 G705 C706 C707 A711 C712 G715 G716 U717 C718 G721 G722 A723 C724 G725 G726 C727 U728 G729 G730 A733 C737 G742 G743 G744 G745 A746 A747 G748 G749 U750 G751 G752 U911 G912 U913 U914 A915 C916 A917 G918 C919 C920 C921 C922
C923 C924 C925 G926 G927 C928 A929 G930 C931 A932 G933 C934 A935 C936 U937 C938 G939 C940 C941 G942 A943 A944 U945 C946 C947 C948 G951 G952 C953 A956 G957 G958 G959 A960 G961 C962 G963 A964 G965 A966 C967 C968 G969 G970 U971 G972 G973 C974 G975 G976 C977 G978 C979 U982 C983 C984 C985
C986 U989 C990 C991 C992 G993 G994 C995 G996 C997 C1047 C1048 C1049 C1050 G1051 G1064 G1065 G1066 G1067 G1068 G1069 G1070 C1071 C1072 G1073 G1074 G1075 C1076 C1081 C1082 U1083 C1084 C1085 C1086 G1090 C1091 G1092 C1093 C1097 G1098 C1099 U1100 C1167 G1170 G1171 C1172 A1175 C1176 U1177 C1180 C1181 C1182 C1183
A1184 G1185 U1186 G1187 C1188 G1189 C1190 C1191 C1192 C1193 G1194 G1195 G1196 C1197 G1198 C1199 G1203 C1204 G1205 C1206 C1207 G1208 U1209 C1210 G1211 G1212 G1213 C1214 C1215 G1219 G1220 G1221 A1222 G1232 G1233 G1234 G1235 C1236 C1237 A1238 C1239 G1240 C1241 G1242 C1243 G1244 C1245 G1246 U1247 C1248 C1249 C1250 C1251 C1252 G1253 A1254 A1255 G1256
A1257 G1258 G1259 G1260 G1261 G1262 A1263 C1264 G1265 G1266 C1267 G1268 G1269 A1270 G1271 C1272 G1273 A1274 G1275 C1276 G1277 C1278 A1279 C1280 G1281 G1282 G1283 G1284 U1285 C1286 G1287 G1288 G1291 C1292 G1293 A1294 C1295 G1296 U1297 C1301 U1302 A1303 C1304 C1308 C1309 C1313 A1322 A1326 C1327 G1328 G1329 A1330 C1331 C1332
A1337 G1338 U1339 C1340 C1344 G1353 A1354 C1357 G1358 G1359 G1360 G1361 G1362 C1363 U1364 C1365 G1366 C1367 A1368 G1369 G1370 A1371 A1372 A1373 G1374 C1375 C1376 G1377 C1378 C1379 G1380 U1381 G1382 G1383 C1384 A1387 G1390 G1394 A1397 A1398 G1399 G1400 C1401 C1402 G1403 G1404 C1405 G1406 C1407 G1408 C1409 U1410
C1411 G1412 C1413 C1414 G1415 G1416 C1417 C1418 G1419 A1420 G1421 G1422 U1423 G1424 G1425 C1429 C1430 C1431 G1432 G1435 C1436 C1437 U1438 C1439 U1440 C1441 C1442 U1445 C1446 C1447 G1448 C1449 C1450 G1454 G1455 C1456 G1457 C1464 G1465 G1466 C1467 C1468 C1472 U1473 C1474 G1475 C1476 C1477 C1478 C1481 G1482 C1483 G1484
C1485 C1486 G1489 A1497 G1498 C1499 A1500 C1501 G1502 A1503 G1504 C1505 G1506 C1507 U1514 A1515 G1516 C1517 A1518 A1523 A1524 A1525 A1533 A1534 C1535 G1539 C1540 C1541 A1547 G1548 G1549 G1550 C1551 C1557 A1563 A1564 A1565 C1566 G1571 U1578 C1579 C1580 G1581 U1582 A1583 G1584 C1585 G1586
U1591 U1596 A1601 U1602 G1612 A1613 C1614 G1619 G1624 G1625 A1631 A1632 G1633 A1634 C1635 U1636 A1637 A1638 U1639 C1640 G1641 A1642 A1643 G1654 C1655 U1656 C1661 C1662 C1663 G1667 A1668 A1669 G1670 U1671 U1672 U1673 C1676 U1677 C1678 A1679 A1682 U1683 A1684 G1685 C1686 U1687 G1688 G1689 C1690
G1691 C1692 U1693 C1694 U1695 C1696 G1697 C1698 A1699 C1718 A1719 C1720 G1721 C1722 A1723 G1724 U1725 U1726 C1732 G1733 G1734 U1735 G1739 C1740 G1741 A1742 A1746 U1747 U1748 A1749 G1750 A1751 G1752 G1753 U1754 C1755 U1756 U1757 G1758 G1759 G1760 G1761 C1762 C1763 G1764 A1765 A1766 A1767 C1768 U1771 C1772 U1773 C1774 A1775 A1776 C1777
A1780 U1781 U1782 C1783 A1787 G1798 G1799 U1800 A1804 A1805 C1808 G1811 C1812 G1815 G1818 G1819 C1820 G1821 U1822 G1823 A1825 G1826 C1827 C1828 G1829 G1830 G1831 C1832 G1833 U1834 G1835 G1836 A1837 A1838 U1839 G1840 G1842 G1846 C1847 C1848 G1854 G1855 C1856 A1867 A1868 G1869 G1872 A1873

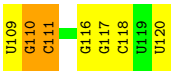




• Molecule 49: 5S ribosomal RNA

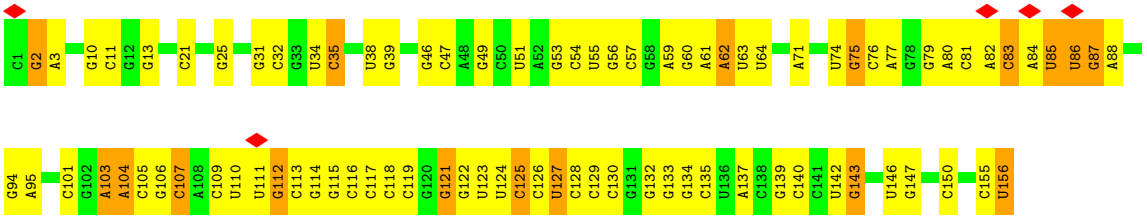
Chain 7:





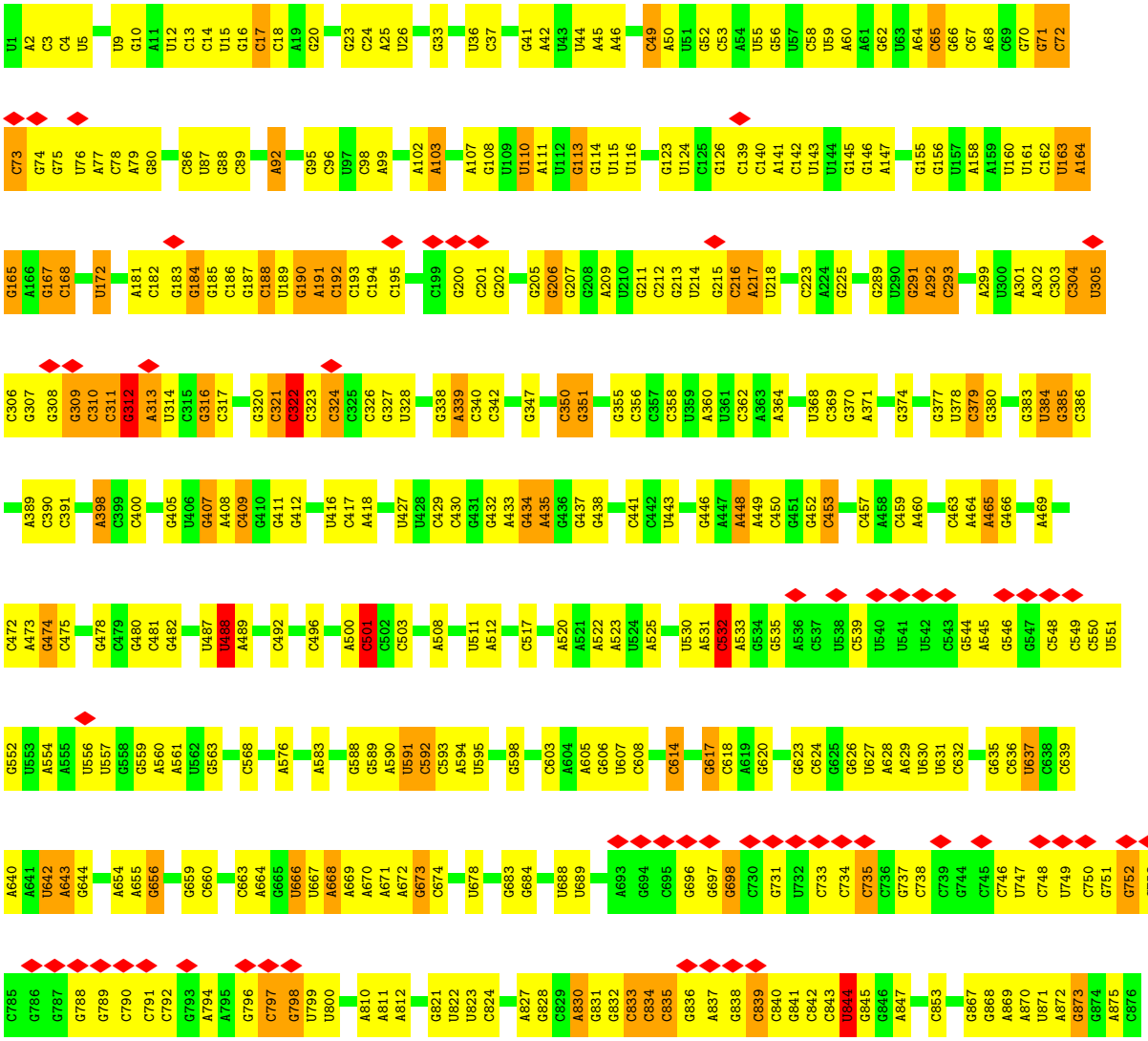
• Molecule 50: 5.8S ribosomal RNA

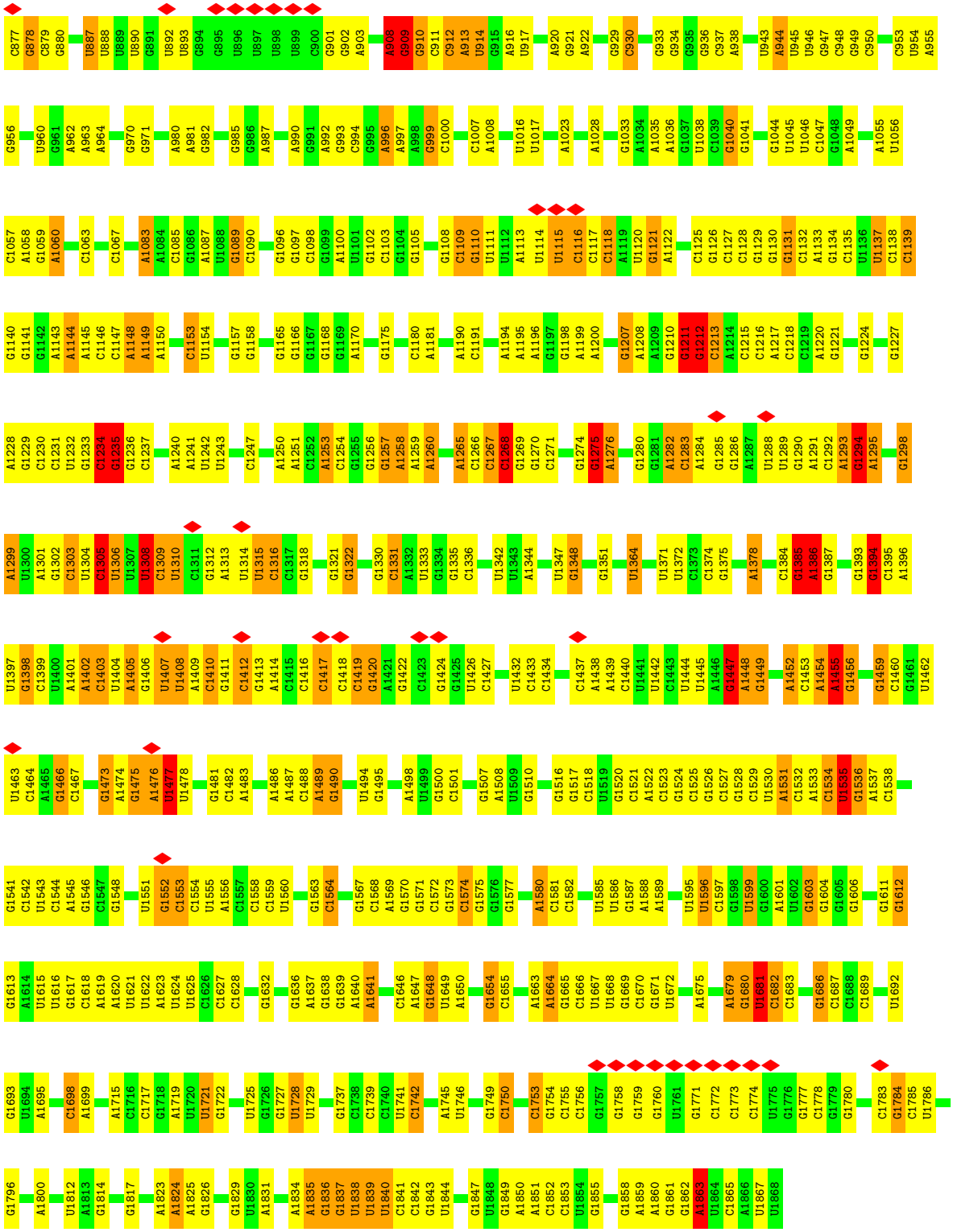
Chain 8:



• Molecule 51: 18S ribosomal RNA

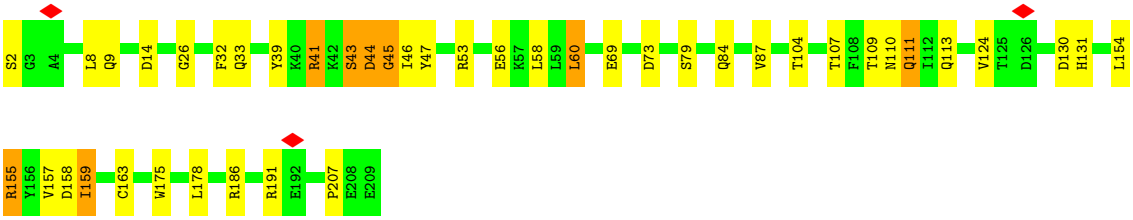
Chain 9:





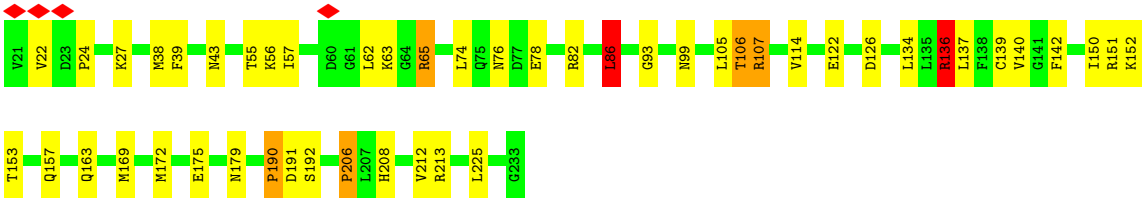
• Molecule 52: uS2

Chain AA:



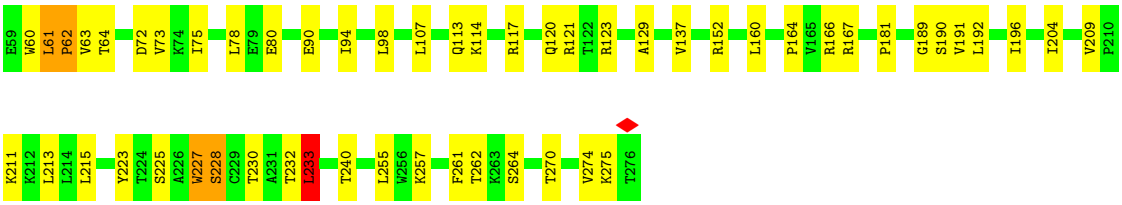
• Molecule 53: eS1

Chain BB:



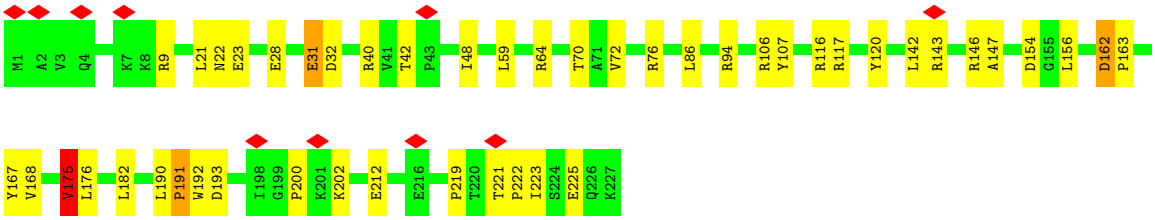
• Molecule 54: uS5

Chain CC:



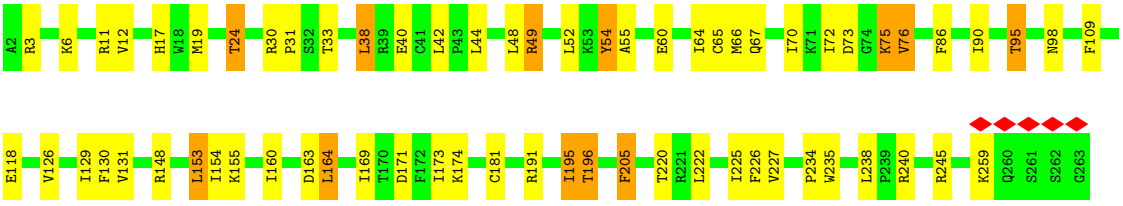
• Molecule 55: uS3

Chain DD:



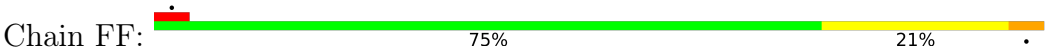
• Molecule 56: eS4

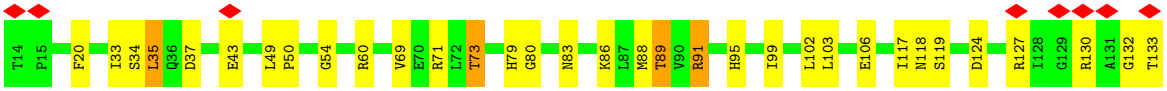
Chain EE:



• Molecule 57: uS7

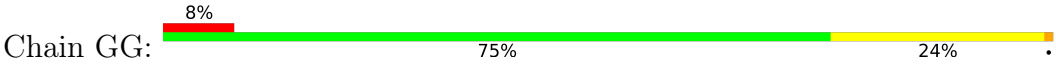
Chain FF:

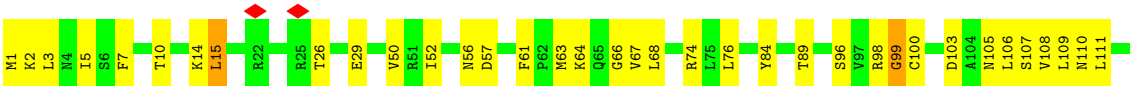




• Molecule 58: eS6

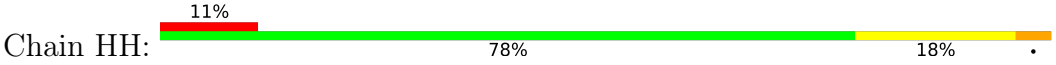
Chain GG:

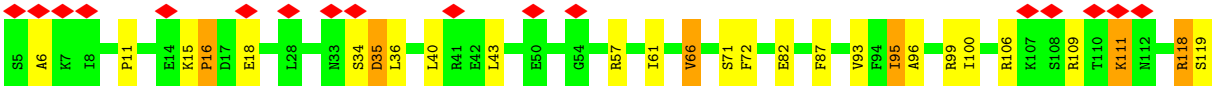




• Molecule 59: eS7

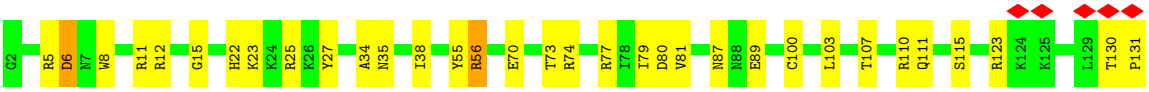
Chain HH:

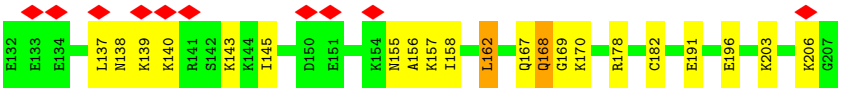




• Molecule 60: eS8

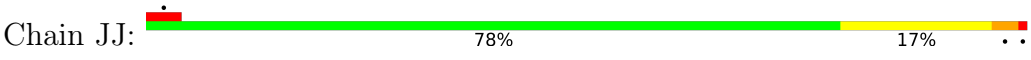
Chain II:

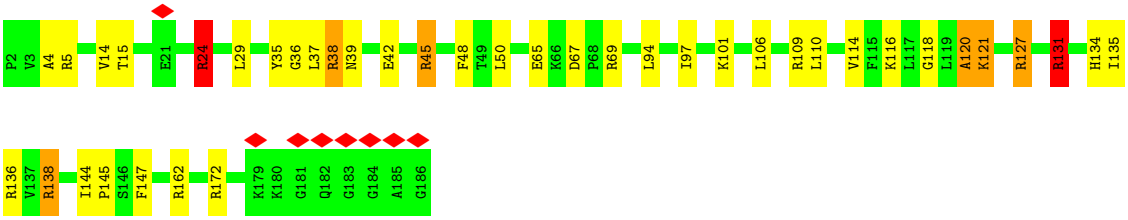




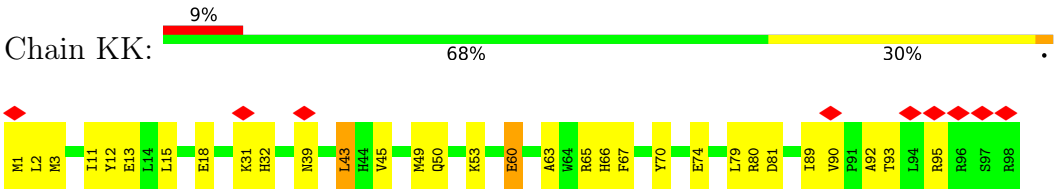
• Molecule 61: uS4

Chain JJ:

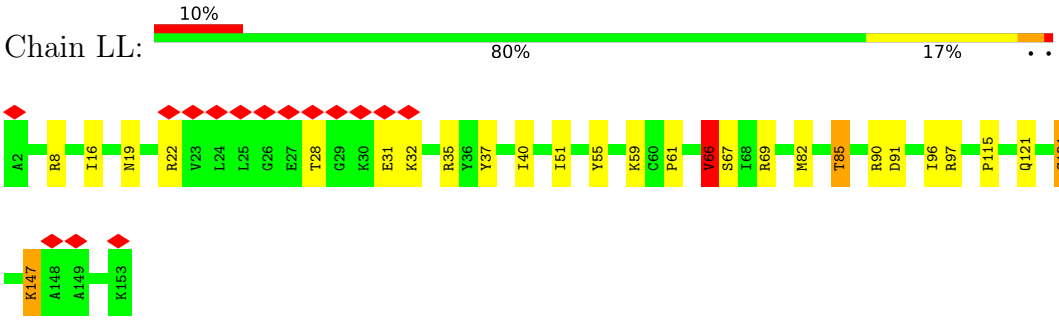




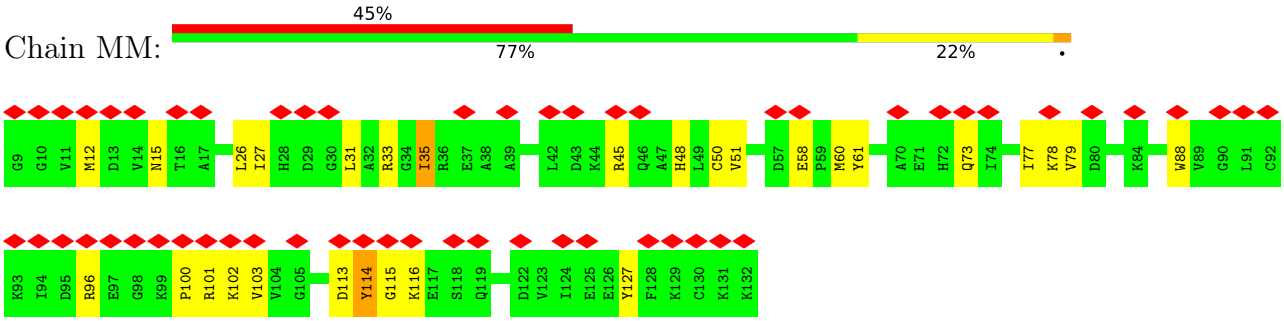
• Molecule 62: eS10



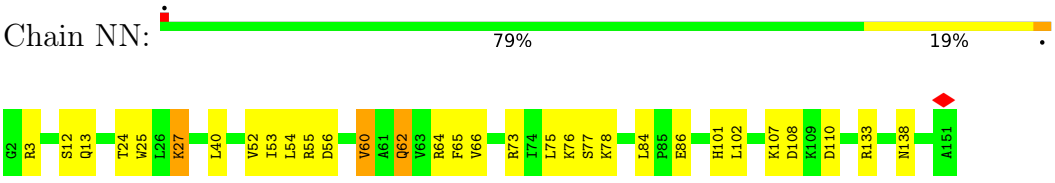
• Molecule 63: uS17



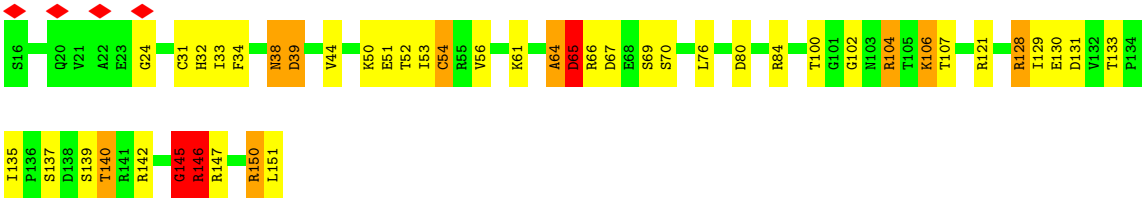
• Molecule 64: eS12



• Molecule 65: uS15

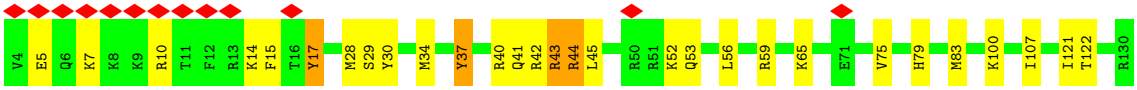


• Molecule 66: uS11



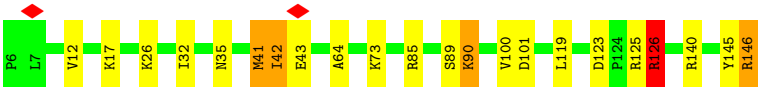
• Molecule 67: uS19

Chain PP:



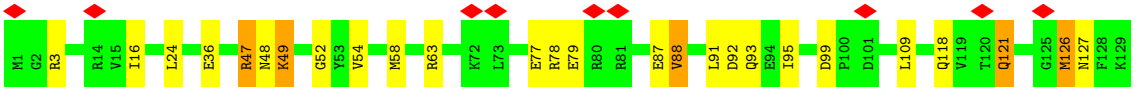
• Molecule 68: uS9

Chain QQ:



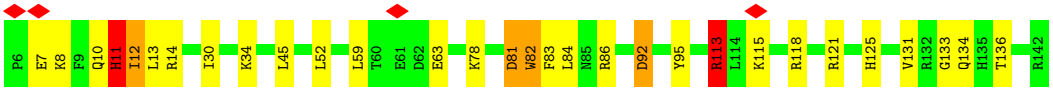
• Molecule 69: eS17

Chain RR:



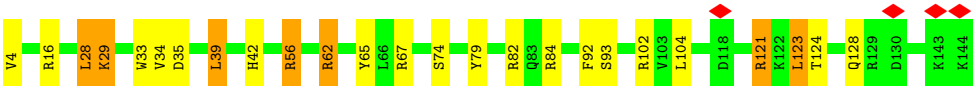
• Molecule 70: uS13

Chain SS:



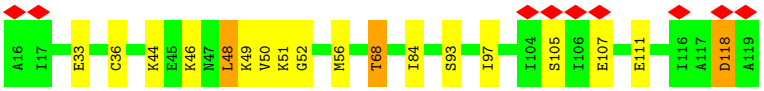
• Molecule 71: eS19

Chain TT:



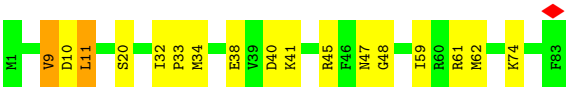
• Molecule 72: uS10

Chain UU:



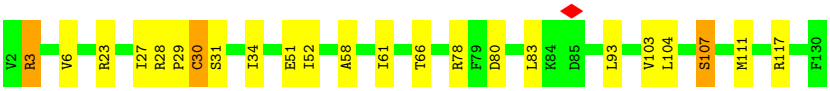
• Molecule 73: eS21

Chain VV:



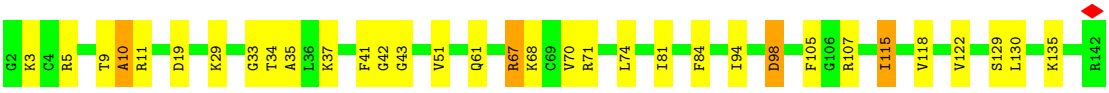
• Molecule 74: uS8

Chain WW:



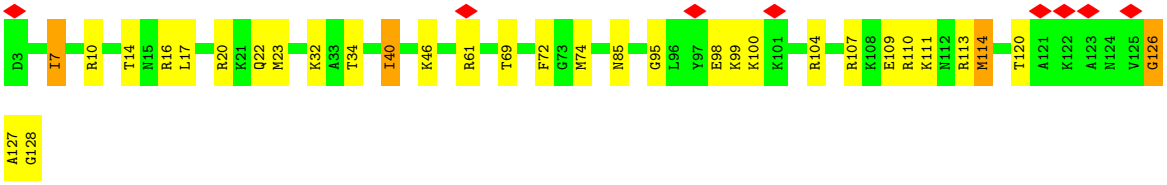
• Molecule 75: uS12

Chain XX:



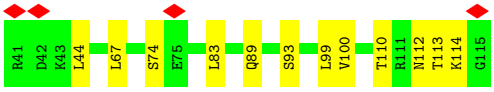
• Molecule 76: eS24

Chain YY:



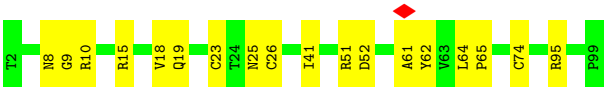
• Molecule 77: eS25

Chain ZZ:



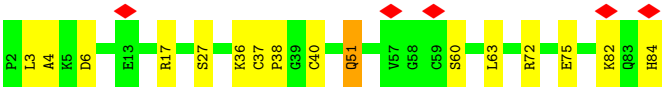
• Molecule 78: eS26

Chain aa:



• Molecule 79: eS27

Chain bb:



• Molecule 80: eS28

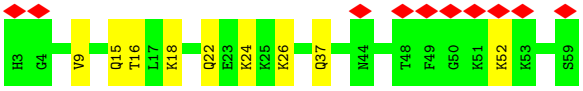
Chain cc:

• Molecule 81: uS14

Chain dd:

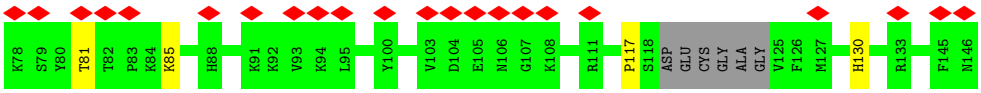
• Molecule 82: eS30

Chain ee:



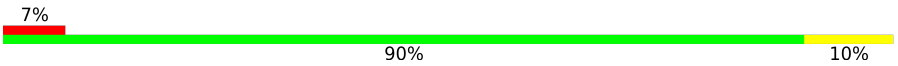
• Molecule 83: eS31

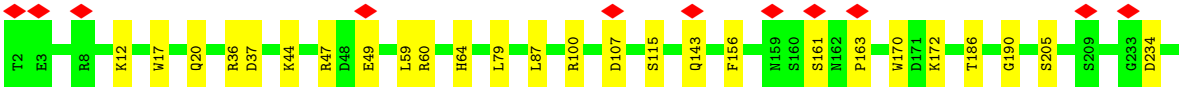
Chain ff:

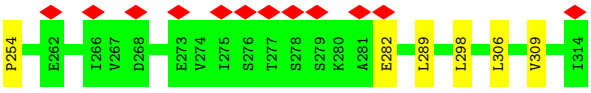


• Molecule 84: RACK1

Chain gg:

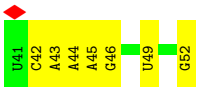






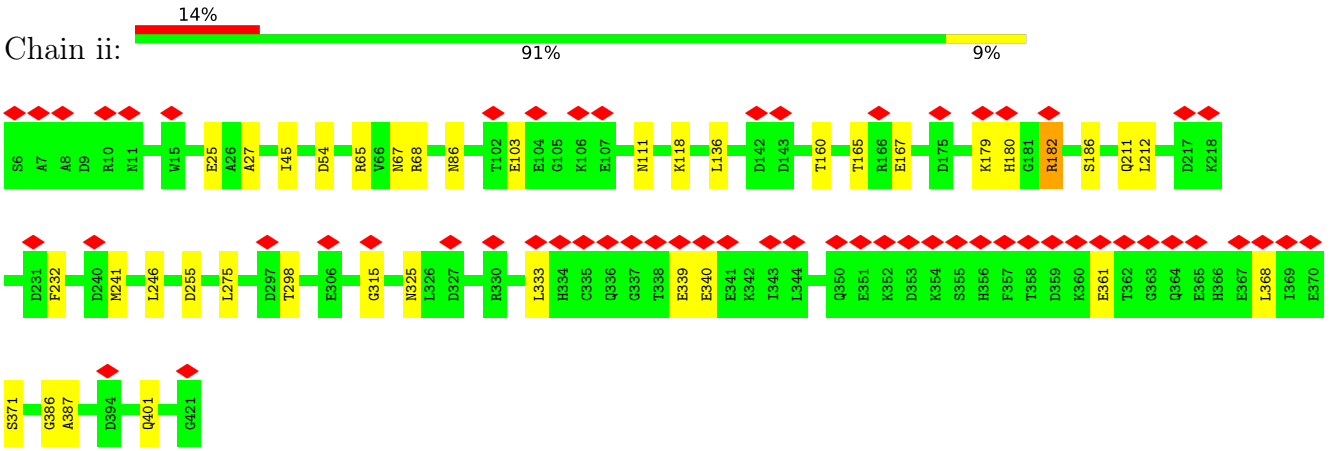
• Molecule 85: mRNA

Chain hh:



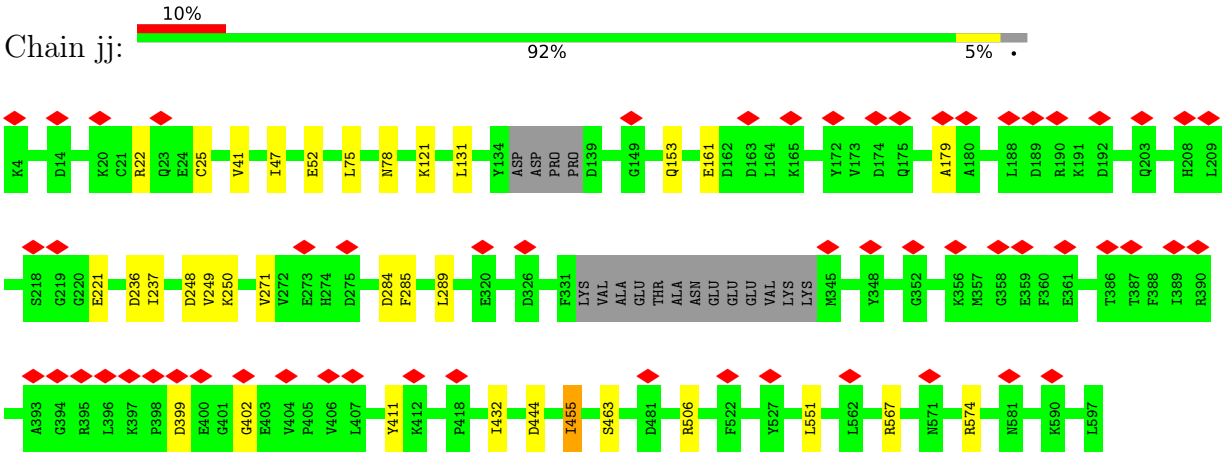
• Molecule 86: eRF1

Chain ii:



• Molecule 87: ABCE1

Chain jj:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	49979	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	
Microscope	FEI TITAN KRIOS, FEI TITAN KRIOS	Depositor
Voltage (kV)	300, 300	Depositor
Electron dose ($e^-/Å^2$)	30	Depositor
Minimum defocus (nm)	2000, 2000	Depositor
Maximum defocus (nm)	3600, 3600	Depositor
Magnification	104478, 104478	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.759	Depositor
Minimum map value	-0.468	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.07	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, ADP, MG, SF4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.47	0/1906	0.78	0/2556
2	B	0.47	0/3216	0.77	2/4311 (0.0%)
3	C	0.48	0/2937	0.81	6/3946 (0.2%)
4	D	0.40	0/2432	0.70	1/3257 (0.0%)
5	E	0.46	0/1936	0.81	2/2600 (0.1%)
6	F	0.45	0/1905	0.75	1/2539 (0.0%)
7	G	0.42	0/1967	0.75	2/2647 (0.1%)
8	H	0.40	0/1535	0.74	1/2063 (0.0%)
9	I	0.40	0/1693	0.68	1/2260 (0.0%)
10	J	0.43	0/1376	0.75	1/1841 (0.1%)
11	L	0.42	0/1734	0.80	0/2317
12	M	0.44	0/1158	0.74	0/1547
13	N	0.46	0/1746	0.79	0/2338
14	O	0.48	1/1671 (0.1%)	0.79	0/2234
15	P	0.49	0/1268	0.75	0/1700
16	Q	0.43	0/1530	0.81	0/2041
17	R	0.43	0/1524	0.80	3/2013 (0.1%)
18	S	0.48	0/1493	0.85	3/2002 (0.1%)
19	T	0.40	0/1326	0.70	0/1770
20	U	0.40	0/822	0.64	0/1103
21	V	0.45	0/993	0.74	0/1332
22	W	0.47	0/541	0.81	1/720 (0.1%)
23	X	0.45	0/993	0.71	0/1334
24	Y	0.44	0/1132	0.79	1/1504 (0.1%)
25	Z	0.41	0/1130	0.71	0/1507
26	a	0.45	0/1191	0.77	0/1590
27	b	0.45	0/619	0.72	0/818
28	c	0.38	0/742	0.66	0/996
29	d	0.44	0/903	0.82	1/1216 (0.1%)
30	e	0.52	0/1071	0.84	0/1429
31	f	0.48	0/895	0.87	0/1198
32	g	0.46	0/916	0.79	1/1220 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	h	0.39	0/1021	0.75	1/1348 (0.1%)
34	i	0.53	1/841 (0.1%)	1.85	7/1112 (0.6%)
35	j	0.50	0/720	0.91	2/952 (0.2%)
36	k	0.39	0/575	0.68	0/761
37	l	0.49	0/454	0.83	0/599
38	m	0.41	0/435	0.79	0/575
39	n	0.46	0/223	0.89	0/284
40	o	0.42	0/864	0.74	0/1140
41	p	0.46	0/718	0.72	0/953
42	r	0.49	0/1017	0.79	0/1364
43	s	0.38	0/1547	0.59	0/2088
44	t	0.41	0/1257	0.70	0/1697
45	1	0.48	0/129	0.61	0/173
46	2	0.26	0/1805	0.71	0/2809
47	3	0.39	1/1777 (0.1%)	0.97	8/2763 (0.3%)
48	5	0.39	2/87790 (0.0%)	0.78	87/136937 (0.1%)
49	7	0.32	0/2858	0.67	0/4455
50	8	0.39	0/3701	0.73	0/5766
51	9	0.33	1/41013 (0.0%)	0.78	43/63919 (0.1%)
52	AA	0.41	0/1679	0.68	0/2283
53	BB	0.40	0/1756	0.76	4/2350 (0.2%)
54	CC	0.40	0/1732	0.75	2/2347 (0.1%)
55	DD	0.41	0/1792	0.72	0/2412
56	EE	0.38	0/2115	0.74	1/2843 (0.0%)
57	FF	0.42	1/1531 (0.1%)	0.74	2/2059 (0.1%)
58	GG	0.43	0/1946	0.75	0/2590
59	HH	0.40	0/1544	0.69	1/2068 (0.0%)
60	II	0.44	0/1715	0.76	0/2287
61	JJ	0.44	0/1550	0.85	5/2069 (0.2%)
62	KK	0.41	0/851	0.72	0/1147
63	LL	0.44	0/1259	0.75	0/1684
64	MM	0.45	0/968	0.64	0/1296
65	NN	0.44	0/1232	0.75	0/1656
66	OO	0.41	0/1029	0.84	1/1380 (0.1%)
67	PP	0.43	0/1079	0.75	1/1437 (0.1%)
68	QQ	0.37	0/1142	0.73	1/1528 (0.1%)
69	RR	0.38	0/1060	0.70	0/1421
70	SS	0.41	0/1157	0.83	2/1548 (0.1%)
71	TT	0.39	0/1120	0.77	2/1499 (0.1%)
72	UU	0.37	0/831	0.69	0/1115
73	VV	0.39	0/645	0.74	0/865
74	WW	0.44	0/1051	0.75	0/1406
75	XX	0.38	0/1116	0.74	0/1490

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
76	YY	0.40	0/1040	0.72	0/1382
77	ZZ	0.38	0/604	0.74	0/810
78	aa	0.39	0/794	0.76	0/1065
79	bb	0.39	0/665	0.64	0/891
80	cc	0.36	0/478	0.76	0/640
81	dd	0.41	0/455	0.81	1/603 (0.2%)
82	ee	0.38	0/462	0.74	0/607
83	ff	0.41	0/538	0.61	0/713
84	gg	0.35	0/2493	0.63	0/3394
85	hh	0.32	0/286	0.74	0/443
86	ii	0.38	0/3333	0.62	1/4483 (0.0%)
87	jj	0.43	1/4633 (0.0%)	0.61	2/6249 (0.0%)
All	All	0.40	8/242727 (0.0%)	0.77	201/355704 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	2
3	C	0	2
5	E	0	1
9	I	0	2
11	L	0	1
17	R	0	1
18	S	0	3
24	Y	0	1
26	a	0	2
31	f	0	2
34	i	0	3
38	m	0	1
42	r	0	1
51	9	0	3
52	AA	0	2
56	EE	0	2
57	FF	0	1
59	HH	0	1
66	OO	0	1
68	QQ	0	1
70	SS	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
71	TT	0	1
72	UU	0	1
73	VV	0	1
74	WW	0	1
75	XX	0	1
86	ii	0	2
All	All	0	42

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	jj	121	LYS	CE-NZ	13.88	1.83	1.49
34	i	91	SER	C-N	-9.54	1.12	1.34
51	9	1306	U	O3'-P	-7.59	1.52	1.61
48	5	957	G	O3'-P	6.93	1.69	1.61
47	3	41	U	C3'-C2'	6.36	1.59	1.52

The worst 5 of 201 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	i	92	SER	CA-C-N	-33.35	43.83	117.20
34	i	91	SER	O-C-N	-30.40	74.06	122.70
34	i	92	SER	C-N-CA	-30.10	46.45	121.70
47	3	70	G	N9-C1'-C2'	-11.69	98.81	114.00
48	5	3753	G	N9-C1'-C2'	-11.37	99.22	114.00

There are no chirality outliers.

5 of 42 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	196	TRP	Peptide
2	B	17	LEU	Peptide
2	B	257	TRP	Peptide
3	C	339	THR	Peptide
3	C	48	ASN	Peptide

5.2 Too-close contacts (i)

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1868	0	1959	19	0
2	B	3148	0	3267	30	0
3	C	2883	0	3053	41	0
4	D	2386	0	2419	23	0
5	E	1898	0	2035	34	0
6	F	1870	0	1994	18	0
7	G	1934	0	2087	36	0
8	H	1516	0	1597	10	0
9	I	1655	0	1704	36	0
10	J	1353	0	1386	16	0
11	L	1703	0	1820	22	0
12	M	1137	0	1211	23	0
13	N	1701	0	1749	16	0
14	O	1638	0	1777	23	0
15	P	1242	0	1274	5	0
16	Q	1506	0	1623	10	0
17	R	1508	0	1664	34	0
18	S	1454	0	1496	11	0
19	T	1298	0	1366	11	0
20	U	808	0	831	3	0
21	V	979	0	1039	3	0
22	W	528	0	541	3	0
23	X	976	0	1053	6	0
24	Y	1115	0	1205	6	0
25	Z	1107	0	1182	11	0
26	a	1162	0	1209	0	0
27	b	609	0	650	0	0
28	c	732	0	769	0	0
29	d	888	0	930	0	0
30	e	1053	0	1147	0	0
31	f	876	0	912	0	0
32	g	906	0	1000	0	0
33	h	1013	0	1147	0	0
34	i	830	0	914	0	0
35	j	705	0	737	0	0
36	k	569	0	637	0	0
37	l	444	0	483	0	0
38	m	429	0	467	0	0
39	n	222	0	264	0	0
40	o	851	0	921	0	0
41	p	708	0	757	0	0
42	r	1001	0	1060	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	s	1523	0	1577	0	0
44	t	1238	0	1295	0	0
45	1	125	0	117	3	0
46	2	1616	0	824	15	0
47	3	1593	0	811	111	0
48	5	78486	0	39661	1252	0
49	7	2558	0	1296	26	0
50	8	3314	0	1683	48	0
51	9	36680	0	18530	603	0
52	AA	1642	0	1646	14	0
53	BB	1729	0	1803	9	0
54	CC	1694	0	1782	35	0
55	DD	1764	0	1863	8	0
56	EE	2073	0	2175	22	0
57	FF	1509	0	1563	34	0
58	GG	1923	0	2089	20	0
59	HH	1521	0	1616	14	0
60	II	1686	0	1772	30	0
61	JJ	1525	0	1640	18	0
62	KK	827	0	854	5	0
63	LL	1238	0	1315	11	0
64	MM	958	0	993	3	0
65	NN	1208	0	1294	6	0
66	OO	1016	0	1039	13	0
67	PP	1060	0	1120	12	0
68	QQ	1124	0	1193	6	0
69	RR	1047	0	1103	17	0
70	SS	1139	0	1191	11	0
71	TT	1102	0	1142	11	0
72	UU	821	0	883	1	0
73	VV	636	0	634	4	0
74	WW	1034	0	1080	5	0
75	XX	1098	0	1167	11	0
76	YY	1023	0	1090	7	0
77	ZZ	598	0	656	3	0
78	aa	781	0	828	0	0
79	bb	651	0	672	0	0
80	cc	475	0	497	0	0
81	dd	445	0	439	0	0
82	ee	457	0	502	0	0
83	ff	527	0	545	0	0
84	gg	2436	0	2393	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	hh	256	0	129	0	0
86	ii	3280	0	3326	0	0
87	jj	4551	0	4687	0	0
88	5	146	0	0	0	0
88	7	5	0	0	0	0
88	8	2	0	0	0	0
88	9	35	0	0	0	0
88	C	1	0	0	0	0
88	I	1	0	0	0	0
88	P	1	0	0	0	0
88	Q	1	0	0	0	0
88	V	1	0	0	0	0
88	g	1	0	0	0	0
88	hh	1	0	0	0	0
89	aa	1	0	0	0	0
89	dd	1	0	0	0	0
89	ff	1	0	0	0	0
89	g	1	0	0	0	0
89	j	1	0	0	0	0
89	m	1	0	0	0	0
89	o	1	0	0	0	0
89	p	1	0	0	0	0
90	jj	16	0	0	0	0
91	jj	54	0	24	0	0
All	All	226469	0	169875	2584	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 2584 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:JJ:121:LYS:NZ	61:JJ:121:LYS:CE	1.49	1.39
57:FF:194:ASP:O	57:FF:198:ARG:HG3	1.28	1.33
48:5:976:G:H2'	48:5:977:C:O4'	1.26	1.30
7:G:29:ASN:OD1	7:G:30:PRO:HD3	1.30	1.28
48:5:4213:A:N1	48:5:4218:U:O4	1.66	1.26

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	242/244 (99%)	215 (89%)	23 (10%)	4 (2%)	9 42
2	B	392/394 (100%)	354 (90%)	33 (8%)	5 (1%)	12 47
3	C	360/362 (99%)	322 (89%)	30 (8%)	8 (2%)	6 37
4	D	290/292 (99%)	263 (91%)	25 (9%)	2 (1%)	22 59
5	E	232/248 (94%)	179 (77%)	34 (15%)	19 (8%)	1 11
6	F	223/225 (99%)	206 (92%)	16 (7%)	1 (0%)	34 69
7	G	239/241 (99%)	206 (86%)	25 (10%)	8 (3%)	4 31
8	H	188/190 (99%)	170 (90%)	16 (8%)	2 (1%)	14 51
9	I	200/213 (94%)	181 (90%)	14 (7%)	5 (2%)	5 35
10	J	167/169 (99%)	144 (86%)	15 (9%)	8 (5%)	2 22
11	L	208/210 (99%)	182 (88%)	15 (7%)	11 (5%)	2 21
12	M	136/138 (99%)	124 (91%)	12 (9%)	0	100 100
13	N	201/203 (99%)	186 (92%)	15 (8%)	0	100 100
14	O	197/199 (99%)	190 (96%)	7 (4%)	0	100 100
15	P	151/153 (99%)	141 (93%)	9 (6%)	1 (1%)	22 59
16	Q	185/187 (99%)	172 (93%)	11 (6%)	2 (1%)	14 51
17	R	178/180 (99%)	166 (93%)	10 (6%)	2 (1%)	14 51
18	S	173/175 (99%)	158 (91%)	11 (6%)	4 (2%)	6 36
19	T	157/159 (99%)	139 (88%)	15 (10%)	3 (2%)	8 40
20	U	97/99 (98%)	84 (87%)	8 (8%)	5 (5%)	2 21
21	V	129/131 (98%)	116 (90%)	12 (9%)	1 (1%)	19 56
22	W	61/63 (97%)	57 (93%)	4 (7%)	0	100 100
23	X	117/119 (98%)	111 (95%)	5 (4%)	1 (1%)	17 54
24	Y	132/134 (98%)	115 (87%)	15 (11%)	2 (2%)	10 44
25	Z	133/135 (98%)	114 (86%)	13 (10%)	6 (4%)	2 23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
26	a	145/147 (99%)	124 (86%)	16 (11%)	5 (3%)	3 30
27	b	73/75 (97%)	66 (90%)	6 (8%)	1 (1%)	11 45
28	c	92/94 (98%)	89 (97%)	3 (3%)	0	100 100
29	d	105/107 (98%)	90 (86%)	13 (12%)	2 (2%)	8 40
30	e	126/128 (98%)	117 (93%)	6 (5%)	3 (2%)	6 35
31	f	107/109 (98%)	93 (87%)	9 (8%)	5 (5%)	2 22
32	g	112/114 (98%)	107 (96%)	5 (4%)	0	100 100
33	h	120/122 (98%)	108 (90%)	8 (7%)	4 (3%)	4 31
34	i	100/102 (98%)	85 (85%)	11 (11%)	4 (4%)	3 26
35	j	84/86 (98%)	73 (87%)	10 (12%)	1 (1%)	13 49
36	k	67/69 (97%)	57 (85%)	7 (10%)	3 (4%)	2 23
37	l	48/50 (96%)	40 (83%)	4 (8%)	4 (8%)	1 10
38	m	50/52 (96%)	46 (92%)	4 (8%)	0	100 100
39	n	21/23 (91%)	21 (100%)	0	0	100 100
40	o	102/104 (98%)	89 (87%)	10 (10%)	3 (3%)	4 32
41	p	89/91 (98%)	79 (89%)	10 (11%)	0	100 100
42	r	123/125 (98%)	100 (81%)	18 (15%)	5 (4%)	3 25
43	s	196/198 (99%)	162 (83%)	24 (12%)	10 (5%)	2 21
44	t	161/163 (99%)	100 (62%)	34 (21%)	27 (17%)	0 2
45	1	13/15 (87%)	10 (77%)	1 (8%)	2 (15%)	0 3
52	AA	206/208 (99%)	174 (84%)	23 (11%)	9 (4%)	2 24
53	BB	211/213 (99%)	172 (82%)	25 (12%)	14 (7%)	1 16
54	CC	216/218 (99%)	187 (87%)	22 (10%)	7 (3%)	4 31
55	DD	225/227 (99%)	187 (83%)	29 (13%)	9 (4%)	3 26
56	EE	260/262 (99%)	215 (83%)	29 (11%)	16 (6%)	1 18
57	FF	189/191 (99%)	163 (86%)	18 (10%)	8 (4%)	3 25
58	GG	235/237 (99%)	205 (87%)	27 (12%)	3 (1%)	12 47
59	HH	187/189 (99%)	153 (82%)	22 (12%)	12 (6%)	1 17
60	II	204/206 (99%)	171 (84%)	26 (13%)	7 (3%)	3 30
61	JJ	183/185 (99%)	156 (85%)	20 (11%)	7 (4%)	3 27
62	KK	96/98 (98%)	64 (67%)	21 (22%)	11 (12%)	0 5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
63	LL	150/152 (99%)	131 (87%)	14 (9%)	5 (3%)	4 31
64	MM	122/124 (98%)	85 (70%)	29 (24%)	8 (7%)	1 16
65	NN	148/150 (99%)	126 (85%)	16 (11%)	6 (4%)	3 25
66	OO	134/136 (98%)	104 (78%)	15 (11%)	15 (11%)	0 5
67	PP	125/127 (98%)	111 (89%)	11 (9%)	3 (2%)	6 35
68	QQ	139/141 (99%)	116 (84%)	17 (12%)	6 (4%)	2 24
69	RR	127/129 (98%)	108 (85%)	14 (11%)	5 (4%)	3 26
70	SS	135/137 (98%)	116 (86%)	11 (8%)	8 (6%)	1 18
71	TT	139/141 (99%)	128 (92%)	8 (6%)	3 (2%)	6 37
72	UU	102/104 (98%)	88 (86%)	8 (8%)	6 (6%)	1 18
73	VV	81/83 (98%)	70 (86%)	7 (9%)	4 (5%)	2 22
74	WW	127/129 (98%)	110 (87%)	10 (8%)	7 (6%)	2 20
75	XX	139/141 (99%)	125 (90%)	10 (7%)	4 (3%)	4 32
76	YY	124/126 (98%)	102 (82%)	15 (12%)	7 (6%)	2 19
77	ZZ	73/75 (97%)	59 (81%)	12 (16%)	2 (3%)	5 33
78	aa	96/98 (98%)	78 (81%)	9 (9%)	9 (9%)	0 9
79	bb	81/83 (98%)	66 (82%)	9 (11%)	6 (7%)	1 13
80	cc	59/61 (97%)	48 (81%)	10 (17%)	1 (2%)	9 42
81	dd	51/53 (96%)	44 (86%)	6 (12%)	1 (2%)	7 39
82	ee	55/57 (96%)	40 (73%)	13 (24%)	2 (4%)	3 29
83	ff	59/69 (86%)	51 (86%)	6 (10%)	2 (3%)	3 30
84	gg	311/313 (99%)	269 (86%)	33 (11%)	9 (3%)	4 32
86	ii	414/416 (100%)	383 (92%)	25 (6%)	6 (1%)	11 45
87	jj	569/594 (96%)	518 (91%)	40 (7%)	11 (2%)	8 40
All	All	12494/12710 (98%)	10874 (87%)	1202 (10%)	418 (3%)	6 31

5 of 418 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	196	TRP
5	E	91	PRO
5	E	95	ASP
5	E	118	PRO
5	E	175	LEU

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	187/187 (100%)	160 (86%)	27 (14%)	3 19
2	B	336/342 (98%)	301 (90%)	35 (10%)	7 30
3	C	302/302 (100%)	260 (86%)	42 (14%)	3 20
4	D	247/247 (100%)	222 (90%)	25 (10%)	7 31
5	E	208/221 (94%)	184 (88%)	24 (12%)	5 27
6	F	194/195 (100%)	166 (86%)	28 (14%)	3 19
7	G	206/206 (100%)	183 (89%)	23 (11%)	6 28
8	H	169/169 (100%)	149 (88%)	20 (12%)	5 26
9	I	174/180 (97%)	155 (89%)	19 (11%)	6 29
10	J	142/142 (100%)	130 (92%)	12 (8%)	10 40
11	L	176/176 (100%)	147 (84%)	29 (16%)	2 14
12	M	117/117 (100%)	100 (86%)	17 (14%)	3 18
13	N	171/171 (100%)	151 (88%)	20 (12%)	5 26
14	O	171/171 (100%)	148 (86%)	23 (14%)	4 21
15	P	134/134 (100%)	121 (90%)	13 (10%)	8 33
16	Q	163/163 (100%)	141 (86%)	22 (14%)	4 21
17	R	159/159 (100%)	139 (87%)	20 (13%)	4 23
18	S	156/156 (100%)	133 (85%)	23 (15%)	3 18
19	T	139/139 (100%)	123 (88%)	16 (12%)	5 27
20	U	89/89 (100%)	81 (91%)	8 (9%)	9 37
21	V	101/101 (100%)	84 (83%)	17 (17%)	2 13
22	W	55/55 (100%)	50 (91%)	5 (9%)	9 37
23	X	107/107 (100%)	96 (90%)	11 (10%)	7 31
24	Y	124/124 (100%)	106 (86%)	18 (14%)	3 18
25	Z	117/117 (100%)	110 (94%)	7 (6%)	19 51
26	a	119/119 (100%)	107 (90%)	12 (10%)	7 31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
27	b	62/62 (100%)	57 (92%)	5 (8%)	11 41
28	c	79/79 (100%)	68 (86%)	11 (14%)	3 20
29	d	98/98 (100%)	81 (83%)	17 (17%)	2 12
30	e	114/114 (100%)	97 (85%)	17 (15%)	3 17
31	f	88/88 (100%)	76 (86%)	12 (14%)	3 21
32	g	98/98 (100%)	85 (87%)	13 (13%)	4 21
33	h	109/109 (100%)	97 (89%)	12 (11%)	6 29
34	i	86/86 (100%)	79 (92%)	7 (8%)	11 41
35	j	73/73 (100%)	64 (88%)	9 (12%)	4 24
36	k	64/64 (100%)	58 (91%)	6 (9%)	8 35
37	l	47/47 (100%)	41 (87%)	6 (13%)	4 22
38	m	48/48 (100%)	37 (77%)	11 (23%)	1 6
39	n	22/22 (100%)	19 (86%)	3 (14%)	3 21
40	o	92/92 (100%)	79 (86%)	13 (14%)	3 19
41	p	74/74 (100%)	68 (92%)	6 (8%)	11 41
42	r	109/109 (100%)	90 (83%)	19 (17%)	2 12
43	s	166/166 (100%)	156 (94%)	10 (6%)	19 51
44	t	136/136 (100%)	126 (93%)	10 (7%)	13 44
45	1	13/13 (100%)	13 (100%)	0	100 100
52	AA	174/174 (100%)	154 (88%)	20 (12%)	5 27
53	BB	194/194 (100%)	166 (86%)	28 (14%)	3 19
54	CC	184/184 (100%)	161 (88%)	23 (12%)	4 23
55	DD	190/190 (100%)	160 (84%)	30 (16%)	2 16
56	EE	223/223 (100%)	191 (86%)	32 (14%)	3 19
57	FF	161/161 (100%)	138 (86%)	23 (14%)	3 19
58	GG	207/207 (100%)	177 (86%)	30 (14%)	3 18
59	HH	169/169 (100%)	153 (90%)	16 (10%)	8 34
60	II	178/178 (100%)	155 (87%)	23 (13%)	4 22
61	JJ	161/161 (100%)	140 (87%)	21 (13%)	4 22
62	KK	89/89 (100%)	76 (85%)	13 (15%)	3 18
63	LL	136/136 (100%)	119 (88%)	17 (12%)	4 23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
64	MM	104/104 (100%)	87 (84%)	17 (16%)	2 14
65	NN	130/130 (100%)	112 (86%)	18 (14%)	3 20
66	OO	106/106 (100%)	81 (76%)	25 (24%)	1 5
67	PP	116/116 (100%)	98 (84%)	18 (16%)	2 16
68	QQ	117/117 (100%)	104 (89%)	13 (11%)	6 28
69	RR	117/117 (100%)	104 (89%)	13 (11%)	6 28
70	SS	119/119 (100%)	100 (84%)	19 (16%)	2 15
71	TT	112/112 (100%)	98 (88%)	14 (12%)	4 23
72	UU	94/94 (100%)	82 (87%)	12 (13%)	4 22
73	VV	67/67 (100%)	59 (88%)	8 (12%)	5 25
74	WW	112/112 (100%)	102 (91%)	10 (9%)	9 38
75	XX	113/113 (100%)	98 (87%)	15 (13%)	4 21
76	YY	108/108 (100%)	87 (81%)	21 (19%)	1 9
77	ZZ	66/66 (100%)	58 (88%)	8 (12%)	5 24
78	aa	85/85 (100%)	76 (89%)	9 (11%)	6 30
79	bb	75/75 (100%)	64 (85%)	11 (15%)	3 18
80	cc	54/54 (100%)	46 (85%)	8 (15%)	3 18
81	dd	47/47 (100%)	39 (83%)	8 (17%)	2 13
82	ee	47/47 (100%)	40 (85%)	7 (15%)	3 17
83	ff	59/62 (95%)	57 (97%)	2 (3%)	37 63
84	gg	272/272 (100%)	249 (92%)	23 (8%)	10 40
86	ii	358/358 (100%)	328 (92%)	30 (8%)	11 40
87	jj	507/522 (97%)	486 (96%)	21 (4%)	30 59
All	All	10892/10936 (100%)	9583 (88%)	1309 (12%)	8 24

5 of 1309 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
60	II	203	LYS
75	XX	3	LYS
62	KK	50	GLN
60	II	196	GLU
67	PP	7	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
5	E	217	GLN
12	M	131	GLN
80	cc	40	HIS
86	ii	325	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
46	2	74/76 (97%)	22 (29%)	1 (1%)
47	3	72/75 (96%)	36 (50%)	13 (18%)
48	5	3645/3662 (99%)	1161 (31%)	270 (7%)
49	7	119/120 (99%)	19 (15%)	1 (0%)
50	8	155/156 (99%)	47 (30%)	6 (3%)
51	9	1710/1719 (99%)	559 (32%)	113 (6%)
85	hh	11/12 (91%)	7 (63%)	0
All	All	5786/5820 (99%)	1851 (31%)	404 (6%)

5 of 1851 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
46	2	5	C
46	2	7	G
46	2	8	U
46	2	9	A
46	2	13	U

5 of 404 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
48	5	4069	U
50	8	51	U
51	9	1721	U
48	5	4121	G
48	5	4656	A

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 207 ligands modelled in this entry, 203 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
91	ADP	jj	602	-	24,29,29	1.05	2 (8%)	29,45,45	1.46	4 (13%)
91	ADP	jj	603	-	24,29,29	1.06	2 (8%)	29,45,45	1.46	4 (13%)
90	SF4	jj	601	87	0,12,12	-	-	-		
90	SF4	jj	600	87	0,12,12	-	-	-		

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
91	ADP	jj	603	-	-	1/12/32/32	0/3/3/3
91	ADP	jj	602	-	-	1/12/32/32	0/3/3/3
90	SF4	jj	600	87	-	-	0/6/5/5
90	SF4	jj	601	87	-	-	0/6/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
91	jj	602	ADP	C5-C4	2.66	1.48	1.40
91	jj	603	ADP	C5-C4	2.63	1.47	1.40
91	jj	603	ADP	C2-N3	2.25	1.35	1.32
91	jj	602	ADP	C2-N3	2.22	1.35	1.32

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
91	jj	602	ADP	N3-C2-N1	-3.78	122.77	128.68
91	jj	603	ADP	N3-C2-N1	-3.72	122.87	128.68
91	jj	603	ADP	C3'-C2'-C1'	3.31	105.97	100.98
91	jj	602	ADP	C3'-C2'-C1'	3.14	105.71	100.98
91	jj	603	ADP	PA-O3A-PB	-2.96	122.67	132.83

There are no chirality outliers.

All (2) torsion outliers are listed below:

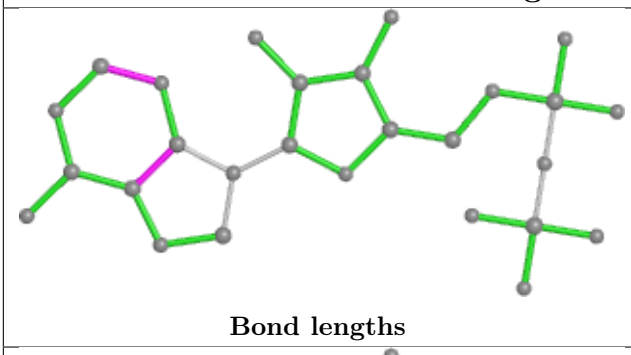
Mol	Chain	Res	Type	Atoms
91	jj	602	ADP	PB-O3A-PA-O1A
91	jj	603	ADP	PB-O3A-PA-O1A

There are no ring outliers.

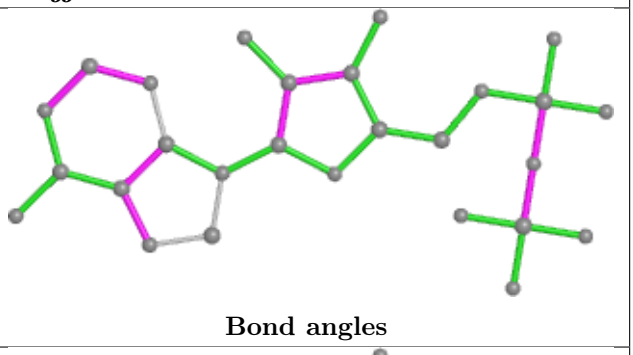
No monomer is involved in short contacts.

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.

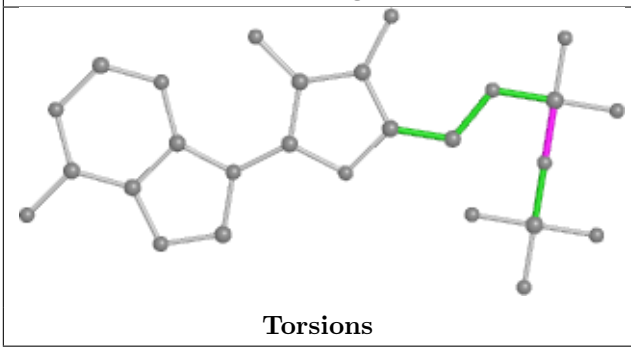
Ligand ADP jj 602



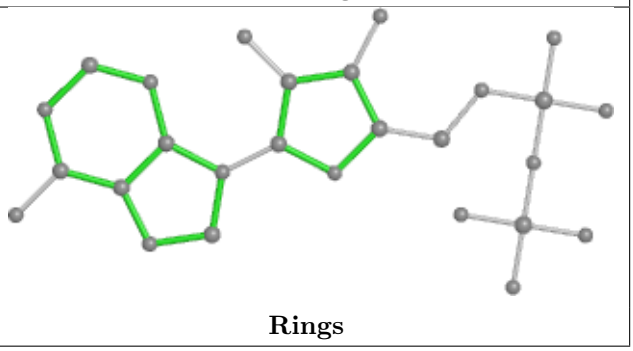
Bond lengths



Bond angles

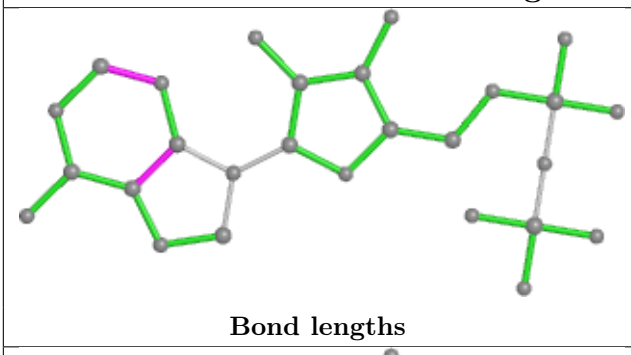


Torsions

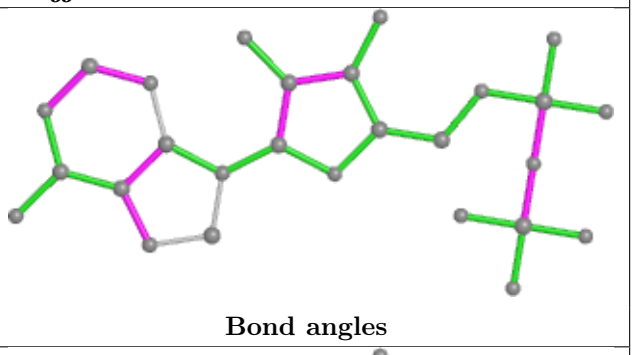


Rings

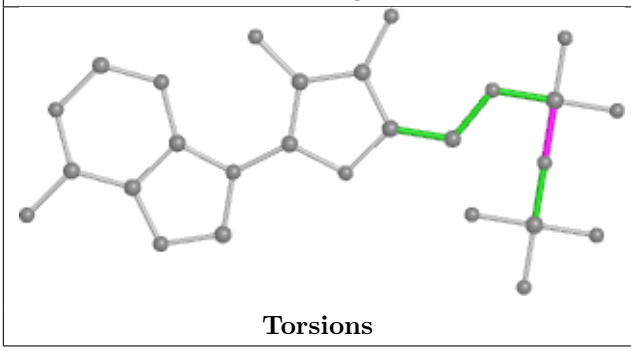
Ligand ADP jj 603



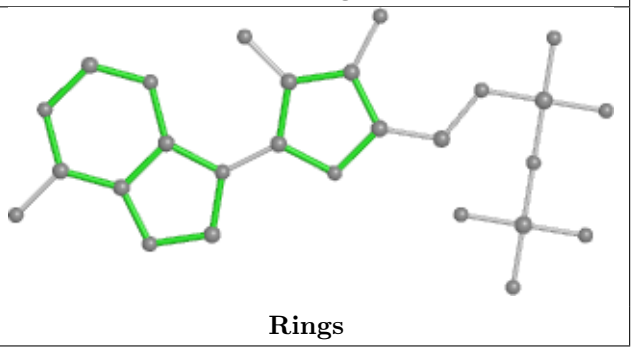
Bond lengths



Bond angles



Torsions



Rings

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	16
51	9	8
47	3	2
46	2	1
87	jj	1
34	i	1

The worst 5 of 29 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	9	753:C	O3'	785:C	P	23.46
1	9	126:G	O3'	139:C	P	21.86
1	9	698:G	O3'	730:C	P	19.70
1	5	4776:G	O3'	4859:C	P	18.03
1	9	1761:U	O3'	1771:G	P	17.54

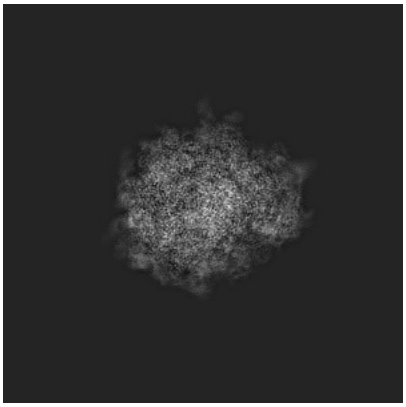
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-3038. These allow visual inspection of the internal detail of the map and identification of artifacts.

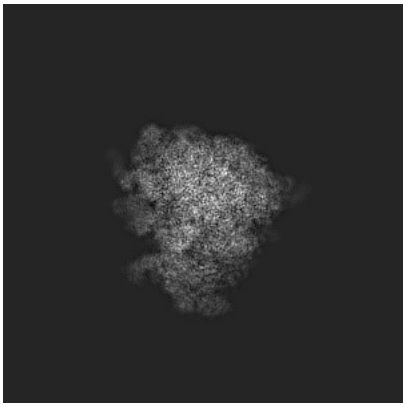
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

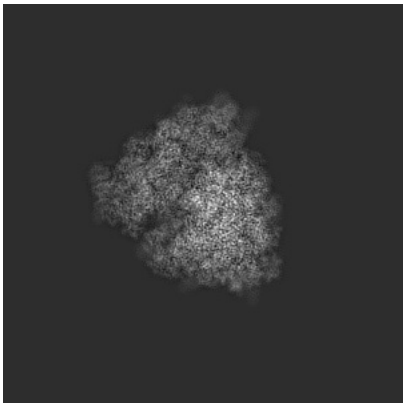
6.1.1 Primary map



X



Y

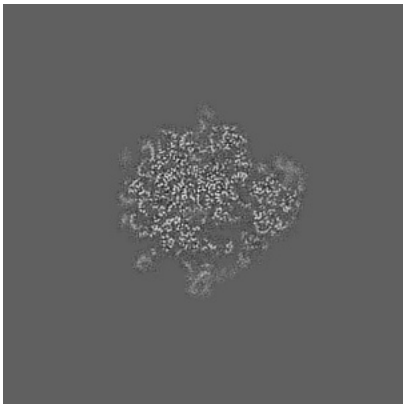


Z

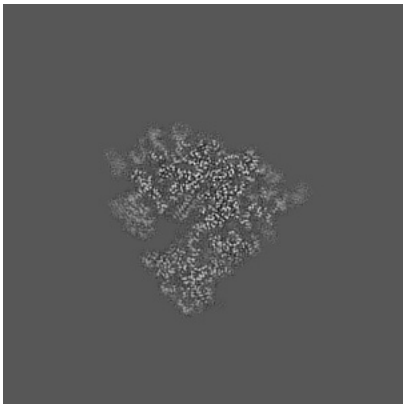
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map



X Index: 210



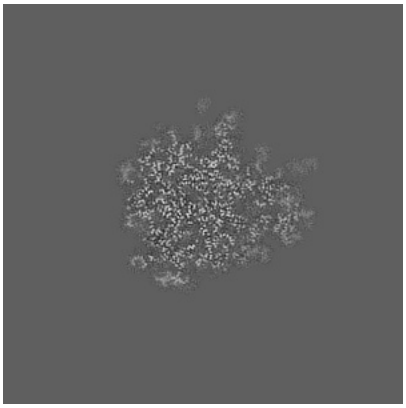
Y Index: 210

Z Index: 210

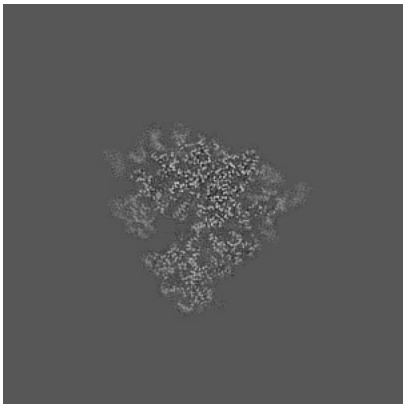
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

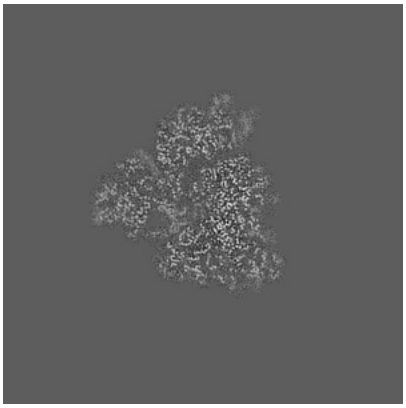
6.3.1 Primary map



X Index: 228



Y Index: 211

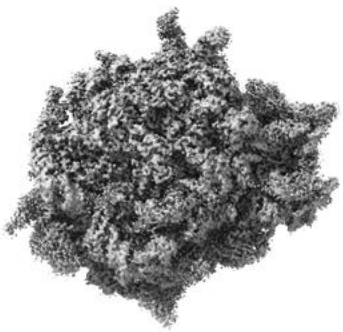


Z Index: 195

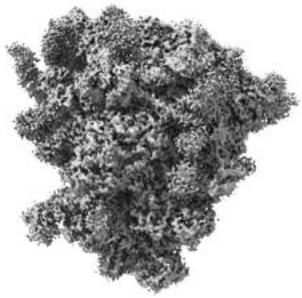
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

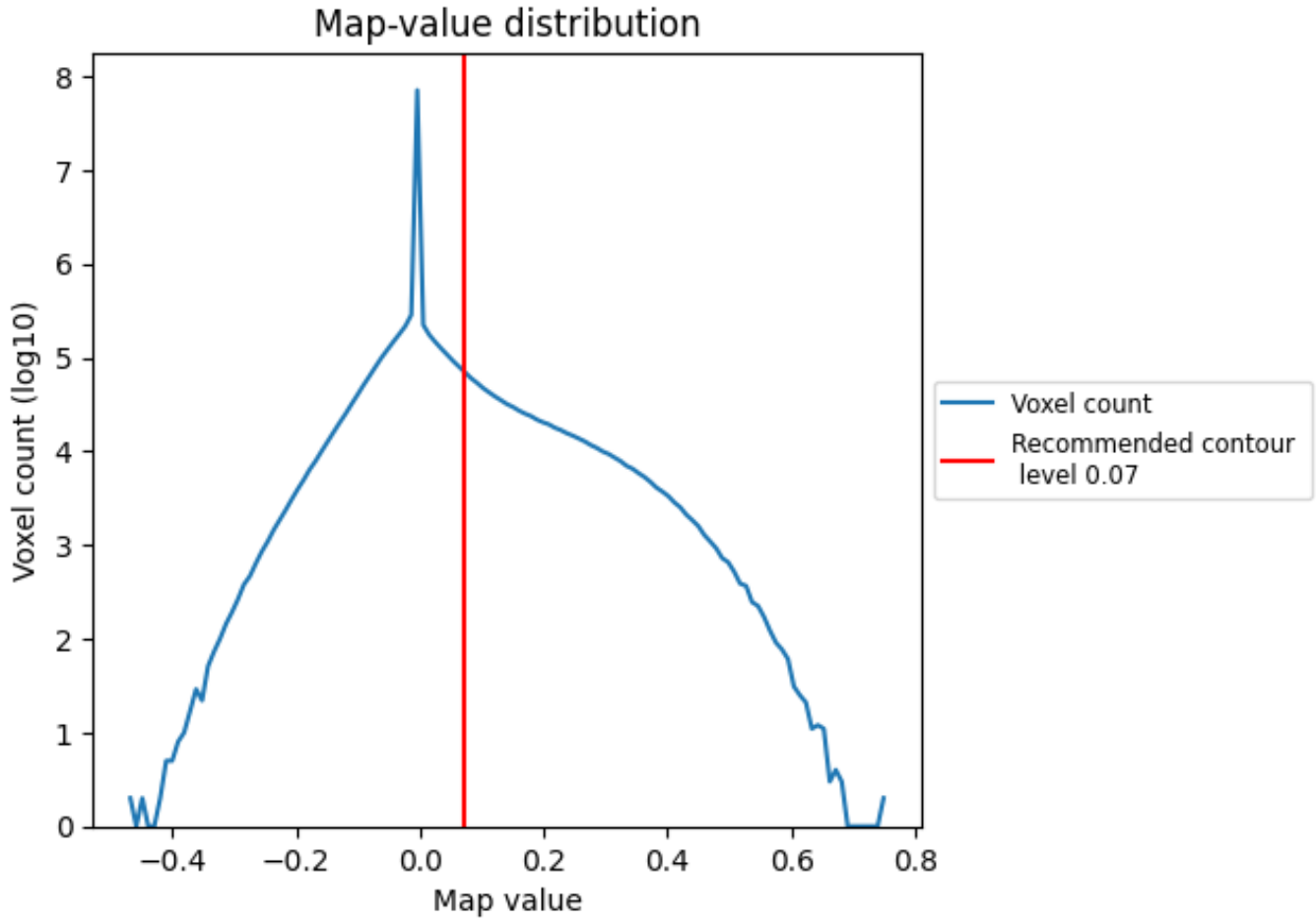
6.5 Mask visualisation (i)

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

7 Map analysis

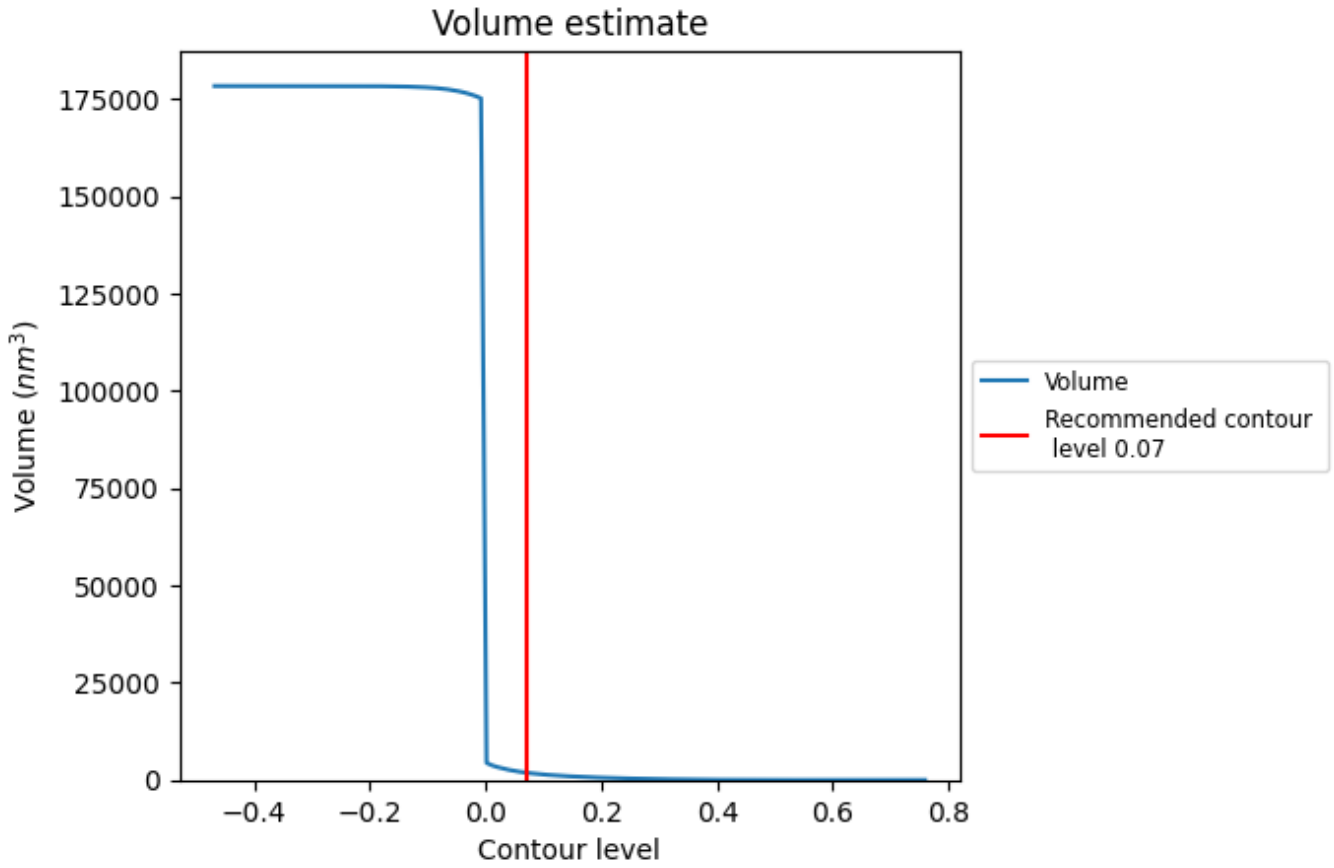
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

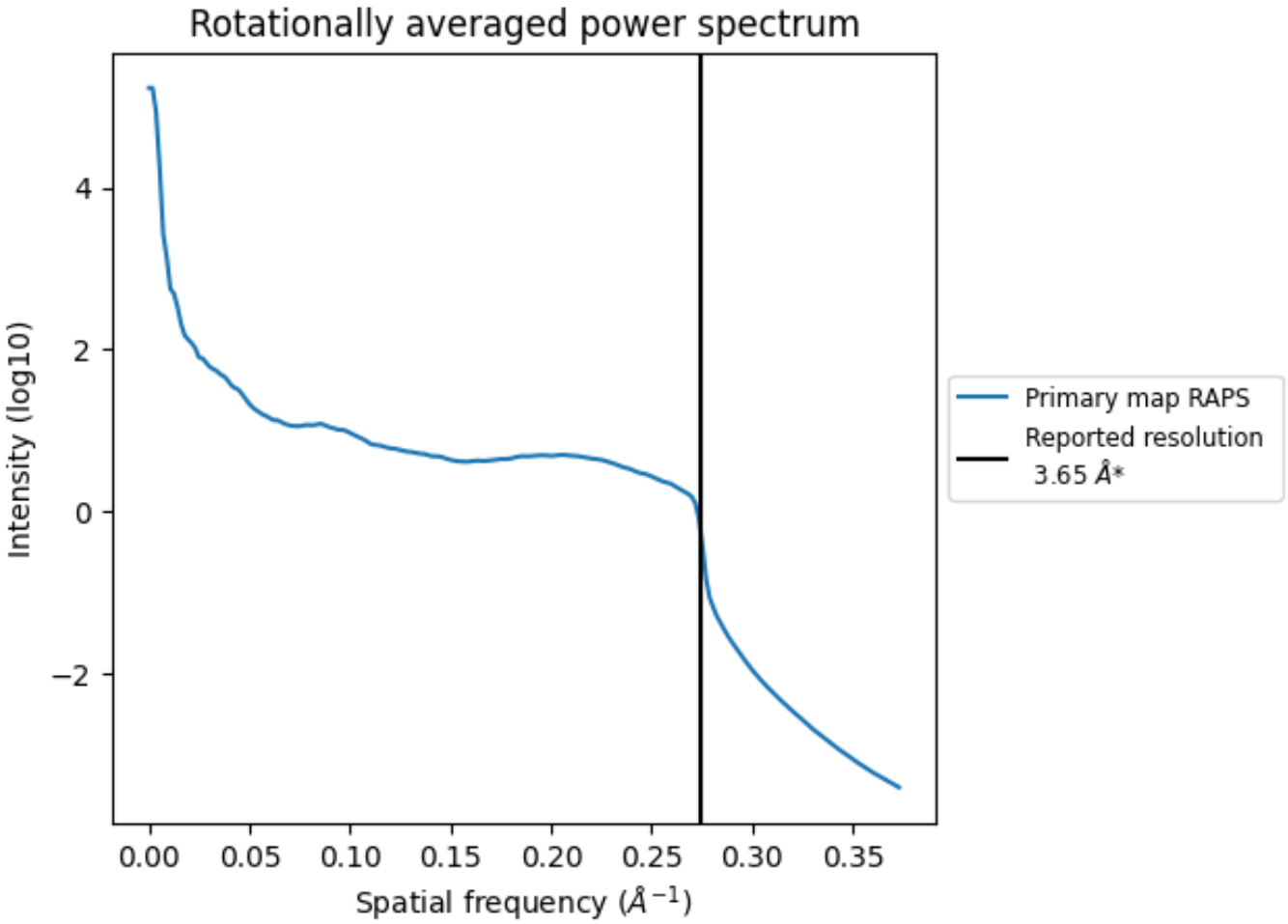
7.2 Volume estimate (i)



The volume at the recommended contour level is 1869 nm^3; this corresponds to an approximate mass of 1688 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)

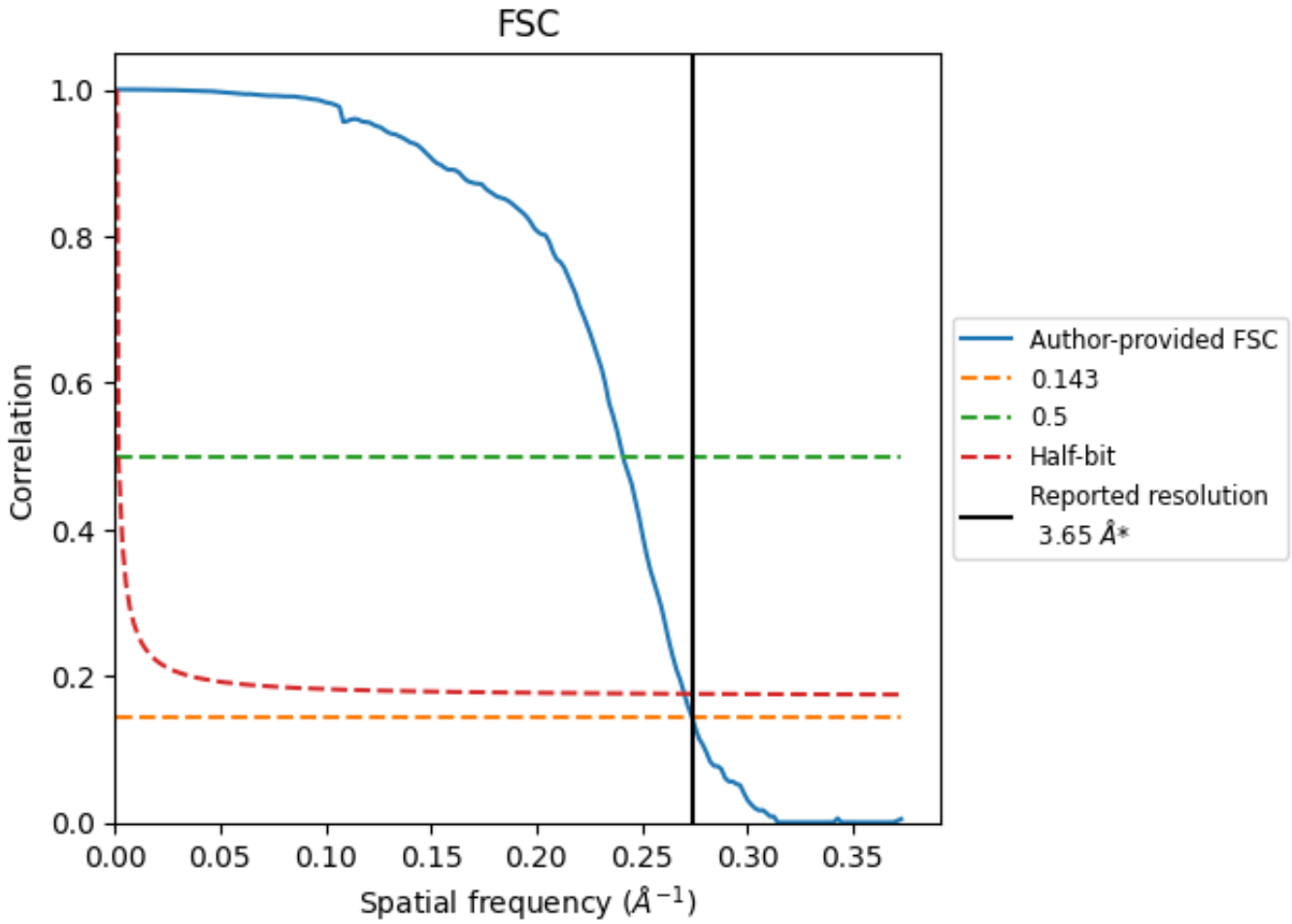


*Reported resolution corresponds to spatial frequency of 0.274 Å^{-1}

8 Fourier-Shell correlation

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



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

8.2 Resolution estimates (i)

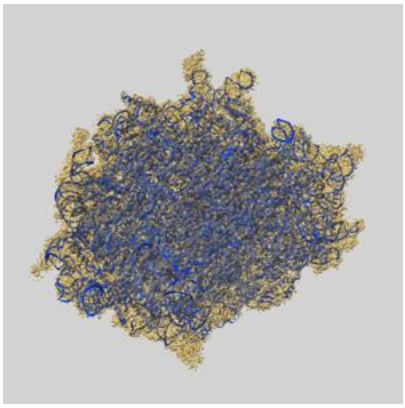
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.65	-	-
Author-provided FSC curve	3.65	4.15	3.70
Unmasked-calculated*	-	-	-

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

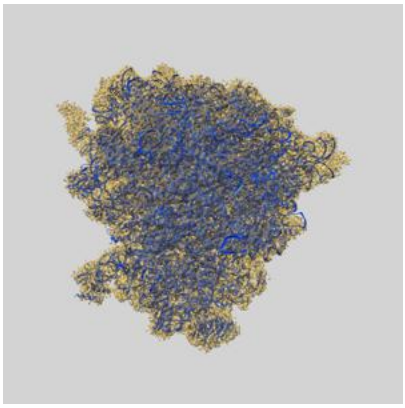
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-3038 and PDB model 3JAG. Per-residue inclusion information can be found in section 3 on page 24.

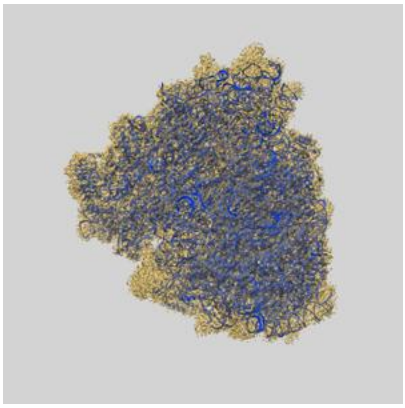
9.1 Map-model overlay



X



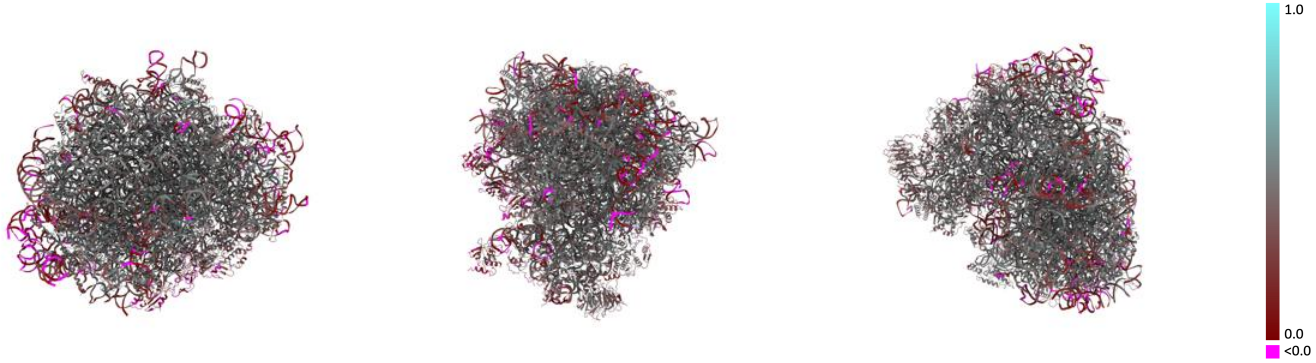
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.07 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.

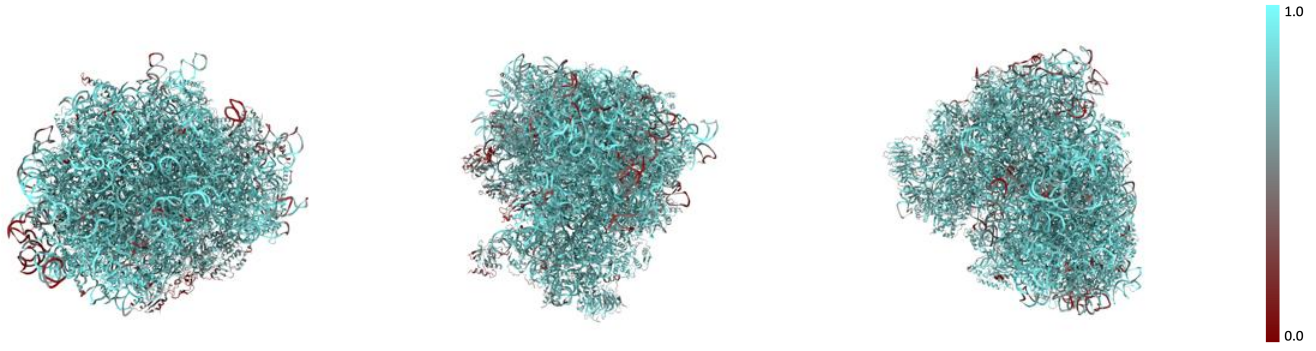
9.2 Q-score mapped to coordinate model



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.

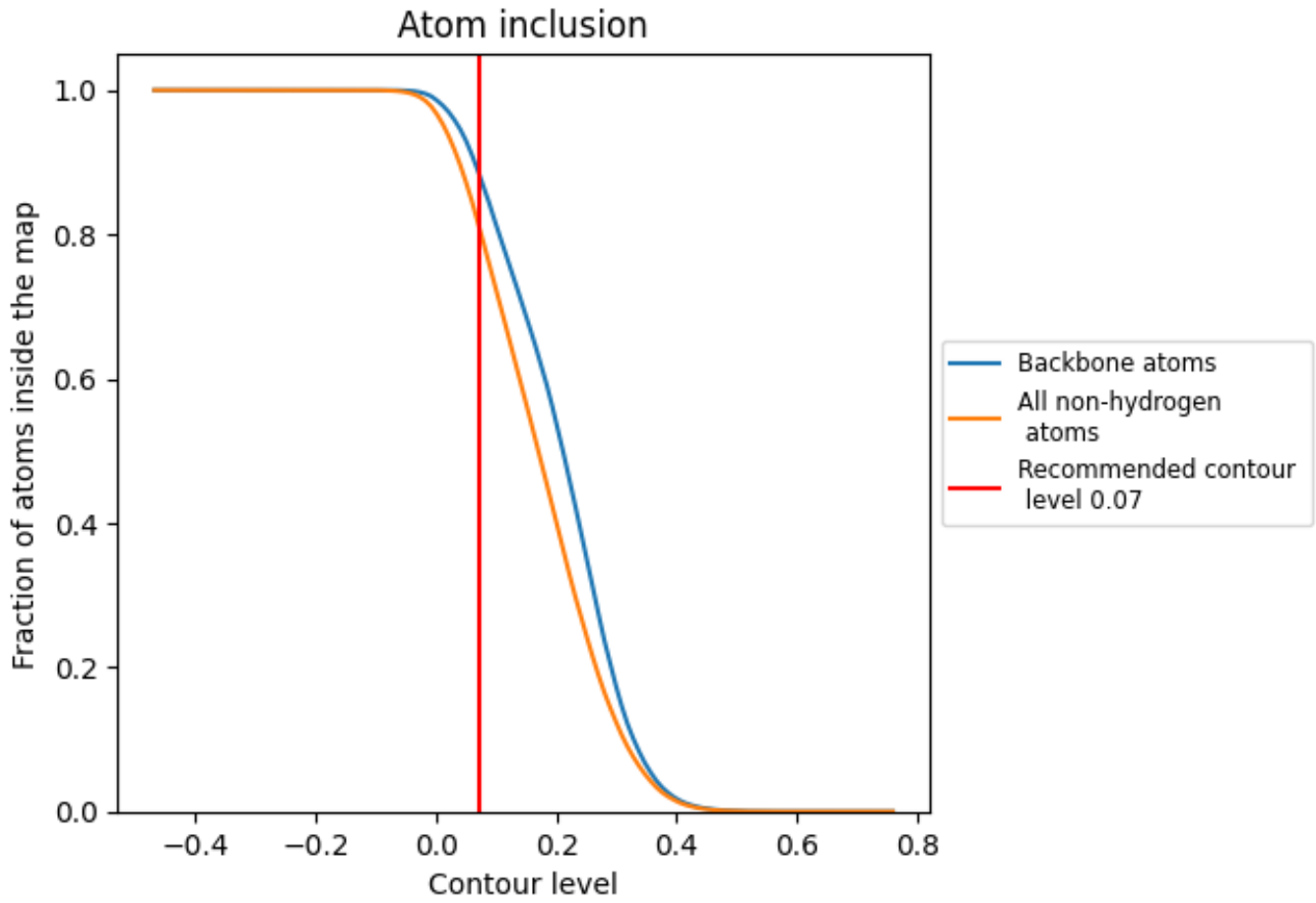
9.3 Atom inclusion mapped to coordinate model



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 (0.07).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8148	0.4070
1	0.6446	0.3920
2	0.8280	0.3460
3	0.5524	0.2200
5	0.8483	0.3910
7	0.9384	0.4610
8	0.8869	0.4200
9	0.8596	0.3980
A	0.8417	0.4900
AA	0.7845	0.4370
B	0.8458	0.4860
BB	0.7816	0.4540
C	0.8438	0.4820
CC	0.7931	0.4590
D	0.8293	0.4450
DD	0.7193	0.3880
E	0.7709	0.4070
EE	0.8162	0.4600
F	0.8401	0.4760
FF	0.7330	0.4060
G	0.7537	0.4060
GG	0.7305	0.3680
H	0.8146	0.4630
HH	0.6816	0.3600
I	0.8157	0.4650
II	0.7769	0.4170
J	0.7873	0.4180
JJ	0.7857	0.4310
KK	0.7143	0.3420
L	0.8092	0.4410
LL	0.7598	0.4370
M	0.8535	0.4690
MM	0.4280	0.1740
N	0.8593	0.4940
NN	0.8055	0.4650

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Chain	Atom inclusion	Q-score
O	0.8332	0.4750
OO	0.7933	0.4520
P	0.8575	0.4900
PP	0.7047	0.3530
Q	0.8504	0.4930
QQ	0.7914	0.4260
R	0.8085	0.4500
RR	0.7105	0.3590
S	0.8529	0.4820
SS	0.7765	0.3960
T	0.8290	0.4660
TT	0.7826	0.4150
U	0.7937	0.4020
UU	0.7000	0.3770
V	0.8142	0.4800
VV	0.7669	0.4250
W	0.8369	0.4770
WW	0.8287	0.4810
X	0.8156	0.4610
XX	0.8095	0.4770
Y	0.8200	0.4590
YY	0.7734	0.4000
Z	0.8397	0.4620
ZZ	0.7358	0.3890
a	0.8759	0.4960
aa	0.8194	0.4660
b	0.7521	0.4230
bb	0.7496	0.4230
c	0.8308	0.4650
cc	0.7202	0.4130
d	0.8180	0.4620
dd	0.8318	0.4550
e	0.8555	0.4900
ee	0.6818	0.3810
f	0.8800	0.4970
ff	0.5010	0.2120
g	0.8175	0.4590
gg	0.7131	0.3710
h	0.7998	0.4410
hh	0.8249	0.4200
i	0.8153	0.4370
ii	0.6316	0.3670

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
j	0.8782	0.4900
jj	0.6426	0.3640
k	0.7648	0.4000
l	0.8440	0.4800
m	0.8293	0.4620
n	0.8209	0.4510
o	0.8208	0.4670
p	0.8041	0.4750
r	0.8631	0.4900
s	0.3311	0.1170
t	0.4515	0.1540