



wwPDB EM Validation Summary Report ⓘ

Aug 3, 2026 – 04:51 PM EDT

PDB ID : 3JAH / pdb_00003jah
EMDB ID : EMD-3039
Title : Structure of a mammalian ribosomal termination complex with ABCE1, eRF1(AAQ), and the UAG stop codon
Authors : Brown, A.; Shao, S.; Murray, J.; Hegde, R.S.; Ramakrishnan, V.
Deposited on : 2015-06-10
Resolution : 3.45 Å(reported)
Based on initial models : 3J7P, 3BK7, 4V51, 1DT9, 3J92

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

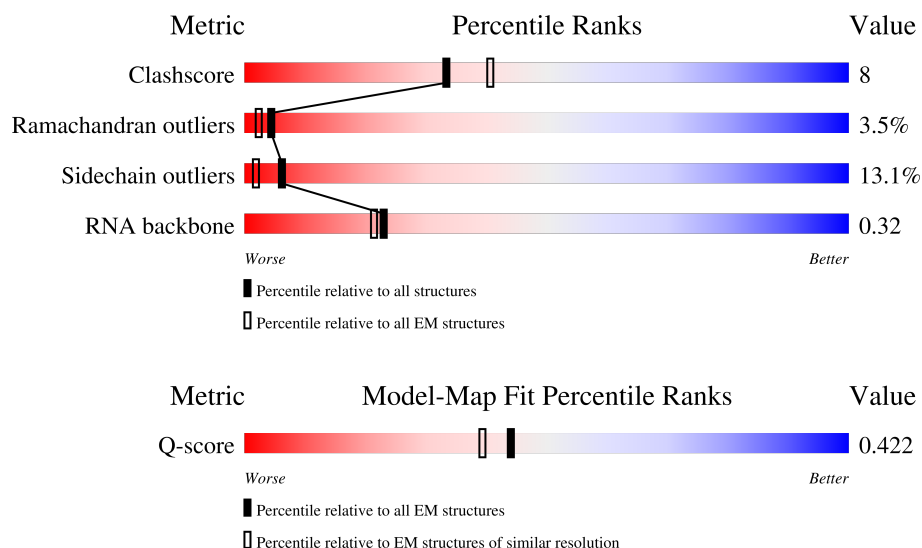
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.45 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



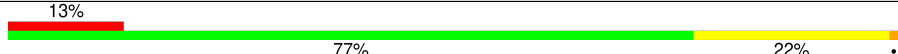
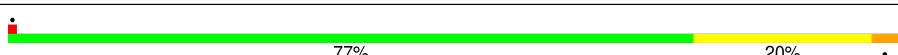
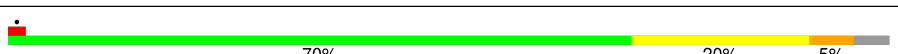
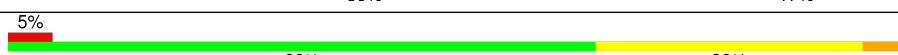
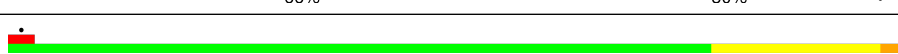
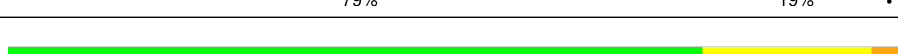
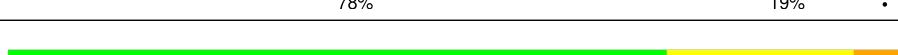
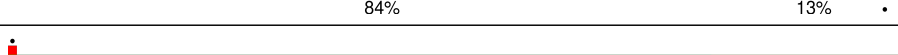
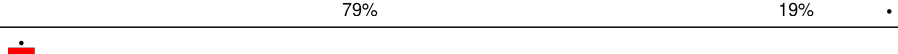
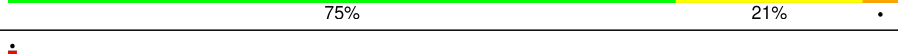
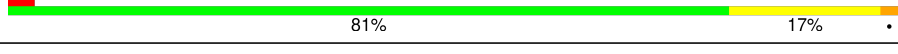
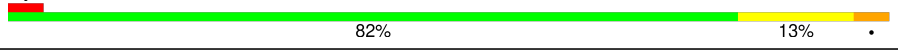
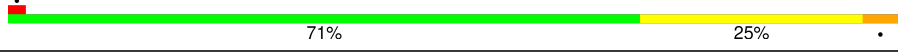
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13836 (2.95 - 3.95)

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

Mol	Chain	Length	Quality of chain
1	A	244	
2	B	394	
3	C	362	

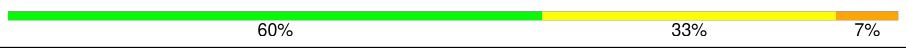
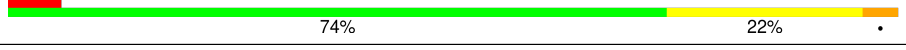
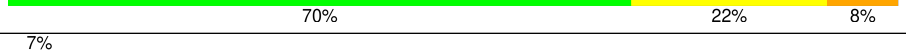
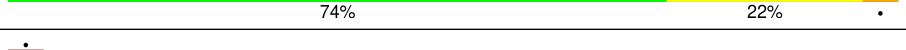
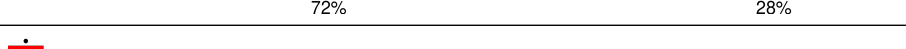
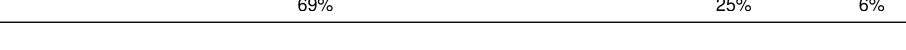
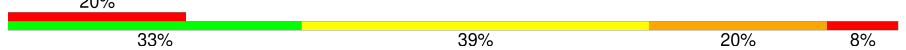
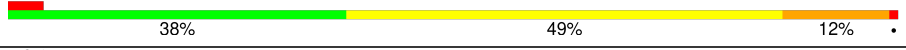
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Mol	Chain	Length	Quality of chain
4	D	292	
5	E	248	
6	F	225	
7	G	241	
8	H	190	
9	I	213	
10	J	169	
11	L	210	
12	M	138	
13	N	203	
14	O	199	
15	P	153	
16	Q	187	
17	R	180	
18	S	175	
19	T	159	
20	U	99	
21	V	131	
22	W	63	
23	X	119	
24	Y	134	
25	Z	135	
26	a	147	
27	b	75	
28	c	94	

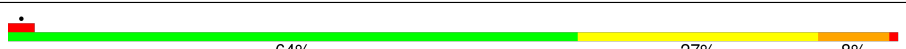
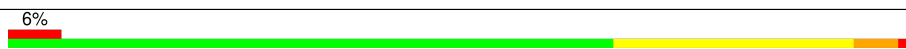
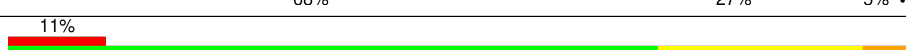
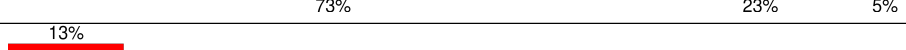
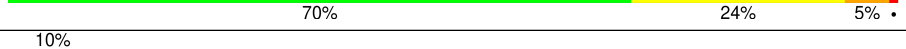
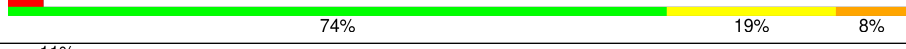
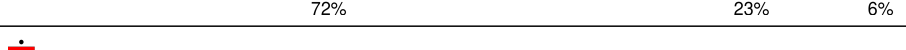
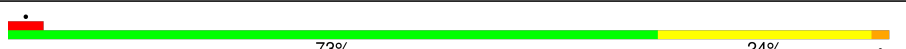
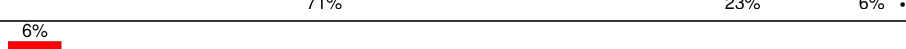
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Mol	Chain	Length	Quality of chain
29	d	107	
30	e	128	
31	f	109	
32	g	114	
33	h	122	
34	i	102	
35	j	86	
36	k	69	
37	l	50	
38	m	52	
39	n	23	
40	o	104	
41	p	91	
42	r	125	
43	s	198	
44	t	163	
45	1	15	
46	2	76	
47	3	75	
48	5	3662	
49	7	120	
50	8	156	
51	9	1719	
52	AA	208	
53	BB	213	

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Mol	Chain	Length	Quality of chain
54	CC	218	
55	DD	227	
56	EE	262	
57	FF	191	
58	GG	237	
59	HH	189	
60	II	206	
61	JJ	185	
62	KK	98	
63	LL	152	
64	MM	124	
65	NN	150	
66	OO	136	
67	PP	127	
68	QQ	141	
69	RR	129	
70	SS	137	
71	TT	141	
72	UU	104	
73	VV	83	
74	WW	129	
75	XX	141	
76	YY	126	
77	ZZ	75	
78	aa	98	

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Mol	Chain	Length	Quality of chain
79	bb	83	
80	cc	61	
81	dd	53	
82	ee	57	
83	ff	68	
84	gg	313	
85	hh	12	
86	ii	416	
87	jj	594	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
89	ZN	o	201	-	-	X	-

2 Entry composition

There are 91 unique types of molecules in this entry. The entry contains 226454 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	244	Total	C	N	O	S	0	0
			1868	1171	382	309	6		

- Molecule 2 is a protein called uL3.

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

- Molecule 3 is a protein called uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	362	Total	C	N	O	S	0	0
			2884	1814	578	478	14		

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	LYS	-	expression tag	UNP G1SVW5
C	363	SER	-	expression tag	UNP G1SVW5

- Molecule 4 is a protein called uL18.

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

- Molecule 5 is a protein called eL6.

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

- 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	776	241	216	9		

- Molecule 16 is a protein called uL14.

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
			1692	1102	287	296	7		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CC	194	ARG	HIS	conflict	UNP G1TUT9
CC	228	GLY	SER	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	62	Total	C	N	O	S	0	0
			520	331	98	85	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
ff	?	-	VAL	deletion	UNP G1SK22

- 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
			257	115	46	84	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	576	Total	C	N	O	S	0	0
			4543	2904	779	829	31		

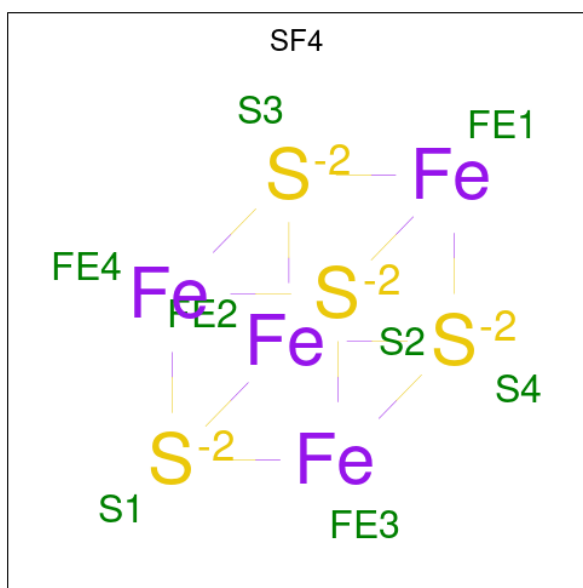
- Molecule 88 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
88	B	1	Total 1	Mg 1	0
88	C	1	Total 1	Mg 1	0
88	I	1	Total 1	Mg 1	0
88	P	1	Total 1	Mg 1	0
88	V	1	Total 1	Mg 1	0
88	g	1	Total 1	Mg 1	0
88	5	146	Total 146	Mg 146	0
88	7	5	Total 5	Mg 5	0
88	8	2	Total 2	Mg 2	0
88	9	34	Total 34	Mg 34	0
88	LL	1	Total 1	Mg 1	0
88	hh	1	Total 1	Mg 1	0

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

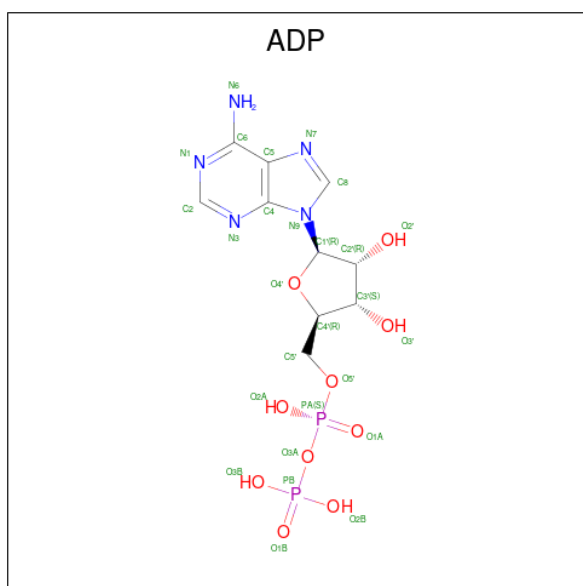
Mol	Chain	Residues	Atoms		AltConf
89	g	1	Total 1	Zn 1	0
89	j	1	Total 1	Zn 1	0
89	m	1	Total 1	Zn 1	0
89	o	1	Total 1	Zn 1	0
89	p	1	Total 1	Zn 1	0
89	aa	1	Total 1	Zn 1	0
89	dd	1	Total 1	Zn 1	0
89	ff	1	Total 1	Zn 1	0

- Molecule 90 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
90	jj	1	Total	Fe	S	0
			8	4	4	
90	jj	1	Total	Fe	S	0
			8	4	4	

- Molecule 91 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$).



Mol	Chain	Residues	Atoms					AltConf
91	jj	1	Total	C	N	O	P	0
			27	10	5	10	2	

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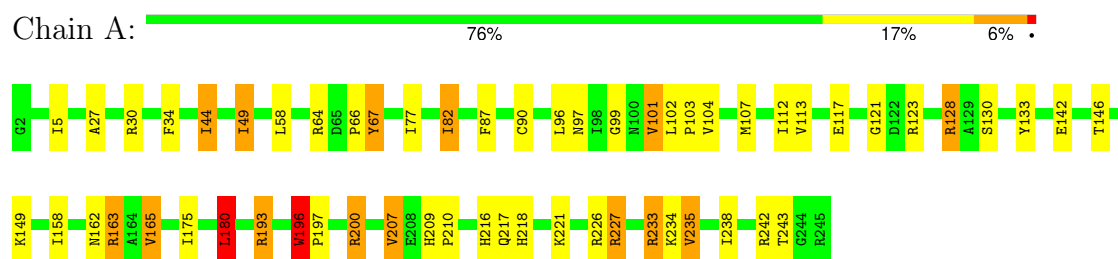
Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
91	jj	1	27	10	5	10	2	0

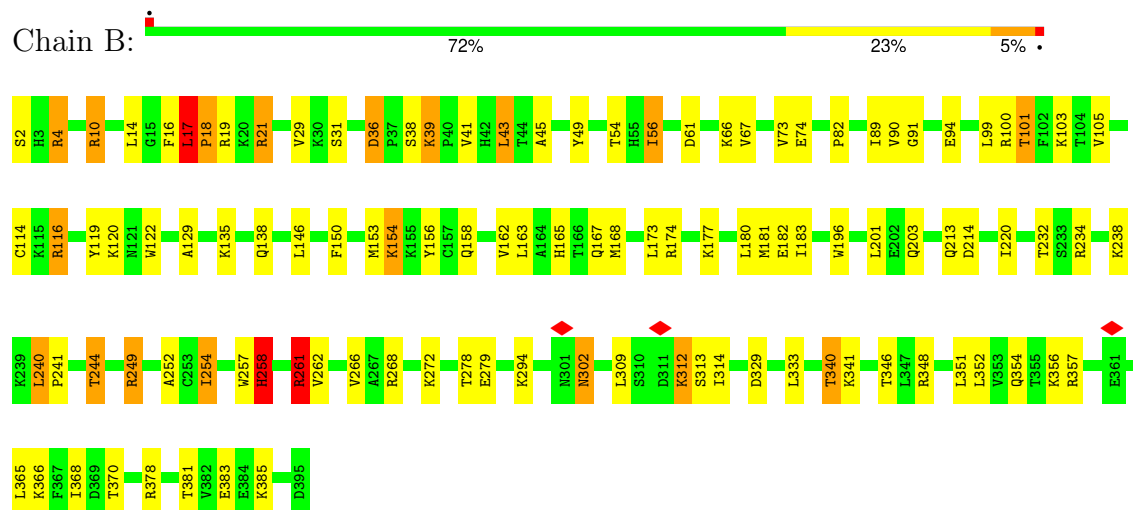
3 Residue-property plots

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

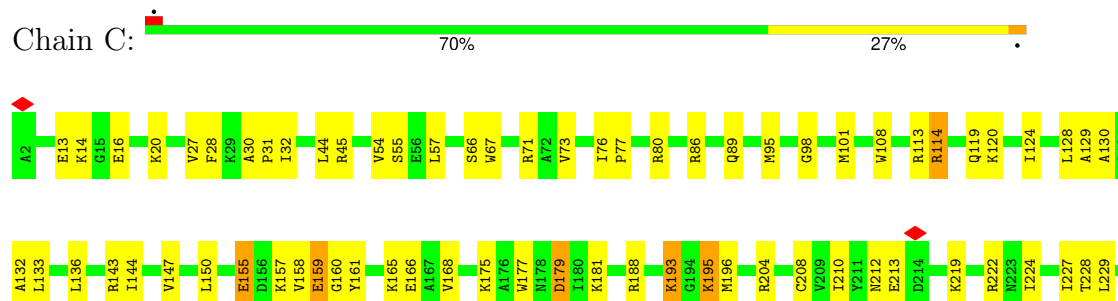
• Molecule 1: uL2

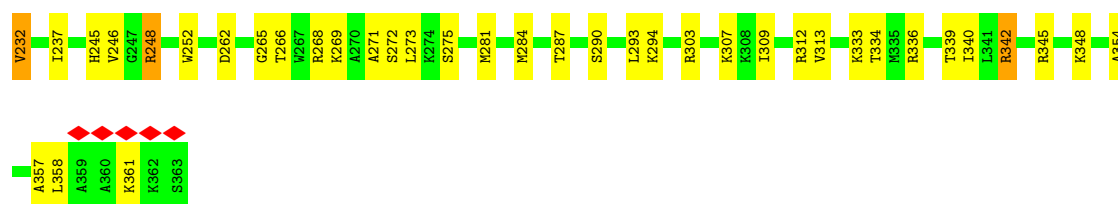


• Molecule 2: uL3

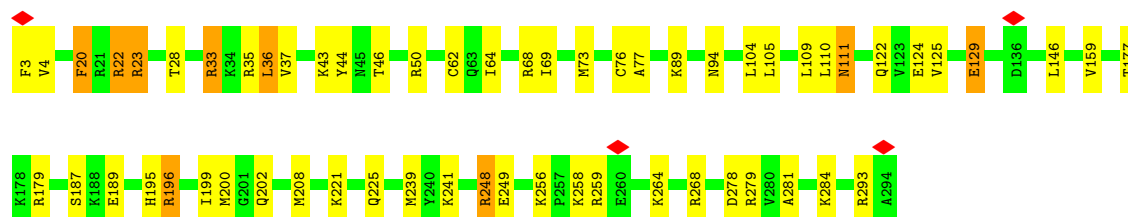
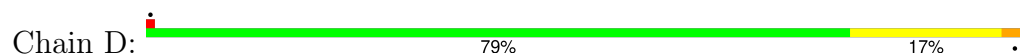


• Molecule 3: uL4

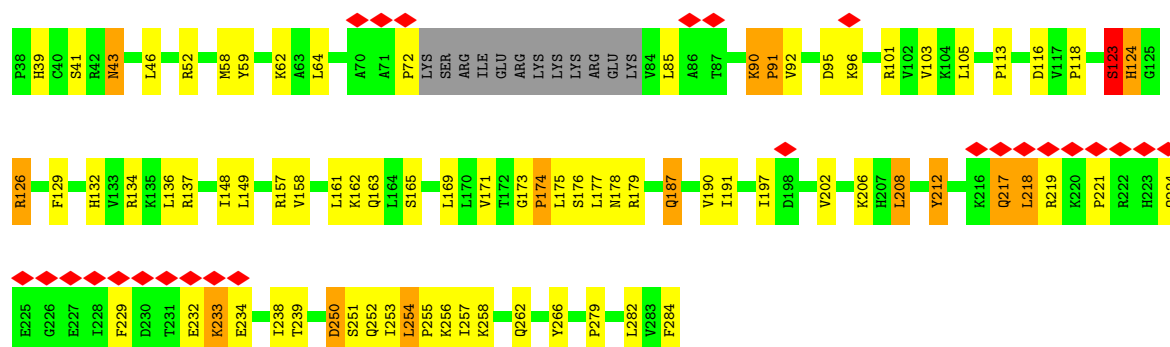




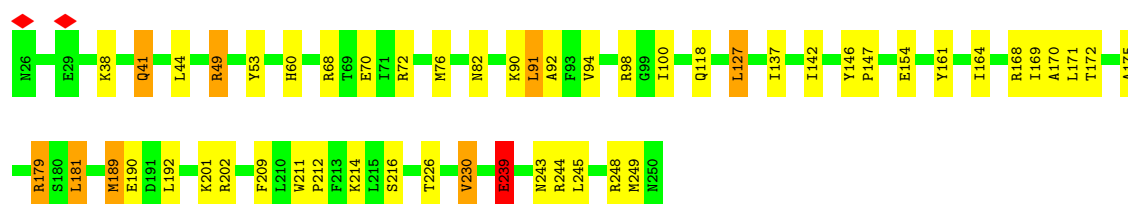
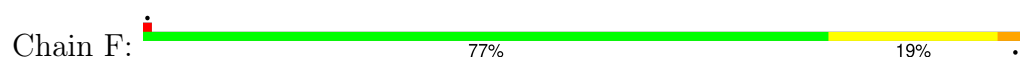
• Molecule 4: uL18



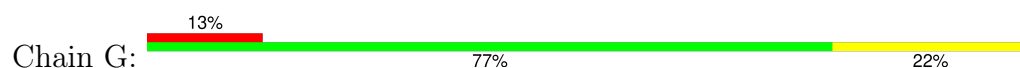
• Molecule 5: eL6

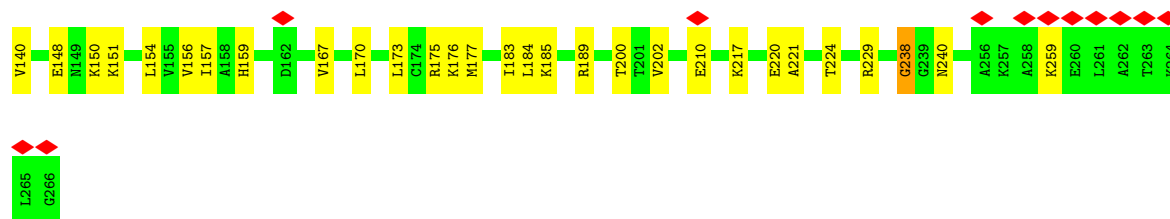


• Molecule 6: uL30

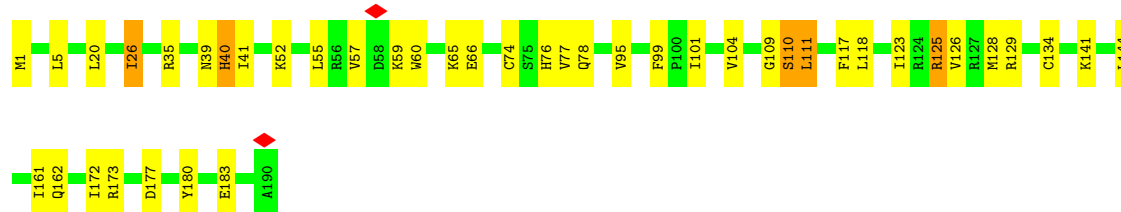
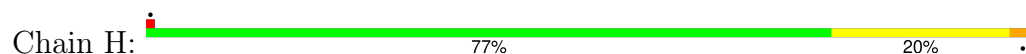


• Molecule 7: eL8

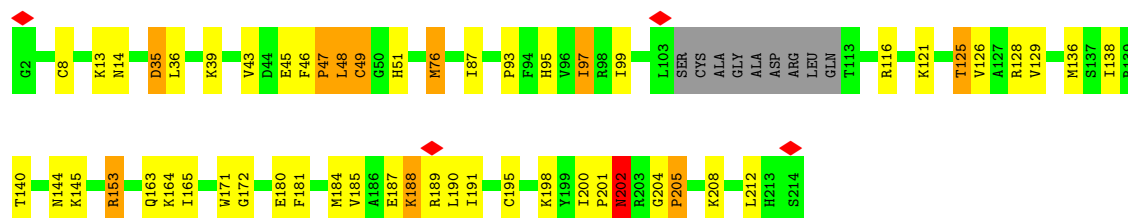




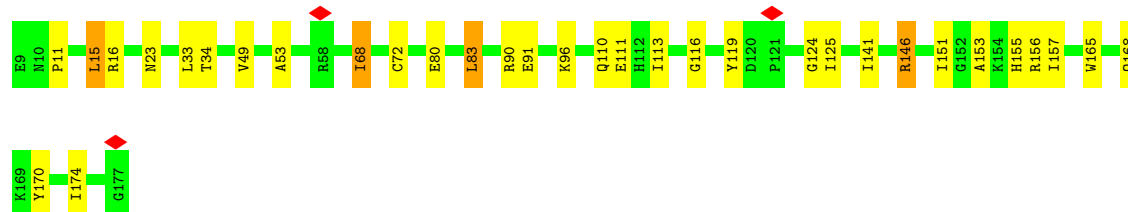
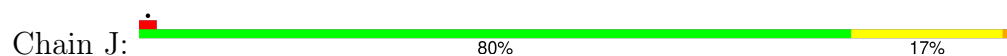
• Molecule 8: uL6



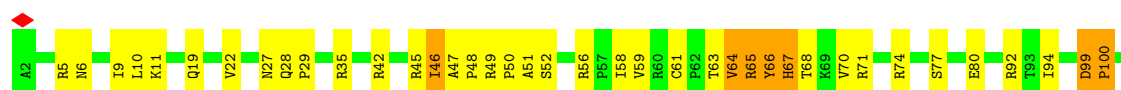
• Molecule 9: uL16

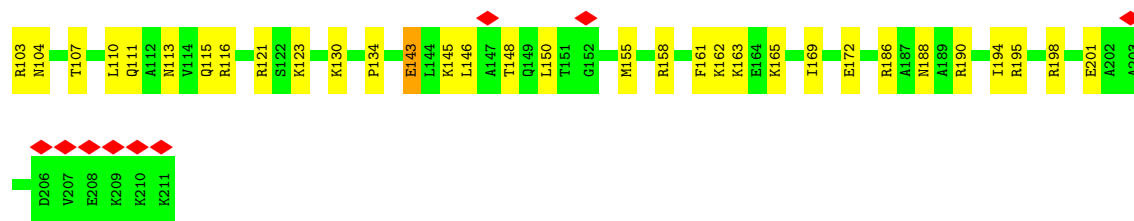


• Molecule 10: uL5

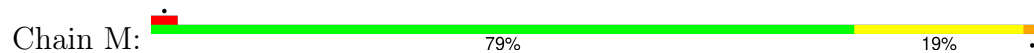


• Molecule 11: eL13

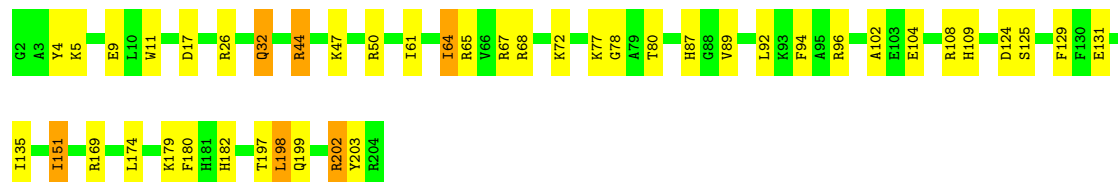
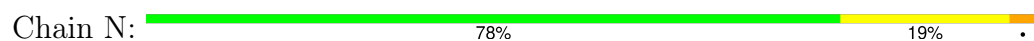




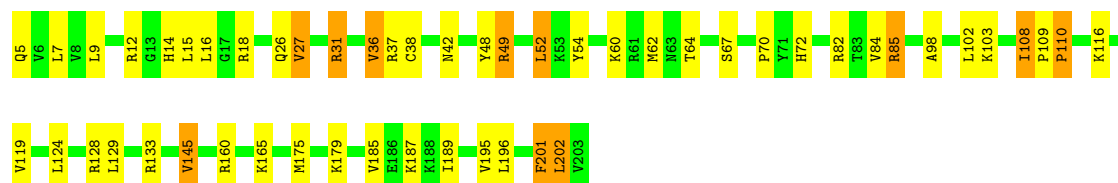
• Molecule 12: eL14



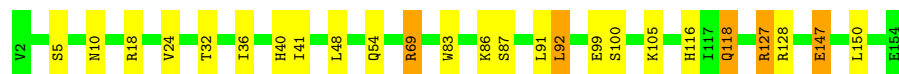
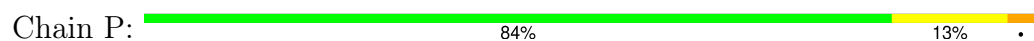
• Molecule 13: eL15



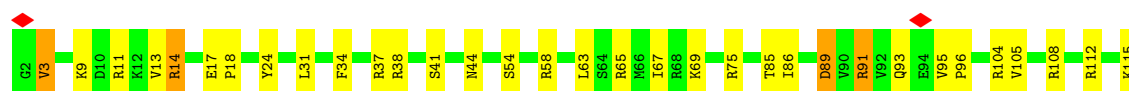
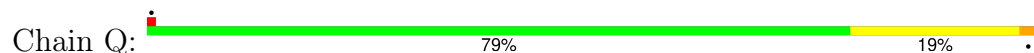
• Molecule 14: uL13

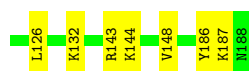


• Molecule 15: uL22



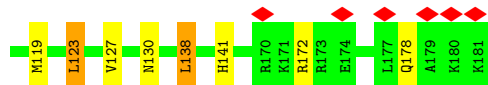
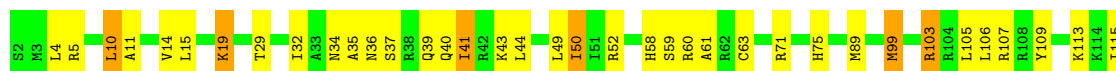
• Molecule 16: uL14





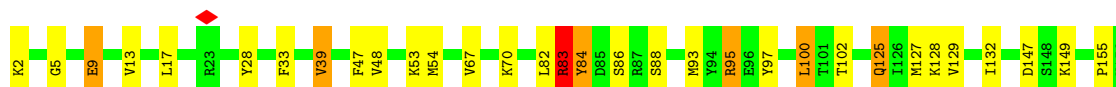
• Molecule 17: eL19

Chain R: 75% 21%



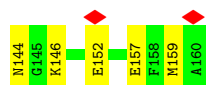
• Molecule 18: eL20

Chain S: 77% 18%



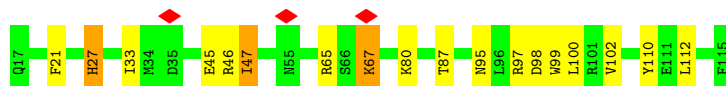
• Molecule 19: eL21

Chain T: 77% 20%



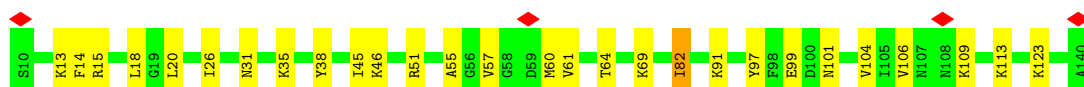
• Molecule 20: eL22

Chain U: 82% 15%



• Molecule 21: uL14

Chain V: 79% 21%



- Molecule 22: eL24

Chain W:  81% 17%



- Molecule 23: uL23

Chain X:  79% 19%



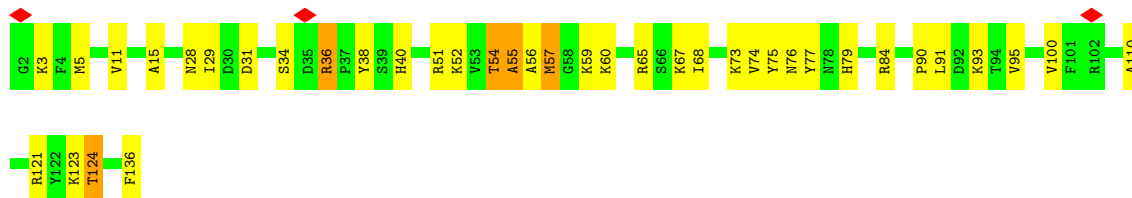
- Molecule 24: uL24

Chain Y:  82% 13%



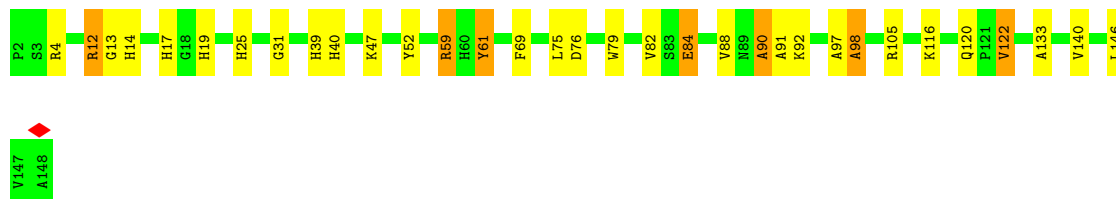
- Molecule 25: eL27

Chain Z:  71% 25%



- Molecule 26: uL15

Chain a:  78% 18% 5%



- Molecule 27: eL29

Chain b:  17% 83% 12% 5%



- Molecule 28: eL30

Chain c:  73% 24%



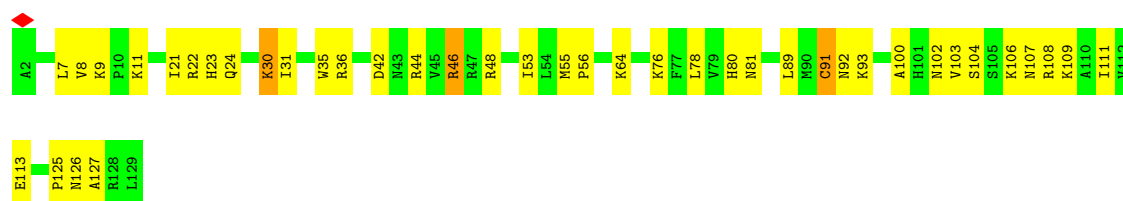
- Molecule 29: eL31

Chain d:  78% 20%



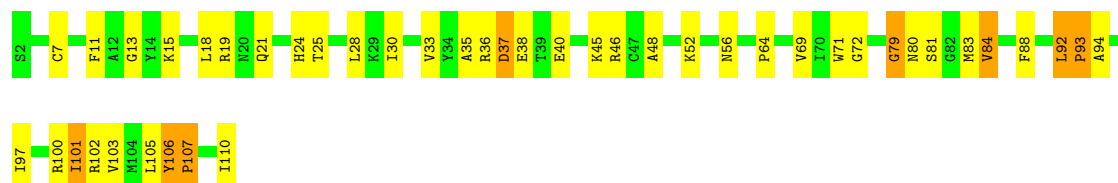
- Molecule 30: eL32

Chain e:  68% 30%



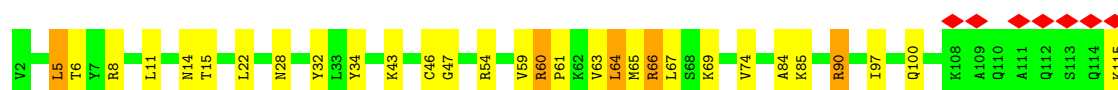
- Molecule 31: eL33

Chain f:  60% 33% 7%



- Molecule 32: eL34

Chain g:  6% 74% 22%

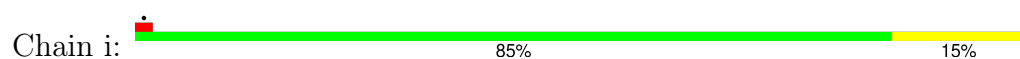


- Molecule 33: uL29

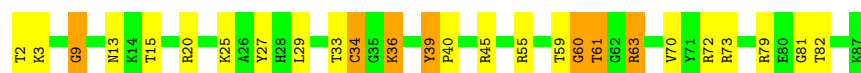
Chain h:  83% 13%



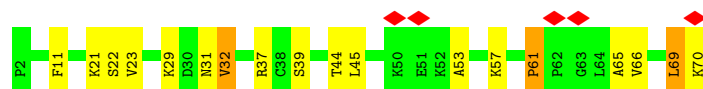
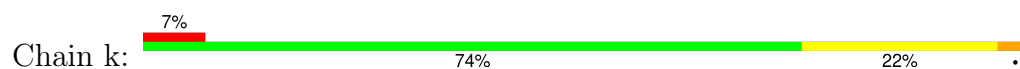
- Molecule 34: eL36



- Molecule 35: eL37



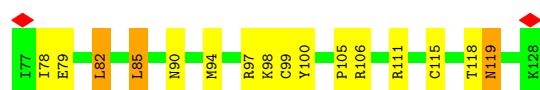
- Molecule 36: eL38



- Molecule 37: eL39



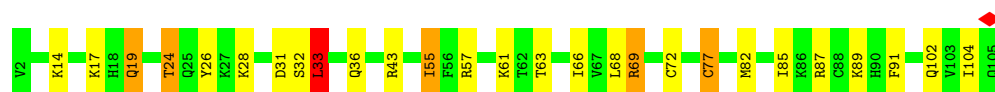
- Molecule 38: eL40



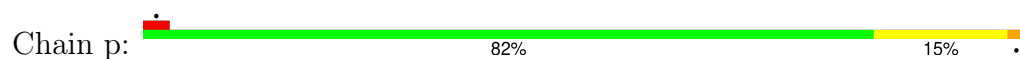
- Molecule 39: eL41



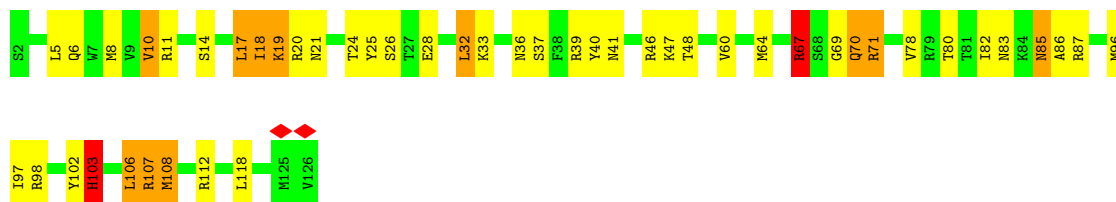
- Molecule 40: eL42



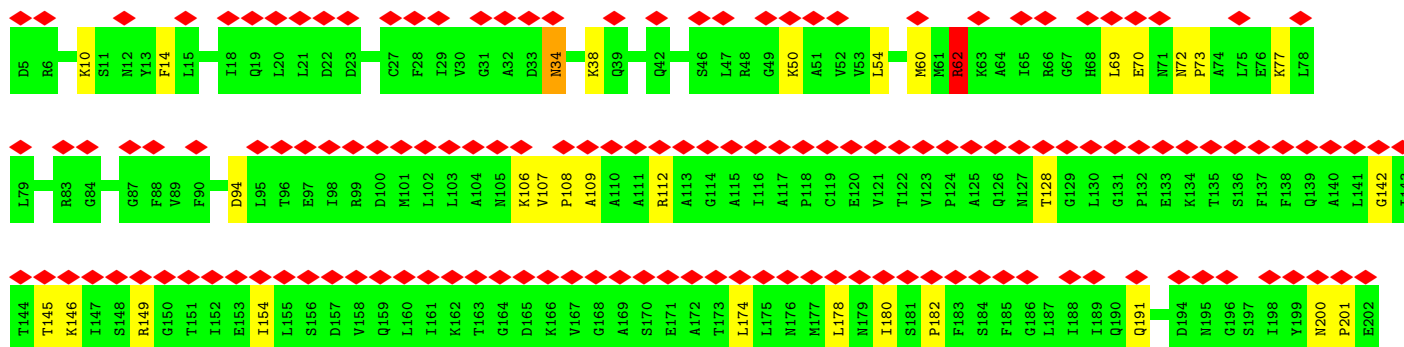
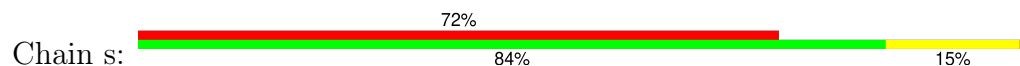
- Molecule 41: eL43



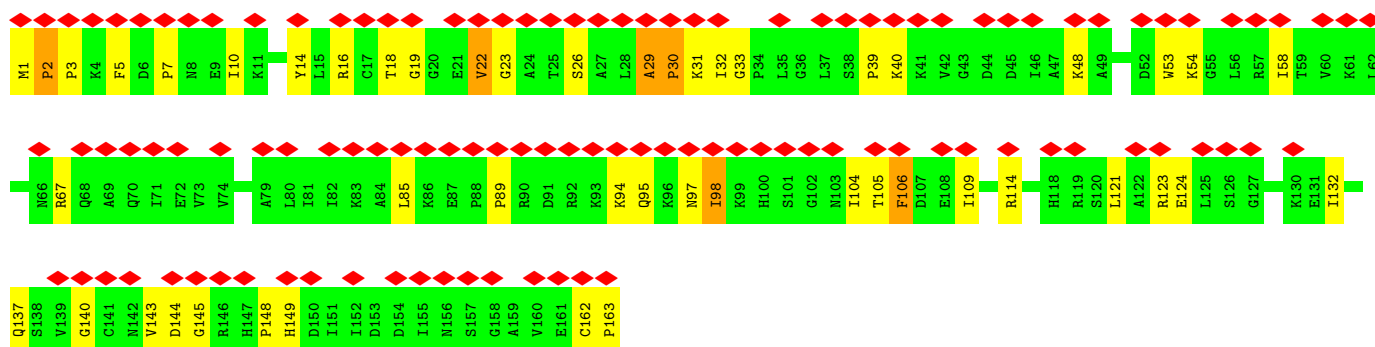
• Molecule 42: eL28



• Molecule 43: uL10

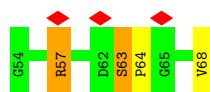


• Molecule 44: uL11

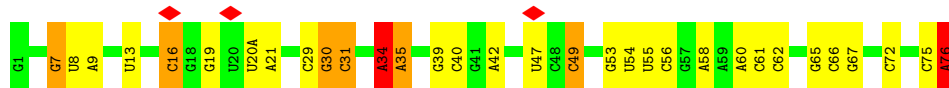


• Molecule 45: peptide

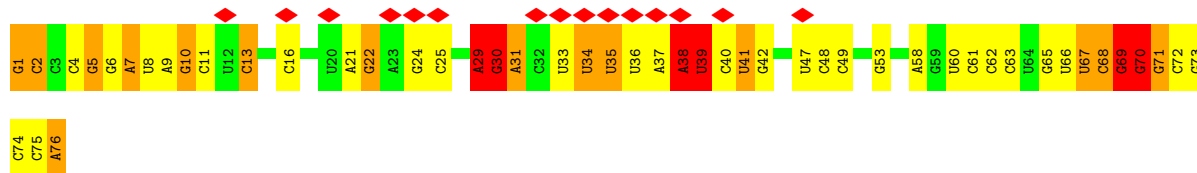




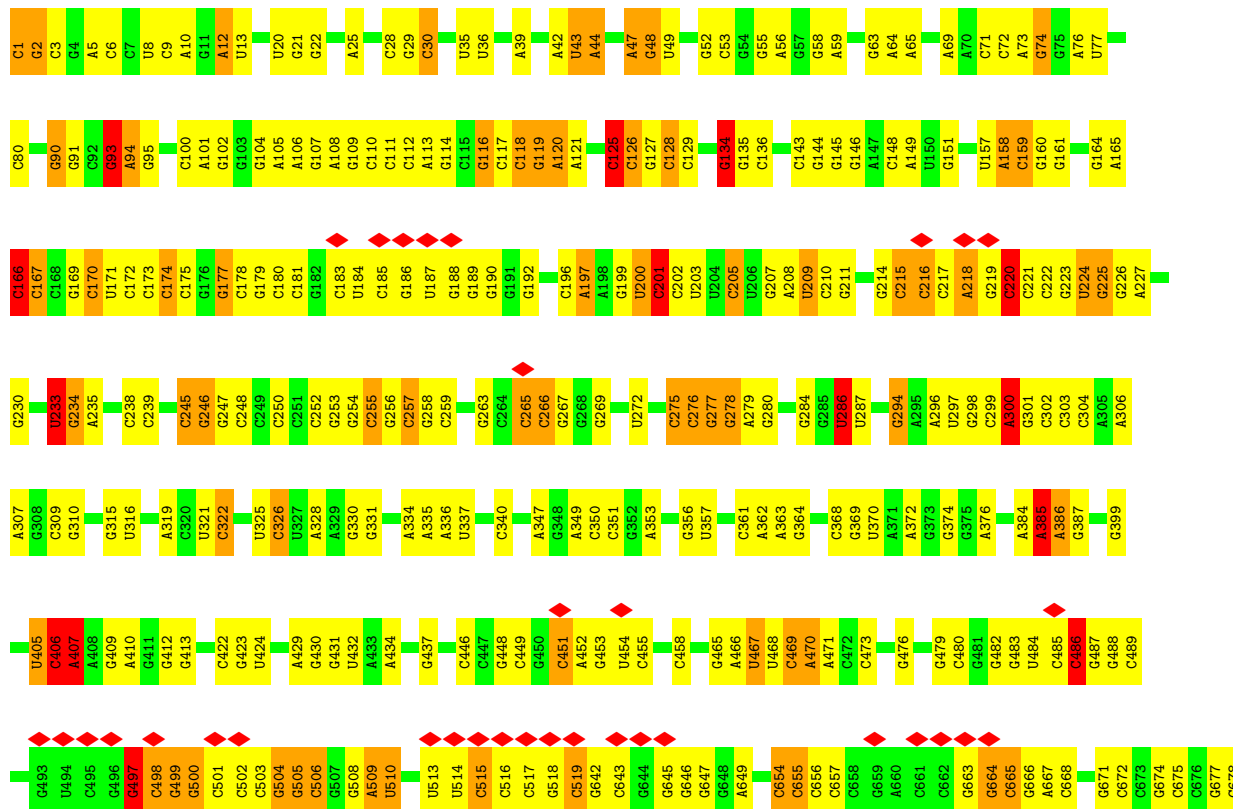
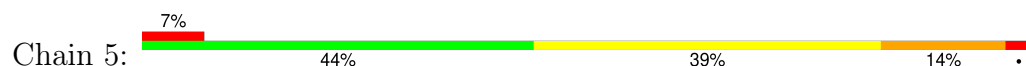
• Molecule 46: tRNA(Val)



• Molecule 47: tRNA(Lys)



• Molecule 48: 28S ribosomal RNA

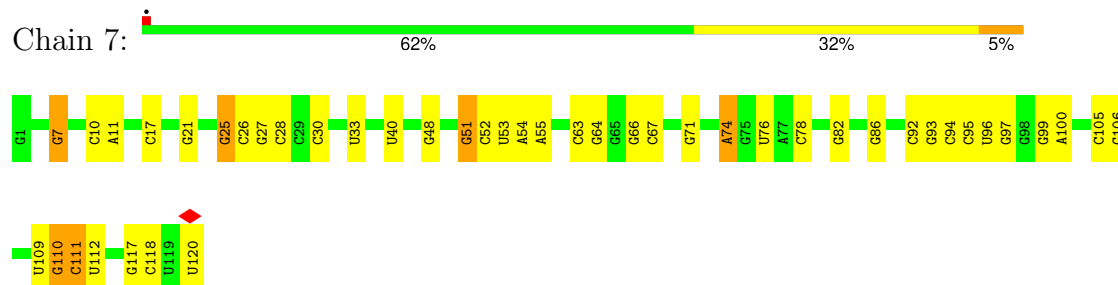


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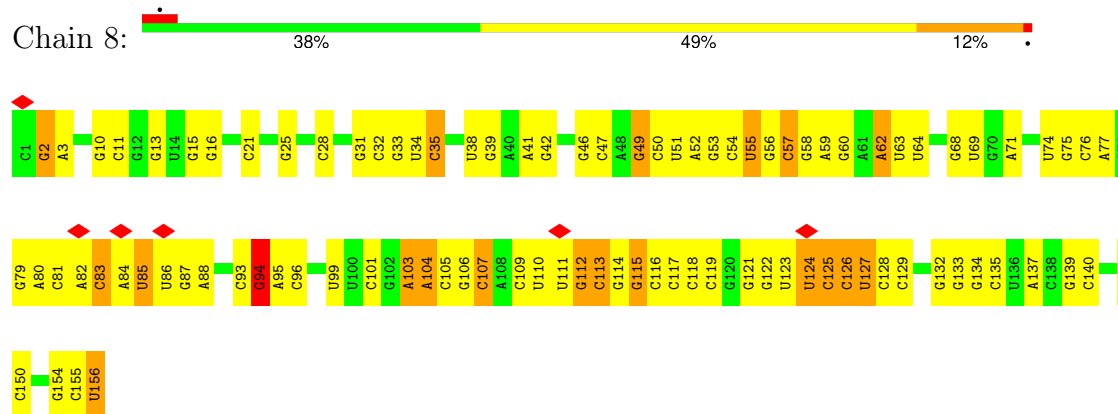


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G4106	G4107	C4108	C4109	C4110	U4111	U4112	U4113	C4114	C4115	C4116	U4117	U4118	C4119	U4120	C4121	C4122	C4123	C4124	C4125	C4126	A4127	A4128	C4129	C4130	C4131	C4132	C4133	C4134	C4135	C4136	C4137	C4138	C4139	C4140	C4141	C4142	C4143	C4144	C4145	C4146	C4147	C4148	C4152	C4153	G4154	C4155	C4158	C4159	C4160	C4161	C4162	U4163	C4164	C4165	G4166	C4168																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
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C4259	U4260	C4261	C4262	C4263	U4264	U4265	G4266	A4268	C4269	C4270	A4271	G4272	A4273	A4274	G4275	G4276	G4277	C4278	A4280	A4281	A4282	G4283	C4284	G4291	G4297	U4301	U4302	C4303	C4304	C4305	U4306	A4307	A4311	U4312	A4313	C4314	A4317	C4318	C4319	C4320	U4321	A4325	G4326	C4327	G4328	C4329	C4330	C4331	C4332	U4333																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
C4335	A4336	C4337	C4338	C4341	C4349	C4350	U4354	U4355	C4356	U4360	G4364	G4367	G4368	U4371	U4372	U4373	U4374	U4375	U4376	A4378	A4379	A4380	C4387	A4388	C4389	A4390	A4391	U4392	U4393	A4394	U4395	A4396	A4397	C4398	U4399	G4400	U4404	C4405	G4408	C4409	G4411	G4416	G4418	U4419	U4420	C4421																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
A4422	U4423	A4424	C4425	C4426	U4430	U4431	U4432	U4433	C4434	U4435	U4438	U4439	U4440	A4441	U4444	U4445	C4447	U4448	U4449	U4450	U4451	U4452	G4454	U4457	C4458	C4461	C4462	U4463	A4464	U4471	G4472	A4473	A4474	C4475	C4476	U4481	U4482	C4483	A4484	C4486	A4487	A4488	C4489	C4490	C4491	U4492	G4495																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
U4500	C4506	C4507	C4508	U4509	A4510	A4511	U4512	U4513	U4514	U4515	U4516	A4517	U4518	U4519	U4520	U4521	A4522	A4523	C4525	U4526	C4527	G4528	U4530	U4531	A4535	C4536	C4537	G4538	C4543	A4548	G4549	U4550	U4555	U4556	U4557	U4558	A4559	C4560	C4561	U4562	U4563	A4564	G4567	A4568	U4569	C4570	U4573	U4574	C4575	U4576																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
U4577	C4578	U4579	U4580	C4583	A4584	U4585	U4586	C4587	A4590	U4591	A4595	U4600	G4606	C4614	C4615	C4616	C4617	C4618	C4625	C4631	U4634	A4635	U4636	C4637	C4640	U4641	G4644	C4645	U4646	C4647	A4648	A4655	A4656	U4657	C4661	C4662	G4663	A4664	A4665	C4666	C4667	C4670	C4671	U4672	C4675	C4676	C4677																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
U4677	A4681	U4682	A4687	A4691	C4694	C4695	C4696	U4699	U4700	A4701	G4702	U4709	G4713	C4714	C4715	C4716	C4717	C4718	C4719	C4720	C4721	G4722	A4723	A4724	C4725	C4730	C4731	G4732	C4733	A4734	C4735	C4736	C4737	C4738	C4739	U4740	C4741	G4742	C4743	C4744	C4745	C4746	C4749	C4750	U4753	C4754	C4756	C4757																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
U4758	C4759	G4760	C4761	A4762	U4763	A4764	C4767	C4768	C4769	U4770	C4771	C4772	C4773	C4774	C4789	C4863	C4868	U4869	C4890	C4891	C4892	C4893	C4894	C4895	C4896	C4897	C4898	C4899	C4900	C4901	C4904	C4905	C4906	C4907	C4908	C4909	C4910	C4911	C4912	C4913	C4914	C4915	C4916	C4917	C4918	C4919	C4920	C4921	C4922	C4923	C4924	C4925	C4926	C4927	C4928	C4929	C4930	C4931	C4932	C4933	C4934	C4935	C4936	C4937	C4938	C4939	C4940	C4941	C4942	C4943	C4944	C4945	C4946	C4947	C4948	C4949	C4950	C4951	C4952	C4953	C4954	C4955	C4956	C4957	C4958	C4959	C4960	C4961	C4962	C4963	C4964	C4965	C4966	C4967	C4968	C4969	C4970	C4971	C4972	C4973	C4974	C4975	C4976	C4977	C4978	C4979	C4980	C4981	C4982	C4983	C4984	C4985	C4986	C4987	C4988	C4989	C4990	C4991	C4992	C4993	C4994	C4995	C4996	C4997	C4998	C4999	C5000	C5001	C5002	C5003	C5004	C5005	C5006	C5007	C5008	C5009	C5010	C5011	C5012	C5013	C5014	C5015	C5016	C5017	C5018	C5019	C5020	C5021	C5022	C5023	C5024	C5025	C5026	C5027	C5028	C5029	C5030	C5031	C5032	C5033	C5034	C5035	C5036	C5037	C5038	C5039	C5040	C5041	C5042	C5043	C5044	C5045	C5046	C5047	C5048	C5049	C5050	C5051	C5052	C5053	C5054	C5055	C5056	C5057	C5058	C5059	C5060	C5061	C5062	C5063	C5064	C5065	C5066	C5067	C5068	C5069	C5070	C5071	C5072	C5073	C5074	C5075	C5076	C5077	C5078	C5079	C5080	C5081	C5082	C5083	C5084	C5085	C5086	C5087	C5088	C5089	C5090	C5091	C5092	C5093	C5094	C5095	C5096	C5097	C5098	C5099	C5100	C5101	C5102	C5103	C5104	C5105	C5106	C5107	C5108	C5109	C5110	C5111	C5112	C5113	C5114	C5115	C5116	C5117	C5118	C5119	C5120	C5121	C5122	C5123	C5124	C5125	C5126	C5127	C5128	C5129	C5130	C5131	C5132	C5133	C5134	C5135	C5136	C5137	C5138	C5139	C5140	C5141	C5142	C5143	C5144	C5145	C5146	C5147	C5148	C5149	C5150	C5151	C5152	C5153	C5154	C5155	C5156	C5157	C5158	C5159	C5160	C5161	C5162	C5163	C5164	C5165	C5166	C5167	C5168	C5169	C5170	C5171	C5172	C5173	C5174	C5175	C5176	C5177	C5178	C5179	C5180	C5181	C5182	C5183	C5184	C5185	C5186	C5187	C5188	C5189	C5190	C5191	C5192	C5193	C5194	C5195	C5196	C5197	C5198	C5199	C5200	C5201	C5202	C5203	C5204	C5205	C5206	C5207	C5208	C5209	C5210	C5211	C5212	C5213	C5214	C5215	C5216	C5217	C5218	C5219	C5220	C5221	C5222	C5223	C5224	C5225	C5226	C5227	C5228	C5229	C5230	C5231	C5232	C5233	C5234	C5235	C5236	C5237	C5238	C5239	C5240	C5241	C5242	C5243	C5244	C5245	C5246	C5247	C5248	C5249	C5250	C5251	C5252	C5253	C5254	C5255	C5256	C5257	C5258	C5259	C5260	C5261	C5262	C5263	C5264	C5265	C5266	C5267	C5268	C5269	C5270	C5271	C5272	C5273	C5274	C5275	C5276	C5277	C5278	C5279	C5280	C5281	C5282	C5283	C5284	C5285	C5286	C5287	C5288	C5289	C5290	C5291	C5292	C5293	C5294	C5295	C5296	C5297	C5298	C5299	C5300	C5301	C5302	C5303	C5304	C5305	C5306	C5307	C5308	C5309	C5310	C5311	C5312	C5313	C5314	C5315	C5316	C5317	C5318	C5319	C5320	C5321	C5322	C5323	C5324	C5325	C5326	C5327	C5328	C5329	C5330	C5331	C5332	C5333	C5334	C5335	C5336	C5337	C5338	C5339	C5340	C5341	C5342	C5343	C5344	C5345	C5346	C5347	C5348	C5349	C5350	C5351	C5352	C5353	C5354	C5355	C5356	C5357	C5358	C5359	C5360	C5361	C5362	C5363	C5364	C5365	C5366	C5367	C5368	C5369	C5370	C5371	C5372	C5373	C5374	C5375	C5376	C5377	C5378	C5379	C5380	C5381	C5382	C5383	C5384	C5385	C5386	C5387	C5388	C5389	C5390	C5391	C5392	C5393	C5394	C5395	C5396	C5397	C5398	C5399	C5400	C5401	C5402	C5403	C5404	C5405	C5406	C5407	C5408	C5409	C5410	C5411	C5412	C5413	C5414	C5415	C5416	C5417	C5418	C5419	C5420	C5421	C5422	C5423	C5424	C5425	C5426	C5427	C5428	C5429	C5430	C5431	C5432	C5433	C5434	C5435	C5436	C5437	C5438	C5439	C5440	C5441	C5442	C5443	C5444	C5445	C5446	C5447	C5448	C5449	C5450	C5451	C5452	C5453	C5454	C5455	C5456	C5457	C5458	C5459	C5460	C5461	C5462	C5463	C5464	C5465	C5466	C5467	C5468	C5469	C5470	C5471	C5472	C5473	C5474	C5475	C5476	C5477	C5478	C5479	C5480	C5481	C5482	C5483	C5484	C5485	C5486	C5487	C5488	C5489	C5490	C5491	C5492	C5493	C5494	C5495	C5496	C5497	C5498	C5499	C5500	C5501	C5502	C5503	C5504	C5505	C5506	C5507	C5508	C5509	C5510	C5511	C5512	C5513	C5514	C5515	C5516	C5517	C5518	C5519	C5520	C5521	C5522	C5523	C5524	C5525	C5526	C5527	C5528	C5529	C5530	C5531	C5532	C5533	C5534	C5535	C5536	C5537	C5538	C5539	C5540	C5541	C5542	C5543	C5544	C5545	C5546	C5547	C5548	C5549	C5550	C5551	C5552	C5553	C5554	C5555	C5556	C5557	C5558	C5559	C5560	C5561	C5562	C5563	C5564	C5565	C5566	C5567	C5568	C5569	C5570	C5571	C5572	C5573	C5574	C5575	C5576	C5577	C5578	C5579	C5580	C5581	C5582	C5583	C5584	C5585	C5586	C5587	C5588	C5589	C5590	C5591	C5592	C5593	C5594	C5595	C5596	C5597	C5598	C5599	C5600	C5601	C5602	C5603	C5604	C5605	C5606	C5607	C5608	C5609	C5610	C5611	C5612	C5613	C5614	C5615	C5616	C5617	C5618	C5619	C5620	C5621	C5622	C5623	C5624	C5625	C5626	C5627	C5628	C5629	C5630	C5631	C5632	C5633	C5634	C5635	C5636	C5637	C5638	C5639	C5640	C5641	C5642	C5643	C5644	C5645	C5646	C5647	C5648	C5649	C5650	C5651	C5652	C5653	C5654	C5655	C5656	C5657	C5658	C5659	C5660	C5661	C5662	C5663	C5664	C5665	C5666	C5667	C5668	C5669	C5670	C5671	C5672	C5673	C5674	C5675	C5676	C5677	C5678	C5679	C5680	C5681	C5682	C5683	C5684	C5685	C5686	C5687	C5688	C5689	C5690	C5691	C5692	C5693	C5694	C5695	C5696	C5697	C5698	C5699	C5700	C5701	C5702	C5703	C5704	C5705	C5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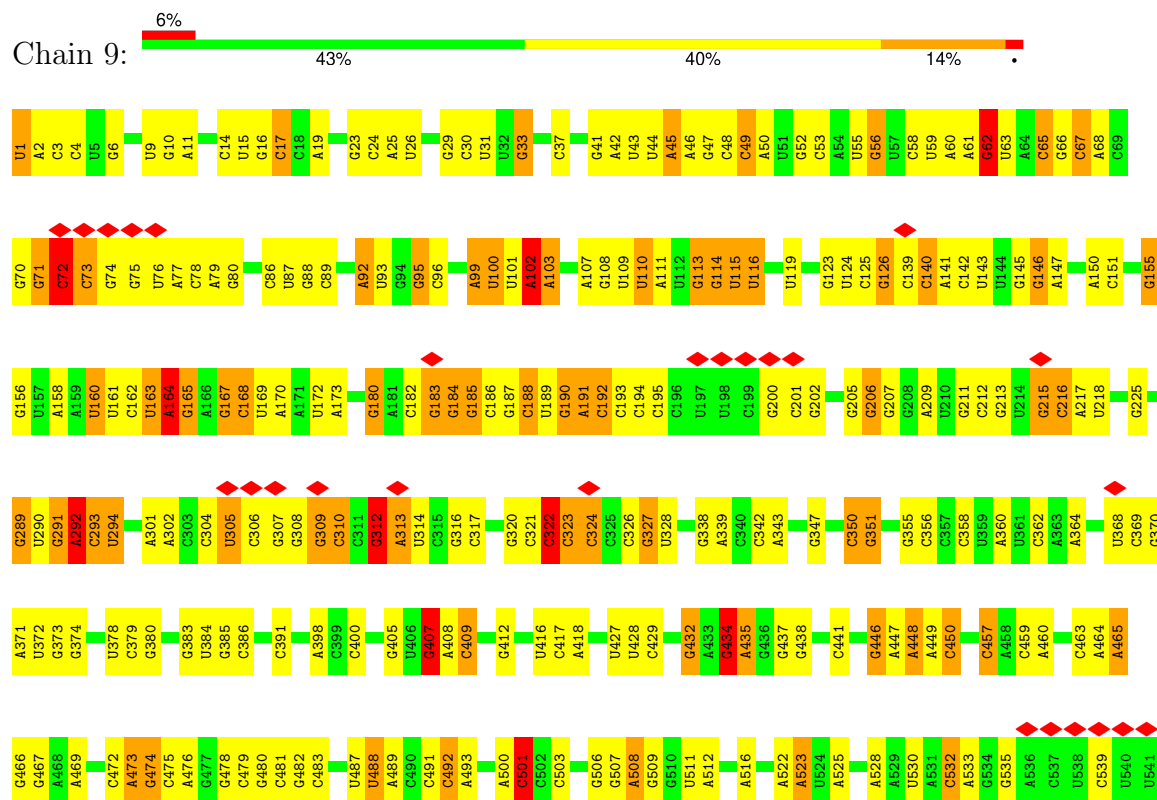
- Molecule 49: 5S ribosomal RNA

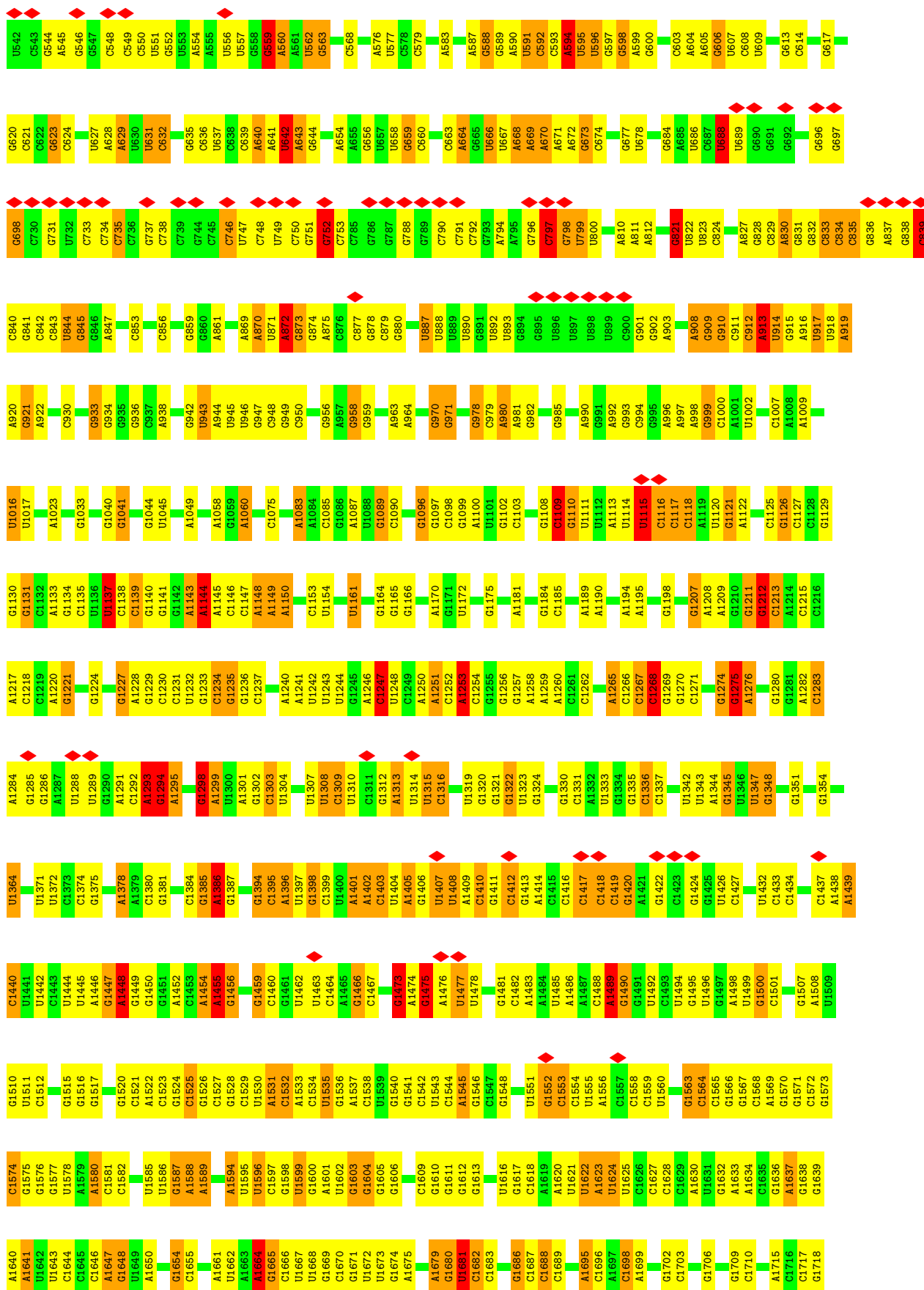


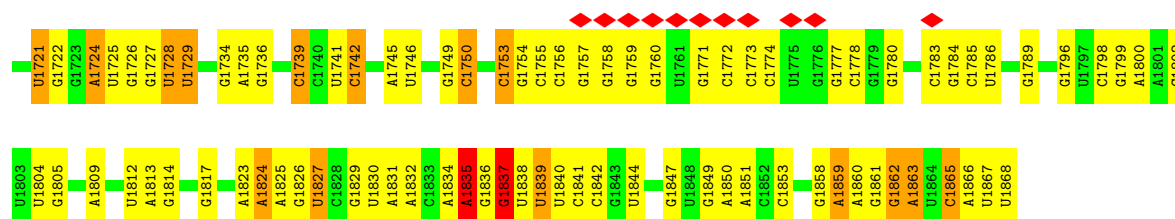
- Molecule 50: 5.8S ribosomal RNA



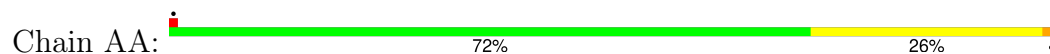
- Molecule 51: 18S ribosomal RNA



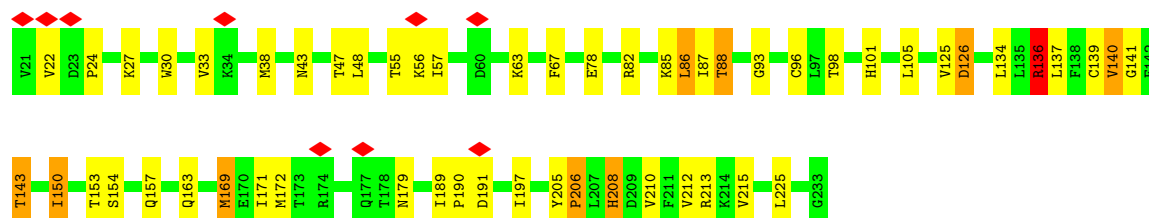
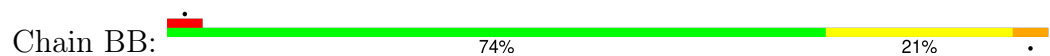




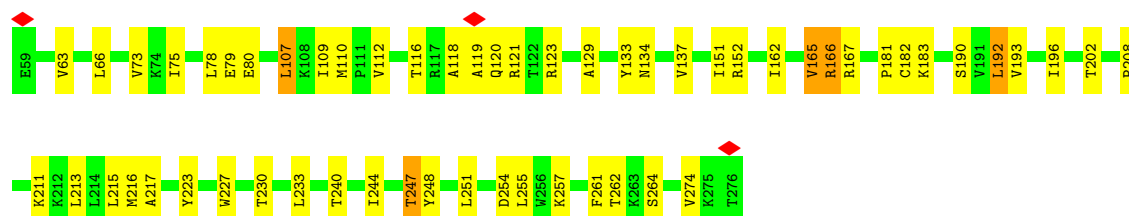
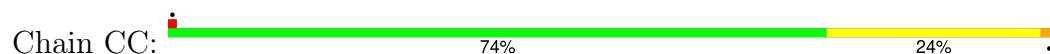
• Molecule 52: uS2



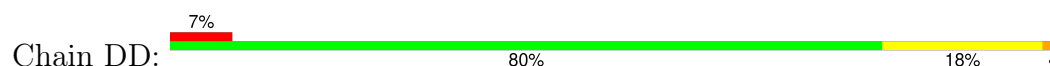
• Molecule 53: eS1

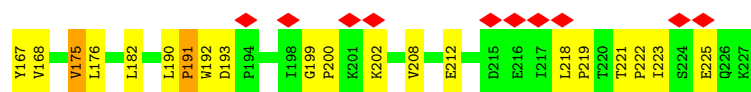


• Molecule 54: uS5

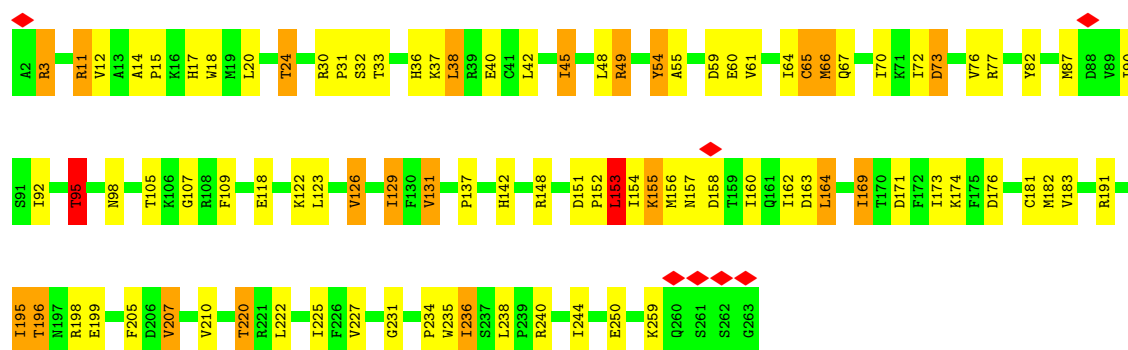


• Molecule 55: uS3

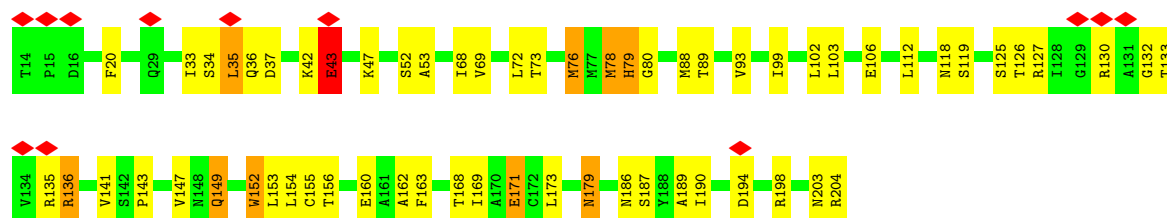




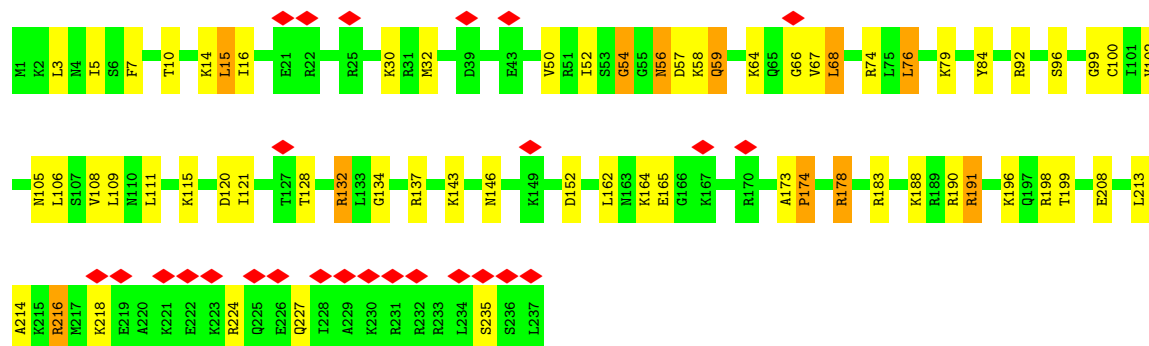
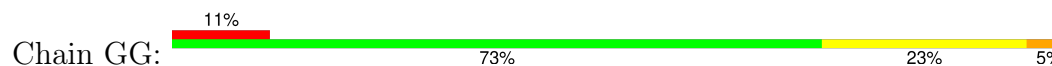
• Molecule 56: eS4



• Molecule 57: uS7

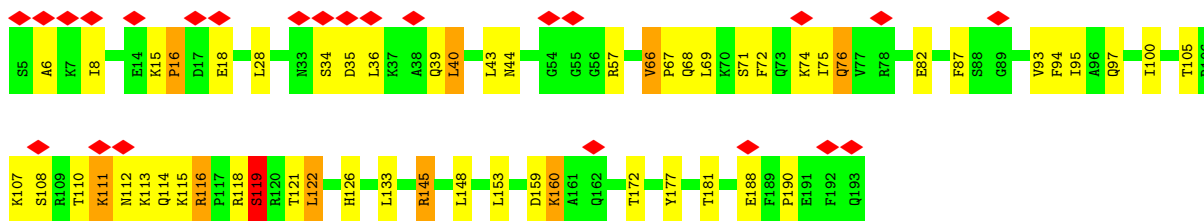


• Molecule 58: eS6

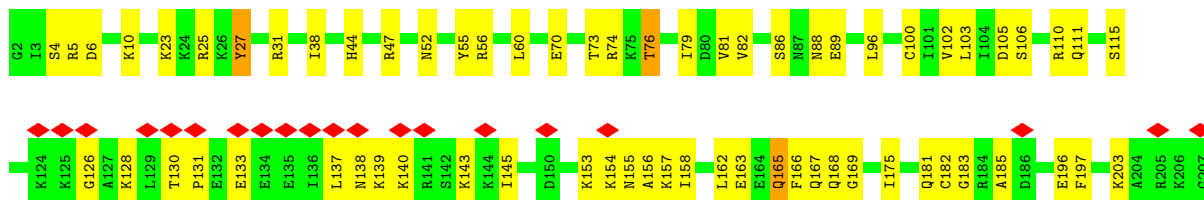


• Molecule 59: eS7

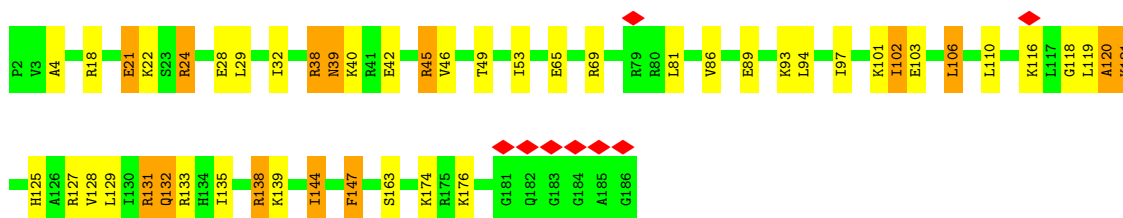
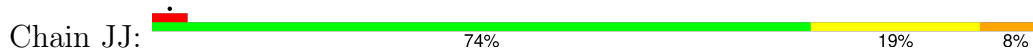




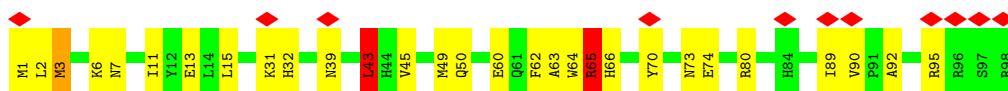
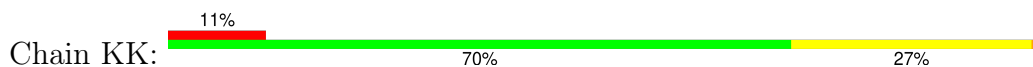
• Molecule 60: eS8



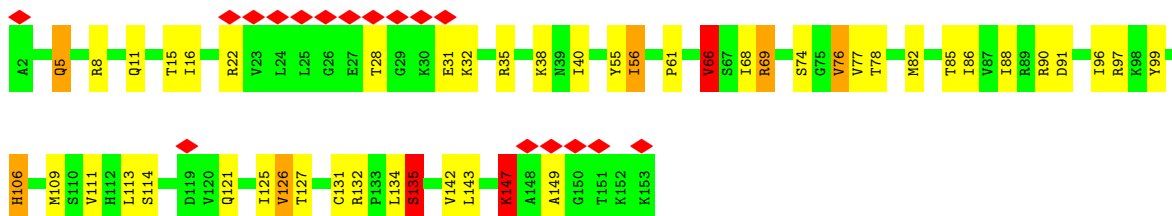
• Molecule 61: uS4



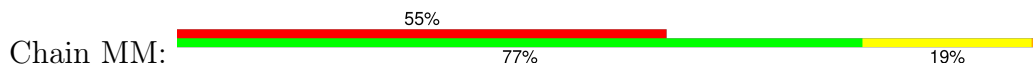
• Molecule 62: eS10

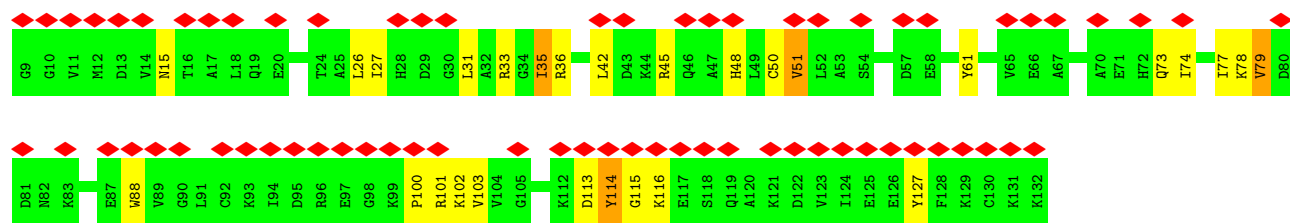


• Molecule 63: uS17



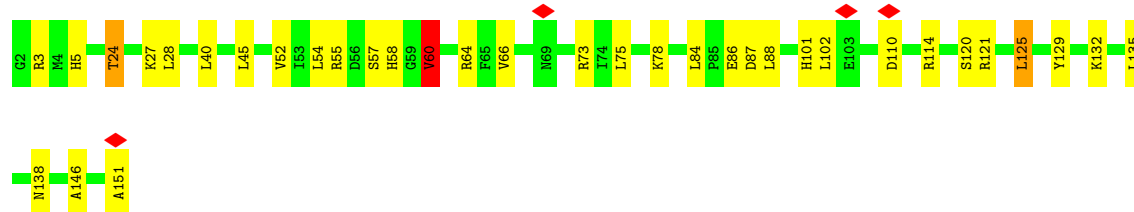
• Molecule 64: eS12





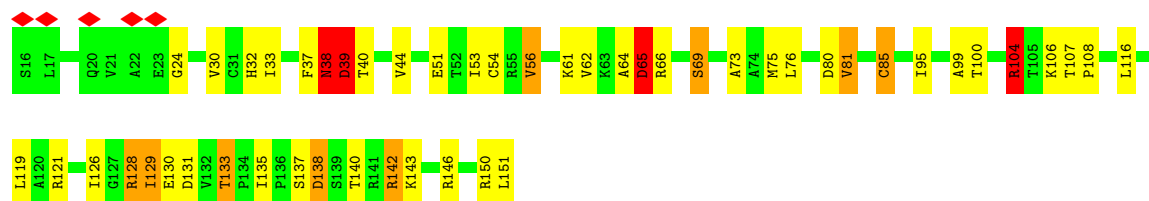
• Molecule 65: uS15

Chain NN: 77% 21% ..



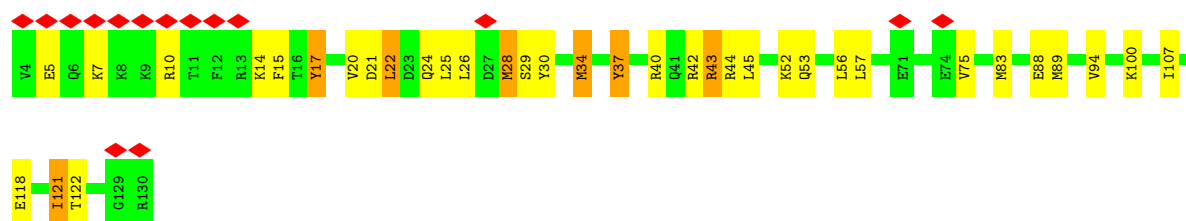
• Molecule 66: uS11

Chain OO: 63% 27% 7% .



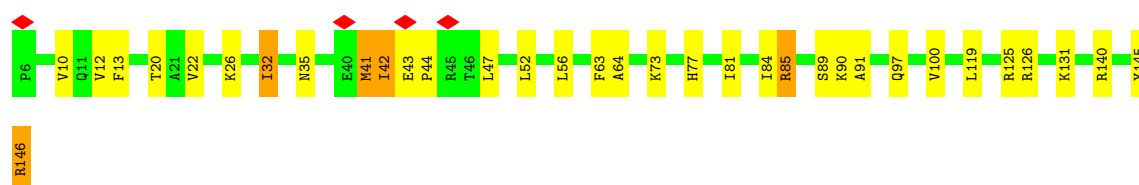
• Molecule 67: uS19

Chain PP: 12% 72% 23% 6%

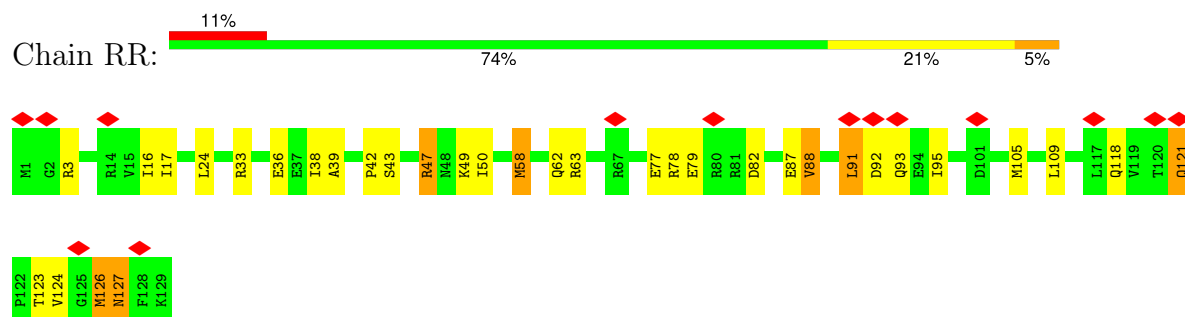


• Molecule 68: uS9

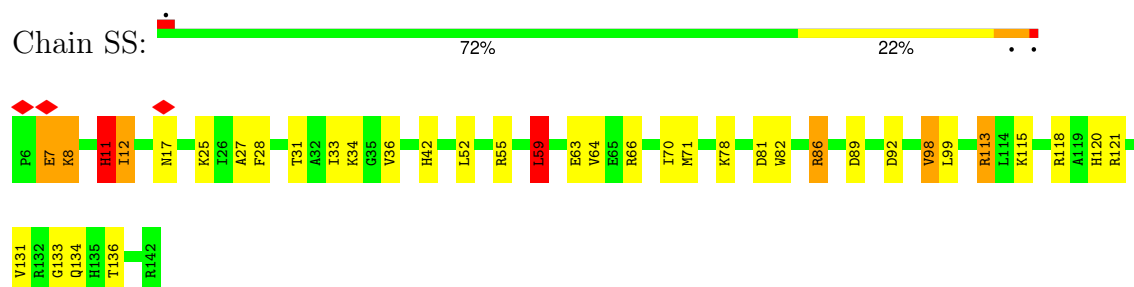
Chain QQ: 76% 21% .



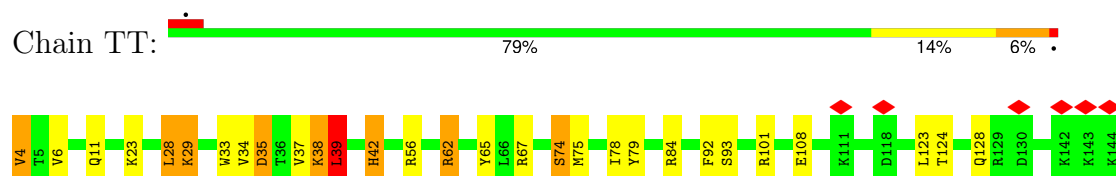
- Molecule 69: eS17



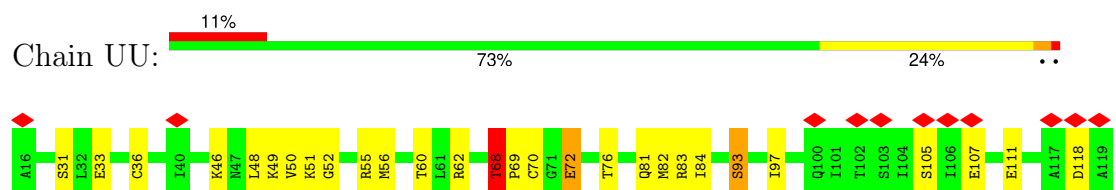
- Molecule 70: uS13



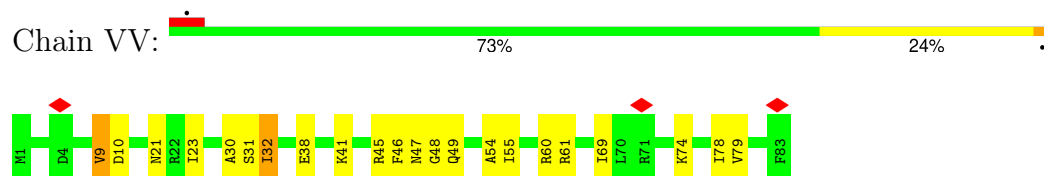
- Molecule 71: eS19

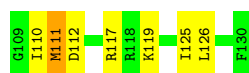


- Molecule 72: uS10



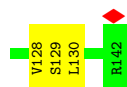
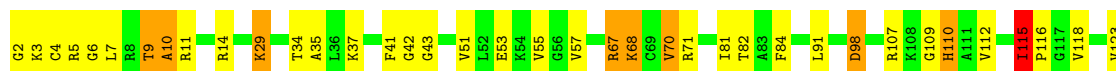
- Molecule 73: eS21





- Molecule 75: uS12

Chain XX: 71% 23% 6%



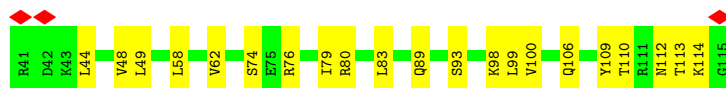
- Molecule 76: eS24

Chain YY: 6% 74% 21% 6%



- Molecule 77: eS25

Chain ZZ: 72% 28%



- Molecule 78: eS26

Chain aa: 65% 27% 8%

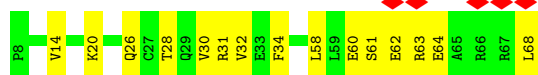
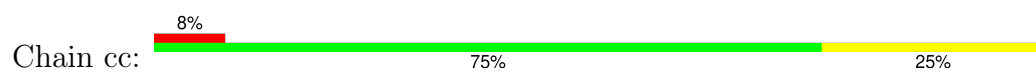


- Molecule 79: eS27

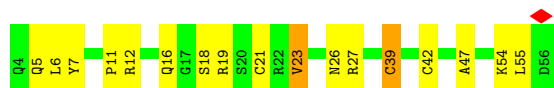
Chain bb: 5% 70% 29% 6%



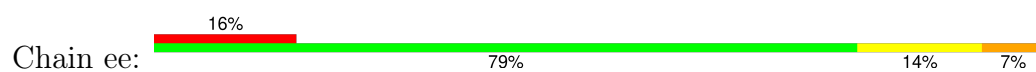
- Molecule 80: eS28



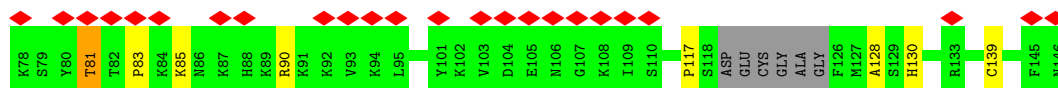
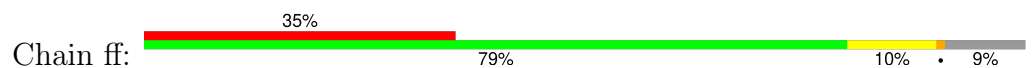
- Molecule 81: uS14



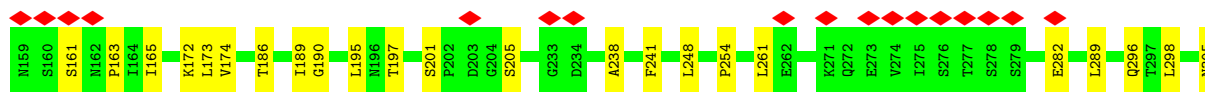
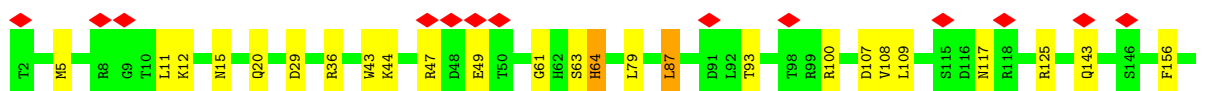
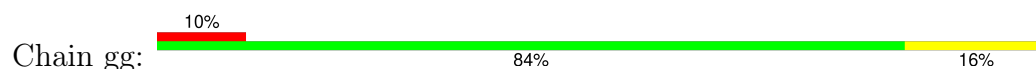
- Molecule 82: eS30



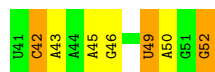
- Molecule 83: eS31



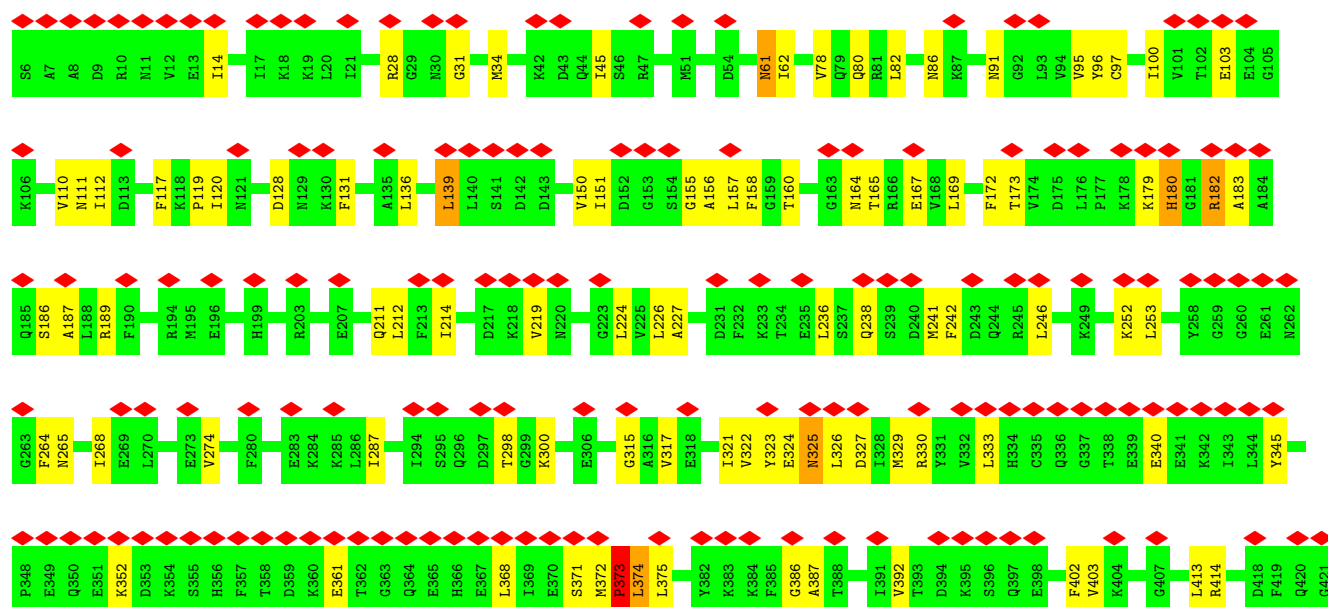
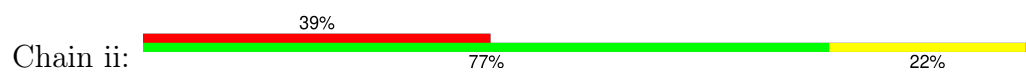
- Molecule 84: RACK1



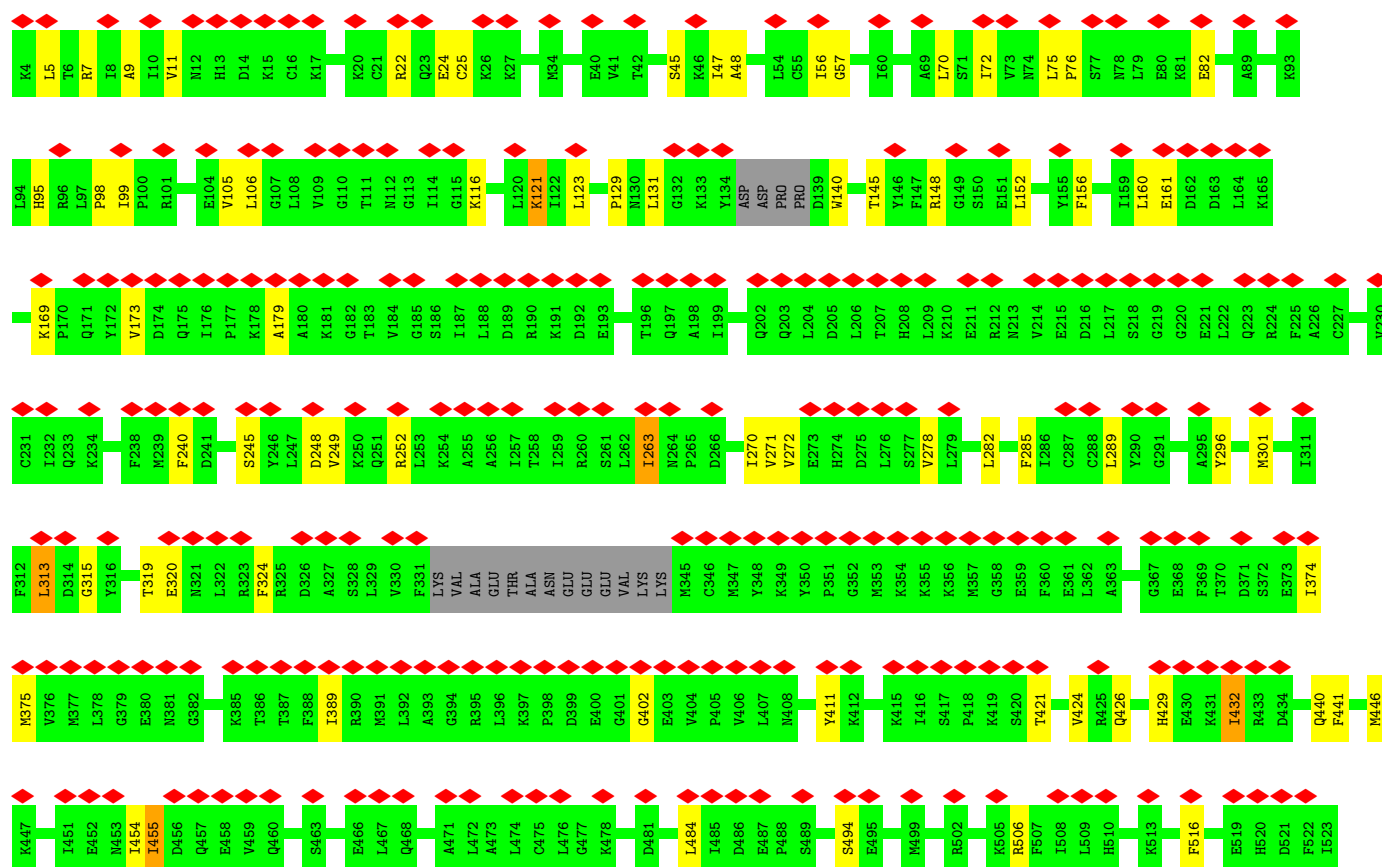
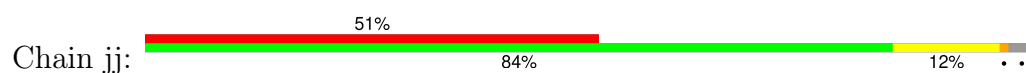
- Molecule 85: mRNA

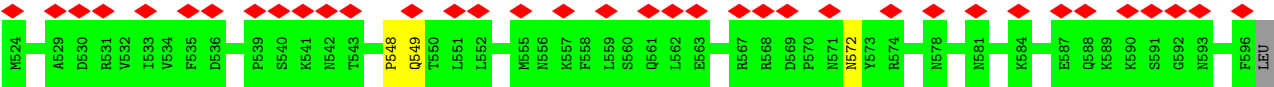


- Molecule 86: eRF1



• Molecule 87: ABCE1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	20515	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	1700	Depositor
Maximum defocus (nm)	3600	Depositor
Magnification	104478	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.528	Depositor
Minimum map value	-0.315	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.07	Depositor
Map size ($\text{\AA}$)	562.8, 562.8, 562.8	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.3399999, 1.3399999, 1.3399999	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ADP, ZN, 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	0.63	3/1906 (0.2%)	0.92	2/2556 (0.1%)
2	B	0.53	0/3216	0.93	14/4311 (0.3%)
3	C	0.56	2/2938 (0.1%)	0.96	3/3946 (0.1%)
4	D	0.48	0/2432	0.86	0/3257
5	E	0.65	3/1936 (0.2%)	1.00	7/2600 (0.3%)
6	F	0.51	0/1905	0.87	0/2539
7	G	0.54	0/1967	0.94	2/2647 (0.1%)
8	H	0.52	1/1535 (0.1%)	0.82	2/2063 (0.1%)
9	I	0.56	1/1693 (0.1%)	0.87	3/2260 (0.1%)
10	J	0.48	0/1376	0.85	1/1841 (0.1%)
11	L	0.55	1/1734 (0.1%)	0.92	1/2317 (0.0%)
12	M	0.49	0/1158	0.94	1/1547 (0.1%)
13	N	0.58	1/1746 (0.1%)	0.96	3/2338 (0.1%)
14	O	0.54	0/1671	0.95	3/2234 (0.1%)
15	P	0.59	3/1268 (0.2%)	0.91	4/1701 (0.2%)
16	Q	0.54	0/1530	0.89	0/2041
17	R	0.58	2/1524 (0.1%)	0.95	2/2013 (0.1%)
18	S	0.52	0/1493	0.94	2/2002 (0.1%)
19	T	0.55	1/1326 (0.1%)	0.84	1/1770 (0.1%)
20	U	0.52	1/822 (0.1%)	0.77	0/1103
21	V	0.55	0/993	0.88	1/1332 (0.1%)
22	W	0.58	0/541	0.94	2/720 (0.3%)
23	X	0.55	1/993 (0.1%)	0.89	0/1334
24	Y	0.48	0/1132	0.91	1/1504 (0.1%)
25	Z	0.51	0/1130	0.90	3/1507 (0.2%)
26	a	0.52	0/1191	0.97	4/1590 (0.3%)
27	b	0.56	1/619 (0.2%)	0.96	1/818 (0.1%)
28	c	0.49	0/742	0.93	0/996
29	d	0.51	0/903	0.87	0/1216
30	e	0.61	1/1071 (0.1%)	0.98	1/1429 (0.1%)
31	f	0.70	3/895 (0.3%)	1.02	7/1198 (0.6%)
32	g	0.55	1/916 (0.1%)	0.89	1/1220 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	h	0.48	0/1021	0.93	1/1348 (0.1%)
34	i	0.57	1/841 (0.1%)	0.94	2/1112 (0.2%)
35	j	0.61	0/720	1.03	1/952 (0.1%)
36	k	0.55	0/575	0.90	1/761 (0.1%)
37	l	0.66	0/454	0.92	0/599
38	m	0.51	0/435	0.89	0/575
39	n	0.55	0/223	0.87	0/284
40	o	0.52	0/864	0.86	0/1140
41	p	0.57	0/718	0.94	1/953 (0.1%)
42	r	0.65	2/1017 (0.2%)	0.98	2/1364 (0.1%)
43	s	0.58	0/1547	0.81	3/2088 (0.1%)
44	t	0.64	0/1257	0.97	4/1697 (0.2%)
45	1	0.58	0/129	1.02	2/173 (1.2%)
46	2	0.37	0/1805	0.79	3/2809 (0.1%)
47	3	0.45	0/1777	1.01	15/2763 (0.5%)
48	5	0.41	1/87790 (0.0%)	0.89	278/136937 (0.2%)
49	7	0.38	0/2858	0.77	1/4455 (0.0%)
50	8	0.40	0/3701	0.82	3/5766 (0.1%)
51	9	0.40	1/41013 (0.0%)	0.86	107/63919 (0.2%)
52	AA	0.50	0/1679	0.91	0/2283
53	BB	0.53	0/1756	0.93	3/2350 (0.1%)
54	CC	0.55	0/1730	0.95	2/2344 (0.1%)
55	DD	0.52	0/1792	0.88	0/2412
56	EE	0.57	2/2115 (0.1%)	0.98	8/2843 (0.3%)
57	FF	0.63	3/1531 (0.2%)	0.99	2/2059 (0.1%)
58	GG	0.53	0/1946	0.88	0/2590
59	HH	0.62	2/1544 (0.1%)	0.94	1/2068 (0.0%)
60	II	0.55	0/1715	0.93	1/2287 (0.0%)
61	JJ	0.55	1/1550 (0.1%)	0.97	3/2069 (0.1%)
62	KK	0.66	1/851 (0.1%)	0.94	0/1147
63	LL	0.53	0/1259	0.88	3/1684 (0.2%)
64	MM	0.64	0/968	0.91	0/1296
65	NN	0.55	1/1232 (0.1%)	1.02	3/1656 (0.2%)
66	OO	0.60	0/1029	1.01	2/1380 (0.1%)
67	PP	0.55	0/1079	0.94	1/1437 (0.1%)
68	QQ	0.50	0/1142	0.87	0/1528
69	RR	0.56	0/1060	0.94	0/1421
70	SS	0.53	0/1157	0.97	1/1548 (0.1%)
71	TT	0.60	2/1120 (0.2%)	1.01	2/1499 (0.1%)
72	UU	0.52	0/831	0.92	2/1115 (0.2%)
73	VV	0.55	0/645	0.95	1/865 (0.1%)
74	WW	0.51	0/1051	0.91	1/1406 (0.1%)
75	XX	0.50	0/1116	1.00	1/1490 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	YY	0.52	0/1040	0.89	0/1382
77	ZZ	0.55	0/604	0.94	0/810
78	aa	0.56	0/794	0.98	0/1065
79	bb	0.51	0/665	0.78	0/891
80	cc	0.47	0/478	0.85	0/640
81	dd	0.52	0/455	0.90	0/603
82	ee	0.62	0/462	0.87	0/607
83	ff	0.55	0/531	0.71	0/703
84	gg	0.52	2/2493 (0.1%)	0.79	2/3394 (0.1%)
85	hh	0.41	0/287	0.87	1/445 (0.2%)
86	ii	0.55	3/3333 (0.1%)	0.89	3/4483 (0.1%)
87	jj	0.58	2/4625 (0.0%)	0.83	0/6238
All	All	0.48	50/242712 (0.0%)	0.89	539/355683 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	4
3	C	0	2
4	D	0	1
5	E	0	1
7	G	0	1
9	I	0	2
11	L	0	3
17	R	0	1
18	S	0	2
19	T	0	1
20	U	0	1
24	Y	0	1
31	f	0	1
42	r	0	2
48	5	0	1
51	9	0	1
52	AA	0	1
56	EE	0	2
57	FF	0	2
59	HH	0	1
60	II	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
61	JJ	0	2
66	OO	0	1
68	QQ	0	1
70	SS	0	1
71	TT	0	1
72	UU	0	2
73	VV	0	1
74	WW	0	2
75	XX	0	1
78	aa	0	1
86	ii	0	3
All	All	0	49

The worst 5 of 50 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	5	1965	G	O3'-P	-18.41	1.33	1.61
87	jj	121	LYS	CE-NZ	16.52	1.99	1.49
51	9	908	A	O3'-P	7.18	1.72	1.61
19	T	3	ASN	CG-OD1	5.80	1.34	1.23
84	gg	64	HIS	ND1-CE1	5.51	1.38	1.32

The worst 5 of 539 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	98	GLY	N-CA-C	-13.80	98.97	111.67
48	5	1358	G	C4'-C3'-O3'	13.61	133.41	113.00
48	5	4975	G	C2'-C3'-O3'	13.14	129.21	109.50
48	5	1357	C	C4'-C3'-O3'	12.91	132.37	113.00
48	5	47	A	C4'-C3'-O3'	11.97	127.36	109.40

There are no chirality outliers.

5 of 49 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
2	B	258	HIS	Peptide
2	B	351	LEU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1868	0	1959	29	0
2	B	3148	0	3267	63	0
3	C	2884	0	3062	47	0
4	D	2386	0	2419	32	0
5	E	1898	0	2035	73	0
6	F	1870	0	1994	28	0
7	G	1934	0	2087	32	0
8	H	1516	0	1597	17	0
9	I	1655	0	1704	43	0
10	J	1353	0	1386	15	0
11	L	1703	0	1820	28	0
12	M	1137	0	1211	16	0
13	N	1701	0	1749	19	0
14	O	1638	0	1777	31	0
15	P	1242	0	1269	12	0
16	Q	1506	0	1623	15	0
17	R	1508	0	1664	26	0
18	S	1454	0	1496	15	0
19	T	1298	0	1366	12	0
20	U	808	0	831	5	0
21	V	979	0	1039	5	0
22	W	528	0	541	5	0
23	X	976	0	1053	8	0
24	Y	1115	0	1205	7	0
25	Z	1107	0	1182	17	0
26	a	1162	0	1209	19	0
27	b	609	0	650	6	0
28	c	732	0	769	11	0
29	d	888	0	930	6	0
30	e	1053	0	1147	12	0
31	f	876	0	912	19	0
32	g	906	0	999	13	0
33	h	1013	0	1147	8	0
34	i	830	0	916	4	0
35	j	705	0	738	16	0
36	k	569	0	637	6	0
37	l	444	0	483	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	m	429	0	466	11	0
39	n	222	0	264	4	0
40	o	851	0	921	11	0
41	p	708	0	756	7	0
42	r	1001	0	1060	50	0
43	s	1523	0	1577	30	0
44	t	1238	0	1295	10	0
45	1	125	0	117	3	0
46	2	1616	0	824	19	0
47	3	1593	0	811	79	0
48	5	78486	0	39663	1372	0
49	7	2558	0	1296	27	0
50	8	3314	0	1683	56	0
51	9	36680	0	18529	640	0
52	AA	1642	0	1646	21	0
53	BB	1729	0	1803	14	0
54	CC	1692	0	1780	22	0
55	DD	1764	0	1863	9	0
56	EE	2073	0	2175	48	0
57	FF	1509	0	1562	30	0
58	GG	1923	0	2089	31	0
59	HH	1521	0	1616	22	0
60	II	1686	0	1772	31	0
61	JJ	1525	0	1640	22	0
62	KK	827	0	854	8	0
63	LL	1238	0	1315	18	0
64	MM	958	0	993	3	0
65	NN	1208	0	1294	13	0
66	OO	1016	0	1039	17	0
67	PP	1060	0	1120	17	0
68	QQ	1124	0	1193	11	0
69	RR	1047	0	1103	14	0
70	SS	1139	0	1191	19	0
71	TT	1102	0	1142	12	0
72	UU	821	0	883	6	0
73	VV	636	0	634	9	0
74	WW	1034	0	1080	27	0
75	XX	1098	0	1167	12	0
76	YY	1023	0	1090	12	0
77	ZZ	598	0	656	6	0
78	aa	781	0	828	17	0
79	bb	651	0	672	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
80	cc	475	0	497	4	0
81	dd	445	0	439	6	0
82	ee	457	0	502	4	0
83	ff	520	0	536	13	0
84	gg	2436	0	2393	12	0
85	hh	257	0	129	2	0
86	ii	3280	0	3326	65	0
87	jj	4543	0	4674	43	0
88	5	146	0	0	0	0
88	7	5	0	0	0	0
88	8	2	0	0	0	0
88	9	34	0	0	0	0
88	B	1	0	0	0	0
88	C	1	0	0	0	0
88	I	1	0	0	0	0
88	LL	1	0	0	0	0
88	P	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	1	0
89	dd	1	0	0	1	0
89	ff	1	0	0	1	0
89	g	1	0	0	0	0
89	j	1	0	0	0	0
89	m	1	0	0	1	0
89	o	1	0	0	2	0
89	p	1	0	0	0	0
90	jj	16	0	0	0	0
91	jj	54	0	24	0	0
All	All	226454	0	169855	3251	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 8.

The worst 5 of 3251 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)
5:E:279:PRO:HG2	31:f:7:CYS:SG	1.65	1.36
51:9:1137:U:O4	51:9:1148:A:N1	1.61	1.34
48:5:976:G:H2'	48:5:977:C:O4'	1.26	1.32

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:172:ARG:NH1	51:9:908:A:H5''	1.47	1.29
48:5:2367:A:N1	48:5:2788:U:O4	1.66	1.29

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%)	209 (86%)	28 (12%)	5 (2%)	5	31
2	B	392/394 (100%)	345 (88%)	42 (11%)	5 (1%)	9	39
3	C	360/362 (99%)	322 (89%)	27 (8%)	11 (3%)	3	25
4	D	290/292 (99%)	262 (90%)	25 (9%)	3 (1%)	12	44
5	E	232/248 (94%)	179 (77%)	36 (16%)	17 (7%)	1	9
6	F	223/225 (99%)	204 (92%)	17 (8%)	2 (1%)	14	46
7	G	239/241 (99%)	203 (85%)	31 (13%)	5 (2%)	5	31
8	H	188/190 (99%)	165 (88%)	20 (11%)	3 (2%)	7	36
9	I	200/213 (94%)	181 (90%)	15 (8%)	4 (2%)	6	32
10	J	167/169 (99%)	147 (88%)	13 (8%)	7 (4%)	2	19
11	L	208/210 (99%)	180 (86%)	16 (8%)	12 (6%)	1	13
12	M	136/138 (99%)	123 (90%)	12 (9%)	1 (1%)	18	51
13	N	201/203 (99%)	181 (90%)	20 (10%)	0	100	100
14	O	197/199 (99%)	184 (93%)	12 (6%)	1 (0%)	24	57
15	P	151/153 (99%)	135 (89%)	16 (11%)	0	100	100
16	Q	185/187 (99%)	169 (91%)	14 (8%)	2 (1%)	11	42
17	R	178/180 (99%)	166 (93%)	9 (5%)	3 (2%)	7	35
18	S	173/175 (99%)	157 (91%)	12 (7%)	4 (2%)	5	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	T	157/159 (99%)	139 (88%)	15 (10%)	3 (2%)	6	33
20	U	97/99 (98%)	82 (84%)	11 (11%)	4 (4%)	2	19
21	V	129/131 (98%)	115 (89%)	13 (10%)	1 (1%)	16	49
22	W	61/63 (97%)	56 (92%)	4 (7%)	1 (2%)	7	36
23	X	117/119 (98%)	109 (93%)	6 (5%)	2 (2%)	7	35
24	Y	132/134 (98%)	114 (86%)	17 (13%)	1 (1%)	16	49
25	Z	133/135 (98%)	113 (85%)	13 (10%)	7 (5%)	1	14
26	a	145/147 (99%)	122 (84%)	19 (13%)	4 (3%)	4	26
27	b	73/75 (97%)	67 (92%)	5 (7%)	1 (1%)	9	38
28	c	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
29	d	105/107 (98%)	91 (87%)	13 (12%)	1 (1%)	12	44
30	e	126/128 (98%)	115 (91%)	6 (5%)	5 (4%)	2	19
31	f	107/109 (98%)	94 (88%)	8 (8%)	5 (5%)	2	17
32	g	112/114 (98%)	103 (92%)	8 (7%)	1 (1%)	14	46
33	h	120/122 (98%)	107 (89%)	9 (8%)	4 (3%)	3	23
34	i	100/102 (98%)	92 (92%)	6 (6%)	2 (2%)	6	32
35	j	84/86 (98%)	70 (83%)	9 (11%)	5 (6%)	1	12
36	k	67/69 (97%)	56 (84%)	7 (10%)	4 (6%)	1	12
37	l	48/50 (96%)	40 (83%)	7 (15%)	1 (2%)	5	31
38	m	50/52 (96%)	44 (88%)	6 (12%)	0	100	100
39	n	21/23 (91%)	21 (100%)	0	0	100	100
40	o	102/104 (98%)	92 (90%)	7 (7%)	3 (3%)	3	26
41	p	89/91 (98%)	80 (90%)	8 (9%)	1 (1%)	11	42
42	r	123/125 (98%)	102 (83%)	14 (11%)	7 (6%)	1	13
43	s	196/198 (99%)	164 (84%)	22 (11%)	10 (5%)	1	15
44	t	161/163 (99%)	102 (63%)	33 (20%)	26 (16%)	0	2
45	1	13/15 (87%)	11 (85%)	0	2 (15%)	0	2
52	AA	206/208 (99%)	173 (84%)	23 (11%)	10 (5%)	1	16
53	BB	211/213 (99%)	165 (78%)	33 (16%)	13 (6%)	1	12
54	CC	216/218 (99%)	184 (85%)	26 (12%)	6 (3%)	4	26
55	DD	225/227 (99%)	181 (80%)	33 (15%)	11 (5%)	1	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
56	EE	260/262 (99%)	200 (77%)	42 (16%)	18 (7%)	1	10
57	FF	189/191 (99%)	160 (85%)	21 (11%)	8 (4%)	2	19
58	GG	235/237 (99%)	198 (84%)	31 (13%)	6 (3%)	4	27
59	HH	187/189 (99%)	148 (79%)	25 (13%)	14 (8%)	1	9
60	II	204/206 (99%)	168 (82%)	28 (14%)	8 (4%)	2	20
61	JJ	183/185 (99%)	153 (84%)	20 (11%)	10 (6%)	1	14
62	KK	96/98 (98%)	65 (68%)	21 (22%)	10 (10%)	0	6
63	LL	150/152 (99%)	125 (83%)	19 (13%)	6 (4%)	2	19
64	MM	122/124 (98%)	87 (71%)	28 (23%)	7 (6%)	1	13
65	NN	148/150 (99%)	126 (85%)	17 (12%)	5 (3%)	3	23
66	OO	134/136 (98%)	99 (74%)	21 (16%)	14 (10%)	0	6
67	PP	125/127 (98%)	107 (86%)	15 (12%)	3 (2%)	4	29
68	QQ	139/141 (99%)	116 (84%)	18 (13%)	5 (4%)	2	22
69	RR	127/129 (98%)	106 (84%)	15 (12%)	6 (5%)	2	17
70	SS	135/137 (98%)	114 (84%)	16 (12%)	5 (4%)	2	21
71	TT	139/141 (99%)	126 (91%)	10 (7%)	3 (2%)	5	30
72	UU	102/104 (98%)	87 (85%)	9 (9%)	6 (6%)	1	13
73	VV	81/83 (98%)	67 (83%)	10 (12%)	4 (5%)	1	16
74	WW	127/129 (98%)	106 (84%)	16 (13%)	5 (4%)	2	20
75	XX	139/141 (99%)	118 (85%)	13 (9%)	8 (6%)	1	13
76	YY	124/126 (98%)	99 (80%)	17 (14%)	8 (6%)	1	11
77	ZZ	73/75 (97%)	59 (81%)	12 (16%)	2 (3%)	4	27
78	aa	96/98 (98%)	73 (76%)	13 (14%)	10 (10%)	0	6
79	bb	81/83 (98%)	61 (75%)	16 (20%)	4 (5%)	1	16
80	cc	59/61 (97%)	47 (80%)	10 (17%)	2 (3%)	3	23
81	dd	51/53 (96%)	45 (88%)	3 (6%)	3 (6%)	1	13
82	ee	55/57 (96%)	40 (73%)	12 (22%)	3 (6%)	1	14
83	ff	58/68 (85%)	50 (86%)	6 (10%)	2 (3%)	3	23
84	gg	311/313 (99%)	269 (86%)	33 (11%)	9 (3%)	3	26
86	ii	414/416 (100%)	380 (92%)	26 (6%)	8 (2%)	6	33
87	jj	568/594 (96%)	513 (90%)	41 (7%)	14 (2%)	4	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	12492/12709 (98%)	10717 (86%)	1333 (11%)	442 (4%)	4	23

5 of 442 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	196	TRP
3	C	273	LEU
5	E	91	PRO
5	E	95	ASP
5	E	118	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	187/187 (100%)	158 (84%)	29 (16%)	2	15
2	B	336/342 (98%)	282 (84%)	54 (16%)	2	14
3	C	302/302 (100%)	261 (86%)	41 (14%)	3	20
4	D	247/247 (100%)	217 (88%)	30 (12%)	5	23
5	E	208/221 (94%)	183 (88%)	25 (12%)	5	23
6	F	194/195 (100%)	168 (87%)	26 (13%)	4	20
7	G	206/206 (100%)	181 (88%)	25 (12%)	5	23
8	H	169/169 (100%)	147 (87%)	22 (13%)	4	21
9	I	174/180 (97%)	151 (87%)	23 (13%)	4	21
10	J	142/142 (100%)	125 (88%)	17 (12%)	5	23
11	L	176/176 (100%)	142 (81%)	34 (19%)	1	8
12	M	117/117 (100%)	101 (86%)	16 (14%)	3	19
13	N	171/171 (100%)	148 (86%)	23 (14%)	4	20
14	O	171/171 (100%)	144 (84%)	27 (16%)	2	15
15	P	134/134 (100%)	121 (90%)	13 (10%)	8	31
16	Q	163/163 (100%)	142 (87%)	21 (13%)	4	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	R	159/159 (100%)	141 (89%)	18 (11%)	5	25
18	S	156/156 (100%)	133 (85%)	23 (15%)	3	17
19	T	139/139 (100%)	120 (86%)	19 (14%)	3	19
20	U	89/89 (100%)	83 (93%)	6 (7%)	15	42
21	V	101/101 (100%)	82 (81%)	19 (19%)	1	9
22	W	55/55 (100%)	48 (87%)	7 (13%)	4	22
23	X	107/107 (100%)	94 (88%)	13 (12%)	5	23
24	Y	124/124 (100%)	109 (88%)	15 (12%)	5	23
25	Z	117/117 (100%)	107 (92%)	10 (8%)	10	35
26	a	119/119 (100%)	108 (91%)	11 (9%)	8	32
27	b	62/62 (100%)	56 (90%)	6 (10%)	8	31
28	c	79/79 (100%)	66 (84%)	13 (16%)	2	14
29	d	98/98 (100%)	80 (82%)	18 (18%)	1	9
30	e	114/114 (100%)	94 (82%)	20 (18%)	2	11
31	f	88/88 (100%)	74 (84%)	14 (16%)	2	15
32	g	98/98 (100%)	84 (86%)	14 (14%)	3	18
33	h	109/109 (100%)	99 (91%)	10 (9%)	8	32
34	i	86/86 (100%)	79 (92%)	7 (8%)	11	36
35	j	73/73 (100%)	63 (86%)	10 (14%)	3	19
36	k	64/64 (100%)	57 (89%)	7 (11%)	6	27
37	l	47/47 (100%)	40 (85%)	7 (15%)	3	17
38	m	48/48 (100%)	40 (83%)	8 (17%)	2	13
39	n	22/22 (100%)	19 (86%)	3 (14%)	3	20
40	o	92/92 (100%)	78 (85%)	14 (15%)	3	16
41	p	74/74 (100%)	66 (89%)	8 (11%)	6	27
42	r	109/109 (100%)	87 (80%)	22 (20%)	1	7
43	s	166/166 (100%)	156 (94%)	10 (6%)	17	45
44	t	136/136 (100%)	127 (93%)	9 (7%)	15	43
45	1	13/13 (100%)	12 (92%)	1 (8%)	12	38
52	AA	174/174 (100%)	153 (88%)	21 (12%)	5	23
53	BB	194/194 (100%)	168 (87%)	26 (13%)	4	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	CC	183/183 (100%)	156 (85%)	27 (15%)	3	17
55	DD	190/190 (100%)	163 (86%)	27 (14%)	3	18
56	EE	223/223 (100%)	181 (81%)	42 (19%)	1	9
57	FF	161/161 (100%)	130 (81%)	31 (19%)	1	8
58	GG	207/207 (100%)	177 (86%)	30 (14%)	3	18
59	HH	169/169 (100%)	151 (89%)	18 (11%)	6	27
60	II	178/178 (100%)	153 (86%)	25 (14%)	3	19
61	JJ	161/161 (100%)	138 (86%)	23 (14%)	3	18
62	KK	89/89 (100%)	75 (84%)	14 (16%)	2	15
63	LL	136/136 (100%)	109 (80%)	27 (20%)	1	7
64	MM	104/104 (100%)	85 (82%)	19 (18%)	2	10
65	NN	130/130 (100%)	112 (86%)	18 (14%)	3	19
66	OO	106/106 (100%)	79 (74%)	27 (26%)	0	3
67	PP	116/116 (100%)	96 (83%)	20 (17%)	2	12
68	QQ	117/117 (100%)	101 (86%)	16 (14%)	3	19
69	RR	117/117 (100%)	99 (85%)	18 (15%)	2	16
70	SS	119/119 (100%)	100 (84%)	19 (16%)	2	14
71	TT	112/112 (100%)	96 (86%)	16 (14%)	3	18
72	UU	94/94 (100%)	79 (84%)	15 (16%)	2	14
73	VV	67/67 (100%)	62 (92%)	5 (8%)	12	38
74	WW	112/112 (100%)	99 (88%)	13 (12%)	5	25
75	XX	113/113 (100%)	92 (81%)	21 (19%)	1	9
76	YY	108/108 (100%)	90 (83%)	18 (17%)	2	13
77	ZZ	66/66 (100%)	55 (83%)	11 (17%)	2	13
78	aa	85/85 (100%)	73 (86%)	12 (14%)	3	19
79	bb	75/75 (100%)	62 (83%)	13 (17%)	2	12
80	cc	54/54 (100%)	47 (87%)	7 (13%)	4	21
81	dd	47/47 (100%)	39 (83%)	8 (17%)	2	12
82	ee	47/47 (100%)	40 (85%)	7 (15%)	3	17
83	ff	58/61 (95%)	56 (97%)	2 (3%)	32	59
84	gg	272/272 (100%)	251 (92%)	21 (8%)	12	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
86	ii	358/358 (100%)	329 (92%)	29 (8%)	11	36
87	jj	506/522 (97%)	490 (97%)	16 (3%)	34	60
All	All	10889/10934 (100%)	9459 (87%)	1430 (13%)	6	21

5 of 1430 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
57	FF	126	THR
67	PP	17	TYR
58	GG	120	ASP
57	FF	125	SER
62	KK	3	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 130 such sidechains are listed below:

Mol	Chain	Res	Type
83	ff	86	ASN
86	ii	79	GLN
23	X	69	ASN
23	X	57	GLN
86	ii	164	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
46	2	74/76 (97%)	20 (27%)	1 (1%)
47	3	72/75 (96%)	36 (50%)	7 (9%)
48	5	3649/3662 (99%)	1202 (32%)	269 (7%)
49	7	119/120 (99%)	20 (16%)	1 (0%)
50	8	155/156 (99%)	52 (33%)	6 (3%)
51	9	1713/1719 (99%)	619 (36%)	129 (7%)
85	hh	11/12 (91%)	7 (63%)	0
All	All	5793/5820 (99%)	1956 (33%)	413 (7%)

5 of 1956 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
46	2	7	G
46	2	8	U

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

5 of 413 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
48	5	4124	G
51	9	3	C
51	9	1646	C
48	5	4378	A
48	5	4889	G

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	-	28,29,29	1.51	5 (17%)	43,45,45	1.90	11 (25%)
90	SF4	jj	601	87	0,12,12	-	-	-		
91	ADP	jj	603	-	28,29,29	1.51	5 (17%)	43,45,45	1.90	11 (25%)
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	602	-	-	1/16/32/32	0/3/3/3
90	SF4	jj	601	87	-	-	0/6/5/5
91	ADP	jj	603	-	-	1/16/32/32	0/3/3/3
90	SF4	jj	600	87	-	-	0/6/5/5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
91	jj	603	ADP	C5-C4	5.01	1.48	1.39
91	jj	602	ADP	C5-C4	4.94	1.47	1.39
91	jj	602	ADP	C5-C6	2.99	1.49	1.41
91	jj	603	ADP	C5-C6	2.97	1.49	1.41
91	jj	602	ADP	C8-N7	2.45	1.36	1.31

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
91	jj	603	ADP	C5-C4-N3	-5.90	118.59	126.72
91	jj	602	ADP	C5-C4-N3	-5.82	118.70	126.72
91	jj	603	ADP	N3-C4-N9	4.71	135.18	127.17
91	jj	602	ADP	N3-C4-N9	4.63	135.04	127.17
91	jj	603	ADP	C2-N3-C4	3.94	121.45	111.83

There are no chirality outliers.

All (2) torsion outliers are listed below:

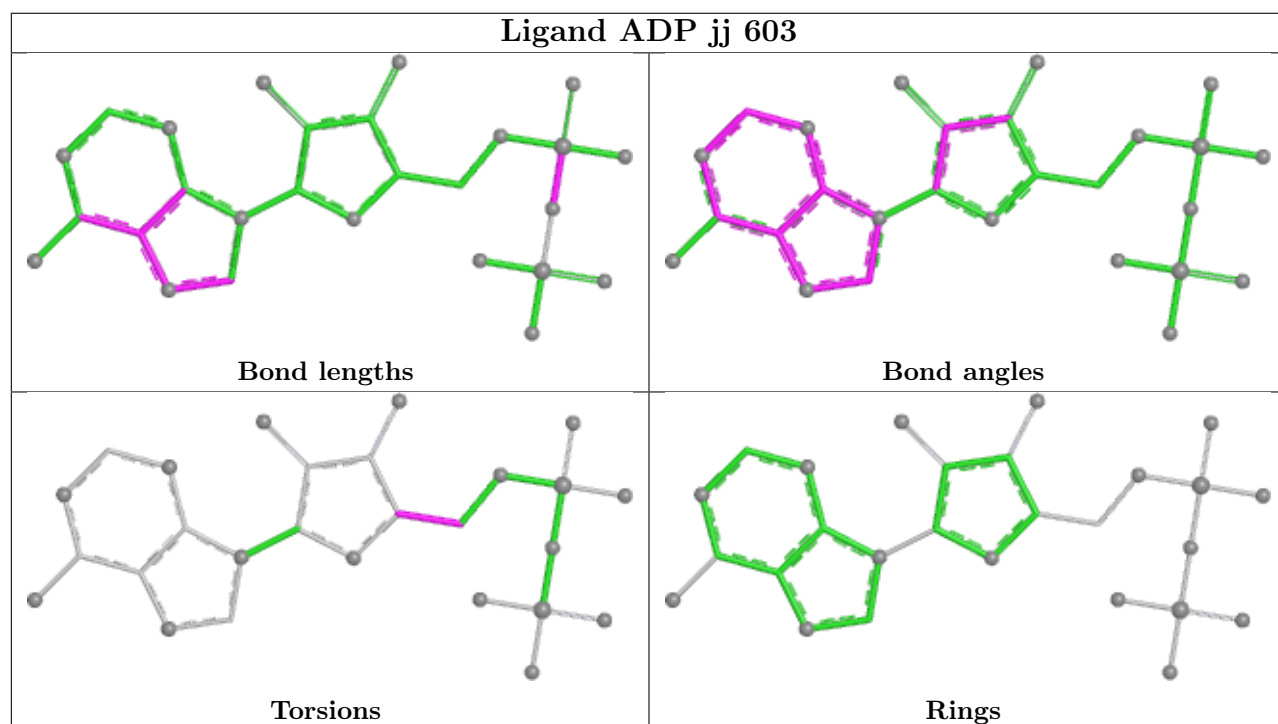
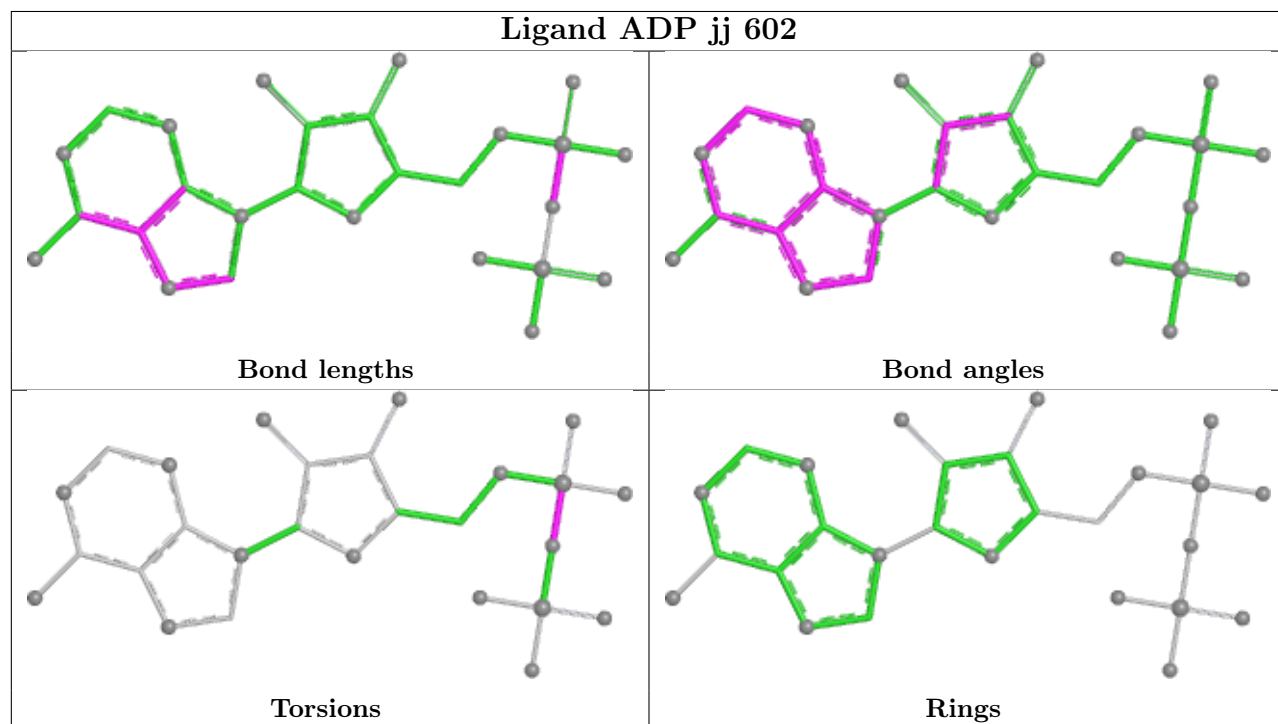
Mol	Chain	Res	Type	Atoms
91	jj	603	ADP	O4'-C4'-C5'-O5'
91	jj	602	ADP	PB-O3A-PA-O1A

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
48	5	17
51	9	8
47	3	2
46	2	1
87	jj	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	23.16
1	9	126:G	O3'	139:C	P	22.33
1	9	698:G	O3'	730:C	P	19.62
1	5	4776:G	O3'	4859:C	P	17.95
1	9	1761:U	O3'	1771:G	P	17.55

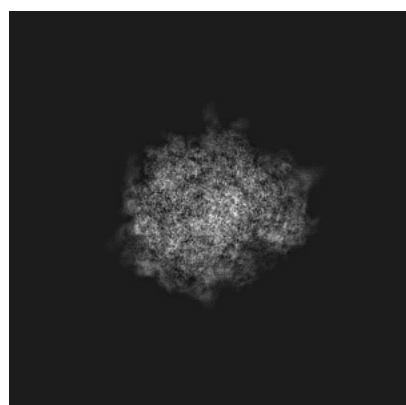
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3039. These allow visual inspection of the internal detail of the map and identification of artifacts.

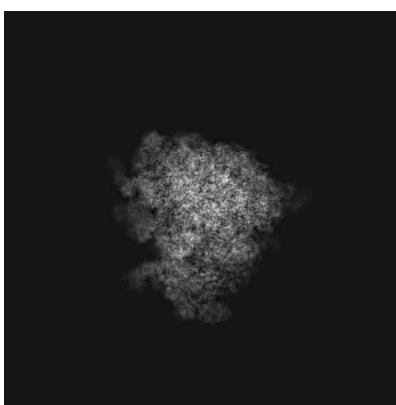
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

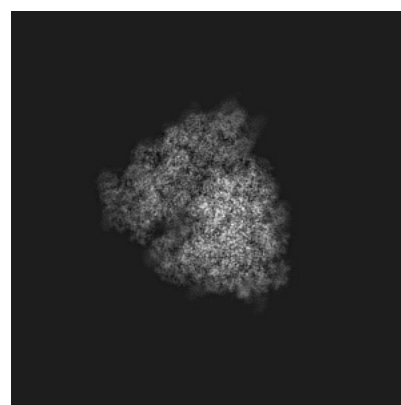
6.1.1 Primary map



X



Y

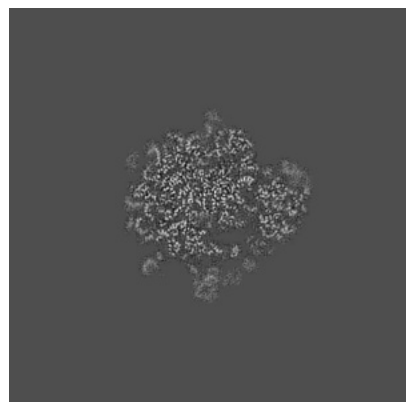


Z

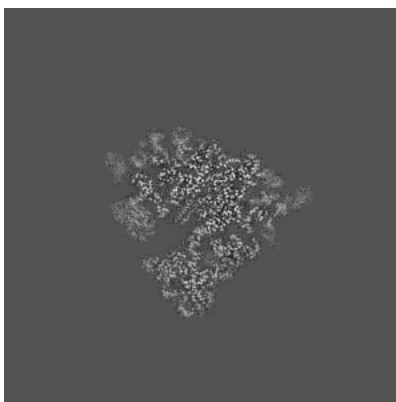
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 210



Y Index: 210

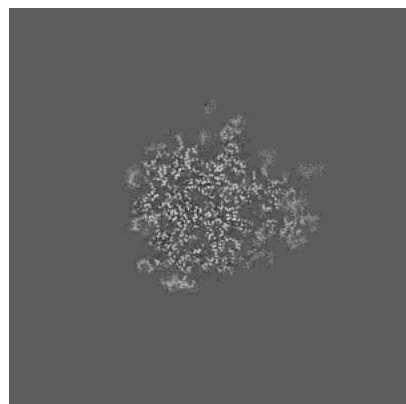


Z Index: 210

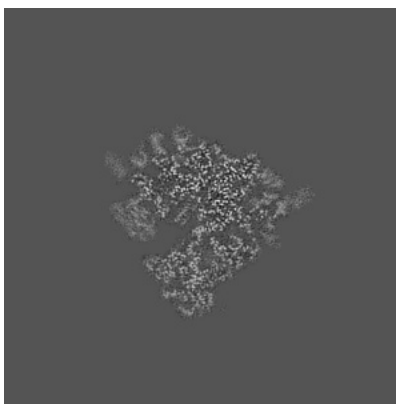
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

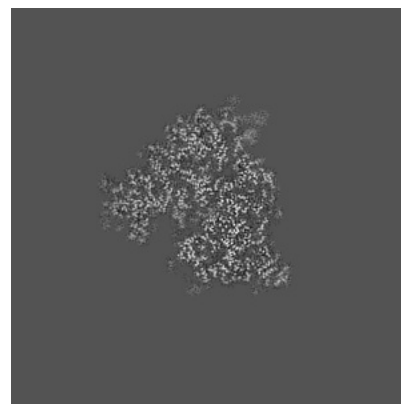
6.3.1 Primary map



X Index: 228



Y Index: 211

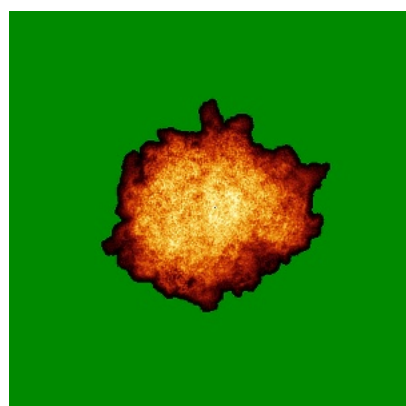


Z Index: 203

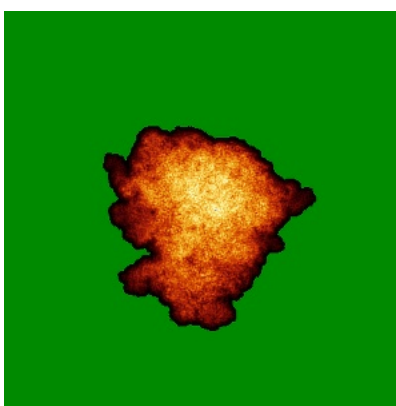
The images above show the largest variance slices of the map in three orthogonal directions.

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

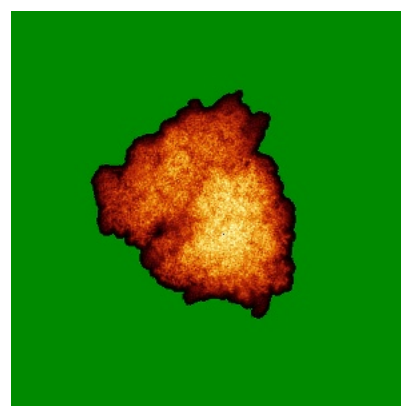
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

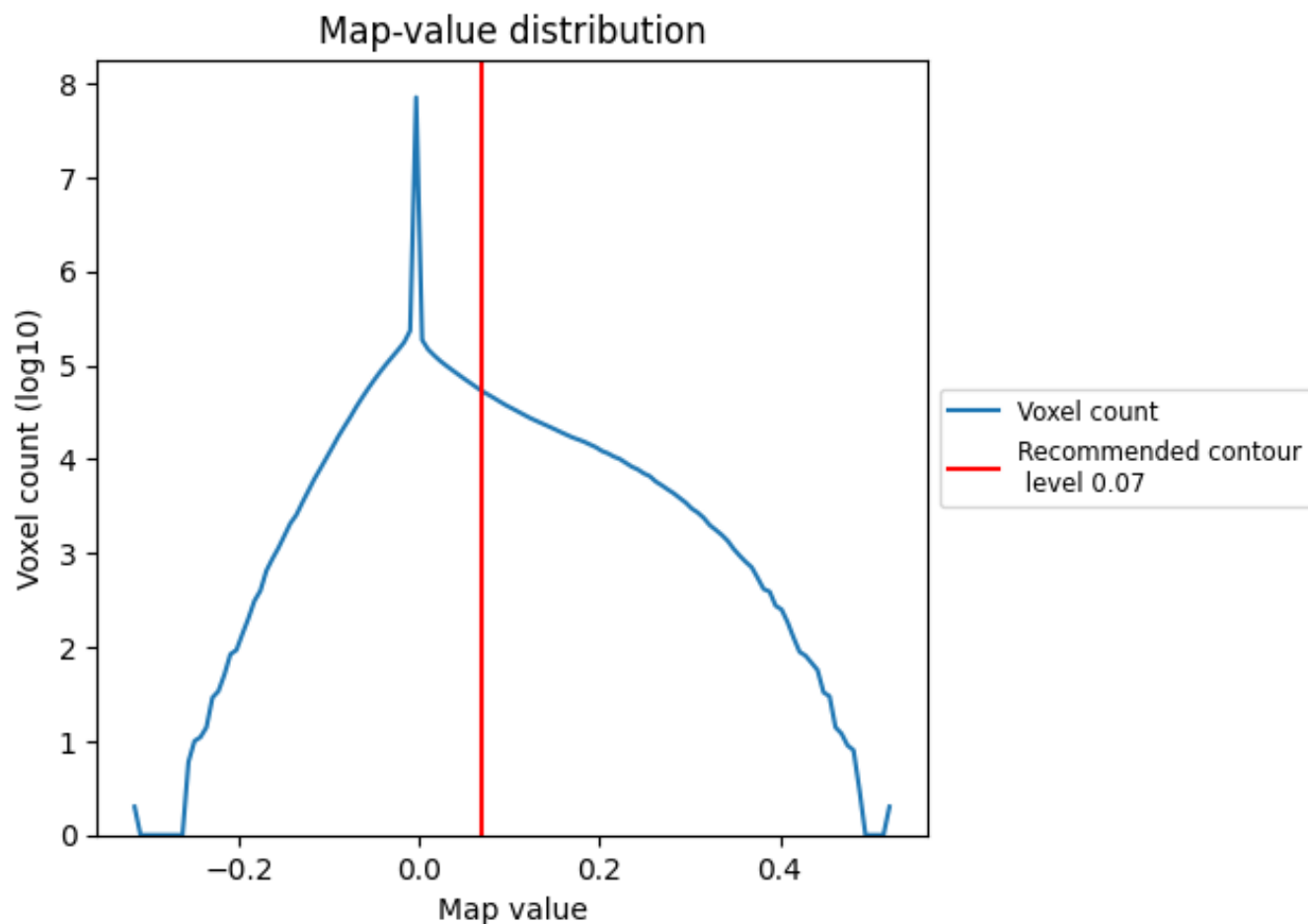
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

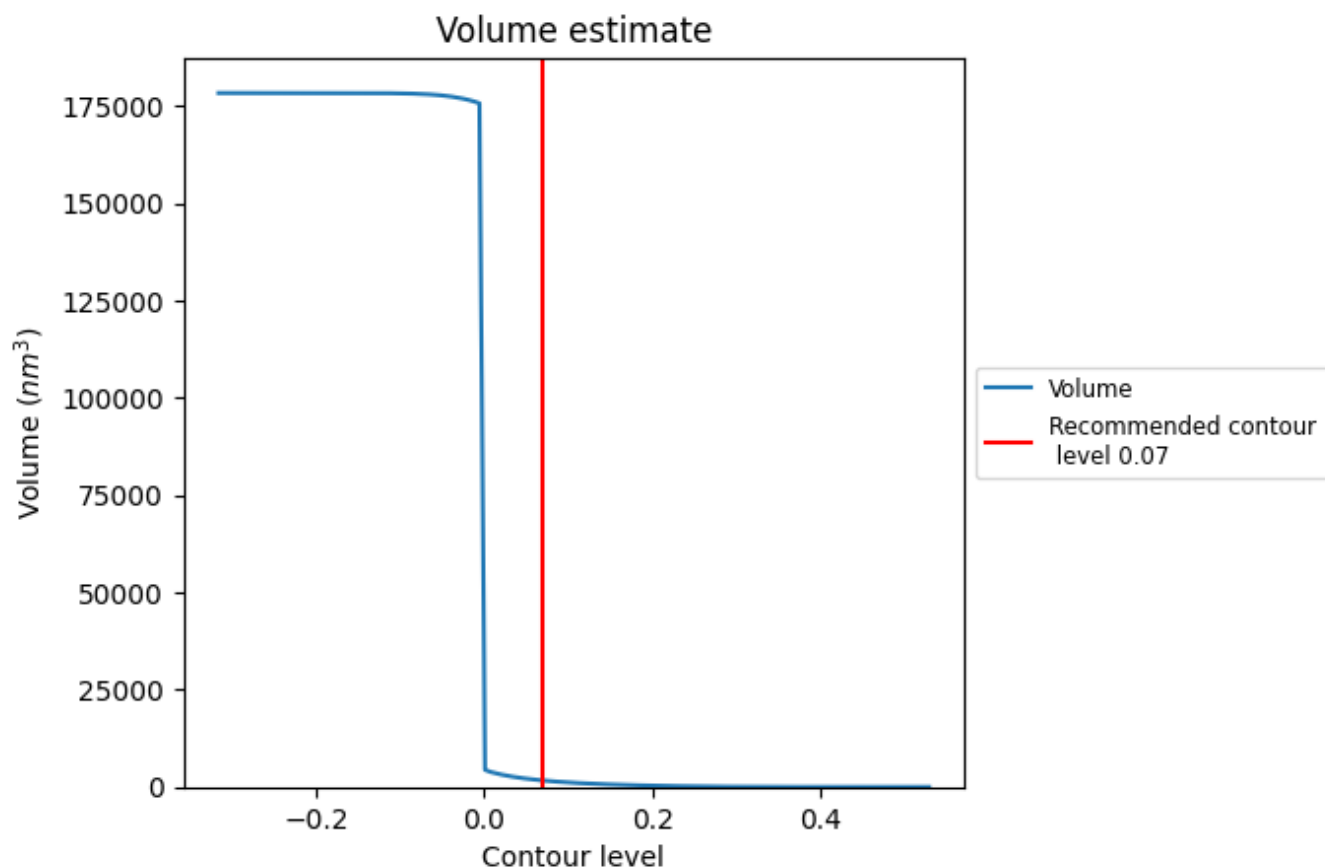
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

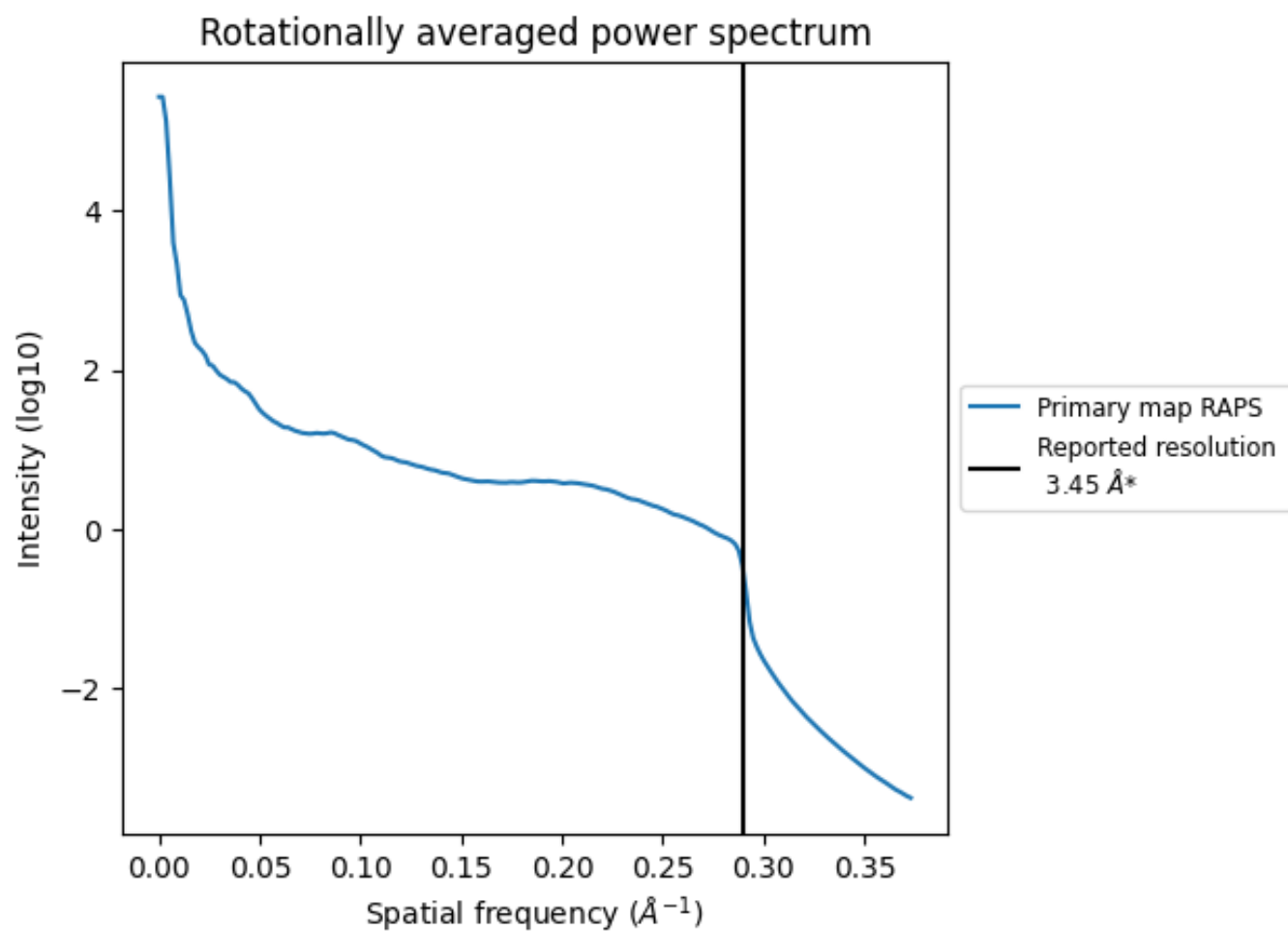
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1656 nm^3 ; this corresponds to an approximate mass of 1496 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

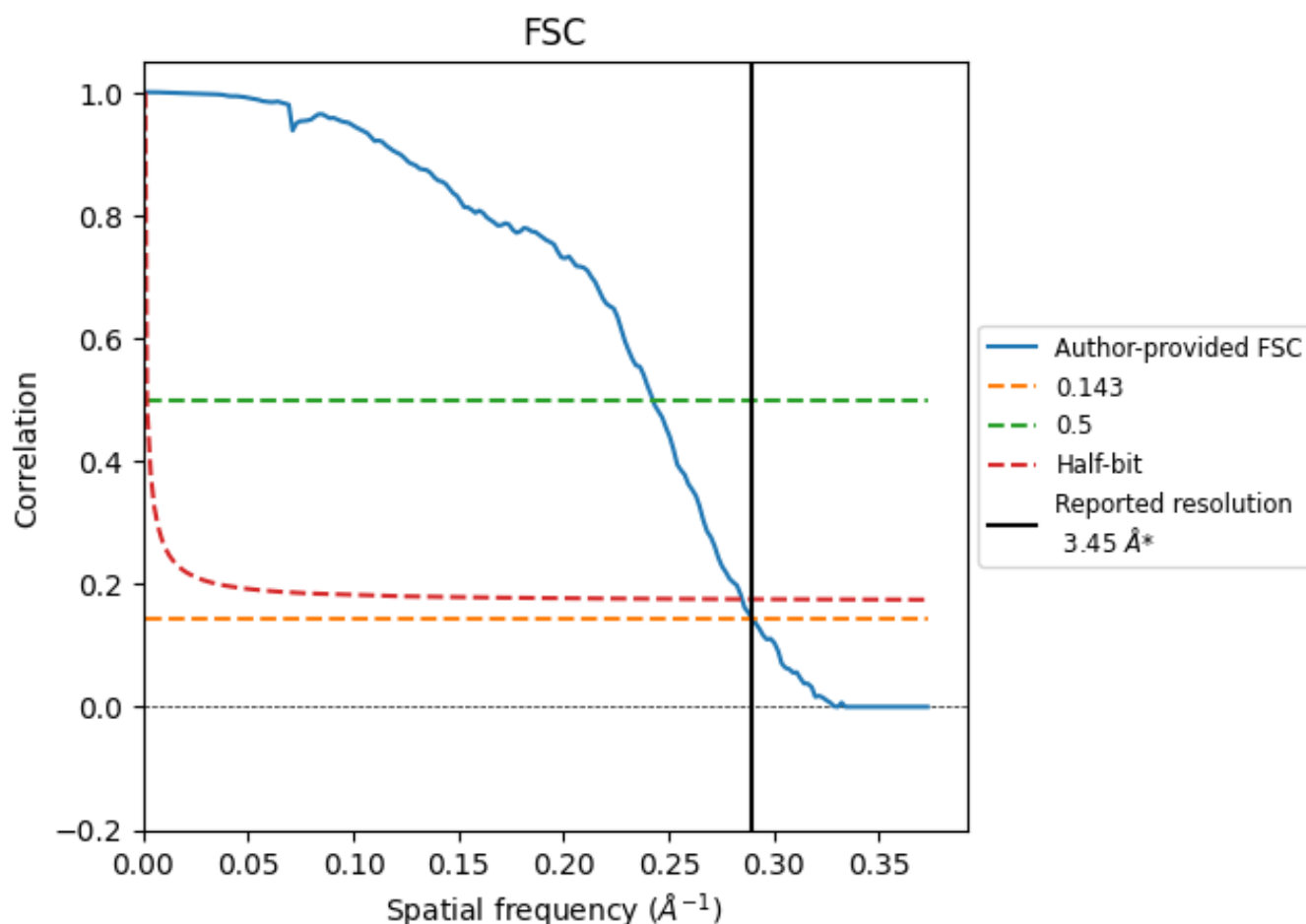


*Reported resolution corresponds to spatial frequency of 0.290 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.290 Å⁻¹

8.2 Resolution estimates [i](#)

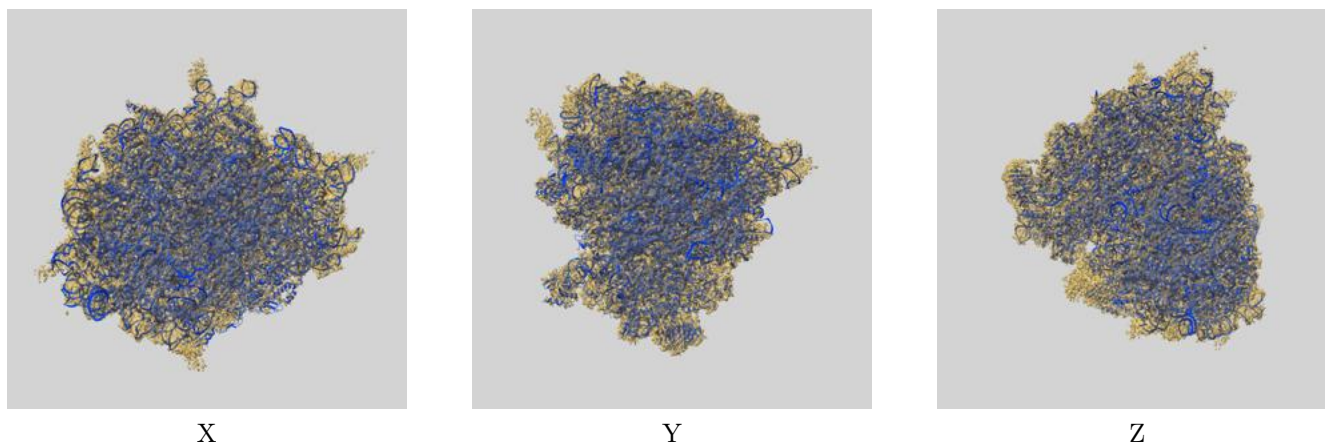
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.45	-	-
Author-provided FSC curve	3.45	4.12	3.51
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

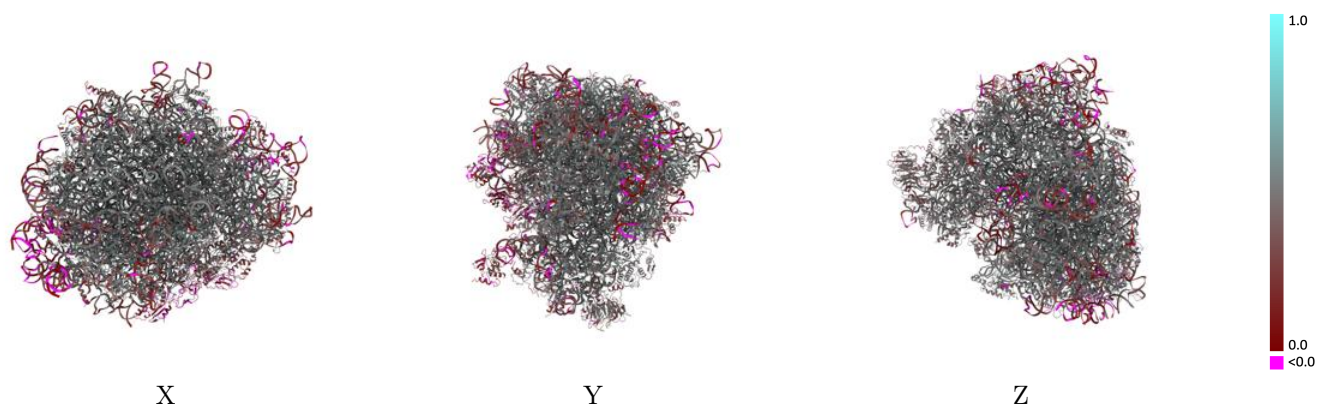
This section contains information regarding the fit between EMDB map EMD-3039 and PDB model 3JAH. Per-residue inclusion information can be found in [section 3](#) on [page 24](#).

9.1 Map-model overlay [i](#)



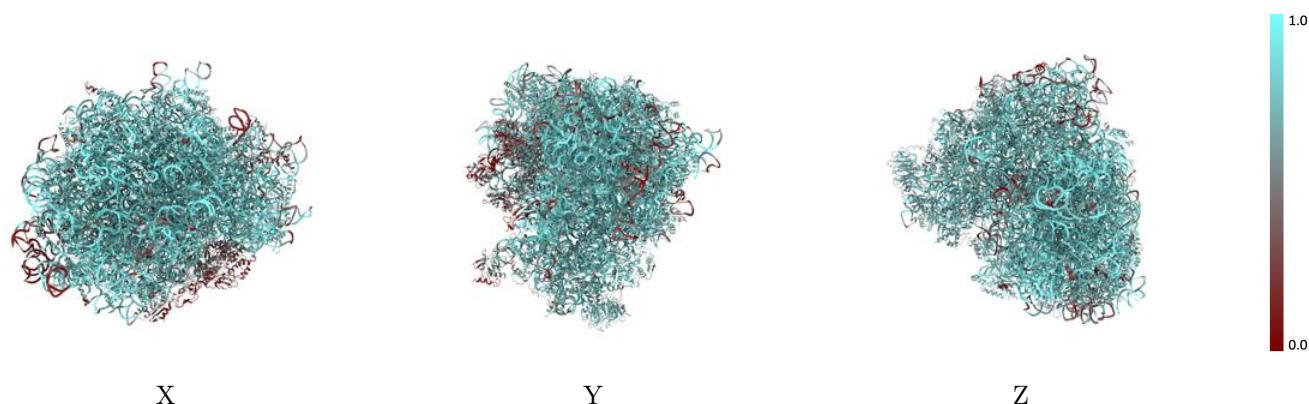
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



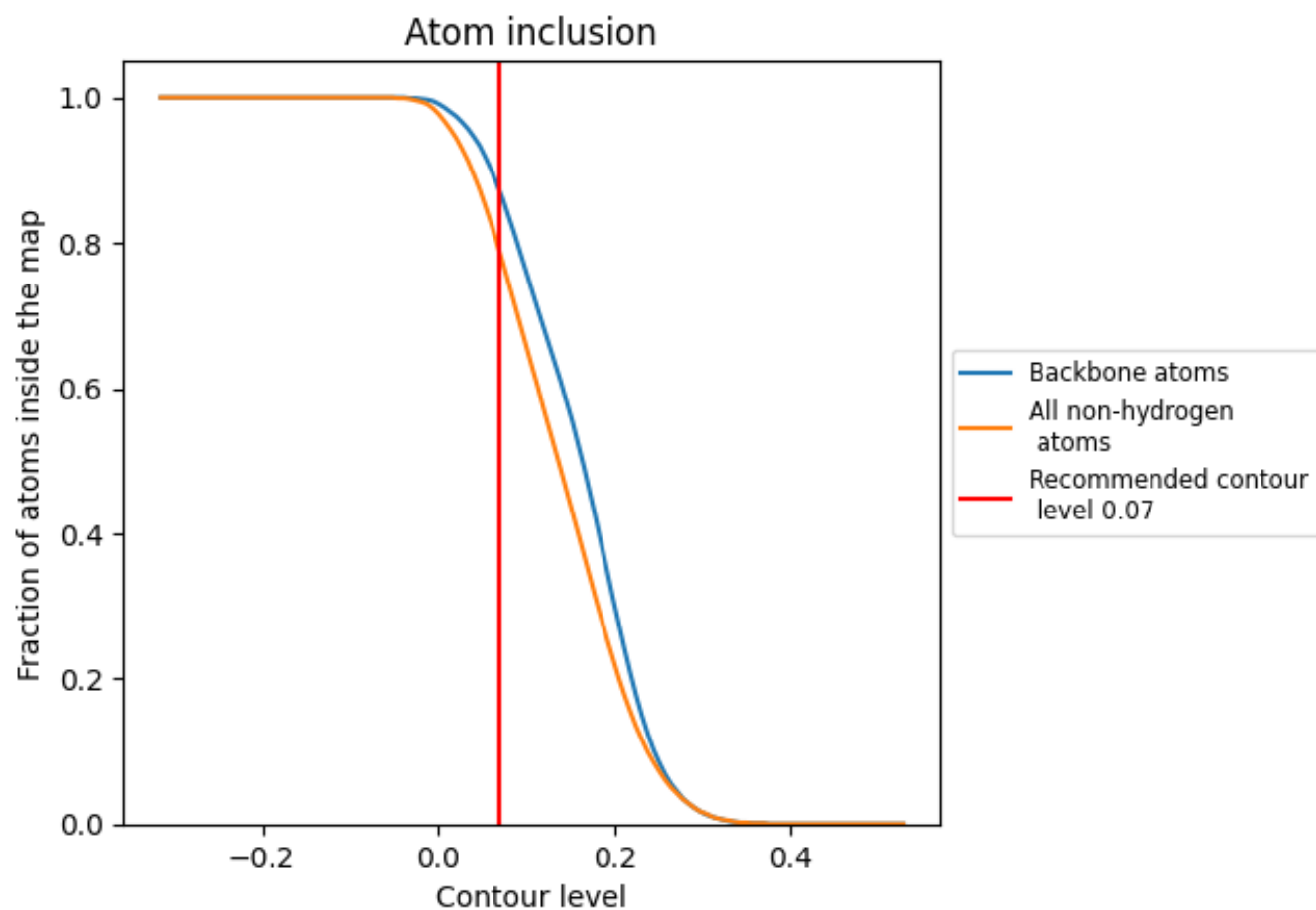
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.07).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 79% 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	 0.7880	 0.4220
1	 0.5790	 0.4150
2	 0.8210	 0.3920
3	 0.5400	 0.2310
5	 0.8440	 0.4100
7	 0.9450	 0.4810
8	 0.8850	 0.4360
9	 0.8580	 0.4170
A	 0.8160	 0.5110
AA	 0.7530	 0.4540
B	 0.8160	 0.4980
BB	 0.7450	 0.4630
C	 0.8040	 0.4910
CC	 0.7680	 0.4710
D	 0.7990	 0.4550
DD	 0.6680	 0.4010
E	 0.7210	 0.4160
EE	 0.7630	 0.4700
F	 0.8050	 0.4870
FF	 0.6990	 0.4280
G	 0.6970	 0.4080
GG	 0.6780	 0.3660
H	 0.7670	 0.4690
HH	 0.6430	 0.3800
I	 0.7880	 0.4810
II	 0.7330	 0.4270
J	 0.7620	 0.4350
JJ	 0.7600	 0.4550
KK	 0.6450	 0.3440
L	 0.7780	 0.4530
LL	 0.7180	 0.4460
M	 0.8000	 0.4560
MM	 0.3720	 0.1710
N	 0.8380	 0.5080
NN	 0.7830	 0.4750



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Chain	Atom inclusion	Q-score
O	 0.8120	 0.4870
OO	 0.7710	 0.4790
P	 0.8190	 0.5040
PP	 0.6510	 0.3750
Q	 0.7960	 0.5000
QQ	 0.7350	 0.4470
R	 0.7630	 0.4520
RR	 0.6690	 0.3950
S	 0.8120	 0.4910
SS	 0.7430	 0.4190
T	 0.7930	 0.4790
TT	 0.7360	 0.4240
U	 0.7490	 0.4220
UU	 0.6610	 0.4020
V	 0.7630	 0.4940
VV	 0.7350	 0.4630
W	 0.8050	 0.4840
WW	 0.7900	 0.4880
X	 0.7780	 0.4670
XX	 0.7700	 0.4960
Y	 0.7910	 0.4670
YY	 0.7370	 0.4160
Z	 0.8100	 0.4740
ZZ	 0.6930	 0.3830
a	 0.8430	 0.5100
aa	 0.7910	 0.4860
b	 0.6880	 0.4000
bb	 0.7140	 0.4450
c	 0.8040	 0.4690
cc	 0.6750	 0.4260
d	 0.7950	 0.4660
dd	 0.7780	 0.4520
e	 0.8040	 0.5000
ee	 0.6540	 0.4090
f	 0.8280	 0.5090
ff	 0.4820	 0.2530
g	 0.7780	 0.4700
gg	 0.6610	 0.3850
h	 0.7890	 0.4630
hh	 0.8100	 0.4440
i	 0.7760	 0.4520
ii	 0.4330	 0.3710

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Chain	Atom inclusion	Q-score
j	 0.8440	 0.5000
jj	 0.3780	 0.3410
k	 0.7240	 0.4200
l	 0.8180	 0.4960
m	 0.7840	 0.4770
n	 0.7960	 0.4730
o	 0.7680	 0.4860
p	 0.7920	 0.4850
r	 0.8220	 0.4860
s	 0.2520	 0.1220
t	 0.2800	 0.1180