



## wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Nov 22, 2016 – 12:30 PM EST

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

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
EM map analysis : **NOT EXECUTED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20028320

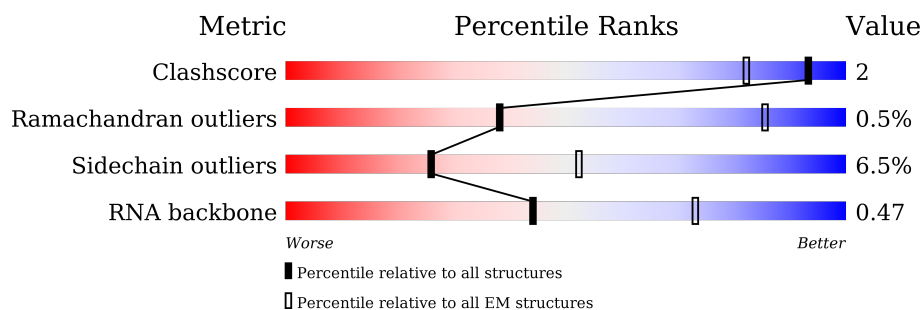
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.65 Å.

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




















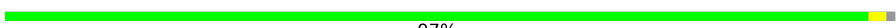







Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	257	82% 14% .
2	B	403	88% 10% .
3	C	425	78% 7% 15%
4	D	297	88% 10% .
5	E	291	66% 7% . 26%
6	F	247	81% 10% 9%
7	G	319	65% 8% . 27%
8	H	192	87% 12% .


























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Mol	Chain	Length	Quality of chain
9	I	214	 88% 7% . .
10	J	178	 86% 10% .
11	L	211	 91% 8%
12	M	218	 54% 8% . 37%
13	N	204	 92% 8%
14	O	203	 85% 12% . .
15	P	184	 76% 7% . 17%
16	Q	188	 91% 8% .
17	R	196	 83% 8% . 8%
18	S	176	 85% 14% .
19	T	160	 91% 8% .
20	U	128	 73% . 23%
21	V	140	 80% 13% . 6%
22	W	157	 65% . . 32%
23	X	156	 71% 5% 24%
24	Y	145	 86% 6% 8%
25	Z	136	 92% 7% .
26	a	148	 97% . .
27	b	245	 41% . 58%
28	c	115	 83% . 15%
29	d	125	 79% 6% 14%
30	e	135	 88% 7% 5%
31	f	110	 92% 7% .
32	g	117	 93% . .
33	h	123	 94% 5% .




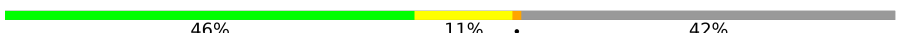



















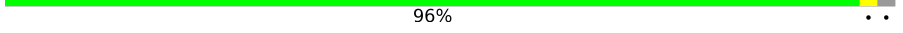

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Mol	Chain	Length	Quality of chain
34	i	105	95% 
35	j	97	84%  5% 11%
36	k	70	96% 
37	l	51	96% 
38	m	102	48%  49%
39	n	25	92% 
40	o	106	92%  6%
41	p	92	97% 
42	r	137	85%  5% 9%
43	s	318	59%  38%
44	t	165	88%  7%
45	1	15	87% 
46	2	76	78%  20%
47	3	75	68%  29%
48	5	3543	71%  26%
49	7	120	86%  13%
50	8	156	73%  21%
51	9	1869	63%  26% 9%
52	AA	295	66%  7% 26%
53	BB	264	67%  13% 19%
54	CC	293	66%  9% 25%
55	DD	243	82%  11% 6%
56	EE	263	85% 
57	FF	204	76%  13% 9%
58	GG	249	85%  9% 5%

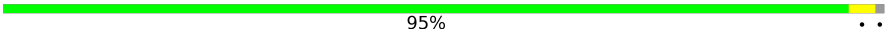



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Mol	Chain	Length	Quality of chain
59	HH	194	
60	II	208	
61	JJ	194	
62	KK	165	
63	LL	158	
64	MM	132	
65	NN	151	
66	OO	168	
67	PP	145	
68	QQ	146	
69	RR	135	
70	SS	152	
71	TT	145	
72	UU	119	
73	VV	83	
74	WW	130	
75	XX	143	
76	YY	130	
77	ZZ	125	
78	aa	115	
79	bb	84	
80	cc	69	
81	dd	56	
82	ee	133	
83	ff	156	

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

## 2 Entry composition

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

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

- Molecule 1 is a protein called uL2.

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

- Molecule 2 is a protein called uL3.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 3 is a protein called uL4.

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

- Molecule 4 is a protein called uL18.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 5 is a protein called eL6.

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

- Molecule 6 is a protein called uL30.

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

There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 7 is a protein called eL8.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 8 is a protein called uL6.

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

- Molecule 9 is a protein called uL16.

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

- Molecule 10 is a protein called uL5.



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

- Molecule 11 is a protein called eL13.

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

- Molecule 12 is a protein called eL14.

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

- Molecule 13 is a protein called eL15.

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

- Molecule 14 is a protein called uL13.

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

- Molecule 15 is a protein called uL22.

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

- Molecule 16 is a protein called eL18.

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

- Molecule 17 is a protein called eL19.

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

- Molecule 18 is a protein called eL20.

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

- Molecule 19 is a protein called eL21.

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

- Molecule 20 is a protein called eL22.

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

- Molecule 21 is a protein called uL14.

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

- Molecule 22 is a protein called eL24.

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

- Molecule 23 is a protein called uL23.

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

- Molecule 24 is a protein called uL24.

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

- Molecule 25 is a protein called eL27.

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

- Molecule 26 is a protein called uL15.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 27 is a protein called eL29.

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

- Molecule 28 is a protein called eL30.

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

- Molecule 29 is a protein called eL31.

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

- Molecule 30 is a protein called eL32.

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

- Molecule 31 is a protein called eL33.

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

- Molecule 32 is a protein called eL34.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 33 is a protein called uL29.

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

- Molecule 34 is a protein called eL36.

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

- Molecule 35 is a protein called eL37.

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

- Molecule 36 is a protein called eL38.

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

- Molecule 37 is a protein called eL39.

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

- Molecule 38 is a protein called eL40.

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

- Molecule 39 is a protein called eL41.

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

- Molecule 40 is a protein called eL42.

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

- Molecule 41 is a protein called eL43.

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

- Molecule 42 is a protein called eL28.

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

- Molecule 43 is a protein called uL10.

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

- Molecule 44 is a protein called uL11.

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

- Molecule 45 is a protein called Nascent chain.

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 52 is a protein called uS2.

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

- Molecule 53 is a protein called eS1.

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

- Molecule 54 is a protein called uS5.

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

- Molecule 55 is a protein called uS3.

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

- Molecule 56 is a protein called eS4.

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

- Molecule 57 is a protein called uS7.

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

- Molecule 58 is a protein called eS6.

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

- Molecule 59 is a protein called eS7.

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

- Molecule 60 is a protein called eS8.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 61 is a protein called uS4.

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

- Molecule 62 is a protein called eS10.

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

- Molecule 63 is a protein called uS17.



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

- Molecule 64 is a protein called eS12.

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

- Molecule 65 is a protein called uS15.

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

- Molecule 66 is a protein called uS11.

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

- Molecule 67 is a protein called uS19.

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

- Molecule 68 is a protein called uS9.

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

- Molecule 69 is a protein called eS17.

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

- Molecule 70 is a protein called uS13.

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

- Molecule 71 is a protein called eS19.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 72 is a protein called uS10.

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

- Molecule 73 is a protein called eS21.

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

- Molecule 74 is a protein called uS8.

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

- Molecule 75 is a protein called uS12.

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

- Molecule 76 is a protein called eS24.

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

- Molecule 77 is a protein called eS25.

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

- Molecule 78 is a protein called eS26.

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

- Molecule 79 is a protein called eS27.

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

- Molecule 80 is a protein called eS28.

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

- Molecule 81 is a protein called uS14.

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

- Molecule 82 is a protein called eS30.

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

- Molecule 83 is a protein called eS31.

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

- Molecule 84 is a protein called RACK1.

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

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

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

- Molecule 86 is a protein called eRF1.

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

There are 22 discrepancies between the modelled and reference sequences:

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

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

- Molecule 87 is a protein called eRF3a.

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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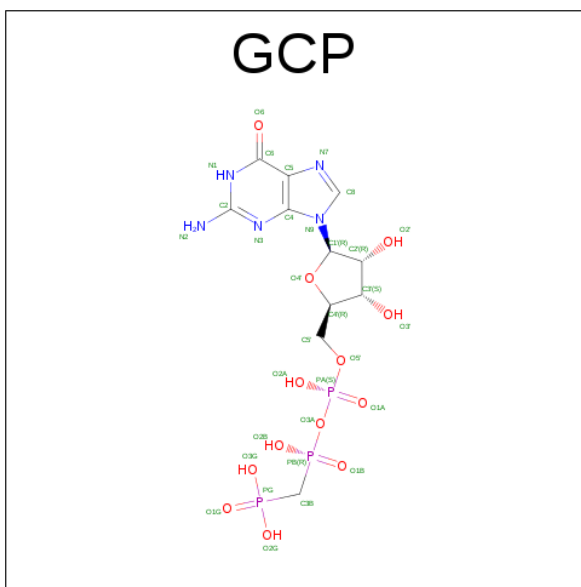
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Mol	Chain	Residues	Atoms		AltConf
88	8	8	Total 8	Mg 8	0
88	9	71	Total 71	Mg 71	0
88	hh	1	Total 1	Mg 1	0

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

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

- Molecule 90 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: C<sub>11</sub>H<sub>18</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).

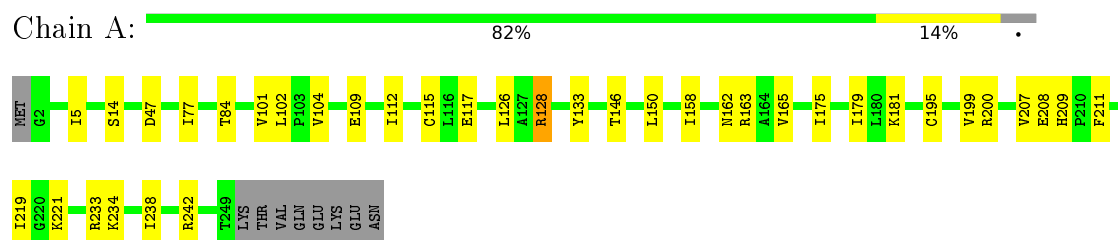


Mol	Chain	Residues	Atoms					AltConf
90	jj	1	Total	C	N	O	P	0
			32	11	5	13	3	

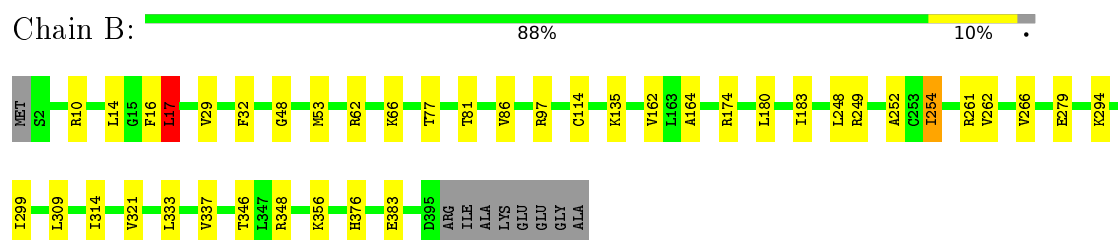
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

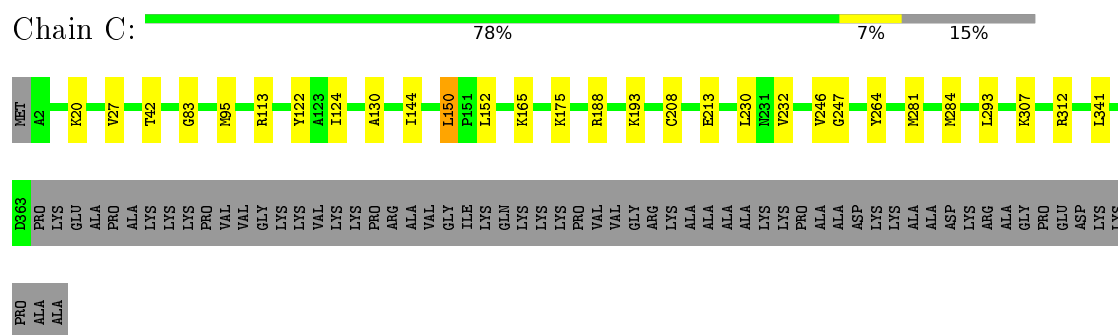
- Molecule 1: uL2



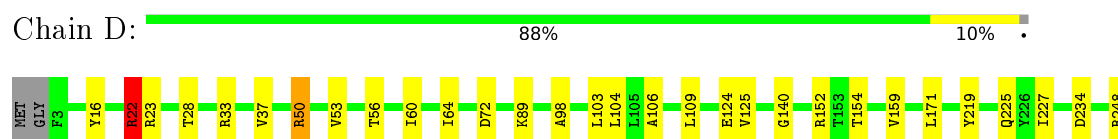
- Molecule 2: uL3



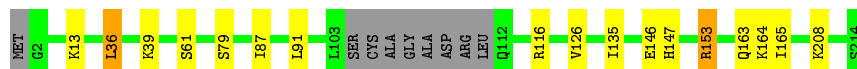
- Molecule 3: uL4



- Molecule 4: uL18







- Molecule 10: uL5

Chain J:  86% 10% .



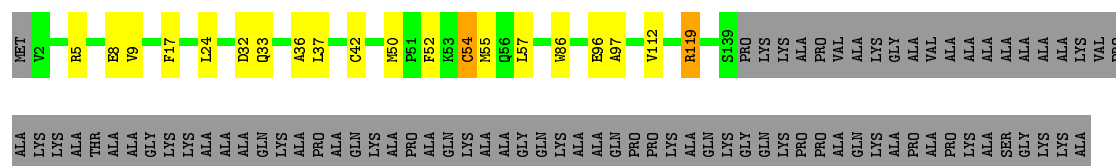
- Molecule 11: eL13

Chain L:  91% 8%



- Molecule 12: eL14

Chain M:  54% 8% 37%



- Molecule 13: eL15

Chain N:  92% 8%



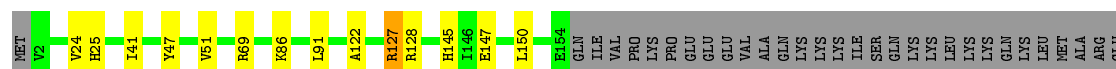
- Molecule 14: uL13

Chain 0:  85% 12% ..



- Molecule 15: uL22

Chain P:  76% 7% 17%




- Molecule 16: eL18

Chain Q:  91% 8%




- Molecule 17: eL19

Chain R:  83% 8% 8%



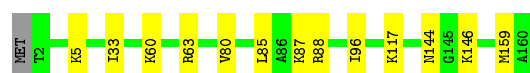
- Molecule 18: eL20

Chain S:  85% 14%



- Molecule 19: eL21

Chain T:  91% 8%




- Molecule 20: eL22

Chain U:  73% 23%



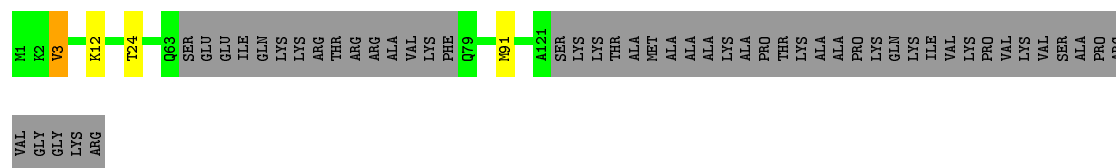
- Molecule 21: uL14

Chain V:  80% 13% 6%



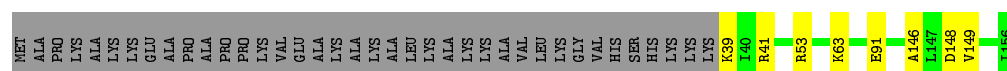
- Molecule 22: eL24

Chain W:  65% 32%




- Molecule 23: uL23

Chain X:  71% 5% 24%



- Molecule 24: uL24

Chain Y:  86% 6% 8%



- Molecule 25: eL27

Chain Z:  92% 7%



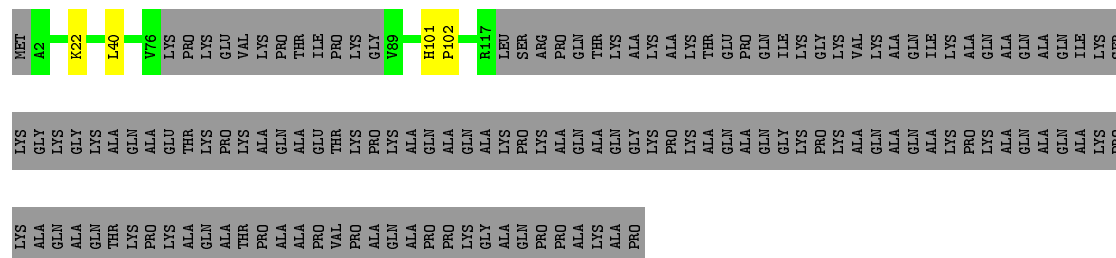
- Molecule 26: uL15

Chain a:  97%

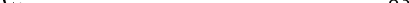


- Molecule 27: eL29

Chain b:  41% . 58%

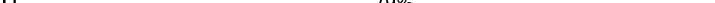


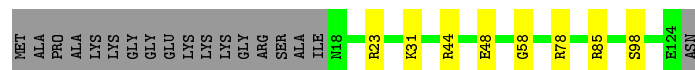
- Molecule 28: eL30

Chain c:  83% • 15%



- Molecule 29: eL31

Chain d:  79% 6% 14%




- Molecule 30: eL32

Chain e:  88% 7% 5%



- Molecule 31: eL33

Chain f:  92% 7%



- Molecule 32: eL34

Chain g:  93%



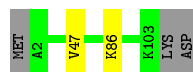
- Molecule 33: uL29

Chain h:  94% 5%




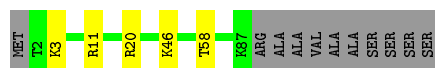
- Molecule 34: eL36

Chain i:  95%



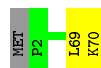
- Molecule 35: eL37

Chain j:  84% 5% 11%



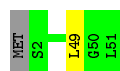
- Molecule 36: eL38

Chain k:  96%



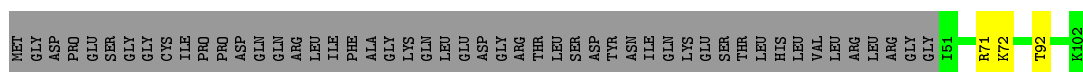
- Molecule 37: eL39

Chain l:  96%



- Molecule 38: eL40

Chain m:  48% 49%



- Molecule 39: eL41



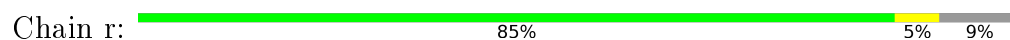
- Molecule 40: eL42



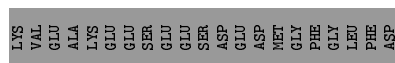
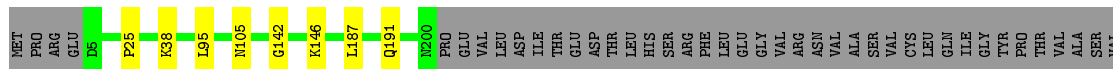
- Molecule 41: eL43



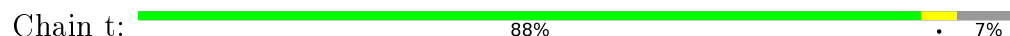
- Molecule 42: eL28



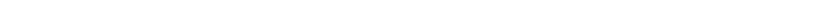
- Molecule 43: uL10



- Molecule 44: uL11




- Molecule 45: Nascent chain

Chain 1:  87% 13%



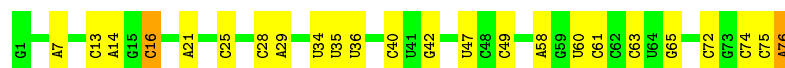
- Molecule 46: P-site tRNA

Chain 2:  78% 20%



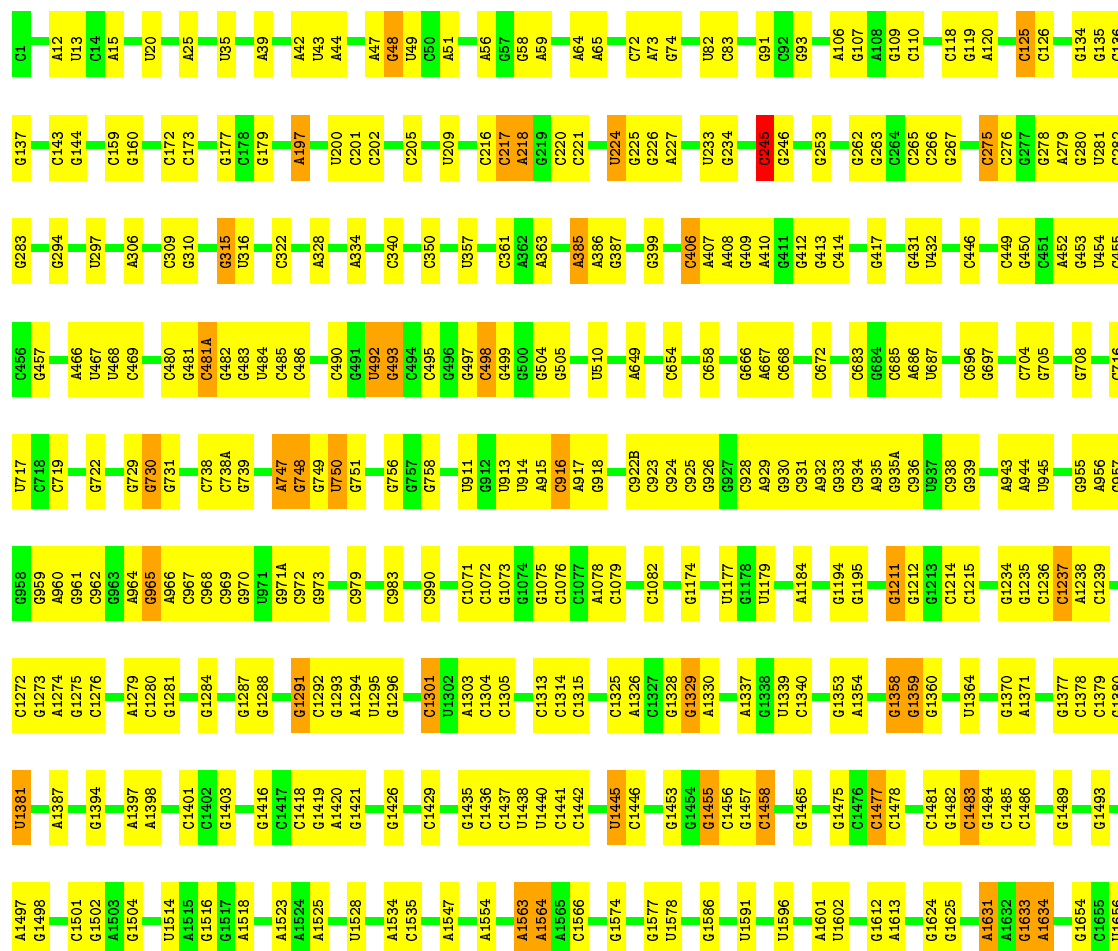
- Molecule 47: E-site tRNA

Chain 3:  68% 29% .



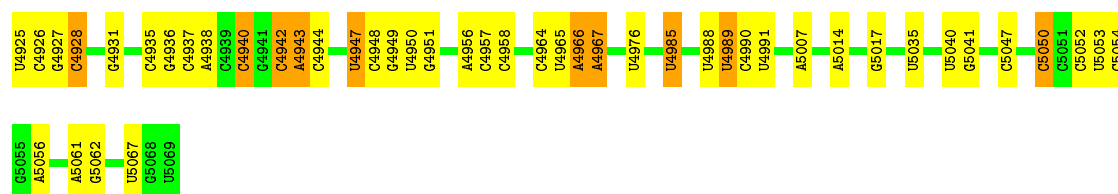
- Molecule 48: 28S ribosomal RNA

Chain 5:  71% 26% .



G4736	G4737	G4745	G4751	G4752	G4753	G4754	G4755	G4756	G4757	G4758	G4759	G4760	G4761	G4765	G4771	G4772	G4868	G4869	G4870	G4871	G4872	G4873	G4874	G4875	G4876	G4877	U4882	G4883	G4884	G4885	G4886	G4887	G4891	G4895	G4896	G4897	A4910	G4912	G4913	G4914	G4915	G4918	G4919	A4920	G4921	G4924																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
A4280	A4281	G4291	G4297	U4301	A4304	G4305	U4306	C4314	A4317	C4318	C4319	G4326	G4329	G4330	G4331	C4335	A4336	A4339	C4349	C4350	U4354	G4355	G4373	A4376	G4377	A4378	A4379	A4380	C4387	G4391	G4392	G4393	A4394	U4395	C4398	G4401	A4415	U4419																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
C4421	A4422	G4440	C4444	G4448	U4449	U4450	C4453	U4457	C4458	U4459	U4460	A4464	A4467	U4471	G4475	A4476	A4477	A4478	A4479	A4488	G4495	U4500	A4510	A4511	A4512	A4513	C4519	G4520	G4524	G4527	G4528	U4531	A4548	G4549	C4560	G4567																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
U4450	A4571	U4572	U4573	U4574	U4575	U4576	U4577	U4578	U4579	U4580	U4581	U4582	U4583	U4584	U4585	U4586	U4587	U4588	U4589	U4590	U4591	U4592	U4593	U4594	U4595	U4596	U4597	U4598	U4599	U4600	U4601	U4602	U4603	U4604	U4605	U4606	U4607	U4608	U4609	U4610	U4611	U4612	U4613	U4614	U4615	U4616	U4617	U4618	U4619	U4620	U4621	U4622	U4623	U4624	U4625	U4626	U4627	U4628	U4629	U4630	U4631	U4632	U4633	U4634	U4635	U4636	U4637	U4638	U4639	U4640	U4641	U4642	U4643	U4644	U4645	U4646	U4647	U4648	U4649	U4650	U4651	U4652	U4653	U4654	U4655	U4656	U4657	U4658	U4659	U4660	U4661	U4662	U4663	U4664	U4665	U4666	U4667	U4668	U4669	U4670	U4671	U4672	U4673	U4674	U4675	U4676	U4677	U4678	U4679	U4680	U4681	U4682	U4683	U4684	U4685	U4686	U4687	U4688	U4689	U4690	U4691	U4692	U4693	U4694	U4695	U4696	U4697	U4698	U4699	U4700	U4701	U4702	U4703	U4704	U4705	U4706	U4707	U4708	U4709	U4710	U4711	U4712	U4713	U4714	U4715	U4716	U4717	U4718	U4719	U4720	U4721	U4722	U4723	U4724	U4725	U4726	U4727	U4728	U4729	U4730	U4731	U4732	U4733	U4734	U4735	U4736	U4737	U4738	U4739	U4740	U4741	U4742	U4743	U4744	U4745	U4746	U4747	U4748	U4749	U4750	U4751	U4752	U4753	U4754	U4755	U4756	U4757	U4758	U4759	U4760	U4761	U4762	U4763	U4764	U4765	U4766	U4767	U4768	U4769	U4770	U4771	U4772	U4773	U4774	U4775	U4776	U4777	U4778	U4779	U4780	U4781	U4782	U4783	U4784	U4785	U4786	U4787	U4788	U4789	U4790	U4791	U4792	U4793	U4794	U4795	U4796	U4797	U4798	U4799	U4800	U4801	U4802	U4803	U4804	U4805	U4806	U4807	U4808	U4809	U4810	U4811	U4812	U4813	U4814	U4815	U4816	U4817	U4818	U4819	U4820	U4821	U4822	U4823	U4824	U4825	U4826	U4827	U4828	U4829	U4830	U4831	U4832	U4833	U4834	U4835	U4836	U4837	U4838	U4839	U4840	U4841	U4842	U4843	U4844	U4845	U4846	U4847	U4848	U4849	U4850	U4851	U4852	U4853	U4854	U4855	U4856	U4857	U4858	U4859	U4860	U4861	U4862	U4863	U4864	U4865	U4866	U4867	U4868	U4869	U4870	U4871	U4872	U4873	U4874	U4875	U4876	U4877	U4878	U4879	U4880	U4881	U4882	U4883	U4884	U4885	U4886	U4887	U4888	U4889	U4890	U4891	U4892	U4893	U4894	U4895	U4896	U4897	U4898	U4899	U4900	U4901	U4902	U4903	U4904	U4905	U4906	U4907	U4908	U4909	U4910	U4911	U4912	U4913	U4914	U4915	U4916	U4917	U4918	U4919	U4920	U4921	U4922	U4923	U4924	U4925	U4926	U4927	U4928	U4929	U4930	U4931	U4932	U4933	U4934	U4935	U4936	U4937	U4938	U4939	U4940	U4941	U4942	U4943	U4944	U4945	U4946	U4947	U4948	U4949	U4950	U4951	U4952	U4953	U4954	U4955	U4956	U4957	U4958	U4959	U4960	U4961	U4962	U4963	U4964	U4965	U4966	U4967	U4968	U4969	U4970	U4971	U4972	U4973	U4974	U4975	U4976	U4977	U4978	U4979	U4980	U4981	U4982	U4983	U4984	U4985	U4986	U4987	U4988	U4989	U4990	U4991	U4992	U4993	U4994	U4995	U4996	U4997	U4998	U4999	U5000	U5001	U5002	U5003	U5004	U5005	U5006	U5007	U5008	U5009	U5010	U5011	U5012	U5013	U5014	U5015	U5016	U5017	U5018	U5019	U5020	U5021	U5022	U5023	U5024	U5025	U5026	U5027	U5028	U5029	U5030	U5031	U5032	U5033	U5034	U5035	U5036	U5037	U5038	U5039	U5040	U5041	U5042	U5043	U5044	U5045	U5046	U5047	U5048	U5049	U5050	U5051	U5052	U5053	U5054	U5055	U5056	U5057	U5058	U5059	U5060	U5061	U5062	U5063	U5064	U5065	U5066	U5067	U5068	U5069	U5070	U5071	U5072	U5073	U5074	U5075	U5076	U5077	U5078	U5079	U5080	U5081	U5082	U5083	U5084	U5085	U5086	U5087	U5088	U5089	U5090	U5091	U5092	U5093	U5094	U5095	U5096	U5097	U5098	U5099	U5100	U5101	U5102	U5103	U5104	U5105	U5106	U5107	U5108	U5109	U5110	U5111	U5112	U5113	U5114	U5115	U5116	U5117	U5118	U5119	U5120	U5121	U5122	U5123	U5124	U5125	U5126	U5127	U5128	U5129	U5130	U5131	U5132	U5133	U5134	U5135	U5136	U5137	U5138	U5139	U5140	U5141	U5142	U5143	U5144	U5145	U5146	U5147	U5148	U5149	U5150	U5151	U5152	U5153	U5154	U5155	U5156	U5157	U5158	U5159	U5160	U5161	U5162	U5163	U5164	U5165	U5166	U5167	U5168	U5169	U5170	U5171	U5172	U5173	U5174	U5175	U5176	U5177	U5178	U5179	U5180	U5181	U5182	U5183	U5184	U5185	U5186	U5187	U5188	U5189	U5190	U5191	U5192	U5193	U5194	U5195	U5196	U5197	U5198	U5199	U5200	U5201	U5202	U5203	U5204	U5205	U5206	U5207	U5208	U5209	U5210	U5211	U5212	U5213	U5214	U5215	U5216	U5217	U5218	U5219	U5220	U5221	U5222	U5223	U5224	U5225	U5226	U5227	U5228	U5229	U5230	U5231	U5232	U5233	U5234	U5235	U5236	U5237	U5238	U5239	U5240	U5241	U5242	U5243	U5244	U5245	U5246	U5247	U5248	U5249	U5250	U5251	U5252	U5253	U5254	U5255	U5256	U5257	U5258	U5259	U5260	U5261	U5262	U5263	U5264	U5265	U5266	U5267	U5268	U5269	U5270	U5271	U5272	U5273	U5274	U5275	U5276	U5277	U5278	U5279	U5280	U5281	U5282	U5283	U5284	U5285	U5286	U5287	U5288	U5289	U5290	U5291	U5292	U5293	U5294	U5295	U5296	U5297	U5298	U5299	U5300	U5301	U5302	U5303	U5304	U5305	U5306	U5307	U5308	U5309	U5310	U5311	U5312	U5313	U5314	U5315	U5316	U5317	U5318	U5319	U5320	U5321	U5322	U5323	U5324	U5325	U5326	U5327	U5328	U5329	U5330	U5331	U5332	U5333	U5334	U5335	U5336	U5337	U5338	U5339	U5340	U5341	U5342	U5343	U5344	U5345	U5346	U5347	U5348	U5349	U5350	U5351	U5352	U5353	U5354	U5355	U5356	U5357	U5358	U5359	U5360	U5361	U5362	U5363	U5364	U5365	U5366	U5367	U5368	U5369	U5370	U5371	U5372	U5373	U5374	U5375	U5376	U5377	U5378	U5379	U5380	U5381	U5382	U5383	U5384	U5385	U5386	U5387	U5388	U5389	U5390	U5391	U5392	U5393	U5394	U5395	U5396	U5397	U5398	U5399	U5400	U5401	U5402	U5403	U5404	U5405	U5406	U5407	U5408	U5409	U5410	U5411	U5412	U5413	U5414	U5415	U5416	U5417	U5418	U5419	U5420	U5421	U5422	U5423	U5424	U5425	U5426	U5427	U5428	U5429	U5430	U5431	U5432	U5433	U5434	U5435	U5436	U5437	U5438	U5439	U5440	U5441	U5442	U5443	U5444	U5445	U5446	U5447	U5448	U5449	U5450	U5451	U5452	U5453	U5454	U5455	U5456	U5457	U5458	U5459	U5460	U5461	U5462	U5463	U5464	U5465	U5466	U5467	U5468	U5469	U5470	U5471	U5472	U5473	U5474	U5475	U5476	U5477	U5478	U5479	U5480	U5481	U5482	U5483	U5484	U5485	U5486	U5487	U5488	U5489	U5490	U5491	U5492	U5493	U5494	U5495	U5496	U5497	U5498	U5499	U5500	U5501	U5502	U5503	U5504	U5505	U5506	U5507	U5508	U5509	U5510	U5511	U5512	U5513	U5514	U5515	U5516	U5517	U5518	U5519	U5520	U5521	U5522	U5523	U5524	U5525	U5526	U5527	U5528	U5529	U5530	U5531	U5532	U5533	U5534	U5535	U5536	U5537	U5538	U5539	U5540	U5541	U5542	U5543	U5544	U5545	U5546	U5547	U5548	U5549	U5550	U5551	U5552	U5553	U5554	U5555	U5556	U5557	U5558	U5559	U5560	U5561	U5562	U5563	U5564	U5565	U5566	U5567	U5568	U5569	U5570	U5571	U5572	U5573	U5574	U5575	U5576	U5577	U5578	U5579	U5580	U5581	U5582	U5583	U5584	U5585	U5586	U5587	U5588	U5589	U5590	U5591	U5592	U5593	U5594	U5595	U5596	U5597	U5598	U5599	U5600	U5601	U5602	U5603	U5604	U5605	U5606	U5607	U5608	U5609	U5610	U5611	U5612	U5613	U5614	U5615	U5616	U5617	U5618	U5619	U5620	U5621	U5622	U5623	U5624	U5625	U5626	U5627	U5628	U5629	U5630	U5631	U5632	U5633	U5634	U5635	U5636	U5637	U5638	U5639	U5640	U5641	U5642	U5643	U5644	U5645	U5646	U5647	U5648	U5649	U5650	U5651	U5652	U5653	U5654	U5655	U5656	U5657	U5658	U5659	U5660	U5661	U5662	U5663	U5664	U5665	U5666	U5667	U5668	U5669	U5670	U5671	U5672	U5673	U5674	U5675	U5676	U5677	U5678	U5679	U5680	U568





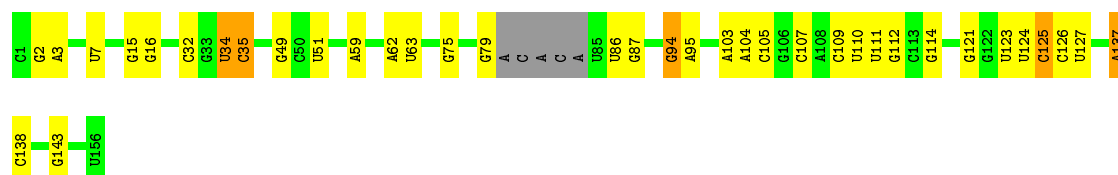
• Molecule 49: 5S ribosomal RNA

Chain 7: 86% 13%



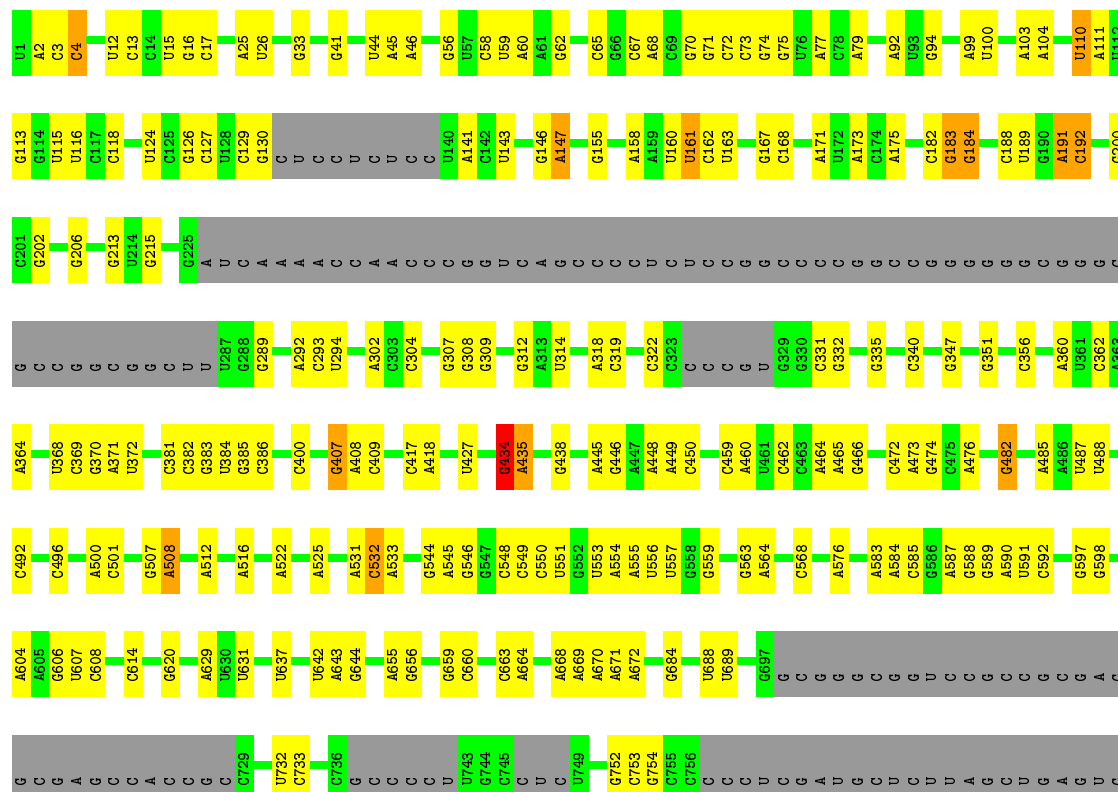
• Molecule 50: 5.8S ribosomal RNA

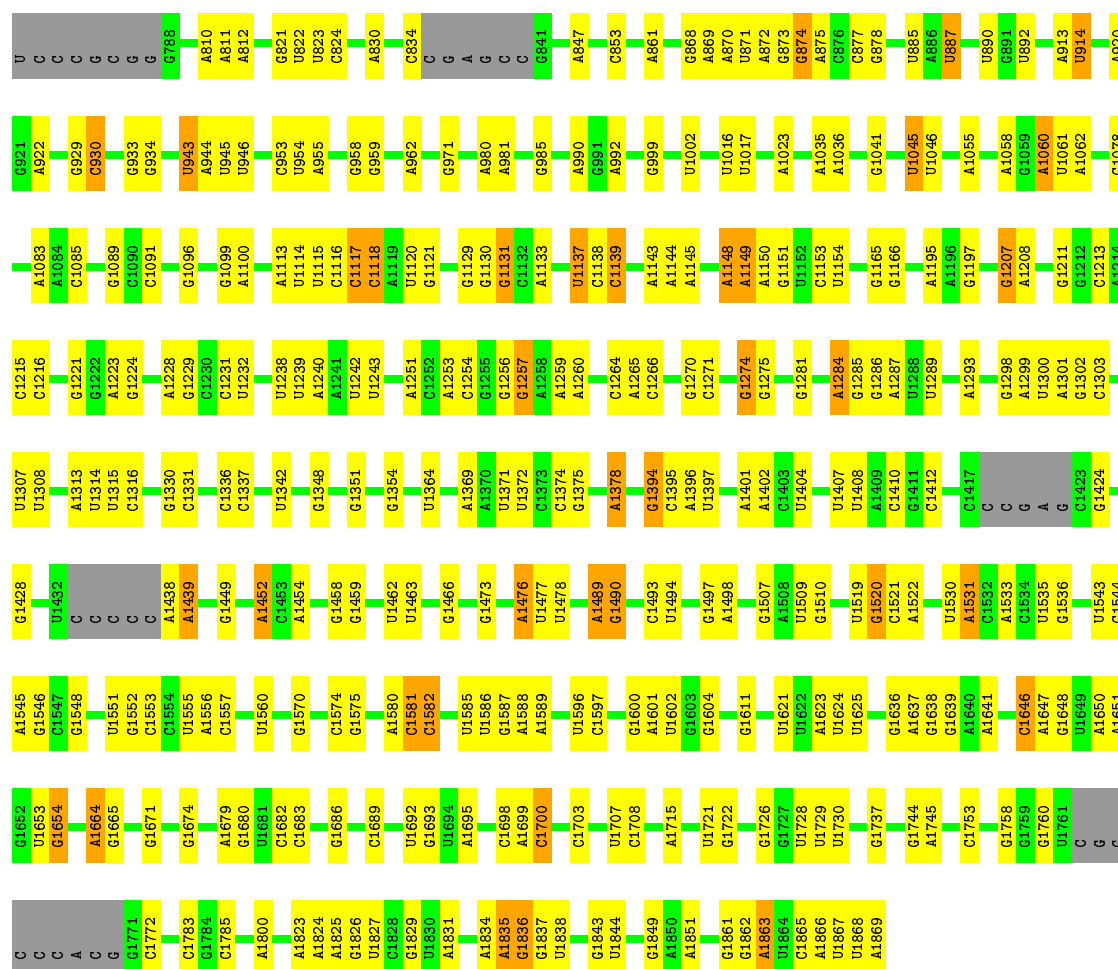
Chain 8: 73% 21%



• Molecule 51: 18S ribosomal RNA

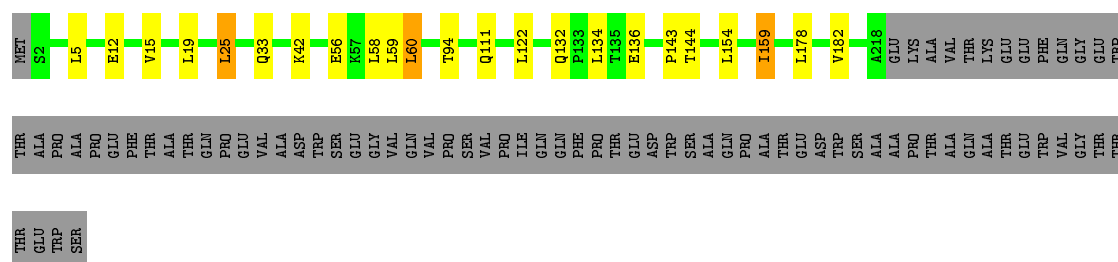
Chain 9: 63% 26% 9%





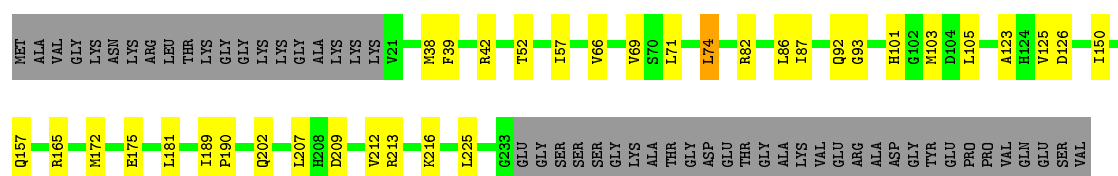
- Molecule 52: uS2

Chain AA: 66% 7% 26%




- Molecule 53: eS1

Chain BB: 67% 13% 19%






- Molecule 59: eS7

Chain HH: 




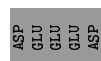
- Molecule 60: eS8

Chain II: 



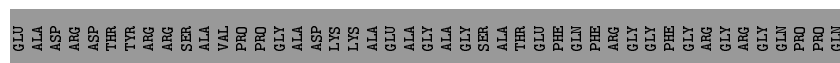
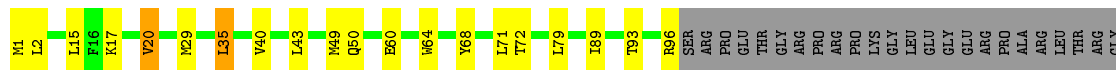
- Molecule 61: uS4

Chain JJ: 




- Molecule 62: eS10

Chain KK: 




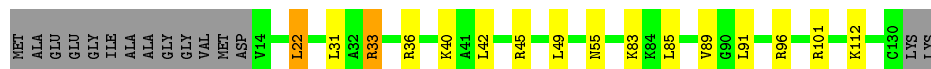
- Molecule 63: uS17

Chain LL: 




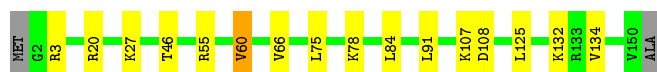
- Molecule 64: eS12

Chain MM: 

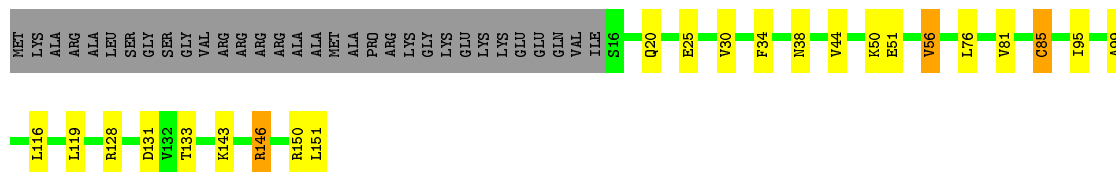


- Molecule 65: uS15

Chain NN: 



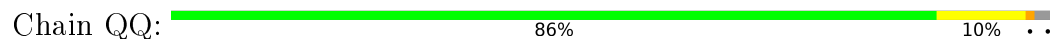
- Molecule 66: uS11



- Molecule 67: uS19



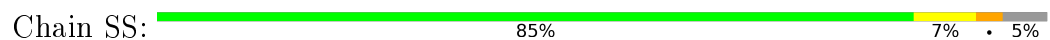
- Molecule 68: uS9



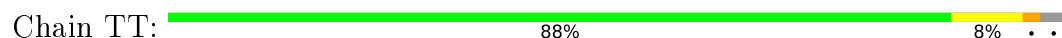
- Molecule 69: eS17



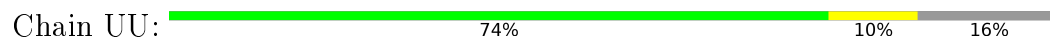
- Molecule 70: uS13



- Molecule 71: eS19



- Molecule 72: uS10





- Molecule 73: eS21

Chain VV: 88% 11% .



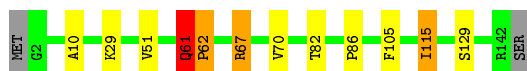
- Molecule 74: uS8

Chain WW: 81% 18% .



- Molecule 75: uS12

Chain XX: 90% 6% ...



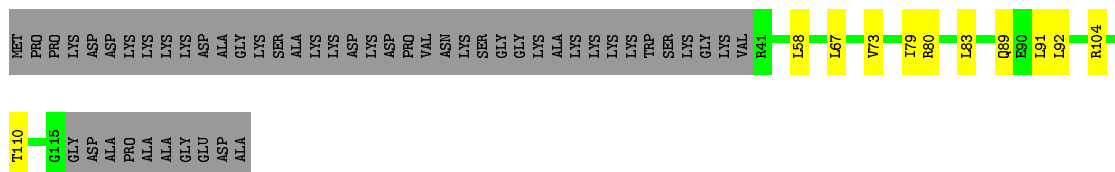
- Molecule 76: eS24

Chain YY: 82% 14% 5%



- Molecule 77: eS25

Chain ZZ: 51% 9% 40%



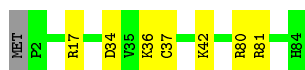
- Molecule 78: eS26

Chain aa: 81% 6% 12%

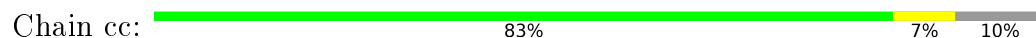


- Molecule 79: eS27

Chain bb: 90% 8% .



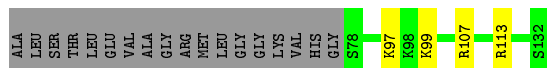
- Molecule 80: eS28



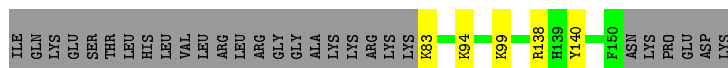
- Molecule 81: uS14



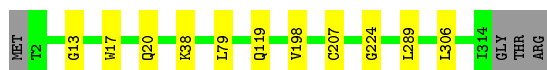
- Molecule 82: eS30



- Molecule 83: eS31



- Molecule 84: RACK1

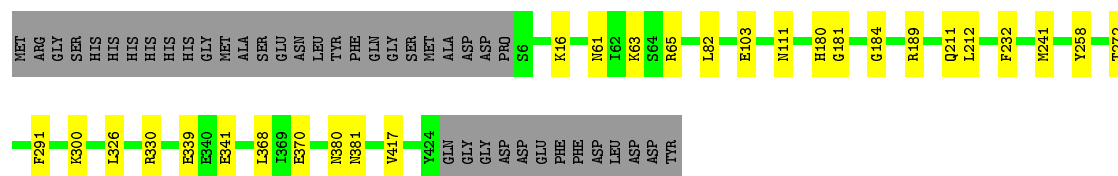


- Molecule 85: mRNA (UGA stop codon)



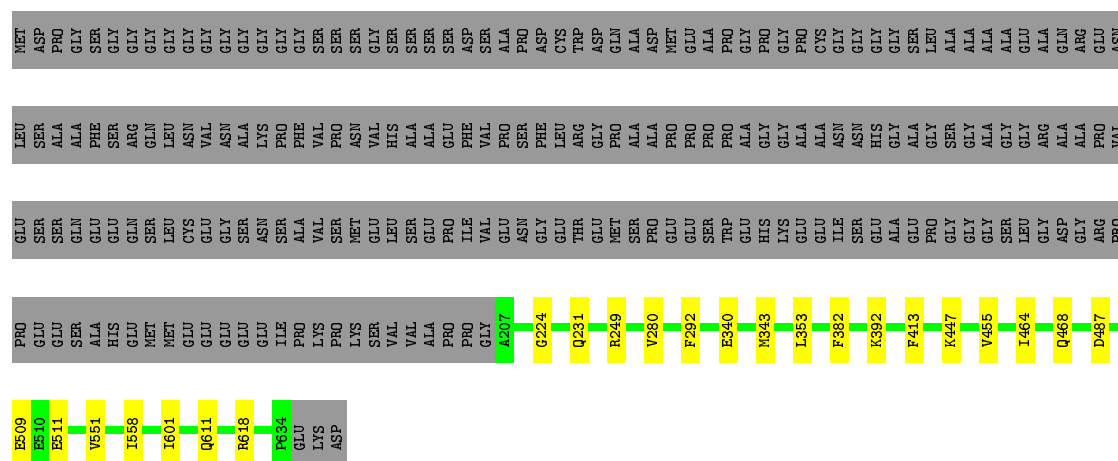
- Molecule 86: eRF1

Chain ii:



- Molecule 87: eRF3a

Chain jj:





## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	61752	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	104478	Depositor
Image detector	Not provided	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GCP, ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	A	0.34	0/1936	0.69	0/2596
10	J	0.33	0/1385	0.61	0/1852
11	L	0.34	0/1733	0.67	0/2316
12	M	0.35	0/1158	0.65	0/1547
13	N	0.35	0/1746	0.67	0/2338
14	O	0.34	0/1662	0.66	0/2222
15	P	0.36	0/1268	0.64	0/1700
16	Q	0.35	0/1539	0.72	0/2054
17	R	0.34	0/1524	0.67	0/2013
18	S	0.37	0/1501	0.68	0/2012
19	T	0.33	0/1326	0.60	0/1770
2	B	0.33	0/3240	0.64	0/4339
20	U	0.35	0/823	0.55	0/1104
21	V	0.34	0/993	0.62	0/1332
22	W	0.34	0/873	0.56	0/1158
23	X	0.33	0/984	0.60	0/1323
24	Y	0.33	0/1132	0.62	0/1504
25	Z	0.34	0/1130	0.61	0/1507
26	a	0.32	0/1191	0.61	0/1590
27	b	0.34	0/861	0.58	0/1138
28	c	0.32	0/771	0.54	0/1034
29	d	0.34	0/903	0.66	0/1216
3	C	0.33	0/2937	0.66	0/3946
30	e	0.34	0/1071	0.66	0/1429
31	f	0.36	0/895	0.69	0/1198
32	g	0.33	0/916	0.67	0/1220
33	h	0.32	0/1021	0.61	0/1348
34	i	0.34	0/841	0.60	0/1112
35	j	0.36	0/720	0.72	0/952
36	k	0.32	0/575	0.55	0/761
37	l	0.35	0/459	0.63	0/608
38	m	0.34	0/435	0.61	0/575

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
39	n	0.34	0/240	0.67	0/305
4	D	0.34	0/2437	0.61	3/3264 (0.1%)
40	o	0.34	0/864	0.61	0/1140
41	p	0.32	0/718	0.62	0/953
42	r	0.35	0/1010	0.69	0/1354
43	s	0.36	0/1530	0.50	0/2064
44	t	0.36	0/1174	0.52	0/1582
45	1	0.41	0/129	0.61	0/173
46	2	0.22	0/1805	0.67	0/2809
47	3	0.21	0/1777	0.66	0/2763
48	5	0.27	0/84973	0.68	22/132508 (0.0%)
49	7	0.26	0/2858	0.67	0/4455
5	E	0.33	0/1762	0.63	0/2362
50	8	0.28	0/3581	0.67	0/5577
51	9	0.25	0/40524	0.69	10/63134 (0.0%)
52	AA	0.33	0/1747	0.60	0/2374
53	BB	0.33	0/1756	0.63	0/2350
54	CC	0.34	0/1753	0.62	0/2369
55	DD	0.35	0/1796	0.61	0/2417
56	EE	0.34	0/2118	0.64	0/2849
57	FF	0.33	0/1492	0.61	0/2005
58	GG	0.35	0/1946	0.67	0/2590
59	HH	0.35	0/1510	0.59	0/2022
6	F	0.36	0/1911	0.66	1/2549 (0.0%)
60	II	0.34	0/1715	0.63	0/2287
61	JJ	0.33	0/1550	0.68	0/2069
62	KK	0.34	0/834	0.59	0/1125
63	LL	0.35	0/1195	0.66	0/1597
64	MM	0.36	0/918	0.61	0/1233
65	NN	0.33	0/1226	0.62	0/1649
66	OO	0.34	0/1029	0.78	1/1380 (0.1%)
67	PP	0.34	0/1017	0.64	0/1358
68	QQ	0.32	0/1146	0.61	0/1534
69	RR	0.33	0/1082	0.60	0/1452
7	G	0.33	0/1910	0.62	0/2569
70	SS	0.34	0/1208	0.68	0/1618
71	TT	0.36	0/1115	0.63	1/1493 (0.1%)
72	UU	0.34	0/805	0.65	0/1081
73	VV	0.36	0/643	0.67	0/860
74	WW	0.34	0/1051	0.69	0/1406
75	XX	0.32	0/1116	0.64	0/1490
76	YY	0.35	0/1028	0.61	0/1366
77	ZZ	0.33	0/604	0.59	0/810

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
78	aa	0.35	0/828	0.74	0/1109
79	bb	0.33	0/665	0.59	0/891
8	H	0.31	0/1535	0.60	0/2063
80	cc	0.33	0/490	0.65	0/656
81	dd	0.37	0/470	0.62	0/623
82	ee	0.35	0/447	0.70	0/587
83	ff	0.36	0/567	0.56	0/753
84	gg	0.32	0/2493	0.55	0/3394
85	hh	0.31	0/353	0.77	0/547
86	ii	0.35	0/3361	0.54	0/4519
87	jj	0.35	0/3435	0.55	0/4633
9	I	0.33	0/1702	0.60	0/2272
All	All	0.30	0/238498	0.66	38/349206 (0.0%)

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

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

There are no bond length outliers.

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

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

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	16	PHE	Peptide
74	WW	27	ILE	Peptide

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Mol	Chain	Res	Type	Group
75	XX	61	GLN	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1898	0	1993	17	0
2	B	3172	0	3310	17	0
3	C	2883	0	3053	7	0
4	D	2391	0	2424	13	0
5	E	1729	0	1887	10	0
6	F	1875	0	1995	10	0
7	G	1879	0	2027	10	0
8	H	1516	0	1597	8	0
9	I	1664	0	1712	5	0
10	J	1362	0	1399	7	0
11	L	1702	0	1820	6	0
12	M	1137	0	1211	9	0
13	N	1701	0	1749	4	0
14	O	1630	0	1778	14	0
15	P	1242	0	1274	4	0
16	Q	1515	0	1634	5	0
17	R	1508	0	1664	5	0
18	S	1462	0	1508	12	0
19	T	1298	0	1366	4	0
20	U	809	0	833	1	0
21	V	979	0	1039	7	0
22	W	860	0	903	3	0
23	X	967	0	1040	1	0
24	Y	1115	0	1205	1	0
25	Z	1107	0	1182	4	0
26	a	1162	0	1209	0	0
27	b	848	0	920	0	0
28	c	761	0	794	0	0
29	d	888	0	930	0	0
30	e	1053	0	1147	0	0
31	f	876	0	912	0	0
32	g	906	0	999	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	h	1013	0	1147	0	0
34	i	830	0	916	0	0
35	j	705	0	737	0	0
36	k	569	0	637	0	0
37	l	447	0	480	0	0
38	m	429	0	465	0	0
39	n	239	0	289	0	0
40	o	851	0	920	0	0
41	p	708	0	758	0	0
42	r	994	0	1051	0	0
43	s	1507	0	1564	0	0
44	t	1160	0	1218	0	0
45	1	125	0	117	1	0
46	2	1616	0	824	5	0
47	3	1593	0	811	3	0
48	5	75972	0	38393	128	0
49	7	2558	0	1296	2	0
50	8	3208	0	1629	6	0
51	9	36249	0	18316	98	0
52	AA	1710	0	1708	10	0
53	BB	1729	0	1803	11	0
54	CC	1716	0	1806	10	0
55	DD	1768	0	1866	9	0
56	EE	2076	0	2177	9	0
57	FF	1471	0	1522	11	0
58	GG	1923	0	2089	9	0
59	HH	1488	0	1582	4	0
60	II	1686	0	1772	6	0
61	JJ	1525	0	1640	12	0
62	KK	810	0	836	8	0
63	LL	1175	0	1249	4	0
64	MM	908	0	939	5	0
65	NN	1202	0	1289	2	0
66	OO	1016	0	1039	5	0
67	PP	997	0	1045	5	0
68	QQ	1128	0	1195	8	0
69	RR	1068	0	1121	5	0
70	SS	1190	0	1249	3	0
71	TT	1097	0	1132	4	0
72	UU	795	0	862	3	0
73	VV	636	0	637	5	0
74	WW	1034	0	1080	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
75	XX	1098	0	1167	4	0
76	YY	1011	0	1083	1	0
77	ZZ	598	0	656	6	0
78	aa	814	0	864	0	0
79	bb	651	0	672	0	0
80	cc	488	0	514	0	0
81	dd	459	0	449	0	0
82	ee	443	0	492	0	0
83	ff	555	0	566	0	0
84	gg	2436	0	2393	0	0
85	hh	317	0	161	0	0
86	ii	3307	0	3346	0	0
87	jj	3368	0	3422	0	0
88	5	185	0	0	0	0
88	7	5	0	0	0	0
88	8	8	0	0	0	0
88	9	71	0	0	0	0
88	A	1	0	0	0	0
88	B	1	0	0	0	0
88	I	1	0	0	0	0
88	P	3	0	0	0	0
88	Q	1	0	0	0	0
88	V	1	0	0	0	0
88	a	1	0	0	0	0
88	g	1	0	0	0	0
88	hh	1	0	0	0	0
88	j	1	0	0	0	0
88	jj	1	0	0	0	0
89	aa	1	0	0	0	0
89	dd	1	0	0	0	0
89	ff	1	0	0	0	0
89	g	1	0	0	0	0
89	j	1	0	0	0	0
89	m	1	0	0	0	0
89	o	1	0	0	0	0
89	p	1	0	0	0	0
90	jj	32	0	14	0	0
All	All	222683	0	167519	523	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 523 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)
48:5:2367:A:N1	48:5:2788:U:O4	1.66	1.25
51:9:1137:U:O4	51:9:1148:A:N1	1.68	1.23
51:9:1137:U:C4	51:9:1148:A:N1	2.11	1.18
51:9:1137:U:O4	51:9:1148:A:C2	2.17	0.98
51:9:1137:U:O4	51:9:1148:A:C6	2.32	0.82

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	246/257 (96%)	218 (89%)	26 (11%)	2 (1%)	24	70
2	B	392/403 (97%)	360 (92%)	29 (7%)	3 (1%)	24	70
3	C	360/425 (85%)	337 (94%)	21 (6%)	2 (1%)	30	74
4	D	291/297 (98%)	275 (94%)	15 (5%)	1 (0%)	46	83
5	E	208/291 (72%)	191 (92%)	17 (8%)	0	100	100
6	F	223/247 (90%)	212 (95%)	10 (4%)	1 (0%)	39	80
7	G	229/319 (72%)	216 (94%)	11 (5%)	2 (1%)	21	68
8	H	188/192 (98%)	178 (95%)	10 (5%)	0	100	100
9	I	201/214 (94%)	185 (92%)	16 (8%)	0	100	100
10	J	168/178 (94%)	161 (96%)	7 (4%)	0	100	100
11	L	208/211 (99%)	196 (94%)	11 (5%)	1 (0%)	34	77
12	M	136/218 (62%)	123 (90%)	12 (9%)	1 (1%)	26	72
13	N	201/204 (98%)	187 (93%)	13 (6%)	1 (0%)	34	77
14	O	197/203 (97%)	188 (95%)	8 (4%)	1 (0%)	34	77
15	P	151/184 (82%)	142 (94%)	9 (6%)	0	100	100
16	Q	185/188 (98%)	173 (94%)	12 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	R	178/196 (91%)	173 (97%)	5 (3%)	0	100	100
18	S	174/176 (99%)	159 (91%)	14 (8%)	1 (1%)	30	74
19	T	157/160 (98%)	147 (94%)	10 (6%)	0	100	100
20	U	97/128 (76%)	87 (90%)	10 (10%)	0	100	100
21	V	129/140 (92%)	120 (93%)	9 (7%)	0	100	100
22	W	102/157 (65%)	97 (95%)	4 (4%)	1 (1%)	19	66
23	X	116/156 (74%)	107 (92%)	9 (8%)	0	100	100
24	Y	132/145 (91%)	122 (92%)	10 (8%)	0	100	100
25	Z	133/136 (98%)	126 (95%)	5 (4%)	2 (2%)	13	59
26	a	145/148 (98%)	131 (90%)	14 (10%)	0	100	100
27	b	100/245 (41%)	94 (94%)	5 (5%)	1 (1%)	19	66
28	c	96/115 (84%)	93 (97%)	3 (3%)	0	100	100
29	d	105/125 (84%)	89 (85%)	15 (14%)	1 (1%)	19	66
30	e	126/135 (93%)	120 (95%)	6 (5%)	0	100	100
31	f	107/110 (97%)	97 (91%)	8 (8%)	2 (2%)	10	55
32	g	112/117 (96%)	105 (94%)	7 (6%)	0	100	100
33	h	120/123 (98%)	118 (98%)	2 (2%)	0	100	100
34	i	100/105 (95%)	94 (94%)	5 (5%)	1 (1%)	19	66
35	j	84/97 (87%)	78 (93%)	6 (7%)	0	100	100
36	k	67/70 (96%)	65 (97%)	2 (3%)	0	100	100
37	l	48/51 (94%)	44 (92%)	4 (8%)	0	100	100
38	m	50/102 (49%)	47 (94%)	3 (6%)	0	100	100
39	n	23/25 (92%)	23 (100%)	0	0	100	100
40	o	102/106 (96%)	98 (96%)	4 (4%)	0	100	100
41	p	89/92 (97%)	83 (93%)	5 (6%)	1 (1%)	17	65
42	r	122/137 (89%)	112 (92%)	9 (7%)	1 (1%)	24	70
43	s	194/318 (61%)	176 (91%)	16 (8%)	2 (1%)	19	66
44	t	151/165 (92%)	135 (89%)	14 (9%)	2 (1%)	15	61
45	l	13/15 (87%)	10 (77%)	2 (15%)	1 (8%)	1	19
52	AA	215/295 (73%)	203 (94%)	11 (5%)	1 (0%)	34	77
53	BB	211/264 (80%)	198 (94%)	12 (6%)	1 (0%)	34	77

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	CC	219/293 (75%)	206 (94%)	13 (6%)	0	100	100
55	DD	226/243 (93%)	213 (94%)	12 (5%)	1 (0%)	39	80
56	EE	260/263 (99%)	246 (95%)	14 (5%)	0	100	100
57	FF	181/204 (89%)	170 (94%)	9 (5%)	2 (1%)	17	65
58	GG	235/249 (94%)	224 (95%)	11 (5%)	0	100	100
59	HH	181/194 (93%)	171 (94%)	10 (6%)	0	100	100
60	II	204/208 (98%)	192 (94%)	11 (5%)	1 (0%)	34	77
61	JJ	183/194 (94%)	177 (97%)	6 (3%)	0	100	100
62	KK	94/165 (57%)	89 (95%)	4 (4%)	1 (1%)	17	65
63	LL	139/158 (88%)	130 (94%)	9 (6%)	0	100	100
64	MM	115/132 (87%)	103 (90%)	12 (10%)	0	100	100
65	NN	147/151 (97%)	142 (97%)	4 (3%)	1 (1%)	26	72
66	OO	134/168 (80%)	123 (92%)	9 (7%)	2 (2%)	13	59
67	PP	118/145 (81%)	105 (89%)	12 (10%)	1 (1%)	24	70
68	QQ	140/146 (96%)	132 (94%)	7 (5%)	1 (1%)	26	72
69	RR	130/135 (96%)	120 (92%)	10 (8%)	0	100	100
70	SS	142/152 (93%)	135 (95%)	7 (5%)	0	100	100
71	TT	139/145 (96%)	130 (94%)	8 (6%)	1 (1%)	26	72
72	UU	98/119 (82%)	91 (93%)	7 (7%)	0	100	100
73	VV	81/83 (98%)	79 (98%)	2 (2%)	0	100	100
74	WW	127/130 (98%)	120 (94%)	5 (4%)	2 (2%)	12	58
75	XX	139/143 (97%)	128 (92%)	8 (6%)	3 (2%)	8	52
76	YY	122/130 (94%)	115 (94%)	7 (6%)	0	100	100
77	ZZ	73/125 (58%)	70 (96%)	3 (4%)	0	100	100
78	aa	99/115 (86%)	93 (94%)	4 (4%)	2 (2%)	9	54
79	bb	81/84 (96%)	75 (93%)	6 (7%)	0	100	100
80	cc	60/69 (87%)	58 (97%)	2 (3%)	0	100	100
81	dd	53/56 (95%)	48 (91%)	5 (9%)	0	100	100
82	ee	53/133 (40%)	51 (96%)	2 (4%)	0	100	100
83	ff	66/156 (42%)	59 (89%)	7 (11%)	0	100	100
84	gg	311/317 (98%)	285 (92%)	24 (8%)	2 (1%)	30	74

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
86	ii	417/459 (91%)	387 (93%)	24 (6%)	6 (1%)	14	60
87	jj	426/637 (67%)	371 (87%)	50 (12%)	5 (1%)	16	63
All	All	12375/14486 (85%)	11531 (93%)	780 (6%)	64 (0%)	38	77

5 of 64 Ramachandran outliers are listed below:

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

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	190/199 (96%)	179 (94%)	11 (6%)	25	67
2	B	342/348 (98%)	325 (95%)	17 (5%)	30	71
3	C	302/347 (87%)	285 (94%)	17 (6%)	26	68
4	D	247/250 (99%)	235 (95%)	12 (5%)	31	71
5	E	190/251 (76%)	177 (93%)	13 (7%)	20	62
6	F	196/215 (91%)	184 (94%)	12 (6%)	23	66
7	G	200/272 (74%)	189 (94%)	11 (6%)	27	69
8	H	169/171 (99%)	157 (93%)	12 (7%)	18	60
9	I	175/181 (97%)	166 (95%)	9 (5%)	29	71
10	J	143/149 (96%)	136 (95%)	7 (5%)	31	71
11	L	175/176 (99%)	167 (95%)	8 (5%)	33	73
12	M	117/161 (73%)	108 (92%)	9 (8%)	16	57
13	N	171/172 (99%)	163 (95%)	8 (5%)	32	73
14	O	171/173 (99%)	160 (94%)	11 (6%)	22	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	P	134/163 (82%)	126 (94%)	8 (6%)	24	66
16	Q	164/165 (99%)	156 (95%)	8 (5%)	31	71
17	R	159/175 (91%)	147 (92%)	12 (8%)	17	58
18	S	157/157 (100%)	146 (93%)	11 (7%)	19	61
19	T	139/140 (99%)	129 (93%)	10 (7%)	18	59
20	U	89/114 (78%)	86 (97%)	3 (3%)	44	79
21	V	101/107 (94%)	93 (92%)	8 (8%)	15	55
22	W	86/126 (68%)	85 (99%)	1 (1%)	78	91
23	X	106/134 (79%)	100 (94%)	6 (6%)	25	68
24	Y	124/135 (92%)	117 (94%)	7 (6%)	26	68
25	Z	117/118 (99%)	114 (97%)	3 (3%)	54	83
26	a	119/120 (99%)	116 (98%)	3 (2%)	55	83
27	b	84/184 (46%)	81 (96%)	3 (4%)	42	78
28	c	84/98 (86%)	81 (96%)	3 (4%)	42	78
29	d	98/110 (89%)	91 (93%)	7 (7%)	18	60
30	e	114/121 (94%)	105 (92%)	9 (8%)	15	55
31	f	88/89 (99%)	82 (93%)	6 (7%)	20	62
32	g	98/100 (98%)	93 (95%)	5 (5%)	29	71
33	h	109/110 (99%)	103 (94%)	6 (6%)	27	69
34	i	86/89 (97%)	85 (99%)	1 (1%)	78	91
35	j	73/80 (91%)	68 (93%)	5 (7%)	20	62
36	k	64/65 (98%)	62 (97%)	2 (3%)	47	81
37	l	47/48 (98%)	46 (98%)	1 (2%)	61	86
38	m	48/90 (53%)	45 (94%)	3 (6%)	22	65
39	n	24/24 (100%)	22 (92%)	2 (8%)	14	53
40	o	92/94 (98%)	86 (94%)	6 (6%)	21	64
41	p	74/75 (99%)	73 (99%)	1 (1%)	74	90
42	r	108/121 (89%)	102 (94%)	6 (6%)	26	68
43	s	164/258 (64%)	158 (96%)	6 (4%)	41	77
44	t	126/137 (92%)	121 (96%)	5 (4%)	38	76
45	l	13/13 (100%)	13 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	AA	180/245 (74%)	168 (93%)	12 (7%)	20	63
53	BB	194/231 (84%)	176 (91%)	18 (9%)	11	49
54	CC	187/225 (83%)	175 (94%)	12 (6%)	22	64
55	DD	190/202 (94%)	174 (92%)	16 (8%)	14	53
56	EE	224/225 (100%)	202 (90%)	22 (10%)	10	45
57	FF	158/170 (93%)	144 (91%)	14 (9%)	12	51
58	GG	207/218 (95%)	192 (93%)	15 (7%)	18	59
59	HH	165/174 (95%)	152 (92%)	13 (8%)	15	55
60	II	178/180 (99%)	163 (92%)	15 (8%)	14	53
61	JJ	161/168 (96%)	146 (91%)	15 (9%)	11	49
62	KK	87/136 (64%)	75 (86%)	12 (14%)	4	29
63	LL	130/142 (92%)	120 (92%)	10 (8%)	16	57
64	MM	99/108 (92%)	85 (86%)	14 (14%)	4	28
65	NN	130/131 (99%)	118 (91%)	12 (9%)	11	49
66	OO	106/130 (82%)	91 (86%)	15 (14%)	4	28
67	PP	109/130 (84%)	98 (90%)	11 (10%)	9	44
68	QQ	117/121 (97%)	110 (94%)	7 (6%)	24	66
69	RR	119/121 (98%)	110 (92%)	9 (8%)	16	57
70	SS	125/132 (95%)	111 (89%)	14 (11%)	7	39
71	TT	111/115 (96%)	103 (93%)	8 (7%)	18	59
72	UU	92/107 (86%)	86 (94%)	6 (6%)	21	64
73	VV	67/67 (100%)	63 (94%)	4 (6%)	24	66
74	WW	112/113 (99%)	103 (92%)	9 (8%)	15	55
75	XX	113/115 (98%)	107 (95%)	6 (5%)	28	70
76	YY	107/112 (96%)	91 (85%)	16 (15%)	3	26
77	ZZ	66/103 (64%)	62 (94%)	4 (6%)	23	66
78	aa	88/98 (90%)	81 (92%)	7 (8%)	15	55
79	bb	75/76 (99%)	68 (91%)	7 (9%)	11	49
80	cc	55/62 (89%)	50 (91%)	5 (9%)	12	50
81	dd	48/49 (98%)	47 (98%)	1 (2%)	61	86
82	ee	46/106 (43%)	42 (91%)	4 (9%)	13	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
83	ff	61/140 (44%)	56 (92%)	5 (8%)	14	54
84	gg	272/275 (99%)	263 (97%)	9 (3%)	45	80
86	ii	361/394 (92%)	339 (94%)	22 (6%)	23	66
87	jj	372/520 (72%)	354 (95%)	18 (5%)	31	72
All	All	10789/12266 (88%)	10088 (94%)	701 (6%)	26	64

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

Mol	Chain	Res	Type
52	AA	56	GLU
56	EE	240	ARG
83	ff	83	LYS
53	BB	38	MET
54	CC	254	ASP

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

Mol	Chain	Res	Type
54	CC	235	ASN
57	FF	118	ASN
87	jj	499	ASN
56	EE	142	HIS
58	GG	13	GLN

### 5.3.3 RNA ⓘ

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

5 of 1387 RNA backbone outliers are listed below:

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

5 of 250 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
48	5	2474	G
48	5	4124	G
51	9	1476	A
48	5	2502	A
48	5	3673	C

## 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 291 ligands modelled in this entry, 290 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
90	GCP	jj	700	88	29,34,34	2.66	9 (31%)	31,54,54	1.17	2 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means

no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
90	GCP	jj	700	88	-	0/18/38/38	0/3/3/3

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
90	jj	700	GCP	C4-N9	-10.50	1.33	1.47
90	jj	700	GCP	C8-N9	-3.75	1.35	1.47
90	jj	700	GCP	PG-O3G	-2.66	1.48	1.54
90	jj	700	GCP	C5-C6	-2.15	1.49	1.53
90	jj	700	GCP	C2-N1	-2.03	1.35	1.44

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
90	jj	700	GCP	C4-C5-N7	2.57	106.68	102.67
90	jj	700	GCP	C8-N9-C4	3.63	108.92	104.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

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

The worst 5 of 40 chain breaks are listed below:



Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	2113:G	O3'	2258:C	P	41.06
1	5	1252:C	O3'	1271:G	P	35.64
1	5	1219:G	O3'	1233:G	P	22.79
1	5	3948:C	O3'	4065:G	P	19.75
1	5	1406(C):G	O3'	1411:C	P	18.65