



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

Mar 2, 2017 – 12:19 pm GMT

PDB ID : 3JAI  
EMDB ID: : EMD-3040  
Title : Structure of a mammalian ribosomal termination complex with ABCE1, eRF1(AAQ), and the UGA stop codon  
Authors : Brown, A.; Shao, S.; Murray, J.; Hegde, R.S.; Ramakrishnan, V.  
Deposited on : 2015-06-10  
Resolution : 3.65 Å(reported)  
Based on PDB ID : 1DT9, 4V51, 3J7P, 3J92, 3BK7

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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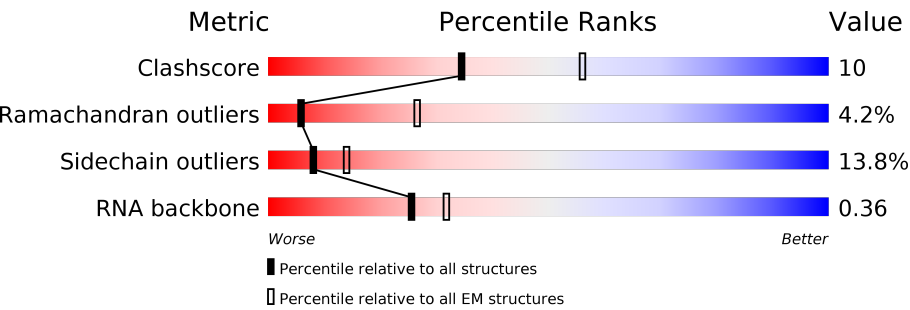
MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc29047

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 3.65 Å.

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

















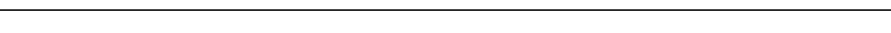




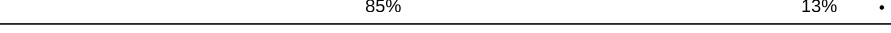





Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

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	244	<div><div>66%</div><div>29%</div><div>5%</div><div>.</div></div>
2	B	394	<div><div>68%</div><div>26%</div><div>5%</div><div>.</div></div>
3	C	361	<div><div>67%</div><div>27%</div><div>5%</div><div>.</div></div>
4	D	292	<div><div>78%</div><div>21%</div><div>.</div></div>
5	E	248	<div><div>57%</div><div>28%</div><div>9%</div><div>5%</div></div>
6	F	225	<div><div>66%</div><div>29%</div><div>5%</div></div>
7	G	241	<div><div>69%</div><div>28%</div><div>.</div></div>
8	H	190	<div><div>72%</div><div>26%</div><div>..</div></div>


























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Mol	Chain	Length	Quality of chain
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	
29	d	107	
30	e	128	
31	f	109	
32	g	114	
33	h	122	


























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Mol	Chain	Length	Quality of chain
34	i	102	 84% 14% •
35	j	86	 78% 20% •
36	k	69	 87% 13%
37	l	50	 82% 18%
38	m	52	 77% 21% •
39	n	23	 87% 13%
40	o	104	 84% 15% •
41	p	91	 82% 18%
42	r	125	 82% 16% ••
43	s	198	 89% 10% •
44	t	163	 79% 20% •
45	1	15	 73% 27%
46	2	76	 46% 45% 8% •
47	3	75	 39% 43% 15% •
48	5	3662	 40% 44% 15% •
49	7	120	 62% 31% 8%
50	8	156	 47% 37% 15%
51	9	1719	 39% 45% 15% •
52	AA	208	 63% 30% 6%
53	BB	213	 69% 27% 5%
54	CC	218	 62% 34% ••
55	DD	227	 70% 25% 6%
56	EE	262	 63% 29% 7%
57	FF	191	 68% 28% 5%
58	GG	237	 68% 27% 5%

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Mol	Chain	Length	Quality of chain
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	
79	bb	83	
80	cc	61	
81	dd	53	
82	ee	57	
83	ff	68	

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Mol	Chain	Length	Quality of chain
84	gg	313	<div><div></div><div>90%10%</div></div>
85	hh	12	<div><div></div><div>50%50%</div></div>
86	ii	416	<div><div></div><div>88%12%</div></div>
87	jj	594	<div><div></div><div>89%7% . .</div></div>

## 2 Entry composition

There are 91 unique types of molecules in this entry. The entry contains 226453 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	361	Total	C	N	O	S	0	0
			2875	1808	576	477	14		

There are 2 discrepancies between the modelled and reference sequences:

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

- 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 eL18.

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

- Molecule 17 is a protein called eL19.

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

- Molecule 18 is a protein called eL20.

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

- Molecule 19 is a protein called eL21.

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

- Molecule 20 is a protein called eL22.

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

- Molecule 21 is a protein called uL14.

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

- Molecule 22 is a protein called eL24.

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

- Molecule 23 is a protein called uL23.

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

- Molecule 24 is a protein called uL24.

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

- Molecule 25 is a protein called eL27.

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

- Molecule 26 is a protein called uL15.

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

- Molecule 27 is a protein called eL29.

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

- Molecule 28 is a protein called eL30.

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

- Molecule 29 is a protein called eL31.

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

- Molecule 30 is a protein called eL32.

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

- Molecule 31 is a protein called eL33.

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

- Molecule 32 is a protein called eL34.

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

- Molecule 33 is a protein called uL29.

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

- Molecule 34 is a protein called eL36.

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

- Molecule 35 is a protein called eL37.

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

- Molecule 36 is a protein called eL38.

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

- Molecule 37 is a protein called eL39.

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

- Molecule 38 is a protein called eL40.

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

- Molecule 39 is a protein called eL41.

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

- Molecule 40 is a protein called eL42.

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

- Molecule 41 is a protein called eL43.

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

- Molecule 42 is a protein called eL28.

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

- Molecule 43 is a protein called uL10.

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

- Molecule 44 is a protein called uL11.

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

- Molecule 45 is a protein called peptide.

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 52 is a protein called uS2.

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

- Molecule 53 is a protein called eS1.

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

- Molecule 54 is a protein called uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	CC	218	Total	C	N	O	S	0	0
			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	577	Total	C	N	O	S	0	0
			4551	2910	780	830	31		

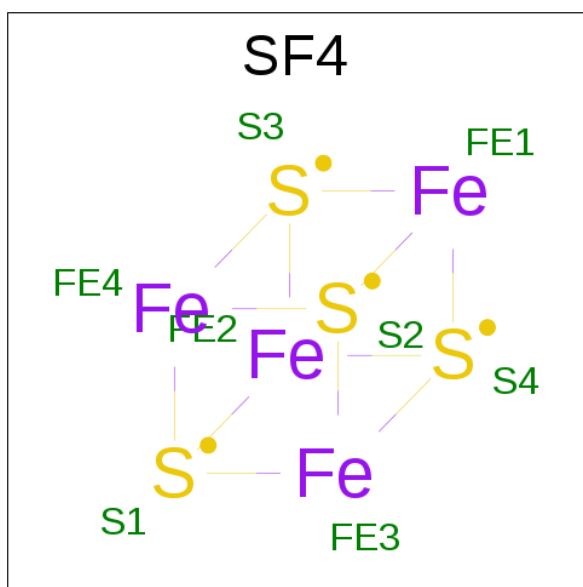
- Molecule 88 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
88	P	1	Total 1	Mg 1	0
88	g	1	Total 1	Mg 1	0
88	I	1	Total 1	Mg 1	0
88	C	1	Total 1	Mg 1	0
88	V	1	Total 1	Mg 1	0
88	7	5	Total 5	Mg 5	0
88	5	147	Total 147	Mg 147	0
88	8	2	Total 2	Mg 2	0
88	9	35	Total 35	Mg 35	0
88	hh	1	Total 1	Mg 1	0

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

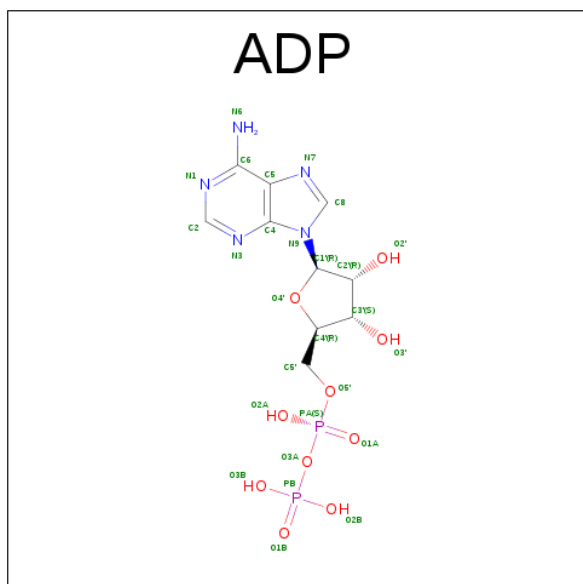
Mol	Chain	Residues	Atoms		AltConf
89	p	1	Total 1	Zn 1	0
89	g	1	Total 1	Zn 1	0
89	j	1	Total 1	Zn 1	0
89	dd	1	Total 1	Zn 1	0
89	ff	1	Total 1	Zn 1	0
89	aa	1	Total 1	Zn 1	0
89	o	1	Total 1	Zn 1	0
89	m	1	Total 1	Zn 1	0

- Molecule 90 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



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

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



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

*Continued on next page...*

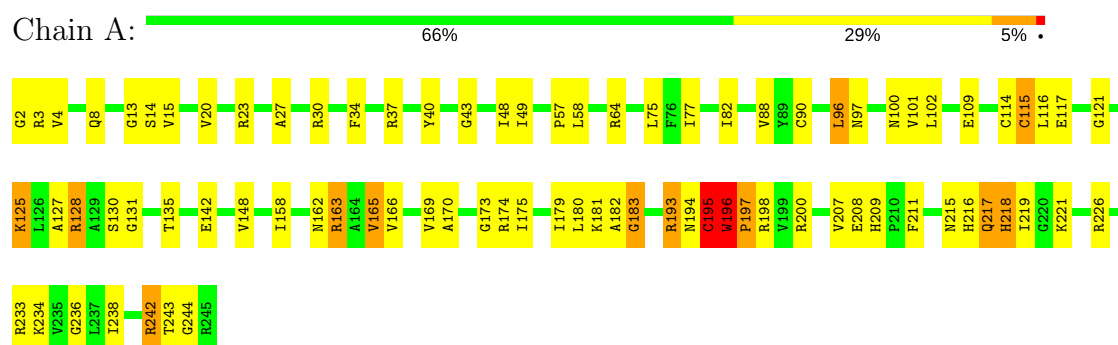
*Continued from previous page...*

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

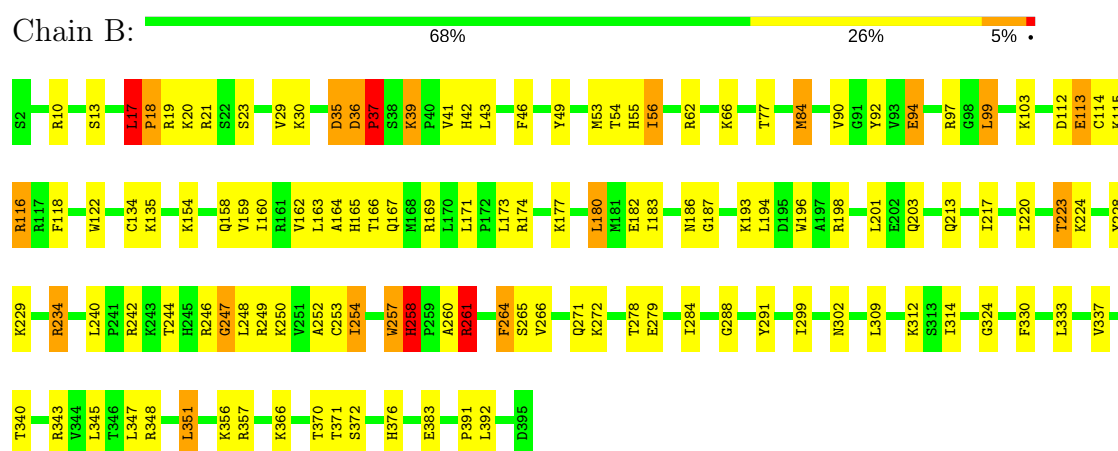
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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

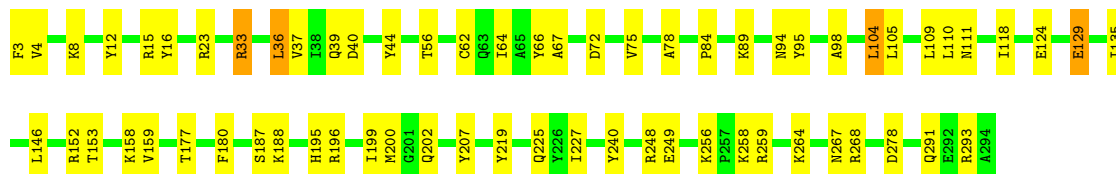






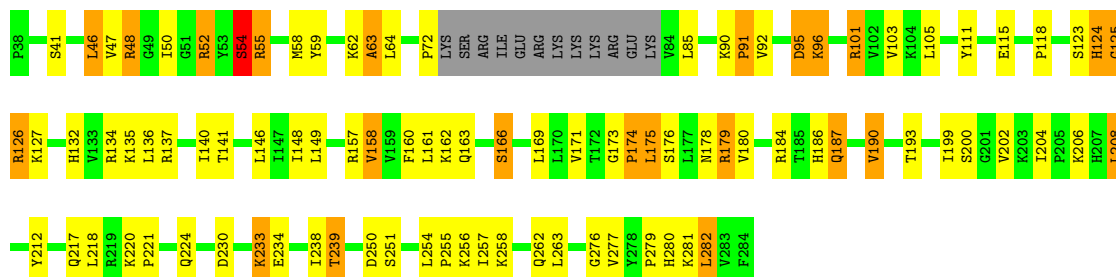
• Molecule 4: uL18

Chain D: 78% 21%



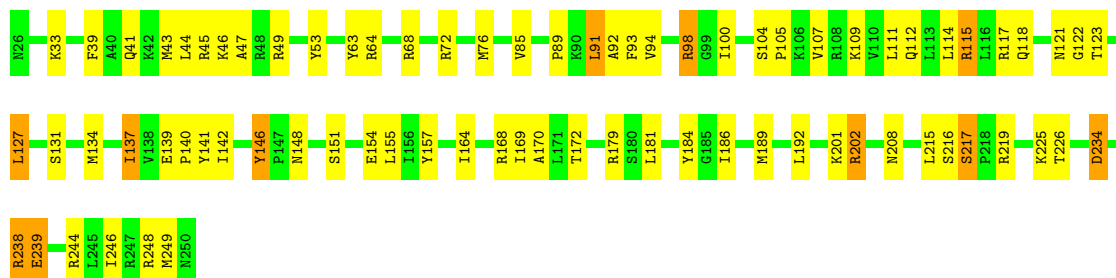
• Molecule 5: eL6

Chain E: 57% 28% 9% 5%



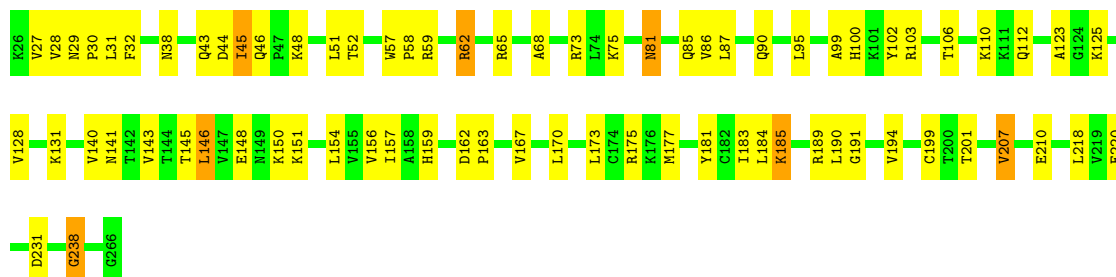
• Molecule 6: uL30

Chain F: 66% 29% 5%



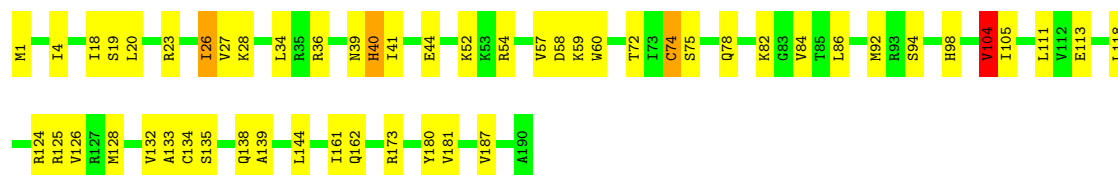
• Molecule 7: eL8

Chain G: 69% 28%



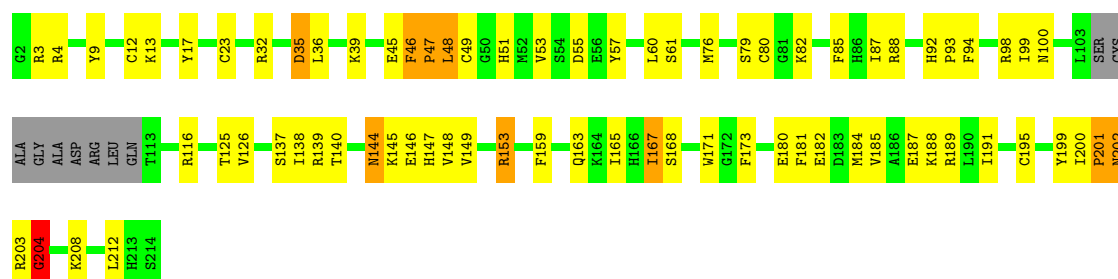
- Molecule 8: uL6

Chain H: 



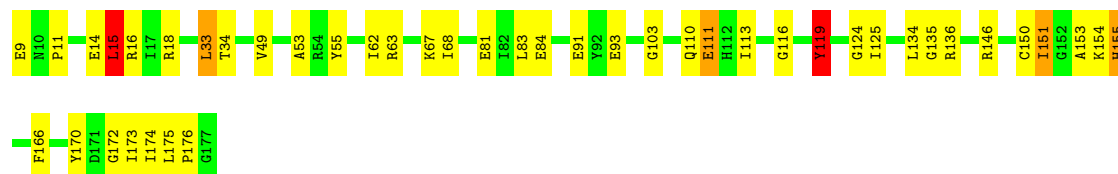
- Molecule 9: uL16

Chain I: 



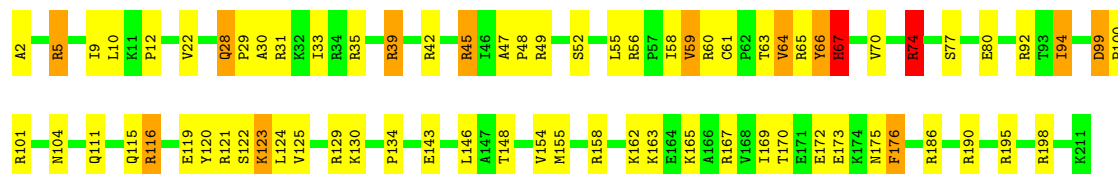
- Molecule 10: uL5

Chain J: 



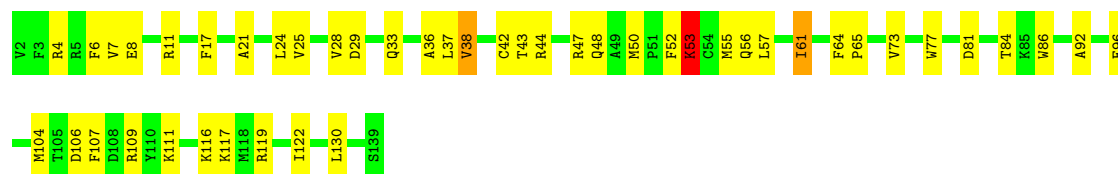
- Molecule 11: eL13

Chain L: 

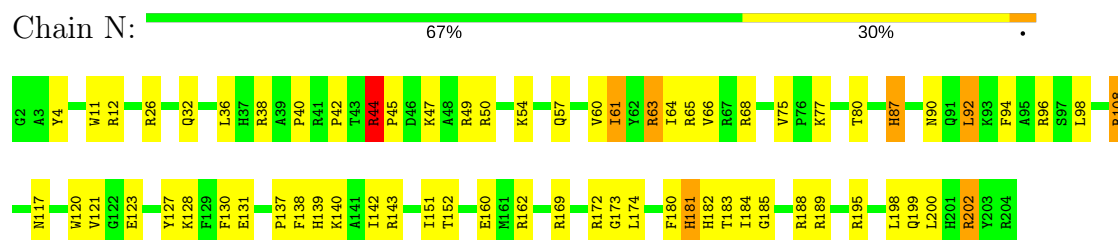


- Molecule 12: eL14

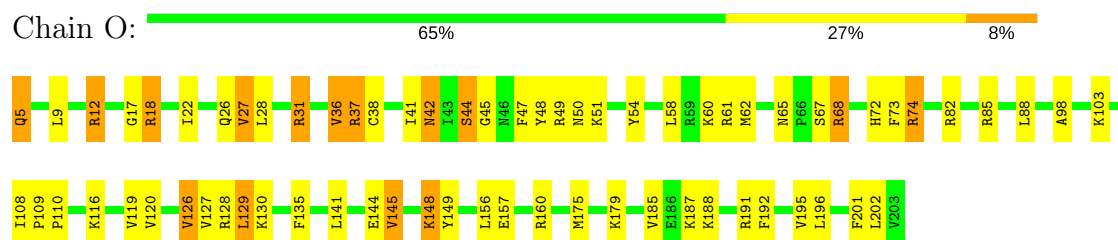
Chain M: 



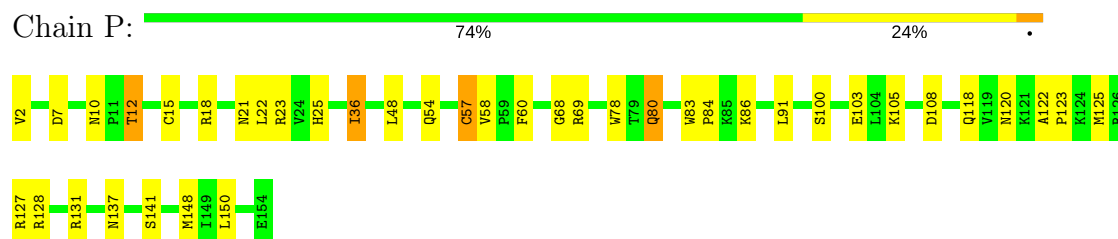
- Molecule 13: eL15



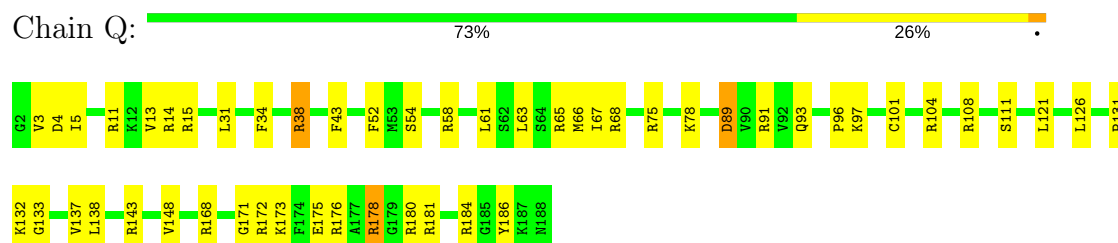
- Molecule 14: uL13



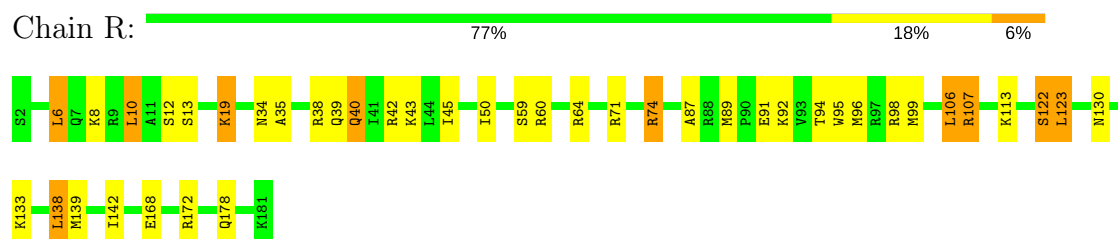
- Molecule 15: uL22



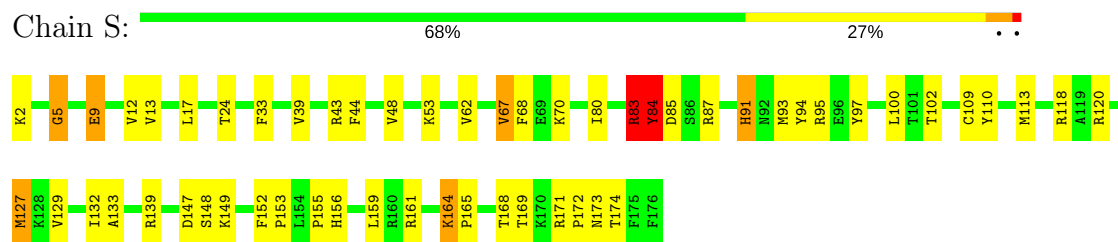
- Molecule 16: eL18



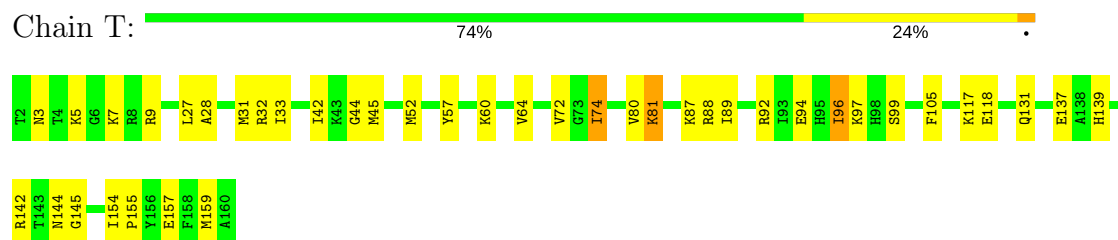
- Molecule 17: eL19



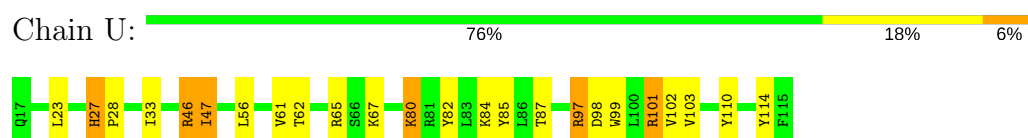
- Molecule 18: eL20



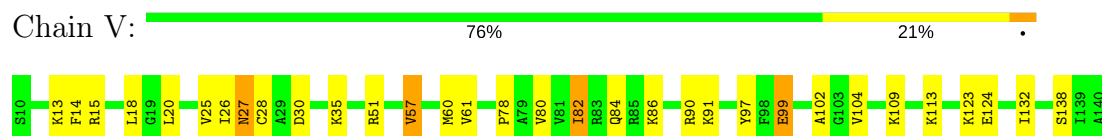
• Molecule 19: eL21



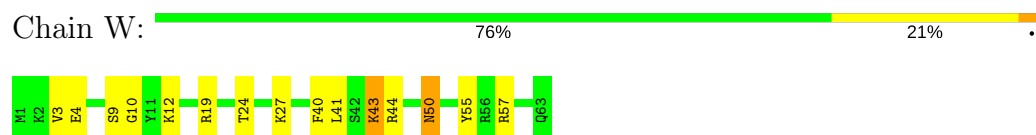
• Molecule 20: eL22



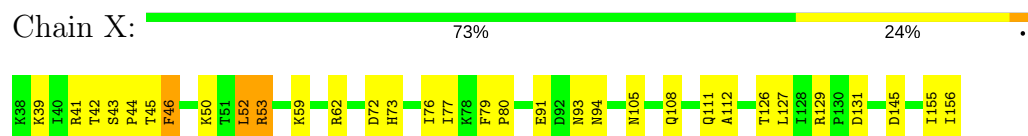
• Molecule 21: uL14



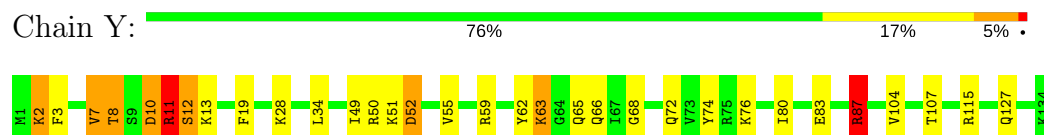
• Molecule 22: eL24



• Molecule 23: uL23

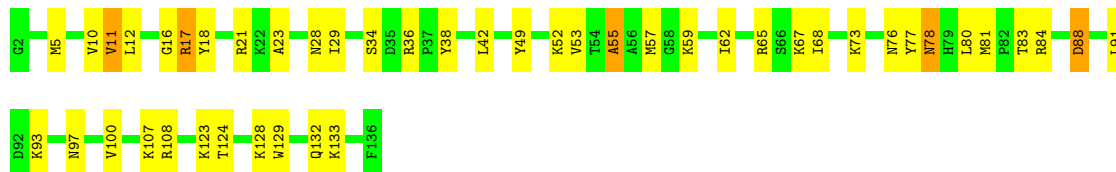


• Molecule 24: uL24




- Molecule 25: eL27

Chain Z:  66% 30% .




- Molecule 26: uL15

Chain a:  88% 9% .




- Molecule 27: eL29

Chain b:  85% 13% .




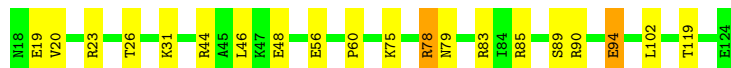
- Molecule 28: eL30

Chain c:  85% 15% .




- Molecule 29: eL31

Chain d:  81% 17% .




- Molecule 30: eL32

Chain e:  82% 17% .




- Molecule 31: eL33

Chain f:  82% 17% .




- Molecule 32: eL34

Chain g:  82% 18%




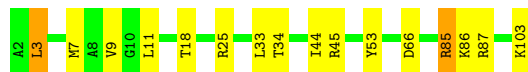
• Molecule 33: uL29

Chain h:  85% 14%



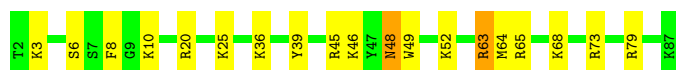
• Molecule 34: eL36

Chain i:  84% 14%




• Molecule 35: eL37

Chain j:  78% 20%




• Molecule 36: eL38

Chain k:  87% 13%




• Molecule 37: eL39

Chain l:  82% 18%




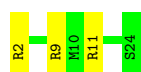
• Molecule 38: eL40

Chain m:  77% 21%



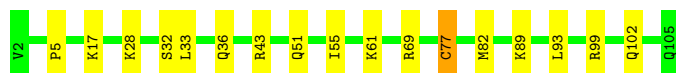
• Molecule 39: eL41

Chain n:  87% 13%



• Molecule 40: eL42

Chain o: 84% 15%



• Molecule 41: eL43

Chain p: 82% 18%



• Molecule 42: eL28

Chain r: 82% 16%



• Molecule 43: uL10

Chain s: 89% 10%



• Molecule 44: uL11

Chain t: 79% 20%



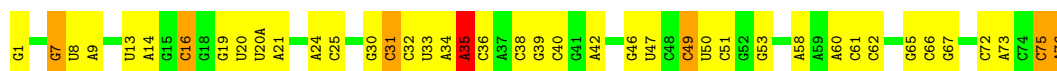
• Molecule 45: peptide

Chain 1: 73% 27%



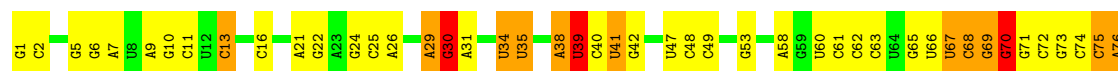
• Molecule 46: tRNA(Val)

Chain 2: 46% 45% 8%



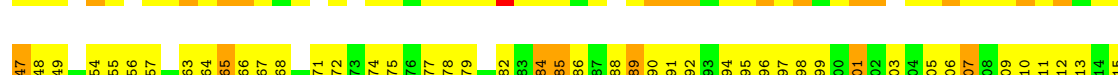
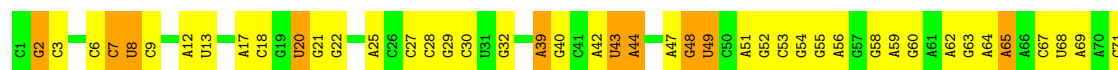
• Molecule 47: tRNA(Lys)

Chain 3: 



• Molecule 48: 28S ribosomal RNA

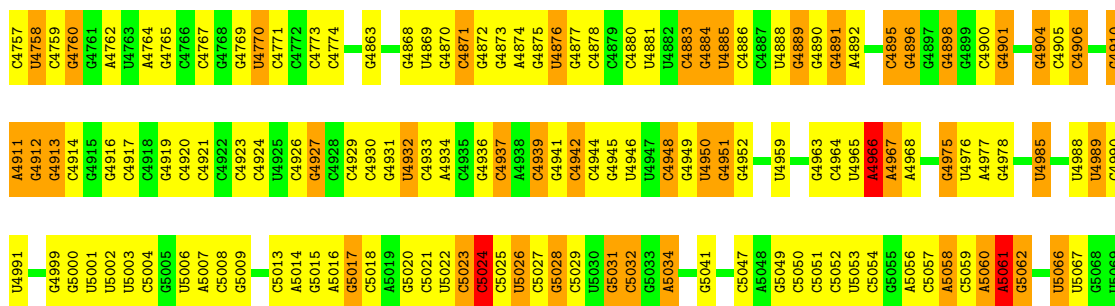
Chain 5: 



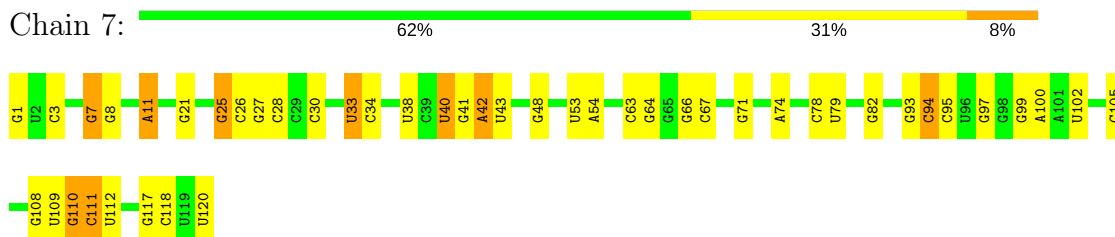


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G2632	G2557	U2485	G2402	G2311	G2126	G2064	U1992	C1921	G1761	G1670	U1591	U1512	G1421	G1360
U2633	G2558	G2486	A2403	G2312	G2127	G2065	C1993	G1922	G1764	U1671	U1596	U1513	G1422	G1361
G2638	C2560	C2488	U2408	A2313	G2128	G2066	C1994	A1923	G1765	U1672	U1597	U1514	U1423	G1362
U2639	G2561	C2489	U2409	G2314	G2129	G2067	G1995	C1924	A1767	G1676	U1598	A1515	G1424	C1363
G2640	G2562	U2490	G2410	G2315	G2130	G2068	G1996	G1925	C1768	U1677	C1598	G1516	G1425	U1364
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	G2566	G2492	G2416		G2244	U2070	A1998	U1927			A1601	U1518		G1366
G2645	C2567	G2493	A2417	G2322	G2245	A2071	A1999	C1928	U1771	G1678	U1602	C1519	C1430	G1367
C2646	G2568	U2494	A2418	G2323	G2246	C2072	G2000	A1929	C1772	U1679	C1603	C1520	C1431	A1368
		U2495		G2324	G2247	C2073	G2001	U1930		G1681				C1369
G2649	C2571	G2496	G2421	G2325	G2248	G2076	A2002	C1931	A1776	U1682	G1612	A1523	G1435	G1370
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	G2574		A2423		G2250	C2078	G2005	A1934			C1615	U1528	C1439	A1373
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C2683	C2589	G2517	G2441	G2345	G2265	A2093	G2024	A1958	U1800	G1719	A1632	C1548		A1387
C2684	G2594	G2518	G2442	G2346	G2266	G2094	A2025	U1959	A1801	G1720	G1633	G1549	G1464	U1388
C2685	U2519	C2519	G2443	A2347	U2267	A2095	A2026	A1960	A1802	G1721	G1634	G1549	G1465	G1390
G2686	G2595	G2520	C2446	G2348	A2268	G2096	U2027	G1961	G1803	C1722	A1634	G1550	G1466	A1391
U2687	G2596	G2521	U2447	U2350	C2269	U2097	C2028	A1962	G1804	G1723	C1635	C1551	C1467	A1392
C2689	G2597	G2522		G2351	G2270		A2029	A1964	A1805	U1725	A1637	A1554	C1468	G1393
			G2450			A2100	U2032	G1965		U1726	A1638		C1469	G1394
	G2601	U2524	A2451	A2360	G2273	G2101	A2033	G1966	G1811		U1639	C1557	G1474	U1395
	C2602				G2274	G2102	A2034	C1967	C1812	C1732	C1640		G1475	G1396
G2693	C2603	A2527		G2364	G2275	G2103	C2035	G1968	G1733	A1564	C1477		C1476	A1397
G2694	G2606	U2530	G2457	G2365	A2276	G2104	G2036	G1969	G1734	A1565	C1478		C1477	A1398
A2695	C2607	C2531	C2458	A2366	G2277	A2105	A2040	G1969	G1819	A1646	U1647		C1478	G1400
A2696	G2608	C2532	U2459	A2367	G2278	G2106	A2041	A1970	C1820	U1741			G1482	G1401
G2698	G2609	U2537	A2460	A2368	A2279	G2107	A2042	G1971	G1821	A1742				
C2699	G2610		G2461	U2369	G2280	G2108		G1972	U1822					
				A2370	U2281	G2109	G2045			A1743	A1653	G1571	C1483	G1404
G2703	A2611	U2538	U2467	A2371	A2282	C2110	G2046	G1975	G1823	U1744	G1654	U1572	C1484	C1405
G2704	C2612	C2539	U2468			G2111	A2047	G1976	G1825	G1745	C1655		C1485	G1406
	C2613		C2469	A2374		G2112	U2048		G1826		U1656	A1575	C1486	C1407
U2708	C2614	G2544	G2470		G2288	G2113	A1979	U1906	C1827	U1748	G1657	G1575	G1408	G1408
C2709	G2615	U2545	G2471	G2390	C2289	G2114	U1980	A1907	C1828	G1749	G1658	G1577	C1409	C1409
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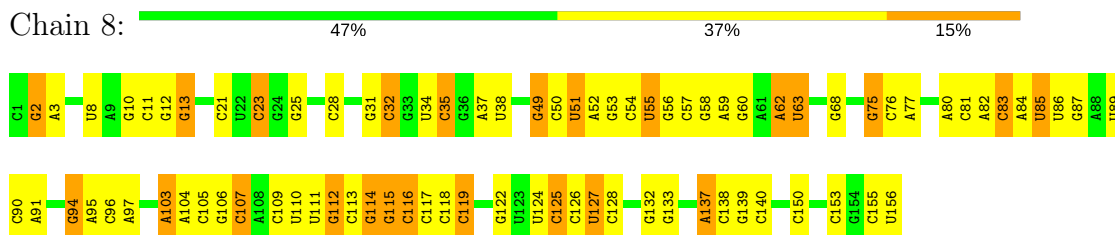
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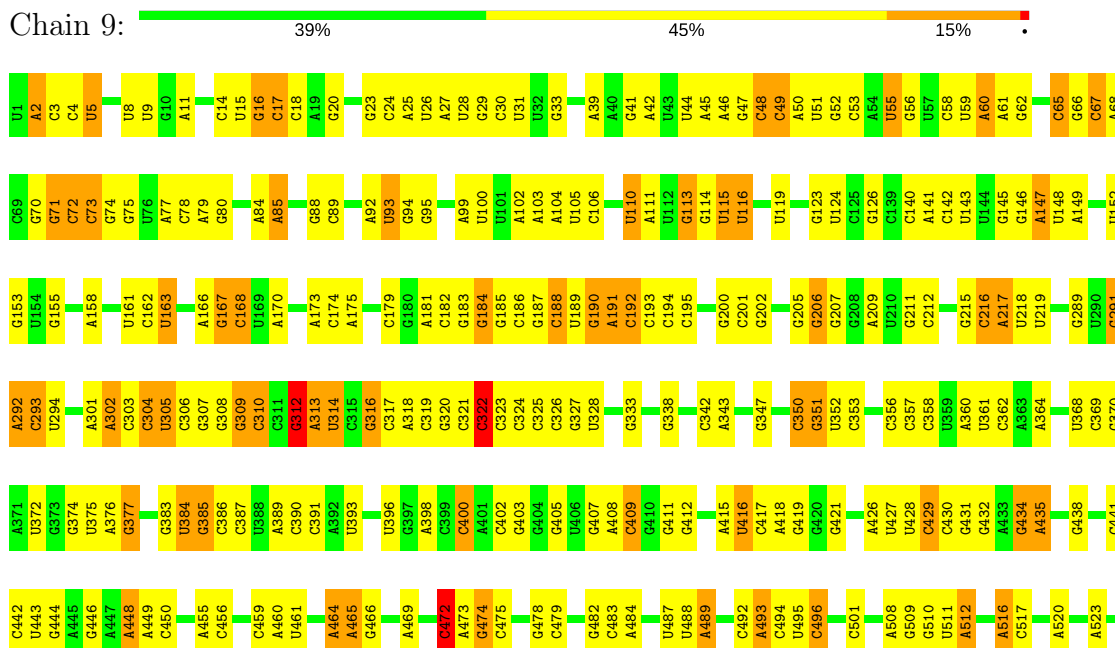
- Molecule 49: 5S ribosomal RNA



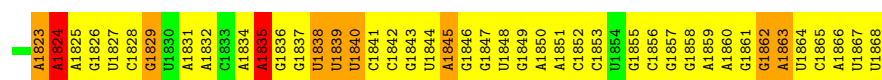
- Molecule 50: 5.8S ribosomal RNA



- Molecule 51: 18S ribosomal RNA

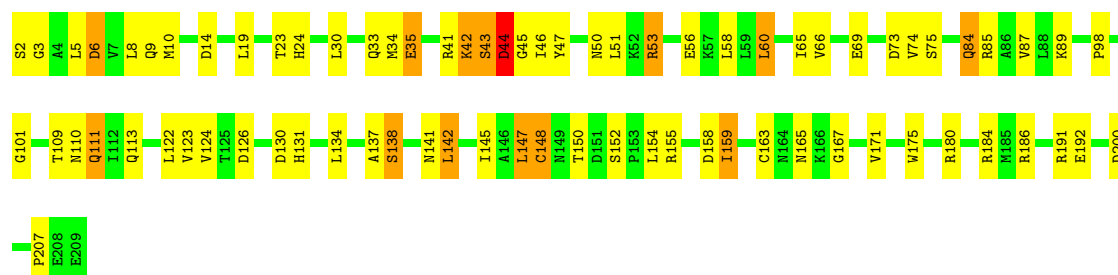


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U1729	U1649	G1573	A1508	C1437	U1372	U1296	G1229	A1149	A1083	A996	C911	G828	A672	A605	U530
U1730	A1650	C1575	U1509	A1438	C1373	U1297	C1230	A1150	A1084	A997	A913	C829	C674	G606	A531
A1731	G1654	U1575	U1510	A1439	C1374	U1298	C1231	G1151	C1085	G998	G915	G831	U914	U607	C532
G1732	C1655	U1578	C1511	U1441	A1376	U1300	G1232	U1152	G1089	G999	G916	G832	G677	C608	A533
A1735	U1651	U1579	U1512	U1442	U1377	A1301	C1234	U1154	C1090	C1000	A917	C833	U915	U609	G534
G1736	A1661	A1580	C1513	C1443	A1378	G1302	G1235	U1157	C1093	U1001	G918	C834	A679	G610	G535
G1737	U1662	U1515	G1514	U1444	C1380	C1303	C1236	G1157	A1093	U1002	A919	C835	G680	C614	C539
C1738	U1663	U1516	G1517	U1445	C1381	U1304	C1237	C1163	G1096	G1005	A920	C836	U681	C615	C540
C1739	A1664	G1518	U1519	G1447	C1382	U1307	A1240	G1164	G1097	C1006	A921	G837	U682	A616	U542
A1745	G1665	U1520	U1521	G1448	G1385	C1308	A1241	G1165	C1098	C1007	G921	G838	G683	G617	U543
U1746	C1666	G1522	C1521	G1449	U1387	U1243	U1242	G1166	G1099	A1011	G925	C840	G684	C618	G544
C1747	U1667	A1588	U1522	A1452	A1386	C1310	U1243	G1167	G1101	A1012	G929	G841	U688	A619	A545
G1749	U1668	U1589	C1523	C1453	C1387	G1312	C1247	G1168	C1099	U1013	C930	G842	U689	G621	A546
C1750	G1670	G1594	G1524	U1454	C1391	A1313	U1248	G1175	G1102	U1016	G933	U844	G696	G622	C548
C1751	A1671	U1595	C1525	A1455	U1392	U1314	C1249	A1181	G1103	U1017	G934	U845	G697	G623	C549
U1672	U1672	U1596	G1526	A1456	G1393	U1315	A1250	A1182	G1104	U1018	G935	U846	G698	G624	C550
G1753	U1673	C1597	U1527	G1459	G1394	C1316	A1251	A1183	G1105	U1019	G936	U847	G699	G625	U551
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C1772	G1683	G1612	C1537	C1469	A1405	G1331	C1266	G1198	C1118	A1034	G953	U857	C745	U637	C568
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G1817	U1725	C1643	C1568	U1499	G1431	U1364	A1291	G1222	A1144		G987	U879	C767		
A1818	G1726	U1645	U1569	C1500	U1432	C1433	C1292	G1223	C1145		A990	U880	C768		
A1819	G1727	C1646	G1570	C1501	C1434	G1365	C1293	G1224	C1146		A992	U881	C769		
			G1571	C1502	C1435		G1294	G1225	C1147			U882	C770		
								G1226				U883	C771		
								G1227				U884	C772		
								G1228				U885	C773		
								G1229				U886	C774		
								G1230				U887	C775		
								G1231				U888	C776		
								G1232				U889	C777		
								G1233				U890	C778		
								G1234				U891	C779		
								G1235				U892	C780		
								G1236				U893	C781		
								G1237				U894	C782		
								G1238				U895	C783		
								G1239				U896	C784		
								G1240				U897	C785		
								G1241				U898	C786		
								G1242				U899	C787		
								G1243				U900	C788		
								G1244				U901	C789		
								G1245				U902	C790		
								G1246				U903	C791		
								G1247				U904	C792		
								G1248				U905	C793		
								G1249				U906	C794		
								G1250				U907	C795		
								G1251				U908	C796		
								G1252				U909	C797		
								G1253				U910	C798		
								G1254				U911	C799		
								G1255				U912	C800		
								G1256				U913	C801		
								G1257				U914	C802		
								G1258				U915	C803		
								G1259				U916	C804		
								G1260				U917	C805		
								G1261				U918	C806		
								G1262				U919	C807		
								G1263				U920	C808		
								G1264				U921	C809		
								G1265				U922	C810		
								G1266				U923	C811		
								G1267				U924	C812		
								G1268				U925	C813		
								G1269				U926	C814		
								G1270				U927	C815		
								G1271				U928	C816		
								G1272				U929	C817		
								G1273				U930	C818		
								G1274				U931	C819		
								G1275				U932	C820		
								G1276				U933	C821		
								G1277				U934	C822		
								G1278				U935	C823		
								G1279				U936	C824		



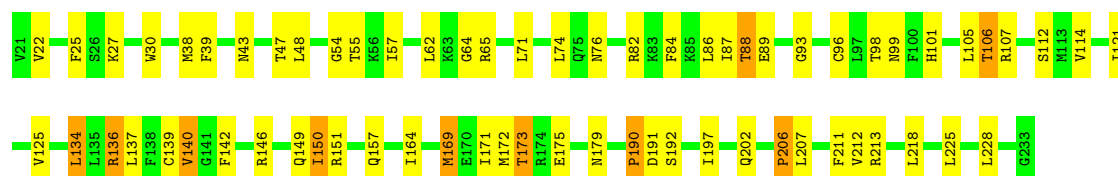
• Molecule 52: uS2

Chain AA: 63% 30% 6%



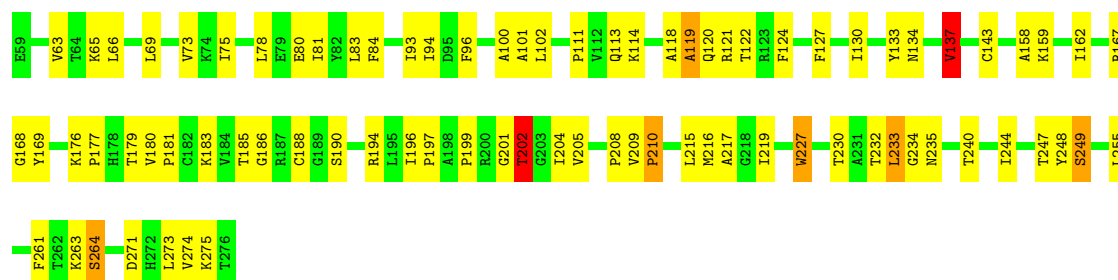
• Molecule 53: eS1

Chain BB: 69% 27% 5%



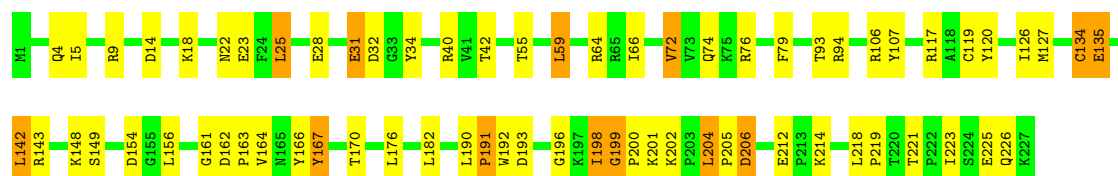
• Molecule 54: uS5

Chain CC: 62% 34% 2%



• Molecule 55: uS3

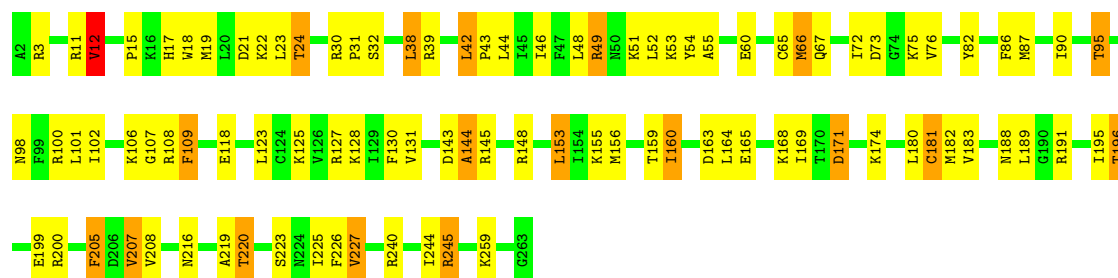
Chain DD: 70% 25% 6%



• Molecule 56: eS4

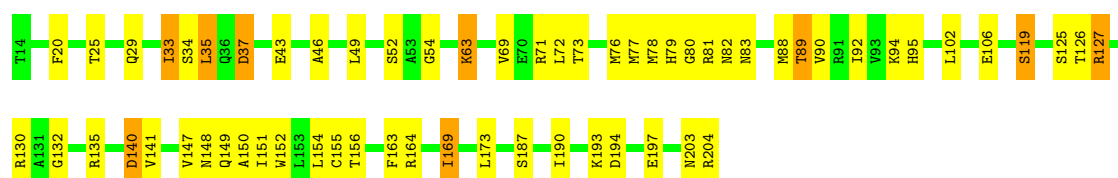
Chain EE: 63% 29% 7%





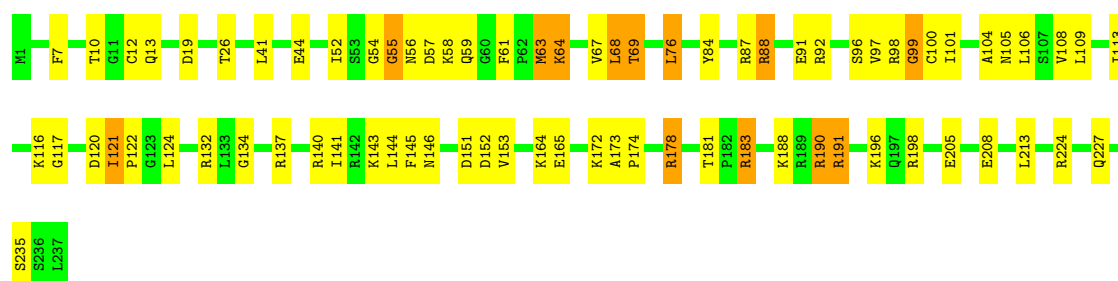
• Molecule 57: uS7

Chain FF: 68% 28% 5%



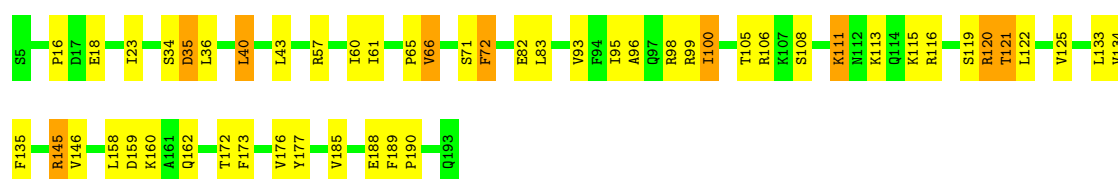
• Molecule 58: eS6

Chain GG: 68% 27% 5%



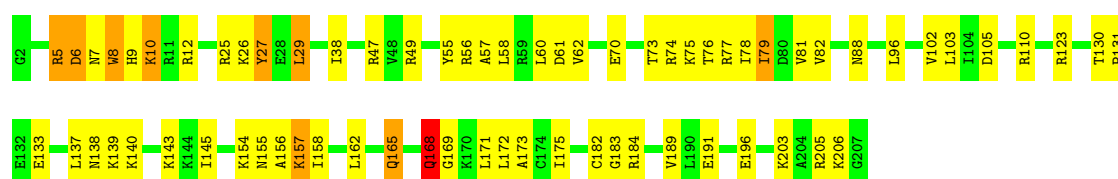
• Molecule 59: eS7

Chain HH: 72% 23% 5%

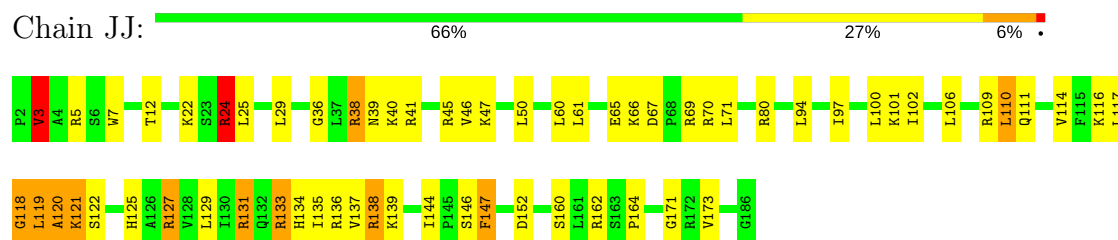


• Molecule 60: eS8

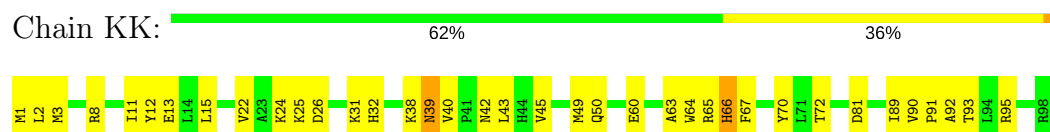
Chain II: 67% 29% 5%



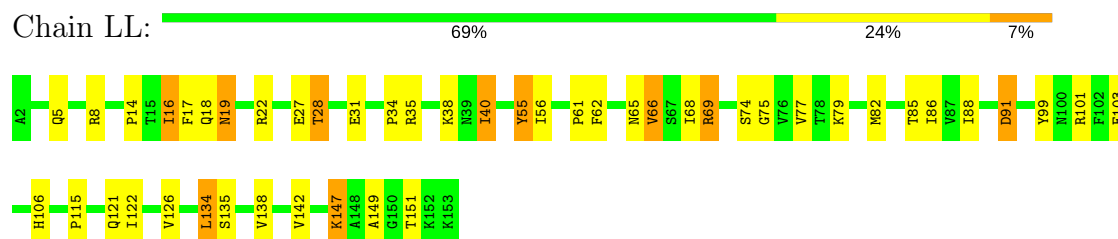
- Molecule 61: uS4



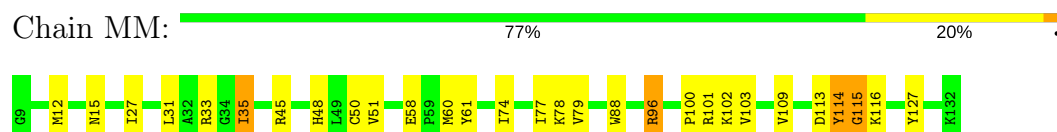
- Molecule 62: eS10



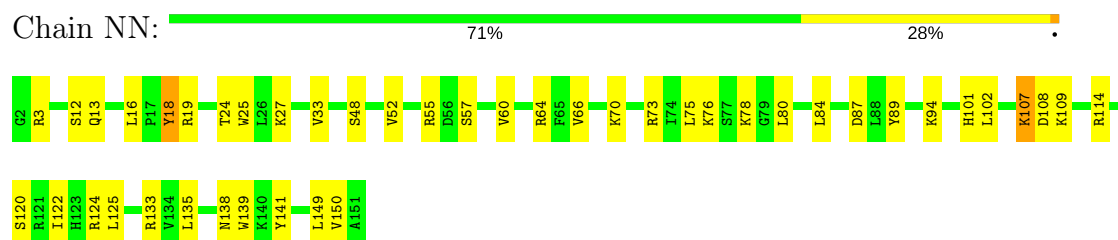
- Molecule 63: uS17



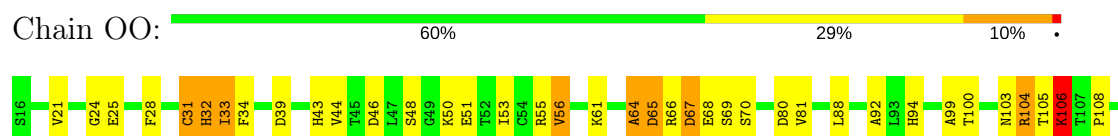
- Molecule 64: eS12



- Molecule 65: uS15



- Molecule 66: uS11





• Molecule 67: uS19

Chain PP: 76% 20% •



• Molecule 68: uS9

Chain QQ: 74% 21% • •



• Molecule 69: eS17

Chain RR: 70% 26% 5%



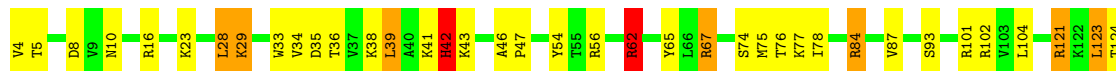
• Molecule 70: uS13

Chain SS: 69% 25% • •



• Molecule 71: eS19

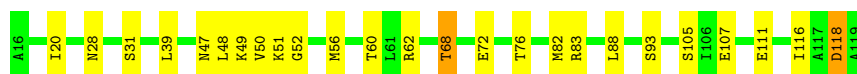
Chain TT: 72% 22% 5% •



• Molecule 72: uS10

Chain UU: 76% 22% •





• Molecule 73: eS21



• Molecule 74: uS8



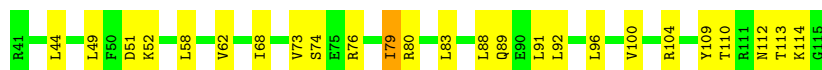
• Molecule 75: uS12



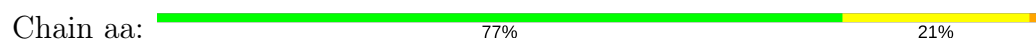
• Molecule 76: eS24



• Molecule 77: eS25

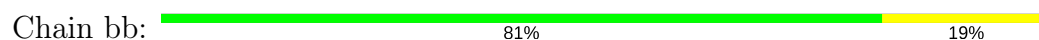


• Molecule 78: eS26





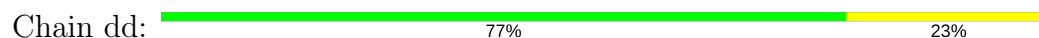
• Molecule 79: eS27



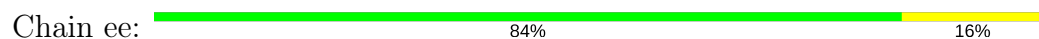
• Molecule 80: eS28



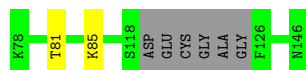
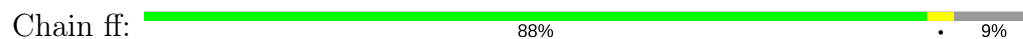
• Molecule 81: uS14



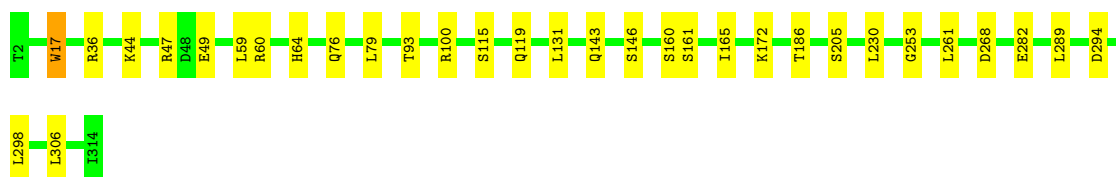
• Molecule 82: eS30



• Molecule 83: eS31



• Molecule 84: RACK1



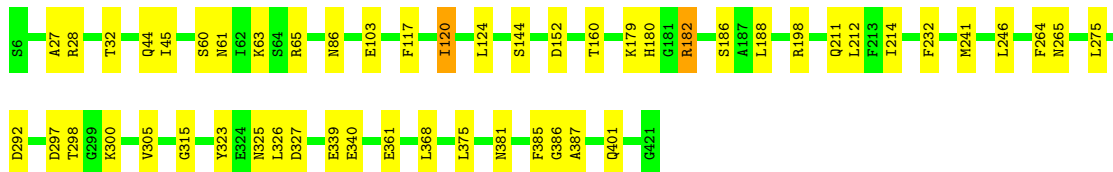
• Molecule 85: mRNA





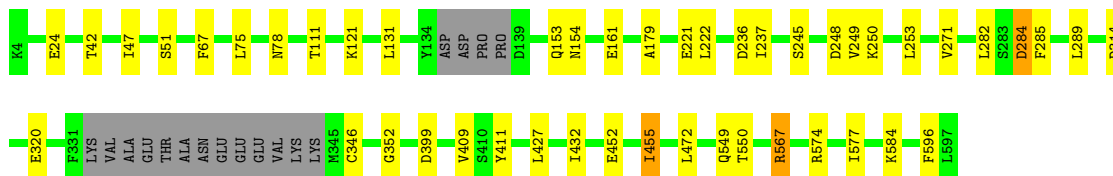
• Molecule 86: eRF1

Chain ii: 88% 12%



• Molecule 87: ABCE1

Chain jj: 89% 7%



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	22058	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	Not provided	Depositor
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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, SF4, ADP

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	0.68	0/1906	0.94	1/2556 (0.0%)
10	J	0.49	0/1376	0.80	2/1841 (0.1%)
11	L	0.59	0/1734	0.92	2/2317 (0.1%)
12	M	0.55	0/1158	0.80	0/1547
13	N	0.67	0/1746	0.99	3/2338 (0.1%)
14	O	0.63	0/1671	0.88	0/2234
15	P	0.67	0/1268	0.87	0/1701
16	Q	0.62	0/1530	0.94	0/2041
17	R	0.54	0/1524	0.88	2/2013 (0.1%)
18	S	0.63	0/1493	0.93	6/2002 (0.3%)
19	T	0.53	0/1326	0.80	0/1770
2	B	0.62	0/3216	0.89	4/4311 (0.1%)
20	U	0.48	0/822	0.75	0/1103
21	V	0.59	0/993	0.84	0/1332
22	W	0.57	0/541	0.86	2/720 (0.3%)
23	X	0.55	0/993	0.84	1/1334 (0.1%)
24	Y	0.54	0/1132	0.90	1/1504 (0.1%)
25	Z	0.58	0/1130	0.84	0/1507
26	a	0.65	0/1191	0.91	1/1590 (0.1%)
27	b	0.56	0/619	0.79	1/818 (0.1%)
28	c	0.55	0/742	0.79	0/996
29	d	0.55	0/903	0.90	1/1216 (0.1%)
3	C	0.65	1/2929 (0.0%)	0.91	5/3935 (0.1%)
30	e	0.59	0/1071	0.93	1/1429 (0.1%)
31	f	0.70	0/895	0.95	0/1198
32	g	0.59	0/916	0.90	3/1220 (0.2%)
33	h	0.51	0/1021	0.84	1/1348 (0.1%)
34	i	0.52	0/841	0.87	2/1112 (0.2%)
35	j	0.73	1/720 (0.1%)	1.09	4/952 (0.4%)
36	k	0.54	0/575	0.79	0/761
37	l	0.66	0/454	0.91	0/599
38	m	0.51	0/435	0.86	0/575

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
39	n	0.56	0/223	1.00	1/284 (0.4%)
4	D	0.50	0/2432	0.76	1/3257 (0.0%)
40	o	0.59	0/864	0.86	0/1140
41	p	0.57	0/718	0.82	0/953
42	r	0.63	0/1017	0.91	2/1364 (0.1%)
43	s	0.41	0/1547	0.60	0/2088
44	t	0.41	0/1257	0.70	0/1697
45	1	0.60	0/129	0.78	0/173
46	2	0.32	0/1805	0.76	3/2809 (0.1%)
47	3	0.34	0/1777	0.88	5/2763 (0.2%)
48	5	0.52	20/87790 (0.0%)	0.86	109/136937 (0.1%)
49	7	0.47	0/2858	0.74	1/4455 (0.0%)
5	E	0.54	0/1936	0.87	2/2600 (0.1%)
50	8	0.53	0/3701	0.78	0/5766
51	9	0.45	10/41013 (0.0%)	0.82	41/63919 (0.1%)
52	AA	0.51	0/1679	0.78	0/2283
53	BB	0.54	0/1756	0.81	1/2350 (0.0%)
54	CC	0.52	0/1730	0.84	1/2344 (0.0%)
55	DD	0.47	0/1792	0.77	0/2412
56	EE	0.49	0/2115	0.87	0/2843
57	FF	0.52	0/1531	0.82	0/2059
58	GG	0.49	0/1946	0.80	0/2590
59	HH	0.46	0/1544	0.74	0/2068
6	F	0.64	0/1905	0.88	2/2539 (0.1%)
60	II	0.52	0/1715	0.86	1/2287 (0.0%)
61	JJ	0.52	0/1550	0.91	3/2069 (0.1%)
62	KK	0.51	0/851	0.78	0/1147
63	LL	0.54	0/1259	0.85	0/1684
64	MM	0.48	0/968	0.65	0/1296
65	NN	0.52	0/1232	0.83	0/1656
66	OO	0.59	0/1029	0.98	2/1380 (0.1%)
67	PP	0.48	0/1079	0.79	0/1437
68	QQ	0.51	0/1142	0.82	1/1528 (0.1%)
69	RR	0.49	0/1060	0.76	0/1421
7	G	0.55	0/1967	0.83	2/2647 (0.1%)
70	SS	0.47	0/1157	0.86	1/1548 (0.1%)
71	TT	0.51	0/1120	0.84	3/1499 (0.2%)
72	UU	0.48	0/831	0.75	0/1115
73	VV	0.53	0/645	0.83	0/865
74	WW	0.59	0/1051	0.88	0/1406
75	XX	0.58	0/1116	0.90	1/1490 (0.1%)
76	YY	0.51	0/1040	0.80	0/1382
77	ZZ	0.49	0/604	0.82	0/810

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
78	aa	0.53	0/794	0.87	0/1065
79	bb	0.43	0/665	0.71	0/891
8	H	0.51	0/1535	0.84	1/2063 (0.0%)
80	cc	0.57	0/478	0.88	0/640
81	dd	0.61	0/455	0.92	1/603 (0.2%)
82	ee	0.57	0/462	0.84	1/607 (0.2%)
83	ff	0.39	0/531	0.65	0/703
84	gg	0.45	0/2493	0.70	1/3394 (0.0%)
85	hh	0.47	0/287	0.78	0/445
86	ii	0.45	0/3333	0.67	1/4483 (0.0%)
87	jj	0.42	0/4633	0.70	3/6249 (0.0%)
9	I	0.55	0/1693	0.79	1/2260 (0.0%)
All	All	0.52	32/242711 (0.0%)	0.84	235/355683 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
11	L	0	1
14	O	0	3
18	S	0	2
19	T	0	1
2	B	0	6
21	V	0	1
23	X	0	1
24	Y	0	1
26	a	0	2
3	C	0	5
31	f	0	1
33	h	0	1
36	k	0	1
38	m	0	1
4	D	0	1
42	r	0	1
5	E	0	4
51	9	0	3
52	AA	0	2
53	BB	0	3
55	DD	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
56	EE	0	2
57	FF	0	1
59	HH	0	1
61	JJ	0	1
63	LL	0	2
66	OO	0	2
68	QQ	0	1
7	G	0	1
70	SS	0	3
71	TT	0	1
72	UU	0	2
73	VV	0	1
74	WW	0	1
75	XX	0	1
76	YY	0	1
78	aa	0	2
86	ii	0	3
87	jj	0	2
9	I	0	4
All	All	0	76

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	5	957	G	O3'-P	9.85	1.73	1.61
48	5	3859	G	O3'-P	-8.08	1.51	1.61
48	5	1847	C	O3'-P	-7.85	1.51	1.61
48	5	956	A	O3'-P	7.22	1.69	1.61
51	9	677	G	O3'-P	-6.35	1.53	1.61

The worst 5 of 235 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	1965	G	P-O3'-C3'	20.40	144.18	119.70
48	5	3753	G	N9-C1'-C2'	-13.34	96.66	114.00
51	9	1235	G	N9-C1'-C2'	-12.87	97.27	114.00
47	3	70	G	N9-C1'-C2'	-12.35	97.94	114.00
51	9	1212	G	N9-C1'-C2'	-11.52	99.03	114.00

There are no chirality outliers.

5 of 76 planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	A	195	CYS	Peptide
1	A	196	TRP	Peptide
2	B	17	LEU	Peptide
2	B	35	ASP	Peptide
2	B	36	ASP	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	44	0
2	B	3148	0	3267	69	0
3	C	2875	0	3049	69	0
4	D	2386	0	2419	29	0
5	E	1898	0	2035	64	0
6	F	1870	0	1994	41	0
7	G	1934	0	2087	40	0
8	H	1516	0	1597	21	0
9	I	1655	0	1704	62	0
10	J	1353	0	1386	19	0
11	L	1703	0	1820	46	0
12	M	1137	0	1211	27	0
13	N	1701	0	1749	42	0
14	O	1638	0	1777	38	0
15	P	1242	0	1269	15	0
16	Q	1506	0	1623	22	0
17	R	1508	0	1664	25	0
18	S	1454	0	1496	33	0
19	T	1298	0	1366	13	0
20	U	808	0	831	10	0
21	V	979	0	1039	10	0
22	W	528	0	541	6	0
23	X	976	0	1053	20	0
24	Y	1115	0	1205	13	0
25	Z	1107	0	1182	20	0
26	a	1162	0	1209	0	0
27	b	609	0	650	0	0
28	c	732	0	769	0	0
29	d	888	0	930	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	e	1053	0	1147	0	0
31	f	876	0	912	0	0
32	g	906	0	998	0	0
33	h	1013	0	1147	0	0
34	i	830	0	916	0	0
35	j	705	0	738	0	0
36	k	569	0	637	0	0
37	l	444	0	483	0	0
38	m	429	0	467	0	0
39	n	222	0	264	0	0
40	o	851	0	922	0	0
41	p	708	0	756	0	0
42	r	1001	0	1060	0	0
43	s	1523	0	1577	0	0
44	t	1238	0	1295	0	0
45	1	125	0	117	2	0
46	2	1616	0	824	22	0
47	3	1593	0	811	48	0
48	5	78486	0	39663	1576	0
49	7	2558	0	1296	30	0
50	8	3314	0	1683	53	0
51	9	36680	0	18530	711	0
52	AA	1642	0	1646	30	0
53	BB	1729	0	1803	28	0
54	CC	1692	0	1780	45	0
55	DD	1764	0	1863	23	0
56	EE	2073	0	2175	45	0
57	FF	1509	0	1563	24	0
58	GG	1923	0	2089	33	0
59	HH	1521	0	1616	27	0
60	II	1686	0	1772	35	0
61	JJ	1525	0	1640	30	0
62	KK	827	0	854	10	0
63	LL	1238	0	1315	20	0
64	MM	958	0	993	4	0
65	NN	1208	0	1294	8	0
66	OO	1016	0	1039	24	0
67	PP	1060	0	1120	12	0
68	QQ	1124	0	1193	13	0
69	RR	1047	0	1103	12	0
70	SS	1139	0	1191	16	0
71	TT	1102	0	1142	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
72	UU	821	0	883	2	0
73	VV	636	0	634	13	0
74	WW	1034	0	1080	19	0
75	XX	1098	0	1167	9	0
76	YY	1023	0	1090	19	0
77	ZZ	598	0	656	9	0
78	aa	781	0	829	0	0
79	bb	651	0	672	0	0
80	cc	475	0	497	0	0
81	dd	445	0	439	0	0
82	ee	457	0	502	0	0
83	ff	520	0	536	0	0
84	gg	2436	0	2393	0	0
85	hh	257	0	129	0	0
86	ii	3280	0	3326	0	0
87	jj	4551	0	4687	0	0
88	5	147	0	0	0	0
88	7	5	0	0	0	0
88	8	2	0	0	0	0
88	9	35	0	0	0	0
88	C	1	0	0	0	0
88	I	1	0	0	0	0
88	P	1	0	0	0	0
88	V	1	0	0	0	0
88	g	1	0	0	0	0
88	hh	1	0	0	0	0
89	aa	1	0	0	0	0
89	dd	1	0	0	0	0
89	ff	1	0	0	0	0
89	g	1	0	0	0	0
89	j	1	0	0	0	0
89	m	1	0	0	0	0
89	o	1	0	0	0	0
89	p	1	0	0	0	0
90	jj	16	0	0	0	0
91	jj	54	0	24	0	0
All	All	226453	0	169859	3455	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 10.

The worst 5 of 3455 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)
9:I:191:ILE:HD12	9:I:200:ILE:CD1	1.25	1.59
9:I:191:ILE:CD1	9:I:200:ILE:HD12	1.17	1.55
48:5:1968:G:H1	48:5:2018:C:N4	1.21	1.34
9:I:191:ILE:CD1	9:I:200:ILE:CD1	1.90	1.34
48:5:976:G:H2'	48:5:977:C:O4'	1.21	1.31

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%)	199 (82%)	34 (14%)	9 (4%)	4	36
2	B	392/394 (100%)	338 (86%)	44 (11%)	10 (3%)	6	44
3	C	359/361 (99%)	302 (84%)	48 (13%)	9 (2%)	6	45
4	D	290/292 (99%)	255 (88%)	31 (11%)	4 (1%)	13	55
5	E	232/248 (94%)	172 (74%)	37 (16%)	23 (10%)	1	11
6	F	223/225 (99%)	204 (92%)	18 (8%)	1 (0%)	38	76
7	G	239/241 (99%)	205 (86%)	26 (11%)	8 (3%)	4	39
8	H	188/190 (99%)	161 (86%)	25 (13%)	2 (1%)	17	61
9	I	200/213 (94%)	178 (89%)	17 (8%)	5 (2%)	6	45
10	J	167/169 (99%)	141 (84%)	18 (11%)	8 (5%)	2	29
11	L	208/210 (99%)	174 (84%)	25 (12%)	9 (4%)	3	32
12	M	136/138 (99%)	123 (90%)	12 (9%)	1 (1%)	25	68
13	N	201/203 (99%)	167 (83%)	32 (16%)	2 (1%)	18	62
14	O	197/199 (99%)	176 (89%)	20 (10%)	1 (0%)	32	73
15	P	151/153 (99%)	134 (89%)	13 (9%)	4 (3%)	6	44
16	Q	185/187 (99%)	161 (87%)	20 (11%)	4 (2%)	8	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	R	178/180 (99%)	151 (85%)	25 (14%)	2 (1%)	17	61
18	S	173/175 (99%)	151 (87%)	18 (10%)	4 (2%)	7	47
19	T	157/159 (99%)	137 (87%)	17 (11%)	3 (2%)	9	51
20	U	97/99 (98%)	82 (84%)	11 (11%)	4 (4%)	3	33
21	V	129/131 (98%)	110 (85%)	19 (15%)	0	100	100
22	W	61/63 (97%)	55 (90%)	5 (8%)	1 (2%)	11	54
23	X	117/119 (98%)	106 (91%)	9 (8%)	2 (2%)	11	53
24	Y	132/134 (98%)	114 (86%)	13 (10%)	5 (4%)	4	35
25	Z	133/135 (98%)	113 (85%)	14 (10%)	6 (4%)	3	30
26	a	145/147 (99%)	114 (79%)	24 (17%)	7 (5%)	2	29
27	b	73/75 (97%)	65 (89%)	5 (7%)	3 (4%)	3	33
28	c	92/94 (98%)	87 (95%)	5 (5%)	0	100	100
29	d	105/107 (98%)	86 (82%)	17 (16%)	2 (2%)	9	51
30	e	126/128 (98%)	110 (87%)	12 (10%)	4 (3%)	5	40
31	f	107/109 (98%)	88 (82%)	12 (11%)	7 (6%)	1	22
32	g	112/114 (98%)	97 (87%)	13 (12%)	2 (2%)	10	52
33	h	120/122 (98%)	106 (88%)	10 (8%)	4 (3%)	4	39
34	i	100/102 (98%)	87 (87%)	11 (11%)	2 (2%)	9	50
35	j	84/86 (98%)	73 (87%)	8 (10%)	3 (4%)	4	37
36	k	67/69 (97%)	53 (79%)	10 (15%)	4 (6%)	2	24
37	l	48/50 (96%)	41 (85%)	5 (10%)	2 (4%)	3	32
38	m	50/52 (96%)	43 (86%)	7 (14%)	0	100	100
39	n	21/23 (91%)	21 (100%)	0	0	100	100
40	o	102/104 (98%)	79 (78%)	19 (19%)	4 (4%)	3	34
41	p	89/91 (98%)	75 (84%)	9 (10%)	5 (6%)	2	25
42	r	123/125 (98%)	104 (85%)	10 (8%)	9 (7%)	1	19
43	s	196/198 (99%)	163 (83%)	21 (11%)	12 (6%)	2	23
44	t	161/163 (99%)	100 (62%)	36 (22%)	25 (16%)	0	4
45	1	13/15 (87%)	10 (77%)	2 (15%)	1 (8%)	1	17
52	AA	206/208 (99%)	153 (74%)	37 (18%)	16 (8%)	1	16
53	BB	211/213 (99%)	165 (78%)	34 (16%)	12 (6%)	2	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	CC	216/218 (99%)	184 (85%)	22 (10%)	10 (5%)	3	30
55	DD	225/227 (99%)	184 (82%)	30 (13%)	11 (5%)	2	28
56	EE	260/262 (99%)	197 (76%)	43 (16%)	20 (8%)	1	17
57	FF	189/191 (99%)	156 (82%)	22 (12%)	11 (6%)	2	24
58	GG	235/237 (99%)	198 (84%)	29 (12%)	8 (3%)	4	39
59	HH	187/189 (99%)	144 (77%)	30 (16%)	13 (7%)	1	20
60	II	204/206 (99%)	169 (83%)	25 (12%)	10 (5%)	2	28
61	JJ	183/185 (99%)	152 (83%)	19 (10%)	12 (7%)	1	22
62	KK	96/98 (98%)	65 (68%)	20 (21%)	11 (12%)	0	7
63	LL	150/152 (99%)	125 (83%)	16 (11%)	9 (6%)	2	24
64	MM	122/124 (98%)	87 (71%)	25 (20%)	10 (8%)	1	15
65	NN	148/150 (99%)	121 (82%)	21 (14%)	6 (4%)	3	33
66	OO	134/136 (98%)	96 (72%)	24 (18%)	14 (10%)	0	10
67	PP	125/127 (98%)	102 (82%)	20 (16%)	3 (2%)	7	46
68	QQ	139/141 (99%)	115 (83%)	14 (10%)	10 (7%)	1	19
69	RR	127/129 (98%)	100 (79%)	18 (14%)	9 (7%)	1	19
70	SS	135/137 (98%)	110 (82%)	15 (11%)	10 (7%)	1	18
71	TT	139/141 (99%)	127 (91%)	9 (6%)	3 (2%)	8	47
72	UU	102/104 (98%)	84 (82%)	12 (12%)	6 (6%)	2	24
73	VV	81/83 (98%)	65 (80%)	9 (11%)	7 (9%)	1	14
74	WW	127/129 (98%)	101 (80%)	21 (16%)	5 (4%)	3	34
75	XX	139/141 (99%)	122 (88%)	8 (6%)	9 (6%)	1	22
76	YY	124/126 (98%)	100 (81%)	15 (12%)	9 (7%)	1	19
77	ZZ	73/75 (97%)	58 (80%)	11 (15%)	4 (6%)	2	26
78	aa	96/98 (98%)	76 (79%)	8 (8%)	12 (12%)	0	7
79	bb	81/83 (98%)	59 (73%)	16 (20%)	6 (7%)	1	18
80	cc	59/61 (97%)	47 (80%)	11 (19%)	1 (2%)	11	53
81	dd	51/53 (96%)	40 (78%)	11 (22%)	0	100	100
82	ee	55/57 (96%)	39 (71%)	14 (26%)	2 (4%)	4	37
83	ff	58/68 (85%)	49 (84%)	8 (14%)	1 (2%)	11	53
84	gg	311/313 (99%)	263 (85%)	40 (13%)	8 (3%)	6	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
86	ii	414/416 (100%)	378 (91%)	25 (6%)	11 (3%)	6	43
87	jj	569/594 (96%)	501 (88%)	54 (10%)	14 (2%)	6	45
All	All	12492/12708 (98%)	10443 (84%)	1523 (12%)	526 (4%)	6	32

5 of 526 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	SER
1	A	196	TRP
1	A	197	PRO
2	B	37	PRO
2	B	302	ASN

### 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%)	159 (85%)	28 (15%)	3	23
2	B	336/342 (98%)	288 (86%)	48 (14%)	4	26
3	C	301/301 (100%)	258 (86%)	43 (14%)	4	26
4	D	247/247 (100%)	218 (88%)	29 (12%)	6	33
5	E	208/221 (94%)	179 (86%)	29 (14%)	4	27
6	F	194/195 (100%)	169 (87%)	25 (13%)	5	29
7	G	206/206 (100%)	176 (85%)	30 (15%)	3	24
8	H	169/169 (100%)	147 (87%)	22 (13%)	5	29
9	I	174/180 (97%)	158 (91%)	16 (9%)	11	45
10	J	142/142 (100%)	127 (89%)	15 (11%)	8	38
11	L	176/176 (100%)	144 (82%)	32 (18%)	2	13
12	M	117/117 (100%)	104 (89%)	13 (11%)	7	36
13	N	171/171 (100%)	149 (87%)	22 (13%)	5	29
14	O	171/171 (100%)	141 (82%)	30 (18%)	2	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	P	134/134 (100%)	118 (88%)	16 (12%)	6	32
16	Q	163/163 (100%)	142 (87%)	21 (13%)	5	29
17	R	159/159 (100%)	139 (87%)	20 (13%)	5	30
18	S	156/156 (100%)	137 (88%)	19 (12%)	6	31
19	T	139/139 (100%)	115 (83%)	24 (17%)	2	15
20	U	89/89 (100%)	79 (89%)	10 (11%)	7	36
21	V	101/101 (100%)	82 (81%)	19 (19%)	2	12
22	W	55/55 (100%)	49 (89%)	6 (11%)	7	37
23	X	107/107 (100%)	95 (89%)	12 (11%)	7	36
24	Y	124/124 (100%)	106 (86%)	18 (14%)	4	24
25	Z	117/117 (100%)	101 (86%)	16 (14%)	4	27
26	a	119/119 (100%)	108 (91%)	11 (9%)	11	45
27	b	62/62 (100%)	54 (87%)	8 (13%)	5	29
28	c	79/79 (100%)	65 (82%)	14 (18%)	2	14
29	d	98/98 (100%)	79 (81%)	19 (19%)	1	11
30	e	114/114 (100%)	95 (83%)	19 (17%)	2	17
31	f	88/88 (100%)	75 (85%)	13 (15%)	3	24
32	g	98/98 (100%)	81 (83%)	17 (17%)	2	15
33	h	109/109 (100%)	96 (88%)	13 (12%)	6	32
34	i	86/86 (100%)	72 (84%)	14 (16%)	3	18
35	j	73/73 (100%)	57 (78%)	16 (22%)	1	8
36	k	64/64 (100%)	60 (94%)	4 (6%)	21	60
37	l	47/47 (100%)	40 (85%)	7 (15%)	3	23
38	m	48/48 (100%)	36 (75%)	12 (25%)	1	5
39	n	22/22 (100%)	20 (91%)	2 (9%)	11	46
40	o	92/92 (100%)	78 (85%)	14 (15%)	3	22
41	p	74/74 (100%)	63 (85%)	11 (15%)	3	23
42	r	109/109 (100%)	93 (85%)	16 (15%)	3	24
43	s	166/166 (100%)	155 (93%)	11 (7%)	19	59
44	t	136/136 (100%)	126 (93%)	10 (7%)	16	54
45	l	13/13 (100%)	11 (85%)	2 (15%)	3	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	AA	174/174 (100%)	142 (82%)	32 (18%)	2	12
53	BB	194/194 (100%)	168 (87%)	26 (13%)	4	28
54	CC	183/183 (100%)	162 (88%)	21 (12%)	6	34
55	DD	190/190 (100%)	151 (80%)	39 (20%)	1	9
56	EE	223/223 (100%)	188 (84%)	35 (16%)	3	21
57	FF	161/161 (100%)	132 (82%)	29 (18%)	2	13
58	GG	207/207 (100%)	174 (84%)	33 (16%)	3	20
59	HH	169/169 (100%)	155 (92%)	14 (8%)	13	49
60	II	178/178 (100%)	150 (84%)	28 (16%)	3	21
61	JJ	161/161 (100%)	139 (86%)	22 (14%)	4	27
62	KK	89/89 (100%)	76 (85%)	13 (15%)	3	24
63	LL	136/136 (100%)	116 (85%)	20 (15%)	3	24
64	MM	104/104 (100%)	88 (85%)	16 (15%)	3	22
65	NN	130/130 (100%)	104 (80%)	26 (20%)	1	10
66	OO	106/106 (100%)	84 (79%)	22 (21%)	1	9
67	PP	116/116 (100%)	97 (84%)	19 (16%)	2	18
68	QQ	117/117 (100%)	100 (86%)	17 (14%)	4	24
69	RR	117/117 (100%)	96 (82%)	21 (18%)	2	14
70	SS	119/119 (100%)	101 (85%)	18 (15%)	3	23
71	TT	112/112 (100%)	94 (84%)	18 (16%)	3	19
72	UU	94/94 (100%)	79 (84%)	15 (16%)	3	20
73	VV	67/67 (100%)	56 (84%)	11 (16%)	2	18
74	WW	112/112 (100%)	98 (88%)	14 (12%)	5	30
75	XX	113/113 (100%)	92 (81%)	21 (19%)	2	12
76	YY	108/108 (100%)	87 (81%)	21 (19%)	1	11
77	ZZ	66/66 (100%)	58 (88%)	8 (12%)	6	32
78	aa	85/85 (100%)	74 (87%)	11 (13%)	5	29
79	bb	75/75 (100%)	65 (87%)	10 (13%)	4	28
80	cc	54/54 (100%)	40 (74%)	14 (26%)	0	5
81	dd	47/47 (100%)	36 (77%)	11 (23%)	1	6
82	ee	47/47 (100%)	41 (87%)	6 (13%)	5	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
83	ff	58/61 (95%)	57 (98%)	1 (2%)	66	87
84	gg	272/272 (100%)	248 (91%)	24 (9%)	12	47
86	ii	358/358 (100%)	319 (89%)	39 (11%)	7	37
87	jj	507/522 (97%)	475 (94%)	32 (6%)	21	60
All	All	10889/10933 (100%)	9386 (86%)	1503 (14%)	8	27

5 of 1503 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
34	i	9	VAL
53	BB	142	PHE
80	cc	68	LEU
35	j	49	TRP
42	r	39	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
5	E	217	GLN
11	L	175	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
46	2	74/76 (97%)	24 (32%)	0
47	3	72/75 (96%)	28 (38%)	0
48	5	3643/3662 (99%)	1236 (33%)	0
49	7	119/120 (99%)	24 (20%)	0
50	8	155/156 (99%)	49 (31%)	0
51	9	1709/1719 (99%)	614 (35%)	0
85	hh	11/12 (91%)	6 (54%)	0
All	All	5783/5820 (99%)	1981 (34%)	0

5 of 1981 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	14	A

There are no RNA pucker outliers to report.

## 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 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	$\# Z  > 2$
90	SF4	jj	600	87	0,12,12	0.00	-	0,24,24	0.00	-
90	SF4	jj	601	87	0,12,12	0.00	-	0,24,24	0.00	-
91	ADP	jj	602	-	25,29,29	1.08	2 (8%)	24,45,45	1.79	2 (8%)
91	ADP	jj	603	-	25,29,29	1.08	2 (8%)	24,45,45	1.79	2 (8%)

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	SF4	jj	600	87	-	0/0/48/48	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
90	SF4	jj	601	87	-	0/0/48/48	0/6/5/5
91	ADP	jj	602	-	-	0/12/32/32	0/3/3/3
91	ADP	jj	603	-	-	0/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
91	jj	602	ADP	C2-N3	2.08	1.35	1.32
91	jj	603	ADP	C2-N3	2.09	1.35	1.32
91	jj	603	ADP	C5-C4	3.29	1.47	1.40
91	jj	602	ADP	C5-C4	3.31	1.48	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
91	jj	602	ADP	N3-C2-N1	-6.98	122.78	128.86
91	jj	603	ADP	N3-C2-N1	-6.89	122.86	128.86
91	jj	602	ADP	C4-C5-N7	-3.18	106.34	109.41
91	jj	603	ADP	C4-C5-N7	-3.15	106.37	109.41

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](#)

There are no chain breaks in this entry.