



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

Mar 2, 2017 – 12:39 pm GMT

PDB ID : 3JAH  
EMDB ID: : EMD-3039  
Title : Structure of a mammalian ribosomal termination complex with ABCE1, eRF1(AAQ), and the UAG stop codon  
Authors : Brown, A.; Shao, S.; Murray, J.; Hegde, R.S.; Ramakrishnan, V.  
Deposited on : 2015-06-10  
Resolution : 3.45 Å(reported)  
Based on 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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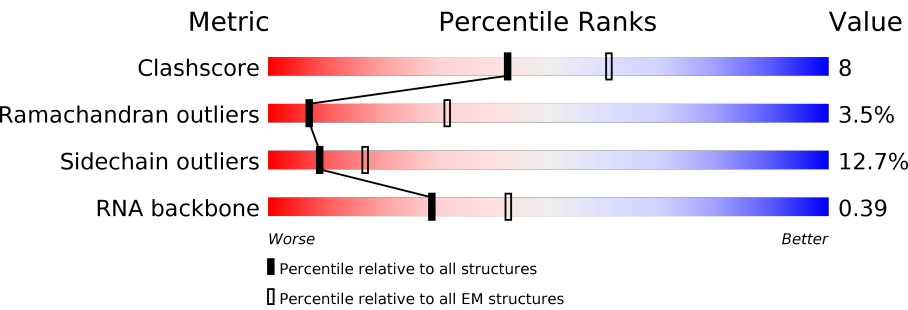
MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc29047

# 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 3.45 Å.

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



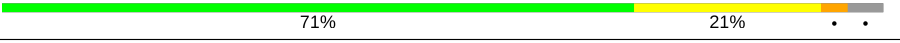















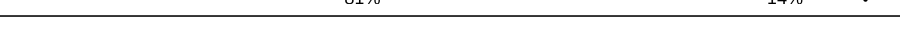
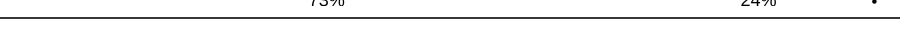
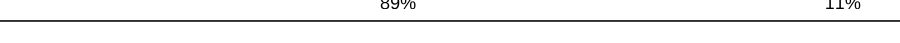
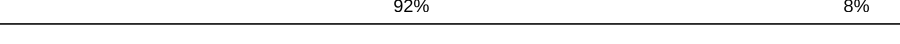
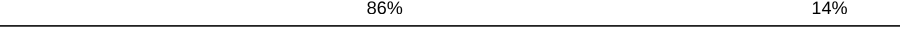
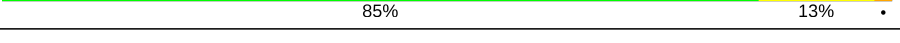



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

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>76%</div><div>18%</div><div>5%</div></div>
2	B	394	<div><div>76%</div><div>21%</div><div>.</div></div>
3	C	362	<div><div>71%</div><div>26%</div><div>.</div></div>
4	D	292	<div><div>79%</div><div>18%</div><div>.</div></div>
5	E	248	<div><div>65%</div><div>25%</div><div>5%</div><div>5%</div></div>
6	F	225	<div><div>76%</div><div>20%</div><div>.</div><div>.</div></div>
7	G	241	<div><div>78%</div><div>22%</div><div>.</div></div>
8	H	190	<div><div>81%</div><div>17%</div><div>.</div></div>














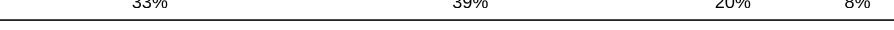


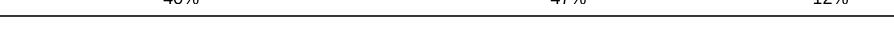

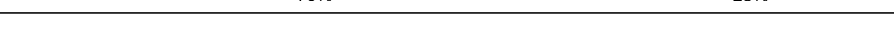
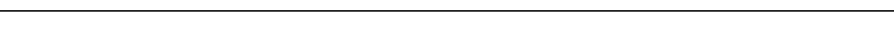
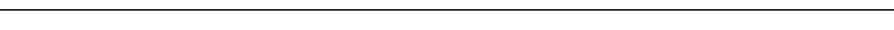
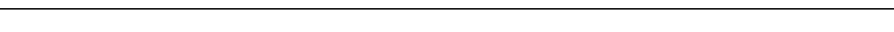
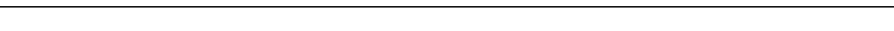
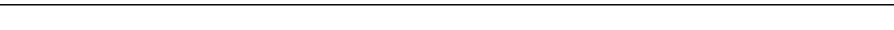

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Mol	Chain	Length	Quality of chain
9	I	213	
10	J	169	
11	L	210	
12	M	138	
13	N	203	
14	O	199	
15	P	153	
16	Q	187	
17	R	180	
18	S	175	
19	T	159	
20	U	99	
21	V	131	
22	W	63	
23	X	119	
24	Y	134	
25	Z	135	
26	a	147	
27	b	75	
28	c	94	
29	d	107	
30	e	128	
31	f	109	
32	g	114	
33	h	122	

















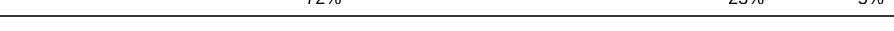

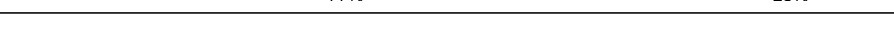
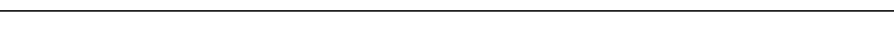
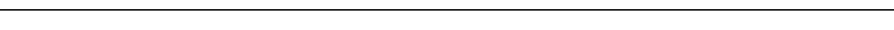
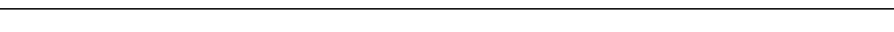
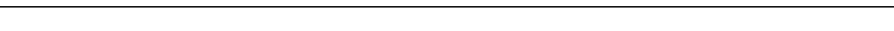
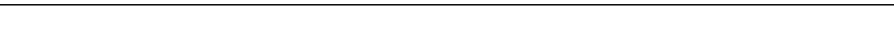

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Mol	Chain	Length	Quality of chain
34	i	102	
35	j	86	
36	k	69	
37	l	50	
38	m	52	
39	n	23	
40	o	104	
41	p	91	
42	r	125	
43	s	198	
44	t	163	
45	1	15	
46	2	76	
47	3	75	
48	5	3662	
49	7	120	
50	8	156	
51	9	1719	
52	AA	208	
53	BB	213	
54	CC	218	
55	DD	227	
56	EE	262	
57	FF	191	
58	GG	237	





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Mol	Chain	Length	Quality of chain
59	HH	189	 71% 24% 5%
60	II	206	 69% 30% .
61	JJ	185	 75% 18% 6% .
62	KK	98	 71% 27% .
63	LL	152	 70% 24% . .
64	MM	124	 75% 24% .
65	NN	150	 76% 22% .
66	OO	136	 67% 23% 7% .
67	PP	127	 75% 21% .
68	QQ	141	 77% 20% .
69	RR	129	 78% 19% .
70	SS	137	 74% 20% . .
71	TT	141	 79% 16% 5% .
72	UU	104	 75% 22% . .
73	VV	83	 73% 24% .
74	WW	129	 65% 29% 5% .
75	XX	141	 72% 23% 5%
76	YY	126	 73% 22% 5%
77	ZZ	75	 77% 23%
78	aa	98	 81% 19%
79	bb	83	 80% 20%
80	cc	61	 80% 20%
81	dd	53	 81% 19%
82	ee	57	 82% 16% .
83	ff	68	 87% . 9%

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Mol	Chain	Length	Quality of chain
84	gg	313	 90%9%
85	hh	12	 42%58%
86	ii	416	 89%10%
87	jj	594	 91%5%•

## 2 Entry composition [i](#)

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

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

- Molecule 1 is a protein called uL2.

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

- Molecule 2 is a protein called uL3.

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

- Molecule 3 is a protein called uL4.

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

There are 3 discrepancies between the modelled and reference sequences:

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

- Molecule 4 is a protein called uL18.

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

- Molecule 5 is a protein called eL6.

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

- Molecule 6 is a protein called uL30.

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

- Molecule 7 is a protein called eL8.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 8 is a protein called uL6.

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

- Molecule 9 is a protein called uL16.

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

- Molecule 10 is a protein called uL5.

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

- Molecule 11 is a protein called eL13.

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

- Molecule 12 is a protein called eL14.

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

- Molecule 13 is a protein called eL15.

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

- Molecule 14 is a protein called uL13.

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

- Molecule 15 is a protein called uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	153	Total	C	N	O	S	0	0
			1242	776	241	216	9		

- Molecule 16 is a protein called uL14.

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

- Molecule 17 is a protein called eL19.

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

- Molecule 18 is a protein called eL20.

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

- Molecule 19 is a protein called eL21.

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

- Molecule 20 is a protein called eL22.

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

- Molecule 21 is a protein called uL14.

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

- Molecule 22 is a protein called eL24.

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

- Molecule 23 is a protein called uL23.

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

- Molecule 24 is a protein called uL24.

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

- Molecule 25 is a protein called eL27.

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

- Molecule 26 is a protein called uL15.

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

- Molecule 27 is a protein called eL29.

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

- Molecule 28 is a protein called eL30.

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

- Molecule 29 is a protein called eL31.

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

- Molecule 30 is a protein called eL32.

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

- Molecule 31 is a protein called eL33.

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

- Molecule 32 is a protein called eL34.

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

- Molecule 33 is a protein called uL29.

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

- Molecule 34 is a protein called eL36.

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

- Molecule 35 is a protein called eL37.

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

- Molecule 36 is a protein called eL38.

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

- Molecule 37 is a protein called eL39.

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

- Molecule 38 is a protein called eL40.

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

- Molecule 39 is a protein called eL41.

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

- Molecule 40 is a protein called eL42.

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

- Molecule 41 is a protein called eL43.

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

- Molecule 42 is a protein called eL28.

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

- Molecule 43 is a protein called uL10.

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

- Molecule 44 is a protein called uL11.

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

- Molecule 45 is a protein called peptide.

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 52 is a protein called uS2.

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

- Molecule 53 is a protein called eS1.

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

- Molecule 54 is a protein called uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	CC	218	Total	C	N	O	S	0	0
			1692	1102	287	296	7		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CC	194	ARG	HIS	CONFLICT	UNP G1TUT9
CC	228	GLY	SER	CONFLICT	UNP G1TUT9

- Molecule 55 is a protein called uS3.

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

- Molecule 56 is a protein called eS4.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 57 is a protein called uS7.

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

- Molecule 58 is a protein called eS6.

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

- Molecule 59 is a protein called eS7.

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

- Molecule 60 is a protein called eS8.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 61 is a protein called uS4.

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

- Molecule 62 is a protein called eS10.

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

- Molecule 63 is a protein called uS17.

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

- Molecule 64 is a protein called eS12.

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

- Molecule 65 is a protein called uS15.

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

- Molecule 66 is a protein called uS11.

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

- Molecule 67 is a protein called uS19.

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

- Molecule 68 is a protein called uS9.

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

- Molecule 69 is a protein called eS17.

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

- Molecule 70 is a protein called uS13.

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

- Molecule 71 is a protein called eS19.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 72 is a protein called uS10.

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

- Molecule 73 is a protein called eS21.

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

There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 74 is a protein called uS8.

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

- Molecule 75 is a protein called uS12.

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

- Molecule 76 is a protein called eS24.

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

- Molecule 77 is a protein called eS25.

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

- Molecule 78 is a protein called eS26.

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

- Molecule 79 is a protein called eS27.

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

- Molecule 80 is a protein called eS28.

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

There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 81 is a protein called uS14.

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

- Molecule 82 is a protein called eS30.

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

- Molecule 83 is a protein called eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	ff	62	Total	C	N	O	S	0	0
			520	331	98	85	6		

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 84 is a protein called RACK1.

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

- Molecule 85 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	hh	12	Total	C	N	O	P	0	0
			257	115	46	84	12		

- Molecule 86 is a protein called eRF1.

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

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 87 is a protein called ABCE1.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	jj	576	Total	C	N	O	S	0	0
			4543	2904	779	829	31		

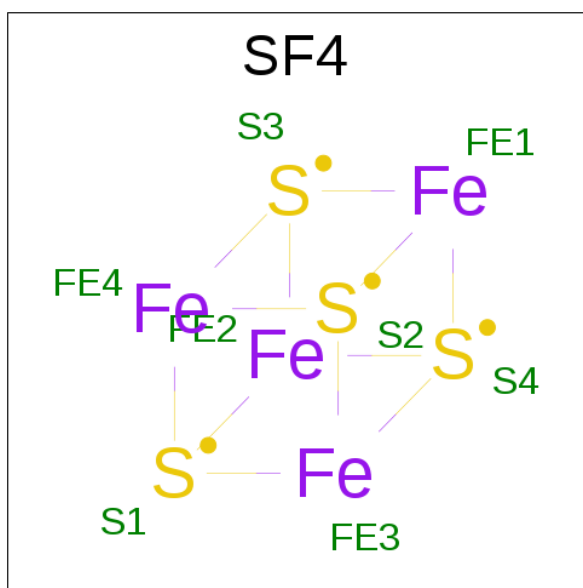
- Molecule 88 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

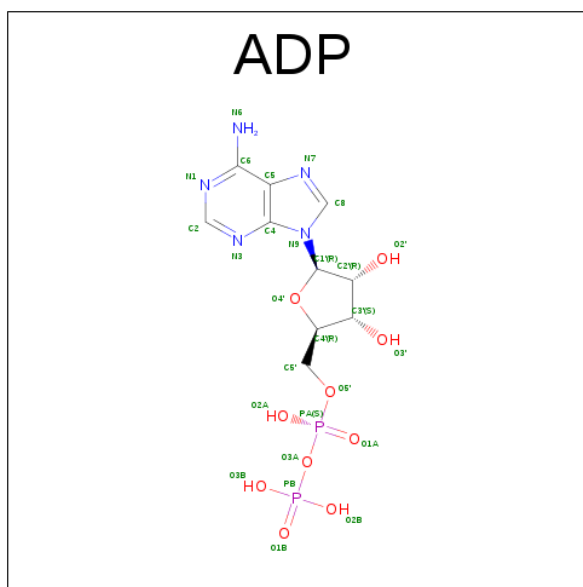
Mol	Chain	Residues	Atoms		AltConf
89	p	1	Total 1	Zn 1	0
89	g	1	Total 1	Zn 1	0
89	j	1	Total 1	Zn 1	0
89	dd	1	Total 1	Zn 1	0
89	ff	1	Total 1	Zn 1	0
89	aa	1	Total 1	Zn 1	0
89	o	1	Total 1	Zn 1	0
89	m	1	Total 1	Zn 1	0

- Molecule 90 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



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

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

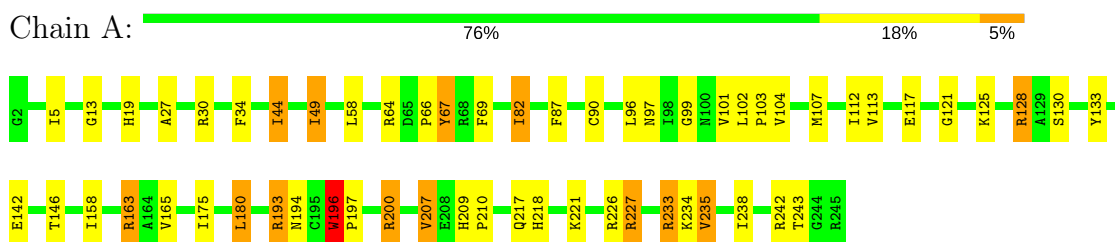


Mol	Chain	Residues	Atoms					AltConf
91	jj	1	Total	C	N	O	P	0
			54	20	10	20	4	
91	jj	1	Total	C	N	O	P	0
			54	20	10	20	4	

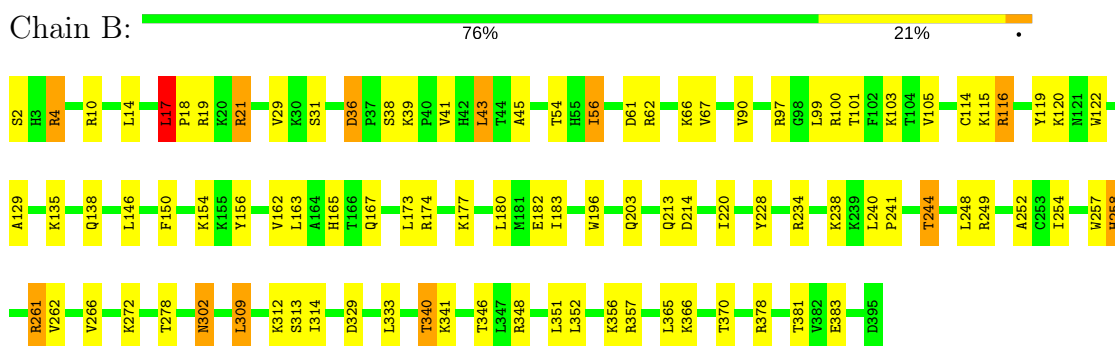
### 3 Residue-property plots

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.

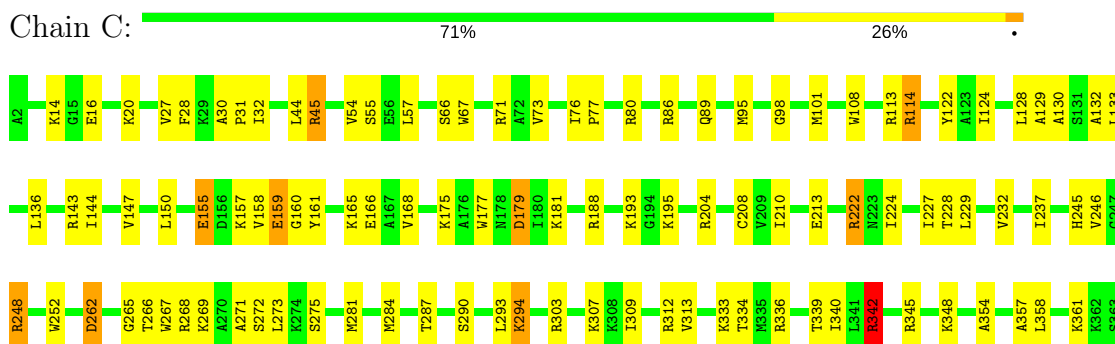
#### • Molecule 1: uL2



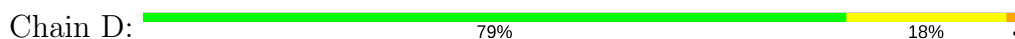
#### • Molecule 2: uL3

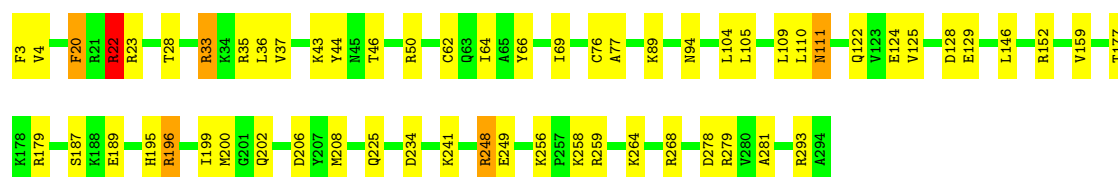


#### • Molecule 3: uL4

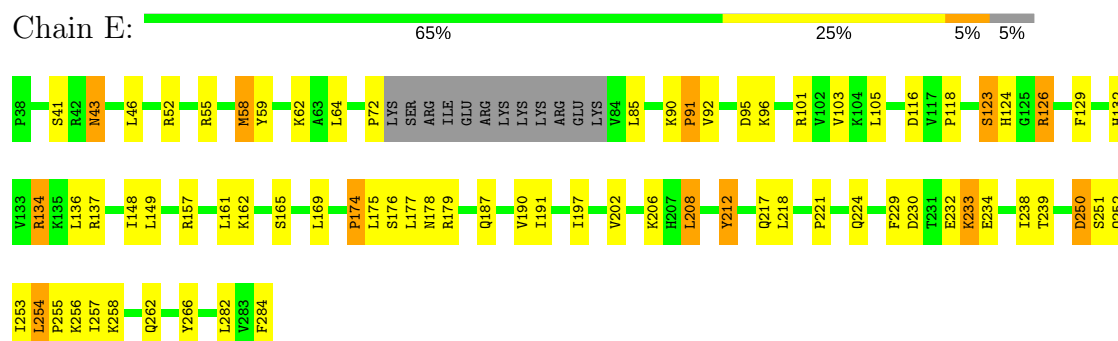


#### • Molecule 4: uL18

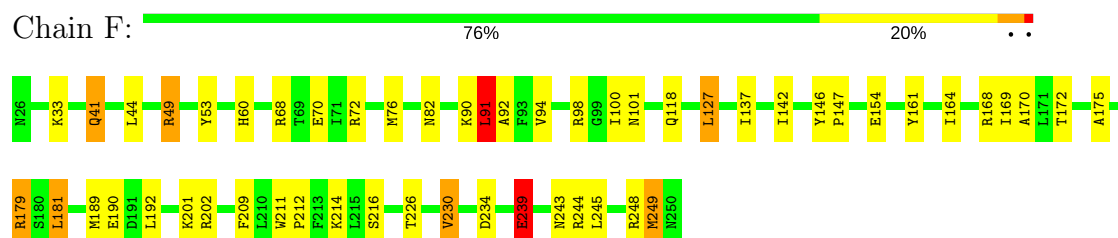




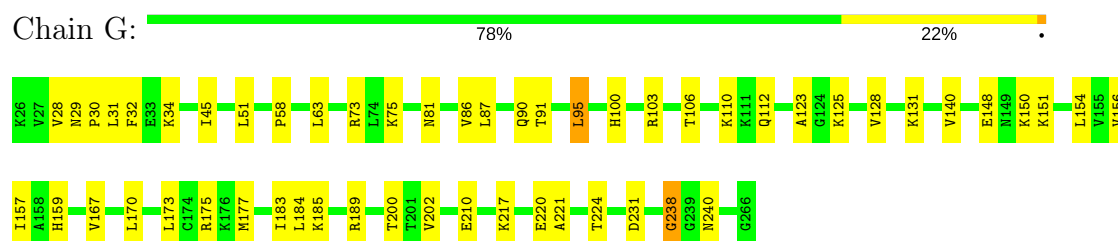
• Molecule 5: eL6



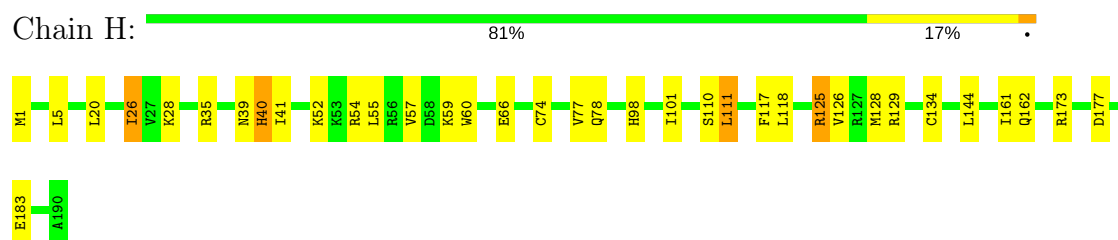
• Molecule 6: uL30



• Molecule 7: eL8

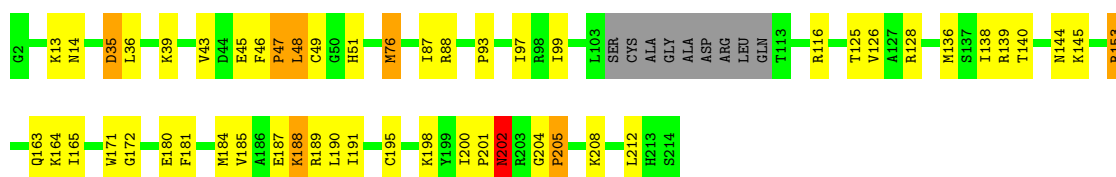


• Molecule 8: uL6



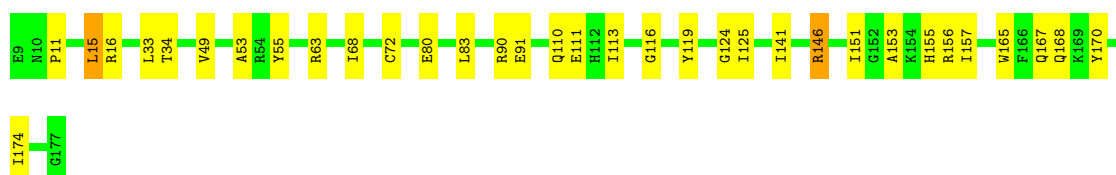
• Molecule 9: uL16





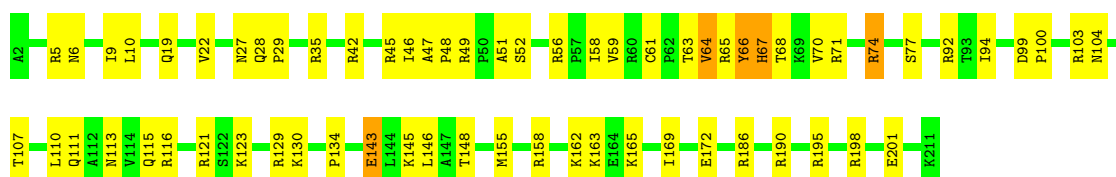
• Molecule 10: uL5

Chain J: 80% 19%



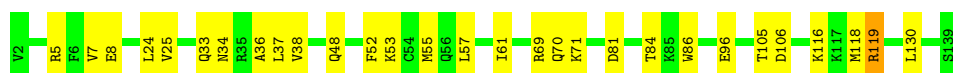
• Molecule 11: eL13

Chain L: 69% 29%



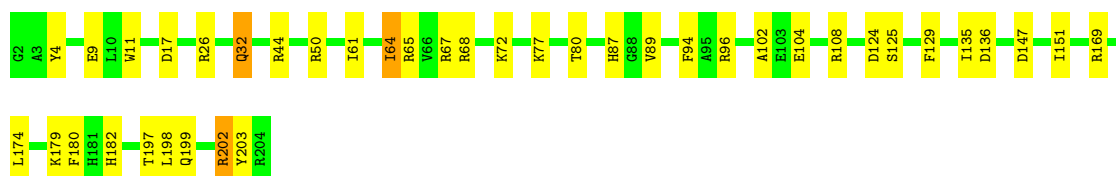
• Molecule 12: eL14

Chain M: 79% 20%



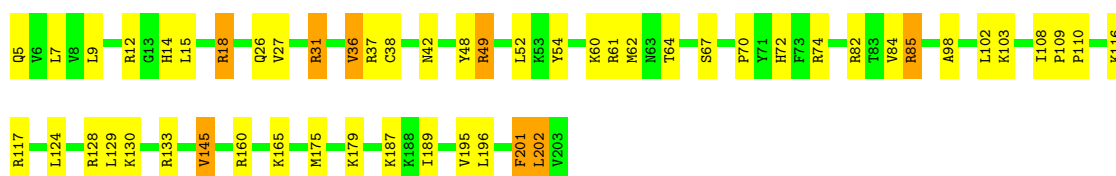
• Molecule 13: eL15

Chain N: 80% 18%




• Molecule 14: uL13

Chain O: 73% 23%




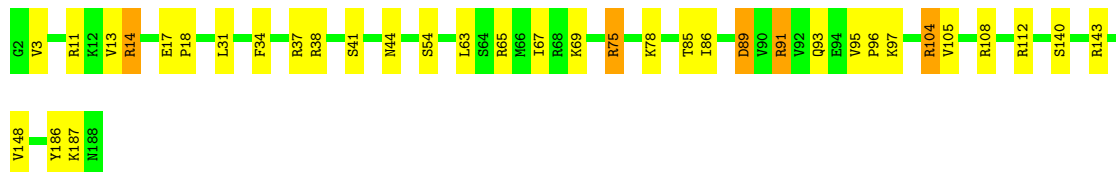
- Molecule 15: uL22

Chain P:  84% 14%



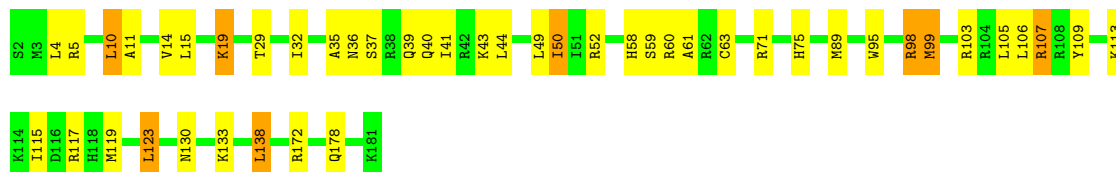
- Molecule 16: uL14

Chain Q:  81% 17%




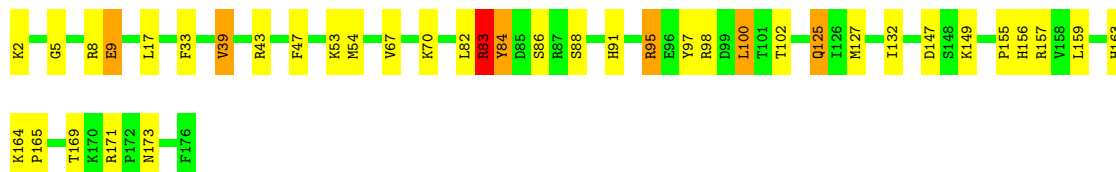
- Molecule 17: eL19

Chain R:  74% 21%




- Molecule 18: eL20

Chain S:  78% 18%




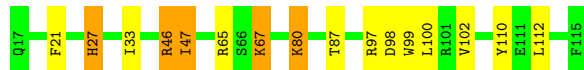
- Molecule 19: eL21

Chain T:  80% 19%




- Molecule 20: eL22

Chain U:  84% 11% 5%




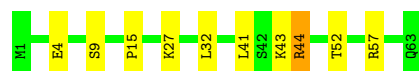
- Molecule 21: uL14

Chain V:  81% 18%




- Molecule 22: eL24

Chain W:  84% 14%




- Molecule 23: uL23

Chain X:  82% 16%



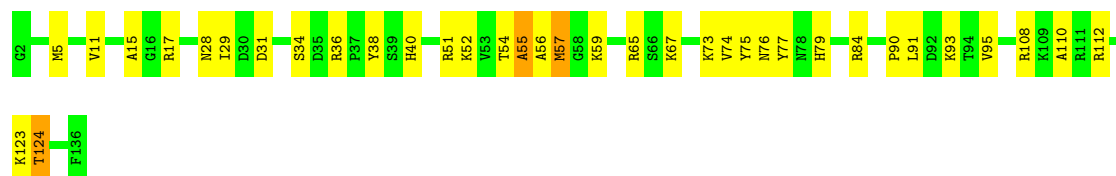
- Molecule 24: uL24

Chain Y:  81% 14%




- Molecule 25: eL27

Chain Z:  73% 24%



- Molecule 26: uL15

Chain a:  89% 11%




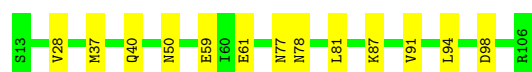
- Molecule 27: eL29

Chain b:  92% 8%




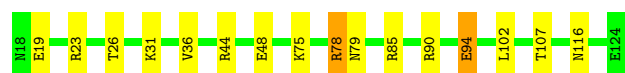
- Molecule 28: eL30

Chain c:  86% 14%




- Molecule 29: eL31

Chain d:  85% 13%




- Molecule 30: eL32

Chain e:  84% 16%




- Molecule 31: eL33

Chain f:  83% 17%



- Molecule 32: eL34

Chain g:  86% 13%




- Molecule 33: uL29

Chain h:  88% 11%




- Molecule 34: eL36

Chain i:  91% 9%

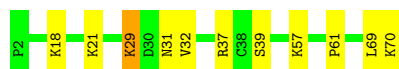
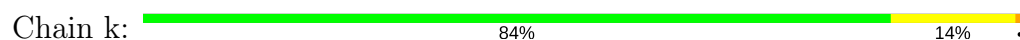


- Molecule 35: eL37

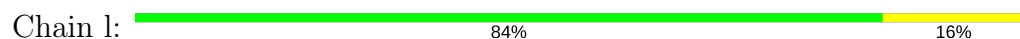
Chain j:  83% 15%



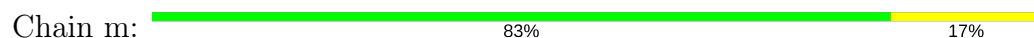
• Molecule 36: eL38



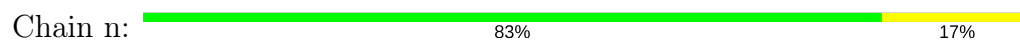
• Molecule 37: eL39



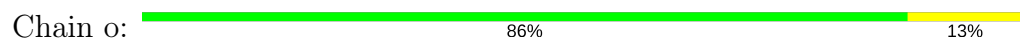
• Molecule 38: eL40



• Molecule 39: eL41



• Molecule 40: eL42




• Molecule 41: eL43

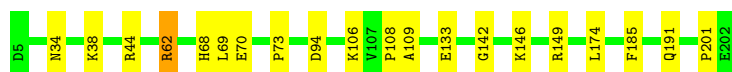


• Molecule 42: eL28




• Molecule 43: uL10

Chain s: 



• Molecule 44: uL11

Chain t: 



• Molecule 45: peptide

Chain 1: 



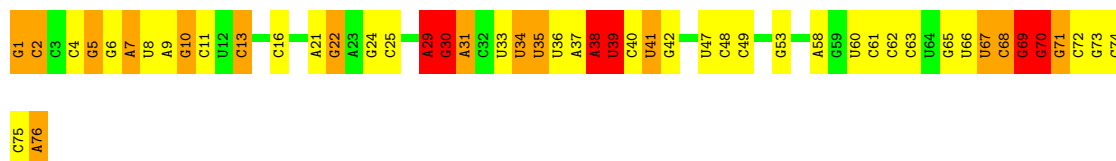
• Molecule 46: tRNA(Val)

Chain 2: 



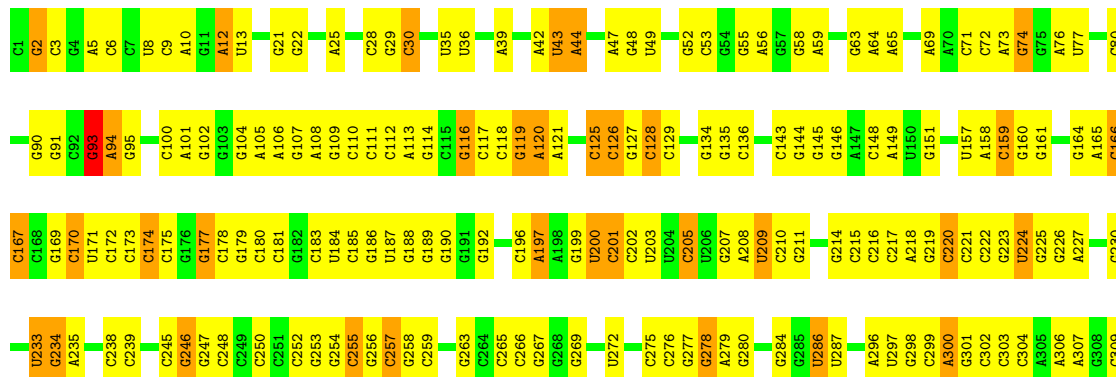
• Molecule 47: tRNA(Lys)

Chain 3: 



• Molecule 48: 28S ribosomal RNA

Chain 5: 

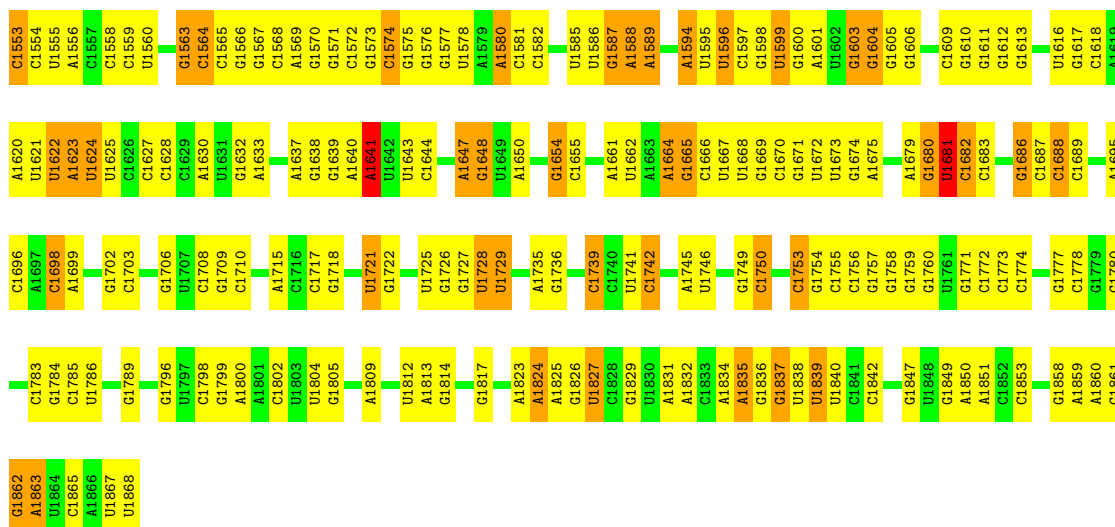


[illegible]

A4224	G4141	G4076	A3775	A3692	G3600	A2825	G2731	G2653	G2566	G2493	G2399	G2295	G2114	G2046
G4225	C4142	C4079	G3776	C3696	C3601	U2826	G2732	C2654	G2567	U2494	G2399	G2296	G2115	A2047
G4226	G4143		G3777	U3697	C3605	U2827	C2733	C2654	G2568	G2495	U2408	G2297	G2116	U2048
U4229	C4144		G3778	G3698	U3606	U2828	U2734	U2661	G2569	G2496	U2409	G2298	G2117	G2049
U4232	G4145		A3779			G2830	U2740	U2662	G2571	C2497	U2409	G2299	G2118	G2050
A4233	G4146		G3780	A3702	A3610	G2831	U2740	G2663	C2572	C2498	A2417	G2300	G2119	C2051
	G4147		C3781		A3611	G2832	A2743	G2664		C2499		G2301	G2120	G2052
	C4148		C3782		C3612	A2835	A2744	G2669	U2575	G2503	C2422	C2302	G2121	G2053
	G4152		A3783	G3705	G3615	U2838	G2752	C2669	G2576	C2504	A2423	C2311	G2122	U2054
	G4153		A3784	C3706	G3615	U2839	G2753	C2670	G2577	C2505	G2424	C2312	G2123	G2055
	G4154		U3785	G3707	G3616	G2842	G2754	C2671	G2578	G2506	U2425	G2313	G2124	G2056
	C4155		U3786	G3708	G3617	U2843	G2755	C2672	C2583	A2507	U2426	G2314	G2125	A2057
			C3788	G3710	C3618	U2844	A2755	G2673			A2428	G2315	G2126	G2058
			U3798	A3711	G3620	A2844	G2756	G2676	G2586	A2512	U2429		G2127	C2059
			A3799	G3712	G3620	U2844	G2757	A2676	U2587	A2513	U2429	G2322	G2128	C2062
			U3802	G3713	G3621	U2847	G2758	G2679	C2588	G2514	G2433	G2323	G2129	G2063
				G3714	A3624	G2847	G2759	U2680	G2590	G2515	G2434	C2324	G2130	G2064
				G3715	G3625	U2847	G2760	G2681	A2591	G2516	U2440	C2325	G2131	G2065
				G3716	G3626	U2855	G2761	G2682		A2517	U2441		G2245	C2066
				A3717	G3628	A2858	G2762	C2683	C2594	U2519	C2441	G2328	G2246	C2067
				A3719	A3630	G2859	U2763	G2686	A2601	G2520	U2447	G2331	C2247	A2068
				G3722		G2862	A2764	G2687	G2602	G2521		G2332	C2248	U2070
				A3723	A3635	U2869	U2767	G2688	G2602	U2524	G2450	C2333	G2250	A2071
				A3724		U2869	C2768	G2689		U2525		C2334	G2251	C2072
				G3725	U3641	U2870	U2769	G2690	G2606	U2526		C2335	G2252	C2073
				A3726	A3644	A2871	G2770	G2691	C2607	G2526	G2457	C2336	G2253	G2076
				A3727	U3644	C2872	G2771	G2692	G2608	C2527	G2458	C2337	G2254	G2077
				A3728	U3645	U2872	G2772	G2693	G2609	C2527	G2459	C2338	G2255	C2078
				A3729	U3646	U2889	G2773	G2694	G2610	U2530		G2345	G2256	C2079
				A3730	A3653	C2890	C2774	G2695	G2611			G2346	G2257	
				A3737	U3657	U2896	C2775	G2696	G2612	C2463		G2347	G2258	
				G3740	G3658	G2897	G2779	G2699	G2613	C2464		G2348	G2259	C2083
				A3748	G3659	G2898	A2783	G2703	G2614	C2465		G2349	G2260	C2084
				C3749	A3662	C2899	C2787	G2704	G2615	C2466		G2350	G2261	C2085
				G3750		U2904	U2788	U2708	G2616	U2467		G2351	G2262	
				G3751	C3668	G2905	U2789	C2709	G2617	C2468		G2352	A2263	A2088
				G3752	C3669	G2906	A2790	G2710	G2618	C2469		G2353	G2264	U2089
				G3753	C3670	G2907	G2793	G2711	G2619	C2470		G2354	G2265	U2090
				C3754	C3671	U2908	G2794	G2712	G2620	C2471		G2355	U2267	C2091
				G3755	G3672	C2909	C2795	G2713	G2621	C2472		G2356	G2268	G2092
				A3756	C3673	G2910	A2796	G2714	U2625	A2543		G2364	G2269	A2093
				A3759	G3674	G3586	G2797	G2715	U2626	G2544		G2367	G2270	G2094
				A3760	G3675	C3587	C2798	G2716	C2627	A2545		G2368	G2271	A2095
								G2720	U2628	G2546		G2369	G2272	G2096
								G2721	U2629	G2547		A2370	G2273	U2097
								G2722	C2629	G2548		G2376	G2274	A2100
								G2723		A2553		A2377	G2275	G2102
								U2724	U2632	U2554		C2377	G2103	G2107
								G2725	U2633	G2555		A2382	G2108	C2107
								G2726	G2638	G2556		A2382	G2109	G2108
								G2727	U2639	G2557		U2382	G2110	G2109
								G2728	G2640	G2558		U2385	G2111	G2110
								U2729	G2645	G2559		A2395	G2112	G2111
								G2730	C2646	G2560		A2396	G2113	G2112
									A2647			C2492	G2294	G2113

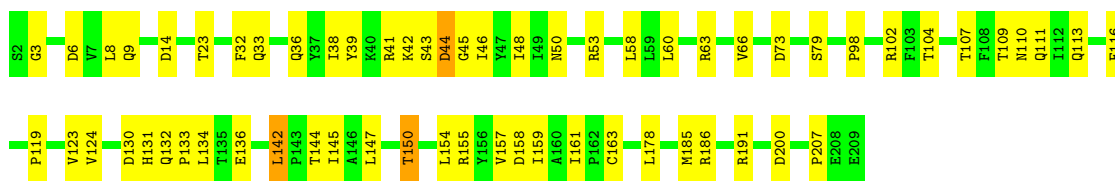


U1485	G1330	G1256	G1181	G1098	G971	G878	C790	U637	A555	G380	A301	U157	G70	U1
A1486	C1331	G1257	A1181	G1099	G978	C879	C791	G638	U556	G383	A302	A158	G71	A2
A1487	U1332	A1258	G1184	A1100	G980	G880	C792	C639	U557	U384	C303	A159	C72	C3
A1488	U1333	A1259	C1185	U1101	G979	G881	C793	A640	G558	G385	C304	U161	C73	C4
A1489	G1334	A1260	C1186	C1102	A980	U887	A794	A641	G559	U386	U305	U162	G74	U5
G1490	G1335	A1261	A1189	G1103	A981	U888	A795	A642	A560	C387	C306	U163	G75	G6
G1491	C1336	C1262	A1190	C1104	G982	U889	C796	A643	A561	C391	C307	U164	U76	U6
U1492	C1337	C1263	A1191	G1105	G983	U890	C797	G644	U562	U392	G308	U165	A77	U9
C1493	U1342	C1264	A1192	C1106	G984	U891	C798	A654	U563	A398	C309	A166	C78	G10
U1494	G1343	C1265	A1193	U1110	A990	U892	U799	U658	G564	U399	C310	G167	A79	A11
U1495	U1344	G1270	A1194	U1111	A991	U893	U800	C663	C568	C400	C311	C168	G80	U12
U1496	G1345	C1271	G1198	U1112	A992	G901	A810	U659	A576	U487	C312	U172	C86	G14
C1497	U1346	C1272	G1199	U1113	A993	G902	A811	C660	U577	U488	A313	A173	U87	U15
A1498	U1347	G1274	G1207	U1114	G993	G903	A812	U667	U578	A489	U314	G180	G88	G16
U1499	G1348	G1275	A1208	U1115	G994	A903	U821	U668	C579	C490	C315	C181	G89	C17
G1500	U1349	A1276	A1209	C1116	G995	G904	U822	A664	C580	C491	C316	A182	C90	C18
C1501	G1350	C1277	G1210	C1117	A996	U908	U823	U669	A583	C492	C317	C183	A92	A19
G1507	G1351	C1278	G1211	C1118	A997	G909	U824	U670	A584	C493	G320	C184	U93	G23
G1510	U1372	G1280	G1212	U1120	A998	G910	U825	U671	A585	U489	C321	C185	U94	G24
G1511	G1354	A1281	C1213	U1121	G999	C911	C924	U672	A586	U490	C322	C186	U95	A25
C1512	U1364	C1282	C1214	A1122	C1000	C912	A827	U673	A587	C495	C323	C187	C96	U26
G1515	U1371	A1283	C1215	U1123	U1002	U914	G828	A670	G590	U418	C324	G187	U99	G29
G1516	U1372	G1285	G1216	C1125	C1007	U915	C829	A671	U591	C325	C325	U188	U100	C30
G1517	U1373	C1286	A1217	C1126	G1008	A916	A830	A672	C592	C326	C326	U189	U101	U31
C1520	G1374	A1287	C1218	C1127	A1009	U917	C831	U674	C593	U427	C327	G190	U102	U32
G1521	U1375	U1288	C1219	U1128	A1010	U918	G832	C675	A594	U428	U328	C191	A103	G32
C1522	G1376	U1289	G1220	C1129	G995	A919	C833	U676	U595	C429	G338	C192	A104	U33
G1523	U1377	G1290	G1221	U1130	U1016	U920	C834	U677	U596	U430	G339	C193	U105	G37
G1524	A1378	A1291	G1222	C1131	U1017	G921	C835	U678	U597	U431	A339	C194	U106	U34
C1525	U1379	C1292	G1223	U1132	A1023	A922	A837	U679	G598	U432	C340	C195	U107	U35
G1526	G1380	A1293	C1224	C1133	C1033	C930	G838	U680	A599	U433	C341	G200	U108	G41
C1527	U1381	G1294	G1225	U1134	G1034	G933	C940	U681	A599	U434	C342	G201	U109	A42
G1528	G1384	A1295	A1228	C1135	U1035	G934	G841	U682	A599	U435	C343	G202	U110	U43
C1529	U1385	C1230	C1229	U1136	G1040	G935	C942	U683	A599	U436	C344	G203	U111	U44
U1530	A1386	C1231	C1230	C1137	G1041	G936	C943	U684	A599	U437	C345	G204	U112	A45
G1531	G1387	U1302	U1232	C1138	G1042	G937	C944	U685	A599	U438	C346	G205	U113	A46
C1532	U1388	A1301	U1233	C1139	G1043	A938	G845	U686	A599	U439	C347	G206	U114	A47
G1533	G1389	C1302	G1234	U1140	U1044	G942	G846	U687	A599	U440	C348	G207	U115	C47
C1534	U1390	C1303	G1235	C1141	U1045	U943	C947	U688	A599	U441	C349	G208	U116	C48
U1535	U1391	U1307	C1236	U1142	A1049	G944	A847	U689	A599	U442	C350	G209	U117	U49
G1536	G1392	U1308	C1237	U1143	G1054	U945	C953	U690	A599	U443	C351	G210	U118	U51
C1537	U1393	C1309	A1240	C1144	U1058	U946	C956	U691	A599	U444	C352	G211	U119	C52
G1538	U1400	U1310	U1241	C1145	A1059	U947	C957	U692	A599	U445	C353	G212	U120	C53
C1539	A1401	C1311	U1242	U1146	G1068	U948	C958	U693	A599	U446	C354	G213	U121	A54
U1540	U1402	G1312	U1243	C1147	A1069	G949	G859	U694	A599	U447	C355	G214	U122	U55
G1541	C1403	A1313	U1244	U1148	A1070	U950	G860	U695	A599	U448	C356	G215	U123	G56
C1542	U1404	G1314	G1245	U1149	C1075	C951	A861	U696	A599	U449	C357	G216	U124	U57
U1543	U1405	U1315	A1246	C1153	A1083	G956	A869	U697	A599	U450	C358	G217	U125	C58
G1544	A1406	C1316	C1247	U1154	A1084	G957	A870	U698	A599	U451	C359	G218	U126	U59
C1545	U1407	U1316	U1248	U1155	C1085	U958	U871	U699	A599	U452	C360	G219	U127	A60
U1546	U1408	G1317	C1249	U1156	C1086	G959	C872	U700	A599	U453	C361	G220	U128	G62
G1547	U1409	C1321	U1250	U1157	C1087	U960	C873	U701	A599	U454	C362	G221	U129	U63
C1548	U1410	U1322	G1251	G1164	G1089	A963	G874	U702	A599	U455	C363	G222	U130	A64
U1551	G1411	U1323	C1252	G1165	C1090	A964	C875	U703	A599	U456	C364	G223	U131	G65
G1552	U1412	U1324	G1253	G1166	C1091	A965	C876	U704	A599	U457	C365	G224	U132	G66
C1553	A1413	U1325	G1254	G1167	C1092	A966	C877	U705	A599	U458	C366	G225	U133	C67
G1554	U1414	G1255	G1255	A1170	C1093	G970	C878	U706	A599	U459	C367	G226	U134	G68



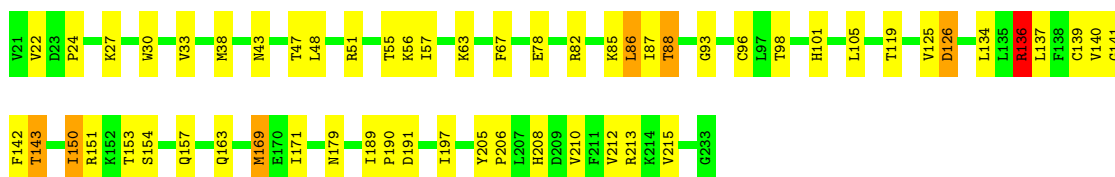
• Molecule 52: uS2

Chain AA: 70% 28%



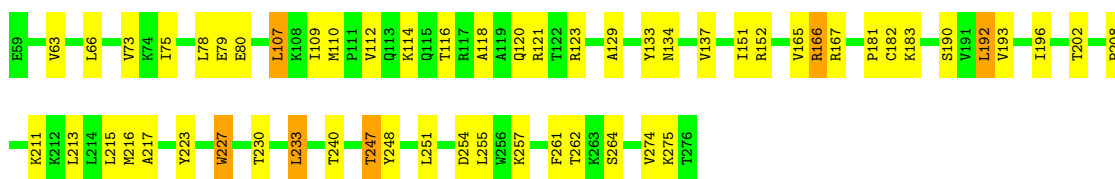
• Molecule 53: eS1

Chain BB: 73% 23%



• Molecule 54: uS5

Chain CC: 74% 23%



• Molecule 55: uS3

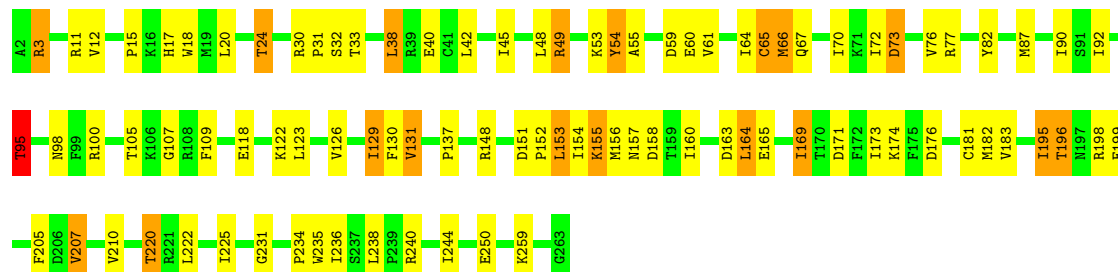
Chain DD: 81% 18%





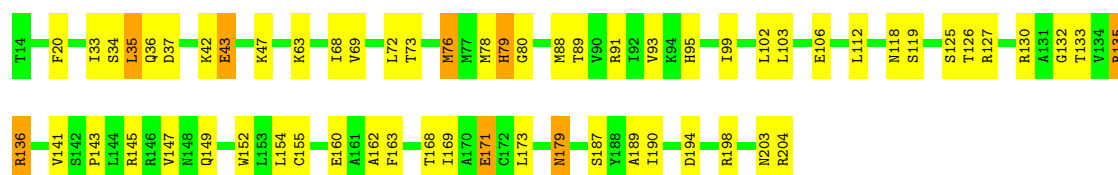
• Molecule 56: eS4

Chain EE: 65% 27% 7%



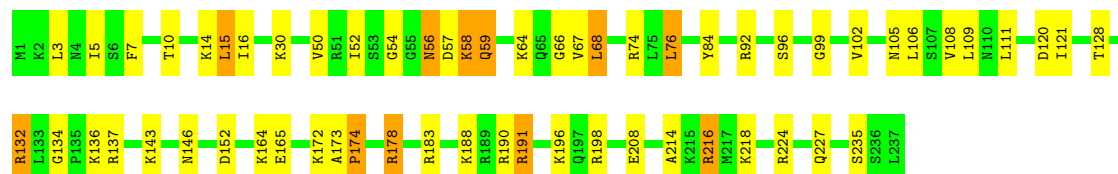
• Molecule 57: uS7

Chain FF: 68% 28% 4%



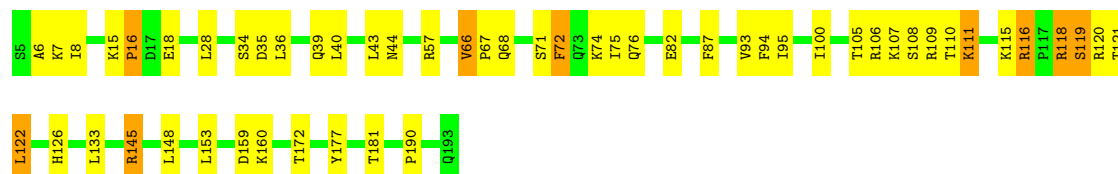
• Molecule 58: eS6

Chain GG: 75% 21% 4%



• Molecule 59: eS7

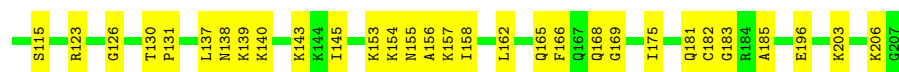
Chain HH: 71% 24% 5%



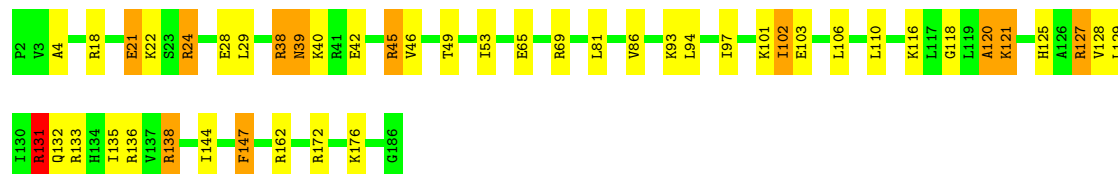
• Molecule 60: eS8

Chain II: 69% 30% 1%





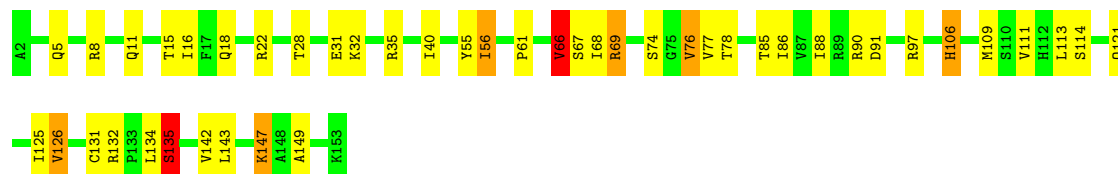
• Molecule 61: uS4



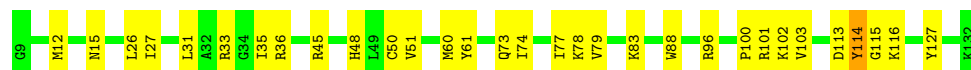
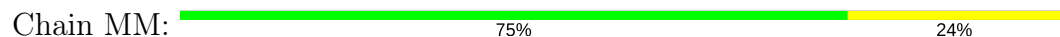
• Molecule 62: eS10



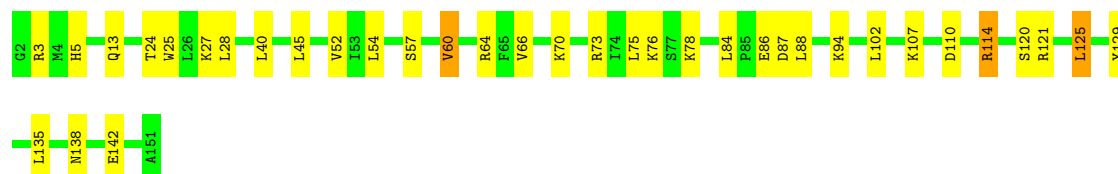
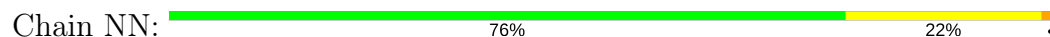
• Molecule 63: uS17



• Molecule 64: eS12

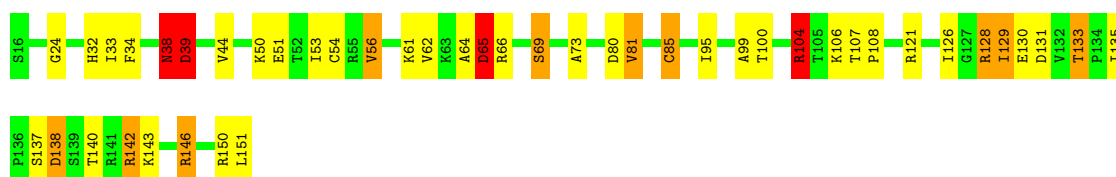


• Molecule 65: uS15



• Molecule 66: uS11





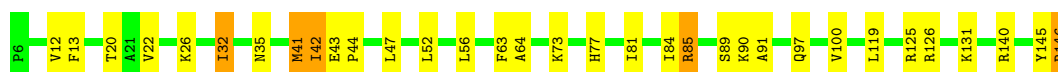
- Molecule 67: uS19

Chain PP: 75% 21% •



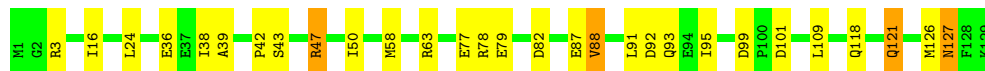
- Molecule 68: uS9

Chain QQ: 77% 20% •



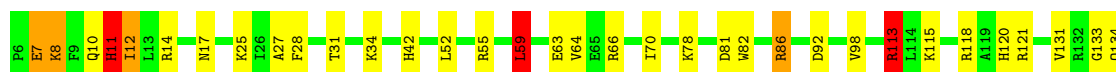
- Molecule 69: eS17

Chain RR: 78% 19% •



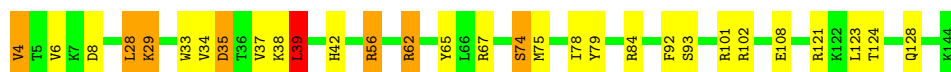
- Molecule 70: uS13

Chain SS: 74% 20% • •



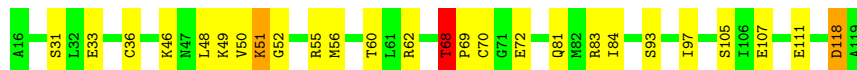
- Molecule 71: eS19

Chain TT: 79% 16% 5% •




- Molecule 72: uS10

Chain UU: 75% 22% • •



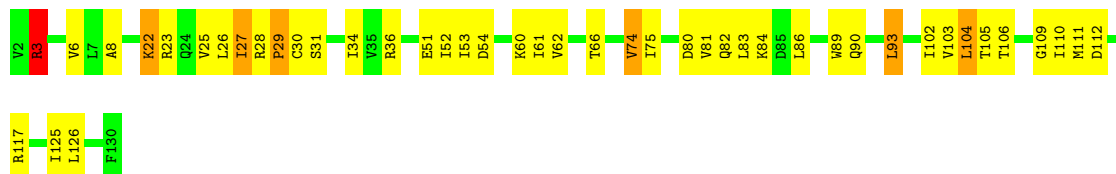
- Molecule 73: eS21

Chain VV:  73% 24% .



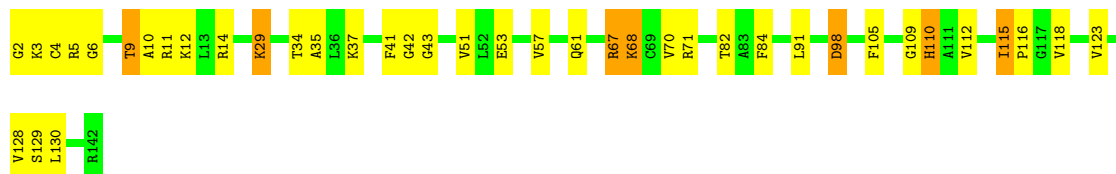
- Molecule 74: uS8

Chain WW:  65% 29% 5% .



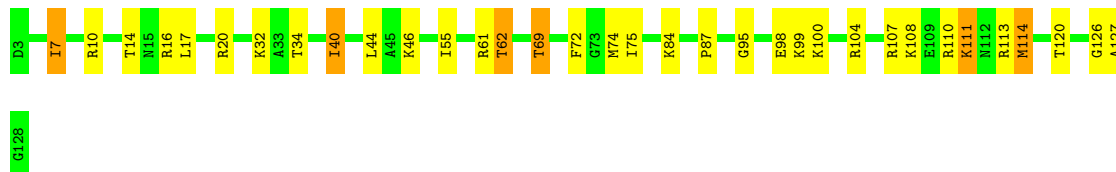
- Molecule 75: uS12

Chain XX:  72% 23% 5%




- Molecule 76: eS24

Chain YY:  73% 22% 5%




- Molecule 77: eS25

Chain ZZ:  77% 23%




- Molecule 78: eS26

Chain aa:  81% 19%



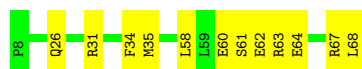
- Molecule 79: eS27

Chain bb:  80% 20%



• Molecule 80: eS28

Chain cc: 80% 20%



• Molecule 81: uS14

Chain dd: 81% 19%



• Molecule 82: eS30

Chain ee: 82% 16%



• Molecule 83: eS31

Chain ff: 87% 9%



• Molecule 84: RACK1

Chain gg: 90% 9%



• Molecule 85: mRNA

Chain hh: 42% 58%



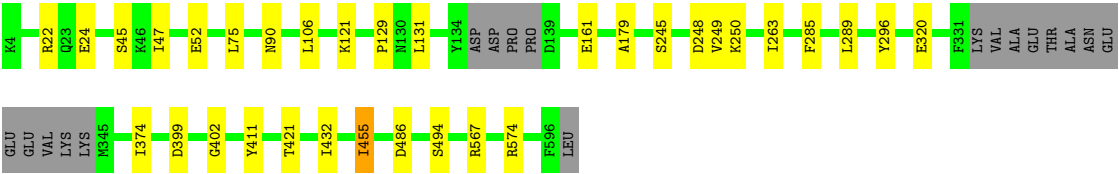
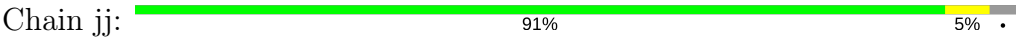
• Molecule 86: eRF1

Chain ii: 89% 10%





● Molecule 87: ABCE1



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	20515	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	0.46	0/1906	0.79	0/2556
10	J	0.38	0/1376	0.73	0/1841
11	L	0.41	0/1734	0.79	0/2317
12	M	0.37	0/1158	0.74	0/1547
13	N	0.43	0/1746	0.83	0/2338
14	O	0.40	0/1671	0.77	0/2234
15	P	0.42	0/1268	0.75	0/1701
16	Q	0.41	0/1530	0.81	1/2041 (0.0%)
17	R	0.41	0/1524	0.79	0/2013
18	S	0.40	0/1493	0.85	3/2002 (0.1%)
19	T	0.41	0/1326	0.72	0/1770
2	B	0.40	0/3216	0.78	1/4311 (0.0%)
20	U	0.41	0/822	0.68	0/1103
21	V	0.40	0/993	0.73	0/1332
22	W	0.48	0/541	0.83	1/720 (0.1%)
23	X	0.42	0/993	0.74	0/1334
24	Y	0.37	0/1132	0.80	2/1504 (0.1%)
25	Z	0.39	0/1130	0.72	0/1507
26	a	0.40	0/1191	0.79	0/1590
27	b	0.44	0/619	0.73	0/818
28	c	0.36	0/742	0.69	0/996
29	d	0.38	0/903	0.81	1/1216 (0.1%)
3	C	0.43	0/2938	0.80	5/3946 (0.1%)
30	e	0.47	0/1071	0.85	0/1429
31	f	0.52	0/895	0.87	0/1198
32	g	0.42	0/916	0.81	1/1220 (0.1%)
33	h	0.36	0/1021	0.77	1/1348 (0.1%)
34	i	0.40	0/841	0.82	2/1112 (0.2%)
35	j	0.45	0/720	0.93	1/952 (0.1%)
36	k	0.37	0/575	0.68	0/761
37	l	0.50	0/454	0.84	0/599
38	m	0.37	0/435	0.76	0/575

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
39	n	0.41	0/223	0.91	0/284
4	D	0.37	0/2432	0.70	2/3257 (0.1%)
40	o	0.39	0/864	0.75	0/1140
41	p	0.42	0/718	0.71	0/953
42	r	0.48	0/1017	0.80	1/1364 (0.1%)
43	s	0.38	0/1547	0.58	0/2088
44	t	0.41	0/1257	0.69	0/1697
45	1	0.45	0/129	0.72	0/173
46	2	0.26	0/1805	0.72	1/2809 (0.0%)
47	3	0.36	0/1777	0.97	10/2763 (0.4%)
48	5	0.37	4/87790 (0.0%)	0.79	75/136937 (0.1%)
49	7	0.30	0/2858	0.69	0/4455
5	E	0.46	0/1936	0.82	2/2600 (0.1%)
50	8	0.36	0/3701	0.74	0/5766
51	9	0.32	1/41013 (0.0%)	0.79	45/63919 (0.1%)
52	AA	0.36	0/1679	0.70	0/2283
53	BB	0.38	0/1756	0.77	4/2350 (0.2%)
54	CC	0.41	0/1730	0.76	1/2344 (0.0%)
55	DD	0.37	0/1792	0.72	0/2412
56	EE	0.39	0/2115	0.78	0/2843
57	FF	0.49	0/1531	0.78	1/2059 (0.0%)
58	GG	0.37	0/1946	0.78	0/2590
59	HH	0.44	0/1544	0.72	1/2068 (0.0%)
6	F	0.40	0/1905	0.75	1/2539 (0.0%)
60	II	0.41	0/1715	0.78	0/2287
61	JJ	0.41	0/1550	0.88	4/2069 (0.2%)
62	KK	0.47	0/851	0.73	0/1147
63	LL	0.40	0/1259	0.78	0/1684
64	MM	0.42	0/968	0.64	0/1296
65	NN	0.39	0/1232	0.77	0/1656
66	OO	0.42	0/1029	0.88	1/1380 (0.1%)
67	PP	0.39	0/1079	0.76	0/1437
68	QQ	0.37	0/1142	0.70	0/1528
69	RR	0.42	0/1060	0.71	0/1421
7	G	0.38	0/1967	0.73	1/2647 (0.0%)
70	SS	0.38	0/1157	0.84	1/1548 (0.1%)
71	TT	0.43	0/1120	0.78	2/1499 (0.1%)
72	UU	0.36	0/831	0.71	0/1115
73	VV	0.39	0/645	0.75	0/865
74	WW	0.38	0/1051	0.79	0/1406
75	XX	0.38	0/1116	0.80	0/1490
76	YY	0.39	0/1040	0.74	0/1382
77	ZZ	0.37	0/604	0.75	0/810

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
78	aa	0.39	0/794	0.83	0/1065
79	bb	0.37	0/665	0.67	0/891
8	H	0.37	0/1535	0.71	0/2063
80	cc	0.36	0/478	0.78	0/640
81	dd	0.40	0/455	0.80	0/603
82	ee	0.46	0/462	0.75	0/607
83	ff	0.39	0/531	0.62	0/703
84	gg	0.37	0/2493	0.65	0/3394
85	hh	0.29	0/287	0.76	0/445
86	ii	0.39	0/3333	0.63	2/4483 (0.0%)
87	jj	0.47	1/4625 (0.0%)	0.58	0/6238
9	I	0.41	0/1693	0.69	0/2260
All	All	0.38	6/242712 (0.0%)	0.78	174/355683 (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
1	A	0	1
11	L	0	3
17	R	0	1
18	S	0	2
19	T	0	1
2	B	0	4
20	U	0	1
24	Y	0	1
3	C	0	2
31	f	0	1
4	D	0	1
42	r	0	2
48	5	0	1
5	E	0	1
51	9	0	1
52	AA	0	1
56	EE	0	2
57	FF	0	2
59	HH	0	1
60	II	0	1
61	JJ	0	2
66	OO	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
68	QQ	0	1
7	G	0	1
70	SS	0	1
71	TT	0	1
72	UU	0	2
73	VV	0	1
74	WW	0	2
75	XX	0	1
78	aa	0	1
86	ii	0	3
9	I	0	2
All	All	0	49

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	5	1965	G	O3'-P	-23.01	1.33	1.61
87	jj	121	LYS	CE-NZ	19.94	1.99	1.49
51	9	908	A	O3'-P	8.98	1.72	1.61
48	5	1847	C	O3'-P	-6.16	1.53	1.61
48	5	957	G	O3'-P	5.62	1.67	1.61

The worst 5 of 174 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	9	909	G	O5'-P-OP2	-16.21	91.11	105.70
47	3	70	G	N9-C1'-C2'	-13.18	96.87	114.00
48	5	3753	G	N9-C1'-C2'	-11.91	98.52	114.00
51	9	1235	G	N9-C1'-C2'	-11.46	99.11	114.00
48	5	3718	A	N9-C1'-C2'	-10.30	100.61	114.00

There are no chirality outliers.

5 of 49 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	196	TRP	Peptide
2	B	17	LEU	Peptide
2	B	257	TRP	Peptide
2	B	258	HIS	Peptide
2	B	351	LEU	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1868	0	1959	31	0
2	B	3148	0	3267	55	0
3	C	2884	0	3062	45	0
4	D	2386	0	2419	31	0
5	E	1898	0	2035	66	0
6	F	1870	0	1994	27	0
7	G	1934	0	2087	32	0
8	H	1516	0	1597	10	0
9	I	1655	0	1704	45	0
10	J	1353	0	1386	16	0
11	L	1703	0	1820	22	0
12	M	1137	0	1211	16	0
13	N	1701	0	1749	18	0
14	O	1638	0	1777	31	0
15	P	1242	0	1269	12	0
16	Q	1506	0	1623	14	0
17	R	1508	0	1664	31	0
18	S	1454	0	1496	14	0
19	T	1298	0	1366	11	0
20	U	808	0	831	5	0
21	V	979	0	1039	5	0
22	W	528	0	541	5	0
23	X	976	0	1053	8	0
24	Y	1115	0	1205	6	0
25	Z	1107	0	1182	16	0
26	a	1162	0	1209	0	0
27	b	609	0	650	0	0
28	c	732	0	769	0	0
29	d	888	0	930	0	0
30	e	1053	0	1147	0	0
31	f	876	0	912	0	0
32	g	906	0	999	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	m	429	0	466	0	0
39	n	222	0	264	0	0
40	o	851	0	921	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	3	0
46	2	1616	0	824	18	0
47	3	1593	0	811	79	0
48	5	78486	0	39663	1322	0
49	7	2558	0	1296	27	0
50	8	3314	0	1683	53	0
51	9	36680	0	18529	615	0
52	AA	1642	0	1646	22	0
53	BB	1729	0	1803	15	0
54	CC	1692	0	1780	22	0
55	DD	1764	0	1863	8	0
56	EE	2073	0	2175	45	0
57	FF	1509	0	1562	28	0
58	GG	1923	0	2089	29	0
59	HH	1521	0	1616	20	0
60	II	1686	0	1772	30	0
61	JJ	1525	0	1640	22	0
62	KK	827	0	854	7	0
63	LL	1238	0	1315	17	0
64	MM	958	0	993	3	0
65	NN	1208	0	1294	8	0
66	OO	1016	0	1039	14	0
67	PP	1060	0	1120	13	0
68	QQ	1124	0	1193	11	0
69	RR	1047	0	1103	9	0
70	SS	1139	0	1191	17	0
71	TT	1102	0	1142	11	0
72	UU	821	0	883	6	0
73	VV	636	0	634	9	0
74	WW	1034	0	1080	23	0
75	XX	1098	0	1167	11	0
76	YY	1023	0	1090	11	0
77	ZZ	598	0	656	6	0
78	aa	781	0	828	0	0
79	bb	651	0	672	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	4543	0	4674	0	0
88	5	146	0	0	0	0
88	7	5	0	0	0	0
88	8	2	0	0	0	0
88	9	34	0	0	0	0
88	B	1	0	0	0	0
88	C	1	0	0	0	0
88	I	1	0	0	0	0
88	LL	1	0	0	0	0
88	P	1	0	0	0	0
88	V	1	0	0	0	0
88	g	1	0	0	0	0
88	hh	1	0	0	0	0
89	aa	1	0	0	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	226454	0	169855	2802	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 2802 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)
51:9:1137:U:O4	51:9:1148:A:N1	1.61	1.34
48:5:976:G:H2'	48:5:977:C:O4'	1.26	1.32
17:R:172:ARG:NH1	51:9:908:A:H5''	1.47	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:2367:A:N1	48:5:2788:U:O4	1.66	1.29
5:E:126:ARG:NH1	48:5:712:C:H1'	1.49	1.27

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	242/244 (99%)	209 (86%)	28 (12%)	5 (2%)	8	44
2	B	392/394 (100%)	345 (88%)	42 (11%)	5 (1%)	14	54
3	C	360/362 (99%)	322 (89%)	27 (8%)	11 (3%)	5	36
4	D	290/292 (99%)	262 (90%)	25 (9%)	3 (1%)	18	60
5	E	232/248 (94%)	179 (77%)	36 (16%)	17 (7%)	1	13
6	F	223/225 (99%)	204 (92%)	17 (8%)	2 (1%)	20	63
7	G	239/241 (99%)	203 (85%)	31 (13%)	5 (2%)	8	44
8	H	188/190 (99%)	165 (88%)	20 (11%)	3 (2%)	11	50
9	I	200/213 (94%)	181 (90%)	15 (8%)	4 (2%)	9	45
10	J	167/169 (99%)	147 (88%)	13 (8%)	7 (4%)	3	28
11	L	208/210 (99%)	180 (86%)	16 (8%)	12 (6%)	2	19
12	M	136/138 (99%)	123 (90%)	12 (9%)	1 (1%)	25	67
13	N	201/203 (99%)	181 (90%)	20 (10%)	0	100	100
14	O	197/199 (99%)	184 (93%)	12 (6%)	1 (0%)	32	73
15	P	151/153 (99%)	135 (89%)	16 (11%)	0	100	100
16	Q	185/187 (99%)	169 (91%)	14 (8%)	2 (1%)	17	58
17	R	178/180 (99%)	166 (93%)	9 (5%)	3 (2%)	11	49
18	S	173/175 (99%)	157 (91%)	12 (7%)	4 (2%)	7	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	T	157/159 (99%)	139 (88%)	15 (10%)	3 (2%)	9	46
20	U	97/99 (98%)	82 (84%)	11 (11%)	4 (4%)	3	29
21	V	129/131 (98%)	115 (89%)	13 (10%)	1 (1%)	22	65
22	W	61/63 (97%)	56 (92%)	4 (7%)	1 (2%)	11	50
23	X	117/119 (98%)	109 (93%)	6 (5%)	2 (2%)	11	49
24	Y	132/134 (98%)	114 (86%)	17 (13%)	1 (1%)	22	65
25	Z	133/135 (98%)	113 (85%)	13 (10%)	7 (5%)	2	21
26	a	145/147 (99%)	122 (84%)	19 (13%)	4 (3%)	6	38
27	b	73/75 (97%)	67 (92%)	5 (7%)	1 (1%)	13	52
28	c	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
29	d	105/107 (98%)	91 (87%)	13 (12%)	1 (1%)	18	60
30	e	126/128 (98%)	115 (91%)	6 (5%)	5 (4%)	3	29
31	f	107/109 (98%)	94 (88%)	8 (8%)	5 (5%)	3	25
32	g	112/114 (98%)	103 (92%)	8 (7%)	1 (1%)	20	63
33	h	120/122 (98%)	107 (89%)	9 (8%)	4 (3%)	4	34
34	i	100/102 (98%)	92 (92%)	6 (6%)	2 (2%)	9	45
35	j	84/86 (98%)	70 (83%)	9 (11%)	5 (6%)	2	18
36	k	67/69 (97%)	56 (84%)	7 (10%)	4 (6%)	2	18
37	l	48/50 (96%)	40 (83%)	7 (15%)	1 (2%)	8	44
38	m	50/52 (96%)	44 (88%)	6 (12%)	0	100	100
39	n	21/23 (91%)	21 (100%)	0	0	100	100
40	o	102/104 (98%)	92 (90%)	7 (7%)	3 (3%)	5	37
41	p	89/91 (98%)	80 (90%)	8 (9%)	1 (1%)	17	58
42	r	123/125 (98%)	102 (83%)	14 (11%)	7 (6%)	2	20
43	s	196/198 (99%)	164 (84%)	22 (11%)	10 (5%)	2	22
44	t	161/163 (99%)	102 (63%)	33 (20%)	26 (16%)	0	2
45	1	13/15 (87%)	11 (85%)	0	2 (15%)	0	3
52	AA	206/208 (99%)	173 (84%)	23 (11%)	10 (5%)	2	23
53	BB	211/213 (99%)	165 (78%)	33 (16%)	13 (6%)	2	18
54	CC	216/218 (99%)	184 (85%)	26 (12%)	6 (3%)	6	38
55	DD	225/227 (99%)	181 (80%)	33 (15%)	11 (5%)	2	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
56	EE	260/262 (99%)	200 (77%)	42 (16%)	18 (7%)	1	15
57	FF	189/191 (99%)	160 (85%)	21 (11%)	8 (4%)	3	28
58	GG	235/237 (99%)	198 (84%)	31 (13%)	6 (3%)	6	39
59	HH	187/189 (99%)	148 (79%)	25 (13%)	14 (8%)	1	13
60	II	204/206 (99%)	168 (82%)	28 (14%)	8 (4%)	3	30
61	JJ	183/185 (99%)	153 (84%)	20 (11%)	10 (6%)	2	20
62	KK	96/98 (98%)	65 (68%)	21 (22%)	10 (10%)	0	7
63	LL	150/152 (99%)	125 (83%)	19 (13%)	6 (4%)	3	29
64	MM	122/124 (98%)	87 (71%)	28 (23%)	7 (6%)	2	20
65	NN	148/150 (99%)	126 (85%)	17 (12%)	5 (3%)	4	34
66	OO	134/136 (98%)	99 (74%)	21 (16%)	14 (10%)	0	7
67	PP	125/127 (98%)	107 (86%)	15 (12%)	3 (2%)	7	42
68	QQ	139/141 (99%)	116 (84%)	18 (13%)	5 (4%)	4	32
69	RR	127/129 (98%)	106 (84%)	15 (12%)	6 (5%)	3	25
70	SS	135/137 (98%)	114 (84%)	16 (12%)	5 (4%)	4	32
71	TT	139/141 (99%)	126 (91%)	10 (7%)	3 (2%)	8	43
72	UU	102/104 (98%)	87 (85%)	9 (9%)	6 (6%)	2	19
73	VV	81/83 (98%)	67 (83%)	10 (12%)	4 (5%)	2	23
74	WW	127/129 (98%)	106 (84%)	16 (13%)	5 (4%)	3	30
75	XX	139/141 (99%)	118 (85%)	13 (9%)	8 (6%)	2	19
76	YY	124/126 (98%)	99 (80%)	17 (14%)	8 (6%)	1	16
77	ZZ	73/75 (97%)	59 (81%)	12 (16%)	2 (3%)	6	39
78	aa	96/98 (98%)	73 (76%)	13 (14%)	10 (10%)	0	7
79	bb	81/83 (98%)	61 (75%)	16 (20%)	4 (5%)	2	23
80	cc	59/61 (97%)	47 (80%)	10 (17%)	2 (3%)	4	34
81	dd	51/53 (96%)	45 (88%)	3 (6%)	3 (6%)	2	19
82	ee	55/57 (96%)	40 (73%)	12 (22%)	3 (6%)	2	20
83	ff	58/68 (85%)	50 (86%)	6 (10%)	2 (3%)	4	34
84	gg	311/313 (99%)	269 (86%)	33 (11%)	9 (3%)	5	37
86	ii	414/416 (100%)	380 (92%)	26 (6%)	8 (2%)	9	46
87	jj	568/594 (96%)	513 (90%)	41 (7%)	14 (2%)	6	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	12492/12709 (98%)	10717 (86%)	1333 (11%)	442 (4%)	7	33

5 of 442 Ramachandran outliers are listed below:

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

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	187/187 (100%)	161 (86%)	26 (14%)	4	22
2	B	336/342 (98%)	291 (87%)	45 (13%)	4	23
3	C	302/302 (100%)	260 (86%)	42 (14%)	4	22
4	D	247/247 (100%)	218 (88%)	29 (12%)	6	28
5	E	208/221 (94%)	185 (89%)	23 (11%)	7	31
6	F	194/195 (100%)	165 (85%)	29 (15%)	3	19
7	G	206/206 (100%)	182 (88%)	24 (12%)	6	28
8	H	169/169 (100%)	148 (88%)	21 (12%)	5	26
9	I	174/180 (97%)	153 (88%)	21 (12%)	6	27
10	J	142/142 (100%)	126 (89%)	16 (11%)	7	30
11	L	176/176 (100%)	145 (82%)	31 (18%)	2	11
12	M	117/117 (100%)	102 (87%)	15 (13%)	5	25
13	N	171/171 (100%)	152 (89%)	19 (11%)	7	31
14	O	171/171 (100%)	144 (84%)	27 (16%)	3	17
15	P	134/134 (100%)	120 (90%)	14 (10%)	8	35
16	Q	163/163 (100%)	145 (89%)	18 (11%)	7	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	R	159/159 (100%)	140 (88%)	19 (12%)	6	27
18	S	156/156 (100%)	132 (85%)	24 (15%)	3	17
19	T	139/139 (100%)	122 (88%)	17 (12%)	6	27
20	U	89/89 (100%)	82 (92%)	7 (8%)	14	48
21	V	101/101 (100%)	84 (83%)	17 (17%)	2	14
22	W	55/55 (100%)	50 (91%)	5 (9%)	11	41
23	X	107/107 (100%)	97 (91%)	10 (9%)	10	40
24	Y	124/124 (100%)	107 (86%)	17 (14%)	4	22
25	Z	117/117 (100%)	109 (93%)	8 (7%)	18	56
26	a	119/119 (100%)	107 (90%)	12 (10%)	9	36
27	b	62/62 (100%)	57 (92%)	5 (8%)	14	47
28	c	79/79 (100%)	66 (84%)	13 (16%)	2	14
29	d	98/98 (100%)	82 (84%)	16 (16%)	3	15
30	e	114/114 (100%)	99 (87%)	15 (13%)	5	24
31	f	88/88 (100%)	76 (86%)	12 (14%)	4	23
32	g	98/98 (100%)	83 (85%)	15 (15%)	3	18
33	h	109/109 (100%)	97 (89%)	12 (11%)	7	32
34	i	86/86 (100%)	81 (94%)	5 (6%)	23	60
35	j	73/73 (100%)	62 (85%)	11 (15%)	3	19
36	k	64/64 (100%)	56 (88%)	8 (12%)	5	26
37	l	47/47 (100%)	40 (85%)	7 (15%)	3	19
38	m	48/48 (100%)	39 (81%)	9 (19%)	2	9
39	n	22/22 (100%)	18 (82%)	4 (18%)	2	10
40	o	92/92 (100%)	79 (86%)	13 (14%)	4	21
41	p	74/74 (100%)	68 (92%)	6 (8%)	14	47
42	r	109/109 (100%)	88 (81%)	21 (19%)	1	8
43	s	166/166 (100%)	155 (93%)	11 (7%)	19	57
44	t	136/136 (100%)	128 (94%)	8 (6%)	23	60
45	1	13/13 (100%)	12 (92%)	1 (8%)	15	49
52	AA	174/174 (100%)	152 (87%)	22 (13%)	5	26
53	BB	194/194 (100%)	169 (87%)	25 (13%)	5	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	CC	183/183 (100%)	155 (85%)	28 (15%)	3	18
55	DD	190/190 (100%)	168 (88%)	22 (12%)	6	29
56	EE	223/223 (100%)	183 (82%)	40 (18%)	2	11
57	FF	161/161 (100%)	126 (78%)	35 (22%)	1	5
58	GG	207/207 (100%)	179 (86%)	28 (14%)	4	23
59	HH	169/169 (100%)	151 (89%)	18 (11%)	8	33
60	II	178/178 (100%)	155 (87%)	23 (13%)	5	25
61	JJ	161/161 (100%)	141 (88%)	20 (12%)	5	26
62	KK	89/89 (100%)	76 (85%)	13 (15%)	3	20
63	LL	136/136 (100%)	110 (81%)	26 (19%)	2	8
64	MM	104/104 (100%)	85 (82%)	19 (18%)	2	10
65	NN	130/130 (100%)	108 (83%)	22 (17%)	2	13
66	OO	106/106 (100%)	81 (76%)	25 (24%)	1	4
67	PP	116/116 (100%)	98 (84%)	18 (16%)	3	17
68	QQ	117/117 (100%)	102 (87%)	15 (13%)	5	25
69	RR	117/117 (100%)	102 (87%)	15 (13%)	5	25
70	SS	119/119 (100%)	100 (84%)	19 (16%)	3	16
71	TT	112/112 (100%)	94 (84%)	18 (16%)	3	16
72	UU	94/94 (100%)	79 (84%)	15 (16%)	3	16
73	VV	67/67 (100%)	61 (91%)	6 (9%)	11	42
74	WW	112/112 (100%)	99 (88%)	13 (12%)	6	29
75	XX	113/113 (100%)	94 (83%)	19 (17%)	2	14
76	YY	108/108 (100%)	88 (82%)	20 (18%)	2	9
77	ZZ	66/66 (100%)	59 (89%)	7 (11%)	8	34
78	aa	85/85 (100%)	77 (91%)	8 (9%)	10	39
79	bb	75/75 (100%)	62 (83%)	13 (17%)	2	12
80	cc	54/54 (100%)	44 (82%)	10 (18%)	2	9
81	dd	47/47 (100%)	40 (85%)	7 (15%)	3	19
82	ee	47/47 (100%)	39 (83%)	8 (17%)	2	13
83	ff	58/61 (95%)	57 (98%)	1 (2%)	66	87
84	gg	272/272 (100%)	250 (92%)	22 (8%)	14	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
86	ii	358/358 (100%)	324 (90%)	34 (10%)	10	39
87	jj	506/522 (97%)	487 (96%)	19 (4%)	38	72
All	All	10889/10934 (100%)	9508 (87%)	1381 (13%)	9	25

5 of 1381 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
34	i	33	LEU
53	BB	212	VAL
79	bb	72	ARG
36	k	37	ARG
42	r	70	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
5	E	217	GLN
7	G	29	ASN
42	r	103	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
46	2	74/76 (97%)	20 (27%)	0
47	3	72/75 (96%)	36 (50%)	0
48	5	3643/3662 (99%)	1179 (32%)	0
49	7	119/120 (99%)	19 (15%)	0
50	8	155/156 (99%)	52 (33%)	0
51	9	1709/1719 (99%)	608 (35%)	0
85	hh	11/12 (91%)	7 (63%)	0
All	All	5783/5820 (99%)	1921 (33%)	0

5 of 1921 RNA backbone outliers are listed below:

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

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Mol	Chain	Res	Type
46	2	16	C

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	1.81	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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	2.07	1.35	1.32
91	jj	603	ADP	C2-N3	2.16	1.35	1.32
91	jj	602	ADP	C5-C4	3.28	1.47	1.40
91	jj	603	ADP	C5-C4	3.34	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	-6.96	122.80	128.86
91	jj	603	ADP	N3-C2-N1	-6.95	122.81	128.86
91	jj	603	ADP	C4-C5-N7	-3.07	106.45	109.41
91	jj	602	ADP	C4-C5-N7	-3.07	106.45	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.