



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 03:09 PM BST

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 EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

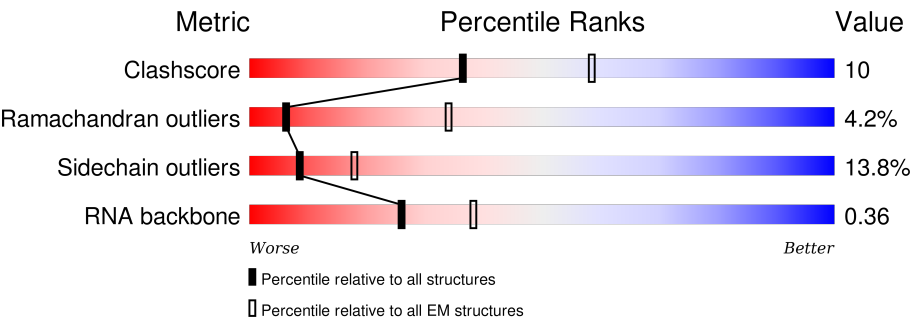
MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 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	66% 29% 5% .
2	B	394	68% 26% 5% .
3	C	361	67% 27% 5%
4	D	292	78% 21% .
5	E	248	57% 28% 9% 5%
6	F	225	66% 29% 5%
7	G	241	69% 28% .
8	H	190	72% 26% ..












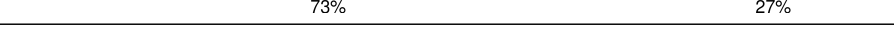







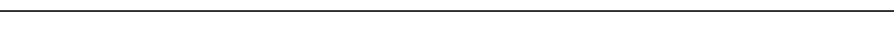

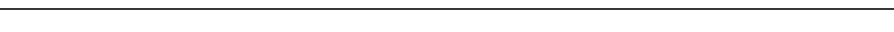
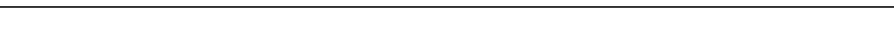


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Mol	Chain	Length	Quality of chain
9	I	213	
10	J	169	
11	L	210	
12	M	138	
13	N	203	
14	O	199	
15	P	153	
16	Q	187	
17	R	180	
18	S	175	
19	T	159	
20	U	99	
21	V	131	
22	W	63	
23	X	119	
24	Y	134	
25	Z	135	
26	a	147	
27	b	75	
28	c	94	
29	d	107	
30	e	128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





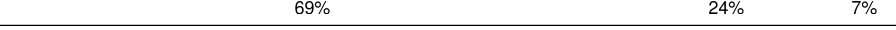
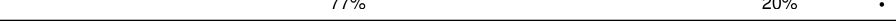

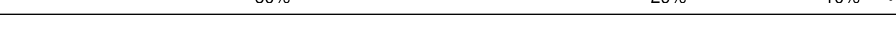
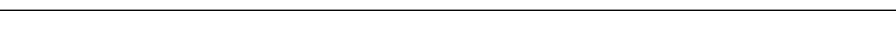
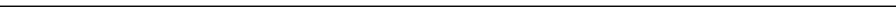















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Mol	Chain	Length	Quality of chain
34	i	102	 84% 14% •
35	j	86	 78% 20% •
36	k	69	 87% 13%
37	l	50	 82% 18%
38	m	52	 77% 21% •
39	n	23	 87% 13%
40	o	104	 84% 15% •
41	p	91	 82% 18%
42	r	125	 82% 16% ••
43	s	198	 89% 10% •
44	t	163	 79% 20% •
45	1	15	 73% 27%
46	2	76	 46% 45% 8% •
47	3	75	 39% 43% 15% •
48	5	3662	 39% 43% 16% •
49	7	120	 62% 29% 9%
50	8	156	 47% 37% 16%
51	9	1719	 38% 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%</div><div>10%</div></div>
85	hh	12	<div><div></div><div>50%</div><div>50%</div></div>
86	ii	416	<div><div></div><div>88%</div><div>12%</div></div>
87	jj	594	<div><div></div><div>89%</div><div>7%</div><div></div><div></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		

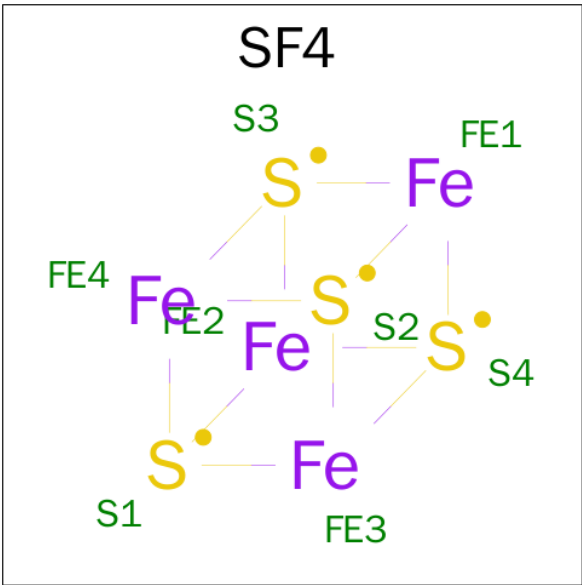
- Molecule 88 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

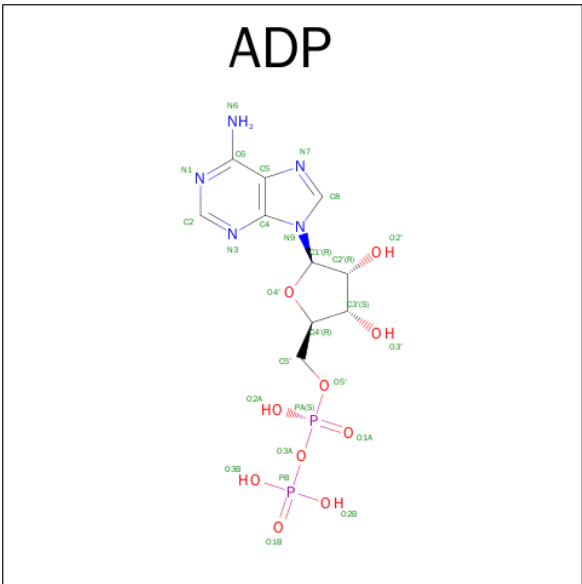
Mol	Chain	Residues	Atoms	AltConf
89	p	1	Total Zn 1 1	0
89	g	1	Total Zn 1 1	0
89	j	1	Total Zn 1 1	0
89	dd	1	Total Zn 1 1	0
89	ff	1	Total Zn 1 1	0
89	aa	1	Total Zn 1 1	0
89	o	1	Total Zn 1 1	0
89	m	1	Total Zn 1 1	0

- Molecule 90 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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

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



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

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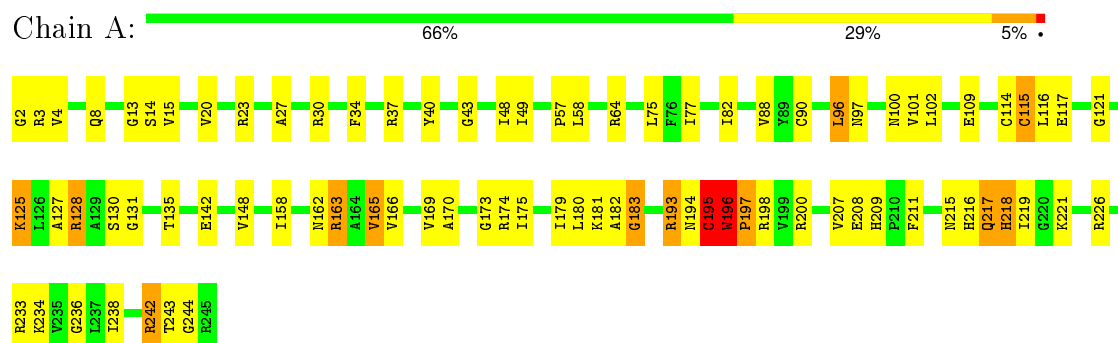
Continued from previous page...

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

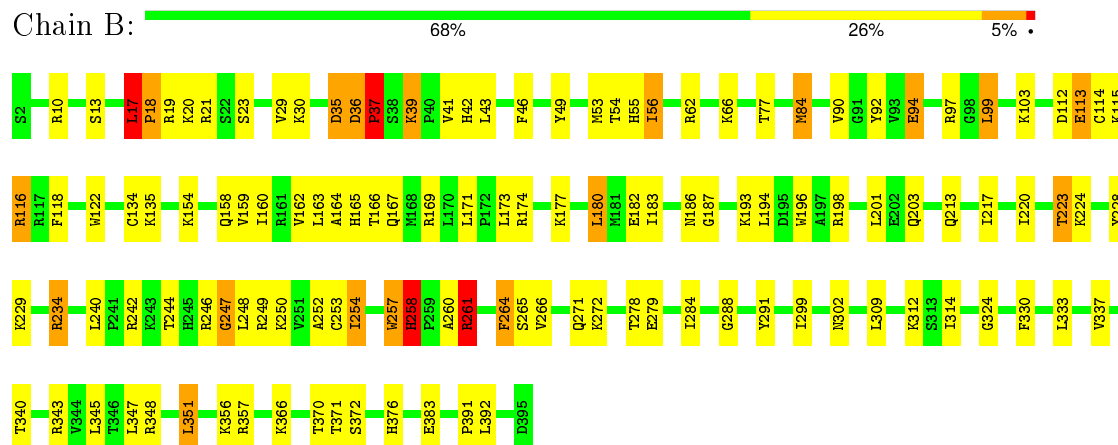
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

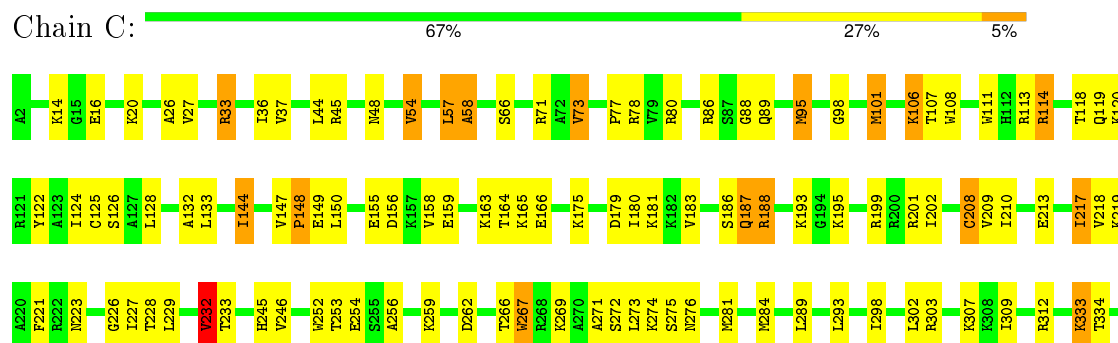
• Molecule 1: uL2



• Molecule 2: uL3

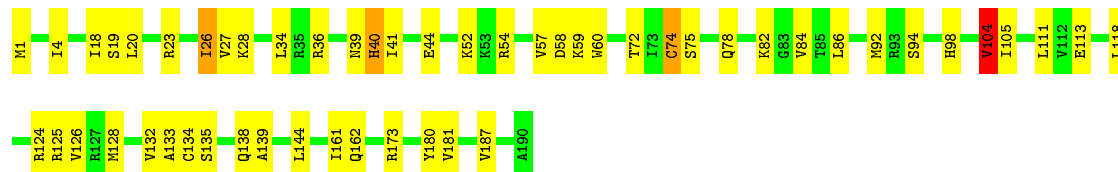


• Molecule 3: uL4



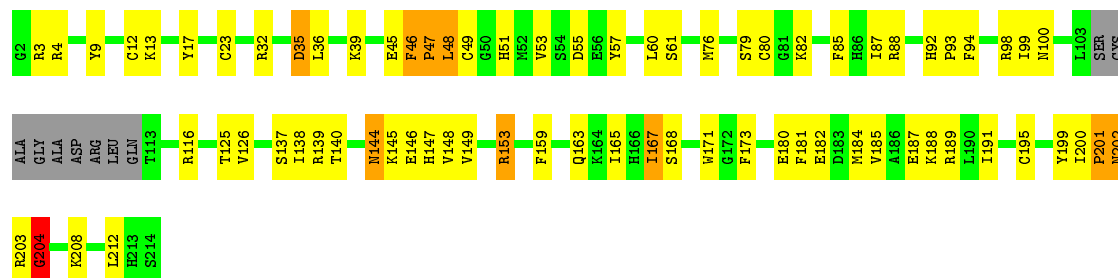
- Molecule 8: uL6

Chain H: 



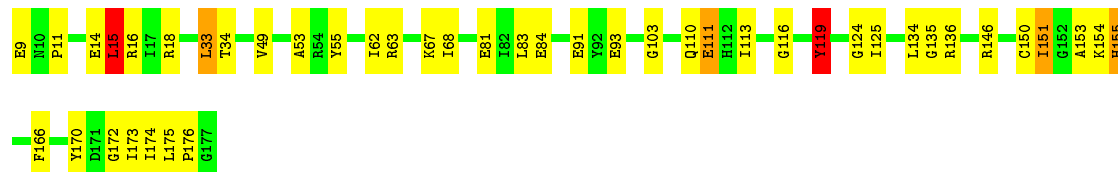
- Molecule 9: uL16

Chain I: 



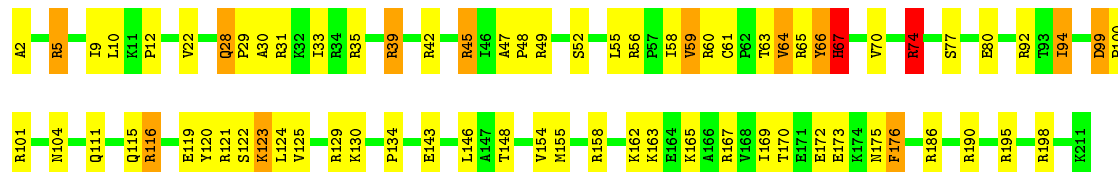
- Molecule 10: uL5

Chain J: 



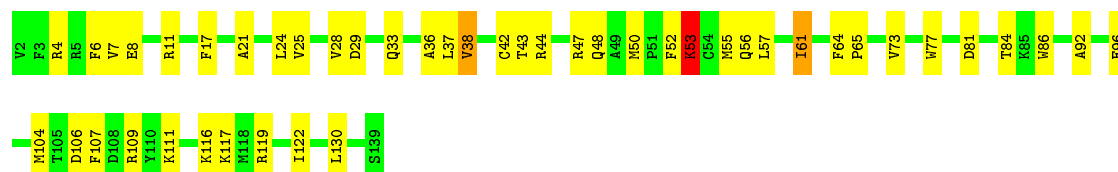
- Molecule 11: eL13

Chain L: 

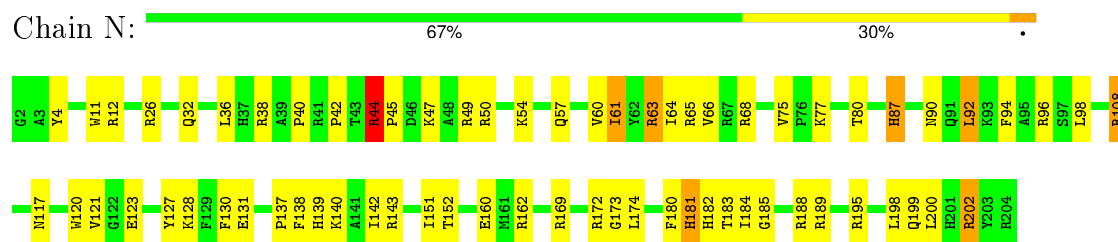


- Molecule 12: eL14

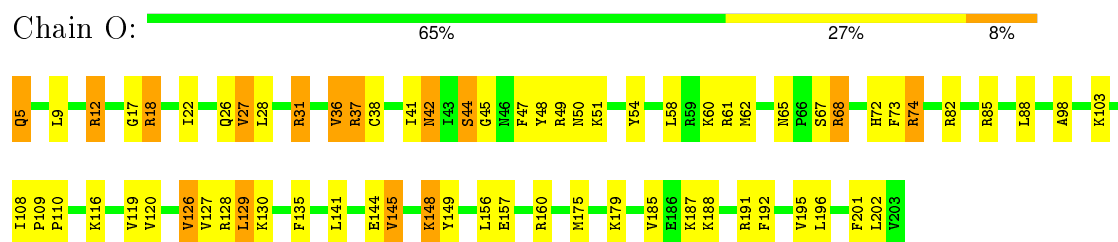
Chain M: 



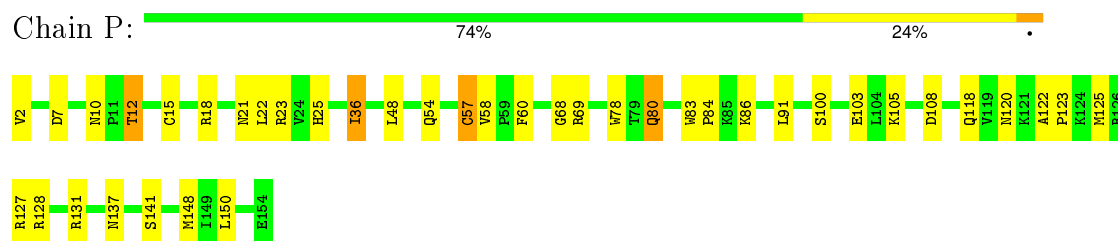
- Molecule 13: eL15



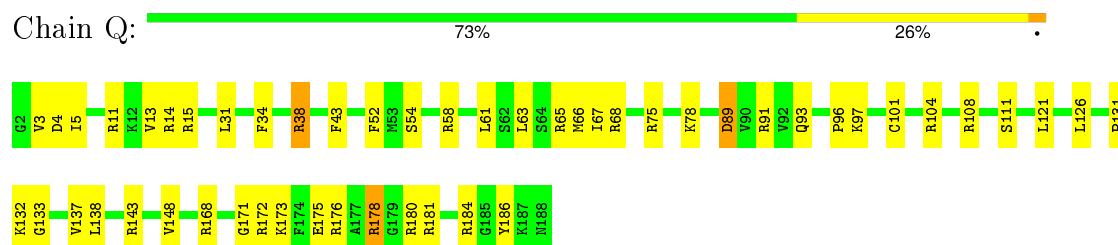
- Molecule 14: uL13



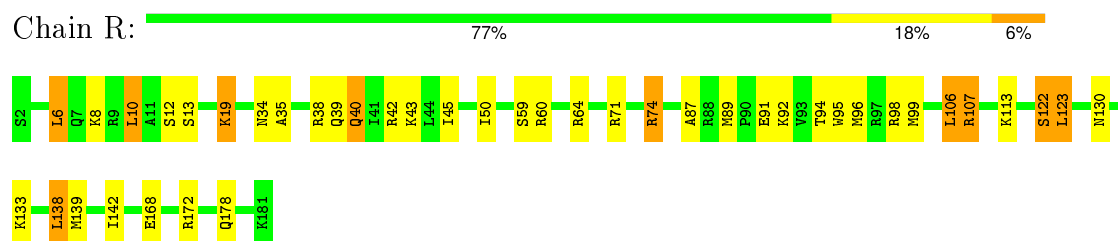
- Molecule 15: uL22



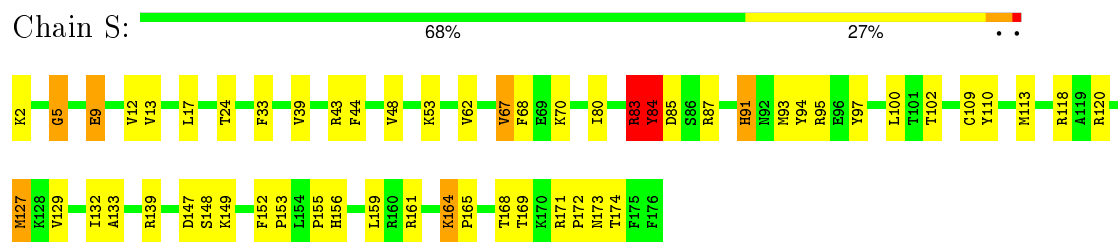
- Molecule 16: eL18



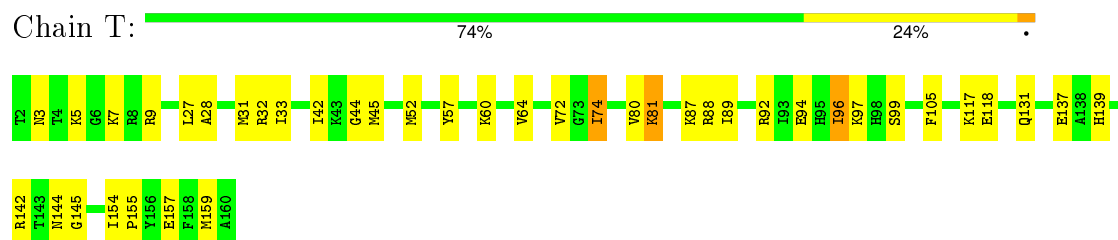
- Molecule 17: eL19



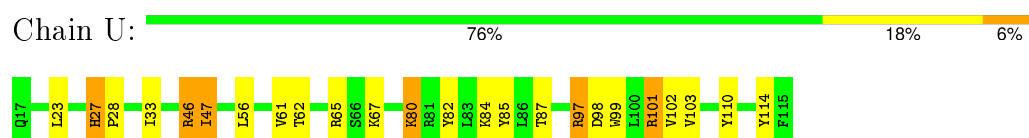
- Molecule 18: eL20



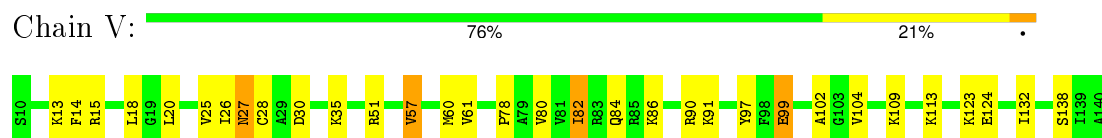
- Molecule 19: eL21



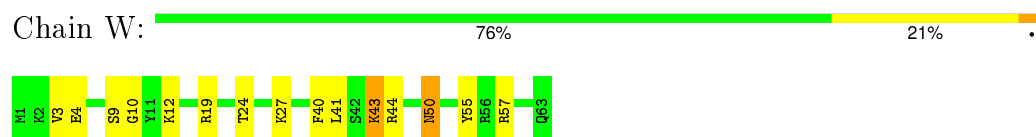
- Molecule 20: eL22



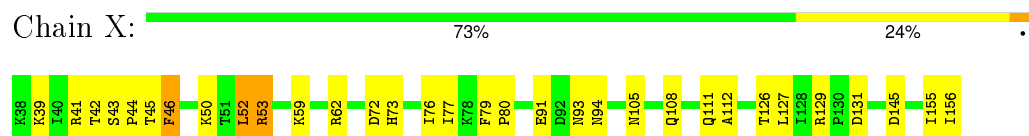
- Molecule 21: uL14



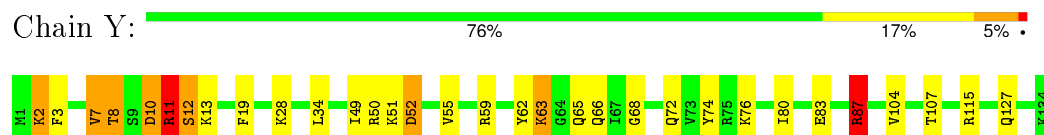
- Molecule 22: eL24



- Molecule 23: uL23

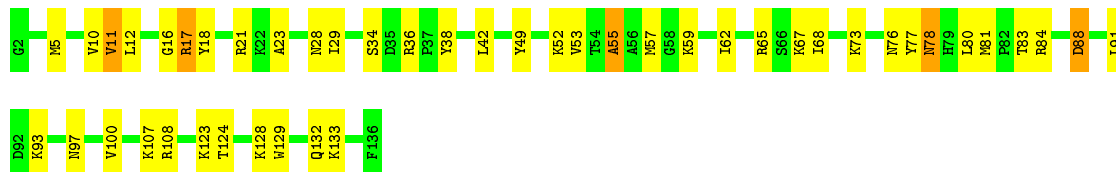


- Molecule 24: uL24




- Molecule 25: eL27

Chain Z:  66% 30% .




- Molecule 26: uL15

Chain a:  88% 9% .




- Molecule 27: eL29

Chain b:  85% 13% .




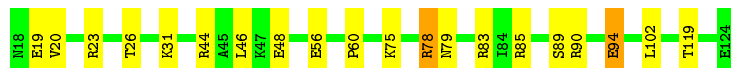
- Molecule 28: eL30

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%




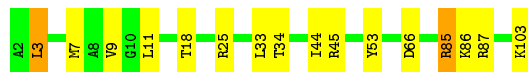
- Molecule 33: uL29

Chain h:  85% 14%




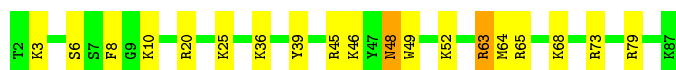
- Molecule 34: eL36

Chain i:  84% 14%




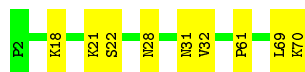
- Molecule 35: eL37

Chain j:  78% 20%




- Molecule 36: eL38

Chain k:  87% 13%




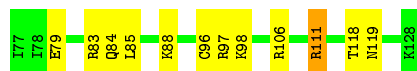
- Molecule 37: eL39

Chain l:  82% 18%




- Molecule 38: eL40

Chain m:  77% 21%



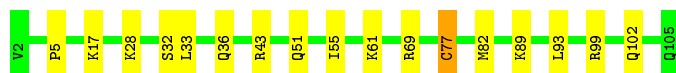
- Molecule 39: eL41

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%



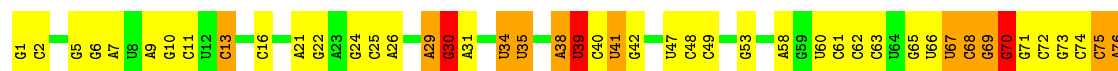
- Molecule 46: tRNA(Val)

Chain 2: 46% 45% 8% .

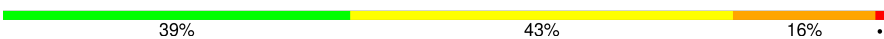


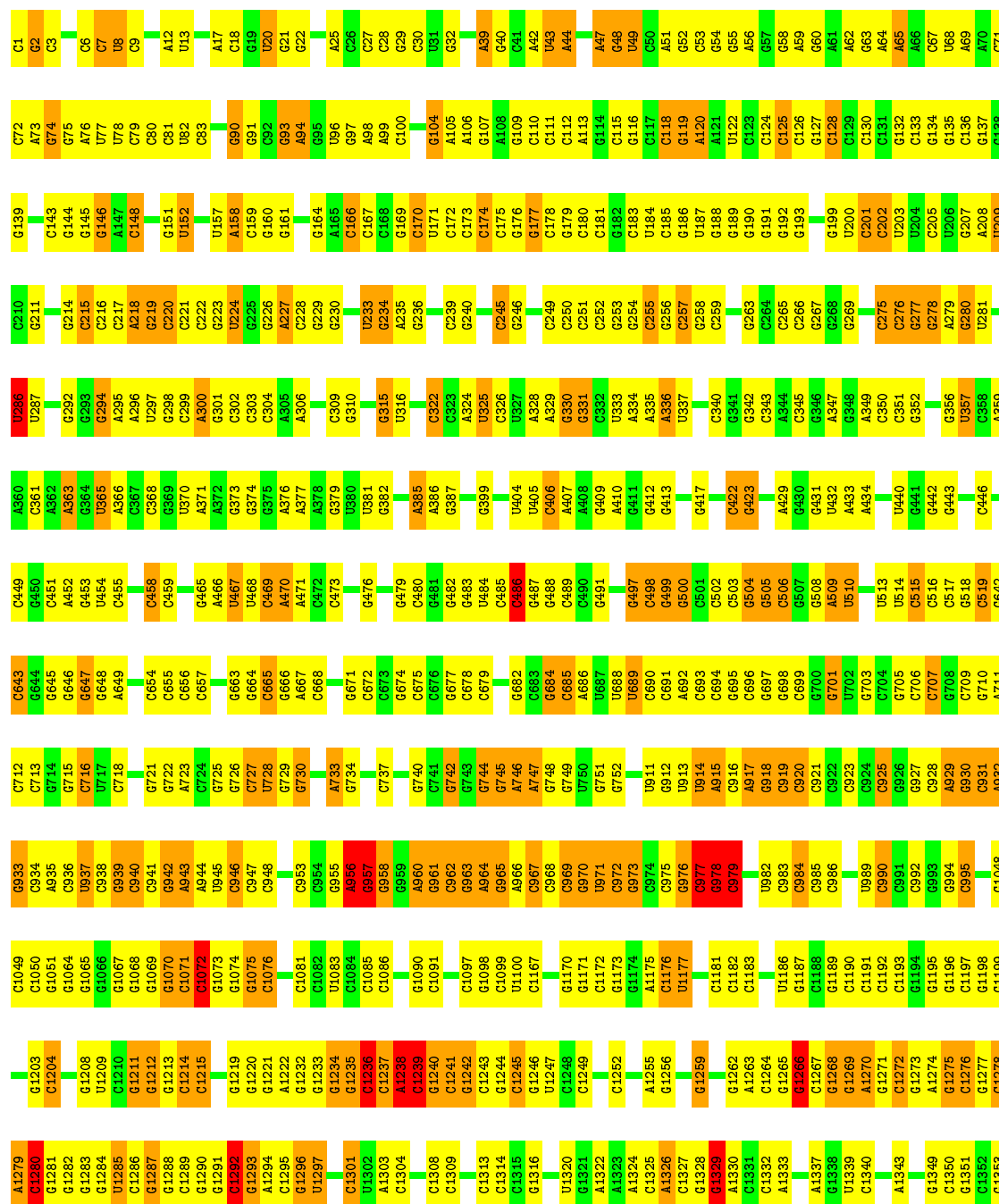
• Molecule 47: tRNA(Lys)

Chain 3: 



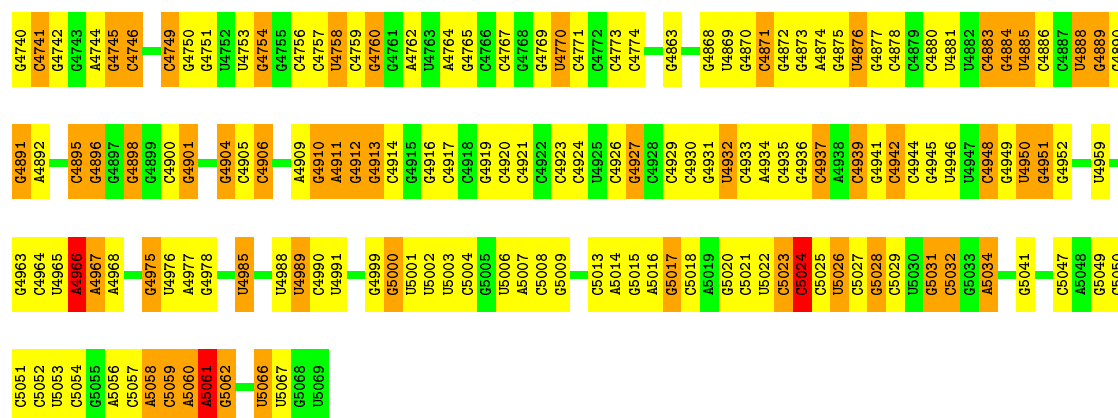
• Molecule 48: 28S ribosomal RNA

Chain 5: 



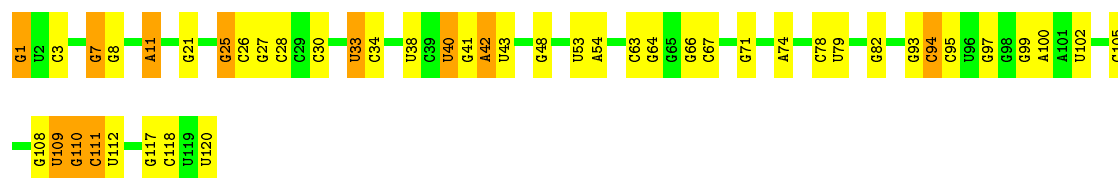
C2614	U2545	C2392	G2294	U2054	G1910	G1752	C1662	U1582	C1505	G1415	A1354
C2615	G2546	C2393	C2295	G2055	C1911	G1753	C1663	A1583	G1506	G1416	G1355
C2617	G2547	G2394	G2296	G2056	C1912	U1754	U1664	G1584	C1507	C1417	G1356
G2618	C2548	A2395	G2297	A2057	C1913	G1755	G1665	G1585	A1508	C1418	C1357
G2619	G2549	A2396	G2298	G2058	C1914	U1756	C1666	U1586	U1511	G1419	G1358
G2620	G2550	G2397	G2299	G2059	A1917	U1757	G1667	U1590	U1512	A1420	G1359
A2621	A2551	U2398	G2301	G2060	U1918	G1758	A1668	U1591	G1513	G1421	G1360
G2622	G2552	G2400	C2302	U2061	U1919	G1759	G1669	U1592	U1514	G1422	G1361
A2623	A2553	A2401	G2306	G2062	C1921	U1760	G1670	U1593	U1515	U1423	G1362
G2624	G2554	G2402	G2307	G2063	U1922	G1761	U1671	U1594	A1516	G1424	C1363
C2627	G2555	A2403	G2311	G2064	U1923	G1762	U1672	U1595	G1517	G1425	G1364
C2628	G2556	U2312	G2312	G2065	C1924	U1764	U1673	U1598	G1518	G1426	G1365
U2629	C2557	G2313	G2313	G2066	U1925	U1767	G1676	A1601	C1519	C1430	G1366
C2630	C2558	G2314	G2314	G2067	G1926	C1768	U1677	U1602	C1520	C1431	G1367
U2633	G2559	G2315	G2315	G2068	C1927	U1769	A1678	G1603	U1521	C1432	C1368
C2634	C2560	G2316	G2316	A2069	U1928	U1770	G1680	U1604	U1522	G1433	C1369
G2638	G2561	G2317	G2317	U2070	C1929	U1771	G1681	C1611	A1523	G1434	G1370
U2639	G2562	G2243	G2243	G2071	U1930	U1772	G1682	G1612	U1524	G1435	A1371
G2640	G2563	G2244	G2244	C2072	U1931	U1773	U1683	G1613	U1525	G1436	A1372
C2645	U2567	G2245	G2245	C2073	U1932	U1774	U1684	U1614	U1526	C1439	G1373
C2646	C2568	G2246	G2246	G2074	A1933	U1775	U1685	G1615	U1527	U1440	G1374
C2649	G2569	G2247	G2247	G2075	U1934	U1776	U1686	U1616	U1528	C1441	C1375
A2652	C2570	G2248	G2248	G2076	U1935	U1777	U1687	U1617	U1529	C1442	C1376
C2654	U2571	G2249	G2249	G2077	U1936	U1778	U1688	G1618	U1530	G1443	G1377
C2655	C2572	G2250	G2250	G2078	A1937	U1779	G1689	U1619	U1531	U1444	C1378
U2658	A2573	G2251	G2251	U2080	U1938	U1780	G1690	U1620	U1532	U1445	C1379
C2659	G2574	G2252	G2252	G2081	G1939	U1781	G1691	U1621	A1533	C1446	G1380
C2660	C2575	G2253	G2253	C2082	U1940	U1782	G1692	U1622	C1534	C1447	C1381
G2668	U2576	G2254	G2254	G2083	A1941	U1783	U1693	U1623	C1535	G1448	G1382
C2671	C2577	G2255	G2255	C2084	U1942	U1784	U1694	G1624	C1536	C1449	C1383
U2661	U2578	G2256	G2256	G2085	A1943	U1785	U1695	G1625	U1537	G1454	G1384
G2662	C2579	G2257	G2257	G2086	U1944	U1786	U1696	U1626	U1538	G1455	G1385
C2669	U2580	G2258	G2258	G2087	U1945	U1787	U1697	U1627	C1539	G1456	C1386
C2670	C2581	G2259	G2259	C2088	U1946	U1788	U1698	U1628	U1540	G1457	A1387
A2676	G2582	G2260	G2260	U2089	U1947	U1789	U1699	G1629	C1541	C1458	A1388
G2677	C2583	G2261	G2261	G2090	U1948	U1790	U1701	U1630	U1542	C1464	G1389
C2681	U2584	G2262	G2262	C2091	U1949	U1791	U1702	G1631	G1543	G1465	G1390
C2682	G2585	G2263	G2263	G2092	U1950	U1792	U1703	G1632	G1544	G1466	A1391
C2683	C2586	G2264	G2264	G2093	U1951	U1793	U1704	G1633	G1545	C1467	A1392
G2684	U2587	G2265	G2265	A2094	U1952	U1794	U1705	G1634	U1546	G1468	G1393
C2685	G2588	G2266	G2266	G2095	U1953	U1795	U1706	G1635	C1547	C1469	G1394
C2686	C2589	U2267	U2267	G2096	U1954	U1796	U1707	G1636	U1548	U1474	U1395
C2687	U2590	G2268	G2268	G2097	U1955	U1797	U1708	G1637	U1549	G1475	G1396
C2688	G2591	G2269	G2269	U2097	U1956	U1798	U1709	U1638	C1550	G1476	A1397
C2689	U2592	G2270	G2270	A2100	U1957	U1799	U1710	U1639	U1551	C1477	A1398
G2693	A2593	G2271	G2271	C2101	U1958	U1800	U1711	G1640	A1552	C1478	G1399
C2694	G2594	G2272	G2272	G2102	U1959	U1801	U1712	G1641	U1553	G1479	G1400
G2695	U2595	G2273	G2273	G2103	U1960	U1802	U1713	A1646	C1554	C1480	C1401
C2696	C2596	G2274	G2274	G2104	U1961	U1803	U1714	U1647	U1555	G1482	G1404
A2697	U2597	G2275	G2275	A2105	U1962	U1804	U1715	U1648	U1556	C1483	C1405
C2698	G2598	G2276	G2276	G2106	U1963	U1805	U1716	U1649	C1557	G1484	G1406
G2699	U2599	G2277	G2277	U2107	U1964	U1806	U1717	U1650	U1558	C1485	C1407
C2703	U2600	G2278	G2278	A2108	U1965	U1807	U1718	U1651	U1559	G1497	G1408
C2704	C2601	G2279	G2279	G2109	U1966	U1808	U1719	U1652	U1560	U1498	C1409
C2705	G2602	G2280	G2280	G2110	U1967	U1809	U1720	U1653	U1561	G1499	C1410
C2706	C2603	G2281	G2281	G2111	U1968	U1810	U1721	U1654	U1562	C1411	C1411
C2707	U2604	G2282	G2282	G2112	U1969	U1811	U1722	U1655	U1563	C1412	C1412
C2708	G2605	G2283	G2283	G2113	U1970	U1812	U1723	U1656	U1564	A1502	C1413
C2709	C2606	G2284	G2284	G2114	U1971	U1813	U1724	U1657	U1565	G1503	C1414
C2710	U2607	G2285	G2285	G2115	U1972	U1814	U1725	U1658	U1566	G1504	C1415
C2711	G2608	G2286	G2286	G2116	U1973	U1815	U1726	U1659	U1567		
C2712	C2609	G2287	G2287	G2117	U1974	U1816	U1727	U1660	U1568		
C2713	U2610	G2288	G2288	G2118	U1975	U1817	U1728	U1661	U1569		
C2714	G2611	G2289	G2289	G2119	U1976	U1818	U1729	U1662	U1570		
C2715	C2612	G2290	G2290	G2120	U1977	U1819	U1730	U1663	U1571		
C2716	U2613	G2291	G2291	G2121	U1978	U1820	U1731	U1664	U1572		
C2717	C2613	G2292	G2292	G2122	U1979	U1821	U1732	U1665	U1573		
C2718	G2614	G2293	G2293	G2123	U1980	U1822	U1733	U1666	U1574		
C2719	C2615	G2294	G2294	G2124	U1981	U1823	U1734	U1667	U1575		
C2720	U2616	G2295	G2295	G2125	U1982	U1824	U1735	U1668	U1576		
C2721	C2617	G2296	G2296	G2126	U1983	U1825	U1736	U1669	U1577		
C2722	G2618	G2297	G2297	G2127	U1984	U1826	U1737	U1670	U1578		
C2723	U2619	G2298	G2298	G2128	U1985	U1827	U1738	U1671	U1579		
C2724	C2620	G2299	G2299	G2129	U1986	U1828	U1739	U1672	U1580		
C2725	A2621	G2300	G2300	G2130	U1987	U1829	U1740	U1673	U1581		
C2726	G2621	G2301	G2301	G2131	U1988	U1830	U1741	U1674	U1582		
C2727	U2622	G2302	G2302	G2132	U1989	U1831	U1742	U1675	U1583		
C2728	C2623	G2303	G2303	G2133	U1990	U1832	U1743	U1676	U1584		
C2729	G2624	G2304	G2304	G2134	U1991	U1833	U1744	U1677	U1585		
C2730	U2624	G2305	G2305	G2135	U1992	U1834	U1745	U1678	U1586		
C2731	C2625	G2306	G2306	G2136	U1993	U1835	U1746	U1679	U1587		
C2732	G2626	G2307	G2307	G2137	U1994	U1836	U1747	U1680	U1588		
C2733	U2626	G2308	G2308	G2138	U1995	U1837	U1748	U1681	U1589		
C2734	C2627	G2309	G2309	G2139	U1996	U1838	U1749	U1682	U1590		
C2735	G2628	G2310	G2310	G2140	U1997	U1839	U1750	U1683	U1591		
C2736	U2627	G2311	G2311	G2141	U1998	U1840	U1751	U1684	U1592		
C2737	C2629	G2312	G2312	G2142	U1999	U1841	U1752	U1685	U1593		
C2738	G2630	G2313	G2313	G2143	U2000	U1842	U1753	U1686	U1594		
C2739	U2630	G2314	G2314	G2144	U2001	U1843	U1754	U1687	U1595		
C2740	C2631	G2315	G2315	G2145	U2002	U1844	U1755	U1688	U1596		
C2741	G2632	G2316	G2316	G2146	U2003	U1845	U1756	U1689	U1597		
C2742	U2632	G2317	G2317	G2147	U2004	U1846	U1757	U1690	U1598		
C2743	C2633	G2318	G2318	G2148	U2005	U1847	U1758	U1691	U1599		
C2744	U2633	G2319	G2319	G2149	U2006	U1848	U1759	U1692	U1600		
C2745	G2634	G2320	G2320	G2150	U2007	U1849	U1760	U1693	U1601		
C2746	C2635	G2321	G2321	G2151	U2008	U1850	U1761	U1694	U1602		
C2747	U2634	G2322	G2322	G2152	U2009	U1851	U1762	U1695	U1603		
C2748	C2636	G2323	G2323	G2153	U2010	U1852	U1763	U1696	U1604		
C2749	U2635	G2324	G2324	G2154	U2011	U1853	U1764	U1697	U1605		
C2750	G2637	G2325	G2325	G2155	U2012	U1854	U1765	U1698	U1606		
C2751	C2638	G2326	G2326	G2156	U2013	U1855	U1766	U1699	U1607		
C2752	U2638	G2327	G2327	G2157	U2014	U1856	U1767	U1700	U1608		
C2753	C2639	G2328	G2328	G2158	U2015	U1857	U1768	U1701	U1609		
C2754	G2640	G2329	G2329	G2159	U2016	U1858	U1769	U1702	U1610		
C2755	U2639	G2330	G2330	G2160	U2017	U1859	U1770	U1703	U1611		
C2756	C2641	G2331	G2331	G2161	U2018	U1860	U1771	U1704	U1612		
C2757	G2642	G2332	G2332	G2162	U2019	U1861	U1772	U1705	U1613		
C2758	U2640	G2333	G2333	G2163	U2020	U1862	U1773	U1706	U1614		
C2759	C2643	G2334	G2334	G2164	U2021	U1863	U1774	U1707	U1615		
C2760	G2644	G2335</									

C4670	A4589	G4515	C4434	G4368	A4268	G4187	C4119	U3925	A3856	A3774	G3703	A3629	G2859		U2708
C4671	A4590	G4516	U4437	A4369	G4269	U4188	U4120	C3926	G3857	A3775	U3704	A3630	G2862		C2709
A4591	C4592	A4518	U4438	G4370	C4270	U4189	G4121	U3927	C3858	G3776	G3705	G3631	G2863		C2710
C4595	G4596	C4519	U4439	A4371	A4271	U4190	G4122	G3933	G3859	G3777	C3706	G3632	G2864		G2711
C4596		G4520	G4440	A4372	G4272	G4191	C4123	G3934	A3860		U3707	A3635	U2865		C2712
		U4521	A4441	G4373	A4273	G4197	C4124	C3937	A3861	C3782	C3708	C3636			C2713
		G4522			G4274	G4198	C4125	G3938	A3862	A3783	U3709	U3637			G2714
		A4523			A4275		C4126	G3939		A3784	G3710		U2874		G2715
					G4276		A4127		A3867		G3711				C2716
							A4128		G3868		A3712				
							G4129	A3943	G3869		A3713				C2720
							C4130	G3944	C3870		G3714				G2721
							G4131	A3945	A3871		U3715				G2722
							C4132	G3946	A3872		C3716				U2723
							C4133								G2724
							G4134	U4069	G3873		A3717				A2725
							G4135	U4070	G3874		A3718				G2726
							C4136		A3875		A3719				C2727
							G4137	A4073	A3876						U2728
							C4138	U4074	A3877		A3723				C2729
							C4139	C4075	C3878		A3724				G2730
							G4140	G4076	G3879		G3725				C2731
							C4141		G3880		A3726				G2732
							G4142	C4079	G3881		A3727				C2733
							C4143	C4080	C3882		A3728				G2734
							G4144	C4081	U3883		U3729				U2735
							C4145				U3730				G2736
							G4146	G4084	G3886		C3731				C2737
							C4147	A4085	C3887		A3732				
							G4148	G4086	G3888						
							C4149	G4087	G3889		G3735				U2740
							C4150	C4088	G3890		A3736				U2741
							G4151		A3891		A3737				G2742
							C4152	G4091	U3892						
							C4153	G4092	C3893		G3740				A2743
							G4154	G4093	A3894		C3741				A2744
							C4155	G4094	G3895						
							C4156	G4095	C3896		A3747				C2749
							C4157	C4096	G3897		A3748				G2750
							G4161	U4097	G3898		C3749				G2751
							C4162	A4098	G3899		G3750				G2752
							U4163	G4099	G3900		G3751				G2753
							C4164	C4100	A3901		G3752				G2754
							C4165	C4101			G3753				A2755
							G4166	C4102	G3904						G2756
							C4167	C4103	A3905		G3754				A2757
							G4168	G4104	A3906		G3755				G2758
							C4169	A4105	G3907		A3756				G2759
							A4170	G4106	A3908						G2760
							C4171	G4107	G3909		A3759				U2761
							A4172	G4108	C3910		A3760				G2762
							G4173	G4109	C3911		C3761				U2763
							C4174	C4110	U3912		U3762				A2764
							A4175	C4111	G3913		A3763				
							G4176	U4111	G3914		U3764				U2767
							C4177	C4112	U3915		A3765				C2768
							G4178	G4113	G3916		U3766				U2769
							A4182	C4114	U3917		A3766				C2770
							G4183	G4115	A3918						G2771
							C4184	C4116	G3919		U3770				C2772
							G4185	U4117	C3919		C3771				G2773
							A4186	U4118			U3772				C2774
							C4196				U3773				



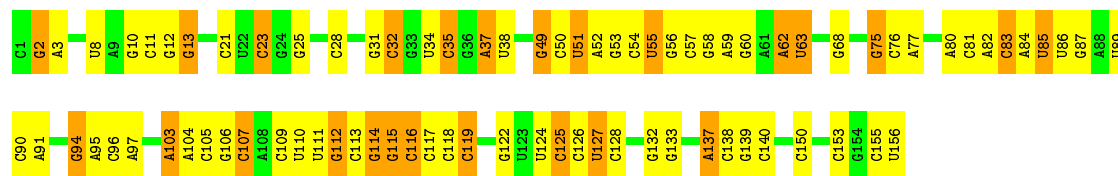
- Molecule 49: 5S ribosomal RNA

Chain 7: 62% 29% 9%



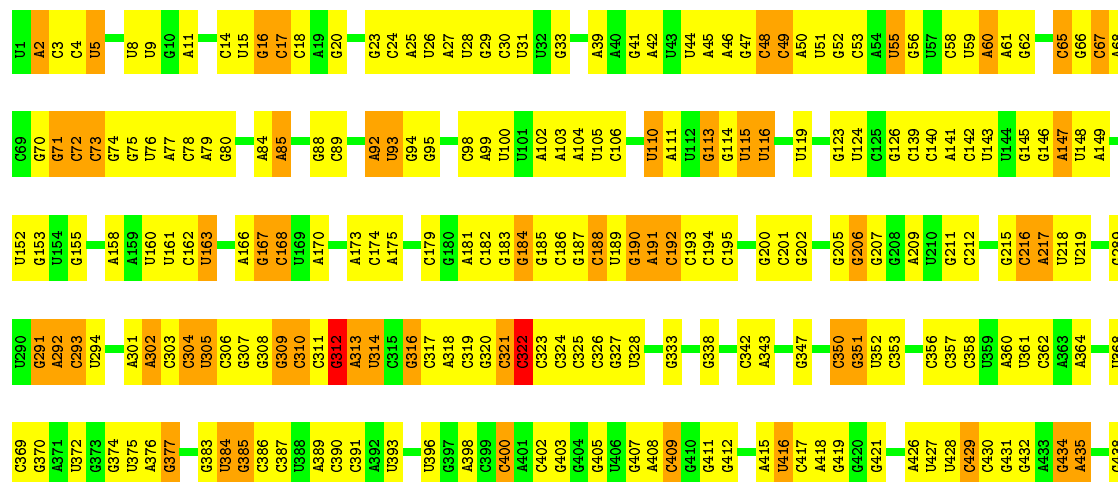
- Molecule 50: 5.8S ribosomal RNA

Chain 8: 47% 37% 16%

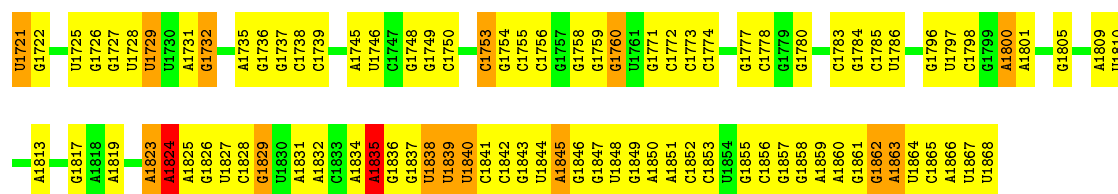


- Molecule 51: 18S ribosomal RNA

Chain 9: 38% 45% 15%

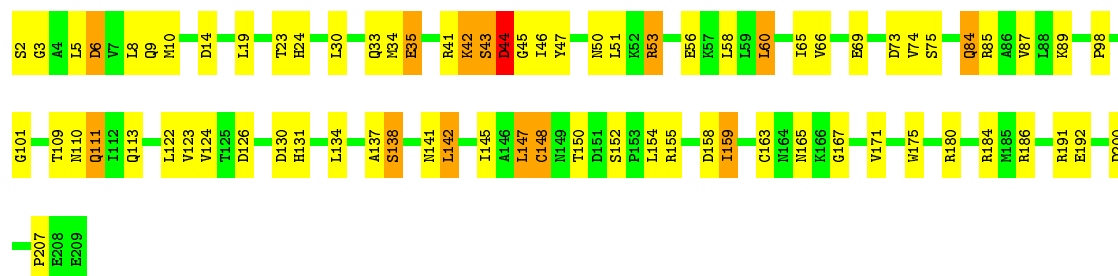




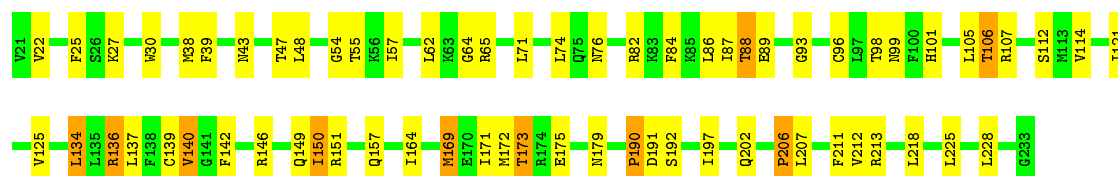
• Molecule 52: uS2

Chain AA: 63% 30% 6%



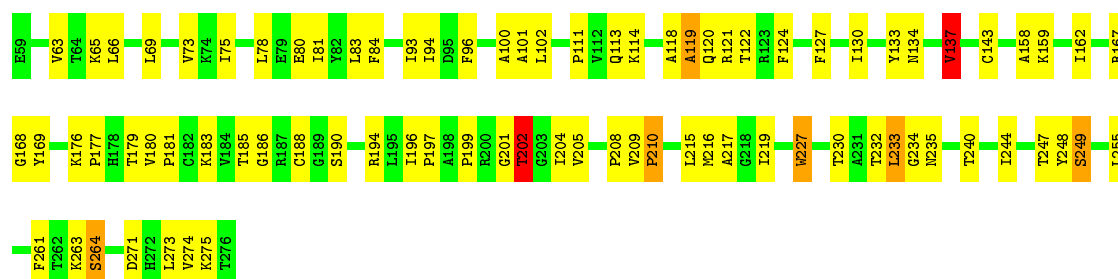
• Molecule 53: eS1

Chain BB: 69% 27% 5%



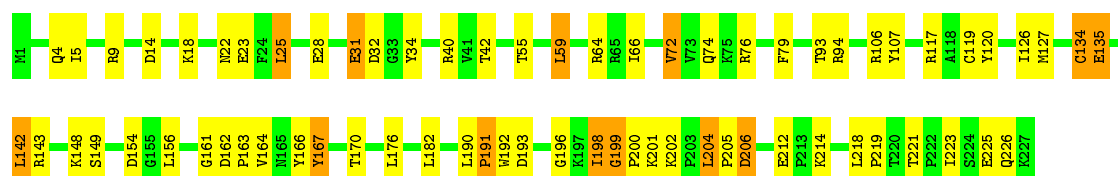
• Molecule 54: uS5

Chain CC: 62% 34% 2%

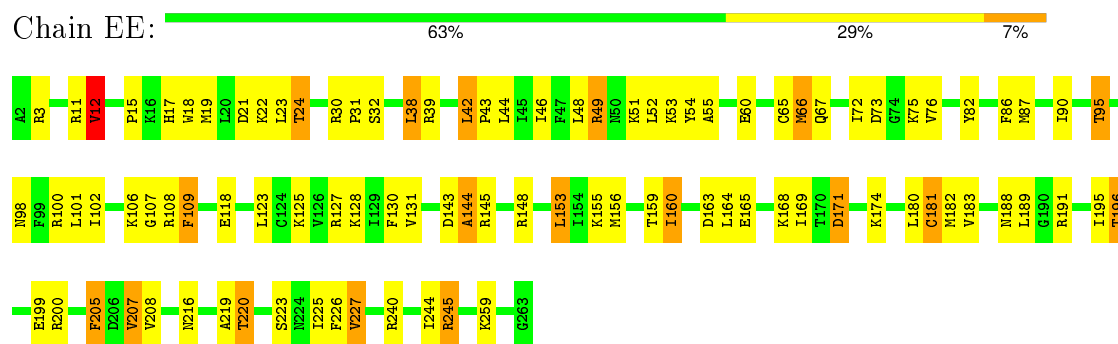


• Molecule 55: uS3

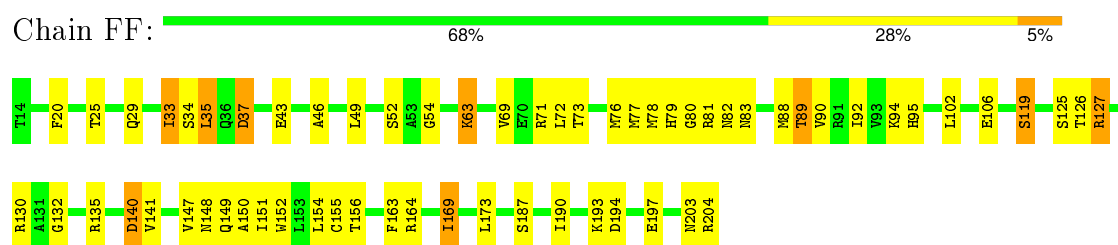
Chain DD: 70% 25% 6%



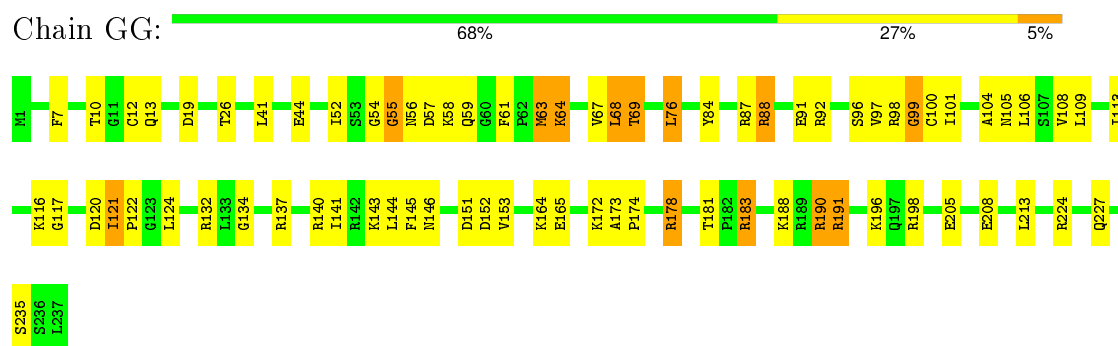
- Molecule 56: eS4



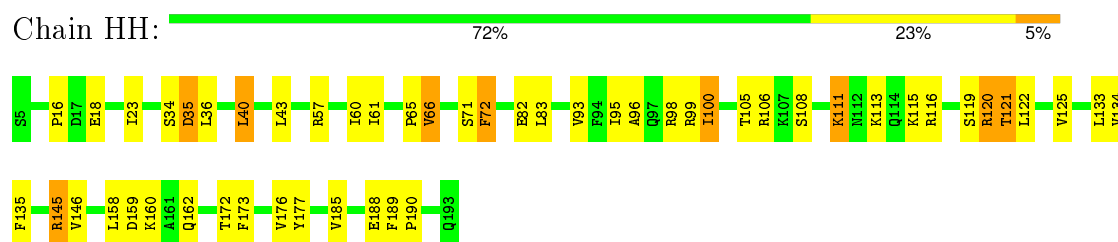
- Molecule 57: uS7



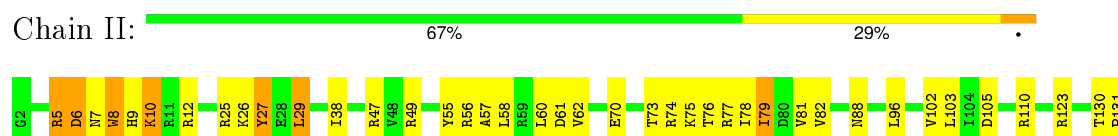
- Molecule 58: eS6

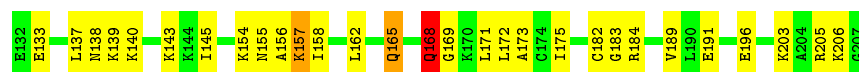


- Molecule 59: eS7



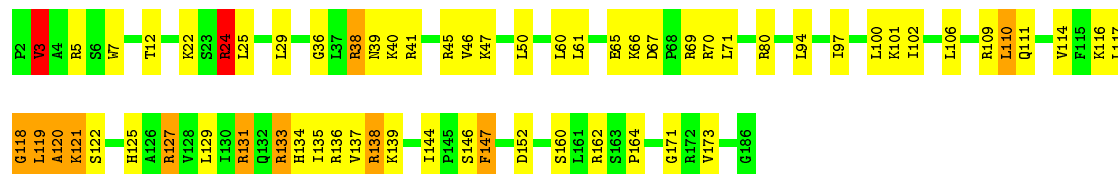
- Molecule 60: eS8





• Molecule 61: uS4

Chain JJ: 66% 27% 6% •



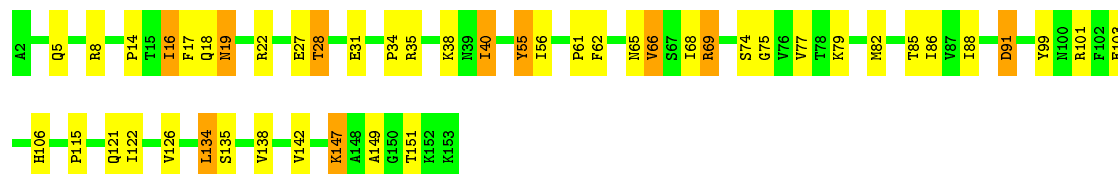
• Molecule 62: eS10

Chain KK: 62% 36% •



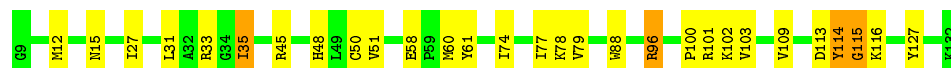
• Molecule 63: uS17

Chain LL: 69% 24% 7% •



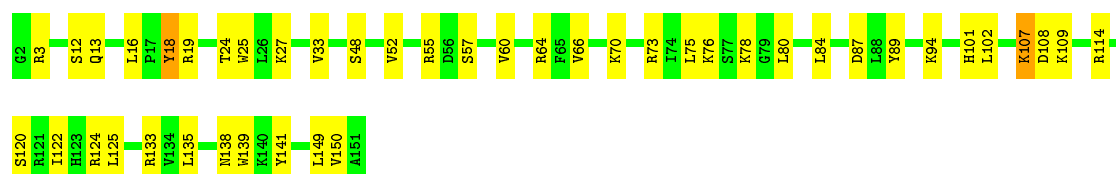
• Molecule 64: eS12

Chain MM: 77% 20% •



• Molecule 65: uS15

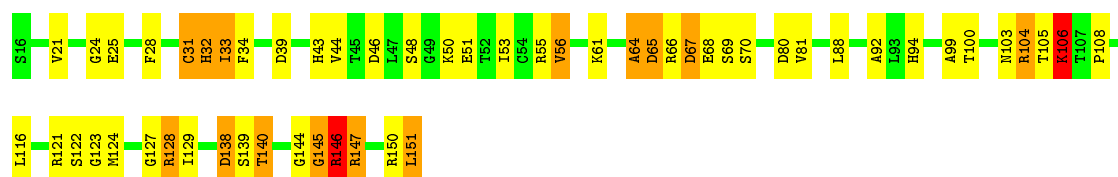
Chain NN: 71% 28% •



• Molecule 66: uS11

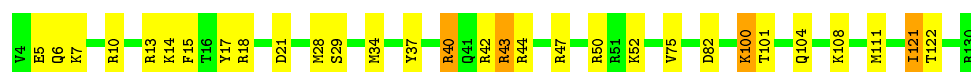
Chain OO: 60% 29% 10% •





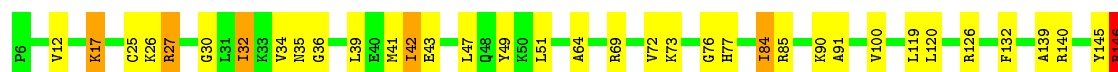
- Molecule 67: uS19

Chain PP: 76% 20% •



- Molecule 68: uS9

Chain QQ: 74% 21% • •



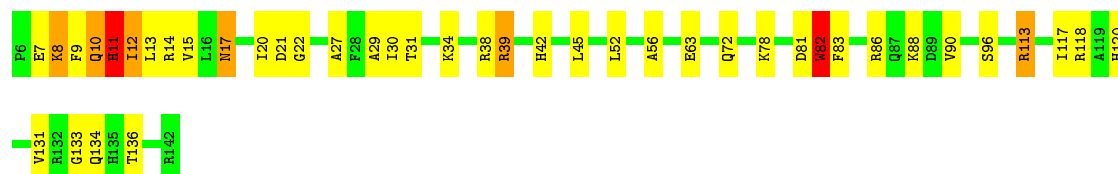
- Molecule 69: eS17

Chain RR: 70% 26% 5% • •



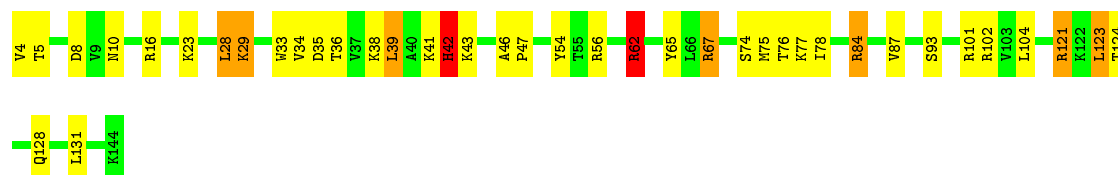
- Molecule 70: uS13

Chain SS: 69% 25% • •




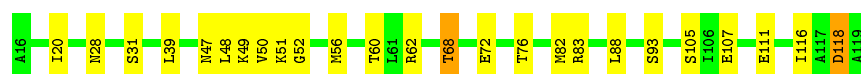
- Molecule 71: eS19

Chain TT: 72% 22% 5% •



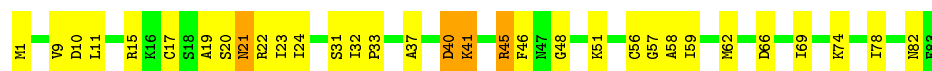
- Molecule 72: uS10

Chain UU:  76% 22% .



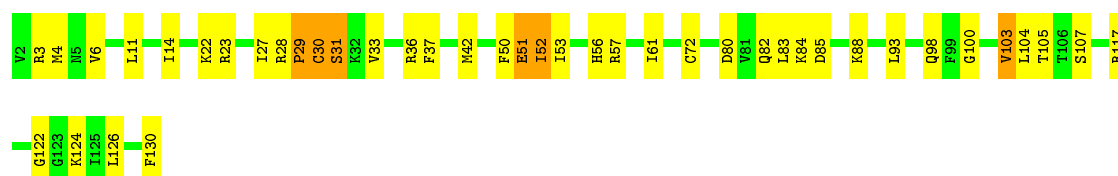
- Molecule 73: eS21

Chain VV:  61% 34% 5%




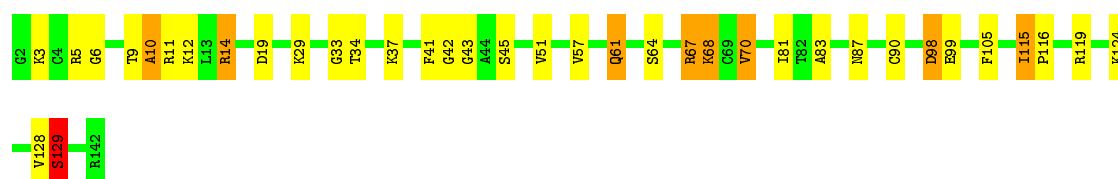
- Molecule 74: uS8

Chain WW:  67% 28% 5%



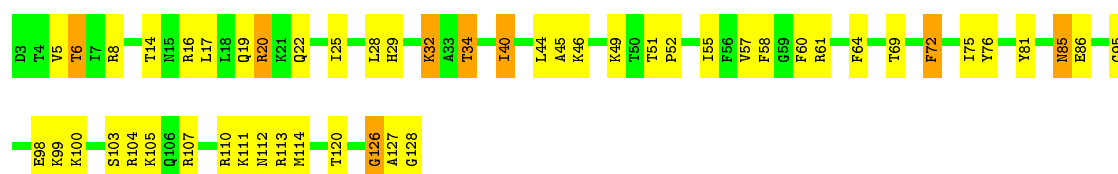
- Molecule 75: uS12

Chain XX:  74% 20% 6% .



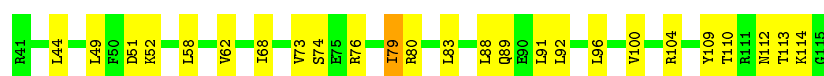
- Molecule 76: eS24

Chain YY:  60% 34% 6%




- Molecule 77: eS25

Chain ZZ:  67% 32% .

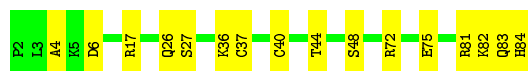
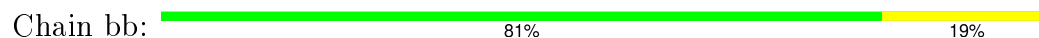


- Molecule 78: eS26

Chain aa:  77% 21% .



- Molecule 79: eS27



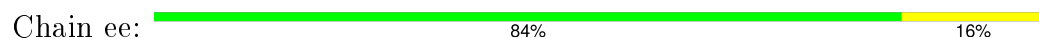
- Molecule 80: eS28



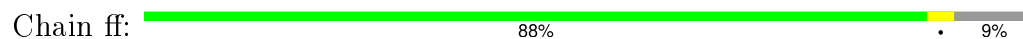
- Molecule 81: uS14



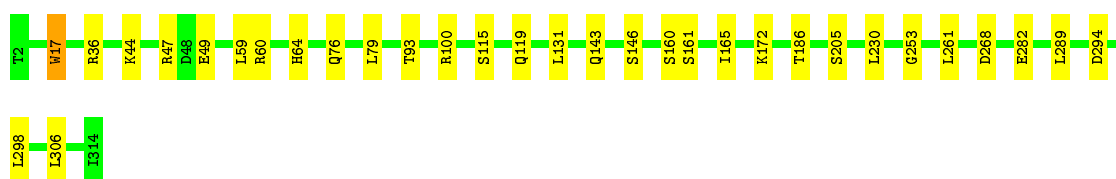
- Molecule 82: eS30



- Molecule 83: eS31



- Molecule 84: RACK1



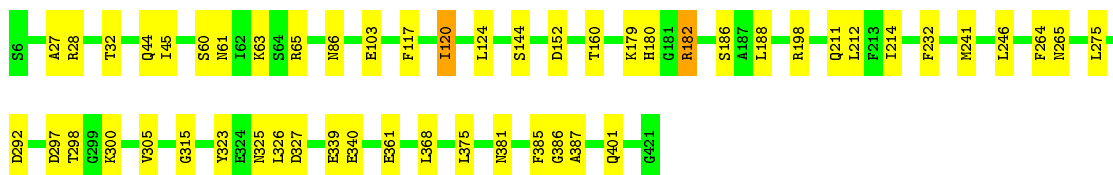
- Molecule 85: mRNA





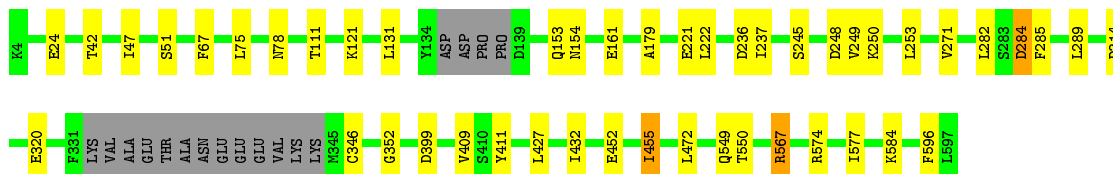
• Molecule 86: eRF1

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 images	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	59000	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
9:I:191:ILE:CD1	9:I:200:ILE:CD1	1.90	1.34
48:5:1968:G:H1	48:5:2018:C:N4	1.21	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	41
2	B	392/394 (100%)	338 (86%)	44 (11%)	10 (3%)	7	48
3	C	359/361 (99%)	302 (84%)	48 (13%)	9 (2%)	7	49
4	D	290/292 (99%)	255 (88%)	31 (11%)	4 (1%)	14	60
5	E	232/248 (94%)	172 (74%)	37 (16%)	23 (10%)	1	13
6	F	223/225 (99%)	204 (92%)	18 (8%)	1 (0%)	39	80
7	G	239/241 (99%)	205 (86%)	26 (11%)	8 (3%)	5	44
8	H	188/190 (99%)	161 (86%)	25 (13%)	2 (1%)	17	65
9	I	200/213 (94%)	178 (89%)	17 (8%)	5 (2%)	7	49
10	J	167/169 (99%)	141 (84%)	18 (11%)	8 (5%)	3	32
11	L	208/210 (99%)	174 (84%)	25 (12%)	9 (4%)	3	35
12	M	136/138 (99%)	123 (90%)	12 (9%)	1 (1%)	26	72
13	N	201/203 (99%)	167 (83%)	32 (16%)	2 (1%)	19	66
14	O	197/199 (99%)	176 (89%)	20 (10%)	1 (0%)	34	77
15	P	151/153 (99%)	134 (89%)	13 (9%)	4 (3%)	7	48
16	Q	185/187 (99%)	161 (87%)	20 (11%)	4 (2%)	8	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	R	178/180 (99%)	151 (85%)	25 (14%)	2 (1%)	17	65
18	S	173/175 (99%)	151 (87%)	18 (10%)	4 (2%)	8	52
19	T	157/159 (99%)	137 (87%)	17 (11%)	3 (2%)	10	55
20	U	97/99 (98%)	82 (84%)	11 (11%)	4 (4%)	3	37
21	V	129/131 (98%)	110 (85%)	19 (15%)	0	100	100
22	W	61/63 (97%)	55 (90%)	5 (8%)	1 (2%)	12	58
23	X	117/119 (98%)	106 (91%)	9 (8%)	2 (2%)	11	57
24	Y	132/134 (98%)	114 (86%)	13 (10%)	5 (4%)	4	39
25	Z	133/135 (98%)	113 (85%)	14 (10%)	6 (4%)	3	34
26	a	145/147 (99%)	114 (79%)	24 (17%)	7 (5%)	3	32
27	b	73/75 (97%)	65 (89%)	5 (7%)	3 (4%)	3	37
28	c	92/94 (98%)	87 (95%)	5 (5%)	0	100	100
29	d	105/107 (98%)	86 (82%)	17 (16%)	2 (2%)	10	55
30	e	126/128 (98%)	110 (87%)	12 (10%)	4 (3%)	5	45
31	f	107/109 (98%)	88 (82%)	12 (11%)	7 (6%)	1	25
32	g	112/114 (98%)	97 (87%)	13 (12%)	2 (2%)	11	56
33	h	120/122 (98%)	106 (88%)	10 (8%)	4 (3%)	5	44
34	i	100/102 (98%)	87 (87%)	11 (11%)	2 (2%)	9	54
35	j	84/86 (98%)	73 (87%)	8 (10%)	3 (4%)	4	41
36	k	67/69 (97%)	53 (79%)	10 (15%)	4 (6%)	2	26
37	l	48/50 (96%)	41 (85%)	5 (10%)	2 (4%)	3	36
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%)	4	38
41	p	89/91 (98%)	75 (84%)	9 (10%)	5 (6%)	2	28
42	r	123/125 (98%)	104 (85%)	10 (8%)	9 (7%)	1	21
43	s	196/198 (99%)	163 (83%)	21 (11%)	12 (6%)	2	26
44	t	161/163 (99%)	100 (62%)	36 (22%)	25 (16%)	0	5
45	l	13/15 (87%)	10 (77%)	2 (15%)	1 (8%)	1	19
52	AA	206/208 (99%)	153 (74%)	37 (18%)	16 (8%)	1	19
53	BB	211/213 (99%)	165 (78%)	34 (16%)	12 (6%)	2	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	CC	216/218 (99%)	184 (85%)	22 (10%)	10 (5%)	3	33
55	DD	225/227 (99%)	184 (82%)	30 (13%)	11 (5%)	3	32
56	EE	260/262 (99%)	197 (76%)	43 (16%)	20 (8%)	1	19
57	FF	189/191 (99%)	156 (82%)	22 (12%)	11 (6%)	2	27
58	GG	235/237 (99%)	198 (84%)	29 (12%)	8 (3%)	5	44
59	HH	187/189 (99%)	144 (77%)	30 (16%)	13 (7%)	1	22
60	II	204/206 (99%)	169 (83%)	25 (12%)	10 (5%)	3	32
61	JJ	183/185 (99%)	152 (83%)	19 (10%)	12 (7%)	1	24
62	KK	96/98 (98%)	65 (68%)	20 (21%)	11 (12%)	0	9
63	LL	150/152 (99%)	125 (83%)	16 (11%)	9 (6%)	2	26
64	MM	122/124 (98%)	87 (71%)	25 (20%)	10 (8%)	1	17
65	NN	148/150 (99%)	121 (82%)	21 (14%)	6 (4%)	3	37
66	OO	134/136 (98%)	96 (72%)	24 (18%)	14 (10%)	1	11
67	PP	125/127 (98%)	102 (82%)	20 (16%)	3 (2%)	7	51
68	QQ	139/141 (99%)	115 (83%)	14 (10%)	10 (7%)	1	21
69	RR	127/129 (98%)	100 (79%)	18 (14%)	9 (7%)	1	22
70	SS	135/137 (98%)	110 (82%)	15 (11%)	10 (7%)	1	20
71	TT	139/141 (99%)	127 (91%)	9 (6%)	3 (2%)	8	52
72	UU	102/104 (98%)	84 (82%)	12 (12%)	6 (6%)	2	27
73	VV	81/83 (98%)	65 (80%)	9 (11%)	7 (9%)	1	16
74	WW	127/129 (98%)	101 (80%)	21 (16%)	5 (4%)	4	38
75	XX	139/141 (99%)	122 (88%)	8 (6%)	9 (6%)	1	25
76	YY	124/126 (98%)	100 (81%)	15 (12%)	9 (7%)	1	21
77	ZZ	73/75 (97%)	58 (80%)	11 (15%)	4 (6%)	2	29
78	aa	96/98 (98%)	76 (79%)	8 (8%)	12 (12%)	0	8
79	bb	81/83 (98%)	59 (73%)	16 (20%)	6 (7%)	1	20
80	cc	59/61 (97%)	47 (80%)	11 (19%)	1 (2%)	11	57
81	dd	51/53 (96%)	40 (78%)	11 (22%)	0	100	100
82	ee	55/57 (96%)	39 (71%)	14 (26%)	2 (4%)	4	41
83	ff	58/68 (85%)	49 (84%)	8 (14%)	1 (2%)	11	57
84	gg	311/313 (99%)	263 (85%)	40 (13%)	8 (3%)	7	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
86	ii	414/416 (100%)	378 (91%)	25 (6%)	11 (3%)	6	48
87	jj	569/594 (96%)	501 (88%)	54 (10%)	14 (2%)	7	49
All	All	12492/12708 (98%)	10443 (84%)	1523 (12%)	526 (4%)	6	36

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	26
2	B	336/342 (98%)	288 (86%)	48 (14%)	4	28
3	C	301/301 (100%)	258 (86%)	43 (14%)	4	28
4	D	247/247 (100%)	218 (88%)	29 (12%)	7	36
5	E	208/221 (94%)	179 (86%)	29 (14%)	4	29
6	F	194/195 (100%)	169 (87%)	25 (13%)	5	32
7	G	206/206 (100%)	176 (85%)	30 (15%)	4	27
8	H	169/169 (100%)	147 (87%)	22 (13%)	5	32
9	I	174/180 (97%)	158 (91%)	16 (9%)	11	49
10	J	142/142 (100%)	127 (89%)	15 (11%)	8	42
11	L	176/176 (100%)	144 (82%)	32 (18%)	2	15
12	M	117/117 (100%)	104 (89%)	13 (11%)	8	40
13	N	171/171 (100%)	149 (87%)	22 (13%)	5	32
14	O	171/171 (100%)	141 (82%)	30 (18%)	2	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	P	134/134 (100%)	118 (88%)	16 (12%)	6	35
16	Q	163/163 (100%)	142 (87%)	21 (13%)	5	32
17	R	159/159 (100%)	139 (87%)	20 (13%)	5	32
18	S	156/156 (100%)	137 (88%)	19 (12%)	6	34
19	T	139/139 (100%)	115 (83%)	24 (17%)	2	17
20	U	89/89 (100%)	79 (89%)	10 (11%)	7	39
21	V	101/101 (100%)	82 (81%)	19 (19%)	2	13
22	W	55/55 (100%)	49 (89%)	6 (11%)	8	41
23	X	107/107 (100%)	95 (89%)	12 (11%)	7	39
24	Y	124/124 (100%)	106 (86%)	18 (14%)	4	27
25	Z	117/117 (100%)	101 (86%)	16 (14%)	4	30
26	a	119/119 (100%)	108 (91%)	11 (9%)	11	49
27	b	62/62 (100%)	54 (87%)	8 (13%)	5	32
28	c	79/79 (100%)	65 (82%)	14 (18%)	2	16
29	d	98/98 (100%)	79 (81%)	19 (19%)	2	12
30	e	114/114 (100%)	95 (83%)	19 (17%)	3	19
31	f	88/88 (100%)	75 (85%)	13 (15%)	4	26
32	g	98/98 (100%)	81 (83%)	17 (17%)	2	17
33	h	109/109 (100%)	96 (88%)	13 (12%)	6	35
34	i	86/86 (100%)	72 (84%)	14 (16%)	3	20
35	j	73/73 (100%)	57 (78%)	16 (22%)	1	9
36	k	64/64 (100%)	60 (94%)	4 (6%)	22	65
37	l	47/47 (100%)	40 (85%)	7 (15%)	4	26
38	m	48/48 (100%)	36 (75%)	12 (25%)	1	6
39	n	22/22 (100%)	20 (91%)	2 (9%)	12	50
40	o	92/92 (100%)	78 (85%)	14 (15%)	3	25
41	p	74/74 (100%)	63 (85%)	11 (15%)	4	26
42	r	109/109 (100%)	93 (85%)	16 (15%)	4	26
43	s	166/166 (100%)	155 (93%)	11 (7%)	21	63
44	t	136/136 (100%)	126 (93%)	10 (7%)	17	58
45	l	13/13 (100%)	11 (85%)	2 (15%)	3	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	AA	174/174 (100%)	142 (82%)	32 (18%)	2	14
53	BB	194/194 (100%)	168 (87%)	26 (13%)	5	30
54	CC	183/183 (100%)	162 (88%)	21 (12%)	7	37
55	DD	190/190 (100%)	151 (80%)	39 (20%)	1	11
56	EE	223/223 (100%)	188 (84%)	35 (16%)	3	23
57	FF	161/161 (100%)	132 (82%)	29 (18%)	2	15
58	GG	207/207 (100%)	174 (84%)	33 (16%)	3	22
59	HH	169/169 (100%)	155 (92%)	14 (8%)	14	53
60	II	178/178 (100%)	150 (84%)	28 (16%)	3	23
61	JJ	161/161 (100%)	139 (86%)	22 (14%)	4	30
62	KK	89/89 (100%)	76 (85%)	13 (15%)	4	27
63	LL	136/136 (100%)	116 (85%)	20 (15%)	4	26
64	MM	104/104 (100%)	88 (85%)	16 (15%)	3	24
65	NN	130/130 (100%)	104 (80%)	26 (20%)	1	12
66	OO	106/106 (100%)	84 (79%)	22 (21%)	1	10
67	PP	116/116 (100%)	97 (84%)	19 (16%)	3	20
68	QQ	117/117 (100%)	100 (86%)	17 (14%)	4	27
69	RR	117/117 (100%)	96 (82%)	21 (18%)	2	16
70	SS	119/119 (100%)	101 (85%)	18 (15%)	3	25
71	TT	112/112 (100%)	94 (84%)	18 (16%)	3	21
72	UU	94/94 (100%)	79 (84%)	15 (16%)	3	22
73	VV	67/67 (100%)	56 (84%)	11 (16%)	3	20
74	WW	112/112 (100%)	98 (88%)	14 (12%)	6	33
75	XX	113/113 (100%)	92 (81%)	21 (19%)	2	14
76	YY	108/108 (100%)	87 (81%)	21 (19%)	2	12
77	ZZ	66/66 (100%)	58 (88%)	8 (12%)	6	34
78	aa	85/85 (100%)	74 (87%)	11 (13%)	5	32
79	bb	75/75 (100%)	65 (87%)	10 (13%)	5	31
80	cc	54/54 (100%)	40 (74%)	14 (26%)	0	6
81	dd	47/47 (100%)	36 (77%)	11 (23%)	1	7
82	ee	47/47 (100%)	41 (87%)	6 (13%)	5	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
83	ff	58/61 (95%)	57 (98%)	1 (2%)	68	89
84	gg	272/272 (100%)	248 (91%)	24 (9%)	12	51
86	ii	358/358 (100%)	319 (89%)	39 (11%)	8	41
87	jj	507/522 (97%)	475 (94%)	32 (6%)	22	65
All	All	10889/10933 (100%)	9386 (86%)	1503 (14%)	8	29

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%)	6 (8%)
48	5	3645/3662 (99%)	1236 (33%)	291 (7%)
49	7	120/120 (100%)	24 (20%)	2 (1%)
50	8	155/156 (99%)	49 (31%)	6 (3%)
51	9	1710/1719 (99%)	614 (35%)	115 (6%)
85	hh	11/12 (91%)	6 (54%)	0
All	All	5787/5820 (99%)	1981 (34%)	420 (7%)

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

5 of 420 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
48	5	2490	U
48	5	4076	G
51	9	1418	C
48	5	2530	U
48	5	2858	A

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

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

5.5 Carbohydrates [i](#)

There are no 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	-	24,29,29	1.07	1 (4%)	23,45,45	1.91	1 (4%)
91	ADP	jj	603	-	24,29,29	1.08	1 (4%)	23,45,45	1.91	1 (4%)

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
91	ADP	jj	603	-	-	0/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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 (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
91	jj	602	ADP	N3-C2-N1	-7.76	122.78	128.87
91	jj	603	ADP	N3-C2-N1	-7.65	122.86	128.87

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.