



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

Nov 22, 2016 – 03:08 PM EST

PDB ID : 5LZX  
EMDB ID: : EMD-4135  
Title : Structure of the mammalian rescue complex with Pelota and Hbs1l assembled on a UGA stop codon.  
Authors : Shao, S.; Murray, J.; Brown, A.; Taunton, J.; Ramakrishnan, V.; Hegde, R.S.  
Deposited on : 2016-10-02  
Resolution : 3.67 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

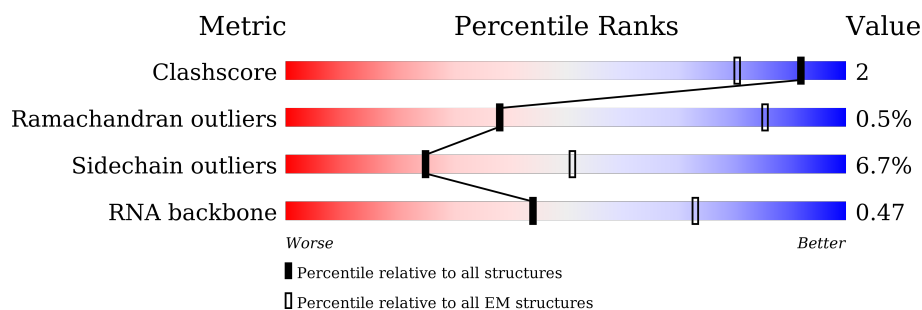
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.67 Å.

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
















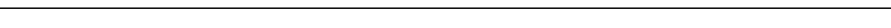




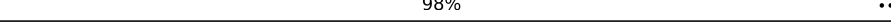




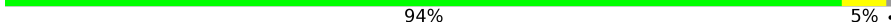

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	257	82% 14% . .
2	B	403	89% 9% .
3	C	425	76% 8% . 15%
4	D	297	89% 9% .
5	E	291	67% 6% . 26%
6	F	247	80% 11% . 9%
7	G	319	65% 8% 27%
8	H	192	89% 10% .

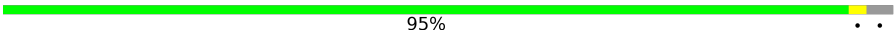

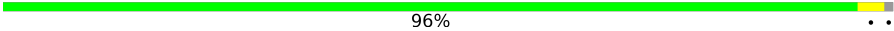
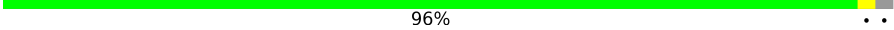



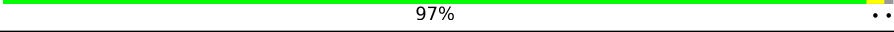



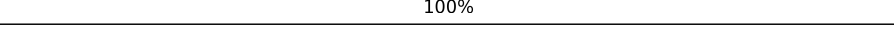







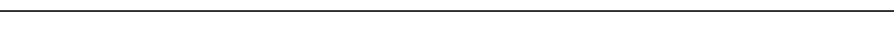

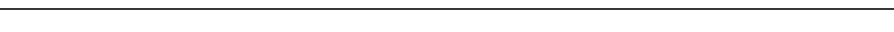
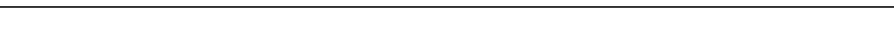


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Mol	Chain	Length	Quality of chain
9	I	214	 88% 7% .
10	J	178	 88% 7% .
11	L	211	 92% 7%
12	M	218	 55% 8% 37%
13	N	204	 89% 10%
14	O	203	 88% 10% .
15	P	184	 78% . . 17%
16	Q	188	 90% 10% .
17	R	196	 82% 9% . 8%
18	S	176	 86% 14%
19	T	160	 91% 9% .
20	U	128	 70% 6% . 23%
21	V	140	 82% 11% . 6%
22	W	157	 62% 6% 32%
23	X	156	 71% . 24%
24	Y	145	 87% 6% 8%
25	Z	136	 90% 10% .
26	a	148	 98% ..
27	b	245	 41% . 58%
28	c	115	 83% . 15%
29	d	125	 77% 9% 14%
30	e	135	 88% 7% 5%
31	f	110	 94% 5% .
32	g	117	 92% 5% .
33	h	123	 95% . .


























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Mol	Chain	Length	Quality of chain
34	i	105	95% 
35	j	97	84%  5% 11%
36	k	70	96% 
37	l	51	96% 
38	m	102	49%  49%
39	n	25	92% 
40	o	106	92%  6%
41	p	92	97% 
42	r	137	82%  8% 9%
43	s	318	59%  38%
44	t	165	90%  7%
45	1	7	100% 
46	2	76	83%  16%
47	3	75	64%  32%
48	5	3543	70%  26%
49	7	120	85%  14%
50	8	156	72%  24%
51	9	1869	62%  26% 9%
52	AA	295	64%  10% 26%
53	BB	264	71%  8% 19%
54	CC	293	67%  8% 25%
55	DD	243	83%  10% 6%
56	EE	263	87% 
57	FF	204	81%  9% 9%
58	GG	249	85%  10% 5%

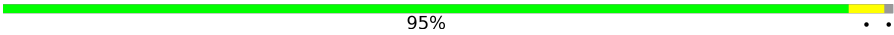



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Mol	Chain	Length	Quality of chain
59	HH	194	
60	II	208	
61	JJ	194	
62	KK	165	
63	LL	158	
64	MM	132	
65	NN	151	
66	OO	168	
67	PP	145	
68	QQ	146	
69	RR	135	
70	SS	152	
71	TT	145	
72	UU	119	
73	VV	83	
74	WW	130	
75	XX	143	
76	YY	130	
77	ZZ	125	
78	aa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

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Mol	Chain	Length	Quality of chain
84	gg	317	 95% . .
85	hh	8	 50% 50%
86	ii	403	 88% . 8%
87	jj	710	 55% . 40%

## 2 Entry composition

There are 90 unique types of molecules in this entry. The entry contains 222005 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called uL2.

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

- Molecule 2 is a protein called U13.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 3 is a protein called uL4.

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

- Molecule 4 is a protein called 60S ribosomal protein L5.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 5 is a protein called 60S ribosomal protein L6.

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

- Molecule 6 is a protein called uL30.

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

There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 7 is a protein called eL8.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 8 is a protein called uL6.

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

- Molecule 9 is a protein called Ribosomal protein L10 (Predicted).

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

- Molecule 10 is a protein called uL5.



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

- Molecule 11 is a protein called eL13.

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

- Molecule 12 is a protein called eL14.

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

- Molecule 13 is a protein called Ribosomal protein L15.

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

- Molecule 14 is a protein called uL13.

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

- Molecule 15 is a protein called uL22.

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

- Molecule 16 is a protein called eL18.

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

- Molecule 17 is a protein called eL19.

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

- Molecule 18 is a protein called eL20.

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

- Molecule 19 is a protein called eL21.

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

- Molecule 20 is a protein called eL22.

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

- Molecule 21 is a protein called uL14.

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

- Molecule 22 is a protein called eL24.

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

- Molecule 23 is a protein called uL23.

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

- Molecule 24 is a protein called uL24.

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

- Molecule 25 is a protein called 60S ribosomal protein L27.

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

- Molecule 26 is a protein called uL15.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 27 is a protein called eL29.

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

- Molecule 28 is a protein called eL30.

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

- Molecule 29 is a protein called eL31.

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

- Molecule 30 is a protein called eL32.

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

- Molecule 31 is a protein called eL33.

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

- Molecule 32 is a protein called eL34.

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

- 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 60S ribosomal protein L36.

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 Ribosomal protein L37.

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

- Molecule 36 is a protein called eL38.

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

- Molecule 37 is a protein called eL39.

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

- Molecule 38 is a protein called eL40.

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

- Molecule 39 is a protein called eL41.

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

- Molecule 40 is a protein called eL42.

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

- Molecule 41 is a protein called eL43.

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

- Molecule 42 is a protein called eL28.

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

- Molecule 43 is a protein called uL10.

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

- Molecule 44 is a protein called uL11.

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

- Molecule 45 is a protein called Nascent chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	1	7	Total	C	N	O	0	0
			49	31	8	10		

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 52 is a protein called uS2.

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

- Molecule 53 is a protein called 40S ribosomal protein S3a.

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

- Molecule 54 is a protein called uS5.

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

- Molecule 55 is a protein called uS3.

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

- Molecule 56 is a protein called eS4.

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

- Molecule 57 is a protein called uS7.

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

- Molecule 58 is a protein called 40S ribosomal protein S6.

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

- Molecule 59 is a protein called eS7.

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

- Molecule 60 is a protein called eS8.

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

- Molecule 61 is a protein called Ribosomal protein S9 (Predicted).

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

- Molecule 62 is a protein called eS10.

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

- Molecule 63 is a protein called uS17.

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

- Molecule 64 is a protein called 40S ribosomal protein S12.

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

- Molecule 65 is a protein called uS15.



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

- Molecule 66 is a protein called uS11.

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

- Molecule 67 is a protein called uS19.

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

- Molecule 68 is a protein called uS9.

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

- Molecule 69 is a protein called eS17.

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

- Molecule 70 is a protein called uS13.

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

- Molecule 71 is a protein called eS19.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 72 is a protein called uS10.

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

- Molecule 73 is a protein called eS21.

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

- Molecule 74 is a protein called uS8.

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

- Molecule 75 is a protein called uS12.

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

- Molecule 76 is a protein called eS24.

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

- Molecule 77 is a protein called eS25.

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

- Molecule 78 is a protein called eS26.

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

- Molecule 79 is a protein called 40S ribosomal protein S27.

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

- Molecule 80 is a protein called eS28.

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

- Molecule 81 is a protein called uS14.

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

- Molecule 82 is a protein called eS30.

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

- Molecule 83 is a protein called eS31.

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

- Molecule 84 is a protein called RACK1.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
85	hh	8	Total	C	N	O	P	0	0
			169	76	29	56	8		

- Molecule 86 is a protein called Protein pelota homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	ii	372	Total	C	N	O	S	0	0
			2947	1844	528	559	16		

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
ii	221	MET	LEU	variant	UNP Q9BRX2
ii	386	GLY	-	expression tag	UNP Q9BRX2
ii	387	SER	-	expression tag	UNP Q9BRX2
ii	388	GLU	-	expression tag	UNP Q9BRX2
ii	389	ASN	-	expression tag	UNP Q9BRX2
ii	390	LEU	-	expression tag	UNP Q9BRX2
ii	391	TYR	-	expression tag	UNP Q9BRX2
ii	392	PHE	-	expression tag	UNP Q9BRX2
ii	393	GLN	-	expression tag	UNP Q9BRX2
ii	394	GLY	-	expression tag	UNP Q9BRX2
ii	395	ALA	-	expression tag	UNP Q9BRX2
ii	396	HIS	-	expression tag	UNP Q9BRX2
ii	397	HIS	-	expression tag	UNP Q9BRX2
ii	398	HIS	-	expression tag	UNP Q9BRX2
ii	399	HIS	-	expression tag	UNP Q9BRX2
ii	400	HIS	-	expression tag	UNP Q9BRX2
ii	401	HIS	-	expression tag	UNP Q9BRX2
ii	402	SER	-	expression tag	UNP Q9BRX2
ii	403	THR	-	expression tag	UNP Q9BRX2

- Molecule 87 is a protein called HBS1-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	jj	425	Total	C	N	O	S	0	0
			3292	2100	565	609	18		

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
jj	-25	MET	-	initiating methionine	UNP Q9Y450
jj	-24	ASP	-	expression tag	UNP Q9Y450

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Chain	Residue	Modelled	Actual	Comment	Reference
jj	-23	TYR	-	expression tag	UNP Q9Y450
jj	-22	LYS	-	expression tag	UNP Q9Y450
jj	-21	ASP	-	expression tag	UNP Q9Y450
jj	-20	HIS	-	expression tag	UNP Q9Y450
jj	-19	ASP	-	expression tag	UNP Q9Y450
jj	-18	GLY	-	expression tag	UNP Q9Y450
jj	-17	ASP	-	expression tag	UNP Q9Y450
jj	-16	TYR	-	expression tag	UNP Q9Y450
jj	-15	LYS	-	expression tag	UNP Q9Y450
jj	-14	ASP	-	expression tag	UNP Q9Y450
jj	-13	HIS	-	expression tag	UNP Q9Y450
jj	-12	ASP	-	expression tag	UNP Q9Y450
jj	-11	ILE	-	expression tag	UNP Q9Y450
jj	-10	ASP	-	expression tag	UNP Q9Y450
jj	-9	TYR	-	expression tag	UNP Q9Y450
jj	-8	LYS	-	expression tag	UNP Q9Y450
jj	-7	ASP	-	expression tag	UNP Q9Y450
jj	-6	ASP	-	expression tag	UNP Q9Y450
jj	-5	ASP	-	expression tag	UNP Q9Y450
jj	-4	ASP	-	expression tag	UNP Q9Y450
jj	-3	LYS	-	expression tag	UNP Q9Y450
jj	-2	ALA	-	expression tag	UNP Q9Y450
jj	-1	GLY	-	expression tag	UNP Q9Y450
jj	0	SER	-	expression tag	UNP Q9Y450

- 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	jj	1	Total Mg 1 1	0
88	V	1	Total Mg 1 1	0
88	7	5	Total Mg 5 5	0
88	a	1	Total Mg 1 1	0
88	5	182	Total Mg 182 182	0
88	8	6	Total Mg 6 6	0

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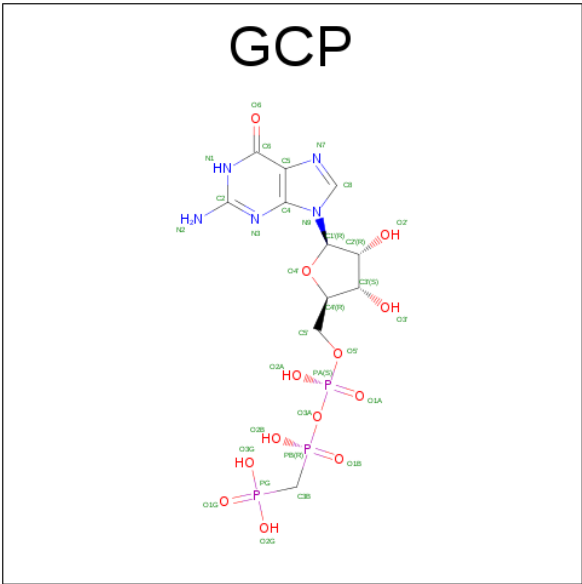
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Mol	Chain	Residues	Atoms		AltConf
88	9	66	Total	Mg	0
			66	66	
88	L	1	Total	Mg	0
			1	1	

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

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

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

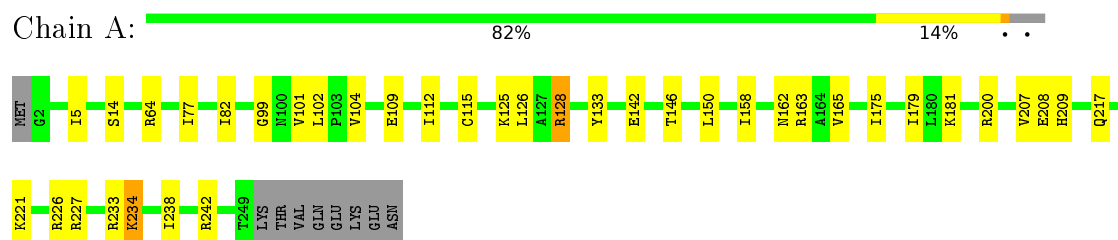


Mol	Chain	Residues	Atoms					AltConf
90	jj	1	Total	C	N	O	P	0
			32	11	5	13	3	

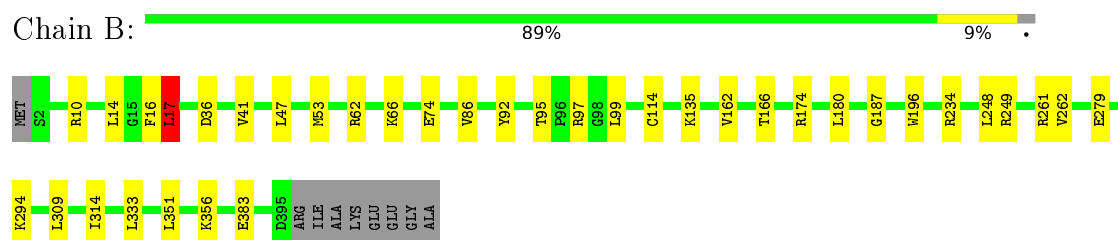
### 3 Residue-property plots

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.

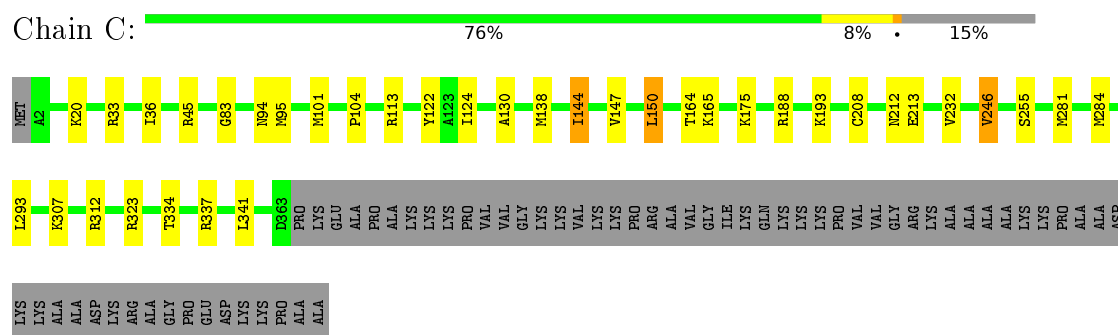
- Molecule 1: uL2



- Molecule 2: U13



- Molecule 3: uL4



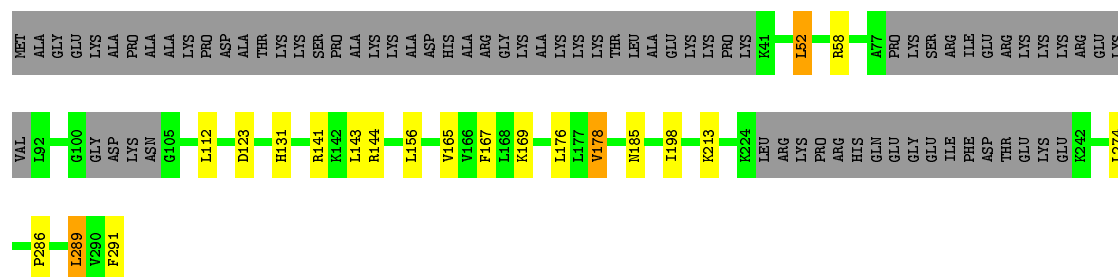
- Molecule 4: 60S ribosomal protein L5




- Molecule 5: 60S ribosomal protein L6

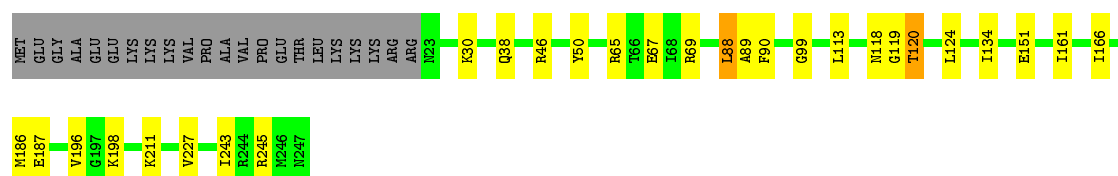


Chain E:  67% 6% 26%



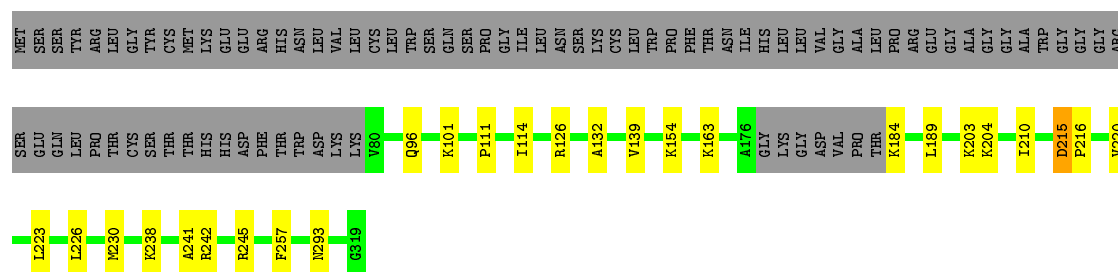
- Molecule 6: uL30

Chain F:  80% 11% 9%




- Molecule 7: eL8

Chain G:  65% 8% 27%




- Molecule 8: uL6

Chain H:  89% 10%




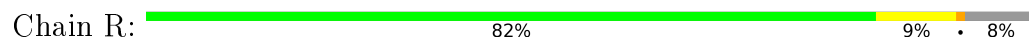
- Molecule 9: Ribosomal protein L10 (Predicted)

Chain I:  88% 7%



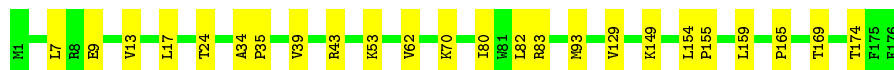
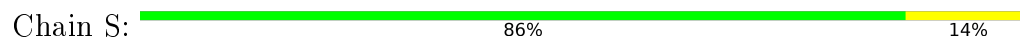
- Molecule 10: uL5

Chain J:  88% 7%

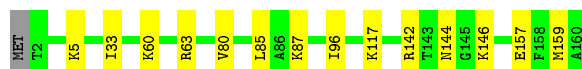




- Molecule 18: eL20



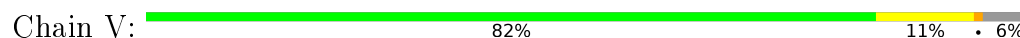
- Molecule 19: eL21



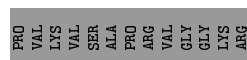
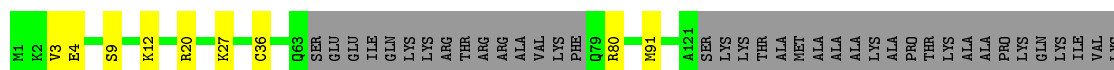
- Molecule 20: eL22



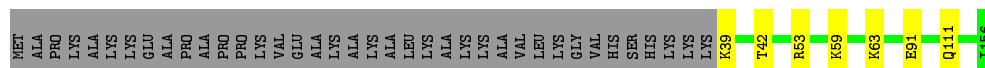
- Molecule 21: uL14



- Molecule 22: eL24



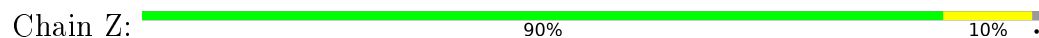
- Molecule 23: uL23



- Molecule 24: uL24



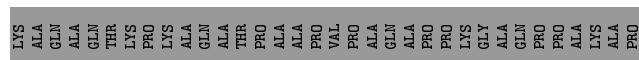
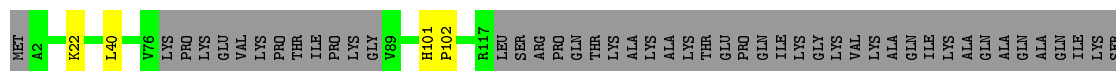
- Molecule 25: 60S ribosomal protein L27



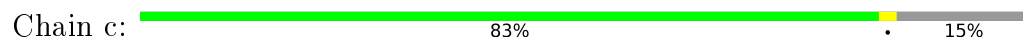
- Molecule 26: uL15



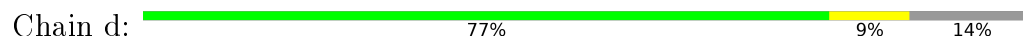
- Molecule 27: eL29



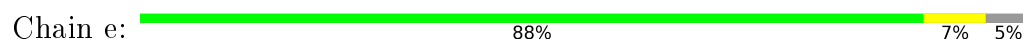
- Molecule 28: eL30



- Molecule 29: eL31



- Molecule 30: eL32



- Molecule 31: eL33

Chain f:  94% 5%



- Molecule 32: eL34

Chain g:  92% 5%



- Molecule 33: uL29

Chain h:  95% . .




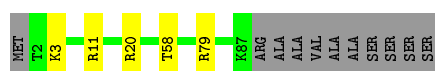
- Molecule 34: 60S ribosomal protein L36

Chain i:  95% . .



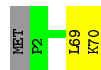
- Molecule 35: Ribosomal protein L37

Chain j:  84% 5% 11%



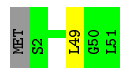
- Molecule 36: eL38

Chain k:  96% . .



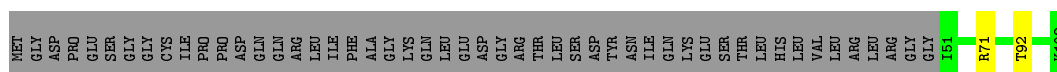
- Molecule 37: eL39

Chain l:  96% . .



- Molecule 38: eL40

Chain m:  49% . 49%



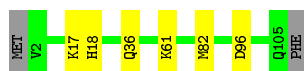
- Molecule 39: eL41

Chain n:



- Molecule 40: eL42

Chain o:



- Molecule 41: eL43

Chain p:



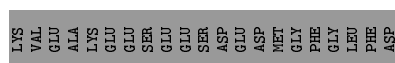
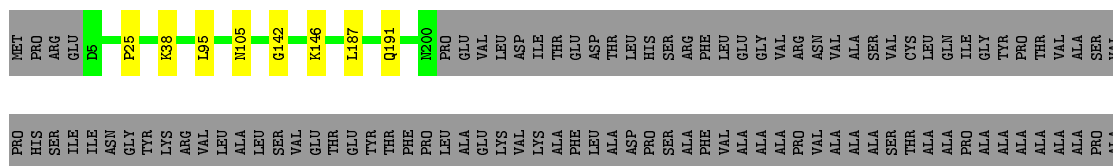
- Molecule 42: eL28

Chain r:



- Molecule 43: uL10

Chain s:



- Molecule 44: uL11

Chain t:




- Molecule 45: Nascent chain

Chain 1:  100%

There are no outlier residues recorded for this chain.

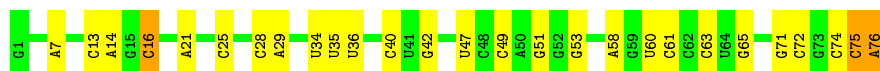
- Molecule 46: P-site tRNA

Chain 2:  83% 16%



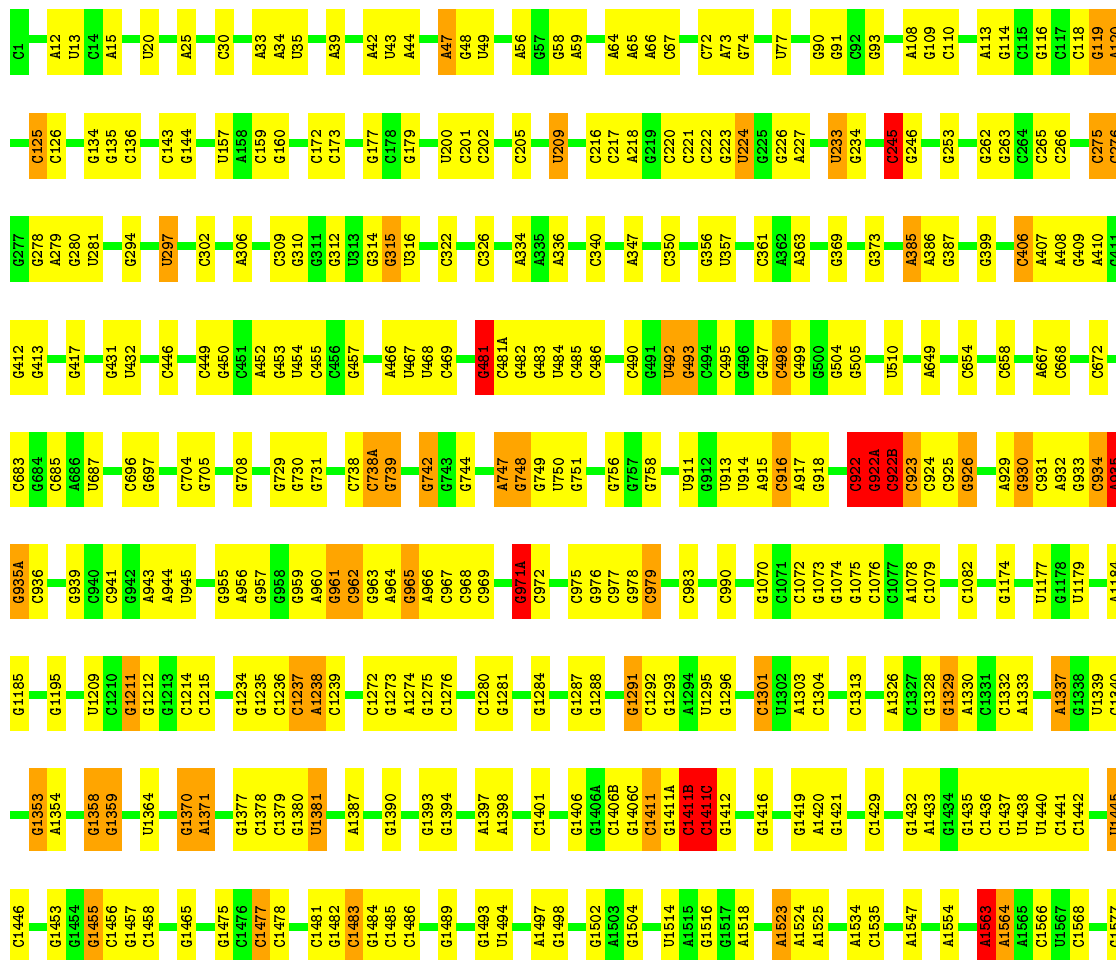
- Molecule 47: E-site tRNA

Chain 3:  64% 32%



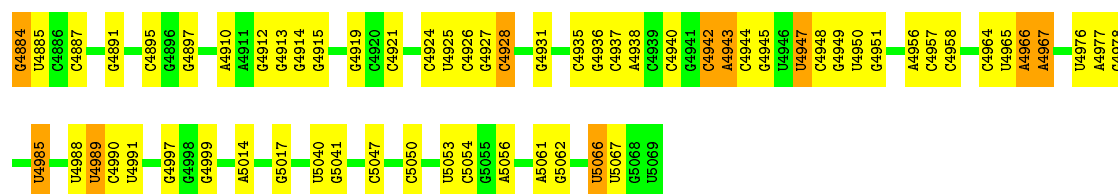
- Molecule 48: 28S ribosomal RNA

Chain 5:  70% 26%



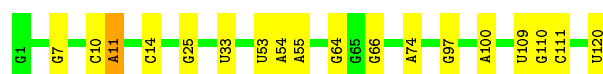
C4670	C4671	C4672	C4673	C4674	C4675	C4676	C4677	C4678	C4679	C4680	C4681	C4682	C4683	C4684	C4685	C4686	C4687	C4688	C4689	C4690	C4691	C4692	C4693	C4694	C4695	C4696	C4697	C4698	C4699	C4700	C4701	C4702	C4703	C4704	C4705	C4706	C4707	C4708	C4709	C4710	C4711	C4712	C4713	C4714	C4715	C4716	C4717	C4718	C4719	C4720	C4721	C4722	C4723	C4724	C4725	C4726	C4727	C4728	C4729	C4730	C4731	C4732	C4733	C4734	C4735	C4736	C4737	C4738	C4739	C4740	C4741	C4742	C4743	C4744	C4745	C4746	C4747	C4748	C4749	C4750	C4751	C4752	C4753	C4754	C4755	C4756	C4757	C4758	C4759	C4760	C4761	C4762	C4763	C4764	C4765	C4766	C4767	C4768	C4769	C4770	C4771	C4772	C4773	C4774	C4775	C4776	C4777	C4778	C4779	C4780	C4781	C4782	C4783	C4784	C4785	C4786	C4787	C4788	C4789	C4790	C4791	C4792	C4793	C4794	C4795	C4796	C4797	C4798	C4799	C4800	C4801	C4802	C4803	C4804	C4805	C4806	C4807	C4808	C4809	C4810	C4811	C4812	C4813	C4814	C4815	C4816	C4817	C4818	C4819	C4820	C4821	C4822	C4823	C4824	C4825	C4826	C4827	C4828	C4829	C4830	C4831	C4832	C4833	C4834	C4835	C4836	C4837	C4838	C4839	C4840	C4841	C4842	C4843	C4844	C4845	C4846	C4847	C4848	C4849	C4850	C4851	C4852	C4853	C4854	C4855	C4856	C4857	C4858	C4859	C4860	C4861	C4862	C4863	C4864	C4865	C4866	C4867	C4868	C4869	C4870	C4871	C4872	C4873	C4874	C4875	C4876	C4877	C4878	C4879	C4880	C4881	C4882	C4883	C4884	C4885	C4886	C4887	C4888	C4889	C4890	C4891	C4892	C4893	C4894	C4895	C4896	C4897	C4898	C4899	C4900	C4901	C4902	C4903	C4904	C4905	C4906	C4907	C4908	C4909	C4910	C4911	C4912	C4913	C4914	C4915	C4916	C4917	C4918	C4919	C4920	C4921	C4922	C4923	C4924	C4925	C4926	C4927	C4928	C4929	C4930	C4931	C4932	C4933	C4934	C4935	C4936	C4937	C4938	C4939	C4940	C4941	C4942	C4943	C4944	C4945	C4946	C4947	C4948	C4949	C4950	C4951	C4952	C4953	C4954	C4955	C4956	C4957	C4958	C4959	C4960	C4961	C4962	C4963	C4964	C4965	C4966	C4967	C4968	C4969	C4970	C4971	C4972	C4973	C4974	C4975	C4976	C4977	C4978	C4979	C4980	C4981	C4982	C4983	C4984	C4985	C4986	C4987	C4988	C4989	C4990	C4991	C4992	C4993	C4994	C4995	C4996	C4997	C4998	C4999	C5000	C5001	C5002	C5003	C5004	C5005	C5006	C5007	C5008	C5009	C5010	C5011	C5012	C5013	C5014	C5015	C5016	C5017	C5018	C5019	C5020	C5021	C5022	C5023	C5024	C5025	C5026	C5027	C5028	C5029	C5030	C5031	C5032	C5033	C5034	C5035	C5036	C5037	C5038	C5039	C5040	C5041	C5042	C5043	C5044	C5045	C5046	C5047	C5048	C5049	C5050	C5051	C5052	C5053	C5054	C5055	C5056	C5057	C5058	C5059	C5060	C5061	C5062	C5063	C5064	C5065	C5066	C5067	C5068	C5069	C5070	C5071	C5072	C5073	C5074	C5075	C5076	C5077	C5078	C5079	C5080	C5081	C5082	C5083	C5084	C5085	C5086	C5087	C5088	C5089	C5090	C5091	C5092	C5093	C5094	C5095	C5096	C5097	C5098	C5099	C5100	C5101	C5102	C5103	C5104	C5105	C5106	C5107	C5108	C5109	C5110	C5111	C5112	C5113	C5114	C5115	C5116	C5117	C5118	C5119	C5120	C5121	C5122	C5123	C5124	C5125	C5126	C5127	C5128	C5129	C5130	C5131	C5132	C5133	C5134	C5135	C5136	C5137	C5138	C5139	C5140	C5141	C5142	C5143	C5144	C5145	C5146	C5147	C5148	C5149	C5150	C5151	C5152	C5153	C5154	C5155	C5156	C5157	C5158	C5159	C5160	C5161	C5162	C5163	C5164	C5165	C5166	C5167	C5168	C5169	C5170	C5171	C5172	C5173	C5174	C5175	C5176	C5177	C5178	C5179	C5180	C5181	C5182	C5183	C5184	C5185	C5186	C5187	C5188	C5189	C5190	C5191	C5192	C5193	C5194	C5195	C5196	C5197	C5198	C5199	C5200	C5201	C5202	C5203	C5204	C5205	C5206	C5207	C5208	C5209	C5210	C5211	C5212	C5213	C5214	C5215	C5216	C5217	C5218	C5219	C5220	C5221	C5222	C5223	C5224	C5225	C5226	C5227	C5228	C5229	C5230	C5231	C5232	C5233	C5234	C5235	C5236	C5237	C5238	C5239	C5240	C5241	C5242	C5243	C5244	C5245	C5246	C5247	C5248	C5249	C5250	C5251	C5252	C5253	C5254	C5255	C5256	C5257	C5258	C5259	C5260	C5261	C5262	C5263	C5264	C5265	C5266	C5267	C5268	C5269	C5270	C5271	C5272	C5273	C5274	C5275	C5276	C5277	C5278	C5279	C5280	C5281	C5282	C5283	C5284	C5285	C5286	C5287	C5288	C5289	C5290	C5291	C5292	C5293	C5294	C5295	C5296	C5297	C5298	C5299	C5300	C5301	C5302	C5303	C5304	C5305	C5306	C5307	C5308	C5309	C5310	C5311	C5312	C5313	C5314	C5315	C5316	C5317	C5318	C5319	C5320	C5321	C5322	C5323	C5324	C5325	C5326	C5327	C5328	C5329	C5330	C5331	C5332	C5333	C5334	C5335	C5336	C5337	C5338	C5339	C5340	C5341	C5342	C5343	C5344	C5345	C5346	C5347	C5348	C5349	C5350	C5351	C5352	C5353	C5354	C5355	C5356	C5357	C5358	C5359	C5360	C5361	C5362	C5363	C5364	C5365	C5366	C5367	C5368	C5369	C5370	C5371	C5372	C5373	C5374	C5375	C5376	C5377	C5378	C5379	C5380	C5381	C5382	C5383	C5384	C5385	C5386	C5387	C5388	C5389	C5390	C5391	C5392	C5393	C5394	C5395	C5396	C5397	C5398	C5399	C5400	C5401	C5402	C5403	C5404	C5405	C5406	C5407	C5408	C5409	C5410	C5411	C5412	C5413	C5414	C5415	C5416	C5417	C5418	C5419	C5420	C5421	C5422	C5423	C5424	C5425	C5426	C5427	C5428	C5429	C5430	C5431	C5432	C5433	C5434	C5435	C5436	C5437	C5438	C5439	C5440	C5441	C5442	C5443	C5444	C5445	C5446	C5447	C5448	C5449	C5450	C5451	C5452	C5453	C5454	C5455	C5456	C5457	C5458	C5459	C5460	C5461	C5462	C5463	C5464	C5465	C5466	C5467	C5468	C5469	C5470	C5471	C5472	C5473	C5474	C5475	C5476	C5477	C5478	C5479	C5480	C5481	C5482	C5483	C5484	C5485	C5486	C5487	C5488	C5489	C5490	C5491	C5492	C5493	C5494	C5495	C5496	C5497	C5498	C5499	C5500	C5501	C5502	C5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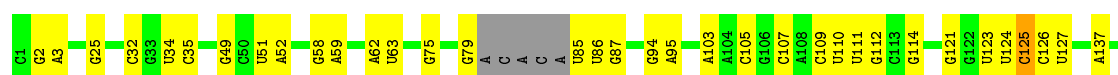
• Molecule 49: 5S ribosomal RNA

Chain 7: 85% 14%



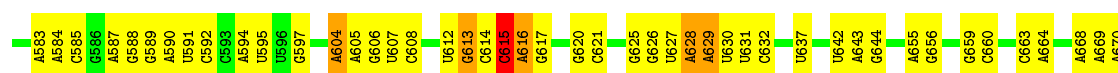
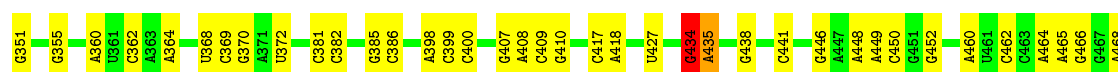
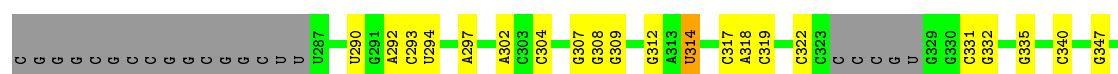
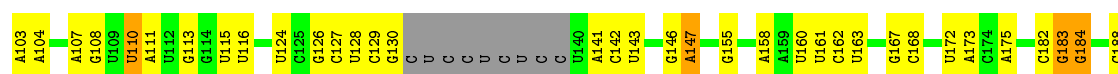
• Molecule 50: 5.8S ribosomal RNA

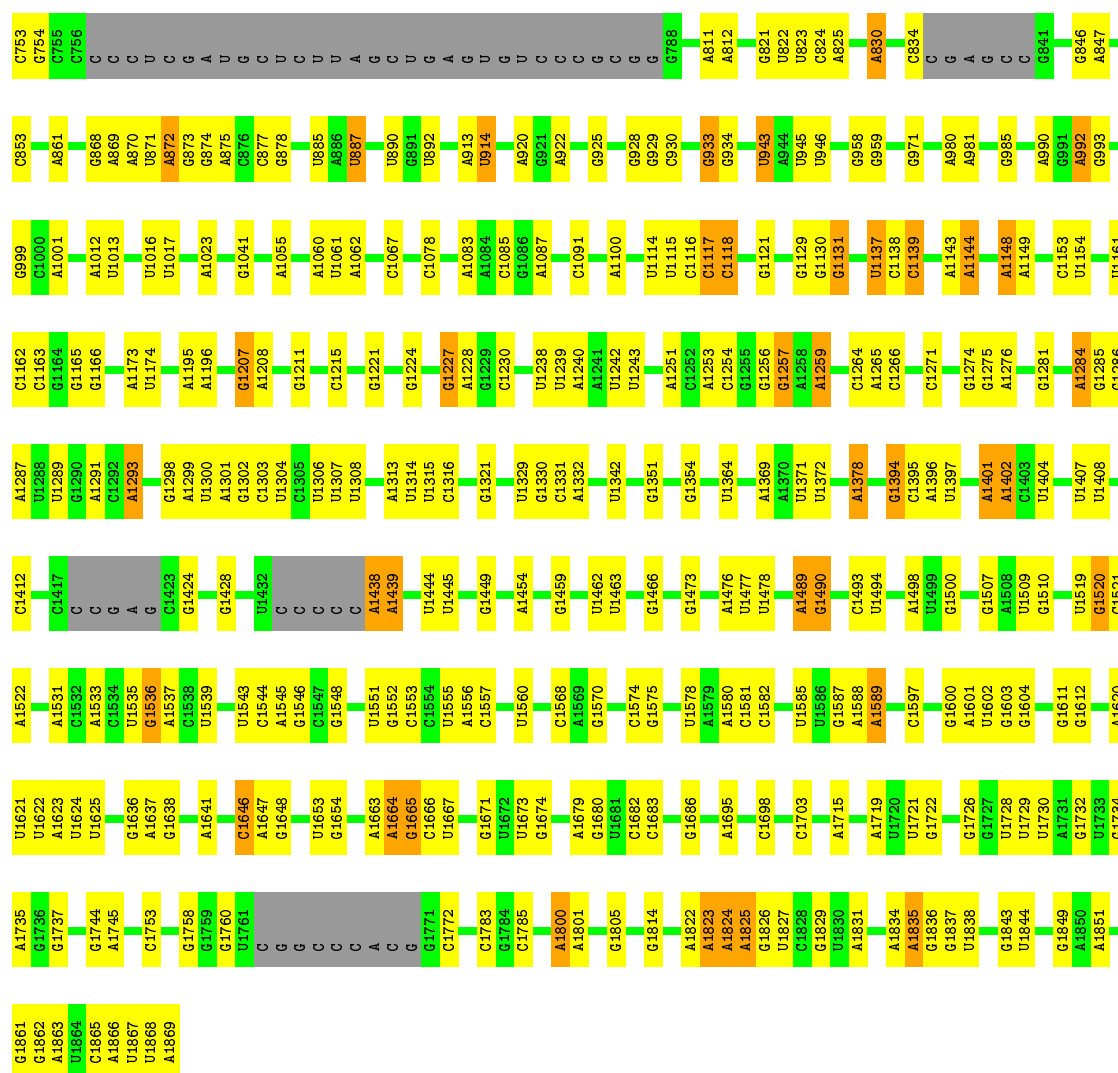
Chain 8: 72% 24%



• Molecule 51: 18S ribosomal RNA

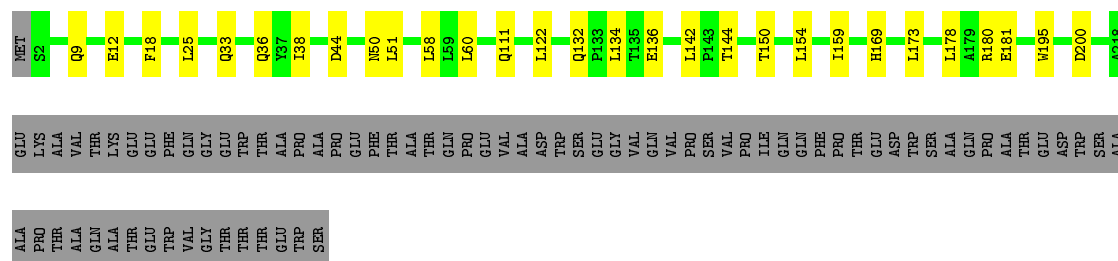
Chain 9: 62% 26% 9%





• Molecule 52: uS2

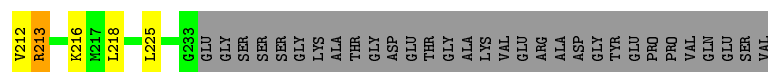
Chain AA: 64% 10% 26%



• Molecule 53: 40S ribosomal protein S3a

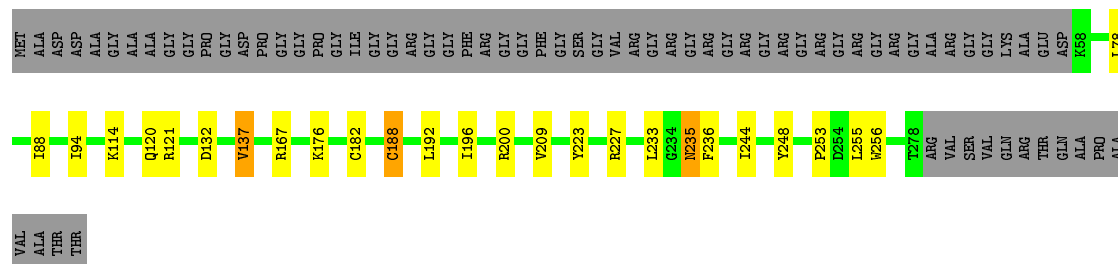
Chain BB: 71% 8% 19%





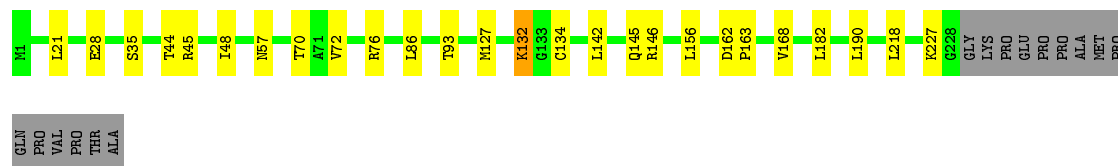
• Molecule 54: uS5

Chain CC: 67% 8% 25%



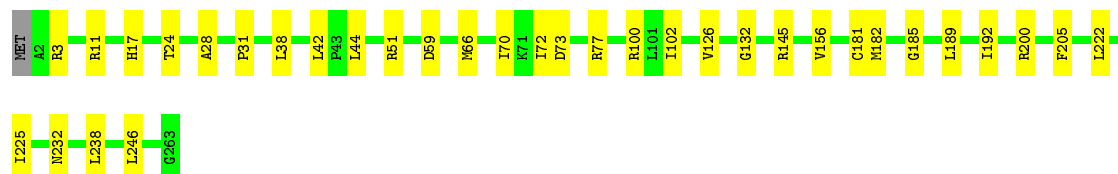
• Molecule 55: uS3

Chain DD: 83% 10% 6%



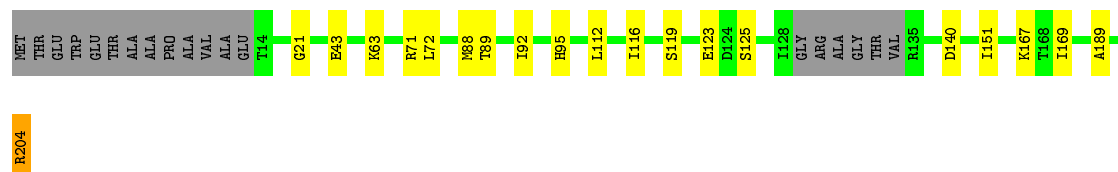
• Molecule 56: eS4

Chain EE: 87% 13%



• Molecule 57: uS7

Chain FF: 81% 9% 9%



• Molecule 58: 40S ribosomal protein S6

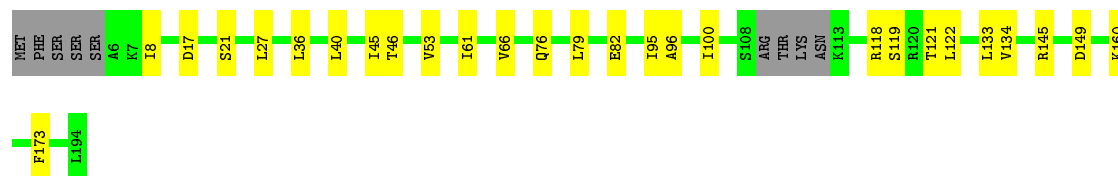
Chain GG: 85% 10% 5%



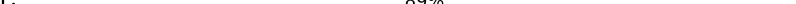
SER  
GLN  
LYS

- Molecule 59: eS7

Chain HH:  81% 14% 5%



- Molecule 60: eS8

Chain II:  89% 10%



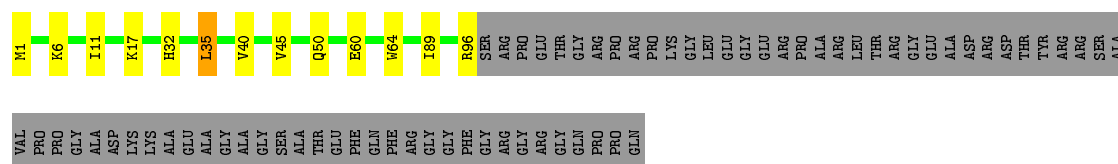
- Molecule 61: Ribosomal protein S9 (Predicted)

Chain JJ:  86% 9% 5%



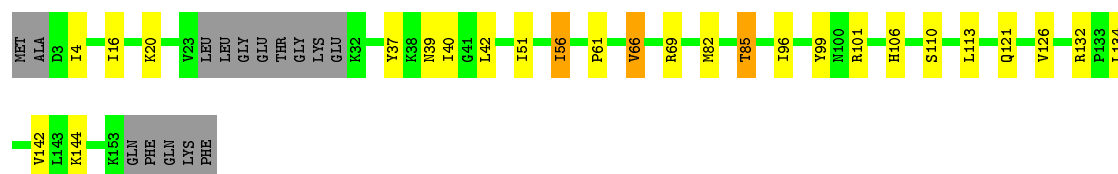
- Molecule 62: eS10

Chain KK: 




- Molecule 63: uS17

Chain LL:  74% 15% • 9%



- Molecule 64: 40S ribosomal protein S12

Chain MM:  77% 12% 11%



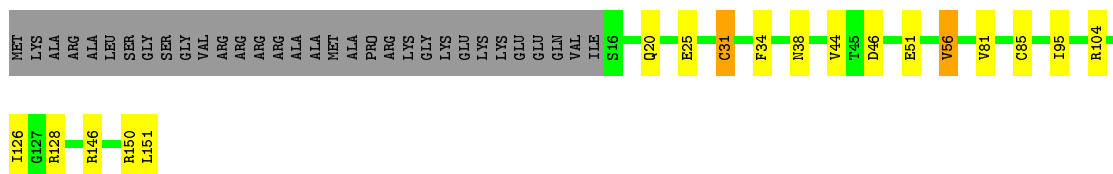
• Molecule 65: uS15

Chain NN: 85% 12% ..



• Molecule 66: uS11

Chain OO: 70% 10% 19%



• Molecule 67: uS19

Chain PP: 74% 9% 17%



• Molecule 68: uS9

Chain QQ: 90% 8%



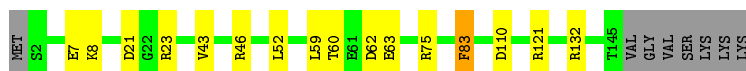
• Molecule 69: eS17

Chain RR: 82% 15% ..



• Molecule 70: uS13

Chain SS: 84% 10% 5%



• Molecule 71: eS19

Chain TT: 88% 8% ..



- Molecule 72: uS10

Chain UU: 76% 8% 16%



- Molecule 73: eS21

Chain VV: 92% 8%



- Molecule 74: uS8

Chain WW: 88% 11% ..



- Molecule 75: uS12

Chain XX: 87% 9% ...



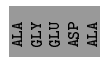
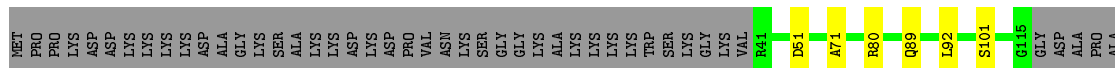
- Molecule 76: eS24

Chain YY: 85% 10% 5%



- Molecule 77: eS25

Chain ZZ: 55% 5% 40%



- Molecule 78: eS26

Chain aa: 80% 7% 12%



- Molecule 79: 40S ribosomal protein S27

Chain bb: 89% 8% ..



- Molecule 80: eS28

Chain cc: 83% 7% 10%



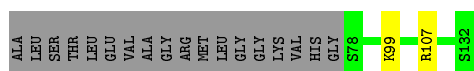
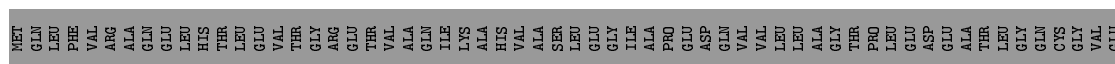
- Molecule 81: uS14

Chain dd: 89% 9% .



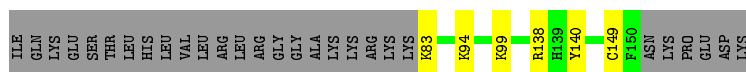
- Molecule 82: eS30

Chain ee: 40% . 59%



- Molecule 83: eS31

Chain ff: 40% . 56%



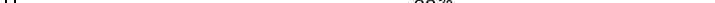
- Molecule 84: RACK1

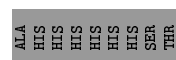
Chain gg: 95% . .



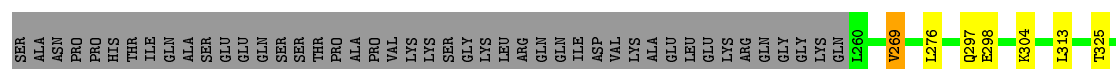
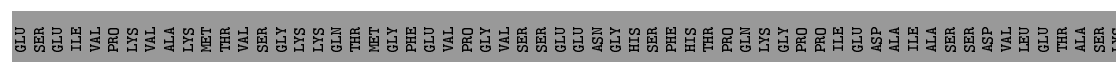
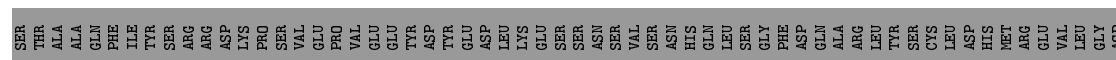
- Molecule 85: mRNA (UGA stop codon)

U41	C42	A43	A44	A45	G46	U47	U48
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- Chain ii:  88% . 8%



- Chain jj:  55% . 40%





## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	37432	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	104478	Depositor
Image detector	Not provided	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	A	0.35	0/1936	0.70	0/2596
10	J	0.34	0/1385	0.61	0/1852
11	L	0.34	0/1733	0.68	0/2316
12	M	0.36	0/1158	0.68	0/1547
13	N	0.35	0/1746	0.67	0/2338
14	O	0.36	0/1662	0.66	0/2222
15	P	0.36	0/1268	0.64	0/1700
16	Q	0.35	0/1539	0.73	0/2054
17	R	0.34	0/1524	0.66	0/2013
18	S	0.35	0/1501	0.65	0/2012
19	T	0.34	0/1326	0.62	0/1770
2	B	0.36	0/3240	0.65	0/4339
20	U	0.35	0/823	0.56	0/1104
21	V	0.34	0/993	0.63	0/1332
22	W	0.35	0/873	0.57	0/1158
23	X	0.31	0/984	0.60	0/1323
24	Y	0.32	0/1132	0.62	0/1504
25	Z	0.36	0/1130	0.63	0/1507
26	a	0.33	0/1191	0.63	0/1590
27	b	0.33	0/861	0.58	0/1138
28	c	0.31	0/771	0.54	0/1034
29	d	0.35	0/903	0.66	0/1216
3	C	0.34	0/2937	0.67	0/3946
30	e	0.34	0/1071	0.64	0/1429
31	f	0.38	0/895	0.70	0/1198
32	g	0.34	0/916	0.69	0/1220
33	h	0.31	0/1021	0.61	0/1348
34	i	0.34	0/841	0.60	0/1112
35	j	0.35	0/720	0.70	0/952
36	k	0.31	0/575	0.54	0/761
37	l	0.35	0/459	0.63	0/608
38	m	0.31	0/435	0.60	0/575

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
39	n	0.36	0/240	0.67	0/305
4	D	0.34	0/2437	0.62	2/3264 (0.1%)
40	o	0.34	0/864	0.62	0/1140
41	p	0.34	0/718	0.59	0/953
42	r	0.34	0/1010	0.65	0/1354
43	s	0.37	0/1530	0.50	0/2064
44	t	0.36	0/1174	0.53	0/1582
45	1	0.44	0/49	0.61	0/65
46	2	0.21	0/1805	0.66	0/2809
47	3	0.21	0/1777	0.65	0/2763
48	5	0.31	14/84961 (0.0%)	0.76	62/132460 (0.0%)
49	7	0.28	0/2858	0.67	0/4455
5	E	0.33	0/1762	0.62	0/2362
50	8	0.27	0/3581	0.67	0/5577
51	9	0.27	1/40523 (0.0%)	0.70	8/63130 (0.0%)
52	AA	0.35	0/1747	0.61	0/2374
53	BB	0.33	0/1756	0.58	0/2350
54	CC	0.34	0/1753	0.63	0/2369
55	DD	0.35	0/1796	0.62	0/2417
56	EE	0.35	0/2118	0.64	0/2849
57	FF	0.34	0/1492	0.61	0/2005
58	GG	0.35	0/1946	0.66	0/2590
59	HH	0.35	0/1510	0.58	0/2022
6	F	0.36	0/1911	0.65	0/2549
60	II	0.34	0/1715	0.66	0/2287
61	JJ	0.34	0/1550	0.70	0/2069
62	KK	0.35	0/834	0.57	0/1125
63	LL	0.34	0/1195	0.69	0/1597
64	MM	0.36	0/918	0.59	0/1233
65	NN	0.33	0/1226	0.64	0/1649
66	OO	0.34	0/1029	0.72	0/1380
67	PP	0.37	0/1017	0.65	0/1358
68	QQ	0.34	0/1146	0.60	0/1534
69	RR	0.35	0/1082	0.61	0/1452
7	G	0.34	0/1910	0.62	0/2569
70	SS	0.35	0/1208	0.66	0/1618
71	TT	0.37	0/1115	0.63	1/1493 (0.1%)
72	UU	0.33	0/805	0.64	0/1081
73	VV	0.36	0/643	0.65	0/860
74	WW	0.34	0/1051	0.68	0/1406
75	XX	0.34	0/1116	0.65	0/1490
76	YY	0.37	0/1028	0.64	0/1366
77	ZZ	0.35	0/604	0.61	0/810

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
78	aa	0.35	0/828	0.73	0/1109
79	bb	0.35	0/665	0.62	0/891
8	H	0.33	0/1535	0.61	0/2063
80	cc	0.33	0/490	0.68	0/656
81	dd	0.38	0/470	0.65	0/623
82	ee	0.35	0/447	0.65	0/587
83	ff	0.37	0/567	0.57	0/753
84	gg	0.33	0/2493	0.55	0/3394
85	hh	0.28	0/188	0.81	0/290
86	ii	0.34	0/2996	0.57	0/4050
87	jj	0.34	0/3352	0.55	0/4523
9	I	0.34	0/1702	0.63	0/2272
All	All	0.32	15/237792 (0.0%)	0.70	73/348210 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
48	5	0	2
75	XX	0	1
78	aa	0	1
All	All	0	5

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	5	935	A	C5-C6	-17.76	1.25	1.41
48	5	922(A)	G	O3'-P	13.89	1.77	1.61
48	5	935	A	C6-N1	-12.33	1.26	1.35
48	5	935	A	C2-N3	10.66	1.43	1.33
48	5	1411(B)	C	O3'-P	9.43	1.72	1.61

The worst 5 of 73 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	481	G	N1-C2-N2	-51.75	69.62	116.20
48	5	481	G	C8-N9-C1'	-51.47	60.09	127.00
48	5	935	A	C5-C6-N6	-47.28	85.88	123.70
48	5	935	A	C6-N1-C2	-34.46	97.92	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
48	5	935	A	N1-C6-N6	-34.37	97.98	118.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
48	5	481	G	Sidechain
48	5	935	A	Sidechain
2	B	16	PHE	Peptide
75	XX	61	GLN	Peptide
78	aa	26	CYS	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1898	0	1993	15	0
2	B	3172	0	3310	12	0
3	C	2883	0	3053	13	0
4	D	2391	0	2424	11	0
5	E	1729	0	1887	7	0
6	F	1875	0	1995	10	0
7	G	1879	0	2027	9	0
8	H	1516	0	1597	6	0
9	I	1664	0	1712	3	0
10	J	1362	0	1399	4	0
11	L	1702	0	1820	4	0
12	M	1137	0	1211	9	0
13	N	1701	0	1749	7	0
14	O	1630	0	1778	9	0
15	P	1242	0	1274	2	0
16	Q	1515	0	1634	4	0
17	R	1508	0	1664	7	0
18	S	1462	0	1508	11	0
19	T	1298	0	1366	2	0
20	U	809	0	833	5	0
21	V	979	0	1039	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	W	860	0	903	4	0
23	X	967	0	1040	1	0
24	Y	1115	0	1205	1	0
25	Z	1107	0	1182	4	0
26	a	1162	0	1209	0	0
27	b	848	0	920	0	0
28	c	761	0	794	0	0
29	d	888	0	930	0	0
30	e	1053	0	1147	0	0
31	f	876	0	912	0	0
32	g	906	0	1000	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	447	0	480	0	0
38	m	429	0	467	0	0
39	n	239	0	289	0	0
40	o	851	0	920	0	0
41	p	708	0	758	0	0
42	r	994	0	1051	0	0
43	s	1507	0	1564	0	0
44	t	1160	0	1218	0	0
45	1	49	0	51	0	0
46	2	1616	0	824	1	0
47	3	1593	0	811	2	0
48	5	75972	0	38400	244	0
49	7	2558	0	1296	4	0
50	8	3208	0	1629	3	0
51	9	36249	0	18317	131	0
52	AA	1710	0	1708	6	0
53	BB	1729	0	1803	9	0
54	CC	1716	0	1806	8	0
55	DD	1768	0	1866	6	0
56	EE	2076	0	2177	12	0
57	FF	1471	0	1522	6	0
58	GG	1923	0	2089	4	0
59	HH	1488	0	1582	7	0
60	II	1686	0	1772	5	0
61	JJ	1525	0	1640	5	0
62	KK	810	0	836	5	0
63	LL	1175	0	1249	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
64	MM	908	0	939	2	0
65	NN	1202	0	1289	5	0
66	OO	1016	0	1039	5	0
67	PP	997	0	1045	1	0
68	QQ	1128	0	1195	2	0
69	RR	1068	0	1121	5	0
70	SS	1190	0	1249	2	0
71	TT	1097	0	1132	3	0
72	UU	795	0	862	1	0
73	VV	636	0	637	2	0
74	WW	1034	0	1080	6	0
75	XX	1098	0	1167	6	0
76	YY	1011	0	1083	1	0
77	ZZ	598	0	656	1	0
78	aa	814	0	863	0	0
79	bb	651	0	672	0	0
80	cc	488	0	514	0	0
81	dd	459	0	448	0	0
82	ee	443	0	492	0	0
83	ff	555	0	567	0	0
84	gg	2436	0	2393	0	0
85	hh	169	0	86	0	0
86	ii	2947	0	2957	0	0
87	jj	3292	0	3371	0	0
88	5	182	0	0	0	0
88	7	5	0	0	0	0
88	8	6	0	0	0	0
88	9	66	0	0	0	0
88	L	1	0	0	0	0
88	P	1	0	0	0	0
88	V	1	0	0	0	0
88	a	1	0	0	0	0
88	jj	1	0	0	0	0
89	aa	1	0	0	0	0
89	dd	1	0	0	0	0
89	ff	1	0	0	0	0
89	g	1	0	0	0	0
89	j	1	0	0	0	0
89	m	1	0	0	0	0
89	o	1	0	0	0	0
89	p	1	0	0	0	0
90	jj	32	0	14	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	222005	0	166949	604	0

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

The worst 5 of 604 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:922:C:C5'	48:5:922(A):G:H3'	1.43	1.44
48:5:3914:U:O4	48:5:4378:A:N1	1.57	1.37
48:5:922:C:H5''	48:5:922(B):C:O5'	1.25	1.32
48:5:922:C:H5'	48:5:922(A):G:C3'	1.57	1.31
51:9:1137:U:O4	51:9:1148:A:N1	1.67	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	246/257 (96%)	224 (91%)	19 (8%)	3 (1%)	16	63
2	B	392/403 (97%)	367 (94%)	24 (6%)	1 (0%)	46	83
3	C	360/425 (85%)	338 (94%)	20 (6%)	2 (1%)	30	74
4	D	291/297 (98%)	279 (96%)	10 (3%)	2 (1%)	26	72
5	E	208/291 (72%)	190 (91%)	18 (9%)	0	100	100
6	F	223/247 (90%)	210 (94%)	11 (5%)	2 (1%)	21	68
7	G	229/319 (72%)	221 (96%)	8 (4%)	0	100	100
8	H	188/192 (98%)	172 (92%)	16 (8%)	0	100	100
9	I	201/214 (94%)	183 (91%)	17 (8%)	1 (0%)	34	77

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	J	168/178 (94%)	161 (96%)	7 (4%)	0	100	100
11	L	208/211 (99%)	196 (94%)	11 (5%)	1 (0%)	34	77
12	M	136/218 (62%)	123 (90%)	13 (10%)	0	100	100
13	N	201/204 (98%)	186 (92%)	14 (7%)	1 (0%)	34	77
14	O	197/203 (97%)	183 (93%)	14 (7%)	0	100	100
15	P	151/184 (82%)	142 (94%)	8 (5%)	1 (1%)	26	72
16	Q	185/188 (98%)	168 (91%)	15 (8%)	2 (1%)	17	65
17	R	178/196 (91%)	170 (96%)	8 (4%)	0	100	100
18	S	174/176 (99%)	163 (94%)	9 (5%)	2 (1%)	17	65
19	T	157/160 (98%)	142 (90%)	15 (10%)	0	100	100
20	U	97/128 (76%)	86 (89%)	10 (10%)	1 (1%)	19	66
21	V	129/140 (92%)	121 (94%)	8 (6%)	0	100	100
22	W	102/157 (65%)	97 (95%)	4 (4%)	1 (1%)	19	66
23	X	116/156 (74%)	111 (96%)	5 (4%)	0	100	100
24	Y	132/145 (91%)	128 (97%)	4 (3%)	0	100	100
25	Z	133/136 (98%)	126 (95%)	5 (4%)	2 (2%)	13	59
26	a	145/148 (98%)	136 (94%)	9 (6%)	0	100	100
27	b	100/245 (41%)	92 (92%)	7 (7%)	1 (1%)	19	66
28	c	96/115 (84%)	93 (97%)	3 (3%)	0	100	100
29	d	105/125 (84%)	90 (86%)	14 (13%)	1 (1%)	19	66
30	e	126/135 (93%)	120 (95%)	6 (5%)	0	100	100
31	f	107/110 (97%)	99 (92%)	6 (6%)	2 (2%)	10	55
32	g	112/117 (96%)	104 (93%)	8 (7%)	0	100	100
33	h	120/123 (98%)	117 (98%)	3 (2%)	0	100	100
34	i	100/105 (95%)	93 (93%)	7 (7%)	0	100	100
35	j	84/97 (87%)	75 (89%)	9 (11%)	0	100	100
36	k	67/70 (96%)	64 (96%)	3 (4%)	0	100	100
37	l	48/51 (94%)	42 (88%)	6 (12%)	0	100	100
38	m	50/102 (49%)	48 (96%)	2 (4%)	0	100	100
39	n	23/25 (92%)	23 (100%)	0	0	100	100
40	o	102/106 (96%)	96 (94%)	5 (5%)	1 (1%)	19	66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	p	89/92 (97%)	81 (91%)	7 (8%)	1 (1%)	17	65
42	r	122/137 (89%)	109 (89%)	11 (9%)	2 (2%)	12	58
43	s	194/318 (61%)	175 (90%)	17 (9%)	2 (1%)	19	66
44	t	151/165 (92%)	135 (89%)	14 (9%)	2 (1%)	15	61
45	1	5/7 (71%)	2 (40%)	3 (60%)	0	100	100
52	AA	215/295 (73%)	198 (92%)	16 (7%)	1 (0%)	34	77
53	BB	211/264 (80%)	201 (95%)	10 (5%)	0	100	100
54	CC	219/293 (75%)	204 (93%)	15 (7%)	0	100	100
55	DD	226/243 (93%)	207 (92%)	17 (8%)	2 (1%)	21	68
56	EE	260/263 (99%)	248 (95%)	11 (4%)	1 (0%)	39	80
57	FF	181/204 (89%)	169 (93%)	10 (6%)	2 (1%)	17	65
58	GG	235/249 (94%)	226 (96%)	8 (3%)	1 (0%)	39	80
59	HH	181/194 (93%)	172 (95%)	9 (5%)	0	100	100
60	II	204/208 (98%)	190 (93%)	13 (6%)	1 (0%)	34	77
61	JJ	183/194 (94%)	176 (96%)	6 (3%)	1 (0%)	34	77
62	KK	94/165 (57%)	87 (93%)	6 (6%)	1 (1%)	17	65
63	LL	139/158 (88%)	127 (91%)	11 (8%)	1 (1%)	26	72
64	MM	115/132 (87%)	100 (87%)	15 (13%)	0	100	100
65	NN	147/151 (97%)	139 (95%)	8 (5%)	0	100	100
66	OO	134/168 (80%)	124 (92%)	9 (7%)	1 (1%)	26	72
67	PP	118/145 (81%)	104 (88%)	14 (12%)	0	100	100
68	QQ	140/146 (96%)	130 (93%)	10 (7%)	0	100	100
69	RR	130/135 (96%)	117 (90%)	12 (9%)	1 (1%)	24	70
70	SS	142/152 (93%)	134 (94%)	8 (6%)	0	100	100
71	TT	139/145 (96%)	130 (94%)	8 (6%)	1 (1%)	26	72
72	UU	98/119 (82%)	92 (94%)	6 (6%)	0	100	100
73	VV	81/83 (98%)	77 (95%)	4 (5%)	0	100	100
74	WW	127/130 (98%)	116 (91%)	10 (8%)	1 (1%)	24	70
75	XX	139/143 (97%)	128 (92%)	8 (6%)	3 (2%)	8	52
76	YY	122/130 (94%)	115 (94%)	7 (6%)	0	100	100
77	ZZ	73/125 (58%)	70 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
78	aa	99/115 (86%)	90 (91%)	7 (7%)	2 (2%)	9	54
79	bb	81/84 (96%)	70 (86%)	10 (12%)	1 (1%)	16	63
80	cc	60/69 (87%)	57 (95%)	3 (5%)	0	100	100
81	dd	53/56 (95%)	48 (91%)	4 (8%)	1 (2%)	10	55
82	ee	53/133 (40%)	51 (96%)	2 (4%)	0	100	100
83	ff	66/156 (42%)	59 (89%)	7 (11%)	0	100	100
84	gg	311/317 (98%)	282 (91%)	26 (8%)	3 (1%)	19	66
86	ii	370/403 (92%)	342 (92%)	27 (7%)	1 (0%)	46	83
87	jj	423/710 (60%)	388 (92%)	31 (7%)	4 (1%)	21	68
All	All	12317/14495 (85%)	11449 (93%)	804 (6%)	64 (0%)	38	77

5 of 64 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
18	S	155	PRO
75	XX	62	PRO
75	XX	86	PRO
1	A	217	GLN
3	C	83	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	190/199 (96%)	175 (92%)	15 (8%)	15	56
2	B	342/348 (98%)	322 (94%)	20 (6%)	25	67
3	C	302/347 (87%)	282 (93%)	20 (7%)	21	63
4	D	247/250 (99%)	235 (95%)	12 (5%)	31	71
5	E	190/251 (76%)	178 (94%)	12 (6%)	22	65
6	F	196/215 (91%)	182 (93%)	14 (7%)	18	60
7	G	200/272 (74%)	188 (94%)	12 (6%)	24	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	H	169/171 (99%)	158 (94%)	11 (6%)	21	64
9	I	175/181 (97%)	165 (94%)	10 (6%)	25	68
10	J	143/149 (96%)	136 (95%)	7 (5%)	31	71
11	L	175/176 (99%)	166 (95%)	9 (5%)	29	71
12	M	117/161 (73%)	110 (94%)	7 (6%)	24	66
13	N	171/172 (99%)	162 (95%)	9 (5%)	28	70
14	O	171/173 (99%)	159 (93%)	12 (7%)	19	61
15	P	134/163 (82%)	125 (93%)	9 (7%)	20	63
16	Q	164/165 (99%)	153 (93%)	11 (7%)	20	63
17	R	159/175 (91%)	148 (93%)	11 (7%)	19	61
18	S	157/157 (100%)	147 (94%)	10 (6%)	22	64
19	T	139/140 (99%)	128 (92%)	11 (8%)	15	56
20	U	89/114 (78%)	87 (98%)	2 (2%)	60	85
21	V	101/107 (94%)	91 (90%)	10 (10%)	10	45
22	W	86/126 (68%)	85 (99%)	1 (1%)	78	91
23	X	106/134 (79%)	100 (94%)	6 (6%)	25	68
24	Y	124/135 (92%)	118 (95%)	6 (5%)	31	72
25	Z	117/118 (99%)	114 (97%)	3 (3%)	54	83
26	a	119/120 (99%)	117 (98%)	2 (2%)	68	89
27	b	84/184 (46%)	81 (96%)	3 (4%)	42	78
28	c	84/98 (86%)	82 (98%)	2 (2%)	57	84
29	d	98/110 (89%)	88 (90%)	10 (10%)	9	44
30	e	114/121 (94%)	105 (92%)	9 (8%)	15	56
31	f	88/89 (99%)	84 (96%)	4 (4%)	34	74
32	g	98/100 (98%)	92 (94%)	6 (6%)	23	66
33	h	109/110 (99%)	104 (95%)	5 (5%)	33	73
34	i	86/89 (97%)	84 (98%)	2 (2%)	58	85
35	j	73/80 (91%)	68 (93%)	5 (7%)	20	62
36	k	64/65 (98%)	62 (97%)	2 (3%)	47	81
37	l	47/48 (98%)	46 (98%)	1 (2%)	61	86
38	m	48/90 (53%)	46 (96%)	2 (4%)	36	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	n	24/24 (100%)	22 (92%)	2 (8%)	14	54
40	o	92/94 (98%)	87 (95%)	5 (5%)	27	69
41	p	74/75 (99%)	73 (99%)	1 (1%)	74	90
42	r	108/121 (89%)	99 (92%)	9 (8%)	14	54
43	s	164/258 (64%)	158 (96%)	6 (4%)	41	77
44	t	126/137 (92%)	123 (98%)	3 (2%)	57	84
45	l	6/6 (100%)	6 (100%)	0	100	100
52	AA	180/245 (74%)	163 (91%)	17 (9%)	11	48
53	BB	194/231 (84%)	180 (93%)	14 (7%)	18	59
54	CC	187/225 (83%)	172 (92%)	15 (8%)	15	55
55	DD	190/202 (94%)	173 (91%)	17 (9%)	12	51
56	EE	224/225 (100%)	211 (94%)	13 (6%)	25	67
57	FF	158/170 (93%)	150 (95%)	8 (5%)	29	71
58	GG	207/218 (95%)	188 (91%)	19 (9%)	11	49
59	HH	165/174 (95%)	150 (91%)	15 (9%)	12	50
60	II	178/180 (99%)	166 (93%)	12 (7%)	20	63
61	JJ	161/168 (96%)	150 (93%)	11 (7%)	20	62
62	KK	87/136 (64%)	79 (91%)	8 (9%)	11	49
63	LL	130/142 (92%)	116 (89%)	14 (11%)	8	41
64	MM	99/108 (92%)	86 (87%)	13 (13%)	5	31
65	NN	130/131 (99%)	114 (88%)	16 (12%)	6	34
66	OO	106/130 (82%)	94 (89%)	12 (11%)	7	39
67	PP	109/130 (84%)	97 (89%)	12 (11%)	8	40
68	QQ	117/121 (97%)	109 (93%)	8 (7%)	20	62
69	RR	119/121 (98%)	106 (89%)	13 (11%)	8	41
70	SS	125/132 (95%)	111 (89%)	14 (11%)	7	39
71	TT	111/115 (96%)	101 (91%)	10 (9%)	12	50
72	UU	92/107 (86%)	84 (91%)	8 (9%)	13	52
73	VV	67/67 (100%)	64 (96%)	3 (4%)	34	74
74	WW	112/113 (99%)	107 (96%)	5 (4%)	34	74
75	XX	113/115 (98%)	106 (94%)	7 (6%)	23	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
76	YY	107/112 (96%)	96 (90%)	11 (10%)	9	43
77	ZZ	66/103 (64%)	61 (92%)	5 (8%)	16	57
78	aa	88/98 (90%)	81 (92%)	7 (8%)	15	55
79	bb	75/76 (99%)	67 (89%)	8 (11%)	8	42
80	cc	55/62 (89%)	50 (91%)	5 (9%)	12	50
81	dd	48/49 (98%)	44 (92%)	4 (8%)	14	54
82	ee	46/106 (43%)	44 (96%)	2 (4%)	35	75
83	ff	61/140 (44%)	55 (90%)	6 (10%)	10	46
84	gg	272/275 (99%)	262 (96%)	10 (4%)	41	77
86	ii	326/353 (92%)	309 (95%)	17 (5%)	29	70
87	jj	358/608 (59%)	330 (92%)	28 (8%)	16	56
All	All	10733/12306 (87%)	10017 (93%)	716 (7%)	25	63

5 of 716 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
43	s	146	LYS
56	EE	200	ARG
84	gg	17	TRP
52	AA	44	ASP
54	CC	121	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
54	CC	235	ASN
61	JJ	111	GLN
86	ii	109	GLN
59	HH	114	GLN
66	OO	20	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
46	2	74/76 (97%)	13 (17%)	0
47	3	72/75 (96%)	27 (37%)	1 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
48	5	3506/3543 (98%)	849 (24%)	165 (4%)
49	7	119/120 (99%)	12 (10%)	2 (1%)
50	8	150/156 (96%)	35 (23%)	7 (4%)
51	9	1680/1869 (89%)	425 (25%)	84 (5%)
85	hh	7/8 (87%)	4 (57%)	0
All	All	5608/5847 (95%)	1365 (24%)	259 (4%)

5 of 1365 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
46	2	8	U
46	2	9	A
46	2	13	U
46	2	16	C
46	2	19	G

5 of 259 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
48	5	2724	G
48	5	4272	G
51	9	1519	U
48	5	2806	A
48	5	3904	G

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 273 ligands modelled in this entry, 272 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length

(or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
90	GCP	jj	700	88	29,34,34	2.51	8 (27%)	31,54,54	1.12	2 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

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

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
90	jj	700	GCP	C4-N9	-10.40	1.33	1.47
90	jj	700	GCP	C8-N9	-3.75	1.35	1.47
90	jj	700	GCP	C5-C6	-2.18	1.49	1.53
90	jj	700	GCP	PB-O2B	2.16	1.61	1.56
90	jj	700	GCP	PG-O2G	2.67	1.61	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
90	jj	700	GCP	C4-C5-N7	2.49	106.55	102.67
90	jj	700	GCP	C8-N9-C4	3.39	108.64	104.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.



## 5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
48	5	43
51	9	8
47	3	2
46	2	1

The worst 5 of 54 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	2113:G	O3'	2258:C	P	40.91
1	5	1252:C	O3'	1271:G	P	35.78
1	5	1405:C	O3'	1406:G	P	23.41
1	5	1219:G	O3'	1233:G	P	22.71
1	5	1406:G	O3'	1406(A):G	P	20.12