



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Nov 22, 2016 – 03:02 PM EST

PDB ID : 5LZY
EMDB ID: : EMD-4136
Title : Structure of the mammalian rescue complex with Pelota and Hbs1l assembled on a polyadenylated mRNA.
Authors : Shao, S.; Murray, J.; Brown, A.; Taunton, J.; Ramakrishnan, V.; Hegde, R.S.
Deposited on : 2016-10-02
Resolution : 3.99 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

A user guide is available at

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

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

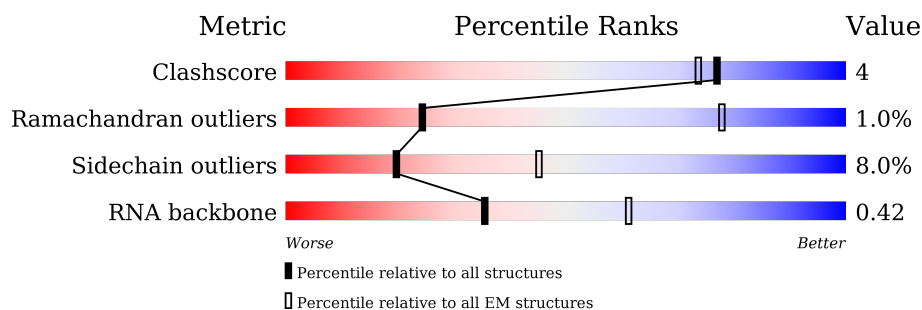
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.99 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.
















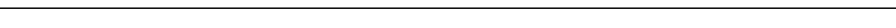




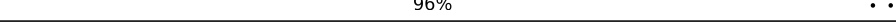






Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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	257	75% 19% . .
2	B	403	79% 18% ..
3	C	425	64% 19% . 15%
4	D	297	88% 10% ..
5	E	291	65% 8% . 26%
6	F	247	73% 16% . 9%
7	G	319	63% 9% 27%
8	H	192	83% 15% ..

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Mol	Chain	Length	Quality of chain
9	I	214	
10	J	178	
11	L	211	
12	M	218	
13	N	204	
14	O	203	
15	P	184	
16	Q	188	
17	R	196	
18	S	176	
19	T	160	
20	U	128	
21	V	140	
22	W	157	
23	X	156	
24	Y	145	
25	Z	136	
26	a	148	
27	b	245	
28	c	115	
29	d	125	
30	e	135	
31	f	110	
32	g	117	
33	h	123	



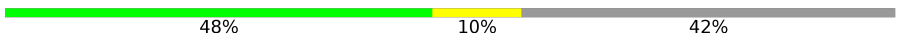






















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Mol	Chain	Length	Quality of chain
34	i	105	94% . .
35	j	97	78% 9% . 11%
36	k	70	91% 7% .
37	l	51	90% 6% . .
38	m	102	45% 6% 49%
39	n	25	92% 8%
40	o	106	92% 7% .
41	p	92	95% . .
42	r	137	80% 10% 9%
43	s	318	59% . 38%
44	t	165	90% . 7%
45	2	75	71% 27% .
45	3	75	68% 29% .
46	5	3543	62% 31% 7%
47	7	120	75% 24% .
48	8	156	57% 35% . .
49	9	1869	56% 30% 5% 9%
50	AA	295	61% 12% . 26%
51	BB	264	69% 12% 19%
52	CC	293	61% 13% . 25%
53	DD	243	84% 9% . 6%
54	EE	263	84% 15%
55	FF	204	75% 14% . 9%
56	GG	249	82% 12% . 5%
57	HH	194	78% 16% . 5%




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Mol	Chain	Length	Quality of chain
58	II	208	
59	JJ	194	
60	KK	165	
61	LL	158	
62	MM	132	
63	NN	151	
64	OO	168	
65	PP	145	
66	QQ	146	
67	RR	135	
68	SS	152	
69	TT	145	
70	UU	119	
71	VV	83	
72	WW	130	
73	XX	143	
74	YY	130	
75	ZZ	125	
76	aa	115	
77	bb	84	
78	cc	69	
79	dd	56	
80	ee	133	
81	ff	156	
82	gg	317	

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Mol	Chain	Length	Quality of chain
83	hh	8	 50%50%
84	ii	403	 88%8%
85	jj	710	 56%40%

2 Entry composition

There are 88 unique types of molecules in this entry. The entry contains 221912 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called uL2.

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

- Molecule 2 is a protein called uL3.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	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 eL14.

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 eL23.

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 eL37.

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

- Molecule 36 is a protein called eL38.

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

- Molecule 37 is a protein called eL39.

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

- Molecule 38 is a protein called eL40.

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

- Molecule 39 is a protein called eL41.

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

- Molecule 40 is a protein called eL42.

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

- Molecule 41 is a protein called eL43.

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

- Molecule 42 is a protein called eL28.

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

- Molecule 43 is a protein called uL10.

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

- Molecule 44 is a protein called uL11.

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

- Molecule 45 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	2	75	Total	C	N	O	P	0	0
			1593	712	281	526	74		
45	3	75	Total	C	N	O	P	0	0
			1593	712	281	526	74		

- Molecule 46 is a RNA chain called 28S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	5	3543	Total	C	N	O	P	0	0
			75972	33833	13910	24686	3543		

- Molecule 47 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	7	120	Total	C	N	O	P	0	0
			2558	1141	456	842	119		

- Molecule 48 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	8	151	Total	C	N	O	P	0	0
			3208	1432	564	1062	150		

- Molecule 49 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	9	1698	Total	C	N	O	P	0	0
			36249	16180	6508	11864	1697		

- Molecule 50 is a protein called uS2.

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

- Molecule 51 is a protein called 40S ribosomal protein S3a.

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

- Molecule 52 is a protein called uS5.

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

- Molecule 53 is a protein called uS3.

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

- Molecule 54 is a protein called eS4.

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

- Molecule 55 is a protein called uS7.

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

- Molecule 56 is a protein called 40S ribosomal protein S6.

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

- Molecule 57 is a protein called eS7.

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

- Molecule 58 is a protein called eS8.

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

- Molecule 59 is a protein called Ribosomal protein S9 (Predicted).

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

- Molecule 60 is a protein called eS10.

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

- Molecule 61 is a protein called uS17.

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

- Molecule 62 is a protein called 40S ribosomal protein S12.

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

- Molecule 63 is a protein called uS15.

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

- Molecule 64 is a protein called uS11.

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

- Molecule 65 is a protein called uS19.

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

- Molecule 66 is a protein called uS9.

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

- Molecule 67 is a protein called eS17.

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

- Molecule 68 is a protein called uS13.

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

- Molecule 69 is a protein called eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	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 70 is a protein called uS10.

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

- Molecule 71 is a protein called eS21.

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

- Molecule 72 is a protein called uS8.

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

- Molecule 73 is a protein called uS12.

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

- Molecule 74 is a protein called eS24.

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

- Molecule 75 is a protein called eS25.

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

- Molecule 76 is a protein called eS26.

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

- Molecule 77 is a protein called 40S ribosomal protein S27.

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

- Molecule 78 is a protein called eS28.

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

- Molecule 79 is a protein called uS14.

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

- Molecule 80 is a protein called eS30.

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

- Molecule 81 is a protein called eS31.

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

- Molecule 82 is a protein called RACK1.

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

- Molecule 83 is a RNA chain called mRNA (polyadenylated).

Mol	Chain	Residues	Atoms					AltConf	Trace
83	hh	8	Total	C	N	O	P	0	0
			176	80	40	48	8		

- Molecule 84 is a protein called Protein pelota homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	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 85 is a protein called HBS1-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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

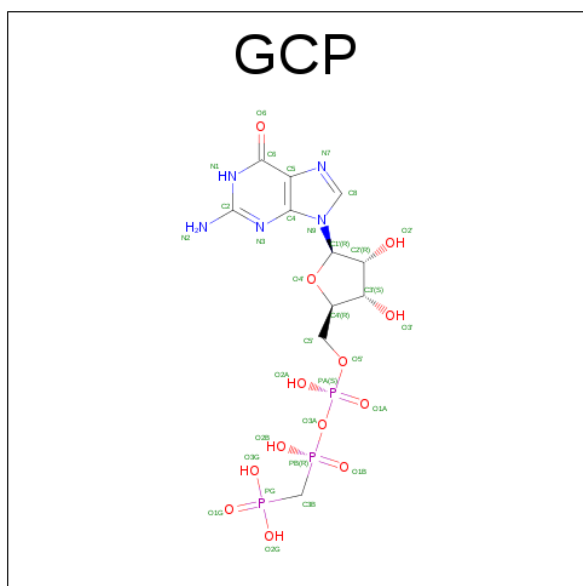
- Molecule 86 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
86	P	1	Total Mg 1 1	0
86	TT	1	Total Mg 1 1	0
86	jj	1	Total Mg 1 1	0
86	I	1	Total Mg 1 1	0
86	V	1	Total Mg 1 1	0
86	7	5	Total Mg 5 5	0
86	a	1	Total Mg 1 1	0
86	5	164	Total Mg 164 164	0
86	8	3	Total Mg 3 3	0
86	9	56	Total Mg 56 56	0
86	L	1	Total Mg 1 1	0
86	hh	1	Total Mg 1 1	0

- Molecule 87 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 88 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).

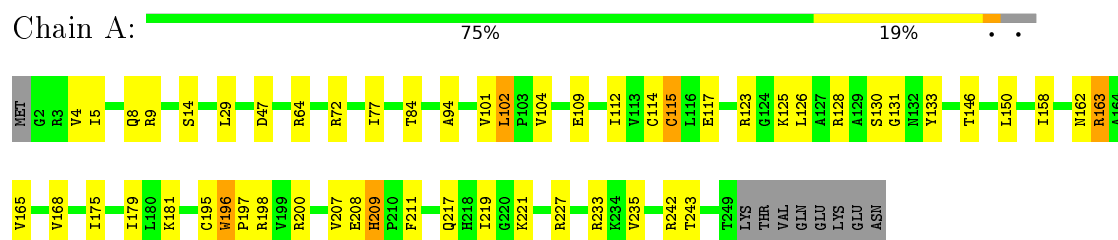


Mol	Chain	Residues	Atoms					AltConf
88	jj	1	Total	C	N	O	P	0
			32	11	5	13	3	

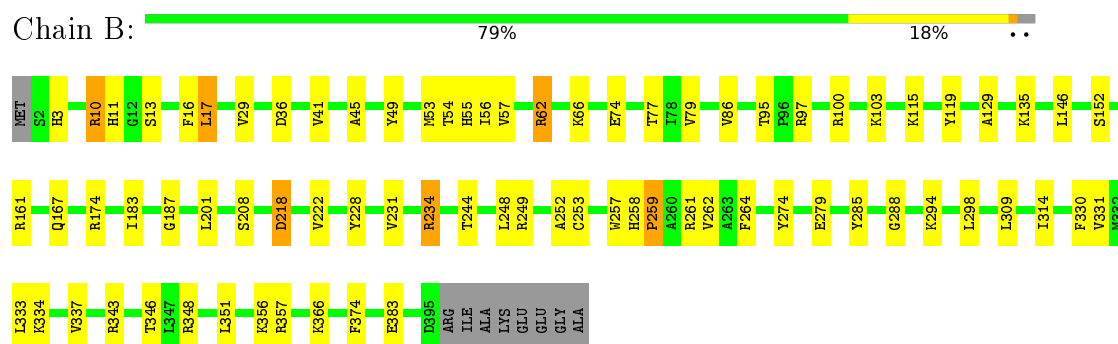
3 Residue-property plots

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.

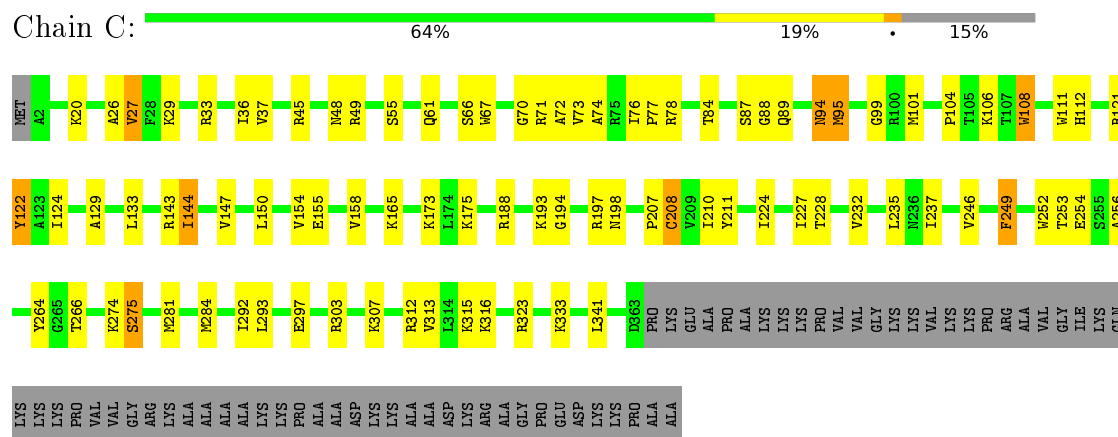
• Molecule 1: uL2



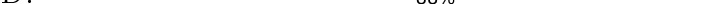
• Molecule 2: uL3

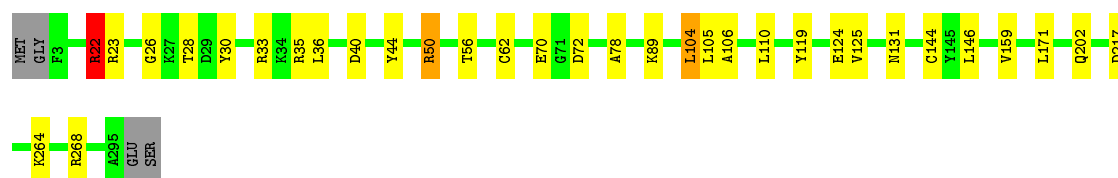


• Molecule 3: uL4



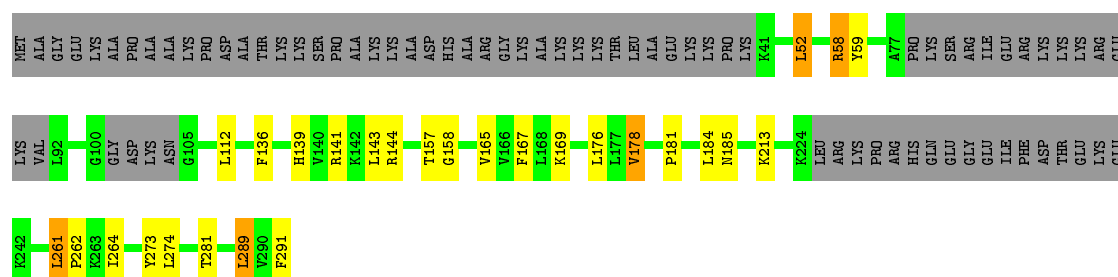
• Molecule 4: 60S ribosomal protein L5

Chain D:  88% 10% ..



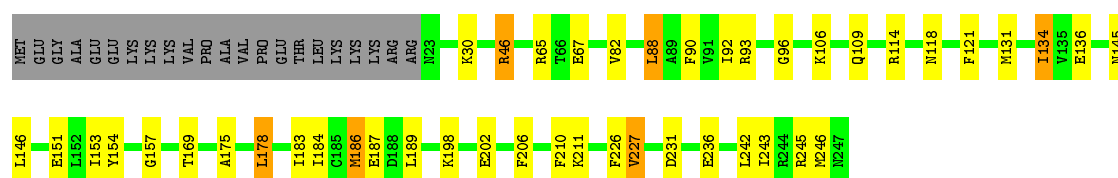
- Molecule 5: 60S ribosomal protein L6

Chain E:  65% 8% • 26%



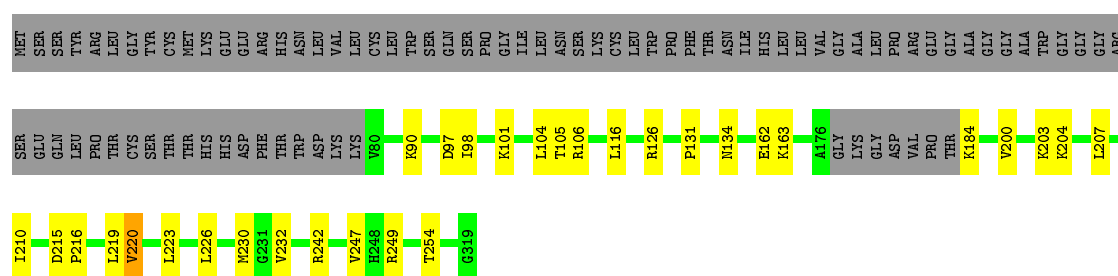
- Molecule 6: uL30

Chain F:  73% 16% 9%

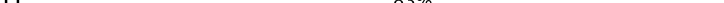


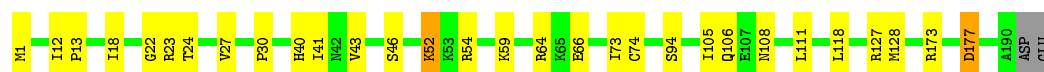
- Molecule 7: eL8

Chain G:  63% 9% 27%

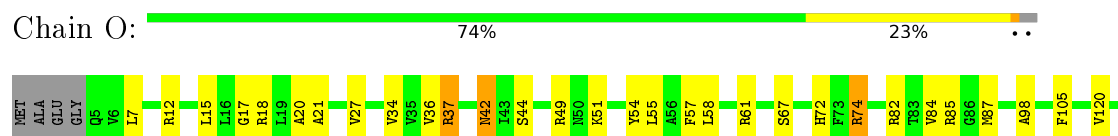


- Molecule 8: uL6

Chain H:  83% 15% ..

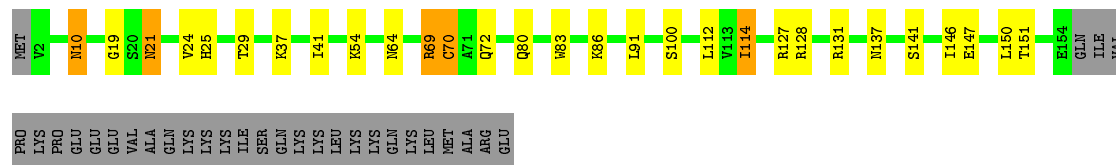


- Molecule 9: Ribosomal protein L10 (Predicted)

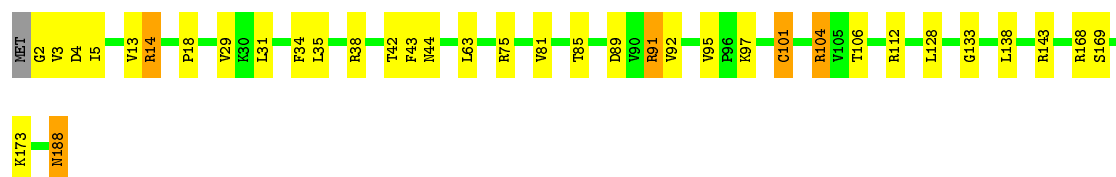
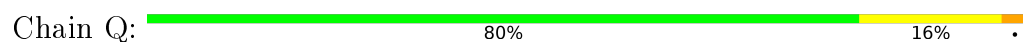




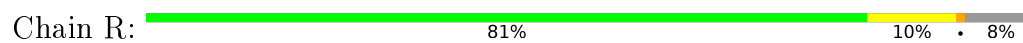
• Molecule 15: uL22



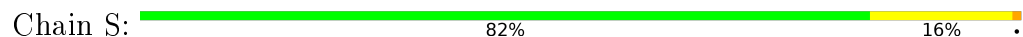
• Molecule 16: eL18



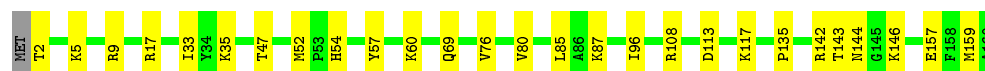
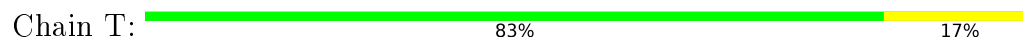
• Molecule 17: eL19



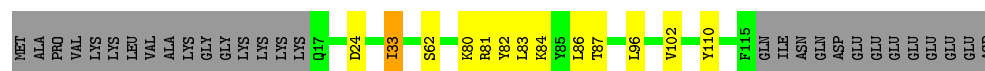
• Molecule 18: eL20



• Molecule 19: eL21

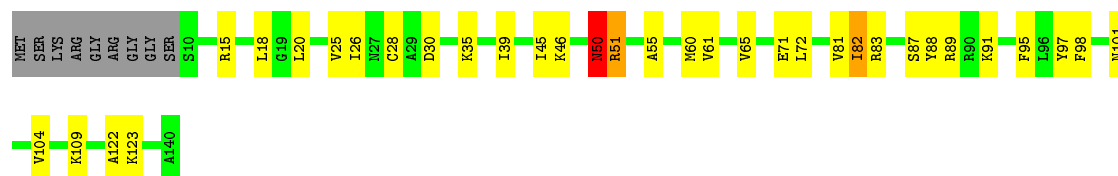


• Molecule 20: eL22



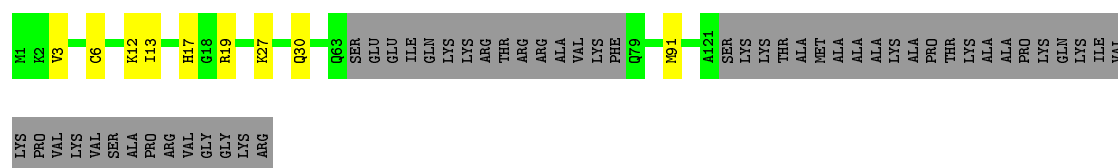
• Molecule 21: eL14

Chain V: 



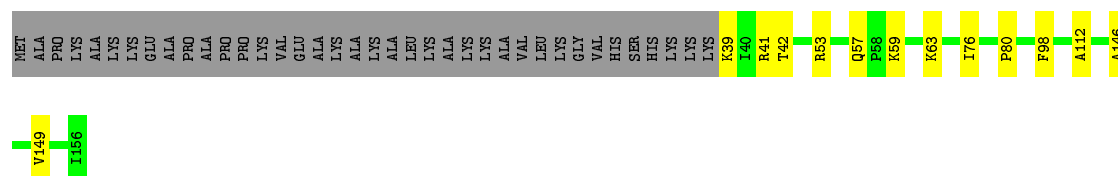
- Molecule 22: eL24

Chain W: 




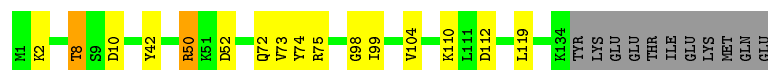
- Molecule 23: eL23

Chain X: 




- Molecule 24: uL24

Chain Y: 



- Molecule 25: 60S ribosomal protein L27

Chain Z: 



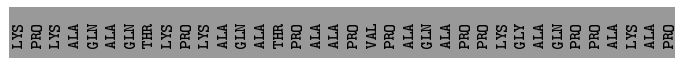
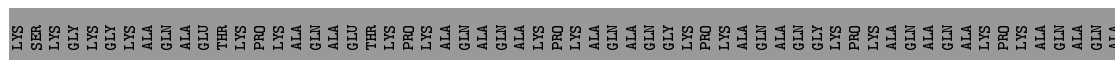
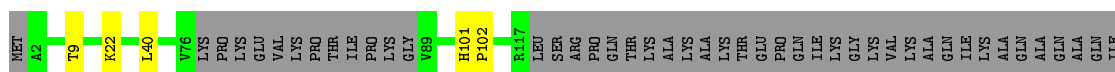
- Molecule 26: uL15

Chain a: 



- Molecule 27: eL29

Chain b: 



- Molecule 28: eL30

Chain c: 80% 5% 15%



- Molecule 29: eL31

Chain d: 77% 9% 14%



- Molecule 30: eL32

Chain e: 87% 8% 5%



- Molecule 31: eL33

Chain f: 89% 9% ..



- Molecule 32: eL34

Chain g: 87% 10% .



- Molecule 33: uL29

Chain h: 95% ..




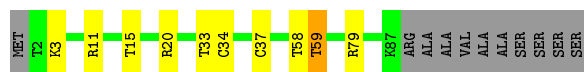
- Molecule 34: 60S ribosomal protein L36

Chain i:  94% . .



- Molecule 35: eL37

Chain j:  78% 9% . 11%




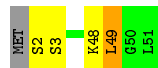
- Molecule 36: eL38

Chain k:  91% 7% .



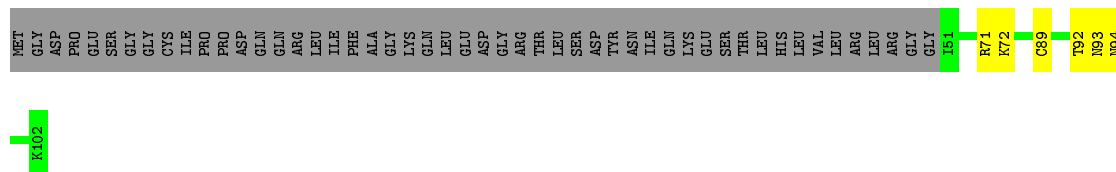
- Molecule 37: eL39

Chain l:  90% 6% . .



- Molecule 38: eL40

Chain m:  45% 6% 49%



- Molecule 39: eL41

Chain n:  92% 8%



- Molecule 40: eL42

Chain o:  92% 7% .




- Molecule 41: eL43

Chain p:  95%



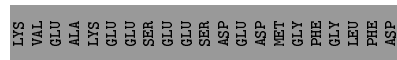
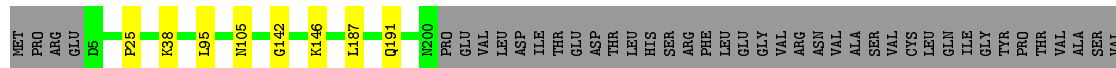
- Molecule 42: eL28

Chain r:  80% 10% 9%




- Molecule 43: uL10

Chain s:  59% 38%



- Molecule 44: uL11

Chain t:  90% 7%



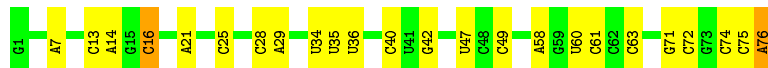
- Molecule 45: tRNA

Chain 2:  71% 27%



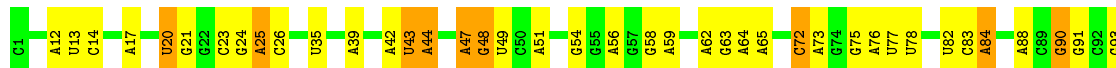
- Molecule 45: tRNA

Chain 3:  68% 29%



- Molecule 46: 28S ribosomal RNA

Chain 5:  62% 31% 7%



G2288	G2289	G2065	G2066	G2067	G2068	A2069	G2077	A2300	G2301	A2307	A2313	G2314	A2332	G2333	G2343	U2344	G2348	A2349	U2350	G2351	U2352	G2098	G2099	G2100	A2101	G2102	A2103	A2104	A2105	G2106	A2107	G2108	A2109	G2110	A2382	A2395	A2396	G2397	U2398	G2265	G2266	A2267	A2268	G2269	G2270	G2271	G2272	G2273	G2274	G2275	G2416	A2417	G2421	G2422																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
G1854	G1855	G1856	G1857	A1858	A1867	G1869	G1872	U1876	G1877	G1882	U1883	A1888	A1891	U1892	C1893	U1897	G1898	A1908	G1909	G1910	G1911	G1912	G1913	G1916	A1917	U1918	G1919	G1921	G1922	A1923	C1928	A1929	U1930	G1931	A1932	G1933	C1938	G2054	G2055	G2056	A2057	G2058	G2062	G2063	A2064	G1854	G1855	G1856	G1857	A1858	A1867	G1869	G1872	U1876	G1877	G1882	U1883	A1888	A1891	U1892	C1893	U1897	G1898	A1908	G1909	G1910	G1911	G1912	G1913	G1916	A1917	U1918	G1919	G1921	G1922	A1923	C1928	A1929	U1930	G1931	A1932	G1933	C1938	G2054	G2055	G2056	A2057	G2058	G2062	G2063	A2064																																																																																																																																																																																																																																																																																																																																																																																																																															
G1750	A1751	G1752	G1753	U1754	G1755	U1756	U1757	G1761	U1762	G1763	G1764	C1768	A1776	A1780	U1781	U1782	C1783	A1786	A1787	A1788	C1789	A1794	G1799	A1802	G1803	A1804	A1805	C1812	G1813	G1814	G1815	G1816	G1817	G1818	G1819	G1820	U1821	U1822	C1828	G1833	U1834	G1835	G1836	A1837	G1842	G1846	C1847	G1750	A1751	G1752	G1753	U1754	G1755	U1756	U1757	G1761	U1762	G1763	G1764	C1768	A1776	A1780	U1781	U1782	C1783	A1786	A1787	A1788	C1789	A1794	G1799	A1802	G1803	A1804	A1805	C1812	G1813	G1814	G1815	G1816	G1817	G1818	G1819	G1820	U1821	U1822	C1828	G1833	U1834	G1835	G1836	A1837	G1842	G1846	C1847																																																																																																																																																																																																																																																																																																																																																																																																																											
G1639	G1640	A1643	G1644	G1645	A1646	G1647	G1648	A1649	A1650	G1651	U1652	A1653	G1654	U1655	U1656	G1657	G1661	U1664	C1665	G1666	A1667	G1670	U1671	U1672	U1673	G1676	U1677	C1678	G1679	G1680	U1683	G1689	G1690	G1691	G1694	G1724	A1729	G1733	G1734	U1735	G1739	G1740	A1742	U1748	A1749	G1639	G1640	A1643	G1644	G1645	A1646	G1647	G1648	A1649	A1650	G1651	U1652	A1653	G1654	U1655	U1656	G1657	G1661	U1664	C1665	G1666	A1667	G1670	U1671	U1672	U1673	G1676	U1677	C1678	G1679	G1680	U1683	G1689	G1690	G1691	G1694	G1724	A1729	G1733	G1734	U1735	G1739	G1740	A1742	U1748	A1749																																																																																																																																																																																																																																																																																																																																																																																																																															
U1428	C1429	G1432	A1433	G1434	G1435	A1436	C1437	U1438	U1440	C1441	C1442	U1445	U1446	G1453	G1454	G1455	U1456	G1457	C1458	G1465	C1468	C1469	U1475	C1476	C1477	C1478	C1481	G1482	C1483	G1484	C1485	C1486	A1497	G1498	G1502	A1503	G1504	U1513	U1514	A1515	U1516	A1517	A1518	A1523	A1524	A1525	U1528	U1428	C1429	G1432	A1433	G1434	G1435	A1436	C1437	U1438	U1440	C1441	C1442	U1445	U1446	G1453	G1454	G1455	U1456	G1457	C1458	G1465	C1468	C1469	U1475	C1476	C1477	C1478	C1481	G1482	C1483	G1484	C1485	C1486	A1497	G1498	G1502	A1503	G1504	U1513	U1514	A1515	U1516	A1517	A1518	A1523	A1524	A1525	U1528																																																																																																																																																																																																																																																																																																																																																																																																																											
G1328	G1329	A1330	A1337	G1338	U1339	C1340	G1343	A1353	G1354	G1358	G1359	U1361	U1364	G1370	A1371	A1372	A1373	G1374	G1375	C1376	G1377	C1378	G1379	G1380	U1381	G1382	G1383	C1384	G1385	C1386	A1387	A1388	G1394	U1395	A1397	A1398	C1401	C1411	G1411A	G1411B	G1411C	G1412	G1416	G1419	A1420	G1421	G1422	G1328	G1329	A1330	A1337	G1338	U1339	C1340	G1343	A1353	G1354	G1358	G1359	U1361	U1364	G1370	A1371	A1372	A1373	G1374	G1375	C1376	G1377	C1378	G1379	G1380	U1381	G1382	G1383	C1384	G1385	C1386	A1387	A1388	G1394	U1395	A1397	A1398	C1401	C1411	G1411A	G1411B	G1411C	G1412	G1416	G1419	A1420	G1421	G1422																																																																																																																																																																																																																																																																																																																																																																																																																											
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G696	G697	C704	G705	G708	A711	C712	G725	U728	G729	G730	G731	C738	C738A	G739	G742	G743	G744	G745	A747	G748	G749	U750	G751	G752	C753	G758	U911	U913	U914	G647	G648	A649	C922	G922A	C922B	G923	C924	C925	G926	A667	G668	G669	G672	C683	G684	A686	G933	G696	G697	C704	G705	G708	A711	C712	G725	U728	G729	G730	G731	C738	C738A	G739	G742	G743	G744	G745	A747	G748	G749	U750	G751	G752	C753	G758	U911	U913	U914	G647	G648	A649	C922	G922A	C922B	G923	C924	C925	G926	A667	G668	G669	G672	C683	G684	A686	G933																																																																																																																																																																																																																																																																																																																																																																																																																											
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A4966	U4881	G4690	U4579	A4397	C4303	G4201	U4067	G3839	A3718	G3604	A2798	G2694	U2537	U2426
A4967	U4882	G4694	U4580	U4398	A4304	U4202	U4068	U3840	G3722	G3605	G2799	A2695	A2538	G2427
U4976	C4883	G4694	C4583	U4399	A4305	U4203	U4069	A3845	A3723	U3606	A2806	A2696	C2539	A2428
A4977	C4884	G4694	A4584	G4400	A4306	A4204	A4073	A3856	A3724	U3613	A2807	G2698	G3546	G2433
A4978	U4885	G4694	U4585	G4401	A4307	A4205	A4074	G3857	G3725	G3614	G2808	C2699	C2547	G2434
U4985	C4886	G4694	U4586	A4415	A4311	A4206	A4075	G3858	G3726	G3615	G2809	C2704	C2548	G2435
U4988	U4887	G4694	A4510	A4416	A4312	A4207	A4076	G3859	G3727	C3618	C2814	U2707	G2549	G2439
U4989	G4694	G4694	A4511	G4418	C4314	A4212	A4077	A3860	G3728	G3619	A2815	U2708	A2553	U2440
C4990	A4512	G4694	U4513	U4419	A4315	A4213	G4076	A3861	G3729	G3620	G2816	C2709	U2554	G2441
U4991	A4514	G4694	G4515	U4420	A4316	U4214	G4077	A3862	A3740	A3621	C2817	C2710	G2555	G2442
G4994	G4516	G4694	U4517	A4422	C4319	A4219	G4078	A3863	A3741	C3622	C2818	G2711	G2566	G2443
U4995	A4518	G4694	A4518	U4423	C4320	A4220	A4079	A3864	A3742	G3623	C2819	G2712	U2567	U2447
C4996	A4519	G4694	C4520	U4424	U4321	A4221	A4080	A3865	A3743	G3624	C2820	C2713	U2575	G2450
U4997	G4521	G4694	U4521	A4425	A4322	A4222	G4081	A3866	G3750	G3625	U2821	G2714	U2576	G2451
G4998	A4522	G4694	G4522	U4426	A4323	A4223	G4082	A3867	G3751	A3635	U2822	C2715	C2583	A2483
C4999	U4523	G4694	U4523	U4427	C4324	A4224	G4083	A3868	A3752	A3636	G2823	C2716	G2584	C2484
U5000	A4524	G4694	G4524	U4428	A4325	A4225	G4084	A3869	A3753	A3637	U2824	C2717	U2585	C2485
G5001	U4525	G4694	U4525	A4429	A4326	A4226	G4085	A3870	A3754	A3638	U2825	C2718	G2586	C2486
U5002	G4526	G4694	G4526	U4430	A4327	A4227	G4086	A3871	A3755	A3639	U2826	C2719	U2587	C2487
A5007	U4527	G4694	U4527	U4431	A4328	A4228	G4087	A3872	A3756	A3640	U2827	C2720	A2601	G2466
C5008	G4528	G4694	G4528	U4432	A4329	U4229	G4088	A3873	A3757	A3641	U2828	C2721	G2608	U2467
G5009	U4529	G4694	U4529	U4433	A4330	U4230	G4089	A3874	A3758	A3642	U2829	C2722	G2609	U2468
C5013	G4530	G4694	G4530	U4434	A4331	A4231	G4090	A3875	A3759	A3643	U2830	C2723	A2611	C2469
A5014	U4531	G4694	U4531	U4435	A4332	A4232	G4091	A3876	A3760	A3644	U2831	C2724	G2612	C2470
G5015	G4532	G4694	G4532	U4436	A4333	A4233	G4092	A3877	A3761	U3645	U2832	C2725	A2472	A2473
A5016	U4533	G4694	U4533	U4437	A4334	A4234	G4093	A3878	A3762	A3646	U2833	C2726	G2620	A2474
G5017	G4534	G4694	G4534	U4438	A4335	A4235	G4094	A3879	A3763	A3647	U2834	C2727	G2621	G2475
U5033	U4535	G4694	U4535	U4439	A4336	A4236	G4095	A3880	A3764	A3648	U2835	C2728	C2622	G2483
A5034	G4536	G4694	G4536	U4440	A4337	A4237	G4096	A3881	A3765	A3649	U2836	C2729	G2623	A2484
U5035	U4537	G4694	U4537	U4441	A4338	A4238	G4097	A3882	A3766	A3650	U2837	C2730	U2639	U2485
U5040	G4538	G4694	G4538	U4442	A4339	A4239	G4098	A3883	A3767	A3651	U2838	C2731	G2640	C2488
G5041	U4539	G4694	U4539	U4443	A4340	A4240	G4099	A3884	A3768	A3652	U2839	C2732	U2641	C2489
C5047	G4540	G4694	G4540	U4444	A4341	A4241	G4100	A3885	A3769	A3653	U2840	C2733	A2647	C2490
U5060	U4541	G4694	U4541	U4445	A4342	A4242	G4101	A3886	A3770	A3654	U2841	C2734	A2660	U2495
C5063	G4542	G4694	G4542	U4446	A4343	A4243	G4102	A3887	A3771	A3655	U2842	C2735	U2661	A2502
G5064	U4543	G4694	U4543	U4447	A4344	A4244	G4103	A3888	A3772	A3656	U2843	C2736	G2662	G2503
A5065	G4544	G4694	G4544	U4448	A4345	A4245	G4104	A3889	A3773	A3657	U2844	C2737	C2663	C2504
C5067	U4545	G4694	U4545	U4449	A4346	A4246	G4105	A3890	A3774	A3658	U2845	C2738	C2664	C2505
U5068	G4546	G4694	G4546	U4450	A4347	A4247	G4106	A3891	A3775	A3659	U2846	C2739	U2665	G2506
A5069	U4547	G4694	U4547	U4451	A4348	A4248	G4107	A3892	A3776	A3660	U2847	C2740	A2666	
U5077	G4548	G4694	G4548	U4452	A4349	A4249	G4108	A3893	A3777	A3661	U2848	C2741	U2667	
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U5093	U4551	G4694	U4551	U4455	A4352	A4252	G4111	A3896	A3780	A3664	U2851	C2744	C2670	C2515
G5094	G4552	G4694	G4552	U4456	A4353	A4253	G4112	A3897	A3781	A3665	U2852	C2745	C2671	G2516
C5097	U4553	G4694	U4553	U4457	A4354	A4254	G4113	A3898	A3782	A3666	U2853	C2746	A2668	A2517
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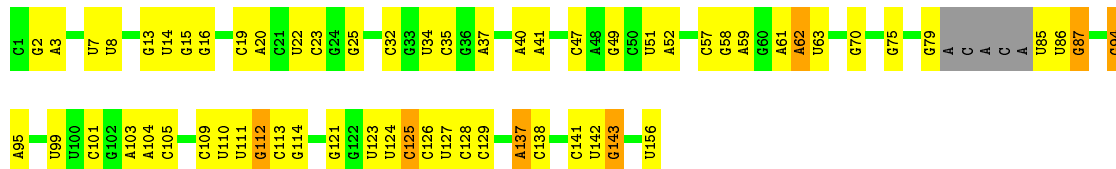
• Molecule 47: 5S ribosomal RNA

Chain 7:  75% 24%



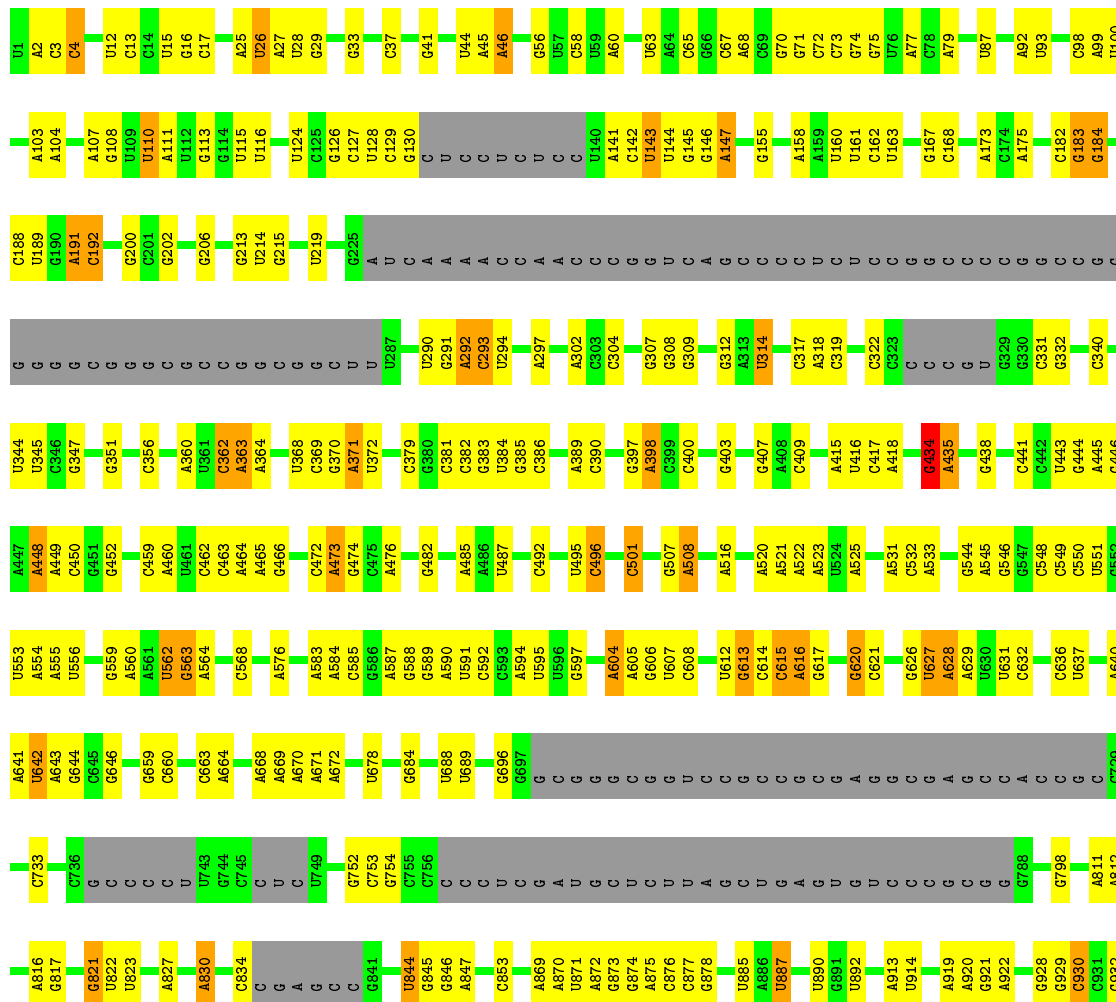
• Molecule 48: 5.8S ribosomal RNA

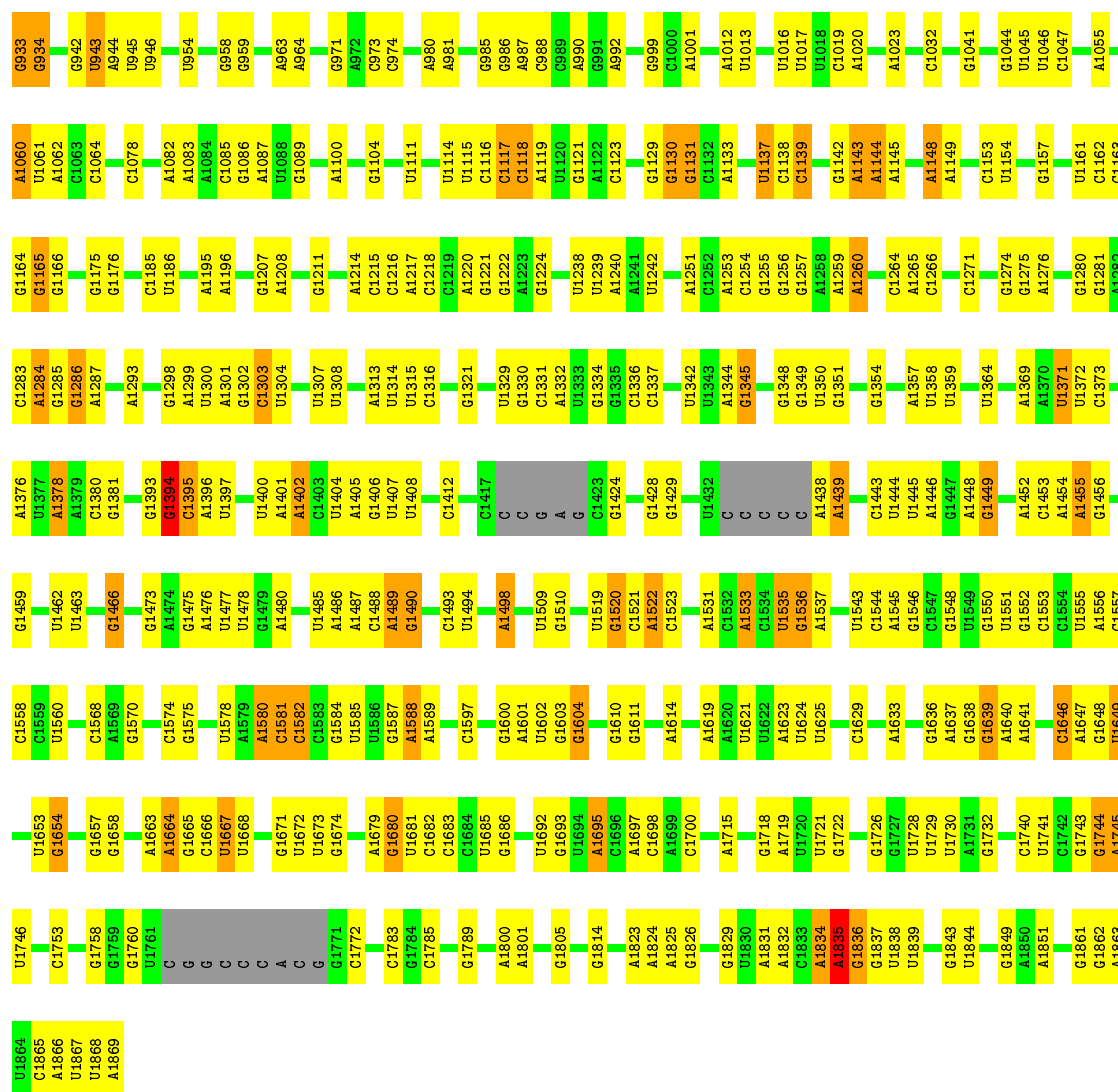
Chain 8:  57% 35%



• Molecule 49: 18S ribosomal RNA

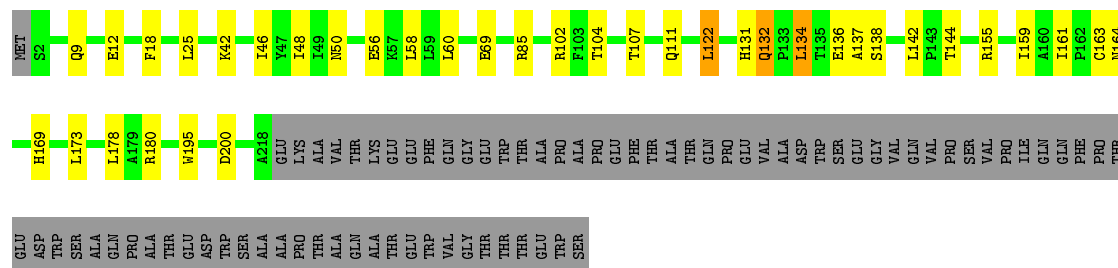
Chain 9:  56% 30% 5% 9%





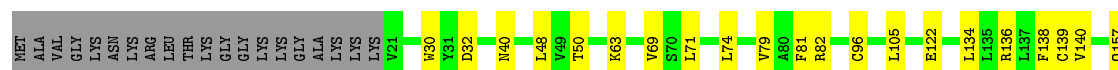
- Molecule 50: uS2

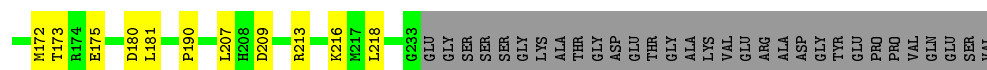
Chain AA: 61% 12% 26%



- Molecule 51: 40S ribosomal protein S3a

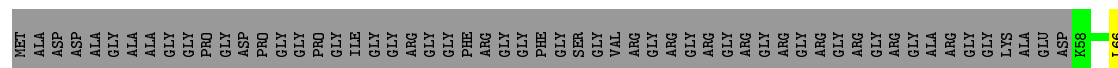
Chain BB: 69% 12% 19%





• Molecule 52: uS5

Chain CC: 61% 13% 25%



• Molecule 53: uS3

Chain DD: 84% 9% 6%



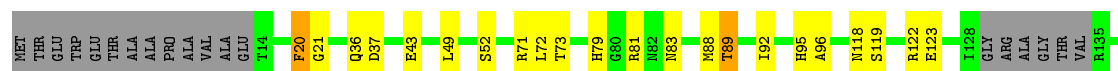
• Molecule 54: eS4

Chain EE: 84% 15%



• Molecule 55: uS7

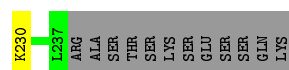
Chain FF: 75% 14% 9%



• Molecule 56: 40S ribosomal protein S6

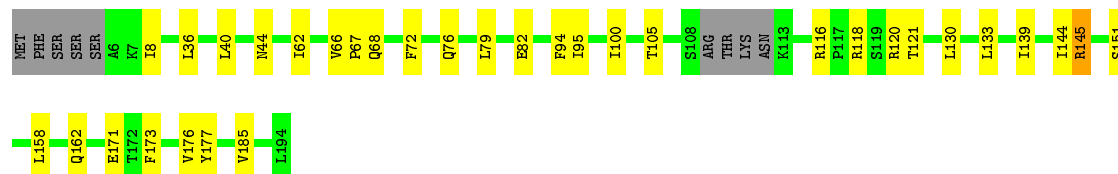
Chain GG: 82% 12% 5%





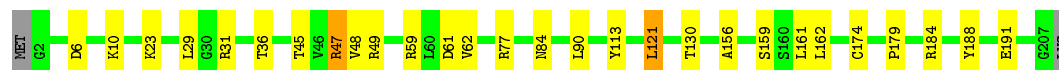
- Molecule 57: eS7

Chain HH: 78% 16% 5%



- Molecule 58: eS8

Chain II: 86% 13% ..



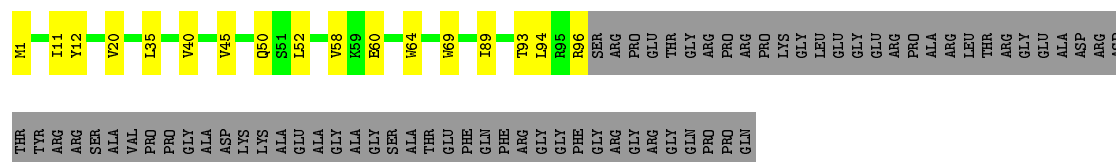
- Molecule 59: Ribosomal protein S9 (Predicted)

Chain JJ: 83% 12% 5%



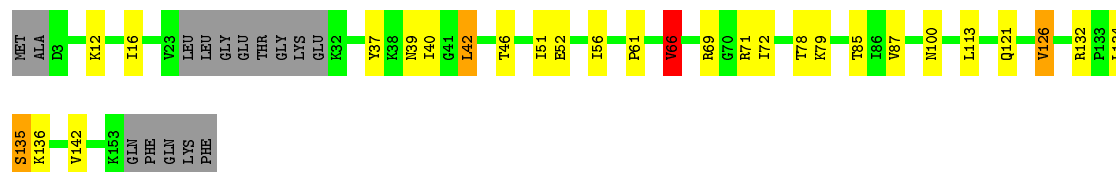
- Molecule 60: eS10

Chain KK: 48% 10% 42%



- Molecule 61: uS17

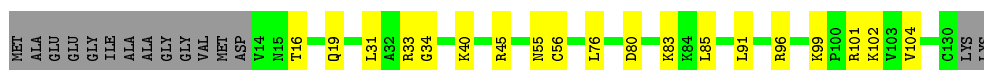
Chain LL: 73% 15% .. 9%



- Molecule 62: 40S ribosomal protein S12

Chain MM: 74% 14% 11%





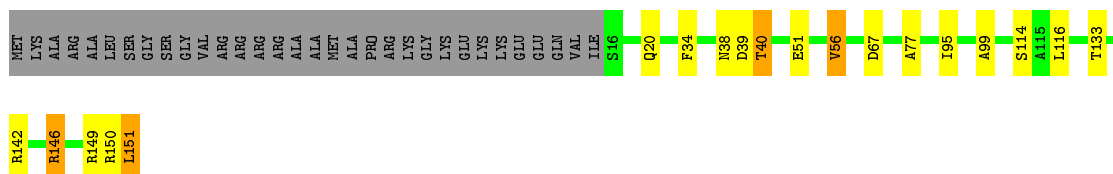
• Molecule 63: uS15

Chain NN: 81% 16% ..



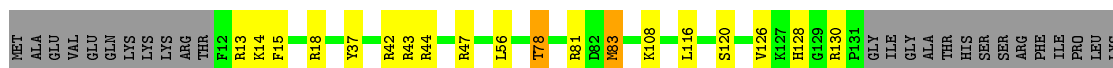
• Molecule 64: uS11

Chain OO: 70% 9% 19%



• Molecule 65: uS19

Chain PP: 70% 12% 17%



• Molecule 66: uS9

Chain QQ: 88% 9% .



• Molecule 67: eS17

Chain RR: 81% 16% ..



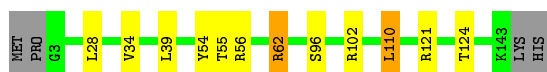
• Molecule 68: uS13

Chain SS: 78% 16% 5%



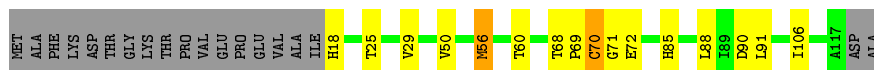
• Molecule 69: eS19

Chain TT: 89% 7% ..



- Molecule 70: uS10

Chain UU: 71% 12% 16%



- Molecule 71: eS21

Chain VV: 88% 12%



- Molecule 72: uS8

Chain WW: 77% 20% 3%



- Molecule 73: uS12

Chain XX: 83% 12% 5%



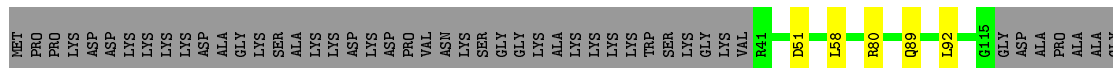
- Molecule 74: eS24

Chain YY: 78% 15% 5%



- Molecule 75: eS25

Chain ZZ: 56% 40% 4%



- Molecule 76: eS26

Chain aa: 77% 11% 12%



- Molecule 77: 40S ribosomal protein S27

Chain bb: 89% 8% ..



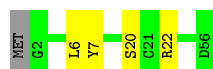
- Molecule 78: eS28

Chain cc: 80% 10% 10%



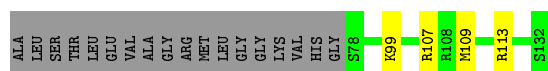
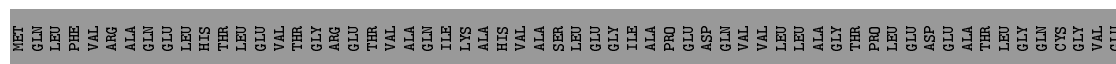
- Molecule 79: uS14

Chain dd: 91% 7% .



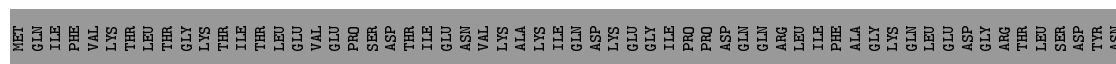
- Molecule 80: eS30

Chain ee: 38% . 59%



- Molecule 81: eS31

Chain ff: 38% 5% 56%



- Molecule 82: RACK1

Chain gg: 93% 5% .



- Molecule 83: mRNA (polyadenylated)

- Molecule 84: Protein pelota homolog

HIS
HIS
HIS
HIS
SER
THR

- Molecule 85: HBS1-like protein

D527	M330	Q361	V369	Q385	H389	M408	L425	F434	R435	R436	R482	R489	Q499	I505	I585	K596	Q605	I613	L616	I617	S618	I640	L653	R664	E684
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	20717	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	0.44	0/1936	0.79	1/2596 (0.0%)
10	J	0.39	0/1385	0.68	0/1852
11	L	0.42	0/1733	0.77	1/2316 (0.0%)
12	M	0.45	0/1158	0.75	0/1547
13	N	0.44	0/1746	0.79	1/2338 (0.0%)
14	O	0.48	0/1662	0.77	0/2222
15	P	0.45	0/1268	0.71	0/1700
16	Q	0.47	0/1539	0.84	1/2054 (0.0%)
17	R	0.40	0/1524	0.74	0/2013
18	S	0.51	0/1501	0.80	0/2012
19	T	0.43	0/1326	0.73	0/1770
2	B	0.45	0/3240	0.77	2/4339 (0.0%)
20	U	0.39	0/823	0.63	0/1104
21	V	0.45	0/993	0.75	0/1332
22	W	0.44	0/873	0.61	0/1158
23	X	0.40	0/984	0.68	0/1323
24	Y	0.38	0/1132	0.69	0/1504
25	Z	0.42	0/1130	0.67	0/1507
26	a	0.46	0/1191	0.77	0/1590
27	b	0.40	0/861	0.68	0/1138
28	c	0.39	0/771	0.63	0/1034
29	d	0.43	0/903	0.75	0/1216
3	C	0.48	0/2937	0.79	0/3946
30	e	0.50	1/1071 (0.1%)	0.74	0/1429
31	f	0.48	0/895	0.80	0/1198
32	g	0.46	0/916	0.79	0/1220
33	h	0.38	0/1021	0.67	0/1348
34	i	0.38	0/841	0.68	0/1112
35	j	0.44	0/720	0.82	0/952
36	k	0.37	0/575	0.64	0/761
37	l	0.44	0/459	0.76	0/608
38	m	0.38	0/435	0.67	0/575

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
39	n	0.38	0/240	0.71	0/305
4	D	0.40	0/2437	0.71	3/3264 (0.1%)
40	o	0.40	0/864	0.68	0/1140
41	p	0.44	0/718	0.68	0/953
42	r	0.42	0/1010	0.73	0/1354
43	s	0.37	0/1530	0.50	0/2064
44	t	0.37	0/1174	0.52	0/1582
45	2	0.23	0/1777	0.68	1/2763 (0.0%)
45	3	0.21	0/1777	0.66	0/2763
46	5	0.39	13/84961 (0.0%)	0.79	56/132460 (0.0%)
47	7	0.33	0/2858	0.67	0/4455
48	8	0.37	0/3581	0.73	0/5577
49	9	0.32	0/40524	0.73	12/63134 (0.0%)
5	E	0.39	0/1762	0.70	0/2362
50	AA	0.40	0/1747	0.68	0/2374
51	BB	0.36	0/1756	0.64	0/2350
52	CC	0.40	0/1753	0.71	0/2369
53	DD	0.38	0/1796	0.67	0/2417
54	EE	0.39	0/2118	0.68	0/2849
55	FF	0.39	0/1492	0.69	1/2005 (0.0%)
56	GG	0.37	0/1946	0.69	0/2590
57	HH	0.38	0/1510	0.64	0/2022
58	II	0.43	0/1715	0.75	0/2287
59	JJ	0.39	0/1550	0.76	0/2069
6	F	0.51	0/1911	0.78	0/2549
60	KK	0.39	0/834	0.60	0/1125
61	LL	0.41	0/1195	0.74	0/1597
62	MM	0.38	0/918	0.57	0/1233
63	NN	0.39	0/1226	0.72	0/1649
64	OO	0.40	0/1029	0.81	1/1380 (0.1%)
65	PP	0.40	0/1017	0.70	0/1358
66	QQ	0.37	0/1146	0.69	0/1534
67	RR	0.41	0/1082	0.64	0/1452
68	SS	0.40	0/1208	0.72	0/1618
69	TT	0.39	0/1115	0.68	1/1493 (0.1%)
7	G	0.37	0/1910	0.67	0/2569
70	UU	0.38	0/805	0.69	0/1081
71	VV	0.41	0/643	0.76	0/860
72	WW	0.41	0/1051	0.77	0/1406
73	XX	0.39	0/1116	0.72	0/1490
74	YY	0.37	0/1028	0.66	0/1366
75	ZZ	0.36	0/604	0.64	0/810
76	aa	0.40	0/828	0.83	1/1109 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
77	bb	0.39	0/665	0.66	0/891
78	cc	0.39	0/490	0.74	0/656
79	dd	0.43	0/470	0.71	0/623
8	H	0.41	0/1535	0.72	0/2063
80	ee	0.37	0/447	0.68	0/587
81	ff	0.38	0/567	0.55	0/753
82	gg	0.35	0/2493	0.58	0/3394
83	hh	0.27	0/199	0.76	0/308
84	ii	0.36	0/2996	0.58	0/4050
85	jj	0.36	0/3352	0.57	0/4523
9	I	0.42	0/1702	0.71	0/2272
All	All	0.39	14/237727 (0.0%)	0.74	82/348121 (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
11	L	0	1
2	B	0	3
31	f	0	1
37	l	0	1
4	D	0	1
46	5	0	2
72	WW	0	1
73	XX	0	1
All	All	0	11

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	5	935	A	C5-C6	-15.76	1.26	1.41
46	5	935	A	C6-N1	-11.91	1.27	1.35
46	5	935	A	C2-N3	10.06	1.42	1.33
46	5	481	G	N1-C2	-9.60	1.30	1.37
46	5	481	G	C2-N2	-9.49	1.25	1.34

The worst 5 of 82 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	5	481	G	N1-C2-N2	-52.72	68.75	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	5	935	A	C5-C6-N6	-48.91	84.57	123.70
46	5	935	A	N1-C6-N6	-35.79	97.12	118.60
46	5	935	A	C6-N1-C2	-31.76	99.55	118.60
46	5	481	G	N3-C2-N2	-29.71	99.10	119.90

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	16	PHE	Peptide
2	B	257	TRP	Peptide
2	B	259	PRO	Peptide
4	D	36	LEU	Peptide
11	L	46	ILE	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	23	0
2	B	3172	0	3310	31	0
3	C	2883	0	3053	50	0
4	D	2391	0	2424	13	0
5	E	1729	0	1887	15	0
6	F	1875	0	1995	23	0
7	G	1879	0	2027	12	0
8	H	1516	0	1597	13	0
9	I	1664	0	1712	15	0
10	J	1362	0	1399	14	0
11	L	1702	0	1820	11	0
12	M	1137	0	1211	18	0
13	N	1701	0	1749	24	0
14	O	1630	0	1778	29	0
15	P	1242	0	1274	14	0
16	Q	1515	0	1634	16	0
17	R	1508	0	1664	7	0
18	S	1462	0	1508	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	T	1298	0	1366	11	0
20	U	809	0	833	9	0
21	V	979	0	1039	13	0
22	W	860	0	903	3	0
23	X	967	0	1040	4	0
24	Y	1115	0	1205	6	0
25	Z	1107	0	1182	8	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	1001	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	466	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	2	1593	0	811	4	0
45	3	1593	0	811	3	0
46	5	75972	0	38399	476	0
47	7	2558	0	1296	7	0
48	8	3208	0	1629	20	0
49	9	36249	0	18316	200	0
50	AA	1710	0	1708	12	0
51	BB	1729	0	1803	10	0
52	CC	1716	0	1806	14	0
53	DD	1768	0	1866	10	0
54	EE	2076	0	2177	13	0
55	FF	1471	0	1522	7	0
56	GG	1923	0	2089	14	0
57	HH	1488	0	1582	13	0
58	II	1686	0	1772	14	0
59	JJ	1525	0	1640	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	KK	810	0	836	6	0
61	LL	1175	0	1249	11	0
62	MM	908	0	939	11	0
63	NN	1202	0	1289	6	0
64	OO	1016	0	1039	7	0
65	PP	997	0	1045	7	0
66	QQ	1128	0	1195	5	0
67	RR	1068	0	1121	5	0
68	SS	1190	0	1249	9	0
69	TT	1097	0	1132	4	0
70	UU	795	0	862	5	0
71	VV	636	0	637	3	0
72	WW	1034	0	1080	13	0
73	XX	1098	0	1167	10	0
74	YY	1011	0	1083	7	0
75	ZZ	598	0	656	0	0
76	aa	814	0	864	0	0
77	bb	651	0	672	0	0
78	cc	488	0	514	0	0
79	dd	459	0	449	0	0
80	ee	443	0	492	0	0
81	ff	555	0	566	0	0
82	gg	2436	0	2393	0	0
83	hh	176	0	89	0	0
84	ii	2947	0	2957	0	0
85	jj	3292	0	3371	0	0
86	5	164	0	0	0	0
86	7	5	0	0	0	0
86	8	3	0	0	0	0
86	9	56	0	0	0	0
86	I	1	0	0	0	0
86	L	1	0	0	0	0
86	P	1	0	0	0	0
86	TT	1	0	0	0	0
86	V	1	0	0	0	0
86	a	1	0	0	0	0
86	hh	1	0	0	0	0
86	jj	1	0	0	0	0
87	aa	1	0	0	0	0
87	dd	1	0	0	0	0
87	ff	1	0	0	0	0
87	g	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
87	j	1	0	0	0	0
87	m	1	0	0	0	0
87	o	1	0	0	0	0
87	p	1	0	0	0	0
88	jj	32	0	14	0	0
All	All	221912	0	166887	1173	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 4.

The worst 5 of 1173 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)
46:5:3914:U:O4	46:5:4378:A:N1	1.60	1.32
49:9:830:A:N1	49:9:844:U:O4	1.71	1.20
46:5:1929:A:N1	46:5:2054:U:O4	1.73	1.20
46:5:77:U:O4	46:5:336:A:N1	1.70	1.20
46:5:922:C:C5'	46:5:922(A):G:H3'	1.74	1.17

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	217 (88%)	25 (10%)	4 (2%)	12	57
2	B	392/403 (97%)	343 (88%)	47 (12%)	2 (0%)	34	76
3	C	360/425 (85%)	319 (89%)	32 (9%)	9 (2%)	7	49
4	D	291/297 (98%)	270 (93%)	18 (6%)	3 (1%)	19	65
5	E	208/291 (72%)	182 (88%)	25 (12%)	1 (0%)	34	76

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	223/247 (90%)	199 (89%)	20 (9%)	4 (2%)	11	55
7	G	229/319 (72%)	212 (93%)	16 (7%)	1 (0%)	39	79
8	H	188/192 (98%)	168 (89%)	18 (10%)	2 (1%)	17	64
9	I	201/214 (94%)	178 (89%)	23 (11%)	0	100	100
10	J	168/178 (94%)	156 (93%)	10 (6%)	2 (1%)	16	62
11	L	208/211 (99%)	185 (89%)	21 (10%)	2 (1%)	19	65
12	M	136/218 (62%)	126 (93%)	7 (5%)	3 (2%)	8	52
13	N	201/204 (98%)	180 (90%)	17 (8%)	4 (2%)	9	54
14	O	197/203 (97%)	176 (89%)	21 (11%)	0	100	100
15	P	151/184 (82%)	138 (91%)	11 (7%)	2 (1%)	15	60
16	Q	185/188 (98%)	163 (88%)	20 (11%)	2 (1%)	17	64
17	R	178/196 (91%)	170 (96%)	8 (4%)	0	100	100
18	S	174/176 (99%)	161 (92%)	11 (6%)	2 (1%)	17	64
19	T	157/160 (98%)	141 (90%)	16 (10%)	0	100	100
20	U	97/128 (76%)	86 (89%)	9 (9%)	2 (2%)	9	53
21	V	129/140 (92%)	117 (91%)	10 (8%)	2 (2%)	12	57
22	W	102/157 (65%)	91 (89%)	10 (10%)	1 (1%)	19	65
23	X	116/156 (74%)	109 (94%)	7 (6%)	0	100	100
24	Y	132/145 (91%)	126 (96%)	6 (4%)	0	100	100
25	Z	133/136 (98%)	126 (95%)	5 (4%)	2 (2%)	13	58
26	a	145/148 (98%)	134 (92%)	11 (8%)	0	100	100
27	b	100/245 (41%)	89 (89%)	10 (10%)	1 (1%)	19	65
28	c	96/115 (84%)	91 (95%)	5 (5%)	0	100	100
29	d	105/125 (84%)	87 (83%)	16 (15%)	2 (2%)	10	54
30	e	126/135 (93%)	116 (92%)	9 (7%)	1 (1%)	24	69
31	f	107/110 (97%)	96 (90%)	8 (8%)	3 (3%)	6	47
32	g	112/117 (96%)	98 (88%)	12 (11%)	2 (2%)	11	55
33	h	120/123 (98%)	112 (93%)	7 (6%)	1 (1%)	24	69
34	i	100/105 (95%)	91 (91%)	9 (9%)	0	100	100
35	j	84/97 (87%)	72 (86%)	11 (13%)	1 (1%)	16	62
36	k	67/70 (96%)	61 (91%)	5 (8%)	1 (2%)	13	58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	l	48/51 (94%)	42 (88%)	5 (10%)	1 (2%)	9	53
38	m	50/102 (49%)	46 (92%)	3 (6%)	1 (2%)	9	54
39	n	23/25 (92%)	23 (100%)	0	0	100	100
40	o	102/106 (96%)	89 (87%)	11 (11%)	2 (2%)	9	54
41	p	89/92 (97%)	81 (91%)	8 (9%)	0	100	100
42	r	122/137 (89%)	103 (84%)	16 (13%)	3 (2%)	7	49
43	s	194/318 (61%)	173 (89%)	19 (10%)	2 (1%)	19	65
44	t	151/165 (92%)	135 (89%)	14 (9%)	2 (1%)	15	60
50	AA	215/295 (73%)	189 (88%)	23 (11%)	3 (1%)	14	59
51	BB	211/264 (80%)	194 (92%)	17 (8%)	0	100	100
52	CC	219/293 (75%)	202 (92%)	14 (6%)	3 (1%)	14	59
53	DD	226/243 (93%)	207 (92%)	18 (8%)	1 (0%)	39	79
54	EE	260/263 (99%)	245 (94%)	13 (5%)	2 (1%)	24	69
55	FF	181/204 (89%)	164 (91%)	14 (8%)	3 (2%)	11	56
56	GG	235/249 (94%)	221 (94%)	13 (6%)	1 (0%)	39	79
57	HH	181/194 (93%)	170 (94%)	11 (6%)	0	100	100
58	II	204/208 (98%)	187 (92%)	17 (8%)	0	100	100
59	JJ	183/194 (94%)	172 (94%)	10 (6%)	1 (0%)	34	76
60	KK	94/165 (57%)	85 (90%)	8 (8%)	1 (1%)	17	64
61	LL	139/158 (88%)	119 (86%)	19 (14%)	1 (1%)	26	71
62	MM	115/132 (87%)	97 (84%)	18 (16%)	0	100	100
63	NN	147/151 (97%)	131 (89%)	16 (11%)	0	100	100
64	OO	134/168 (80%)	116 (87%)	17 (13%)	1 (1%)	26	71
65	PP	118/145 (81%)	103 (87%)	15 (13%)	0	100	100
66	QQ	140/146 (96%)	131 (94%)	8 (6%)	1 (1%)	26	71
67	RR	130/135 (96%)	114 (88%)	15 (12%)	1 (1%)	24	69
68	SS	142/152 (93%)	134 (94%)	6 (4%)	2 (1%)	14	59
69	TT	139/145 (96%)	130 (94%)	8 (6%)	1 (1%)	26	71
70	UU	98/119 (82%)	90 (92%)	7 (7%)	1 (1%)	19	65
71	VV	81/83 (98%)	76 (94%)	5 (6%)	0	100	100
72	WW	127/130 (98%)	112 (88%)	12 (9%)	3 (2%)	7	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
73	XX	139/143 (97%)	126 (91%)	10 (7%)	3 (2%)	8	52
74	YY	122/130 (94%)	116 (95%)	6 (5%)	0	100	100
75	ZZ	73/125 (58%)	71 (97%)	2 (3%)	0	100	100
76	aa	99/115 (86%)	84 (85%)	13 (13%)	2 (2%)	9	54
77	bb	81/84 (96%)	71 (88%)	9 (11%)	1 (1%)	16	62
78	cc	60/69 (87%)	55 (92%)	4 (7%)	1 (2%)	11	56
79	dd	53/56 (95%)	44 (83%)	8 (15%)	1 (2%)	10	54
80	ee	53/133 (40%)	48 (91%)	5 (9%)	0	100	100
81	ff	66/156 (42%)	60 (91%)	4 (6%)	2 (3%)	5	45
82	gg	311/317 (98%)	281 (90%)	27 (9%)	3 (1%)	19	65
84	ii	370/403 (92%)	342 (92%)	28 (8%)	0	100	100
85	jj	423/710 (60%)	383 (90%)	35 (8%)	5 (1%)	16	62
All	All	12312/14488 (85%)	11148 (90%)	1047 (8%)	117 (1%)	24	65

5 of 117 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	196	TRP
3	C	254	GLU
7	G	105	THR
18	S	155	PRO
29	d	58	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%)	170 (90%)	20 (10%)	8	40
2	B	342/348 (98%)	308 (90%)	34 (10%)	10	43
3	C	302/347 (87%)	275 (91%)	27 (9%)	12	48
4	D	247/250 (99%)	233 (94%)	14 (6%)	25	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	190/251 (76%)	178 (94%)	12 (6%)	22	61
6	F	196/215 (91%)	181 (92%)	15 (8%)	16	55
7	G	200/272 (74%)	186 (93%)	14 (7%)	19	58
8	H	169/171 (99%)	154 (91%)	15 (9%)	12	48
9	I	175/181 (97%)	161 (92%)	14 (8%)	15	53
10	J	143/149 (96%)	136 (95%)	7 (5%)	31	69
11	L	175/176 (99%)	164 (94%)	11 (6%)	22	61
12	M	117/161 (73%)	107 (92%)	10 (8%)	13	51
13	N	171/172 (99%)	158 (92%)	13 (8%)	16	55
14	O	171/173 (99%)	156 (91%)	15 (9%)	12	48
15	P	134/163 (82%)	122 (91%)	12 (9%)	12	47
16	Q	164/165 (99%)	147 (90%)	17 (10%)	9	40
17	R	159/175 (91%)	145 (91%)	14 (9%)	12	48
18	S	157/157 (100%)	145 (92%)	12 (8%)	16	55
19	T	139/140 (99%)	125 (90%)	14 (10%)	9	41
20	U	89/114 (78%)	87 (98%)	2 (2%)	60	84
21	V	101/107 (94%)	87 (86%)	14 (14%)	4	29
22	W	86/126 (68%)	83 (96%)	3 (4%)	43	76
23	X	106/134 (79%)	100 (94%)	6 (6%)	25	65
24	Y	124/135 (92%)	117 (94%)	7 (6%)	26	65
25	Z	117/118 (99%)	112 (96%)	5 (4%)	35	72
26	a	119/120 (99%)	114 (96%)	5 (4%)	36	72
27	b	84/184 (46%)	80 (95%)	4 (5%)	31	69
28	c	84/98 (86%)	78 (93%)	6 (7%)	18	58
29	d	98/110 (89%)	89 (91%)	9 (9%)	11	46
30	e	114/121 (94%)	105 (92%)	9 (8%)	15	54
31	f	88/89 (99%)	80 (91%)	8 (9%)	12	47
32	g	98/100 (98%)	88 (90%)	10 (10%)	9	41
33	h	109/110 (99%)	105 (96%)	4 (4%)	41	75
34	i	86/89 (97%)	83 (96%)	3 (4%)	43	76
35	j	73/80 (91%)	63 (86%)	10 (14%)	4	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	k	64/65 (98%)	60 (94%)	4 (6%)	22	61
37	l	47/48 (98%)	44 (94%)	3 (6%)	22	61
38	m	48/90 (53%)	43 (90%)	5 (10%)	9	40
39	n	24/24 (100%)	22 (92%)	2 (8%)	14	51
40	o	92/94 (98%)	87 (95%)	5 (5%)	27	67
41	p	74/75 (99%)	70 (95%)	4 (5%)	27	67
42	r	108/121 (89%)	97 (90%)	11 (10%)	9	41
43	s	164/258 (64%)	158 (96%)	6 (4%)	41	75
44	t	126/137 (92%)	123 (98%)	3 (2%)	57	82
50	AA	180/245 (74%)	161 (89%)	19 (11%)	8	39
51	BB	194/231 (84%)	176 (91%)	18 (9%)	11	46
52	CC	187/225 (83%)	168 (90%)	19 (10%)	9	41
53	DD	190/202 (94%)	178 (94%)	12 (6%)	22	61
54	EE	224/225 (100%)	205 (92%)	19 (8%)	13	51
55	FF	158/170 (93%)	140 (89%)	18 (11%)	7	36
56	GG	207/218 (95%)	187 (90%)	20 (10%)	10	43
57	HH	165/174 (95%)	150 (91%)	15 (9%)	12	47
58	II	178/180 (99%)	169 (95%)	9 (5%)	29	68
59	JJ	161/168 (96%)	146 (91%)	15 (9%)	11	46
60	KK	87/136 (64%)	82 (94%)	5 (6%)	25	65
61	LL	130/142 (92%)	116 (89%)	14 (11%)	8	39
62	MM	99/108 (92%)	84 (85%)	15 (15%)	3	25
63	NN	130/131 (99%)	113 (87%)	17 (13%)	5	30
64	OO	106/130 (82%)	96 (91%)	10 (9%)	11	45
65	PP	109/130 (84%)	99 (91%)	10 (9%)	11	46
66	QQ	117/121 (97%)	111 (95%)	6 (5%)	29	68
67	RR	119/121 (98%)	102 (86%)	17 (14%)	4	28
68	SS	125/132 (95%)	110 (88%)	15 (12%)	6	33
69	TT	111/115 (96%)	105 (95%)	6 (5%)	27	67
70	UU	92/107 (86%)	84 (91%)	8 (9%)	13	48
71	VV	67/67 (100%)	63 (94%)	4 (6%)	24	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
72	WW	112/113 (99%)	104 (93%)	8 (7%)	18	58
73	XX	113/115 (98%)	103 (91%)	10 (9%)	12	48
74	YY	107/112 (96%)	92 (86%)	15 (14%)	4	29
75	ZZ	66/103 (64%)	61 (92%)	5 (8%)	16	55
76	aa	88/98 (90%)	78 (89%)	10 (11%)	7	36
77	bb	75/76 (99%)	67 (89%)	8 (11%)	8	39
78	cc	55/62 (89%)	49 (89%)	6 (11%)	8	38
79	dd	48/49 (98%)	45 (94%)	3 (6%)	22	61
80	ee	46/106 (43%)	42 (91%)	4 (9%)	13	48
81	ff	61/140 (44%)	55 (90%)	6 (10%)	10	43
82	gg	272/275 (99%)	258 (95%)	14 (5%)	29	68
84	ii	326/353 (92%)	310 (95%)	16 (5%)	31	69
85	jj	358/608 (59%)	332 (93%)	26 (7%)	17	57
All	All	10727/12300 (87%)	9867 (92%)	860 (8%)	20	53

5 of 860 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
35	j	33	THR
52	CC	137	VAL
80	ee	99	LYS
37	l	3	SER
44	t	98	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
19	T	98	HIS
32	g	14	ASN
73	XX	77	ASN
19	T	131	GLN
22	W	30	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
45	2	72/75 (96%)	17 (23%)	1 (1%)
45	3	72/75 (96%)	21 (29%)	1 (1%)
46	5	3506/3543 (98%)	921 (26%)	179 (5%)
47	7	119/120 (99%)	19 (15%)	3 (2%)
48	8	149/156 (95%)	39 (26%)	6 (4%)
49	9	1679/1869 (89%)	452 (26%)	88 (5%)
83	hh	7/8 (87%)	4 (57%)	0
All	All	5604/5846 (95%)	1473 (26%)	278 (4%)

5 of 1473 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
45	2	7	A
45	2	13	C
45	2	16	C
45	2	21	A
45	2	25	C

5 of 278 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
46	5	2724	G
46	5	4254	G
49	9	1519	U
46	5	2806	A
46	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 245 ligands modelled in this entry, 244 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	$\# Z > 2$
88	GCP	jj	700	86	29,34,34	2.50	8 (27%)	31,54,54	1.07	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
88	GCP	jj	700	86	-	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)
88	jj	700	GCP	C4-N9	-10.26	1.34	1.47
88	jj	700	GCP	C8-N9	-3.77	1.35	1.47
88	jj	700	GCP	C5-C6	-2.10	1.49	1.53
88	jj	700	GCP	PB-C3B	2.03	1.82	1.80
88	jj	700	GCP	PB-O2B	2.07	1.61	1.56

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	jj	700	GCP	C4-C5-N7	2.32	106.29	102.67
88	jj	700	GCP	C8-N9-C4	3.06	108.27	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
46	5	42
49	9	7
45	2	2
45	3	2

The worst 5 of 53 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	40.66
1	5	1252:C	O3'	1271:G	P	36.39
1	5	1405:C	O3'	1406:G	P	23.89
1	5	1219:G	O3'	1233:G	P	22.08
1	5	1406:G	O3'	1406(A):G	P	20.74