



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Aug 17, 2017 – 01:38 PM EDT

PDB ID : 5LZZ
EMDB ID: : EMD-4137
Title : Structure of the mammalian rescue complex with Pelota and Hbs1l (combined)
Authors : Shao, S.; Murray, J.; Brown, A.; Taunton, J.; Ramakrishnan, V.; Hegde, R.S.
Deposited on : unknown
Resolution : 3.47 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.

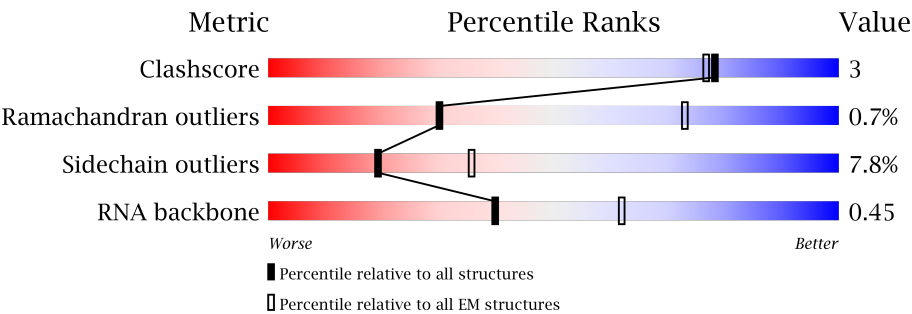
MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.47 Å.

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




















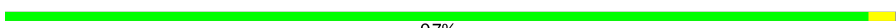







Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 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	<div><div>79%</div><div>16%</div><div>.</div><div>.</div></div>
2	B	403	<div><div>80%</div><div>17%</div><div>.</div><div>.</div></div>
3	C	425	<div><div>69%</div><div>15%</div><div>.</div><div>15%</div></div>
4	D	297	<div><div>88%</div><div>9%</div><div>.</div><div>.</div></div>
5	E	291	<div><div>68%</div><div>.</div><div>.</div><div>26%</div></div>
6	F	247	<div><div>74%</div><div>17%</div><div>.</div><div>9%</div></div>
7	G	319	<div><div>64%</div><div>8%</div><div>.</div><div>27%</div></div>
8	H	192	<div><div>82%</div><div>16%</div><div>.</div><div>.</div></div>







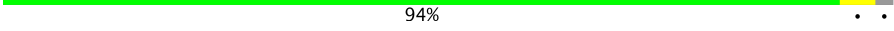




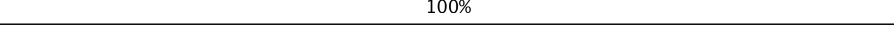







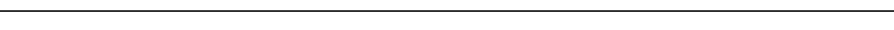

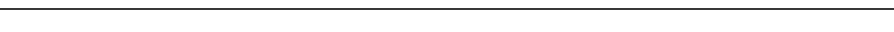
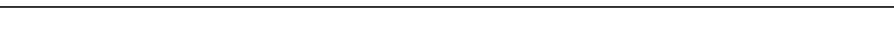


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Mol	Chain	Length	Quality of chain
9	I	214	
10	J	178	
11	L	211	
12	M	218	
13	N	204	
14	O	203	
15	P	184	
16	Q	188	
17	R	196	
18	S	176	
19	T	160	
20	U	128	
21	V	140	
22	W	157	
23	X	156	
24	Y	145	
25	Z	136	
26	a	148	
27	b	245	
28	c	115	
29	d	125	
30	e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


























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Mol	Chain	Length	Quality of chain
34	i	105	 93% . .
35	j	97	 82% 6% 11%
36	k	70	 93% 6% .
37	l	51	 94% . .
38	m	102	 47% . 49%
39	n	25	 92% 8%
40	o	106	 94% . .
41	p	92	 92% 7% .
42	r	137	 80% 11% 9%
43	s	318	 59% . 38%
44	t	165	 89% . 7%
45	1	7	 100%
46	2	76	 79% 20% .
47	3	75	 68% 29% .
48	5	3543	 67% 28% 5%
49	7	120	 81% 19%
50	8	156	 63% 30% . .
51	9	1869	 58% 28% . 9%
52	AA	295	 58% 15% . 26%
53	BB	264	 67% 13% . 19%
54	CC	293	 63% 12% 25%
55	DD	243	 82% 11% . 6%
56	EE	263	 84% 16%
57	FF	204	 80% 9% . 9%
58	GG	249	 81% 14% 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	 93%6% •
85	hh	8	 50%50%
86	ii	403	 88% •8%
87	jj	710	 56% •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 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 Uncharacterized protein.

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 60S ribosomal protein L7a,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 Uncharacterized protein.

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 40S ribosomal protein S8.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 61 is a protein called 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 Uncharacterized protein.

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 Uncharacterized protein.

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 40S ribosomal protein S24.

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.

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
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	g	1	Total Mg 1 1	0
88	j	1	Total Mg 1 1	0
88	e	1	Total Mg 1 1	0
88	B	1	Total Mg 1 1	0
88	I	1	Total Mg 1 1	0

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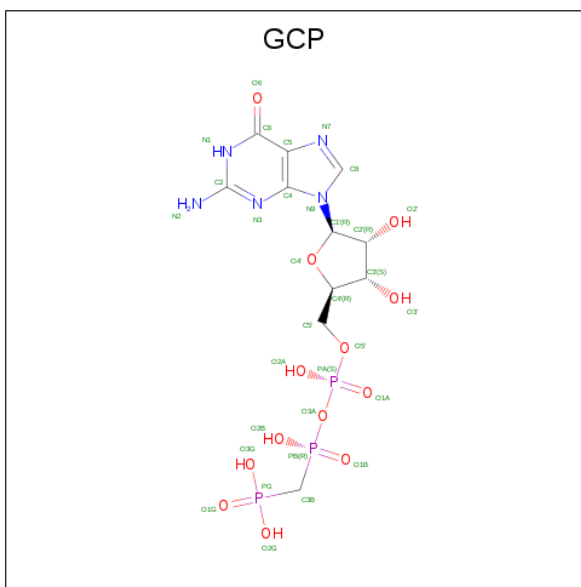
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
88	jj	1	Total 1	Mg 1	0
88	V	1	Total 1	Mg 1	0
88	7	5	Total 5	Mg 5	0
88	a	1	Total 1	Mg 1	0
88	5	178	Total 178	Mg 178	0
88	8	5	Total 5	Mg 5	0
88	9	66	Total 66	Mg 66	0
88	L	1	Total 1	Mg 1	0

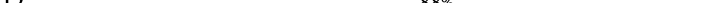
- Molecule 89 is ZINC ION (three-letter code: ZN) (formula: Zn).

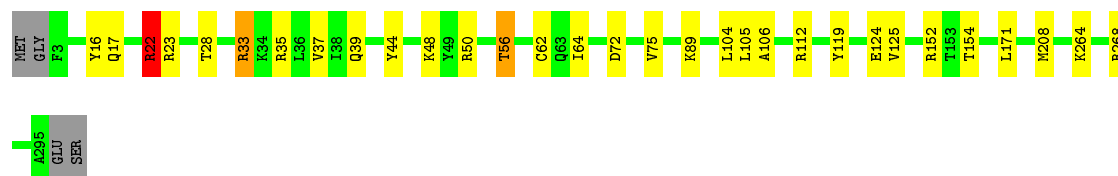
Mol	Chain	Residues	Atoms		AltConf
89	p	1	Total 1	Zn 1	0
89	g	1	Total 1	Zn 1	0
89	j	1	Total 1	Zn 1	0
89	dd	1	Total 1	Zn 1	0
89	ff	1	Total 1	Zn 1	0
89	aa	1	Total 1	Zn 1	0
89	o	1	Total 1	Zn 1	0
89	m	1	Total 1	Zn 1	0

- Molecule 90 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: C₁₁H₁₈N₅O₁₃P₃).



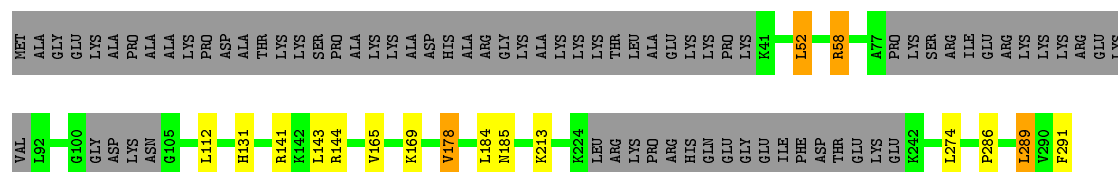
Mol	Chain	Residues	Atoms					AltConf
90	jj	1	Total	C	N	O	P	0
			32	11	5	13	3	

Chain D:  88% 9% ..



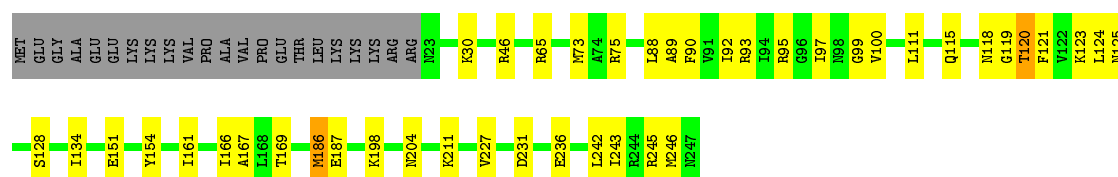
- Molecule 5: 60S ribosomal protein L6

Chain E:  68% . . 26%



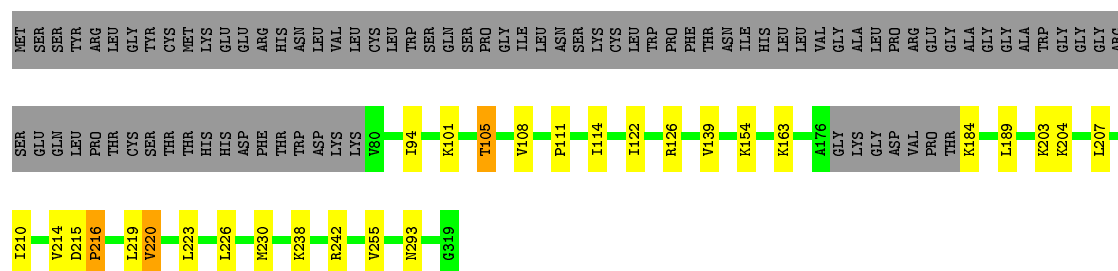
- Molecule 6: Uncharacterized protein

Chain F:  74% 17% 9%




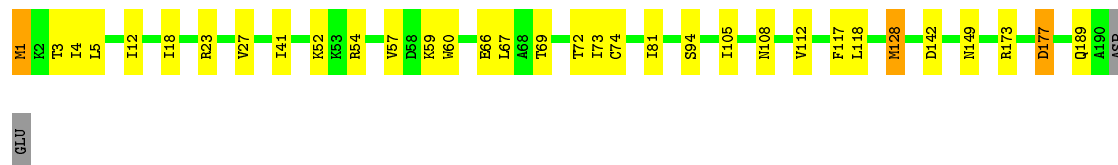
- Molecule 7: 60S ribosomal protein L7a,eL8

Chain G:  64% 8% 27%




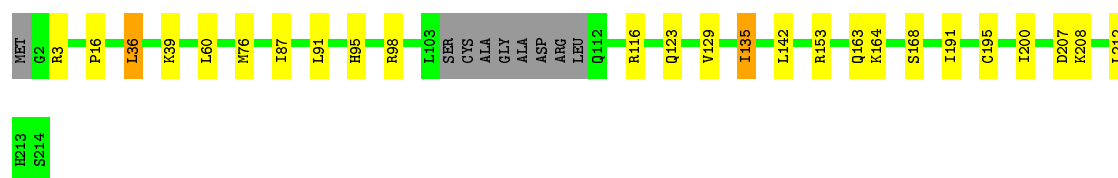
- Molecule 8: uL6

Chain H:  82% 16%




- Molecule 9: Ribosomal protein L10 (Predicted)

Chain I:  84% 11% . .



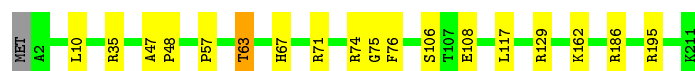
- Molecule 10: uL5

Chain J:  82% 12% . .



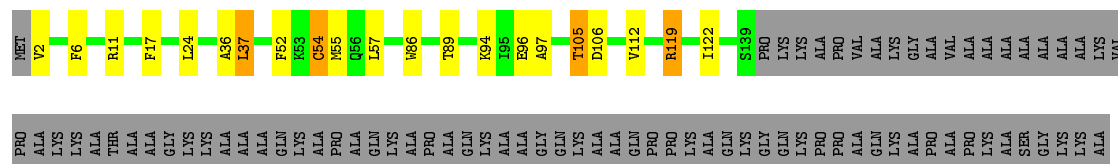
- Molecule 11: eL13

Chain L:  91% 8%




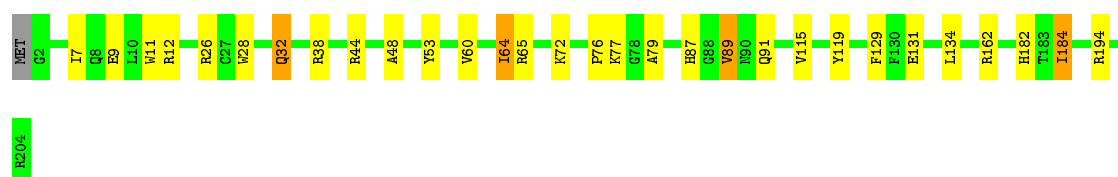
- Molecule 12: eL14

Chain M:  54% 8% 37%




- Molecule 13: Ribosomal protein L15

Chain N:  85% 13%



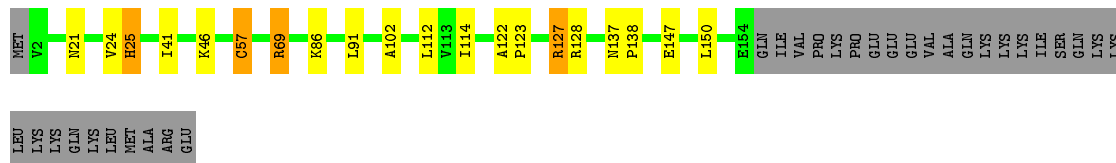
- Molecule 14: uL13

Chain O:  79% 16%




- Molecule 15: uL22

Chain P:  72% 9% 17%




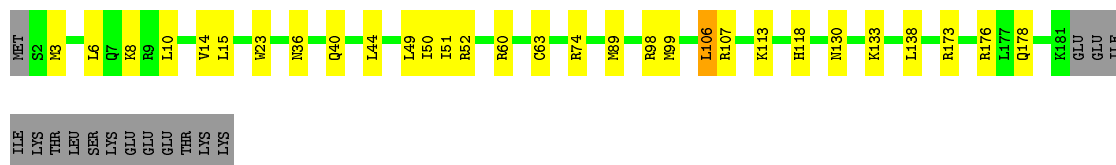
- Molecule 16: eL18

Chain Q:  84% 15%




- Molecule 17: eL19

Chain R:  77% 15% 8%




- Molecule 18: eL20

Chain S:  81% 18%



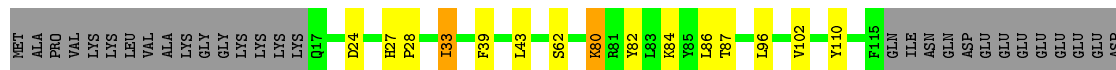
- Molecule 19: eL21

Chain T:  83% 16%



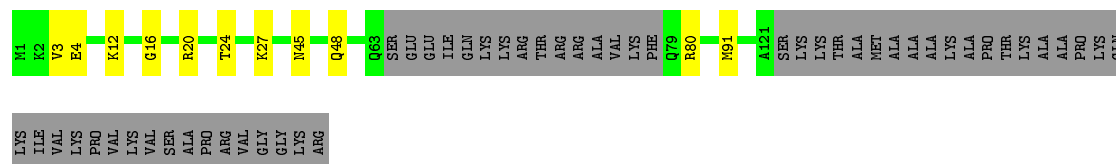
- Molecule 20: eL22

Chain U:  66% 10% 23%

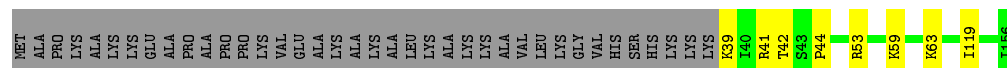


- Molecule 21: uL14

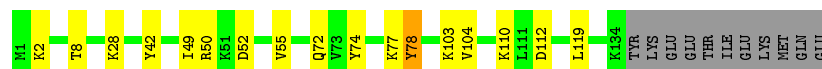
- Molecule 22: eL24



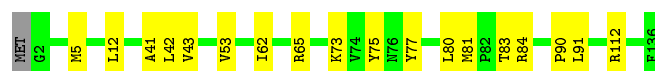
- Molecule 23: uL23



- Molecule 24: uL24



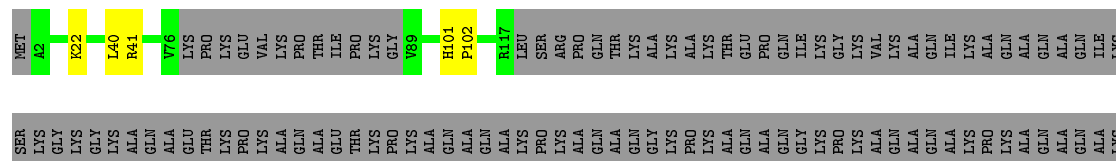
- Molecule 25: 60S ribosomal protein L27



- Molecule 26: uL15




- Molecule 27: eL29



PRO LYS ALA GLN ALA GLN THR PRO LYS LYS ALA GLN ALA THR PRO ALA ALA PRO VAL VAL ALA GLN ALA PRO LYS LYS GLY ALA PRO GLN GLN PRO ALA LYS ALA LYS ALA PRO

• Molecule 28: eL30

Chain c:  79% 6% 15%


MET VAL ALA ALA LYS LYS THR LYS LYS S10 M37 N50 N78 L81 G82 T83 R90 V91 C92 S107 MET PRO GLU GLN THR GLY LYS

• Molecule 29: eL31

Chain d:  74% 11% 14%


MET ALA PRO ALA LYS LYS GLY GLU LYS LYS LYS GLY ANG SER SER ALA ALA ILE N18 R23 T26 K31 R44 E48 E56 M57 G58 R78 N79 R83 T84 R85 R90 S98 L117 E124 ASN

• Molecule 30: eL32

Chain e:  89% 6% 5%

MET A2 I21 R22 R48 R64 L78 E86 K106 R128 L129 ARG SER GLU ASN GLU

• Molecule 31: eL33

Chain f:  90% 9% .

MET S2 R16 R23 L28 V33 K52 S90 I101 L105 Y106 P107 I110

• Molecule 32: eL34

Chain g:  91% 6% .

MET V2 L22 V48 R54 R60 R66 R90 Q114 K115 ALA LYS

• Molecule 33: uL29

Chain h:  95% . .


MET A2 E16 L28 E87 K77 R89 A123

• Molecule 34: 60S ribosomal protein L36

Chain i:  93% . .

MET A2 T34 C48 K36 E89 K103 LYS ASP

- Molecule 35: Ribosomal protein L37

Chain j:  82% 6% 11%



- Molecule 36: eL38

Chain k:  93% 6% .



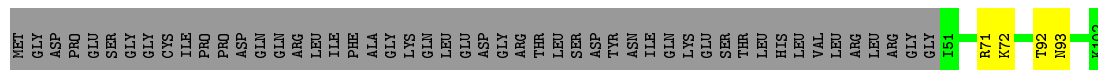
- Molecule 37: eL39

Chain l:  94% . .



- Molecule 38: eL40

Chain m:  47% . 49%



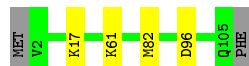
- Molecule 39: eL41

Chain n:  92% 8%



- Molecule 40: eL42

Chain o:  94% . .



- Molecule 41: eL43

Chain p:  92% 7% .



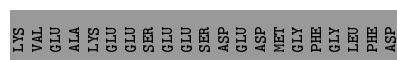
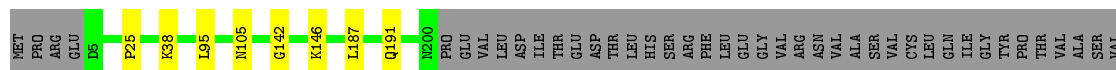
- Molecule 42: eL28

Chain r:  80% 11% 9%



- Molecule 43: uL10

Chain s: 59% 38%



- Molecule 44: uL11

Chain t: 89% 7%



- Molecule 45: Nascent chain

Chain 1: 100%

There are no outlier residues recorded for this chain.

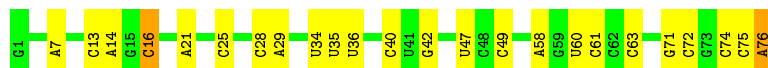
- Molecule 46: P-site tRNA

Chain 2: 79% 20%



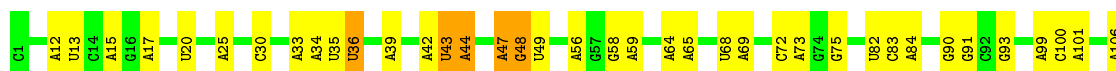
- Molecule 47: E-site tRNA

Chain 3: 68% 29%

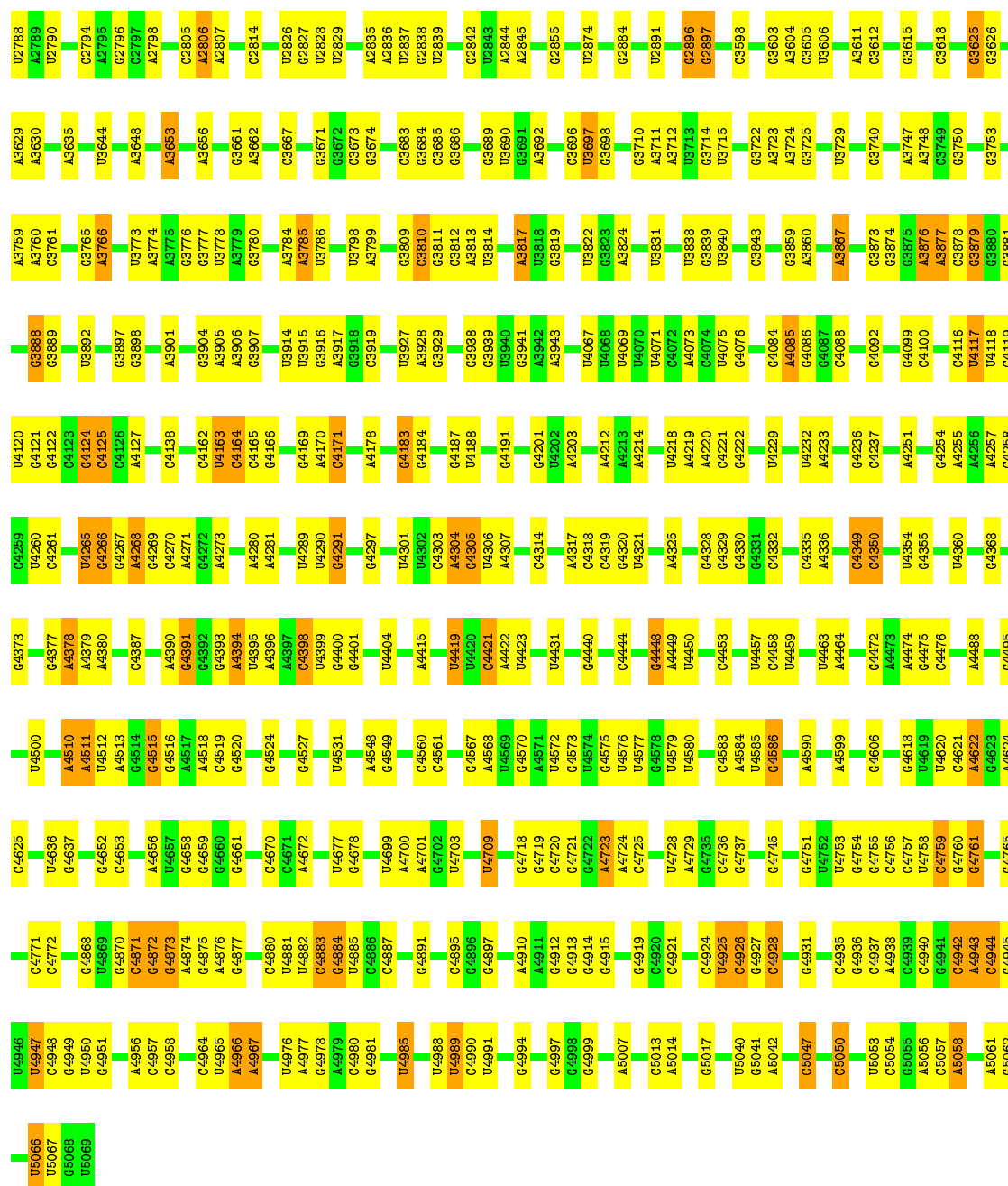


- Molecule 48: 28S ribosomal RNA

Chain 5: 67% 28% 5%

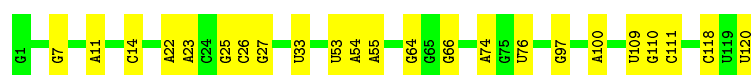


G2686	G2687	A2513	G2514	G2399	G2262	C2031	A1923	G1799	C1676	C1546	G1432	A1326	G1075	A917	G497	G387	G234
G2693	G2694	U2519	G2520	U2409	G2266	A2032	C1928	G1803	C1678	A1554	G1433	C1327	G1076	G918	C498	G399	A235
G2694	G2521	G2521	G2522	U2409	U2267	G2034	C1931	A1804	A1679	A1554	G1435	G1328	A1077	C922	G499	G399	G236
A2695	A2696	G2522	G2523	G2416	A2268	G2044	A1932	A1805	G1685	A1563	C1436	A1330	C1079	C922A	G500	G401	G245
		U2524	U2524	A2417	G2270	G2045	C1935	G1813	C1686	A1564	C1437	A1337	C1082	C922B	G504	G401	G246
C2704	U2707	A2529	U2530	G2421	G2274	G2046	C1938	G1819	G1691	A1565	U1440	G1338	C1082	C923	G647	U404	G253
U2708	U2709	G2422	G2423	G2424	G2275	A2047	C1939	U1820	G1694	U1567	U1441	G1339	G1174	C924	G648	U405	
G2710	G2711	A2428	U2425	U2426	G2276	U2048	U1947	U1821	C1694	U1568	U1442	C1340	G1177	G926	A649	A408	G262
G2712	G2713	G2433	G2434	U2427	G2277	G2052	U1948	U1822	G1724	U1577	U1445	G1353	U1177	A929	C654	U404	G265
G2714	G2715	G2439	U2440	U2441	G2278	G2055	G1948	C1828	G1729	U1578	U1446	A1354	U1179	G930	C658	A410	C266
G2716	G2717	U2442	U2443	U2444	G2279	G2056	G1951	G1833	A1729	G1586	G1453	G1358	G1195	C931	G666	G411	G267
C2719	G2720	G2443	U2444	U2445	G2280	A2057	G1952	U1834	G1733	U1591	G1454	G1359	G1195	A932	G667	G412	C275
G2721	G2722	G2444	U2445	U2446	G2281	A2058	G1953	G1835	G1734	U1591	G1455	G1360	U1209	C934	A667	G413	C276
G2723	G2724	G2445	U2446	U2447	G2282	C2062	G1961	G1836	C1740	U1596	G1456	U1364	C1210	A935	C668	G417	G277
A2725	G2726	G2446	U2447	U2448	G2283	G2063	A1962	U1837	G1741	U1613	G1457	G1370	G1212	C936	C672	G423	G278
G2727	G2728	G2447	U2448	U2449	G2284	G2064	A1963	G1842	A1742	A1601	G1458	A1371	G1213	U937	G683	U424	A279
C2729	U2730	G2448	U2449	U2450	G2285	G2065	G1966	G1843	U1744	U1602	C1478	G1377	G1214	C938	G684	G431	G280
G2731	G2732	G2449	U2450	U2451	G2286	G2066	A1967	G1844	G1745	U1602	C1479	G1378	C1215	G939	G685	U432	U281
G2733	G2734	G2450	U2451	U2452	G2287	G2067	G1976	G1845	A1746	U1612	C1480	G1380	G1234	C940	G686	U433	U297
A2735	G2736	G2451	U2452	U2453	G2288	G2068	C1977	G1846	U1747	U1613	C1481	U1381	G1235	C941	G687	A441	A306
G2737	G2738	G2452	U2453	U2454	G2289	G2069	C1978	G1847	U1748	A1613	G1482	G1382	G1236	A943	C696	G444	A307
G2739	G2740	G2453	U2454	U2455	G2290	G2070	C1979	G1848	U1749	A1614	G1483	G1383	C1237	U945	G697	G445	G308
U2743	U2744	G2454	U2455	U2456	G2291	G2071	C1980	G1849	U1750	G1624	G1484	G1384	C1238	C942	G704	U446	G309
G2750	G2751	G2455	U2456	U2457	G2292	G2072	C1981	G1850	G1751	G1625	G1485	A1387	C1239	G955	G705	C446	G310
G2752	G2753	G2456	U2457	U2458	G2293	G2073	C1982	G1851	G1752	G1626	G1486	A1397	G1280	C962	C738	U454	U321
G2754	G2755	G2457	U2458	U2459	G2294	G2074	C1983	G1852	G1753	G1627	G1487	A1398	G1281	C963	C739	C455	C322
G2756	G2757	G2458	U2459	U2460	G2295	G2075	C1984	G1853	U1754	G1628	G1488	G1399	G1282	A964	C740	C456	A334
G2758	G2759	G2459	U2460	U2461	G2296	G2076	C1985	G1854	G1755	G1629	G1489	G1401	G1283	A965	G741	G457	A335
G2760	G2761	G2460	U2461	U2462	G2297	G2077	C1986	G1855	U1756	G1630	G1490	C1401	G1284	A966	G742	C458	A336
U2762	U2763	G2461	U2462	U2463	G2298	G2078	C1987	G1856	G1757	G1631	G1491	C1401	G1285	C967	C743	A466	C340
G2764	G2765	G2462	U2463	U2464	G2299	G2079	C1988	G1857	U1758	G1632	G1492	C1401	G1286	C968	C744	U467	C347
G2766	G2767	G2463	U2464	U2465	G2300	G2080	C1989	G1858	G1759	G1633	G1493	C1401	G1287	C969	C745	U468	C350
U2768	U2769	G2464	U2465	U2466	G2301	G2081	C1990	G1859	U1760	G1634	G1494	C1401	G1288	C970	C746	C469	C357
G2770	G2771	G2465	U2466	U2467	G2302	G2082	C1991	G1860	G1761	G1635	G1495	C1401	G1289	C971	C747	C470	G356
G2772	G2773	G2466	U2467	U2468	G2303	G2083	C1992	G1861	G1762	G1636	G1496	C1401	G1290	C972	C748	C471	U357
G2774	G2775	G2467	U2468	U2469	G2304	G2084	C1993	G1862	U1763	G1637	G1497	C1401	G1291	C973	C749	C472	C361
G2776	G2777	G2468	U2469	U2470	G2305	G2085	C1994	G1863	G1764	G1638	G1498	C1401	G1292	C974	C750	C473	A362
G2778	G2779	G2469	U2470	U2471	G2306	G2086	C1995	G1864	U1765	G1639	G1499	C1401	G1293	C975	C751	C474	A363
G2780	G2781	G2470	U2471	U2472	G2307	G2087	C1996	G1865	G1766	G1640	G1500	C1401	G1294	C976	C752	C475	G366
G2782	G2783	G2471	U2472	U2473	G2308	G2088	C1997	G1866	U1767	G1641	G1501	C1401	G1295	C977	C753	C476	U357
G2784	G2785	G2472	U2473	U2474	G2309	G2089	C1998	G1867	G1768	G1642	G1502	C1401	G1296	C978	C754	C477	C361
G2786	G2787	G2473	U2474	U2475	G2310	G2090	C1999	G1868	U1769	G1643	G1503	C1401	G1297	C979	C755	C478	A362
G2788	G2789	G2474	U2475	U2476	G2311	G2091	C2000	G1869	G1770	G1644	G1504	C1401	G1298	C980	C756	C479	A363
G2790	G2791	G2475	U2476	U2477	G2312	G2092	C2001	G1870	U1771	G1645	G1505	C1401	G1299	C981	C757	C480	U365
G2792	G2793	G2476	U2477	U2478	G2313	G2093	C2002	G1871	G1772	G1646	G1506	C1401	G1300	C982	C758	C481	G492
G2794	G2795	G2477	U2478	U2479	G2314	G2094	C2003	G1872	U1773	G1647	G1507	C1401	G1301	C983	C759	C482	G493
G2796	G2797	G2478	U2479	U2480	G2315	G2095	C2004	G1873	G1774	G1648	G1508	C1401	G1302	C984	C760	C483	C494
G2798	G2799	G2479	U2480	U2481	G2316	G2096	C2005	G1874	U1775	G1649	G1509	C1401	G1303	C985	C761	C484	C495
G2800	G2801	G2480	U2481	U2482	G2317	G2097	C2006	G1875	G1776	G1650	G1510	C1401	G1304	C986	C762	C485	G496
G2802	G2803	G2481	U2482	U2483	G2318	G2098	C2007	G1876	U1777	G1651	G1511	C1401	G1305	C987	C763	C486	
G2804	G2805	G2482	U2483	U2484	G2319	G2099	C2008	G1877	U1778	G1652	G1512	C1401	G1306	C988	C764	C487	
G2806	G2807	G2483	U2484	U2485	G2320	G2100	C2009	G1878	U1779	G1653	G1513	C1401	G1307	C989	C765	C488	
G2808	G2809	G2484	U2485	U2486	G2321	G2101	C2010	G1879	U1780	G1654	G1514	C1401	G1308	C990	C766	C489	
G2810	G2811	G2485	U2486	U2487	G2322	G2102	C2011	G1880	U1781	G1655	G1515	C1401	G1309	C991	C767	C490	
G2812	G2813	G2486	U2487	U2488	G2323	G2103	C2012	G1881	U1782	G1656	G1516	C1401	G1310	C992	C768	C491	
G2814	G2815	G2487	U2488	U2489	G2324	G2104	C2013	G1882	U1783	G1657	G1517	C1401	G1311	C993	C769	C492	
G2816	G2817	G2488	U2489	U2490	G2325	G2105	C2014	G1883	U1784	G1658	G1518	C1401	G1312	C994	C770	C493	
G2818	G2819	G2489	U2490	U2491	G2326	G2106	C2015	G1884	U1785	G1659	G1519	C1401	G1313	C995	C771	C494	
G2820	G2821	G2490	U2491	U2492	G2327	G2107	C2016	G1885	U1786	G1660	G1520	C1401	G1314	C996	C772	C495	
G2822	G2823	G2491	U2492	U2493	G2328	G2108	C2017	G1886	U1787	G1661	G1521	C1401	G1315	C997	C773	C496	
G2824	G2825	G2492	U2493	U2494	G2329	G2109	C2018	G1887	U1788	G1662	G1522	C1401	G1316	C998	C774	C497	
G2826	G2827	G2493	U2494	U2495	G2330	G2110	C2019	G1888	U1789	G1663	G1523	C1401	G1317	C999	C775	C498	
G2828	G2829	G2494	U2495	U2496	G2331	G2111	C2020	G1889	U1790	G1664	G1524	C1401	G1318	C1000	C776	C499	
G2830	G2831	G2495	U2496	U2497	G2332	G2112	C2021	G1890	U1791	G1665	G1525	C1401	G1319	C1001	C777	C500	
G2832	G2833	G2496	U2497	U2498	G2333	G2113	C2022	G1891	U1792	G1666	G1526	C1401	G1320	C1002	C778	C501	
G2834	G2835	G2497	U2498	U2499	G2334	G2114	C2023	G1892	U1793	G1667	G1527	C1401	G1321	C1003	C779	C502	
G2836	G2837	G2498	U2499	U2500	G2335	G2115	C2024	G1893	U1794	G1668	G1528	C1401	G1322	C1004	C780	C503	
G2838	G2839	G2499	U2500	U2501	G2336	G2116	C2025	G1894	U1795	G1669	G1529	C1401	G1323	C1005	C781	C504	
G2840	G2841	G2500	U2501	U2502	G2337	G2117	C2026	G1895	U1796	G1670	G1530	C1401	G1324	C1006	C782	C505	
G2842	G2843	G2501	U2502	U2503	G2338	G2118	C2027	G1896	U1797	G1671	G1531	C1401	G1325	C1007	C783	C506	
G2844	G2845	G2502	U2503	U2504	G2339	G2119	C2028	G1897	U1798	G1672	G1532	C1401	G1326	C1008	C784	C507	
G2846	G2847	G2503	U2504	U2505	G2340	G2120	C2029	G1898	U1799	G1673	G1533	C1401	G1327	C1009	C785	C508	
G2848	G2849	G2504	U2505	U2506	G2341	G2121	C2030	G1899	U1800	G1674	G1534	C1401	G1328	C1010	C786	C509	
G2850	G2851	G2505	U2506	U2507	G2342	G2122	C2031	G1900	U1801	G1675	G1535	C1401	G1329	C1011	C787	C510	
G2852	G2853	G2506	U2507	U25													



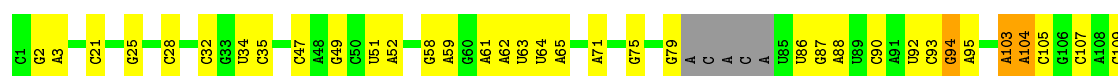
- Molecule 49: 5S ribosomal RNA

Chain 7: 81% 19%



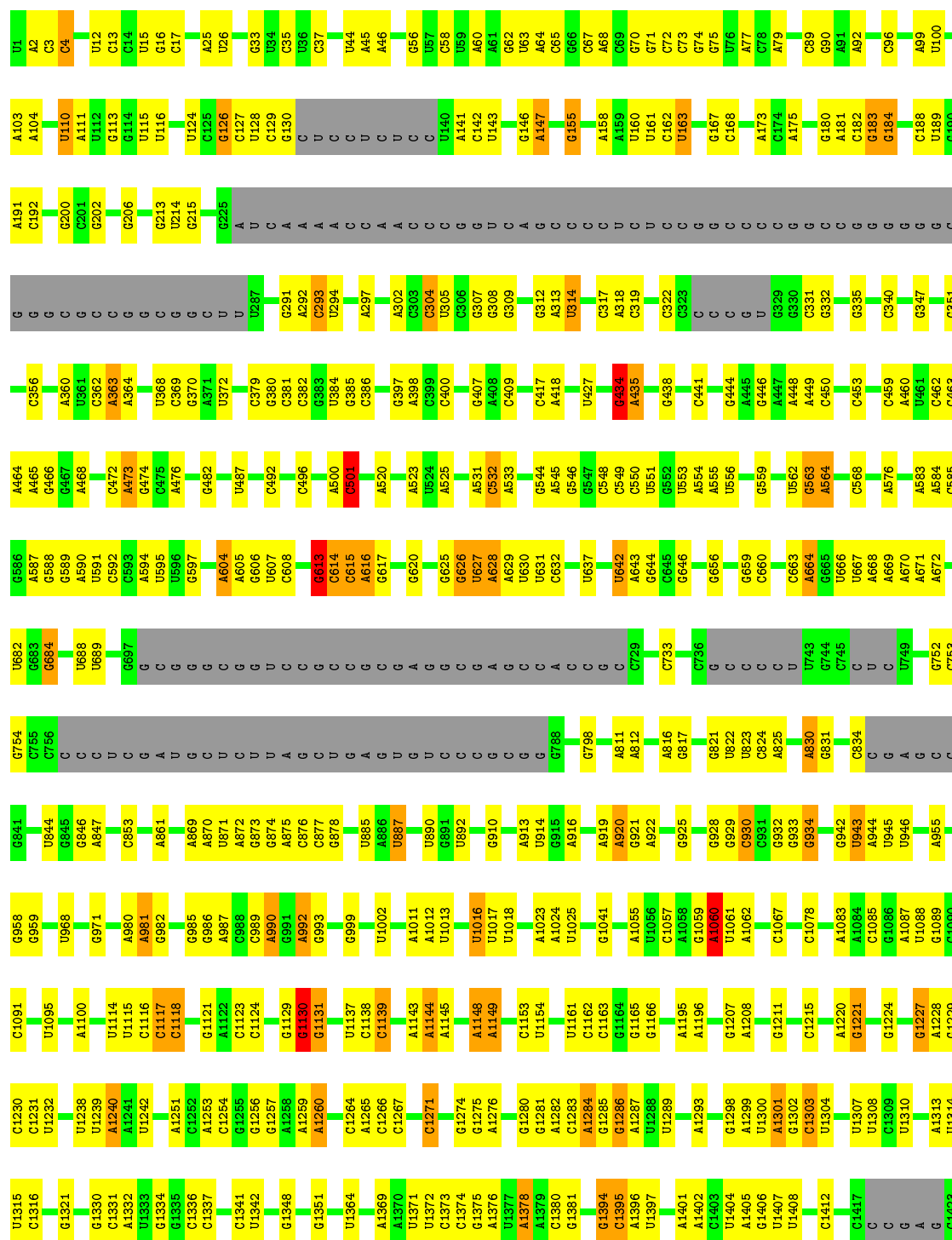
- Molecule 50: 5.8S ribosomal RNA

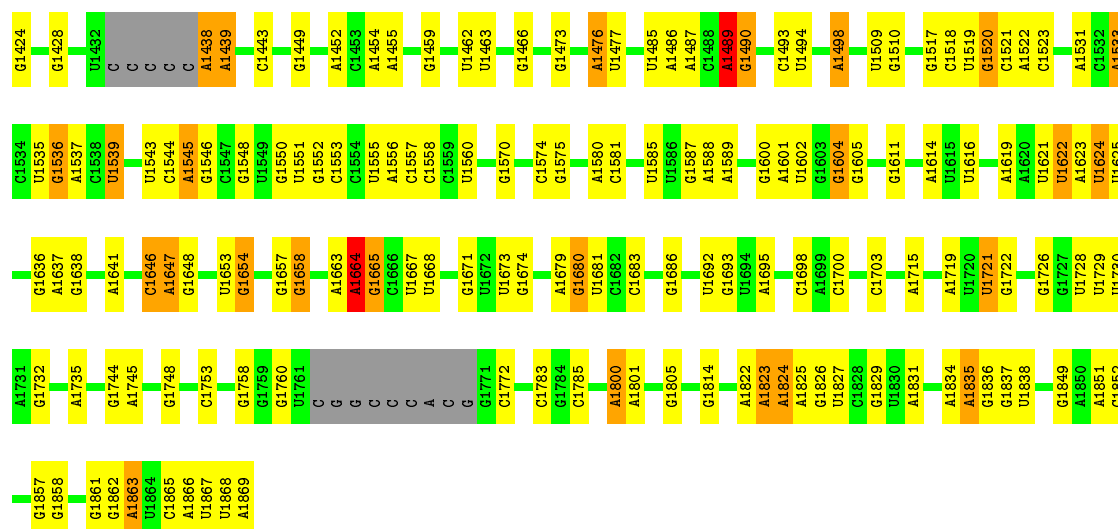
Chain 8: 63% 30%



- Molecule 51: 18S ribosomal RNA

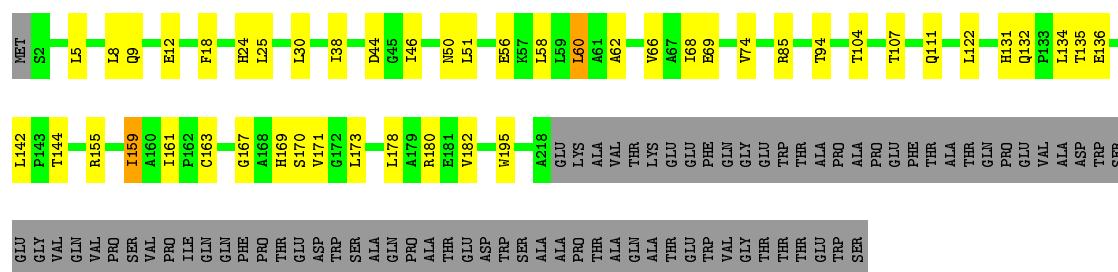
Chain 9:  58% 28% 0% 9%





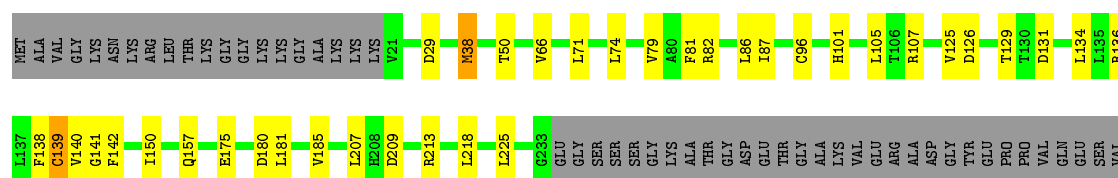
- Molecule 52: uS2

Chain AA: 58% 15% 26%



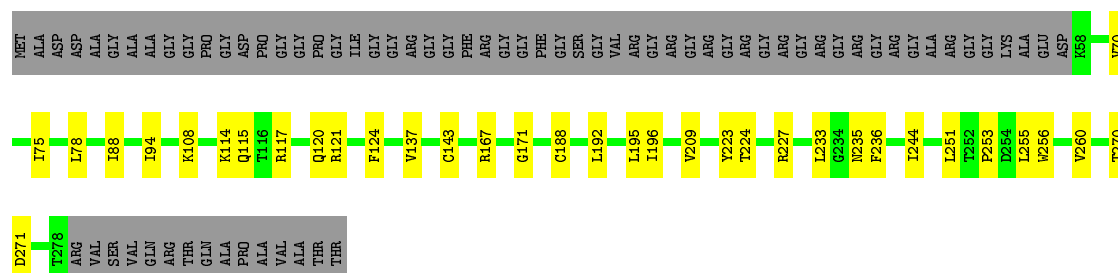
- Molecule 53: 40S ribosomal protein S3a

Chain BB: 67% 13% 19%

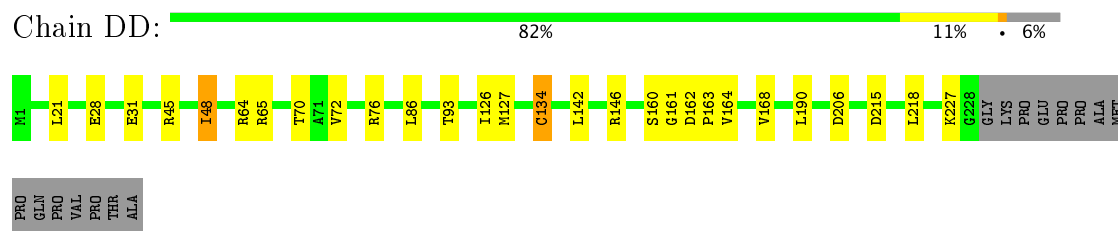


- Molecule 54: uS5

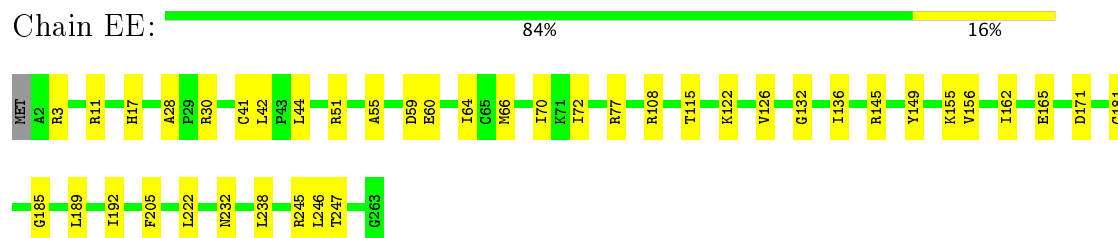
Chain CC: 63% 12% 25%



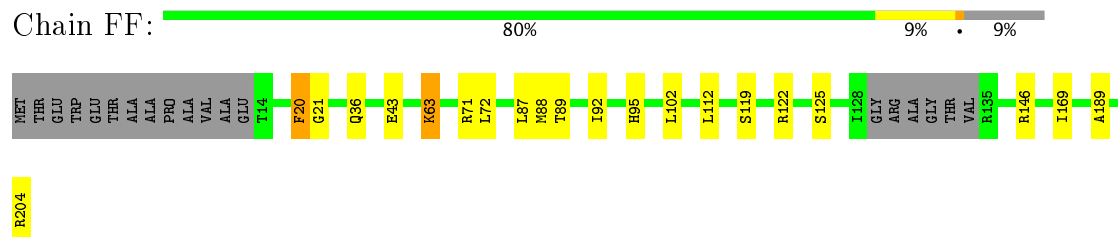
- Molecule 55: Uncharacterized protein



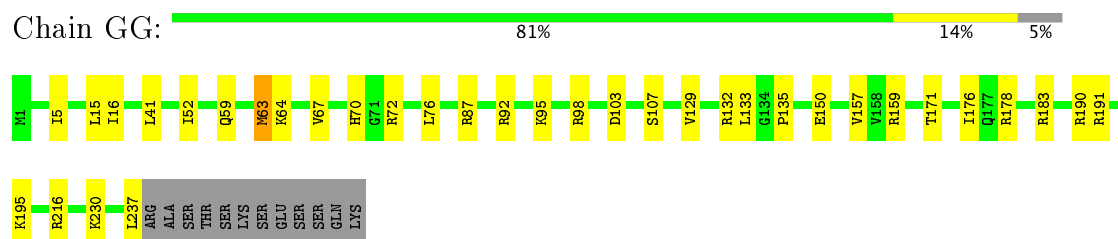
- Molecule 56: eS4



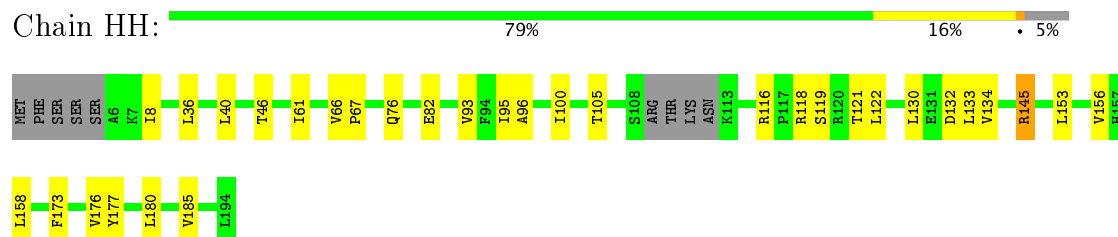
- Molecule 57: uS7



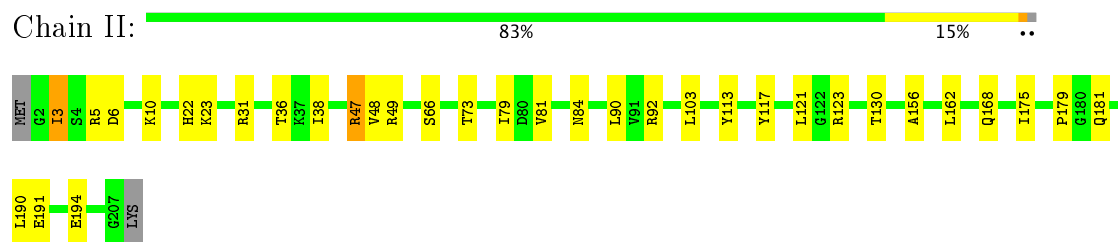
- Molecule 58: 40S ribosomal protein S6



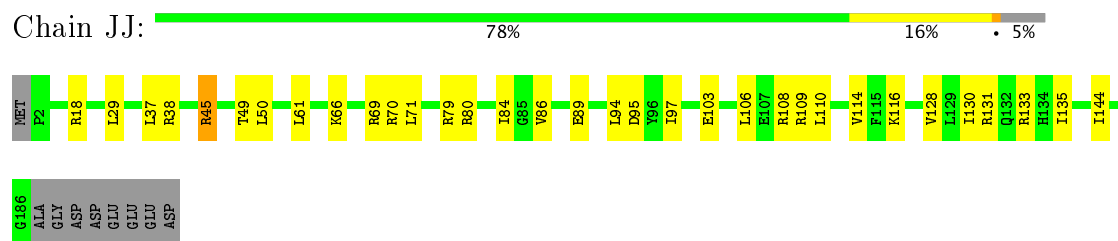
- Molecule 59: eS7



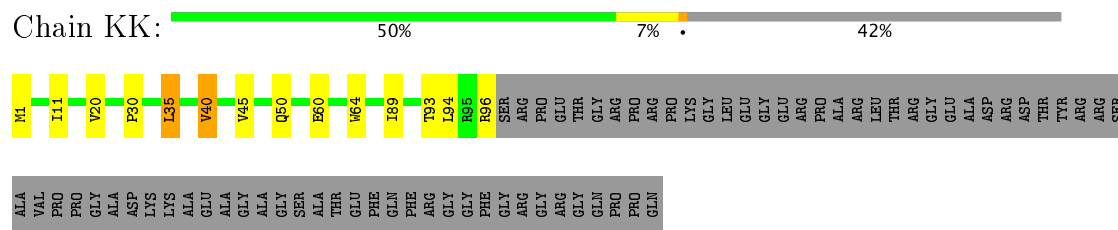
- Molecule 60: 40S ribosomal protein S8



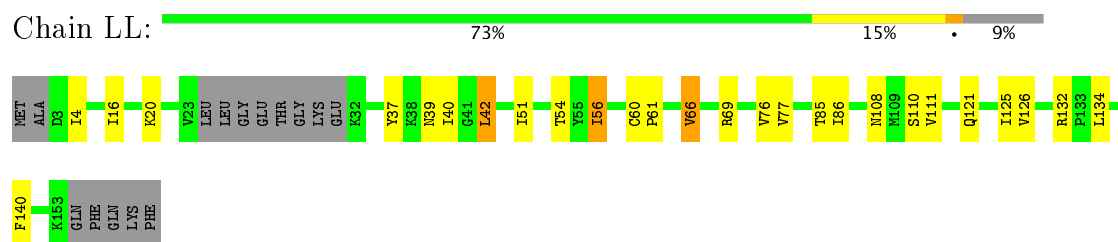
- Molecule 61: Ribosomal protein S9 (Predicted)



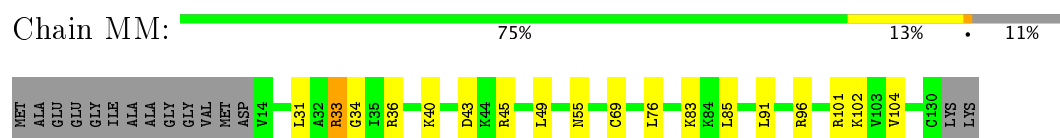
- Molecule 62: Uncharacterized protein



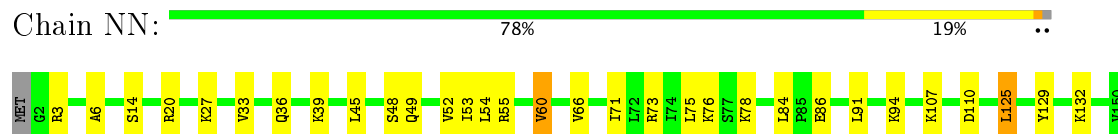
- Molecule 63: Uncharacterized protein



- Molecule 64: 40S ribosomal protein S12



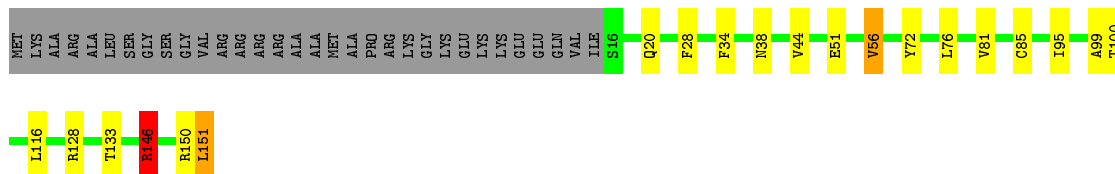
- Molecule 65: uS15



ALA

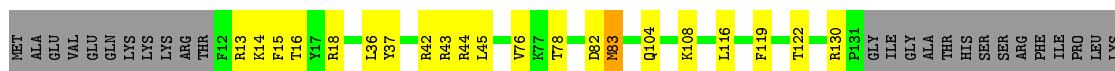
- Molecule 66: uS11

Chain OO:  69% 10% .. 19%




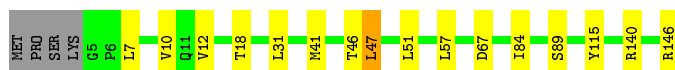
- Molecule 67: uS19

Chain PP:  68% 14% . 17%




- Molecule 68: uS9

Chain QQ:  86% 10% ..



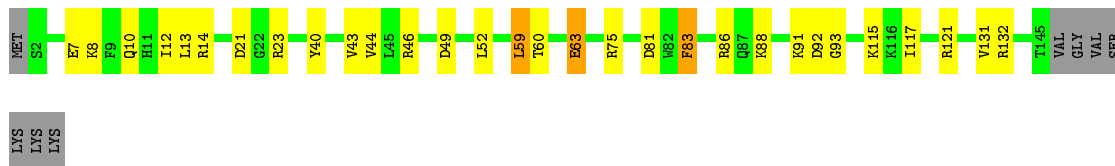
- Molecule 69: eS17

Chain RR:  83% 13% ..



- Molecule 70: uS13

Chain SS:  75% 18% . 5%



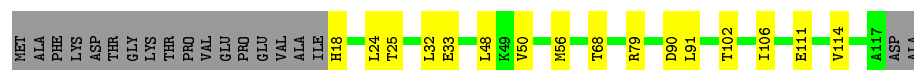
- Molecule 71: eS19

Chain TT:  88% 8% ..



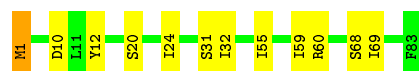
- Molecule 72: uS10

Chain UU:  71% 13% 16%




- Molecule 73: eS21

Chain VV: 86% 13%



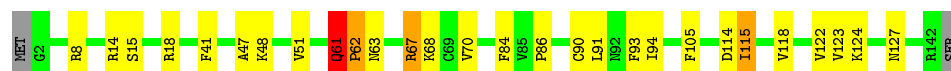
- Molecule 74: uS8

Chain WW:  76% 22% .




- Molecule 75: uS12

Chain XX: 79% 17% ...



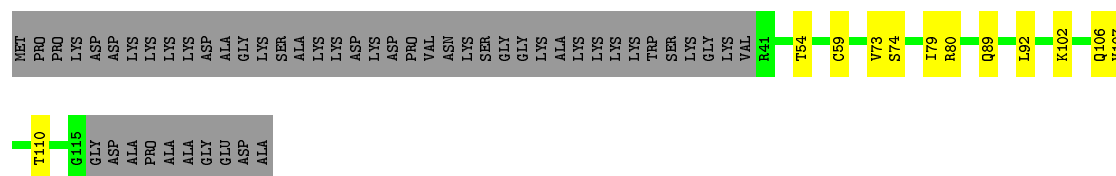
- Molecule 76: 40S ribosomal protein S24

Chain YY:  81% 15% 5%



- Molecule 77: eS25

Chain ZZ: 

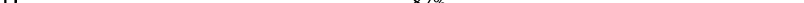


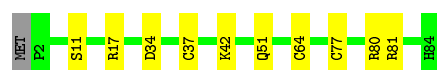
- Molecule 78: eS26

Chain aa:

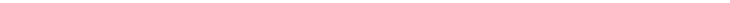


- Molecule 79: 40S ribosomal protein S27

Chain bb:  87% 12%



- Molecule 80: eS28

Chain cc:  77% 10% • 10%



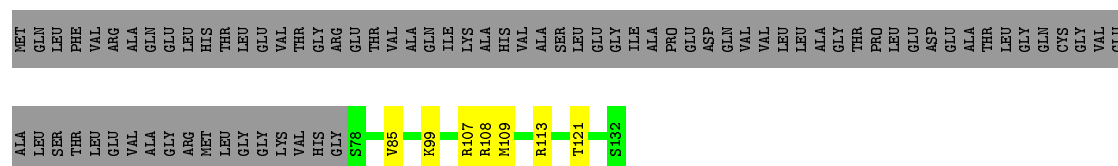
- Molecule 81: uS14

Chain dd: 91% 7%



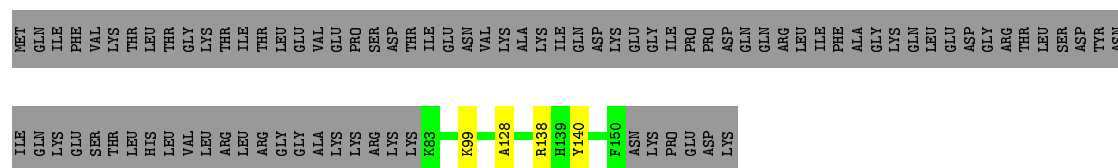
- Molecule 82: eS30

Chain ee: 36% 5% 59%



- Molecule 83: eS31

Chain ff:  41% 0% 56%



- Molecule 84: RACK1

Chain gg:  93% 6%



- Molecule 85: mRNA

Chain hh:  50% 50%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	58773	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	104478	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0/2596
10	J	0.40	0/1385	0.70	0/1852
11	L	0.41	0/1733	0.74	0/2316
12	M	0.44	0/1158	0.72	0/1547
13	N	0.43	0/1746	0.78	0/2338
14	O	0.44	0/1662	0.73	0/2222
15	P	0.49	0/1268	0.73	0/1700
16	Q	0.44	0/1539	0.82	0/2054
17	R	0.41	0/1524	0.74	1/2013 (0.0%)
18	S	0.54	0/1501	0.79	1/2012 (0.0%)
19	T	0.42	0/1326	0.70	0/1770
2	B	0.48	0/3240	0.75	1/4339 (0.0%)
20	U	0.39	0/823	0.64	0/1104
21	V	0.45	0/993	0.72	0/1332
22	W	0.45	0/873	0.62	0/1158
23	X	0.37	0/984	0.66	0/1323
24	Y	0.42	0/1132	0.72	0/1504
25	Z	0.44	0/1130	0.70	0/1507
26	a	0.44	0/1191	0.72	0/1590
27	b	0.37	0/861	0.63	0/1138
28	c	0.40	0/771	0.60	0/1034
29	d	0.44	0/903	0.75	0/1216
3	C	0.46	0/2937	0.77	2/3946 (0.1%)
30	e	0.45	0/1071	0.74	0/1429
31	f	0.48	0/895	0.78	0/1198
32	g	0.42	0/916	0.74	0/1220
33	h	0.36	0/1021	0.66	0/1348
34	i	0.43	0/841	0.69	0/1112
35	j	0.45	0/720	0.77	0/952
36	k	0.35	0/575	0.60	0/761
37	l	0.43	0/459	0.70	0/608
38	m	0.47	0/435	0.72	0/575

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
39	n	0.39	0/240	0.77	0/305
4	D	0.39	0/2437	0.69	2/3264 (0.1%)
40	o	0.44	0/864	0.70	0/1140
41	p	0.47	0/718	0.70	0/953
42	r	0.47	0/1010	0.76	0/1354
43	s	0.37	0/1530	0.49	0/2064
44	t	0.36	0/1174	0.52	0/1582
45	1	0.48	0/49	0.59	0/65
46	2	0.26	0/1805	0.66	0/2809
47	3	0.23	0/1777	0.66	0/2763
48	5	0.41	15/84961 (0.0%)	0.78	53/132460 (0.0%)
49	7	0.37	0/2858	0.67	0/4455
5	E	0.38	0/1762	0.69	0/2362
50	8	0.38	0/3581	0.70	0/5577
51	9	0.37	3/40523 (0.0%)	0.73	14/63130 (0.0%)
52	AA	0.40	0/1747	0.67	0/2374
53	BB	0.38	0/1756	0.64	0/2350
54	CC	0.40	0/1753	0.70	0/2369
55	DD	0.37	0/1796	0.65	0/2417
56	EE	0.37	0/2118	0.69	0/2849
57	FF	0.35	0/1492	0.66	0/2005
58	GG	0.37	0/1946	0.69	0/2590
59	HH	0.36	0/1510	0.61	0/2022
6	F	0.54	0/1911	0.79	0/2549
60	II	0.40	0/1715	0.72	0/2287
61	JJ	0.40	0/1550	0.76	0/2069
62	KK	0.39	0/834	0.61	0/1125
63	LL	0.41	0/1195	0.73	0/1597
64	MM	0.37	0/918	0.62	0/1233
65	NN	0.40	0/1226	0.74	0/1649
66	OO	0.42	0/1029	0.83	1/1380 (0.1%)
67	PP	0.40	0/1017	0.71	0/1358
68	QQ	0.36	0/1146	0.66	0/1534
69	RR	0.37	0/1082	0.65	0/1452
7	G	0.40	0/1910	0.68	0/2569
70	SS	0.37	0/1208	0.70	0/1618
71	TT	0.37	0/1115	0.66	0/1493
72	UU	0.37	0/805	0.68	0/1081
73	VV	0.41	0/643	0.73	0/860
74	WW	0.45	0/1051	0.79	2/1406 (0.1%)
75	XX	0.43	0/1116	0.75	1/1490 (0.1%)
76	YY	0.37	0/1028	0.67	0/1366
77	ZZ	0.36	0/604	0.66	0/810

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
78	aa	0.42	0/828	0.80	0/1109
79	bb	0.37	0/665	0.65	0/891
8	H	0.42	0/1535	0.69	0/2063
80	cc	0.37	0/490	0.73	0/656
81	dd	0.43	0/470	0.72	0/623
82	ee	0.38	0/447	0.70	0/587
83	ff	0.37	0/567	0.53	0/753
84	gg	0.34	0/2493	0.59	0/3394
85	hh	0.28	0/188	0.79	0/290
86	ii	0.34	0/2996	0.58	0/4050
87	jj	0.34	0/3352	0.57	0/4523
9	I	0.43	0/1702	0.69	0/2272
All	All	0.40	18/237792 (0.0%)	0.73	78/348210 (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
11	L	0	1
13	N	0	1
2	B	0	2
3	C	0	1
31	f	0	1
48	5	0	2
56	EE	0	1
74	WW	0	1
75	XX	0	1
78	aa	0	1
80	cc	0	1
All	All	0	13

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	5	935	A	C5-C6	-15.99	1.26	1.41
48	5	935	A	C6-N1	-12.18	1.27	1.35
48	5	935	A	C2-N3	10.23	1.42	1.33
48	5	481	G	N1-C2	-9.91	1.29	1.37
48	5	922(A)	G	O3'-P	9.08	1.72	1.61

The worst 5 of 78 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	481	G	N1-C2-N2	-52.63	68.83	116.20
48	5	935	A	C5-C6-N6	-48.73	84.72	123.70
48	5	935	A	N1-C6-N6	-35.80	97.12	118.60
48	5	935	A	C6-N1-C2	-31.95	99.43	118.60
48	5	481	G	N3-C2-N2	-29.88	98.98	119.90

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	16	PHE	Peptide
2	B	257	TRP	Peptide
3	C	90	GLY	Peptide
11	L	71	ARG	Peptide
13	N	184	ILE	Peptide

5.2 Too-close contacts [i](#)

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	29	0
3	C	2883	0	3053	34	0
4	D	2391	0	2424	16	0
5	E	1729	0	1887	8	0
6	F	1875	0	1995	16	0
7	G	1879	0	2027	14	0
8	H	1516	0	1597	19	0
9	I	1664	0	1712	9	0
10	J	1362	0	1399	10	0
11	L	1702	0	1820	4	0
12	M	1137	0	1211	13	0
13	N	1701	0	1749	16	0
14	O	1630	0	1778	23	0
15	P	1242	0	1274	8	0
16	Q	1515	0	1634	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	R	1508	0	1664	10	0
18	S	1462	0	1508	19	0
19	T	1298	0	1366	11	0
20	U	809	0	833	7	0
21	V	979	0	1039	7	0
22	W	860	0	903	9	0
23	X	967	0	1040	2	0
24	Y	1115	0	1205	5	0
25	Z	1107	0	1182	9	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	1002	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	756	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	2	0
47	3	1593	0	811	3	0
48	5	75972	0	38398	321	0
49	7	2558	0	1296	7	0
50	8	3208	0	1629	14	0
51	9	36249	0	18317	196	0
52	AA	1710	0	1708	18	0
53	BB	1729	0	1803	14	0
54	CC	1716	0	1806	11	0
55	DD	1768	0	1866	9	0
56	EE	2076	0	2177	13	0
57	FF	1471	0	1522	7	0
58	GG	1923	0	2089	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	HH	1488	0	1582	15	0
60	II	1686	0	1772	14	0
61	JJ	1525	0	1640	10	0
62	KK	810	0	836	7	0
63	LL	1175	0	1249	8	0
64	MM	908	0	939	16	0
65	NN	1202	0	1289	11	0
66	OO	1016	0	1039	11	0
67	PP	997	0	1045	19	0
68	QQ	1128	0	1195	8	0
69	RR	1068	0	1121	7	0
70	SS	1190	0	1249	22	0
71	TT	1097	0	1132	3	0
72	UU	795	0	862	4	0
73	VV	636	0	637	5	0
74	WW	1034	0	1080	13	0
75	XX	1098	0	1167	13	0
76	YY	1011	0	1083	3	0
77	ZZ	598	0	656	3	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	449	0	0
82	ee	443	0	492	0	0
83	ff	555	0	565	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	178	0	0	0	0
88	7	5	0	0	0	0
88	8	5	0	0	0	0
88	9	66	0	0	0	0
88	B	1	0	0	0	0
88	I	1	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	e	1	0	0	0	0
88	g	1	0	0	0	0
88	j	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
All	All	222005	0	166945	992	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 3.

The worst 5 of 992 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)
48:5:3914:U:O4	48:5:4378:A:N1	1.58	1.35
48:5:922:C:C5'	48:5:922(A):G:H3'	1.59	1.31
48:5:922:C:H5''	48:5:922(B):C:O5'	1.38	1.23
51:9:1283:C:N4	64:MM:102:LYS:HE3	1.52	1.21
48:5:1411:C:H4'	48:5:1411(C):C:O4'	1.41	1.16

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%)	220 (89%)	24 (10%)	2 (1%)	22	65
2	B	392/403 (97%)	355 (91%)	35 (9%)	2 (0%)	32	73

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	360/425 (85%)	332 (92%)	23 (6%)	5 (1%)	13	52
4	D	291/297 (98%)	278 (96%)	10 (3%)	3 (1%)	18	60
5	E	208/291 (72%)	189 (91%)	19 (9%)	0	100	100
6	F	223/247 (90%)	204 (92%)	16 (7%)	3 (1%)	14	54
7	G	229/319 (72%)	216 (94%)	11 (5%)	2 (1%)	20	63
8	H	188/192 (98%)	172 (92%)	16 (8%)	0	100	100
9	I	201/214 (94%)	177 (88%)	23 (11%)	1 (0%)	32	73
10	J	168/178 (94%)	157 (94%)	9 (5%)	2 (1%)	15	56
11	L	208/211 (99%)	193 (93%)	14 (7%)	1 (0%)	32	73
12	M	136/218 (62%)	125 (92%)	11 (8%)	0	100	100
13	N	201/204 (98%)	181 (90%)	19 (10%)	1 (0%)	32	73
14	O	197/203 (97%)	183 (93%)	13 (7%)	1 (0%)	32	73
15	P	151/184 (82%)	140 (93%)	9 (6%)	2 (1%)	14	54
16	Q	185/188 (98%)	168 (91%)	16 (9%)	1 (0%)	32	73
17	R	178/196 (91%)	171 (96%)	6 (3%)	1 (1%)	28	70
18	S	174/176 (99%)	159 (91%)	12 (7%)	3 (2%)	11	48
19	T	157/160 (98%)	142 (90%)	15 (10%)	0	100	100
20	U	97/128 (76%)	86 (89%)	9 (9%)	2 (2%)	8	44
21	V	129/140 (92%)	113 (88%)	16 (12%)	0	100	100
22	W	102/157 (65%)	93 (91%)	8 (8%)	1 (1%)	18	60
23	X	116/156 (74%)	109 (94%)	6 (5%)	1 (1%)	20	63
24	Y	132/145 (91%)	126 (96%)	5 (4%)	1 (1%)	22	65
25	Z	133/136 (98%)	123 (92%)	8 (6%)	2 (2%)	12	51
26	a	145/148 (98%)	135 (93%)	10 (7%)	0	100	100
27	b	100/245 (41%)	93 (93%)	6 (6%)	1 (1%)	18	60
28	c	96/115 (84%)	89 (93%)	7 (7%)	0	100	100
29	d	105/125 (84%)	94 (90%)	10 (10%)	1 (1%)	18	60
30	e	126/135 (93%)	121 (96%)	5 (4%)	0	100	100
31	f	107/110 (97%)	97 (91%)	8 (8%)	2 (2%)	9	45
32	g	112/117 (96%)	103 (92%)	8 (7%)	1 (1%)	20	63
33	h	120/123 (98%)	116 (97%)	3 (2%)	1 (1%)	22	65

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	i	100/105 (95%)	92 (92%)	8 (8%)	0	100	100
35	j	84/97 (87%)	74 (88%)	9 (11%)	1 (1%)	15	56
36	k	67/70 (96%)	63 (94%)	3 (4%)	1 (2%)	12	51
37	l	48/51 (94%)	41 (85%)	7 (15%)	0	100	100
38	m	50/102 (49%)	46 (92%)	4 (8%)	0	100	100
39	n	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
40	o	102/106 (96%)	92 (90%)	9 (9%)	1 (1%)	18	60
41	p	89/92 (97%)	81 (91%)	7 (8%)	1 (1%)	17	58
42	r	122/137 (89%)	104 (85%)	14 (12%)	4 (3%)	4	34
43	s	194/318 (61%)	174 (90%)	18 (9%)	2 (1%)	18	60
44	t	151/165 (92%)	134 (89%)	15 (10%)	2 (1%)	14	54
45	1	5/7 (71%)	2 (40%)	3 (60%)	0	100	100
52	AA	215/295 (73%)	195 (91%)	19 (9%)	1 (0%)	32	73
53	BB	211/264 (80%)	199 (94%)	12 (6%)	0	100	100
54	CC	219/293 (75%)	202 (92%)	16 (7%)	1 (0%)	32	73
55	DD	226/243 (93%)	206 (91%)	18 (8%)	2 (1%)	20	63
56	EE	260/263 (99%)	242 (93%)	18 (7%)	0	100	100
57	FF	181/204 (89%)	168 (93%)	10 (6%)	3 (2%)	11	48
58	GG	235/249 (94%)	217 (92%)	17 (7%)	1 (0%)	38	77
59	HH	181/194 (93%)	168 (93%)	13 (7%)	0	100	100
60	II	204/208 (98%)	191 (94%)	11 (5%)	2 (1%)	18	60
61	JJ	183/194 (94%)	175 (96%)	8 (4%)	0	100	100
62	KK	94/165 (57%)	85 (90%)	6 (6%)	3 (3%)	5	34
63	LL	139/158 (88%)	124 (89%)	14 (10%)	1 (1%)	25	67
64	MM	115/132 (87%)	99 (86%)	16 (14%)	0	100	100
65	NN	147/151 (97%)	134 (91%)	13 (9%)	0	100	100
66	OO	134/168 (80%)	120 (90%)	13 (10%)	1 (1%)	25	67
67	PP	118/145 (81%)	103 (87%)	14 (12%)	1 (1%)	22	65
68	QQ	140/146 (96%)	132 (94%)	8 (6%)	0	100	100
69	RR	130/135 (96%)	115 (88%)	14 (11%)	1 (1%)	22	65
70	SS	142/152 (93%)	134 (94%)	8 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
71	TT	139/145 (96%)	131 (94%)	7 (5%)	1 (1%)	25	67
72	UU	98/119 (82%)	92 (94%)	6 (6%)	0	100	100
73	VV	81/83 (98%)	76 (94%)	5 (6%)	0	100	100
74	WW	127/130 (98%)	116 (91%)	9 (7%)	2 (2%)	11	49
75	XX	139/143 (97%)	124 (89%)	12 (9%)	3 (2%)	8	43
76	YY	122/130 (94%)	116 (95%)	6 (5%)	0	100	100
77	ZZ	73/125 (58%)	71 (97%)	2 (3%)	0	100	100
78	aa	99/115 (86%)	88 (89%)	9 (9%)	2 (2%)	9	45
79	bb	81/84 (96%)	73 (90%)	7 (9%)	1 (1%)	15	56
80	cc	60/69 (87%)	55 (92%)	3 (5%)	2 (3%)	4	34
81	dd	53/56 (95%)	48 (91%)	5 (9%)	0	100	100
82	ee	53/133 (40%)	50 (94%)	3 (6%)	0	100	100
83	ff	66/156 (42%)	60 (91%)	5 (8%)	1 (2%)	12	51
84	gg	311/317 (98%)	284 (91%)	24 (8%)	3 (1%)	18	60
86	ii	370/403 (92%)	343 (93%)	26 (7%)	1 (0%)	44	81
87	jj	423/710 (60%)	381 (90%)	38 (9%)	4 (1%)	20	63
All	All	12317/14495 (85%)	11302 (92%)	923 (8%)	92 (1%)	30	67

5 of 92 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	236	GLU
18	S	155	PRO
31	f	107	PRO
75	XX	62	PRO
87	jj	605	GLN

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%)	176 (93%)	14 (7%)	16	51
2	B	342/348 (98%)	312 (91%)	30 (9%)	12	43
3	C	302/347 (87%)	278 (92%)	24 (8%)	14	48
4	D	247/250 (99%)	236 (96%)	11 (4%)	32	68
5	E	190/251 (76%)	179 (94%)	11 (6%)	23	60
6	F	196/215 (91%)	177 (90%)	19 (10%)	9	37
7	G	200/272 (74%)	186 (93%)	14 (7%)	18	54
8	H	169/171 (99%)	155 (92%)	14 (8%)	13	45
9	I	175/181 (97%)	161 (92%)	14 (8%)	14	48
10	J	143/149 (96%)	134 (94%)	9 (6%)	21	58
11	L	175/176 (99%)	165 (94%)	10 (6%)	24	61
12	M	117/161 (73%)	109 (93%)	8 (7%)	18	55
13	N	171/172 (99%)	161 (94%)	10 (6%)	23	60
14	O	171/173 (99%)	156 (91%)	15 (9%)	12	43
15	P	134/163 (82%)	124 (92%)	10 (8%)	16	51
16	Q	164/165 (99%)	149 (91%)	15 (9%)	11	41
17	R	159/175 (91%)	143 (90%)	16 (10%)	9	36
18	S	157/157 (100%)	145 (92%)	12 (8%)	15	50
19	T	139/140 (99%)	126 (91%)	13 (9%)	10	39
20	U	89/114 (78%)	87 (98%)	2 (2%)	57	83
21	V	101/107 (94%)	90 (89%)	11 (11%)	7	32
22	W	86/126 (68%)	85 (99%)	1 (1%)	75	90
23	X	106/134 (79%)	101 (95%)	5 (5%)	30	67
24	Y	124/135 (92%)	116 (94%)	8 (6%)	20	57
25	Z	117/118 (99%)	112 (96%)	5 (4%)	33	69
26	a	119/120 (99%)	115 (97%)	4 (3%)	42	75
27	b	84/184 (46%)	80 (95%)	4 (5%)	30	66
28	c	84/98 (86%)	77 (92%)	7 (8%)	13	45
29	d	98/110 (89%)	85 (87%)	13 (13%)	4	24
30	e	114/121 (94%)	106 (93%)	8 (7%)	18	54
31	f	88/89 (99%)	81 (92%)	7 (8%)	14	48
32	g	98/100 (98%)	92 (94%)	6 (6%)	22	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	h	109/110 (99%)	104 (95%)	5 (5%)	31	67
34	i	86/89 (97%)	82 (95%)	4 (5%)	30	67
35	j	73/80 (91%)	68 (93%)	5 (7%)	18	55
36	k	64/65 (98%)	61 (95%)	3 (5%)	30	67
37	l	47/48 (98%)	45 (96%)	2 (4%)	33	69
38	m	48/90 (53%)	44 (92%)	4 (8%)	13	45
39	n	24/24 (100%)	22 (92%)	2 (8%)	13	45
40	o	92/94 (98%)	89 (97%)	3 (3%)	43	75
41	p	74/75 (99%)	69 (93%)	5 (7%)	18	55
42	r	108/121 (89%)	97 (90%)	11 (10%)	8	35
43	s	164/258 (64%)	158 (96%)	6 (4%)	39	73
44	t	126/137 (92%)	122 (97%)	4 (3%)	44	76
45	l	6/6 (100%)	6 (100%)	0	100	100
52	AA	180/245 (74%)	161 (89%)	19 (11%)	8	33
53	BB	194/231 (84%)	176 (91%)	18 (9%)	10	40
54	CC	187/225 (83%)	170 (91%)	17 (9%)	11	41
55	DD	190/202 (94%)	173 (91%)	17 (9%)	11	42
56	EE	224/225 (100%)	204 (91%)	20 (9%)	11	42
57	FF	158/170 (93%)	147 (93%)	11 (7%)	18	54
58	GG	207/218 (95%)	185 (89%)	22 (11%)	8	33
59	HH	165/174 (95%)	152 (92%)	13 (8%)	14	48
60	II	178/180 (99%)	167 (94%)	11 (6%)	21	59
61	JJ	161/168 (96%)	142 (88%)	19 (12%)	6	28
62	KK	87/136 (64%)	81 (93%)	6 (7%)	18	55
63	LL	130/142 (92%)	114 (88%)	16 (12%)	5	26
64	MM	99/108 (92%)	86 (87%)	13 (13%)	5	24
65	NN	130/131 (99%)	114 (88%)	16 (12%)	5	26
66	OO	106/130 (82%)	97 (92%)	9 (8%)	12	44
67	PP	109/130 (84%)	97 (89%)	12 (11%)	7	32
68	QQ	117/121 (97%)	110 (94%)	7 (6%)	22	59
69	RR	119/121 (98%)	109 (92%)	10 (8%)	13	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
70	SS	125/132 (95%)	107 (86%)	18 (14%)	4	20
71	TT	111/115 (96%)	102 (92%)	9 (8%)	14	47
72	UU	92/107 (86%)	83 (90%)	9 (10%)	9	37
73	VV	67/67 (100%)	63 (94%)	4 (6%)	22	59
74	WW	112/113 (99%)	103 (92%)	9 (8%)	14	48
75	XX	113/115 (98%)	105 (93%)	8 (7%)	17	54
76	YY	107/112 (96%)	92 (86%)	15 (14%)	4	21
77	ZZ	66/103 (64%)	59 (89%)	7 (11%)	8	33
78	aa	88/98 (90%)	75 (85%)	13 (15%)	3	19
79	bb	75/76 (99%)	66 (88%)	9 (12%)	6	27
80	cc	55/62 (89%)	47 (86%)	8 (14%)	4	20
81	dd	48/49 (98%)	44 (92%)	4 (8%)	13	45
82	ee	46/106 (43%)	39 (85%)	7 (15%)	3	18
83	ff	61/140 (44%)	58 (95%)	3 (5%)	29	65
84	gg	272/275 (99%)	257 (94%)	15 (6%)	25	62
86	ii	326/353 (92%)	310 (95%)	16 (5%)	29	65
87	jj	358/608 (59%)	331 (92%)	27 (8%)	16	51
All	All	10733/12306 (87%)	9892 (92%)	841 (8%)	19	48

5 of 841 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
41	p	47	MET
55	DD	190	LEU
82	ee	109	MET
42	r	67	ARG
53	BB	82	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 60 such sidechains are listed below:

Mol	Chain	Res	Type
43	s	34	ASN
56	EE	98	ASN
86	ii	109	GLN
54	CC	235	ASN

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Mol	Chain	Res	Type
57	FF	118	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
46	2	74/76 (97%)	15 (20%)	0
47	3	72/75 (96%)	21 (29%)	1 (1%)
48	5	3506/3543 (98%)	881 (25%)	182 (5%)
49	7	119/120 (99%)	13 (10%)	1 (0%)
50	8	149/156 (95%)	38 (25%)	6 (4%)
51	9	1680/1869 (89%)	435 (25%)	85 (5%)
85	hh	7/8 (87%)	4 (57%)	0
All	All	5607/5847 (95%)	1407 (25%)	275 (4%)

5 of 1407 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
46	2	9	A
46	2	13	U
46	2	14	A
46	2	16	C
46	2	19	G

5 of 275 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
48	5	2754	G
48	5	4221	C
51	9	1438	A
48	5	2874	U
48	5	3809	G

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	25,34,34	2.60	7 (28%)	28,54,54	0.93	1 (3%)

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 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
90	jj	700	GCP	C4-N9	-10.51	1.33	1.47
90	jj	700	GCP	C8-N9	-3.89	1.35	1.46
90	jj	700	GCP	C5-C6	-2.26	1.48	1.53
90	jj	700	GCP	PB-O2B	2.28	1.61	1.56
90	jj	700	GCP	PB-O3A	2.54	1.61	1.58

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
90	jj	700	GCP	PA-O3A-PB	-2.64	123.88	132.39

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	42
51	9	8
47	3	2
46	2	1

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	40.91
1	5	1252:C	O3'	1271:G	P	36.05
1	5	1405:C	O3'	1406:G	P	23.79
1	5	1219:G	O3'	1233:G	P	22.30
1	5	1406:G	O3'	1406(A):G	P	20.51