



wwPDB EM Map/Model Validation Report ⓘ

May 11, 2016 – 11:51 AM EDT

PDB ID : 5IT7
EMDB ID: : EMD-8123
Title : Structure of the Kluyveromyces lactis 80S ribosome in complex with the cricket paralysis virus IRES and eEF2
Authors : Murray, J.; Savva, C.G.; Shin, B.S.; Dever, T.E.; Ramakrishnan, V.; Fernandez, I.S.
Deposited on : 2016-03-16
Resolution : 3.60 Å(reported)
Based on PDB ID : ?

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

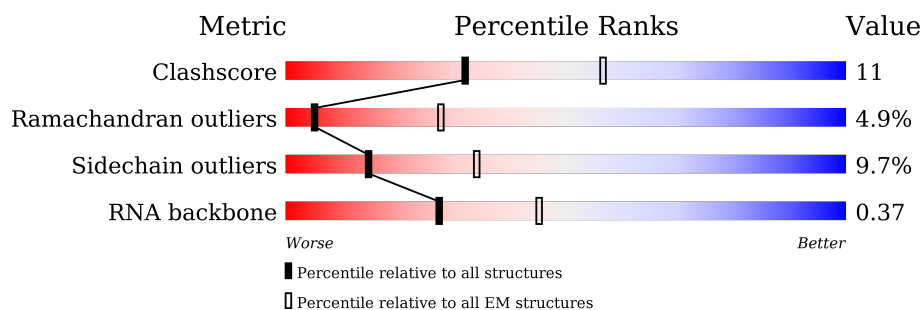
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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.
















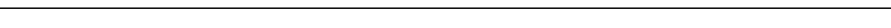

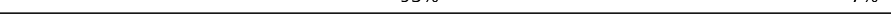

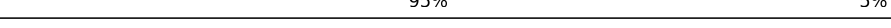




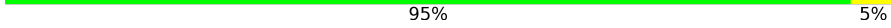
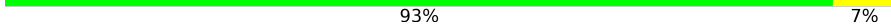

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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	5	3270	46% 41% 11% .
2	7	121	63% 34% .
3	8	157	50% 43% 5% .
4	AA	249	69% 24% 6%
5	BB	384	65% 28% 7%
6	CC	360	68% 24% 8%
7	DD	295	76% 22% .
8	EE	170	76% 12% 6% . 5%



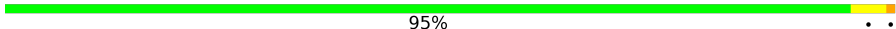










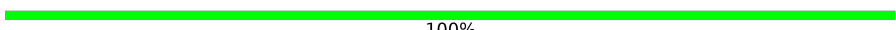











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Mol	Chain	Length	Quality of chain
9	FF	222	 74% 19% 6%
10	GG	233	 80% 17% .
11	HH	191	 79% 19% .
12	II	216	 75% 19% . .
13	JJ	168	 81% 15% .
14	LL	197	 79% 17% .
15	MM	136	 79% 18% .
16	NN	202	 77% 19% .
17	OO	198	 10% 51% 35% .
18	PP	180	 73% 22% .
19	QQ	184	 78% 18% .
20	RR	188	 84% 14% .
21	SS	169	 80% 19% .
22	TT	158	 72% 24% .
23	UU	100	 93% 7%
24	VV	132	 70% 23% 7%
25	WW	62	 95% 5%
26	XX	121	 82% 16% .
27	YY	125	 82% 15% . .
28	ZZ	134	 72% 24% .
29	aa	147	 85% 15%
30	bb	57	 95% 5%
31	cc	97	 93% 7%
32	dd	106	 89% 11%
33	ee	122	 94% 6%


















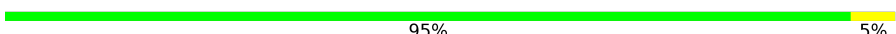
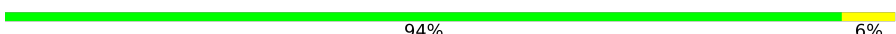






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Mol	Chain	Length	Quality of chain
34	ff	105	 92% 8%
35	gg	121	 91% 8% .
36	hh	116	 95% . .
37	ii	98	 86% 14%
38	jj	85	 87% 13%
39	kk	76	 91% 8% .
40	ll	49	 88% 12%
41	mm	51	 90% 10%
42	nn	25	 84% 16%
43	oo	101	 87% 12% .
44	pp	87	 77% 18% 5%
45	qq	217	 83% 14% .
46	rr	195	 85% 14% .
47	KK	147	 100%
48	A	206	 76% 19% . .
49	B	214	 81% 16% .
50	C	217	 76% 19% 5% .
51	D	223	 85% 12% .
52	E	260	 84% 13% .
53	F	206	 85% 14% .
54	G	226	 83% 15% .
55	H	184	 82% 17% .
56	I	200	 75% 19% . 6%
57	J	182	 74% 21% 5%
58	K	96	 83% 15% .

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Mol	Chain	Length	Quality of chain
59	L	155	 74%21%5%
60	M	122	 92%7%.
61	N	150	 84%14%.
62	O	127	 80%19%.
63	P	123	 80%14%7%
64	Q	141	 81%18%.
65	R	129	 80%18%.
66	S	145	 82%17%..
67	T	143	 87%13%.
68	U	106	 89%11%
69	V	87	 76%22%.
70	W	129	 69%24%7%
71	X	145	 71%21%7%.
72	Y	134	 82%16%.
73	Z	70	 90%9%.
74	a	100	 72%23%..
75	b	82	 91%7%.
76	c	63	 95%5%
77	d	53	 94%6%
78	e	55	 89%11%
79	f	69	 78%17%.
80	g	324	 90%7%..
81	2	1798	 34%51%13%..
82	4	190	 39%41%18%.
83	1	827	 67%24%7%.

2 Entry composition

There are 87 unique types of molecules in this entry. The entry contains 215768 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 DNA/RNA hybrid called 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	5	3270	Total	C	N	O	P	0	0
			69896	31222	12579	22825	3270		

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	7	121	Total	C	N	O	P	0	0
			2579	1152	461	845	121		

- Molecule 3 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	8	157	Total	C	N	O	P	0	0
			3326	1488	573	1108	157		

- Molecule 4 is a protein called KLLA0D16027p.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AA	249	Total	C	N	O	S	0	0
			1892	1176	385	330	1		

- Molecule 5 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	BB	384	Total	C	N	O	S	0	0
			3064	1946	580	533	5		

- Molecule 6 is a protein called KLLA0B07139p.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	CC	359	Total	C	N	O	S	0	0
			2731	1715	522	491	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CC	3	ARG	ILE	conflict	UNP Q6CW41

- Molecule 7 is a protein called KLLA0D06941p.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	DD	295	Total	C	N	O	S	0	0
			2384	1510	417	456	1		

- Molecule 8 is a protein called KLLA0B04686p.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	EE	161	Total	C	N	O	S	0	0
			1300	834	243	223			

- Molecule 9 is a protein called KLLA0D03410p.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	FF	222	Total	C	N	O	S	0	0
			1774	1138	319	316	1		

- Molecule 10 is a protein called KLLA0E00573p.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	GG	233	Total	C	N	O	S	0	0
			1817	1160	324	330	3		

- Molecule 11 is a protein called KLLA0F04499p.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	HH	191	Total	C	N	O	S	0	0
			1528	965	277	284	2		

- Molecule 12 is a protein called KLLA0D05643p.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	II	207	Total	C	N	O	S	0	0
			1690	1074	319	292	5		

- Molecule 13 is a protein called KLLA0F08261p.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	JJ	168	Total	C	N	O	S	0	0
			1349	845	255	245	4		

- Molecule 14 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LL	197	Total	C	N	O		0	0
			1581	988	317	276			

- Molecule 15 is a protein called KLLA0B13409p.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	MM	136	Total	C	N	O		0	0
			1045	666	196	183			

- Molecule 16 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	NN	202	Total	C	N	O	S	0	0
			1709	1069	359	280	1		

- Molecule 17 is a protein called KLLA0F04675p.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	OO	198	Total	C	N	O	S	196	0
			1571	1013	290	267	1		

- Molecule 18 is a protein called KLLA0A06336p.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	PP	180	Total	C	N	O		0	0
			1432	885	287	260			

- Molecule 19 is a protein called KLLA0A07227p.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	QQ	184	Total	C	N	O		0	0
			1444	911	290	243			

- Molecule 20 is a protein called KLLA0E12453p.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	RR	188	Total	C	N	O	S	0	0
			1522	933	328	259	2		

- Molecule 21 is a protein called 60S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	SS	169	Total	C	N	O	S	0	0
			1416	916	259	238	3		

- Molecule 22 is a protein called KLLA0E23651p.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	TT	158	Total	C	N	O	S	0	0
			1262	797	240	220	5		

- Molecule 23 is a protein called KLLA0D05181p.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	UU	100	Total	C	N	O	0	0
			807	524	131	152		

- Molecule 24 is a protein called KLLA0E06997p.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	VV	132	Total	C	N	O	S	0	0
			976	612	182	174	8		

- Molecule 25 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	WW	62	Total	C	N	O	0	0
			515	330	103	82		

- Molecule 26 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	XX	121	Total	C	N	O	S	0	0
			964	620	169	174	1		

- Molecule 27 is a protein called KLLA0B05742p.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	YY	125	Total	C	N	O	0	0
			992	622	189	181		

- Molecule 28 is a protein called KLLA0E03455p.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	ZZ	134	Total	C	N	O	0	0
			1089	708	199	182		

- Molecule 29 is a protein called RPL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	aa	147	Total	C	N	O	S	0	0
			1156	740	225	189	2		

- Molecule 30 is a protein called KLLA0D16071p.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	bb	57	Total	C	N	O	0	0
			458	287	99	72		

- Molecule 31 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	cc	97	Total	C	N	O	S	0	0
			740	477	125	137	1		

- Molecule 32 is a protein called KLLA0B02937p.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	dd	106	Total	C	N	O	S	0	0
			869	553	167	147	2		

- Molecule 33 is a protein called KLLA0E06843p.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	ee	122	Total	C	N	O	S	0	0
			980	618	198	162	2		

- Molecule 34 is a protein called KLLA0D07405p.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	ff	105	Total	C	N	O	S	0	0
			837	531	161	144	1		

- Molecule 35 is a protein called KLLA0C08371p.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	gg	121	Total	C	N	O	S	0	0
			951	591	192	167	1		

- Molecule 36 is a protein called KLLA0F05247p.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	hh	116	Total	C	N	O	S	0	0
			961	608	187	166			

- Molecule 37 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	ii	98	Total	C	N	O	S	0	0
			766	479	155	131	1		

- Molecule 38 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	jj	85	Total	C	N	O	S	0	0
			675	410	148	111	6		

- Molecule 39 is a protein called KLLA0C18216p.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	kk	76	Total	C	N	O	S	0	0
			619	398	114	107			

- Molecule 40 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	ll	49	Total	C	N	O	S	0	0
			428	266	96	64	2		

- Molecule 41 is a protein called Ubiquitin fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	mm	51	Total	C	N	O	S	0	0
			410	254	85	66	5		

- Molecule 42 is a protein called 60S ribosomal protein L41-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	nn	25	Total	C	N	O	S	0	0
			233	142	63	27	1		

- Molecule 43 is a protein called 60S ribosomal protein L44.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	oo	101	Total	C	N	O	S	0	0
			814	509	163	136	6		

- Molecule 44 is a protein called KLLA0E05941p.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	pp	87	Total	C	N	O	S	0	0
			660	404	133	117	6		

- Molecule 45 is a protein called Ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	qq	217	Total	C	N	O	S	0	0
			1721	1100	300	312	9		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
qq	11	GLU	ASP	conflict	UNP Q6CWR9
qq	12	HIS	ASN	conflict	UNP Q6CWR9
qq	152	ARG	LYS	conflict	UNP Q6CWR9

- Molecule 46 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	rr	195	Total	C	N	O	S	0	0
			1508	968	258	278	4		

- Molecule 47 is a protein called uL11.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	KK	147	Total	C	N	O	0	0
			735	441	147	147		

- Molecule 48 is a protein called 40S ribosomal protein S0.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	A	206	Total	C	N	O	S	0	0
			1616	1035	285	294	2		

- Molecule 49 is a protein called 40S ribosomal protein S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	B	214	Total	C	N	O	S	0	0
			1722	1089	313	317	3		

- Molecule 50 is a protein called KLLA0F09812p.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	C	217	Total	C	N	O	S	0	0
			1629	1041	287	297	4		

- Molecule 51 is a protein called KLLA0D08305p.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	D	223	Total	C	N	O	S	0	0
			1744	1108	313	318	5		

- Molecule 52 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	E	260	Total	C	N	O	S	0	0
			2078	1322	393	359	4		

- Molecule 53 is a protein called KLLA0D10659p.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	F	206	Total	C	N	O	S	0	0
			1609	1008	298	300	3		

- Molecule 54 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	G	226	Total	C	N	O	S	0	0
			1812	1134	348	326	4		

- Molecule 55 is a protein called KLLA0C13519p.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	H	184	Total	C	N	O		0	0
			1483	950	270	263			

- Molecule 56 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	I	188	Total	C	N	O	S	0	0
			1493	926	301	265	1		

- Molecule 57 is a protein called KLLA0E23673p.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	J	182	Total	C	N	O	S	0	0
			1471	929	287	254	1		

- Molecule 58 is a protein called KLLA0B08173p.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	K	96	Total	C	N	O	S	0	0
			809	533	129	146	1		

- Molecule 59 is a protein called KLLA0A10483p.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	L	155	Total	C	N	O	S	0	0
			1248	798	237	210	3		

- Molecule 60 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	M	122	Total	C	N	O		0	0
			922	575	167	180			

- Molecule 61 is a protein called KLLA0F18040p.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	N	150	Total	C	N	O	S	0	0
			1187	756	223	206	2		

- Molecule 62 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	O	127	Total	C	N	O	S	0	0
			942	578	188	173	3		

- Molecule 63 is a protein called KLLA0F07843p.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	P	123	Total	C	N	O	S	0	0
			980	628	179	168	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	130	ALA	-	expression tag	UNP Q6CKV4

- Molecule 64 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms				AltConf	Trace
64	Q	141	Total	C	N	O	0	0
			1105	709	204	192		

- Molecule 65 is a protein called KLLA0B01474p.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	R	129	Total	C	N	O	S	0	0
			1031	641	193	194	3		

- Molecule 66 is a protein called KLLA0B01562p.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	S	145	Total	C	N	O	S	0	0
			1193	741	240	210	2		

- Molecule 67 is a protein called KLLA0A07194p.

Mol	Chain	Residues	Atoms				AltConf	Trace
67	T	143	Total	C	N	O	0	0
			1110	693	210	207		

- Molecule 68 is a protein called KLLA0F25542p.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	U	106	Total	C	N	O	S	0	0
			845	540	152	152	1		

- Molecule 69 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	V	87	Total	C	N	O	S	0	0
			687	424	126	135	2		

- Molecule 70 is a protein called 40S ribosomal protein S22.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	W	129	Total	C	N	O	S	0	0
			1021	651	187	180	3		

- Molecule 71 is a protein called RPS23.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	X	145	Total	C	N	O	S	0	0
			1127	713	219	192	3		

- Molecule 72 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms				AltConf	Trace
72	Y	134	Total	C	N	O	0	0
			1061	665	207	189		

- Molecule 73 is a protein called KLLA0B06182p.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	Z	70	Total	C	N	O	S	0	0
			558	355	104	98	1		

- Molecule 74 is a protein called KLLA0D05115p.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	a	100	Total	C	N	O	S	0	0
			798	491	170	131	6		

- Molecule 75 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	b	82	Total	C	N	O	S	0	0
			617	384	113	114	6		

- Molecule 76 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	c	63	Total	C	N	O	S	0	0
			494	305	98	90	1		

- Molecule 77 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	d	53	Total	C	N	O	S	0	0
			446	280	89	76	1		

- Molecule 78 is a protein called KLLA0C04809p.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	e	55	Total	C	N	O	S	0	0
			443	276	90	76	1		

- Molecule 79 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	f	69	Total	C	N	O	S	0	0
			549	352	102	91	4		

- Molecule 80 is a protein called KLLA0E12277p.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	g	318	Total	C	N	O	S	0	0
			2466	1561	430	470	5		

- Molecule 81 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	2	1780	Total	C	N	O	P	0	0
			37797	16892	6658	12467	1780		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	676	G	U	conflict	GB 49642208
2	678	U	G	conflict	GB 49642208

- Molecule 82 is DNA/RNA hybrid called cricket paralysis virus IRES.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	4	190	Total	C	N	O	P	0	0
			3950	1768	667	1325	190		

- Molecule 83 is a protein called Eft2p.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	1	827	Total	C	N	O	S	0	0
			6421	4070	1106	1216	29		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	310	GLU	ASP	conflict	UNP W7R097

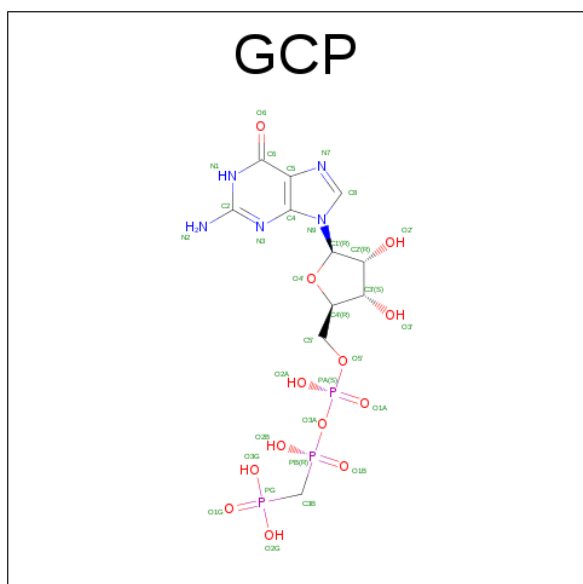
- Molecule 84 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
84	2	75	Total	Mg	0
			75	75	
84	1	1	Total	Mg	0
			1	1	
84	f	1	Total	Mg	0
			1	1	
84	N	1	Total	Mg	0
			1	1	
84	5	2	Total	Mg	0
			2	2	

- Molecule 85 is ZINC ION (three-letter code: ZN) (formula: Zn).

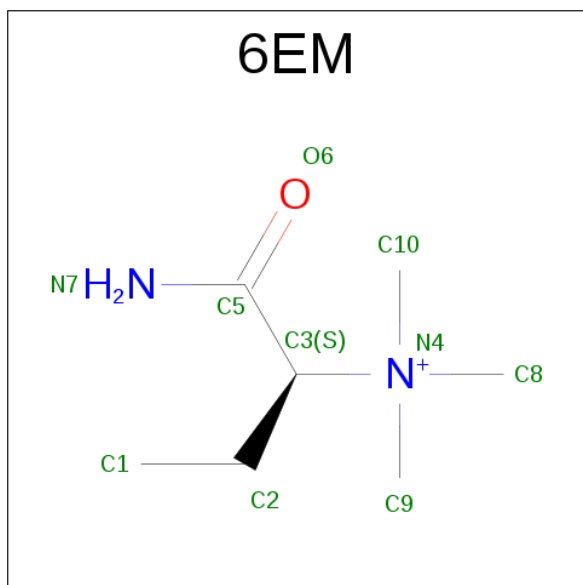
Mol	Chain	Residues	Atoms		AltConf
85	oo	1	Total	Zn	0
			1	1	
85	b	1	Total	Zn	0
			1	1	
85	mm	1	Total	Zn	0
			1	1	
85	jj	1	Total	Zn	0
			1	1	
85	a	1	Total	Zn	0
			1	1	
85	f	1	Total	Zn	0
			1	1	

- Molecule 86 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
86	1	1	Total	C	N	O	P	0
			32	11	5	13	3	

- Molecule 87 is (2S)-1-amino-N,N,N-trimethyl-1-oxobutan-2-aminium (three-letter code: 6EM) (formula: $C_7H_{17}N_2O$).

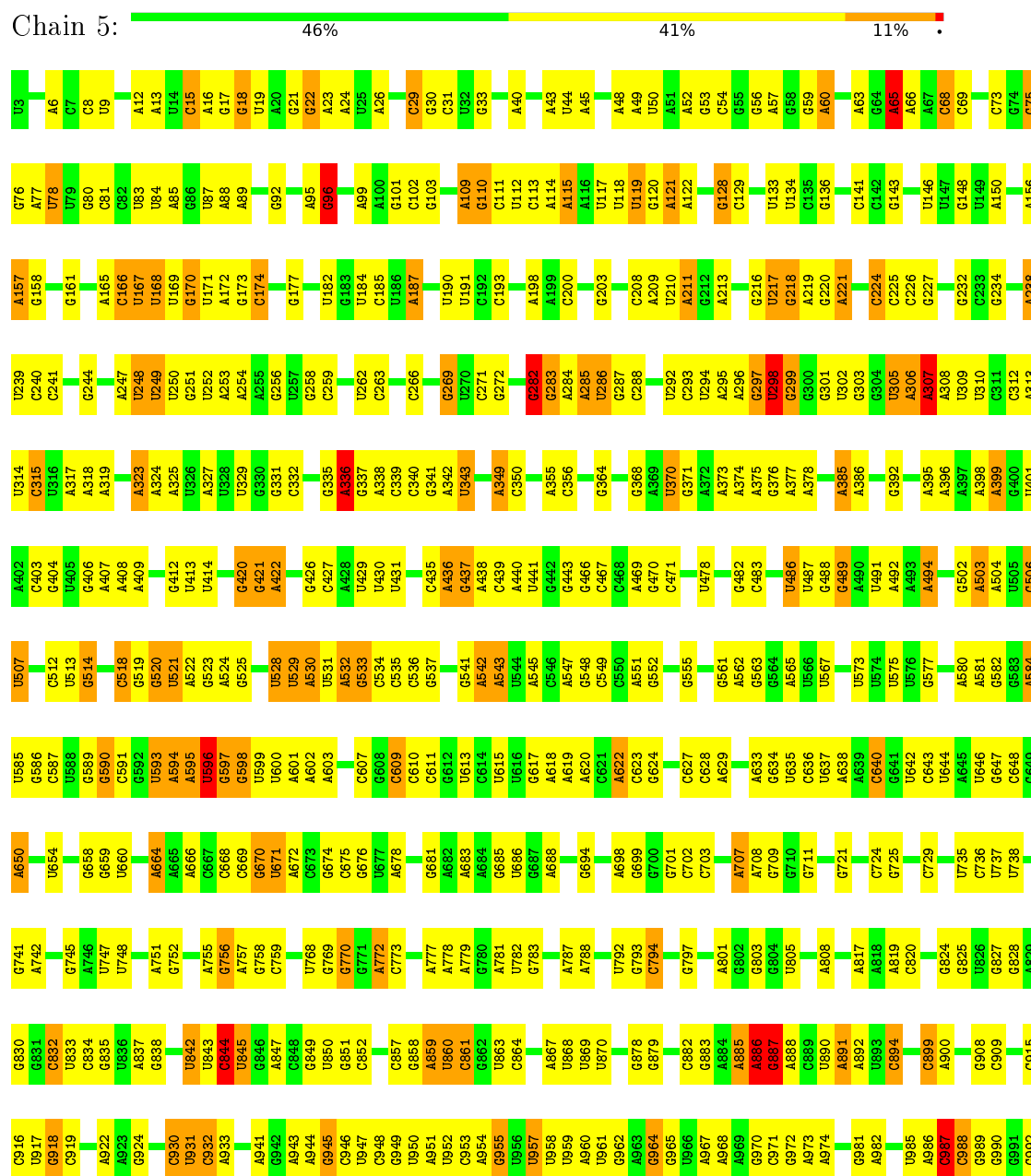


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
87	1	1	10	7	2	1	0

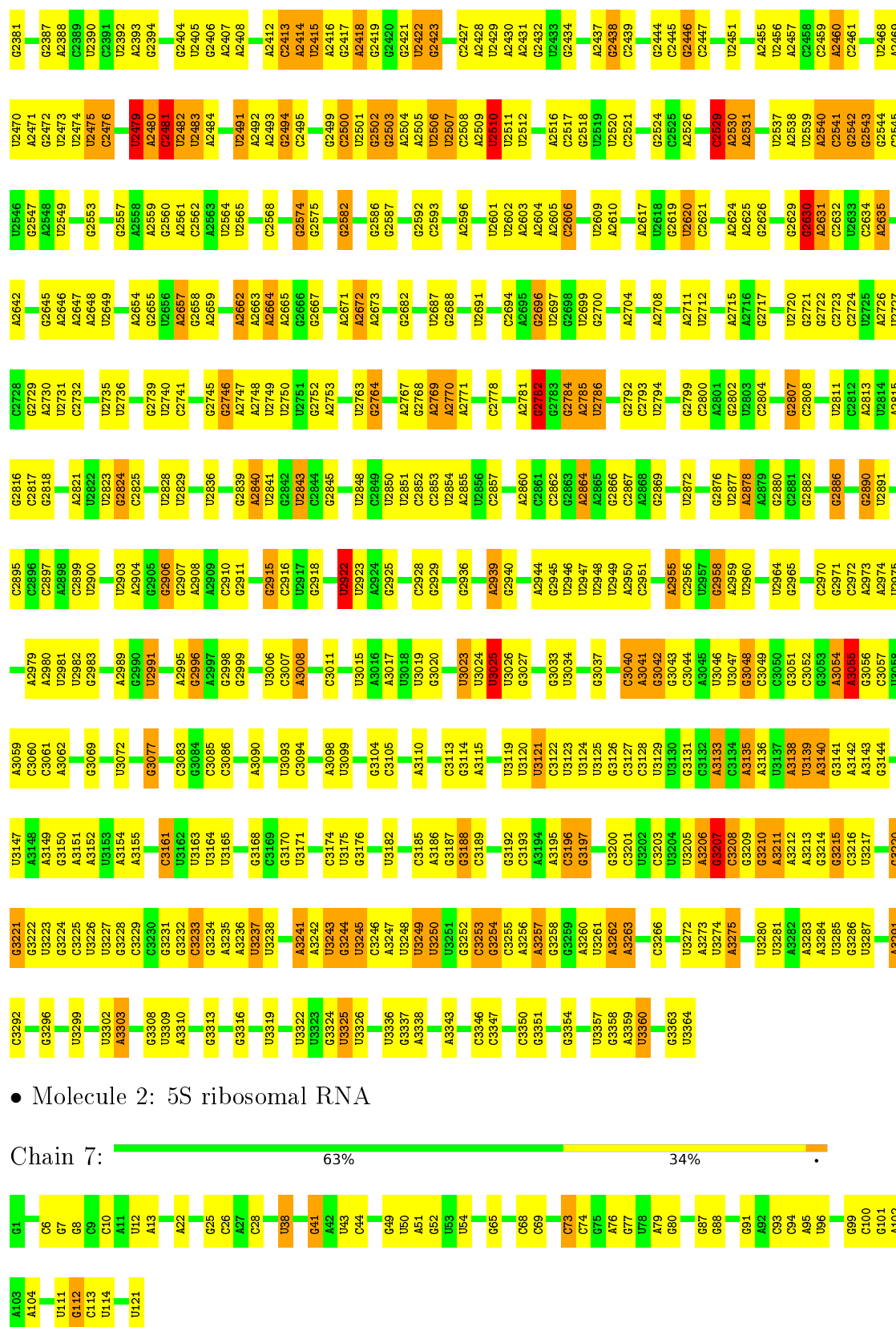
3 Residue-property plots [i](#)

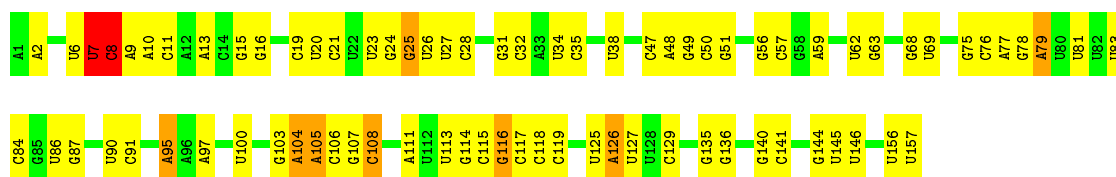
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric 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: 25S ribosomal RNA



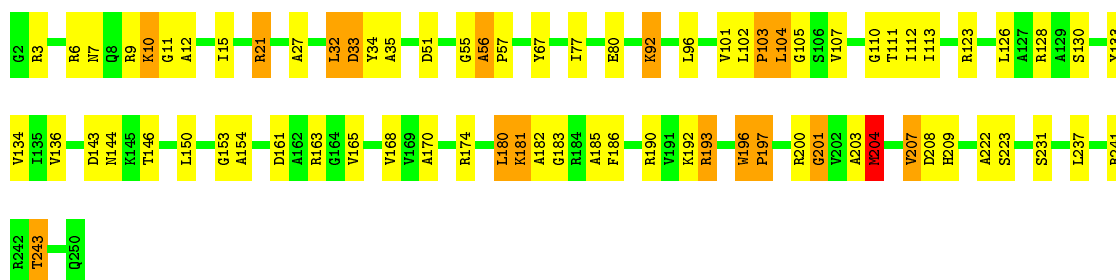
A2301	A2224	U2139	A2050	G1871	U1793	G1720	C1632	A1558	G1484	A1404	G1317	G1235	C1160	G1086	U993
C2302	A2225	G2140	U2051	U1872	C1794	A1721	C1633	G1559	G1485	G1405	U1318	G1236	A1161	G1087	U994
G2303	C2226	U2303	G2052	C1873	C1795	G1722	C1634	G1560			U1319	G1237	A1162	G1088	G995
G2304	U2227	G2149	G2053	G1874	C1796	C1723				C1408	A1320		C1163	G1089	A996
U2305	A2228	C2150	U2054	A1875	G1797	G1724	G1637	A1562	G1491	C1409	A1321	C1248	A1164	C1089	A997
	U2229	A2151	G2055	C1876	G1798	C1725	C1638	A1563	U1493	U1410	U1322	A1249	G1165	G1090	A998
C2308	G2230	G2154	A2056	A1877	G1799	A1726	U1641	U1564	A1495	G1411	A1323	C1250	A1166	U1091	A999
U2313	A2231	U2155	C2057	U1878	U1800	G1727	G1642	C1565	A1496	G1414	U1324	C1254	A1168	U1092	G1000
A2314	U2233	U2155	U2058	A1882	C1801	C1728	G1643	A1572	U1497		G1325	C1255		U1093	C1003
C2315	C2234	U2159	U2059		G1807	G1729	G1644	U1573	C1498	A1417	U1327	G1256	C1172	G1097	U1004
U2316	U2235	U2160	U2060	C1886	A1808	U1731	A1645	A1574	G1499	G1418	G1328	A1257	A1173		U1005
	C2236	C2161	A2062	C1887	U1809	U1732	G1646	U1575			C1329		A1174	G1102	G1006
G2324	U2237	U2162	G2063		A1810	G1733		U1576		C1503	G1333	A1261	G1177	G1105	A1017
A2325	C2238	G2163	G2064	G1896	A1811	U1734	U1651	C1577	U1504	G1421	A1334	A1262	A1178	A1018	A1018
A2326	C2239	C2164	A2065		C1812	G1735	A1652	C1578		C1422	A1335	C1263	U1179	A1019	A1019
A2327	A2240	C2165		U1909			U1656	G1579	G1507		G1336		G1180	C1108	C1020
C2328	G2241	C2166	A2069	C1910	C1815	G1739	U1657	A1581		A1425	A1337	G1266	U1186	U1109	
	C2242	A2167	U2070	U1911	A1816		U1658			G1514	U1338	C1267	U1187	G1110	A1025
C2331	U2243	C2168	U2071	C1912	G1817	C1742		C1584	G1513	A1427	U1339	C1268	C1187	G1111	A1026
A2332	A2244	U2169	A2072	C1913	C1818	C1743	U1664	U1585	G1514		A1340	C1269		C1112	
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	C2246	C2171		C1917			A1666	G1587			U1191	A1272	A1114		U1031
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	A2248	C2173	U2078		U1824	C1748	C1670	U1589	G1522	A1436	C1347	A1274	G1116		A1033
G2339	A2249	U2174	G2079	G1922	C1825	G1749	U1671	A1590	G1523	U1442	G1350	A1275	G1193		G1034
G2340	A2250	C2175	G2080	C1923	C1826	C1750	A1671	A1590	G1524		G1351	U1276	C1195		A1035
A2341	U2251	U2081	A1924	U2081	A1827	C1751	U1672		U1524	A1446	A1352	G1277	A1196	G1120	A1036
A2342	G2252	U2180	A2082	C1925	A1828	C1752	A1673	C1597	U1525		G1353	G1278	G1197		
C2343		C2181	C2083	U1926		G1753	U1674	U1598	U1526	G1447	C1354		C1198	A1121	
G2344	G2257	A2182		G1927	A1833	C1754		U1599	A1528	A1448	U1355	U1280		G1122	G1043
	A2260	C2183	A2086	A1928	A1834	G1755	C1678	C1600	A1529		U1356	A1281	A1202	G1123	U1044
G2346	C2261	G2345	C2087	G1929	C1835	A1756	C1679	A1601	A1530	A1482	C1356	G1281	C1203	A1124	U1045
C2347	C2262	A2191	A2088	U2061	A1836			C1602	G1531		A1357	G1282	C1203	A1125	
	U2263	U2194	G2089	G1941	G1837	U1763	A1684	G1603	G1532	G1453	C1283	C1283	C1203	C1126	
	A2264		U2090	U1942		U1764	U1685	G1604	G1533	G1454	A1361	G1284	U1206	G1127	U1049
C2352		C2198	G2092	C1943	U1840	G1765	U1686		C1534	U1455	U1378		U1207	C1128	
A2353	U2267	C2199	G2093	G2025	A1843	A1766	G1687	C1608	U1535		A1370	A1288	G1207	G1129	U1052
G2354	C2268	C2200	A2094	A2026	G1844	A1769	G1688	G1609	U1536	G1457	C1371	A1289	C1208	A1130	U1053
C2358	G2269	A2201	A2095	C2027	U1845	U1770	U1690	U1610	A1536	G1458	G1372	G1290	C1209	A1130	G1054
		A2202		G2028	U1846	U1770	U1691	A1611	A1537	G1459	C1373	C1291	C1210	A1055	A1055
C2361	G2274	G2203	A2100	G2028	U1847	A1773	U1692	A1612	U1538		U1378		U1212	U1138	A1056
G2362	C2275	C2204	U2106	G2029	G1847	C1774	A1693	C1613	U1539		A1378	U1296	U1213	U1139	G1057
G2365	G2276	C2204	U2107	C2030	A1848	C1774	C1694	U1614	U1540	A1297	G1213	A1297	G1214	A1140	G1058
A2366	G2277	G2208	A2107	U2032	U1849	G1777		A1616	U1541	U1465	G1214	C1298	G1215	A1141	
A2367	U2279		A2108	U2033	A1850		A1700	U1617	U1543	U1300	G1216	U1300	G1217	A1064	A1064
		A2211		G2034	A1855	G1780	G1701	U1618	A1544	A1301	U1218	A1301	G1218	U1065	U1065
A2368	G2280	C2212	G2035	U2036		G1781			G1544			U1302		U1066	U1066
G2369	A2281	A2213	C2369	U2036	U1859	G1782	G1704	G1621	G1546	C1470	G1221	C1303	G1221	C1147	G1067
A2370	C2214	C2213	A2112	A2037	A1860	A1783	G1705	G1622	C1547	C1470	A1222	C1304	A1150	G1148	A1069
A2371	G2215	G2214	A2114	U1784	G1861	C1784	A1785	A1623	G1548	U1395	A1223	U1305	A1151		
G2372	G2216	G2216	G2038	U1862	A1861	A1785	A1710	G1624	A1549	C1396	A1224	C1306	A1151	U1073	G1072
			G2039	A1862	G1862	A1785		U1625	A1549	U1397	U1224	C1307	A1152	A1074	A1074
A2373	G2285	C2217	G2126	U2040	U1863	G1786		C1626	C1551	A1398	G1225	C1307	A1153	G1075	
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	U2287	G2219	U2042	U2042	A1865	U1788	C1714	G1627	G1478	A1399	U1229		G1154	G1076	
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	C2300		G2046		G1867	C1791	A1718	G1630	A1480	U1401	G1233	G1315	G1158	G1079	
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			C2040												





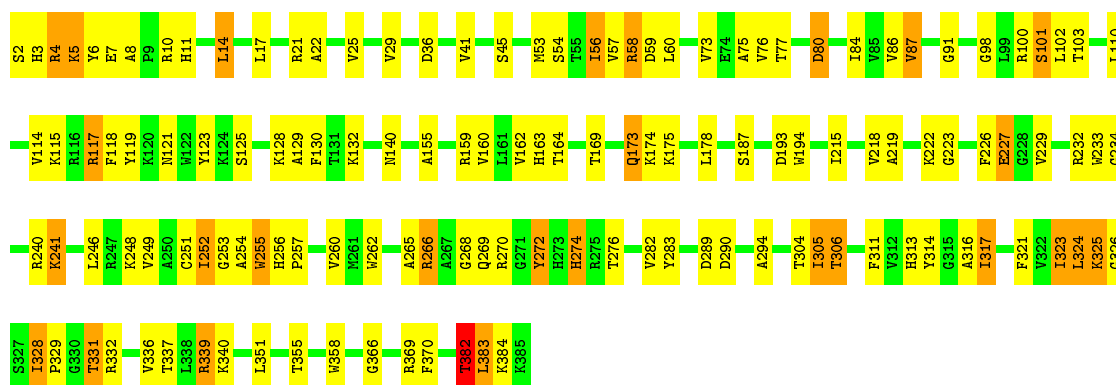
• Molecule 4: KLLA0D16027p

Chain AA: 69% 24% 6%



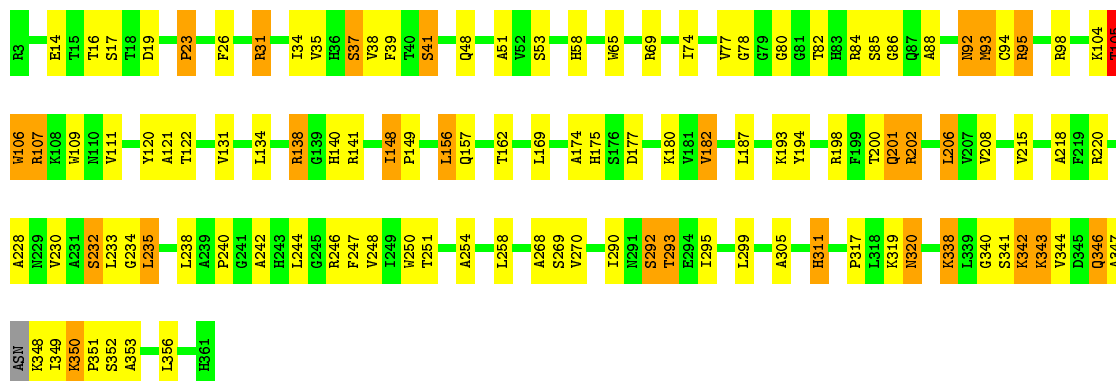
• Molecule 5: 60S ribosomal protein L3

Chain BB: 65% 28% 7%

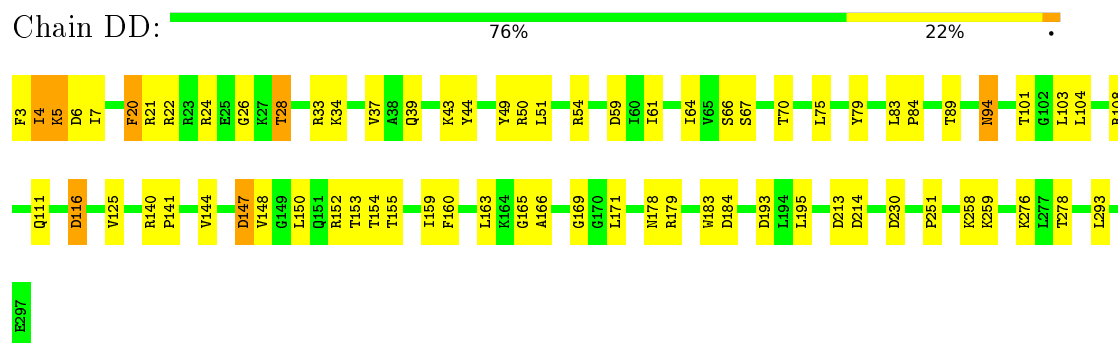


• Molecule 6: KLLA0B07139p

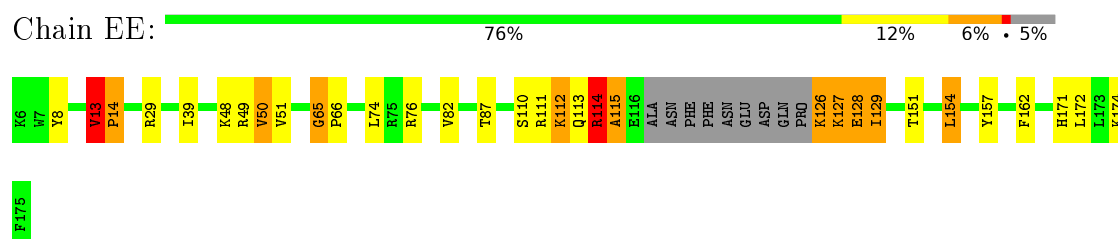
Chain CC: 68% 24% 8%



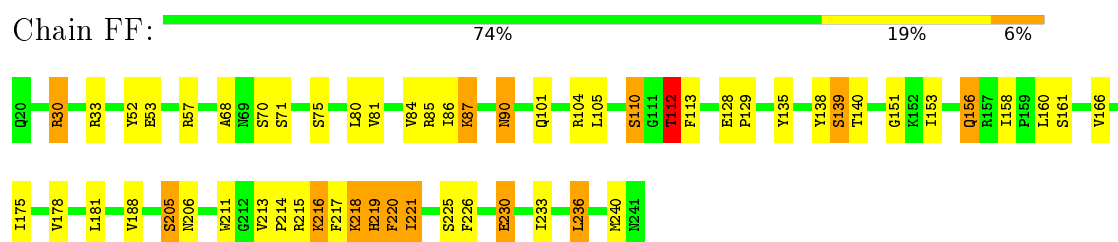
• Molecule 7: KLLA0D06941p



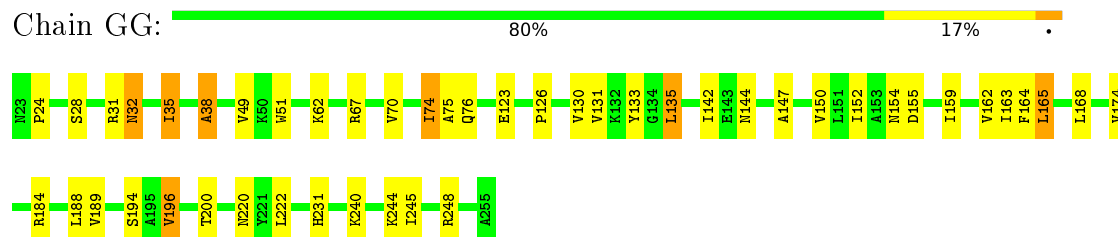
- Molecule 8: KLLA0B04686p



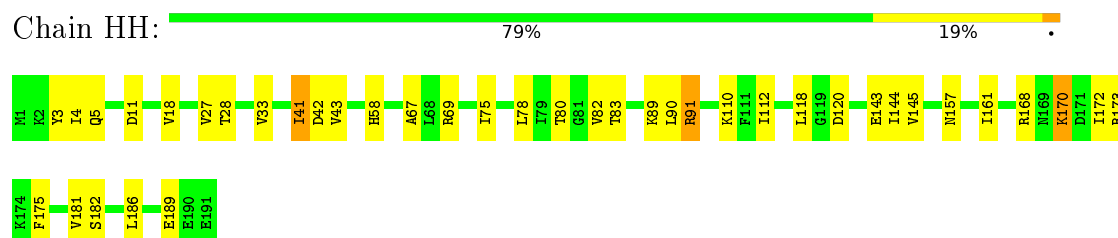
- Molecule 9: KLLA0D03410p



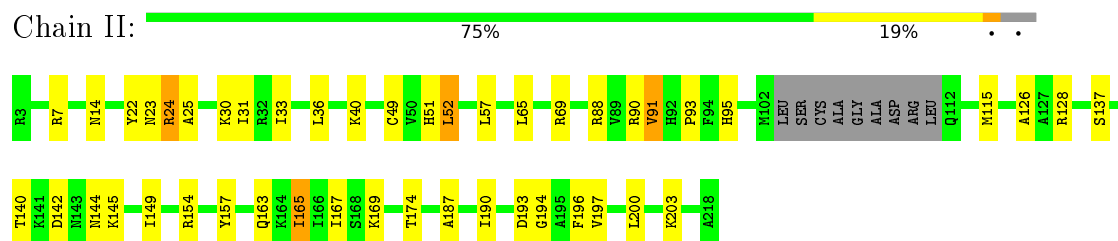
- Molecule 10: KLLA0E00573p



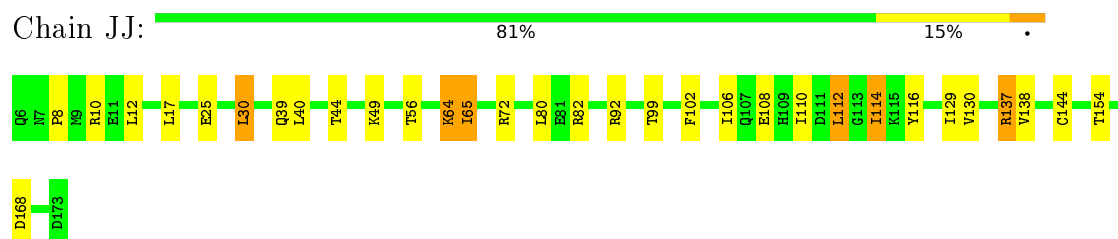
- Molecule 11: KLLA0F04499p



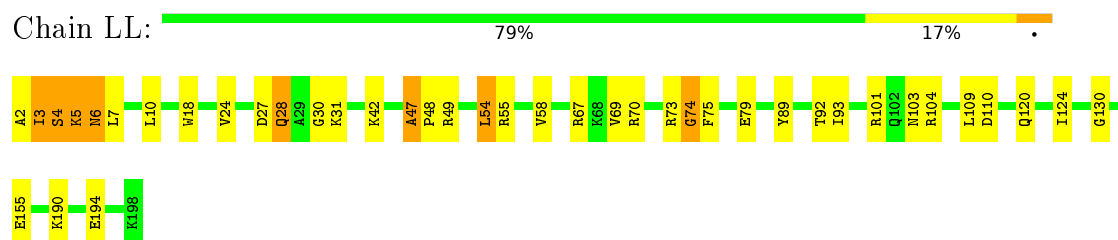
- Molecule 12: KLLA0D05643p



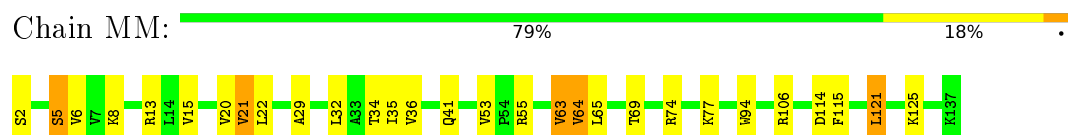
- Molecule 13: KLLA0F08261p



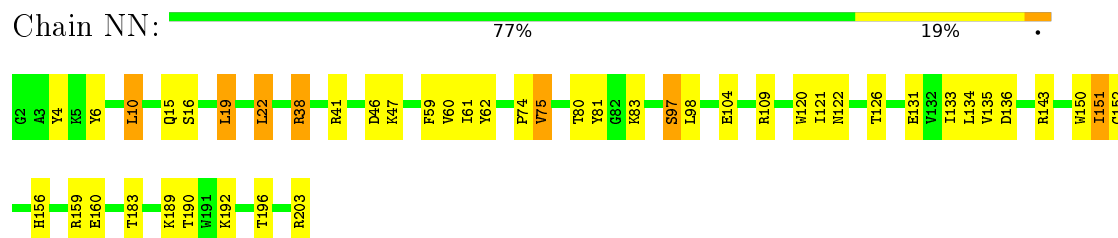
- Molecule 14: 60S ribosomal protein L13



- Molecule 15: KLLA0B13409p

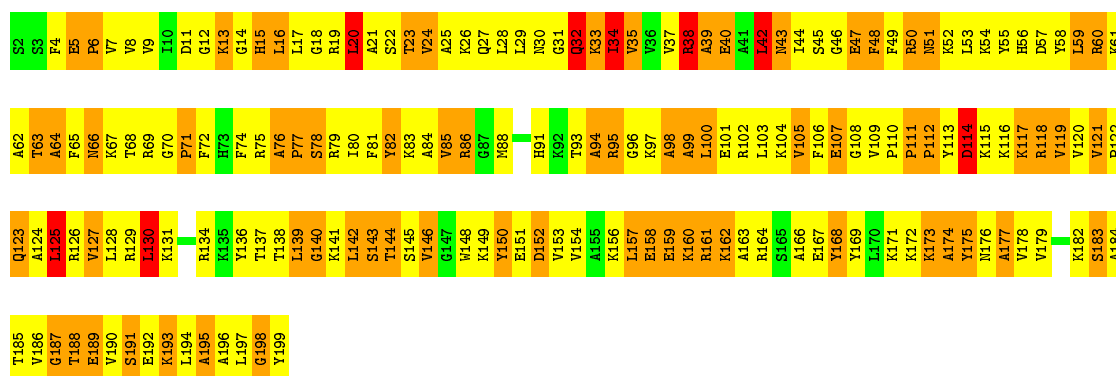


- Molecule 16: Ribosomal protein L15



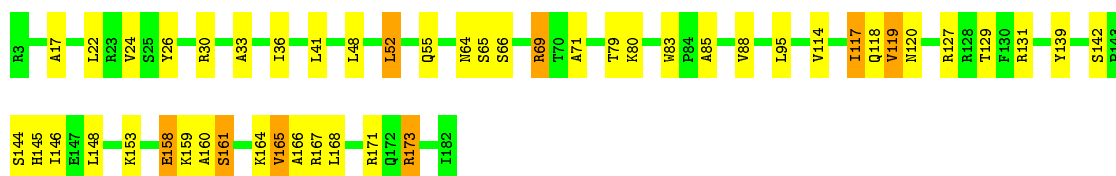
- Molecule 17: KLLA0F04675p





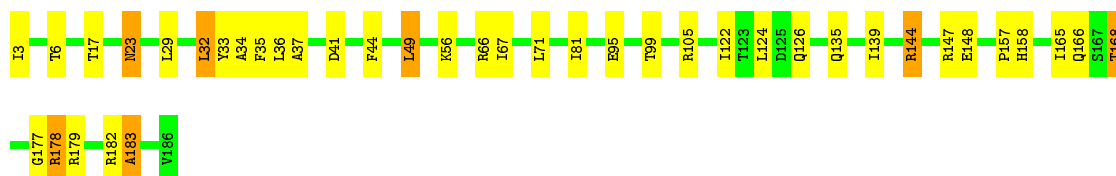
• Molecule 18: KLLA0A06336p

Chain PP: 73% 22% .



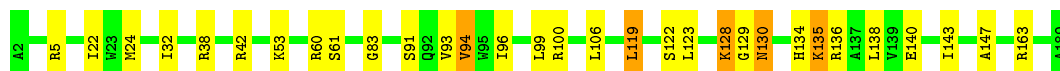
• Molecule 19: KLLA0A07227p

Chain QQ: 78% 18% .



• Molecule 20: KLLA0E12453p

Chain RR: 84% 14% .



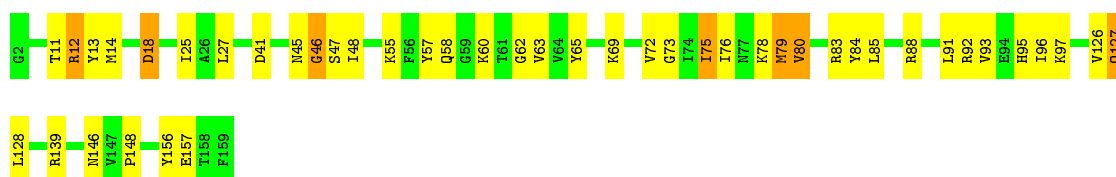
• Molecule 21: 60S ribosomal protein L20

Chain SS: 80% 19% .



• Molecule 22: KLLA0E23651p

Chain TT: 72% 24% .



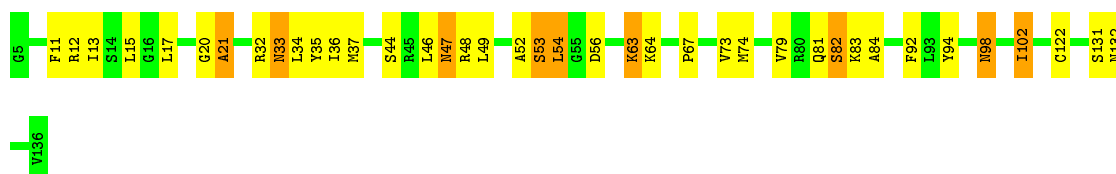
- Molecule 23: KLLA0D05181p

Chain UU: 93% 7%



- Molecule 24: KLLA0E06997p

Chain VV: 70% 23% 7%



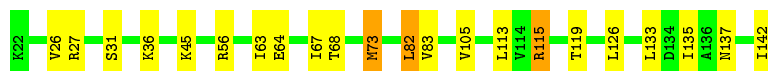
- Molecule 25: 60S ribosomal protein L24

Chain WW: 95% 5%



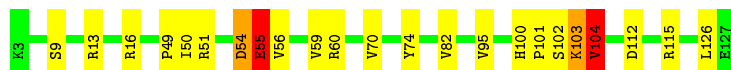
- Molecule 26: 60S ribosomal protein L25

Chain XX: 82% 16% 2%



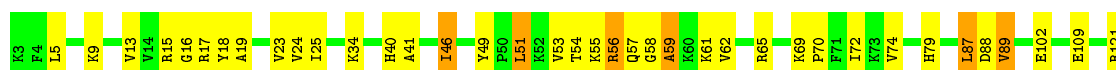
- Molecule 27: KLLA0B05742p

Chain YY: 82% 15% 3%




- Molecule 28: KLLA0E03455p

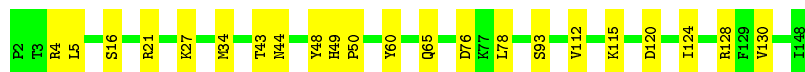
Chain ZZ: 72% 24% 4%





- Molecule 29: RPL28

Chain aa:  85% 15%



- Molecule 30: KLLA0D16071p

Chain bb:  95% 5%



- Molecule 31: 60S ribosomal protein L30

Chain cc:  93% 7%



- Molecule 32: KLLA0B02937p

Chain dd:  89% 11%



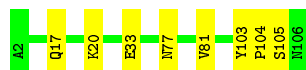
- Molecule 33: KLLA0E06843p

Chain ee:  94% 6%



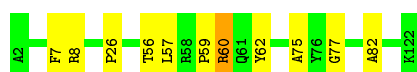
- Molecule 34: KLLA0D07405p

Chain ff:  92% 8%



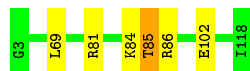
- Molecule 35: KLLA0C08371p

Chain gg:  91% 8%



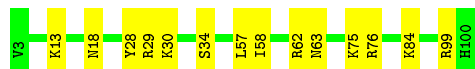
- Molecule 36: KLLA0F05247p

Chain hh:  95%




- Molecule 37: 60S ribosomal protein L36

Chain ii:  86%



- Molecule 38: Ribosomal protein L37

Chain jj:  87%




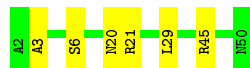
- Molecule 39: KLLA0C18216p

Chain kk:  91%



- Molecule 40: 60S ribosomal protein L39

Chain ll:  88%




- Molecule 41: Ubiquitin fusion protein

Chain mm:  90%




- Molecule 42: 60S ribosomal protein L41-A

Chain nn:  84%




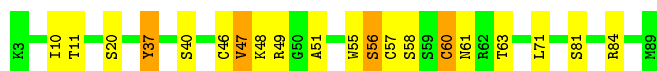
- Molecule 43: 60S ribosomal protein L44

Chain oo:  87% 12%




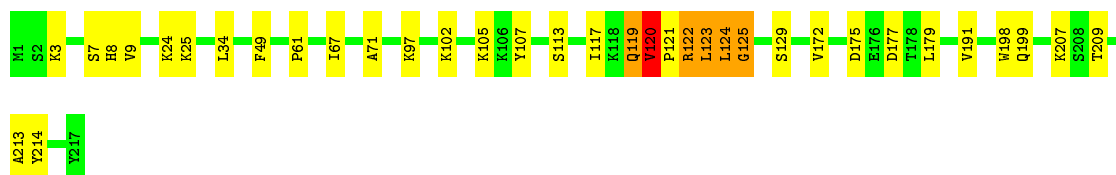
- Molecule 44: KLLA0E05941p

Chain pp:  77% 18% 5%




- Molecule 45: Ribosomal protein

Chain qq:  83% 14%



- Molecule 46: 60S acidic ribosomal protein P0

Chain rr:  85% 14%



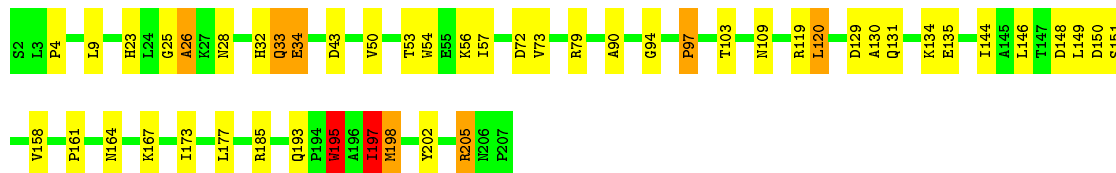
- Molecule 47: uL11

Chain KK:  100%


There are no outlier residues recorded for this chain.

- Molecule 48: 40S ribosomal protein S0

Chain A:  76% 19%



- Molecule 49: 40S ribosomal protein S1

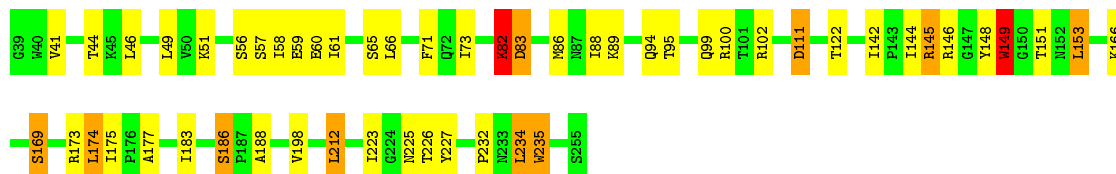
Chain B:  81% 16%





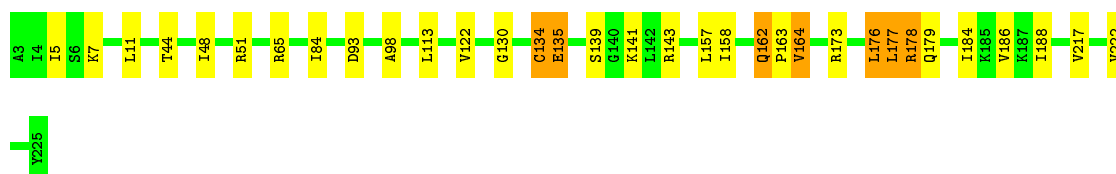
- Molecule 50: KLLA0F09812p

Chain C: 76% 19% 5% •



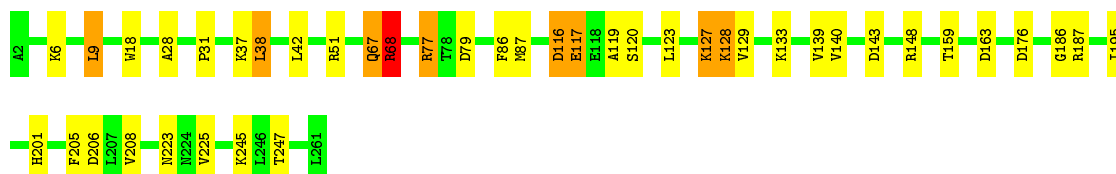
- Molecule 51: KLLA0D08305p

Chain D: 85% 12% •



- Molecule 52: 40S ribosomal protein S4

Chain E: 84% 13% •



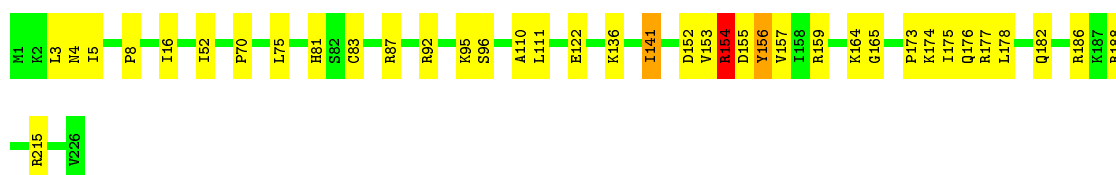
- Molecule 53: KLLA0D10659p

Chain F: 85% 14% •

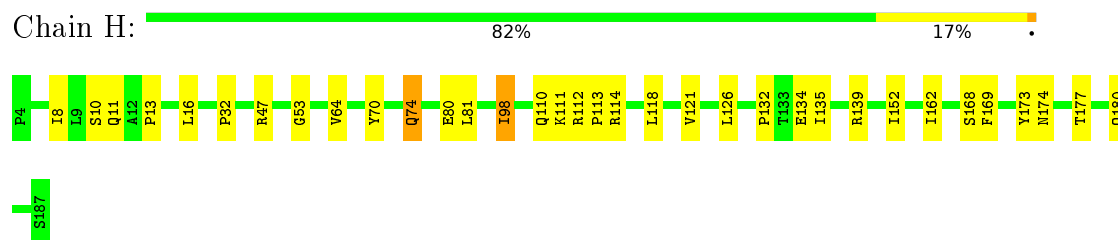


- Molecule 54: 40S ribosomal protein S6

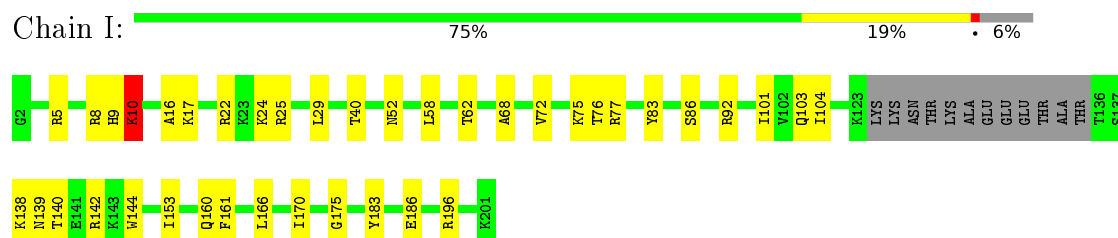
Chain G: 83% 15% •



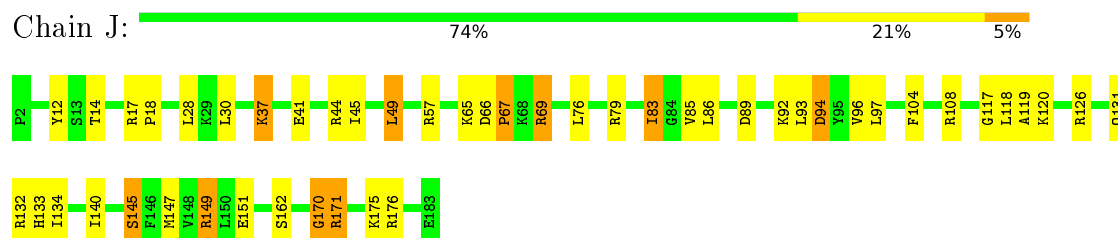
- Molecule 55: KLLA0C13519p



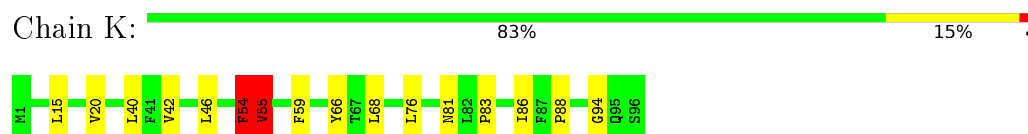
- Molecule 56: 40S ribosomal protein S8



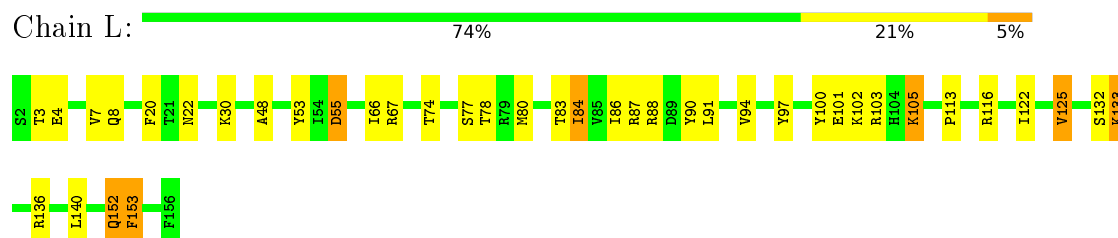
- Molecule 57: KLLA0E23673p



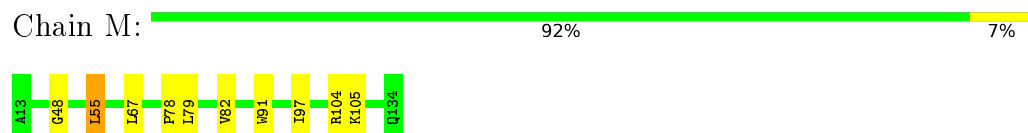
- Molecule 58: KLLA0B08173p



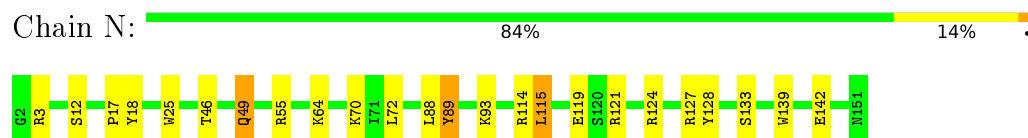
- Molecule 59: KLLA0A10483p



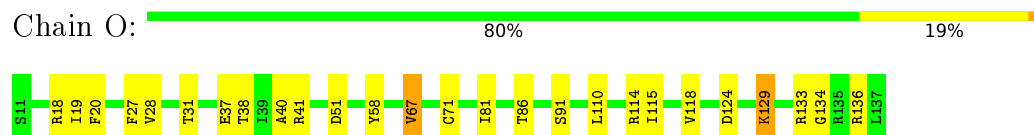
- Molecule 60: 40S ribosomal protein S12



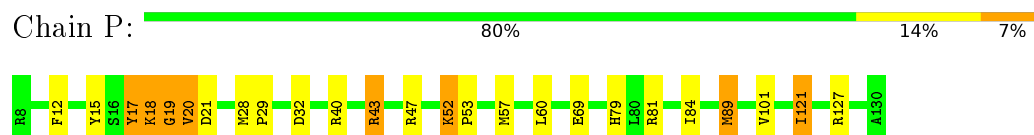
- Molecule 61: KLLA0F18040p



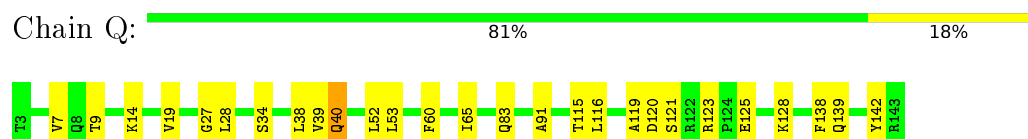
- Molecule 62: 40S ribosomal protein S14



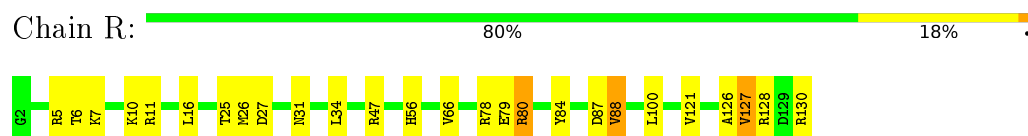
- Molecule 63: KLLA0F07843p



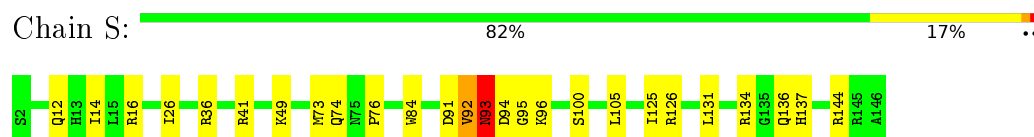
- Molecule 64: 40S ribosomal protein S16



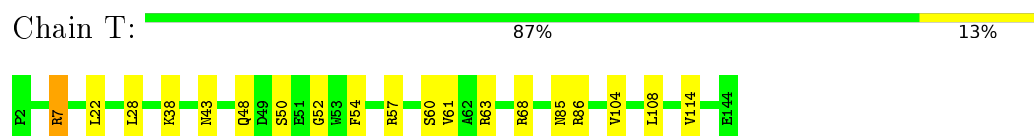
- Molecule 65: KLLA0B01474p




- Molecule 66: KLLA0B01562p



- Molecule 67: KLLA0A07194p




- Molecule 68: KLLA0F25542p

Chain U:  89% 11%



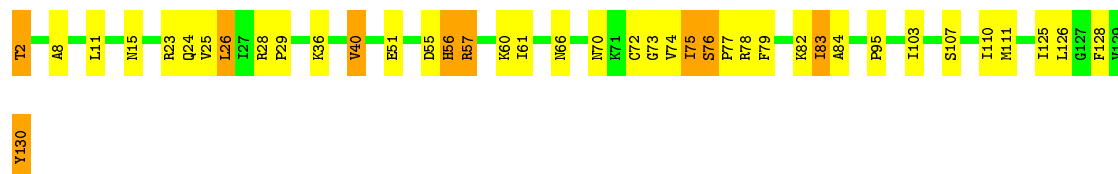
- Molecule 69: 40S ribosomal protein S21

Chain V:  76% 22% .



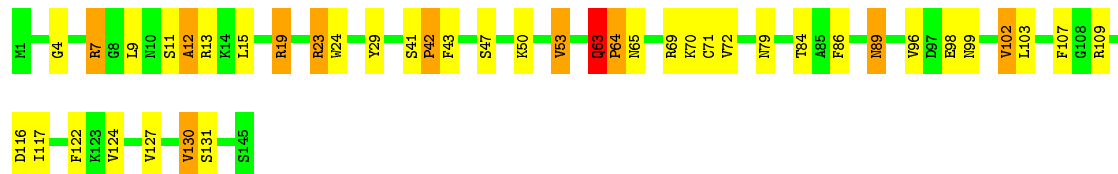
- Molecule 70: 40S ribosomal protein S22

Chain W:  69% 24% 7%




- Molecule 71: RPS23

Chain X:  71% 21% 7% .




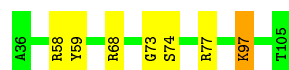
- Molecule 72: 40S ribosomal protein S24

Chain Y:  82% 16% .



- Molecule 73: KLLA0B06182p

Chain Z:  90% 9% .



- Molecule 74: KLLA0D05115p

Chain a:  72% 23% . .



- Molecule 75: 40S ribosomal protein S27

Chain b: 91% 7% .



- Molecule 76: 40S ribosomal protein S28

Chain c: 95% 5%



- Molecule 77: 40S ribosomal protein S29

Chain d: 94% 6%



- Molecule 78: KLLA0C04809p

Chain e: 89% 11%



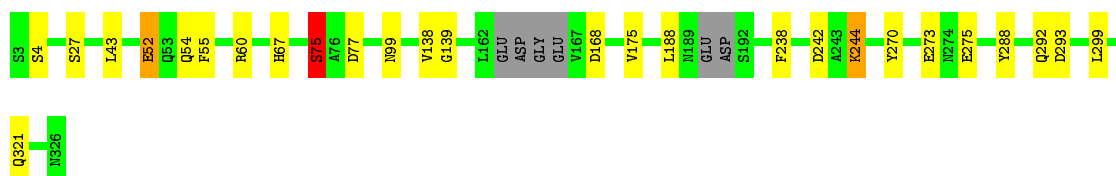
- Molecule 79: Ubiquitin-40S ribosomal protein S27a

Chain f: 78% 17% .



- Molecule 80: KLLA0E12277p

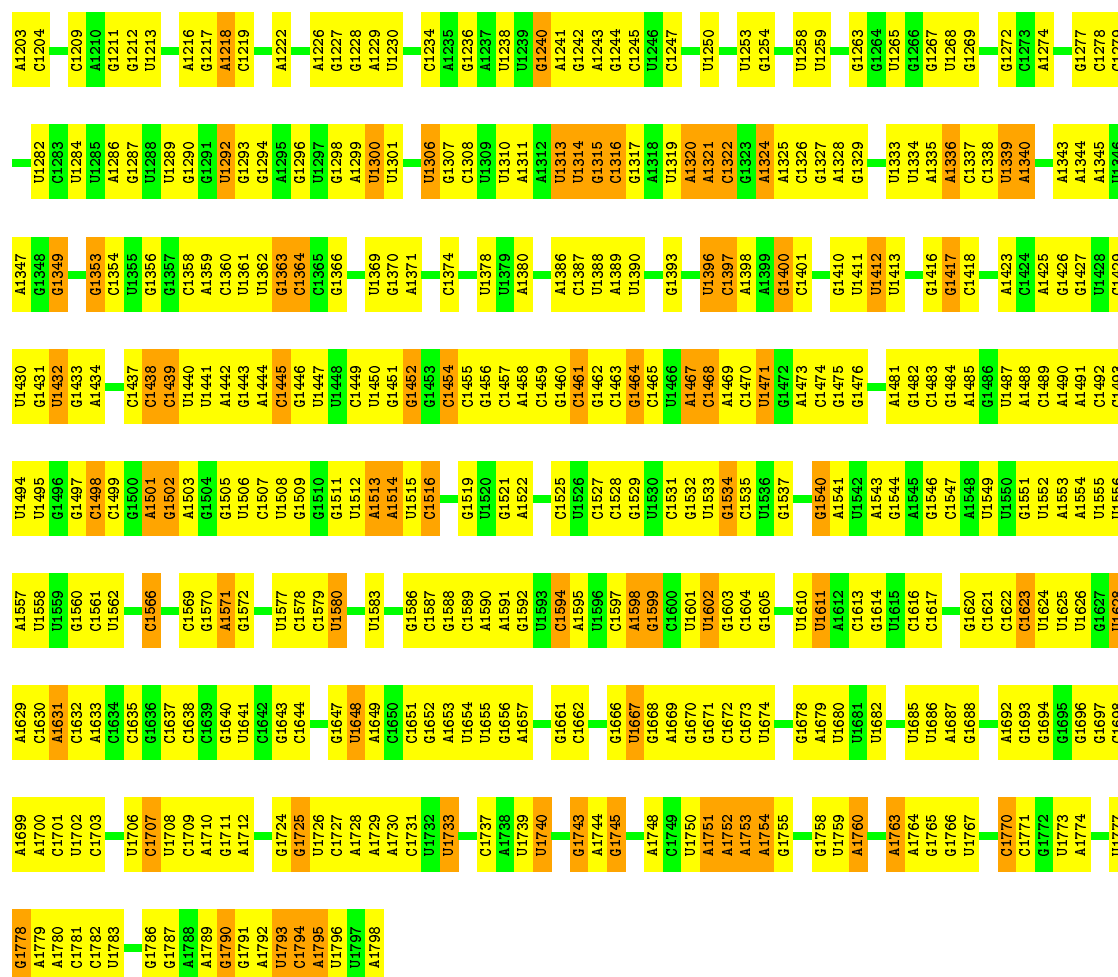
Chain g: 90% 7% ..



- Molecule 81: 18S ribosomal RNA

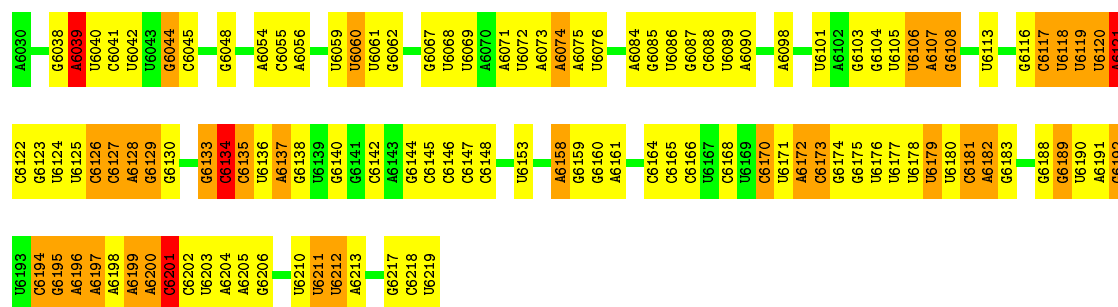
Chain 2: 34% 51% 13% ..

G1127	U1056	C990	U856	G786	U715	G642	G573	U507	G431	U367	U291	A216	A46	U1
U1128	A991	A992	G857	A787	C716	G647	C574	G508	C432	A368	U292	A217	A146	A2
G1129	C1058	G993	A858	A788	U717	U648	G575	G509	G433	A369	C293	A218	U147	U3
A1130	G993	A932	U859	U789	U718	U649	G576	A510	A436	G370	A294	A219	C148	C4
A1131	U1059	A994	A860	A790	U719	U650	U577	A511	A437	G371	A295	A220	U149	U5
A1132	U1060		A861	U791	G720	C652	A578	U512	A438	G372	A296	A221	G150	U6
A1136	G1063	C999	A862	A792	U721	G653	A579	G513	U438	U373	A297	A222	U151	U8
A1137	G1001	C937	U863	U793	G722	G654	U580	A514	U439		A300	A223	G152	U9
G1138	A1002	A938	A864	U794	G723	G655	U581	G515	A440	G376	U301	A224	G153	G10
G1139	U1003	A939		A795	G724	U656	C582		C441	A377	U302	A225	U154	A11
G1140	A1004	A940	U872			C657	C583	C518	C442		U303	G227	A155	A78
A1141	G1073	G941	G874	U798	C727	C	A584	A519	C443	C380	C304	C228	G156	C13
A1142	G1074	C942	G875	U799		G	G585		A444	C381	C305	C229	G157	G14
G1145	A1075	U943	G876	G800	C731	A	C586	G522	C447	G383	G307	U230	U158	U15
A1146	G1008	U944	G877	G801	G732	C		U523		A384	C308	C232	C159	G16
C1147	G1009	U945	G878	A802	G733	U	G591	A524	A451	A385	C309	G233	A161	C18
G1148	U1010	U946	C879	G809	A734	U	A593	A525	U452	A386	U310	G234	G162	A19
G1149	U1011	G947		A810	C735	U	G594	A526	U453	G387	A311			G20
G1150	A1012	C948	C882	A811	A737	A	C595	C530	C454	G388	U312	C239	C165	U21
G1153	U1014	A950	A883	A812	G738	U	G596	U531	A455	G389	C313	U240	U166	A22
G1154	A1085	A951	U884	G814	A740	G		U532	G458	A390	A314	U241	A167	G23
	A1086	G952	A886	G815	C741	U	A600	A533	A459	G391	A315		U168	U24
A1087	U1017	G953	U887	A816	U742	C	U602	A534	G460	C392		U248	U169	C25
	A1018	G954	U888	C817	U743	C	A603	C585		C393	U319	C249	A170	A26
G1157	A1090	C955	C889	G818	U744	G	A604	G596	A463	U394	C320			U29
C1158	A1091	G956	U819	A819	U745	C	A605	A537	A464	G395	G321	A253	U173	G30
A1159	A1092	U957	U820	U821	U746	A	G606	G598	A467	A396	A322	U254	C175	U101
A1162	G1093	U958	C896	U822	U749	C	U607	G599	A468	G397	G325	A255	U176	C31
G1163	U1094	U959	A897	G823	U750	A	U608	A540	A469	A398	U326	C257	U177	U32
	G1095	U960	G898	G824		G676	G609	A541		A400	A327	U258	U178	U33
G1166	U1096	C961	A899	U824	A753	G677	U610	C542	A473	C401	G328	U259	A179	G34
A1170	U1097	A962	G900	U825	A754	U679	C613	A543	A474	G402	G329	U260	A180	C38
C1171	G1099	U964	U902	U826		U679	A614	A544	A475	G403	A330		U181	A39
C1172	G1100	A965	G903	U827	A760	C683	G615	C545	A476	C404	U331	A254	C183	A40
C1173	U1030	A966	A904	U829	A762	A684		U546	A477	H405	U332	A265	U184	A41
U1174	U1031	U967	A905	U830	G763	U691	A618	G547	C478	A406	G333	U266	G185	G42
C1175	C1032	C968	U907	U831	U764	C692	A619	G548	G479	C407	U334	C287	G186	U45
G1176	G1034	A970	U908	U832	G765	U693	A620	C553	A480	C408	G335	C288	C187	A46
G1177	U1035	G971	C909	U834	U767	U695	A621	C554	C483	A411	C337	C289	C190	A47
G1178	G1036	A972	U910	U835	C768	C696	A622	A555		A412	C342	G273	U191	A48
C1179	U1037		U911	G837	A769	C697	G623	G556	G487	C413		C274	U192	G49
U1184	A1038	G975	G912		A770	U698	U625	U557		C414	U349	C275	U193	C50
U1185	G1039	A976	G913	U840	A771	U699	C626	U559	C490	A415	G350	U276	G194	A51
	U1113	A977	A914	C841		C700	G627	U560	A491	A416	G351	U277	G195	U52
A1188	G1041	A978	U915	U842	A774	U701	U628	G561	U492	G417	A351	U278	G196	G53
A1193	U1042	G979	U916		G775		A629	U562	C494	G418		U279	A197	C54
C1194	U1043	U980		G845	G776	C704	G630	G563		G421	G356	G280	G198	C57
A1195	G1044	U981	U920		G777	U705	U631	C564	G497	C422	U357	C281	A199	U58
C1196	G1045	A982	G921	C848	G778		C565	U568	U498	C423	A359	U282	G203	
G1197	G1046	G983	A922	U850	A779	C708	A566	C567	C499	A424	C360	G283	G204	A61
G1198	G1047	G984	A923	U851	G780	C709	G567	U500	U500	G425	C361	C285	A205	A62
G1199	U1048	G985	G924	C851	A781	U710	C568	U503	U503	C426	G362	G286	U206	G63
G1200	A1123	G986	A925	G852	G782	G711	A569	U504	U504	A427	G363	A287	U207	U64
A1201	A1124	A987	C926	U853	U783	U712	G570	C571	A504	G428	G364	U288	G208	A65
A1202	G1126	C989	A928	A855	G785	C714	G641	C572	U506	G429	A365	U289	A209	U66



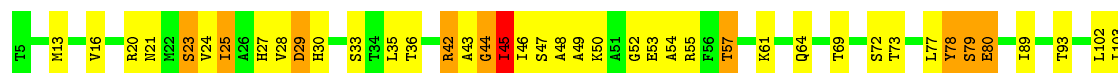
• Molecule 82: cricket paralysis virus IRES

Chain 4: 39% 41% 18%



• Molecule 83: Eft2p

Chain 1: 67% 24% 7%






4 Experimental information ⓘ

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	37844	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	Not provided	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, 6EM, 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	5	0.51	19/78233 (0.0%)	0.81	74/121966 (0.1%)
10	GG	0.44	0/1846	0.69	0/2486
11	HH	0.43	0/1547	0.73	0/2083
12	II	0.48	0/1725	0.74	0/2310
13	JJ	0.40	0/1370	0.71	0/1835
14	LL	0.48	0/1607	0.78	0/2156
15	MM	0.44	0/1060	0.74	0/1430
16	NN	0.69	0/1746	0.88	0/2339
17	OO	0.72	0/1602	0.79	0/2151
18	PP	0.58	0/1455	0.79	1/1952 (0.1%)
19	QQ	0.48	0/1469	0.81	1/1970 (0.1%)
2	7	0.38	0/2883	0.71	0/4491
20	RR	0.47	0/1539	0.78	0/2047
21	SS	0.52	0/1452	0.76	0/1956
22	TT	0.51	0/1286	0.76	0/1722
23	UU	0.38	0/824	0.59	0/1113
24	VV	0.58	0/991	0.84	0/1331
25	WW	0.51	0/528	0.74	0/703
26	XX	0.47	0/979	0.75	0/1320
27	YY	0.45	0/1003	0.78	0/1339
28	ZZ	0.46	0/1114	0.75	0/1493
29	aa	0.57	0/1186	0.83	1/1590 (0.1%)
3	8	0.47	0/3714	0.78	2/5781 (0.0%)
30	bb	0.43	0/468	0.68	0/621
31	cc	0.45	0/748	0.68	0/1005
32	dd	0.48	0/885	0.72	0/1186
33	ee	0.59	0/998	0.78	0/1332
34	ff	0.64	0/855	0.83	0/1150
35	gg	0.52	0/961	0.84	0/1281
36	hh	0.43	0/970	0.71	0/1291
37	ii	0.43	0/773	0.79	0/1029
38	jj	0.73	0/690	0.93	2/913 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
39	kk	0.47	0/626	0.82	0/835
4	AA	0.62	0/1926	0.92	3/2588 (0.1%)
40	ll	0.60	0/435	0.93	1/577 (0.2%)
41	mm	0.49	0/416	0.78	0/552
42	nn	0.43	0/234	0.91	0/300
43	oo	0.47	0/825	0.81	0/1086
44	pp	0.62	0/667	0.95	1/891 (0.1%)
45	qq	0.60	4/1748 (0.2%)	0.83	7/2350 (0.3%)
46	rr	0.41	0/1535	0.67	0/2077
48	A	0.40	0/1656	0.71	0/2264
49	B	0.40	0/1747	0.69	0/2353
5	BB	0.61	0/3136	0.86	1/4225 (0.0%)
50	C	0.45	0/1659	0.81	4/2252 (0.2%)
51	D	0.37	0/1769	0.61	0/2378
52	E	0.42	0/2122	0.75	0/2861
53	F	0.37	0/1628	0.65	2/2198 (0.1%)
54	G	0.45	2/1835 (0.1%)	0.70	0/2451
55	H	0.37	0/1507	0.66	0/2028
56	I	0.42	0/1519	0.73	0/2033
57	J	0.56	2/1495 (0.1%)	0.82	2/2001 (0.1%)
58	K	0.39	0/831	0.57	1/1123 (0.1%)
59	L	0.43	0/1276	0.76	0/1718
6	CC	0.54	0/2780	0.83	2/3760 (0.1%)
60	M	0.40	0/929	0.59	0/1255
61	N	0.41	0/1210	0.71	0/1628
62	O	0.42	0/953	0.75	1/1279 (0.1%)
63	P	0.50	1/1000 (0.1%)	0.71	1/1343 (0.1%)
64	Q	0.38	0/1125	0.61	0/1510
65	R	0.37	0/1042	0.70	0/1399
66	S	0.43	0/1212	0.69	1/1629 (0.1%)
67	T	0.36	0/1129	0.60	0/1520
68	U	0.35	0/857	0.60	0/1158
69	V	0.40	0/696	0.68	0/938
7	DD	0.43	0/2436	0.71	0/3292
70	W	0.51	0/1039	0.81	0/1399
71	X	0.48	0/1145	0.83	1/1526 (0.1%)
72	Y	0.39	0/1075	0.65	0/1433
73	Z	0.39	0/567	0.63	0/762
74	a	0.48	0/810	0.92	1/1084 (0.1%)
75	b	0.36	0/627	0.68	0/847
76	c	0.36	0/496	0.69	0/666
77	d	0.38	0/457	0.61	0/607
78	e	0.36	0/450	0.65	0/599

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
79	f	0.43	0/562	0.65	0/751
8	EE	0.43	0/1322	0.79	2/1776 (0.1%)
80	g	0.36	0/2521	0.58	0/3431
81	2	0.36	6/42269 (0.0%)	0.78	20/65862 (0.0%)
82	4	0.30	0/4407	0.84	6/6849 (0.1%)
83	1	0.42	1/6540 (0.0%)	0.80	10/8853 (0.1%)
9	FF	0.58	0/1810	0.80	0/2440
All	All	0.47	35/230565 (0.0%)	0.78	148/338109 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	5	0	6
14	LL	0	1
21	SS	0	1
27	YY	0	1
28	ZZ	0	1
29	aa	0	1
34	ff	0	1
35	gg	0	2
4	AA	0	2
44	pp	0	3
45	qq	0	3
46	rr	0	1
48	A	0	2
49	B	0	1
5	BB	0	1
50	C	0	3
51	D	0	1
52	E	0	3
53	F	0	1
58	K	0	1
59	L	0	1
6	CC	0	3
62	O	0	1
63	P	0	1
64	Q	0	1
65	R	0	2
69	V	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
7	DD	0	1
70	W	0	2
71	X	0	1
74	a	0	4
79	f	0	2
8	EE	0	3
80	g	0	1
82	4	1	0
83	1	0	16
9	FF	0	2
All	All	1	78

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	2219	G	O3'-P	-16.66	1.41	1.61
57	J	170	GLY	CA-C	11.07	1.69	1.51
81	2	510	A	O3'-P	9.75	1.72	1.61
45	qq	123	LEU	N-CA	7.99	1.62	1.46
1	5	2239	A	O3'-P	-7.87	1.51	1.61

The worst 5 of 148 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	1	581	ASN	N-CA-CB	18.89	144.59	110.60
1	5	2049	G	N9-C1'-C2'	-12.44	97.83	114.00
81	2	511	A	P-O5'-C5'	10.73	138.07	120.90
83	1	580	PRO	N-CA-C	10.27	138.81	112.10
81	2	23	G	N9-C1'-C2'	-10.23	100.70	114.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
82	4	6205	DA	C4'

5 of 78 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	5	1178	G	Sidechain
1	5	2049	G	Sidechain
1	5	2218	G	Sidechain
1	5	2219	G	Sidechain

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Mol	Chain	Res	Type	Group
1	5	2285	G	Sidechain

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	5	69896	0	35118	1364	0
2	7	2579	0	1304	23	0
3	8	3326	0	1680	65	0
4	AA	1892	0	1954	47	0
5	BB	3064	0	3140	80	0
6	CC	2731	0	2842	84	0
7	DD	2384	0	2337	27	0
8	EE	1300	0	1393	25	0
9	FF	1774	0	1832	31	0
10	GG	1817	0	1927	32	0
11	HH	1528	0	1596	19	0
12	II	1690	0	1729	20	0
13	JJ	1349	0	1382	8	0
14	LL	1581	0	1661	37	0
15	MM	1045	0	1126	11	0
16	NN	1709	0	1763	20	0
17	OO	1571	0	1663	417	0
18	PP	1432	0	1465	27	0
19	QQ	1444	0	1541	27	0
20	RR	1522	0	1624	20	0
21	SS	1416	0	1461	15	0
22	TT	1262	0	1309	19	0
23	UU	807	0	821	5	0
24	VV	976	0	1021	28	0
25	WW	515	0	532	2	0
26	XX	964	0	1031	7	0
27	YY	992	0	1070	12	0
28	ZZ	1089	0	1150	23	0
29	aa	1156	0	1206	0	0
30	bb	458	0	486	0	0
31	cc	740	0	792	0	0
32	dd	869	0	920	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	ee	980	0	1048	0	0
34	ff	837	0	861	0	0
35	gg	951	0	1036	0	0
36	hh	961	0	1062	0	0
37	ii	766	0	840	0	0
38	jj	675	0	679	0	0
39	kk	619	0	675	0	0
40	ll	428	0	464	0	0
41	mm	410	0	446	0	0
42	nn	233	0	284	0	0
43	oo	814	0	875	0	0
44	pp	660	0	690	0	0
45	qq	1721	0	1820	0	0
46	rr	1508	0	1542	0	0
47	KK	735	0	177	0	0
48	A	1616	0	1636	22	0
49	B	1722	0	1793	17	0
50	C	1629	0	1710	19	0
51	D	1744	0	1826	8	0
52	E	2078	0	2157	9	0
53	F	1609	0	1679	7	0
54	G	1812	0	1911	35	0
55	H	1483	0	1579	8	0
56	I	1493	0	1515	12	0
57	J	1471	0	1553	36	0
58	K	809	0	810	6	0
59	L	1248	0	1311	18	0
60	M	922	0	953	1	0
61	N	1187	0	1251	8	0
62	O	942	0	979	8	0
63	P	980	0	1029	12	0
64	Q	1105	0	1170	9	0
65	R	1031	0	1082	7	0
66	S	1193	0	1217	9	0
67	T	1110	0	1124	7	0
68	U	845	0	913	3	0
69	V	687	0	682	7	0
70	W	1021	0	1056	21	0
71	X	1127	0	1210	23	0
72	Y	1061	0	1111	7	0
73	Z	558	0	585	2	0
74	a	798	0	854	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
75	b	617	0	643	0	0
76	c	494	0	534	0	0
77	d	446	0	436	0	0
78	e	443	0	481	0	0
79	f	549	0	564	0	0
80	g	2466	0	2406	0	0
81	2	37797	0	19015	680	0
82	4	3950	0	1982	120	0
83	1	6421	0	6490	456	0
84	1	1	0	0	0	0
84	2	75	0	0	0	0
84	5	2	0	0	0	0
84	N	1	0	0	0	0
84	f	1	0	0	0	0
85	a	1	0	0	0	0
85	b	1	0	0	0	0
85	f	1	0	0	0	0
85	jj	1	0	0	0	0
85	mm	1	0	0	0	0
85	oo	1	0	0	0	0
86	1	32	0	14	1	0
87	1	10	0	0	2	0
All	All	215768	0	160636	3748	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 11.

The worst 5 of 3748 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)
81:2:884:G:H2'	81:2:885:U:C1'	1.20	1.64
83:1:698:ILE:HG22	83:1:699:HIS:CD2	1.33	1.58
1:5:2217:C:C3'	1:5:2218:G:H5'	1.16	1.57
83:1:576:LEU:HD21	83:1:587:TYR:CD1	1.36	1.57
1:5:2217:C:H3'	1:5:2218:G:C5'	1.12	1.54

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	
4	AA	247/249 (99%)	198 (80%)	35 (14%)	14 (6%)	2	25
5	BB	382/384 (100%)	311 (81%)	52 (14%)	19 (5%)	3	29
6	CC	357/360 (99%)	273 (76%)	57 (16%)	27 (8%)	1	17
7	DD	293/295 (99%)	254 (87%)	27 (9%)	12 (4%)	3	34
8	EE	157/170 (92%)	127 (81%)	22 (14%)	8 (5%)	2	28
9	FF	220/222 (99%)	182 (83%)	25 (11%)	13 (6%)	2	24
10	GG	231/233 (99%)	198 (86%)	25 (11%)	8 (4%)	4	40
11	HH	189/191 (99%)	168 (89%)	19 (10%)	2 (1%)	17	64
12	II	203/216 (94%)	179 (88%)	20 (10%)	4 (2%)	9	53
13	JJ	166/168 (99%)	136 (82%)	20 (12%)	10 (6%)	2	24
14	LL	195/197 (99%)	170 (87%)	17 (9%)	8 (4%)	3	34
15	MM	134/136 (98%)	124 (92%)	5 (4%)	5 (4%)	4	38
16	NN	200/202 (99%)	172 (86%)	25 (12%)	3 (2%)	13	57
17	OO	196/198 (99%)	88 (45%)	40 (20%)	68 (35%)	0	0
18	PP	178/180 (99%)	152 (85%)	19 (11%)	7 (4%)	4	36
19	QQ	182/184 (99%)	155 (85%)	23 (13%)	4 (2%)	8	51
20	RR	186/188 (99%)	155 (83%)	25 (13%)	6 (3%)	5	42
21	SS	167/169 (99%)	144 (86%)	18 (11%)	5 (3%)	5	44
22	TT	156/158 (99%)	126 (81%)	22 (14%)	8 (5%)	2	28
23	UU	98/100 (98%)	86 (88%)	12 (12%)	0	100	100
24	VV	130/132 (98%)	115 (88%)	10 (8%)	5 (4%)	4	37
25	WW	60/62 (97%)	53 (88%)	7 (12%)	0	100	100
26	XX	119/121 (98%)	107 (90%)	11 (9%)	1 (1%)	24	69
27	YY	123/125 (98%)	104 (85%)	16 (13%)	3 (2%)	7	49
28	ZZ	132/134 (98%)	107 (81%)	17 (13%)	8 (6%)	2	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	aa	145/147 (99%)	121 (83%)	17 (12%)	7 (5%)	3	30
30	bb	55/57 (96%)	48 (87%)	5 (9%)	2 (4%)	4	39
31	cc	95/97 (98%)	83 (87%)	12 (13%)	0	100	100
32	dd	104/106 (98%)	90 (86%)	9 (9%)	5 (5%)	3	30
33	ee	120/122 (98%)	104 (87%)	15 (12%)	1 (1%)	24	69
34	ff	103/105 (98%)	94 (91%)	8 (8%)	1 (1%)	19	66
35	gg	119/121 (98%)	102 (86%)	9 (8%)	8 (7%)	1	21
36	hh	114/116 (98%)	100 (88%)	11 (10%)	3 (3%)	7	46
37	ii	96/98 (98%)	75 (78%)	16 (17%)	5 (5%)	2	27
38	jj	83/85 (98%)	66 (80%)	16 (19%)	1 (1%)	16	62
39	kk	74/76 (97%)	55 (74%)	16 (22%)	3 (4%)	3	34
40	ll	47/49 (96%)	38 (81%)	7 (15%)	2 (4%)	3	33
41	mm	49/51 (96%)	41 (84%)	7 (14%)	1 (2%)	9	53
42	nn	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
43	oo	99/101 (98%)	74 (75%)	21 (21%)	4 (4%)	4	35
44	pp	85/87 (98%)	62 (73%)	14 (16%)	9 (11%)	0	10
45	qq	215/217 (99%)	166 (77%)	33 (15%)	16 (7%)	1	18
46	rr	193/195 (99%)	147 (76%)	30 (16%)	16 (8%)	1	15
48	A	204/206 (99%)	160 (78%)	31 (15%)	13 (6%)	2	23
49	B	212/214 (99%)	162 (76%)	43 (20%)	7 (3%)	5	41
50	C	215/217 (99%)	170 (79%)	34 (16%)	11 (5%)	2	28
51	D	221/223 (99%)	190 (86%)	24 (11%)	7 (3%)	5	42
52	E	258/260 (99%)	220 (85%)	26 (10%)	12 (5%)	3	30
53	F	204/206 (99%)	168 (82%)	29 (14%)	7 (3%)	5	41
54	G	224/226 (99%)	188 (84%)	28 (12%)	8 (4%)	4	39
55	H	182/184 (99%)	149 (82%)	21 (12%)	12 (7%)	1	22
56	I	184/200 (92%)	148 (80%)	29 (16%)	7 (4%)	4	37
57	J	180/182 (99%)	151 (84%)	19 (11%)	10 (6%)	2	26
58	K	94/96 (98%)	78 (83%)	12 (13%)	4 (4%)	3	33
59	L	153/155 (99%)	122 (80%)	24 (16%)	7 (5%)	3	31
60	M	120/122 (98%)	94 (78%)	22 (18%)	4 (3%)	5	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
61	N	148/150 (99%)	129 (87%)	17 (12%)	2 (1%)	14	59
62	O	125/127 (98%)	104 (83%)	18 (14%)	3 (2%)	7	49
63	P	121/123 (98%)	98 (81%)	16 (13%)	7 (6%)	2	25
64	Q	139/141 (99%)	120 (86%)	12 (9%)	7 (5%)	3	29
65	R	127/129 (98%)	99 (78%)	23 (18%)	5 (4%)	4	36
66	S	143/145 (99%)	117 (82%)	21 (15%)	5 (4%)	4	40
67	T	141/143 (99%)	126 (89%)	13 (9%)	2 (1%)	14	59
68	U	104/106 (98%)	92 (88%)	9 (9%)	3 (3%)	6	44
69	V	85/87 (98%)	66 (78%)	14 (16%)	5 (6%)	2	24
70	W	127/129 (98%)	104 (82%)	18 (14%)	5 (4%)	4	36
71	X	143/145 (99%)	112 (78%)	20 (14%)	11 (8%)	1	16
72	Y	132/134 (98%)	111 (84%)	13 (10%)	8 (6%)	2	24
73	Z	68/70 (97%)	57 (84%)	8 (12%)	3 (4%)	3	32
74	a	98/100 (98%)	68 (69%)	13 (13%)	17 (17%)	0	3
75	b	80/82 (98%)	61 (76%)	15 (19%)	4 (5%)	3	29
76	c	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
77	d	51/53 (96%)	40 (78%)	11 (22%)	0	100	100
78	e	53/55 (96%)	46 (87%)	4 (8%)	3 (6%)	2	25
79	f	67/69 (97%)	49 (73%)	12 (18%)	6 (9%)	1	13
80	g	312/324 (96%)	251 (80%)	50 (16%)	11 (4%)	4	40
83	1	825/827 (100%)	654 (79%)	120 (14%)	51 (6%)	2	24
All	All	12121/12322 (98%)	9932 (82%)	1590 (13%)	599 (5%)	5	29

5 of 599 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	AA	10	LYS
4	AA	34	TYR
4	AA	92	LYS
4	AA	181	LYS
4	AA	197	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	AA	190/190 (100%)	174 (92%)	16 (8%)	14	52
5	BB	323/323 (100%)	272 (84%)	51 (16%)	3	22
6	CC	288/291 (99%)	253 (88%)	35 (12%)	6	32
7	DD	243/243 (100%)	215 (88%)	28 (12%)	7	36
8	EE	139/147 (95%)	128 (92%)	11 (8%)	15	54
9	FF	188/188 (100%)	167 (89%)	21 (11%)	7	38
10	GG	192/194 (99%)	175 (91%)	17 (9%)	12	50
11	HH	173/173 (100%)	155 (90%)	18 (10%)	9	42
12	II	177/185 (96%)	156 (88%)	21 (12%)	6	34
13	JJ	144/144 (100%)	130 (90%)	14 (10%)	10	45
14	LL	162/162 (100%)	149 (92%)	13 (8%)	15	54
15	MM	109/109 (100%)	93 (85%)	16 (15%)	4	25
16	NN	175/175 (100%)	156 (89%)	19 (11%)	8	39
17	OO	163/163 (100%)	136 (83%)	27 (17%)	3	19
18	PP	148/148 (100%)	132 (89%)	16 (11%)	8	40
19	QQ	150/150 (100%)	139 (93%)	11 (7%)	17	58
20	RR	152/152 (100%)	147 (97%)	5 (3%)	45	80
21	SS	154/154 (100%)	145 (94%)	9 (6%)	25	66
22	TT	135/135 (100%)	118 (87%)	17 (13%)	5	31
23	UU	90/90 (100%)	90 (100%)	0	100	100
24	VV	101/101 (100%)	90 (89%)	11 (11%)	8	39
25	WW	54/54 (100%)	52 (96%)	2 (4%)	41	77
26	XX	106/106 (100%)	91 (86%)	15 (14%)	4	27
27	YY	111/111 (100%)	102 (92%)	9 (8%)	15	54
28	ZZ	115/115 (100%)	106 (92%)	9 (8%)	16	55
29	aa	117/117 (100%)	104 (89%)	13 (11%)	8	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	bb	45/45 (100%)	44 (98%)	1 (2%)	60	86
31	cc	79/79 (100%)	72 (91%)	7 (9%)	12	50
32	dd	95/95 (100%)	88 (93%)	7 (7%)	17	57
33	ee	106/106 (100%)	100 (94%)	6 (6%)	25	67
34	ff	90/90 (100%)	84 (93%)	6 (7%)	20	62
35	gg	102/102 (100%)	100 (98%)	2 (2%)	63	87
36	hh	104/104 (100%)	100 (96%)	4 (4%)	40	77
37	ii	79/79 (100%)	70 (89%)	9 (11%)	7	36
38	jj	69/69 (100%)	61 (88%)	8 (12%)	7	36
39	kk	68/68 (100%)	63 (93%)	5 (7%)	17	57
40	ll	44/44 (100%)	41 (93%)	3 (7%)	20	61
41	mm	46/46 (100%)	42 (91%)	4 (9%)	13	51
42	nn	23/23 (100%)	19 (83%)	4 (17%)	2	17
43	oo	86/86 (100%)	76 (88%)	10 (12%)	7	36
44	pp	69/69 (100%)	58 (84%)	11 (16%)	3	21
45	qq	198/198 (100%)	181 (91%)	17 (9%)	13	51
46	rr	162/162 (100%)	147 (91%)	15 (9%)	11	48
48	A	174/174 (100%)	159 (91%)	15 (9%)	13	51
49	B	196/196 (100%)	178 (91%)	18 (9%)	11	48
50	C	176/176 (100%)	152 (86%)	24 (14%)	5	29
51	D	185/185 (100%)	165 (89%)	20 (11%)	8	40
52	E	223/223 (100%)	199 (89%)	24 (11%)	8	40
53	F	174/174 (100%)	165 (95%)	9 (5%)	29	69
54	G	192/192 (100%)	179 (93%)	13 (7%)	20	61
55	H	164/164 (100%)	152 (93%)	12 (7%)	17	58
56	I	148/158 (94%)	131 (88%)	17 (12%)	7	36
57	J	153/153 (100%)	137 (90%)	16 (10%)	8	41
58	K	88/88 (100%)	81 (92%)	7 (8%)	15	54
59	L	136/136 (100%)	123 (90%)	13 (10%)	10	45
60	M	97/97 (100%)	92 (95%)	5 (5%)	29	69
61	N	127/127 (100%)	112 (88%)	15 (12%)	6	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
62	O	96/96 (100%)	87 (91%)	9 (9%)	11	47
63	P	105/105 (100%)	92 (88%)	13 (12%)	6	32
64	Q	117/117 (100%)	111 (95%)	6 (5%)	29	70
65	R	117/117 (100%)	107 (92%)	10 (8%)	13	52
66	S	128/128 (100%)	112 (88%)	16 (12%)	6	32
67	T	117/117 (100%)	110 (94%)	7 (6%)	24	65
68	U	96/96 (100%)	92 (96%)	4 (4%)	36	75
69	V	73/73 (100%)	65 (89%)	8 (11%)	8	39
70	W	110/110 (100%)	94 (86%)	16 (14%)	4	26
71	X	120/120 (100%)	107 (89%)	13 (11%)	8	40
72	Y	108/108 (100%)	99 (92%)	9 (8%)	14	52
73	Z	60/60 (100%)	57 (95%)	3 (5%)	30	70
74	a	85/85 (100%)	73 (86%)	12 (14%)	4	28
75	b	72/72 (100%)	68 (94%)	4 (6%)	26	68
76	c	55/55 (100%)	52 (94%)	3 (6%)	27	68
77	d	46/46 (100%)	43 (94%)	3 (6%)	21	63
78	e	49/49 (100%)	46 (94%)	3 (6%)	23	65
79	f	58/60 (97%)	48 (83%)	10 (17%)	2	17
80	g	265/270 (98%)	246 (93%)	19 (7%)	18	58
83	1	700/702 (100%)	612 (87%)	88 (13%)	5	31
All	All	10374/10414 (100%)	9367 (90%)	1007 (10%)	15	45

5 of 1007 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
36	hh	85	THR
49	B	89	ASP
83	1	64	GLN
38	jj	15	SER
45	qq	3	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 98 such sidechains are listed below:

Mol	Chain	Res	Type
32	dd	57	GLN
46	rr	39	GLN
83	1	30	HIS
33	ee	35	GLN
38	jj	69	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	5	3265/3270 (99%)	984 (30%)	198 (6%)
2	7	120/121 (99%)	22 (18%)	4 (3%)
3	8	156/157 (99%)	40 (25%)	6 (3%)
81	2	1778/1798 (98%)	790 (44%)	127 (7%)
82	4	184/190 (96%)	90 (48%)	24 (13%)
All	All	5503/5536 (99%)	1926 (34%)	359 (6%)

5 of 1926 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	5	6	A
1	5	15	C
1	5	18	G
1	5	21	G
1	5	22	G

5 of 359 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	5	2769	A
2	7	76	A
81	2	1763	A
1	5	2866	G
1	5	3186	A

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 88 ligands modelled in this entry, 86 are monoatomic - leaving 2 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
86	GCP	1	902	84	29,34,34	2.80	8 (27%)	31,54,54	1.19	3 (9%)
87	6EM	1	903	83	7,9,9	1.05	1 (14%)	9,13,13	2.12	2 (22%)

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
86	GCP	1	902	84	-	0/18/38/38	0/3/3/3
87	6EM	1	903	83	-	0/12/12/12	0/0/0/0

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	1	902	GCP	C4-N9	-11.20	1.32	1.47
86	1	902	GCP	C8-N9	-3.81	1.35	1.47
86	1	902	GCP	PG-O3G	-3.00	1.47	1.54
86	1	902	GCP	C5-C6	-2.53	1.48	1.53
87	1	903	6EM	C3-C5	-2.11	1.50	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	1	902	GCP	C4-C5-N7	2.46	106.51	102.67
86	1	902	GCP	O2G-PG-C3B	2.84	112.85	106.13
86	1	902	GCP	C8-N9-C4	3.02	108.22	104.78
87	1	903	6EM	C1-C2-C3	3.77	125.06	112.66
87	1	903	6EM	C9-N4-C3	4.21	120.13	110.57

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	1	902	GCP	1	0
87	1	903	6EM	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
47	KK	2
1	5	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	443:G	O3'	466:G	P	31.65
1	5	1948:C	O3'	2019:G	P	17.88
1	KK	23:UNK	C	28:UNK	N	3.41
1	KK	52:UNK	C	54:UNK	N	3.29