Full wwPDB EM Validation Report ⓘ

Dec 11, 2022 – 12:41 am GMT

PDB ID	:	6R5Q
EMDB ID	:	EMD-4729
Title	:	Structure of XBP1u-paused ribosome nascent chain complex (post-state)
Authors	:	Shanmuganathan, V.; Cheng, J.; Berninghausen, O.; Beckmann, R.
Deposited on	:	2019-03-25
Resolution	:	3.00 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

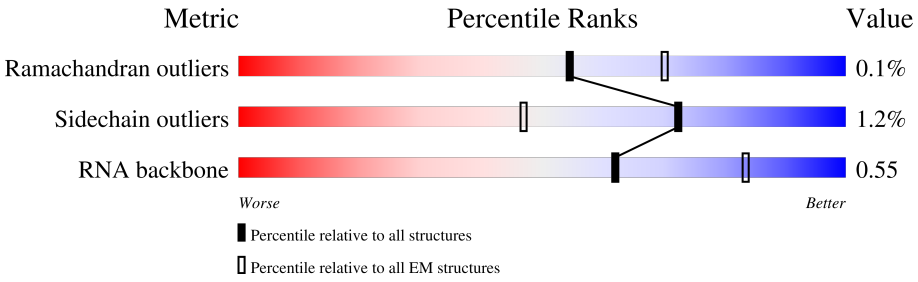
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 3.00 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	3	75	80% 75% 24% ·
2	1	24	· 79% 17% ·
3	2	76	16% 54% 42% ·
4	5	3543	16% 75% 22% ·
5	7	120	· 85% 15%
6	8	151	8% 76% 22% ·
7	A	248	· 98% ·
8	B	394	8% 97% ·

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Mol	Chain	Length	Quality of chain
9	C	362	7% 98%
10	D	293	13% 99%
11	E	251	18% 85% 14%
12	F	225	8% 100%
13	G	233	24% 98%
14	H	190	13% 98%
15	I	205	8% 98%
16	J	170	19% 100%
17	L	210	18% 99%
18	M	138	7% 99%
19	N	203	98%
20	O	199	5% 99%
21	P	153	5% 99%
22	Q	187	5% 99%
23	R	180	15% 98%
24	S	176	100%
25	T	159	17% 99%
26	U	99	40% 99%
27	V	131	98%
28	W	121	40% 88% 12%
29	X	118	9% 99%
30	Y	134	11% 99%
31	Z	135	19% 100%
32	a	147	7% 99%
33	b	104	45% 98%

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Mol	Chain	Length	Quality of chain
34	c	98	11% 99%
35	d	107	13% 98%
36	e	128	5% 99%
37	f	109	6% 99%
38	g	114	11% 98%
39	h	122	8% 100%
40	i	102	20% 99%
41	j	86	5% 99%
42	k	69	42% 100%
43	l	50	12% 98%
44	m	52	8% 100%
45	n	25	8% 100%
46	o	104	9% 99%
47	p	91	7% 99%
48	r	124	10% 98%
49	s	196	100% 100%
50	t	153	100% 100%
51	K	1698	25% 76% 22%
52	q	217	55% 99%
53	u	213	34% 98%
54	v	221	38% 100%
55	w	228	79% 97%
56	x	262	65% 98%
57	y	191	40% 97%
58	z	237	87% 99%

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Mol	Chain	Length	Quality of chain
59	BB	189	73% 97%
60	CC	206	34% 99%
61	DD	185	63% 98%
62	SS	96	95% 99%
63	EE	151	23% 93% 5%
64	RR	117	100% 99%
65	QQ	149	20% 99%
66	MM	135	18% 99%
67	WW	120	79% 98%
68	UU	142	65% 99%
69	KK	132	76% 100%
70	II	144	51% 99%
71	PP	141	66% 99%
72	GG	100	82% 99%
73	HH	83	57% 99%
74	TT	129	18% 100%
75	VV	141	16% 99%
76	NN	124	92% 99%
77	OO	75	68% 100%
78	LL	101	28% 99%
79	JJ	83	57% 99%
80	FF	62	50% 98%
81	9	55	42% 100%
82	4	6	17% 50% 33% 17%
83	0	68	100% 99%

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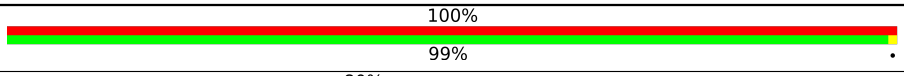
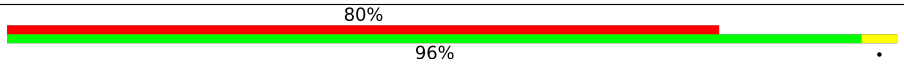
Mol	Chain	Length	Quality of chain
84	6	313	
85	AA	55	

2 Entry composition

There are 87 unique types of molecules in this entry. The entry contains 215870 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 RNA chain called E-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	3	75	Total	C	N	O	P	0	0
			1597	714	287	522	74		

- Molecule 2 is a protein called X-box-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	24	Total	C	N	O	S	0	0
			204	137	35	30	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	255	ALA	SER	conflict	UNP P17861

- Molecule 3 is a RNA chain called P-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	76	Total	C	N	O	P	0	0
			1614	722	287	530	75		

- Molecule 4 is a RNA chain called 28S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	3543	Total	C	N	O	P	0	0
			75972	33833	13910	24686	3543		

- Molecule 5 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	7	120	Total	C	N	O	P	0	0
			2558	1141	456	842	119		

- Molecule 6 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	8	151	Total	C	N	O	P	0	0
			3208	1432	564	1062	150		

- Molecule 7 is a protein called uL2.

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

- Molecule 8 is a protein called uL3.

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

- Molecule 9 is a protein called uL4.

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

- Molecule 10 is a protein called 60S ribosomal protein L5.

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

- Molecule 11 is a protein called 60S ribosomal protein L6.

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

- Molecule 12 is a protein called uL30.

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

- Molecule 13 is a protein called eL8.

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

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	?	-	GLY	deletion	UNP G1STW0
G	?	-	LYS	deletion	UNP G1STW0
G	?	-	GLY	deletion	UNP G1STW0
G	?	-	ASP	deletion	UNP G1STW0
G	?	-	VAL	deletion	UNP G1STW0
G	?	-	PRO	deletion	UNP G1STW0
G	?	-	THR	deletion	UNP G1STW0
G	244	GLY	CYS	conflict	UNP G1STW0

- Molecule 14 is a protein called uL6.

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

- Molecule 15 is a protein called Ribosomal protein L10 (Predicted).

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

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	?	-	LEU	deletion	UNP B7NZQ2
I	?	-	SER	deletion	UNP B7NZQ2
I	?	-	CYS	deletion	UNP B7NZQ2
I	?	-	ALA	deletion	UNP B7NZQ2
I	?	-	GLY	deletion	UNP B7NZQ2
I	?	-	ALA	deletion	UNP B7NZQ2
I	?	-	ASP	deletion	UNP B7NZQ2
I	?	-	ARG	deletion	UNP B7NZQ2

- Molecule 16 is a protein called Ribosomal protein L11.

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

- Molecule 17 is a protein called 60S ribosomal protein L13.

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

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	47	ALA	-	insertion	UNP G1TPV0
L	48	PRO	-	insertion	UNP G1TPV0
L	49	ARG	-	insertion	UNP G1TPV0
L	50	PRO	-	insertion	UNP G1TPV0
L	51	ALA	-	insertion	UNP G1TPV0
L	52	ALA	-	insertion	UNP G1TPV0
L	53	GLY	-	insertion	UNP G1TPV0
L	54	PRO	-	insertion	UNP G1TPV0
L	55	ILE	-	insertion	UNP G1TPV0

- Molecule 18 is a protein called Ribosomal protein L14.

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

- Molecule 19 is a protein called Ribosomal protein L15.

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

- Molecule 20 is a protein called uL13.

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

- Molecule 21 is a protein called uL22.

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

- Molecule 22 is a protein called eL18.

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

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	6	ARG	LEU	conflict	UNP G1TX70
Q	14	ARG	TRP	conflict	UNP G1TX70
Q	23	ILE	MET	conflict	UNP G1TX70
Q	24	TYR	CYS	conflict	UNP G1TX70
Q	38	ARG	HIS	conflict	UNP G1TX70
Q	57	ASN	LYS	conflict	UNP G1TX70
Q	66	MET	VAL	conflict	UNP G1TX70
Q	74	GLY	ASP	conflict	UNP G1TX70
Q	75	ARG	PRO	conflict	UNP G1TX70
Q	86	VAL	ILE	conflict	UNP G1TX70
Q	110	ARG	HIS	conflict	UNP G1TX70
Q	117	GLY	GLU	conflict	UNP G1TX70
Q	124	ASP	HIS	conflict	UNP G1TX70
Q	150	ARG	GLN	conflict	UNP G1TX70
Q	172	ARG	GLY	conflict	UNP G1TX70
Q	184	ARG	TRP	conflict	UNP G1TX70

- Molecule 23 is a protein called eL19.

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

- Molecule 24 is a protein called eL20.

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

- Molecule 25 is a protein called eL21.

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

- Molecule 26 is a protein called eL22.

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

- Molecule 27 is a protein called eL14.

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

- Molecule 28 is a protein called Ribosomal protein L24.

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

- Molecule 29 is a protein called uL23.

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

- Molecule 30 is a protein called Ribosomal protein L26.

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

- Molecule 31 is a protein called 60S ribosomal protein L27.

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

- Molecule 32 is a protein called uL15.

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

- Molecule 33 is a protein called eL29.

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

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b	?	-	LYS	deletion	UNP G1SGR6
b	?	-	PRO	deletion	UNP G1SGR6
b	?	-	LYS	deletion	UNP G1SGR6
b	?	-	GLU	deletion	UNP G1SGR6
b	?	-	VAL	deletion	UNP G1SGR6
b	?	-	LYS	deletion	UNP G1SGR6
b	?	-	PRO	deletion	UNP G1SGR6
b	?	-	THR	deletion	UNP G1SGR6
b	?	-	ILE	deletion	UNP G1SGR6
b	?	-	PRO	deletion	UNP G1SGR6
b	?	-	LYS	deletion	UNP G1SGR6
b	?	-	GLY	deletion	UNP G1SGR6

- Molecule 34 is a protein called eL30.

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

- Molecule 35 is a protein called eL31.

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

- Molecule 36 is a protein called eL32.

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

- Molecule 37 is a protein called eL33.

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

- Molecule 38 is a protein called eL34.

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

- Molecule 39 is a protein called uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	h	122	Total	C	N	O	S	0	0
			1013	640	204	168	1		

- Molecule 40 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	i	102	Total	C	N	O	S	0	0
			830	520	176	129	5		

- Molecule 41 is a protein called Ribosomal protein L37.

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

- Molecule 42 is a protein called eL38.

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

- Molecule 43 is a protein called eL39.

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

- Molecule 44 is a protein called eL40.

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

- Molecule 45 is a protein called 60s ribosomal protein l41.

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

- Molecule 46 is a protein called eL42.

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

- Molecule 47 is a protein called ribosomal protein eL43.

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

- Molecule 48 is a protein called eL28.

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

- Molecule 49 is a protein called 60S acidic ribosomal protein P0.

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

- Molecule 50 is a protein called uL11.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
51	K	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	q	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	u	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	v	221	Total	C	N	O	S	0	0
			1716	1111	295	301	9		

- Molecule 55 is a protein called Ribosomal protein S3.

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

- Molecule 56 is a protein called 40S ribosomal protein S4.

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

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
x	25	GLY	SER	conflict	UNP G1TK17
x	51	ARG	LYS	conflict	UNP G1TK17
x	78	THR	ALA	conflict	UNP G1TK17
x	156	VAL	MET	conflict	UNP G1TK17

- Molecule 57 is a protein called Ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	y	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	z	237	Total	C	N	O	S	0	0
			1923	1200	387	329	7		

- Molecule 59 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	BB	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	CC	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
CC	47	ARG	GLY	conflict	UNP G1TJW1

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

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

- Molecule 62 is a protein called eS10.

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

- Molecule 63 is a protein called Ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	EE	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	RR	117	Total	C	N	O	S	0	0
			908	570	161	169	8		

- Molecule 65 is a protein called ribosomal protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	QQ	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	MM	135	Total	C	N	O	S	0	0
			1004	614	196	188	6		

- Molecule 67 is a protein called uS17.

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

- Molecule 68 is a protein called Ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	UU	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	KK	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	II	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	PP	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
PP	119	GLY	TRP	conflict	UNP G1TN62

- Molecule 72 is a protein called uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	GG	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	HH	83	Total	C	N	O	S	0	0
			636	393	117	121	5		

- Molecule 74 is a protein called Ribosomal protein S15a.

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

- Molecule 75 is a protein called Ribosomal protein S23.

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

- Molecule 76 is a protein called eS24.

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

- Molecule 77 is a protein called ribosomal protein eS25.

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

- Molecule 80 is a protein called Ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	FF	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	9	55	Total	C	N	O	S	0	0
			459	286	94	74	5		

- Molecule 82 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	4	6	Total	C	N	O	P	0	0
			127	57	21	43	6		

- Molecule 83 is a protein called eS31.

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

- Molecule 84 is a protein called ribosomal protein RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	6	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

- Molecule 85 is a protein called 40S ribosomal protein S30.

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

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

Mol	Chain	Residues	Atoms		AltConf
86	5	201	Total	Mg	0
			201	201	
86	7	6	Total	Mg	0
			6	6	
86	8	5	Total	Mg	0
			5	5	
86	I	1	Total	Mg	0
			1	1	
86	P	2	Total	Mg	0
			2	2	
86	V	1	Total	Mg	0
			1	1	
86	a	1	Total	Mg	0
			1	1	
86	e	1	Total	Mg	0
			1	1	
86	g	1	Total	Mg	0
			1	1	
86	j	1	Total	Mg	0
			1	1	
86	K	78	Total	Mg	0
			78	78	
86	PP	1	Total	Mg	0
			1	1	

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

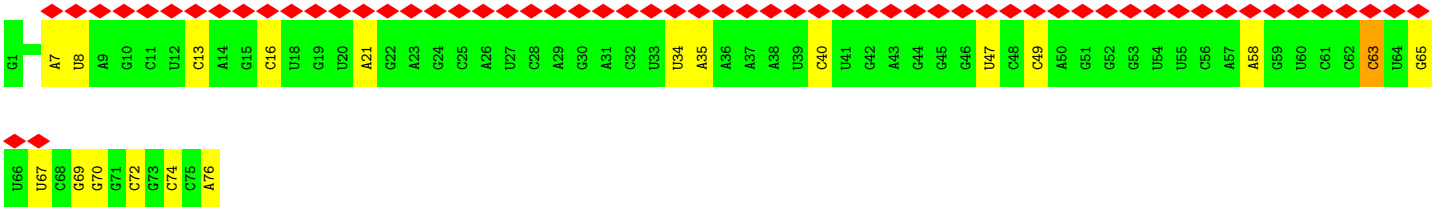
Mol	Chain	Residues	Atoms	AltConf
87	g	1	Total Zn 1 1	0
87	j	1	Total Zn 1 1	0
87	m	1	Total Zn 1 1	0
87	o	1	Total Zn 1 1	0
87	p	1	Total Zn 1 1	0
87	LL	1	Total Zn 1 1	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. 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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

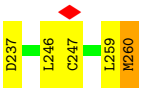
• Molecule 1: E-tRNA

Chain 3:



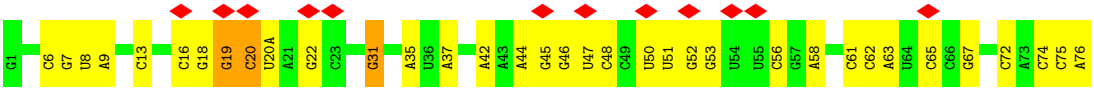
• Molecule 2: X-box-binding protein 1

Chain 1:



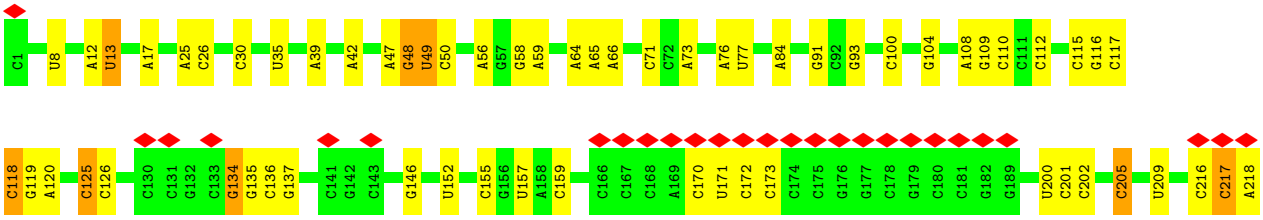
• Molecule 3: P-tRNA

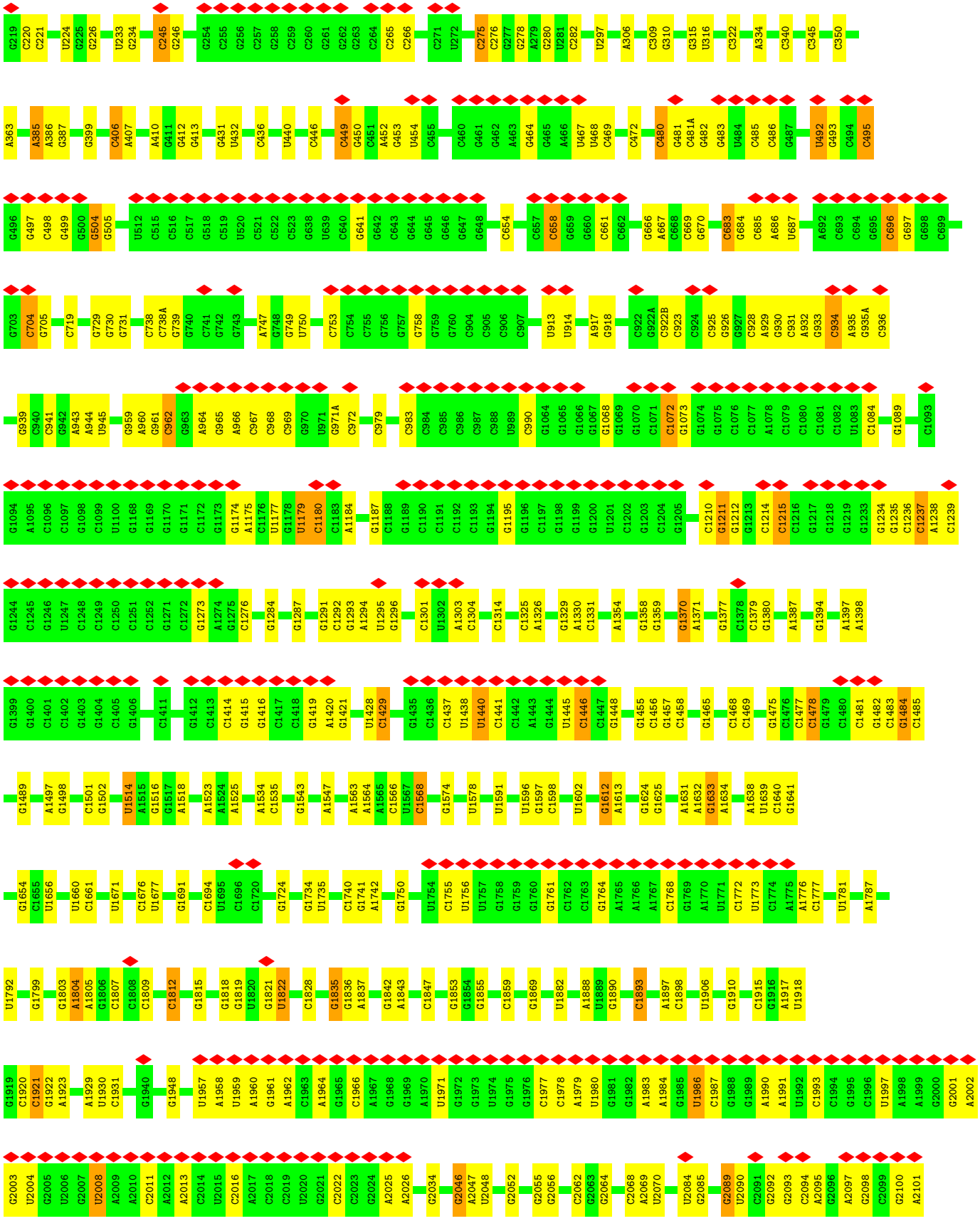
Chain 2:

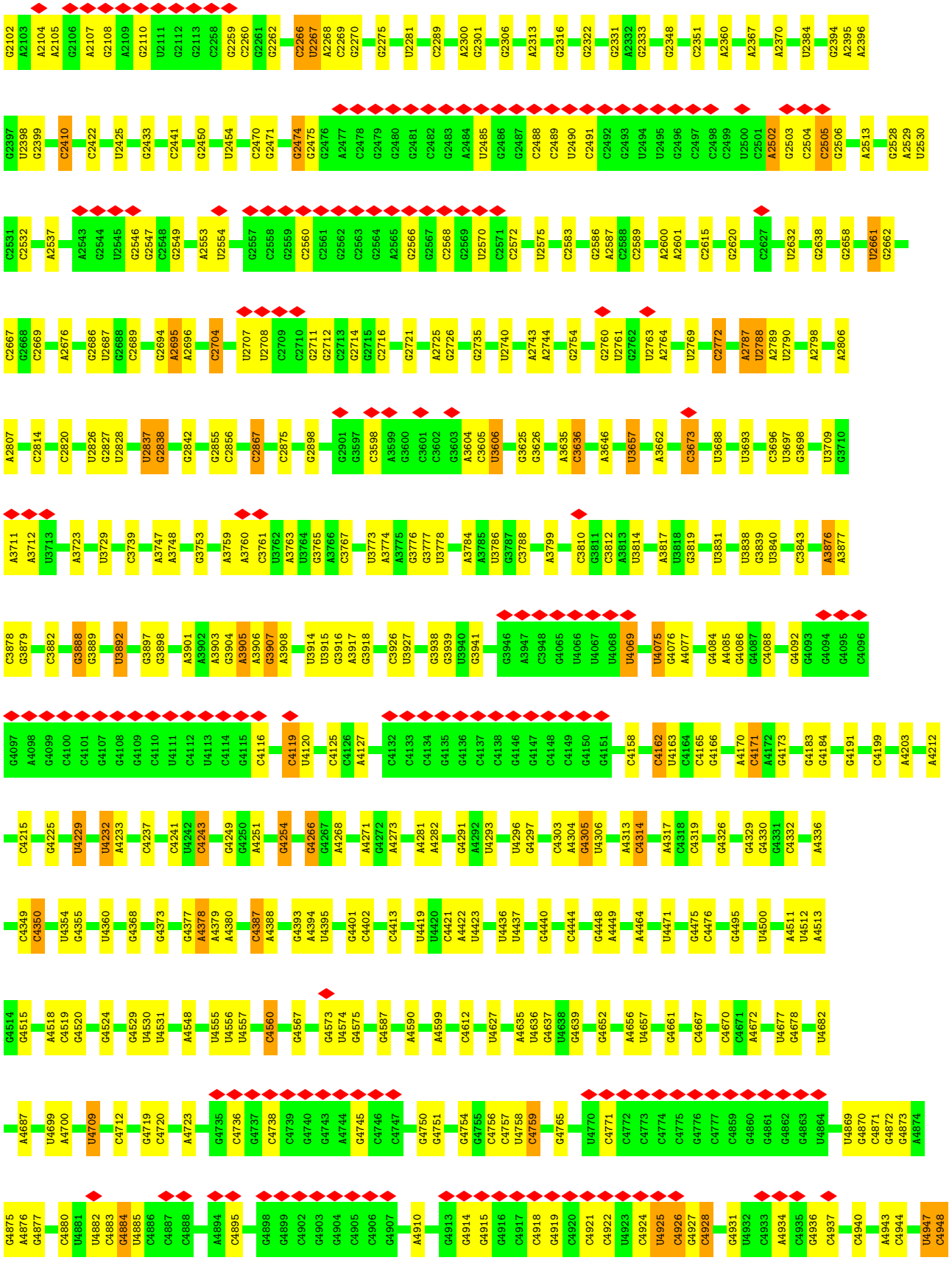


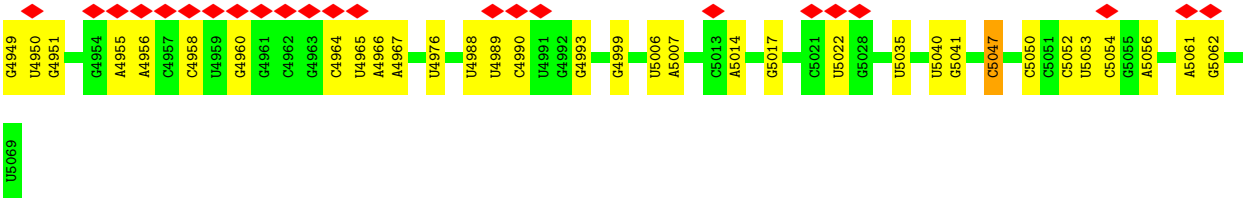
• Molecule 4: 28S ribosomal RNA

Chain 5:



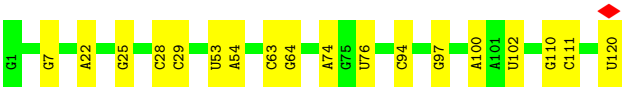

G219 C220 C221 U224 G225 G226 U233 G234 C245 G246 G254 C255 G256 C257 G258 C259 C260 G261 G262 G263 C264 C265 C266 C271 U272 C275 C276 G277 G278 A279 G280 U281 C282 U297 A306 C309 G310 G315 U316 C322 A334 C340 C345 C350
A363 A385 A386 G387 G399 C406 A407 A410 G411 G412 G413 G431 U432 C436 U440 C446 C449 G450 C451 A452 G453 U454 C455 C460 G461 G462 A463 G464 G465 A466 U467 U468 C469 C472 C480 G481 C481A G482 G483 U484 C485 C486 G487 U492 G493 C494 C495
G496 G497 C498 G499 G500 G504 G505 U512 C515 C516 C517 G518 C519 U520 C521 C522 C523 G638 U639 C640 G641 G642 C643 G644 G645 G646 G647 G648 C654 C657 C658 G659 G660 C661 C662 G666 A667 C668 C669 G670 C683 G684 C685 A686 U687 A692 C693 C694 G695 C696 G697 G698 C699
G703 C704 G705 C719 G729 G730 G731 C738 C738A G739 G740 C741 G742 G743 A747 G748 G749 U750 C753 C754 C755 G756 G757 G758 G759 G760 C904 C905 C906 C907 U913 U914 A917 G918 C922 G922A C922B C923 C924 C925 G926 G927 C928 A929 G930 C931 A932 G933 C934 A935 G935A C936
G939 C940 C941 G942 A943 A944 U945 G959 A960 G961 C962 G963 A964 G965 A966 C967 C968 C969 G970 U971 G971A C972 C979 C983 C984 C985 C986 C987 C988 U989 C990 G1064 G1065 G1066 G1067 G1068 G1069 G1070 C1071 C1072 G1073 G1074 G1075 C1076 C1077 A1078 C1079 C1080 C1081 C1082 U1083 C1084 G1089 C1093
G1094 A1095 C1096 C1097 G1098 C1099 U1100 G1168 G1169 G1170 G1171 C1172 G1173 G1174 A1175 C1176 U1177 G1178 U1179 C1180 C1183 A1184 G1187 C1188 G1189 C1190 C1191 C1192 C1193 G1194 G1195 G1196 C1197 G1198 G1199 G1200 U1201 C1202 G1203 C1204 G1205 C1210 G1211 G1212 G1213 C1214 C1215 C1216 G1217 G1218 G1219 G1233 G1234 G1235 C1236 C1237 A1238 C1239
G1244 C1245 G1246 U1247 C1248 C1249 C1250 C1251 C1252 G1271 C1272 G1273 A1274 G1275 C1276 G1284 G1287 G1291 C1292 G1293 A1294 U1295 G1296 C1301 U1302 A1303 C1304 C1314 C1325 A1326 G1329 A1330 C1331 A1354 G1358 G1359 G1370 A1371 G1377 C1378 C1379 G1380 A1387 G1394 A1397 A1398
G1399 G1400 C1401 C1402 G1403 G1404 C1405 G1406 C1411 G1412 C1413 C1414 G1415 G1416 C1417 C1418 G1419 A1420 G1421 U1428 C1429 G1435 C1436 C1437 U1438 U1440 C1441 C1442 A1443 G1444 U1445 C1446 C1447 G1448 G1455 C1456 G1457 C1458 G1465 C1468 C1469 G1475 C1476 C1477 C1478 G1479 C1480 C1481 G1482 C1483 G1484 C1485
G1489 A1497 G1498 C1501 G1502 U1514 A1515 G1516 G1517 A1518 A1523 A1524 A1525 A1534 C1535 G1543 A1547 A1563 A1564 A1565 C1566 U1567 C1568 G1574 U1578 U1591 U1596 G1597 C1598 U1602 G1612 A1613 G1624 G1625 A1631 A1632 G1633 A1634 A1638 U1639 C1640 G1641
G1654 C1655 U1656 U1660 C1661 U1671 C1676 U1677 G1691 C1694 U1695 C1696 C1720 G1724 G1734 U1735 C1740 G1741 A1742 G1750 U1754 C1755 U1756 U1757 G1758 G1759 G1760 G1761 C1762 C1763 G1764 A1765 A1766 A1767 C1768 G1769 A1770 U1771 C1772 U1773 C1774 A1775 A1776 C1777 U1781 A1787
U1792 G1799 G1803 A1804 A1805 G1806 C1807 C1808 C1809 C1812 G1815 G1818 G1819 U1820 G1821 U1822 C1828 G1835 G1836 A1837 G1842 A1843 C1847 G1853 G1854 G1855 C1859 G1869 U1882 A1888 U1889 G1890 C1893 A1897 C1898 U1906 G1910 C1915 G1916 A1917 U1918
G1919 C1920 C1921 G1922 A1923 A1929 U1930 C1931 G1940 G1948 U1957 A1958 U1959 A1960 G1961 A1962 C1963 A1964 G1965 C1966 A1967 G1968 G1969 A1970 U1971 G1972 G1973 U1974 G1975 G1976 C1977 C1978 A1979 U1980 G1981 G1982 A1983 A1984 G1985 U1986 C1987 G1988 G1989 A1990 A1991 U1992 C1993 C1994 G1995 C1996 U1997 A1998 A1999 G2000 G2001 A2002
G2003 U2004 G2005 U2006 G2007 U2008 A2009 A2010 C2011 A2012 A2013 C2014 U2015 C2016 A2017 C2018 C2019 U2020 G2021 C2022 C2023 G2024 A2025 A2026 G2034 G2046 A2047 U2048 G2052 G2055 G2056 C2062 G2063 G2064 C2068 A2069 U2070 U2084 G2085 G2089 U2090 C2091 G2092 G2093 C2094 A2095 G2096 A2097 G2098 C2099 G2100 A2101





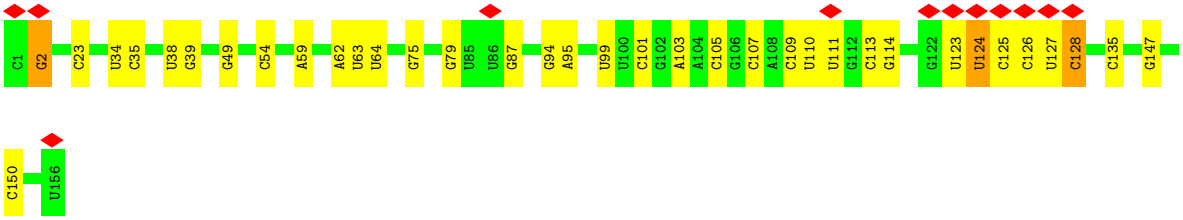
• Molecule 5: 5S rRNA

Chain 7:



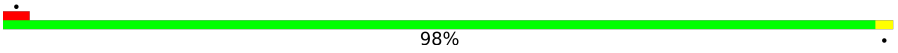
• Molecule 6: 5.8S ribosomal RNA

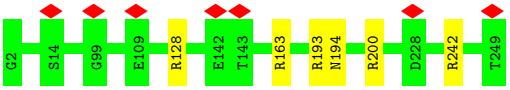
Chain 8:



• Molecule 7: uL2

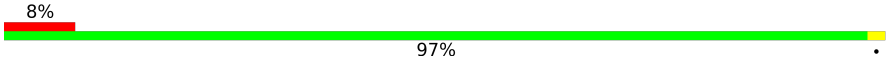
Chain A:

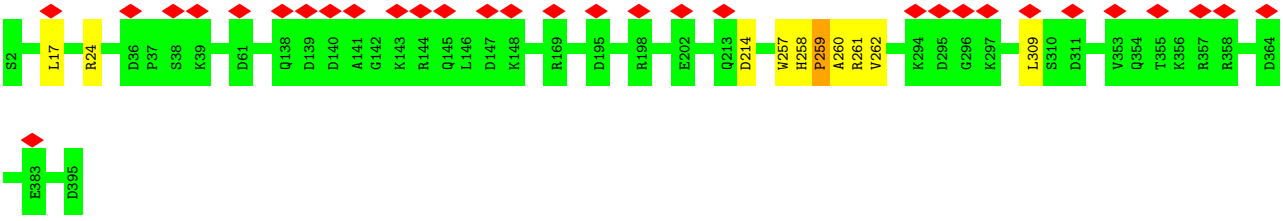




• Molecule 8: uL3

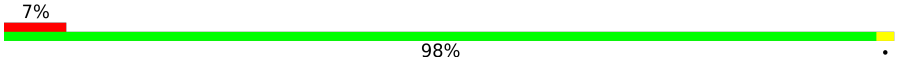
Chain B:

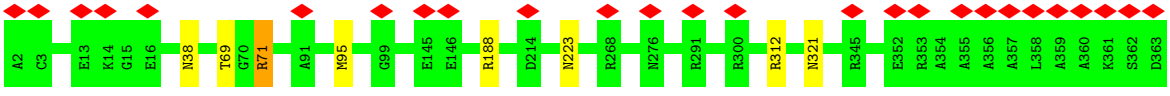




• Molecule 9: uL4

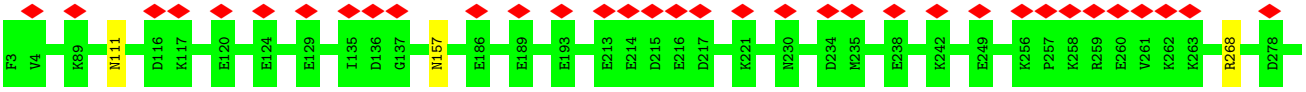
Chain C:

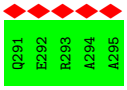




• Molecule 10: 60S ribosomal protein L5

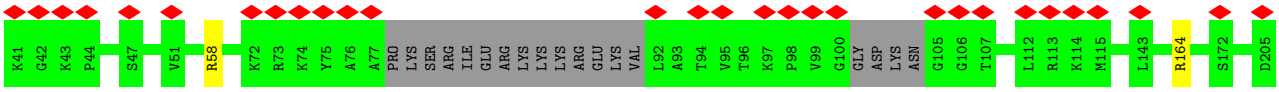
Chain D:

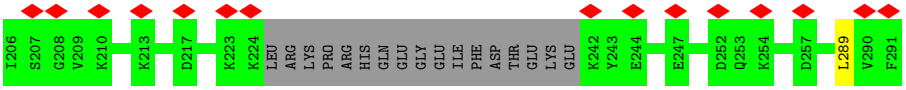




• Molecule 11: 60S ribosomal protein L6

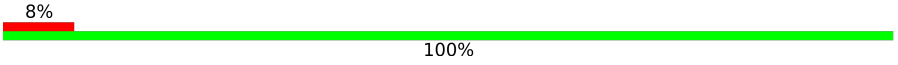
Chain E:

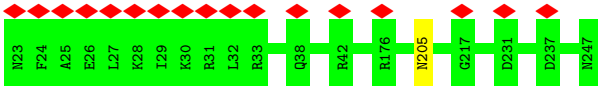




• Molecule 12: uL30

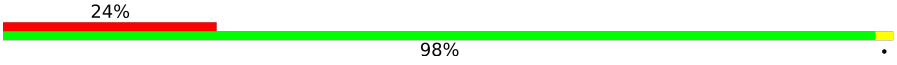
Chain F:

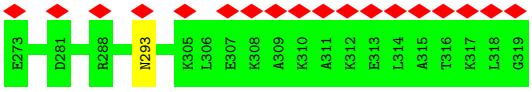




• Molecule 13: eL8

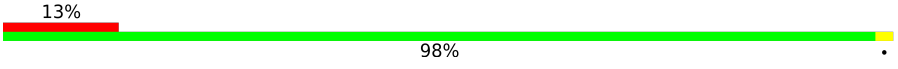
Chain G:

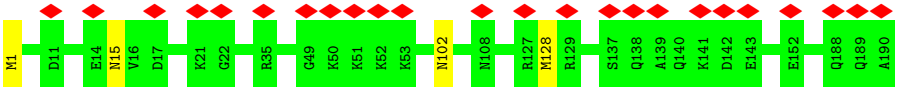




• Molecule 14: uL6

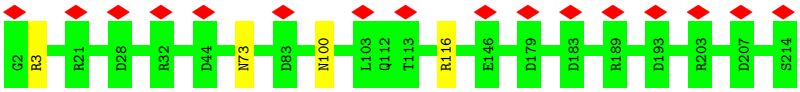
Chain H:





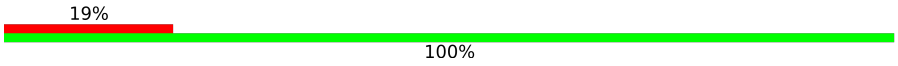
• Molecule 15: Ribosomal protein L10 (Predicted)

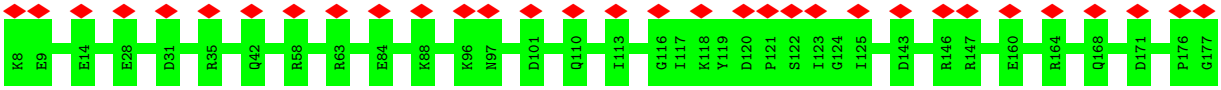
Chain I:



• Molecule 16: Ribosomal protein L11

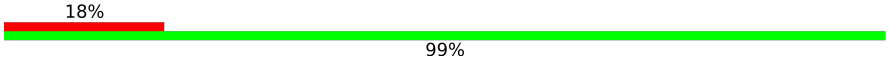
Chain J:

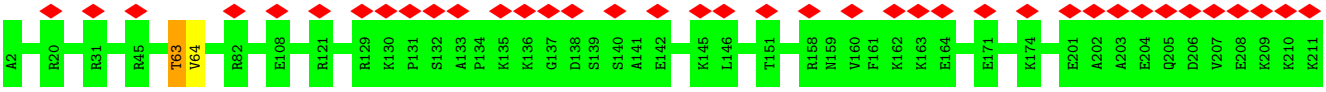




• Molecule 17: 60S ribosomal protein L13

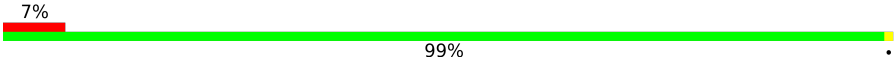
Chain L:

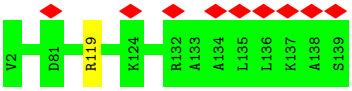




• Molecule 18: Ribosomal protein L14

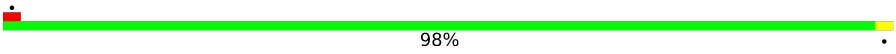
Chain M:

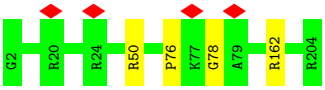




• Molecule 19: Ribosomal protein L15

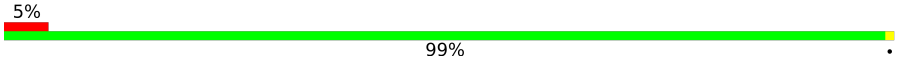
Chain N:

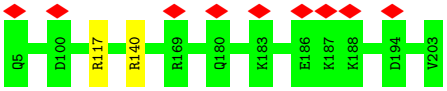




• Molecule 20: uL13

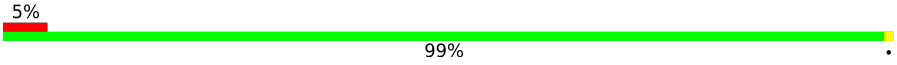
Chain O:

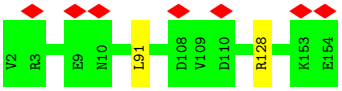




• Molecule 21: uL22

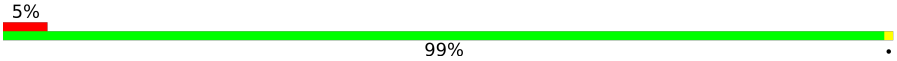
Chain P:

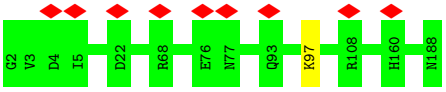




• Molecule 22: eL18

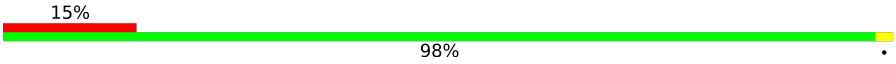
Chain Q:

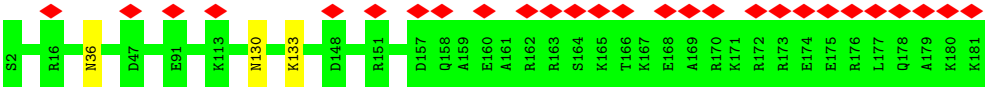




• Molecule 23: eL19

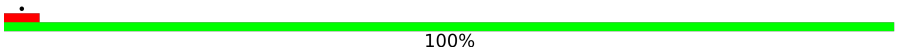
Chain R:

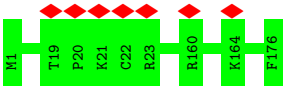




• Molecule 24: eL20

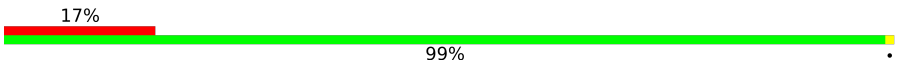
Chain S:

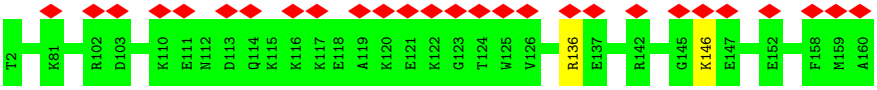




• Molecule 25: eL21

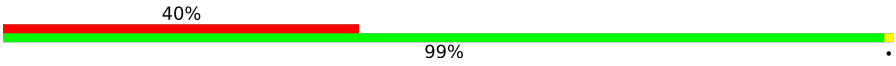
Chain T:

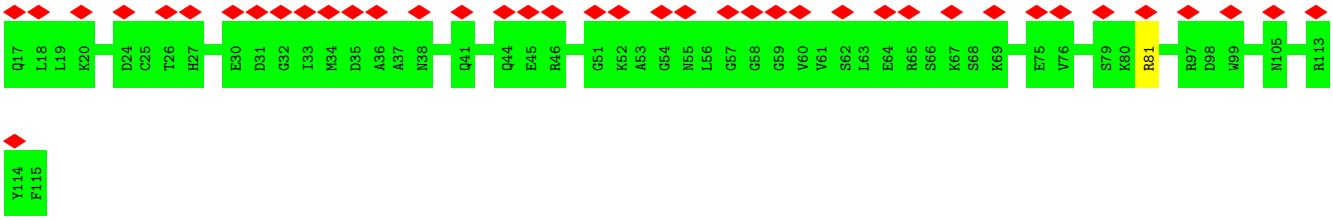




• Molecule 26: eL22

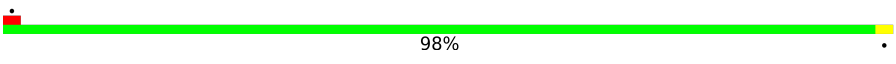
Chain U:

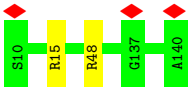




• Molecule 27: eL14

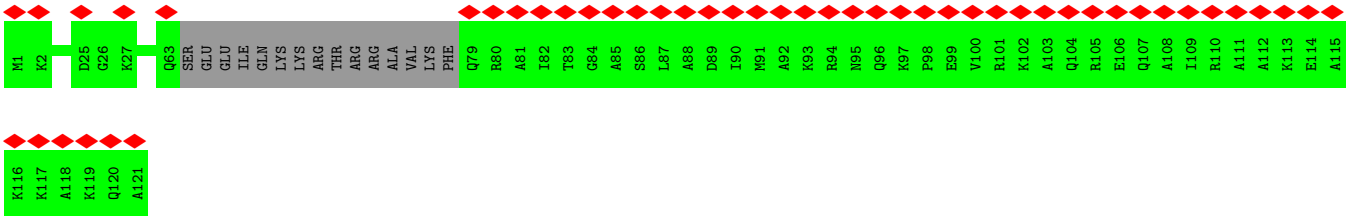
Chain V:





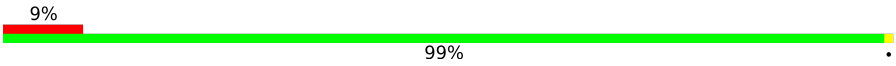
• Molecule 28: Ribosomal protein L24

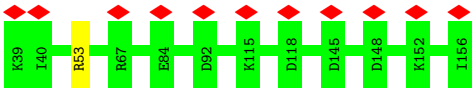
Chain W:



• Molecule 29: uL23

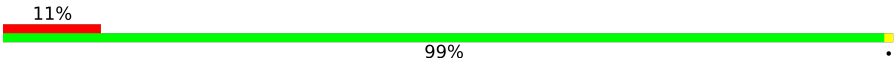
Chain X:

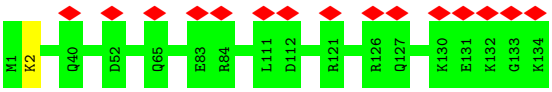




• Molecule 30: Ribosomal protein L26

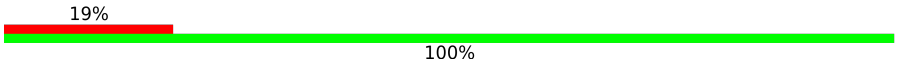
Chain Y:

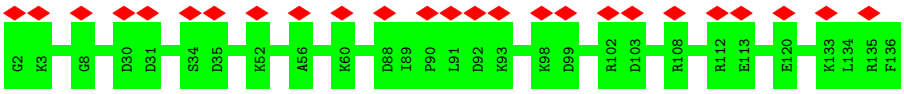




• Molecule 31: 60S ribosomal protein L27

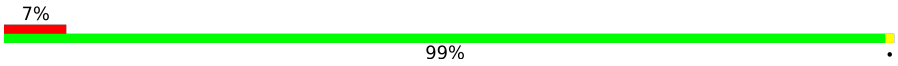
Chain Z:

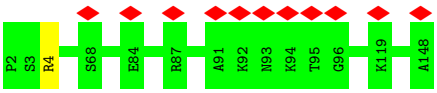




• Molecule 32: uL15

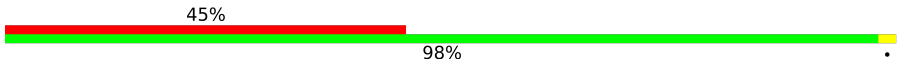
Chain a:

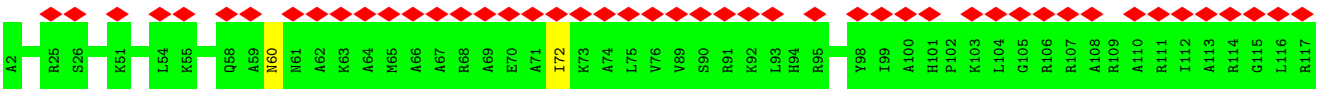




• Molecule 33: eL29

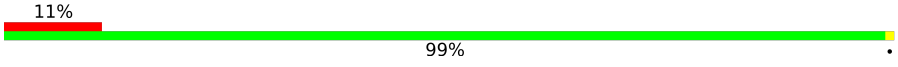
Chain b:

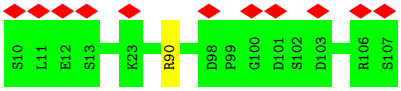




• Molecule 34: eL30

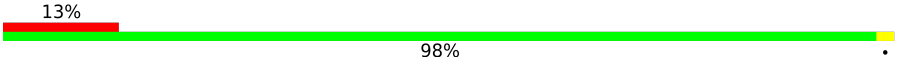
Chain c:

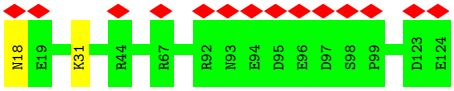




• Molecule 35: eL31

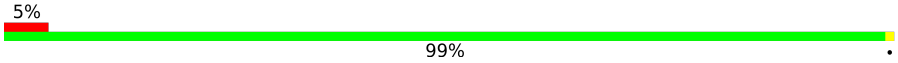
Chain d:

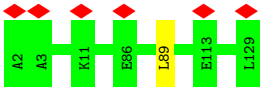




• Molecule 36: eL32

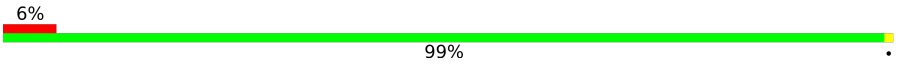
Chain e:

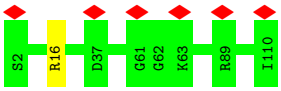




• Molecule 37: eL33

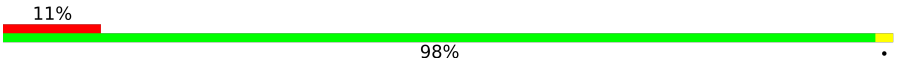
Chain f:

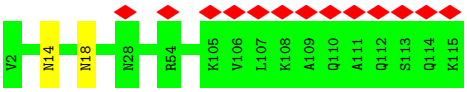




• Molecule 38: eL34

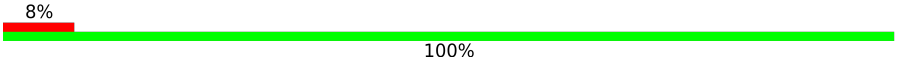
Chain g:

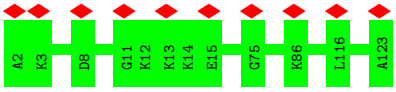




• Molecule 39: uL29

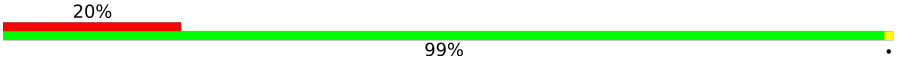
Chain h:

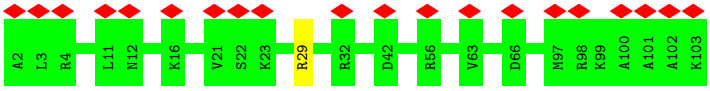




• Molecule 40: 60S ribosomal protein L36

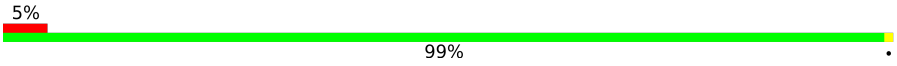
Chain i:

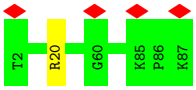




• Molecule 41: Ribosomal protein L37

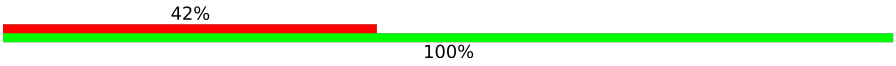
Chain j:

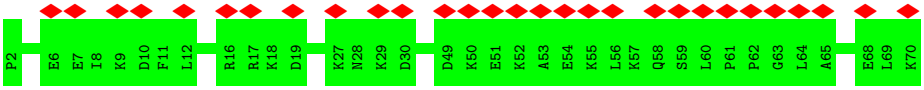




• Molecule 42: eL38

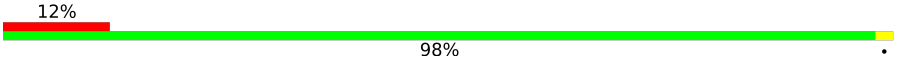
Chain k:

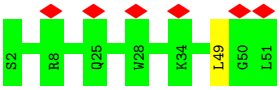




• Molecule 43: eL39

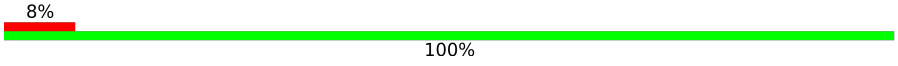
Chain l:

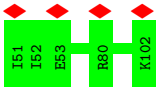




• Molecule 44: eL40

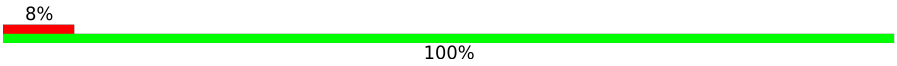
Chain m:

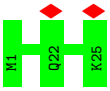




• Molecule 45: 60s ribosomal protein l41

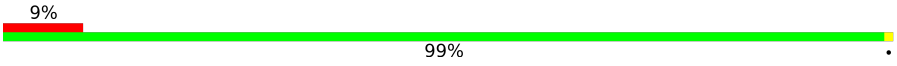
Chain n:

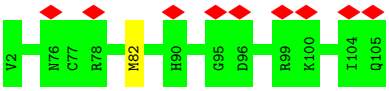




• Molecule 46: eL42

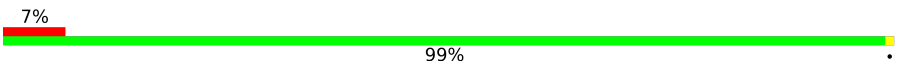
Chain o:

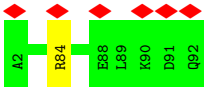




• Molecule 47: ribosomal protein eL43

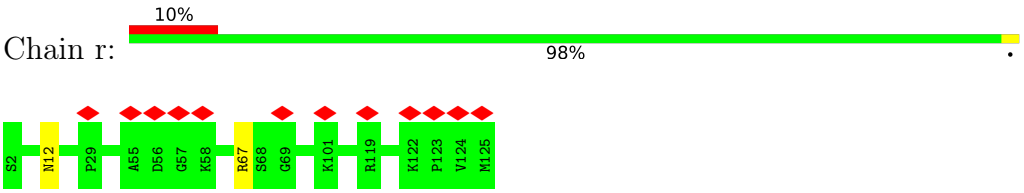
Chain p:





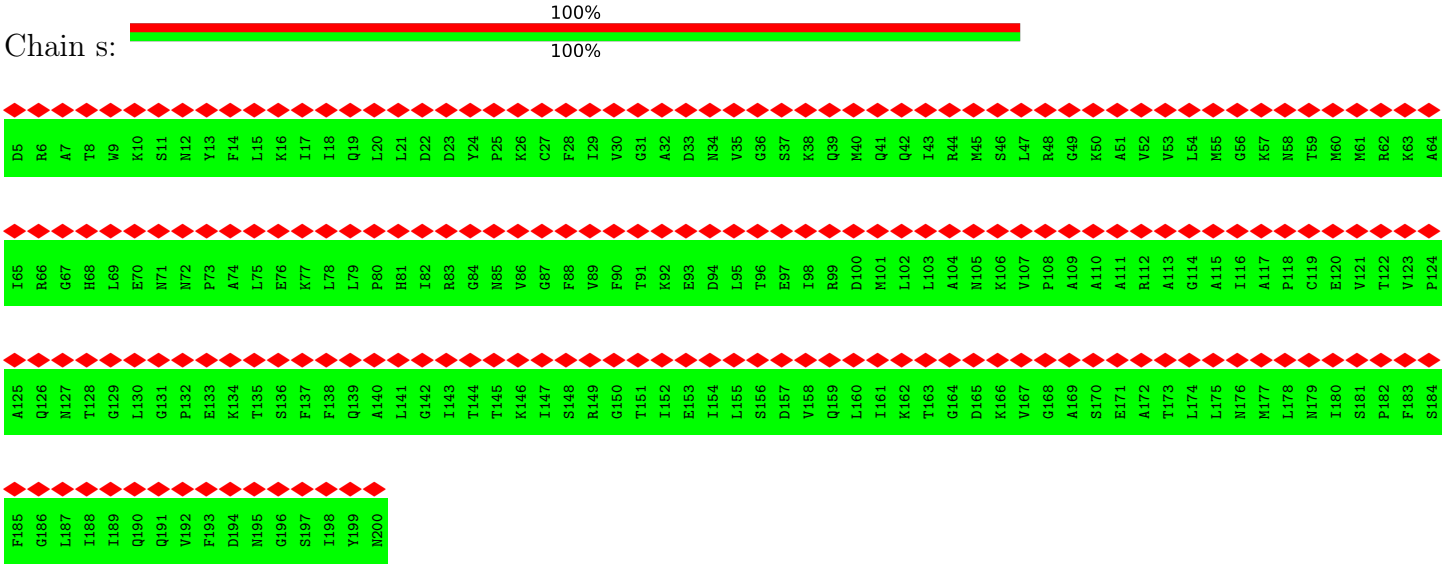
• Molecule 48: eL28

Chain r:



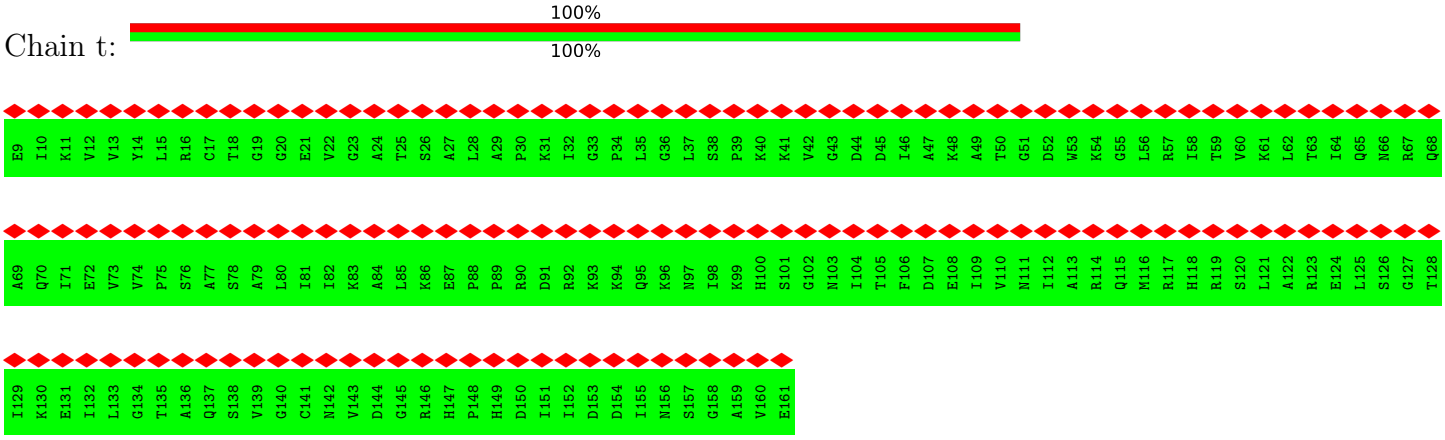
• Molecule 49: 60S acidic ribosomal protein P0

Chain s:



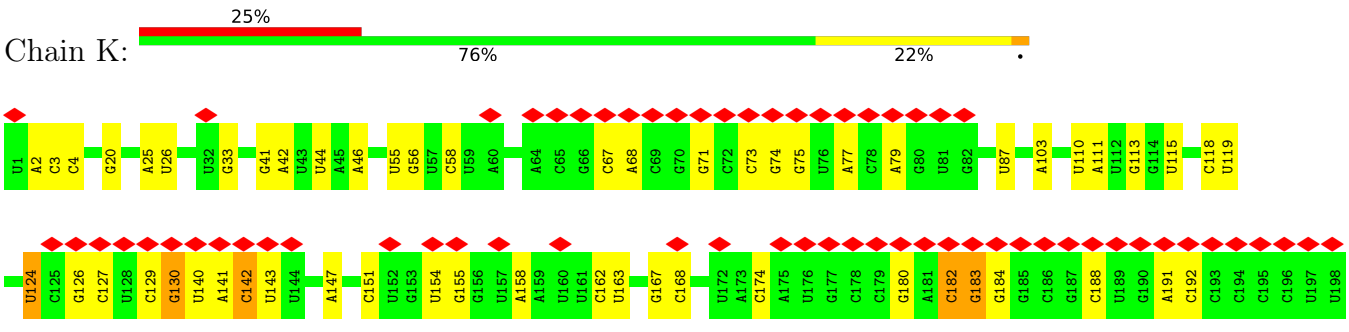
• Molecule 50: uL11

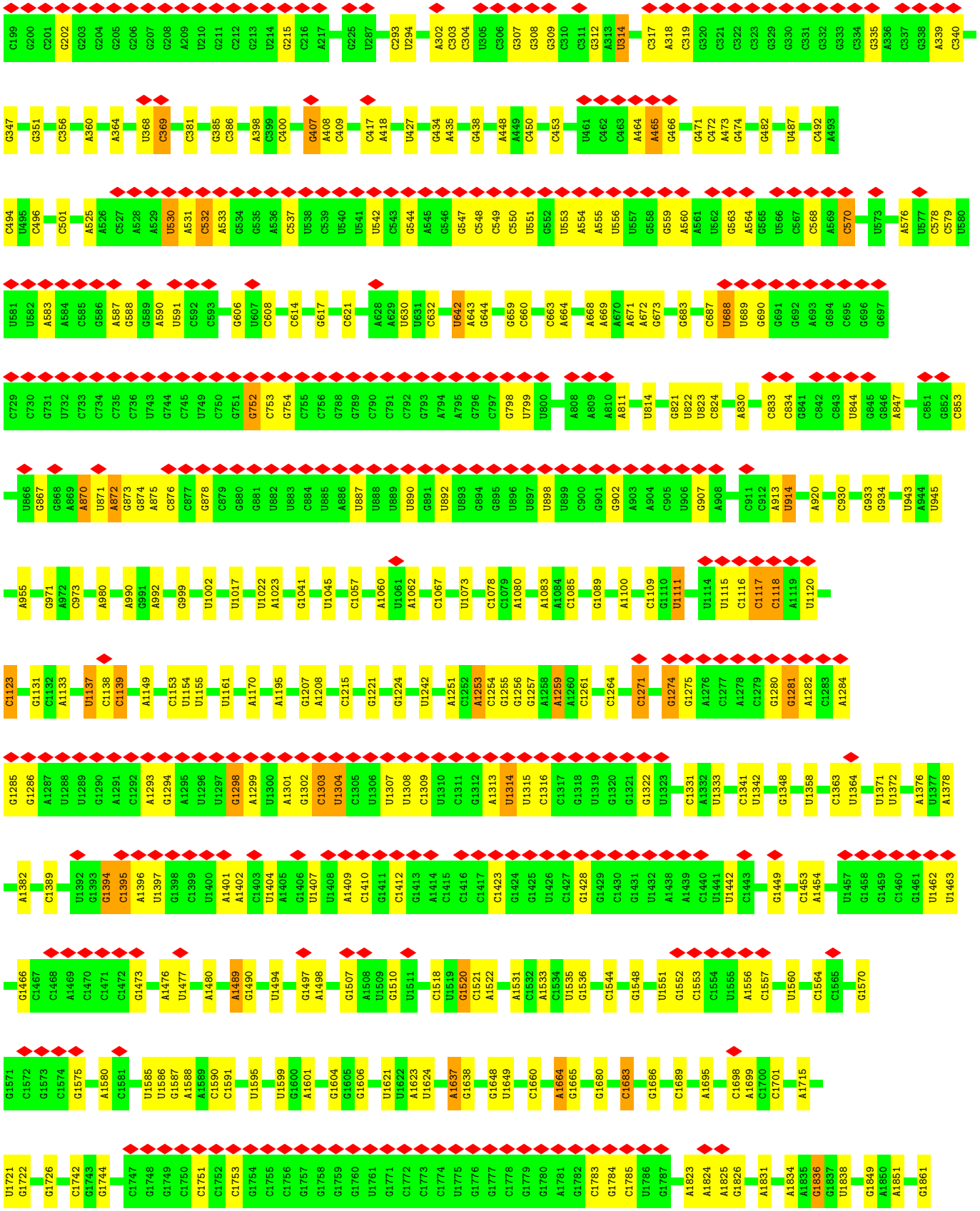
Chain t:

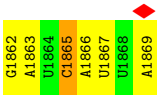


• Molecule 51: 18S ribosomal RNA

Chain K:

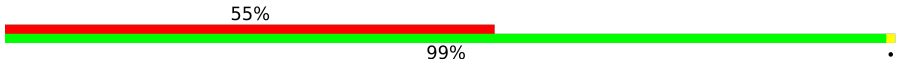


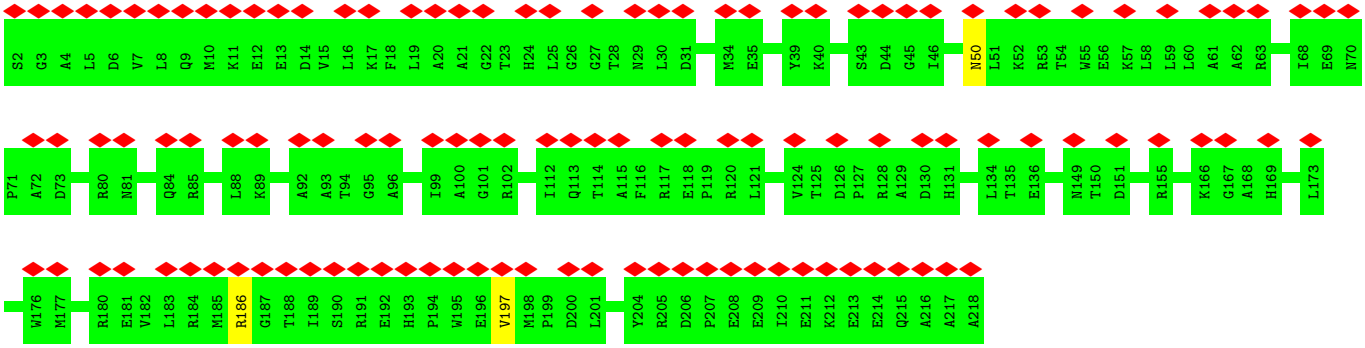

C199 G200 C201 G202 G203 G204 G205 G206 G207 G208 A209 U210 G211 C212 G213 U214 G215 C216 A217 G225 U287 C293 U294 A302 C303 C304 U305 C306 G307 G308 G309 C310 C311 G312 A313 U314 C317 A318 C319 G320 C321 C322 C323 G329 G330 C331 G332 G333 C334 G335 A336 C337 G338 A339 C340
G347 G351 C356 A360 A364 U368 C369 C381 G385 C386 A398 C399 C400 G407 A408 C409 C417 A418 U427 G434 A435 G438 A448 A449 C450 C453 U461 C462 C463 A464 A465 G466 G471 C472 A473 G474 G482 U487 C492 A493
C494 U495 C496 C501 A525 A526 C527 A528 A529 U530 A531 C532 A533 G534 G535 A536 C537 G538 C539 U540 U541 U542 G543 G544 A545 G546 G547 C548 C549 C550 U551 G552 U553 A554 A555 U556 G557 G558 G559 A560 A561 U562 G563 A564 G565 U566 C567 C568 A569 C570 U573 A576 U577 C578 C579 U580
U581 U582 A583 A584 C585 G586 A587 G588 G589 A590 U591 C592 C593 G606 U607 C608 C614 G617 C621 A628 A629 U630 U631 C632 U642 A643 G644 G659 C660 C663 A664 A668 A669 A670 A671 A672 G673 G683 C687 U688 U689 G690 G691 G692 A693 G694 C695 G696 G697
C729 C730 G731 U732 C733 C734 C735 C736 U743 G744 C745 U749 C750 G751 G752 C753 G754 C755 C756 G788 G789 C790 C791 C792 G793 A794 A795 G796 C797 G798 U799 U800 A808 A809 A810 A811 U814 G821 U822 U823 C824 A830 C833 C834 G841 C842 C843 U844 G845 G846 A847 C851 G852 C853
U866 G867 G868 A869 A870 U871 A872 G873 G874 A875 C876 C877 G878 C879 G880 G881 U882 U883 C884 U885 A886 U887 U888 U889 U890 G891 U892 U893 G894 G895 U896 U897 U898 U899 C900 G901 G902 A903 A904 C905 U906 G907 A908 C911 C912 A913 U914 A920 C930 G933 G934 U943 A944 U945
A955 G971 A972 C973 A980 A990 G991 A992 G999 U1002 U1017 U1022 A1023 G1041 U1045 C1057 A1060 U1061 A1062 C1067 U1073 C1078 C1079 A1080 A1083 A1084 C1085 G1089 A1100 C1109 G1110 U1111 U1114 U1115 C1116 C1117 C1118 A1119 U1120
C1123 G1131 C1132 A1133 U1137 C1138 C1139 A1149 C1153 U1154 U1155 U1161 A1170 A1195 G1207 A1208 C1215 G1221 G1224 U1242 A1251 C1252 A1253 C1254 G1255 G1256 G1257 A1258 A1259 A1260 C1261 C1264 C1271 G1274 G1275 A1276 C1277 A1278 C1279 G1280 G1281 A1282 C1283 A1284
G1285 G1286 A1287 U1288 U1289 G1290 A1291 C1292 A1293 G1294 A1295 U1296 U1297 G1298 A1299 U1300 A1301 G1302 C1303 U1304 C1305 U1306 U1307 U1308 C1309 U1310 C1311 G1312 A1313 U1314 U1315 C1316 C1317 G1318 U1319 G1320 G1321 G1322 U1323 C1331 A1332 U1333 C1341 U1342 G1348 U1358 C1363 U1364 U1371 U1372 A1376 U1377 A1378
A1382 C1389 U1392 G1393 G1394 C1395 A1396 U1397 G1398 C1399 U1400 A1401 A1402 C1403 U1404 A1405 G1406 U1407 U1408 A1409 C1410 G1411 C1412 G1413 A1414 C1415 C1416 C1417 C1423 G1424 G1425 U1426 C1427 G1428 G1429 C1430 G1431 U1432 A1438 A1439 C1440 U1441 U1442 C1443 G1449 C1453 A1454 U1457 G1458 G1459 C1460 G1461 U1462 U1463
G1466 C1467 C1468 A1469 C1470 C1471 C1472 G1473 A1476 U1477 A1480 A1489 G1490 U1494 G1497 A1498 G1507 A1508 U1509 G1510 U1511 C1518 U1519 G1520 C1521 A1522 A1531 C1532 A1533 C1534 U1535 G1536 C1544 G1548 U1551 G1552 C1553 C1554 U1555 A1556 C1557 U1560 C1564 C1565 G1570
G1571 C1572 G1573 C1574 G1575 A1580 C1581 U1585 U1586 G1587 A1588 A1589 C1590 C1591 U1595 U1599 G1600 A1601 G1604 G1605 G1606 U1621 U1622 A1623 U1624 A1637 G1638 G1648 U1649 C1660 A1664 G1665 G1680 C1683 G1686 C1689 A1695 C1698 A1699 C1700 C1701 A1715
U1721 G1722 G1726 C1742 G1743 G1744 C1747 G1748 G1749 G1750 C1751 C1752 C1753 G1754 C1755 C1756 G1757 G1758 G1759 G1760 U1761 G1771 C1772 C1773 C1774 U1775 G1776 G1777 C1778 G1779 G1780 A1781 G1782 C1783 G1784 C1785 U1786 G1787 A1823 A1824 A1825 G1826 A1831 A1834 A1835 G1836 G1837 U1838 G1849 A1850 A1851 G1861



• Molecule 52: uS2

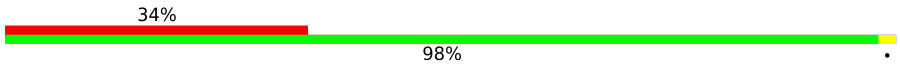
Chain q:

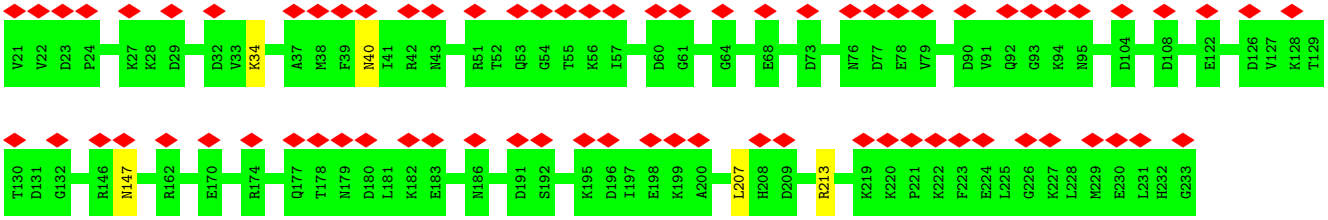




• Molecule 53: 40S ribosomal protein S3a

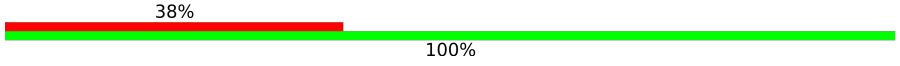
Chain u:

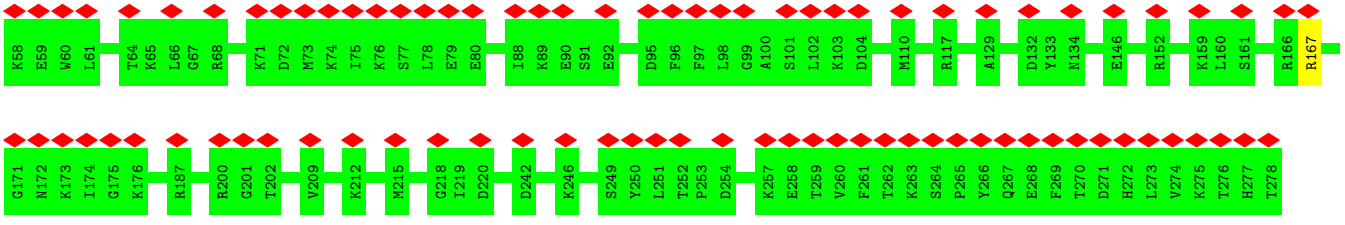




• Molecule 54: uS5

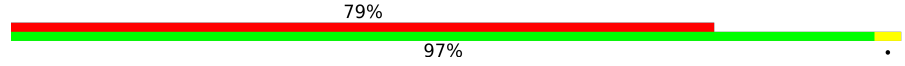
Chain v:

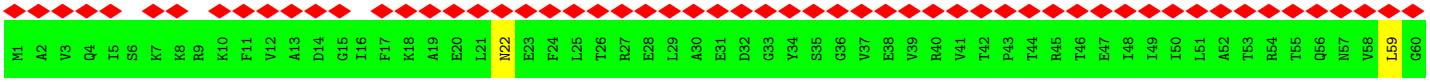


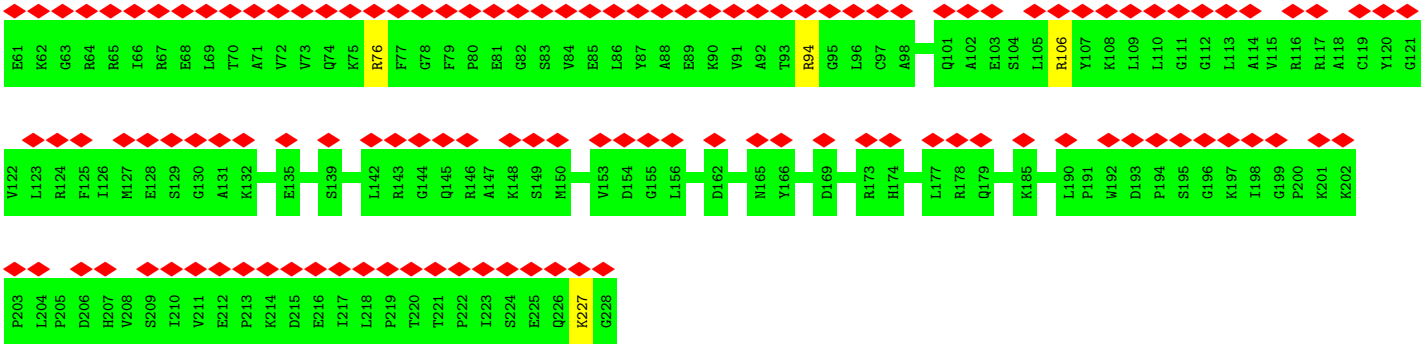


• Molecule 55: Ribosomal protein S3

Chain w:

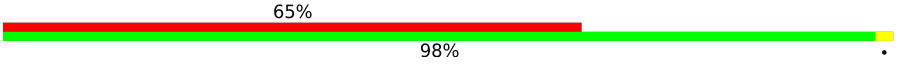


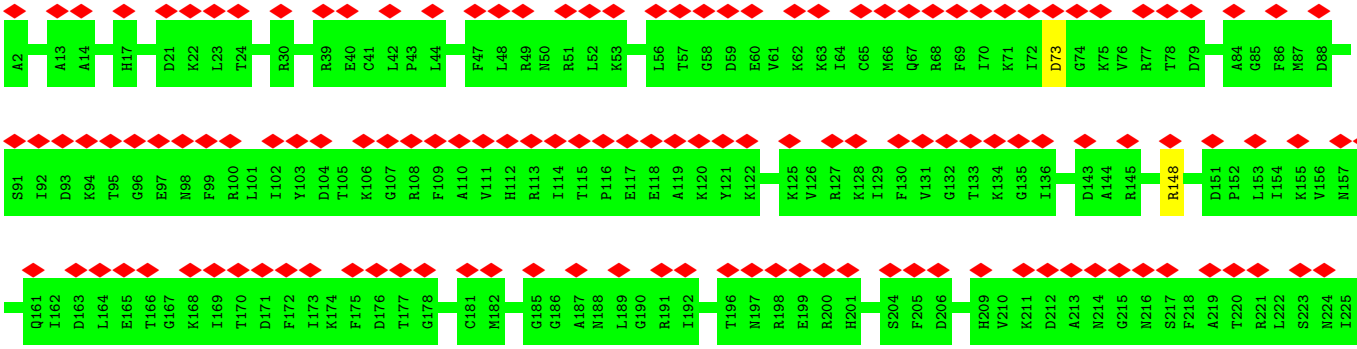




• Molecule 56: 40S ribosomal protein S4

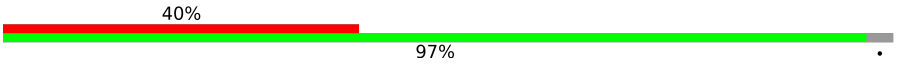
Chain x:

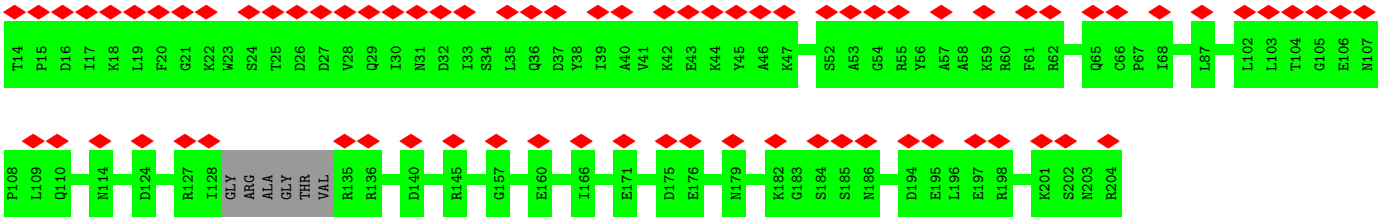




• Molecule 57: Ribosomal protein S5

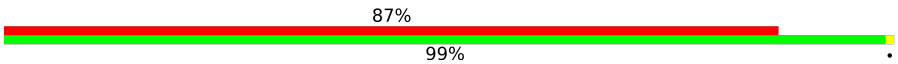
Chain y:

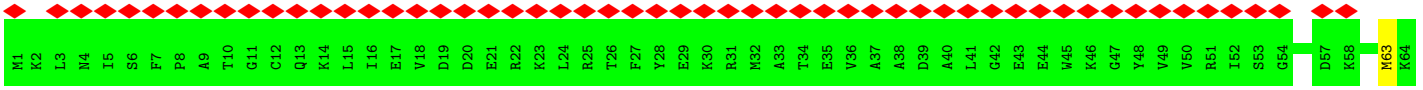


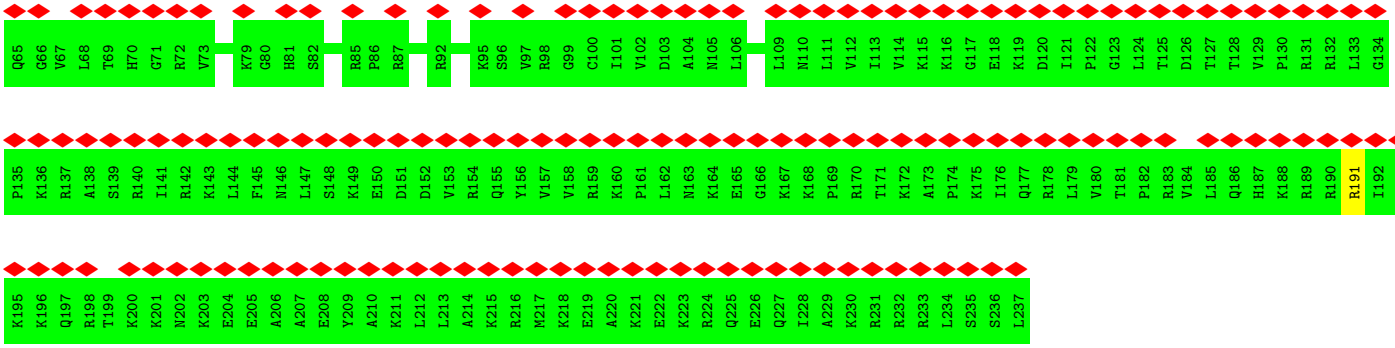


• Molecule 58: 40S ribosomal protein S6

Chain z:

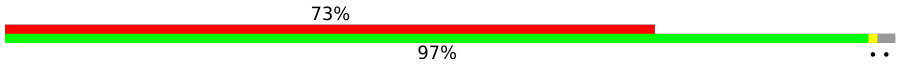


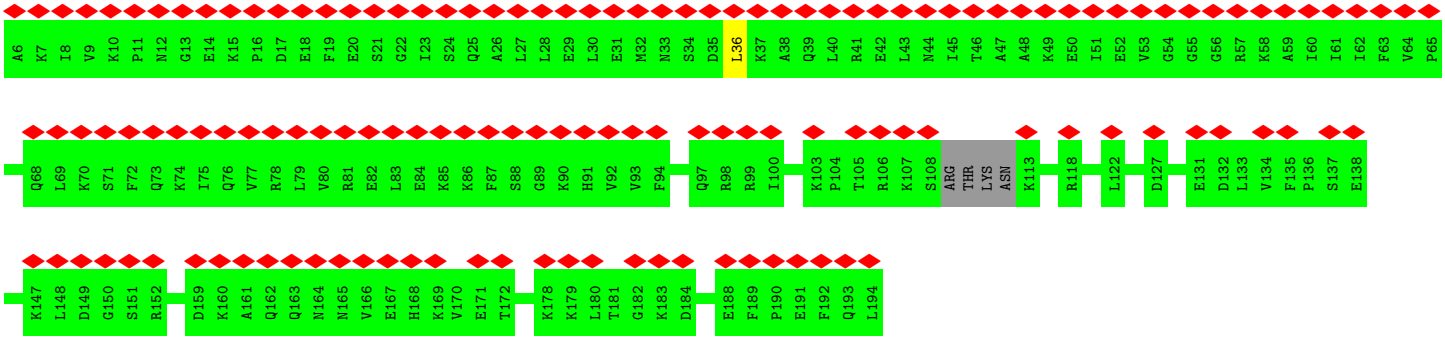




• Molecule 59: 40S ribosomal protein S7

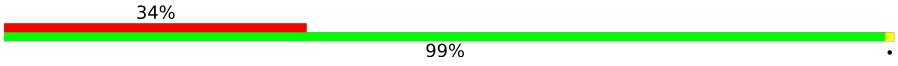
Chain BB:

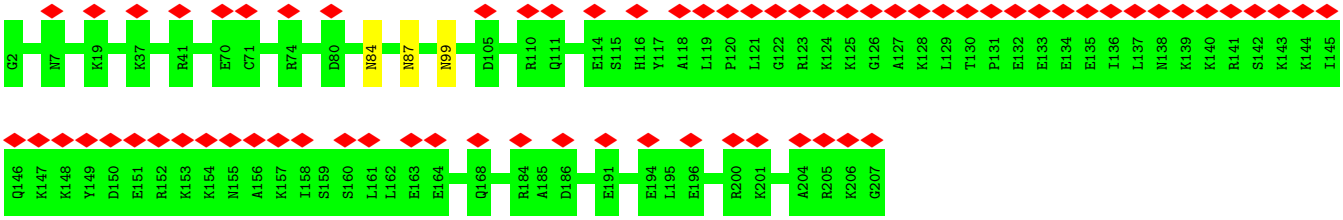




• Molecule 60: 40S ribosomal protein S8

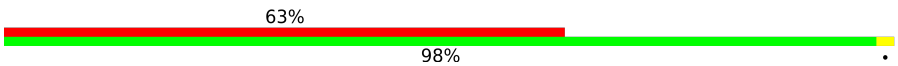
Chain CC:

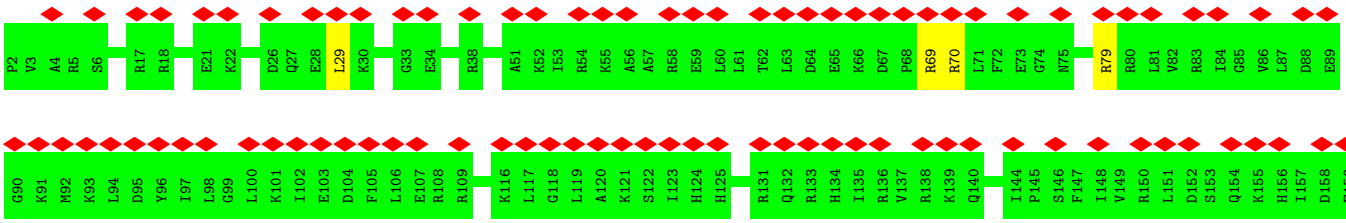


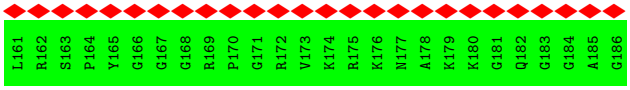


• Molecule 61: Ribosomal protein S9 (Predicted)

Chain DD:

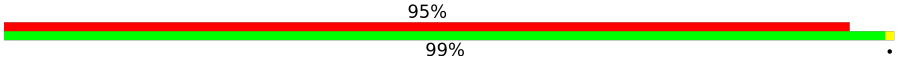


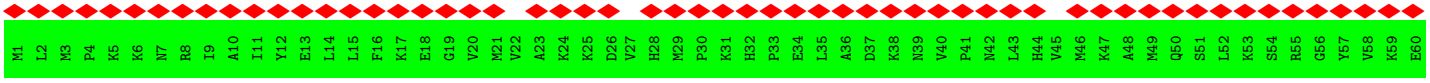


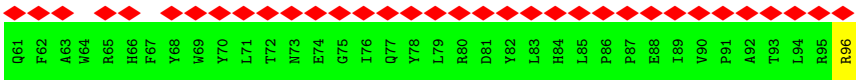


• Molecule 62: eS10

Chain SS:

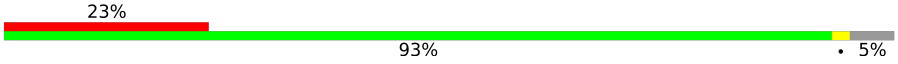


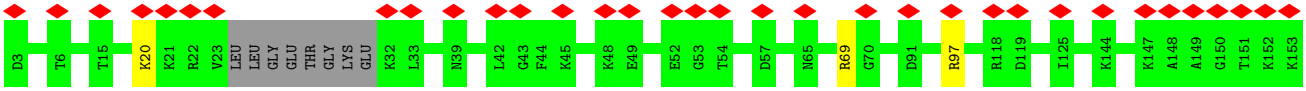




• Molecule 63: Ribosomal protein S11

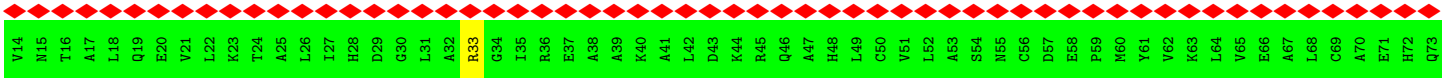
Chain EE:

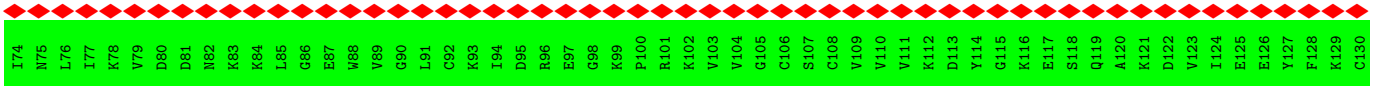




• Molecule 64: 40S ribosomal protein S12

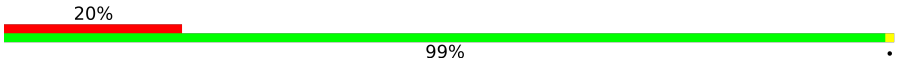
Chain RR:

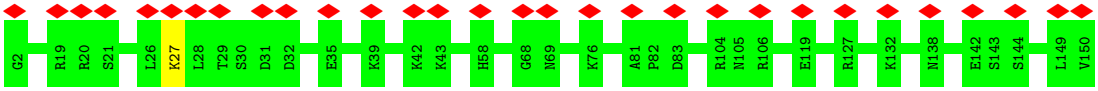




• Molecule 65: ribosomal protein uS15

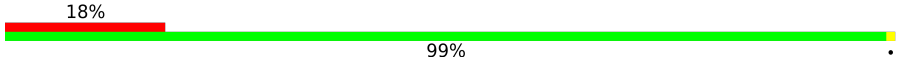
Chain QQ:

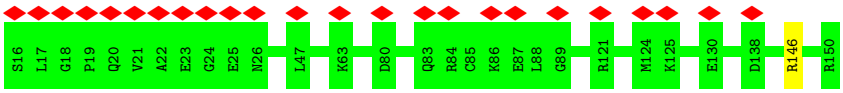




• Molecule 66: uS11

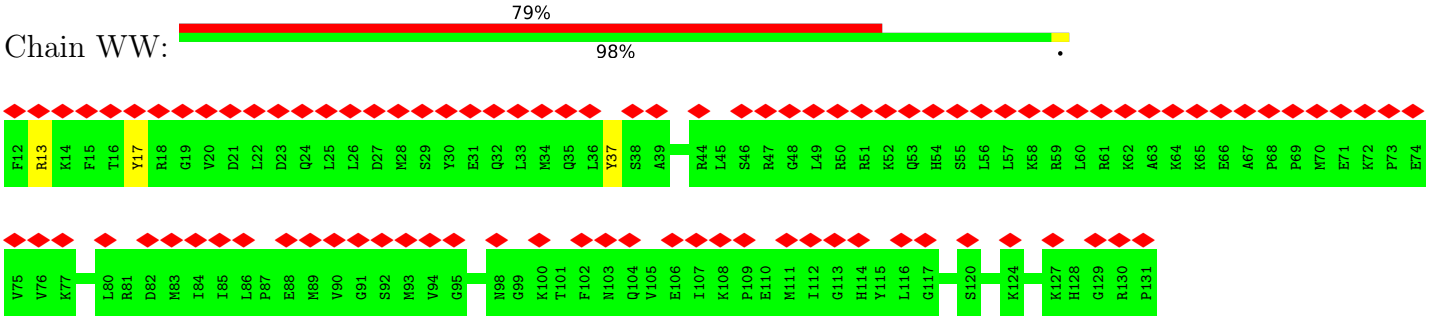
Chain MM:





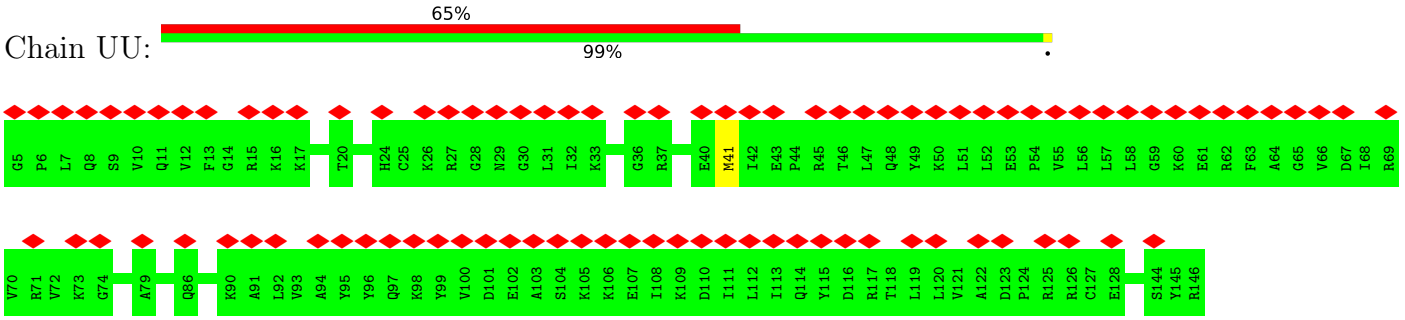
• Molecule 67: uS17

Chain WW:



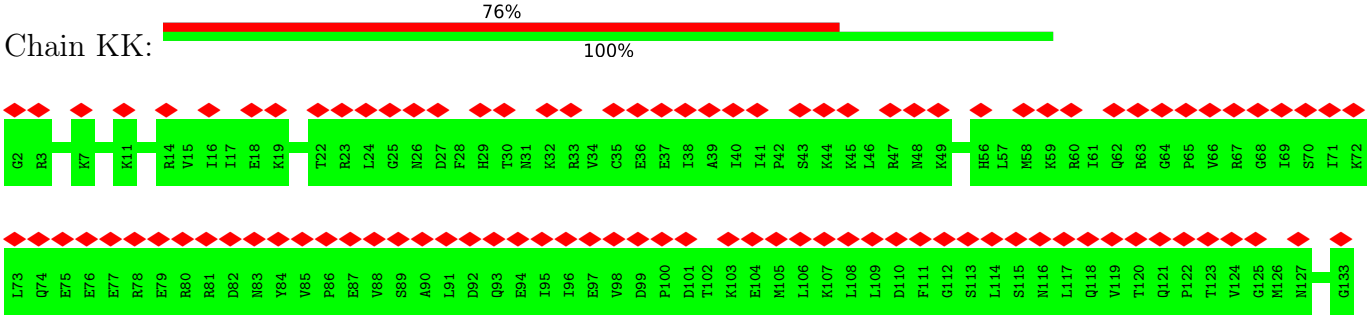
• Molecule 68: Ribosomal protein S16

Chain UU:



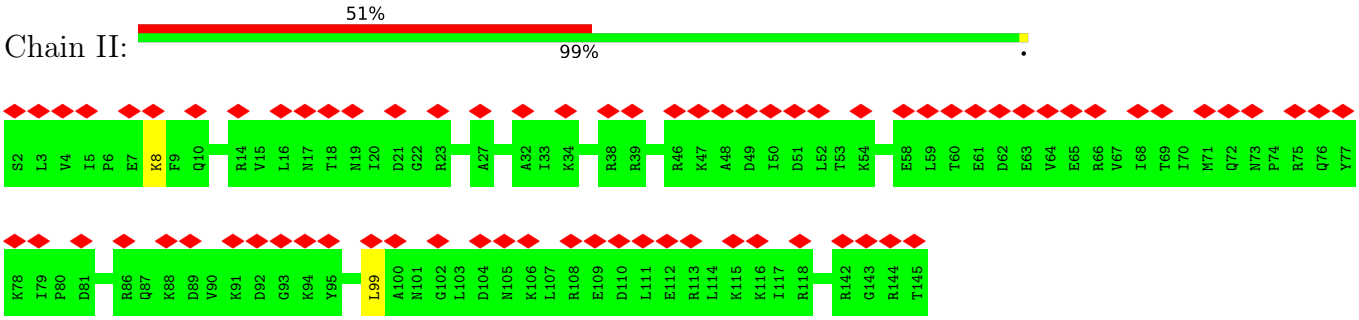
• Molecule 69: eS17

Chain KK:



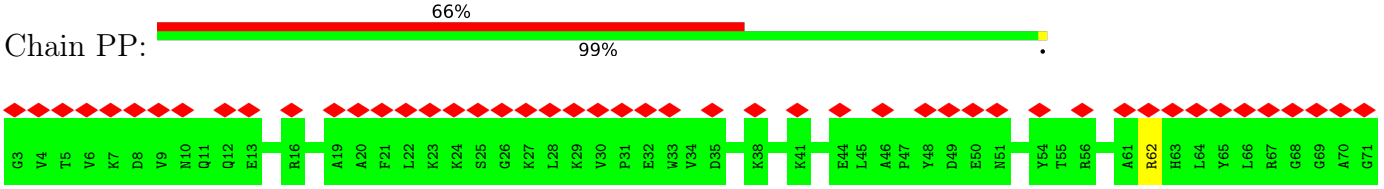
• Molecule 70: uS13

Chain II:



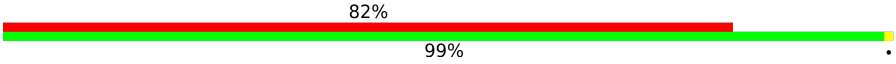
• Molecule 71: eS19

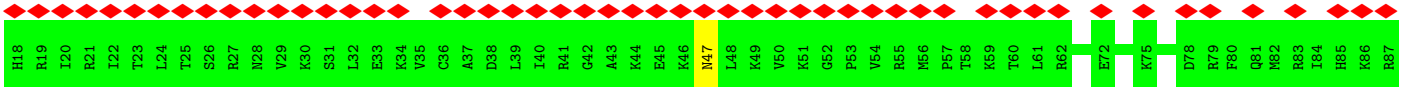
Chain PP:

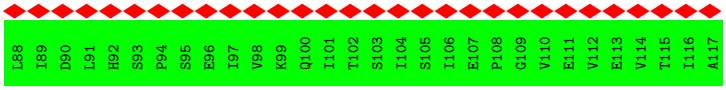


• Molecule 72: uS10

Chain GG:

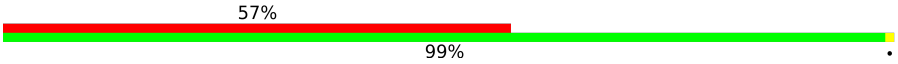


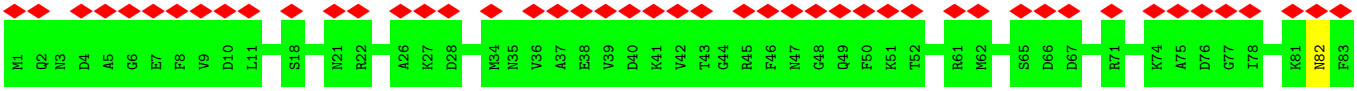




• Molecule 73: eS21

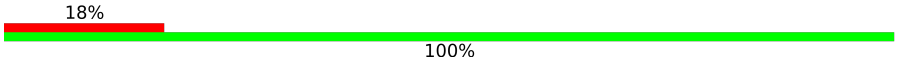
Chain HH:

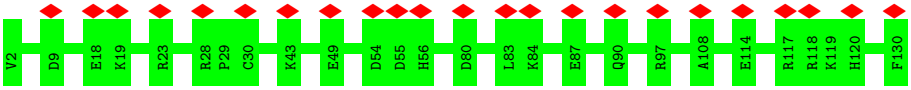




• Molecule 74: Ribosomal protein S15a

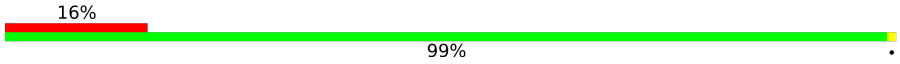
Chain TT:

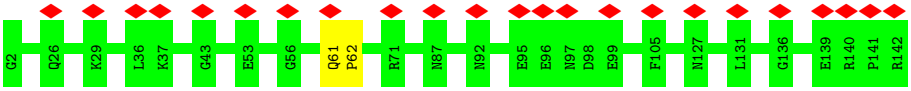




• Molecule 75: Ribosomal protein S23

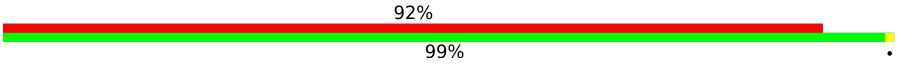
Chain VV:

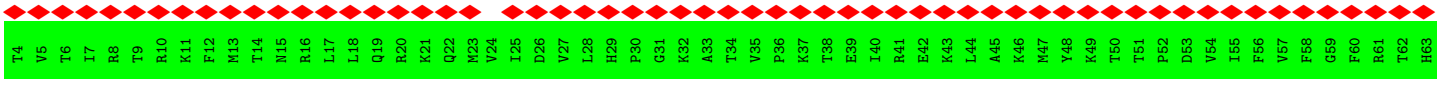


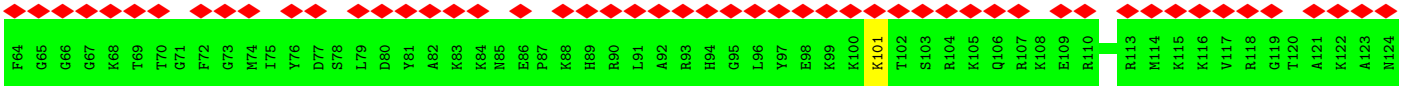


• Molecule 76: eS24

Chain NN:

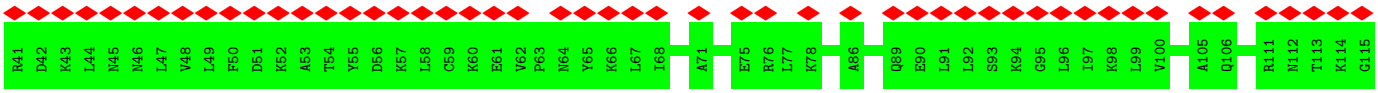






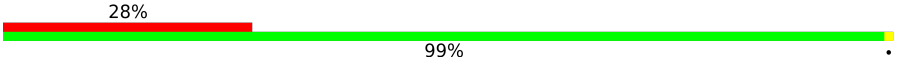
• Molecule 77: ribosomal protein eS25

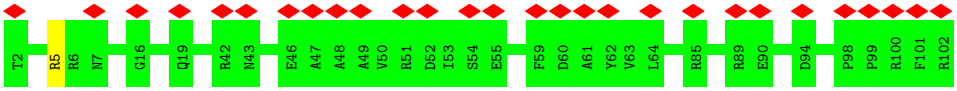
Chain OO:



• Molecule 78: eS26

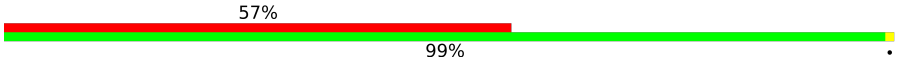
Chain LL:

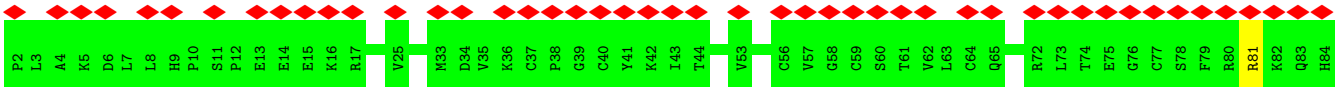




• Molecule 79: 40S ribosomal protein S27

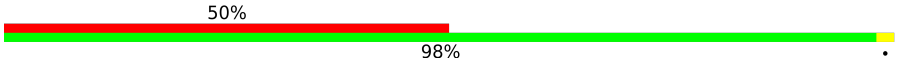
Chain JJ:

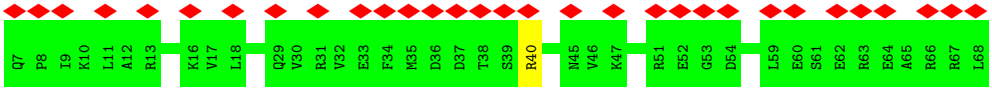




• Molecule 80: Ribosomal protein S28

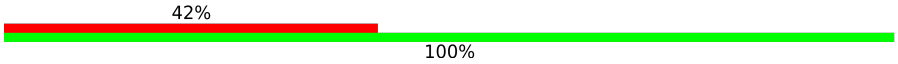
Chain FF:

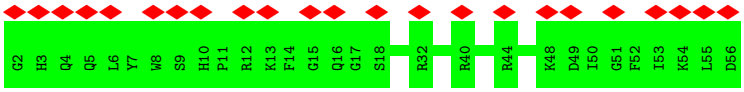




• Molecule 81: uS14

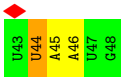
Chain 9:





• Molecule 82: mRNA

Chain 4:



• Molecule 83: eS31

Chain 0:

K83 S84 Y85 T86 T87 P88 K89 K90 N91 K92 H93 K94 R95 K96 K97 V98 K99 L100 A101 V102 L103 K104 Y105 Y106 K107 V108 D109 E110 N111 G112 K113 I114 S115 R116 L117 R118 R119 E120 C121 P122 S123 D124 E125 C126 G127 A128 G129 V130 F131 M132 A133 S134 H135 F136 D137 R138 H139 Y140 C141 G142

K143 C144 C145 L146 T147 Y148 C149 F150

• Molecule 84: ribosomal protein RACK1

Chain 6:

T2 E3 Q4 M5 T6 L7 R8 G9 T10 L11 K12 G13 H14 N15 G16 W17 V18 T19 Q20 I21 A22 T23 T24 P25 Q26 F27 P28 D29 M30 I31 L32 S33 A34 S35 R36 D37 K38 T39 I40 I41 M42 W43 K44 L45 T46 R47 D48 E49 T50 N51 Y52 G53 I54 P55 Q56 R57 A58 L59 R60 G61

H62 S63 H64 F65 V66 S67 D68 V69 V70 I71 S72 S73 D74 G75 Q76 F77 A78 L79 S80 G81 S82 W83 D84 G85 T86 L87 R88 L89 W90 D91 L92 T93 T94 G95 T96 T97 T98 R99 R100 F101 V102 G103 H104 T105 K106 D107 V108 L109 S110 V111 A112 F113 S114 S115 D116 N117 R118 Q119 I120 V121

S122 G123 S124 R125 D126 K127 T128 I129 K130 L131 W132 N133 T134 L135 G136 V137 C138 K139 Y140 T141 V142 Q143 D144 E145 S146 H147 S148 E149 W150 V151 S152 C153 V154 R155 F156 S157 P158 N159 S160 S161 N162 P163 I164 I165 V166 S167 C168 G169 W170 D171 K172 L173 V174 K175 V176 W177 N178 L179 A180 N181

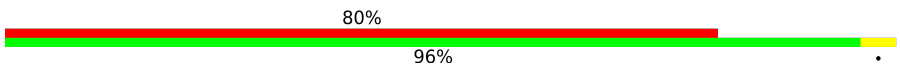
C182 K183 L184 K185 T186 N187 H188 I189 G190 H191 T192 G193 Y194 L195 N196 T197 V198 T199 V200 S201 P202 D203 G204 S205 L206 C207 A208 S209 G210 G211 K212 D213 G214 Q215 A216 M217 L218 W219 D220 L221 N222 E223 G224 K225 H226 L227 Y228 T229 L230 D231 G232 G233 D234 I235 I236 N237 A238 L239 C240 F241

S242 P243 N244 R245 Y246 W247 L248 C249 A250 A251 T252 G253 P254 S255 I256 K257 I258 W259 D260 L261 E262 G263 K264 I265 I266 V267 D268 E269 L270 K271 Q272 E273 V274 I275 S276 T277 S278 S279 K280 A281 E282 P283 P284 Q285 C286 T287 S288 L289 A290 W291 S292 A293 D294 G295 Q296 T297 L298 F299 A300 G301

Y302 T303 D304 N305 L306 V307 R308 V309 W310 Q311 V312 T313 I314

• Molecule 85: 40S ribosomal protein S30

Chain AA:



S78 L79 A80 R81 V82 G83 R86 G87 Q88 T89 L90 K91 V92 A93 K94 Q95 E96 K97 K98 K99 K100 R101 R104 A105 K106 R107 R108 M109 Q110 Y111 N112 R113 R114 F115 V116 N117 V118 V119 P120 T121 F122 G123 K124 K125 K126 G127 P128 N129 A130 N131 S132

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	223773	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	28	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	1.338	Depositor
Minimum map value	-0.753	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.035	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	429.264, 429.264, 429.264	wwPDB
Map dimensions	396, 396, 396	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.084, 1.084, 1.084	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	3	0.30	0/1783	1.04	10/2773 (0.4%)
2	1	0.78	1/216 (0.5%)	0.76	0/298
3	2	0.62	4/1801 (0.2%)	0.83	1/2800 (0.0%)
4	5	0.32	7/84978 (0.0%)	1.05	386/132528 (0.3%)
5	7	0.28	0/2858	1.01	12/4455 (0.3%)
6	8	0.30	0/3581	1.04	14/5577 (0.3%)
7	A	0.28	0/1936	0.53	0/2596
8	B	0.28	0/3240	0.59	6/4339 (0.1%)
9	C	0.28	0/2937	0.49	0/3946
10	D	0.26	0/2437	0.47	0/3264
11	E	0.26	0/1762	0.52	0/2362
12	F	0.27	0/1911	0.49	0/2549
13	G	0.27	0/1910	0.51	0/2569
14	H	0.27	0/1535	0.52	0/2063
15	I	0.26	0/1702	0.49	0/2272
16	J	0.27	0/1385	0.52	0/1852
17	L	0.27	0/1733	0.49	0/2316
18	M	0.27	0/1158	0.49	0/1547
19	N	0.27	0/1746	0.50	0/2338
20	O	0.27	0/1662	0.49	0/2222
21	P	0.26	0/1268	0.48	1/1700 (0.1%)
22	Q	0.25	0/1539	0.51	0/2054
23	R	0.26	0/1524	0.48	0/2013
24	S	0.27	0/1501	0.51	0/2012
25	T	0.27	0/1326	0.46	0/1770
26	U	0.26	0/823	0.52	0/1104
27	V	0.27	0/993	0.50	0/1332
28	W	0.26	0/873	0.44	0/1158
29	X	0.25	0/984	0.48	0/1323
30	Y	0.26	0/1132	0.47	0/1504
31	Z	0.28	0/1130	0.48	0/1507
32	a	0.25	0/1191	0.47	0/1590

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	b	0.24	0/861	0.44	0/1138
34	c	0.26	0/771	0.47	0/1034
35	d	0.28	0/903	0.53	0/1216
36	e	0.25	0/1071	0.50	1/1429 (0.1%)
37	f	0.27	0/895	0.52	0/1198
38	g	0.25	0/916	0.51	0/1220
39	h	0.26	0/1021	0.45	0/1348
40	i	0.26	0/841	0.46	0/1112
41	j	0.25	0/720	0.49	0/952
42	k	0.24	0/575	0.50	0/761
43	l	0.24	0/459	0.50	1/608 (0.2%)
44	m	0.24	0/435	0.46	0/575
45	n	0.22	0/240	0.43	0/305
46	o	0.25	0/864	0.49	0/1140
47	p	0.27	0/718	0.49	0/953
48	r	0.26	0/1010	0.54	0/1354
49	s	0.26	0/1530	0.49	0/2064
50	t	0.25	0/1174	0.53	0/1582
51	K	0.31	2/40531 (0.0%)	1.07	223/63162 (0.4%)
52	q	0.27	0/1747	0.53	1/2374 (0.0%)
53	u	0.26	0/1756	0.54	1/2350 (0.0%)
54	v	0.26	0/1753	0.51	0/2369
55	w	0.27	0/1796	0.54	1/2417 (0.0%)
56	x	0.25	0/2118	0.50	1/2849 (0.0%)
57	y	0.26	0/1492	0.49	0/2005
58	z	0.25	0/1946	0.49	0/2590
59	BB	0.26	0/1510	0.52	1/2022 (0.0%)
60	CC	0.25	0/1715	0.49	0/2287
61	DD	0.26	0/1550	0.50	0/2069
62	SS	0.27	0/834	0.55	0/1125
63	EE	0.26	0/1195	0.50	0/1597
64	RR	0.26	0/918	0.54	0/1233
65	QQ	0.25	0/1226	0.47	0/1649
66	MM	0.27	0/1017	0.53	0/1365
67	WW	0.26	0/1017	0.53	0/1358
68	UU	0.26	0/1146	0.52	0/1534
69	KK	0.24	0/1082	0.45	0/1452
70	II	0.27	0/1208	0.54	0/1618
71	PP	0.27	0/1115	0.51	1/1493 (0.1%)
72	GG	0.26	0/805	0.50	0/1081
73	HH	0.27	0/643	0.54	0/860
74	TT	0.27	0/1051	0.52	0/1406
75	VV	0.25	0/1116	0.51	0/1490

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
76	NN	0.25	0/1028	0.47	0/1366
77	OO	0.25	0/604	0.51	0/810
78	LL	0.25	0/828	0.49	0/1109
79	JJ	0.24	0/665	0.47	0/891
80	FF	0.24	0/490	0.49	0/656
81	9	0.26	0/470	0.44	0/623
82	4	0.45	0/141	1.00	1/217 (0.5%)
83	0	0.25	0/567	0.48	0/753
84	6	0.26	0/2493	0.54	0/3394
85	AA	0.26	0/447	0.43	0/587
All	All	0.30	14/231579 (0.0%)	0.89	662/339883 (0.2%)

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
8	B	1	1
17	L	0	1
19	N	0	2
67	WW	0	2
70	II	0	1
75	VV	0	1
All	All	1	8

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	5	4388	A	O3'-P	-15.59	1.42	1.61
4	5	4387	C	O3'-P	-10.72	1.48	1.61
4	5	3903	A	O3'-P	-10.15	1.49	1.61
4	5	3907	G	O3'-P	-7.34	1.52	1.61
3	2	19	G	O3'-P	-6.78	1.53	1.61
3	2	20	C	O3'-P	6.51	1.69	1.61
4	5	3905	A	O3'-P	-5.99	1.53	1.61
3	2	31	G	O3'-P	-5.78	1.54	1.61
2	1	260	MET	CA-C	5.63	1.67	1.52
51	K	1836	G	O3'-P	-5.46	1.54	1.61
4	5	4529	G	O3'-P	-5.41	1.54	1.61
4	5	2367	A	C6-N1	-5.28	1.31	1.35
3	2	37	A	O3'-P	-5.01	1.55	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	K	1520	G	N9-C4	5.01	1.42	1.38

All (662) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	5	2788	U	C5-C4-O4	21.78	138.97	125.90
4	5	2788	U	N3-C4-O4	-20.51	105.04	119.40
4	5	3914	U	C5-C4-O4	19.68	137.71	125.90
4	5	3914	U	N3-C4-O4	-18.68	106.32	119.40
4	5	2367	A	N1-C6-N6	-13.56	110.46	118.60
4	5	2505	C	C6-N1-C2	-11.22	115.81	120.30
4	5	2505	C	N1-C2-O2	10.81	125.39	118.90
4	5	4378	A	N1-C6-N6	-10.64	112.21	118.60
8	B	258	HIS	C-N-CD	-10.39	97.75	120.60
51	K	1520	G	N3-C4-C5	-9.83	123.69	128.60
4	5	2505	C	N3-C2-O2	-9.75	115.08	121.90
4	5	100	C	C2-N1-C1'	9.66	129.43	118.80
51	K	1139	C	N1-C2-O2	9.52	124.61	118.90
51	K	853	C	C2-N1-C1'	9.40	129.14	118.80
8	B	258	HIS	N-CA-C	9.01	135.32	111.00
51	K	1303	C	N1-C2-O2	8.99	124.29	118.90
4	5	2367	A	C5-C6-N6	8.97	130.87	123.70
51	K	1303	C	C2-N1-C1'	8.88	128.56	118.80
51	K	293	C	N1-C2-O2	8.83	124.20	118.90
4	5	4119	C	N1-C2-O2	8.69	124.12	118.90
51	K	853	C	N1-C2-O2	8.66	124.09	118.90
4	5	4314	C	N1-C2-O2	8.59	124.06	118.90
4	5	4759	C	N1-C2-O2	8.58	124.05	118.90
51	K	1520	G	C2-N3-C4	8.56	116.18	111.90
4	5	4314	C	N3-C2-O2	-8.51	115.94	121.90
4	5	4119	C	C2-N1-C1'	8.50	128.15	118.80
51	K	174	C	N3-C2-O2	-8.49	115.95	121.90
4	5	2022	C	N3-C2-O2	-8.48	115.97	121.90
4	5	100	C	N1-C2-O2	8.45	123.97	118.90
4	5	2022	C	N1-C2-O2	8.41	123.94	118.90
52	q	197	VAL	C-N-CA	8.41	142.72	121.70
51	K	1139	C	C2-N1-C1'	8.34	127.97	118.80
4	5	2367	A	N1-C2-N3	-8.32	125.14	129.30
6	8	128	C	N1-C2-O2	8.30	123.88	118.90
51	K	570	C	N1-C2-O2	8.27	123.86	118.90
4	5	2505	C	C5-C6-N1	8.25	125.12	121.00
51	K	1453	C	C2-N1-C1'	8.20	127.82	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	K	1123	C	N1-C2-O2	8.20	123.82	118.90
4	5	4759	C	C2-N1-C1'	8.14	127.76	118.80
8	B	259	PRO	N-CA-C	-8.14	90.93	112.10
3	2	20	C	C4'-C3'-O3'	8.12	129.25	113.00
51	K	1453	C	N1-C2-O2	8.12	123.77	118.90
4	5	1671	U	N3-C2-O2	-8.12	116.52	122.20
51	K	1551	U	C2-N1-C1'	8.11	127.44	117.70
51	K	1139	C	N3-C2-O2	-8.10	116.23	121.90
4	5	2505	C	C2-N1-C1'	8.10	127.71	118.80
4	5	1639	U	C2-N1-C1'	7.99	127.29	117.70
51	K	1520	G	C8-N9-C4	-7.93	103.23	106.40
4	5	472	C	N1-C2-O2	7.87	123.62	118.90
51	K	293	C	C2-N1-C1'	7.86	127.44	118.80
4	5	4388	A	P-O3'-C3'	7.81	129.07	119.70
4	5	1429	C	N1-C2-O2	7.80	123.58	118.90
51	K	1364	U	N1-C2-O2	7.79	128.26	122.80
51	K	823	U	C2-N1-C1'	7.71	126.95	117.70
51	K	1551	U	N1-C2-O2	7.70	128.19	122.80
4	5	1084	C	N1-C2-O2	7.70	123.52	118.90
4	5	4880	C	C2-N1-C1'	7.69	127.26	118.80
4	5	1237	C	N1-C2-O2	7.68	123.51	118.90
51	K	914	U	C2-N1-C1'	7.64	126.86	117.70
4	5	220	C	C2-N1-C1'	7.61	127.17	118.80
4	5	3636	C	N3-C2-O2	-7.59	116.58	121.90
4	5	4423	U	C2-N1-C1'	7.59	126.80	117.70
4	5	1671	U	N1-C2-O2	7.58	128.11	122.80
51	K	823	U	N1-C2-O2	7.57	128.10	122.80
51	K	823	U	N3-C2-O2	-7.51	116.94	122.20
4	5	1612	G	N3-C4-N9	7.50	130.50	126.00
5	7	29	C	N1-C2-O2	7.49	123.39	118.90
51	K	1364	U	C2-N1-C1'	7.47	126.66	117.70
51	K	1591	C	N1-C2-O2	7.43	123.36	118.90
51	K	1520	G	C4-N9-C1'	7.42	136.15	126.50
4	5	1639	U	N1-C2-O2	7.40	127.98	122.80
51	K	1624	U	C2-N1-C1'	7.36	126.53	117.70
4	5	1177	U	C2-N1-C1'	7.30	126.47	117.70
51	K	1303	C	N3-C2-O2	-7.30	116.79	121.90
4	5	2820	C	N1-C2-O2	7.26	123.26	118.90
4	5	152	U	N3-C2-O2	-7.25	117.12	122.20
4	5	4738	C	N1-C2-O2	7.23	123.24	118.90
4	5	1484	G	C4-N9-C1'	7.21	135.88	126.50
4	5	4305	G	C4-N9-C1'	7.20	135.86	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	5	1978	C	N1-C2-O2	7.19	123.21	118.90
51	K	1551	U	N3-C2-O2	-7.18	117.17	122.20
4	5	4925	U	OP2-P-O3'	7.15	120.94	105.20
4	5	4709	U	N1-C2-O2	7.12	127.79	122.80
51	K	1118	C	C2-N1-C1'	7.10	126.61	118.80
4	5	1237	C	C2-N1-C1'	7.10	126.61	118.80
51	K	1364	U	N3-C2-O2	-7.08	117.24	122.20
4	5	4413	C	C2-N1-C1'	7.08	126.59	118.80
4	5	2788	U	C2-N3-C4	7.07	131.24	127.00
4	5	2046	G	P-O3'-C3'	7.06	128.17	119.70
4	5	2568	C	N1-C2-O2	7.06	123.13	118.90
4	5	4925	U	P-O3'-C3'	7.05	128.17	119.70
4	5	100	C	N3-C2-O2	-7.04	116.97	121.90
4	5	495	C	N1-C2-O2	7.04	123.12	118.90
4	5	77	U	N3-C2-O2	-7.01	117.30	122.20
51	K	1520	G	N3-C4-N9	7.00	130.20	126.00
51	K	340	C	N1-C2-O2	7.00	123.10	118.90
4	5	2695	A	P-O3'-C3'	7.00	128.09	119.70
51	K	853	C	N3-C2-O2	-6.99	117.00	121.90
4	5	1484	G	N3-C4-C5	-6.97	125.11	128.60
4	5	1612	G	C4-N9-C1'	6.93	135.51	126.50
4	5	1177	U	N1-C2-O2	6.92	127.65	122.80
51	K	174	C	N1-C2-O2	6.90	123.04	118.90
4	5	1484	G	N3-C4-N9	6.90	130.14	126.00
51	K	1123	C	N3-C2-O2	-6.88	117.09	121.90
51	K	1683	C	N1-C2-O2	6.88	123.03	118.90
51	K	1274	G	C4-N9-C1'	6.87	135.43	126.50
51	K	688	U	P-O3'-C3'	6.87	127.94	119.70
5	7	94	C	N1-C2-O2	6.86	123.02	118.90
51	K	151	C	C2-N1-C1'	6.86	126.34	118.80
51	K	914	U	C5-C4-O4	-6.85	121.79	125.90
51	K	1139	C	C6-N1-C2	-6.84	117.56	120.30
4	5	4880	C	N1-C2-O2	6.84	123.00	118.90
4	5	4759	C	N3-C2-O2	-6.84	117.11	121.90
51	K	293	C	N3-C2-O2	-6.83	117.12	121.90
4	5	472	C	C2-N1-C1'	6.82	126.31	118.80
4	5	1477	C	C2-N1-C1'	6.82	126.30	118.80
4	5	1735	U	N1-C2-O2	6.81	127.57	122.80
51	K	1261	C	N1-C2-O2	6.81	122.99	118.90
4	5	4423	U	N1-C2-O2	6.81	127.56	122.80
4	5	1812	C	N1-C2-O2	6.80	122.98	118.90
51	K	1664	A	P-O3'-C3'	6.79	127.85	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	5	4119	C	N3-C2-O2	-6.78	117.15	121.90
51	K	1123	C	C6-N1-C2	-6.78	117.59	120.30
4	5	1177	U	N3-C2-O2	-6.77	117.46	122.20
4	5	1978	C	C2-N1-C1'	6.77	126.25	118.80
4	5	3914	U	C2-N3-C4	6.77	131.06	127.00
6	8	128	C	N3-C2-O2	-6.76	117.17	121.90
4	5	1639	U	N3-C2-O2	-6.75	117.48	122.20
51	K	530	U	C2-N1-C1'	6.71	125.76	117.70
51	K	1624	U	N1-C2-O2	6.71	127.50	122.80
51	K	1453	C	N3-C2-O2	-6.70	117.21	121.90
4	5	2008	U	C2-N1-C1'	6.70	125.74	117.70
51	K	1274	G	N3-C4-C5	-6.70	125.25	128.60
51	K	183	G	C4-N9-C1'	6.68	135.19	126.50
4	5	48	G	P-O3'-C3'	6.68	127.72	119.70
51	K	570	C	N3-C2-O2	-6.68	117.23	121.90
4	5	1469	C	N3-C2-O2	-6.65	117.24	121.90
4	5	1612	G	N3-C4-C5	-6.65	125.28	128.60
4	5	3636	C	N1-C2-O2	6.64	122.89	118.90
4	5	4229	U	N3-C2-O2	-6.63	117.56	122.20
8	B	309	LEU	CA-CB-CG	6.63	130.56	115.30
51	K	1057	C	C2-N1-C1'	6.62	126.08	118.80
5	7	102	U	N1-C2-O2	6.62	127.43	122.80
51	K	943	U	C2-N1-C1'	6.62	125.64	117.70
4	5	1807	C	C2-N1-C1'	6.61	126.07	118.80
4	5	3914	U	N1-C2-O2	6.61	127.42	122.80
4	5	4709	U	N3-C2-O2	-6.60	117.58	122.20
4	5	100	C	C6-N1-C1'	-6.60	112.88	120.80
51	K	1624	U	N3-C2-O2	-6.60	117.58	122.20
4	5	112	C	C2-N1-C1'	6.60	126.06	118.80
4	5	683	C	N1-C2-O2	6.58	122.85	118.90
4	5	4423	U	N3-C2-O2	-6.56	117.61	122.20
51	K	1274	G	N3-C4-N9	6.56	129.94	126.00
4	5	658	C	N1-C2-O2	6.55	122.83	118.90
51	K	1298	G	N3-C4-N9	6.54	129.92	126.00
4	5	4928	C	N1-C2-O2	6.53	122.82	118.90
51	K	752	G	P-O3'-C3'	6.52	127.53	119.70
4	5	4305	G	N3-C4-N9	6.52	129.91	126.00
4	5	4555	U	O5'-P-OP2	-6.52	99.83	105.70
51	K	183	G	N3-C4-C5	-6.51	125.34	128.60
4	5	1847	C	C2-N1-C1'	6.51	125.96	118.80
43	l	49	LEU	CA-CB-CG	6.51	130.27	115.30
51	K	930	C	N1-C2-O2	6.51	122.81	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	K	494	C	N1-C2-O2	6.51	122.80	118.90
4	5	100	C	C6-N1-C2	-6.50	117.70	120.30
4	5	2410	C	C2-N1-C1'	6.50	125.95	118.80
4	5	2661	U	P-O3'-C3'	6.49	127.49	119.70
51	K	1123	C	C2-N1-C1'	6.49	125.94	118.80
4	5	1598	C	N1-C2-O2	6.49	122.79	118.90
51	K	973	C	N1-C2-O2	6.49	122.79	118.90
51	K	1120	U	C2-N1-C1'	6.49	125.48	117.70
51	K	853	C	C6-N1-C1'	-6.48	113.02	120.80
4	5	1735	U	N3-C2-O2	-6.47	117.67	122.20
4	5	1072	C	P-O3'-C3'	6.45	127.44	119.70
4	5	2474	G	P-O3'-C3'	6.45	127.43	119.70
51	K	1298	G	N3-C4-C5	-6.44	125.38	128.60
51	K	183	G	N3-C4-N9	6.43	129.86	126.00
4	5	4232	U	P-O3'-C3'	6.43	127.41	119.70
51	K	501	C	N1-C2-O2	6.43	122.76	118.90
4	5	1535	C	N1-C2-O2	6.42	122.75	118.90
4	5	1210	C	N1-C2-O2	6.42	122.75	118.90
51	K	578	C	N1-C2-O2	6.42	122.75	118.90
4	5	2013	A	C6-N1-C2	-6.42	114.75	118.60
4	5	4229	U	N1-C2-O2	6.41	127.28	122.80
51	K	570	C	C2-N1-C1'	6.40	125.84	118.80
4	5	1812	C	C2-N1-C1'	6.38	125.82	118.80
5	7	29	C	N3-C2-O2	-6.38	117.43	121.90
4	5	3914	U	C4-C5-C6	-6.37	115.88	119.70
4	5	2788	U	N1-C2-N3	-6.37	111.08	114.90
4	5	4243	C	C6-N1-C2	-6.36	117.75	120.30
4	5	4928	C	C2-N1-C1'	6.36	125.79	118.80
4	5	2856	C	N1-C2-O2	6.36	122.71	118.90
51	K	537	C	C2-N1-C1'	6.35	125.79	118.80
4	5	2089	G	P-O3'-C3'	6.34	127.30	119.70
4	5	4948	C	C2-N1-C1'	6.33	125.76	118.80
51	K	914	U	C6-N1-C1'	-6.32	112.35	121.20
1	3	63	C	N1-C2-O2	6.31	122.69	118.90
4	5	4305	G	N3-C4-C5	-6.31	125.44	128.60
4	5	1237	C	N3-C2-O2	-6.31	117.48	121.90
4	5	4215	C	N1-C2-O2	6.31	122.68	118.90
4	5	2568	C	C2-N1-C1'	6.30	125.73	118.80
1	3	40	C	C2-N1-C1'	6.30	125.73	118.80
6	8	128	C	C2-N1-C1'	6.29	125.72	118.80
4	5	1429	C	C2-N1-C1'	6.29	125.72	118.80
4	5	2008	U	N1-C2-O2	6.28	127.20	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	5	1446	C	N1-C2-O2	6.28	122.67	118.90
4	5	4388	A	OP1-P-O3'	6.28	119.02	105.20
4	5	4303	C	C2-N1-C1'	6.28	125.71	118.80
5	7	29	C	C2-N1-C1'	6.27	125.70	118.80
51	K	1315	U	N3-C2-O2	-6.27	117.81	122.20
51	K	1689	C	C2-N1-C1'	6.27	125.70	118.80
4	5	4241	C	N1-C2-O2	6.27	122.66	118.90
4	5	4924	C	N3-C2-O2	-6.26	117.52	121.90
4	5	1632	A	C2-N3-C4	6.26	113.73	110.60
4	5	2788	U	C4-C5-C6	-6.26	115.95	119.70
51	K	151	C	C6-N1-C2	-6.24	117.81	120.30
51	K	1637	A	P-O3'-C3'	6.23	127.18	119.70
51	K	1315	U	N1-C2-O2	6.23	127.16	122.80
51	K	814	U	N1-C2-O2	6.23	127.16	122.80
6	8	128	C	C6-N1-C2	-6.22	117.81	120.30
4	5	4165	C	C2-N1-C1'	6.21	125.64	118.80
4	5	1966	C	N1-C2-O2	6.21	122.63	118.90
51	K	1261	C	C2-N1-C1'	6.18	125.60	118.80
4	5	1429	C	N3-C2-O2	-6.18	117.57	121.90
51	K	356	C	C2-N1-C1'	6.17	125.59	118.80
51	K	118	C	N1-C2-O2	6.16	122.60	118.90
51	K	853	C	C6-N1-C2	-6.16	117.84	120.30
6	8	2	G	C4-N9-C1'	6.15	134.50	126.50
4	5	472	C	N3-C2-O2	-6.15	117.59	121.90
4	5	2867	C	C2-N1-C1'	6.15	125.56	118.80
5	7	102	U	N3-C2-O2	-6.15	117.90	122.20
4	5	115	C	C2-N1-C1'	6.14	125.56	118.80
51	K	1591	C	N3-C2-O2	-6.14	117.60	121.90
4	5	4413	C	N1-C2-O2	6.13	122.58	118.90
51	K	1057	C	N1-C2-O2	6.13	122.58	118.90
4	5	1478	C	C2-N1-C1'	6.13	125.54	118.80
4	5	1612	G	C8-N9-C1'	-6.13	119.04	127.00
51	K	1590	C	N1-C2-O2	6.12	122.57	118.90
4	5	1514	U	N1-C2-O2	6.12	127.08	122.80
51	K	130	G	C4-N9-C1'	6.12	134.45	126.50
4	5	2661	U	OP1-P-O3'	6.11	118.65	105.20
4	5	4758	U	C2-N1-C1'	6.11	125.04	117.70
51	K	130	G	N3-C4-C5	-6.11	125.54	128.60
4	5	2528	G	C4-N9-C1'	6.11	134.44	126.50
51	K	579	C	N1-C2-O2	6.11	122.57	118.90
51	K	1518	C	C2-N1-C1'	6.11	125.52	118.80
51	K	814	U	N3-C2-O2	-6.10	117.93	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	K	1303	C	C6-N1-C1'	-6.10	113.48	120.80
51	K	537	C	N1-C2-O2	6.10	122.56	118.90
4	5	1210	C	C2-N1-C1'	6.09	125.50	118.80
4	5	696	C	P-O3'-C3'	6.08	127.00	119.70
4	5	4305	G	C8-N9-C1'	-6.08	119.09	127.00
4	5	3882	C	N1-C2-O2	6.07	122.54	118.90
51	K	130	G	N3-C4-N9	6.06	129.64	126.00
4	5	1414	C	N1-C2-O2	6.06	122.54	118.90
4	5	4709	U	C2-N1-C1'	6.05	124.96	117.70
51	K	1261	C	C6-N1-C2	-6.05	117.88	120.30
4	5	406	C	P-O3'-C3'	6.04	126.95	119.70
51	K	55	U	C2-N1-C1'	6.04	124.94	117.70
4	5	49	U	N1-C2-O2	6.04	127.02	122.80
51	K	1664	A	OP1-P-O3'	6.04	118.48	105.20
4	5	4075	U	P-O3'-C3'	6.03	126.93	119.70
4	5	661	C	C2-N1-C1'	6.02	125.42	118.80
5	7	94	C	N3-C2-O2	-6.02	117.69	121.90
51	K	1118	C	N1-C2-O2	6.02	122.51	118.90
4	5	1484	G	C8-N9-C1'	-6.01	119.19	127.00
4	5	30	C	C2-N1-C1'	6.00	125.40	118.80
4	5	1084	C	N3-C2-O2	-6.00	117.70	121.90
4	5	1777	C	N1-C2-O2	6.00	122.50	118.90
4	5	1777	C	C2-N1-C1'	5.98	125.38	118.80
4	5	77	U	N1-C2-O2	5.98	126.98	122.80
4	5	5035	U	N3-C2-O2	-5.98	118.02	122.20
4	5	1859	C	N1-C2-O2	5.98	122.48	118.90
4	5	1481	C	N1-C2-O2	5.97	122.48	118.90
51	K	1271	C	N1-C2-O2	5.97	122.48	118.90
4	5	1514	U	C2-N1-C1'	5.97	124.86	117.70
51	K	1303	C	C6-N1-C2	-5.97	117.91	120.30
51	K	1564	C	C2-N1-C1'	5.97	125.36	118.80
4	5	4243	C	N1-C2-O2	5.96	122.48	118.90
4	5	2820	C	N3-C2-O2	-5.95	117.74	121.90
4	5	4682	U	N3-C2-O2	-5.94	118.04	122.20
51	K	1022	U	C2-N1-C1'	5.93	124.82	117.70
4	5	282	C	N1-C2-O2	5.93	122.46	118.90
4	5	683	C	C2-N1-C1'	5.92	125.31	118.80
51	K	1298	G	C4-N9-C1'	5.92	134.19	126.50
51	K	945	U	C2-N1-C1'	5.92	124.80	117.70
51	K	1453	C	C6-N1-C2	-5.92	117.93	120.30
4	5	2772	C	C6-N1-C2	-5.92	117.93	120.30
51	K	943	U	C5-C6-N1	5.91	125.66	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	5	2772	C	C2-N1-C1'	5.91	125.30	118.80
4	5	4926	C	C2-N1-C1'	5.91	125.30	118.80
4	5	2632	U	N3-C2-O2	-5.90	118.07	122.20
51	K	1423	C	N1-C2-O2	5.89	122.43	118.90
4	5	4880	C	N3-C2-O2	-5.88	117.78	121.90
4	5	1469	C	C6-N1-C2	-5.88	117.95	120.30
51	K	465	A	P-O3'-C3'	5.88	126.75	119.70
4	5	4119	C	C6-N1-C1'	-5.87	113.75	120.80
51	K	407	G	C4-N9-C1'	5.87	134.13	126.50
4	5	3914	U	N1-C2-N3	-5.86	111.38	114.90
51	K	1274	G	C8-N9-C1'	-5.86	119.38	127.00
4	5	220	C	C6-N1-C2	-5.86	117.96	120.30
4	5	1428	U	N1-C2-O2	5.86	126.90	122.80
4	5	1514	U	N3-C2-O2	-5.85	118.10	122.20
4	5	4254	G	N3-C4-C5	-5.85	125.67	128.60
51	K	119	U	N1-C2-O2	5.85	126.89	122.80
4	5	134	G	P-O3'-C3'	5.84	126.71	119.70
51	K	1520	G	N7-C8-N9	5.83	116.02	113.10
51	K	632	C	C2-N1-C1'	5.83	125.21	118.80
51	K	531	A	P-O3'-C3'	5.83	126.69	119.70
51	K	1660	C	C2-N1-C1'	5.83	125.21	118.80
4	5	1414	C	C2-N1-C1'	5.82	125.20	118.80
4	5	3636	C	C6-N1-C2	-5.82	117.97	120.30
4	5	495	C	N3-C2-O2	-5.80	117.84	121.90
4	5	1084	C	C2-N1-C1'	5.80	125.18	118.80
51	K	1314	U	C2-N1-C1'	5.80	124.66	117.70
6	8	124	U	P-O3'-C3'	5.79	126.65	119.70
59	BB	36	LEU	CA-CB-CG	5.79	128.61	115.30
51	K	151	C	C5-C6-N1	5.78	123.89	121.00
4	5	2266	C	P-O3'-C3'	5.78	126.64	119.70
4	5	4476	C	C2-N1-C1'	5.78	125.16	118.80
51	K	407	G	N3-C4-C5	-5.78	125.71	128.60
4	5	1370	G	P-O3'-C3'	5.78	126.63	119.70
4	5	4199	C	N1-C2-O2	5.78	122.37	118.90
4	5	449	C	P-O3'-C3'	5.77	126.62	119.70
4	5	492	U	P-O3'-C3'	5.76	126.61	119.70
4	5	217	C	C2-N1-C1'	5.75	125.12	118.80
4	5	686	A	C2-N3-C4	5.75	113.47	110.60
4	5	1694	C	C6-N1-C2	-5.74	118.00	120.30
4	5	1804	A	P-O3'-C3'	5.73	126.58	119.70
4	5	4266	G	N3-C4-C5	-5.73	125.73	128.60
4	5	2474	G	OP1-P-O3'	5.73	117.80	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	5	2837	U	N1-C2-O2	5.72	126.81	122.80
4	5	1633	G	P-O3'-C3'	5.72	126.56	119.70
4	5	2367	A	C6-N1-C2	5.72	122.03	118.60
51	K	182	C	P-O3'-C3'	5.72	126.56	119.70
4	5	4627	U	N1-C2-O2	5.71	126.80	122.80
51	K	980	A	C6-N1-C2	-5.71	115.17	118.60
4	5	155	C	N3-C2-O2	-5.71	117.91	121.90
51	K	407	G	N3-C4-N9	5.71	129.42	126.00
4	5	4738	C	N3-C2-O2	-5.70	117.91	121.90
4	5	1792	U	N1-C2-O2	5.69	126.79	122.80
4	5	217	C	P-O3'-C3'	5.69	126.53	119.70
4	5	220	C	C5-C6-N1	5.69	123.84	121.00
4	5	704	C	C2-N1-C1'	5.68	125.05	118.80
4	5	3767	C	C2-N1-C1'	5.68	125.05	118.80
4	5	49	U	N3-C2-O2	-5.68	118.22	122.20
6	8	99	U	C2-N1-C1'	5.68	124.52	117.70
4	5	2568	C	N3-C2-O2	-5.68	117.93	121.90
51	K	1073	U	N3-C2-O2	-5.67	118.23	122.20
4	5	4378	A	C5-C6-N6	5.67	128.23	123.70
6	8	101	C	C2-N1-C1'	5.67	125.03	118.80
51	K	1261	C	N3-C2-O2	-5.67	117.93	121.90
4	5	1966	C	N3-C2-O2	-5.66	117.94	121.90
4	5	2615	C	N1-C2-O2	5.66	122.30	118.90
51	K	119	U	N3-C2-O2	-5.65	118.24	122.20
51	K	124	U	N1-C2-O2	5.65	126.75	122.80
4	5	2281	U	N1-C2-O2	5.63	126.74	122.80
5	7	29	C	C6-N1-C2	-5.63	118.05	120.30
4	5	2008	U	N3-C2-O2	-5.63	118.26	122.20
51	K	1315	U	C2-N1-C1'	5.62	124.45	117.70
4	5	2528	G	N3-C4-N9	5.62	129.37	126.00
51	K	501	C	C6-N1-C2	-5.61	118.06	120.30
51	K	1078	C	C2-N1-C1'	5.60	124.96	118.80
4	5	1211	G	P-O3'-C3'	5.60	126.42	119.70
4	5	4682	U	N1-C2-O2	5.60	126.72	122.80
4	5	220	C	N1-C2-O2	5.59	122.25	118.90
4	5	2016	C	C6-N1-C2	-5.59	118.07	120.30
4	5	2532	C	C2-N1-C1'	5.59	124.95	118.80
4	5	1835	G	P-O3'-C3'	5.58	126.40	119.70
4	5	2787	A	C2-N3-C4	5.58	113.39	110.60
4	5	4758	U	N1-C2-O2	5.58	126.71	122.80
4	5	1671	U	C2-N1-C1'	5.58	124.40	117.70
4	5	4254	G	C4-N9-C1'	5.58	133.75	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	5	50	C	N1-C2-O2	5.58	122.25	118.90
51	K	930	C	C2-N1-C1'	5.57	124.93	118.80
4	5	4069	U	N1-C2-O2	5.57	126.70	122.80
4	5	1084	C	C6-N1-C2	-5.57	118.07	120.30
51	K	183	G	C8-N9-C1'	-5.57	119.77	127.00
51	K	151	C	N1-C2-O2	5.56	122.23	118.90
8	B	17	LEU	CA-CB-CG	5.55	128.07	115.30
4	5	3788	C	N1-C2-O2	5.55	122.23	118.90
4	5	4759	C	C6-N1-C1'	-5.55	114.14	120.80
51	K	340	C	N3-C2-O2	-5.55	118.02	121.90
4	5	658	C	N3-C2-O2	-5.55	118.02	121.90
51	K	630	U	C2-N1-C1'	5.54	124.35	117.70
51	K	356	C	N1-C2-O2	5.54	122.23	118.90
51	K	659	G	C4-N9-C1'	5.54	133.71	126.50
4	5	1921	C	P-O3'-C3'	5.54	126.35	119.70
4	5	2528	G	N3-C4-C5	-5.54	125.83	128.60
51	K	1111	U	N1-C2-O2	5.54	126.68	122.80
4	5	1978	C	N3-C2-O2	-5.54	118.02	121.90
4	5	472	C	C6-N1-C2	-5.54	118.09	120.30
51	K	1535	U	C2-N1-C1'	5.53	124.34	117.70
4	5	155	C	N1-C2-O2	5.53	122.22	118.90
4	5	1180	C	N1-C2-O2	5.53	122.22	118.90
51	K	1111	U	N3-C2-O2	-5.52	118.33	122.20
4	5	2632	U	N1-C2-O2	5.52	126.66	122.80
4	5	436	C	N1-C2-O2	5.52	122.21	118.90
51	K	183	G	C2-N3-C4	5.52	114.66	111.90
6	8	2	G	N3-C4-N9	5.52	129.31	126.00
4	5	4119	C	C6-N1-C2	-5.51	118.09	120.30
4	5	1792	U	N3-C2-O2	-5.51	118.34	122.20
51	K	1161	U	N3-C2-O2	-5.51	118.34	122.20
4	5	4738	C	C2-N1-C1'	5.51	124.86	118.80
4	5	4759	C	C6-N1-C2	-5.51	118.10	120.30
51	K	501	C	N3-C2-O2	-5.50	118.05	121.90
4	5	2704	C	N1-C2-O2	5.50	122.20	118.90
4	5	4266	G	C4-N9-C1'	5.50	133.65	126.50
4	5	4350	C	N1-C2-O2	5.50	122.20	118.90
4	5	385	A	P-O3'-C3'	5.49	126.29	119.70
4	5	4266	G	N3-C4-N9	5.49	129.30	126.00
4	5	4948	C	N1-C2-O2	5.49	122.19	118.90
51	K	532	C	P-O3'-C3'	5.49	126.29	119.70
4	5	1237	C	C6-N1-C2	-5.48	118.11	120.30
51	K	1683	C	N3-C2-O2	-5.48	118.06	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	5	4560	C	N1-C2-O2	5.48	122.19	118.90
4	5	4682	U	C2-N1-C1'	5.48	124.28	117.70
51	K	453	C	C2-N1-C1'	5.48	124.83	118.80
51	K	293	C	C6-N1-C2	-5.48	118.11	120.30
4	5	118	C	C2-N1-C1'	5.48	124.83	118.80
4	5	4627	U	N3-C2-O2	-5.48	118.37	122.20
51	K	1123	C	C5-C6-N1	5.48	123.74	121.00
51	K	1161	U	N1-C2-O2	5.47	126.63	122.80
4	5	2267	U	C2-N1-C1'	5.47	124.27	117.70
4	5	2667	C	N1-C2-O2	5.47	122.18	118.90
4	5	661	C	C6-N1-C2	-5.47	118.11	120.30
4	5	1694	C	C2-N1-C1'	5.47	124.81	118.80
4	5	1915	C	N1-C2-O2	5.46	122.18	118.90
51	K	1453	C	C6-N1-C1'	-5.46	114.24	120.80
4	5	3739	C	N1-C2-O2	5.46	122.18	118.90
1	3	67	U	N1-C2-O2	5.46	126.62	122.80
4	5	934	C	N1-C2-O2	5.46	122.18	118.90
51	K	140	U	C2-N1-C1'	5.46	124.25	117.70
1	3	67	U	N3-C2-O2	-5.46	118.38	122.20
51	K	870	A	P-O3'-C3'	5.46	126.25	119.70
36	e	89	LEU	CA-CB-CG	5.45	127.84	115.30
51	K	1057	C	N3-C2-O2	-5.45	118.08	121.90
4	5	1215	C	N1-C2-O2	5.45	122.17	118.90
8	B	214	ASP	CB-CG-OD1	5.45	123.20	118.30
4	5	1428	U	N3-C2-O2	-5.45	118.39	122.20
4	5	1847	C	N1-C2-O2	5.45	122.17	118.90
4	5	2837	U	N3-C2-O2	-5.44	118.39	122.20
4	5	1568	C	N1-C2-O2	5.43	122.16	118.90
51	K	1683	C	C6-N1-C2	-5.43	118.13	120.30
4	5	3767	C	C6-N1-C2	-5.43	118.13	120.30
51	K	1624	U	O4'-C1'-N1	5.43	112.54	108.20
4	5	1468	C	N1-C2-O2	5.43	122.16	118.90
4	5	1847	C	C6-N1-C2	-5.42	118.13	120.30
4	5	4947	U	P-O3'-C3'	5.42	126.21	119.70
4	5	922(B)	C	P-O3'-C3'	5.42	126.21	119.70
4	5	1929	A	C4-N9-C1'	5.42	136.06	126.30
4	5	2867	C	N1-C2-O2	5.42	122.15	118.90
4	5	2013	A	C5-C6-N1	5.42	120.41	117.70
51	K	687	C	N1-C2-O2	5.42	122.15	118.90
4	5	2470	C	N1-C2-O2	5.41	122.15	118.90
4	5	4303	C	N1-C2-O2	5.41	122.15	118.90
4	5	4243	C	C2-N1-C1'	5.41	124.75	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	K	124	U	N3-C2-O2	-5.41	118.42	122.20
1	3	67	U	C2-N1-C1'	5.41	124.19	117.70
4	5	115	C	N1-C2-O2	5.41	122.14	118.90
4	5	1179	U	C2-N1-C1'	5.41	124.19	117.70
4	5	1429	C	C6-N1-C2	-5.41	118.14	120.30
4	5	2502	A	OP1-P-O3'	5.41	117.09	105.20
4	5	5047	C	N1-C2-O2	5.41	122.14	118.90
6	8	54	C	N1-C2-O2	5.41	122.14	118.90
51	K	1118	C	C6-N1-C2	-5.41	118.14	120.30
51	K	1298	G	C8-N9-C1'	-5.40	119.98	127.00
4	5	3767	C	C5-C6-N1	5.40	123.70	121.00
5	7	28	C	N3-C2-O2	-5.39	118.12	121.90
4	5	495	C	C6-N1-C2	-5.38	118.15	120.30
4	5	4880	C	C6-N1-C2	-5.38	118.15	120.30
51	K	1742	C	C2-N1-C1'	5.38	124.72	118.80
51	K	1751	C	N1-C2-O2	5.38	122.13	118.90
4	5	1735	U	C2-N1-C1'	5.38	124.15	117.70
51	K	427	U	C2-N1-C1'	5.38	124.15	117.70
4	5	1481	C	C2-N1-C1'	5.38	124.71	118.80
51	K	1304	U	N3-C2-O2	-5.38	118.44	122.20
4	5	4171	C	N1-C2-O2	5.38	122.12	118.90
6	8	2	G	N3-C4-C5	-5.37	125.92	128.60
4	5	1847	C	C5-C6-N1	5.37	123.69	121.00
4	5	2410	C	C5-C6-N1	5.37	123.69	121.00
4	5	4869	U	C2-N1-C1'	5.37	124.14	117.70
5	7	28	C	N1-C2-O2	5.37	122.12	118.90
4	5	1929	A	C2-N3-C4	5.36	113.28	110.60
4	5	4360	U	N3-C2-O2	-5.36	118.45	122.20
4	5	1993	C	C2-N1-C1'	5.35	124.69	118.80
51	K	1253	A	P-O3'-C3'	5.35	126.12	119.70
4	5	4069	U	N3-C2-O2	-5.35	118.46	122.20
51	K	824	C	N1-C2-O2	5.35	122.11	118.90
51	K	1389	C	C2-N1-C1'	5.35	124.68	118.80
5	7	28	C	C6-N1-C2	-5.35	118.16	120.30
51	K	1118	C	N3-C2-O2	-5.35	118.16	121.90
4	5	3606	U	C2-N1-C1'	5.34	124.11	117.70
4	5	4241	C	C2-N1-C1'	5.34	124.68	118.80
4	5	1210	C	N3-C2-O2	-5.34	118.16	121.90
4	5	962	C	N1-C2-O2	5.34	122.10	118.90
51	K	1139	C	C6-N1-C1'	-5.34	114.39	120.80
4	5	1986	U	C2-N3-C4	-5.33	123.80	127.00
4	5	2772	C	C5-C6-N1	5.33	123.66	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	K	1865	C	C6-N1-C2	-5.32	118.17	120.30
4	5	2410	C	C6-N1-C2	-5.32	118.17	120.30
4	5	100	C	O4'-C1'-N1	5.32	112.46	108.20
4	5	3892	U	N1-C2-O2	5.32	126.52	122.80
4	5	4069	U	C2-N1-C1'	5.32	124.08	117.70
51	K	578	C	N3-C2-O2	-5.32	118.18	121.90
4	5	245	C	P-O3'-C3'	5.32	126.08	119.70
4	5	2838	G	C4-N9-C1'	5.32	133.41	126.50
6	8	64	U	N3-C2-O2	-5.32	118.48	122.20
4	5	4928	C	N3-C2-O2	-5.31	118.18	121.90
51	K	1518	C	N1-C2-O2	5.31	122.09	118.90
4	5	1325	C	N1-C2-O2	5.31	122.09	118.90
4	5	1893	C	C2-N1-C1'	5.31	124.64	118.80
4	5	3657	U	N3-C2-O2	-5.30	118.49	122.20
51	K	1599	U	N3-C2-O2	-5.30	118.49	122.20
4	5	4350	C	N3-C2-O2	-5.30	118.19	121.90
56	x	73	ASP	CB-CG-OD1	5.30	123.07	118.30
51	K	570	C	C6-N1-C2	-5.30	118.18	120.30
4	5	2560	C	N1-C2-O2	5.30	122.08	118.90
4	5	2454	U	N1-C2-O2	5.29	126.50	122.80
51	K	293	C	C6-N1-C1'	-5.29	114.45	120.80
4	5	2568	C	C6-N1-C2	-5.29	118.19	120.30
51	K	1358	U	N3-C2-O2	-5.28	118.50	122.20
4	5	100	C	C5-C6-N1	5.28	123.64	121.00
51	K	632	C	C5-C6-N1	5.28	123.64	121.00
51	K	1649	U	N1-C2-O2	5.28	126.49	122.80
4	5	3723	A	C6-N1-C2	-5.28	115.44	118.60
4	5	3778	U	N1-C2-O2	5.28	126.49	122.80
51	K	531	A	OP1-P-O3'	5.27	116.80	105.20
4	5	4476	C	N1-C2-O2	5.27	122.06	118.90
4	5	5035	U	N1-C2-O2	5.27	126.49	122.80
4	5	1792	U	C2-N1-C1'	5.26	124.02	117.70
51	K	853	C	C5-C6-N1	5.26	123.63	121.00
4	5	469	C	N1-C2-O2	5.26	122.06	118.90
51	K	1407	U	C2-N1-C1'	5.26	124.01	117.70
4	5	1812	C	N3-C2-O2	-5.25	118.22	121.90
4	5	3914	U	C5-C6-N1	5.25	125.33	122.70
51	K	1395	C	P-O3'-C3'	5.25	126.00	119.70
4	5	275	C	P-O3'-C3'	5.25	126.00	119.70
4	5	3876	A	P-O3'-C3'	5.25	126.00	119.70
4	5	1639	U	C6-N1-C1'	-5.23	113.88	121.20
6	8	135	C	C2-N1-C1'	5.23	124.56	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	K	1331	C	N1-C2-O2	5.23	122.04	118.90
51	K	1304	U	N1-C2-O2	5.23	126.46	122.80
4	5	205	C	N1-C2-O2	5.23	122.04	118.90
6	8	2	G	C8-N9-C1'	-5.23	120.20	127.00
4	5	4413	C	C6-N1-C1'	-5.23	114.53	120.80
4	5	922(B)	C	OP1-P-O3'	5.22	116.68	105.20
4	5	1598	C	N3-C2-O2	-5.22	118.25	121.90
4	5	3657	U	C2-N1-C1'	5.22	123.96	117.70
4	5	3892	U	N3-C2-O2	-5.22	118.55	122.20
4	5	2502	A	P-O3'-C3'	5.22	125.96	119.70
4	5	4758	U	N3-C2-O2	-5.22	118.55	122.20
53	u	34	LYS	C-N-CA	5.21	134.73	121.70
51	K	1595	U	N1-C2-O2	5.21	126.45	122.80
4	5	654	C	N1-C2-O2	5.21	122.02	118.90
4	5	3693	U	N1-C2-O2	5.21	126.44	122.80
4	5	3882	C	C2-N1-C1'	5.21	124.53	118.80
4	5	1812	C	C6-N1-C2	-5.21	118.22	120.30
4	5	2454	U	N3-C2-O2	-5.21	118.56	122.20
4	5	3709	U	C2-N1-C1'	5.20	123.94	117.70
4	5	4880	C	C6-N1-C1'	-5.20	114.56	120.80
4	5	3888	G	P-O3'-C3'	5.20	125.93	119.70
4	5	4612	C	N1-C2-O2	5.19	122.02	118.90
4	5	2528	G	C8-N9-C1'	-5.19	120.25	127.00
51	K	1551	U	C6-N1-C1'	-5.19	113.94	121.20
4	5	4948	C	N3-C2-O2	-5.18	118.27	121.90
51	K	1394	G	P-O3'-C3'	5.18	125.92	119.70
51	K	1591	C	C6-N1-C2	-5.18	118.23	120.30
1	3	74	C	C2-N1-C1'	5.18	124.50	118.80
51	K	1834	A	C8-N9-C4	-5.18	103.73	105.80
4	5	1446	C	N3-C2-O2	-5.17	118.28	121.90
4	5	4243	C	N3-C2-O2	-5.17	118.28	121.90
4	5	2787	A	C4-N9-C1'	5.17	135.61	126.30
4	5	3831	U	N1-C2-O2	5.17	126.42	122.80
51	K	1259	A	C2-N3-C4	5.17	113.19	110.60
4	5	3693	U	N3-C2-O2	-5.17	118.58	122.20
4	5	1822	U	N1-C2-O2	5.16	126.41	122.80
51	K	369	C	N1-C2-O2	5.16	122.00	118.90
4	5	217	C	N1-C2-O2	5.16	121.99	118.90
1	3	63	C	N3-C2-O2	-5.15	118.29	121.90
51	K	973	C	N3-C2-O2	-5.15	118.30	121.90
4	5	4402	C	N1-C2-O2	5.14	121.98	118.90
51	K	1834	A	N7-C8-N9	5.14	116.37	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	5	4314	C	C6-N1-C2	-5.14	118.25	120.30
4	5	112	C	C6-N1-C2	-5.13	118.25	120.30
4	5	3761	C	N1-C2-O2	5.13	121.98	118.90
51	K	752	G	OP1-P-O3'	5.13	116.49	105.20
4	5	13	U	N1-C2-O2	5.13	126.39	122.80
51	K	876	C	C2-N1-C1'	5.13	124.44	118.80
51	K	1751	C	C2-N1-C1'	5.13	124.44	118.80
1	3	63	C	C6-N1-C2	-5.12	118.25	120.30
51	K	142	C	N1-C2-O2	5.12	121.97	118.90
51	K	314	U	N3-C2-O2	-5.12	118.61	122.20
4	5	1853	G	C4-N9-C1'	5.11	133.15	126.50
51	K	130	G	C8-N9-C1'	-5.11	120.35	127.00
51	K	1281	G	C4-N9-C1'	5.11	133.15	126.50
4	5	504	G	P-O3'-C3'	5.11	125.83	119.70
51	K	55	U	N3-C2-O2	-5.11	118.62	122.20
21	P	91	LEU	CA-CB-CG	5.11	127.05	115.30
51	K	1683	C	C2-N1-C1'	5.11	124.42	118.80
4	5	2787	A	N3-C4-N9	5.11	131.49	127.40
4	5	4092	G	C4-N9-C1'	5.11	133.14	126.50
51	K	872	A	C5-C6-N6	-5.10	119.62	123.70
82	4	44	U	C2-N1-C1'	5.10	123.83	117.70
51	K	1303	C	O4'-C1'-N1	5.10	112.28	108.20
1	3	8	U	C2-N1-C1'	5.10	123.82	117.70
4	5	1535	C	N3-C2-O2	-5.10	118.33	121.90
4	5	1807	C	N1-C2-O2	5.10	121.96	118.90
4	5	4254	G	N3-C4-N9	5.09	129.06	126.00
51	K	1590	C	N3-C2-O2	-5.09	118.33	121.90
51	K	1261	C	C5-C6-N1	5.09	123.54	121.00
4	5	4884	G	P-O3'-C3'	5.09	125.81	119.70
51	K	1309	C	C2-N1-C1'	5.09	124.39	118.80
51	K	55	U	N1-C2-O2	5.08	126.36	122.80
71	PP	110	LEU	CA-CB-CG	5.08	126.99	115.30
4	5	3673	C	N1-C2-O2	5.08	121.95	118.90
4	5	4119	C	P-O3'-C3'	5.08	125.80	119.70
4	5	4360	U	N1-C2-O2	5.07	126.35	122.80
4	5	26	C	N1-C2-O2	5.07	121.94	118.90
51	K	1489	A	P-O3'-C3'	5.07	125.78	119.70
51	K	494	C	N3-C2-O2	-5.07	118.35	121.90
4	5	4237	C	C6-N1-C2	-5.07	118.27	120.30
51	K	872	A	N9-C4-C5	-5.07	103.77	105.80
51	K	1137	U	P-O3'-C3'	5.07	125.78	119.70
4	5	704	C	N1-C2-O2	5.06	121.94	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	5	4162	C	C2-N1-C1'	5.06	124.37	118.80
55	w	59	LEU	CA-CB-CG	5.06	126.94	115.30
4	5	1656	U	N1-C2-O2	5.06	126.34	122.80
51	K	1139	C	C5-C6-N1	5.06	123.53	121.00
51	K	1117	C	N1-C2-O2	5.06	121.93	118.90
4	5	3905	A	O5'-P-OP1	-5.05	101.15	105.70
4	5	4293	U	N3-C2-O2	-5.05	118.66	122.20
4	5	125	C	P-O3'-C3'	5.05	125.76	119.70
4	5	4723	A	C6-N1-C2	-5.05	115.57	118.60
4	5	1485	C	N1-C2-O2	5.05	121.93	118.90
51	K	494	C	C2-N1-C1'	5.05	124.35	118.80
5	7	102	U	C2-N1-C1'	5.04	123.75	117.70
51	K	1358	U	N1-C2-O2	5.04	126.33	122.80
4	5	683	C	N3-C2-O2	-5.04	118.37	121.90
4	5	1440	U	P-O3'-C3'	5.04	125.75	119.70
4	5	220	C	C6-N1-C1'	-5.04	114.75	120.80
1	3	72	C	N1-C2-O2	5.04	121.92	118.90
4	5	4712	C	C6-N1-C2	-5.04	118.28	120.30
51	K	898	U	N1-C2-O2	5.04	126.33	122.80
51	K	501	C	C2-N1-C1'	5.04	124.34	118.80
4	5	753	C	N1-C2-O2	5.03	121.92	118.90
51	K	973	C	C6-N1-C2	-5.03	118.29	120.30
4	5	4215	C	N3-C2-O2	-5.03	118.38	121.90
51	K	530	U	N1-C2-O2	5.02	126.32	122.80
51	K	930	C	N3-C2-O2	-5.02	118.38	121.90
51	K	1364	U	C5-C6-N1	5.02	125.21	122.70
51	K	1590	C	C6-N1-C2	-5.02	118.29	120.30
4	5	2704	C	C2-N1-C1'	5.02	124.32	118.80
4	5	1179	U	N1-C2-O2	5.01	126.31	122.80
51	K	87	U	N3-C2-O2	-5.01	118.69	122.20
4	5	1485	C	C2-N1-C1'	5.01	124.31	118.80
51	K	340	C	C2-N1-C1'	5.01	124.31	118.80
51	K	642	U	P-O3'-C3'	5.01	125.71	119.70
4	5	480	C	P-O3'-C3'	5.01	125.71	119.70
4	5	1859	C	N3-C2-O2	-5.00	118.40	121.90
4	5	1990	A	OP1-P-O3'	5.00	116.21	105.20
4	5	2016	C	C2-N1-C1'	5.00	124.31	118.80

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	B	258	HIS	CA

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	B	257	TRP	Mainchain
70	II	99	LEU	Peptide
17	L	63	THR	Peptide
19	N	76	PRO	Peptide
19	N	78	GLY	Peptide
75	VV	61	GLN	Peptide
67	WW	17	TYR	Peptide
67	WW	37	TYR	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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
2	1	22/24 (92%)	19 (86%)	2 (9%)	1 (4%)	2 14
7	A	246/248 (99%)	233 (95%)	13 (5%)	0	100 100
8	B	392/394 (100%)	374 (95%)	16 (4%)	2 (0%)	29 68
9	C	360/362 (99%)	349 (97%)	10 (3%)	1 (0%)	41 76
10	D	291/293 (99%)	283 (97%)	8 (3%)	0	100 100
11	E	208/251 (83%)	199 (96%)	9 (4%)	0	100 100
12	F	223/225 (99%)	212 (95%)	11 (5%)	0	100 100
13	G	229/233 (98%)	219 (96%)	10 (4%)	0	100 100
14	H	188/190 (99%)	181 (96%)	7 (4%)	0	100 100
15	I	201/205 (98%)	195 (97%)	6 (3%)	0	100 100
16	J	168/170 (99%)	162 (96%)	6 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	L	208/210 (99%)	200 (96%)	6 (3%)	2 (1%)	15	53
18	M	136/138 (99%)	129 (95%)	7 (5%)	0	100	100
19	N	201/203 (99%)	191 (95%)	10 (5%)	0	100	100
20	O	197/199 (99%)	192 (98%)	5 (2%)	0	100	100
21	P	151/153 (99%)	148 (98%)	3 (2%)	0	100	100
22	Q	185/187 (99%)	178 (96%)	7 (4%)	0	100	100
23	R	178/180 (99%)	174 (98%)	4 (2%)	0	100	100
24	S	174/176 (99%)	167 (96%)	7 (4%)	0	100	100
25	T	157/159 (99%)	152 (97%)	5 (3%)	0	100	100
26	U	97/99 (98%)	94 (97%)	3 (3%)	0	100	100
27	V	129/131 (98%)	124 (96%)	5 (4%)	0	100	100
28	W	102/121 (84%)	99 (97%)	3 (3%)	0	100	100
29	X	116/118 (98%)	115 (99%)	1 (1%)	0	100	100
30	Y	132/134 (98%)	130 (98%)	2 (2%)	0	100	100
31	Z	133/135 (98%)	127 (96%)	6 (4%)	0	100	100
32	a	145/147 (99%)	141 (97%)	4 (3%)	0	100	100
33	b	100/104 (96%)	95 (95%)	5 (5%)	0	100	100
34	c	96/98 (98%)	95 (99%)	1 (1%)	0	100	100
35	d	105/107 (98%)	100 (95%)	5 (5%)	0	100	100
36	e	126/128 (98%)	123 (98%)	3 (2%)	0	100	100
37	f	107/109 (98%)	105 (98%)	2 (2%)	0	100	100
38	g	112/114 (98%)	111 (99%)	1 (1%)	0	100	100
39	h	120/122 (98%)	118 (98%)	2 (2%)	0	100	100
40	i	100/102 (98%)	98 (98%)	2 (2%)	0	100	100
41	j	84/86 (98%)	81 (96%)	3 (4%)	0	100	100
42	k	67/69 (97%)	67 (100%)	0	0	100	100
43	l	48/50 (96%)	46 (96%)	2 (4%)	0	100	100
44	m	50/52 (96%)	49 (98%)	1 (2%)	0	100	100
45	n	23/25 (92%)	23 (100%)	0	0	100	100
46	o	102/104 (98%)	99 (97%)	3 (3%)	0	100	100
47	p	89/91 (98%)	87 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	r	122/124 (98%)	116 (95%)	6 (5%)	0	100	100
49	s	194/196 (99%)	185 (95%)	9 (5%)	0	100	100
50	t	151/153 (99%)	136 (90%)	15 (10%)	0	100	100
52	q	215/217 (99%)	208 (97%)	7 (3%)	0	100	100
53	u	211/213 (99%)	205 (97%)	6 (3%)	0	100	100
54	v	219/221 (99%)	212 (97%)	7 (3%)	0	100	100
55	w	226/228 (99%)	220 (97%)	6 (3%)	0	100	100
56	x	260/262 (99%)	250 (96%)	10 (4%)	0	100	100
57	y	181/191 (95%)	170 (94%)	11 (6%)	0	100	100
58	z	235/237 (99%)	231 (98%)	4 (2%)	0	100	100
59	BB	181/189 (96%)	176 (97%)	5 (3%)	0	100	100
60	CC	204/206 (99%)	194 (95%)	10 (5%)	0	100	100
61	DD	183/185 (99%)	182 (100%)	1 (0%)	0	100	100
62	SS	94/96 (98%)	89 (95%)	5 (5%)	0	100	100
63	EE	139/151 (92%)	133 (96%)	6 (4%)	0	100	100
64	RR	115/117 (98%)	107 (93%)	8 (7%)	0	100	100
65	QQ	147/149 (99%)	147 (100%)	0	0	100	100
66	MM	133/135 (98%)	127 (96%)	6 (4%)	0	100	100
67	WW	118/120 (98%)	109 (92%)	9 (8%)	0	100	100
68	UU	140/142 (99%)	135 (96%)	5 (4%)	0	100	100
69	KK	130/132 (98%)	127 (98%)	3 (2%)	0	100	100
70	II	142/144 (99%)	135 (95%)	7 (5%)	0	100	100
71	PP	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
72	GG	98/100 (98%)	93 (95%)	5 (5%)	0	100	100
73	HH	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
74	TT	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
75	VV	139/141 (99%)	134 (96%)	4 (3%)	1 (1%)	22	60
76	NN	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
77	OO	73/75 (97%)	72 (99%)	1 (1%)	0	100	100
78	LL	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
79	JJ	81/83 (98%)	78 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
80	FF	60/62 (97%)	59 (98%)	1 (2%)	0	100 100
81	9	53/55 (96%)	52 (98%)	1 (2%)	0	100 100
83	0	66/68 (97%)	62 (94%)	4 (6%)	0	100 100
84	6	311/313 (99%)	289 (93%)	22 (7%)	0	100 100
85	AA	53/55 (96%)	53 (100%)	0	0	100 100
All	All	11540/11784 (98%)	11118 (96%)	415 (4%)	7 (0%)	54 85

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	C	71	ARG
2	1	247	CYS
8	B	260	ALA
17	L	64	VAL
8	B	259	PRO
17	L	63	THR
75	VV	62	PRO

5.3.2 Protein sidechains (i)

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
2	1	22/22 (100%)	18 (82%)	4 (18%)	1 9
7	A	190/190 (100%)	184 (97%)	6 (3%)	39 74
8	B	342/342 (100%)	339 (99%)	3 (1%)	78 92
9	C	302/302 (100%)	294 (97%)	8 (3%)	46 78
10	D	247/247 (100%)	244 (99%)	3 (1%)	71 90
11	E	190/223 (85%)	187 (98%)	3 (2%)	62 86
12	F	196/196 (100%)	195 (100%)	1 (0%)	88 96
13	G	200/200 (100%)	196 (98%)	4 (2%)	55 83
14	H	169/169 (100%)	165 (98%)	4 (2%)	49 79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
15	I	175/175 (100%)	171 (98%)	4 (2%)	50 80
16	J	143/143 (100%)	143 (100%)	0	100 100
17	L	175/175 (100%)	175 (100%)	0	100 100
18	M	117/117 (100%)	116 (99%)	1 (1%)	78 92
19	N	171/171 (100%)	169 (99%)	2 (1%)	71 90
20	O	171/171 (100%)	169 (99%)	2 (1%)	71 90
21	P	134/134 (100%)	133 (99%)	1 (1%)	84 94
22	Q	164/164 (100%)	163 (99%)	1 (1%)	86 95
23	R	159/159 (100%)	156 (98%)	3 (2%)	57 84
24	S	157/157 (100%)	157 (100%)	0	100 100
25	T	139/139 (100%)	137 (99%)	2 (1%)	67 88
26	U	89/89 (100%)	88 (99%)	1 (1%)	73 90
27	V	101/101 (100%)	99 (98%)	2 (2%)	55 83
28	W	86/100 (86%)	86 (100%)	0	100 100
29	X	106/106 (100%)	105 (99%)	1 (1%)	78 92
30	Y	124/124 (100%)	123 (99%)	1 (1%)	81 93
31	Z	117/117 (100%)	117 (100%)	0	100 100
32	a	119/119 (100%)	118 (99%)	1 (1%)	81 93
33	b	84/84 (100%)	82 (98%)	2 (2%)	49 79
34	c	84/84 (100%)	83 (99%)	1 (1%)	71 90
35	d	98/98 (100%)	96 (98%)	2 (2%)	55 83
36	e	114/114 (100%)	114 (100%)	0	100 100
37	f	88/88 (100%)	87 (99%)	1 (1%)	73 90
38	g	98/98 (100%)	96 (98%)	2 (2%)	55 83
39	h	109/109 (100%)	109 (100%)	0	100 100
40	i	86/86 (100%)	85 (99%)	1 (1%)	71 90
41	j	73/73 (100%)	72 (99%)	1 (1%)	67 88
42	k	64/64 (100%)	64 (100%)	0	100 100
43	l	47/47 (100%)	47 (100%)	0	100 100
44	m	48/48 (100%)	48 (100%)	0	100 100
45	n	24/24 (100%)	24 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
46	o	92/92 (100%)	91 (99%)	1 (1%)	73 90
47	p	74/74 (100%)	73 (99%)	1 (1%)	67 88
48	r	108/108 (100%)	106 (98%)	2 (2%)	57 84
49	s	164/164 (100%)	164 (100%)	0	100 100
50	t	126/126 (100%)	126 (100%)	0	100 100
52	q	180/181 (99%)	178 (99%)	2 (1%)	73 90
53	u	194/194 (100%)	190 (98%)	4 (2%)	53 82
54	v	187/187 (100%)	186 (100%)	1 (0%)	88 96
55	w	190/190 (100%)	185 (97%)	5 (3%)	46 78
56	x	224/224 (100%)	221 (99%)	3 (1%)	69 89
57	y	158/161 (98%)	158 (100%)	0	100 100
58	z	207/207 (100%)	205 (99%)	2 (1%)	76 91
59	BB	165/169 (98%)	165 (100%)	0	100 100
60	CC	178/178 (100%)	175 (98%)	3 (2%)	60 85
61	DD	161/161 (100%)	157 (98%)	4 (2%)	47 79
62	SS	87/87 (100%)	86 (99%)	1 (1%)	73 90
63	EE	130/136 (96%)	127 (98%)	3 (2%)	50 80
64	RR	99/99 (100%)	98 (99%)	1 (1%)	76 91
65	QQ	130/130 (100%)	129 (99%)	1 (1%)	81 93
66	MM	104/105 (99%)	103 (99%)	1 (1%)	76 91
67	WW	109/109 (100%)	108 (99%)	1 (1%)	78 92
68	UU	117/117 (100%)	116 (99%)	1 (1%)	78 92
69	KK	119/119 (100%)	119 (100%)	0	100 100
70	II	125/125 (100%)	124 (99%)	1 (1%)	81 93
71	PP	111/111 (100%)	110 (99%)	1 (1%)	78 92
72	GG	92/92 (100%)	91 (99%)	1 (1%)	73 90
73	HH	67/67 (100%)	66 (98%)	1 (2%)	65 87
74	TT	112/112 (100%)	112 (100%)	0	100 100
75	VV	113/113 (100%)	113 (100%)	0	100 100
76	NN	107/107 (100%)	106 (99%)	1 (1%)	78 92
77	OO	66/66 (100%)	66 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
78	LL	88/88 (100%)	87 (99%)	1 (1%)	73 90
79	JJ	75/75 (100%)	74 (99%)	1 (1%)	69 89
80	FF	55/55 (100%)	54 (98%)	1 (2%)	59 85
81	9	48/48 (100%)	48 (100%)	0	100 100
83	0	61/61 (100%)	60 (98%)	1 (2%)	62 86
84	6	272/272 (100%)	270 (99%)	2 (1%)	84 94
85	AA	46/46 (100%)	44 (96%)	2 (4%)	29 66
All	All	10063/10125 (99%)	9945 (99%)	118 (1%)	72 90

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	1	237	ASP
2	1	246	LEU
2	1	259	LEU
2	1	260	MET
7	A	128	ARG
7	A	163	ARG
7	A	193	ARG
7	A	194	ASN
7	A	200	ARG
7	A	242	ARG
8	B	24	ARG
8	B	261	ARG
8	B	262	VAL
9	C	38	ASN
9	C	69	THR
9	C	71	ARG
9	C	95	MET
9	C	188	ARG
9	C	223	ASN
9	C	312	ARG
9	C	321	ASN
10	D	111	ASN
10	D	157	ASN
10	D	268	ARG
11	E	58	ARG
11	E	164	ARG
11	E	289	LEU
12	F	205	ASN

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Mol	Chain	Res	Type
13	G	134	ASN
13	G	242	ARG
13	G	249	ARG
13	G	293	ASN
14	H	1	MET
14	H	15	ASN
14	H	102	ASN
14	H	128	MET
15	I	3	ARG
15	I	73	ASN
15	I	100	ASN
15	I	116	ARG
18	M	119	ARG
19	N	50	ARG
19	N	162	ARG
20	O	117	ARG
20	O	140	ARG
21	P	128	ARG
22	Q	97	LYS
23	R	36	ASN
23	R	130	ASN
23	R	133	LYS
25	T	136	ARG
25	T	146	LYS
26	U	81	ARG
27	V	15	ARG
27	V	48	ARG
29	X	53	ARG
30	Y	2	LYS
32	a	4	ARG
33	b	60	ASN
33	b	72	ILE
34	c	90	ARG
35	d	18	ASN
35	d	31	LYS
37	f	16	ARG
38	g	14	ASN
38	g	18	ASN
40	i	29	ARG
41	j	20	ARG
46	o	82	MET
47	p	84	ARG

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Mol	Chain	Res	Type
48	r	12	ASN
48	r	67	ARG
52	q	50	ASN
52	q	186	ARG
53	u	40	ASN
53	u	147	ASN
53	u	207	LEU
53	u	213	ARG
54	v	167	ARG
55	w	22	ASN
55	w	76	ARG
55	w	94	ARG
55	w	106	ARG
55	w	227	LYS
56	x	148	ARG
56	x	232	ASN
56	x	240	ARG
58	z	63	MET
58	z	191	ARG
60	CC	84	ASN
60	CC	87	ASN
60	CC	99	ASN
61	DD	29	LEU
61	DD	69	ARG
61	DD	70	ARG
61	DD	79	ARG
62	SS	96	ARG
63	EE	20	LYS
63	EE	69	ARG
63	EE	97	ARG
64	RR	33	ARG
65	QQ	27	LYS
66	MM	146	ARG
67	WW	13	ARG
68	UU	41	MET
70	II	8	LYS
71	PP	62	ARG
72	GG	47	ASN
73	HH	82	ASN
76	NN	101	LYS
78	LL	5	ARG
79	JJ	81	ARG

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Mol	Chain	Res	Type
80	FF	40	ARG
83	0	138	ARG
84	6	159	ASN
84	6	178	ASN
85	AA	99	LYS
85	AA	104	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (95) such sidechains are listed below:

Mol	Chain	Res	Type
2	1	253	GLN
7	A	194	ASN
8	B	258	HIS
9	C	38	ASN
9	C	60	HIS
9	C	321	ASN
10	D	138	GLN
10	D	157	ASN
10	D	202	GLN
11	E	193	HIS
12	F	38	GLN
12	F	79	ASN
12	F	109	GLN
12	F	130	ASN
12	F	205	ASN
13	G	99	GLN
13	G	134	ASN
13	G	293	ASN
14	H	15	ASN
14	H	102	ASN
15	I	73	ASN
15	I	95	HIS
15	I	163	GLN
16	J	98	ASN
16	J	104	ASN
17	L	19	GLN
18	M	83	ASN
19	N	8	GLN
19	N	32	GLN
19	N	201	HIS
21	P	64	ASN
21	P	75	GLN

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Mol	Chain	Res	Type
21	P	80	GLN
21	P	120	ASN
21	P	137	ASN
23	R	36	ASN
23	R	58	HIS
23	R	178	GLN
24	S	50	GLN
25	T	127	GLN
27	V	77	HIS
28	W	17	HIS
29	X	93	ASN
29	X	111	GLN
30	Y	14	ASN
32	a	60	HIS
32	a	67	GLN
32	a	120	GLN
33	b	12	GLN
33	b	101	HIS
34	c	19	GLN
35	d	18	ASN
38	g	14	ASN
38	g	18	ASN
38	g	114	GLN
39	h	63	GLN
48	r	12	ASN
49	s	68	HIS
52	q	141	ASN
53	u	124	HIS
53	u	147	ASN
53	u	157	GLN
54	v	113	GLN
54	v	136	HIS
54	v	272	HIS
55	w	22	ASN
56	x	232	ASN
57	y	31	ASN
57	y	114	ASN
58	z	81	HIS
60	CC	84	ASN
60	CC	87	ASN
60	CC	99	ASN
60	CC	165	GLN

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Mol	Chain	Res	Type
62	SS	7	ASN
62	SS	44	HIS
64	RR	82	ASN
66	MM	94	HIS
67	WW	104	GLN
68	UU	80	GLN
68	UU	86	GLN
68	UU	97	GLN
69	KK	62	GLN
72	GG	47	ASN
73	HH	82	ASN
74	TT	56	HIS
74	TT	113	HIS
80	FF	26	GLN
80	FF	29	GLN
84	6	104	HIS
84	6	133	ASN
84	6	159	ASN
84	6	178	ASN
84	6	296	GLN
85	AA	117	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	3	72/75 (96%)	14 (19%)	0
3	2	74/76 (97%)	30 (40%)	10 (13%)
4	5	3519/3543 (99%)	745 (21%)	64 (1%)
5	7	119/120 (99%)	14 (11%)	0
51	K	1686/1698 (99%)	338 (20%)	22 (1%)
6	8	149/151 (98%)	30 (20%)	1 (0%)
82	4	5/6 (83%)	3 (60%)	0
All	All	5624/5669 (99%)	1174 (20%)	97 (1%)

All (1174) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	3	7	A
1	3	13	C
1	3	16	C
1	3	21	A

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Mol	Chain	Res	Type
1	3	34	U
1	3	35	A
1	3	47	U
1	3	49	C
1	3	58	A
1	3	63	C
1	3	65	G
1	3	69	G
1	3	70	G
1	3	76	A
3	2	7	G
3	2	8	U
3	2	9	A
3	2	13	C
3	2	16	C
3	2	19	G
3	2	20	C
3	2	20(A)	U
3	2	22	G
3	2	31	G
3	2	35	A
3	2	42	A
3	2	44	A
3	2	45	G
3	2	47	U
3	2	48	C
3	2	51	U
3	2	52	G
3	2	53	G
3	2	56	C
3	2	58	A
3	2	61	C
3	2	62	C
3	2	63	A
3	2	65	C
3	2	67	G
3	2	72	C
3	2	74	C
3	2	75	C
3	2	76	A
4	5	8	U
4	5	12	A

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Mol	Chain	Res	Type
4	5	13	U
4	5	17	A
4	5	25	A
4	5	35	U
4	5	39	A
4	5	42	A
4	5	48	G
4	5	49	U
4	5	56	A
4	5	58	G
4	5	59	A
4	5	64	A
4	5	65	A
4	5	66	A
4	5	71	C
4	5	73	A
4	5	76	A
4	5	84	A
4	5	91	G
4	5	93	G
4	5	104	G
4	5	108	A
4	5	109	G
4	5	110	C
4	5	116	G
4	5	117	C
4	5	118	C
4	5	119	G
4	5	120	A
4	5	126	C
4	5	134	G
4	5	135	G
4	5	136	C
4	5	137	G
4	5	146	G
4	5	157	U
4	5	159	C
4	5	170	C
4	5	171	U
4	5	172	C
4	5	173	C
4	5	200	U

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Mol	Chain	Res	Type
4	5	201	C
4	5	202	C
4	5	205	C
4	5	209	U
4	5	216	C
4	5	217	C
4	5	218	A
4	5	221	C
4	5	224	U
4	5	226	G
4	5	233	U
4	5	234	G
4	5	246	G
4	5	265	C
4	5	266	C
4	5	276	C
4	5	278	G
4	5	280	G
4	5	297	U
4	5	306	A
4	5	309	C
4	5	310	G
4	5	315	G
4	5	316	U
4	5	322	C
4	5	334	A
4	5	340	C
4	5	345	C
4	5	350	C
4	5	363	A
4	5	386	A
4	5	387	G
4	5	399	G
4	5	407	A
4	5	410	A
4	5	412	G
4	5	413	G
4	5	431	G
4	5	432	U
4	5	440	U
4	5	446	C
4	5	449	C

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Mol	Chain	Res	Type
4	5	450	G
4	5	452	A
4	5	453	G
4	5	454	U
4	5	464	G
4	5	467	U
4	5	468	U
4	5	481	G
4	5	481(A)	C
4	5	482	G
4	5	483	G
4	5	485	C
4	5	486	C
4	5	492	U
4	5	493	G
4	5	495	C
4	5	497	G
4	5	498	C
4	5	499	G
4	5	505	G
4	5	641	G
4	5	658	C
4	5	666	G
4	5	667	A
4	5	669	C
4	5	670	G
4	5	683	C
4	5	684	G
4	5	685	C
4	5	687	U
4	5	696	C
4	5	697	G
4	5	704	C
4	5	705	G
4	5	719	C
4	5	729	G
4	5	730	G
4	5	731	G
4	5	738	C
4	5	738(A)	C
4	5	739	G
4	5	747	A

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Mol	Chain	Res	Type
4	5	749	G
4	5	750	U
4	5	758	G
4	5	913	U
4	5	914	U
4	5	917	A
4	5	918	G
4	5	923	C
4	5	925	C
4	5	926	G
4	5	928	C
4	5	929	A
4	5	931	C
4	5	932	A
4	5	933	G
4	5	934	C
4	5	935	A
4	5	935(A)	G
4	5	936	C
4	5	939	G
4	5	941	C
4	5	943	A
4	5	944	A
4	5	945	U
4	5	959	G
4	5	960	A
4	5	961	G
4	5	962	C
4	5	964	A
4	5	965	G
4	5	966	A
4	5	967	C
4	5	968	C
4	5	969	C
4	5	972	C
4	5	979	C
4	5	983	C
4	5	990	C
4	5	1068	G
4	5	1072	C
4	5	1073	G
4	5	1089	G

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Mol	Chain	Res	Type
4	5	1175	A
4	5	1179	U
4	5	1180	C
4	5	1184	A
4	5	1187	G
4	5	1195	G
4	5	1211	G
4	5	1212	G
4	5	1214	C
4	5	1215	C
4	5	1234	G
4	5	1235	G
4	5	1236	C
4	5	1237	C
4	5	1238	A
4	5	1239	C
4	5	1273	G
4	5	1276	C
4	5	1284	G
4	5	1287	G
4	5	1292	C
4	5	1293	G
4	5	1294	A
4	5	1295	U
4	5	1296	G
4	5	1301	C
4	5	1303	A
4	5	1304	C
4	5	1314	C
4	5	1326	A
4	5	1330	A
4	5	1331	C
4	5	1354	A
4	5	1358	G
4	5	1359	G
4	5	1371	A
4	5	1377	G
4	5	1379	C
4	5	1380	G
4	5	1387	A
4	5	1394	G
4	5	1397	A

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Mol	Chain	Res	Type
4	5	1398	A
4	5	1415	G
4	5	1416	G
4	5	1419	G
4	5	1420	A
4	5	1421	G
4	5	1429	C
4	5	1437	C
4	5	1438	U
4	5	1441	C
4	5	1445	U
4	5	1446	C
4	5	1448	G
4	5	1456	C
4	5	1457	G
4	5	1458	C
4	5	1465	G
4	5	1475	G
4	5	1478	C
4	5	1482	G
4	5	1483	C
4	5	1484	G
4	5	1489	G
4	5	1497	A
4	5	1498	G
4	5	1501	C
4	5	1502	G
4	5	1514	U
4	5	1516	G
4	5	1518	A
4	5	1523	A
4	5	1525	A
4	5	1534	A
4	5	1543	G
4	5	1547	A
4	5	1563	A
4	5	1564	A
4	5	1566	C
4	5	1568	C
4	5	1574	G
4	5	1578	U
4	5	1591	U

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Mol	Chain	Res	Type
4	5	1596	U
4	5	1597	G
4	5	1602	U
4	5	1612	G
4	5	1613	A
4	5	1624	G
4	5	1625	G
4	5	1631	A
4	5	1633	G
4	5	1634	A
4	5	1638	A
4	5	1640	C
4	5	1641	G
4	5	1654	G
4	5	1660	U
4	5	1661	C
4	5	1676	C
4	5	1677	U
4	5	1691	G
4	5	1724	G
4	5	1734	G
4	5	1740	C
4	5	1741	G
4	5	1742	A
4	5	1750	G
4	5	1755	C
4	5	1756	U
4	5	1761	G
4	5	1764	G
4	5	1768	C
4	5	1772	C
4	5	1773	U
4	5	1776	A
4	5	1781	U
4	5	1787	A
4	5	1799	G
4	5	1803	G
4	5	1804	A
4	5	1805	A
4	5	1809	C
4	5	1812	C
4	5	1815	G

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Mol	Chain	Res	Type
4	5	1819	G
4	5	1821	G
4	5	1822	U
4	5	1828	C
4	5	1835	G
4	5	1836	G
4	5	1837	A
4	5	1842	G
4	5	1843	A
4	5	1855	G
4	5	1869	G
4	5	1882	U
4	5	1888	A
4	5	1890	G
4	5	1893	C
4	5	1897	A
4	5	1898	C
4	5	1906	U
4	5	1910	G
4	5	1917	A
4	5	1918	U
4	5	1920	C
4	5	1921	C
4	5	1922	G
4	5	1923	A
4	5	1930	U
4	5	1931	C
4	5	1948	G
4	5	1957	U
4	5	1958	A
4	5	1959	U
4	5	1960	A
4	5	1961	G
4	5	1962	A
4	5	1964	A
4	5	1971	U
4	5	1977	C
4	5	1980	U
4	5	1983	A
4	5	1984	A
4	5	1986	U
4	5	1987	C

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Mol	Chain	Res	Type
4	5	1991	A
4	5	1997	U
4	5	2001	G
4	5	2002	A
4	5	2003	G
4	5	2004	U
4	5	2008	U
4	5	2011	C
4	5	2025	A
4	5	2026	A
4	5	2034	G
4	5	2047	A
4	5	2048	U
4	5	2052	G
4	5	2055	G
4	5	2056	G
4	5	2062	C
4	5	2064	G
4	5	2069	A
4	5	2070	U
4	5	2084	U
4	5	2085	G
4	5	2089	G
4	5	2090	U
4	5	2092	G
4	5	2093	G
4	5	2094	C
4	5	2095	A
4	5	2097	A
4	5	2098	G
4	5	2100	G
4	5	2101	A
4	5	2102	G
4	5	2104	A
4	5	2105	A
4	5	2107	A
4	5	2108	G
4	5	2110	G
4	5	2259	G
4	5	2260	C
4	5	2262	G
4	5	2266	C

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Mol	Chain	Res	Type
4	5	2267	U
4	5	2268	A
4	5	2269	C
4	5	2270	G
4	5	2275	G
4	5	2289	C
4	5	2300	A
4	5	2301	G
4	5	2306	G
4	5	2313	A
4	5	2316	G
4	5	2322	G
4	5	2331	G
4	5	2333	G
4	5	2348	G
4	5	2351	C
4	5	2360	A
4	5	2370	A
4	5	2384	U
4	5	2394	G
4	5	2395	A
4	5	2396	A
4	5	2398	U
4	5	2399	G
4	5	2410	C
4	5	2422	C
4	5	2425	U
4	5	2433	G
4	5	2441	C
4	5	2450	G
4	5	2471	G
4	5	2475	G
4	5	2485	U
4	5	2488	C
4	5	2489	C
4	5	2490	U
4	5	2491	C
4	5	2503	G
4	5	2504	C
4	5	2505	C
4	5	2506	G
4	5	2513	A

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Mol	Chain	Res	Type
4	5	2529	A
4	5	2530	U
4	5	2537	A
4	5	2546	G
4	5	2547	G
4	5	2549	G
4	5	2553	A
4	5	2554	U
4	5	2566	G
4	5	2570	U
4	5	2572	C
4	5	2575	U
4	5	2583	C
4	5	2586	G
4	5	2587	A
4	5	2589	C
4	5	2600	A
4	5	2601	A
4	5	2620	G
4	5	2638	G
4	5	2658	G
4	5	2661	U
4	5	2662	G
4	5	2669	C
4	5	2676	A
4	5	2686	G
4	5	2687	U
4	5	2689	C
4	5	2694	G
4	5	2695	A
4	5	2696	A
4	5	2704	C
4	5	2707	U
4	5	2708	U
4	5	2711	G
4	5	2712	G
4	5	2714	G
4	5	2716	C
4	5	2721	G
4	5	2725	A
4	5	2726	G
4	5	2735	G

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Mol	Chain	Res	Type
4	5	2740	U
4	5	2743	A
4	5	2744	A
4	5	2754	G
4	5	2760	G
4	5	2761	U
4	5	2763	U
4	5	2764	A
4	5	2769	U
4	5	2772	C
4	5	2787	A
4	5	2788	U
4	5	2789	A
4	5	2790	U
4	5	2798	A
4	5	2806	A
4	5	2807	A
4	5	2814	C
4	5	2826	U
4	5	2827	G
4	5	2828	U
4	5	2837	U
4	5	2838	G
4	5	2842	G
4	5	2855	G
4	5	2867	C
4	5	2875	C
4	5	2898	G
4	5	3598	C
4	5	3604	A
4	5	3605	C
4	5	3606	U
4	5	3625	G
4	5	3626	G
4	5	3635	A
4	5	3636	C
4	5	3646	A
4	5	3657	U
4	5	3662	A
4	5	3673	C
4	5	3688	U
4	5	3696	C

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Mol	Chain	Res	Type
4	5	3698	G
4	5	3711	A
4	5	3712	A
4	5	3729	U
4	5	3747	A
4	5	3748	A
4	5	3753	G
4	5	3759	A
4	5	3760	A
4	5	3763	A
4	5	3765	G
4	5	3773	U
4	5	3774	A
4	5	3776	G
4	5	3777	G
4	5	3784	A
4	5	3786	U
4	5	3799	A
4	5	3810	C
4	5	3812	C
4	5	3814	U
4	5	3817	A
4	5	3819	G
4	5	3838	U
4	5	3839	G
4	5	3840	U
4	5	3843	C
4	5	3877	A
4	5	3878	C
4	5	3879	G
4	5	3889	G
4	5	3892	U
4	5	3897	G
4	5	3898	G
4	5	3901	A
4	5	3905	A
4	5	3906	A
4	5	3907	G
4	5	3908	A
4	5	3915	U
4	5	3916	G
4	5	3917	A

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Mol	Chain	Res	Type
4	5	3918	G
4	5	3926	C
4	5	3927	U
4	5	3938	G
4	5	3939	G
4	5	3941	G
4	5	4069	U
4	5	4076	G
4	5	4077	A
4	5	4084	G
4	5	4085	A
4	5	4086	G
4	5	4088	C
4	5	4116	C
4	5	4119	C
4	5	4120	U
4	5	4125	C
4	5	4127	A
4	5	4158	C
4	5	4162	C
4	5	4163	U
4	5	4166	G
4	5	4171	C
4	5	4173	G
4	5	4183	G
4	5	4184	G
4	5	4191	G
4	5	4203	A
4	5	4212	A
4	5	4225	G
4	5	4229	U
4	5	4232	U
4	5	4233	A
4	5	4243	C
4	5	4249	G
4	5	4251	A
4	5	4254	G
4	5	4266	G
4	5	4268	A
4	5	4271	A
4	5	4273	A
4	5	4281	A

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Mol	Chain	Res	Type
4	5	4282	A
4	5	4291	G
4	5	4296	U
4	5	4297	G
4	5	4304	A
4	5	4305	G
4	5	4306	U
4	5	4313	A
4	5	4314	C
4	5	4317	A
4	5	4319	C
4	5	4326	G
4	5	4329	G
4	5	4330	G
4	5	4332	C
4	5	4336	A
4	5	4349	C
4	5	4350	C
4	5	4354	U
4	5	4355	G
4	5	4368	G
4	5	4373	G
4	5	4377	G
4	5	4378	A
4	5	4379	A
4	5	4380	A
4	5	4387	C
4	5	4393	G
4	5	4394	A
4	5	4395	U
4	5	4401	G
4	5	4419	U
4	5	4421	C
4	5	4422	A
4	5	4436	U
4	5	4437	U
4	5	4440	G
4	5	4444	C
4	5	4448	G
4	5	4449	A
4	5	4464	A
4	5	4471	U

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Mol	Chain	Res	Type
4	5	4475	G
4	5	4495	G
4	5	4500	U
4	5	4511	A
4	5	4512	U
4	5	4513	A
4	5	4515	G
4	5	4518	A
4	5	4519	C
4	5	4520	G
4	5	4524	G
4	5	4530	U
4	5	4531	U
4	5	4548	A
4	5	4556	U
4	5	4557	U
4	5	4560	C
4	5	4567	G
4	5	4573	G
4	5	4574	U
4	5	4575	G
4	5	4587	G
4	5	4590	A
4	5	4599	A
4	5	4635	A
4	5	4636	U
4	5	4637	G
4	5	4639	G
4	5	4652	G
4	5	4656	A
4	5	4657	U
4	5	4661	G
4	5	4667	C
4	5	4670	C
4	5	4672	A
4	5	4677	U
4	5	4678	G
4	5	4687	A
4	5	4700	A
4	5	4709	U
4	5	4719	G
4	5	4720	C

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Mol	Chain	Res	Type
4	5	4736	C
4	5	4745	G
4	5	4750	G
4	5	4751	G
4	5	4754	G
4	5	4756	C
4	5	4757	C
4	5	4759	C
4	5	4765	G
4	5	4771	C
4	5	4870	G
4	5	4871	C
4	5	4872	G
4	5	4873	G
4	5	4875	G
4	5	4876	A
4	5	4877	G
4	5	4882	U
4	5	4883	C
4	5	4885	U
4	5	4895	C
4	5	4910	A
4	5	4914	G
4	5	4915	G
4	5	4918	C
4	5	4919	G
4	5	4921	C
4	5	4922	C
4	5	4925	U
4	5	4926	C
4	5	4927	G
4	5	4928	C
4	5	4931	G
4	5	4934	A
4	5	4937	C
4	5	4940	C
4	5	4943	A
4	5	4944	C
4	5	4948	C
4	5	4949	G
4	5	4950	U
4	5	4951	G

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Mol	Chain	Res	Type
4	5	4955	A
4	5	4956	A
4	5	4958	C
4	5	4960	G
4	5	4964	C
4	5	4965	U
4	5	4966	A
4	5	4967	A
4	5	4976	U
4	5	4988	U
4	5	4989	U
4	5	4990	C
4	5	4993	G
4	5	4999	G
4	5	5006	U
4	5	5007	A
4	5	5014	A
4	5	5017	G
4	5	5022	U
4	5	5040	U
4	5	5041	G
4	5	5047	C
4	5	5050	C
4	5	5052	C
4	5	5053	U
4	5	5054	C
4	5	5056	A
4	5	5061	A
4	5	5062	G
5	7	7	G
5	7	22	A
5	7	25	G
5	7	53	U
5	7	54	A
5	7	63	C
5	7	64	G
5	7	74	A
5	7	76	U
5	7	97	G
5	7	100	A
5	7	110	G
5	7	111	C

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Mol	Chain	Res	Type
5	7	120	U
6	8	2	G
6	8	23	C
6	8	34	U
6	8	35	C
6	8	38	U
6	8	39	G
6	8	49	G
6	8	59	A
6	8	62	A
6	8	63	U
6	8	75	G
6	8	79	G
6	8	87	G
6	8	94	G
6	8	95	A
6	8	103	A
6	8	105	C
6	8	107	C
6	8	109	C
6	8	110	U
6	8	111	U
6	8	113	C
6	8	114	G
6	8	123	U
6	8	125	C
6	8	126	C
6	8	127	U
6	8	128	C
6	8	147	G
6	8	150	C
51	K	2	A
51	K	3	C
51	K	4	C
51	K	20	G
51	K	25	A
51	K	26	U
51	K	33	G
51	K	41	G
51	K	42	A
51	K	44	U
51	K	46	A

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Mol	Chain	Res	Type
51	K	56	G
51	K	58	C
51	K	67	C
51	K	68	A
51	K	71	G
51	K	73	C
51	K	74	G
51	K	75	G
51	K	77	A
51	K	79	A
51	K	103	A
51	K	111	A
51	K	113	G
51	K	115	U
51	K	124	U
51	K	126	G
51	K	127	C
51	K	129	C
51	K	130	G
51	K	141	A
51	K	142	C
51	K	143	U
51	K	147	A
51	K	154	U
51	K	155	G
51	K	158	A
51	K	162	C
51	K	163	U
51	K	167	G
51	K	168	C
51	K	180	G
51	K	182	C
51	K	183	G
51	K	184	G
51	K	188	C
51	K	191	A
51	K	192	C
51	K	202	G
51	K	215	G
51	K	294	U
51	K	302	A
51	K	304	C

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Mol	Chain	Res	Type
51	K	307	G
51	K	308	G
51	K	309	G
51	K	312	G
51	K	314	U
51	K	317	C
51	K	318	A
51	K	319	C
51	K	335	G
51	K	339	A
51	K	347	G
51	K	351	G
51	K	360	A
51	K	364	A
51	K	368	U
51	K	369	C
51	K	381	C
51	K	385	G
51	K	386	C
51	K	398	A
51	K	400	C
51	K	407	G
51	K	408	A
51	K	409	C
51	K	417	C
51	K	418	A
51	K	435	A
51	K	438	G
51	K	448	A
51	K	450	C
51	K	464	A
51	K	465	A
51	K	466	G
51	K	471	G
51	K	472	C
51	K	473	A
51	K	474	G
51	K	482	G
51	K	487	U
51	K	492	C
51	K	496	C
51	K	525	A

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Mol	Chain	Res	Type
51	K	530	U
51	K	532	C
51	K	533	A
51	K	542	U
51	K	544	G
51	K	547	G
51	K	548	C
51	K	549	C
51	K	550	C
51	K	551	U
51	K	554	A
51	K	555	A
51	K	556	U
51	K	559	G
51	K	560	A
51	K	563	G
51	K	564	A
51	K	568	C
51	K	570	C
51	K	576	A
51	K	583	A
51	K	587	A
51	K	588	G
51	K	590	A
51	K	591	U
51	K	606	G
51	K	608	C
51	K	614	C
51	K	617	G
51	K	621	C
51	K	643	A
51	K	644	G
51	K	660	C
51	K	663	C
51	K	664	A
51	K	668	A
51	K	669	A
51	K	671	A
51	K	672	A
51	K	673	G
51	K	683	G
51	K	688	U

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Mol	Chain	Res	Type
51	K	689	U
51	K	690	G
51	K	752	G
51	K	753	C
51	K	754	G
51	K	798	G
51	K	799	U
51	K	811	A
51	K	821	G
51	K	822	U
51	K	830	A
51	K	833	C
51	K	834	C
51	K	844	U
51	K	847	A
51	K	867	G
51	K	870	A
51	K	871	U
51	K	872	A
51	K	873	G
51	K	874	G
51	K	875	A
51	K	878	G
51	K	887	U
51	K	890	U
51	K	892	U
51	K	902	G
51	K	907	G
51	K	913	A
51	K	914	U
51	K	920	A
51	K	933	G
51	K	934	G
51	K	955	A
51	K	971	G
51	K	990	A
51	K	992	A
51	K	999	G
51	K	1002	U
51	K	1017	U
51	K	1023	A
51	K	1041	G

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Mol	Chain	Res	Type
51	K	1045	U
51	K	1060	A
51	K	1062	A
51	K	1067	C
51	K	1080	A
51	K	1083	A
51	K	1085	C
51	K	1089	G
51	K	1100	A
51	K	1109	C
51	K	1111	U
51	K	1115	U
51	K	1116	C
51	K	1117	C
51	K	1118	C
51	K	1123	C
51	K	1131	G
51	K	1133	A
51	K	1138	C
51	K	1139	C
51	K	1149	A
51	K	1153	C
51	K	1154	U
51	K	1155	U
51	K	1170	A
51	K	1195	A
51	K	1207	G
51	K	1208	A
51	K	1215	C
51	K	1221	G
51	K	1224	G
51	K	1242	U
51	K	1251	A
51	K	1253	A
51	K	1254	C
51	K	1255	G
51	K	1256	G
51	K	1257	G
51	K	1259	A
51	K	1264	C
51	K	1271	C
51	K	1274	G

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Mol	Chain	Res	Type
51	K	1275	G
51	K	1280	G
51	K	1281	G
51	K	1282	A
51	K	1284	A
51	K	1285	G
51	K	1286	G
51	K	1293	A
51	K	1294	G
51	K	1298	G
51	K	1299	A
51	K	1301	A
51	K	1302	G
51	K	1303	C
51	K	1304	U
51	K	1307	U
51	K	1308	U
51	K	1313	A
51	K	1314	U
51	K	1316	C
51	K	1322	G
51	K	1333	U
51	K	1341	C
51	K	1342	U
51	K	1348	G
51	K	1363	C
51	K	1371	U
51	K	1372	U
51	K	1376	A
51	K	1378	A
51	K	1382	A
51	K	1395	C
51	K	1396	A
51	K	1397	U
51	K	1401	A
51	K	1402	A
51	K	1404	U
51	K	1409	A
51	K	1410	C
51	K	1412	C
51	K	1428	G
51	K	1442	U

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Mol	Chain	Res	Type
51	K	1449	G
51	K	1454	A
51	K	1462	U
51	K	1463	U
51	K	1466	G
51	K	1473	G
51	K	1476	A
51	K	1477	U
51	K	1480	A
51	K	1489	A
51	K	1490	G
51	K	1494	U
51	K	1497	G
51	K	1498	A
51	K	1507	G
51	K	1510	G
51	K	1521	C
51	K	1522	A
51	K	1531	A
51	K	1533	A
51	K	1536	G
51	K	1544	C
51	K	1548	G
51	K	1552	G
51	K	1553	C
51	K	1556	A
51	K	1557	C
51	K	1560	U
51	K	1570	G
51	K	1575	G
51	K	1580	A
51	K	1585	U
51	K	1586	U
51	K	1587	G
51	K	1588	A
51	K	1601	A
51	K	1604	G
51	K	1606	G
51	K	1621	U
51	K	1623	A
51	K	1637	A
51	K	1638	G

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Mol	Chain	Res	Type
51	K	1648	G
51	K	1665	G
51	K	1680	G
51	K	1683	C
51	K	1686	G
51	K	1695	A
51	K	1698	C
51	K	1699	A
51	K	1701	C
51	K	1715	A
51	K	1721	U
51	K	1722	G
51	K	1726	G
51	K	1744	G
51	K	1753	C
51	K	1783	C
51	K	1784	G
51	K	1785	C
51	K	1823	A
51	K	1825	A
51	K	1826	G
51	K	1831	A
51	K	1836	G
51	K	1838	U
51	K	1849	G
51	K	1851	A
51	K	1861	G
51	K	1862	G
51	K	1863	A
51	K	1865	C
51	K	1866	A
51	K	1867	U
51	K	1869	A
82	4	44	U
82	4	45	A
82	4	46	A

All (97) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	2	6	C
3	2	7	G

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Mol	Chain	Res	Type
3	2	18	G
3	2	20	C
3	2	31	G
3	2	44	A
3	2	46	G
3	2	48	C
3	2	50	U
3	2	75	C
4	5	47	A
4	5	48	G
4	5	125	C
4	5	134	G
4	5	217	C
4	5	245	C
4	5	265	C
4	5	275	C
4	5	385	A
4	5	406	C
4	5	449	C
4	5	480	C
4	5	485	C
4	5	492	U
4	5	504	G
4	5	696	C
4	5	930	G
4	5	959	G
4	5	966	A
4	5	971(A)	G
4	5	1072	C
4	5	1174	G
4	5	1211	G
4	5	1236	C
4	5	1238	A
4	5	1291	G
4	5	1329	G
4	5	1370	G
4	5	1440	U
4	5	1445	U
4	5	1455	G
4	5	1633	G
4	5	1804	A
4	5	1818	G

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Mol	Chain	Res	Type
4	5	1835	G
4	5	1921	C
4	5	1979	A
4	5	1983	A
4	5	2046	G
4	5	2068	C
4	5	2089	G
4	5	2266	C
4	5	2474	G
4	5	2502	A
4	5	2546	G
4	5	2661	U
4	5	2695	A
4	5	3625	G
4	5	3697	U
4	5	3876	A
4	5	3888	G
4	5	3904	G
4	5	4075	U
4	5	4119	C
4	5	4170	A
4	5	4232	U
4	5	4448	G
4	5	4556	U
4	5	4699	U
4	5	4719	G
4	5	4884	G
4	5	4925	U
4	5	4936	G
4	5	4947	U
6	8	124	U
51	K	110	U
51	K	182	C
51	K	303	C
51	K	434	G
51	K	465	A
51	K	532	C
51	K	553	U
51	K	642	U
51	K	688	U
51	K	752	G
51	K	798	G

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Mol	Chain	Res	Type
51	K	870	A
51	K	1137	U
51	K	1253	A
51	K	1394	G
51	K	1395	C
51	K	1396	A
51	K	1489	A
51	K	1520	G
51	K	1637	A
51	K	1664	A
51	K	1824	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 305 ligands modelled in this entry, 305 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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 (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	5	25
51	K	11
1	3	2
3	2	2
33	b	1
13	G	1
6	8	1
15	I	1

All 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	41.44
1	b	76:VAL	C	89:VAL	N	37.48
1	5	1252:C	O3'	1271:G	P	36.52
1	5	1219:G	O3'	1233:G	P	22.30
1	5	3948:C	O3'	4065:G	P	19.38
1	K	697:G	O3'	729:C	P	18.46
1	5	1406(C):G	O3'	1411:C	P	18.45
1	K	1761:U	O3'	1771:G	P	18.04
1	5	990:C	O3'	1064:G	P	17.96
1	K	756:C	O3'	788:G	P	17.67
1	5	4101:C	O3'	4107:G	P	17.58
1	5	523:C	O3'	638:G	P	17.53
1	5	4138:C	O3'	4146:G	P	17.26
1	K	834:C	O3'	841:G	P	17.17
1	G	176:ALA	C	184:LYS	N	17.10
1	K	323:C	O3'	329:G	P	16.81
1	5	4777:C	O3'	4859:C	P	16.58
1	K	130:G	O3'	140:U	P	15.95
1	K	1417:C	O3'	1423:C	P	15.74
1	5	1696:C	O3'	1720:C	P	14.92
1	5	760:G	O3'	904:C	P	14.76
1	5	5022:U	O3'	5028:G	P	14.42
1	5	2901:G	O3'	3597:G	P	13.64
1	5	182:G	O3'	189:G	P	13.49
1	5	1364:U	O3'	1368:A	P	13.11
1	8	79:G	O3'	85:U	P	12.22
1	5	4729:A	O3'	4735:G	P	9.79
1	I	103:LEU	C	112:GLN	N	9.41
1	5	1180:C	O3'	1183:C	P	9.34
1	5	512:U	O3'	515:C	P	9.08
1	K	225:G	O3'	287:U	P	7.92
1	K	745:C	O3'	749:U	P	7.91

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	K	736:C	O3'	743:U	P	6.77
1	3	19:G	O3'	20:U	P	6.14
1	5	1239:C	O3'	1244:G	P	5.77
1	5	500:G	O3'	504:G	P	5.75
1	5	1100:U	O3'	1168:G	P	5.33
1	5	4740:G	O3'	4743:G	P	4.67
1	3	16:C	O3'	18:U	P	4.43
1	2	16:C	O3'	18:G	P	4.14
1	K	1432:U	O3'	1438:A	P	4.12
1	5	1438:U	O3'	1440:U	P	3.36
1	5	4899:G	O3'	4902:C	P	3.32
1	2	20(A):U	O3'	21:A	P	3.19

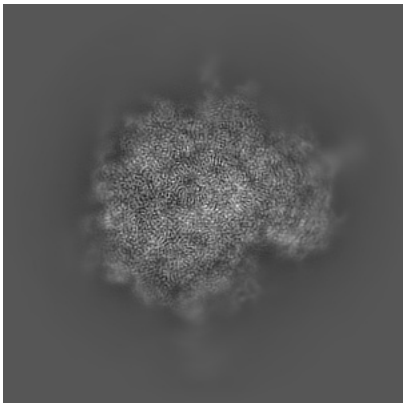
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4729. These allow visual inspection of the internal detail of the map and identification of artifacts.

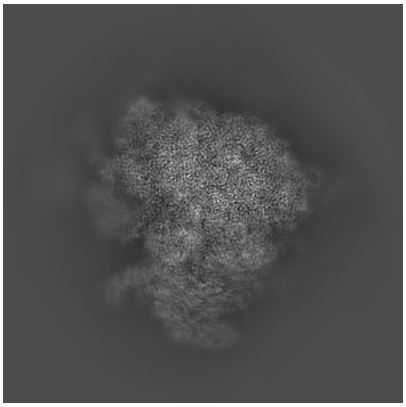
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

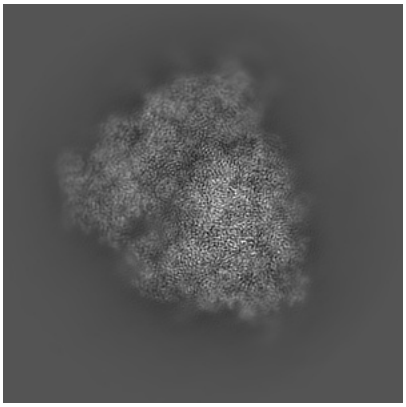
6.1.1 Primary map



X



Y

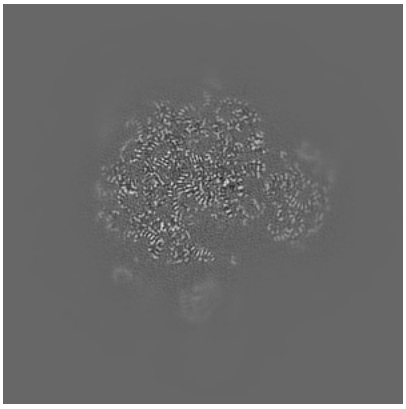


Z

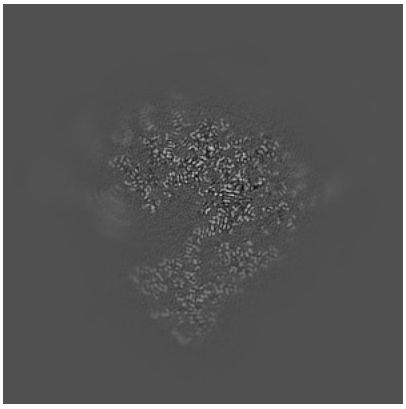
The images above show the map projected in three orthogonal directions.

6.2 Central slices

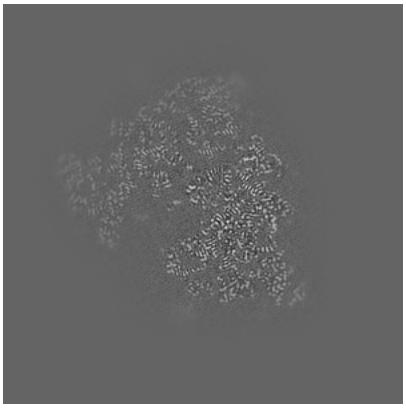
6.2.1 Primary map



X Index: 198



Y Index: 198

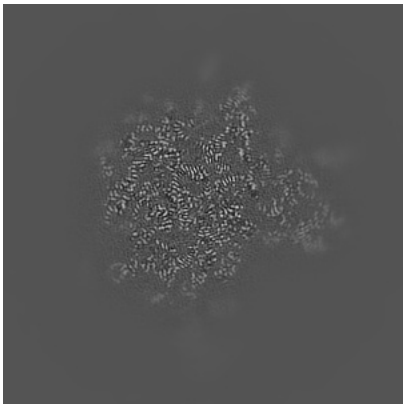


Z Index: 198

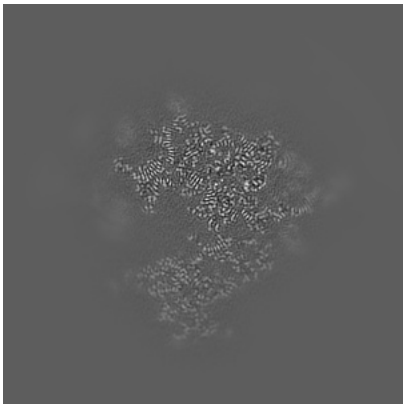
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

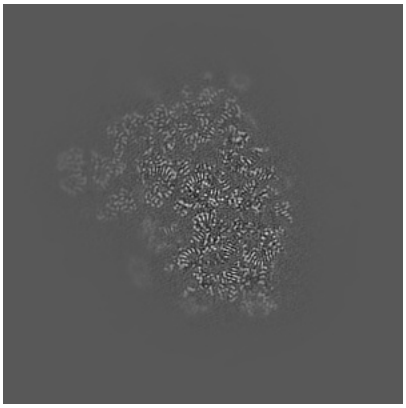
6.3.1 Primary map



X Index: 218



Y Index: 205



Z Index: 216

The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

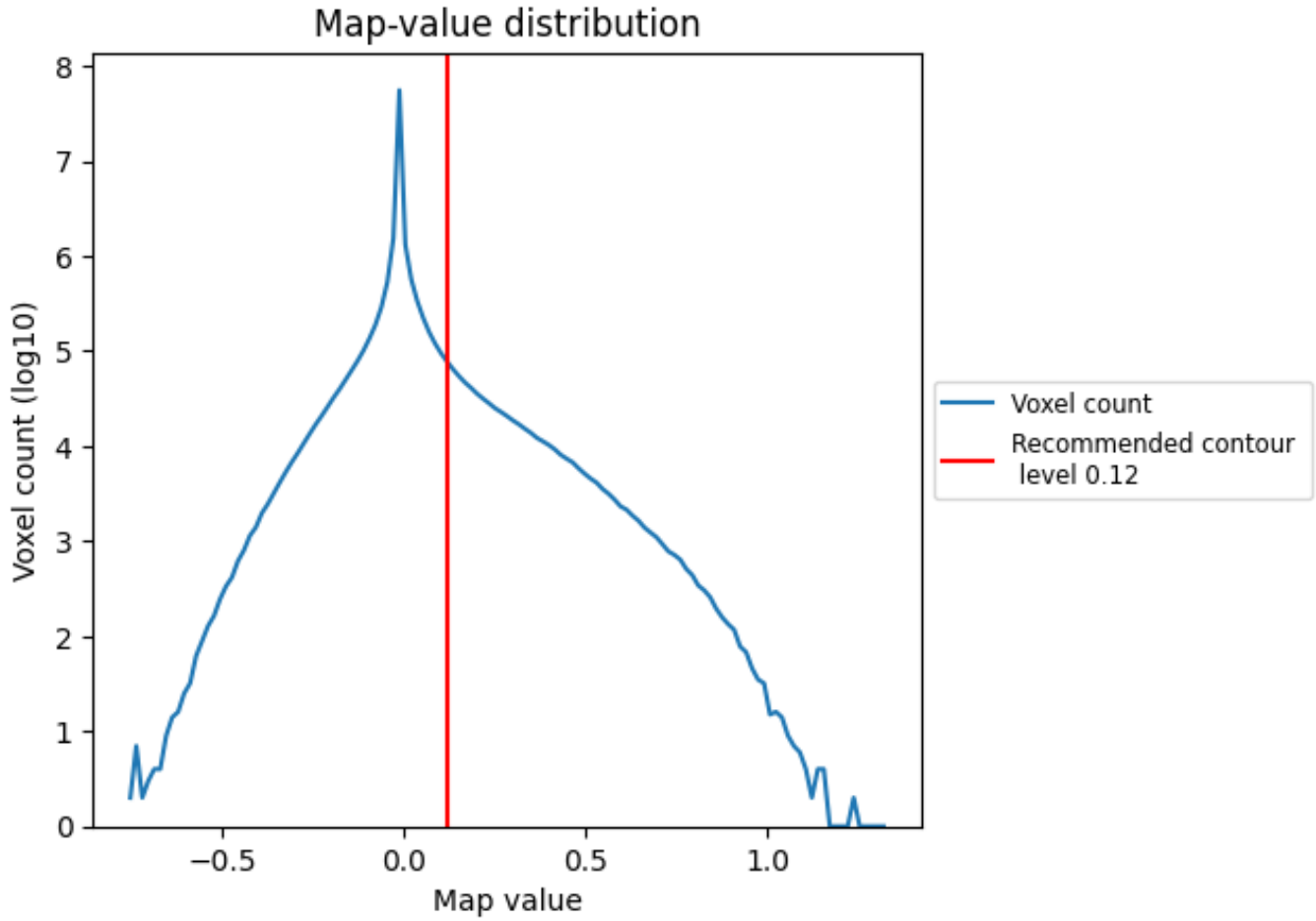
6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

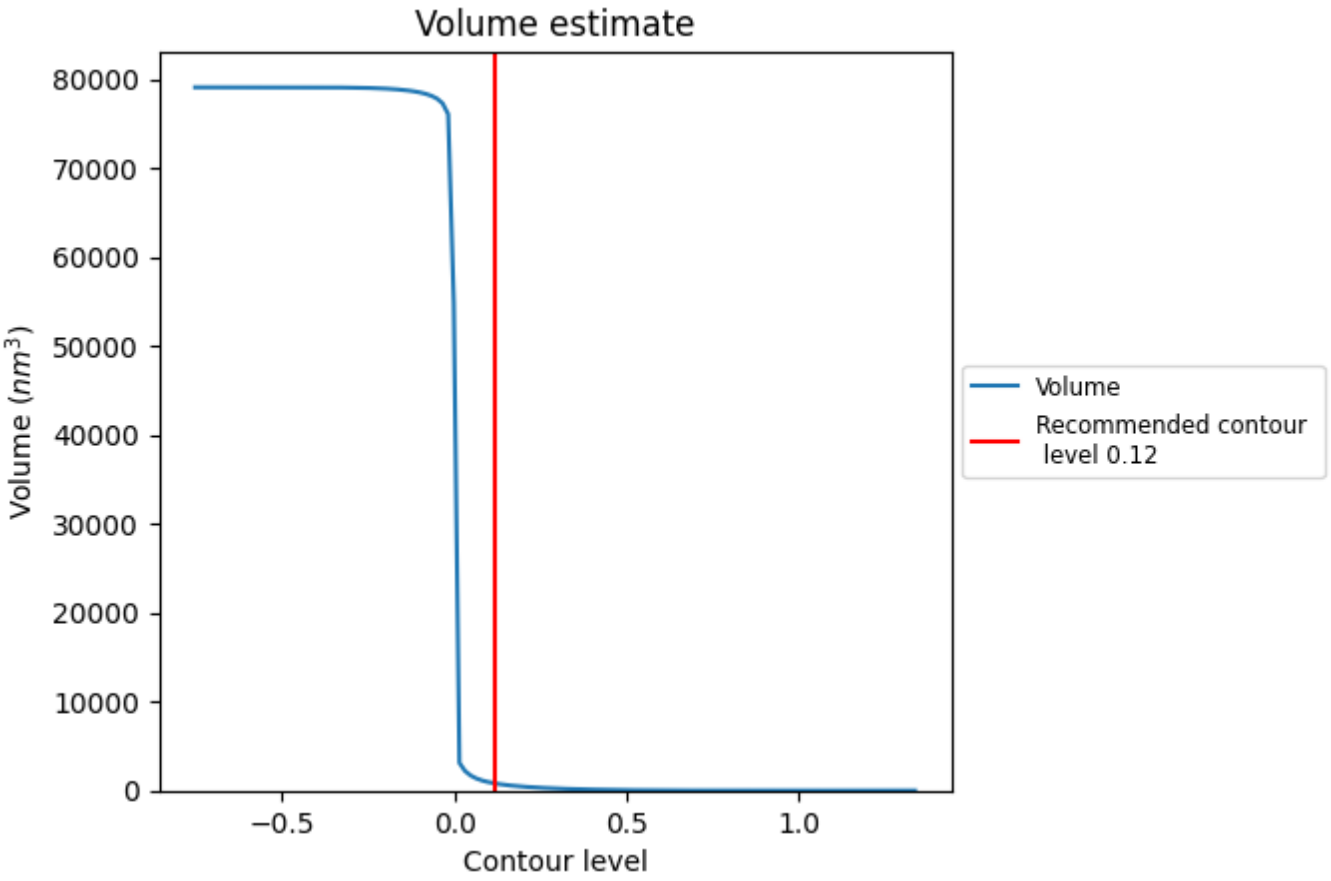
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

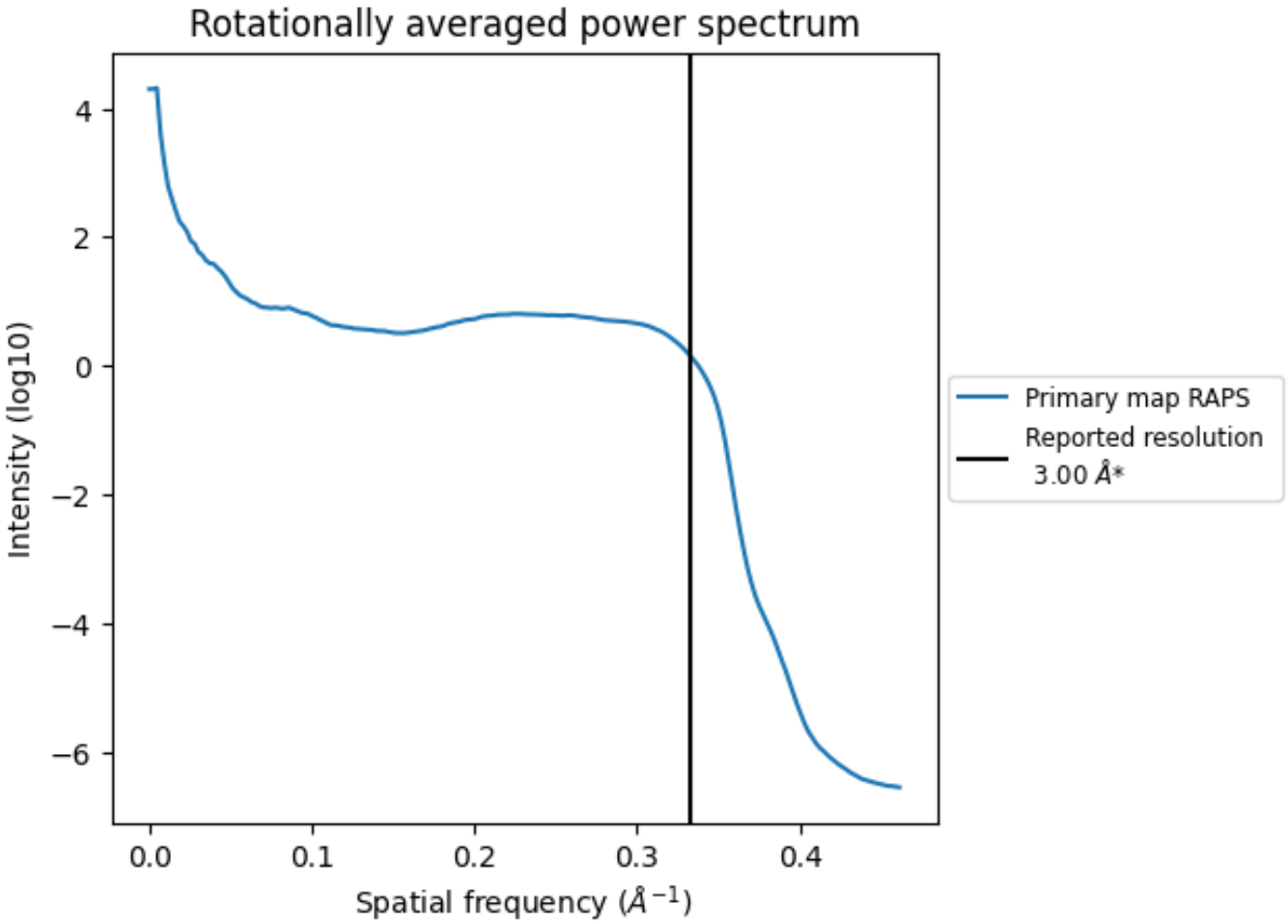
7.2 Volume estimate



The volume at the recommended contour level is 792 nm^3; this corresponds to an approximate mass of 716 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

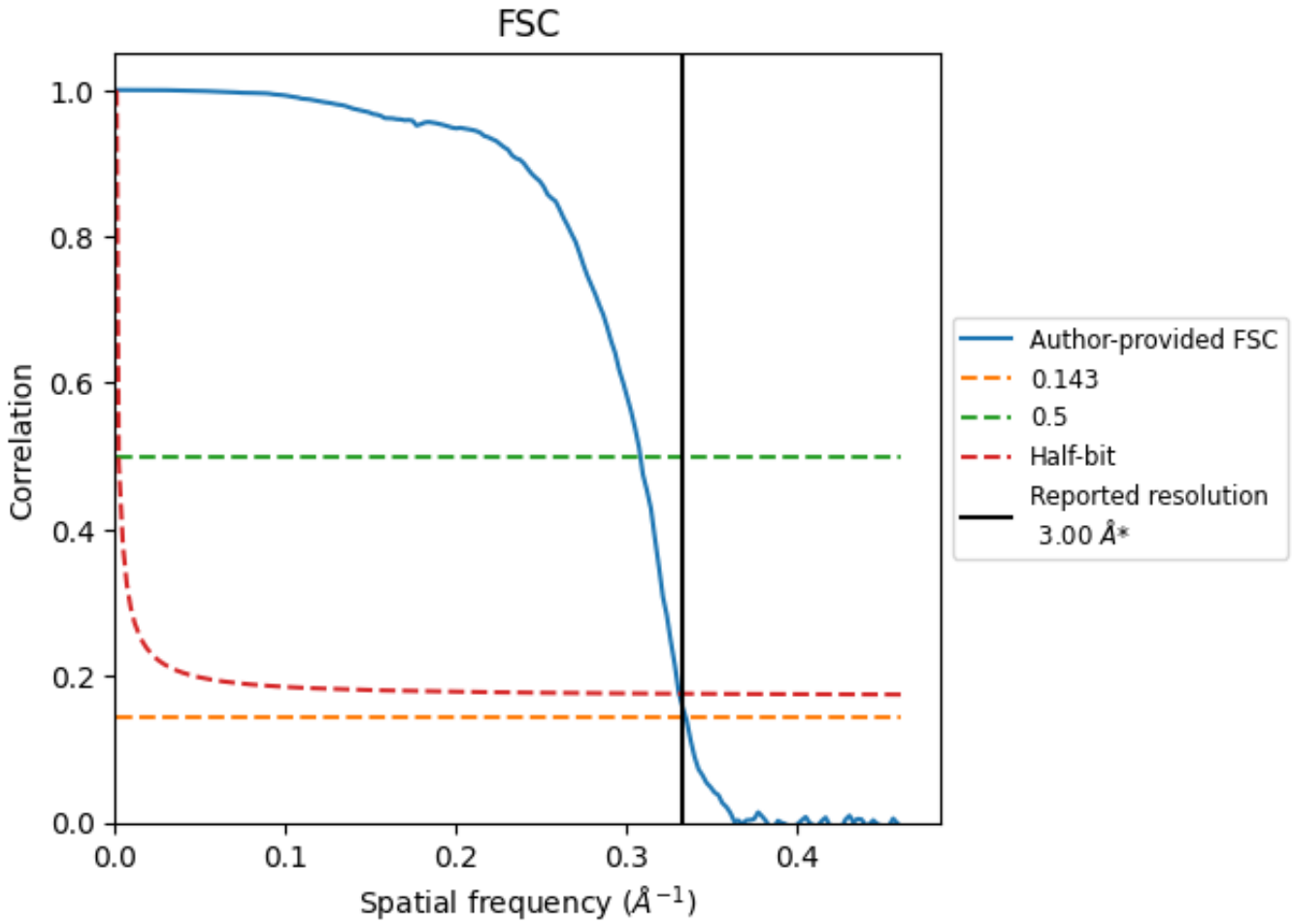


*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

8.2 Resolution estimates (i)

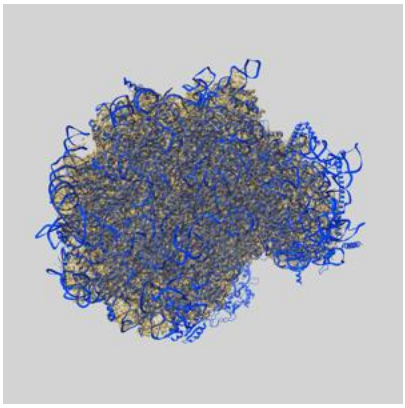
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	2.99	3.24	3.02
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

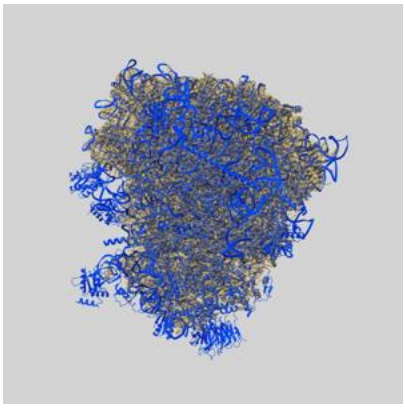
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4729 and PDB model 6R5Q. Per-residue inclusion information can be found in section 3 on page 23.

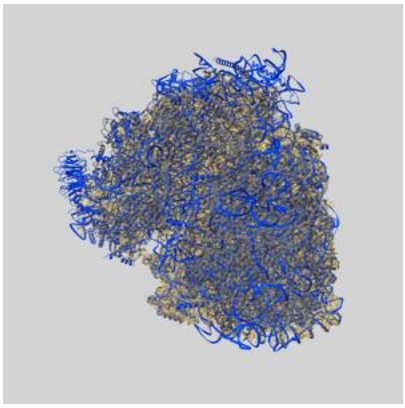
9.1 Map-model overlay



X



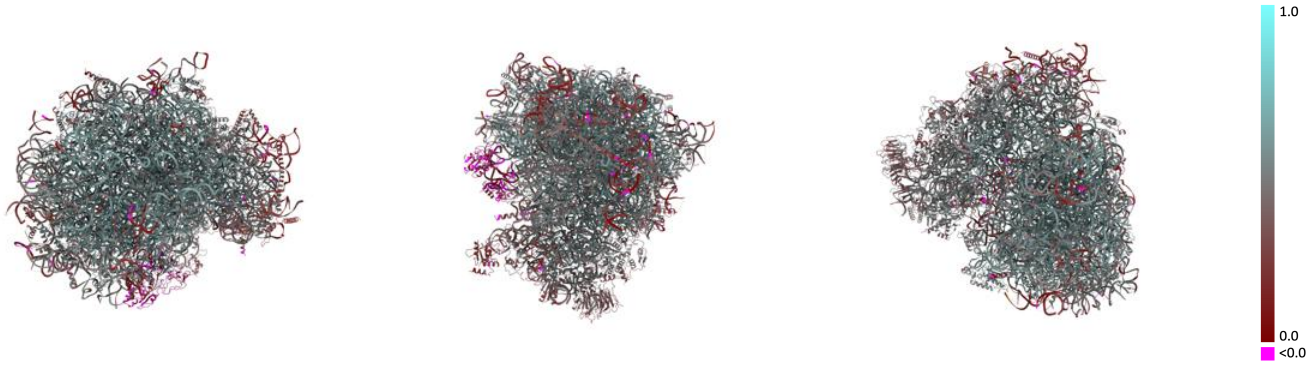
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

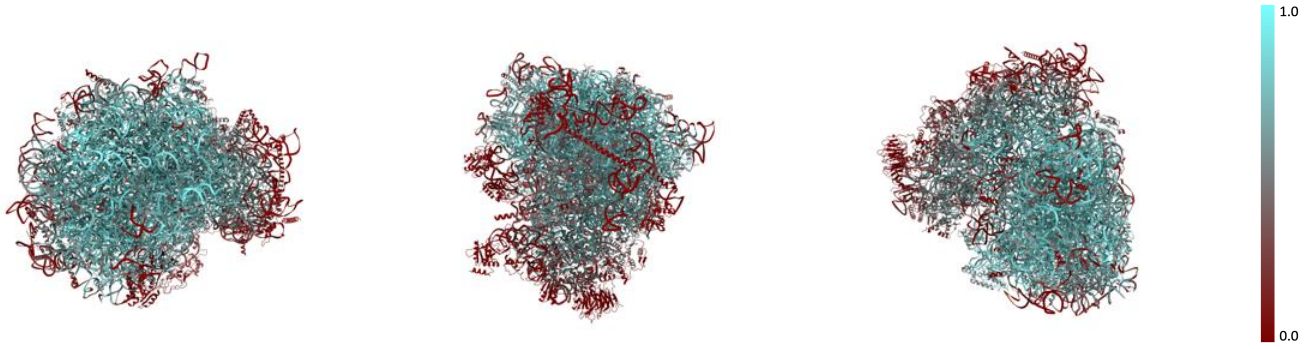
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

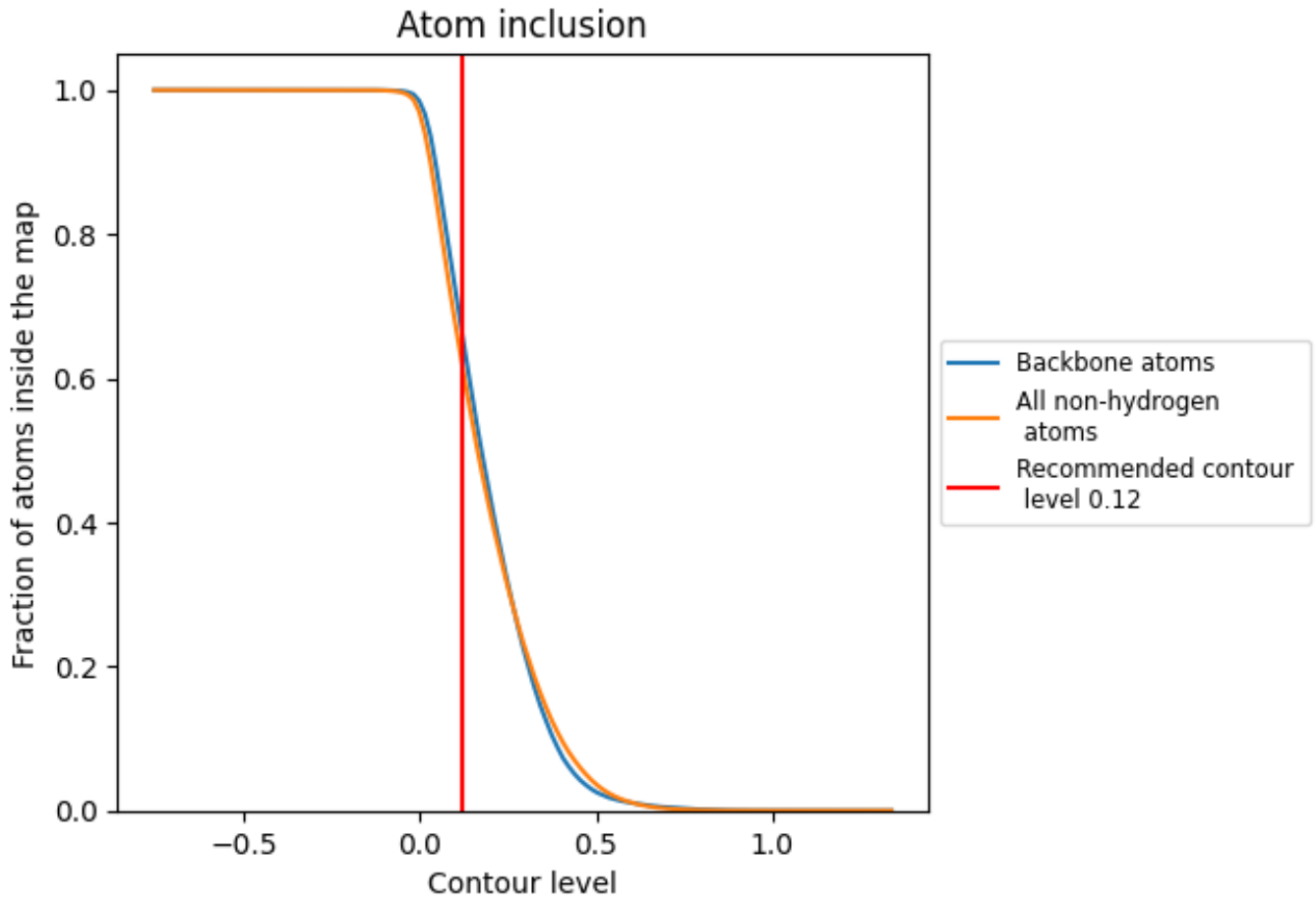
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.12).

9.4 Atom inclusion (i)



At the recommended contour level, 66% of all backbone atoms, 62% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6187	0.4860
0	0.0000	0.2780
1	0.8040	0.5990
2	0.5818	0.5070
3	0.2142	0.3410
4	0.6378	0.5550
5	0.7442	0.5220
6	0.0209	0.3470
7	0.8752	0.5810
8	0.8098	0.5430
9	0.4558	0.4440
A	0.7940	0.5470
AA	0.2418	0.3540
B	0.7368	0.5220
BB	0.2272	0.3960
C	0.7295	0.5180
CC	0.4837	0.4490
D	0.6787	0.5050
DD	0.3597	0.4330
E	0.5956	0.4620
EE	0.5816	0.4930
F	0.7448	0.5190
FF	0.3723	0.4330
G	0.5786	0.4650
GG	0.1899	0.3820
H	0.6543	0.4950
HH	0.3569	0.4460
I	0.7207	0.5180
II	0.3869	0.4160
J	0.6162	0.4700
JJ	0.3912	0.4480
K	0.5796	0.4810
KK	0.2380	0.4180
L	0.6285	0.4740
LL	0.5691	0.4750

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Chain	Atom inclusion	Q-score
M	0.6906	0.5040
MM	0.5640	0.4830
N	0.8130	0.5500
NN	0.1998	0.4040
O	0.7552	0.5270
OO	0.2796	0.4080
P	0.7483	0.5250
PP	0.3052	0.4210
Q	0.7414	0.5110
QQ	0.5969	0.5010
R	0.6357	0.4880
RR	0.0000	0.2170
S	0.7585	0.5180
SS	0.1127	0.3770
T	0.6675	0.4920
TT	0.5475	0.4850
U	0.4703	0.4290
UU	0.3288	0.4330
V	0.7505	0.5390
VV	0.5826	0.4960
W	0.4416	0.4040
WW	0.2311	0.3820
X	0.6691	0.4960
Y	0.6800	0.5000
Z	0.6319	0.4670
a	0.7874	0.5470
b	0.4687	0.4210
c	0.6478	0.5040
d	0.6709	0.4920
e	0.7525	0.5260
f	0.7886	0.5370
g	0.7015	0.5150
h	0.6660	0.4950
i	0.6168	0.4810
j	0.7982	0.5380
k	0.5081	0.4580
l	0.7377	0.5110
m	0.7284	0.5070
n	0.7064	0.4620
o	0.7010	0.5250
p	0.7155	0.5220
q	0.3793	0.4420

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Chain	Atom inclusion	Q-score
r	0.7147	0.5160
s	0.0007	0.0470
t	0.0000	0.0430
u	0.4820	0.4700
v	0.4567	0.4570
w	0.2128	0.3890
x	0.3432	0.4430
y	0.4197	0.4420
z	0.1558	0.3270