



Full wwPDB EM Validation Report ⓘ

Nov 10, 2024 – 12:24 pm 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:

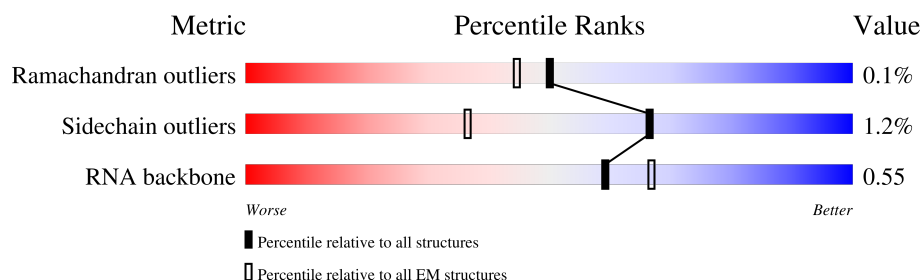
EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

1 Overall quality at a glance

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

The reported resolution of this entry is 3.00 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	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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 $\leq 5\%$. 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	<p>80% 75% 24%</p>
2	1	24	<p>79% 17%</p>
3	2	76	<p>16% 54% 42%</p>
4	5	3543	<p>16% 75% 22%</p>
5	7	120	<p>85% 15%</p>
6	8	151	<p>8% 76% 22%</p>
7	A	248	<p>98%</p>
8	B	394	<p>8% 97%</p>

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

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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%
50	t	153	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	<div><div></div><div>100%</div><div></div></div> <div><div></div><div>99%</div><div></div></div> <div>.</div>
85	AA	55	<div><div></div><div>80%</div><div></div></div> <div><div></div><div>96%</div><div></div></div> <div>.</div>

2 Entry composition [i](#)

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	

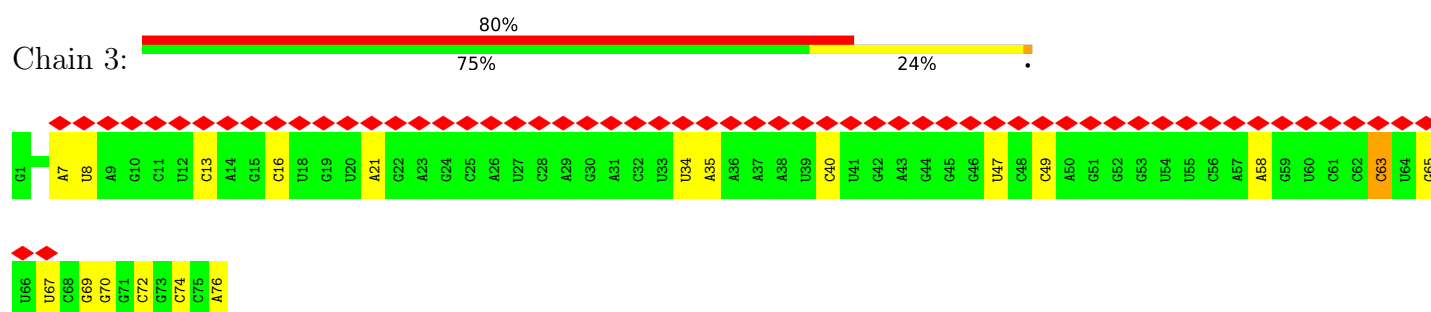
- Molecule 87 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

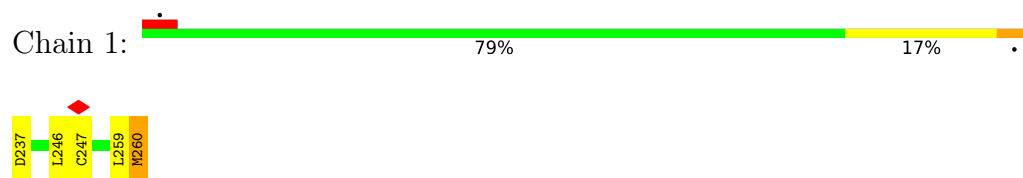
3 Residue-property plots [i](#)

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.

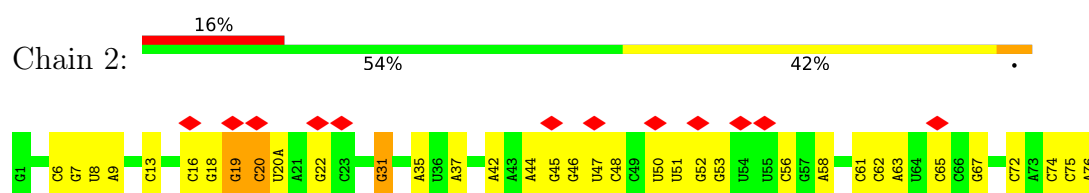
• Molecule 1: E-tRNA



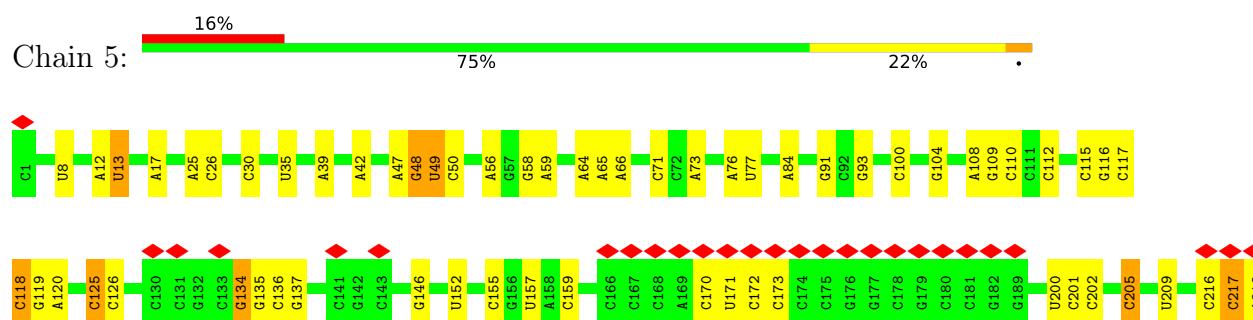
• Molecule 2: X-box-binding protein 1

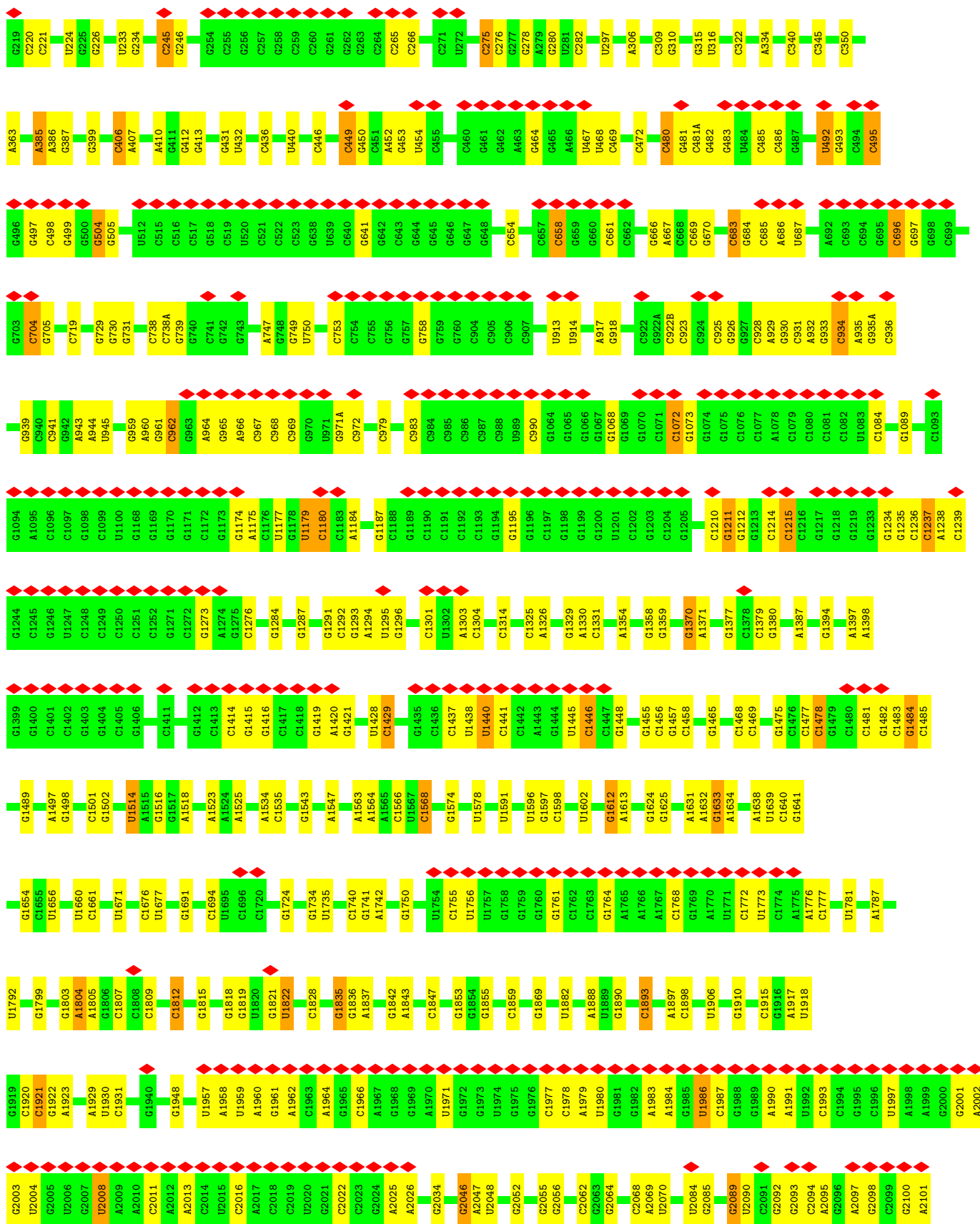


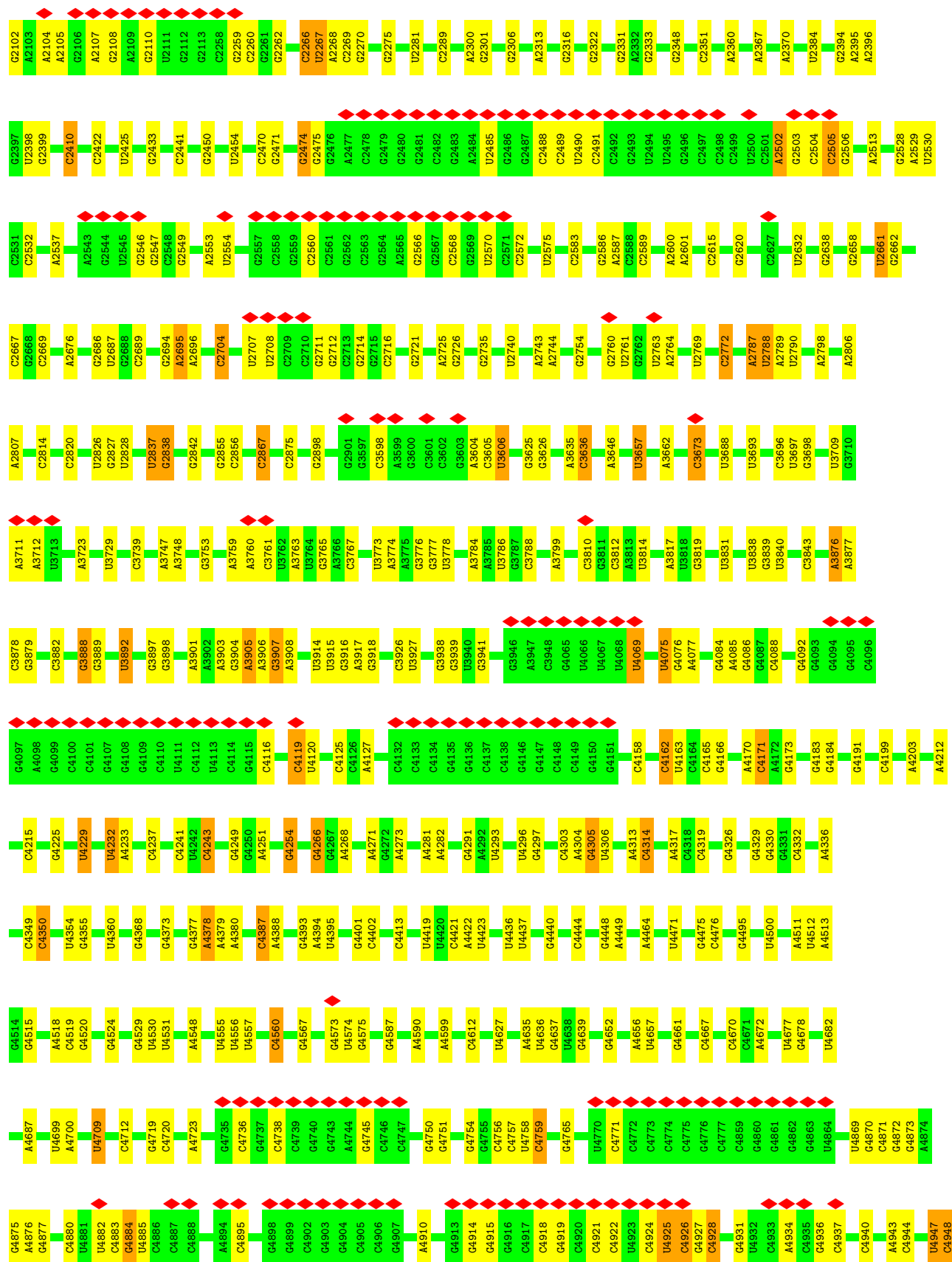
• Molecule 3: P-tRNA

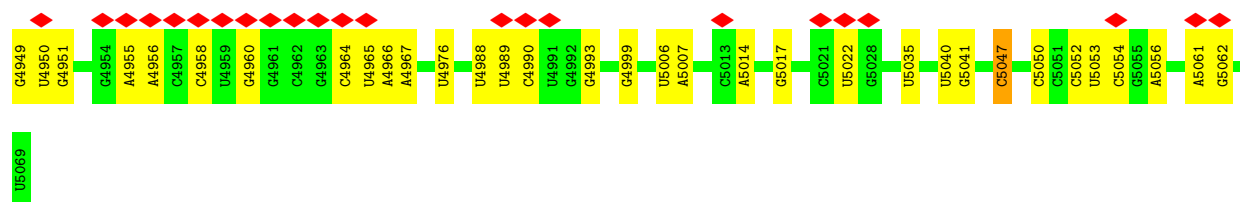


• Molecule 4: 28S ribosomal RNA

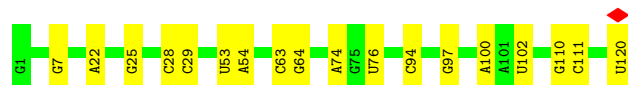
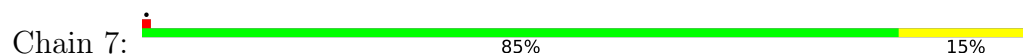




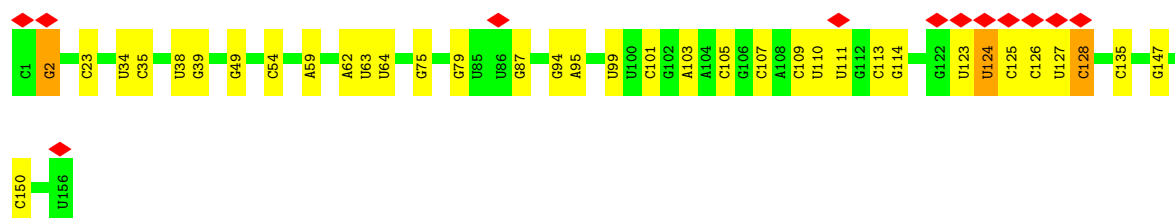
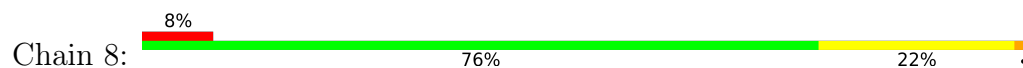




- Molecule 5: 5S rRNA



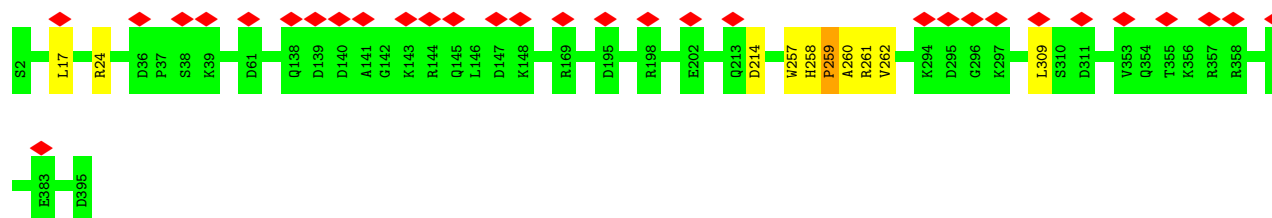
- Molecule 6: 5.8S ribosomal RNA



- Molecule 7: uL2



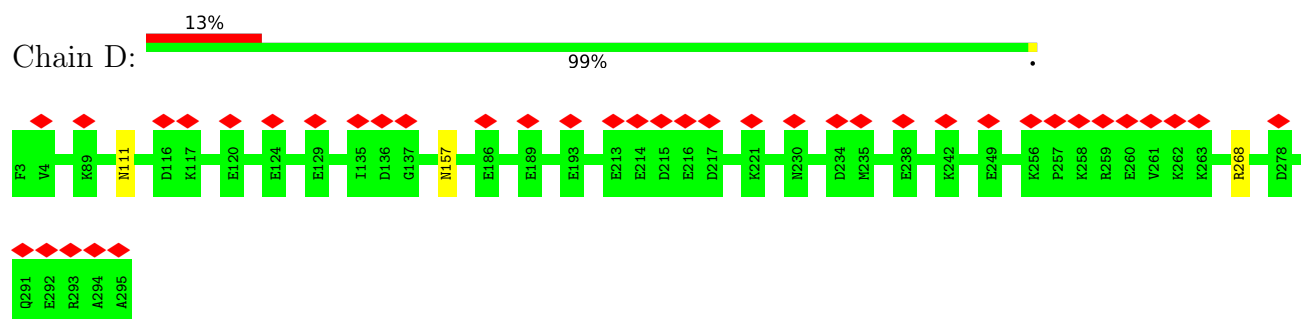
- Molecule 8: uL3



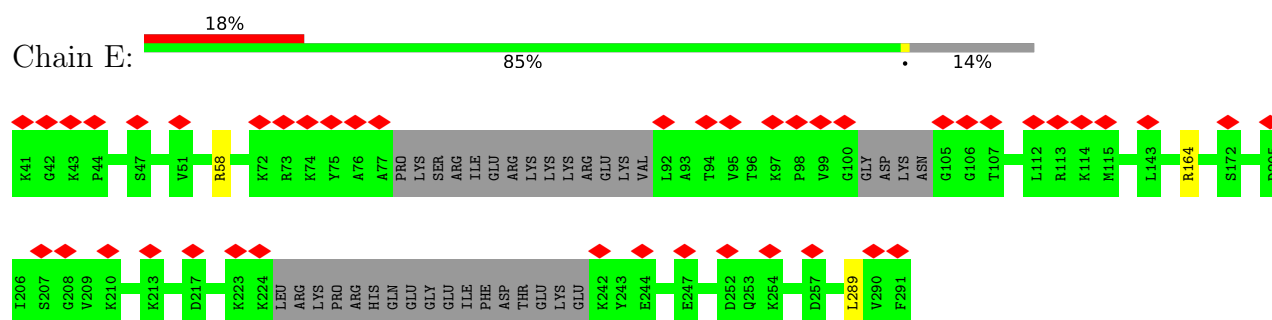
- Molecule 9: uL4



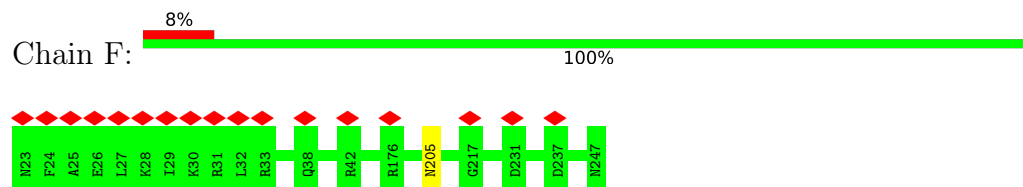
- Molecule 10: 60S ribosomal protein L5



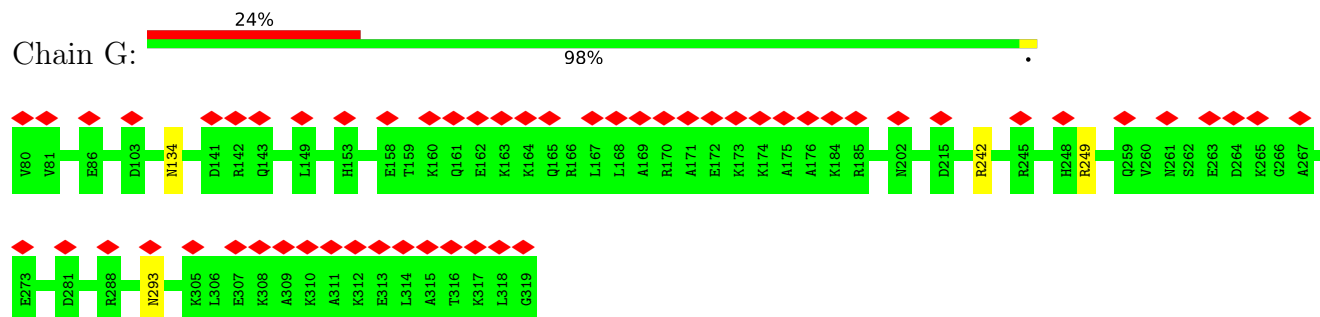
- Molecule 11: 60S ribosomal protein L6



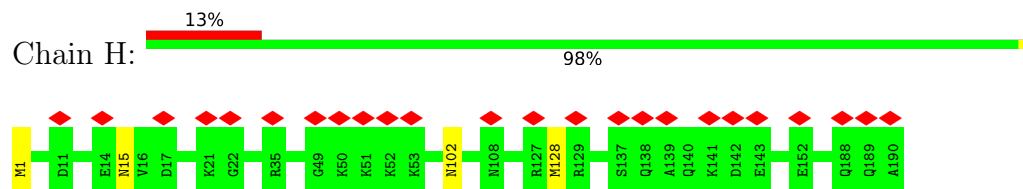
- Molecule 12: uL30



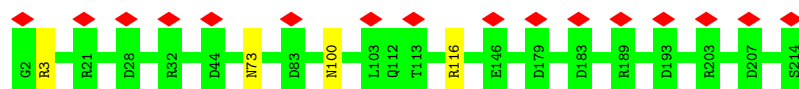
- Molecule 13: eL8



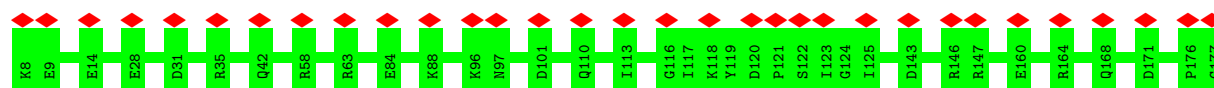
- Molecule 14: uL6



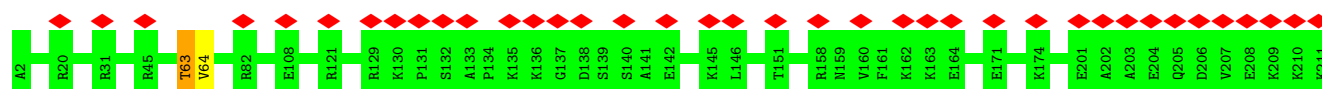
- Molecule 15: Ribosomal protein L10 (Predicted)



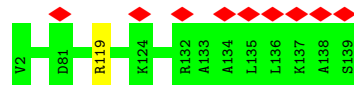
- Molecule 16: Ribosomal protein L11



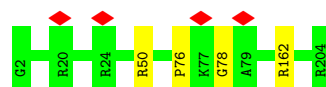
- Molecule 17: 60S ribosomal protein L13



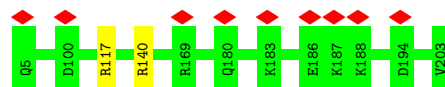
- Molecule 18: Ribosomal protein L14



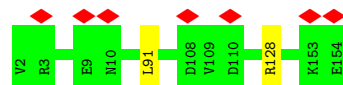
- Molecule 19: Ribosomal protein L15



- Molecule 20: uL13



- Molecule 21: uL22



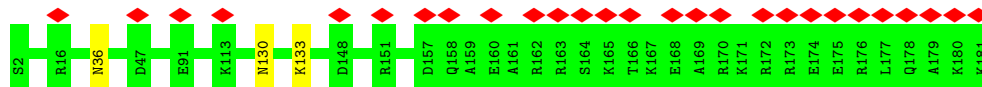
- Molecule 22: eL18

Chain Q:  5% 99%



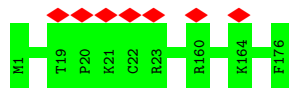
- Molecule 23: eL19

Chain R:  15% 98%



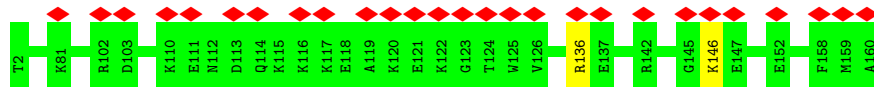
- Molecule 24: eL20

Chain S:  1% 100%




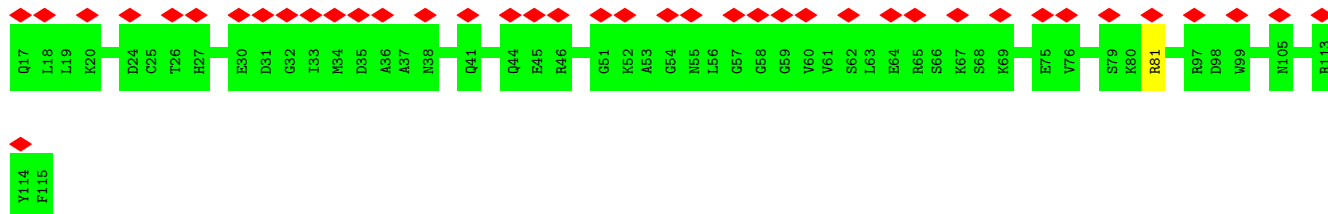
- Molecule 25: eL21

Chain T:  17% 99%



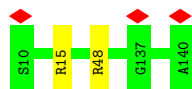
- Molecule 26: eL22

Chain U:  40% 99%

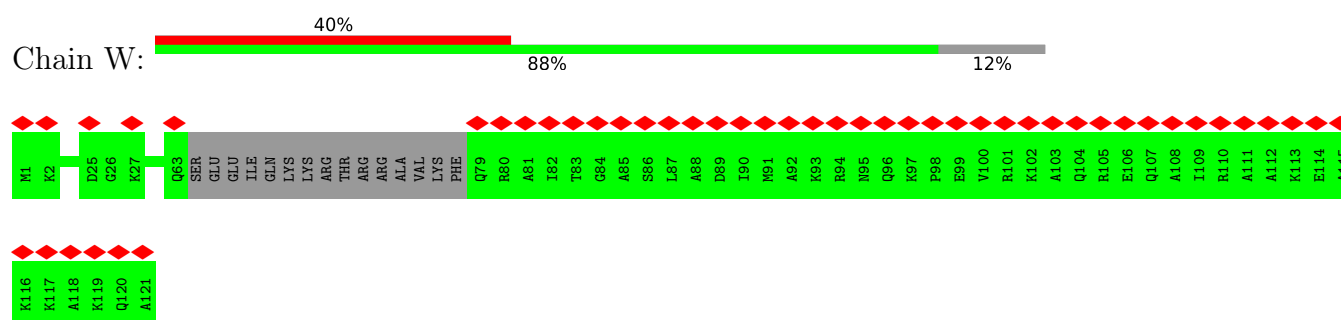


- Molecule 27: eL14

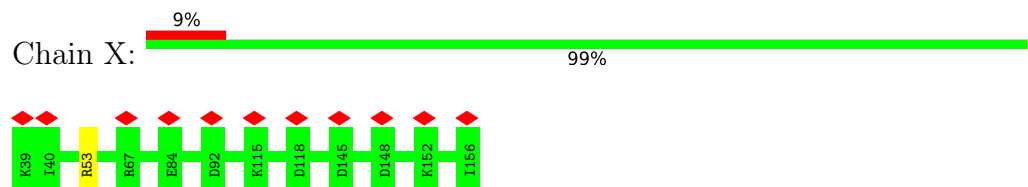
Chain V:  1% 98%



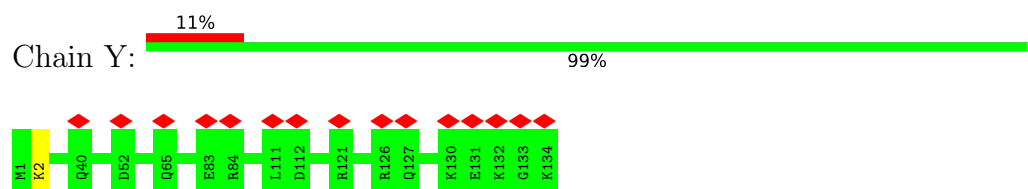
- Molecule 28: Ribosomal protein L24



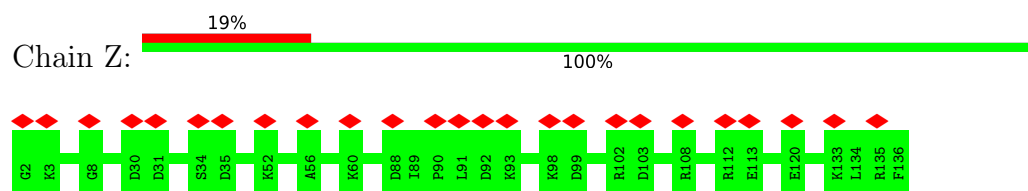
- Molecule 29: uL23



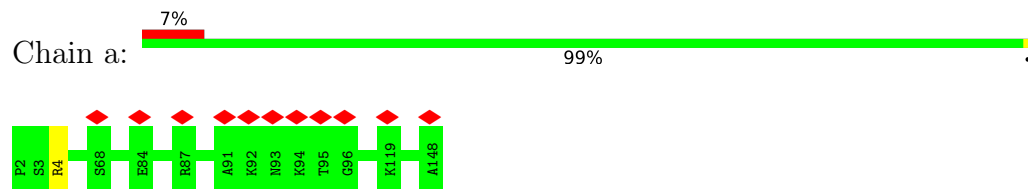
- Molecule 30: Ribosomal protein L26



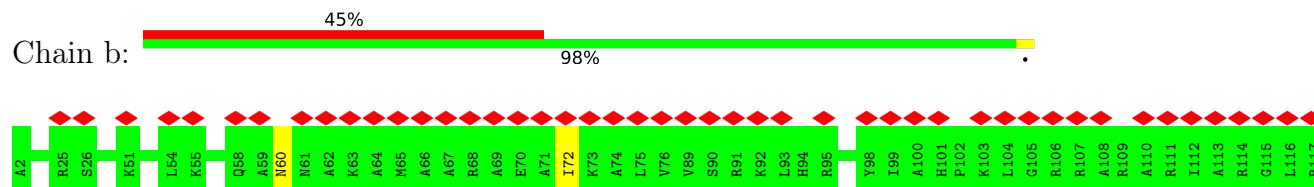
- Molecule 31: 60S ribosomal protein L27



- Molecule 32: uL15

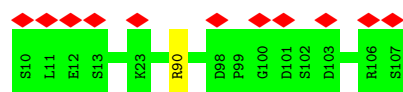


- Molecule 33: eL29

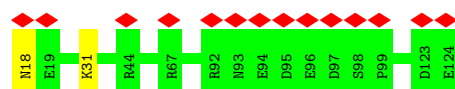


- Molecule 34: eL30

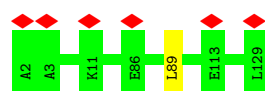




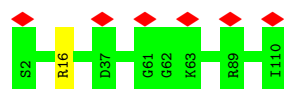
- Molecule 35: eL31



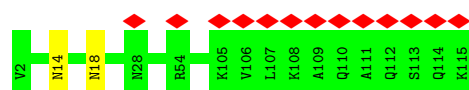
- Molecule 36: eL32



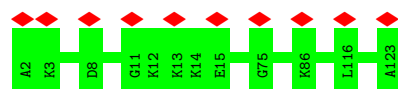
- Molecule 37: eL33



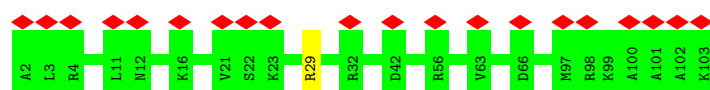
- Molecule 38: eL34



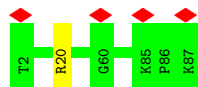
- Molecule 39: uL29



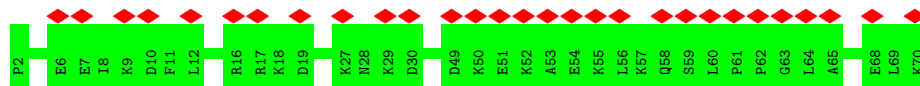
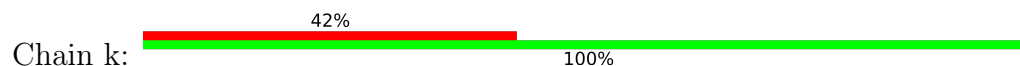
- Molecule 40: 60S ribosomal protein L36



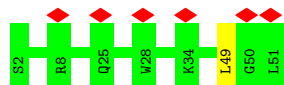
- Molecule 41: Ribosomal protein L37



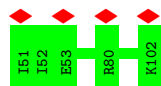
- Molecule 42: eL38



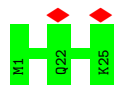
- Molecule 43: eL39



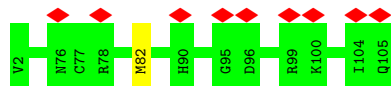
- Molecule 44: eL40



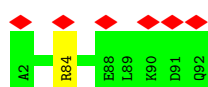
- Molecule 45: 60s ribosomal protein l41



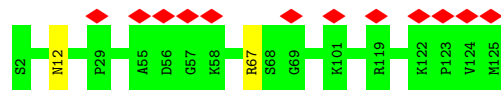
- Molecule 46: eL42



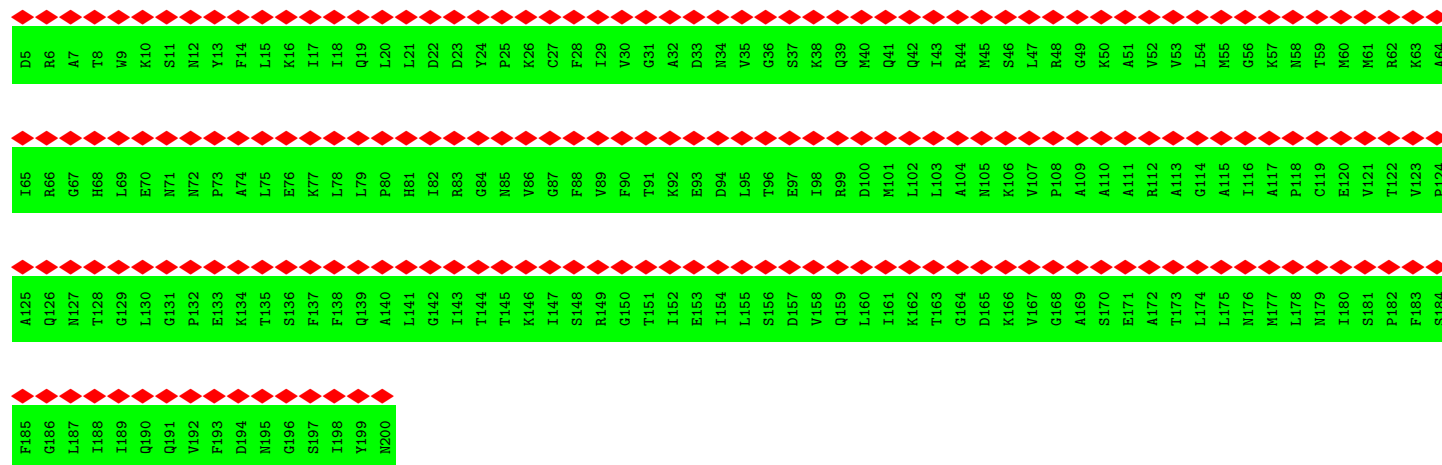
- Molecule 47: ribosomal protein eL43



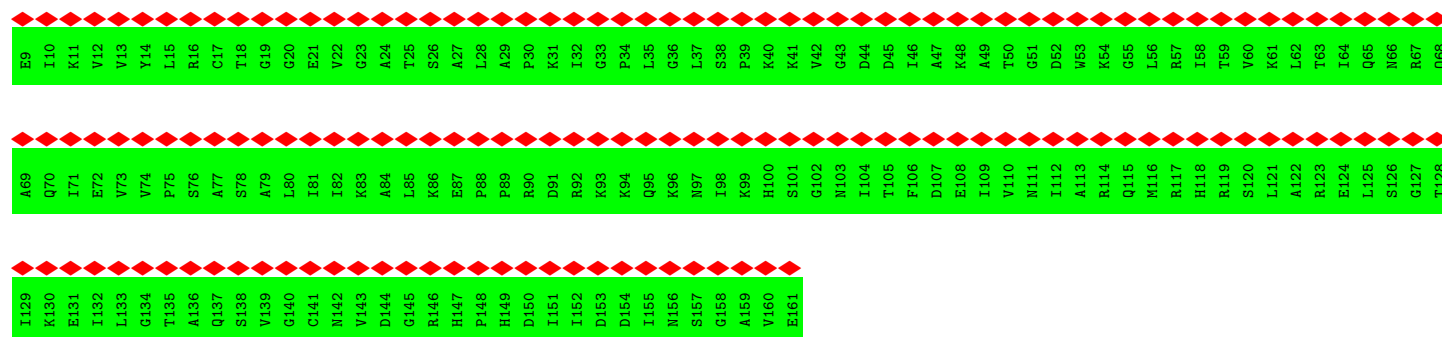
- Molecule 48: eL28



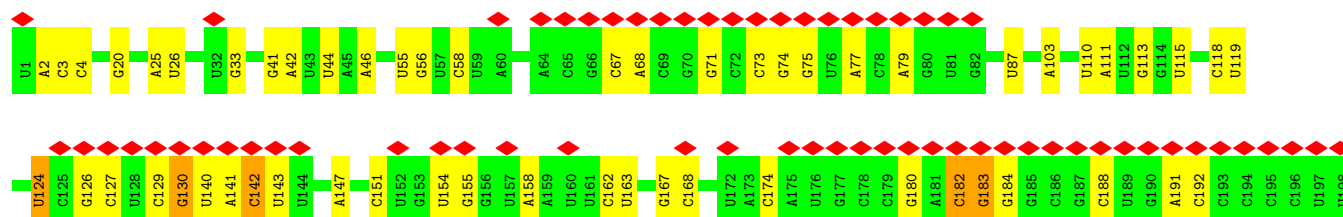
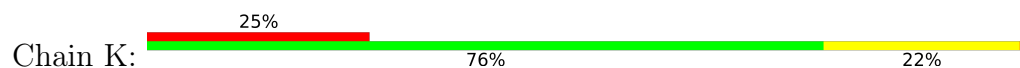
- Molecule 49: 60S acidic ribosomal protein P0

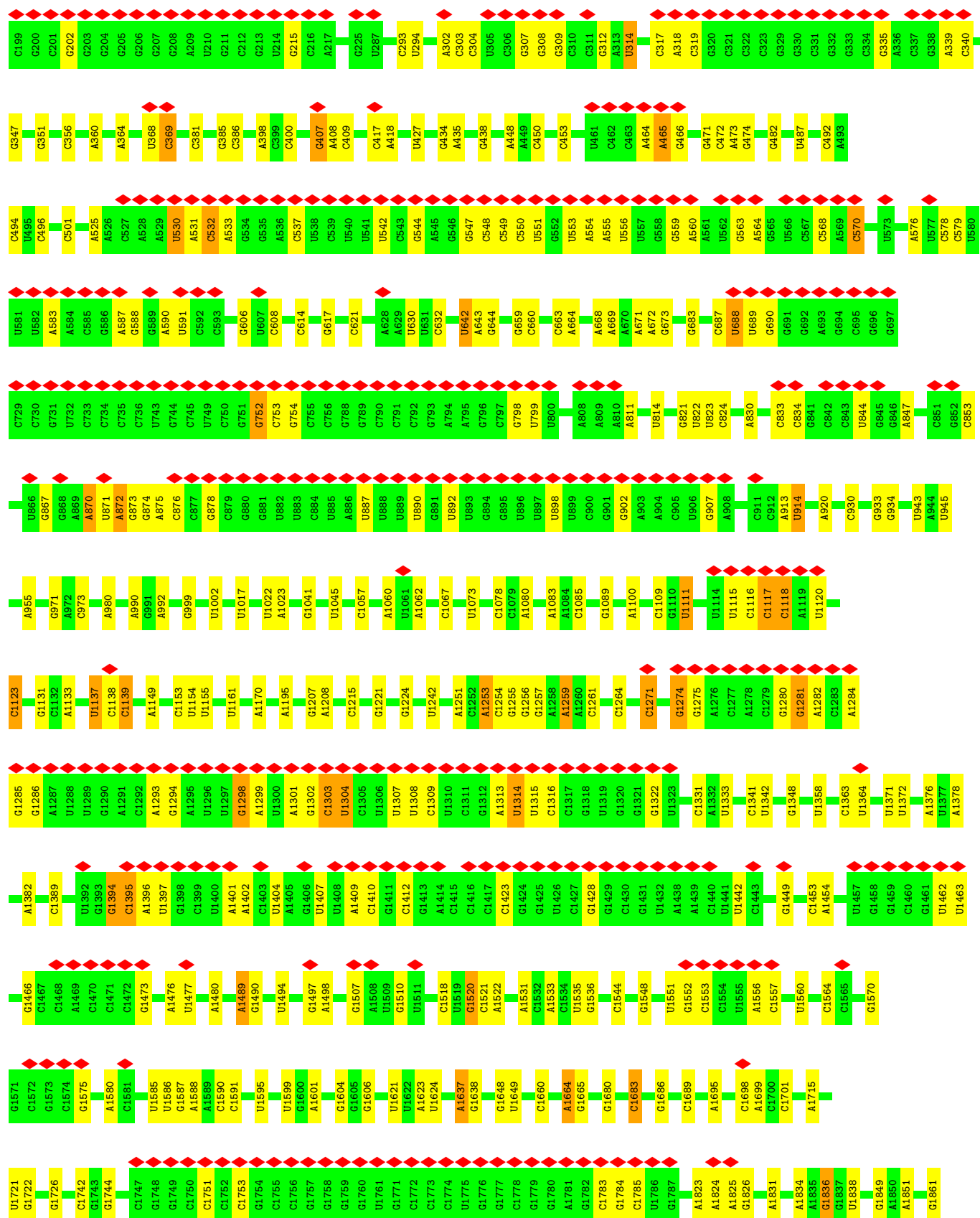


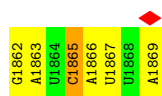
- Molecule 50: uL11



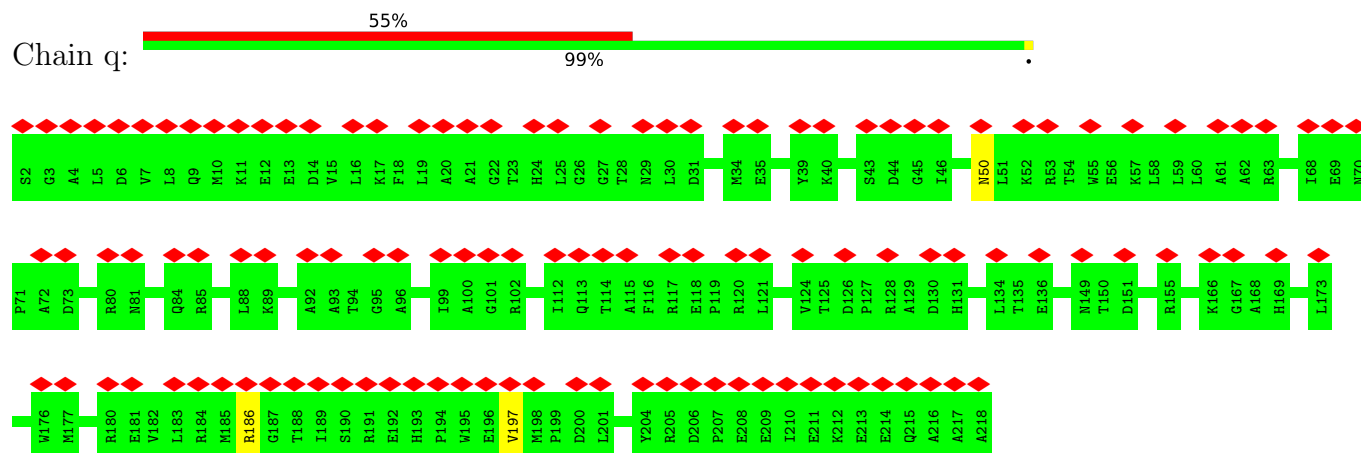
- Molecule 51: 18S ribosomal RNA



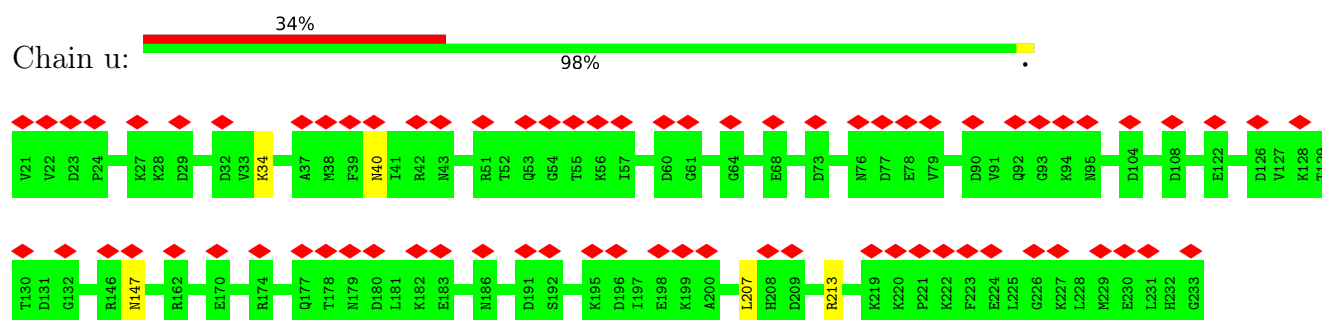




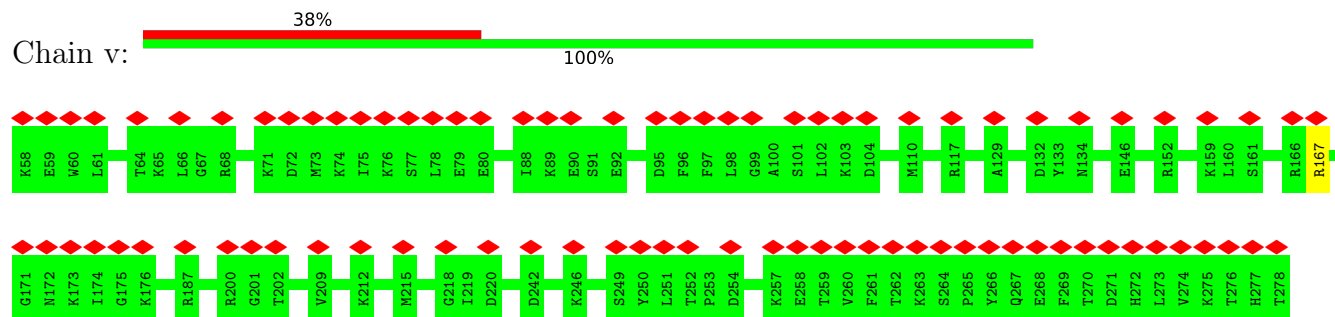
• Molecule 52: uS2



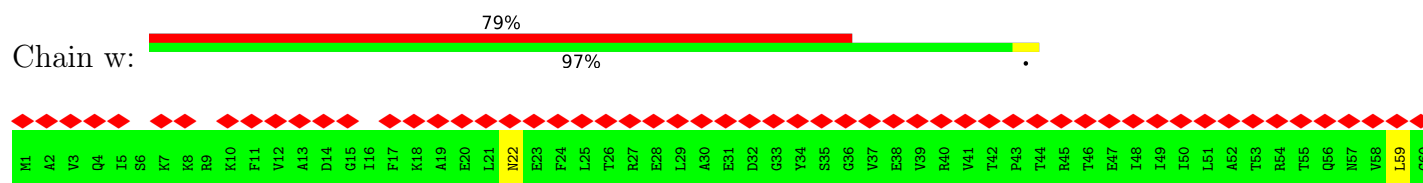
• Molecule 53: 40S ribosomal protein S3a

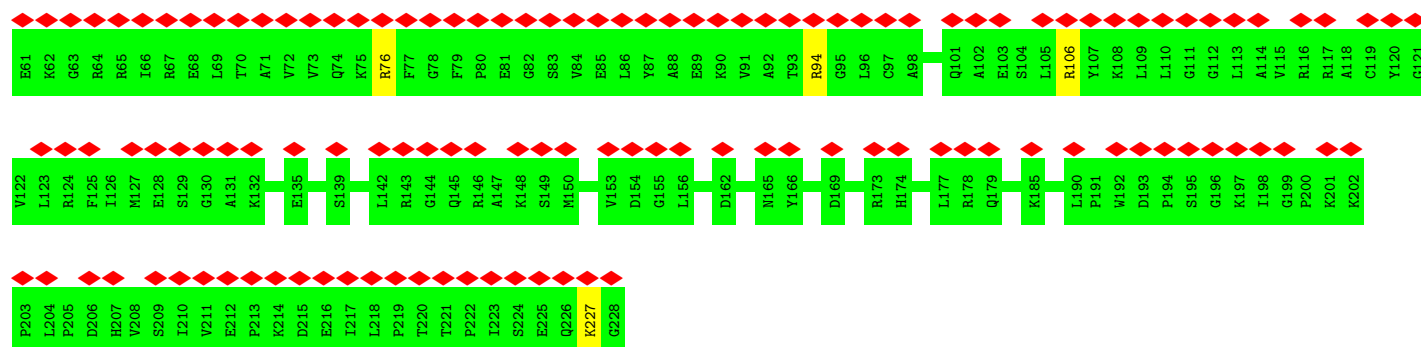


• Molecule 54: uS5

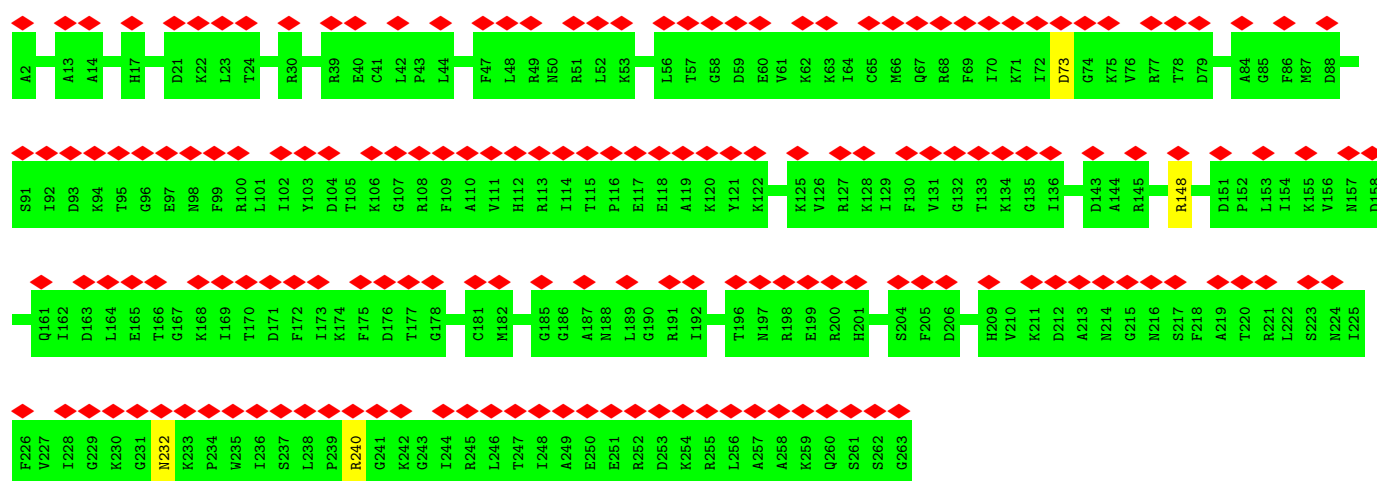


• Molecule 55: Ribosomal protein S3

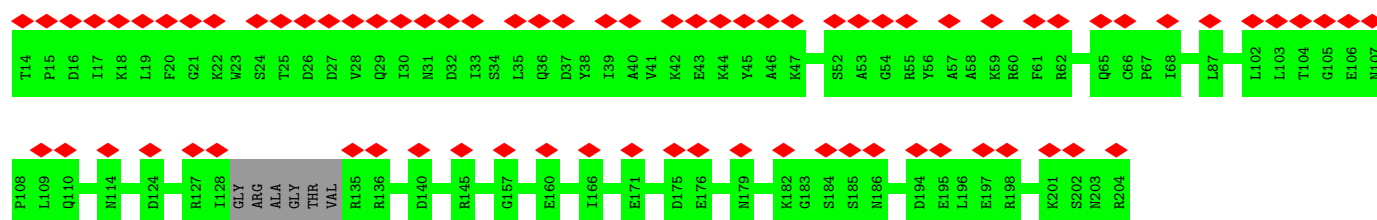
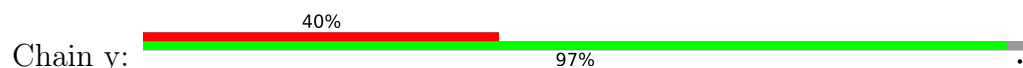




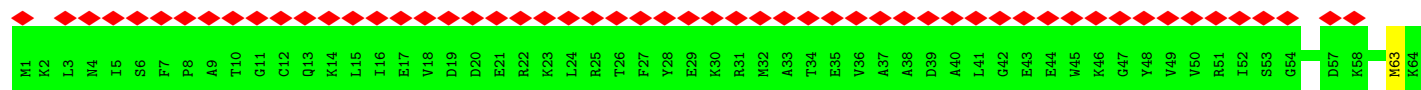
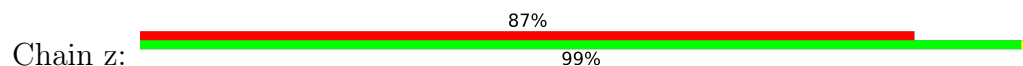
• Molecule 56: 40S ribosomal protein S4

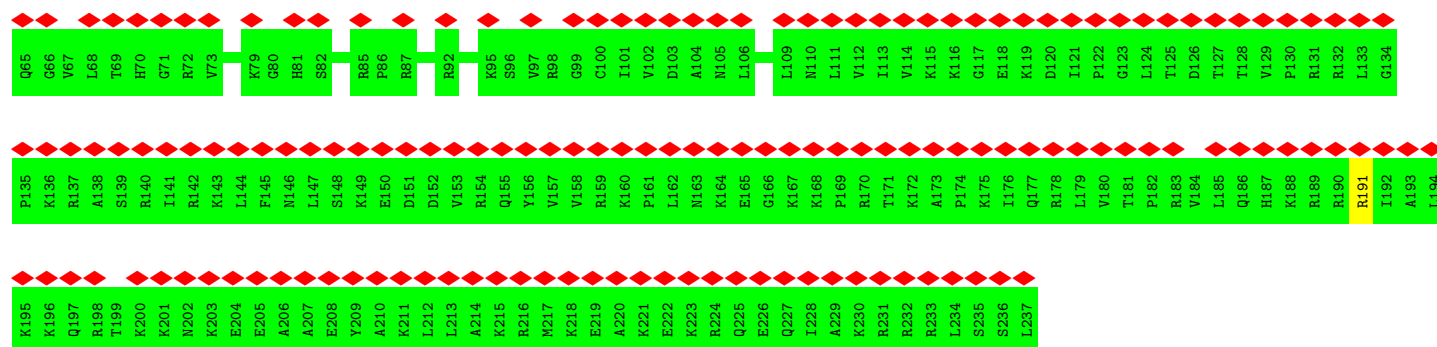


• Molecule 57: Ribosomal protein S5



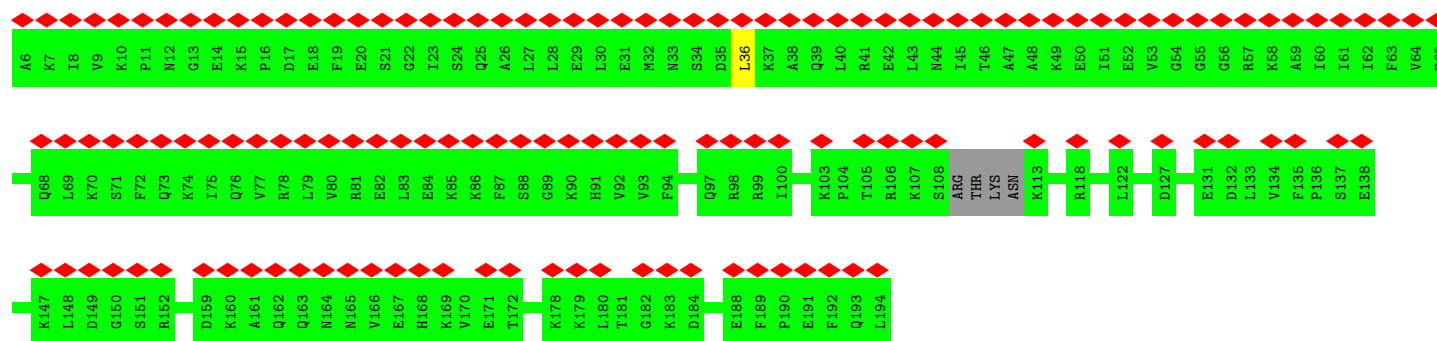
• Molecule 58: 40S ribosomal protein S6





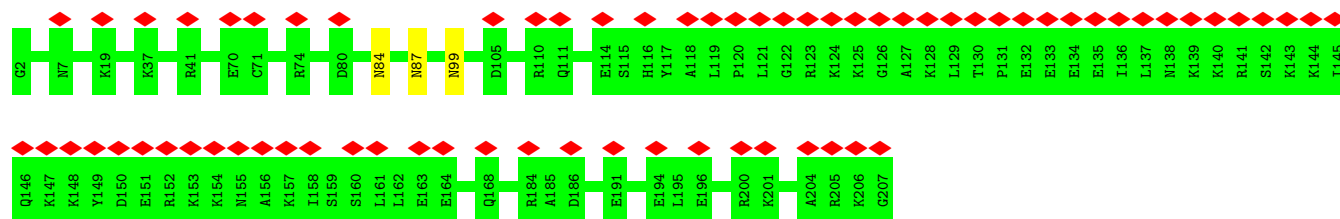
- Molecule 59: 40S ribosomal protein S7

Chain BB: 73% 97%



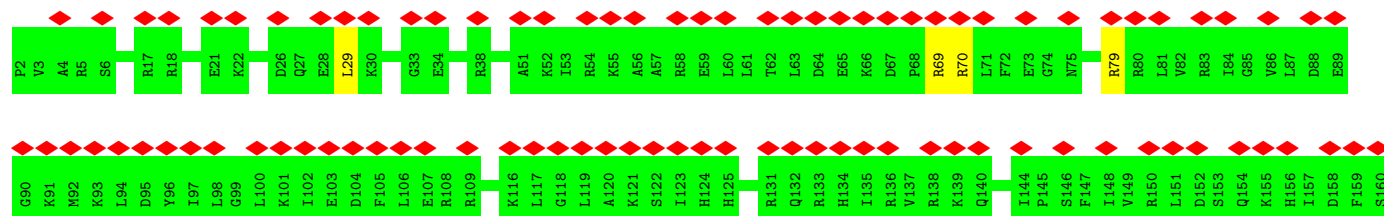
- Molecule 60: 40S ribosomal protein S8

Chain CC: 34% 99%



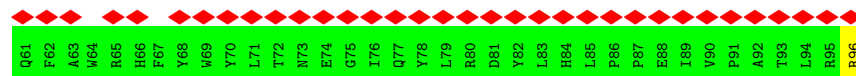
- Molecule 61: Ribosomal protein S9 (Predicted)

Chain DD: 63% 98%

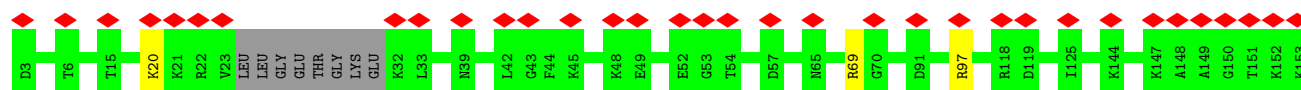




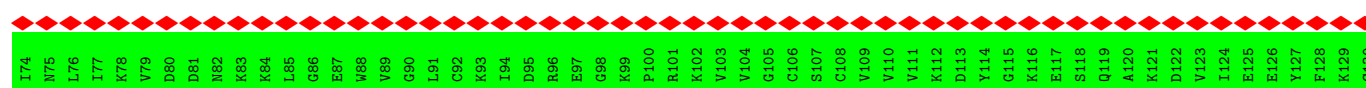
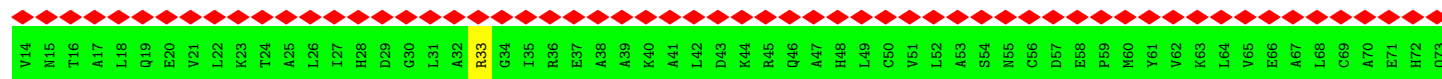
• Molecule 62: eS10



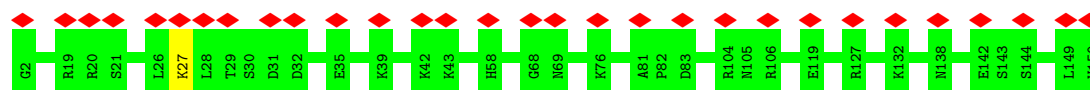
• Molecule 63: Ribosomal protein S11



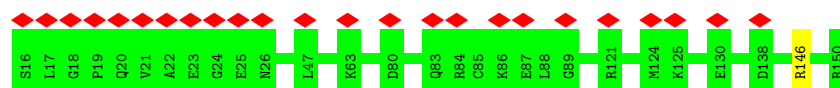
• Molecule 64: 40S ribosomal protein S12



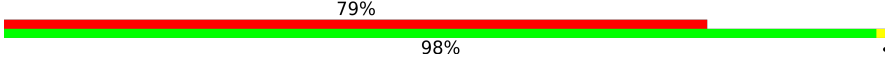
• Molecule 65: ribosomal protein uS15

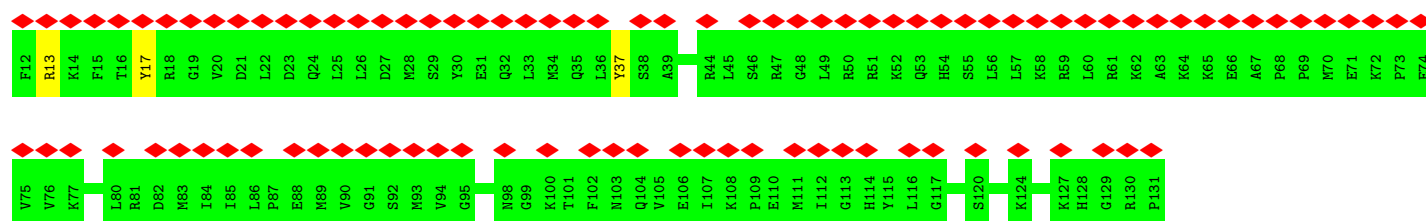


• Molecule 66: uS11



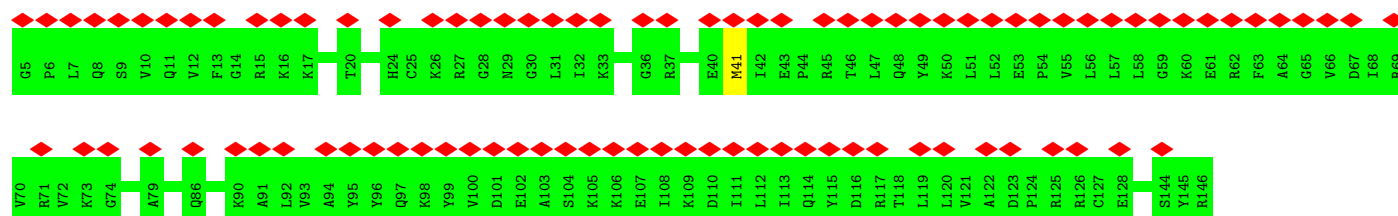
• Molecule 67: uS17

Chain WW: 

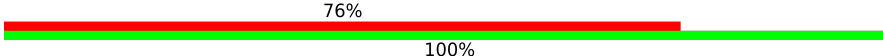


• Molecule 68: Ribosomal protein S16

Chain UU: 



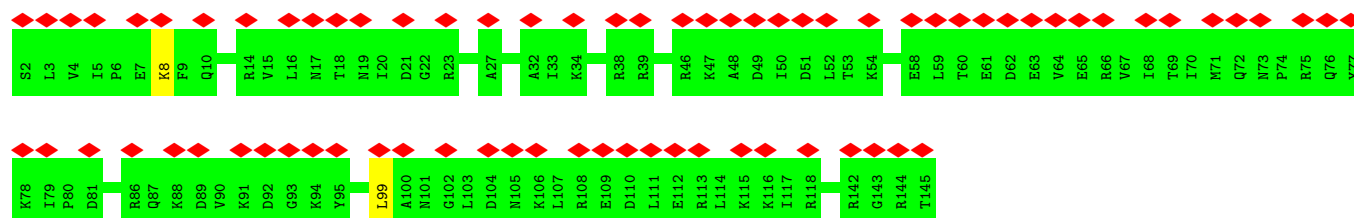
• Molecule 69: eS17

Chain KK: 



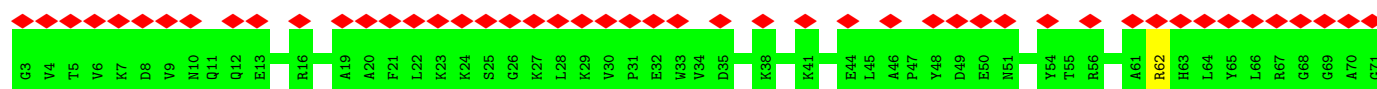
• Molecule 70: uS13

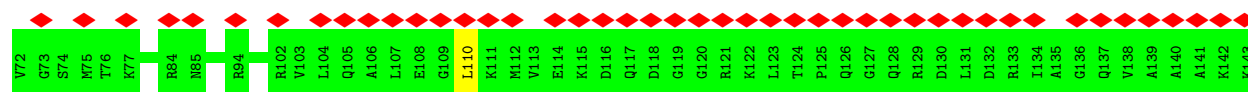
Chain II: 



• Molecule 71: eS19

Chain PP: 

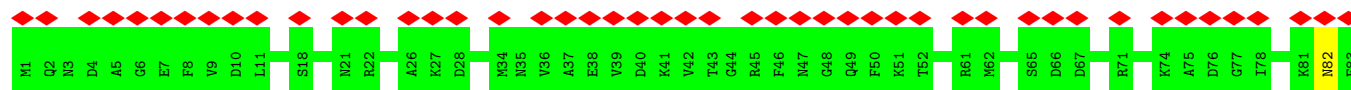
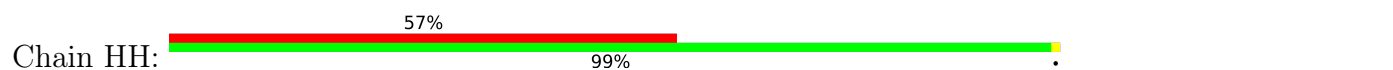




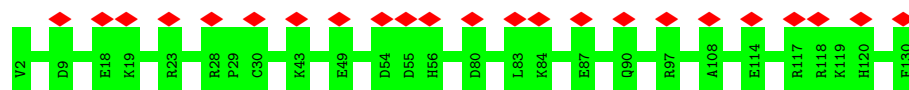
- Molecule 72: uS10



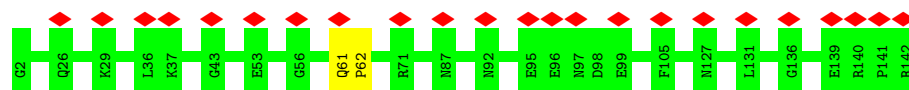
- Molecule 73: eS21



- Molecule 74: Ribosomal protein S15a



- Molecule 75: Ribosomal protein S23

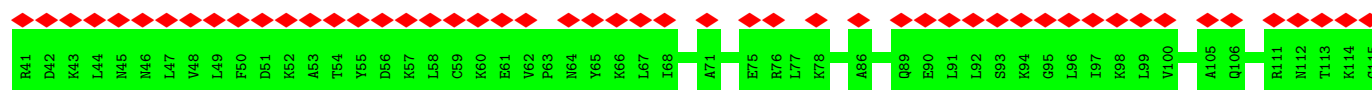


- Molecule 76: eS24

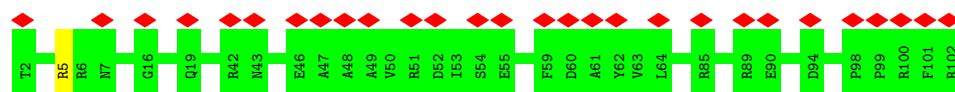




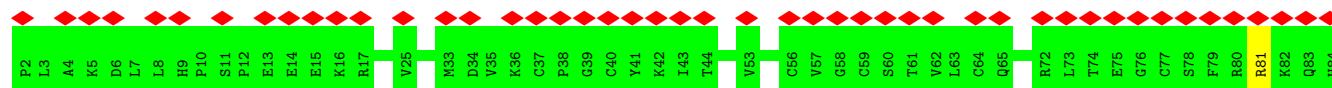
- Molecule 77: ribosomal protein eS25



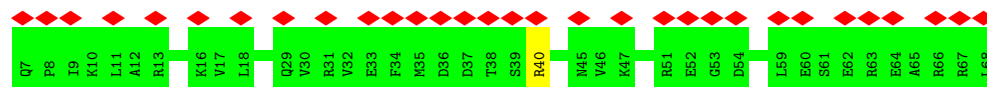
- Molecule 78: eS26



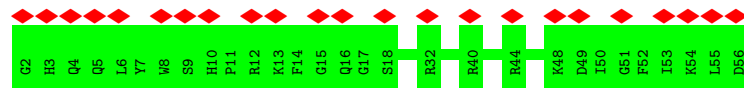
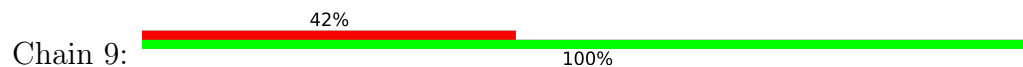
- Molecule 79: 40S ribosomal protein S27



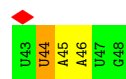
- Molecule 80: Ribosomal protein S28



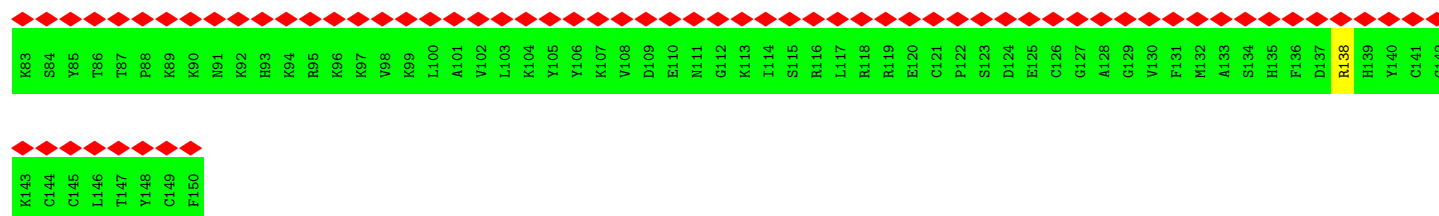
- Molecule 81: uS14



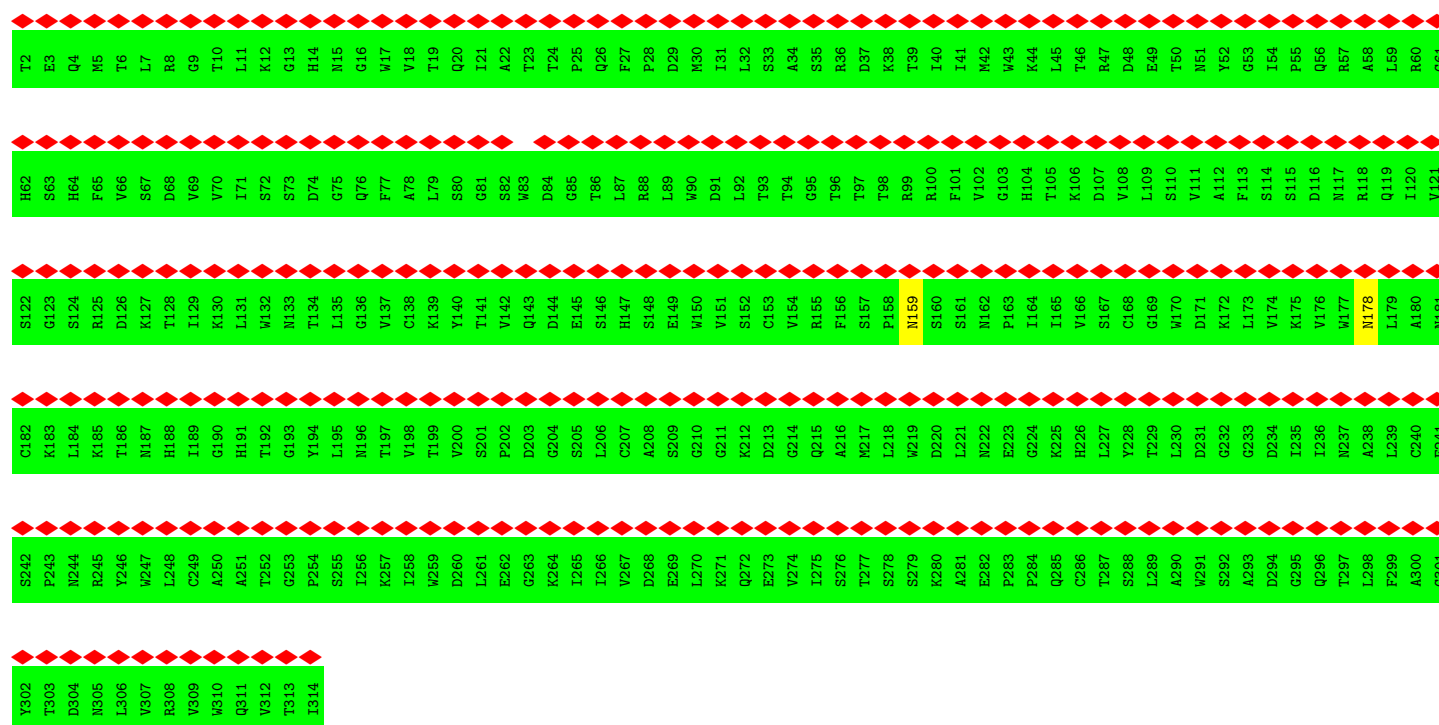
- Molecule 82: mRNA



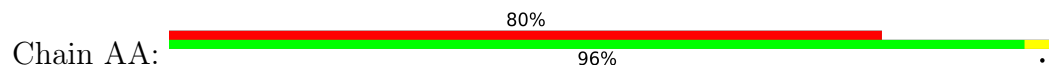
- Molecule 83: eS31



• Molecule 84: ribosomal protein RACK1



• Molecule 85: 40S ribosomal protein S30



4 Experimental information

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 ($e^-/\text{\AA}^2$)	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 (\AA)	429.264, 429.264, 429.264	wwPDB
Map dimensions	396, 396, 396	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.084, 1.084, 1.084	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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(°)	Ideal(°)
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(°)	Ideal(°)
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(°)	Ideal(°)
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(°)	Ideal(°)
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(°)	Ideal(°)
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(°)	Ideal(°)
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(°)	Ideal(°)
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(°)	Ideal(°)
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(°)	Ideal(°)
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(°)	Ideal(°)
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(°)	Ideal(°)
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(°)	Ideal(°)
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(°)	Ideal(°)
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(°)	Ideal(°)
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(°)	Ideal(°)
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(°)	Ideal(°)
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	12
7	A	246/248 (99%)	233 (95%)	13 (5%)	0	100	100
8	B	392/394 (100%)	374 (95%)	16 (4%)	2 (0%)	25	61
9	C	360/362 (99%)	349 (97%)	10 (3%)	1 (0%)	37	70
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%)	13	46
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%)	19	54
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%)	50	81

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 ⓘ

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	7
7	A	190/190 (100%)	184 (97%)	6 (3%)	34	67
8	B	342/342 (100%)	339 (99%)	3 (1%)	75	89
9	C	302/302 (100%)	294 (97%)	8 (3%)	41	72
10	D	247/247 (100%)	244 (99%)	3 (1%)	67	86
11	E	190/223 (85%)	187 (98%)	3 (2%)	58	82
12	F	196/196 (100%)	195 (100%)	1 (0%)	86	94
13	G	200/200 (100%)	196 (98%)	4 (2%)	50	78
14	H	169/169 (100%)	165 (98%)	4 (2%)	44	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	I	175/175 (100%)	171 (98%)	4 (2%)	45	75
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%)	75	89
19	N	171/171 (100%)	169 (99%)	2 (1%)	67	86
20	O	171/171 (100%)	169 (99%)	2 (1%)	67	86
21	P	134/134 (100%)	133 (99%)	1 (1%)	81	91
22	Q	164/164 (100%)	163 (99%)	1 (1%)	84	93
23	R	159/159 (100%)	156 (98%)	3 (2%)	52	79
24	S	157/157 (100%)	157 (100%)	0	100	100
25	T	139/139 (100%)	137 (99%)	2 (1%)	62	83
26	U	89/89 (100%)	88 (99%)	1 (1%)	70	87
27	V	101/101 (100%)	99 (98%)	2 (2%)	50	78
28	W	86/100 (86%)	86 (100%)	0	100	100
29	X	106/106 (100%)	105 (99%)	1 (1%)	75	89
30	Y	124/124 (100%)	123 (99%)	1 (1%)	79	90
31	Z	117/117 (100%)	117 (100%)	0	100	100
32	a	119/119 (100%)	118 (99%)	1 (1%)	79	90
33	b	84/84 (100%)	82 (98%)	2 (2%)	44	74
34	c	84/84 (100%)	83 (99%)	1 (1%)	67	86
35	d	98/98 (100%)	96 (98%)	2 (2%)	50	78
36	e	114/114 (100%)	114 (100%)	0	100	100
37	f	88/88 (100%)	87 (99%)	1 (1%)	70	87
38	g	98/98 (100%)	96 (98%)	2 (2%)	50	78
39	h	109/109 (100%)	109 (100%)	0	100	100
40	i	86/86 (100%)	85 (99%)	1 (1%)	67	86
41	j	73/73 (100%)	72 (99%)	1 (1%)	62	83
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%)	70	87
47	p	74/74 (100%)	73 (99%)	1 (1%)	62	83
48	r	108/108 (100%)	106 (98%)	2 (2%)	52	79
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%)	70	87
53	u	194/194 (100%)	190 (98%)	4 (2%)	48	77
54	v	187/187 (100%)	186 (100%)	1 (0%)	86	94
55	w	190/190 (100%)	185 (97%)	5 (3%)	41	72
56	x	224/224 (100%)	221 (99%)	3 (1%)	65	85
57	y	158/161 (98%)	158 (100%)	0	100	100
58	z	207/207 (100%)	205 (99%)	2 (1%)	73	88
59	BB	165/169 (98%)	165 (100%)	0	100	100
60	CC	178/178 (100%)	175 (98%)	3 (2%)	56	81
61	DD	161/161 (100%)	157 (98%)	4 (2%)	42	73
62	SS	87/87 (100%)	86 (99%)	1 (1%)	70	87
63	EE	130/136 (96%)	127 (98%)	3 (2%)	45	75
64	RR	99/99 (100%)	98 (99%)	1 (1%)	73	88
65	QQ	130/130 (100%)	129 (99%)	1 (1%)	79	90
66	MM	104/105 (99%)	103 (99%)	1 (1%)	73	88
67	WW	109/109 (100%)	108 (99%)	1 (1%)	75	89
68	UU	117/117 (100%)	116 (99%)	1 (1%)	75	89
69	KK	119/119 (100%)	119 (100%)	0	100	100
70	II	125/125 (100%)	124 (99%)	1 (1%)	79	90
71	PP	111/111 (100%)	110 (99%)	1 (1%)	75	89
72	GG	92/92 (100%)	91 (99%)	1 (1%)	70	87
73	HH	67/67 (100%)	66 (98%)	1 (2%)	60	83
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%)	75	89
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%)	70	87
79	JJ	75/75 (100%)	74 (99%)	1 (1%)	65	85
80	FF	55/55 (100%)	54 (98%)	1 (2%)	54	80
81	9	48/48 (100%)	48 (100%)	0	100	100
83	0	61/61 (100%)	60 (98%)	1 (2%)	58	82
84	6	272/272 (100%)	270 (99%)	2 (1%)	81	91
85	AA	46/46 (100%)	44 (96%)	2 (4%)	25	58
All	All	10063/10125 (99%)	9945 (99%)	118 (1%)	66	86

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 ⓘ

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 [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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

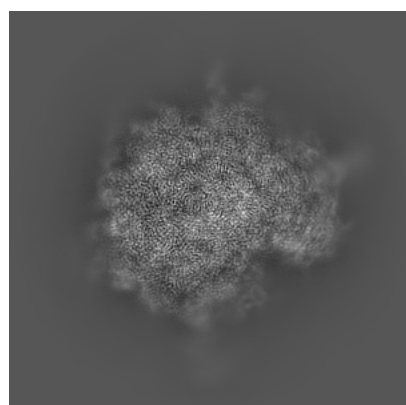
6 Map visualisation [i](#)

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.

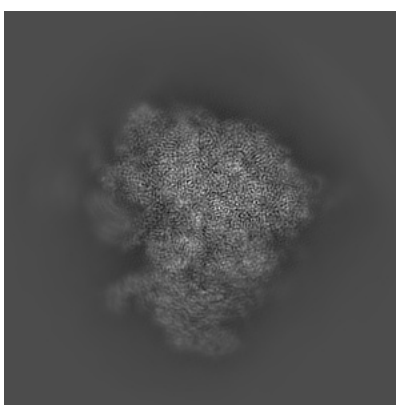
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

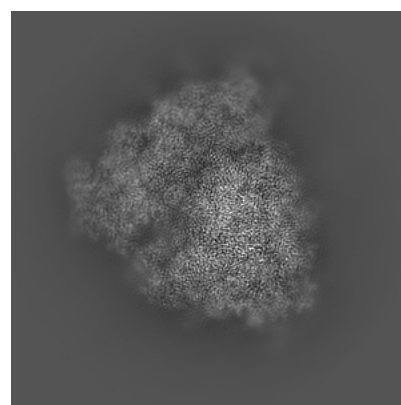
6.1.1 Primary map



X



Y

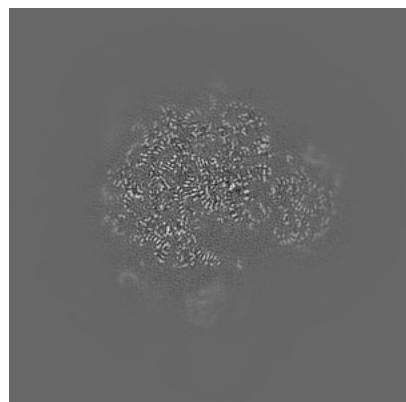


Z

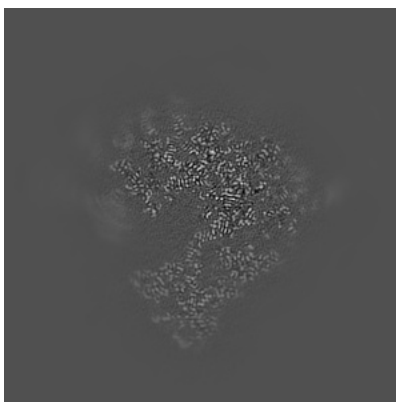
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 198



Y Index: 198

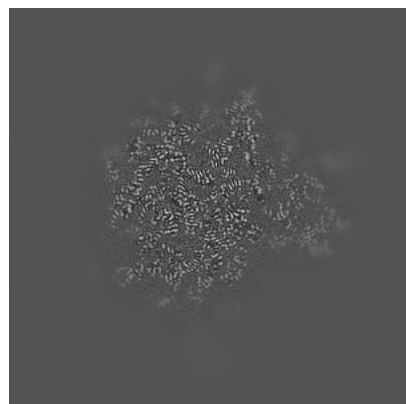


Z Index: 198

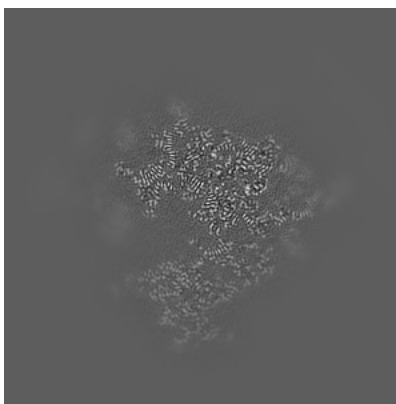
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

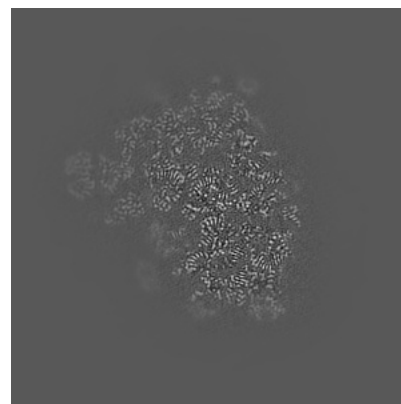
6.3.1 Primary map



X Index: 218



Y Index: 205

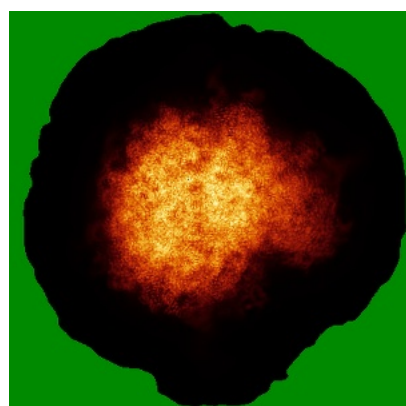


Z Index: 216

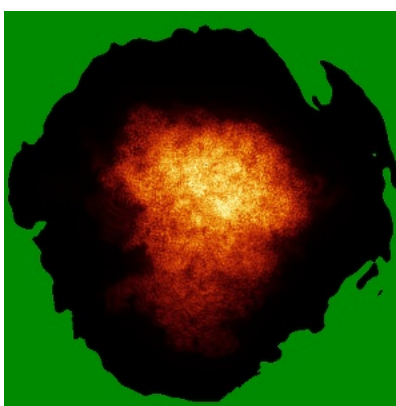
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

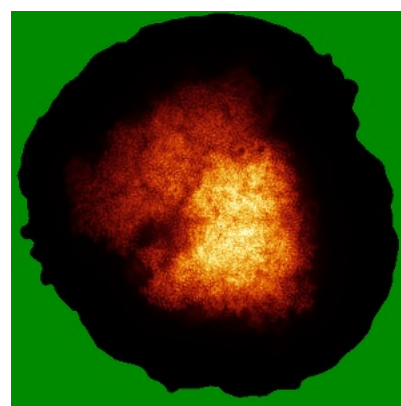
6.4.1 Primary map



X



Y

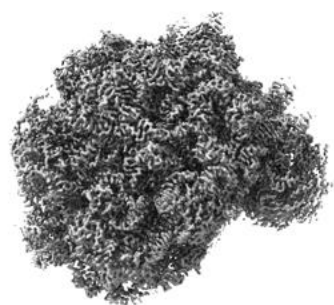


Z

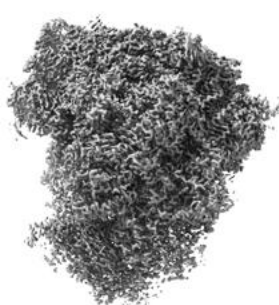
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 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.

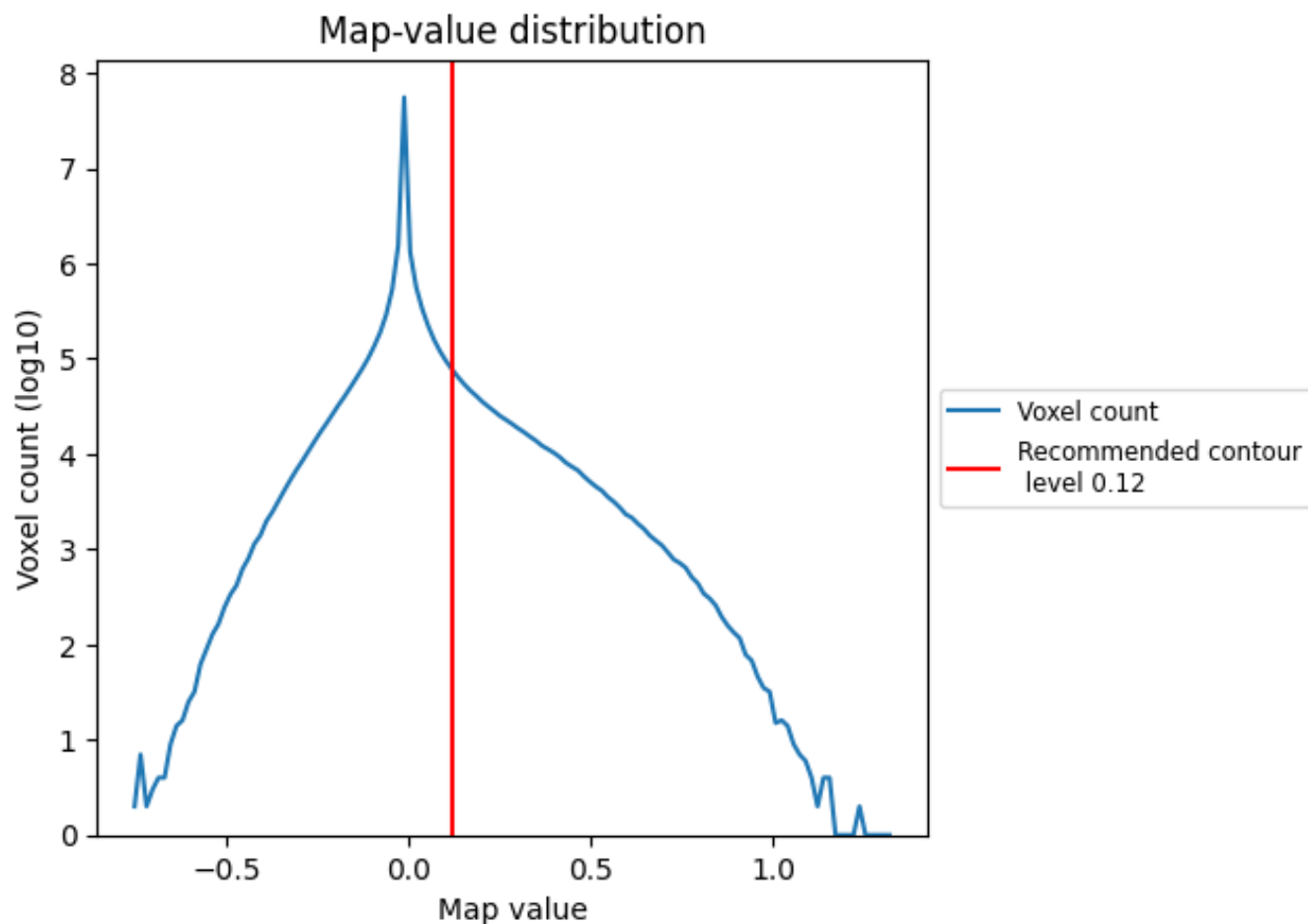
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

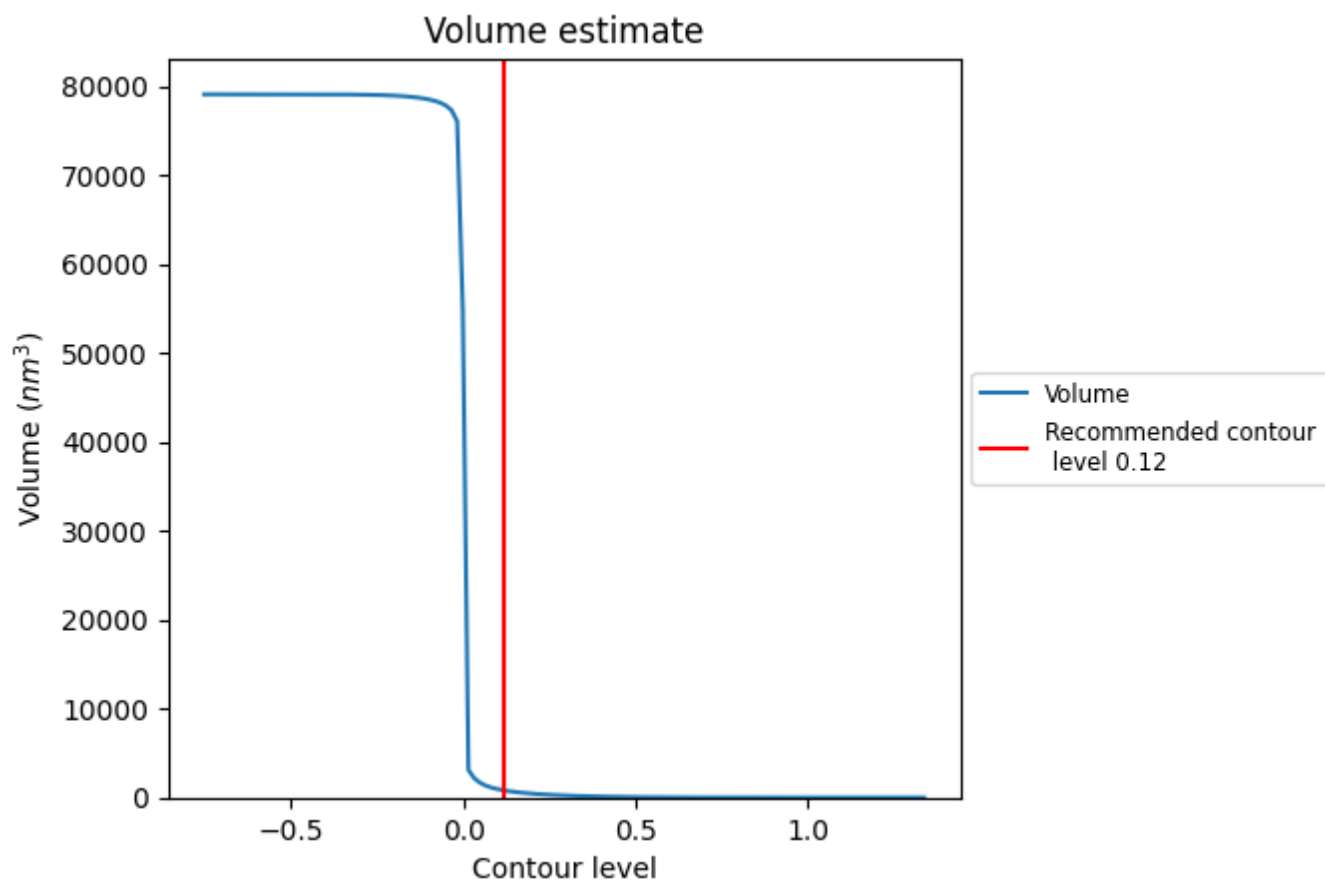
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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.

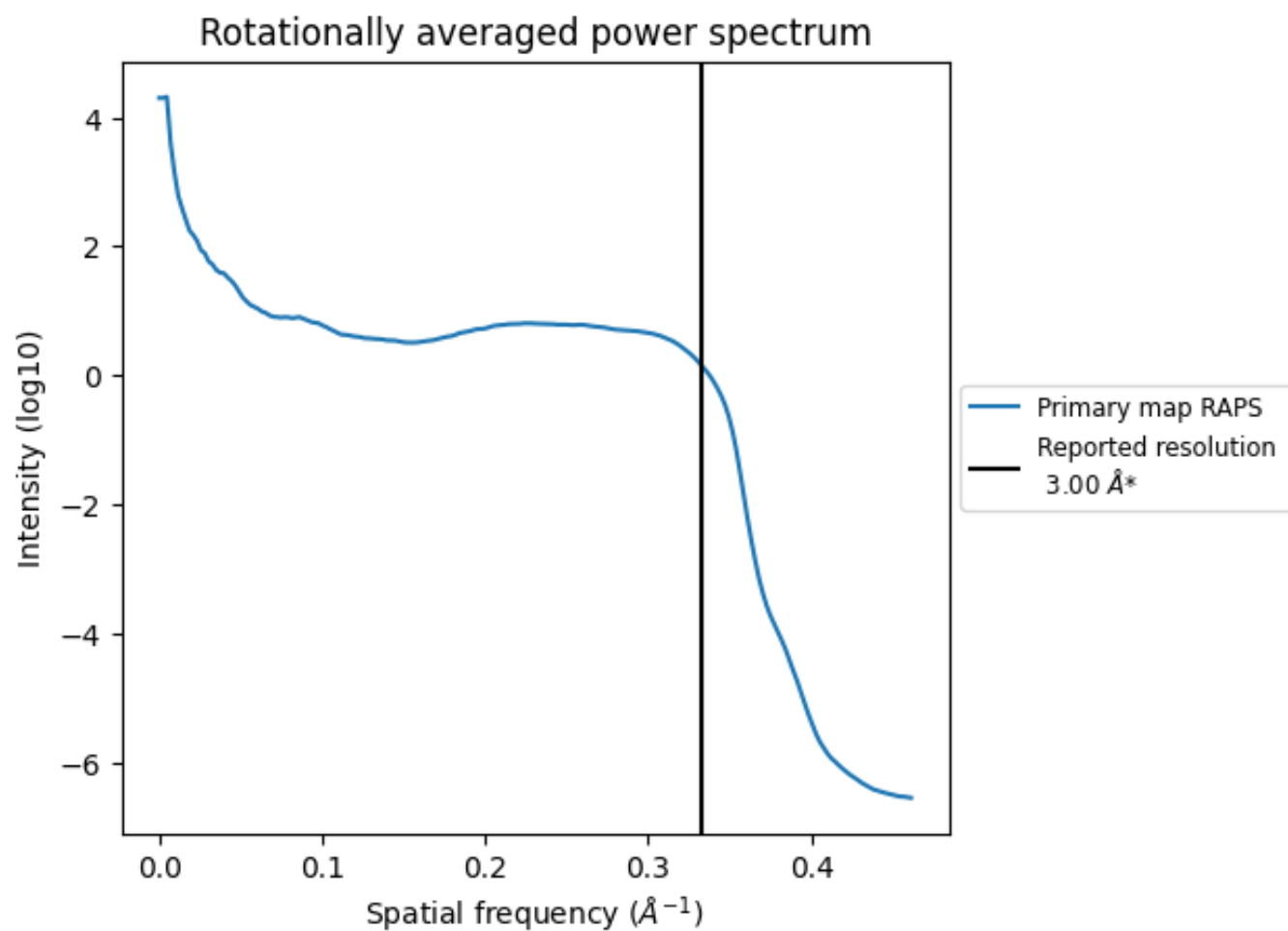
7.2 Volume estimate [i](#)



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 ⓘ

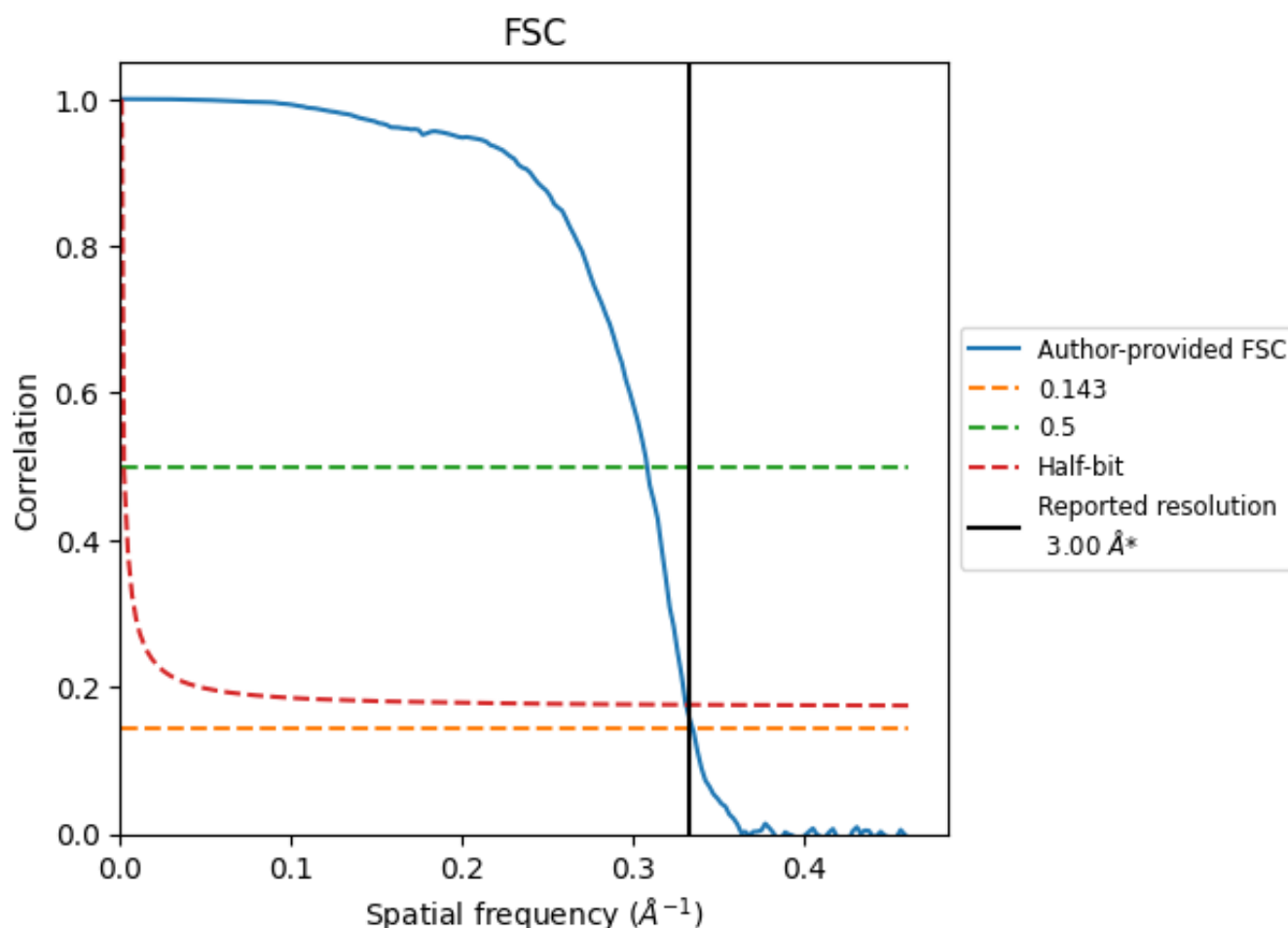


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

8 Fourier-Shell correlation [i](#)

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 [i](#)



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

8.2 Resolution estimates [i](#)

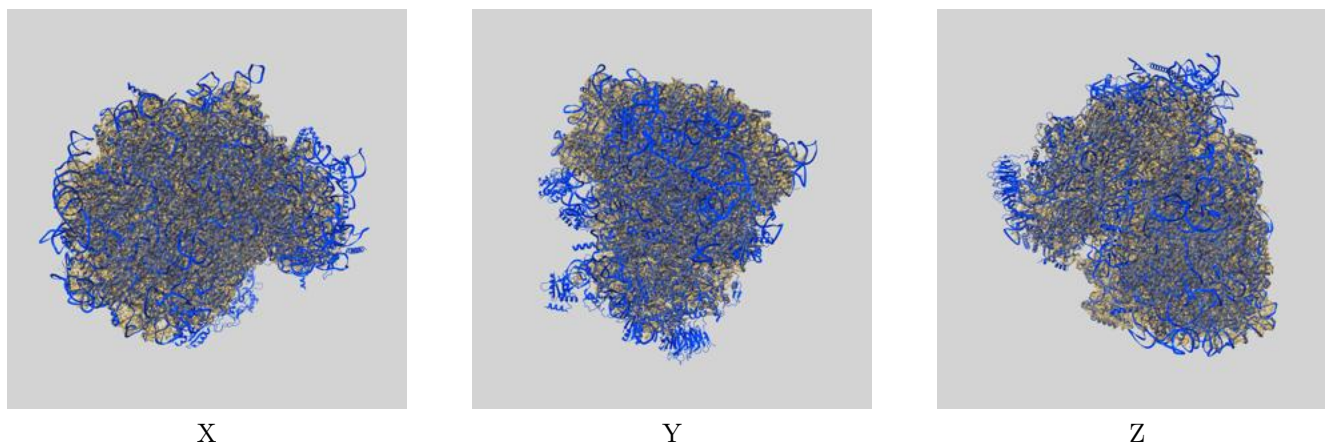
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	2.99	3.24	3.02
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

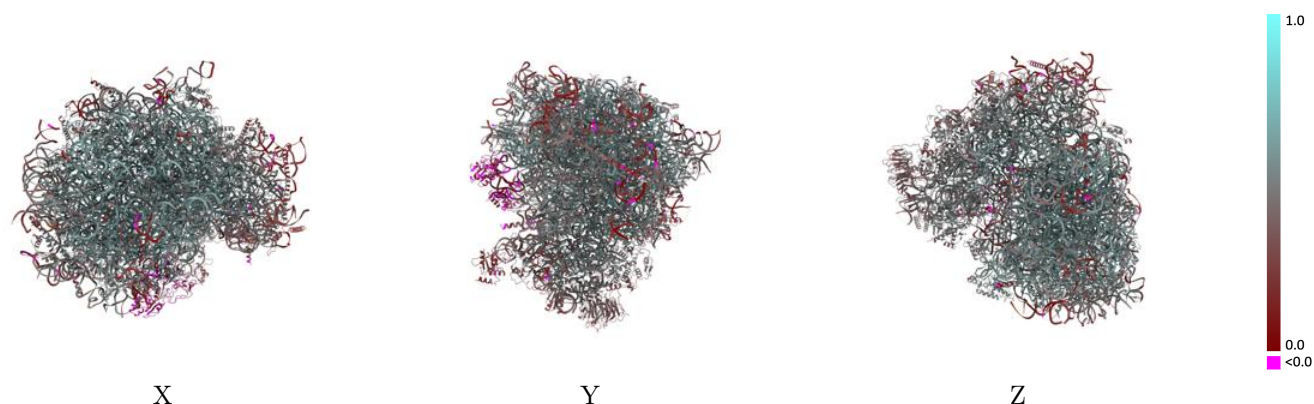
This section contains information regarding the fit between EMDB map EMD-4729 and PDB model 6R5Q. Per-residue inclusion information can be found in section [3](#) on page [23](#).

9.1 Map-model overlay [i](#)



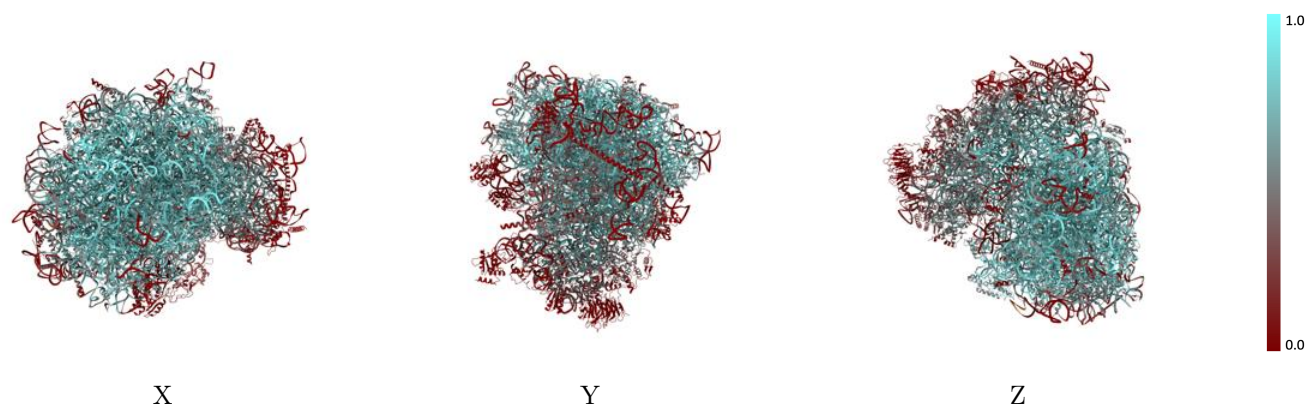
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



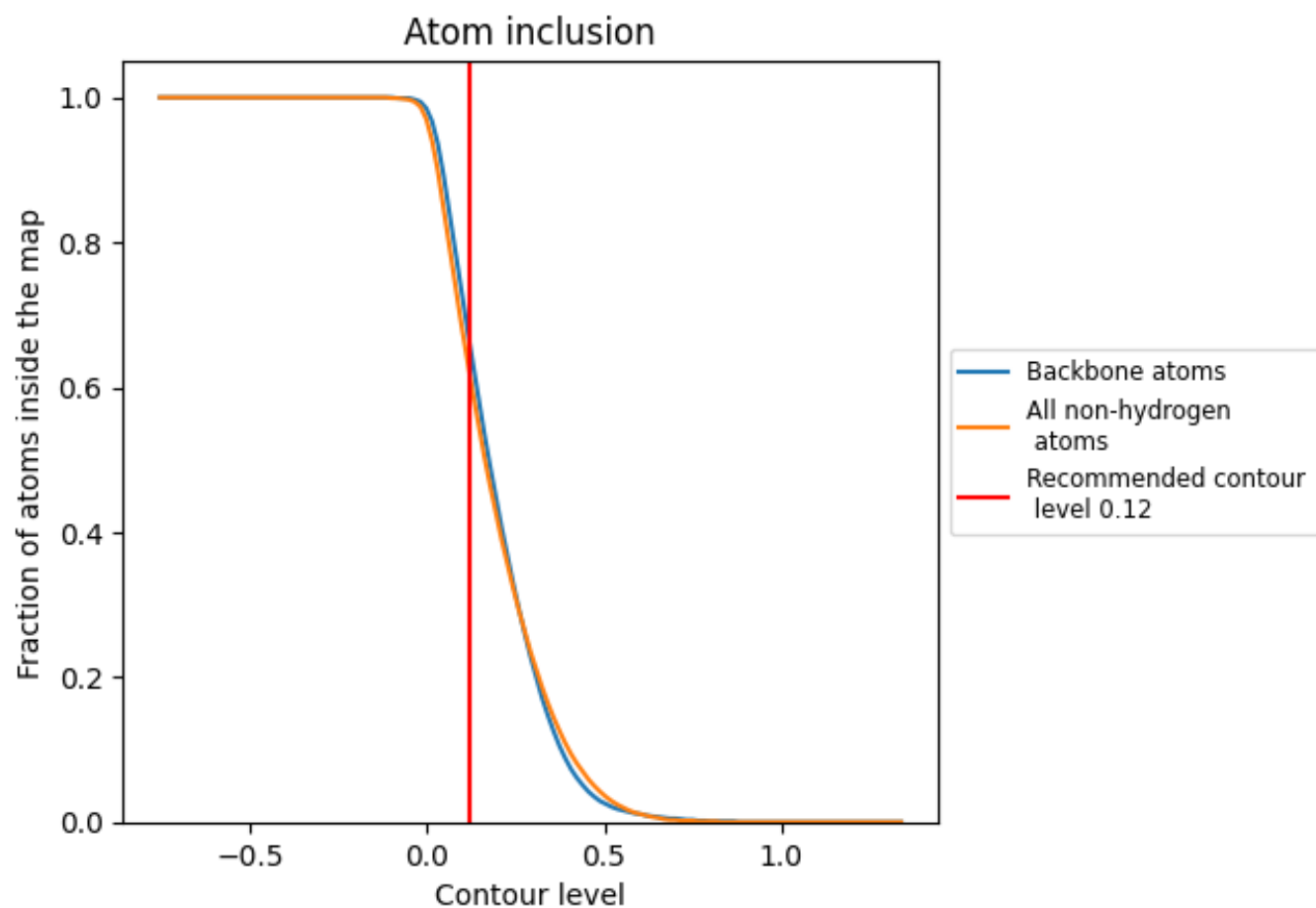
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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	 0.6190	 0.4860
0	 0.0000	 0.2780
1	 0.8040	 0.5990
2	 0.5820	 0.5070
3	 0.2140	 0.3410
4	 0.6380	 0.5550
5	 0.7440	 0.5220
6	 0.0210	 0.3460
7	 0.8750	 0.5810
8	 0.8100	 0.5430
9	 0.4560	 0.4440
A	 0.7940	 0.5470
AA	 0.2420	 0.3540
B	 0.7370	 0.5220
BB	 0.2270	 0.3960
C	 0.7300	 0.5180
CC	 0.4840	 0.4490
D	 0.6790	 0.5050
DD	 0.3600	 0.4330
E	 0.5960	 0.4620
EE	 0.5820	 0.4930
F	 0.7450	 0.5190
FF	 0.3720	 0.4330
G	 0.5790	 0.4650
GG	 0.1900	 0.3820
H	 0.6540	 0.4950
HH	 0.3570	 0.4460
I	 0.7210	 0.5180
II	 0.3870	 0.4160
J	 0.6160	 0.4700
JJ	 0.3910	 0.4480
K	 0.5800	 0.4810
KK	 0.2380	 0.4180
L	 0.6280	 0.4740
LL	 0.5690	 0.4750





















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Chain	Atom inclusion	Q-score
M	 0.6910	 0.5040
MM	 0.5640	 0.4830
N	 0.8130	 0.5500
NN	 0.2000	 0.4040
O	 0.7550	 0.5270
OO	 0.2800	 0.4080
P	 0.7480	 0.5250
PP	 0.3050	 0.4210
Q	 0.7410	 0.5110
QQ	 0.5970	 0.5010
R	 0.6360	 0.4880
RR	 0.0000	 0.2170
S	 0.7580	 0.5180
SS	 0.1130	 0.3770
T	 0.6670	 0.4920
TT	 0.5470	 0.4850
U	 0.4700	 0.4290
UU	 0.3290	 0.4330
V	 0.7500	 0.5390
VV	 0.5830	 0.4960
W	 0.4420	 0.4040
WW	 0.2310	 0.3820
X	 0.6690	 0.4960
Y	 0.6800	 0.5000
Z	 0.6320	 0.4670
a	 0.7870	 0.5470
b	 0.4690	 0.4210
c	 0.6480	 0.5040
d	 0.6710	 0.4920
e	 0.7520	 0.5260
f	 0.7890	 0.5370
g	 0.7020	 0.5150
h	 0.6660	 0.4950
i	 0.6170	 0.4810
j	 0.7980	 0.5380
k	 0.5080	 0.4580
l	 0.7380	 0.5110
m	 0.7280	 0.5070
n	 0.7060	 0.4620
o	 0.7010	 0.5250
p	 0.7160	 0.5220
q	 0.3790	 0.4420

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Chain	Atom inclusion	Q-score
r	 0.7150	 0.5160
s	 0.0010	 0.0470
t	 0.0000	 0.0430
u	 0.4820	 0.4700
v	 0.4570	 0.4570
w	 0.2130	 0.3890
x	 0.3430	 0.4430
y	 0.4200	 0.4420
z	 0.1560	 0.3270