



Full wwPDB EM Validation Report ⓘ

May 19, 2024 – 08:39 am BST

PDB ID : 6R7Q
EMDB ID : EMD-4745
Title : Structure of XBP1u-paused ribosome nascent chain complex with Sec61.
Authors : Shanmuganathan, V.; Cheng, J.; Braunger, K.; Berninghausen, O.; Beatrix, B.; Beckmann, R.
Deposited on : 2019-03-29
Resolution : 3.90 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:

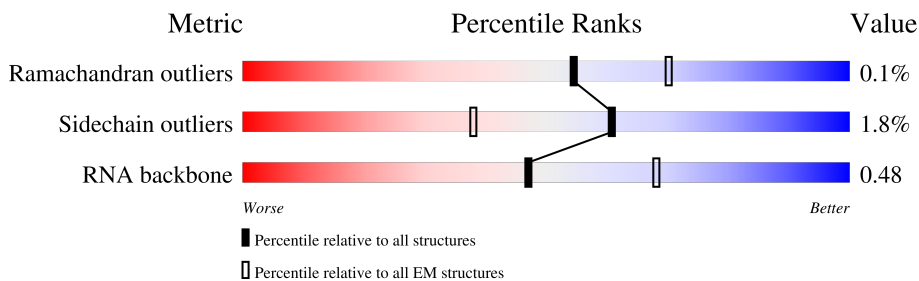
EMDB validation analysis : 0.0.1.dev92
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

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 3.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	AA	55	
2	BB	189	
3	CC	206	
4	DD	185	
5	EE	151	
6	FF	62	
7	GG	100	
8	HH	83	

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Mol	Chain	Length	Quality of chain
9	II	144	56% 99%
10	JJ	83	51% 99%
11	KK	132	61% 100%
12	LL	101	36% 99%
13	MM	136	39% 98%
14	0	68	84% 99%
15	1	24	67% 54% 46%
16	2	75	71% 56% 43%
17	3	75	72% 75% 21%
18	4	6	67% 67% 33%
19	5	3544	11% 67% 28% 5%
20	6	313	91% 99%
21	7	120	79% 19%
22	8	151	7% 73% 25%
23	9	55	53% 100%
24	NN	124	67% 98%
25	OO	75	48% 100%
26	PP	141	64% 99%
27	QQ	149	30% 99%
28	RR	117	92% 99%
29	A	248	7% 97%
30	B	394	9% 98%
31	C	362	9% 97%
32	D	293	12% 99%
33	E	251	18% 82% 14%

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Mol	Chain	Length	Quality of chain
34	F	225	10% 98%
35	G	240	21% 95%
36	H	190	9% 97%
37	I	213	14% 95%
38	J	170	16% 99%
39	K	1698	18% 69% 27%
40	L	210	14% 98%
41	M	138	10% 96%
42	N	203	5% 97%
43	O	199	• 98%
44	P	153	6% 99%
45	Q	187	6% 98%
46	R	180	17% 98%
47	S	176	6% 98%
48	T	159	14% 98%
49	U	99	28% 99%
50	V	131	11% 97%
51	W	121	42% 88% 12%
52	X	118	12% 97%
53	Y	134	11% 99%
54	Z	135	13% 99%
55	SS	96	79% 98%
56	a	147	7% 99%
57	b	116	43% 87% 10%
58	c	98	13% 99%

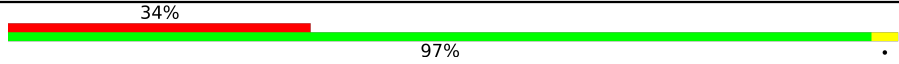
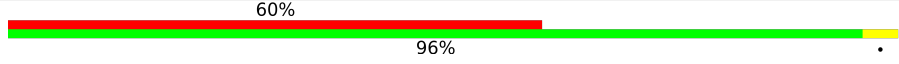

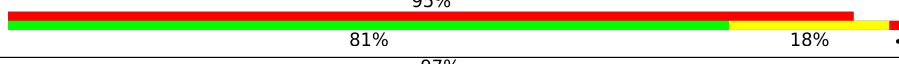

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Mol	Chain	Length	Quality of chain
59	d	107	17% 97%
60	e	128	7% 98%
61	f	109	9% 97%
62	g	114	11% 97%
63	h	122	17% 100%
64	i	102	15% 98%
65	j	86	5% 99%
66	k	69	28% 99%
67	l	50	14% 98%
68	m	52	8% 98%
69	n	25	20% 96%
70	o	104	17% 98%
71	p	91	13% 98%
72	q	217	51% 98%
73	r	124	9% 98%
74	s	196	98% 100%
75	t	153	100% 100%
76	u	213	38% 97%
77	v	221	37% 99%
78	w	228	73% 97%
79	x	262	61% 98%
80	y	191	61% 97%
81	z	237	72% 99%
82	TT	129	43% 99%
83	UU	142	67% 99%

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Mol	Chain	Length	Quality of chain
84	VV	141	
85	WW	120	
86	XX	461	
87	YY	62	
88	ZZ	29	

2 Entry composition [i](#)

There are 90 unique types of molecules in this entry. The entry contains 219898 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 40S ribosomal protein S30.

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

- Molecule 2 is a protein called 40S ribosomal protein S7.

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

- Molecule 3 is a protein called 40S ribosomal protein S8.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 4 is a protein called Ribosomal protein S9 (Predicted).

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

- Molecule 5 is a protein called Ribosomal protein S11.

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

- Molecule 6 is a protein called Ribosomal protein S28.

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

- Molecule 7 is a protein called uS10.

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

- Molecule 8 is a protein called eS21.

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

- Molecule 9 is a protein called uS13.

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

- Molecule 10 is a protein called 40S ribosomal protein S27.

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

- Molecule 11 is a protein called eS17.

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

- Molecule 12 is a protein called eS26.

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

- Molecule 13 is a protein called uS11.

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

- Molecule 14 is a protein called eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	0	68	Total	C	N	O	S	0	0
			555	351	103	94	7		

- Molecule 15 is a protein called X-box-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	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 16 is a RNA chain called P-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	2	75	Total	C	N	O	P	0	0
			1594	713	285	522	74		

- Molecule 17 is a RNA chain called E-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	3	75	Total	C	N	O	P	0	0
			1597	714	287	522	74		

- Molecule 18 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	4	6	Total	C	N	O	P	0	0
			127	57	21	43	6		

- Molecule 19 is a RNA chain called 28S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
19	5	3543	75972	33833	13910	24686	3543	0	0

- Molecule 20 is a protein called ribosomal protein RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	6	313	2436	1535	424	465	12	0	0

- Molecule 21 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
21	7	120	2558	1141	456	842	119	0	0

- Molecule 22 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
22	8	151	3208	1432	564	1062	150	0	0

- Molecule 23 is a protein called uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	9	55	459	286	94	74	5	0	0

- Molecule 24 is a protein called eS24.

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

- Molecule 25 is a protein called ribosomal protein eS25.

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

- Molecule 26 is a protein called eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	PP	141	1097	688	211	195	3	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
PP	119	GLY	TRP	conflict	UNP G1TN62

- Molecule 27 is a protein called ribosomal protein uS15.

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

- Molecule 28 is a protein called 40S ribosomal protein S12.

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

- Molecule 29 is a protein called uL2.

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

- Molecule 30 is a protein called uL3.

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

- Molecule 31 is a protein called uL4.

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

- Molecule 32 is a protein called 60S ribosomal protein L5.

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

- Molecule 33 is a protein called 60S ribosomal protein L6.

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

- Molecule 34 is a protein called uL30.

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

- Molecule 35 is a protein called eL8.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	244	GLY	CYS	conflict	UNP G1STW0

- Molecule 36 is a protein called uL6.

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

- Molecule 37 is a protein called Ribosomal protein L10 (Predicted).

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

- Molecule 38 is a protein called Ribosomal protein L11.

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

- Molecule 39 is a RNA chain called 18S ribosomal RNA.

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

- Molecule 40 is a protein called 60S ribosomal protein L13.

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

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 41 is a protein called Ribosomal protein L14.

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

- Molecule 42 is a protein called Ribosomal protein L15.

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

- Molecule 43 is a protein called uL13.

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

- Molecule 44 is a protein called uL22.

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

- Molecule 45 is a protein called eL18.

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

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 46 is a protein called eL19.

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

- Molecule 47 is a protein called eL20.

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

- Molecule 48 is a protein called eL21.

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

- Molecule 49 is a protein called eL22.

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

- Molecule 50 is a protein called eL14.

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

- Molecule 51 is a protein called Ribosomal protein L24.

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

- Molecule 52 is a protein called uL23.

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

- Molecule 53 is a protein called Ribosomal protein L26.

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

- Molecule 54 is a protein called 60S ribosomal protein L27.

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

- Molecule 55 is a protein called eS10.

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

- Molecule 56 is a protein called uL15.

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

- Molecule 57 is a protein called eL29.

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

- Molecule 58 is a protein called eL30.

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

- Molecule 59 is a protein called eL31.

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

- Molecule 60 is a protein called eL32.

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

- Molecule 61 is a protein called eL33.

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

- Molecule 62 is a protein called eL34.

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

- Molecule 63 is a protein called uL29.

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

- Molecule 64 is a protein called 60S ribosomal protein L36.

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

- Molecule 65 is a protein called Ribosomal protein L37.

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

- Molecule 66 is a protein called eL38.

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

- Molecule 67 is a protein called eL39.

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

- Molecule 68 is a protein called eL40.

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

- Molecule 69 is a protein called 60s ribosomal protein l41.

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

- Molecule 70 is a protein called eL42.

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

- Molecule 71 is a protein called ribosomal protein eL43.

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

- Molecule 72 is a protein called uS2.

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

- Molecule 73 is a protein called eL28.

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

- Molecule 74 is a protein called 60S acidic ribosomal protein P0.

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

- Molecule 75 is a protein called uL11.

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

- Molecule 76 is a protein called 40S ribosomal protein S3a.

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

- Molecule 77 is a protein called uS5.

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

- Molecule 78 is a protein called Ribosomal protein S3.

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

- Molecule 79 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	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 80 is a protein called Ribosomal protein S5.

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

- Molecule 81 is a protein called 40S ribosomal protein S6.

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

- Molecule 82 is a protein called Ribosomal protein S15a.

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

- Molecule 83 is a protein called Ribosomal protein S16.

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

- Molecule 84 is a protein called Ribosomal protein S23.

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

- Molecule 85 is a protein called uS19.

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

- Molecule 86 is a protein called Protein transport protein Sec61 subunit alpha isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
86	XX	426	3313	2181	535	576	21	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
XX	145	SER	THR	conflict	UNP P38377

- Molecule 87 is a protein called Protein transport protein Sec61 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	YY	62	Total	C	N	O	S	0	0
			494	326	86	79	3		

- Molecule 88 is a protein called Protein transport protein Sec61 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
88	ZZ	29	Total	C	N	O	S	0	0
			229	157	36	34	2		

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

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

- Molecule 90 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
90	5	201	Total	Mg	0
			201	201	
90	7	7	Total	Mg	0
			7	7	
90	8	4	Total	Mg	0
			4	4	
90	B	1	Total	Mg	0
			1	1	
90	K	78	Total	Mg	0
			78	78	
90	P	2	Total	Mg	0
			2	2	
90	V	1	Total	Mg	0
			1	1	

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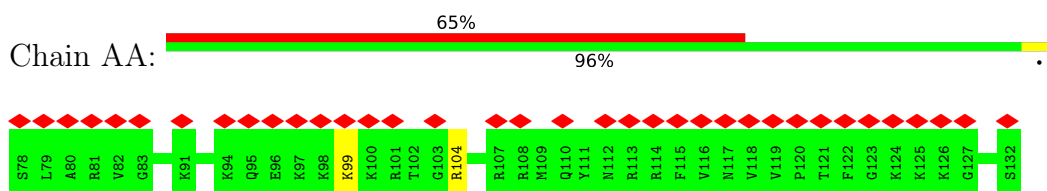
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Mol	Chain	Residues	Atoms		AltConf
90	a	1	Total 1	Mg 1	0
90	e	1	Total 1	Mg 1	0
90	g	1	Total 1	Mg 1	0
90	j	1	Total 1	Mg 1	0
90	y	1	Total 1	Mg 1	0

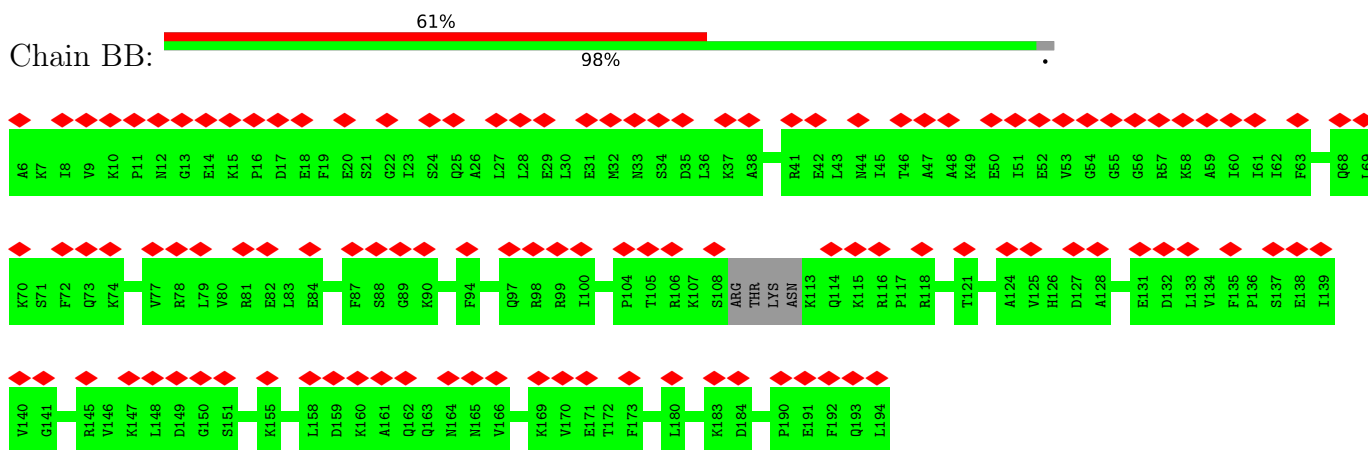
3 Residue-property plots [i](#)

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.

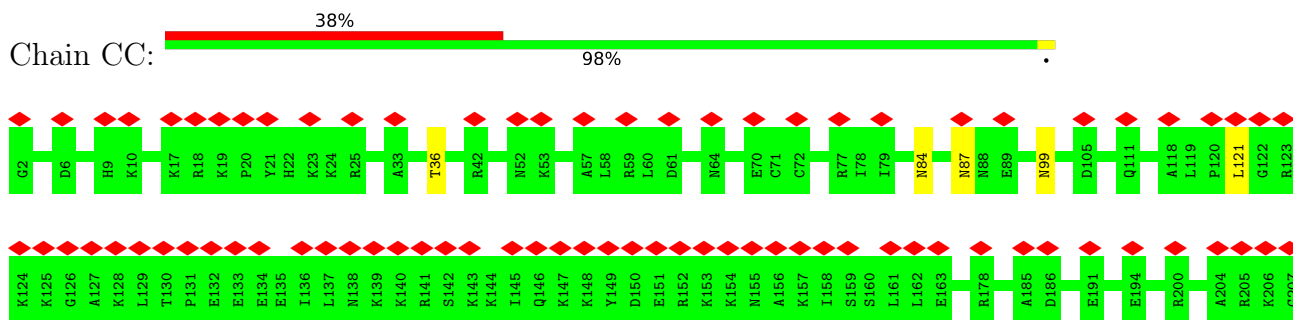
- Molecule 1: 40S ribosomal protein S30



- Molecule 2: 40S ribosomal protein S7

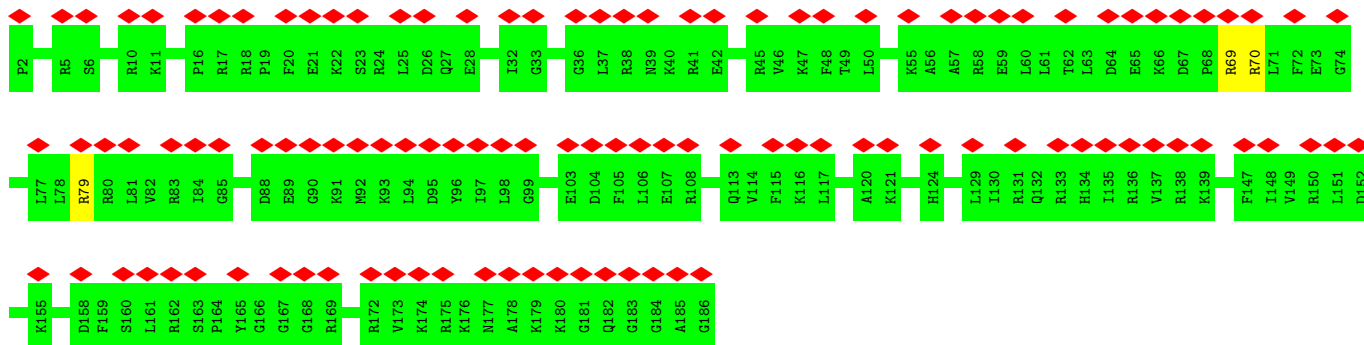


- Molecule 3: 40S ribosomal protein S8

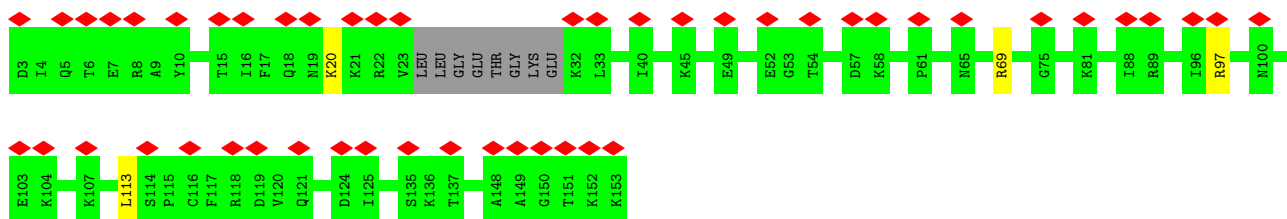


- Molecule 4: Ribosomal protein S9 (Predicted)

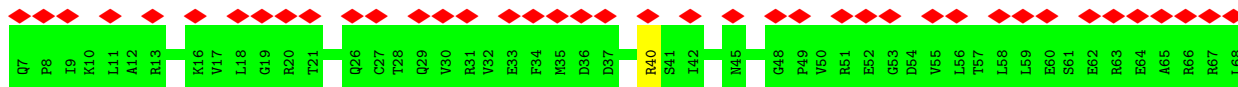




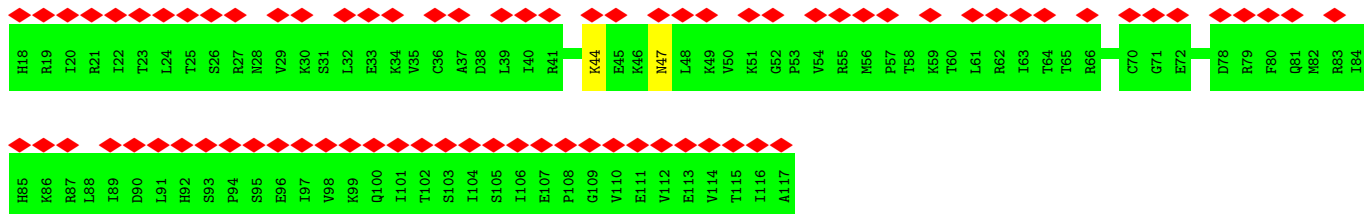
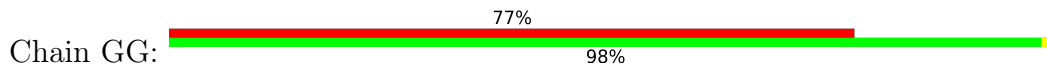
• Molecule 5: Ribosomal protein S11



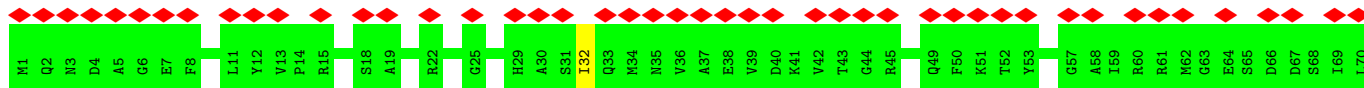
• Molecule 6: Ribosomal protein S28

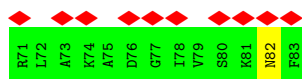


• Molecule 7: uS10

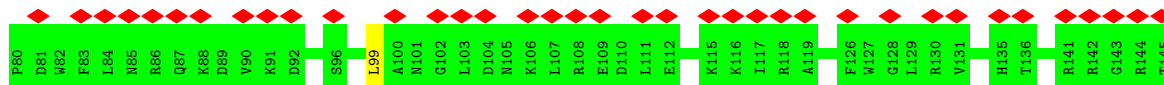
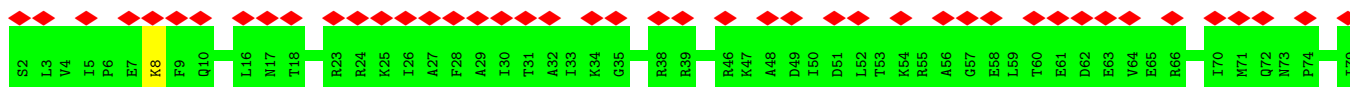


• Molecule 8: eS21

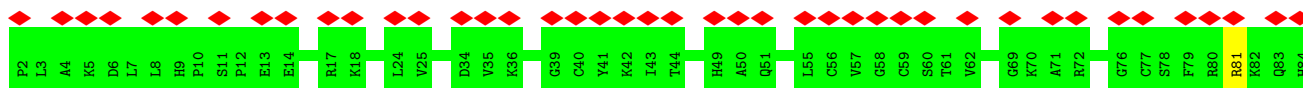




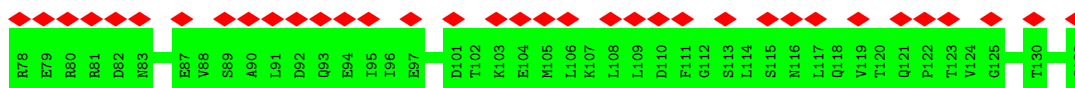
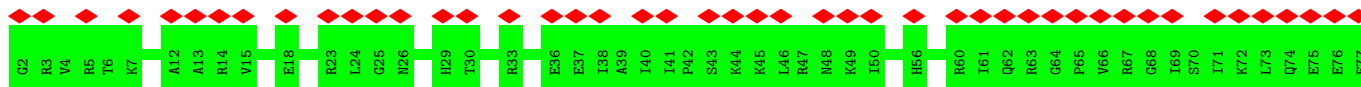
- Molecule 9: uS13



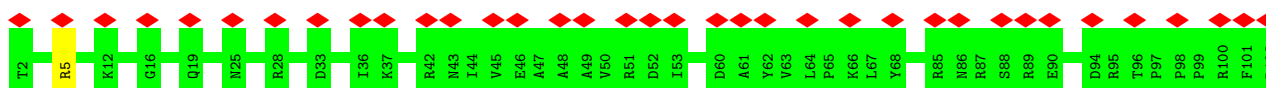
- Molecule 10: 40S ribosomal protein S27



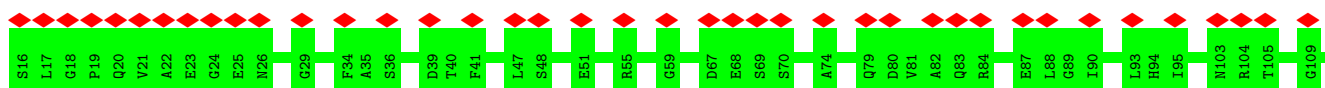
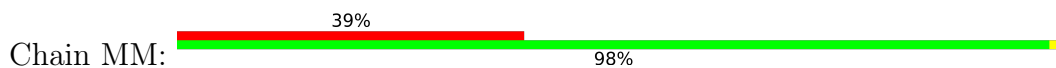
- Molecule 11: eS17

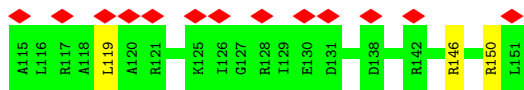


- Molecule 12: eS26

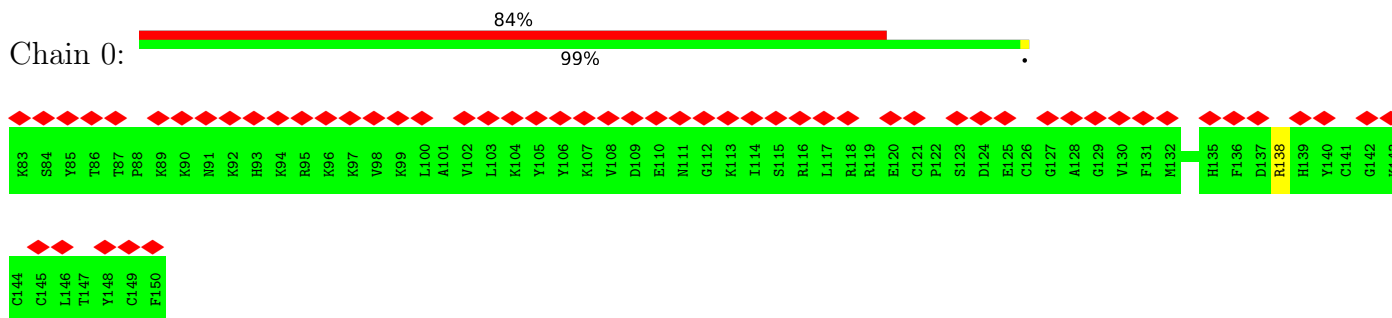


- Molecule 13: uS11





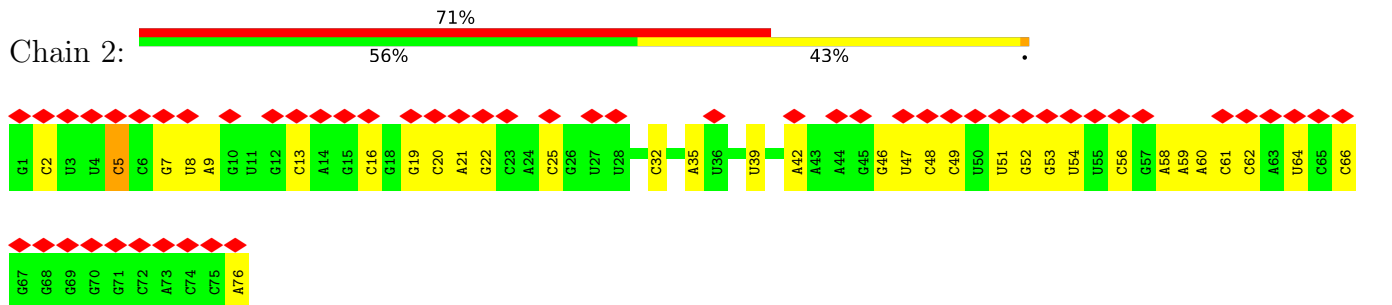
• Molecule 14: eS31



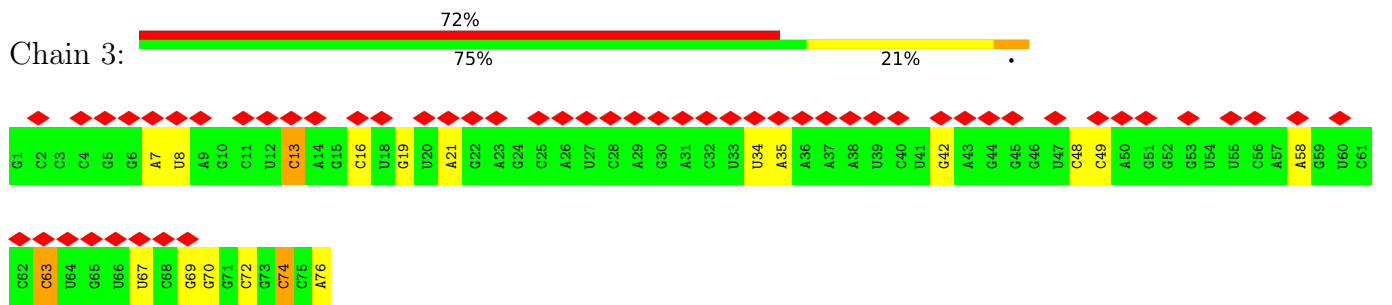
• Molecule 15: X-box-binding protein 1



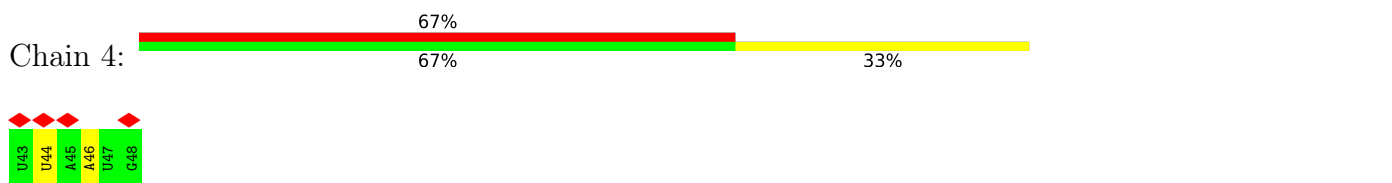
• Molecule 16: P-tRNA



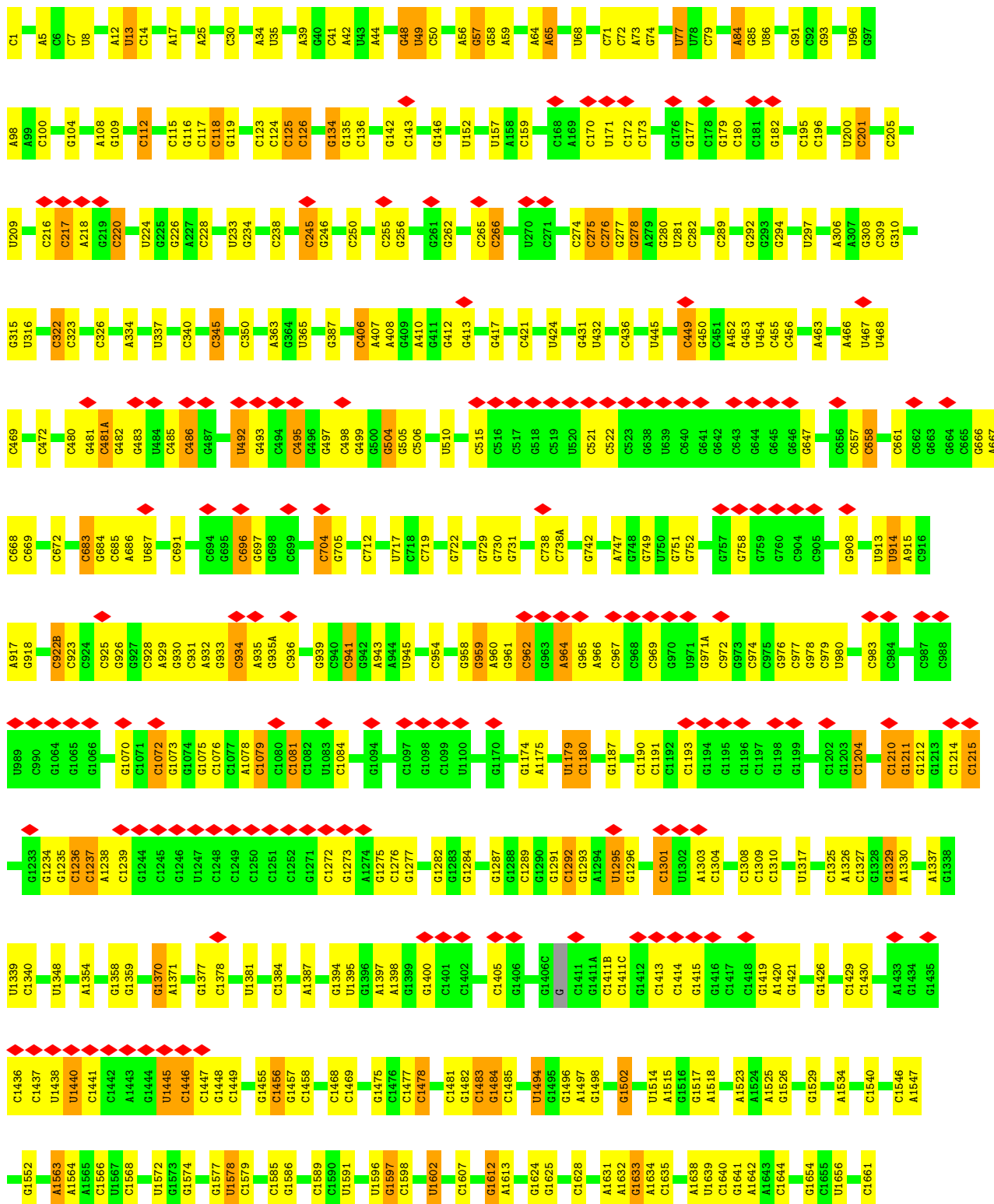
• Molecule 17: E-tRNA

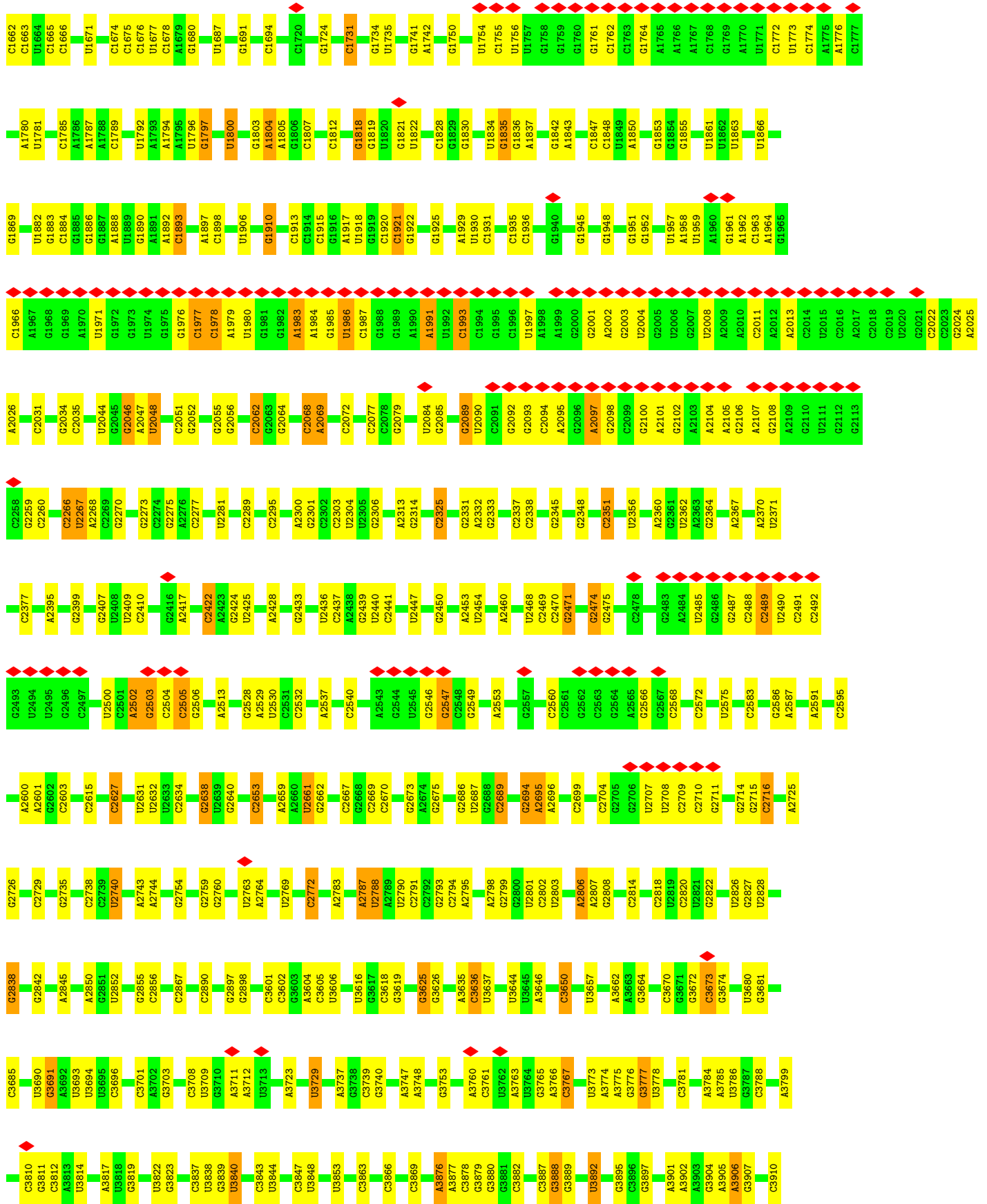


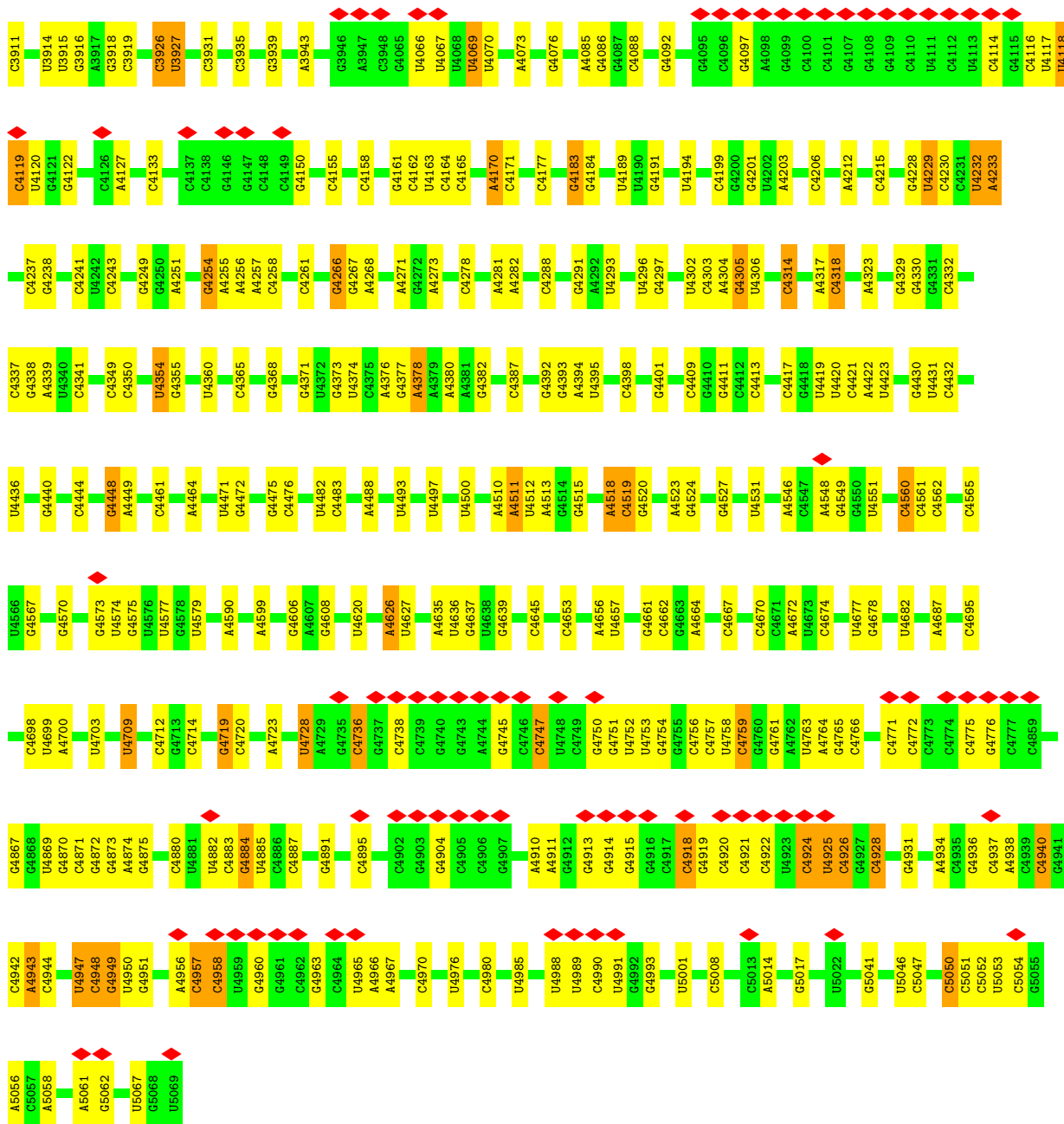
• Molecule 18: messenger RNA



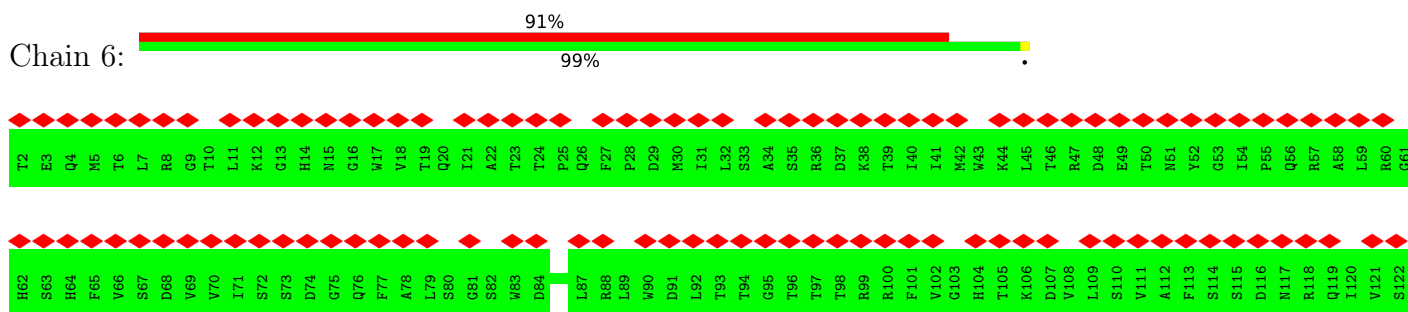
• Molecule 19: 28S ribosomal RNA

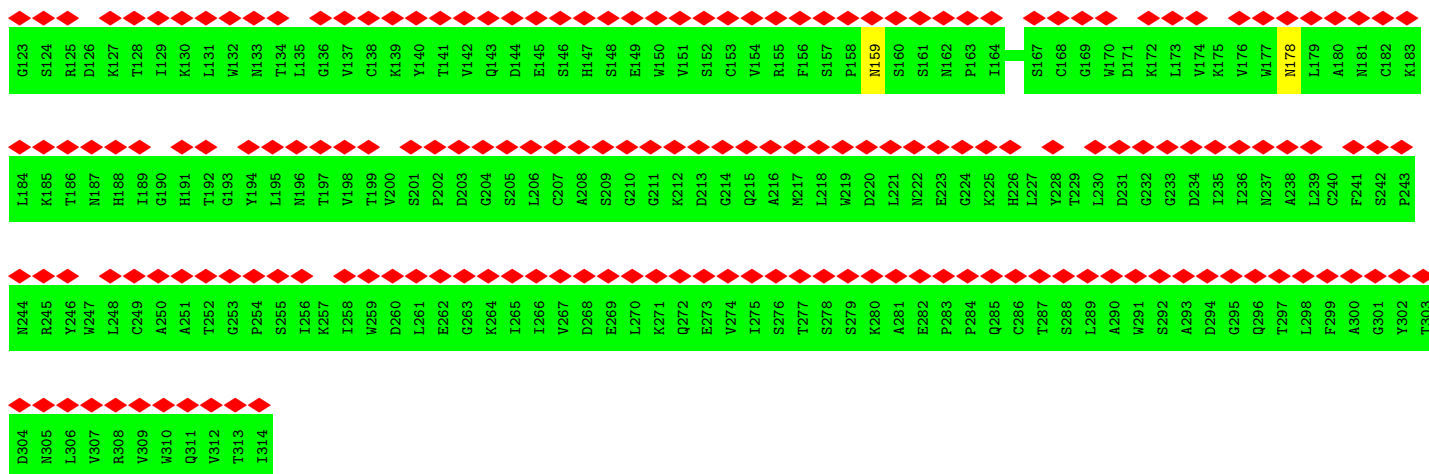




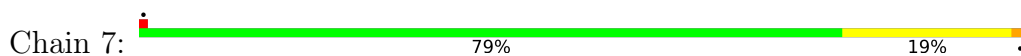


● Molecule 20: ribosomal protein RACK1

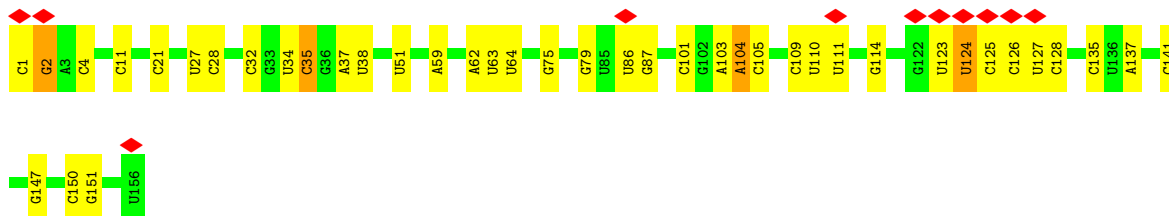




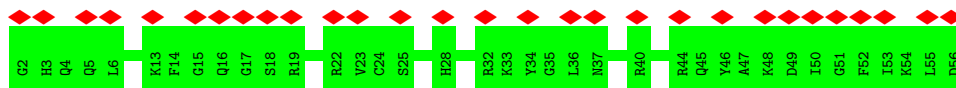
• Molecule 21: 5S ribosomal RNA



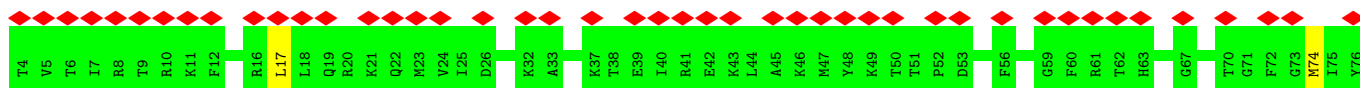
• Molecule 22: 5.8S ribosomal RNA

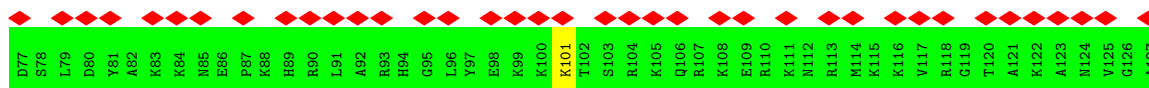


• Molecule 23: uS14

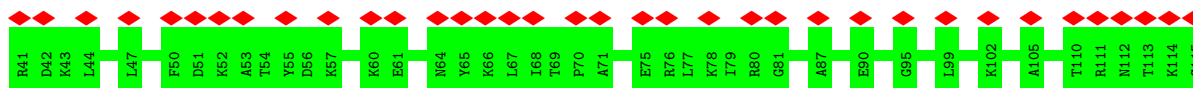


• Molecule 24: eS24

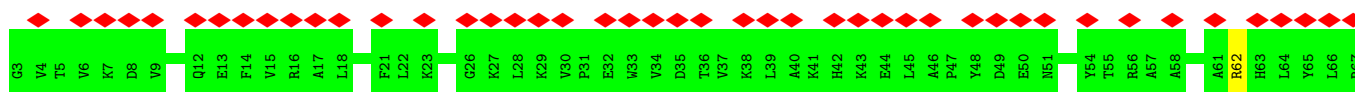




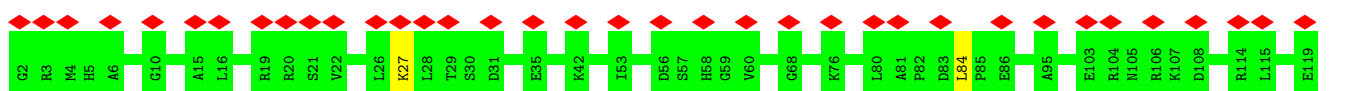
- Molecule 25: ribosomal protein eS25



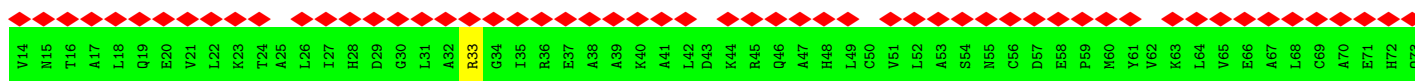
- Molecule 26: eS19



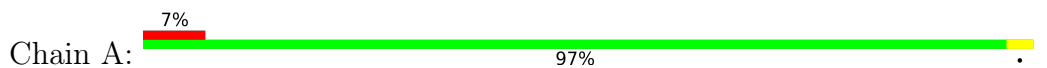
- Molecule 27: ribosomal protein uS15



- Molecule 28: 40S ribosomal protein S12

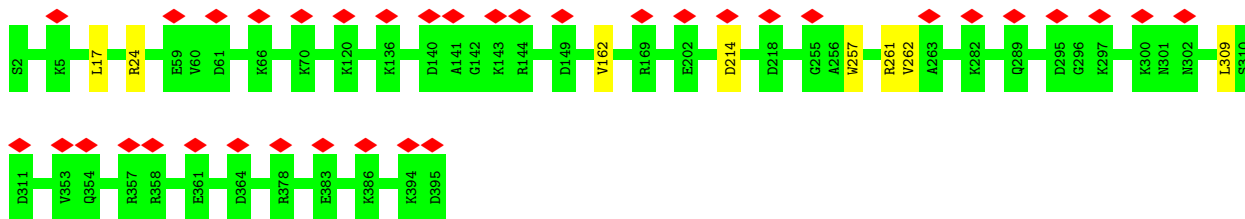


- Molecule 29: uL2

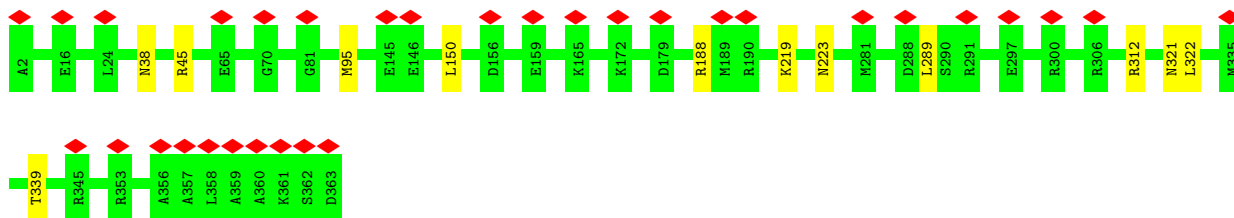




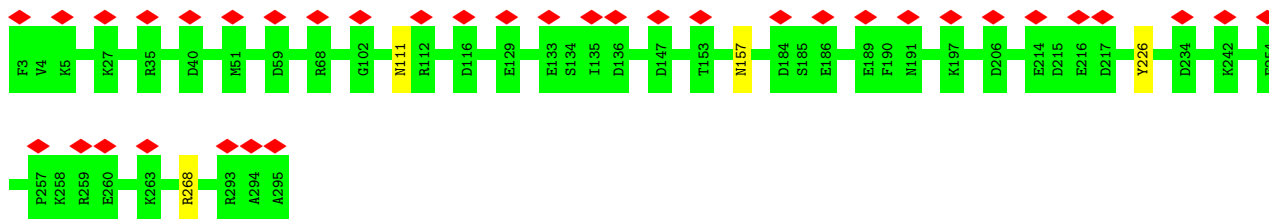
• Molecule 30: uL3



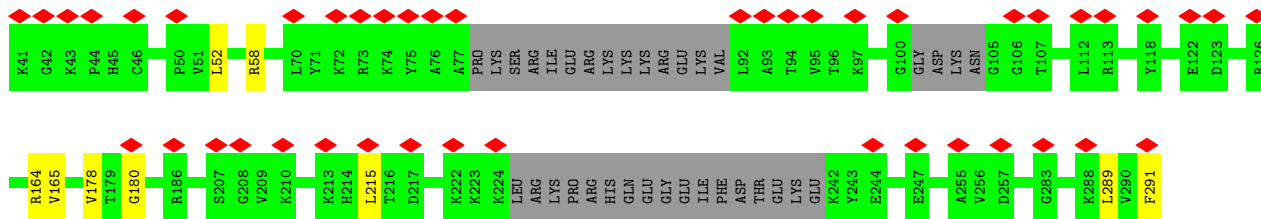
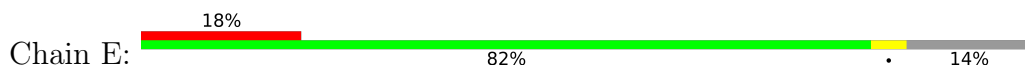
• Molecule 31: uL4



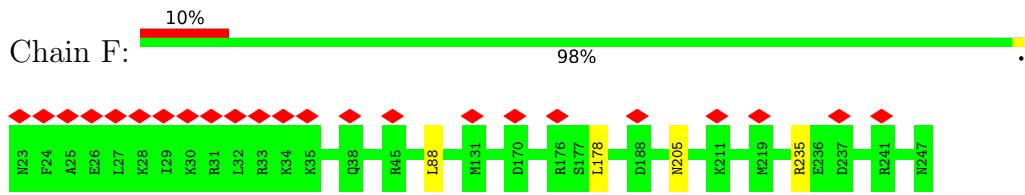
• Molecule 32: 60S ribosomal protein L5



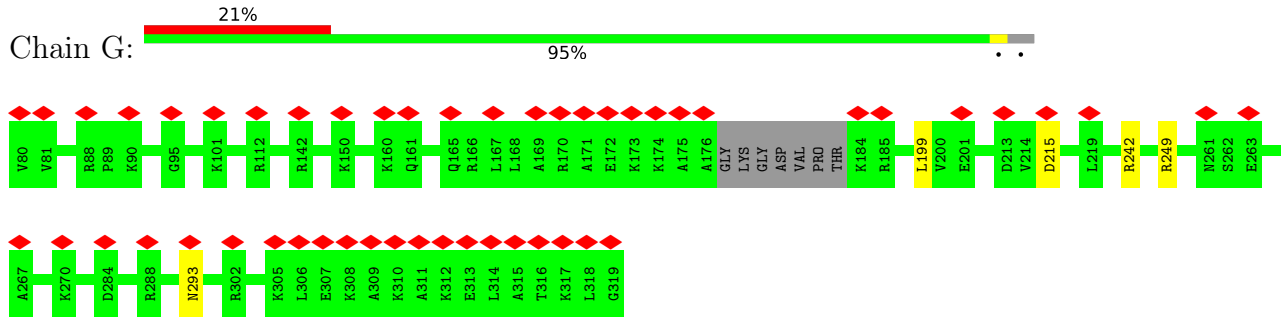
• Molecule 33: 60S ribosomal protein L6



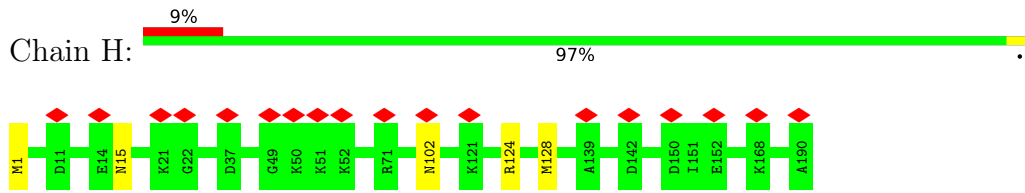
• Molecule 34: uL30



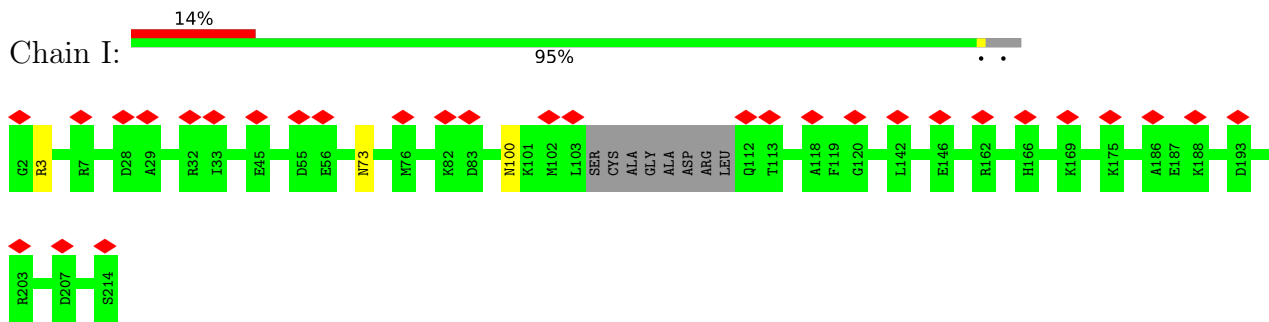
• Molecule 35: eL8



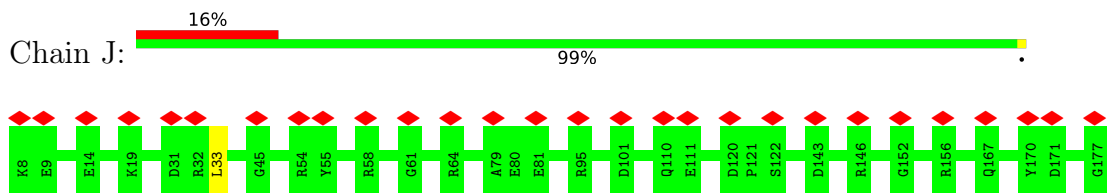
• Molecule 36: uL6



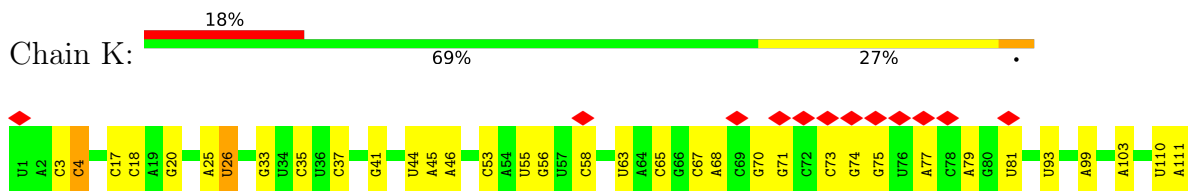
• Molecule 37: Ribosomal protein L10 (Predicted)

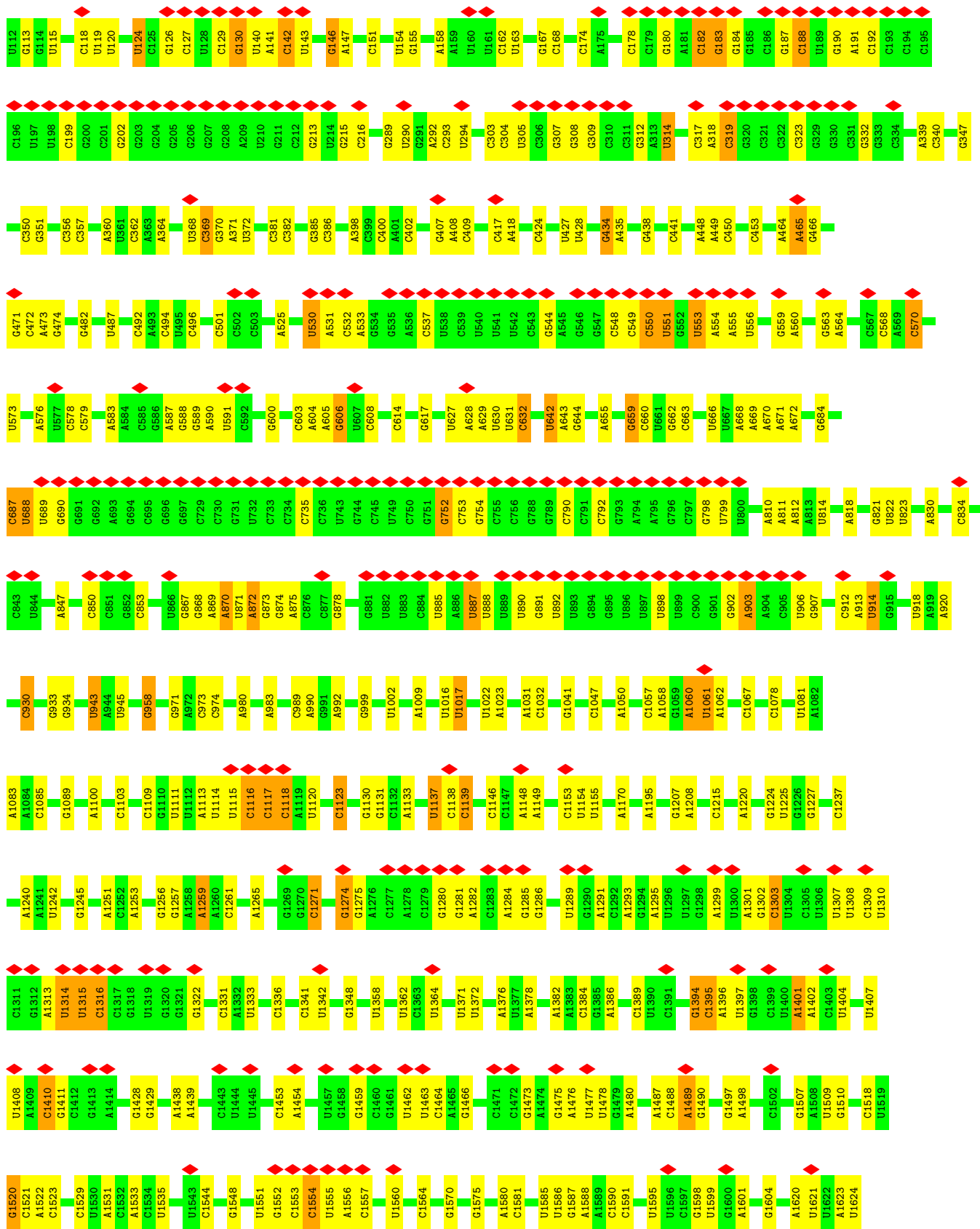


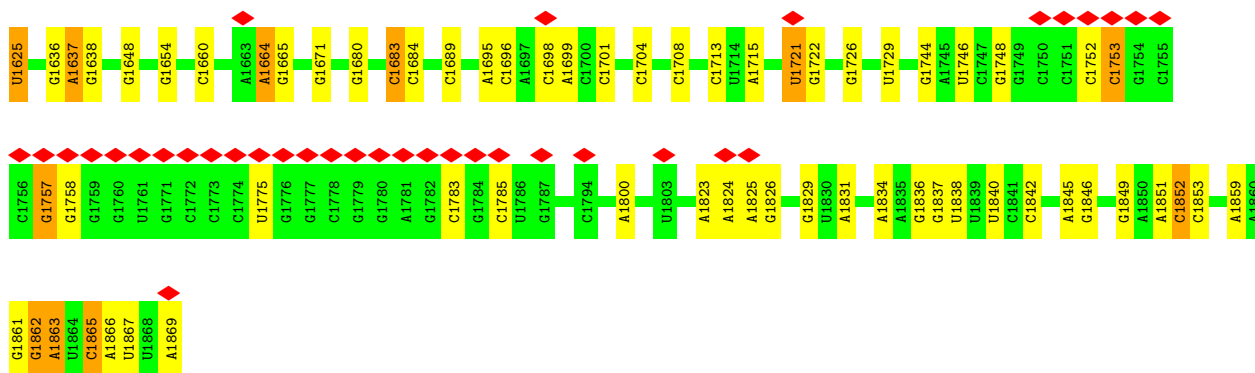
• Molecule 38: Ribosomal protein L11



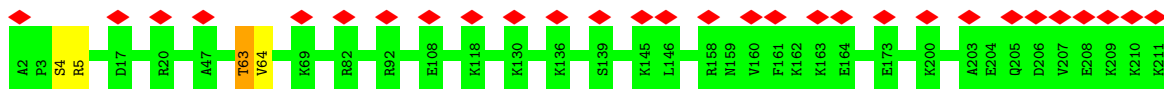
• Molecule 39: 18S ribosomal RNA



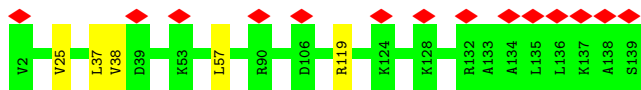




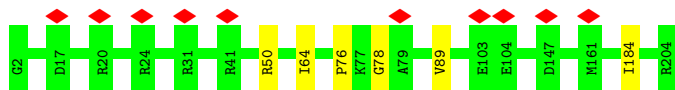
• Molecule 40: 60S ribosomal protein L13



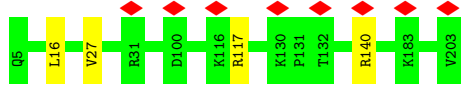
• Molecule 41: Ribosomal protein L14



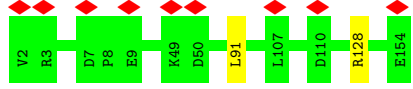
• Molecule 42: Ribosomal protein L15



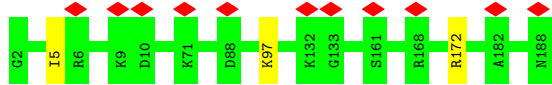
• Molecule 43: uL13



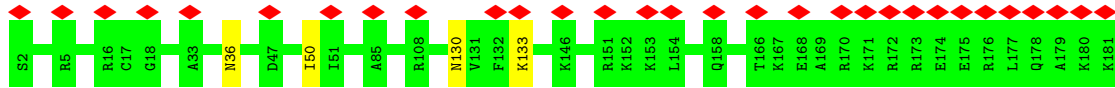
• Molecule 44: uL22



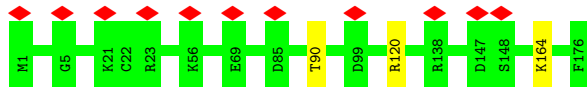
• Molecule 45: eL18



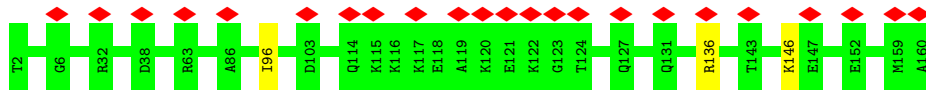
• Molecule 46: eL19



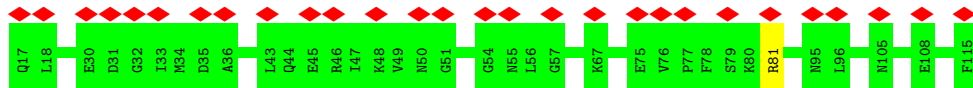
• Molecule 47: eL20



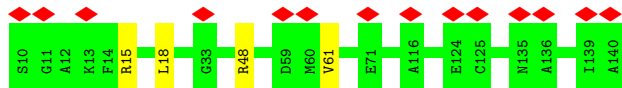
• Molecule 48: eL21



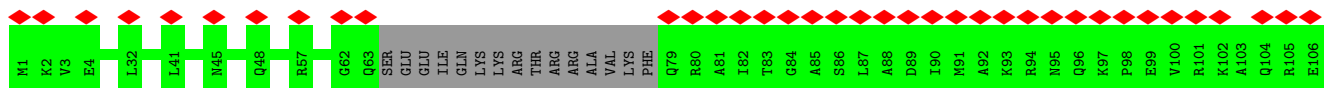
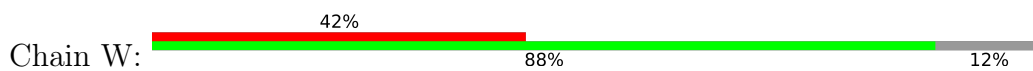
• Molecule 49: eL22

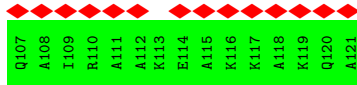


• Molecule 50: eL14

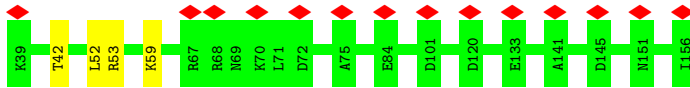


• Molecule 51: Ribosomal protein L24

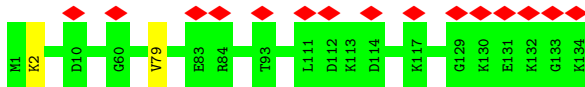




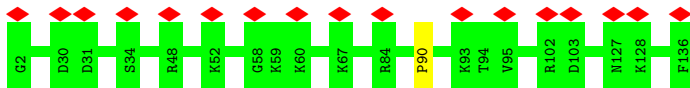
- Molecule 52: uL23



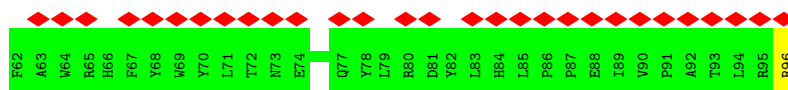
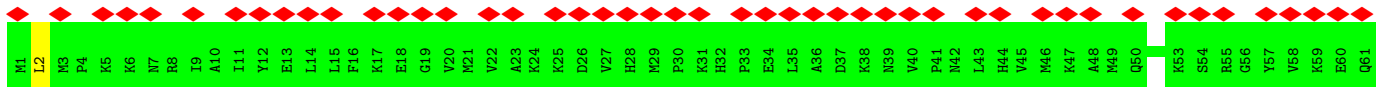
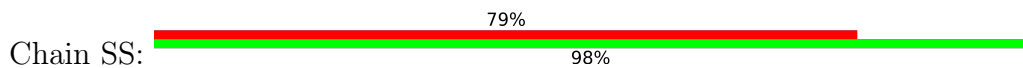
- Molecule 53: Ribosomal protein L26



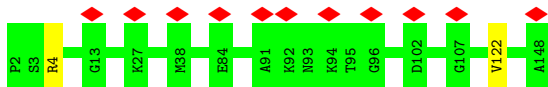
- Molecule 54: 60S ribosomal protein L27



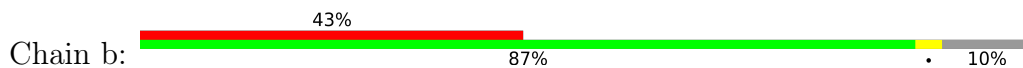
- Molecule 55: eS10

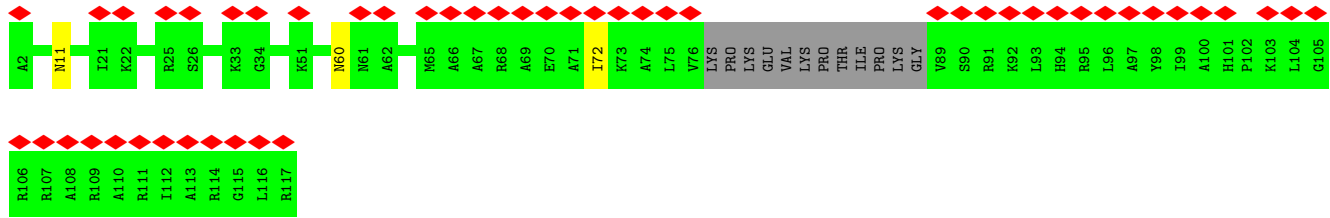


- Molecule 56: uL15



- Molecule 57: eL29

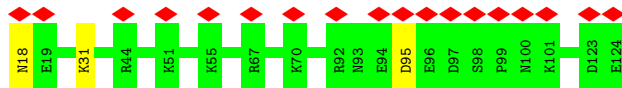




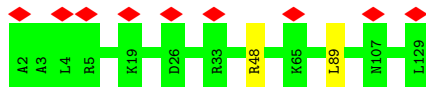
- Molecule 58: eL30



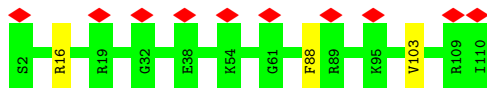
- Molecule 59: eL31



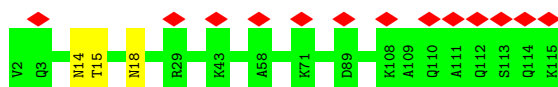
- Molecule 60: eL32



- Molecule 61: eL33

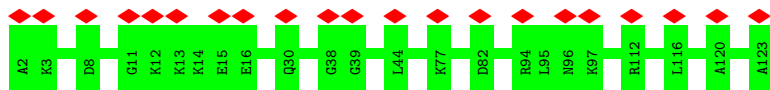


- Molecule 62: eL34

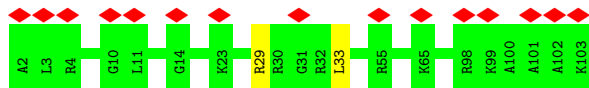


- Molecule 63: uL29

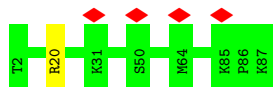




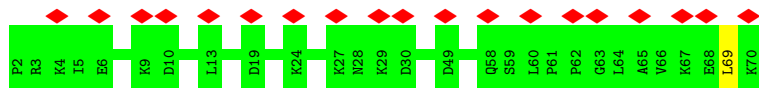
- Molecule 64: 60S ribosomal protein L36



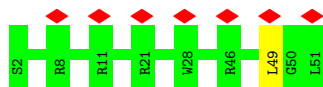
- Molecule 65: Ribosomal protein L37



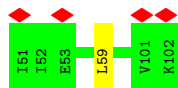
- Molecule 66: eL38



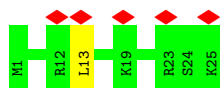
- Molecule 67: eL39



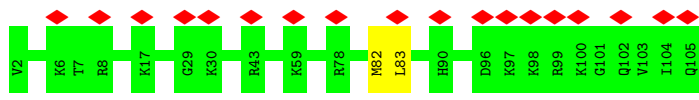
- Molecule 68: eL40



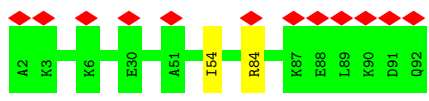
- Molecule 69: 60s ribosomal protein l41



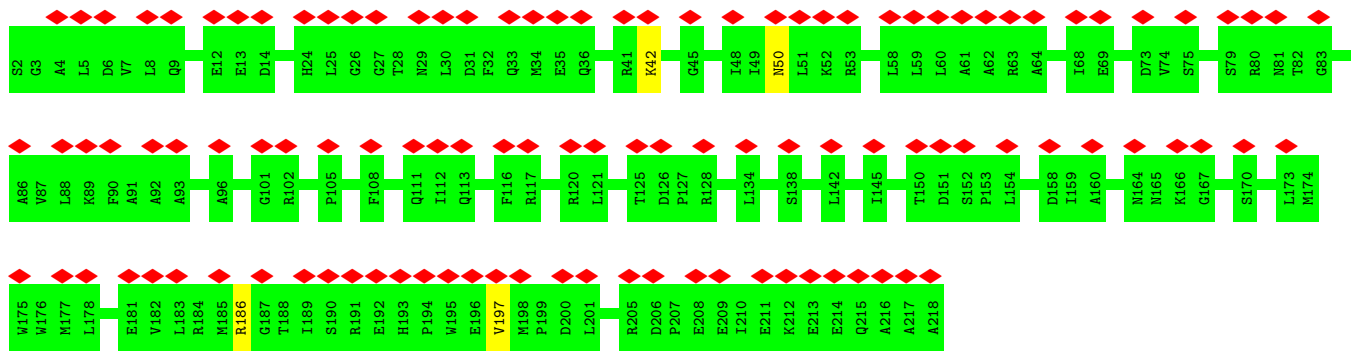
- Molecule 70: eL42



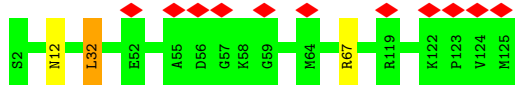
• Molecule 71: ribosomal protein eL43



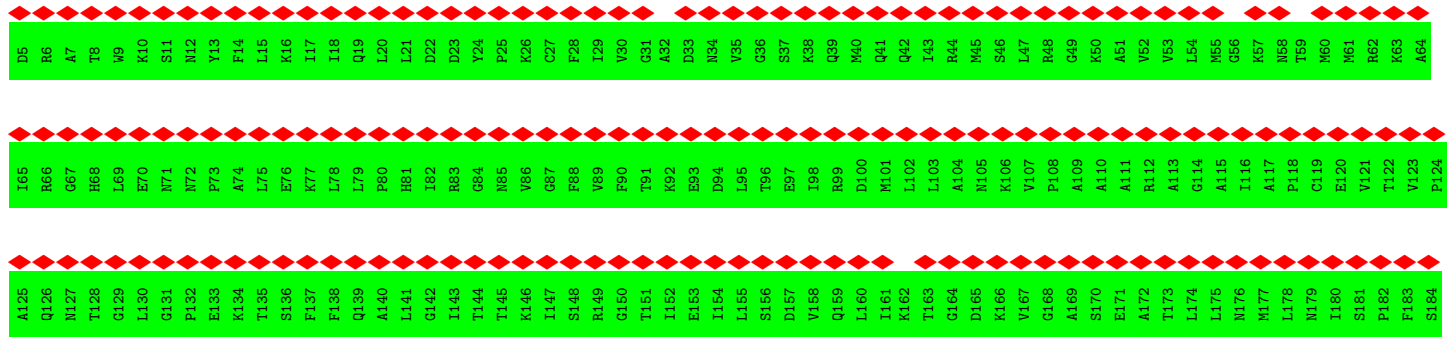
• Molecule 72: uS2

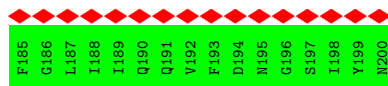


• Molecule 73: eL28

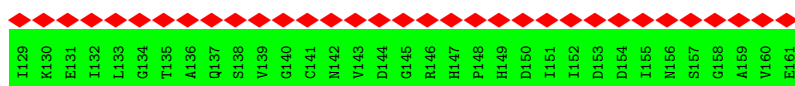
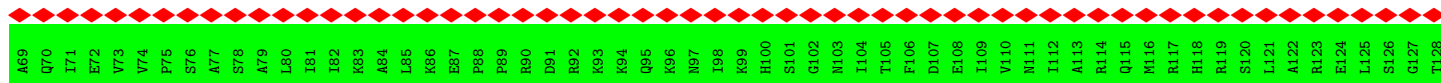


• Molecule 74: 60S acidic ribosomal protein P0

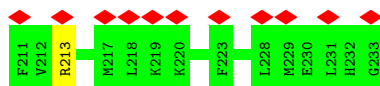
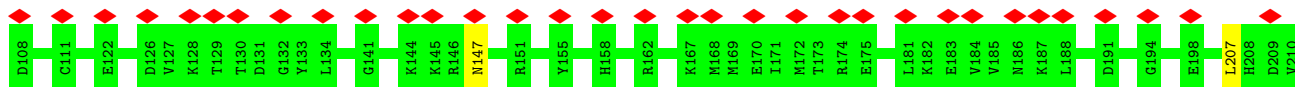
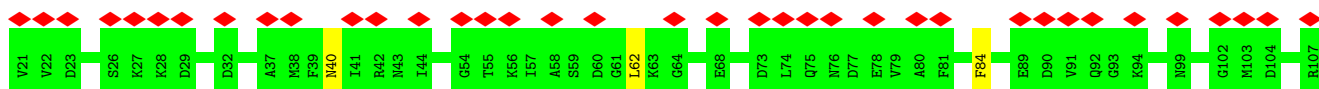
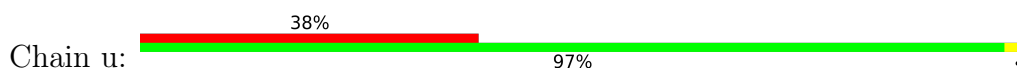




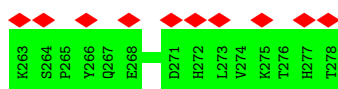
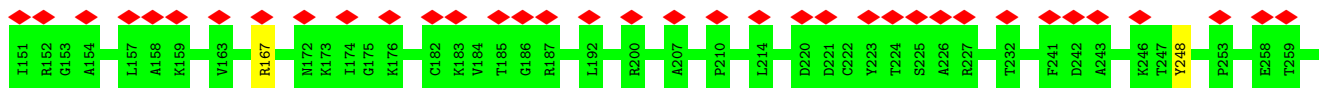
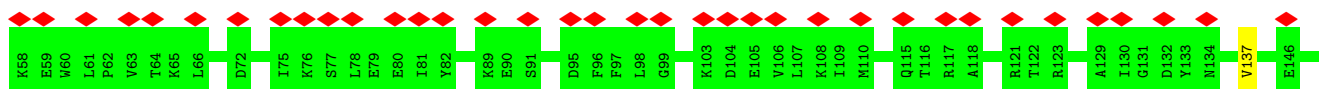
- Molecule 75: uL11



- Molecule 76: 40S ribosomal protein S3a



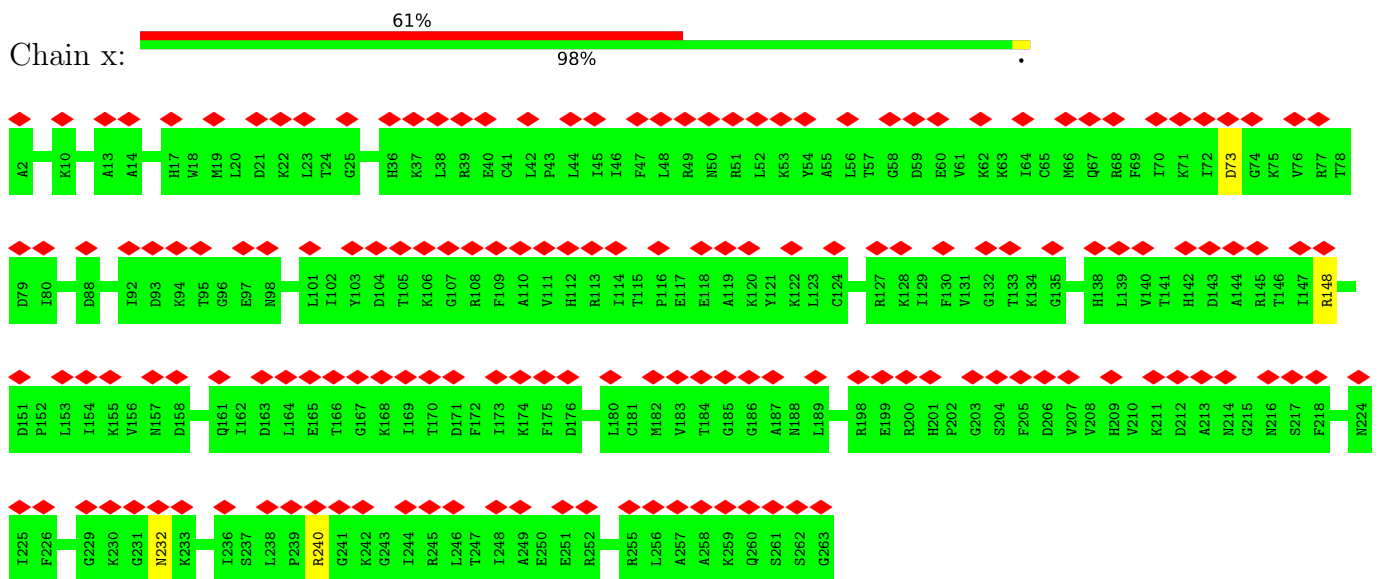
- Molecule 77: uS5



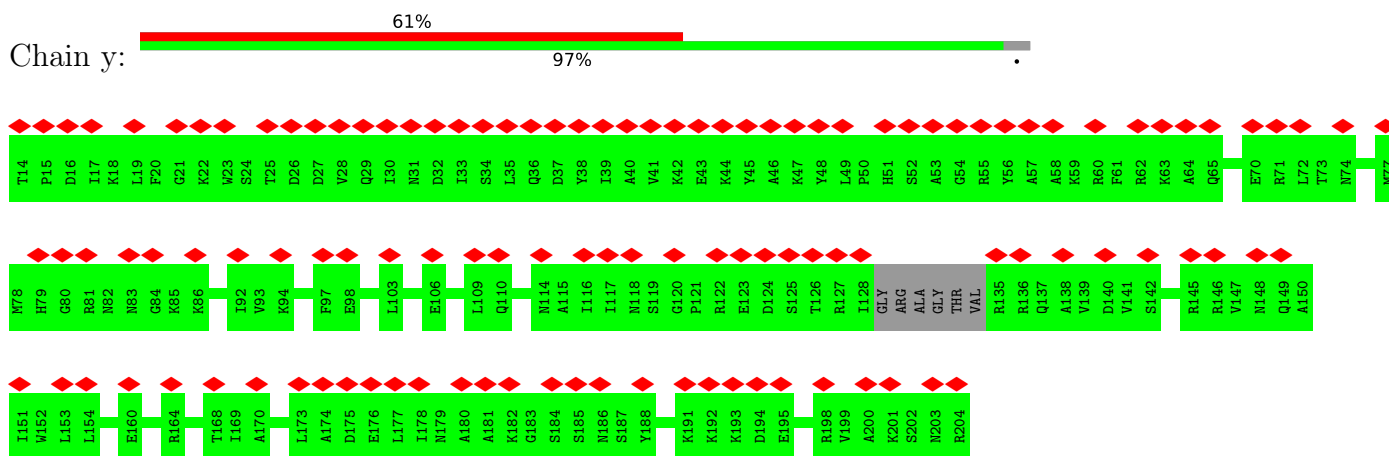
- Molecule 78: Ribosomal protein S3



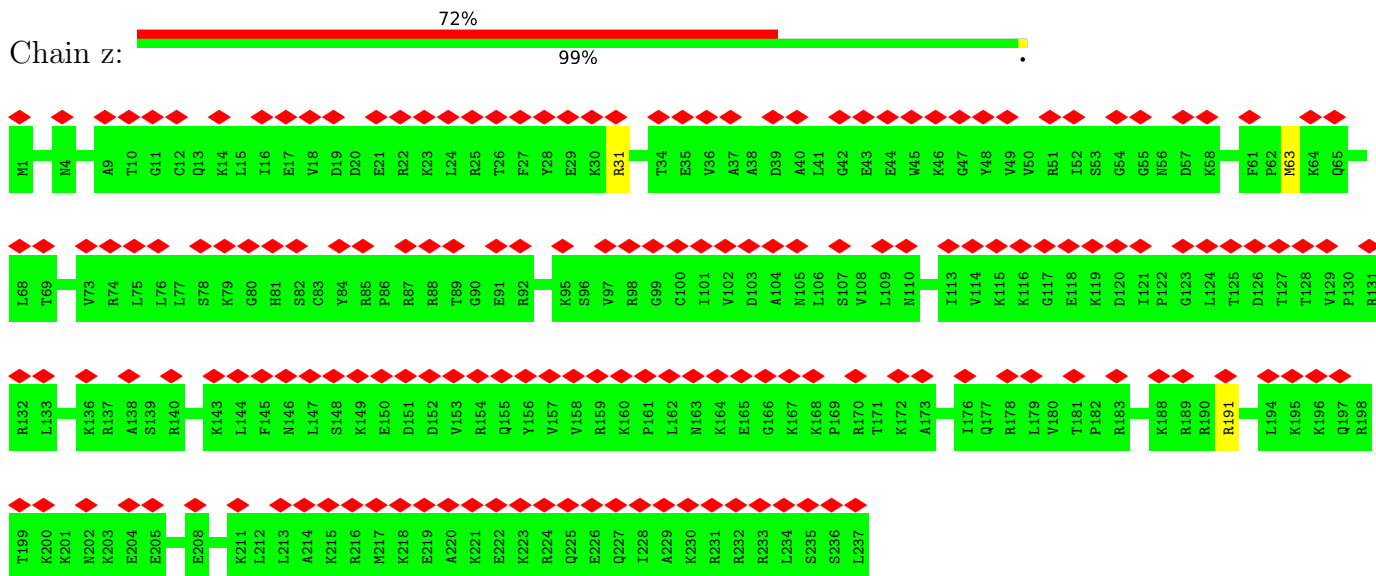
• Molecule 79: 40S ribosomal protein S4



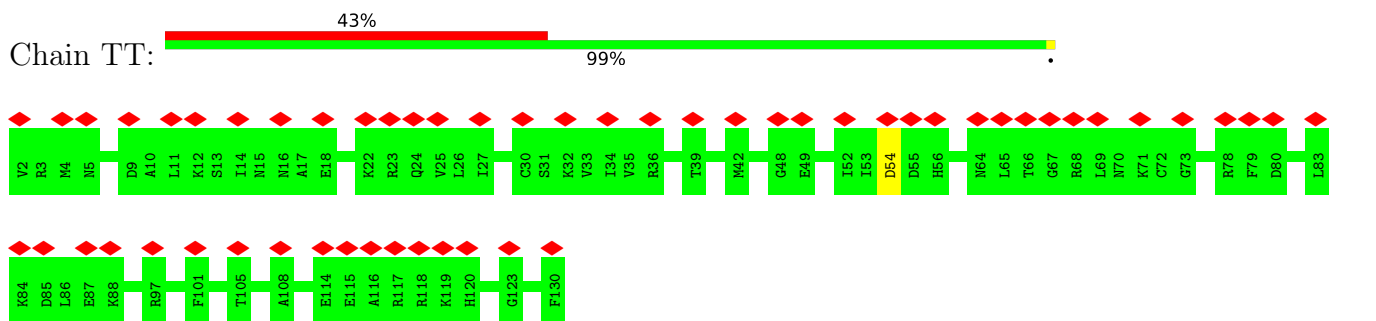
• Molecule 80: Ribosomal protein S5



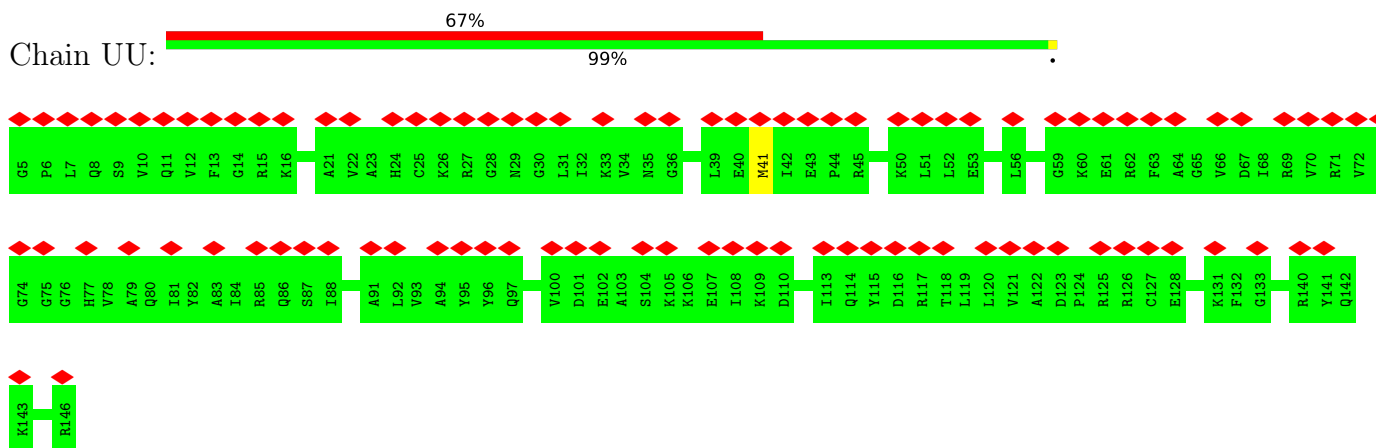
• Molecule 81: 40S ribosomal protein S6



• Molecule 82: Ribosomal protein S15a

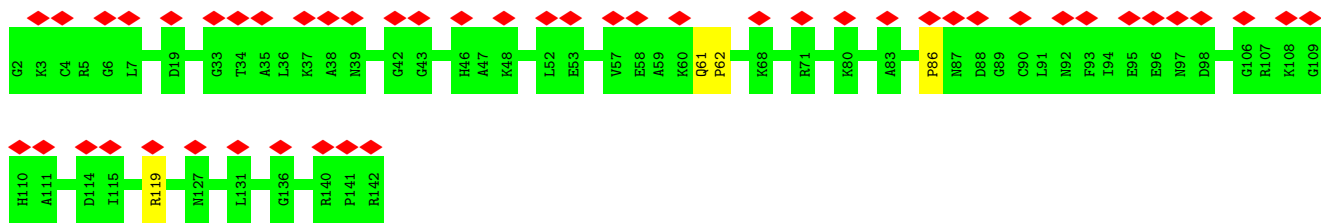


• Molecule 83: Ribosomal protein S16

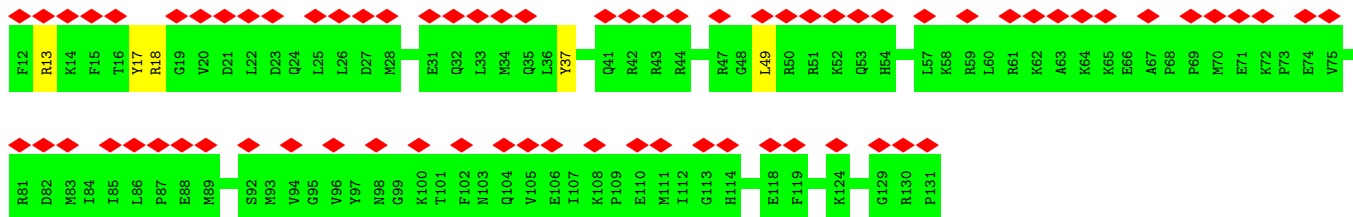


• Molecule 84: Ribosomal protein S23

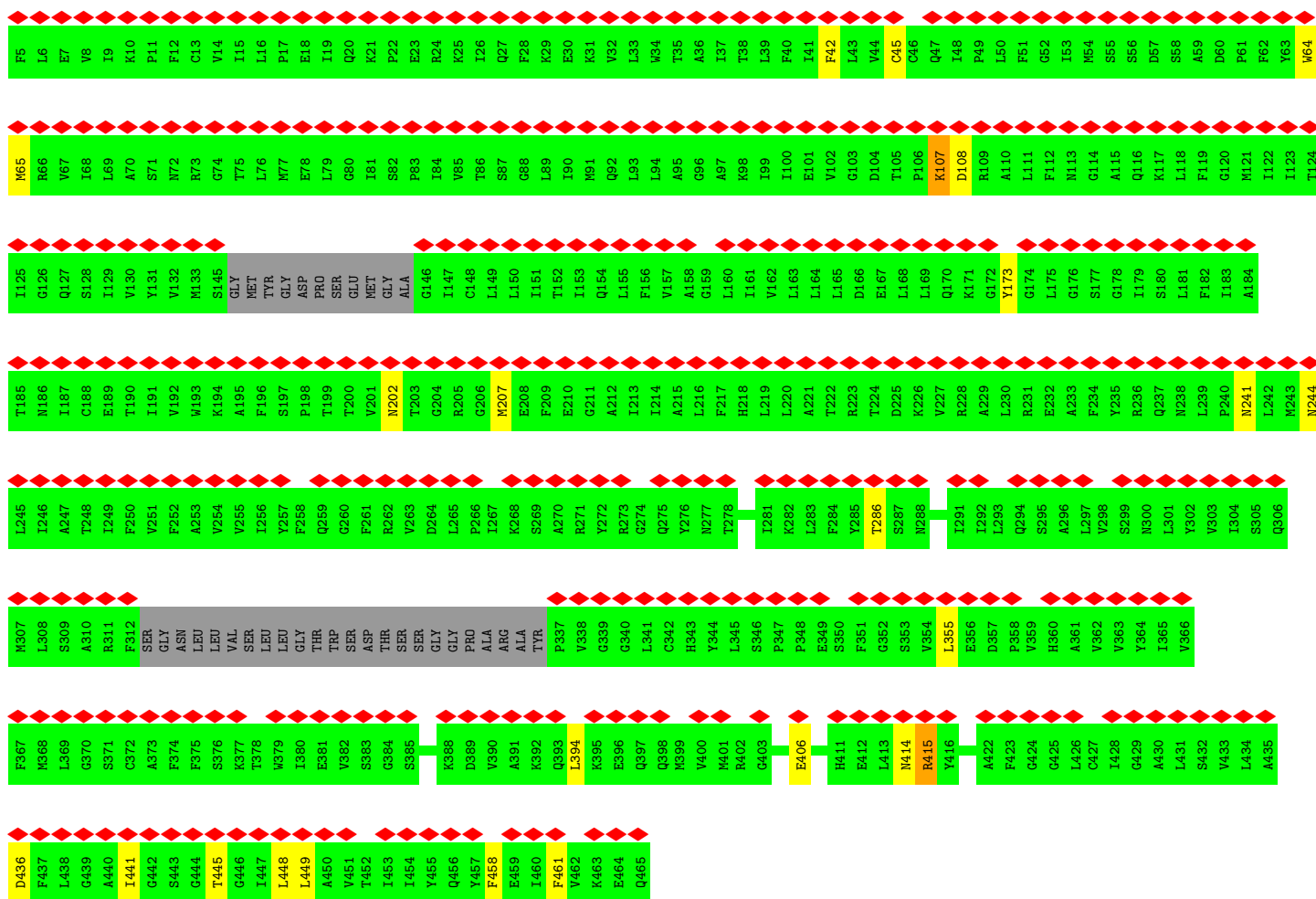
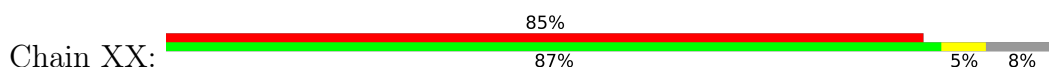




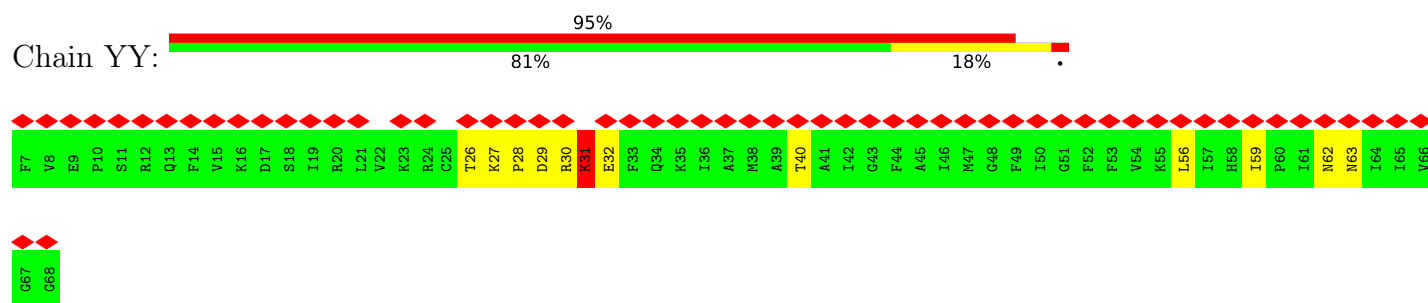
• Molecule 85: uS19



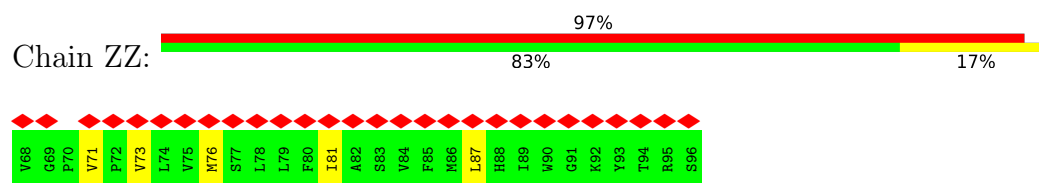
• Molecule 86: Protein transport protein Sec61 subunit alpha isoform 1



- Molecule 87: Protein transport protein Sec61 subunit gamma



- Molecule 88: Protein transport protein Sec61 subunit beta



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	12749	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	0.460	Depositor
Minimum map value	-0.305	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.08	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 i

5.1 Standard geometry i

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	AA	0.34	0/447	0.51	0/587
2	BB	0.33	0/1510	0.59	0/2022
3	CC	0.42	0/1715	0.60	1/2287 (0.0%)
4	DD	0.37	0/1550	0.59	0/2069
5	EE	0.45	0/1195	0.60	1/1597 (0.1%)
6	FF	0.35	0/490	0.57	0/656
7	GG	0.32	0/805	0.57	0/1081
8	HH	0.36	0/643	0.62	0/860
9	II	0.36	0/1208	0.60	0/1618
10	JJ	0.35	0/665	0.59	0/891
11	KK	0.31	0/1082	0.54	0/1452
12	LL	0.42	0/828	0.62	0/1109
13	MM	0.44	0/1029	0.64	1/1380 (0.1%)
14	0	0.30	0/567	0.55	0/753
15	1	0.47	0/216	0.80	0/298
16	2	0.63	2/1780 (0.1%)	1.06	14/2770 (0.5%)
17	3	0.53	0/1783	1.13	12/2773 (0.4%)
18	4	0.71	0/141	1.36	3/217 (1.4%)
19	5	1.05	19/84978 (0.0%)	1.30	964/132528 (0.7%)
20	6	0.29	0/2493	0.58	0/3394
21	7	1.03	0/2858	1.20	25/4455 (0.6%)
22	8	1.04	0/3581	1.24	29/5577 (0.5%)
23	9	0.40	0/470	0.51	0/623
24	NN	0.34	0/1028	0.54	0/1366
25	OO	0.33	0/604	0.58	0/810
26	PP	0.34	0/1115	0.56	0/1493
27	QQ	0.40	0/1226	0.59	1/1649 (0.1%)
28	RR	0.29	0/918	0.61	0/1233
29	A	0.62	0/1936	0.73	0/2596
30	B	0.56	0/3240	0.73	4/4339 (0.1%)
31	C	0.53	0/2937	0.67	2/3946 (0.1%)
32	D	0.51	0/2437	0.61	0/3264

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	E	0.49	2/1762 (0.1%)	0.69	3/2362 (0.1%)
34	F	0.55	0/1911	0.65	2/2549 (0.1%)
35	G	0.49	0/1910	0.69	1/2569 (0.0%)
36	H	0.51	0/1535	0.69	1/2063 (0.0%)
37	I	0.53	0/1702	0.61	0/2272
38	J	0.46	0/1385	0.66	0/1852
39	K	0.72	0/40531	1.21	397/63162 (0.6%)
40	L	0.50	0/1733	0.65	0/2316
41	M	0.51	0/1158	0.67	1/1547 (0.1%)
42	N	0.63	0/1746	0.70	0/2338
43	O	0.59	1/1662 (0.1%)	0.70	1/2222 (0.0%)
44	P	0.55	0/1268	0.70	1/1700 (0.1%)
45	Q	0.57	0/1539	0.71	0/2054
46	R	0.49	0/1524	0.69	0/2013
47	S	0.60	0/1501	0.65	0/2012
48	T	0.59	0/1326	0.63	0/1770
49	U	0.42	0/823	0.64	0/1104
50	V	0.58	0/993	0.70	0/1332
51	W	0.48	0/873	0.56	0/1158
52	X	0.50	1/984 (0.1%)	0.63	1/1323 (0.1%)
53	Y	0.53	0/1132	0.64	0/1504
54	Z	0.55	0/1130	0.66	0/1507
55	SS	0.31	0/834	0.62	1/1125 (0.1%)
56	a	0.61	0/1191	0.69	0/1590
57	b	0.40	0/861	0.56	0/1138
58	c	0.53	0/771	0.62	0/1034
59	d	0.55	0/903	0.68	0/1216
60	e	0.58	0/1071	0.67	1/1429 (0.1%)
61	f	0.63	0/895	0.75	2/1198 (0.2%)
62	g	0.54	0/916	0.68	0/1220
63	h	0.48	0/1021	0.60	0/1348
64	i	0.46	0/841	0.64	1/1112 (0.1%)
65	j	0.58	0/720	0.72	0/952
66	k	0.44	0/575	0.60	0/761
67	l	0.50	0/459	0.61	1/608 (0.2%)
68	m	0.57	0/435	0.67	1/575 (0.2%)
69	n	0.54	0/240	0.74	0/305
70	o	0.55	0/864	0.66	1/1140 (0.1%)
71	p	0.57	0/718	0.68	0/953
72	q	0.39	1/1747 (0.1%)	0.59	1/2374 (0.0%)
73	r	0.55	0/1010	0.73	1/1354 (0.1%)
74	s	0.29	0/1530	0.53	0/2064
75	t	0.27	0/1174	0.56	0/1582

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	u	0.41	0/1756	0.63	1/2350 (0.0%)
77	v	0.41	0/1753	0.61	0/2369
78	w	0.34	0/1796	0.60	1/2417 (0.0%)
79	x	0.35	0/2118	0.58	1/2849 (0.0%)
80	y	0.34	0/1492	0.58	0/2005
81	z	0.31	0/1946	0.57	0/2590
82	TT	0.42	0/1051	0.63	0/1406
83	UU	0.35	0/1146	0.61	0/1534
84	VV	0.41	0/1116	0.62	0/1490
85	WW	0.35	0/1017	0.59	1/1358 (0.1%)
86	XX	0.68	1/3379 (0.0%)	0.83	5/4572 (0.1%)
87	YY	0.47	0/504	0.73	1/673 (0.1%)
88	ZZ	0.42	0/236	0.74	0/321
All	All	0.79	27/235689 (0.0%)	1.07	1485/345434 (0.4%)

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	HH	0	1
9	II	0	1
30	B	0	1
31	C	0	1
33	E	0	1
34	F	0	1
35	G	0	1
40	L	0	1
41	M	0	1
42	N	0	3
47	S	0	1
57	b	0	1
59	d	0	1
72	q	0	1
73	r	0	1
82	TT	0	1
84	VV	0	1
85	WW	0	2
86	XX	0	3
87	YY	0	1
All	All	0	25

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	XX	107	LYS	C-N	26.26	1.94	1.34
16	2	7	G	C1'-N9	-7.47	1.36	1.46
19	5	2367	A	C6-N1	-6.84	1.30	1.35
19	5	3914	U	N3-C4	-6.18	1.32	1.38
43	O	27	VAL	CB-CG1	-6.16	1.40	1.52
19	5	1577	G	C2-N3	-6.00	1.27	1.32
33	E	165	VAL	CB-CG1	-5.85	1.40	1.52
19	5	1890	G	N9-C4	-5.79	1.33	1.38
19	5	4378	A	C6-N1	-5.69	1.31	1.35
19	5	2694	G	N9-C4	-5.69	1.33	1.38
16	2	66	C	C1'-N1	5.53	1.57	1.48
19	5	1337	A	N9-C4	-5.46	1.34	1.37
19	5	4579	U	C2-N3	5.42	1.41	1.37
19	5	3906	A	N9-C4	-5.41	1.34	1.37
19	5	2638	G	N9-C4	-5.28	1.33	1.38
19	5	4560	C	N3-C4	-5.28	1.30	1.33
19	5	2783	A	N9-C4	-5.26	1.34	1.37
19	5	4305	G	C2-N3	-5.26	1.28	1.32
19	5	4194	U	N3-C4	-5.18	1.33	1.38
33	E	178	VAL	CB-CG1	-5.15	1.42	1.52
19	5	3895	G	C2-N3	-5.14	1.28	1.32
19	5	4194	U	C2-N3	-5.13	1.34	1.37
19	5	3914	U	C4-O4	-5.09	1.19	1.23
72	q	197	VAL	C-N	-5.08	1.22	1.34
19	5	2638	G	C2-N3	-5.08	1.28	1.32
52	X	42	THR	C-N	-5.07	1.22	1.34
19	5	3914	U	C2-N3	-5.05	1.34	1.37

All (1485) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	5	3914	U	C5-C4-O4	21.58	138.85	125.90
19	5	2788	U	C5-C4-O4	21.53	138.82	125.90
19	5	2788	U	N3-C4-O4	-21.23	104.54	119.40
19	5	3914	U	N3-C4-O4	-20.58	104.99	119.40
86	XX	107	LYS	O-C-N	-15.28	98.25	122.70
19	5	4378	A	N1-C6-N6	-13.92	110.25	118.60
19	5	2367	A	N1-C6-N6	-13.67	110.40	118.60
39	K	501	C	N1-C2-O2	12.92	126.65	118.90
39	K	914	U	C5-C4-O4	-11.71	118.87	125.90
19	5	2505	C	C6-N1-C2	-11.52	115.69	120.30
19	5	1483	C	N1-C2-O2	11.26	125.66	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	K	914	U	C2-N1-C1'	10.93	130.81	117.70
19	5	2505	C	N1-C2-O2	10.90	125.44	118.90
39	K	501	C	C2-N1-C1'	10.81	130.70	118.80
19	5	4194	U	N3-C2-O2	-10.75	114.67	122.20
19	5	1236	C	C6-N1-C2	-10.70	116.02	120.30
19	5	1483	C	N3-C2-O2	-10.68	114.42	121.90
39	K	293	C	N1-C2-O2	10.64	125.29	118.90
19	5	2505	C	N3-C2-O2	-10.64	114.45	121.90
39	K	903	A	O5'-P-OP1	-10.31	96.42	105.70
19	5	704	C	N1-C2-O2	10.31	125.08	118.90
19	5	1237	C	N1-C2-O2	10.29	125.07	118.90
19	5	4303	C	N3-C2-O2	-10.24	114.73	121.90
19	5	704	C	C2-N1-C1'	10.13	129.94	118.80
19	5	4354	U	C5-C6-N1	10.11	127.75	122.70
19	5	2638	G	N3-C2-N2	-10.04	112.87	119.90
19	5	2627	C	N1-C2-O2	9.94	124.86	118.90
19	5	100	C	C2-N1-C1'	9.93	129.72	118.80
39	K	1139	C	N3-C2-O2	-9.93	114.95	121.90
39	K	1016	U	N1-C2-O2	9.87	129.71	122.80
19	5	2820	C	N1-C2-O2	9.82	124.79	118.90
19	5	417	G	O4'-C1'-N9	9.82	116.06	108.20
19	5	2022	C	N1-C2-O2	9.82	124.79	118.90
19	5	1237	C	N3-C2-O2	-9.82	115.03	121.90
39	K	1520	G	C8-N9-C4	-9.81	102.47	106.40
39	K	55	U	C2-N1-C1'	9.79	129.45	117.70
19	5	1483	C	C6-N1-C2	-9.77	116.39	120.30
39	K	1016	U	N3-C2-O2	-9.76	115.37	122.20
39	K	319	C	O5'-P-OP1	9.63	122.25	110.70
19	5	2783	A	C6-N1-C2	9.58	124.35	118.60
19	5	4354	U	C2-N1-C1'	9.57	129.18	117.70
39	K	501	C	N3-C2-O2	-9.55	115.22	121.90
19	5	4759	C	N1-C2-O2	9.50	124.60	118.90
19	5	2694	G	N3-C4-C5	9.49	133.35	128.60
39	K	1520	G	C2-N3-C4	9.46	116.63	111.90
19	5	1381	U	N3-C2-O2	-9.45	115.59	122.20
19	5	4928	C	N1-C2-O2	9.37	124.52	118.90
19	5	2638	G	N3-C4-N9	-9.36	120.39	126.00
39	K	1520	G	N3-C4-C5	-9.31	123.94	128.60
19	5	4241	C	N1-C2-O2	9.27	124.46	118.90
19	5	4413	C	N1-C2-O2	9.24	124.44	118.90
39	K	1139	C	C2-N1-C1'	9.24	128.96	118.80
19	5	1429	C	N1-C2-O2	9.21	124.43	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	5	4723	A	C6-N1-C2	-9.19	113.08	118.60
19	5	2410	C	C5-C6-N1	9.10	125.55	121.00
39	K	914	U	C6-N1-C1'	-9.09	108.48	121.20
19	5	2367	A	C5-C6-N6	9.07	130.96	123.70
19	5	4119	C	C2-N1-C1'	9.07	128.78	118.80
39	K	853	C	C2-N1-C1'	9.06	128.77	118.80
19	5	1612	G	N3-C4-N9	9.01	131.41	126.00
19	5	4413	C	C2-N1-C1'	9.00	128.71	118.80
19	5	2806	A	O4'-C1'-N9	9.00	115.40	108.20
19	5	4709	U	N1-C2-O2	8.98	129.09	122.80
86	XX	449	LEU	CA-CB-CG	-8.98	94.64	115.30
39	K	1303	C	C2-N1-C1'	8.95	128.64	118.80
19	5	1237	C	C6-N1-C2	-8.93	116.73	120.30
39	K	1139	C	N1-C2-O2	8.93	124.25	118.90
39	K	1453	C	C2-N1-C1'	8.92	128.62	118.80
19	5	2409	U	C4-C5-C6	8.89	125.04	119.70
19	5	1663	C	C5-C6-N1	8.89	125.45	121.00
39	K	1535	U	C2-N1-C1'	8.89	128.37	117.70
19	5	1483	C	C2-N1-C1'	8.84	128.52	118.80
19	5	481(A)	C	C6-N1-C2	-8.84	116.77	120.30
39	K	293	C	C2-N1-C1'	8.81	128.49	118.80
19	5	2022	C	N3-C2-O2	-8.80	115.74	121.90
19	5	1084	C	N1-C2-O2	8.78	124.17	118.90
19	5	2627	C	N3-C2-O2	-8.76	115.77	121.90
19	5	2627	C	C2-N1-C1'	8.70	128.37	118.80
39	K	853	C	N1-C2-O2	8.70	124.12	118.90
19	5	1639	U	C2-N1-C1'	8.68	128.12	117.70
39	K	293	C	N3-C2-O2	-8.65	115.85	121.90
19	5	1847	C	C6-N1-C2	-8.60	116.86	120.30
39	K	1865	C	C6-N1-C2	-8.59	116.86	120.30
39	K	1535	U	N1-C2-O2	8.58	128.81	122.80
39	K	1551	U	N3-C2-O2	-8.56	116.21	122.20
39	K	853	C	N3-C2-O2	-8.55	115.91	121.90
19	5	1978	C	N1-C2-O2	8.54	124.02	118.90
19	5	100	C	C6-N1-C2	-8.52	116.89	120.30
39	K	1060	A	O4'-C1'-N9	8.51	115.00	108.20
39	K	1303	C	N1-C2-O2	8.50	124.00	118.90
19	5	1639	U	N1-C2-O2	8.50	128.75	122.80
19	5	4243	C	C6-N1-C2	-8.50	116.90	120.30
39	K	537	C	C2-N1-C1'	8.50	128.15	118.80
19	5	4709	U	N3-C2-O2	-8.49	116.26	122.20
19	5	4759	C	N3-C2-O2	-8.47	115.97	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	K	1834	A	N7-C8-N9	8.45	118.03	113.80
19	5	4378	A	C5-C6-N6	8.43	130.44	123.70
39	K	1364	U	C2-N1-C1'	8.42	127.81	117.70
19	5	4560	C	C2-N1-C1'	8.42	128.06	118.80
19	5	4119	C	N1-C2-O2	8.41	123.94	118.90
19	5	4759	C	C2-N1-C1'	8.41	128.05	118.80
19	5	1381	U	C2-N1-C1'	8.38	127.76	117.70
19	5	4293	U	N3-C2-O2	-8.38	116.33	122.20
39	K	1624	U	C2-N1-C1'	8.38	127.76	117.70
19	5	4928	C	N3-C2-O2	-8.35	116.05	121.90
19	5	2820	C	N3-C2-O2	-8.35	116.06	121.90
19	5	1847	C	C5-C6-N1	8.33	125.17	121.00
19	5	4928	C	C2-N1-C1'	8.33	127.96	118.80
19	5	481(A)	C	N1-C2-O2	8.30	123.88	118.90
39	K	1139	C	C6-N1-C2	-8.28	116.99	120.30
39	K	1303	C	N3-C2-O2	-8.27	116.11	121.90
19	5	1237	C	C2-N1-C1'	8.26	127.88	118.80
39	K	853	C	C6-N1-C2	-8.23	117.01	120.30
19	5	2051	C	C6-N1-C2	-8.22	117.01	120.30
19	5	115	C	C2-N1-C1'	8.21	127.83	118.80
19	5	4562	C	C6-N1-C2	-8.21	117.02	120.30
39	K	314	U	N3-C2-O2	-8.19	116.46	122.20
19	5	1301	C	C6-N1-C2	-8.17	117.03	120.30
21	7	67	C	C6-N1-C2	-8.16	117.04	120.30
19	5	1552	G	O4'-C1'-N9	8.15	114.72	108.20
39	K	1453	C	N1-C2-O2	8.15	123.79	118.90
39	K	1551	U	N1-C2-O2	8.12	128.49	122.80
19	5	2410	C	C2-N1-C1'	8.12	127.73	118.80
19	5	1812	C	C6-N1-C2	-8.12	117.05	120.30
19	5	1384	C	C6-N1-C2	-8.11	117.06	120.30
19	5	4423	U	C2-N1-C1'	8.10	127.42	117.70
19	5	1309	C	C6-N1-C2	-8.10	117.06	120.30
39	K	356	C	C2-N1-C1'	8.10	127.70	118.80
19	5	220	C	C5-C6-N1	8.07	125.04	121.00
19	5	220	C	C6-N1-C2	-8.05	117.08	120.30
19	5	1484	G	C4-N9-C1'	8.04	136.94	126.50
39	K	1551	U	C2-N1-C1'	8.03	127.34	117.70
39	K	1274	G	N3-C4-N9	8.02	130.81	126.00
39	K	174	C	N3-C2-O2	-8.02	116.29	121.90
19	5	472	C	N1-C2-O2	7.96	123.68	118.90
39	K	1016	U	C2-N1-C1'	7.96	127.25	117.70
19	5	1835	G	O5'-P-OP2	-7.94	98.55	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	5	1977	C	N1-C2-O2	7.93	123.66	118.90
19	5	2638	G	N3-C4-C5	7.90	132.55	128.60
19	5	4423	U	N3-C2-O2	-7.89	116.68	122.20
39	K	427	U	C2-N1-C1'	7.88	127.15	117.70
19	5	220	C	C2-N1-C1'	7.87	127.46	118.80
19	5	1978	C	C2-N1-C1'	7.87	127.46	118.80
39	K	1274	G	N3-C4-C5	-7.86	124.67	128.60
39	K	1274	G	C4-N9-C1'	7.86	136.71	126.50
19	5	4758	U	C2-N1-C1'	7.85	127.12	117.70
19	5	1847	C	C2-N1-C1'	7.84	127.43	118.80
39	K	1453	C	C6-N1-C2	-7.83	117.17	120.30
22	8	21	C	N1-C2-O2	7.82	123.59	118.90
19	5	4229	U	N1-C2-O2	7.79	128.25	122.80
19	5	1612	G	N3-C4-C5	-7.79	124.71	128.60
19	5	4738	C	N1-C2-O2	7.78	123.57	118.90
19	5	1484	G	N3-C4-N9	7.77	130.66	126.00
39	K	1364	U	N1-C2-O2	7.77	128.24	122.80
19	5	704	C	C6-N1-C1'	-7.76	111.48	120.80
19	5	4241	C	N3-C2-O2	-7.76	116.47	121.90
19	5	4709	U	C2-N1-C1'	7.76	127.01	117.70
39	K	140	U	C2-N1-C1'	7.76	127.01	117.70
19	5	217	C	N1-C2-O2	7.76	123.56	118.90
19	5	1890	G	N3-C4-C5	7.75	132.48	128.60
19	5	1309	C	C5-C6-N1	7.75	124.87	121.00
39	K	943	U	C2-N1-C1'	7.75	127.00	117.70
19	5	3788	C	N1-C2-O2	7.75	123.55	118.90
19	5	3914	U	C4-C5-C6	-7.74	115.05	119.70
19	5	5050	C	N1-C2-O2	7.74	123.55	118.90
19	5	4653	C	C6-N1-C2	-7.74	117.20	120.30
19	5	3723	A	C6-N1-C2	-7.74	113.96	118.60
19	5	2505	C	C5-C6-N1	7.73	124.86	121.00
19	5	4880	C	N1-C2-O2	7.72	123.53	118.90
39	K	427	U	N3-C2-O2	-7.72	116.80	122.20
19	5	436	C	N3-C2-O2	-7.71	116.50	121.90
39	K	823	U	C2-N1-C1'	7.70	126.94	117.70
19	5	2367	A	N1-C2-N3	-7.69	125.45	129.30
19	5	1236	C	C5-C6-N1	7.68	124.84	121.00
39	K	980	A	C6-N1-C2	-7.67	114.00	118.60
39	K	55	U	N3-C2-O2	-7.63	116.86	122.20
19	5	3914	U	C2-N3-C4	7.63	131.58	127.00
19	5	2505	C	C2-N1-C1'	7.61	127.17	118.80
19	5	4206	C	C6-N1-C2	-7.61	117.26	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	5	1639	U	N3-C2-O2	-7.59	116.88	122.20
19	5	4579	U	C2-N3-C4	-7.58	122.45	127.00
39	K	55	U	N1-C2-O2	7.58	128.11	122.80
19	5	3657	U	N3-C2-O2	-7.58	116.90	122.20
39	K	537	C	N1-C2-O2	7.58	123.44	118.90
19	5	1210	C	N1-C2-O2	7.57	123.44	118.90
39	K	501	C	C6-N1-C1'	-7.56	111.72	120.80
19	5	1469	C	C6-N1-C2	-7.56	117.28	120.30
19	5	112	C	C2-N1-C1'	7.55	127.11	118.80
19	5	4303	C	N1-C2-O2	7.54	123.43	118.90
16	2	5	C	N1-C2-O2	7.54	123.43	118.90
22	8	35	C	C6-N1-C2	-7.54	117.29	120.30
39	K	1057	C	N3-C2-O2	-7.52	116.64	121.90
19	5	1612	G	C4-N9-C1'	7.50	136.25	126.50
17	3	63	C	N1-C2-O2	7.50	123.40	118.90
19	5	4869	U	C2-N1-C1'	7.50	126.70	117.70
39	K	823	U	N3-C2-O2	-7.50	116.95	122.20
39	K	1591	C	N1-C2-O2	7.50	123.40	118.90
19	5	1456	C	C6-N1-C2	-7.49	117.30	120.30
19	5	4562	C	C5-C6-N1	7.48	124.74	121.00
17	3	63	C	C6-N1-C2	-7.48	117.31	120.30
19	5	4293	U	N1-C2-O2	7.46	128.02	122.80
19	5	4314	C	N3-C2-O2	-7.45	116.69	121.90
19	5	2694	G	C4-C5-N7	7.44	113.77	110.80
39	K	1520	G	C4-N9-C1'	7.42	136.15	126.50
39	K	1535	U	N3-C2-O2	-7.42	117.00	122.20
19	5	1429	C	C6-N1-C2	-7.42	117.33	120.30
19	5	2409	U	C5-C6-N1	-7.42	118.99	122.70
19	5	1589	C	C6-N1-C2	-7.41	117.34	120.30
19	5	436	C	N1-C2-O2	7.41	123.34	118.90
19	5	4958	C	N1-C2-O2	7.40	123.34	118.90
19	5	1429	C	C2-N1-C1'	7.40	126.94	118.80
19	5	3672	G	N3-C4-N9	-7.39	121.57	126.00
39	K	356	C	N1-C2-O2	7.36	123.32	118.90
19	5	4461	C	C6-N1-C2	-7.36	117.36	120.30
19	5	4682	U	N3-C2-O2	-7.34	117.06	122.20
39	K	1520	G	N7-C8-N9	7.34	116.77	113.10
44	P	91	LEU	CA-CB-CG	7.34	132.19	115.30
39	K	945	U	C2-N1-C1'	7.34	126.51	117.70
39	K	1453	C	N3-C2-O2	-7.34	116.76	121.90
19	5	4303	C	C6-N1-C2	-7.34	117.36	120.30
39	K	1590	C	N1-C2-O2	7.33	123.30	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	5	1812	C	N1-C2-O2	7.33	123.30	118.90
21	7	67	C	C5-C6-N1	7.32	124.66	121.00
19	5	1429	C	C5-C6-N1	7.32	124.66	121.00
19	5	4948	C	C2-N1-C1'	7.32	126.85	118.80
19	5	1666	C	C6-N1-C2	-7.31	117.37	120.30
19	5	2716	C	C6-N1-C2	-7.31	117.38	120.30
19	5	4314	C	N1-C2-O2	7.31	123.29	118.90
19	5	4758	U	N3-C2-O2	-7.30	117.09	122.20
19	5	4880	C	C2-N1-C1'	7.30	126.83	118.80
19	5	4413	C	C6-N1-C1'	-7.29	112.05	120.80
19	5	495	C	N1-C2-O2	7.29	123.27	118.90
19	5	4233	A	O5'-P-OP1	-7.28	99.15	105.70
22	8	51	U	N3-C2-O2	-7.28	117.11	122.20
19	5	3935	C	C6-N1-C2	-7.28	117.39	120.30
86	XX	415	ARG	O-C-N	-7.27	111.07	122.70
39	K	1022	U	N1-C2-O2	7.26	127.88	122.80
39	K	914	U	C2-N3-C4	-7.26	122.64	127.00
21	7	29	C	N1-C2-O2	7.26	123.25	118.90
39	K	1057	C	C2-N1-C1'	7.24	126.76	118.80
19	5	2046	G	P-O3'-C3'	7.24	128.38	119.70
39	K	1315	U	N1-C2-O2	7.23	127.86	122.80
19	5	481(A)	C	C5-C6-N1	7.23	124.61	121.00
39	K	1261	C	C6-N1-C2	-7.23	117.41	120.30
19	5	1568	C	C6-N1-C2	-7.22	117.41	120.30
19	5	3848	U	N3-C2-O2	-7.22	117.15	122.20
19	5	4194	U	N1-C2-O2	7.22	127.85	122.80
19	5	2351	C	N1-C2-O2	7.21	123.22	118.90
19	5	481(A)	C	N3-C2-O2	-7.20	116.86	121.90
19	5	2627	C	C6-N1-C2	-7.19	117.42	120.30
22	8	150	C	N1-C2-O2	7.19	123.22	118.90
39	K	1022	U	C2-N1-C1'	7.18	126.32	117.70
19	5	2410	C	C6-N1-C2	-7.17	117.43	120.30
39	K	1130	G	O4'-C1'-N9	7.17	113.94	108.20
39	K	293	C	C6-N1-C2	-7.17	117.43	120.30
19	5	1579	C	C6-N1-C2	-7.16	117.44	120.30
19	5	980	U	C5-C6-N1	7.16	126.28	122.70
19	5	2568	C	N1-C2-O2	7.16	123.19	118.90
19	5	2850	A	C8-N9-C4	-7.15	102.94	105.80
19	5	115	C	N1-C2-O2	7.15	123.19	118.90
19	5	3775	A	O4'-C1'-N9	7.15	113.92	108.20
19	5	4318	C	C6-N1-C2	-7.15	117.44	120.30
19	5	4682	U	N1-C2-O2	7.15	127.80	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	K	1274	G	C8-N9-C1'	-7.15	117.71	127.00
19	5	1963	C	N1-C2-O2	7.14	123.19	118.90
19	5	125	C	C6-N1-C2	-7.14	117.44	120.30
19	5	1598	C	N1-C2-O2	7.13	123.18	118.90
19	5	2704	C	N3-C2-O2	-7.13	116.91	121.90
19	5	1884	C	N1-C2-O2	7.13	123.18	118.90
19	5	1469	C	N3-C2-O2	-7.13	116.91	121.90
39	K	630	U	C2-N1-C1'	7.13	126.25	117.70
19	5	217	C	C2-N1-C1'	7.12	126.64	118.80
19	5	1084	C	C2-N1-C1'	7.12	126.64	118.80
21	7	29	C	N3-C2-O2	-7.12	116.92	121.90
19	5	294	G	N3-C4-N9	7.11	130.27	126.00
19	5	77	U	N3-C2-O2	-7.11	117.22	122.20
39	K	632	C	C2-N1-C1'	7.11	126.62	118.80
19	5	1632	A	C2-N3-C4	7.10	114.15	110.60
39	K	1364	U	N3-C2-O2	-7.10	117.23	122.20
19	5	1484	G	C8-N9-C1'	-7.09	117.78	127.00
19	5	2035	C	C6-N1-C2	-7.09	117.46	120.30
39	K	632	C	C6-N1-C2	-7.09	117.46	120.30
22	8	11	C	C6-N1-C2	-7.08	117.47	120.30
16	2	5	C	C2-N1-C1'	7.08	126.59	118.80
39	K	570	C	N1-C2-O2	7.07	123.14	118.90
39	K	37	C	C6-N1-C2	-7.07	117.47	120.30
39	K	1316	C	N1-C2-O2	7.07	123.14	118.90
39	K	1624	U	N1-C2-O2	7.06	127.74	122.80
19	5	4747	C	C2-N1-C1'	7.05	126.56	118.80
19	5	2409	U	N1-C2-N3	7.05	119.13	114.90
19	5	1381	U	C6-N1-C2	-7.04	116.78	121.00
19	5	2008	U	C2-N1-C1'	7.04	126.14	117.70
30	B	309	LEU	CA-CB-CG	7.03	131.48	115.30
19	5	1084	C	C6-N1-C2	-7.03	117.49	120.30
19	5	2788	U	C4-C5-C6	-7.03	115.48	119.70
19	5	4880	C	N3-C2-O2	-7.01	116.99	121.90
39	K	943	U	C5-C4-O4	-7.01	121.69	125.90
19	5	4266	G	N3-C4-C5	-7.00	125.10	128.60
19	5	4925	U	OP2-P-O3'	7.00	120.61	105.20
30	B	214	ASP	CB-CG-OD1	7.00	124.60	118.30
19	5	4266	G	C4-N9-C1'	7.00	135.60	126.50
39	K	1518	C	C2-N1-C1'	7.00	126.50	118.80
39	K	1261	C	N1-C2-O2	7.00	123.10	118.90
19	5	2695	A	P-O3'-C3'	7.00	128.09	119.70
19	5	2603	C	C5-C6-N1	6.99	124.50	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	5	3767	C	C6-N1-C2	-6.99	117.50	120.30
19	5	4170	A	P-O3'-C3'	6.98	128.08	119.70
19	5	4177	C	C6-N1-C2	-6.98	117.51	120.30
39	K	501	C	C6-N1-C2	-6.97	117.51	120.30
39	K	130	G	N3-C4-N9	6.96	130.18	126.00
19	5	4229	U	N3-C2-O2	-6.96	117.33	122.20
19	5	2362	U	N3-C2-O2	-6.96	117.33	122.20
19	5	4758	U	N1-C2-O2	6.96	127.67	122.80
19	5	3895	G	N3-C2-N2	-6.95	115.03	119.90
39	K	1863	A	N7-C8-N9	6.94	117.27	113.80
19	5	2890	C	C6-N1-C2	-6.94	117.52	120.30
19	5	2802	C	C6-N1-C2	-6.94	117.52	120.30
39	K	1664	A	P-O3'-C3'	6.93	128.02	119.70
19	5	2489	C	N1-C2-O2	6.93	123.06	118.90
19	5	2802	C	C5-C6-N1	6.93	124.46	121.00
19	5	275	C	C6-N1-C2	-6.92	117.53	120.30
19	5	1502	G	N3-C4-C5	6.92	132.06	128.60
19	5	4258	C	C5-C6-N1	6.92	124.46	121.00
19	5	1890	G	N3-C4-N9	-6.92	121.85	126.00
19	5	1977	C	C5-C6-N1	6.91	124.46	121.00
19	5	2661	U	P-O3'-C3'	6.91	127.99	119.70
39	K	1123	C	C2-N1-C1'	6.91	126.40	118.80
22	8	51	U	N1-C2-O2	6.90	127.63	122.80
39	K	1389	C	C2-N1-C1'	6.89	126.38	118.80
19	5	4924	C	N3-C2-O2	-6.89	117.08	121.90
39	K	885	U	C2-N1-C1'	6.89	125.97	117.70
19	5	1084	C	N3-C2-O2	-6.88	117.09	121.90
19	5	4432	C	C6-N1-C2	-6.87	117.55	120.30
19	5	4241	C	C2-N1-C1'	6.86	126.34	118.80
19	5	1484	G	N3-C4-C5	-6.85	125.17	128.60
19	5	4305	G	N3-C2-N2	-6.84	115.11	119.90
19	5	100	C	N3-C2-O2	-6.84	117.11	121.90
19	5	4662	C	C6-N1-C2	-6.83	117.57	120.30
19	5	672	C	N1-C2-O2	6.83	123.00	118.90
19	5	2407	G	O5'-P-OP1	-6.83	99.55	105.70
19	5	3636	C	N1-C2-O2	6.83	123.00	118.90
39	K	1315	U	N3-C2-O2	-6.82	117.42	122.20
19	5	3636	C	C6-N1-C2	-6.81	117.58	120.30
19	5	1884	C	N3-C2-O2	-6.81	117.13	121.90
16	2	5	C	N3-C2-O2	-6.81	117.14	121.90
19	5	3927	U	N3-C2-O2	-6.80	117.44	122.20
19	5	1812	C	N3-C2-O2	-6.79	117.15	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	5	4476	C	C2-N1-C1'	6.78	126.26	118.80
39	K	1032	C	C6-N1-C2	-6.78	117.59	120.30
19	5	1477	C	C2-N1-C1'	6.78	126.25	118.80
19	5	1635	C	C6-N1-C2	-6.77	117.59	120.30
39	K	130	G	C4-N9-C1'	6.77	135.31	126.50
19	5	4354	U	C6-N1-C2	-6.77	116.94	121.00
19	5	1597	G	O4'-C1'-N9	6.77	113.62	108.20
19	5	1210	C	C2-N1-C1'	6.76	126.24	118.80
39	K	1057	C	N1-C2-O2	6.76	122.95	118.90
19	5	1429	C	N3-C2-O2	-6.75	117.17	121.90
19	5	1236	C	C6-N1-C1'	6.75	128.90	120.80
19	5	4302	U	N1-C2-O2	6.75	127.53	122.80
39	K	314	U	N1-C2-O2	6.75	127.53	122.80
39	K	1123	C	C6-N1-C2	-6.75	117.60	120.30
19	5	4303	C	C2-N1-C1'	6.75	126.22	118.80
39	K	1407	U	C2-N1-C1'	6.75	125.80	117.70
19	5	1514	U	N1-C2-O2	6.74	127.52	122.80
39	K	1564	C	C2-N1-C1'	6.74	126.22	118.80
39	K	943	U	C5-C6-N1	6.74	126.07	122.70
19	5	2740	U	N1-C2-O2	6.73	127.51	122.80
39	K	1081	U	N3-C2-O2	-6.72	117.49	122.20
19	5	3739	C	C2-N1-C1'	6.72	126.19	118.80
21	7	29	C	C6-N1-C2	-6.72	117.61	120.30
19	5	2013	A	C6-N1-C2	-6.72	114.57	118.60
19	5	704	C	N3-C2-O2	-6.71	117.20	121.90
19	5	3636	C	N3-C2-O2	-6.71	117.20	121.90
19	5	2704	C	N1-C2-O2	6.71	122.92	118.90
19	5	1340	C	C5-C6-N1	6.71	124.35	121.00
19	5	4709	U	C5-C6-N1	6.70	126.05	122.70
39	K	407	G	N3-C4-C5	-6.70	125.25	128.60
19	5	472	C	C2-N1-C1'	6.70	126.17	118.80
19	5	4302	U	N3-C2-O2	-6.70	117.51	122.20
39	K	199	C	N1-C2-O2	6.69	122.92	118.90
22	8	64	U	N3-C2-O2	-6.69	117.52	122.20
39	K	898	U	N1-C2-O2	6.68	127.48	122.80
39	K	1120	U	C2-N1-C1'	6.68	125.72	117.70
19	5	4354	U	N1-C2-O2	6.68	127.47	122.80
16	2	56	C	C2-N1-C1'	6.68	126.14	118.80
19	5	962	C	N1-C2-O2	6.67	122.91	118.90
19	5	1792	U	N3-C2-O2	-6.67	117.53	122.20
19	5	4254	G	N3-C4-C5	-6.67	125.26	128.60
39	K	303	C	N1-C2-O2	6.67	122.90	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	K	1111	U	N1-C2-O2	6.67	127.47	122.80
19	5	1210	C	N3-C2-O2	-6.67	117.23	121.90
19	5	4682	U	C2-N1-C1'	6.66	125.69	117.70
39	K	1721	U	C2-N1-C1'	6.66	125.69	117.70
19	5	4232	U	P-O3'-C3'	6.65	127.68	119.70
19	5	1612	G	C8-N9-C1'	-6.65	118.35	127.00
39	K	427	U	N1-C2-O2	6.65	127.46	122.80
19	5	2281	U	N1-C2-O2	6.65	127.45	122.80
21	7	26	C	C6-N1-C2	-6.65	117.64	120.30
19	5	4925	U	P-O3'-C3'	6.64	127.67	119.70
19	5	4958	C	C2-N1-C1'	6.63	126.10	118.80
19	5	4423	U	N1-C2-O2	6.63	127.44	122.80
39	K	823	U	N1-C2-O2	6.63	127.44	122.80
39	K	1315	U	C2-N1-C1'	6.63	125.65	117.70
19	5	1977	C	C6-N1-C2	-6.63	117.65	120.30
19	5	1663	C	C6-N1-C2	-6.62	117.65	120.30
19	5	1762	C	C6-N1-C2	-6.62	117.65	120.30
19	5	2716	C	C5-C6-N1	6.62	124.31	121.00
39	K	130	G	N3-C4-C5	-6.61	125.29	128.60
39	K	303	C	N3-C2-O2	-6.61	117.27	121.90
39	K	958	G	O4'-C1'-N9	6.61	113.49	108.20
39	K	188	C	C2-N1-C1'	6.61	126.07	118.80
39	K	407	G	C4-N9-C1'	6.61	135.09	126.50
39	K	735	C	C6-N1-C2	-6.61	117.66	120.30
19	5	1978	C	N3-C2-O2	-6.60	117.28	121.90
19	5	3680	U	N1-C2-O2	6.60	127.42	122.80
39	K	1111	U	C2-N1-C1'	6.60	125.62	117.70
39	K	1846	G	N9-C4-C5	-6.60	102.76	105.40
19	5	3914	U	N1-C2-O2	6.59	127.42	122.80
19	5	2740	U	N3-C2-O2	-6.59	117.59	122.20
39	K	1116	C	N1-C2-O2	6.59	122.85	118.90
19	5	4119	C	C6-N1-C1'	-6.58	112.90	120.80
19	5	1496	G	N9-C4-C5	6.58	108.03	105.40
19	5	696	C	P-O3'-C3'	6.58	127.59	119.70
39	K	55	U	C6-N1-C1'	-6.58	112.00	121.20
33	E	52	LEU	CA-CB-CG	6.57	130.41	115.30
19	5	2547	G	O5'-P-OP1	-6.56	99.79	105.70
39	K	885	U	N3-C2-O2	-6.56	117.61	122.20
39	K	1111	U	N3-C2-O2	-6.56	117.61	122.20
39	K	1842	C	O5'-P-OP2	-6.56	99.80	105.70
19	5	1496	G	N3-C4-N9	-6.55	122.07	126.00
19	5	217	C	N3-C2-O2	-6.55	117.31	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	5	3767	C	C5-C6-N1	6.55	124.28	121.00
39	K	688	U	P-O3'-C3'	6.55	127.56	119.70
19	5	4261	C	C6-N1-C2	-6.54	117.68	120.30
16	2	56	C	N1-C2-O2	6.54	122.83	118.90
19	5	1568	C	N1-C2-O2	6.54	122.83	118.90
19	5	2069	A	O5'-P-OP1	-6.54	99.81	105.70
21	7	28	C	C6-N1-C2	-6.54	117.68	120.30
19	5	1812	C	C2-N1-C1'	6.54	126.00	118.80
39	K	903	A	C5'-C4'-O4'	6.54	116.95	109.10
39	K	814	U	N3-C2-O2	-6.54	117.62	122.20
39	K	1261	C	N3-C2-O2	-6.54	117.32	121.90
39	K	1599	U	N3-C2-O2	-6.54	117.62	122.20
19	5	1215	C	N1-C2-O2	6.54	122.82	118.90
39	K	980	A	C5-C6-N1	6.53	120.97	117.70
39	K	885	U	N1-C2-O2	6.52	127.37	122.80
19	5	1671	U	N3-C2-O2	-6.52	117.64	122.20
39	K	973	C	N1-C2-O2	6.52	122.81	118.90
19	5	41	C	C6-N1-C2	-6.51	117.69	120.30
19	5	1072	C	P-O3'-C3'	6.51	127.52	119.70
19	5	3840	U	N3-C2-O2	-6.51	117.64	122.20
39	K	752	G	P-O3'-C3'	6.51	127.52	119.70
16	2	5	C	C6-N1-C2	-6.51	117.70	120.30
39	K	1261	C	C2-N1-C1'	6.51	125.96	118.80
19	5	1325	C	N3-C2-O2	-6.51	117.35	121.90
19	5	4237	C	N1-C2-O2	6.51	122.80	118.90
19	5	3788	C	N3-C2-O2	-6.50	117.35	121.90
19	5	3694	U	C2-N1-C1'	6.50	125.50	117.70
19	5	1179	U	N1-C2-O2	6.50	127.35	122.80
19	5	115	C	N3-C2-O2	-6.49	117.35	121.90
19	5	4266	G	N3-C4-N9	6.49	129.90	126.00
19	5	974	C	N3-C2-O2	-6.48	117.36	121.90
19	5	1597	G	N1-C6-O6	-6.48	116.01	119.90
19	5	4119	C	N3-C2-O2	-6.48	117.37	121.90
19	5	1853	G	C4-N9-C1'	6.47	134.92	126.50
39	K	1834	A	C8-N9-C4	-6.47	103.21	105.80
19	5	134	G	P-O3'-C3'	6.47	127.46	119.70
19	5	3602	C	C5-C6-N1	6.46	124.23	121.00
39	K	183	G	C4-N9-C1'	6.46	134.90	126.50
19	5	2799	G	C6-C5-N7	-6.46	126.53	130.40
21	7	39	C	C6-N1-C2	-6.46	117.72	120.30
39	K	1683	C	N1-C2-O2	6.45	122.77	118.90
19	5	1282	G	C8-N9-C4	-6.45	103.82	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	5	658	C	N1-C2-O2	6.44	122.76	118.90
19	5	282	C	N1-C2-O2	6.44	122.76	118.90
21	7	94	C	N1-C2-O2	6.43	122.76	118.90
19	5	2267	U	C2-N1-C1'	6.43	125.42	117.70
19	5	1329	G	C8-N9-C4	-6.43	103.83	106.40
19	5	1607	C	N3-C2-O2	-6.42	117.40	121.90
19	5	2281	U	N3-C2-O2	-6.42	117.71	122.20
19	5	41	C	C5-C6-N1	6.42	124.21	121.00
19	5	4237	C	C5-C6-N1	6.42	124.21	121.00
19	5	4579	U	N1-C2-N3	6.42	118.75	114.90
19	5	661	C	C2-N1-C1'	6.41	125.86	118.80
19	5	4723	A	C5-C6-N1	6.41	120.91	117.70
19	5	4305	G	N1-C2-N2	6.41	121.97	116.20
19	5	1628	C	C6-N1-C2	-6.40	117.74	120.30
19	5	1179	U	C2-N1-C1'	6.40	125.38	117.70
39	K	898	U	N3-C2-O2	-6.40	117.72	122.20
19	5	1674	C	C6-N1-C2	-6.40	117.74	120.30
19	5	1339	U	C5-C6-N1	6.40	125.90	122.70
19	5	4560	C	C4-C5-C6	6.40	120.60	117.40
19	5	2502	A	OP1-P-O3'	6.39	119.27	105.20
39	K	371	A	O5'-P-OP2	-6.39	99.95	105.70
19	5	3914	U	N1-C2-N3	-6.39	111.07	114.90
19	5	100	C	O4'-C1'-N1	6.38	113.31	108.20
19	5	2638	G	C2-N3-C4	-6.38	108.71	111.90
19	5	4241	C	C6-N1-C2	-6.38	117.75	120.30
39	K	1464	C	N1-C2-O2	6.38	122.73	118.90
39	K	1721	U	N1-C2-O2	6.38	127.27	122.80
19	5	1411(B)	C	C5-C6-N1	6.38	124.19	121.00
19	5	2528	G	C4-N9-C1'	6.38	134.79	126.50
39	K	872	A	C2-N3-C4	6.37	113.79	110.60
19	5	1963	C	C2-N1-C1'	6.37	125.81	118.80
19	5	977	C	N3-C2-O2	-6.36	117.45	121.90
19	5	3602	C	C6-N1-C2	-6.36	117.75	120.30
39	K	537	C	C6-N1-C1'	-6.36	113.17	120.80
19	5	1381	U	N1-C2-O2	6.35	127.25	122.80
19	5	1910	G	C4-N9-C1'	6.35	134.76	126.50
19	5	4305	G	C4-N9-C1'	6.35	134.75	126.50
39	K	1118	C	C2-N1-C1'	6.35	125.78	118.80
39	K	1057	C	C6-N1-C2	-6.35	117.76	120.30
39	K	1309	C	C5-C6-N1	6.34	124.17	121.00
39	K	1834	A	C5-N7-C8	-6.34	100.73	103.90
21	7	102	U	N1-C2-O2	6.34	127.24	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	5	3672	G	N3-C4-C5	6.33	131.77	128.60
19	5	1445	U	C5-C6-N1	6.33	125.87	122.70
17	3	13	C	C6-N1-C2	-6.33	117.77	120.30
19	5	1662	C	C6-N1-C2	-6.33	117.77	120.30
19	5	2068	C	OP1-P-O3'	6.32	119.11	105.20
19	5	1	C	N1-C2-O2	6.32	122.69	118.90
39	K	1863	A	O4'-C1'-N9	6.32	113.25	108.20
86	XX	448	LEU	CA-CB-CG	6.32	129.82	115.30
19	5	4926	C	C2-N1-C1'	6.31	125.75	118.80
19	5	4254	G	C2-N3-C4	6.31	115.06	111.90
39	K	1123	C	N1-C2-O2	6.31	122.69	118.90
19	5	4162	C	C2-N1-C1'	6.31	125.74	118.80
39	K	1303	C	C6-N1-C2	-6.30	117.78	120.30
19	5	4215	C	N1-C2-O2	6.30	122.68	118.90
19	5	1514	U	C2-N1-C1'	6.30	125.26	117.70
39	K	814	U	N1-C2-O2	6.30	127.21	122.80
19	5	2856	C	C6-N1-C2	-6.29	117.78	120.30
19	5	4118	U	N3-C2-O2	-6.29	117.79	122.20
19	5	1612	G	C6-C5-N7	-6.29	126.62	130.40
19	5	2653	C	C6-N1-C2	-6.29	117.78	120.30
39	K	630	U	N1-C2-O2	6.29	127.20	122.80
19	5	2532	C	C2-N1-C1'	6.29	125.72	118.80
19	5	4069	U	N1-C2-O2	6.29	127.20	122.80
21	7	57	C	C5-C6-N1	6.29	124.14	121.00
17	3	63	C	N3-C2-O2	-6.29	117.50	121.90
22	8	128	C	N1-C2-O2	6.29	122.67	118.90
39	K	630	U	N3-C2-O2	-6.29	117.80	122.20
19	5	4635	A	N7-C8-N9	6.29	116.94	113.80
19	5	3775	A	N7-C8-N9	6.28	116.94	113.80
19	5	4736	C	C2-N1-C1'	6.28	125.71	118.80
19	5	495	C	N3-C2-O2	-6.28	117.50	121.90
19	5	521	C	C6-N1-C2	-6.28	117.79	120.30
39	K	1591	C	N3-C2-O2	-6.28	117.51	121.90
19	5	2068	C	P-O3'-C3'	6.27	127.23	119.70
19	5	4970	C	C6-N1-C2	-6.27	117.79	120.30
19	5	1577	G	C2-N3-C4	6.27	115.03	111.90
31	C	322	LEU	CA-CB-CG	6.27	129.71	115.30
19	5	4703	U	N3-C2-O2	-6.26	117.81	122.20
19	5	2890	C	C5-C6-N1	6.26	124.13	121.00
39	K	407	G	N3-C4-N9	6.26	129.76	126.00
39	K	1535	U	C6-N1-C1'	-6.26	112.44	121.20
19	5	100	C	C6-N1-C1'	-6.25	113.30	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	K	1637	A	P-O3'-C3'	6.25	127.20	119.70
17	3	63	C	C5-C6-N1	6.24	124.12	121.00
19	5	469	C	N1-C2-O2	6.24	122.64	118.90
64	i	33	LEU	CA-CB-CG	6.24	129.65	115.30
39	K	872	A	C5-C6-N1	6.24	120.82	117.70
19	5	3637	U	N3-C2-O2	-6.24	117.83	122.20
39	K	632	C	C5-C6-N1	6.24	124.12	121.00
19	5	2791	C	C6-N1-C2	-6.23	117.81	120.30
19	5	5008	C	C6-N1-C2	-6.23	117.81	120.30
19	5	1282	G	N7-C8-N9	6.23	116.21	113.10
19	5	4215	C	N3-C2-O2	-6.23	117.54	121.90
19	5	2787	A	N3-C4-N9	6.22	132.38	127.40
19	5	2694	G	N3-C4-N9	-6.22	122.27	126.00
39	K	402	C	C6-N1-C2	-6.22	117.81	120.30
39	K	1624	U	N3-C2-O2	-6.22	117.84	122.20
19	5	1977	C	C2-N1-C1'	6.22	125.64	118.80
17	3	74	C	C2-N1-C1'	6.22	125.64	118.80
19	5	4747	C	N1-C2-O2	6.22	122.63	118.90
19	5	4341	C	C6-N1-C2	-6.21	117.81	120.30
22	8	2	G	C4-N9-C1'	6.21	134.58	126.50
41	M	57	LEU	CA-CB-CG	6.21	129.59	115.30
39	K	1358	U	N3-C2-O2	-6.21	117.85	122.20
19	5	1485	C	C2-N1-C1'	6.21	125.63	118.80
19	5	1735	U	C5-C6-N1	6.21	125.80	122.70
39	K	1271	C	N1-C2-O2	6.21	122.62	118.90
19	5	322	C	C5-C6-N1	6.20	124.10	121.00
19	5	65	A	C5-C6-N1	6.20	120.80	117.70
18	4	44	U	C2-N1-C1'	6.20	125.14	117.70
19	5	3657	U	N1-C2-O2	6.19	127.14	122.80
19	5	2528	G	N3-C4-N9	6.19	129.72	126.00
19	5	1214	C	N1-C2-O2	6.19	122.61	118.90
39	K	1620	A	O4'-C1'-N9	6.19	113.15	108.20
19	5	1295	U	N3-C2-O2	-6.19	117.87	122.20
39	K	453	C	N1-C2-O2	6.18	122.61	118.90
16	2	32	C	N1-C2-O2	6.18	122.61	118.90
19	5	4183	G	N3-C4-C5	-6.18	125.51	128.60
19	5	1483	C	C5-C6-N1	6.18	124.09	121.00
19	5	661	C	C6-N1-C2	-6.18	117.83	120.30
19	5	2568	C	N3-C2-O2	-6.18	117.58	121.90
19	5	1687	U	N1-C2-O2	6.17	127.12	122.80
19	5	2267	U	N1-C2-O2	6.17	127.12	122.80
39	K	530	U	C2-N1-C1'	6.17	125.10	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	K	1863	A	C8-N9-C4	-6.17	103.33	105.80
19	5	1579	C	C5-C6-N1	6.17	124.08	121.00
19	5	1792	U	C2-N1-C1'	6.16	125.10	117.70
19	5	1848	C	C6-N1-C2	-6.16	117.83	120.30
19	5	1081	C	N1-C2-O2	6.16	122.59	118.90
19	5	2783	A	N1-C2-N3	-6.16	126.22	129.30
39	K	1590	C	N3-C2-O2	-6.16	117.59	121.90
39	K	579	C	N1-C2-O2	6.15	122.59	118.90
19	5	4698	C	N1-C2-O2	6.15	122.59	118.90
19	5	2470	C	N1-C2-O2	6.15	122.59	118.90
19	5	4518	A	P-O3'-C3'	6.15	127.08	119.70
39	K	1757	G	C4-N9-C1'	6.15	134.49	126.50
39	K	119	U	N3-C2-O2	-6.14	117.90	122.20
39	K	1721	U	N3-C2-O2	-6.14	117.90	122.20
19	5	49	U	N1-C2-O2	6.14	127.10	122.80
19	5	472	C	N3-C2-O2	-6.14	117.60	121.90
39	K	501	C	C5-C6-N1	6.13	124.07	121.00
19	5	4980	C	C5-C6-N1	6.13	124.07	121.00
39	K	1309	C	C2-N1-C1'	6.13	125.54	118.80
39	K	1401	A	C6-N1-C2	-6.13	114.92	118.60
19	5	1325	C	N1-C2-O2	6.12	122.57	118.90
19	5	1633	G	P-O3'-C3'	6.12	127.05	119.70
39	K	1518	C	N1-C2-O2	6.12	122.57	118.90
19	5	294	G	C2-N3-C4	6.12	114.96	111.90
19	5	2266	C	P-O3'-C3'	6.12	127.04	119.70
19	5	1906	U	N3-C2-O2	-6.12	117.92	122.20
39	K	1259	A	C2-N3-C4	6.12	113.66	110.60
19	5	1853	G	C8-N9-C1'	-6.12	119.05	127.00
19	5	696	C	OP2-P-O3'	6.11	118.65	105.20
19	5	4579	U	C2-N1-C1'	6.11	125.03	117.70
19	5	1411(B)	C	C6-N1-C2	-6.11	117.86	120.30
19	5	4958	C	N3-C2-O2	-6.10	117.63	121.90
19	5	4177	C	C5-C6-N1	6.10	124.05	121.00
19	5	4560	C	N3-C2-O2	-6.10	117.63	121.90
19	5	1986	U	C2-N3-C4	-6.10	123.34	127.00
19	5	238	C	C6-N1-C2	-6.09	117.86	120.30
19	5	2089	G	P-O3'-C3'	6.09	127.01	119.70
17	3	8	U	C2-N1-C1'	6.09	125.01	117.70
19	5	2856	C	C5-C6-N1	6.09	124.05	121.00
19	5	4752	U	N1-C2-O2	6.09	127.06	122.80
19	5	1906	U	N1-C2-O2	6.09	127.06	122.80
19	5	2062	C	C6-N1-C2	-6.09	117.87	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	5	3690	U	N3-C2-O2	-6.08	117.94	122.20
19	5	4431	U	N1-C2-O2	6.08	127.06	122.80
19	5	683	C	N1-C2-O2	6.08	122.55	118.90
39	K	1303	C	C6-N1-C1'	-6.08	113.51	120.80
19	5	124	C	C6-N1-C2	-6.08	117.87	120.30
19	5	1589	C	C5-C6-N1	6.07	124.04	121.00
19	5	2008	U	N1-C2-O2	6.07	127.05	122.80
19	5	964	A	N7-C8-N9	6.07	116.83	113.80
16	2	13	C	N3-C2-O2	-6.06	117.66	121.90
19	5	1340	C	C6-N1-C2	-6.06	117.88	120.30
19	5	1910	G	C8-N9-C1'	-6.06	119.12	127.00
19	5	100	C	N1-C2-O2	6.06	122.53	118.90
39	K	1846	G	C4-C5-N7	6.05	113.22	110.80
39	K	1047	C	C6-N1-C2	-6.05	117.88	120.30
19	5	4980	C	C6-N1-C2	-6.05	117.88	120.30
19	5	2303	C	C6-N1-C2	-6.04	117.88	120.30
19	5	4560	C	C6-N1-C1'	-6.04	113.55	120.80
39	K	119	U	N1-C2-O2	6.04	127.03	122.80
39	K	850	C	N1-C2-O2	6.04	122.53	118.90
19	5	3690	U	N1-C2-O2	6.04	127.03	122.80
22	8	128	C	N3-C2-O2	-6.04	117.67	121.90
19	5	4155	C	N1-C2-O2	6.04	122.52	118.90
39	K	146	G	C5-C6-O6	6.04	132.22	128.60
19	5	2704	C	C6-N1-C2	-6.03	117.89	120.30
19	5	48	G	P-O3'-C3'	6.03	126.94	119.70
19	5	3926	C	C6-N1-C2	-6.03	117.89	120.30
19	5	322	C	C6-N1-C2	-6.03	117.89	120.30
19	5	2560	C	N1-C2-O2	6.03	122.52	118.90
19	5	49	U	N3-C2-O2	-6.02	117.99	122.20
19	5	1327	C	C6-N1-C2	-6.02	117.89	120.30
19	5	2661	U	OP1-P-O3'	6.02	118.44	105.20
39	K	973	C	C5-C6-N1	6.02	124.01	121.00
39	K	914	U	O4'-C1'-N1	6.01	113.01	108.20
19	5	4305	G	C8-N9-C4	-6.01	104.00	106.40
19	5	1807	C	C6-N1-C2	-6.00	117.90	120.30
19	5	1084	C	C5-C6-N1	6.00	124.00	121.00
19	5	4365	C	C6-N1-C2	-6.00	117.90	120.30
39	K	1518	C	N3-C2-O2	-6.00	117.70	121.90
19	5	2838	G	C4-N9-C1'	5.99	134.29	126.50
19	5	4409	C	C6-N1-C2	-5.99	117.90	120.30
39	K	356	C	C6-N1-C1'	-5.99	113.61	120.80
19	5	3709	U	N3-C2-O2	-5.99	118.01	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	5	365	U	N1-C2-O2	5.99	126.99	122.80
19	5	4958	C	C6-N1-C2	-5.99	117.91	120.30
19	5	1883	G	C4-C5-N7	5.98	113.19	110.80
19	5	4258	C	C6-N1-C2	-5.98	117.91	120.30
39	K	1529	C	C5-C6-N1	5.98	123.99	121.00
19	5	2694	G	C5-N7-C8	-5.98	101.31	104.30
19	5	220	C	N1-C2-O2	5.98	122.48	118.90
19	5	201	C	C6-N1-C2	-5.97	117.91	120.30
19	5	4165	C	C2-N1-C1'	5.97	125.37	118.80
39	K	1625	U	C2-N1-C1'	5.97	124.86	117.70
19	5	1204	C	N1-C2-O2	5.97	122.48	118.90
21	7	14	C	C5-C6-N1	5.96	123.98	121.00
19	5	449	C	P-O3'-C3'	5.96	126.85	119.70
19	5	4448	G	P-O3'-C3'	5.96	126.85	119.70
19	5	4928	C	C6-N1-C2	-5.96	117.92	120.30
19	5	276	C	C6-N1-C2	-5.95	117.92	120.30
39	K	216	C	C6-N1-C2	-5.95	117.92	120.30
19	5	1978	C	C6-N1-C2	-5.95	117.92	120.30
21	7	94	C	N3-C2-O2	-5.95	117.73	121.90
39	K	1336	C	C6-N1-C2	-5.95	117.92	120.30
19	5	495	C	C6-N1-C2	-5.95	117.92	120.30
19	5	152	U	N3-C2-O2	-5.94	118.04	122.20
30	B	17	LEU	CB-CG-CD2	-5.94	100.90	111.00
16	2	49	C	C6-N1-C2	-5.94	117.92	120.30
19	5	3866	C	C5-C6-N1	5.94	123.97	121.00
39	K	1314	U	C2-N1-C1'	5.94	124.82	117.70
19	5	4360	U	N3-C2-O2	-5.93	118.05	122.20
39	K	1708	C	C6-N1-C2	-5.93	117.93	120.30
19	5	1446	C	N1-C2-O2	5.93	122.46	118.90
19	5	1310	C	C6-N1-C2	-5.93	117.93	120.30
19	5	3650	C	C6-N1-C2	-5.93	117.93	120.30
19	5	1514	U	C5-C6-N1	5.92	125.66	122.70
39	K	902	G	C4'-C3'-O3'	5.92	124.85	113.00
19	5	922(B)	C	P-O3'-C3'	5.92	126.81	119.70
19	5	4354	U	N3-C2-O2	-5.92	118.05	122.20
19	5	4431	U	N3-C2-O2	-5.92	118.06	122.20
19	5	1295	U	N1-C2-O2	5.92	126.94	122.80
19	5	3636	C	C5-C6-N1	5.92	123.96	121.00
19	5	1179	U	N3-C2-O2	-5.92	118.06	122.20
39	K	1022	U	N3-C2-O2	-5.92	118.06	122.20
19	5	1568	C	C5-C6-N1	5.91	123.95	121.00
33	E	215	LEU	CA-CB-CG	5.91	128.88	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	5	661	C	C5-C6-N1	5.90	123.95	121.00
19	5	4497	U	N1-C2-N3	5.90	118.44	114.90
39	K	120	U	N3-C2-O2	-5.90	118.07	122.20
73	r	32	LEU	CA-CB-CG	5.90	128.86	115.30
19	5	1639	U	C6-N1-C1'	-5.89	112.95	121.20
19	5	469	C	C6-N1-C2	-5.89	117.94	120.30
39	K	1358	U	N1-C2-O2	5.89	126.92	122.80
19	5	1568	C	N3-C2-O2	-5.89	117.78	121.90
19	5	1966	C	N1-C2-O2	5.89	122.43	118.90
39	K	1078	C	C6-N1-C2	-5.89	117.95	120.30
19	5	2699	C	C6-N1-C2	-5.88	117.95	120.30
19	5	3823	G	N7-C8-N9	5.88	116.04	113.10
21	7	29	C	C2-N1-C1'	5.88	125.27	118.80
39	K	1775	U	C5-C6-N1	5.88	125.64	122.70
19	5	4237	C	C6-N1-C2	-5.88	117.95	120.30
19	5	228	C	C6-N1-C2	-5.87	117.95	120.30
19	5	1929	A	C4-N9-C1'	5.87	136.87	126.30
22	8	4	C	C5-C6-N1	5.87	123.94	121.00
39	K	199	C	C2-N1-C1'	5.87	125.26	118.80
19	5	115	C	C6-N1-C1'	-5.87	113.76	120.80
19	5	1804	A	P-O3'-C3'	5.86	126.73	119.70
19	5	4413	C	N3-C2-O2	-5.86	117.80	121.90
39	K	37	C	C5-C6-N1	5.86	123.93	121.00
19	5	365	U	N3-C2-O2	-5.86	118.10	122.20
39	K	853	C	C5-C6-N1	5.85	123.93	121.00
19	5	1789	C	C2-N1-C1'	5.85	125.24	118.80
19	5	1977	C	N3-C2-O2	-5.85	117.80	121.90
19	5	2867	C	C2-N1-C1'	5.85	125.24	118.80
19	5	4350	C	C6-N1-C2	-5.85	117.96	120.30
19	5	4940	C	N1-C2-O2	5.85	122.41	118.90
39	K	1123	C	C5-C6-N1	5.85	123.92	121.00
19	5	2788	U	C2-N3-C4	5.85	130.51	127.00
39	K	983	A	N3-C4-N9	5.84	132.07	127.40
19	5	2267	U	N3-C2-O2	-5.83	118.12	122.20
19	5	2615	C	N1-C2-O2	5.83	122.40	118.90
19	5	4887	C	N1-C2-O2	5.83	122.40	118.90
39	K	317	C	C2-N1-C1'	5.83	125.21	118.80
39	K	494	C	N1-C2-O2	5.83	122.40	118.90
43	O	16	LEU	CA-CB-CG	5.83	128.71	115.30
21	7	28	C	N3-C2-O2	-5.83	117.82	121.90
31	C	289	LEU	CA-CB-CG	5.83	128.70	115.30
39	K	903	A	O4'-C1'-N9	5.83	112.86	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	5	1929	A	C2-N3-C4	5.82	113.51	110.60
19	5	3723	A	C5-C6-N1	5.82	120.61	117.70
19	5	4759	C	C6-N1-C1'	-5.82	113.82	120.80
19	5	1598	C	N3-C2-O2	-5.82	117.83	121.90
19	5	3844	U	N1-C2-O2	5.81	126.87	122.80
68	m	59	LEU	CA-CB-CG	5.81	128.67	115.30
19	5	126	C	C5-C6-N1	5.81	123.90	121.00
39	K	1713	C	C6-N1-C2	-5.81	117.98	120.30
19	5	4869	U	O4'-C1'-N1	5.80	112.84	108.20
39	K	1078	C	C2-N1-C1'	5.80	125.19	118.80
19	5	4067	U	C5-C6-N1	5.80	125.60	122.70
30	B	17	LEU	CA-CB-CG	5.79	128.62	115.30
19	5	4712	C	C6-N1-C2	-5.79	117.98	120.30
19	5	180	C	C5-C6-N1	5.79	123.89	121.00
19	5	1602	U	N3-C2-O2	-5.79	118.15	122.20
19	5	4948	C	N3-C2-O2	-5.79	117.85	121.90
19	5	4747	C	C5-C6-N1	5.78	123.89	121.00
19	5	1735	U	C6-N1-C2	-5.78	117.53	121.00
39	K	1636	G	C4-N9-C1'	5.78	134.01	126.50
19	5	77	U	N1-C2-O2	5.78	126.84	122.80
39	K	356	C	N3-C2-O2	-5.78	117.86	121.90
39	K	659	G	C4-N9-C1'	5.78	134.01	126.50
87	YY	56	LEU	CA-CB-CG	5.78	128.58	115.30
19	5	294	G	N3-C4-C5	-5.77	125.71	128.60
19	5	1079	C	N1-C2-O2	5.77	122.36	118.90
19	5	2410	C	N1-C2-O2	5.77	122.36	118.90
19	5	974	C	N1-C2-O2	5.77	122.36	118.90
19	5	1484	G	C6-C5-N7	-5.77	126.94	130.40
39	K	1683	C	C6-N1-C2	-5.77	117.99	120.30
39	K	151	C	C6-N1-C2	-5.76	118.00	120.30
19	5	4728	U	N1-C2-O2	5.76	126.83	122.80
19	5	1665	C	C6-N1-C2	-5.76	118.00	120.30
19	5	2077	C	C6-N1-C2	-5.76	118.00	120.30
19	5	4476	C	C6-N1-C2	-5.76	118.00	120.30
67	l	49	LEU	CA-CB-CG	5.75	128.53	115.30
39	K	124	U	N1-C2-O2	5.75	126.83	122.80
19	5	1411(C)	C	C5-C6-N1	5.75	123.87	121.00
39	K	1752	C	C2-N1-C1'	5.75	125.12	118.80
39	K	1704	C	C6-N1-C2	-5.75	118.00	120.30
39	K	1624	U	C6-N1-C1'	-5.74	113.16	121.20
19	5	1237	C	C5-C6-N1	5.74	123.87	121.00
19	5	2500	U	N1-C2-O2	5.74	126.82	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	K	1752	C	N1-C2-O2	5.74	122.34	118.90
19	5	57	G	C5-C6-O6	5.74	132.04	128.60
39	K	1564	C	N1-C2-O2	5.74	122.34	118.90
39	K	1660	C	C2-N1-C1'	5.74	125.11	118.80
19	5	201	C	C5-C6-N1	5.73	123.87	121.00
19	5	1413	C	N3-C2-O2	-5.73	117.89	121.90
19	5	2022	C	C6-N1-C2	-5.73	118.01	120.30
19	5	3847	C	N1-C2-O2	5.73	122.34	118.90
19	5	4378	A	N1-C2-N3	-5.73	126.43	129.30
19	5	1585	C	C6-N1-C2	-5.73	118.01	120.30
39	K	570	C	N3-C2-O2	-5.73	117.89	121.90
19	5	266	C	O5'-P-OP2	-5.73	100.54	105.70
19	5	3935	C	C5-C6-N1	5.73	123.86	121.00
22	8	28	C	C6-N1-C2	-5.73	118.01	120.30
19	5	1370	G	P-O3'-C3'	5.72	126.57	119.70
39	K	130	G	C8-N9-C1'	-5.72	119.56	127.00
19	5	196	C	C6-N1-C2	-5.72	118.01	120.30
39	K	1389	C	C6-N1-C2	-5.72	118.01	120.30
19	5	934	C	N1-C2-O2	5.71	122.33	118.90
22	8	2	G	N3-C4-C5	-5.71	125.74	128.60
19	5	4943	A	O5'-P-OP1	-5.71	100.56	105.70
19	5	1413	C	N1-C2-O2	5.71	122.33	118.90
19	5	3882	C	N1-C2-O2	5.71	122.33	118.90
39	K	35	C	C6-N1-C2	-5.71	118.02	120.30
19	5	217	C	P-O3'-C3'	5.71	126.55	119.70
19	5	4360	U	N1-C2-O2	5.71	126.79	122.80
21	7	102	U	N3-C2-O2	-5.71	118.21	122.20
19	5	289	C	C5-C6-N1	5.70	123.85	121.00
19	5	294	G	C5-C6-O6	-5.70	125.18	128.60
33	E	289	LEU	CA-CB-CG	5.70	128.41	115.30
39	K	1520	G	N3-C4-N9	5.70	129.42	126.00
19	5	1301	C	N3-C2-O2	-5.70	117.91	121.90
19	5	4949	G	O4'-C1'-N9	5.70	112.76	108.20
19	5	1675	C	N3-C2-O2	-5.69	117.92	121.90
19	5	4635	A	C8-N9-C4	-5.69	103.52	105.80
19	5	1694	C	C6-N1-C2	-5.69	118.02	120.30
19	5	4254	G	C8-N9-C4	-5.69	104.12	106.40
19	5	4738	C	C2-N1-C1'	5.69	125.06	118.80
19	5	959	G	P-O3'-C3'	5.68	126.52	119.70
19	5	3657	U	C2-N1-C1'	5.68	124.52	117.70
19	5	3788	C	C6-N1-C2	-5.68	118.03	120.30
39	K	1316	C	N3-C2-O2	-5.68	117.92	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	K	1591	C	C6-N1-C2	-5.68	118.03	120.30
19	5	914	U	O4'-C1'-N1	5.68	112.74	108.20
19	5	2667	C	N1-C2-O2	5.67	122.31	118.90
39	K	314	U	C2-N1-C1'	5.67	124.51	117.70
19	5	2492	C	C6-N1-C2	-5.67	118.03	120.30
19	5	1481	C	N1-C2-O2	5.67	122.30	118.90
19	5	5050	C	N3-C2-O2	-5.67	117.93	121.90
39	K	1362	U	N3-C2-O2	-5.67	118.23	122.20
19	5	4476	C	N3-C2-O2	-5.67	117.93	121.90
19	5	2787	A	C4-N9-C1'	5.67	136.50	126.30
19	5	1991	A	O5'-P-OP1	5.66	117.50	110.70
39	K	1852	C	C5-C6-N1	5.66	123.83	121.00
19	5	4199	C	C6-N1-C2	-5.66	118.03	120.30
39	K	1022	U	C6-N1-C1'	-5.66	113.27	121.20
39	K	1139	C	C6-N1-C1'	-5.66	114.01	120.80
39	K	1664	A	OP1-P-O3'	5.66	117.65	105.20
39	K	659	G	C8-N9-C1'	-5.66	119.64	127.00
19	5	1936	C	C6-N1-C2	-5.66	118.04	120.30
39	K	974	C	C6-N1-C2	-5.66	118.04	120.30
61	f	88	PHE	CB-CG-CD1	5.65	124.76	120.80
19	5	1915	C	C2-N1-C1'	5.65	125.02	118.80
19	5	4719	G	OP1-P-O3'	5.65	117.63	105.20
19	5	1384	C	C5-C6-N1	5.65	123.82	121.00
19	5	4635	A	C5-N7-C8	-5.65	101.08	103.90
39	K	140	U	N1-C2-O2	5.65	126.75	122.80
39	K	606	G	C4-N9-C1'	5.65	133.84	126.50
39	K	142	C	N1-C2-O2	5.65	122.29	118.90
39	K	958	G	C6-C5-N7	-5.65	127.01	130.40
72	q	197	VAL	C-N-CA	5.65	135.81	121.70
19	5	1893	C	C2-N1-C1'	5.64	125.01	118.80
19	5	2772	C	C5-C6-N1	5.64	123.82	121.00
19	5	481(A)	C	C2-N1-C1'	5.64	125.01	118.80
19	5	2783	A	C5-C6-N1	-5.64	114.88	117.70
19	5	469	C	C2-N1-C1'	5.64	125.00	118.80
19	5	704	C	C5-C6-N1	5.64	123.82	121.00
19	5	289	C	N1-C2-O2	5.63	122.28	118.90
19	5	2838	G	C8-N9-C1'	-5.63	119.67	127.00
19	5	1	C	C2-N1-C1'	5.63	124.99	118.80
19	5	1762	C	C5-C6-N1	5.63	123.81	121.00
39	K	1261	C	C5-C6-N1	5.63	123.81	121.00
19	5	117	C	N1-C2-O2	5.63	122.28	118.90
19	5	2072	C	C5-C6-N1	5.63	123.81	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	5	4653	C	C5-C6-N1	5.63	123.81	121.00
39	K	870	A	P-O3'-C3'	5.63	126.45	119.70
19	5	3680	U	C5-C6-N1	5.62	125.51	122.70
39	K	1729	U	N1-C2-O2	5.62	126.74	122.80
39	K	1081	U	N1-C2-O2	5.62	126.73	122.80
19	5	2489	C	N3-C2-O2	-5.62	117.97	121.90
22	8	124	U	P-O3'-C3'	5.62	126.44	119.70
19	5	3672	G	N3-C2-N2	-5.61	115.97	119.90
19	5	4948	C	N1-C2-O2	5.61	122.27	118.90
19	5	1735	U	C2-N1-C1'	5.61	124.44	117.70
39	K	1757	G	N3-C4-N9	5.61	129.37	126.00
19	5	96	U	N3-C2-O2	-5.61	118.27	122.20
19	5	282	C	N3-C2-O2	-5.61	117.98	121.90
19	5	1308	C	C5-C6-N1	5.61	123.80	121.00
19	5	1411(C)	C	C6-N1-C2	-5.61	118.06	120.30
19	5	4759	C	C6-N1-C2	-5.61	118.06	120.30
19	5	2409	U	C2-N3-C4	-5.60	123.64	127.00
39	K	293	C	C6-N1-C1'	-5.60	114.08	120.80
19	5	1936	C	C2-N1-C1'	5.60	124.96	118.80
22	8	51	U	C2-N1-C1'	5.60	124.42	117.70
19	5	57	G	N3-C4-N9	-5.60	122.64	126.00
39	K	1061	U	P-O3'-C3'	5.60	126.42	119.70
19	5	112	C	C6-N1-C2	-5.59	118.06	120.30
19	5	1607	C	C6-N1-C2	-5.59	118.06	120.30
19	5	1893	C	N1-C2-O2	5.59	122.25	118.90
39	K	983	A	C5-C6-N1	5.59	120.50	117.70
22	8	2	G	N3-C4-N9	5.59	129.35	126.00
39	K	1453	C	C5-C6-N1	5.58	123.79	121.00
22	8	32	C	N3-C2-O2	-5.58	117.99	121.90
19	5	1540	C	C6-N1-C2	-5.58	118.07	120.30
19	5	2422	C	N1-C2-O2	5.58	122.25	118.90
19	5	14	C	C6-N1-C2	-5.58	118.07	120.30
19	5	345	C	C5-C6-N1	5.58	123.79	121.00
19	5	4928	C	C6-N1-C1'	-5.58	114.11	120.80
39	K	666	U	C5-C6-N1	5.58	125.49	122.70
19	5	1204	C	N3-C2-O2	-5.57	118.00	121.90
39	K	872	A	C6-N1-C2	-5.57	115.26	118.60
39	K	1834	A	N1-C2-N3	5.57	132.09	129.30
39	K	687	C	C2-N1-C1'	5.57	124.93	118.80
19	5	1477	C	C5-C6-N1	5.57	123.78	121.00
19	5	1671	U	C5-C6-N1	5.56	125.48	122.70
19	5	2351	C	C2-N1-C1'	5.56	124.92	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	5	2439	G	N3-C4-N9	5.56	129.34	126.00
21	7	28	C	N1-C2-O2	5.56	122.24	118.90
39	K	453	C	C2-N1-C1'	5.56	124.92	118.80
39	K	1660	C	N1-C2-O2	5.56	122.23	118.90
19	5	1481	C	C2-N1-C1'	5.55	124.91	118.80
19	5	2818	C	C6-N1-C2	-5.55	118.08	120.30
39	K	183	G	O4'-C1'-N9	5.55	112.64	108.20
19	5	2540	C	C6-N1-C2	-5.55	118.08	120.30
19	5	2528	G	C8-N9-C1'	-5.55	119.79	127.00
39	K	1696	C	C6-N1-C2	-5.55	118.08	120.30
39	K	293	C	C5-C6-N1	5.55	123.77	121.00
39	K	752	G	OP1-P-O3'	5.55	117.40	105.20
19	5	978	G	C2-N3-C4	-5.54	109.13	111.90
19	5	4738	C	N3-C2-O2	-5.54	118.02	121.90
39	K	407	G	C2-N3-C4	5.54	114.67	111.90
19	5	3673	C	C2-N1-C1'	5.54	124.90	118.80
19	5	2035	C	C5-C6-N1	5.54	123.77	121.00
19	5	2351	C	C5-C6-N1	5.54	123.77	121.00
39	K	872	A	N3-C4-N9	5.54	131.83	127.40
39	K	1684	C	N1-C2-O2	5.54	122.22	118.90
39	K	174	C	N1-C2-O2	5.54	122.22	118.90
39	K	1331	C	C2-N1-C1'	5.54	124.89	118.80
19	5	1325	C	C6-N1-C2	-5.53	118.09	120.30
19	5	1210	C	C6-N1-C2	-5.53	118.09	120.30
19	5	4305	G	C2-N3-C4	5.53	114.66	111.90
39	K	872	A	P-O3'-C3'	5.52	126.33	119.70
19	5	2356	U	N3-C2-O2	-5.52	118.33	122.20
19	5	2772	C	N1-C2-O2	5.52	122.21	118.90
19	5	112	C	C5-C6-N1	5.52	123.76	121.00
19	5	962	C	N3-C2-O2	-5.51	118.04	121.90
19	5	2627	C	C6-N1-C1'	-5.51	114.18	120.80
39	K	20	G	N1-C6-O6	-5.51	116.59	119.90
39	K	850	C	N3-C2-O2	-5.51	118.04	121.90
19	5	4266	G	C8-N9-C4	-5.51	104.20	106.40
39	K	853	C	C6-N1-C1'	-5.51	114.19	120.80
39	K	973	C	C6-N1-C2	-5.51	118.09	120.30
19	5	205	C	N1-C2-O2	5.51	122.20	118.90
19	5	672	C	N3-C2-O2	-5.51	118.05	121.90
39	K	1636	G	N7-C8-N9	5.51	115.85	113.10
19	5	323	C	C6-N1-C2	-5.50	118.10	120.30
16	2	56	C	N3-C2-O2	-5.50	118.05	121.90
19	5	2454	U	N3-C2-O2	-5.50	118.35	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	5	4189	U	C5-C6-N1	5.50	125.45	122.70
19	5	4577	U	N3-C2-O2	-5.50	118.35	122.20
19	5	4698	C	N3-C2-O2	-5.50	118.05	121.90
39	K	1032	C	C5-C6-N1	5.50	123.75	121.00
39	K	140	U	N3-C2-O2	-5.50	118.35	122.20
19	5	1572	U	C5-C6-N1	5.50	125.45	122.70
39	K	1410	C	C2-N1-C1'	5.49	124.84	118.80
39	K	1453	C	C6-N1-C1'	-5.49	114.21	120.80
19	5	86	U	N3-C2-O2	-5.49	118.36	122.20
19	5	2572	C	C6-N1-C2	-5.49	118.11	120.30
19	5	4254	G	P-O3'-C3'	5.49	126.28	119.70
19	5	1993	C	C2-N1-C1'	5.49	124.83	118.80
19	5	4114	C	C2-N1-C1'	5.49	124.83	118.80
19	5	13	U	N3-C2-O2	-5.48	118.36	122.20
19	5	96	U	N1-C2-O2	5.48	126.64	122.80
19	5	2568	C	C2-N1-C1'	5.48	124.83	118.80
19	5	941	C	C6-N1-C2	-5.48	118.11	120.30
39	K	182	C	P-O3'-C3'	5.48	126.27	119.70
39	K	958	G	C4-N9-C1'	5.48	133.62	126.50
19	5	13	U	N1-C2-O2	5.48	126.63	122.80
19	5	2013	A	N1-C6-N6	-5.48	115.31	118.60
39	K	914	U	N3-C4-O4	5.48	123.23	119.40
19	5	521	C	N3-C2-O2	-5.47	118.07	121.90
19	5	2362	U	N1-C2-O2	5.47	126.63	122.80
39	K	1130	G	N3-C4-N9	5.47	129.28	126.00
39	K	1775	U	C2-N1-C1'	5.47	124.27	117.70
19	5	326	C	C6-N1-C2	-5.47	118.11	120.30
22	8	1	C	N1-C2-O2	5.47	122.18	118.90
39	K	465	A	P-O3'-C3'	5.47	126.27	119.70
39	K	1116	C	N3-C2-O2	-5.47	118.07	121.90
39	K	1753	C	C6-N1-C2	-5.47	118.11	120.30
39	K	1846	G	N3-C4-N9	5.47	129.28	126.00
19	5	3703	G	N3-C4-C5	-5.47	125.86	128.60
39	K	1683	C	N3-C2-O2	-5.47	118.07	121.90
19	5	1633	G	OP1-P-O3'	5.47	117.23	105.20
17	3	72	C	N1-C2-O2	5.46	122.18	118.90
19	5	1310	C	C5-C6-N1	5.46	123.73	121.00
39	K	1116	C	C2-N1-C1'	5.46	124.81	118.80
39	K	1237	C	C6-N1-C2	-5.46	118.11	120.30
39	K	1314	U	C5-C6-N1	5.46	125.43	122.70
19	5	4114	C	N1-C2-O2	5.46	122.18	118.90
39	K	1865	C	C2-N1-C1'	5.46	124.81	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	5	976	G	N7-C8-N9	5.46	115.83	113.10
19	5	3910	C	N3-C2-O2	-5.46	118.08	121.90
39	K	790	C	N1-C2-O2	5.46	122.17	118.90
22	8	141	C	C6-N1-C2	-5.46	118.12	120.30
39	K	537	C	C5-C6-N1	5.46	123.73	121.00
19	5	4948	C	C6-N1-C1'	-5.45	114.26	120.80
39	K	1364	U	C6-N1-C1'	-5.45	113.57	121.20
19	5	3892	U	N3-C2-O2	-5.45	118.39	122.20
22	8	37	A	N1-C2-N3	-5.45	126.58	129.30
39	K	26	U	C5-C6-N1	5.45	125.42	122.70
39	K	1729	U	C2-N1-C1'	5.45	124.24	117.70
19	5	323	C	C5-C6-N1	5.45	123.72	121.00
19	5	436	C	C6-N1-C2	-5.45	118.12	120.30
19	5	4069	U	C2-N1-C1'	5.45	124.23	117.70
27	QQ	84	LEU	CA-CB-CG	5.44	127.82	115.30
19	5	4354	U	C6-N1-C1'	-5.44	113.58	121.20
19	5	1797	G	N3-C4-N9	5.44	129.26	126.00
19	5	1812	C	C5-C6-N1	5.44	123.72	121.00
39	K	4	C	C6-N1-C2	-5.44	118.12	120.30
39	K	872	A	C5-C6-N6	-5.44	119.35	123.70
19	5	3919	C	C6-N1-C2	-5.44	118.12	120.30
19	5	48	G	O4'-C1'-N9	5.44	112.55	108.20
19	5	278	G	O4'-C1'-N9	-5.44	103.85	108.20
19	5	2474	G	P-O3'-C3'	5.44	126.23	119.70
19	5	3882	C	N3-C2-O2	-5.44	118.09	121.90
19	5	50	C	C6-N1-C2	-5.43	118.13	120.30
19	5	4766	C	C2-N1-C1'	5.43	124.78	118.80
19	5	4243	C	C2-N1-C1'	5.43	124.77	118.80
19	5	1796	U	N3-C2-O2	-5.43	118.40	122.20
19	5	3781	C	C6-N1-C2	-5.43	118.13	120.30
19	5	2803	U	N1-C2-O2	5.43	126.60	122.80
19	5	5001	U	N3-C2-O2	-5.42	118.40	122.20
39	K	199	C	N3-C2-O2	-5.42	118.10	121.90
39	K	1309	C	C6-N1-C2	-5.42	118.13	120.30
19	5	100	C	C5-C6-N1	5.42	123.71	121.00
19	5	4206	C	C2-N1-C1'	5.42	124.77	118.80
19	5	4241	C	C5-C6-N1	5.42	123.71	121.00
19	5	4869	U	N3-C2-O2	-5.42	118.41	122.20
39	K	1683	C	C2-N1-C1'	5.42	124.76	118.80
19	5	57	G	N1-C6-O6	-5.42	116.65	119.90
19	5	1494	U	N3-C2-O2	-5.42	118.41	122.20
19	5	4561	C	N1-C2-O2	5.42	122.15	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	K	887	U	C2-N1-C1'	5.42	124.20	117.70
19	5	4709	U	C6-N1-C2	-5.41	117.75	121.00
18	4	44	U	N3-C2-O2	-5.41	118.41	122.20
39	K	914	U	N3-C4-C5	5.41	117.85	114.60
18	4	44	U	N1-C2-O2	5.41	126.59	122.80
19	5	49	U	C2-N1-C1'	5.41	124.19	117.70
19	5	1607	C	N1-C2-O2	5.41	122.14	118.90
19	5	3910	C	N1-C2-O2	5.41	122.14	118.90
19	5	1445	U	C2-N1-C1'	5.41	124.19	117.70
19	5	1794	A	C2-N3-C4	5.41	113.30	110.60
19	5	4712	C	C5-C6-N1	5.41	123.70	121.00
34	F	88	LEU	CA-CB-CG	5.40	127.73	115.30
19	5	4230	C	C6-N1-C2	-5.40	118.14	120.30
19	5	2097	A	C2-N3-C4	5.40	113.30	110.60
19	5	3927	U	C6-N1-C2	-5.40	117.76	121.00
19	5	4114	C	C6-N1-C2	-5.40	118.14	120.30
19	5	495	C	C2-N1-C1'	5.40	124.74	118.80
19	5	3672	G	C2-N3-C4	-5.40	109.20	111.90
19	5	4392	G	N1-C6-O6	-5.40	116.66	119.90
19	5	3693	U	N3-C2-O2	-5.40	118.42	122.20
19	5	424	U	C5-C6-N1	5.40	125.40	122.70
19	5	35	U	N3-C2-O2	-5.39	118.42	122.20
19	5	3888	G	P-O3'-C3'	5.39	126.17	119.70
39	K	550	C	N1-C2-O2	5.39	122.14	118.90
19	5	1190	C	N1-C2-O2	5.39	122.14	118.90
19	5	4162	C	C6-N1-C2	-5.39	118.14	120.30
39	K	402	C	C5-C6-N1	5.39	123.70	121.00
22	8	104	A	C4-C5-C6	-5.39	114.30	117.00
39	K	1863	A	N1-C2-N3	5.39	132.00	129.30
19	5	3775	A	C2-N3-C4	-5.39	107.91	110.60
22	8	32	C	N1-C2-O2	5.39	122.13	118.90
39	K	735	C	C5-C6-N1	5.39	123.69	121.00
39	K	792	C	C6-N1-C2	-5.39	118.14	120.30
39	K	943	U	N3-C4-O4	5.39	123.17	119.40
39	K	1757	G	N3-C4-C5	-5.39	125.91	128.60
19	5	1789	C	C6-N1-C2	-5.39	118.14	120.30
19	5	2787	A	C8-N9-C1'	-5.39	118.00	127.70
36	H	124	ARG	NE-CZ-NH2	-5.38	117.61	120.30
39	K	53	C	C6-N1-C2	-5.38	118.15	120.30
39	K	1489	A	P-O3'-C3'	5.38	126.16	119.70
19	5	1440	U	P-O3'-C3'	5.38	126.16	119.70
19	5	2304	U	N3-C2-O2	-5.38	118.43	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	K	453	C	C6-N1-C2	-5.38	118.15	120.30
21	7	68	C	C6-N1-C2	-5.37	118.15	120.30
39	K	1395	C	P-O3'-C3'	5.37	126.15	119.70
39	K	1865	C	N3-C2-O2	-5.37	118.14	121.90
19	5	3691	G	N3-C4-N9	5.37	129.22	126.00
19	5	4432	C	C5-C6-N1	5.37	123.69	121.00
19	5	71	C	C6-N1-C2	-5.37	118.15	120.30
39	K	578	C	N1-C2-O2	5.37	122.12	118.90
19	5	1180	C	N1-C2-O2	5.37	122.12	118.90
19	5	1517	G	C2-N3-C4	5.37	114.58	111.90
22	8	21	C	N3-C2-O2	-5.37	118.14	121.90
19	5	4620	U	C6-N1-C2	-5.37	117.78	121.00
22	8	150	C	N3-C2-O2	-5.37	118.14	121.90
39	K	551	U	C5-C6-N1	5.37	125.38	122.70
19	5	323	C	C2-N1-C1'	5.36	124.70	118.80
19	5	2338	C	C6-N1-C2	-5.36	118.16	120.30
39	K	93	U	N3-C2-O2	-5.36	118.45	122.20
19	5	1915	C	N3-C2-O2	-5.36	118.15	121.90
19	5	4926	C	O4'-C1'-N1	5.36	112.49	108.20
19	5	281	U	N3-C2-O2	-5.35	118.45	122.20
19	5	1301	C	N1-C2-O2	5.35	122.11	118.90
19	5	2632	U	N3-C2-O2	-5.35	118.45	122.20
19	5	4066	U	N3-C2-O2	-5.35	118.45	122.20
19	5	4199	C	N1-C2-O2	5.35	122.11	118.90
39	K	1520	G	P-O3'-C3'	5.35	126.12	119.70
60	e	89	LEU	CA-CB-CG	5.35	127.61	115.30
19	5	1215	C	C2-N1-C1'	5.35	124.68	118.80
39	K	983	A	C2-N3-C4	5.35	113.27	110.60
19	5	337	U	N3-C2-O2	-5.34	118.46	122.20
19	5	469	C	N3-C2-O2	-5.34	118.16	121.90
39	K	216	C	C5-C6-N1	5.34	123.67	121.00
39	K	1408	U	C5-C6-N1	5.34	125.37	122.70
19	5	2638	G	N1-C2-N2	5.34	121.01	116.20
39	K	1303	C	O4'-C1'-N1	5.34	112.47	108.20
39	K	1842	C	C6-N1-C2	-5.34	118.16	120.30
19	5	4461	C	C5-C6-N1	5.34	123.67	121.00
21	7	76	U	C5-C6-N1	5.34	125.37	122.70
19	5	1494	U	N1-C2-O2	5.33	126.53	122.80
19	5	922(B)	C	OP1-P-O3'	5.33	116.93	105.20
19	5	1807	C	C2-N1-C1'	5.33	124.67	118.80
19	5	2787	A	N9-C4-C5	-5.33	103.67	105.80
19	5	1514	U	N3-C2-O2	-5.33	118.47	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	7	39	C	C5-C6-N1	5.33	123.67	121.00
19	5	1983	A	P-O3'-C3'	5.33	126.09	119.70
19	5	3926	C	C2-N1-C1'	5.33	124.66	118.80
19	5	123	C	C6-N1-C2	-5.33	118.17	120.30
19	5	515	C	C6-N1-C2	-5.33	118.17	120.30
19	5	964	A	C8-N9-C4	-5.33	103.67	105.80
19	5	2362	U	C2-N1-C1'	5.33	124.09	117.70
19	5	4957	C	N1-C2-O2	5.32	122.09	118.90
19	5	4719	G	N3-C4-C5	5.32	131.26	128.60
19	5	4627	U	N3-C2-O2	-5.32	118.48	122.20
19	5	1395	U	N3-C2-O2	-5.31	118.48	122.20
39	K	434	G	C8-N9-C4	-5.31	104.28	106.40
39	K	1689	C	C6-N1-C2	-5.31	118.17	120.30
19	5	3888	G	C2'-C3'-O3'	5.31	122.20	113.70
39	K	1660	C	N3-C2-O2	-5.31	118.18	121.90
19	5	1325	C	C2-N1-C1'	5.31	124.64	118.80
19	5	4119	C	P-O3'-C3'	5.31	126.07	119.70
19	5	1978	C	C6-N1-C1'	-5.31	114.43	120.80
19	5	2500	U	N3-C2-O2	-5.30	118.49	122.20
19	5	4162	C	N3-C2-O2	-5.30	118.19	121.90
19	5	4527	G	O4'-C1'-N9	5.30	112.44	108.20
19	5	4118	U	N1-C2-O2	5.30	126.51	122.80
39	K	1696	C	C2-N1-C1'	5.30	124.63	118.80
19	5	2013	A	C5-C6-N1	5.30	120.35	117.70
19	5	1449	C	C6-N1-C2	-5.30	118.18	120.30
19	5	3876	A	P-O3'-C3'	5.30	126.06	119.70
39	K	642	U	P-O3'-C3'	5.30	126.06	119.70
39	K	1149	A	C2-N3-C4	5.30	113.25	110.60
39	K	1840	U	C5-C6-N1	5.29	125.35	122.70
39	K	1862	G	OP1-P-O3'	5.29	116.84	105.20
19	5	1563	A	C3'-C2'-C1'	5.29	105.73	101.50
19	5	4577	U	N1-C2-O2	5.29	126.50	122.80
70	o	83	LEU	CA-CB-CG	5.29	127.47	115.30
19	5	1893	C	C5-C6-N1	5.29	123.64	121.00
19	5	245	C	P-O3'-C3'	5.29	126.04	119.70
19	5	691	C	C6-N1-C2	-5.29	118.19	120.30
39	K	853	C	O4'-C1'-N1	5.29	112.43	108.20
39	K	151	C	C2-N1-C1'	5.28	124.61	118.80
39	K	666	U	C2-N1-C1'	5.28	124.04	117.70
39	K	1289	U	N1-C2-O2	5.28	126.50	122.80
39	K	1394	G	P-O3'-C3'	5.28	126.04	119.70
19	5	2595	C	C6-N1-C2	-5.28	118.19	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	K	407	G	C8-N9-C1'	-5.28	120.13	127.00
19	5	1348	U	N3-C2-O2	-5.28	118.50	122.20
19	5	3777	G	N3-C2-N2	-5.28	116.21	119.90
19	5	2838	G	C6-C5-N7	-5.28	127.23	130.40
19	5	152	U	C6-N1-C2	-5.27	117.84	121.00
19	5	1861	U	N3-C2-O2	-5.27	118.51	122.20
19	5	2325	C	N1-C2-O2	5.27	122.06	118.90
17	3	63	C	C2-N1-C1'	5.27	124.60	118.80
19	5	2788	U	N1-C2-N3	-5.27	111.74	114.90
19	5	4165	C	C5-C6-N1	5.27	123.63	121.00
19	5	1456	C	N3-C2-O2	-5.27	118.21	121.90
19	5	5008	C	C5-C6-N1	5.27	123.63	121.00
39	K	1271	C	N3-C2-O2	-5.27	118.21	121.90
19	5	1963	C	N3-C2-O2	-5.27	118.21	121.90
3	CC	121	LEU	CA-CB-CG	5.26	127.41	115.30
19	5	3701	C	N3-C4-C5	5.26	124.01	121.90
19	5	79	C	C6-N1-C2	-5.26	118.19	120.30
19	5	1993	C	N1-C2-O2	5.26	122.06	118.90
19	5	4183	G	C2-N3-C4	5.26	114.53	111.90
19	5	2689	C	C6-N1-C2	-5.26	118.20	120.30
19	5	3693	U	N1-C2-O2	5.26	126.48	122.80
19	5	4667	C	N1-C2-O2	5.26	122.06	118.90
19	5	2729	C	C6-N1-C2	-5.26	118.20	120.30
19	5	1215	C	N3-C2-O2	-5.26	118.22	121.90
19	5	2560	C	C6-N1-C2	-5.25	118.20	120.30
19	5	2638	G	C8-N9-C1'	5.25	133.83	127.00
19	5	4626	A	O4'-C1'-N9	5.25	112.40	108.20
39	K	183	G	N3-C4-C5	-5.25	125.97	128.60
39	K	1123	C	N3-C2-O2	-5.25	118.22	121.90
19	5	3709	U	C2-N1-C1'	5.25	124.00	117.70
19	5	657	C	C2-N1-C1'	5.25	124.57	118.80
19	5	4266	G	C8-N9-C1'	-5.25	120.18	127.00
17	3	67	U	C2-N1-C1'	5.24	123.99	117.70
22	8	2	G	C8-N9-C1'	-5.24	120.18	127.00
19	5	1663	C	C4-C5-C6	-5.24	114.78	117.40
19	5	3625	G	P-O3'-C3'	5.24	125.99	119.70
39	K	1333	U	N3-C2-O2	-5.24	118.53	122.20
19	5	2667	C	C6-N1-C2	-5.24	118.20	120.30
39	K	1624	U	O4'-C1'-N1	5.24	112.39	108.20
19	5	1478	C	C6-N1-C2	-5.24	118.21	120.30
39	K	1775	U	N1-C2-O2	5.24	126.47	122.80
19	5	1568	C	C2-N1-C1'	5.23	124.56	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	5	4206	C	C5-C6-N1	5.23	123.62	121.00
19	5	308	G	O4'-C1'-N9	5.23	112.38	108.20
19	5	3778	U	C2-N1-C1'	5.23	123.98	117.70
19	5	195	C	C6-N1-C2	-5.23	118.21	120.30
39	K	1031	A	N1-C2-N3	-5.23	126.69	129.30
39	K	1289	U	N3-C2-O2	-5.23	118.54	122.20
19	5	717	U	N3-C2-O2	-5.22	118.54	122.20
19	5	2787	A	C6-C5-N7	-5.22	128.64	132.30
39	K	424	C	C6-N1-C2	-5.22	118.21	120.30
19	5	1792	U	N1-C2-O2	5.22	126.46	122.80
19	5	3840	U	N1-C2-O2	5.22	126.46	122.80
19	5	486	C	C6-N1-C2	-5.22	118.21	120.30
19	5	1910	G	C6-C5-N7	-5.22	127.27	130.40
19	5	3876	A	N9-C4-C5	5.22	107.89	105.80
16	2	39	U	N1-C2-O2	5.22	126.45	122.80
19	5	2822	G	N3-C4-N9	5.22	129.13	126.00
39	K	1117	C	C2-N1-C1'	5.22	124.54	118.80
19	5	2850	A	C4-N9-C1'	5.21	135.69	126.30
19	5	4561	C	C2-N1-C1'	5.21	124.54	118.80
39	K	1146	C	C6-N1-C2	-5.21	118.21	120.30
19	5	4546	A	N9-C4-C5	-5.21	103.72	105.80
19	5	2295	C	C6-N1-C2	-5.21	118.22	120.30
19	5	2325	C	N3-C2-O2	-5.21	118.25	121.90
19	5	2367	A	C6-N1-C2	5.21	121.72	118.60
19	5	976	G	C8-N9-C4	-5.21	104.32	106.40
39	K	1438	A	C6-N1-C2	-5.21	115.48	118.60
13	MM	119	LEU	CA-CB-CG	5.20	127.27	115.30
19	5	1446	C	N3-C2-O2	-5.20	118.26	121.90
39	K	1704	C	C5-C6-N1	5.20	123.60	121.00
19	5	3853	U	N3-C2-O2	-5.20	118.56	122.20
19	5	1430	C	C6-N1-C2	-5.20	118.22	120.30
34	F	178	LEU	CB-CG-CD2	-5.20	102.16	111.00
19	5	2471	G	C4-C5-N7	5.20	112.88	110.80
19	5	3739	C	N1-C2-O2	5.20	122.02	118.90
16	2	13	C	N1-C2-O2	5.20	122.02	118.90
19	5	2454	U	N1-C2-O2	5.20	126.44	122.80
39	K	37	C	C2-N1-C1'	5.20	124.52	118.80
39	K	1529	C	C6-N1-C2	-5.20	118.22	120.30
76	u	62	LEU	CA-CB-CG	5.19	127.25	115.30
19	5	3887	C	C5-C6-N1	5.19	123.60	121.00
19	5	1578	U	N3-C2-O2	-5.19	118.57	122.20
39	K	183	G	C8-N9-C1'	-5.19	120.26	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	5	1572	U	C2-N1-C1'	5.18	123.92	117.70
19	5	1598	C	C2-N1-C1'	5.18	124.50	118.80
39	K	537	C	N3-C2-O2	-5.18	118.27	121.90
19	5	1687	U	N3-C2-O2	-5.18	118.57	122.20
19	5	2031	C	N1-C2-O2	5.18	122.01	118.90
21	7	26	C	C5-C6-N1	5.18	123.59	121.00
19	5	1800	U	N3-C2-O2	-5.18	118.58	122.20
19	5	4069	U	N3-C2-O2	-5.18	118.58	122.20
19	5	7	C	C6-N1-C2	-5.18	118.23	120.30
19	5	1853	G	N3-C4-N9	5.18	129.10	126.00
19	5	3778	U	N1-C2-O2	5.18	126.42	122.80
22	8	27	U	C5-C6-N1	5.18	125.29	122.70
19	5	2532	C	C5-C6-N1	5.17	123.59	121.00
19	5	504	G	P-O3'-C3'	5.17	125.91	119.70
19	5	1517	G	N3-C4-C5	-5.17	126.01	128.60
21	7	28	C	C5-C6-N1	5.17	123.59	121.00
39	K	1017	U	N3-C2-O2	-5.17	118.58	122.20
19	5	1662	C	C5-C6-N1	5.17	123.58	121.00
19	5	2783	A	C5-N7-C8	-5.17	101.32	103.90
19	5	4371	G	O4'-C1'-N9	5.17	112.33	108.20
19	5	1292	C	C2-N1-C1'	5.16	124.48	118.80
19	5	2528	G	N3-C4-C5	-5.16	126.02	128.60
19	5	3761	C	N1-C2-O2	5.16	122.00	118.90
19	5	3788	C	C2-N1-C1'	5.16	124.48	118.80
35	G	199	LEU	CA-CB-CG	5.16	127.17	115.30
19	5	274	C	C2-N1-C1'	5.16	124.47	118.80
19	5	1308	C	C6-N1-C2	-5.16	118.24	120.30
19	5	1598	C	C6-N1-C2	-5.16	118.24	120.30
19	5	4565	C	C6-N1-C2	-5.16	118.24	120.30
19	5	4736	C	C5-C4-N4	-5.16	116.59	120.20
19	5	4497	U	N3-C2-O2	-5.16	118.59	122.20
19	5	3911	C	N1-C2-O2	5.16	121.99	118.90
39	K	124	U	N3-C2-O2	-5.16	118.59	122.20
19	5	35	U	C5-C6-N1	5.15	125.28	122.70
19	5	492	U	P-O3'-C3'	5.15	125.88	119.70
19	5	68	U	N3-C2-O2	-5.15	118.59	122.20
19	5	1671	U	C6-N1-C2	-5.15	117.91	121.00
19	5	3823	G	C6-C5-N7	-5.15	127.31	130.40
19	5	4483	C	C6-N1-C2	-5.15	118.24	120.30
19	5	4493	U	N3-C2-O2	-5.15	118.59	122.20
19	5	1890	G	C2-N3-C4	-5.15	109.33	111.90
19	5	3837	C	C6-N1-C2	-5.15	118.24	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	K	319	C	OP1-P-OP2	-5.14	111.88	119.60
19	5	1818	G	C4-N9-C1'	5.14	133.18	126.50
19	5	1447	C	C2-N1-C1'	5.14	124.45	118.80
19	5	1963	C	C6-N1-C2	-5.14	118.24	120.30
19	5	1329	G	N3-C4-C5	-5.14	126.03	128.60
19	5	1540	C	N1-C2-O2	5.14	121.98	118.90
39	K	930	C	N1-C2-O2	5.14	121.98	118.90
19	5	250	C	C5-C6-N1	5.14	123.57	121.00
19	5	326	C	C2-N1-C1'	5.14	124.45	118.80
19	5	1936	C	C5-C6-N1	5.14	123.57	121.00
17	3	8	U	N1-C2-O2	5.13	126.39	122.80
39	K	1117	C	N1-C2-O2	5.13	121.98	118.90
39	K	18	C	C5-C6-N1	5.13	123.57	121.00
19	5	2471	G	C5-N7-C8	-5.13	101.73	104.30
39	K	1554	C	C6-N1-C2	-5.13	118.25	120.30
19	5	86	U	N1-C2-O2	5.13	126.39	122.80
19	5	1656	U	C2-N1-C1'	5.13	123.86	117.70
19	5	4698	C	C6-N1-C2	-5.13	118.25	120.30
39	K	1227	G	N3-C4-N9	5.13	129.08	126.00
55	SS	2	LEU	CA-CB-CG	5.13	127.10	115.30
21	7	80	U	C5-C6-N1	5.13	125.26	122.70
19	5	2627	C	C5-C6-N1	5.12	123.56	121.00
19	5	125	C	P-O3'-C3'	5.12	125.85	119.70
19	5	1735	U	N3-C2-O2	-5.12	118.61	122.20
19	5	4667	C	C2-N1-C1'	5.12	124.44	118.80
19	5	4775	C	C5-C6-N1	5.12	123.56	121.00
19	5	1792	U	C6-N1-C2	-5.12	117.93	121.00
19	5	1915	C	N1-C2-O2	5.12	121.97	118.90
19	5	4674	C	C6-N1-C2	-5.12	118.25	120.30
39	K	65	C	C6-N1-C2	-5.12	118.25	120.30
79	x	73	ASP	CB-CG-OD1	5.12	122.91	118.30
19	5	112	C	C6-N1-C1'	-5.12	114.66	120.80
19	5	217	C	OP2-P-O3'	5.12	116.46	105.20
19	5	1411(B)	C	C2-N1-C1'	5.12	124.43	118.80
19	5	1632	A	C4-N9-C1'	5.12	135.51	126.30
19	5	2503	G	OP1-P-OP2	-5.12	111.92	119.60
39	K	1757	G	C8-N9-C1'	-5.12	120.35	127.00
39	K	1852	C	C2-N1-C1'	5.12	124.43	118.80
19	5	406	C	P-O3'-C3'	5.12	125.84	119.70
19	5	1644	C	C5-C6-N1	5.12	123.56	121.00
19	5	4942	C	N1-C2-O2	5.12	121.97	118.90
39	K	1595	U	N1-C2-O2	5.12	126.38	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	3	72	C	C2-N1-C1'	5.12	124.43	118.80
19	5	1405	C	C6-N1-C2	-5.12	118.25	120.30
19	5	1978	C	C5-C6-N1	5.12	123.56	121.00
19	5	4880	C	C6-N1-C2	-5.12	118.25	120.30
16	2	39	U	N3-C2-O2	-5.11	118.62	122.20
39	K	1225	U	N3-C2-O2	-5.11	118.62	122.20
19	5	2532	C	N1-C2-O2	5.11	121.97	118.90
19	5	1301	C	C2-N1-C1'	5.11	124.42	118.80
21	7	67	C	C2-N1-C1'	5.11	124.42	118.80
61	f	103	VAL	CG1-CB-CG2	-5.11	102.73	110.90
19	5	2667	C	N3-C2-O2	-5.11	118.33	121.90
19	5	2325	C	C6-N1-C2	-5.10	118.26	120.30
19	5	4423	U	C6-N1-C1'	-5.10	114.05	121.20
19	5	3708	C	C6-N1-C2	-5.10	118.26	120.30
19	5	3761	C	C6-N1-C2	-5.10	118.26	120.30
39	K	140	U	C6-N1-C1'	-5.10	114.06	121.20
19	5	2351	C	C2-N3-C4	5.10	122.45	119.90
19	5	1081	C	C2-N1-C1'	5.10	124.41	118.80
19	5	3729	U	C2-N3-C4	-5.10	123.94	127.00
85	WW	49	LEU	CA-CB-CG	5.10	127.03	115.30
19	5	1478	C	C5-C6-N1	5.10	123.55	121.00
19	5	2337	C	C5-C6-N1	5.10	123.55	121.00
22	8	135	C	C6-N1-C2	-5.10	118.26	120.30
39	K	1475	G	C4-N9-C1'	5.10	133.12	126.50
39	K	553	U	P-O3'-C3'	5.09	125.81	119.70
19	5	3657	U	C5-C6-N1	5.09	125.25	122.70
19	5	4350	C	C5-C6-N1	5.09	123.55	121.00
39	K	1139	C	O4'-C1'-N1	5.09	112.27	108.20
19	5	180	C	C6-N1-C2	-5.09	118.27	120.30
19	5	2694	G	C2-N3-C4	-5.08	109.36	111.90
19	5	4519	C	O5'-P-OP1	5.08	116.80	110.70
16	2	5	C	C5-C6-N1	5.08	123.54	121.00
19	5	4133	C	C2-N1-C1'	5.08	124.39	118.80
19	5	4758	U	C6-N1-C1'	-5.08	114.09	121.20
19	5	3761	C	N3-C2-O2	-5.08	118.35	121.90
19	5	3685	C	C6-N1-C2	-5.07	118.27	120.30
39	K	118	C	N1-C2-O2	5.07	121.94	118.90
39	K	453	C	N3-C2-O2	-5.07	118.35	121.90
86	XX	394	LEU	CA-CB-CG	-5.07	103.63	115.30
19	5	492	U	N3-C2-O2	-5.07	118.65	122.20
19	5	712	C	C6-N1-C2	-5.07	118.27	120.30
19	5	1468	C	N1-C2-O2	5.07	121.94	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	5	1469	C	N1-C2-N3	5.07	122.75	119.20
19	5	1731	C	N1-C2-O2	5.07	121.94	118.90
19	5	2048	U	N1-C2-O2	5.07	126.35	122.80
19	5	2371	U	N3-C2-O2	-5.07	118.65	122.20
19	5	4884	G	P-O3'-C3'	5.07	125.78	119.70
19	5	281	U	N1-C2-O2	5.07	126.35	122.80
19	5	1671	U	N1-C2-O2	5.07	126.35	122.80
19	5	4766	C	C5-C6-N1	5.07	123.53	121.00
39	K	369	C	N1-C2-O2	5.07	121.94	118.90
19	5	2850	A	N7-C8-N9	5.07	116.33	113.80
19	5	3709	U	N1-C2-O2	5.07	126.35	122.80
39	K	891	G	N3-C4-C5	-5.07	126.07	128.60
19	5	118	C	C5-C6-N1	5.06	123.53	121.00
19	5	1339	U	C2-N1-C1'	5.06	123.78	117.70
19	5	1502	G	N3-C4-N9	-5.06	122.96	126.00
19	5	4288	C	C6-N1-C2	-5.06	118.28	120.30
39	K	434	G	P-O3'-C3'	5.06	125.77	119.70
19	5	492	U	N1-C2-O2	5.06	126.34	122.80
22	8	101	C	N3-C2-O2	-5.06	118.36	121.90
19	5	1289	C	N1-C2-O2	5.06	121.93	118.90
19	5	4337	C	C6-N1-C2	-5.06	118.28	120.30
19	5	4747	C	C6-N1-C2	-5.06	118.28	120.30
39	K	790	C	N3-C2-O2	-5.06	118.36	121.90
19	5	4423	U	O4'-C1'-N1	5.06	112.24	108.20
19	5	1211	G	P-O3'-C3'	5.05	125.77	119.70
19	5	4645	C	C6-N1-C2	-5.05	118.28	120.30
19	5	3785	A	O4'-C1'-N9	5.05	112.24	108.20
39	K	1407	U	C5-C4-O4	-5.05	122.87	125.90
19	5	421	C	C6-N1-C2	-5.05	118.28	120.30
19	5	934	C	N3-C2-O2	-5.05	118.36	121.90
19	5	1529	G	N1-C6-O6	-5.05	116.87	119.90
19	5	1612	G	C4-C5-N7	5.05	112.82	110.80
19	5	2470	C	N3-C2-O2	-5.05	118.36	121.90
19	5	4119	C	O4'-C1'-N1	5.05	112.24	108.20
19	5	1	C	N3-C2-O2	-5.05	118.37	121.90
19	5	1317	U	N3-C2-O2	-5.05	118.67	122.20
39	K	146	G	N1-C6-O6	-5.05	116.87	119.90
39	K	891	G	N3-C4-N9	5.05	129.03	126.00
39	K	943	U	C6-N1-C1'	-5.05	114.13	121.20
39	K	1137	U	P-O3'-C3'	5.05	125.76	119.70
19	5	2634	C	C6-N1-C2	-5.04	118.28	120.30
19	5	1921	C	P-O3'-C3'	5.04	125.75	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	5	3931	C	C6-N1-C2	-5.04	118.28	120.30
52	X	52	LEU	CA-CB-CG	5.04	126.90	115.30
78	w	59	LEU	CA-CB-CG	5.04	126.90	115.30
19	5	472	C	C6-N1-C2	-5.04	118.28	120.30
19	5	978	G	N1-C2-N3	5.04	126.92	123.90
19	5	84	A	OP1-P-O3'	5.04	116.29	105.20
19	5	3673	C	N1-C2-O2	5.04	121.92	118.90
39	K	1401	A	C5-C6-N1	5.04	120.22	117.70
19	5	124	C	C5-C6-N1	5.04	123.52	121.00
19	5	2410	C	C6-N1-C1'	-5.04	114.75	120.80
21	7	111	C	C6-N1-C2	-5.04	118.28	120.30
22	8	35	C	C5-C6-N1	5.04	123.52	121.00
19	5	2277	C	N3-C2-O2	-5.04	118.37	121.90
19	5	4918	C	C2-N1-C1'	5.04	124.34	118.80
39	K	663	C	C5-C6-N1	5.04	123.52	121.00
39	K	1853	C	C5-C6-N1	5.04	123.52	121.00
39	K	357	C	C6-N1-C2	-5.03	118.29	120.30
39	K	1464	C	N3-C2-O2	-5.03	118.38	121.90
19	5	1991	A	OP1-P-OP2	-5.03	112.05	119.60
19	5	4511	A	C8-N9-C4	-5.03	103.79	105.80
19	5	4752	U	N3-C2-O2	-5.03	118.68	122.20
19	5	1214	C	C2-N1-C1'	5.03	124.33	118.80
19	5	4417	C	N3-C2-O2	-5.03	118.38	121.90
19	5	4714	C	C6-N1-C2	-5.03	118.29	120.30
19	5	5046	U	N3-C2-O2	-5.03	118.68	122.20
39	K	1591	C	C2-N1-C1'	5.03	124.33	118.80
19	5	2867	C	N1-C2-O2	5.02	121.91	118.90
39	K	1636	G	N3-C4-C5	-5.02	126.09	128.60
19	5	4947	U	P-O3'-C3'	5.02	125.73	119.70
19	5	4695	C	N1-C2-O2	5.02	121.91	118.90
19	5	1913	C	C6-N1-C2	-5.02	118.29	120.30
5	EE	113	LEU	CA-CB-CG	5.02	126.84	115.30
19	5	5051	C	C6-N1-C2	-5.02	118.29	120.30
19	5	3863	C	C5-C6-N1	5.02	123.51	121.00
39	K	1475	G	C6-C5-N7	-5.01	127.39	130.40
19	5	954	C	C6-N1-C2	-5.01	118.30	120.30
39	K	1331	C	N1-C2-O2	5.01	121.91	118.90
19	5	2852	U	C5-C6-N1	5.01	125.20	122.70
19	5	4551	U	N3-C2-O2	-5.01	118.70	122.20
19	5	4719	G	N3-C4-N9	-5.01	123.00	126.00
19	5	2838	G	C4-C5-N7	5.00	112.80	110.80
19	5	4305	G	N7-C8-N9	5.00	115.60	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	K	340	C	N1-C2-O2	5.00	121.90	118.90
19	5	1526	G	N9-C4-C5	-5.00	103.40	105.40
19	5	2351	C	C6-N1-C2	-5.00	118.30	120.30
39	K	1103	C	C6-N1-C2	-5.00	118.30	120.30

There are no chirality outliers.

All (25) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	B	257	TRP	Peptide
31	C	339	THR	Peptide
33	E	180	GLY	Peptide
34	F	235	ARG	Peptide
35	G	215	ASP	Peptide
8	HH	32	ILE	Peptide
9	II	99	LEU	Peptide
40	L	4	SER	Peptide
41	M	37	LEU	Peptide
42	N	184	ILE	Peptide
42	N	76	PRO	Peptide
42	N	78	GLY	Peptide
47	S	164	LYS	Peptide
82	TT	54	ASP	Peptide
84	VV	61	GLN	Peptide
85	WW	17	TYR	Peptide
85	WW	37	TYR	Peptide
86	XX	173	TYR	Peptide
86	XX	415	ARG	Mainchain
86	XX	42	PHE	Peptide
87	YY	31	LYS	Peptide
57	b	11	ASN	Peptide
59	d	95	ASP	Peptide
72	q	42	LYS	Peptide
73	r	32	LEU	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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AA	53/55 (96%)	51 (96%)	2 (4%)	0	100	100
2	BB	181/189 (96%)	174 (96%)	7 (4%)	0	100	100
3	CC	204/206 (99%)	194 (95%)	10 (5%)	0	100	100
4	DD	183/185 (99%)	179 (98%)	4 (2%)	0	100	100
5	EE	139/151 (92%)	132 (95%)	7 (5%)	0	100	100
6	FF	60/62 (97%)	57 (95%)	3 (5%)	0	100	100
7	GG	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
8	HH	81/83 (98%)	76 (94%)	5 (6%)	0	100	100
9	II	142/144 (99%)	135 (95%)	7 (5%)	0	100	100
10	JJ	81/83 (98%)	77 (95%)	4 (5%)	0	100	100
11	KK	130/132 (98%)	123 (95%)	7 (5%)	0	100	100
12	LL	99/101 (98%)	91 (92%)	8 (8%)	0	100	100
13	MM	134/136 (98%)	126 (94%)	8 (6%)	0	100	100
14	0	66/68 (97%)	61 (92%)	5 (8%)	0	100	100
15	1	22/24 (92%)	13 (59%)	7 (32%)	2 (9%)	1	12
20	6	311/313 (99%)	283 (91%)	28 (9%)	0	100	100
23	9	53/55 (96%)	51 (96%)	2 (4%)	0	100	100
24	NN	122/124 (98%)	119 (98%)	3 (2%)	0	100	100
25	OO	73/75 (97%)	70 (96%)	3 (4%)	0	100	100
26	PP	139/141 (99%)	130 (94%)	9 (6%)	0	100	100
27	QQ	147/149 (99%)	145 (99%)	2 (1%)	0	100	100
28	RR	115/117 (98%)	104 (90%)	11 (10%)	0	100	100
29	A	246/248 (99%)	231 (94%)	15 (6%)	0	100	100
30	B	392/394 (100%)	368 (94%)	24 (6%)	0	100	100
31	C	360/362 (99%)	341 (95%)	19 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	D	291/293 (99%)	281 (97%)	10 (3%)	0	100	100
33	E	208/251 (83%)	195 (94%)	13 (6%)	0	100	100
34	F	223/225 (99%)	214 (96%)	9 (4%)	0	100	100
35	G	229/240 (95%)	222 (97%)	7 (3%)	0	100	100
36	H	188/190 (99%)	178 (95%)	10 (5%)	0	100	100
37	I	201/213 (94%)	191 (95%)	10 (5%)	0	100	100
38	J	168/170 (99%)	162 (96%)	6 (4%)	0	100	100
40	L	208/210 (99%)	198 (95%)	7 (3%)	3 (1%)	11	46
41	M	136/138 (99%)	130 (96%)	6 (4%)	0	100	100
42	N	201/203 (99%)	189 (94%)	12 (6%)	0	100	100
43	O	197/199 (99%)	191 (97%)	6 (3%)	0	100	100
44	P	151/153 (99%)	145 (96%)	6 (4%)	0	100	100
45	Q	185/187 (99%)	177 (96%)	8 (4%)	0	100	100
46	R	178/180 (99%)	175 (98%)	3 (2%)	0	100	100
47	S	174/176 (99%)	165 (95%)	9 (5%)	0	100	100
48	T	157/159 (99%)	147 (94%)	10 (6%)	0	100	100
49	U	97/99 (98%)	91 (94%)	6 (6%)	0	100	100
50	V	129/131 (98%)	123 (95%)	6 (5%)	0	100	100
51	W	102/121 (84%)	98 (96%)	4 (4%)	0	100	100
52	X	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
53	Y	132/134 (98%)	129 (98%)	3 (2%)	0	100	100
54	Z	133/135 (98%)	128 (96%)	4 (3%)	1 (1%)	19	57
55	SS	94/96 (98%)	88 (94%)	6 (6%)	0	100	100
56	a	145/147 (99%)	139 (96%)	6 (4%)	0	100	100
57	b	100/116 (86%)	96 (96%)	4 (4%)	0	100	100
58	c	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
59	d	105/107 (98%)	97 (92%)	8 (8%)	0	100	100
60	e	126/128 (98%)	122 (97%)	4 (3%)	0	100	100
61	f	107/109 (98%)	102 (95%)	5 (5%)	0	100	100
62	g	112/114 (98%)	110 (98%)	2 (2%)	0	100	100
63	h	120/122 (98%)	117 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
64	i	100/102 (98%)	97 (97%)	3 (3%)	0	100	100
65	j	84/86 (98%)	82 (98%)	2 (2%)	0	100	100
66	k	67/69 (97%)	66 (98%)	1 (2%)	0	100	100
67	l	48/50 (96%)	45 (94%)	3 (6%)	0	100	100
68	m	50/52 (96%)	49 (98%)	1 (2%)	0	100	100
69	n	23/25 (92%)	23 (100%)	0	0	100	100
70	o	102/104 (98%)	97 (95%)	5 (5%)	0	100	100
71	p	89/91 (98%)	86 (97%)	3 (3%)	0	100	100
72	q	215/217 (99%)	202 (94%)	13 (6%)	0	100	100
73	r	122/124 (98%)	113 (93%)	9 (7%)	0	100	100
74	s	194/196 (99%)	181 (93%)	13 (7%)	0	100	100
75	t	151/153 (99%)	135 (89%)	16 (11%)	0	100	100
76	u	211/213 (99%)	202 (96%)	9 (4%)	0	100	100
77	v	219/221 (99%)	213 (97%)	6 (3%)	0	100	100
78	w	226/228 (99%)	218 (96%)	8 (4%)	0	100	100
79	x	260/262 (99%)	249 (96%)	11 (4%)	0	100	100
80	y	181/191 (95%)	169 (93%)	12 (7%)	0	100	100
81	z	235/237 (99%)	228 (97%)	7 (3%)	0	100	100
82	TT	127/129 (98%)	119 (94%)	8 (6%)	0	100	100
83	UU	140/142 (99%)	133 (95%)	7 (5%)	0	100	100
84	VV	139/141 (99%)	132 (95%)	5 (4%)	2 (1%)	11	46
85	WW	118/120 (98%)	111 (94%)	6 (5%)	1 (1%)	19	57
86	XX	412/461 (89%)	363 (88%)	45 (11%)	4 (1%)	15	52
87	YY	60/62 (97%)	50 (83%)	8 (13%)	2 (3%)	4	31
88	ZZ	27/29 (93%)	25 (93%)	1 (4%)	1 (4%)	3	29
All	All	12040/12364 (97%)	11420 (95%)	604 (5%)	16 (0%)	54	84

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	1	249	TRP
86	XX	107	LYS
86	XX	108	ASP

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Mol	Chain	Res	Type
86	XX	445	THR
40	L	64	VAL
84	VV	62	PRO
15	1	258	PRO
40	L	5	ARG
40	L	63	THR
86	XX	286	THR
87	YY	31	LYS
84	VV	86	PRO
85	WW	18	ARG
54	Z	90	PRO
87	YY	28	PRO
88	ZZ	71	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AA	46/46 (100%)	44 (96%)	2 (4%)	29	57
2	BB	165/169 (98%)	165 (100%)	0	100	100
3	CC	178/178 (100%)	174 (98%)	4 (2%)	52	71
4	DD	161/161 (100%)	158 (98%)	3 (2%)	57	75
5	EE	130/136 (96%)	127 (98%)	3 (2%)	50	71
6	FF	55/55 (100%)	54 (98%)	1 (2%)	59	77
7	GG	92/92 (100%)	90 (98%)	2 (2%)	52	71
8	HH	67/67 (100%)	66 (98%)	1 (2%)	65	80
9	II	125/125 (100%)	124 (99%)	1 (1%)	81	89
10	JJ	75/75 (100%)	74 (99%)	1 (1%)	69	82
11	KK	119/119 (100%)	119 (100%)	0	100	100
12	LL	88/88 (100%)	87 (99%)	1 (1%)	73	84
13	MM	106/106 (100%)	104 (98%)	2 (2%)	57	75
14	0	61/61 (100%)	60 (98%)	1 (2%)	62	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	1	22/22 (100%)	13 (59%)	9 (41%)	0	0
20	6	272/272 (100%)	270 (99%)	2 (1%)	84	90
23	9	48/48 (100%)	48 (100%)	0	100	100
24	NN	107/107 (100%)	104 (97%)	3 (3%)	43	66
25	OO	66/66 (100%)	66 (100%)	0	100	100
26	PP	111/111 (100%)	109 (98%)	2 (2%)	59	77
27	QQ	130/130 (100%)	129 (99%)	1 (1%)	81	89
28	RR	99/99 (100%)	98 (99%)	1 (1%)	76	86
29	A	190/190 (100%)	182 (96%)	8 (4%)	30	57
30	B	342/342 (100%)	338 (99%)	4 (1%)	71	83
31	C	302/302 (100%)	293 (97%)	9 (3%)	41	64
32	D	247/247 (100%)	243 (98%)	4 (2%)	62	79
33	E	190/223 (85%)	187 (98%)	3 (2%)	62	79
34	F	196/196 (100%)	195 (100%)	1 (0%)	88	93
35	G	200/205 (98%)	197 (98%)	3 (2%)	65	80
36	H	169/169 (100%)	165 (98%)	4 (2%)	49	69
37	I	175/180 (97%)	172 (98%)	3 (2%)	60	78
38	J	143/143 (100%)	142 (99%)	1 (1%)	84	90
40	L	175/175 (100%)	174 (99%)	1 (1%)	86	91
41	M	117/117 (100%)	114 (97%)	3 (3%)	46	68
42	N	171/171 (100%)	168 (98%)	3 (2%)	59	77
43	O	171/171 (100%)	169 (99%)	2 (1%)	71	83
44	P	134/134 (100%)	133 (99%)	1 (1%)	84	90
45	Q	164/164 (100%)	161 (98%)	3 (2%)	59	77
46	R	159/159 (100%)	155 (98%)	4 (2%)	47	69
47	S	157/157 (100%)	155 (99%)	2 (1%)	69	82
48	T	139/139 (100%)	136 (98%)	3 (2%)	52	71
49	U	89/89 (100%)	88 (99%)	1 (1%)	73	84
50	V	101/101 (100%)	97 (96%)	4 (4%)	31	58
51	W	86/100 (86%)	86 (100%)	0	100	100
52	X	106/106 (100%)	104 (98%)	2 (2%)	57	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	Y	124/124 (100%)	122 (98%)	2 (2%)	62	79
54	Z	117/117 (100%)	117 (100%)	0	100	100
55	SS	87/87 (100%)	86 (99%)	1 (1%)	73	84
56	a	119/119 (100%)	117 (98%)	2 (2%)	60	78
57	b	84/95 (88%)	82 (98%)	2 (2%)	49	69
58	c	84/84 (100%)	83 (99%)	1 (1%)	71	83
59	d	98/98 (100%)	96 (98%)	2 (2%)	55	74
60	e	114/114 (100%)	113 (99%)	1 (1%)	78	87
61	f	88/88 (100%)	87 (99%)	1 (1%)	73	84
62	g	98/98 (100%)	95 (97%)	3 (3%)	40	64
63	h	109/109 (100%)	109 (100%)	0	100	100
64	i	86/86 (100%)	85 (99%)	1 (1%)	71	83
65	j	73/73 (100%)	72 (99%)	1 (1%)	67	81
66	k	64/64 (100%)	63 (98%)	1 (2%)	62	79
67	l	47/47 (100%)	47 (100%)	0	100	100
68	m	48/48 (100%)	48 (100%)	0	100	100
69	n	24/24 (100%)	23 (96%)	1 (4%)	30	57
70	o	92/92 (100%)	91 (99%)	1 (1%)	73	84
71	p	74/74 (100%)	72 (97%)	2 (3%)	44	67
72	q	180/181 (99%)	178 (99%)	2 (1%)	73	84
73	r	108/108 (100%)	106 (98%)	2 (2%)	57	75
74	s	164/164 (100%)	164 (100%)	0	100	100
75	t	126/126 (100%)	126 (100%)	0	100	100
76	u	194/194 (100%)	189 (97%)	5 (3%)	46	68
77	v	187/187 (100%)	184 (98%)	3 (2%)	62	79
78	w	190/190 (100%)	185 (97%)	5 (3%)	46	68
79	x	224/224 (100%)	221 (99%)	3 (1%)	69	82
80	y	158/161 (98%)	158 (100%)	0	100	100
81	z	207/207 (100%)	204 (99%)	3 (1%)	67	81
82	TT	112/112 (100%)	112 (100%)	0	100	100
83	UU	117/117 (100%)	116 (99%)	1 (1%)	78	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
84	VV	113/113 (100%)	112 (99%)	1 (1%)	78	87
85	WW	109/109 (100%)	108 (99%)	1 (1%)	78	87
86	XX	360/387 (93%)	346 (96%)	14 (4%)	32	59
87	YY	53/53 (100%)	43 (81%)	10 (19%)	1	10
88	ZZ	26/26 (100%)	22 (85%)	4 (15%)	2	17
All	All	10504/10613 (99%)	10319 (98%)	185 (2%)	61	77

All (185) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AA	99	LYS
1	AA	104	ARG
3	CC	36	THR
3	CC	84	ASN
3	CC	87	ASN
3	CC	99	ASN
4	DD	69	ARG
4	DD	70	ARG
4	DD	79	ARG
5	EE	20	LYS
5	EE	69	ARG
5	EE	97	ARG
6	FF	40	ARG
7	GG	44	LYS
7	GG	47	ASN
8	HH	82	ASN
9	II	8	LYS
10	JJ	81	ARG
12	LL	5	ARG
13	MM	146	ARG
13	MM	150	ARG
14	0	138	ARG
15	1	237	ASP
15	1	239	VAL
15	1	241	TYR
15	1	246	LEU
15	1	247	CYS
15	1	251	ARG
15	1	253	GLN
15	1	257	LYS

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Mol	Chain	Res	Type
15	1	259	LEU
20	6	159	ASN
20	6	178	ASN
24	NN	17	LEU
24	NN	74	MET
24	NN	101	LYS
26	PP	62	ARG
26	PP	124	THR
27	QQ	27	LYS
28	RR	33	ARG
29	A	125	LYS
29	A	128	ARG
29	A	193	ARG
29	A	194	ASN
29	A	200	ARG
29	A	207	VAL
29	A	242	ARG
29	A	243	THR
30	B	24	ARG
30	B	162	VAL
30	B	261	ARG
30	B	262	VAL
31	C	38	ASN
31	C	45	ARG
31	C	95	MET
31	C	150	LEU
31	C	188	ARG
31	C	219	LYS
31	C	223	ASN
31	C	312	ARG
31	C	321	ASN
32	D	111	ASN
32	D	157	ASN
32	D	226	TYR
32	D	268	ARG
33	E	58	ARG
33	E	164	ARG
33	E	291	PHE
34	F	205	ASN
35	G	242	ARG
35	G	249	ARG
35	G	293	ASN

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Mol	Chain	Res	Type
36	H	1	MET
36	H	15	ASN
36	H	102	ASN
36	H	128	MET
37	I	3	ARG
37	I	73	ASN
37	I	100	ASN
38	J	33	LEU
40	L	63	THR
41	M	25	VAL
41	M	38	VAL
41	M	119	ARG
42	N	50	ARG
42	N	64	ILE
42	N	89	VAL
43	O	117	ARG
43	O	140	ARG
44	P	128	ARG
45	Q	5	ILE
45	Q	97	LYS
45	Q	172	ARG
46	R	36	ASN
46	R	50	ILE
46	R	130	ASN
46	R	133	LYS
47	S	90	THR
47	S	120	ARG
48	T	96	ILE
48	T	136	ARG
48	T	146	LYS
49	U	81	ARG
50	V	15	ARG
50	V	18	LEU
50	V	48	ARG
50	V	61	VAL
52	X	53	ARG
52	X	59	LYS
53	Y	2	LYS
53	Y	79	VAL
55	SS	96	ARG
56	a	4	ARG
56	a	122	VAL

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Mol	Chain	Res	Type
57	b	60	ASN
57	b	72	ILE
58	c	90	ARG
59	d	18	ASN
59	d	31	LYS
60	e	48	ARG
61	f	16	ARG
62	g	14	ASN
62	g	15	THR
62	g	18	ASN
64	i	29	ARG
65	j	20	ARG
66	k	69	LEU
69	n	13	LEU
70	o	82	MET
71	p	54	ILE
71	p	84	ARG
72	q	50	ASN
72	q	186	ARG
73	r	12	ASN
73	r	67	ARG
76	u	40	ASN
76	u	84	PHE
76	u	147	ASN
76	u	207	LEU
76	u	213	ARG
77	v	137	VAL
77	v	167	ARG
77	v	248	TYR
78	w	22	ASN
78	w	76	ARG
78	w	94	ARG
78	w	106	ARG
78	w	227	LYS
79	x	148	ARG
79	x	232	ASN
79	x	240	ARG
81	z	31	ARG
81	z	63	MET
81	z	191	ARG
83	UU	41	MET
84	VV	119	ARG

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Mol	Chain	Res	Type
85	WW	13	ARG
86	XX	45	CYS
86	XX	64	TRP
86	XX	65	MET
86	XX	202	ASN
86	XX	207	MET
86	XX	241	ASN
86	XX	244	ASN
86	XX	355	LEU
86	XX	406	GLU
86	XX	414	ASN
86	XX	436	ASP
86	XX	441	ILE
86	XX	458	PHE
86	XX	461	PHE
87	YY	26	THR
87	YY	27	LYS
87	YY	29	ASP
87	YY	30	ARG
87	YY	31	LYS
87	YY	32	GLU
87	YY	40	THR
87	YY	59	ILE
87	YY	62	ASN
87	YY	63	ASN
88	ZZ	73	VAL
88	ZZ	76	MET
88	ZZ	81	ILE
88	ZZ	87	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (113) such sidechains are listed below:

Mol	Chain	Res	Type
1	AA	88	GLN
2	BB	126	HIS
2	BB	168	HIS
3	CC	7	ASN
3	CC	84	ASN
3	CC	87	ASN
3	CC	99	ASN
4	DD	154	GLN
5	EE	11	GLN

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Mol	Chain	Res	Type
5	EE	19	ASN
6	FF	26	GLN
6	FF	29	GLN
7	GG	47	ASN
10	JJ	26	GLN
11	KK	62	GLN
13	MM	94	HIS
15	1	252	HIS
15	1	253	GLN
20	6	133	ASN
20	6	159	ASN
20	6	178	ASN
20	6	196	ASN
23	9	26	ASN
24	NN	15	ASN
27	QQ	105	ASN
28	RR	48	HIS
29	A	194	ASN
29	A	216	HIS
31	C	38	ASN
31	C	223	ASN
31	C	321	ASN
32	D	111	ASN
32	D	138	GLN
32	D	222	GLN
33	E	45	HIS
33	E	193	HIS
34	F	38	GLN
34	F	130	ASN
34	F	205	ASN
35	G	117	GLN
35	G	293	ASN
36	H	8	GLN
36	H	15	ASN
36	H	78	GLN
36	H	102	ASN
37	I	73	ASN
37	I	95	HIS
37	I	100	ASN
38	J	98	ASN
40	L	19	GLN
40	L	67	HIS

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Mol	Chain	Res	Type
40	L	113	ASN
41	M	83	ASN
42	N	8	GLN
42	N	196	ASN
44	P	120	ASN
44	P	137	ASN
46	R	36	ASN
46	R	130	ASN
46	R	178	GLN
48	T	98	HIS
48	T	139	HIS
50	V	77	HIS
51	W	50	ASN
51	W	120	GLN
52	X	93	ASN
52	X	105	ASN
52	X	111	GLN
52	X	151	ASN
53	Y	14	ASN
55	SS	7	ASN
55	SS	44	HIS
59	d	18	ASN
59	d	30	HIS
62	g	14	ASN
62	g	18	ASN
62	g	114	GLN
64	i	15	HIS
65	j	76	HIS
70	o	45	GLN
71	p	33	GLN
72	q	141	ASN
73	r	12	ASN
73	r	45	HIS
76	u	147	ASN
76	u	157	GLN
76	u	186	ASN
77	v	272	HIS
78	w	22	ASN
79	x	112	HIS
79	x	138	HIS
79	x	142	HIS
79	x	232	ASN

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Mol	Chain	Res	Type
80	y	31	ASN
80	y	114	ASN
81	z	81	HIS
81	z	186	GLN
82	TT	56	HIS
82	TT	113	HIS
83	UU	11	GLN
83	UU	80	GLN
83	UU	97	GLN
85	WW	41	GLN
85	WW	104	GLN
86	XX	116	GLN
86	XX	202	ASN
86	XX	241	ASN
86	XX	244	ASN
86	XX	300	ASN
86	XX	414	ASN
86	XX	465	GLN
87	YY	58	HIS
87	YY	63	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
16	2	73/75 (97%)	26 (35%)	2 (2%)
17	3	72/75 (96%)	16 (22%)	0
18	4	5/6 (83%)	1 (20%)	0
19	5	3519/3544 (99%)	840 (23%)	73 (2%)
21	7	119/120 (99%)	14 (11%)	0
22	8	149/151 (98%)	26 (17%)	1 (0%)
39	K	1686/1698 (99%)	396 (23%)	25 (1%)
All	All	5623/5669 (99%)	1319 (23%)	101 (1%)

All (1319) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
16	2	2	C
16	2	5	C
16	2	8	U
16	2	9	A
16	2	16	C

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Mol	Chain	Res	Type
16	2	19	G
16	2	20	C
16	2	21	A
16	2	22	G
16	2	25	C
16	2	35	A
16	2	42	A
16	2	46	G
16	2	47	U
16	2	48	C
16	2	51	U
16	2	52	G
16	2	53	G
16	2	54	U
16	2	58	A
16	2	59	A
16	2	60	A
16	2	61	C
16	2	62	C
16	2	64	U
16	2	76	A
17	3	7	A
17	3	13	C
17	3	16	C
17	3	19	G
17	3	21	A
17	3	34	U
17	3	35	A
17	3	42	G
17	3	48	C
17	3	49	C
17	3	58	A
17	3	63	C
17	3	69	G
17	3	70	G
17	3	74	C
17	3	76	A
18	4	46	A
19	5	5	A
19	5	8	U
19	5	12	A
19	5	13	U

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Mol	Chain	Res	Type
19	5	17	A
19	5	25	A
19	5	30	C
19	5	34	A
19	5	39	A
19	5	42	A
19	5	44	A
19	5	48	G
19	5	49	U
19	5	56	A
19	5	57	G
19	5	58	G
19	5	59	A
19	5	64	A
19	5	65	A
19	5	72	C
19	5	73	A
19	5	74	G
19	5	77	U
19	5	84	A
19	5	85	G
19	5	91	G
19	5	93	G
19	5	98	A
19	5	104	G
19	5	108	A
19	5	109	G
19	5	112	C
19	5	116	G
19	5	118	C
19	5	119	G
19	5	126	C
19	5	134	G
19	5	135	G
19	5	136	C
19	5	142	G
19	5	143	C
19	5	146	G
19	5	157	U
19	5	159	C
19	5	170	C
19	5	171	U

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Mol	Chain	Res	Type
19	5	172	C
19	5	173	C
19	5	177	G
19	5	179	G
19	5	182	G
19	5	200	U
19	5	201	C
19	5	209	U
19	5	216	C
19	5	218	A
19	5	220	C
19	5	224	U
19	5	226	G
19	5	233	U
19	5	234	G
19	5	245	C
19	5	246	G
19	5	255	C
19	5	256	G
19	5	262	G
19	5	265	C
19	5	266	C
19	5	276	C
19	5	277	G
19	5	278	G
19	5	280	G
19	5	292	G
19	5	297	U
19	5	306	A
19	5	309	C
19	5	310	G
19	5	315	G
19	5	316	U
19	5	322	C
19	5	334	A
19	5	340	C
19	5	345	C
19	5	350	C
19	5	363	A
19	5	387	G
19	5	407	A
19	5	410	A

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Mol	Chain	Res	Type
19	5	412	G
19	5	413	G
19	5	431	G
19	5	432	U
19	5	445	U
19	5	449	C
19	5	450	G
19	5	452	A
19	5	453	G
19	5	454	U
19	5	455	C
19	5	456	C
19	5	463	A
19	5	466	A
19	5	467	U
19	5	468	U
19	5	481	G
19	5	481(A)	C
19	5	482	G
19	5	483	G
19	5	485	C
19	5	486	C
19	5	492	U
19	5	493	G
19	5	495	C
19	5	497	G
19	5	498	C
19	5	499	G
19	5	505	G
19	5	506	C
19	5	510	U
19	5	522	C
19	5	647	G
19	5	658	C
19	5	666	G
19	5	667	A
19	5	668	C
19	5	669	C
19	5	683	C
19	5	684	G
19	5	685	C
19	5	686	A

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Mol	Chain	Res	Type
19	5	687	U
19	5	696	C
19	5	697	G
19	5	704	C
19	5	705	G
19	5	719	C
19	5	722	G
19	5	729	G
19	5	730	G
19	5	731	G
19	5	738	C
19	5	738(A)	C
19	5	742	G
19	5	747	A
19	5	749	G
19	5	751	G
19	5	752	G
19	5	758	G
19	5	908	G
19	5	913	U
19	5	914	U
19	5	915	A
19	5	917	A
19	5	918	G
19	5	923	C
19	5	925	C
19	5	926	G
19	5	928	C
19	5	929	A
19	5	931	C
19	5	932	A
19	5	933	G
19	5	934	C
19	5	935	A
19	5	935(A)	G
19	5	936	C
19	5	939	G
19	5	941	C
19	5	943	A
19	5	945	U
19	5	958	G
19	5	959	G

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Mol	Chain	Res	Type
19	5	960	A
19	5	961	G
19	5	962	C
19	5	964	A
19	5	965	G
19	5	966	A
19	5	967	C
19	5	969	C
19	5	971(A)	G
19	5	972	C
19	5	979	C
19	5	983	C
19	5	1070	G
19	5	1072	C
19	5	1073	G
19	5	1075	G
19	5	1076	C
19	5	1078	A
19	5	1079	C
19	5	1081	C
19	5	1175	A
19	5	1179	U
19	5	1180	C
19	5	1187	G
19	5	1191	C
19	5	1193	C
19	5	1204	C
19	5	1210	C
19	5	1211	G
19	5	1212	G
19	5	1215	C
19	5	1234	G
19	5	1235	G
19	5	1236	C
19	5	1237	C
19	5	1238	A
19	5	1239	C
19	5	1272	C
19	5	1273	G
19	5	1275	G
19	5	1276	C
19	5	1277	G

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Mol	Chain	Res	Type
19	5	1284	G
19	5	1287	G
19	5	1292	C
19	5	1293	G
19	5	1295	U
19	5	1296	G
19	5	1301	C
19	5	1303	A
19	5	1304	C
19	5	1326	A
19	5	1330	A
19	5	1354	A
19	5	1358	G
19	5	1359	G
19	5	1370	G
19	5	1371	A
19	5	1377	G
19	5	1378	C
19	5	1387	A
19	5	1394	G
19	5	1397	A
19	5	1398	A
19	5	1400	G
19	5	1414	C
19	5	1415	G
19	5	1419	G
19	5	1420	A
19	5	1421	G
19	5	1426	G
19	5	1436	C
19	5	1437	C
19	5	1438	U
19	5	1441	C
19	5	1445	U
19	5	1446	C
19	5	1448	G
19	5	1456	C
19	5	1457	G
19	5	1458	C
19	5	1475	G
19	5	1478	C
19	5	1482	G

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Mol	Chain	Res	Type
19	5	1483	C
19	5	1484	G
19	5	1494	U
19	5	1497	A
19	5	1498	G
19	5	1502	G
19	5	1515	A
19	5	1518	A
19	5	1523	A
19	5	1525	A
19	5	1534	A
19	5	1546	C
19	5	1547	A
19	5	1563	A
19	5	1564	A
19	5	1566	C
19	5	1574	G
19	5	1578	U
19	5	1586	G
19	5	1591	U
19	5	1596	U
19	5	1597	G
19	5	1602	U
19	5	1612	G
19	5	1613	A
19	5	1624	G
19	5	1625	G
19	5	1631	A
19	5	1633	G
19	5	1634	A
19	5	1638	A
19	5	1640	C
19	5	1641	G
19	5	1642	A
19	5	1654	G
19	5	1661	C
19	5	1676	C
19	5	1677	U
19	5	1678	C
19	5	1680	G
19	5	1691	G
19	5	1724	G

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Mol	Chain	Res	Type
19	5	1731	C
19	5	1734	G
19	5	1741	G
19	5	1742	A
19	5	1750	G
19	5	1754	U
19	5	1755	C
19	5	1756	U
19	5	1761	G
19	5	1764	G
19	5	1772	C
19	5	1773	U
19	5	1774	C
19	5	1776	A
19	5	1780	A
19	5	1781	U
19	5	1785	C
19	5	1787	A
19	5	1797	G
19	5	1800	U
19	5	1803	G
19	5	1804	A
19	5	1805	A
19	5	1819	G
19	5	1821	G
19	5	1822	U
19	5	1828	C
19	5	1830	G
19	5	1834	U
19	5	1835	G
19	5	1836	G
19	5	1837	A
19	5	1842	G
19	5	1843	A
19	5	1850	A
19	5	1855	G
19	5	1863	U
19	5	1866	U
19	5	1869	G
19	5	1882	U
19	5	1886	G
19	5	1888	A

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Mol	Chain	Res	Type
19	5	1892	A
19	5	1893	C
19	5	1897	A
19	5	1898	C
19	5	1910	G
19	5	1917	A
19	5	1918	U
19	5	1920	C
19	5	1921	C
19	5	1922	G
19	5	1925	G
19	5	1930	U
19	5	1931	C
19	5	1935	C
19	5	1945	G
19	5	1948	G
19	5	1951	G
19	5	1952	G
19	5	1957	U
19	5	1958	A
19	5	1959	U
19	5	1961	G
19	5	1962	A
19	5	1964	A
19	5	1971	U
19	5	1976	G
19	5	1977	C
19	5	1978	C
19	5	1980	U
19	5	1983	A
19	5	1984	A
19	5	1985	G
19	5	1986	U
19	5	1987	C
19	5	1991	A
19	5	1993	C
19	5	1997	U
19	5	2001	G
19	5	2002	A
19	5	2003	G
19	5	2004	U
19	5	2011	C

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Mol	Chain	Res	Type
19	5	2024	G
19	5	2025	A
19	5	2026	A
19	5	2034	G
19	5	2044	U
19	5	2046	G
19	5	2047	A
19	5	2048	U
19	5	2052	G
19	5	2055	G
19	5	2056	G
19	5	2062	C
19	5	2064	G
19	5	2069	A
19	5	2079	G
19	5	2084	U
19	5	2085	G
19	5	2089	G
19	5	2090	U
19	5	2092	G
19	5	2093	G
19	5	2094	C
19	5	2095	A
19	5	2097	A
19	5	2098	G
19	5	2100	G
19	5	2101	A
19	5	2102	G
19	5	2104	A
19	5	2105	A
19	5	2106	G
19	5	2107	A
19	5	2108	G
19	5	2259	G
19	5	2260	C
19	5	2267	U
19	5	2268	A
19	5	2270	G
19	5	2273	G
19	5	2275	G
19	5	2289	C
19	5	2300	A

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Mol	Chain	Res	Type
19	5	2301	G
19	5	2306	G
19	5	2313	A
19	5	2314	G
19	5	2325	C
19	5	2331	G
19	5	2332	A
19	5	2333	G
19	5	2345	G
19	5	2348	G
19	5	2351	C
19	5	2360	A
19	5	2364	G
19	5	2370	A
19	5	2377	C
19	5	2395	A
19	5	2399	G
19	5	2417	A
19	5	2422	C
19	5	2424	G
19	5	2425	U
19	5	2428	A
19	5	2433	G
19	5	2436	U
19	5	2437	C
19	5	2440	U
19	5	2441	C
19	5	2447	U
19	5	2450	G
19	5	2453	A
19	5	2460	A
19	5	2469	C
19	5	2471	G
19	5	2474	G
19	5	2475	G
19	5	2485	U
19	5	2487	G
19	5	2488	C
19	5	2489	C
19	5	2490	U
19	5	2491	C
19	5	2503	G

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Mol	Chain	Res	Type
19	5	2504	C
19	5	2505	C
19	5	2506	G
19	5	2513	A
19	5	2529	A
19	5	2530	U
19	5	2537	A
19	5	2546	G
19	5	2547	G
19	5	2549	G
19	5	2553	A
19	5	2566	G
19	5	2575	U
19	5	2583	C
19	5	2586	G
19	5	2587	A
19	5	2591	A
19	5	2600	A
19	5	2601	A
19	5	2627	C
19	5	2631	U
19	5	2638	G
19	5	2640	G
19	5	2653	C
19	5	2659	A
19	5	2661	U
19	5	2662	G
19	5	2669	C
19	5	2670	C
19	5	2673	G
19	5	2675	G
19	5	2686	G
19	5	2687	U
19	5	2689	C
19	5	2694	G
19	5	2695	A
19	5	2696	A
19	5	2707	U
19	5	2708	U
19	5	2709	C
19	5	2710	C
19	5	2711	G

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Mol	Chain	Res	Type
19	5	2714	G
19	5	2715	G
19	5	2716	C
19	5	2725	A
19	5	2726	G
19	5	2735	G
19	5	2738	C
19	5	2740	U
19	5	2743	A
19	5	2744	A
19	5	2754	G
19	5	2759	G
19	5	2760	G
19	5	2763	U
19	5	2764	A
19	5	2769	U
19	5	2772	C
19	5	2787	A
19	5	2788	U
19	5	2790	U
19	5	2793	G
19	5	2794	C
19	5	2795	A
19	5	2798	A
19	5	2801	U
19	5	2806	A
19	5	2807	A
19	5	2808	G
19	5	2814	C
19	5	2826	U
19	5	2827	G
19	5	2828	U
19	5	2838	G
19	5	2842	G
19	5	2845	A
19	5	2855	G
19	5	2897	G
19	5	2898	G
19	5	3601	C
19	5	3604	A
19	5	3605	C
19	5	3606	U

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Mol	Chain	Res	Type
19	5	3616	U
19	5	3618	C
19	5	3619	G
19	5	3625	G
19	5	3626	G
19	5	3635	A
19	5	3636	C
19	5	3644	U
19	5	3646	A
19	5	3650	C
19	5	3662	A
19	5	3664	G
19	5	3670	C
19	5	3673	C
19	5	3674	G
19	5	3681	G
19	5	3691	G
19	5	3696	C
19	5	3711	A
19	5	3712	A
19	5	3729	U
19	5	3737	A
19	5	3740	G
19	5	3747	A
19	5	3748	A
19	5	3753	G
19	5	3760	A
19	5	3763	A
19	5	3766	A
19	5	3767	C
19	5	3773	U
19	5	3774	A
19	5	3776	G
19	5	3777	G
19	5	3784	A
19	5	3786	U
19	5	3799	A
19	5	3810	C
19	5	3811	G
19	5	3812	C
19	5	3814	U
19	5	3817	A

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Mol	Chain	Res	Type
19	5	3819	G
19	5	3822	U
19	5	3838	U
19	5	3839	G
19	5	3840	U
19	5	3843	C
19	5	3869	C
19	5	3877	A
19	5	3878	C
19	5	3879	G
19	5	3880	G
19	5	3889	G
19	5	3892	U
19	5	3897	G
19	5	3901	A
19	5	3902	A
19	5	3904	G
19	5	3905	A
19	5	3906	A
19	5	3907	G
19	5	3915	U
19	5	3916	G
19	5	3918	G
19	5	3926	C
19	5	3927	U
19	5	3939	G
19	5	3943	A
19	5	4069	U
19	5	4070	U
19	5	4073	A
19	5	4076	G
19	5	4085	A
19	5	4086	G
19	5	4088	C
19	5	4092	G
19	5	4097	G
19	5	4116	C
19	5	4117	U
19	5	4118	U
19	5	4119	C
19	5	4120	U
19	5	4122	G

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Mol	Chain	Res	Type
19	5	4127	A
19	5	4150	G
19	5	4158	C
19	5	4161	G
19	5	4163	U
19	5	4164	C
19	5	4171	C
19	5	4183	G
19	5	4184	G
19	5	4191	G
19	5	4201	G
19	5	4203	A
19	5	4212	A
19	5	4228	G
19	5	4229	U
19	5	4232	U
19	5	4233	A
19	5	4238	G
19	5	4249	G
19	5	4251	A
19	5	4254	G
19	5	4255	A
19	5	4256	A
19	5	4257	A
19	5	4266	G
19	5	4267	G
19	5	4268	A
19	5	4271	A
19	5	4273	A
19	5	4278	C
19	5	4281	A
19	5	4282	A
19	5	4291	G
19	5	4296	U
19	5	4297	G
19	5	4304	A
19	5	4305	G
19	5	4306	U
19	5	4314	C
19	5	4317	A
19	5	4318	C
19	5	4323	A

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Mol	Chain	Res	Type
19	5	4329	G
19	5	4330	G
19	5	4332	C
19	5	4338	G
19	5	4339	A
19	5	4349	C
19	5	4354	U
19	5	4355	G
19	5	4368	G
19	5	4373	G
19	5	4374	U
19	5	4376	A
19	5	4377	G
19	5	4378	A
19	5	4380	A
19	5	4382	G
19	5	4387	C
19	5	4393	G
19	5	4394	A
19	5	4395	U
19	5	4398	C
19	5	4401	G
19	5	4411	G
19	5	4419	U
19	5	4420	U
19	5	4421	C
19	5	4422	A
19	5	4430	G
19	5	4436	U
19	5	4440	G
19	5	4444	C
19	5	4448	G
19	5	4449	A
19	5	4464	A
19	5	4471	U
19	5	4472	G
19	5	4475	G
19	5	4482	U
19	5	4488	A
19	5	4500	U
19	5	4510	A
19	5	4511	A

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Mol	Chain	Res	Type
19	5	4512	U
19	5	4513	A
19	5	4515	G
19	5	4518	A
19	5	4519	C
19	5	4520	G
19	5	4523	A
19	5	4524	G
19	5	4531	U
19	5	4548	A
19	5	4549	G
19	5	4560	C
19	5	4567	G
19	5	4570	G
19	5	4573	G
19	5	4574	U
19	5	4575	G
19	5	4590	A
19	5	4599	A
19	5	4606	G
19	5	4608	G
19	5	4626	A
19	5	4636	U
19	5	4637	G
19	5	4639	G
19	5	4656	A
19	5	4657	U
19	5	4661	G
19	5	4664	A
19	5	4670	C
19	5	4672	A
19	5	4677	U
19	5	4678	G
19	5	4687	A
19	5	4700	A
19	5	4709	U
19	5	4719	G
19	5	4720	C
19	5	4728	U
19	5	4736	C
19	5	4745	G
19	5	4747	C

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Mol	Chain	Res	Type
19	5	4750	G
19	5	4751	G
19	5	4753	U
19	5	4754	G
19	5	4756	C
19	5	4757	C
19	5	4759	C
19	5	4761	G
19	5	4763	U
19	5	4764	A
19	5	4765	G
19	5	4771	C
19	5	4772	C
19	5	4776	G
19	5	4867	G
19	5	4870	G
19	5	4871	C
19	5	4872	G
19	5	4873	G
19	5	4874	A
19	5	4875	G
19	5	4882	U
19	5	4883	C
19	5	4885	U
19	5	4891	G
19	5	4895	C
19	5	4904	G
19	5	4910	A
19	5	4911	A
19	5	4913	G
19	5	4914	G
19	5	4915	G
19	5	4918	C
19	5	4919	G
19	5	4920	C
19	5	4921	C
19	5	4922	C
19	5	4924	C
19	5	4925	U
19	5	4926	C
19	5	4928	C
19	5	4931	G

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Mol	Chain	Res	Type
19	5	4934	A
19	5	4937	C
19	5	4938	A
19	5	4940	C
19	5	4943	A
19	5	4944	C
19	5	4948	C
19	5	4949	G
19	5	4950	U
19	5	4951	G
19	5	4956	A
19	5	4957	C
19	5	4958	C
19	5	4960	G
19	5	4963	G
19	5	4965	U
19	5	4966	A
19	5	4967	A
19	5	4976	U
19	5	4985	U
19	5	4988	U
19	5	4989	U
19	5	4990	C
19	5	4991	U
19	5	4993	G
19	5	5014	A
19	5	5017	G
19	5	5041	G
19	5	5047	C
19	5	5050	C
19	5	5052	C
19	5	5053	U
19	5	5054	C
19	5	5056	A
19	5	5058	A
19	5	5061	A
19	5	5062	G
19	5	5067	U
21	7	7	G
21	7	25	G
21	7	42	A
21	7	53	U

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Mol	Chain	Res	Type
21	7	54	A
21	7	64	G
21	7	74	A
21	7	76	U
21	7	97	G
21	7	100	A
21	7	109	U
21	7	110	G
21	7	111	C
21	7	120	U
22	8	2	G
22	8	34	U
22	8	35	C
22	8	38	U
22	8	59	A
22	8	62	A
22	8	63	U
22	8	75	G
22	8	79	G
22	8	86	U
22	8	87	G
22	8	103	A
22	8	104	A
22	8	105	C
22	8	109	C
22	8	110	U
22	8	111	U
22	8	114	G
22	8	123	U
22	8	124	U
22	8	125	C
22	8	126	C
22	8	127	U
22	8	137	A
22	8	147	G
22	8	151	G
39	K	3	C
39	K	4	C
39	K	17	C
39	K	25	A
39	K	26	U
39	K	33	G

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Mol	Chain	Res	Type
39	K	41	G
39	K	44	U
39	K	45	A
39	K	46	A
39	K	56	G
39	K	58	C
39	K	63	U
39	K	67	C
39	K	68	A
39	K	70	G
39	K	71	G
39	K	73	C
39	K	74	G
39	K	75	G
39	K	77	A
39	K	79	A
39	K	81	U
39	K	99	A
39	K	103	A
39	K	111	A
39	K	113	G
39	K	115	U
39	K	124	U
39	K	126	G
39	K	127	C
39	K	129	C
39	K	130	G
39	K	141	A
39	K	142	C
39	K	143	U
39	K	146	G
39	K	147	A
39	K	154	U
39	K	155	G
39	K	158	A
39	K	162	C
39	K	163	U
39	K	167	G
39	K	168	C
39	K	178	C
39	K	180	G
39	K	182	C

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Mol	Chain	Res	Type
39	K	183	G
39	K	184	G
39	K	187	G
39	K	188	C
39	K	190	G
39	K	191	A
39	K	192	C
39	K	202	G
39	K	213	G
39	K	215	G
39	K	289	G
39	K	290	U
39	K	292	A
39	K	294	U
39	K	304	C
39	K	305	U
39	K	307	G
39	K	308	G
39	K	309	G
39	K	312	G
39	K	314	U
39	K	318	A
39	K	319	C
39	K	323	C
39	K	332	G
39	K	339	A
39	K	347	G
39	K	350	C
39	K	351	G
39	K	360	A
39	K	362	C
39	K	364	A
39	K	368	U
39	K	369	C
39	K	370	G
39	K	372	U
39	K	381	C
39	K	382	C
39	K	385	G
39	K	386	C
39	K	398	A
39	K	400	C

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Mol	Chain	Res	Type
39	K	408	A
39	K	409	C
39	K	417	C
39	K	418	A
39	K	428	U
39	K	435	A
39	K	438	G
39	K	441	C
39	K	448	A
39	K	449	A
39	K	450	C
39	K	464	A
39	K	465	A
39	K	466	G
39	K	471	G
39	K	472	C
39	K	473	A
39	K	474	G
39	K	482	G
39	K	487	U
39	K	492	C
39	K	496	C
39	K	525	A
39	K	530	U
39	K	531	A
39	K	532	C
39	K	533	A
39	K	544	G
39	K	548	C
39	K	549	C
39	K	550	C
39	K	551	U
39	K	554	A
39	K	555	A
39	K	556	U
39	K	559	G
39	K	560	A
39	K	563	G
39	K	564	A
39	K	568	C
39	K	570	C
39	K	573	U

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Mol	Chain	Res	Type
39	K	576	A
39	K	583	A
39	K	587	A
39	K	588	G
39	K	589	G
39	K	590	A
39	K	591	U
39	K	600	G
39	K	603	C
39	K	604	A
39	K	605	A
39	K	606	G
39	K	608	C
39	K	614	C
39	K	617	G
39	K	627	U
39	K	628	A
39	K	629	A
39	K	631	U
39	K	632	C
39	K	643	A
39	K	644	G
39	K	655	A
39	K	659	G
39	K	660	C
39	K	662	G
39	K	668	A
39	K	669	A
39	K	670	A
39	K	671	A
39	K	672	A
39	K	684	G
39	K	687	C
39	K	688	U
39	K	689	U
39	K	690	G
39	K	752	G
39	K	753	C
39	K	754	G
39	K	798	G
39	K	799	U
39	K	810	A

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Mol	Chain	Res	Type
39	K	811	A
39	K	812	A
39	K	818	A
39	K	821	G
39	K	822	U
39	K	830	A
39	K	834	C
39	K	847	A
39	K	867	G
39	K	868	G
39	K	869	A
39	K	870	A
39	K	871	U
39	K	872	A
39	K	873	G
39	K	874	G
39	K	875	A
39	K	878	G
39	K	887	U
39	K	888	U
39	K	890	U
39	K	892	U
39	K	903	A
39	K	906	U
39	K	907	G
39	K	913	A
39	K	914	U
39	K	918	U
39	K	920	A
39	K	930	C
39	K	933	G
39	K	934	G
39	K	943	U
39	K	958	G
39	K	971	G
39	K	989	C
39	K	990	A
39	K	992	A
39	K	999	G
39	K	1002	U
39	K	1009	A
39	K	1017	U

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Mol	Chain	Res	Type
39	K	1023	A
39	K	1041	G
39	K	1050	A
39	K	1058	A
39	K	1060	A
39	K	1062	A
39	K	1067	C
39	K	1083	A
39	K	1085	C
39	K	1089	G
39	K	1100	A
39	K	1109	C
39	K	1113	A
39	K	1115	U
39	K	1116	C
39	K	1117	C
39	K	1118	C
39	K	1123	C
39	K	1131	G
39	K	1133	A
39	K	1138	C
39	K	1139	C
39	K	1148	A
39	K	1153	C
39	K	1154	U
39	K	1155	U
39	K	1170	A
39	K	1195	A
39	K	1207	G
39	K	1208	A
39	K	1215	C
39	K	1220	A
39	K	1224	G
39	K	1240	A
39	K	1242	U
39	K	1245	G
39	K	1251	A
39	K	1253	A
39	K	1256	G
39	K	1257	G
39	K	1259	A
39	K	1265	A

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Mol	Chain	Res	Type
39	K	1271	C
39	K	1274	G
39	K	1275	G
39	K	1280	G
39	K	1281	G
39	K	1282	A
39	K	1284	A
39	K	1285	G
39	K	1286	G
39	K	1291	A
39	K	1293	A
39	K	1295	A
39	K	1299	A
39	K	1301	A
39	K	1302	G
39	K	1303	C
39	K	1307	U
39	K	1308	U
39	K	1310	U
39	K	1313	A
39	K	1314	U
39	K	1315	U
39	K	1316	C
39	K	1322	G
39	K	1341	C
39	K	1342	U
39	K	1348	G
39	K	1371	U
39	K	1372	U
39	K	1376	A
39	K	1378	A
39	K	1382	A
39	K	1384	C
39	K	1386	A
39	K	1395	C
39	K	1396	A
39	K	1397	U
39	K	1401	A
39	K	1402	A
39	K	1404	U
39	K	1410	C
39	K	1411	G

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Mol	Chain	Res	Type
39	K	1428	G
39	K	1429	G
39	K	1439	A
39	K	1454	A
39	K	1459	G
39	K	1462	U
39	K	1463	U
39	K	1466	G
39	K	1473	G
39	K	1476	A
39	K	1477	U
39	K	1478	U
39	K	1480	A
39	K	1487	A
39	K	1488	C
39	K	1489	A
39	K	1490	G
39	K	1497	G
39	K	1498	A
39	K	1507	G
39	K	1509	U
39	K	1510	G
39	K	1521	C
39	K	1522	A
39	K	1523	C
39	K	1531	A
39	K	1533	A
39	K	1544	C
39	K	1548	G
39	K	1552	G
39	K	1553	C
39	K	1554	C
39	K	1555	U
39	K	1556	A
39	K	1557	C
39	K	1560	U
39	K	1570	G
39	K	1575	G
39	K	1580	A
39	K	1581	C
39	K	1585	U
39	K	1586	U

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Mol	Chain	Res	Type
39	K	1587	G
39	K	1588	A
39	K	1598	G
39	K	1601	A
39	K	1604	G
39	K	1621	U
39	K	1623	A
39	K	1625	U
39	K	1637	A
39	K	1638	G
39	K	1648	G
39	K	1654	G
39	K	1664	A
39	K	1665	G
39	K	1671	G
39	K	1680	G
39	K	1683	C
39	K	1695	A
39	K	1698	C
39	K	1699	A
39	K	1701	C
39	K	1715	A
39	K	1721	U
39	K	1722	G
39	K	1726	G
39	K	1744	G
39	K	1746	U
39	K	1748	G
39	K	1753	C
39	K	1757	G
39	K	1758	G
39	K	1783	C
39	K	1785	C
39	K	1800	A
39	K	1823	A
39	K	1825	A
39	K	1826	G
39	K	1829	G
39	K	1831	A
39	K	1836	G
39	K	1837	G
39	K	1838	U

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Mol	Chain	Res	Type
39	K	1845	A
39	K	1849	G
39	K	1851	A
39	K	1852	C
39	K	1859	A
39	K	1861	G
39	K	1862	G
39	K	1863	A
39	K	1865	C
39	K	1866	A
39	K	1867	U
39	K	1869	A

All (101) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
16	2	20	C
16	2	60	A
19	5	48	G
19	5	125	C
19	5	134	G
19	5	217	C
19	5	224	U
19	5	245	C
19	5	265	C
19	5	275	C
19	5	406	C
19	5	408	A
19	5	449	C
19	5	480	C
19	5	485	C
19	5	492	U
19	5	504	G
19	5	685	C
19	5	696	C
19	5	922(B)	C
19	5	930	G
19	5	959	G
19	5	966	A
19	5	971(A)	G
19	5	1072	C
19	5	1174	G

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Mol	Chain	Res	Type
19	5	1211	G
19	5	1236	C
19	5	1238	A
19	5	1291	G
19	5	1329	G
19	5	1370	G
19	5	1440	U
19	5	1445	U
19	5	1455	G
19	5	1563	A
19	5	1633	G
19	5	1804	A
19	5	1818	G
19	5	1834	U
19	5	1921	C
19	5	1979	A
19	5	1983	A
19	5	2046	G
19	5	2068	C
19	5	2089	G
19	5	2266	C
19	5	2468	U
19	5	2474	G
19	5	2502	A
19	5	2513	A
19	5	2529	A
19	5	2546	G
19	5	2587	A
19	5	2661	U
19	5	2695	A
19	5	3625	G
19	5	3765	G
19	5	3876	A
19	5	3888	G
19	5	3904	G
19	5	4119	C
19	5	4170	A
19	5	4232	U
19	5	4254	G
19	5	4354	U
19	5	4448	G
19	5	4464	A

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Mol	Chain	Res	Type
19	5	4510	A
19	5	4699	U
19	5	4719	G
19	5	4884	G
19	5	4925	U
19	5	4936	G
19	5	4947	U
22	8	124	U
39	K	110	U
39	K	182	C
39	K	369	C
39	K	434	G
39	K	465	A
39	K	532	C
39	K	553	U
39	K	642	U
39	K	688	U
39	K	752	G
39	K	870	A
39	K	872	A
39	K	874	G
39	K	912	C
39	K	1061	U
39	K	1114	U
39	K	1137	U
39	K	1394	G
39	K	1395	C
39	K	1396	A
39	K	1489	A
39	K	1520	G
39	K	1637	A
39	K	1664	A
39	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 monosaccharides 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 [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
19	5	24
39	K	11
86	XX	6
17	3	2
22	8	1
16	2	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	41.14
1	5	1252:C	O3'	1271:G	P	36.47
1	5	1219:G	O3'	1233:G	P	20.39
1	K	697:G	O3'	729:C	P	18.51
1	5	3948:C	O3'	4065:G	P	18.39
1	K	834:C	O3'	841:G	P	18.02
1	K	756:C	O3'	788:G	P	17.51
1	5	523:C	O3'	638:G	P	17.16
1	5	990:C	O3'	1064:G	P	17.06
1	K	1761:U	O3'	1771:G	P	17.03
1	5	4101:C	O3'	4107:G	P	16.93

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	K	323:C	O3'	329:G	P	16.68
1	5	4777:C	O3'	4859:C	P	16.43
1	5	4138:C	O3'	4146:G	P	16.19
1	K	1417:C	O3'	1423:C	P	15.71
1	K	130:G	O3'	140:U	P	15.19
1	5	5022:U	O3'	5028:G	P	14.70
1	5	1696:C	O3'	1720:C	P	14.56
1	5	2901:G	O3'	3597:G	P	13.53
1	5	760:G	O3'	904:C	P	13.50
1	5	1364:U	O3'	1368:A	P	13.46
1	5	182:G	O3'	189:G	P	13.44
1	8	79:G	O3'	85:U	P	12.67
1	5	512:U	O3'	515:C	P	10.15
1	5	1180:C	O3'	1183:C	P	9.83
1	5	4729:A	O3'	4735:G	P	9.21
1	K	225:G	O3'	287:U	P	8.51
1	K	745:C	O3'	749:U	P	8.30
1	XX	133:MET	C	145:SER	N	7.02
1	K	736:C	O3'	743:U	P	6.46
1	5	500:G	O3'	504:G	P	5.93
1	2	16:C	O3'	18:G	P	5.89
1	3	19:G	O3'	20:U	P	5.81
1	5	1100:U	O3'	1168:G	P	5.29
1	5	4740:G	O3'	4743:G	P	5.03
1	5	1239:C	O3'	1244:G	P	5.01
1	K	1432:U	O3'	1438:A	P	4.66
1	5	1438:U	O3'	1440:U	P	4.07
1	3	16:C	O3'	18:U	P	3.95
1	XX	101:GLU	C	102:VAL	N	3.60
1	5	4899:G	O3'	4902:C	P	3.56
1	XX	77:MET	C	78:GLU	N	2.76
1	XX	442:GLY	C	443:SER	N	2.47
1	XX	439:GLY	C	440:ALA	N	2.23
1	XX	107:LYS	C	108:ASP	N	1.94

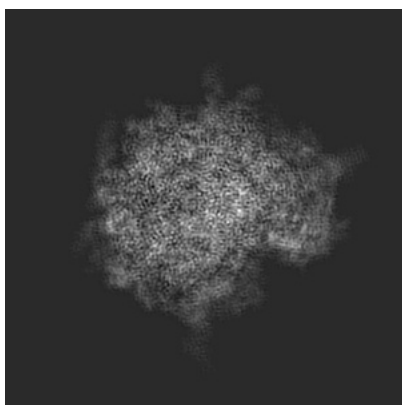
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4745. These allow visual inspection of the internal detail of the map and identification of artifacts.

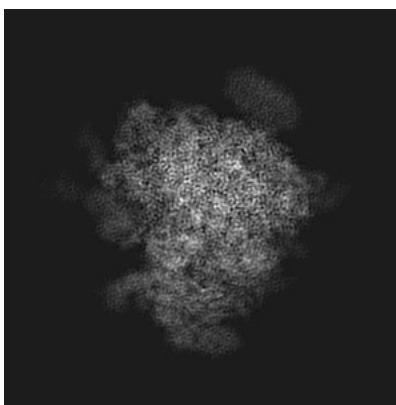
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

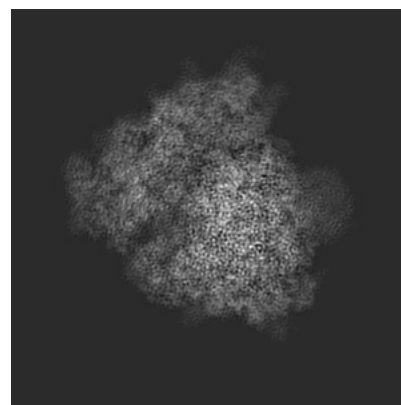
6.1.1 Primary map



X



Y

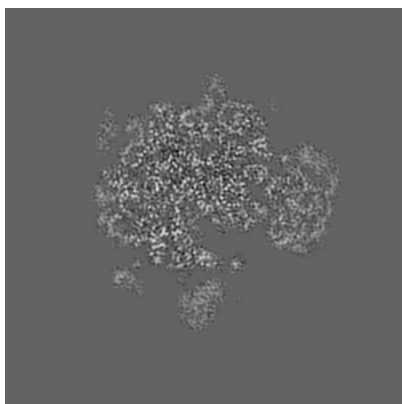


Z

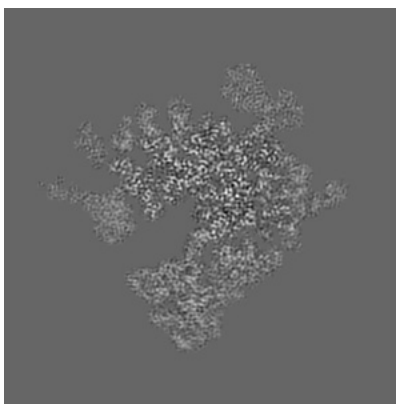
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

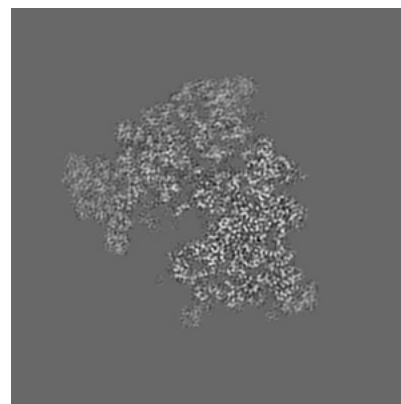
6.2.1 Primary map



X Index: 198



Y Index: 198

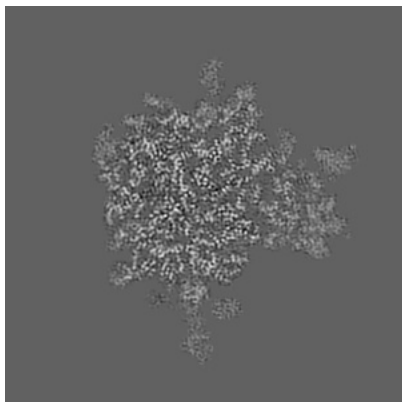


Z Index: 198

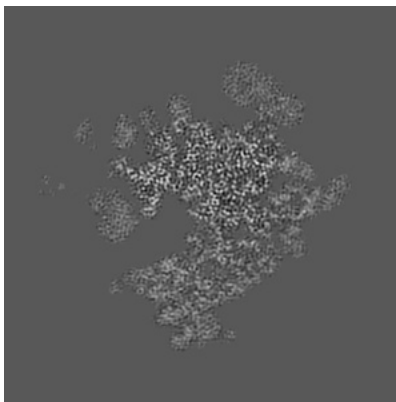
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

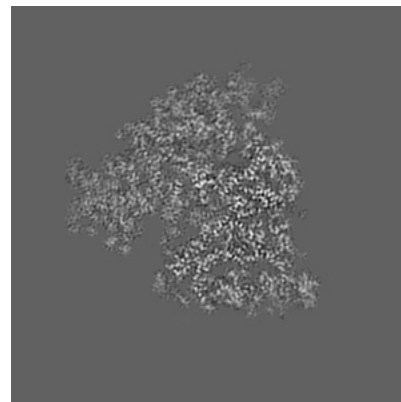
6.3.1 Primary map



X Index: 215



Y Index: 204

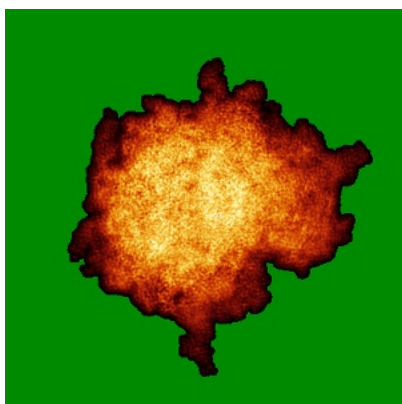


Z Index: 191

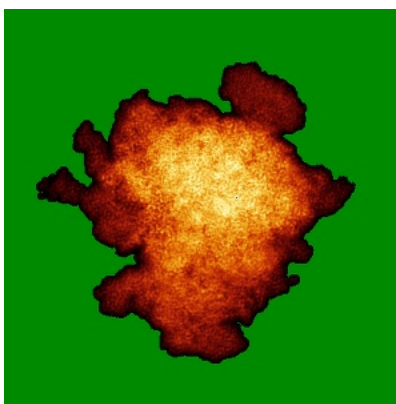
The images above show the largest variance slices of the map in three orthogonal directions.

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

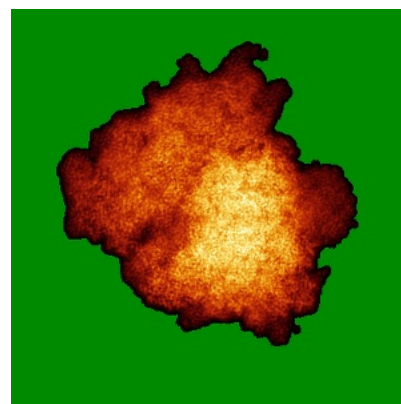
6.4.1 Primary map



X



Y

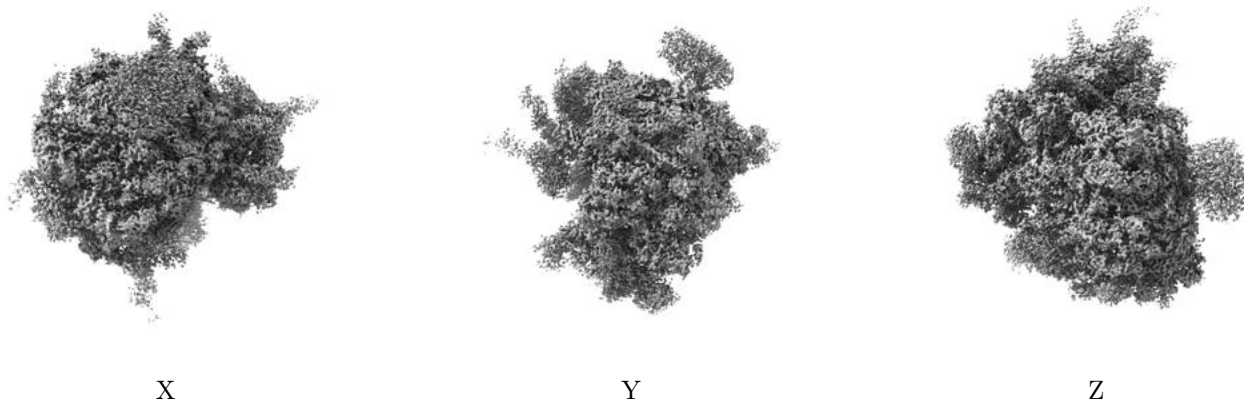


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

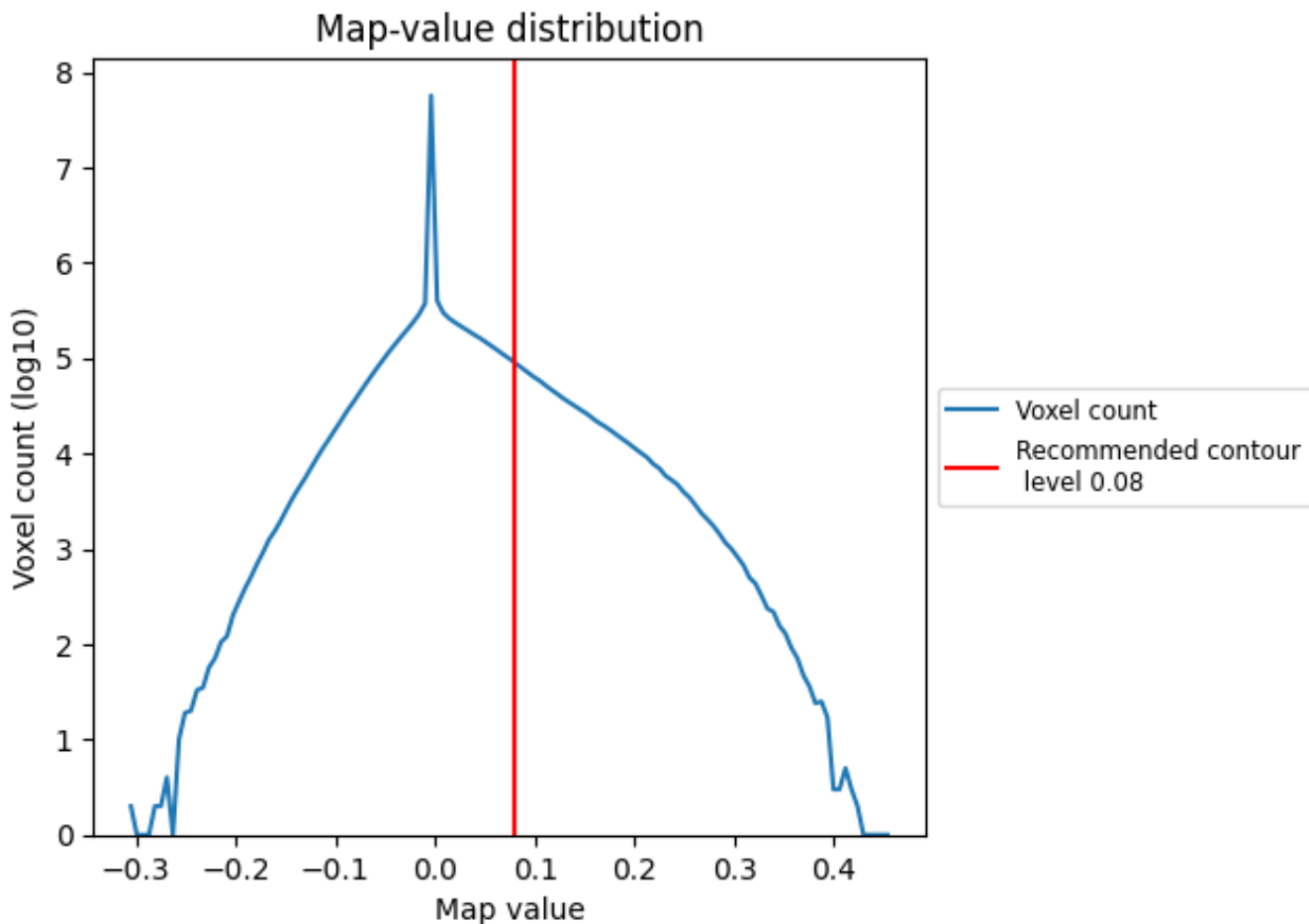
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

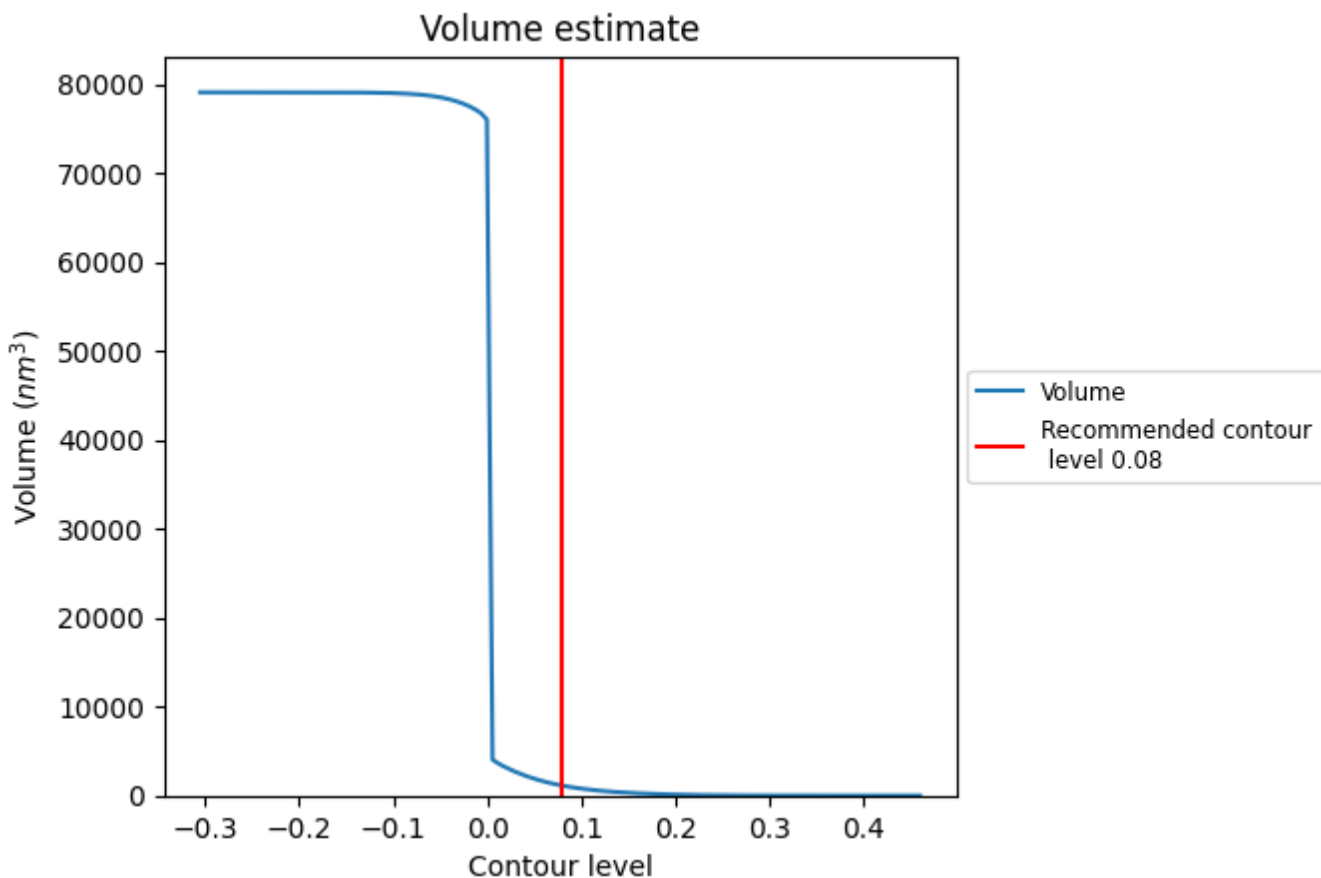
This section contains the results of statistical analysis of the map.

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.

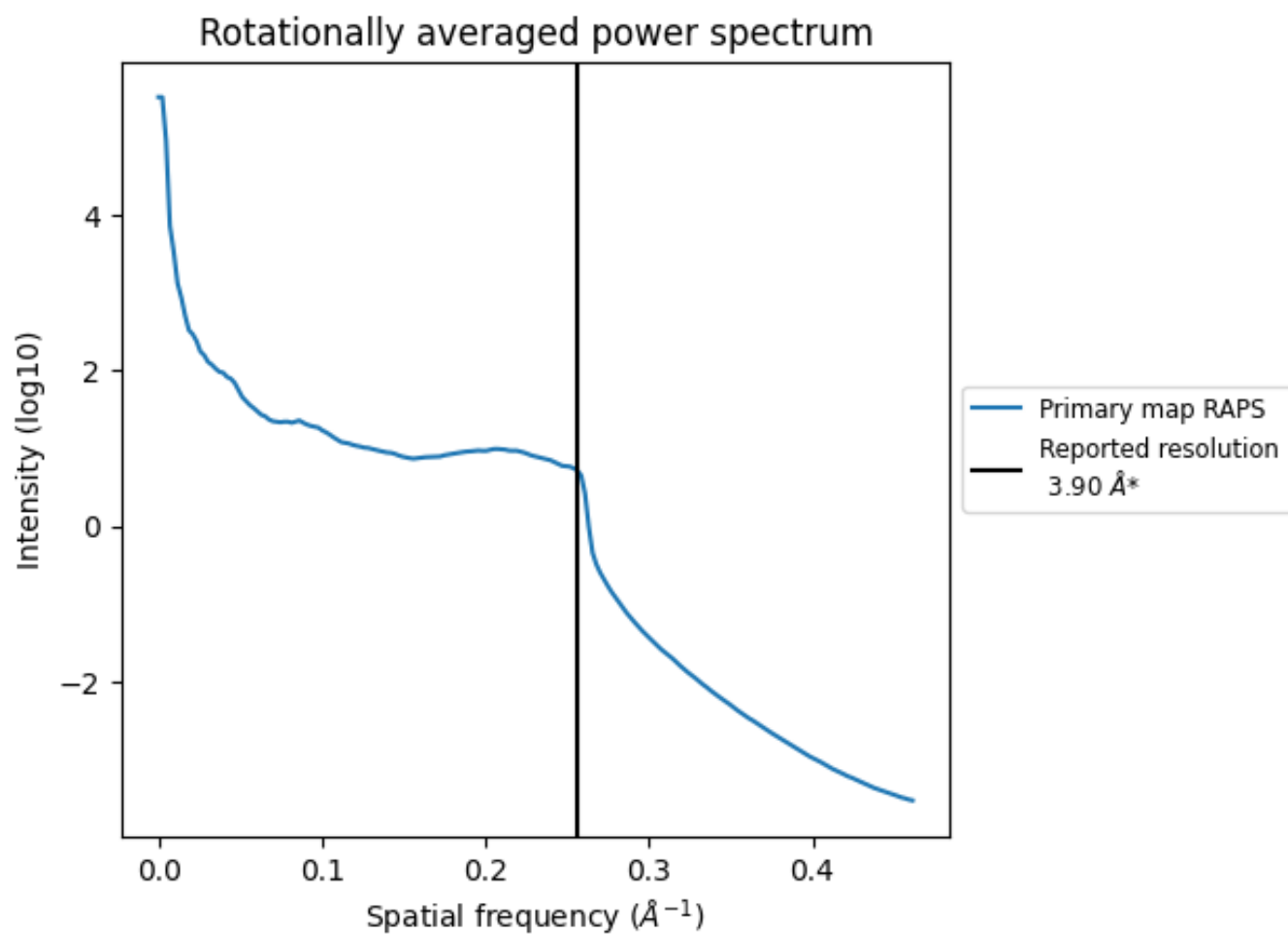
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 11111 nm³; this corresponds to an approximate mass of 1003 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

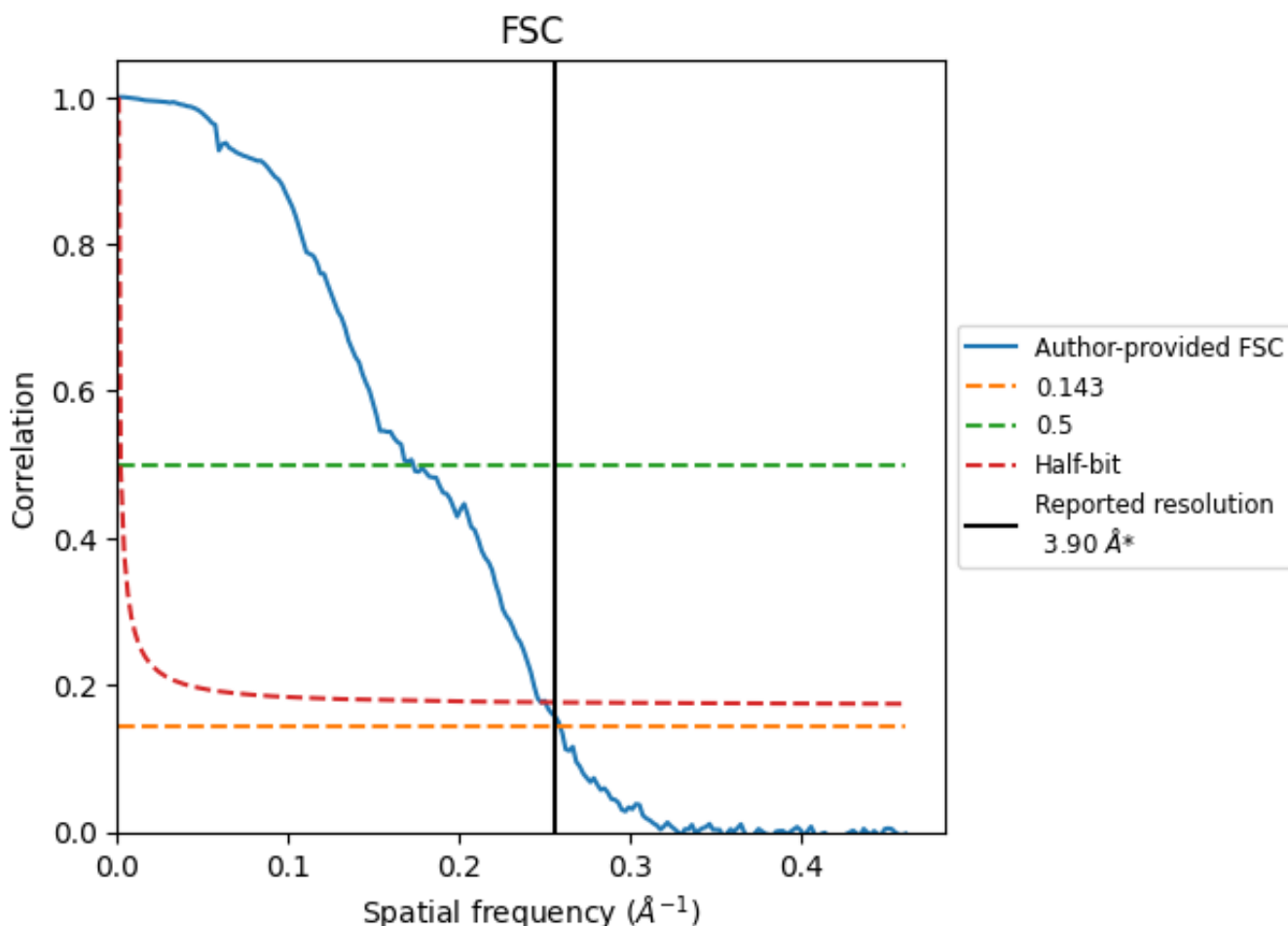


*Reported resolution corresponds to spatial frequency of 0.256\AA^{-1}

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 0.256 Å⁻¹

8.2 Resolution estimates [i](#)

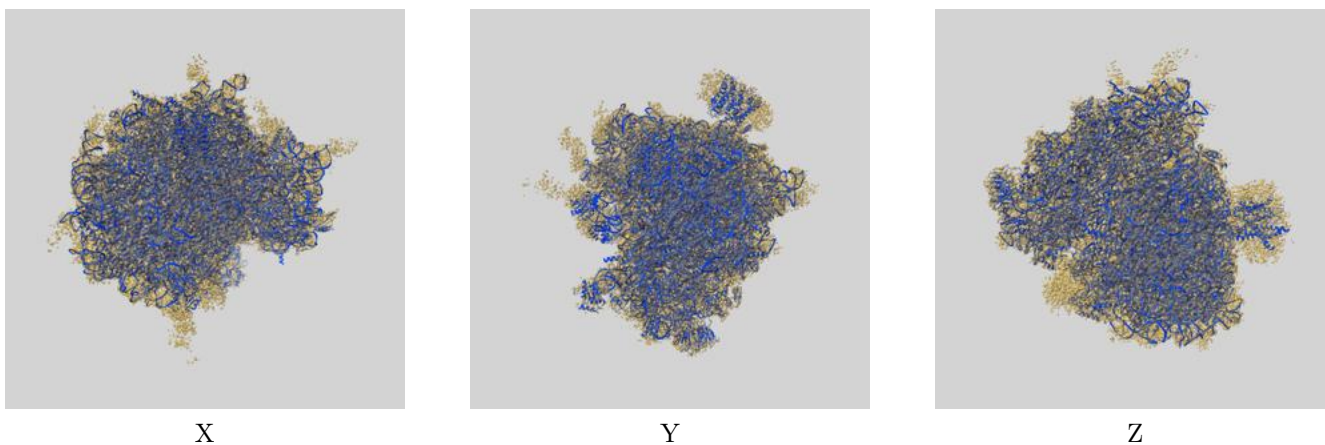
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.86	5.78	4.03
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

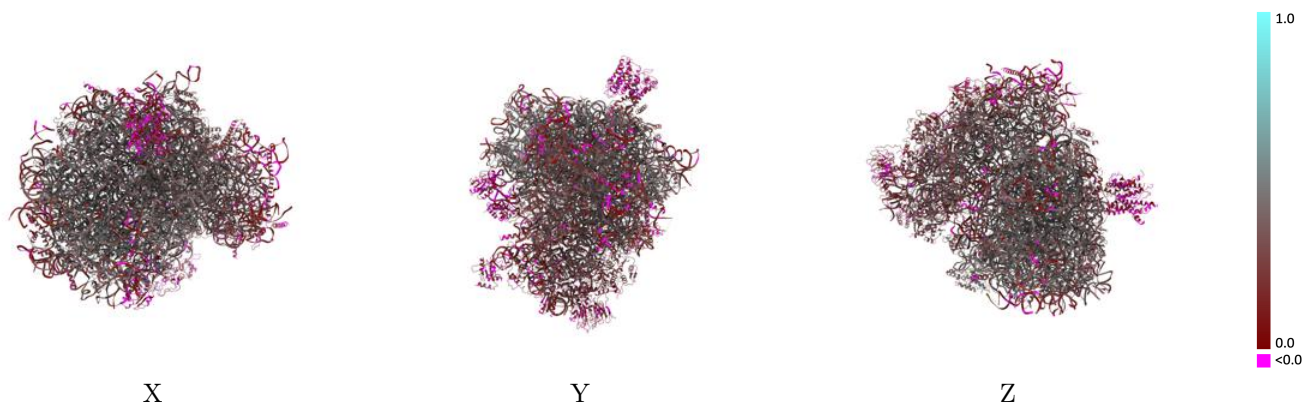
This section contains information regarding the fit between EMDB map EMD-4745 and PDB model 6R7Q. Per-residue inclusion information can be found in section 3 on page 23.

9.1 Map-model overlay [i](#)



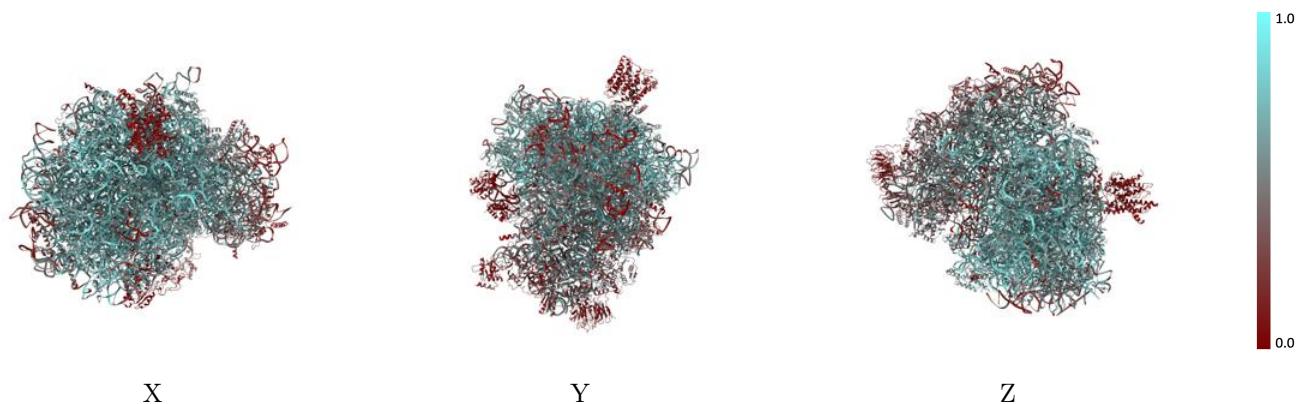
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



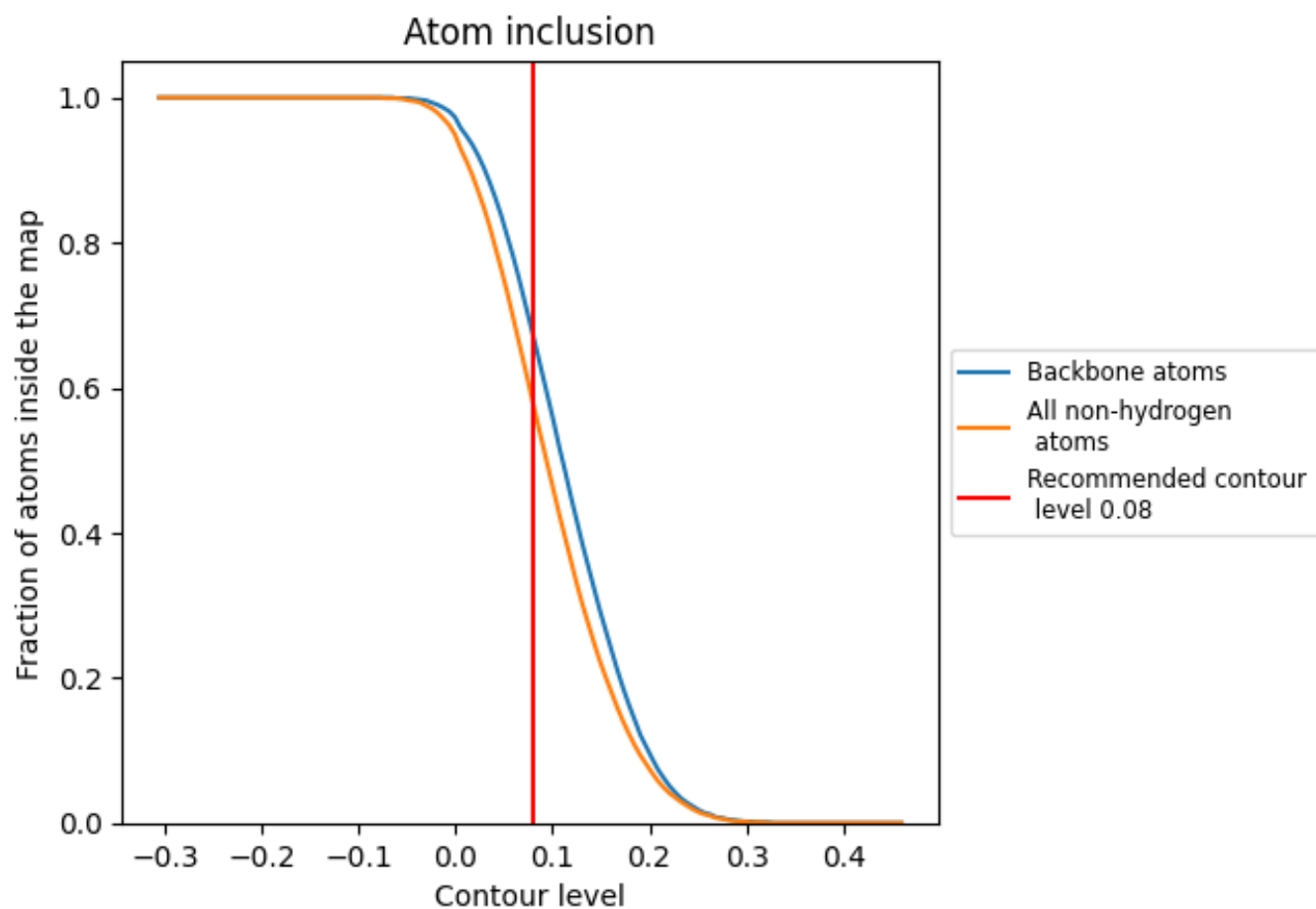
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.08).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 67% of all backbone atoms, 58% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5780	 0.3400
0	 0.1760	 0.1040
1	 0.3220	 0.4330
2	 0.3340	 0.2960
3	 0.2930	 0.1640
4	 0.3390	 0.2880
5	 0.7010	 0.3720
6	 0.1490	 0.1330
7	 0.7970	 0.4190
8	 0.7300	 0.3840
9	 0.4150	 0.3180
A	 0.6390	 0.4340
AA	 0.3070	 0.2330
B	 0.6480	 0.4220
BB	 0.3580	 0.2450
C	 0.6450	 0.4320
CC	 0.4470	 0.3300
D	 0.6060	 0.3800
DD	 0.3710	 0.2580
E	 0.5530	 0.3860
EE	 0.4820	 0.3610
F	 0.6040	 0.4130
FF	 0.3190	 0.2800
G	 0.5440	 0.3470
GG	 0.2530	 0.1790
H	 0.6130	 0.3950
HH	 0.3600	 0.2930
I	 0.6100	 0.4150
II	 0.3970	 0.2740
J	 0.5930	 0.3740
JJ	 0.4290	 0.2860
K	 0.5880	 0.3130
KK	 0.3390	 0.2560
L	 0.6090	 0.3820
LL	 0.4810	 0.3380



























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Chain	Atom inclusion	Q-score
M	0.6370	0.4130
MM	0.4770	0.3470
N	0.6800	0.4340
NN	0.3210	0.2400
O	0.6620	0.4220
OO	0.3960	0.2500
P	0.6480	0.4360
PP	0.3480	0.2300
Q	0.6360	0.4320
QQ	0.5050	0.3570
R	0.5840	0.3650
RR	0.1330	0.0970
S	0.6580	0.4410
SS	0.2850	0.2010
T	0.5990	0.4100
TT	0.4430	0.3440
U	0.5250	0.3240
UU	0.3310	0.2460
V	0.6280	0.4260
VV	0.4710	0.3640
W	0.4080	0.2810
WW	0.3440	0.2270
X	0.6120	0.3900
XX	0.1230	0.0920
Y	0.6210	0.3910
YY	0.1230	0.1000
Z	0.6040	0.3780
ZZ	0.0490	0.0370
a	0.6620	0.4470
b	0.4240	0.3220
c	0.5600	0.3640
d	0.5950	0.3920
e	0.6320	0.4420
f	0.6640	0.4550
g	0.6020	0.4040
h	0.6090	0.3760
i	0.5970	0.3500
j	0.6650	0.4390
k	0.5280	0.3480
l	0.5860	0.4060
m	0.6370	0.4030
n	0.5960	0.3640

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Chain	Atom inclusion	Q-score
o	 0.5990	 0.4160
p	 0.6010	 0.4010
q	 0.4050	 0.2870
r	 0.6250	 0.4290
s	 0.0600	 0.0260
t	 0.0160	 0.0130
u	 0.4530	 0.3290
v	 0.4510	 0.3160
w	 0.2850	 0.2200
x	 0.3640	 0.2840
y	 0.3610	 0.2740
z	 0.3060	 0.2220