



Full wwPDB EM Validation Report ⓘ

Dec 18, 2022 – 03:02 am GMT

PDB ID : 7A5G
EMDB ID : EMD-11642
Title : Structure of the elongating human mitoribosome bound to mtEF-Tu.GMPPCP and A/T mt-tRNA
Authors : Desai, N.; Yang, H.; Chandrasekaran, V.; Kazi, R.; Minczuk, M.; Ramakrishnan, V.
Deposited on : 2020-08-21
Resolution : 4.33 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

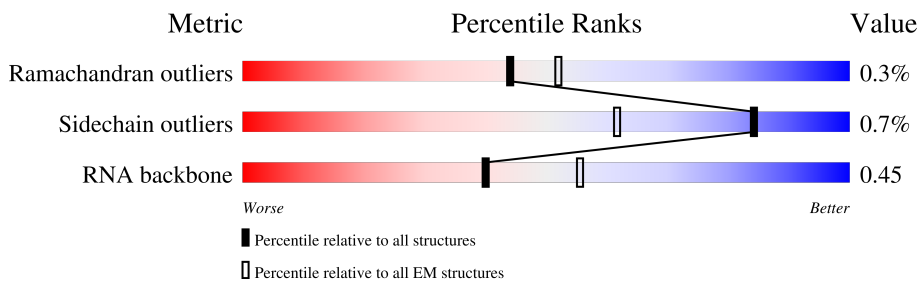
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.33 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	Y2	29	<div style="display: flex; justify-content: space-between;"> <div style="width: 90%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="width: 93%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> </div>
2	A3	1559	<div style="display: flex; justify-content: space-between;"> <div style="width: 7%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="width: 62%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="width: 29%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="width: 6%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> </div>
3	B3	69	<div style="display: flex; justify-content: space-between;"> <div style="width: 13%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="width: 51%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="width: 28%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="width: 19%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> </div>
4	D3	305	<div style="display: flex; justify-content: space-between;"> <div style="width: 12%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="width: 76%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="width: 23%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> </div>
5	E3	348	<div style="display: flex; justify-content: space-between;"> <div style="width: 13%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="width: 83%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="width: 14%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> </div>
6	F3	311	<div style="display: flex; justify-content: space-between;"> <div style="width: 13%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="width: 79%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="width: 20%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> </div>
7	D	267	<div style="display: flex; justify-content: space-between;"> <div style="width: 29%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="width: 29%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="width: 70%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> </div>
7	H3	267	<div style="display: flex; justify-content: space-between;"> <div style="width: 16%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="width: 35%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="width: 64%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> </div>

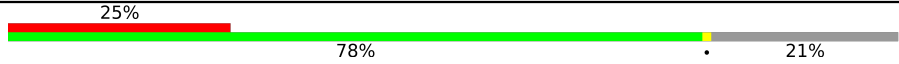

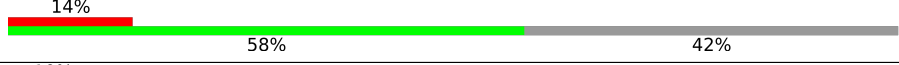

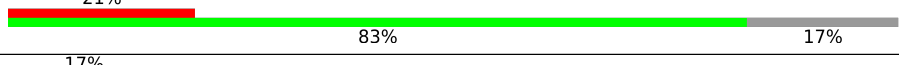
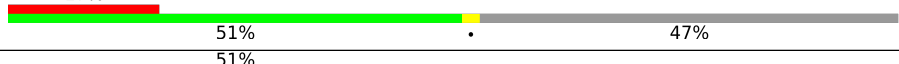
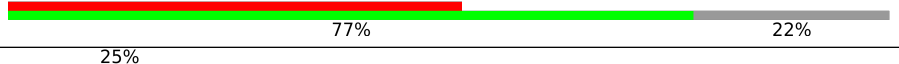

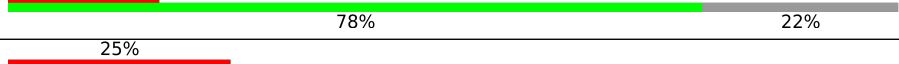





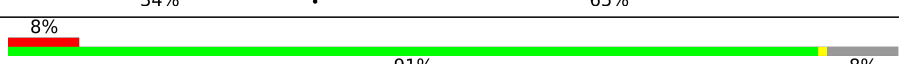
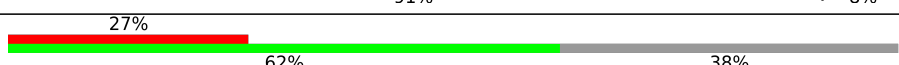
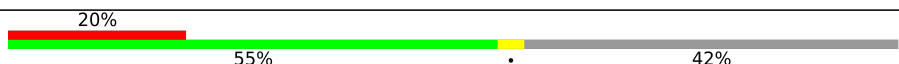
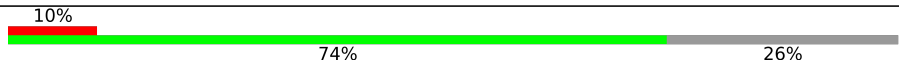
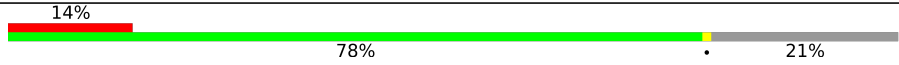
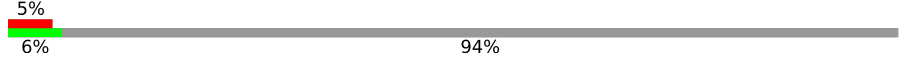
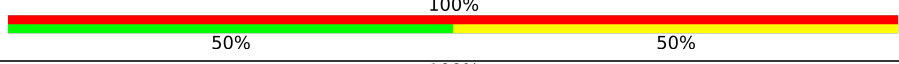
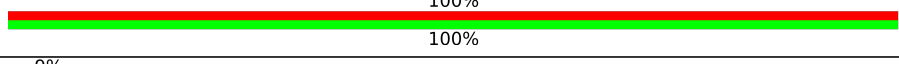
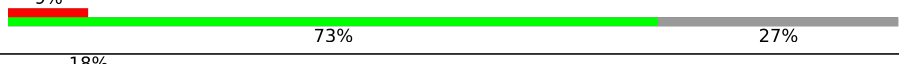


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Mol	Chain	Length	Quality of chain
8	I3	261	37% 61% 39%
9	J3	192	59% 72% 27%
10	K3	178	11% 98%
11	L3	145	23% 79% 21%
12	M3	296	20% 94%
13	N3	251	18% 81% 18%
14	O3	175	10% 86% 13%
15	P3	180	12% 72% 26%
16	Q3	292	20% 73% 25%
17	R3	149	10% 93% 6%
18	S3	205	7% 76% 24%
19	T3	206	15% 80% 19%
20	U3	153	10% 73% 27%
21	V3	216	28% 83% 5% 12%
22	W3	148	9% 74% 25%
23	X3	256	25% 90% 5% 5%
24	Y3	250	12% 70% 30%
25	Z3	161	7% 74% 25%
26	03	188	12% 56% 43%
27	13	65	29% 77% 20%
28	23	92	50% 50%
29	33	188	5% 51% 49%
30	43	103	35% 65%
31	53	423	16% 87% 11%
32	63	380	24% 84% 14%

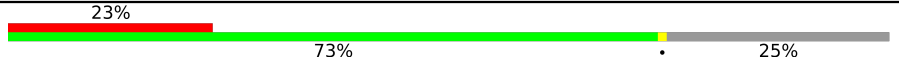
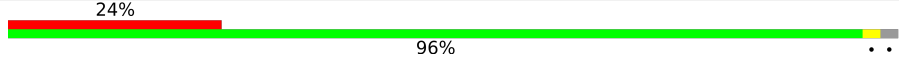
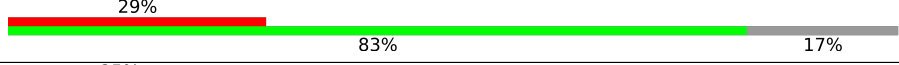

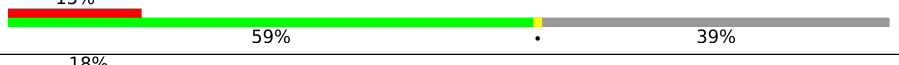
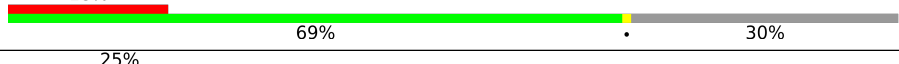
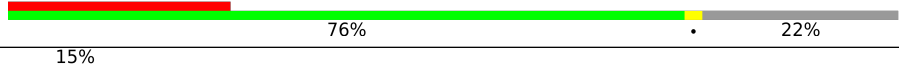

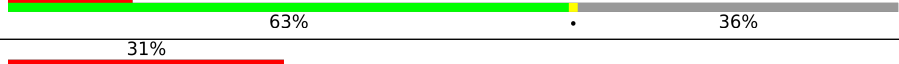


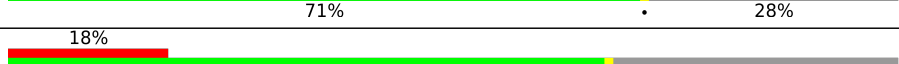
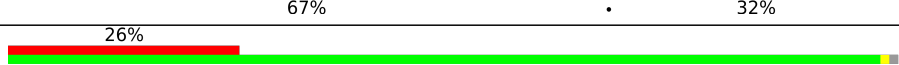
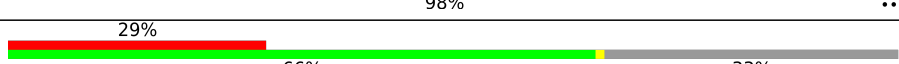

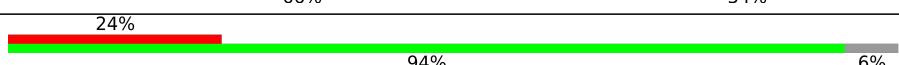
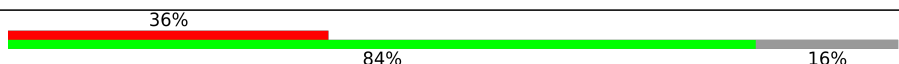




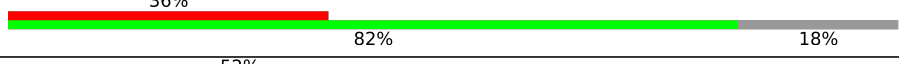
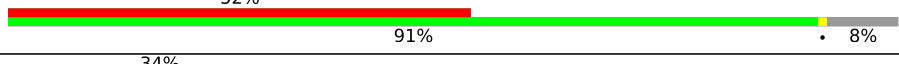


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Mol	Chain	Length	Quality of chain
33	73	338	
34	93	137	
35	a3	142	
36	b3	215	
37	c3	332	
38	d3	306	
39	e3	279	
40	f3	212	
41	g3	166	
42	h3	158	
43	i3	128	
44	j3	123	
45	k3	112	
46	l3	138	
47	m3	128	
48	o3	102	
49	p3	206	
50	q3	222	
51	r3	196	
52	s3	467	
52	t3	467	
53	u3	2	
54	A5	28	
55	B6	296	
56	C6	167	

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Mol	Chain	Length	Quality of chain
57	D6	430	
58	E6	125	
59	F6	242	
60	G6	396	
61	H6	201	
62	I6	194	
63	J6	138	
64	K6	128	
65	L6	257	
66	M6	137	
67	N6	130	
68	O6	258	
69	P6	142	
70	Q6	87	
71	R6	360	
72	S6	190	
73	T6	173	
74	U6	205	
75	V6	414	
76	W6	187	
77	X6	398	
78	Y6	395	
79	Z6	106	
80	a6	218	
81	b6	323	

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Mol	Chain	Length	Quality of chain
82	c6	118	
83	d6	199	
84	e6	689	
85	A6	954	
86	24	73	
86	C	73	
87	i4	10	
88	A	206	
89	Z	452	
90	j	76	
91	n	229	

2 Entry composition [i](#)

There are 101 unique types of molecules in this entry. The entry contains 170507 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 nascent chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	Y2	29	145	87	29	29	0	0

- Molecule 2 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	A3	1503	31913	14319	5761	10330	1503	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A3	3107	U	UNK	conflict	GB 1025814679

- Molecule 3 is a RNA chain called mt-tRNAVal.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	B3	56	1191	534	214	387	56	0	0

- Molecule 4 is a protein called 39S ribosomal protein L2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D3	236	1842	1145	373	315	9	0	0

- Molecule 5 is a protein called 39S ribosomal protein L3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E3	300	2365	1523	410	422	10	0	0

- Molecule 6 is a protein called 39S ribosomal protein L4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F3	250	Total	C	N	O	S	0	0
			2013	1294	365	348	6		

- Molecule 7 is a protein called 39S ribosomal protein L9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H3	95	Total	C	N	O		0	0
			784	498	152	134			
7	D	80	Total	C	N	O	S	0	0
			648	421	111	112	4		

- Molecule 8 is a protein called 39S ribosomal protein L10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I3	158	Total	C	N	O	S	0	0
			1283	828	235	210	10		

- Molecule 9 is a protein called 39S ribosomal protein L11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J3	140	Total	C	N	O	S	0	0
			1061	680	192	187	2		

- Molecule 10 is a protein called 39S ribosomal protein L13, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K3	177	Total	C	N	O	S	0	0
			1451	934	259	251	7		

- Molecule 11 is a protein called 39S ribosomal protein L14, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L3	115	Total	C	N	O	S	0	0
			889	559	171	154	5		

- Molecule 12 is a protein called 39S ribosomal protein L15, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M3	287	Total	C	N	O	S	0	0
			2305	1472	425	402	6		

- Molecule 13 is a protein called 39S ribosomal protein L16, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	N3	205	1654	1056	308	280	10	0	0

- Molecule 14 is a protein called 39S ribosomal protein L17, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	O3	152	1245	784	239	215	7	0	0

- Molecule 15 is a protein called 39S ribosomal protein L18, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	P3	133	1080	677	209	189	5	0	0

- Molecule 16 is a protein called 39S ribosomal protein L19, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	Q3	219	1822	1168	322	323	9	0	0

- Molecule 17 is a protein called 39S ribosomal protein L20, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	R3	140	1153	732	231	186	4	0	0

- Molecule 18 is a protein called 39S ribosomal protein L21, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	S3	156	1251	806	222	219	4	0	0

- Molecule 19 is a protein called 39S ribosomal protein L22, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	T3	166	1368	875	254	232	7	0	0

- Molecule 20 is a protein called 39S ribosomal protein L23, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	U3	111	922	591	176	153	2	0	0

- Molecule 21 is a protein called 39S ribosomal protein L24, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	V3	189	1551	987	278	278	8	0	0

- Molecule 22 is a protein called 39S ribosomal protein L27, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	W3	111	871	558	164	146	3	0	0

- Molecule 23 is a protein called 39S ribosomal protein L28, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	X3	243	2027	1310	350	362	5	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X3	148	ALA	THR	conflict	UNP Q13084
X3	149	SER	PRO	conflict	UNP Q13084
X3	150	GLY	LYS	conflict	UNP Q13084

- Molecule 24 is a protein called 39S ribosomal protein L47, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	Y3	176	1517	970	291	252	4	0	0

- Molecule 25 is a protein called 39S ribosomal protein L30, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	Z3	120	978	626	183	166	3	0	0

- Molecule 26 is a protein called 39S ribosomal protein L32, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	03	108	880	545	172	157	6	0	0

- Molecule 27 is a protein called 39S ribosomal protein L33, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	13	52	433	278	83	70	2	0	0

- Molecule 28 is a protein called 39S ribosomal protein L34, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	23	46	376	233	83	59	1	0	0

- Molecule 29 is a protein called 39S ribosomal protein L35, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	33	95	831	539	162	127	3	0	0

- Molecule 30 is a protein called 39S ribosomal protein L36, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	43	36	322	203	70	46	3	0	0

- Molecule 31 is a protein called 39S ribosomal protein L37, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	53	376	3064	1987	529	538	10	0	0

- Molecule 32 is a protein called 39S ribosomal protein L38, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	63	325	2636	1692	465	470	9	0	0

- Molecule 33 is a protein called 39S ribosomal protein L39, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	73	266	2158	1383	371	388	16	0	0

- Molecule 34 is a protein called 39S ribosomal protein L41, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	93	109	873	565	152	154	2	0	0

- Molecule 35 is a protein called 39S ribosomal protein L42, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	a3	82	686	434	124	123	5	0	0

- Molecule 36 is a protein called 39S ribosomal protein L43, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	b3	148	1178	733	229	213	3	0	0

- Molecule 37 is a protein called 39S ribosomal protein L44, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	c3	275	2217	1415	383	410	9	0	0

- Molecule 38 is a protein called 39S ribosomal protein L45, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	d3	162	1347	870	234	235	8	0	0

- Molecule 39 is a protein called 39S ribosomal protein L46, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	e3	217	1762	1124	310	323	5	0	0

- Molecule 40 is a protein called 39S ribosomal protein L48, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	f3	131	1039	663	169	203	4	0	0

- Molecule 41 is a protein called 39S ribosomal protein L49, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	g3	129	1067	690	185	190	2	0	0

- Molecule 42 is a protein called 39S ribosomal protein L50, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	h3	100	827	524	146	155	2	0	0

- Molecule 43 is a protein called 39S ribosomal protein L51, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	i3	97	827	532	165	126	4	0	0

- Molecule 44 is a protein called 39S ribosomal protein L52, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	j3	85	684	423	133	126	2	0	0

- Molecule 45 is a protein called 39S ribosomal protein L53, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	k3	84	655	407	122	121	5	0	0

- Molecule 46 is a protein called 39S ribosomal protein L54, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
46	l3	23	221	137	52	32	0	0

- Molecule 47 is a protein called 39S ribosomal protein L55, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	m3	45	372	232	76	62	2	0	0

- Molecule 48 is a protein called Ribosomal protein 63, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	o3	94	797	501	165	128	3	0	0

- Molecule 49 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	p3	127	1058	661	201	192	4	0	0

- Molecule 50 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	q3	128	1076	671	208	192	5	0	0

- Molecule 51 is a protein called 39S ribosomal protein S18a, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	r3	146	1203	764	232	199	8	0	0

- Molecule 52 is a protein called 39S ribosomal protein S30, mitochondrial,39S ribosomal protein S30, mitochondrial,mL65.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	s3	370	3036	1946	542	534	14	0	0
52	t3	28	140	84	28	28		0	0

- Molecule 53 is a RNA chain called RNA (5'-R(P*CP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
53	u3	2	42	19	8	13	2	0	0

- Molecule 54 is a protein called Oxa1L tail.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
54	A5	28	140	84	28	28	0	0

- Molecule 55 is a protein called 28S ribosomal protein S2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	B6	217	1768	1131	321	306	10	0	0

- Molecule 56 is a protein called 28S ribosomal protein S24, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	C6	132	1082	699	195	184	4	0	0

- Molecule 57 is a protein called 28S ribosomal protein S5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	D6	322	2557	1611	476	457	13	0	0

- Molecule 58 is a protein called 28S ribosomal protein S6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
58	E6	122	972	614	177	177	4	0	0

- Molecule 59 is a protein called 28S ribosomal protein S7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
59	F6	201	1668	1069	305	283	11	0	0

- Molecule 60 is a protein called 28S ribosomal protein S9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
60	G6	305	2516	1599	448	455	14	0	0

- Molecule 61 is a protein called 28S ribosomal protein S10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	H6	122	Total	C	N	O	S	0	0
			999	643	168	185	3		

- Molecule 62 is a protein called 28S ribosomal protein S11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	I6	136	Total	C	N	O	S	0	0
			1011	637	192	178	4		

- Molecule 63 is a protein called 28S ribosomal protein S12, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	J6	108	Total	C	N	O	S	0	0
			838	521	169	142	6		

- Molecule 64 is a protein called 28S ribosomal protein S14, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	K6	101	Total	C	N	O	S	0	0
			861	537	179	140	5		

- Molecule 65 is a protein called 28S ribosomal protein S15, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	L6	164	Total	C	N	O	S	0	0
			1382	883	257	235	7		

- Molecule 66 is a protein called 28S ribosomal protein S16, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	M6	116	Total	C	N	O	S	0	0
			920	582	182	150	6		

- Molecule 67 is a protein called 28S ribosomal protein S17, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	N6	107	Total	C	N	O	S	0	0
			846	549	153	141	3		

- Molecule 68 is a protein called 28S ribosomal protein S18b, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
68	O6	185	1528	970	285	267	6	0	0

- Molecule 69 is a protein called 28S ribosomal protein S18c, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
69	P6	96	774	498	133	135	8	0	0

- Molecule 70 is a protein called 28S ribosomal protein S21, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
70	Q6	86	740	458	150	124	8	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q6	50	ARG	CYS	conflict	UNP P82921

- Molecule 71 is a protein called 28S ribosomal protein S22, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
71	R6	242	2008	1285	343	372	8	0	0

- Molecule 72 is a protein called 28S ribosomal protein S23, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
72	S6	126	1042	673	183	185	1	0	0

- Molecule 73 is a protein called 28S ribosomal protein S25, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
73	T6	162	1330	850	231	238	11	0	0

- Molecule 74 is a protein called 28S ribosomal protein S26, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	U6	173	Total	C	N	O	S	0	0
			1461	900	294	263	4		

- Molecule 75 is a protein called 28S ribosomal protein S27, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	V6	328	Total	C	N	O	S	0	0
			2702	1737	452	502	11		

- Molecule 76 is a protein called 28S ribosomal protein S28, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	W6	97	Total	C	N	O	S	0	0
			766	486	137	139	4		

- Molecule 77 is a protein called 28S ribosomal protein S29, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	X6	316	Total	C	N	O	S	0	0
			2531	1625	440	455	11		

- Molecule 78 is a protein called 28S ribosomal protein S31, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Y6	108	Total	C	N	O	S	0	0
			914	593	150	169	2		

- Molecule 79 is a protein called 28S ribosomal protein S33, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Z6	87	Total	C	N	O	S	0	0
			740	473	133	130	4		

- Molecule 80 is a protein called 28S ribosomal protein S34, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	a6	201	Total	C	N	O	S	0	0
			1684	1065	322	292	5		

- Molecule 81 is a protein called 28S ribosomal protein S35, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
81	b6	256	2076	1321	350	395	10	0	0

- Molecule 82 is a protein called Coiled-coil-helix-coiled-coil-helix domain-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
82	c6	116	925	574	181	162	8	0	0

- Molecule 83 is a protein called Aurora kinase A-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
83	d6	69	610	393	130	86	1	0	0

- Molecule 84 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
84	e6	414	2838	1805	490	529	14	0	0

- Molecule 85 is a RNA chain called 12S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
85	A6	928	19716	8840	3560	6388	928	0	0

- Molecule 86 is a RNA chain called P tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
86	24	73	1547	696	280	499	72	0	0
86	C	73	1547	696	280	499	72	0	0

- Molecule 87 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
87	i4	10	216	97	41	68	10	0	0

- Molecule 88 is a protein called 39S ribosomal protein L40, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
88	A	162	1375	876	247	249	3	0	0

- Molecule 89 is a protein called Elongation factor Tu, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
89	Z	394	3042	1923	538	566	15	0	0

- Molecule 90 is a RNA chain called E tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
90	j	76	1616	723	291	527	75	0	0

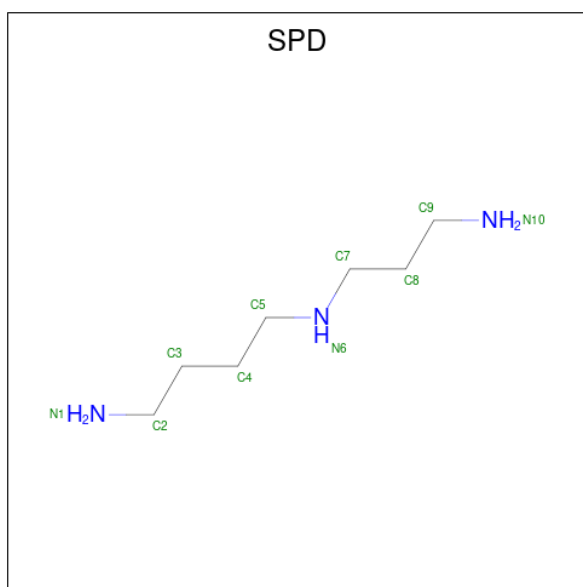
- Molecule 91 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
91	n	228	1767	1121	321	322	3	4	0

- Molecule 92 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
92	A3	95	Total	Mg	0
			95	95	
92	D3	1	Total	Mg	0
			1	1	
92	M3	1	Total	Mg	0
			1	1	
92	g3	1	Total	Mg	0
			1	1	
92	o3	1	Total	Mg	0
			1	1	
92	A6	28	Total	Mg	0
			28	28	
92	n	1	Total	Mg	0
			1	1	

- Molecule 93 is SPERMIDINE (three-letter code: SPD) (formula: C₇H₁₉N₃).



Mol	Chain	Residues	Atoms			AltConf
93	A3	1	Total	C	N	0
			10	7	3	

- Molecule 94 is ZINC ION (three-letter code: ZN) (formula: Zn).

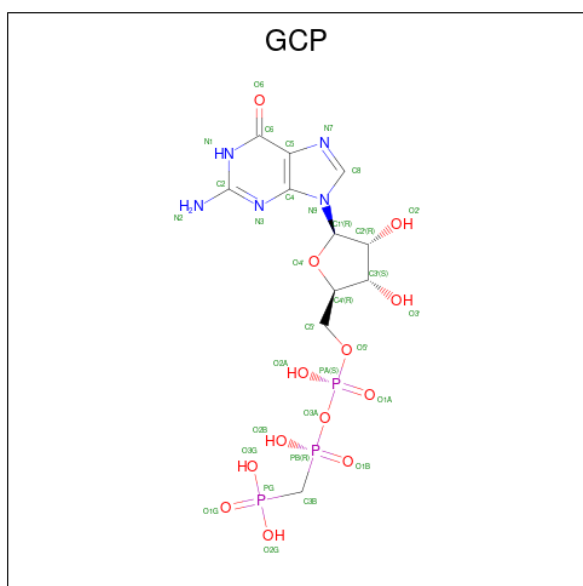
Mol	Chain	Residues	Atoms		AltConf
94	03	1	Total	Zn	0
			1	1	
94	43	1	Total	Zn	0
			1	1	
94	r3	1	Total	Zn	0
			1	1	
94	B6	1	Total	Zn	0
			1	1	
94	O6	1	Total	Zn	0
			1	1	
94	P6	1	Total	Zn	0
			1	1	
94	T6	1	Total	Zn	0
			1	1	

- Molecule 95 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
95	X6	1	28	10	5	11	2	0

- Molecule 96 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).

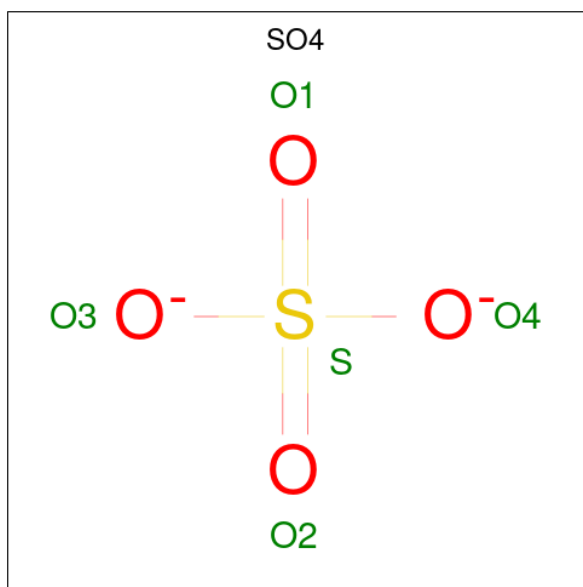


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
96	Z	1	32	11	5	13	3	0

- Molecule 97 is SODIUM ION (three-letter code: NA) (formula: Na).

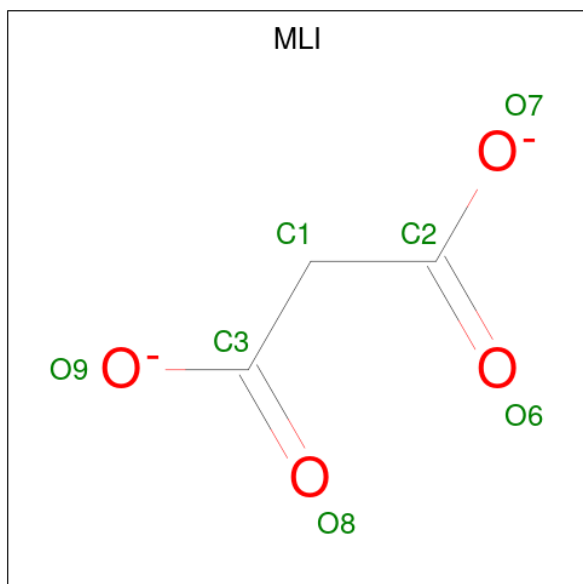
Mol	Chain	Residues	Atoms		AltConf
97	D	2	Total	Na	0
			2	2	
97	n	2	Total	Na	0
			2	2	

- Molecule 98 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			AltConf
98	n	1	Total	O	S	0
			5	4	1	

- Molecule 99 is MALONATE ION (three-letter code: MLI) (formula: C₃H₂O₄).



Mol	Chain	Residues	Atoms			AltConf
99	n	1	Total	C	O	0
			21	9	12	
99	n	1	Total	C	O	0
			21	9	12	
99	n	1	Total	C	O	0
			21	9	12	

- Molecule 100 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
100	n	2	Total	Cl	0
			2	2	

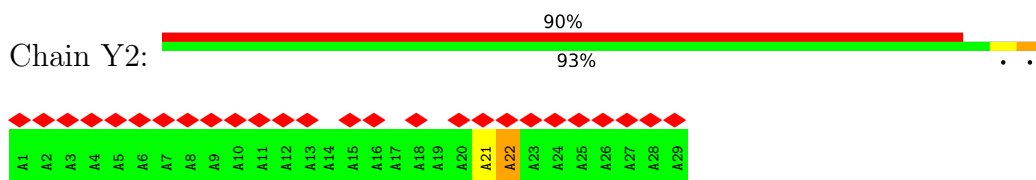
- Molecule 101 is water.

Mol	Chain	Residues	Atoms		AltConf
101	A3	3	Total	O	0
			3	3	
101	D	9	Total	O	0
			9	9	
101	n	67	Total	O	0
			67	67	

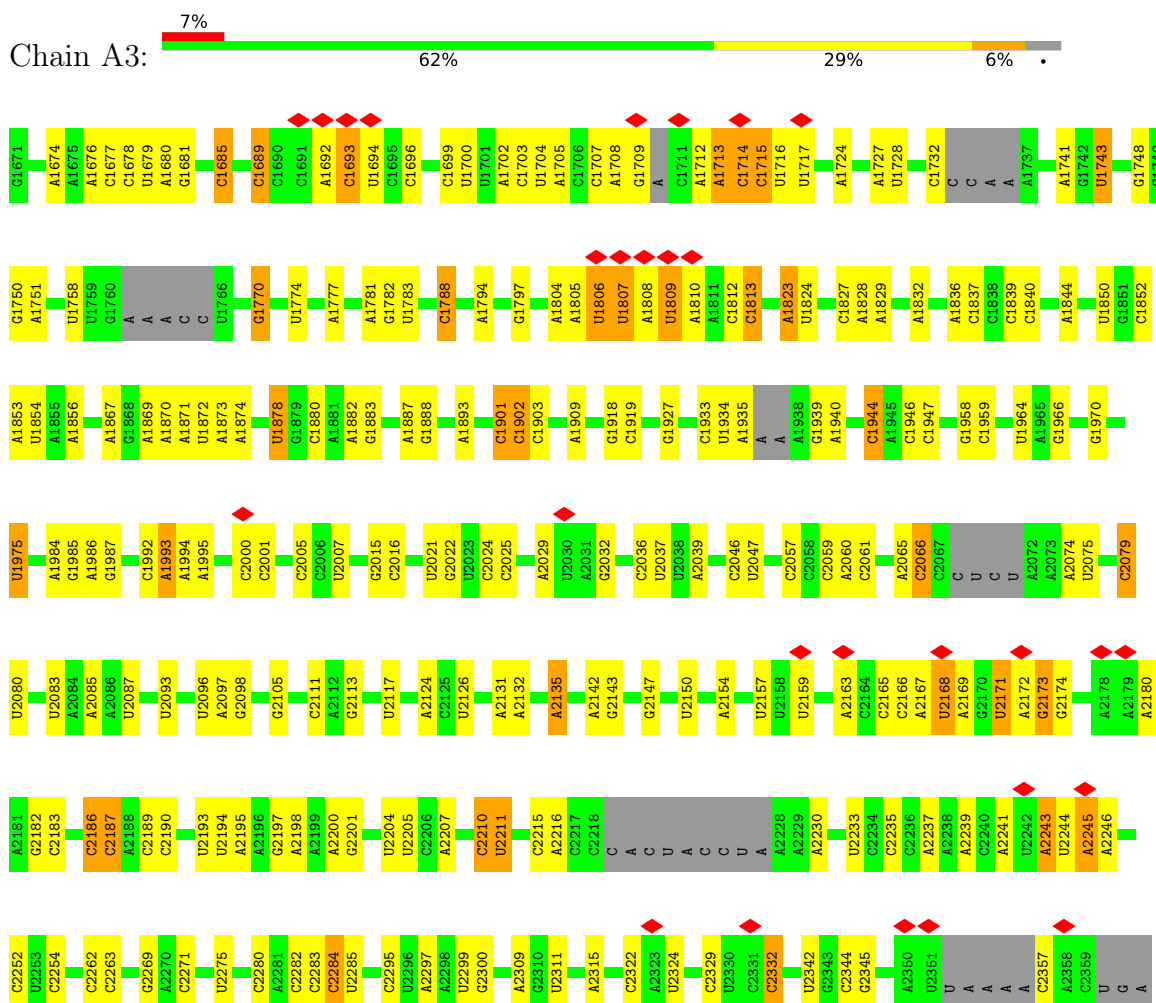
3 Residue-property plots

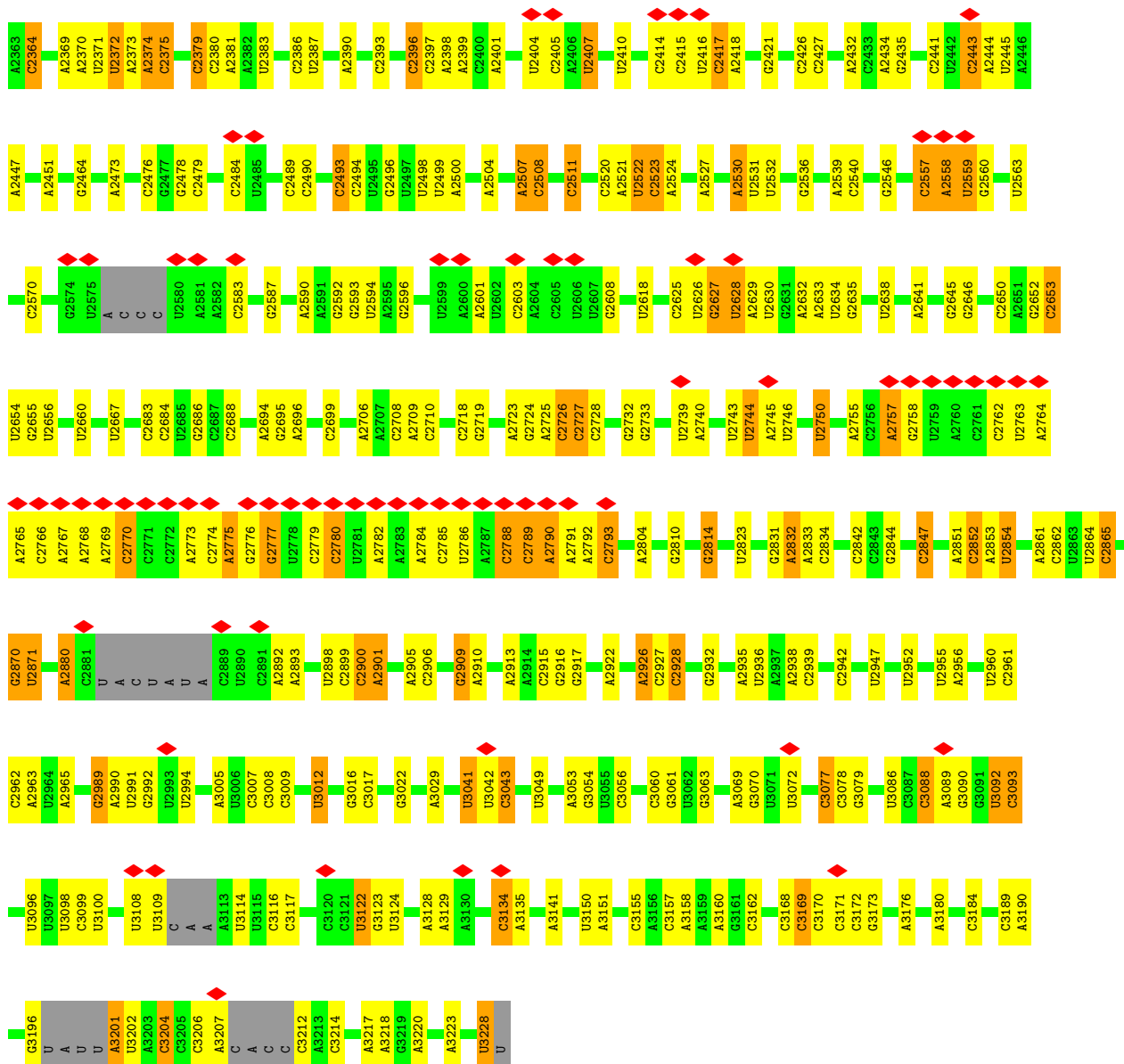
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: nascent chain



- Molecule 2: 16S rRNA

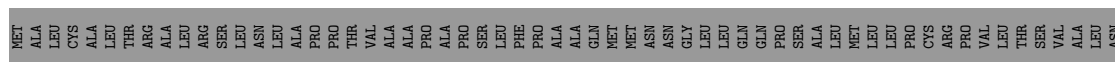
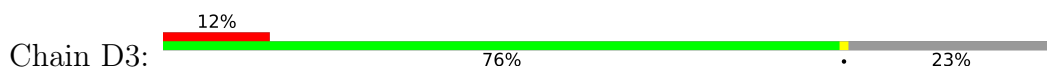


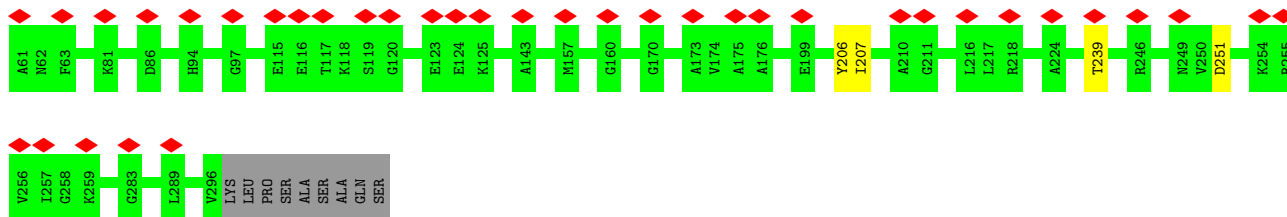


- Molecule 3: mt-tRNAVal

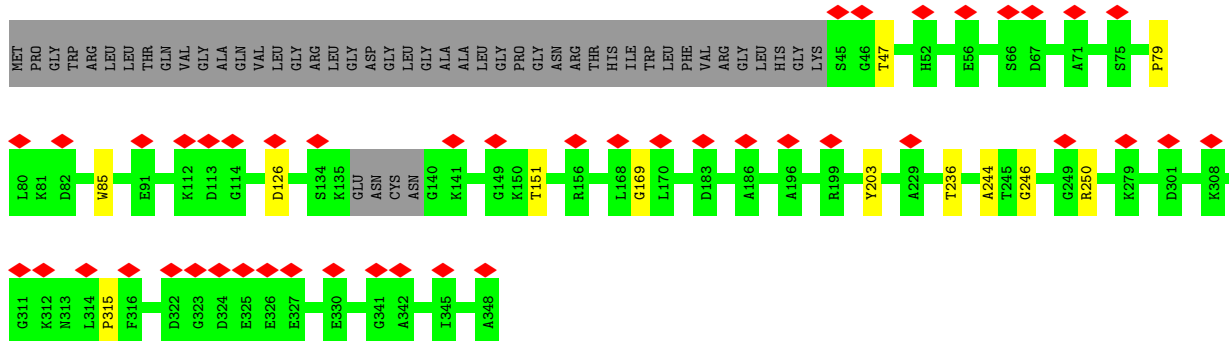
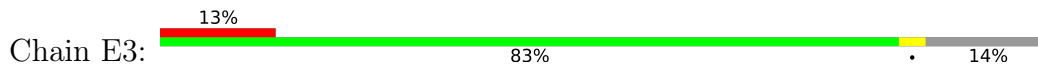


- Molecule 4: 39S ribosomal protein L2, mitochondrial

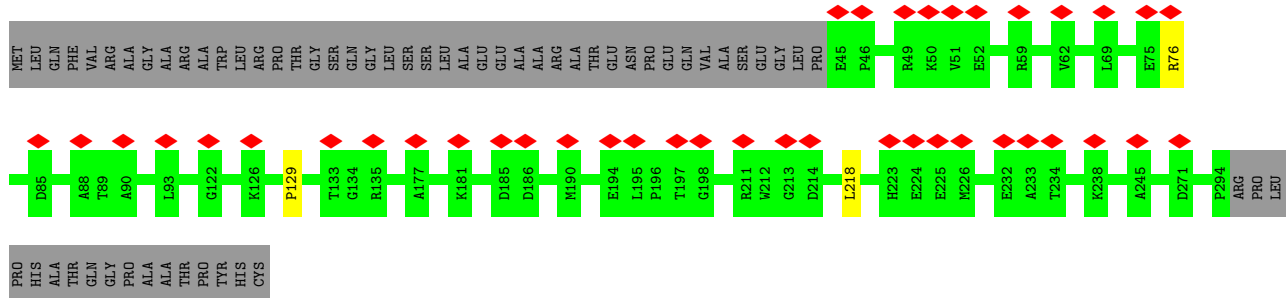
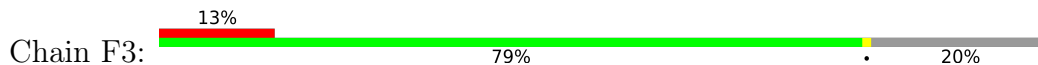




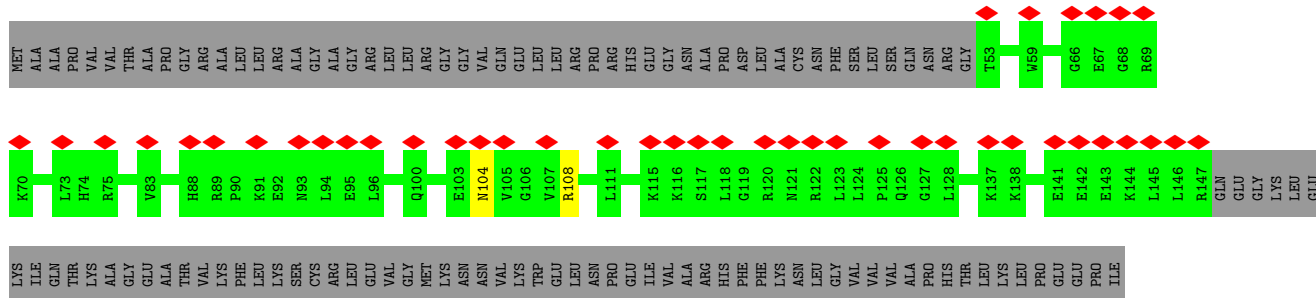
• Molecule 5: 39S ribosomal protein L3, mitochondrial

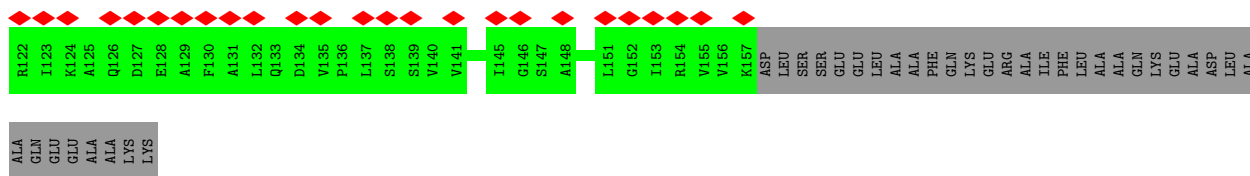


• Molecule 6: 39S ribosomal protein L4, mitochondrial

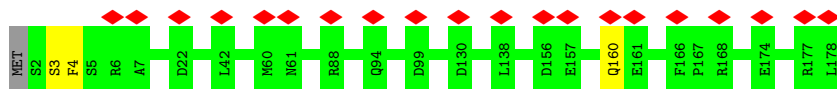


• Molecule 7: 39S ribosomal protein L9, mitochondrial

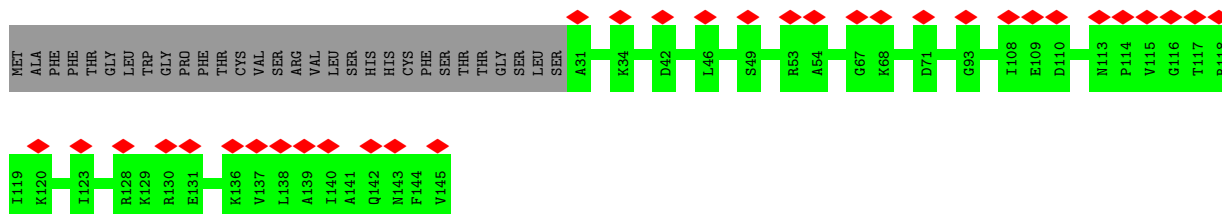
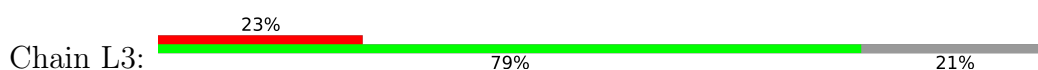




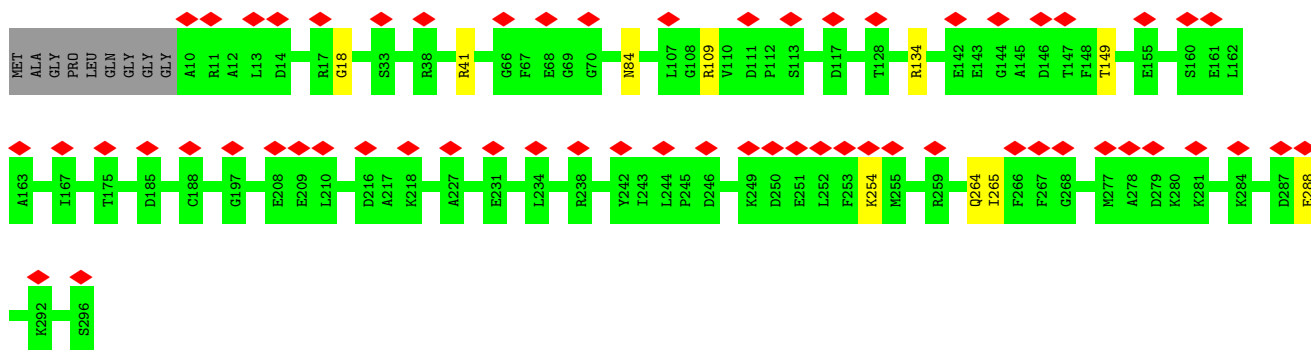
• Molecule 10: 39S ribosomal protein L13, mitochondrial



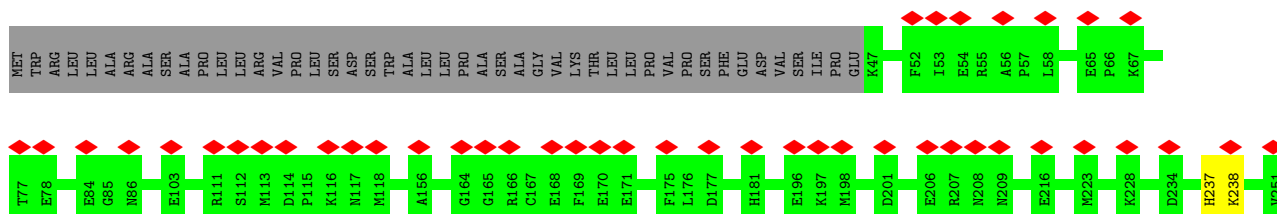
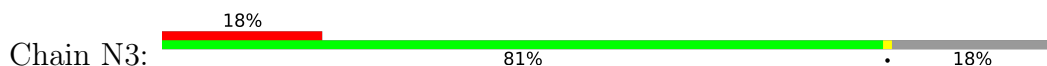
• Molecule 11: 39S ribosomal protein L14, mitochondrial



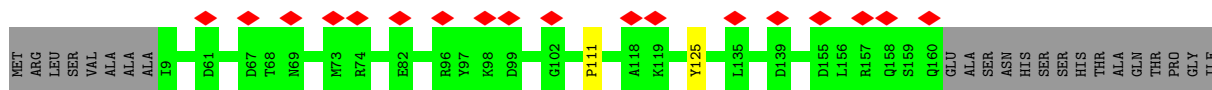
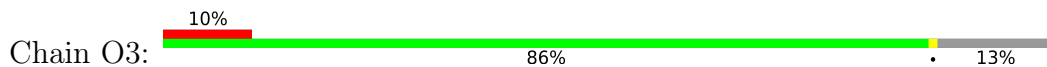
• Molecule 12: 39S ribosomal protein L15, mitochondrial



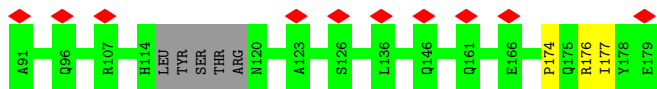
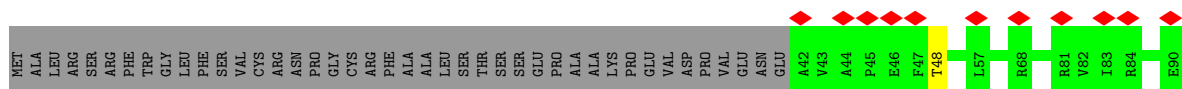
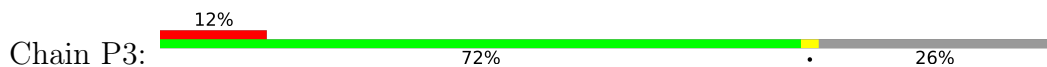
• Molecule 13: 39S ribosomal protein L16, mitochondrial



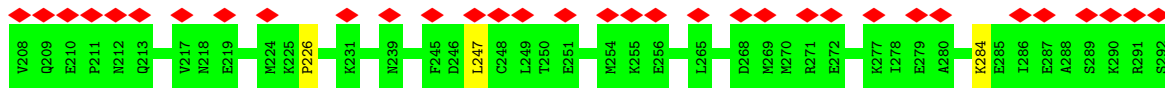
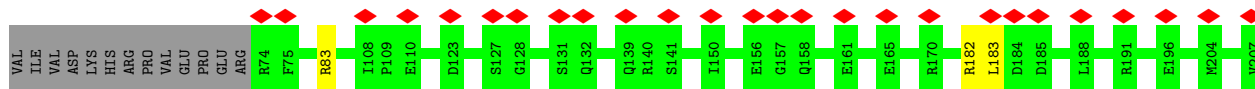
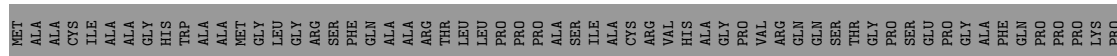
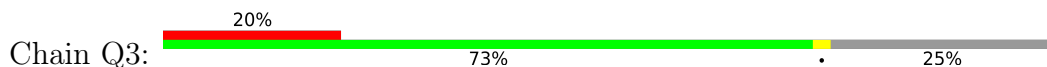
• Molecule 14: 39S ribosomal protein L17, mitochondrial



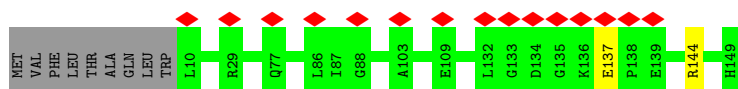
• Molecule 15: 39S ribosomal protein L18, mitochondrial



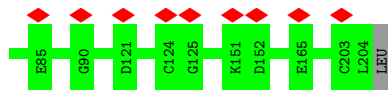
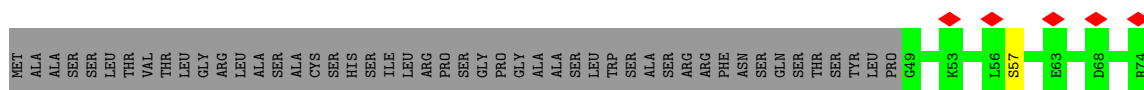
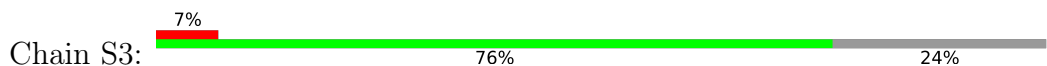
• Molecule 16: 39S ribosomal protein L19, mitochondrial



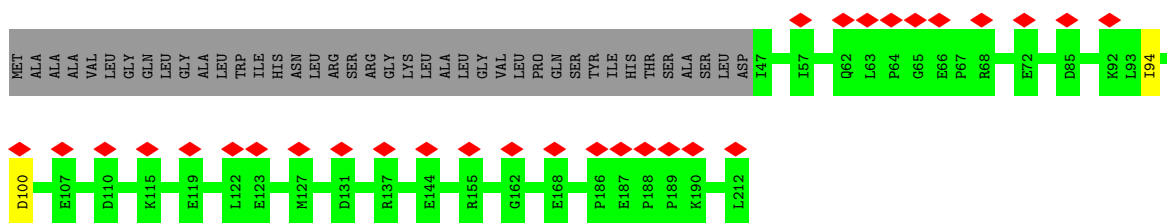
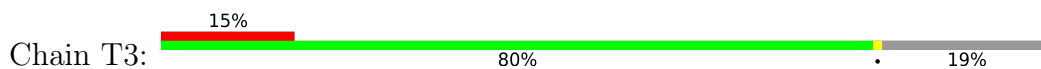
• Molecule 17: 39S ribosomal protein L20, mitochondrial



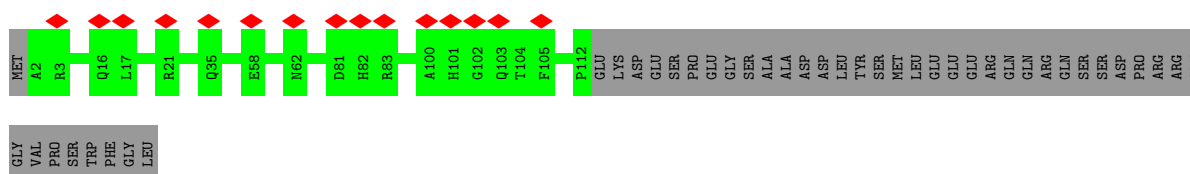
• Molecule 18: 39S ribosomal protein L21, mitochondrial



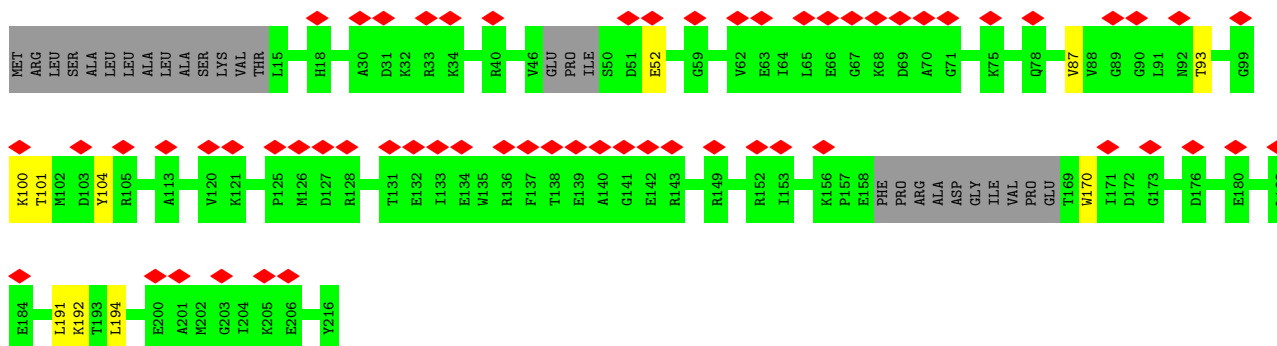
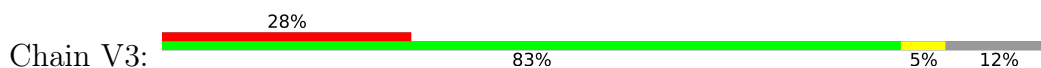
- Molecule 19: 39S ribosomal protein L22, mitochondrial



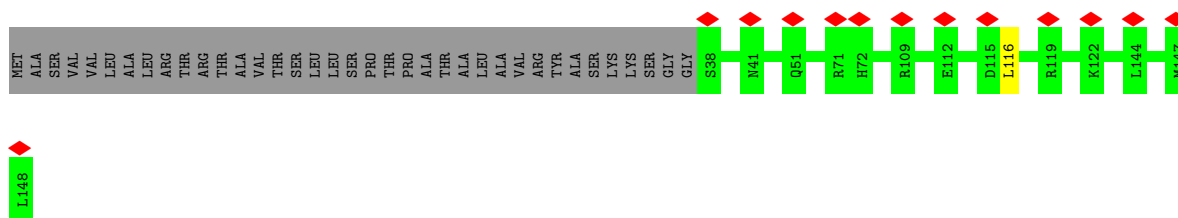
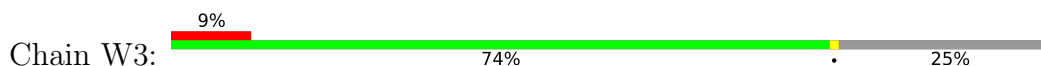
- Molecule 20: 39S ribosomal protein L23, mitochondrial



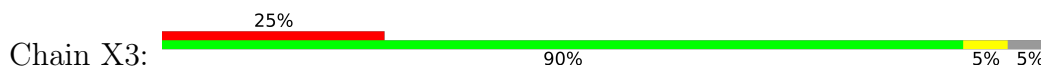
- Molecule 21: 39S ribosomal protein L24, mitochondrial

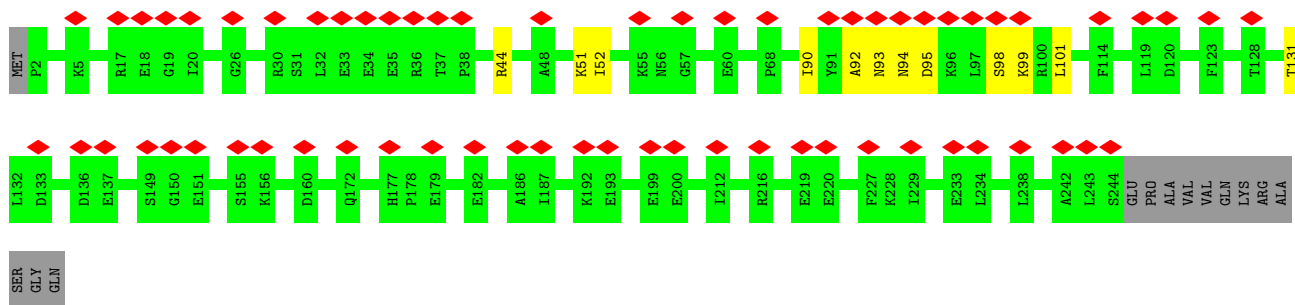


- Molecule 22: 39S ribosomal protein L27, mitochondrial

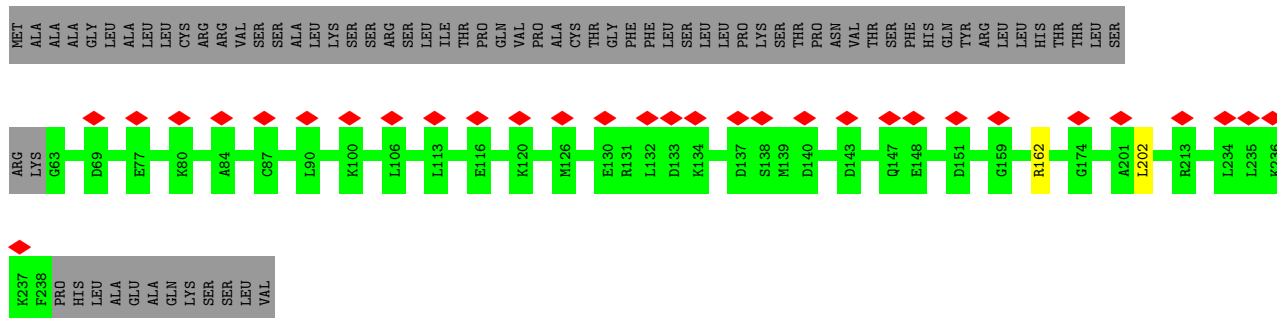


- Molecule 23: 39S ribosomal protein L28, mitochondrial

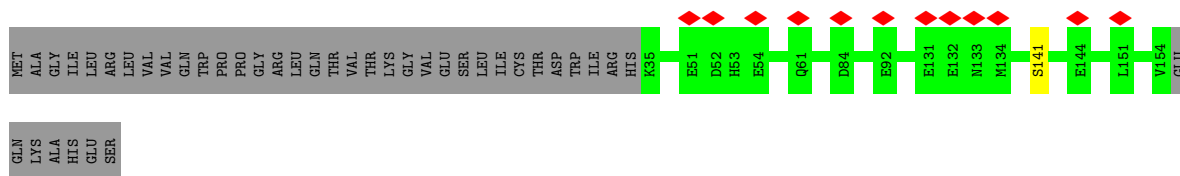
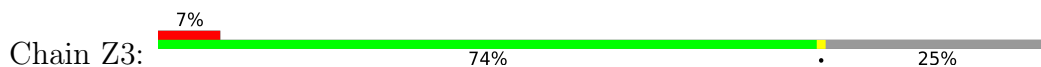




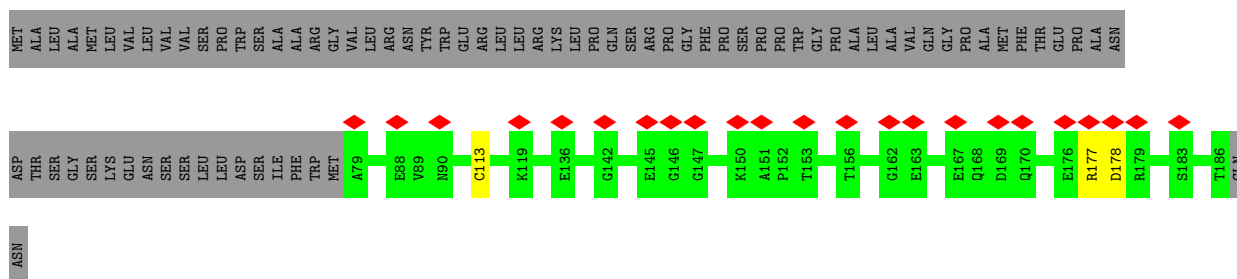
• Molecule 24: 39S ribosomal protein L47, mitochondrial



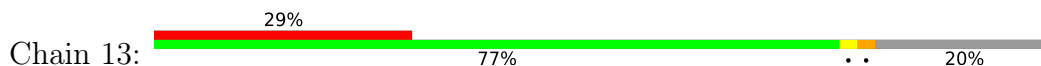
• Molecule 25: 39S ribosomal protein L30, mitochondrial

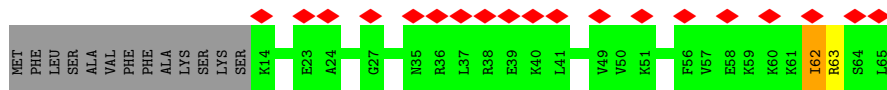


• Molecule 26: 39S ribosomal protein L32, mitochondrial

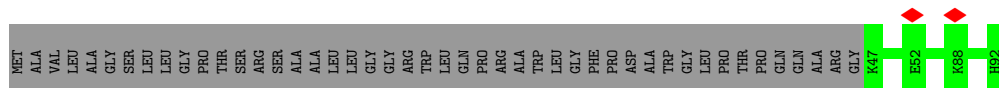


• Molecule 27: 39S ribosomal protein L33, mitochondrial

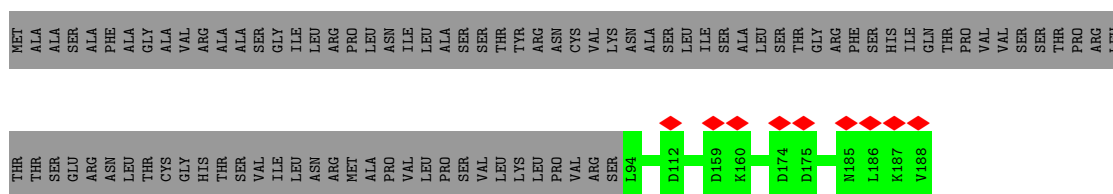




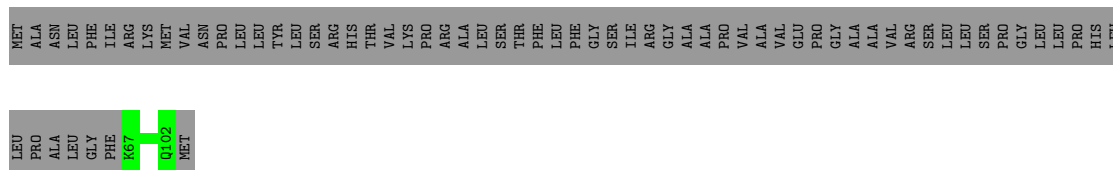
- Molecule 28: 39S ribosomal protein L34, mitochondrial



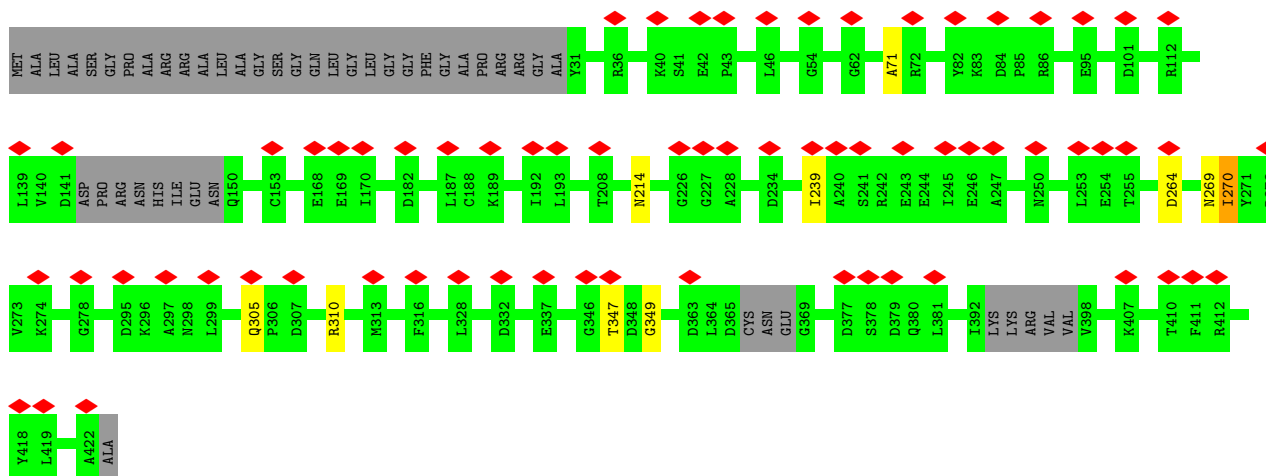
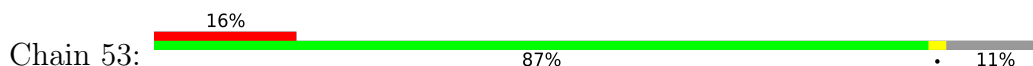
- Molecule 29: 39S ribosomal protein L35, mitochondrial



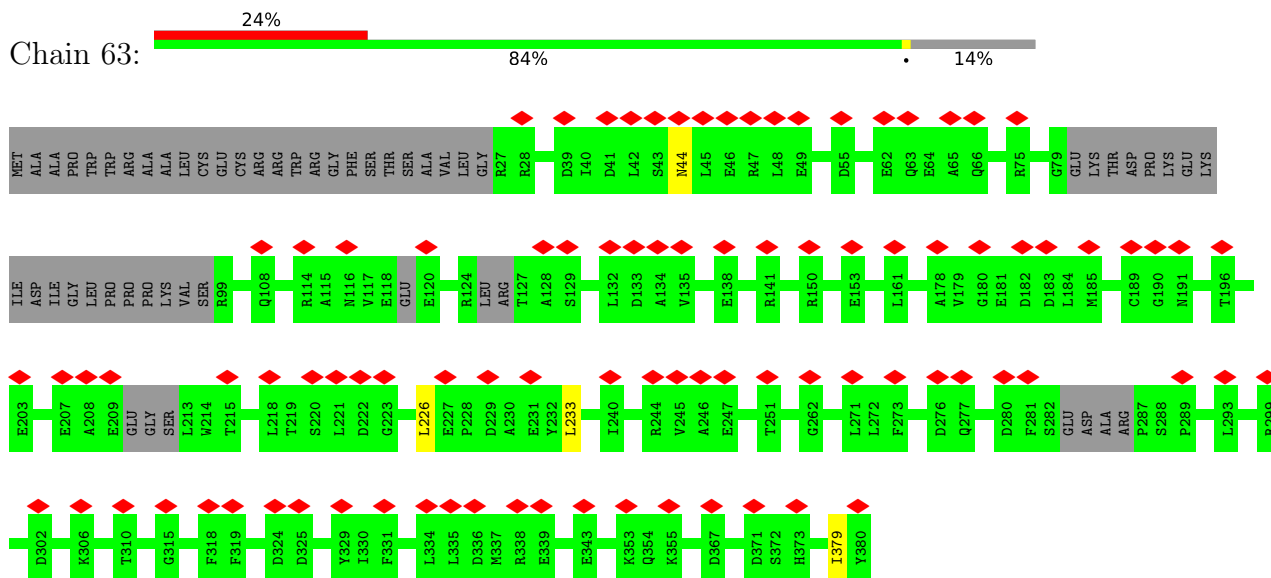
- Molecule 30: 39S ribosomal protein L36, mitochondrial



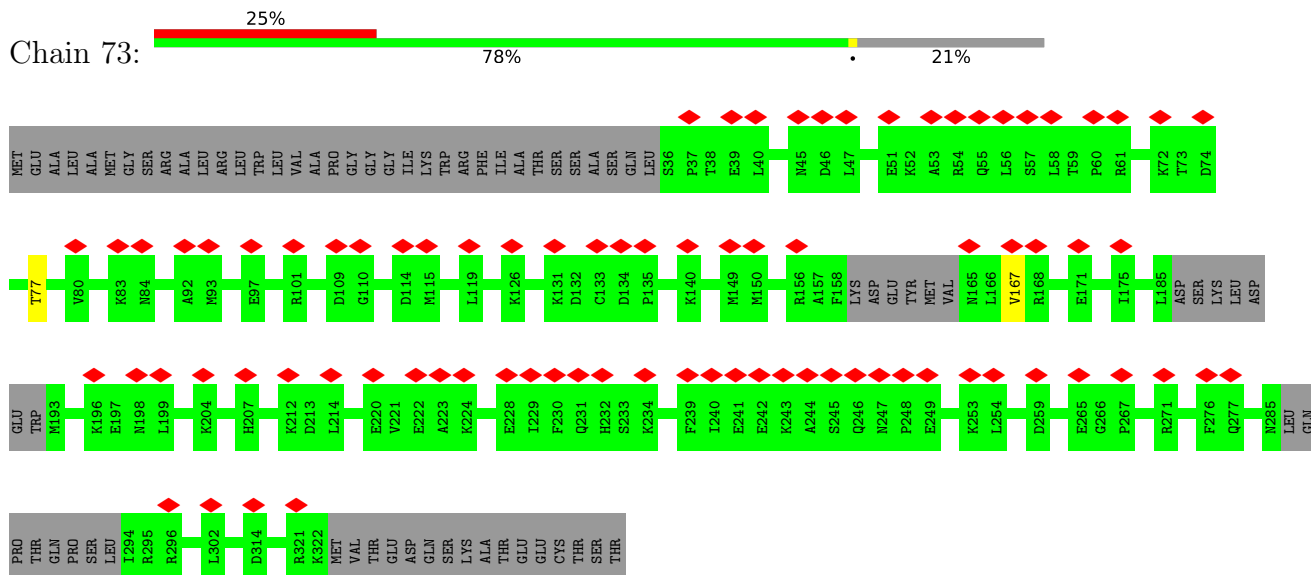
- Molecule 31: 39S ribosomal protein L37, mitochondrial



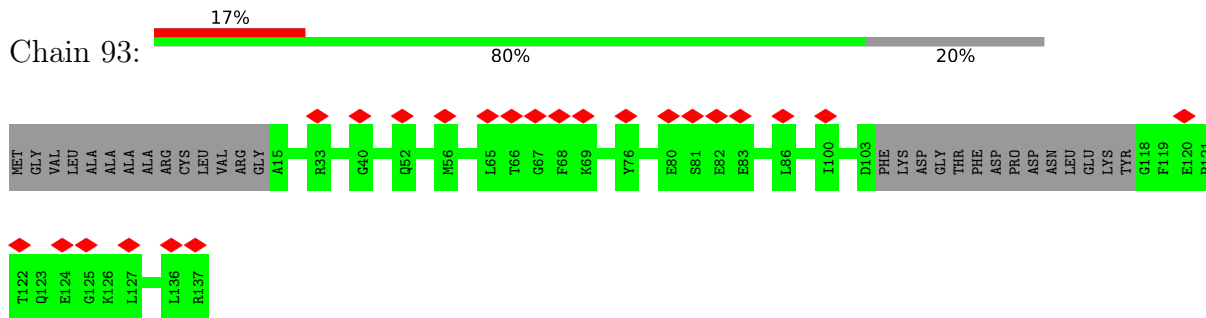
- Molecule 32: 39S ribosomal protein L38, mitochondrial



• Molecule 33: 39S ribosomal protein L39, mitochondrial

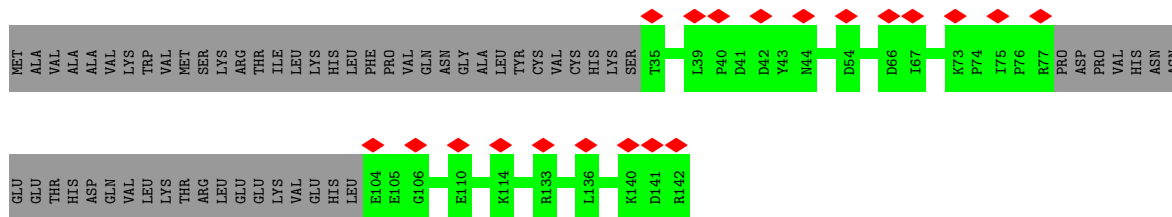


• Molecule 34: 39S ribosomal protein L41, mitochondrial

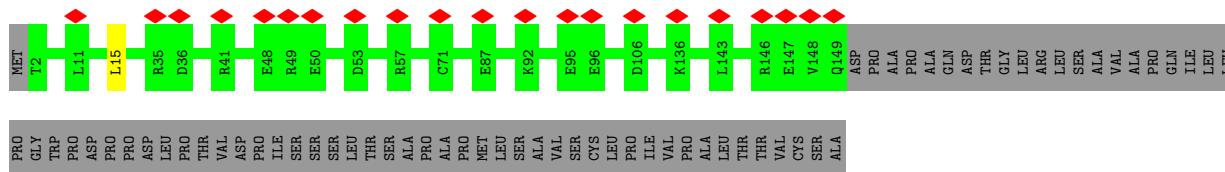


• Molecule 35: 39S ribosomal protein L42, mitochondrial

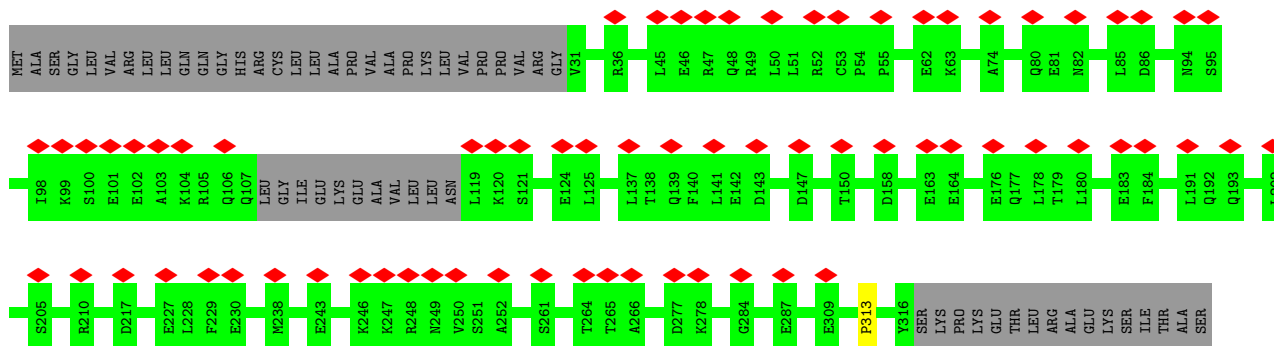
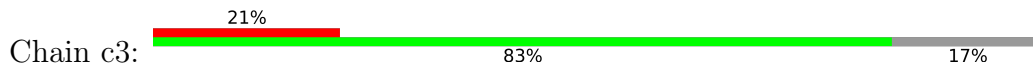




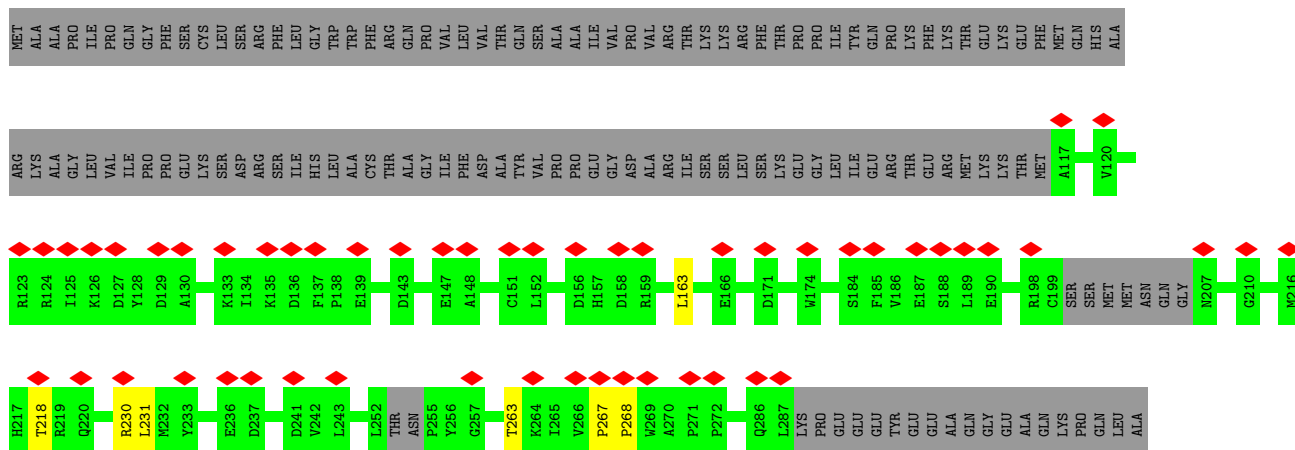
• Molecule 36: 39S ribosomal protein L43, mitochondrial



• Molecule 37: 39S ribosomal protein L44, mitochondrial

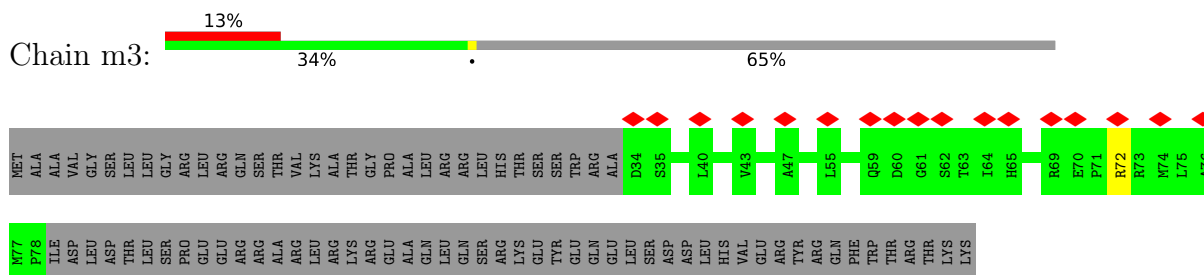


• Molecule 38: 39S ribosomal protein L45, mitochondrial

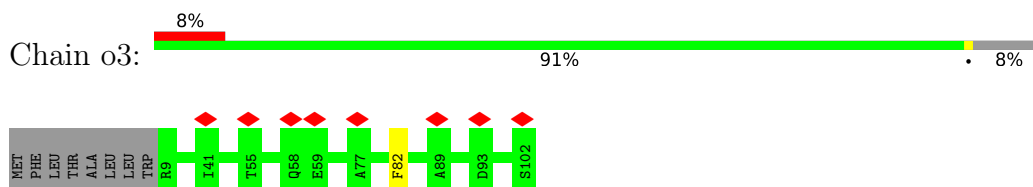


• Molecule 39: 39S ribosomal protein L46, mitochondrial

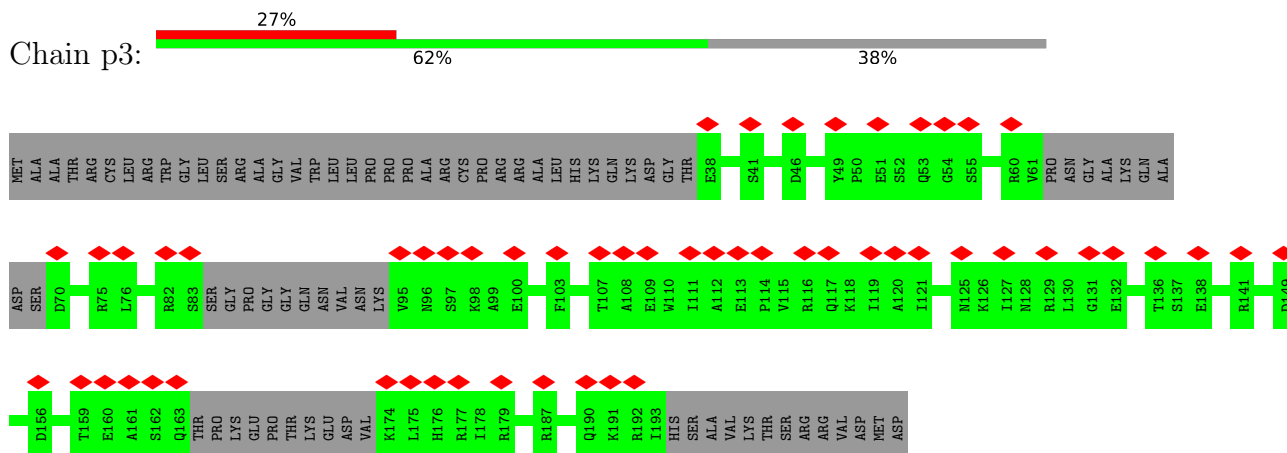
- Molecule 47: 39S ribosomal protein L55, mitochondrial



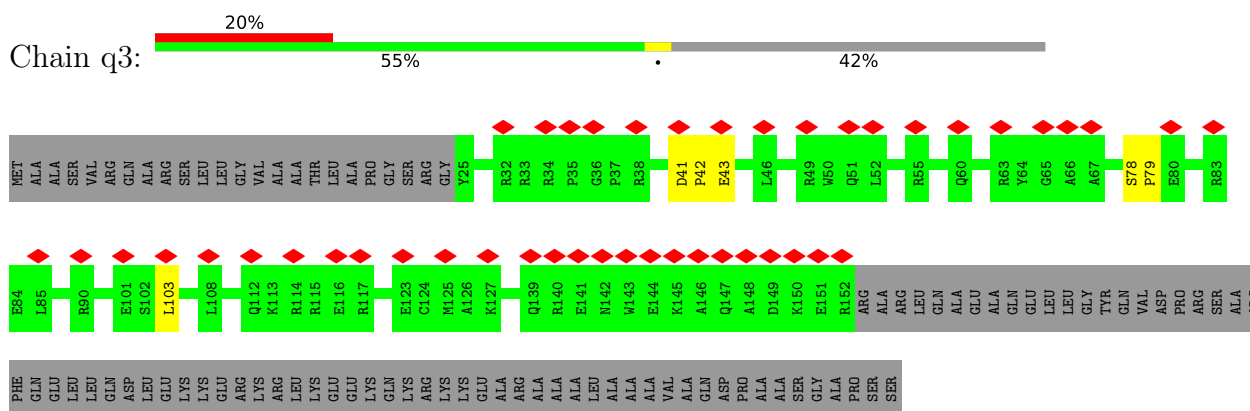
- Molecule 48: Ribosomal protein 63, mitochondrial



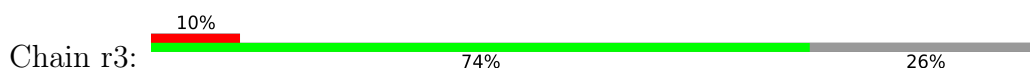
- Molecule 49: Peptidyl-tRNA hydrolase ICT1, mitochondrial

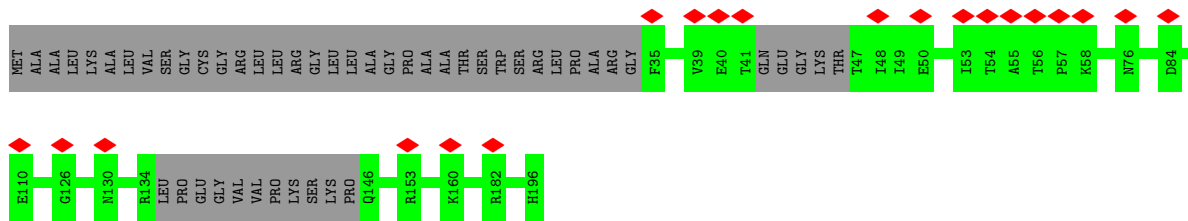


- Molecule 50: Growth arrest and DNA damage-inducible proteins-interacting protein 1

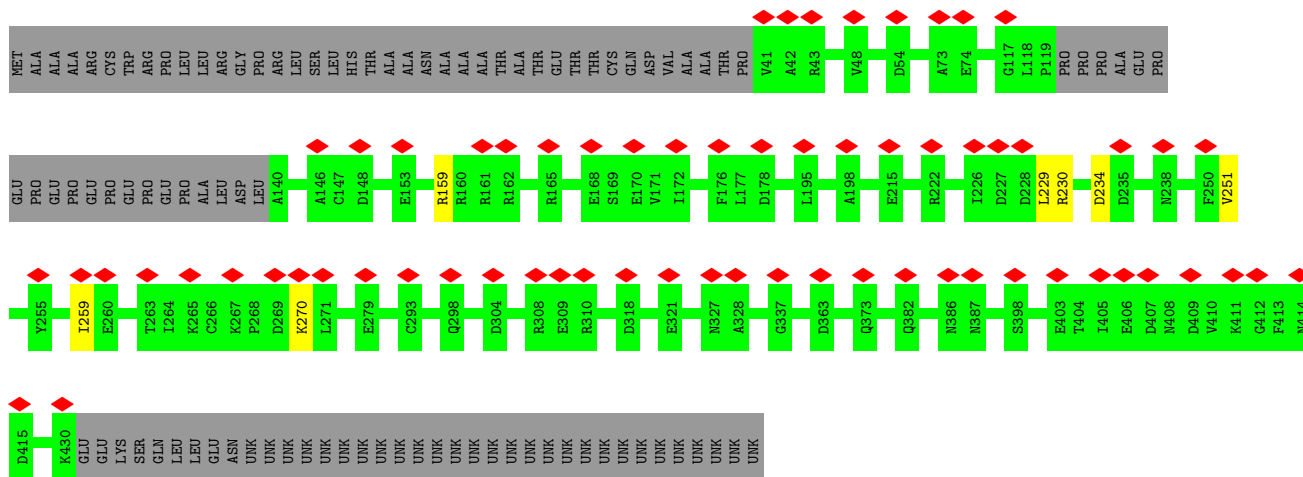
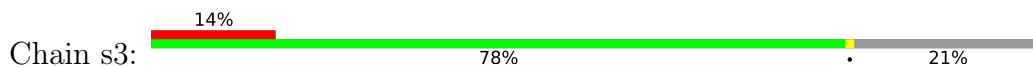


- Molecule 51: 39S ribosomal protein S18a, mitochondrial

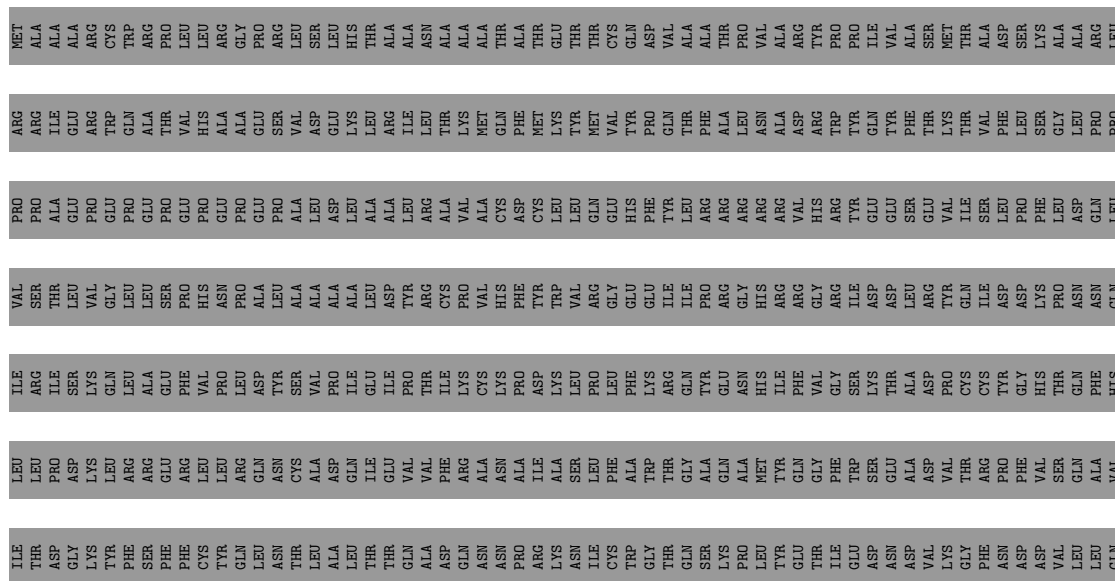


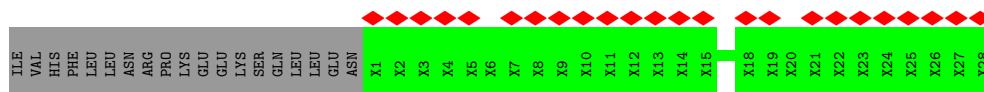


- Molecule 52: 39S ribosomal protein S30, mitochondrial,39S ribosomal protein S30, mitochondrial,mL65



- Molecule 52: 39S ribosomal protein S30, mitochondrial,39S ribosomal protein S30, mitochondrial,mL65





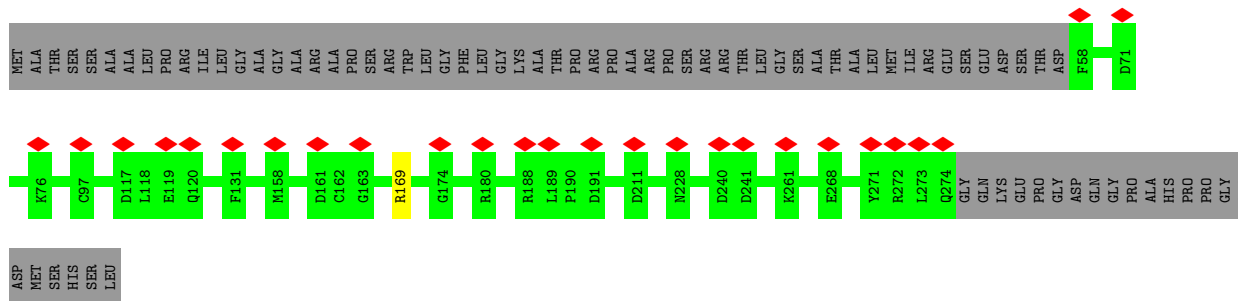
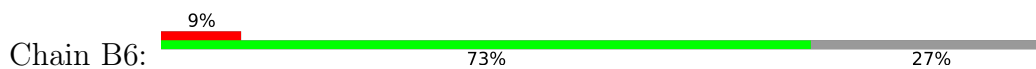
• Molecule 53: RNA (5'-R(P*CP*A)-3')



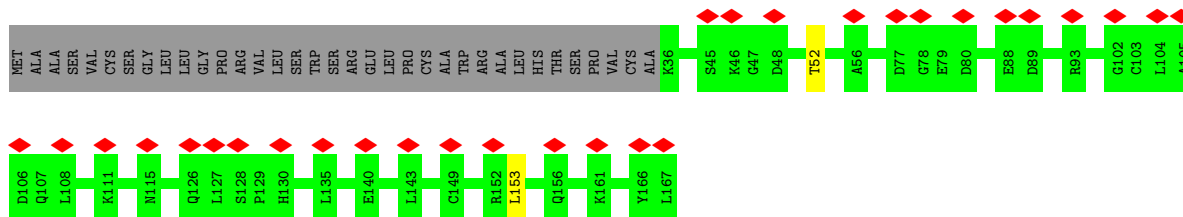
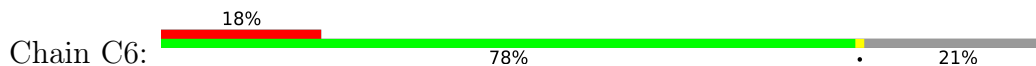
• Molecule 54: Oxa1L tail



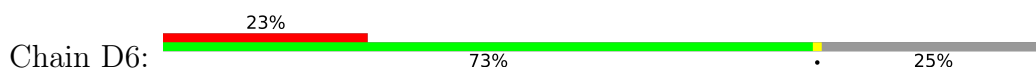
• Molecule 55: 28S ribosomal protein S2, mitochondrial

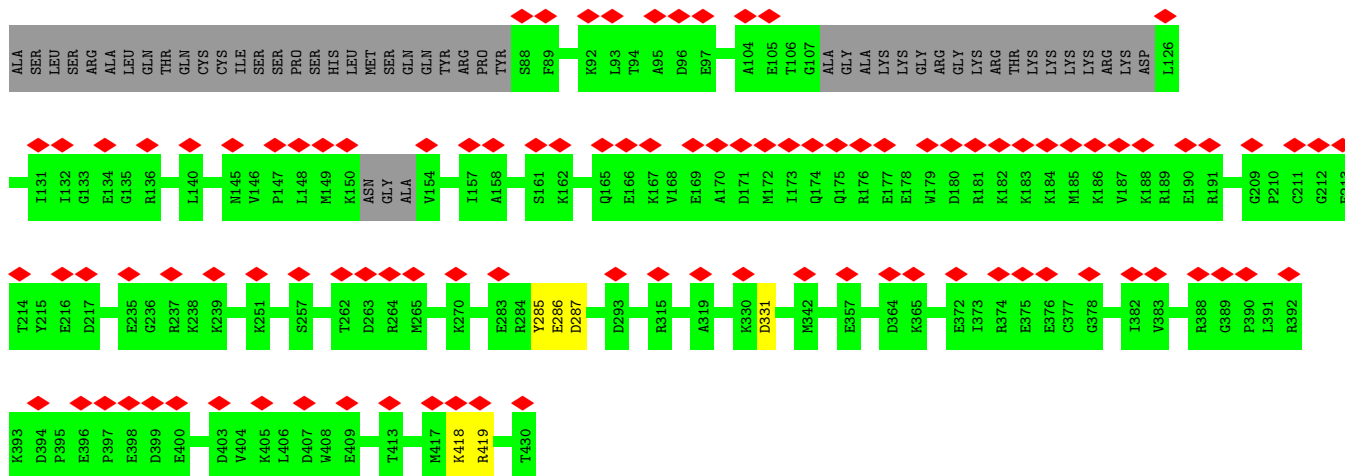


• Molecule 56: 28S ribosomal protein S24, mitochondrial

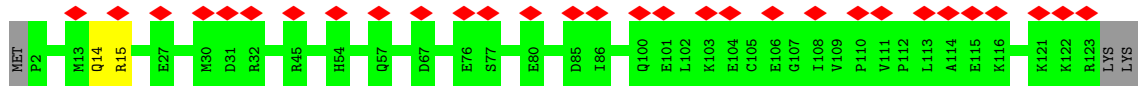


• Molecule 57: 28S ribosomal protein S5, mitochondrial

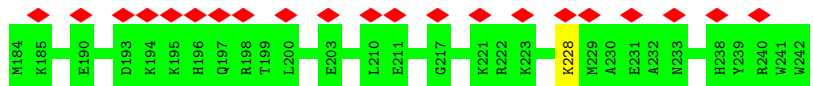
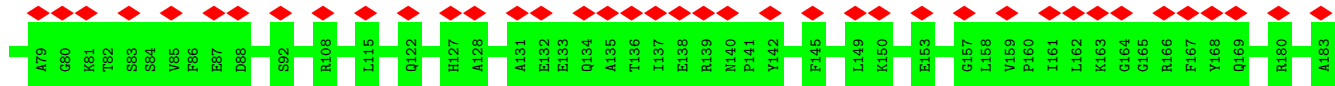
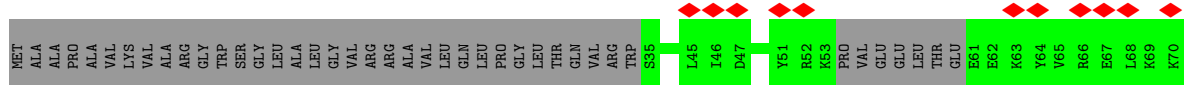
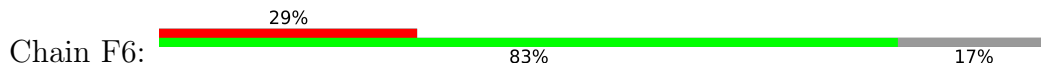




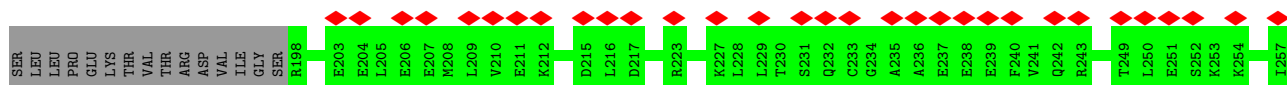
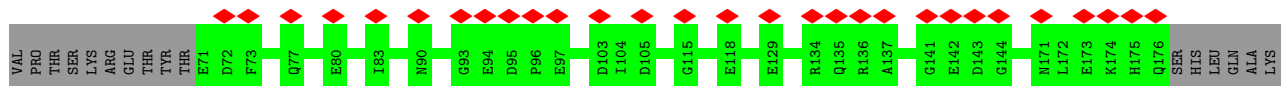
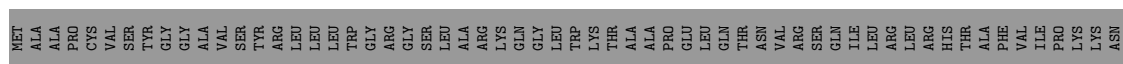
• Molecule 58: 28S ribosomal protein S6, mitochondrial

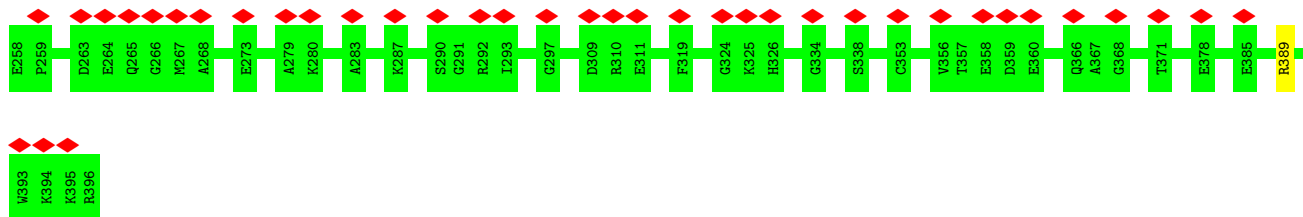


• Molecule 59: 28S ribosomal protein S7, mitochondrial

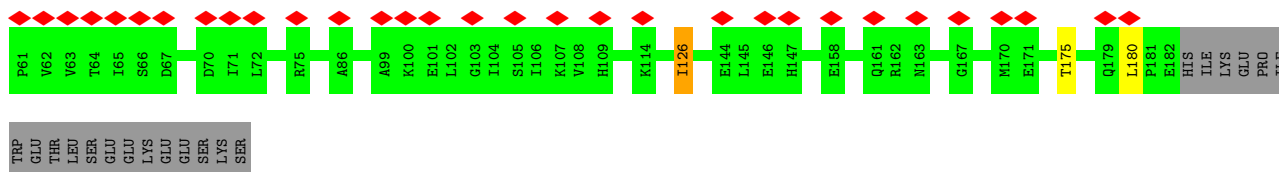


• Molecule 60: 28S ribosomal protein S9, mitochondrial

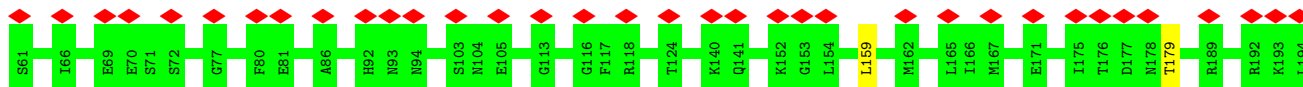
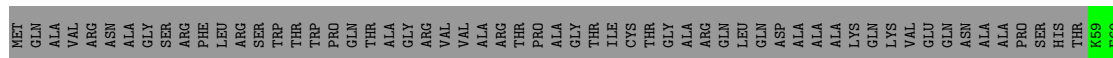




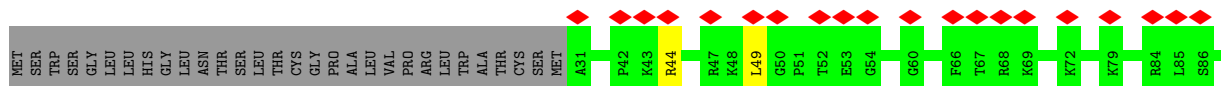
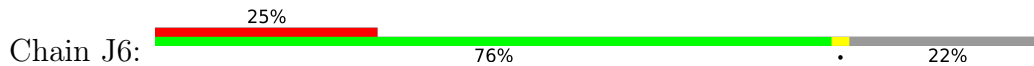
- Molecule 61: 28S ribosomal protein S10, mitochondrial



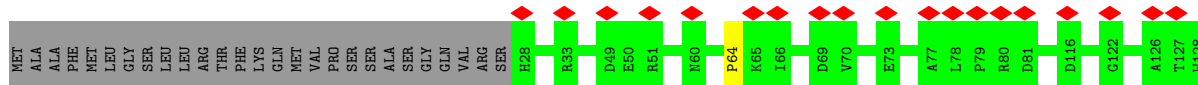
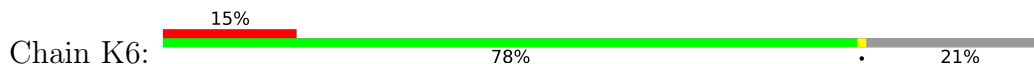
- Molecule 62: 28S ribosomal protein S11, mitochondrial



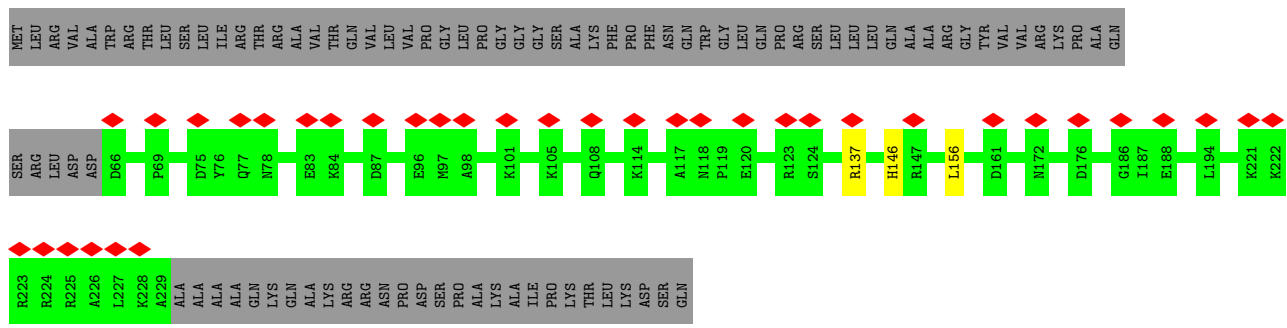
- Molecule 63: 28S ribosomal protein S12, mitochondrial



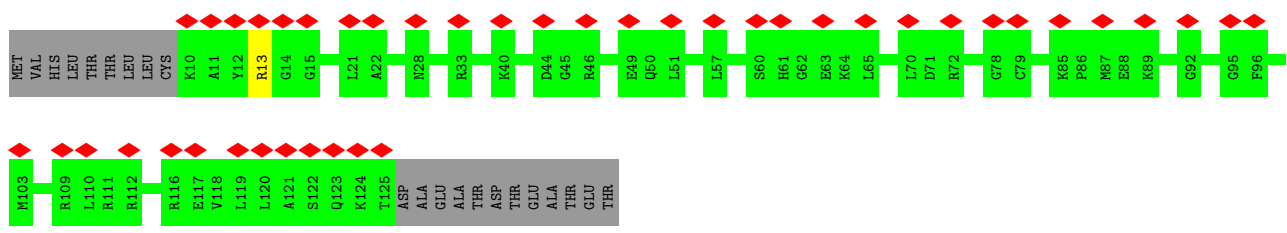
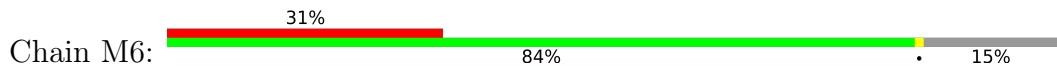
- Molecule 64: 28S ribosomal protein S14, mitochondrial



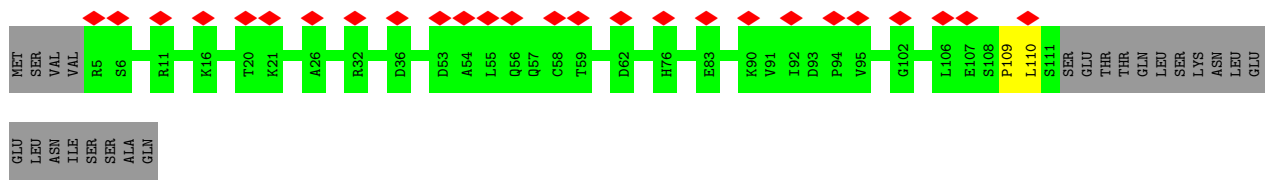
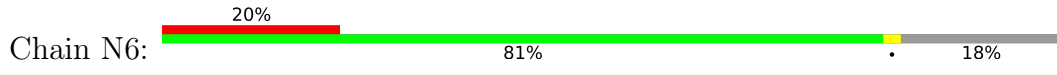
- Molecule 65: 28S ribosomal protein S15, mitochondrial



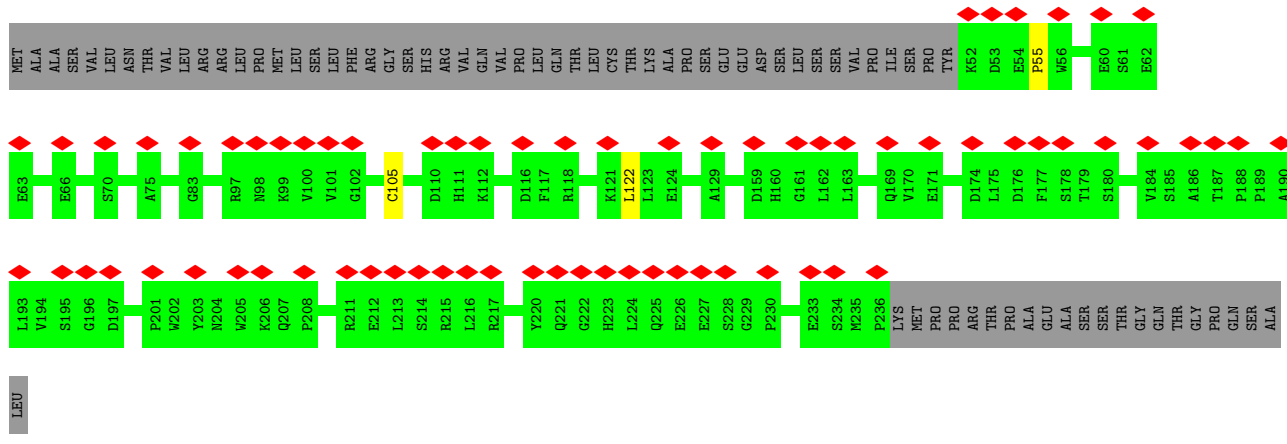
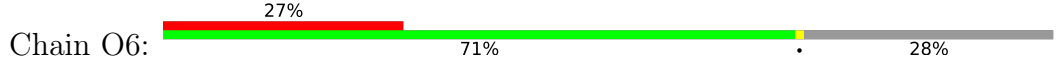
• Molecule 66: 28S ribosomal protein S16, mitochondrial



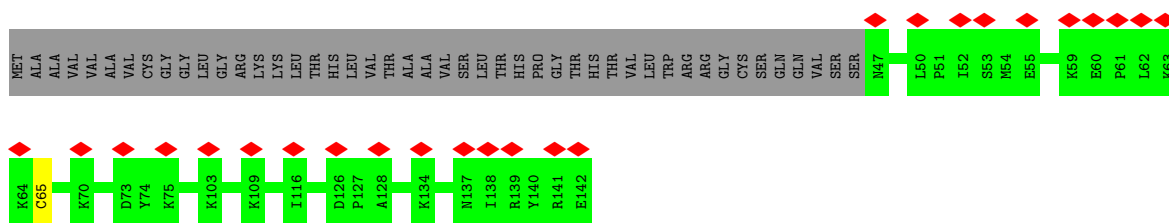
• Molecule 67: 28S ribosomal protein S17, mitochondrial



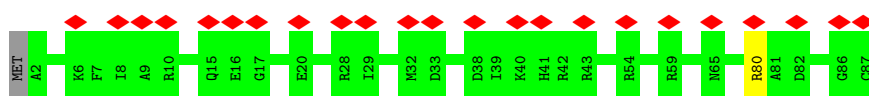
• Molecule 68: 28S ribosomal protein S18b, mitochondrial



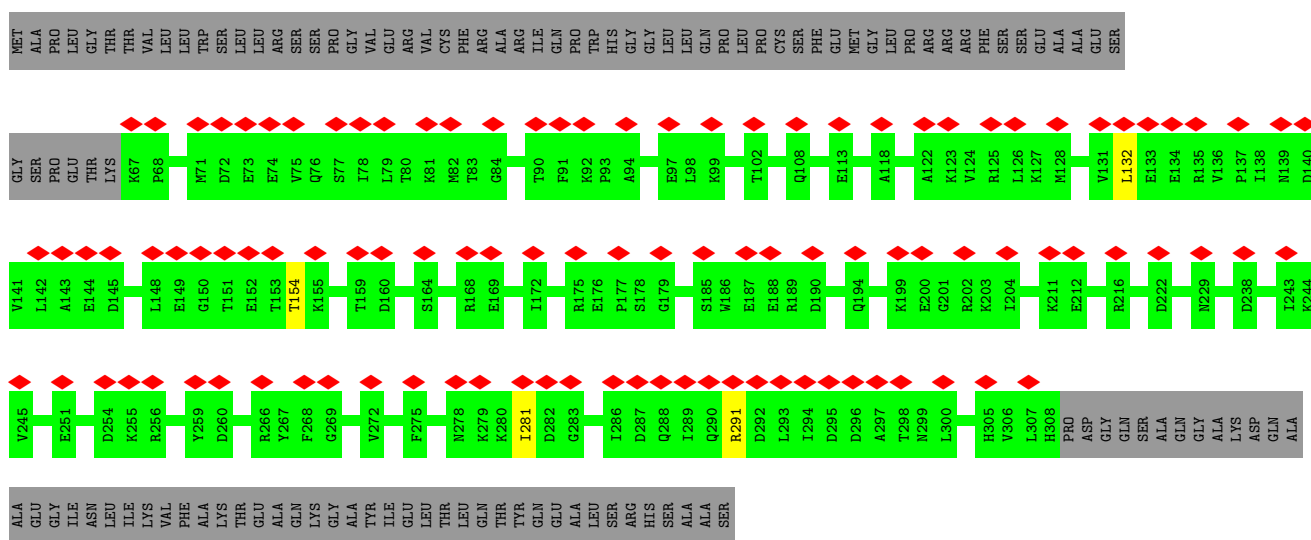
• Molecule 69: 28S ribosomal protein S18c, mitochondrial



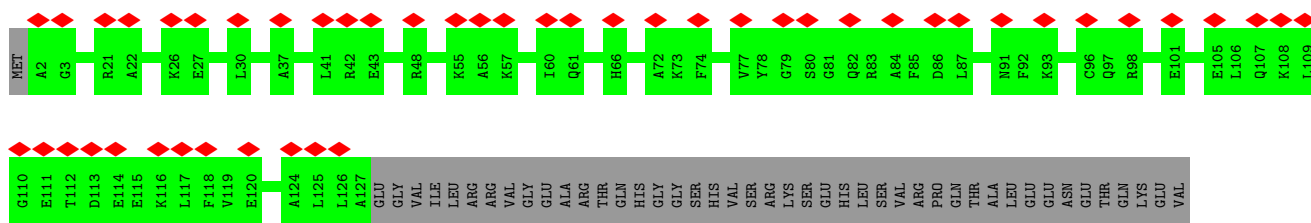
• Molecule 70: 28S ribosomal protein S21, mitochondrial



• Molecule 71: 28S ribosomal protein S22, mitochondrial

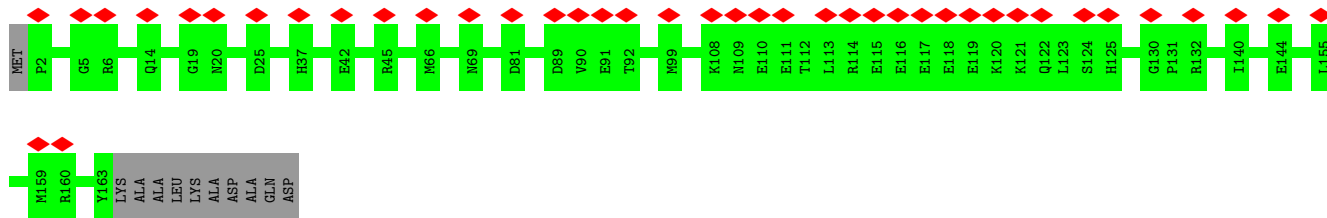


• Molecule 72: 28S ribosomal protein S23, mitochondrial

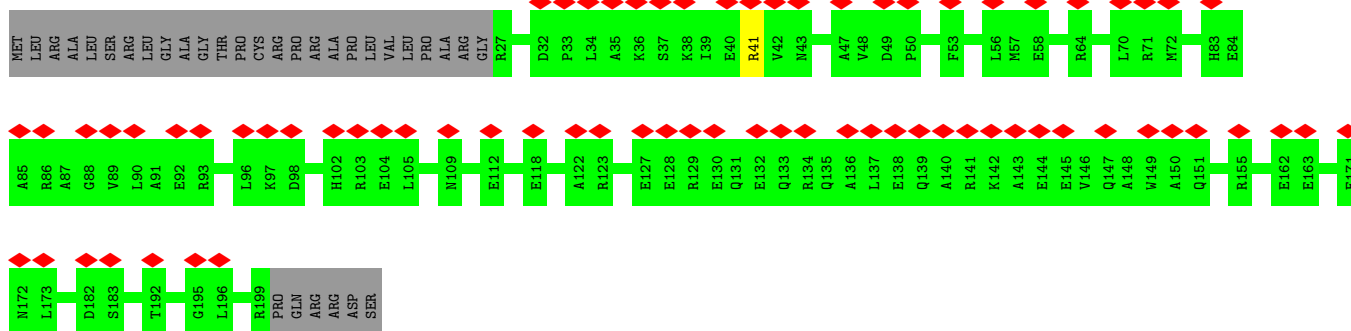
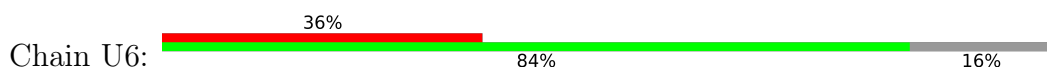


PRO
GLN
ASP
GLN
HIS
LEU
GLU
ALA
PRO
ASP
GLN
SER
LYS
GLY
LEU
LEU
PRO
PRO

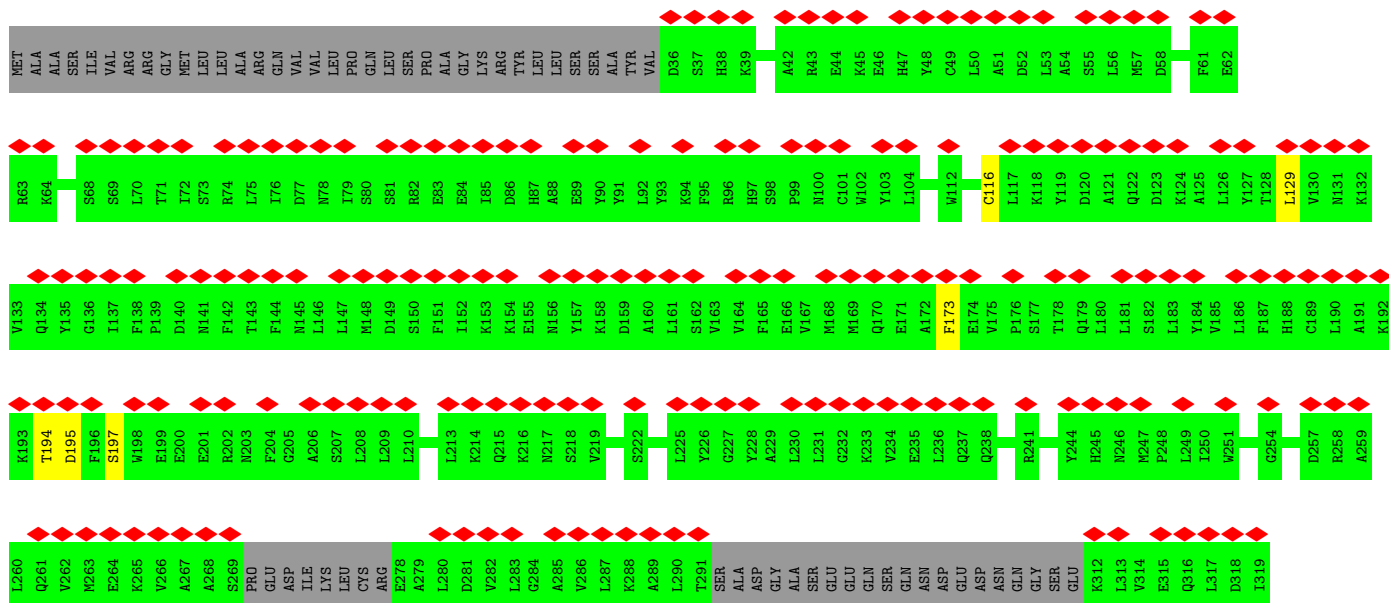
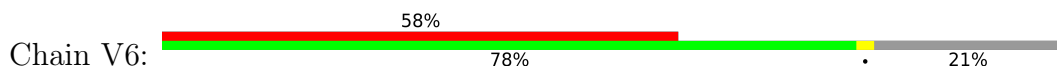
- Molecule 73: 28S ribosomal protein S25, mitochondrial

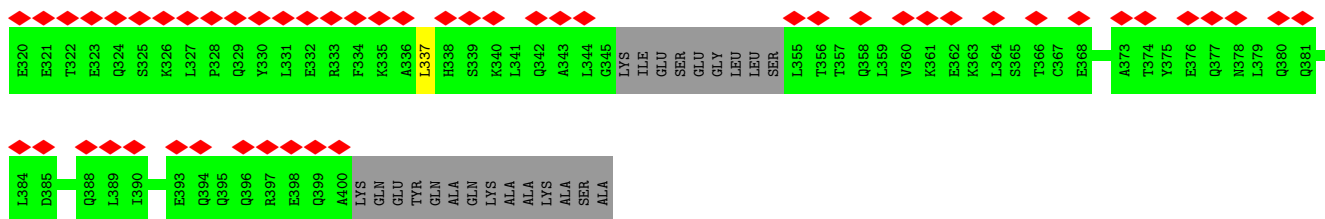


- Molecule 74: 28S ribosomal protein S26, mitochondrial

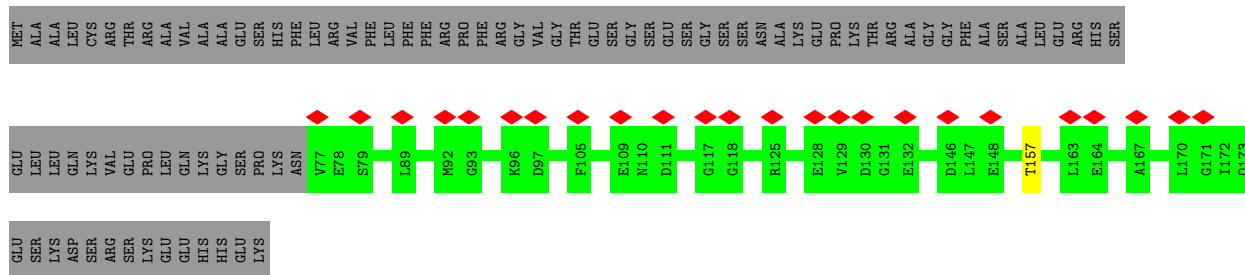


- Molecule 75: 28S ribosomal protein S27, mitochondrial

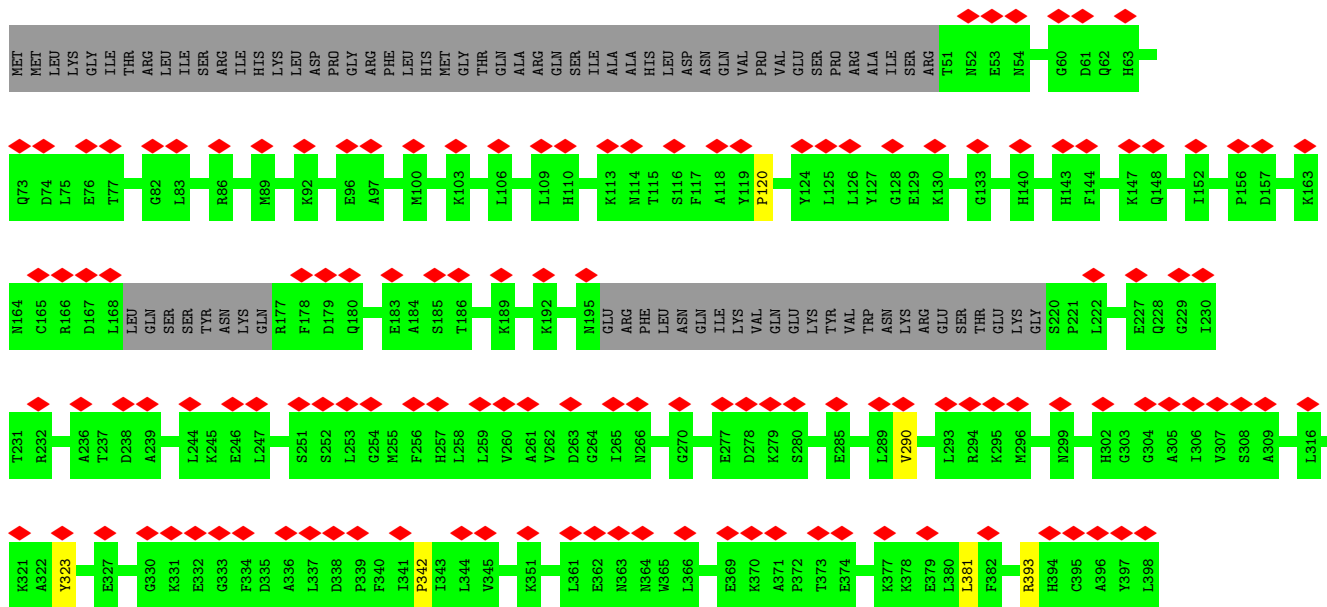
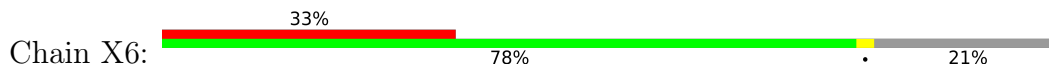




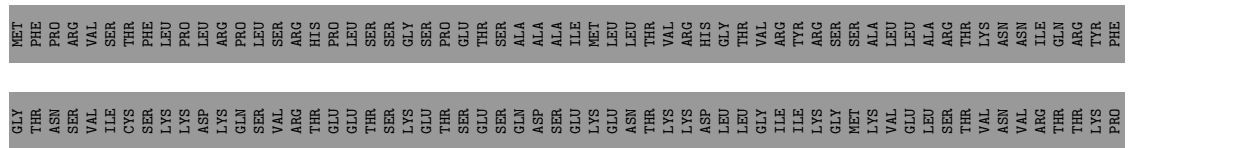
• Molecule 76: 28S ribosomal protein S28, mitochondrial

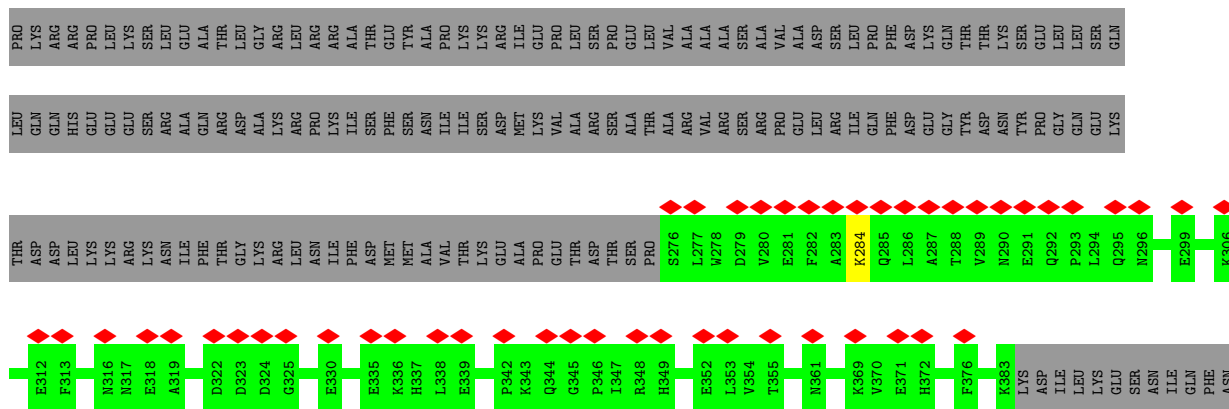


• Molecule 77: 28S ribosomal protein S29, mitochondrial

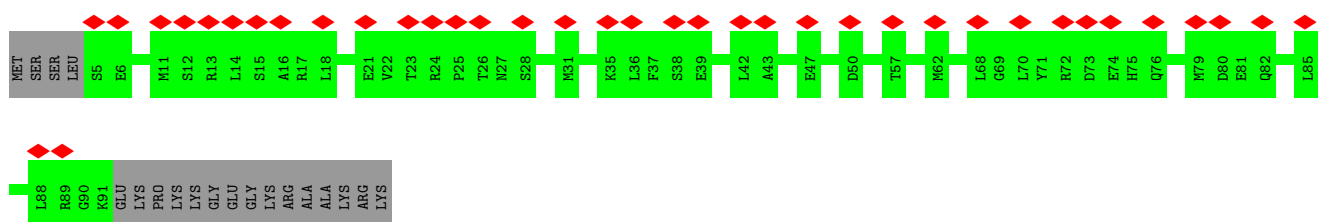
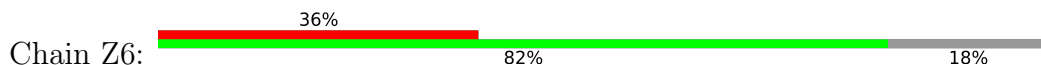


• Molecule 78: 28S ribosomal protein S31, mitochondrial

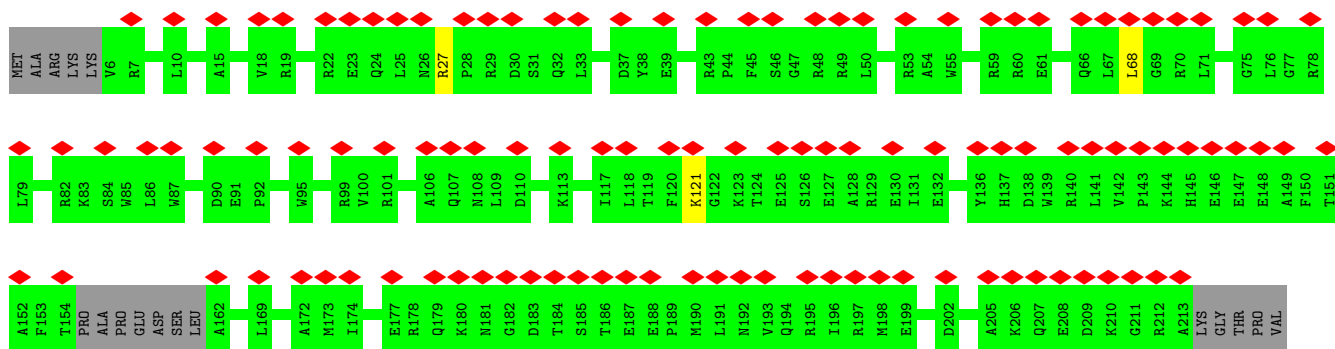
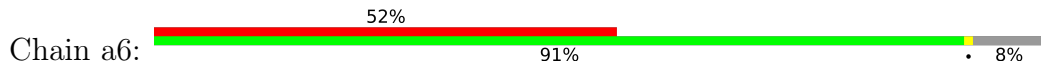




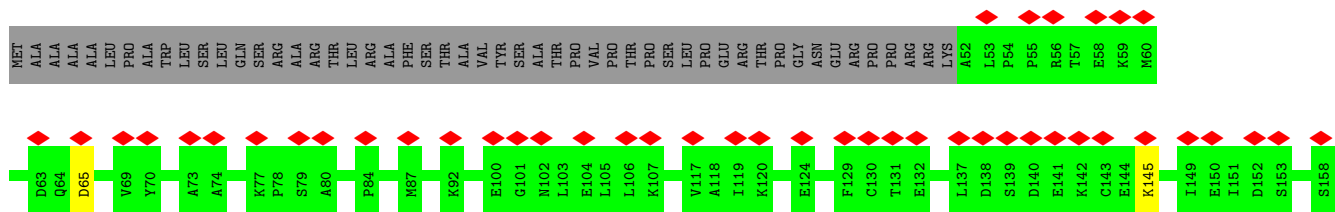
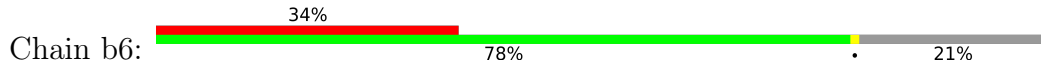
• Molecule 79: 28S ribosomal protein S33, mitochondrial

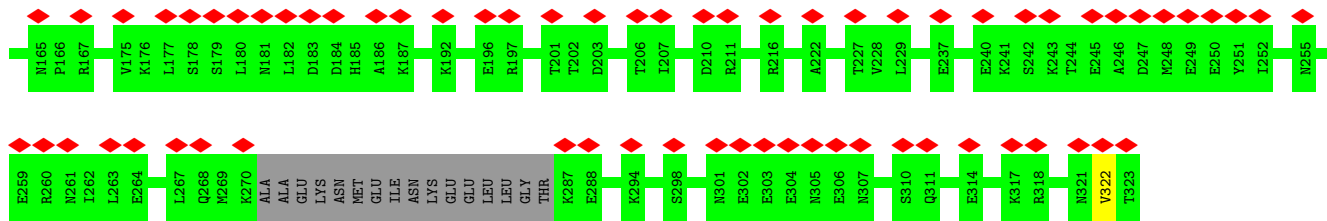


• Molecule 80: 28S ribosomal protein S34, mitochondrial

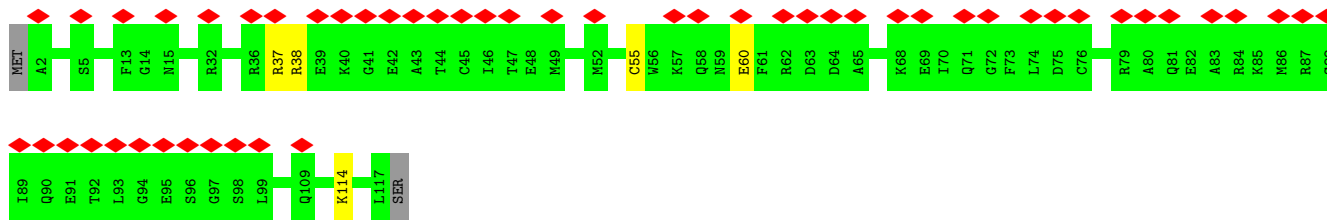
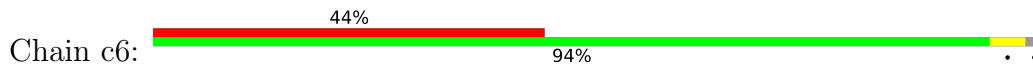


• Molecule 81: 28S ribosomal protein S35, mitochondrial

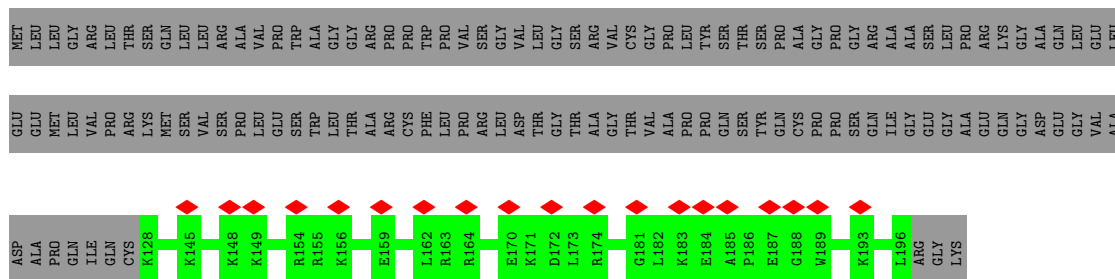




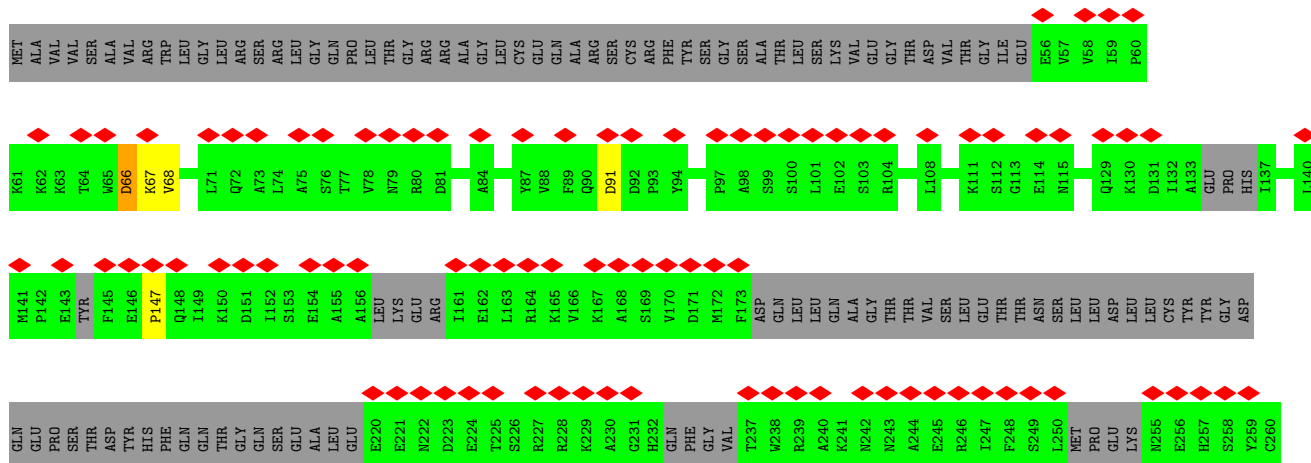
• Molecule 82: Coiled-coil-helix-coiled-coil-helix domain-containing protein 1

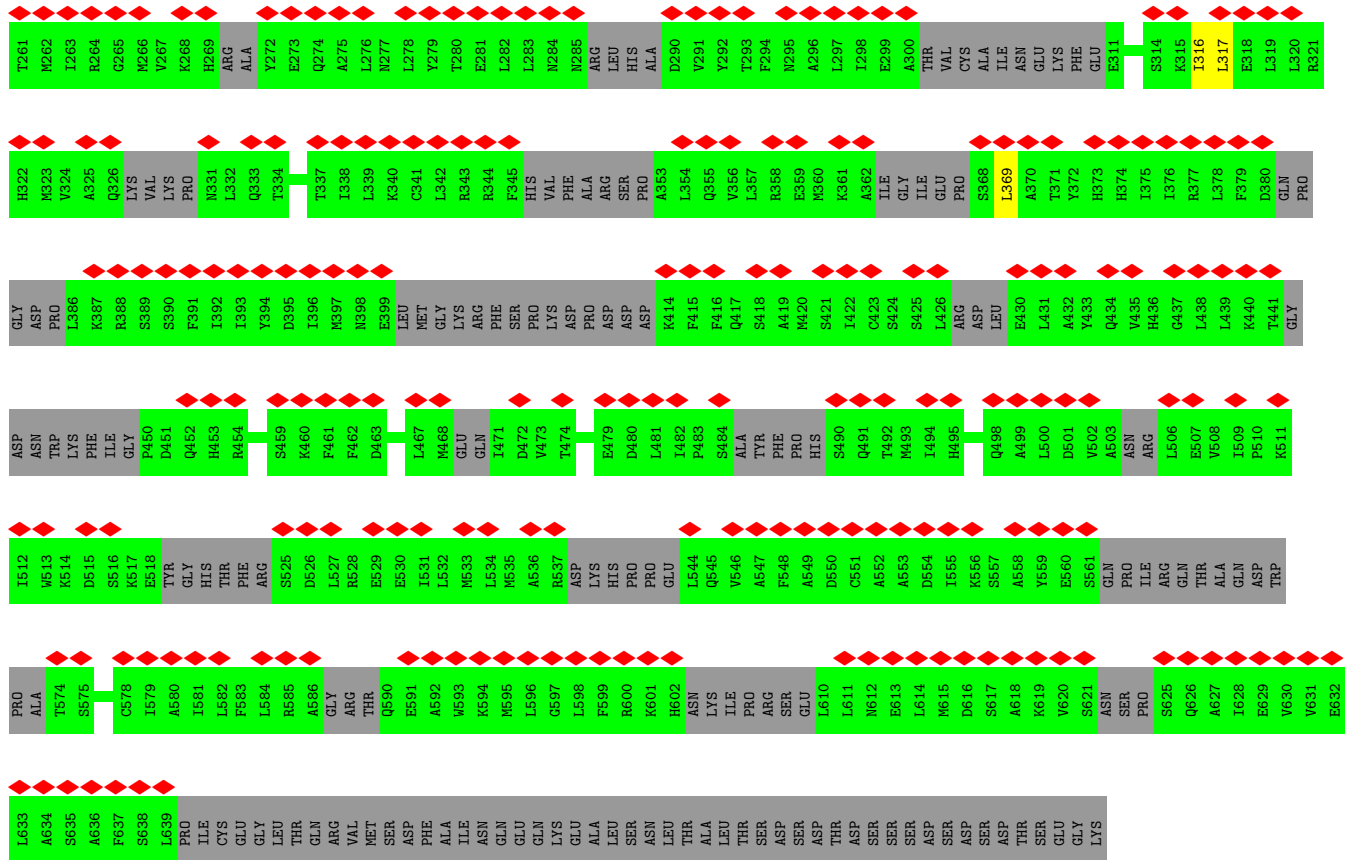


• Molecule 83: Aurora kinase A-interacting protein

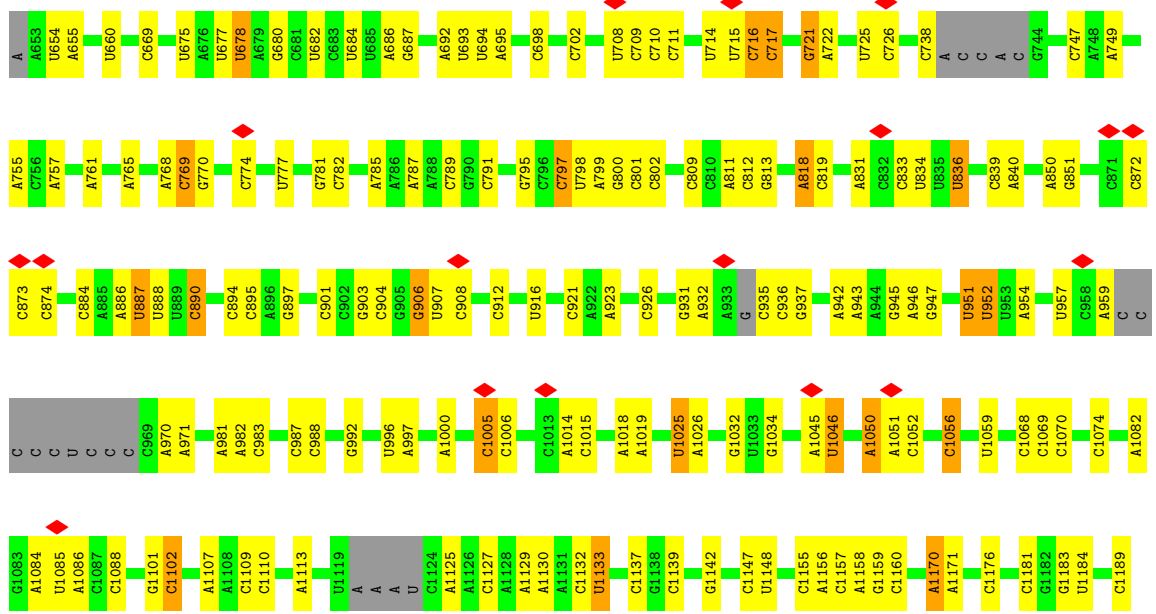


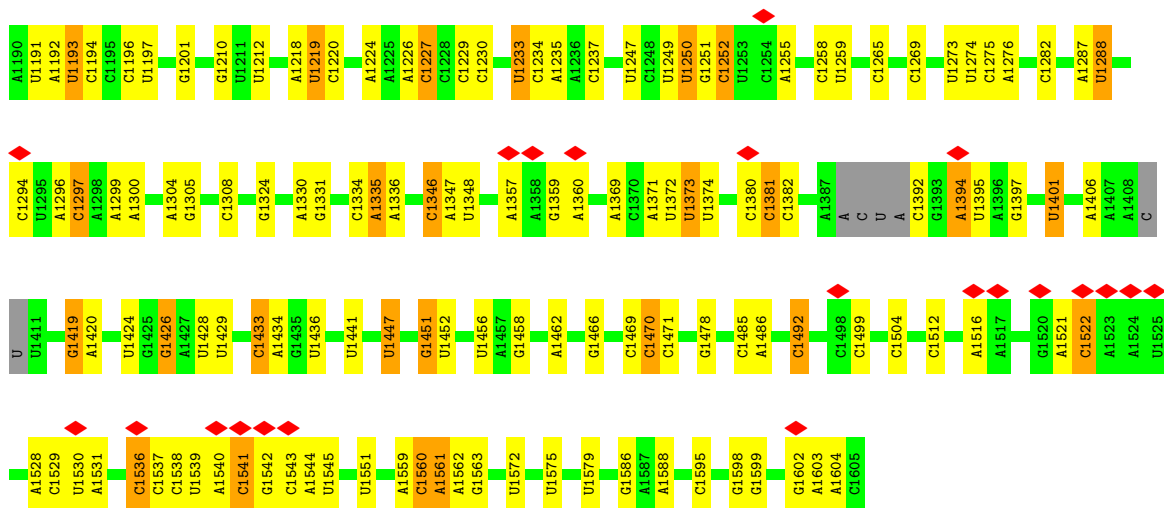
• Molecule 84: Pentatricopeptide repeat domain-containing protein 3, mitochondrial



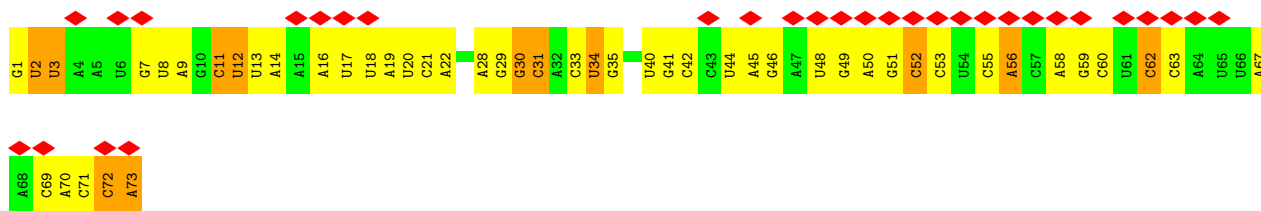
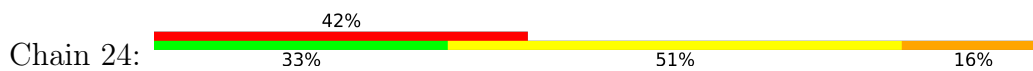


• Molecule 85: 12S rRNA

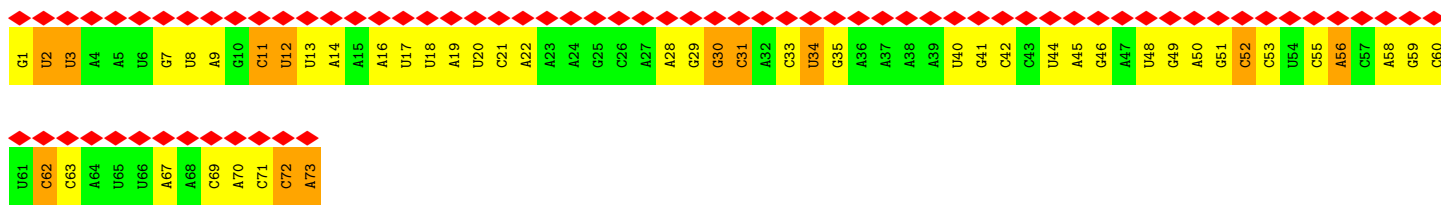




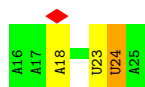
• Molecule 86: P tRNA



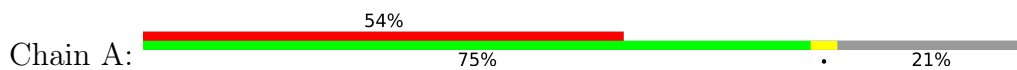
• Molecule 86: P tRNA

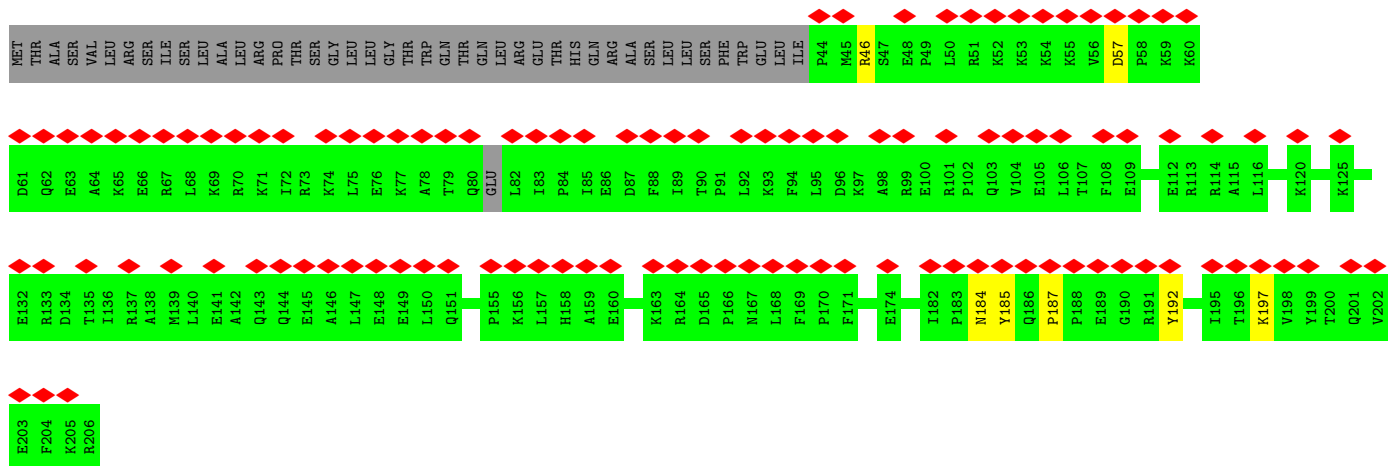


• Molecule 87: mRNA

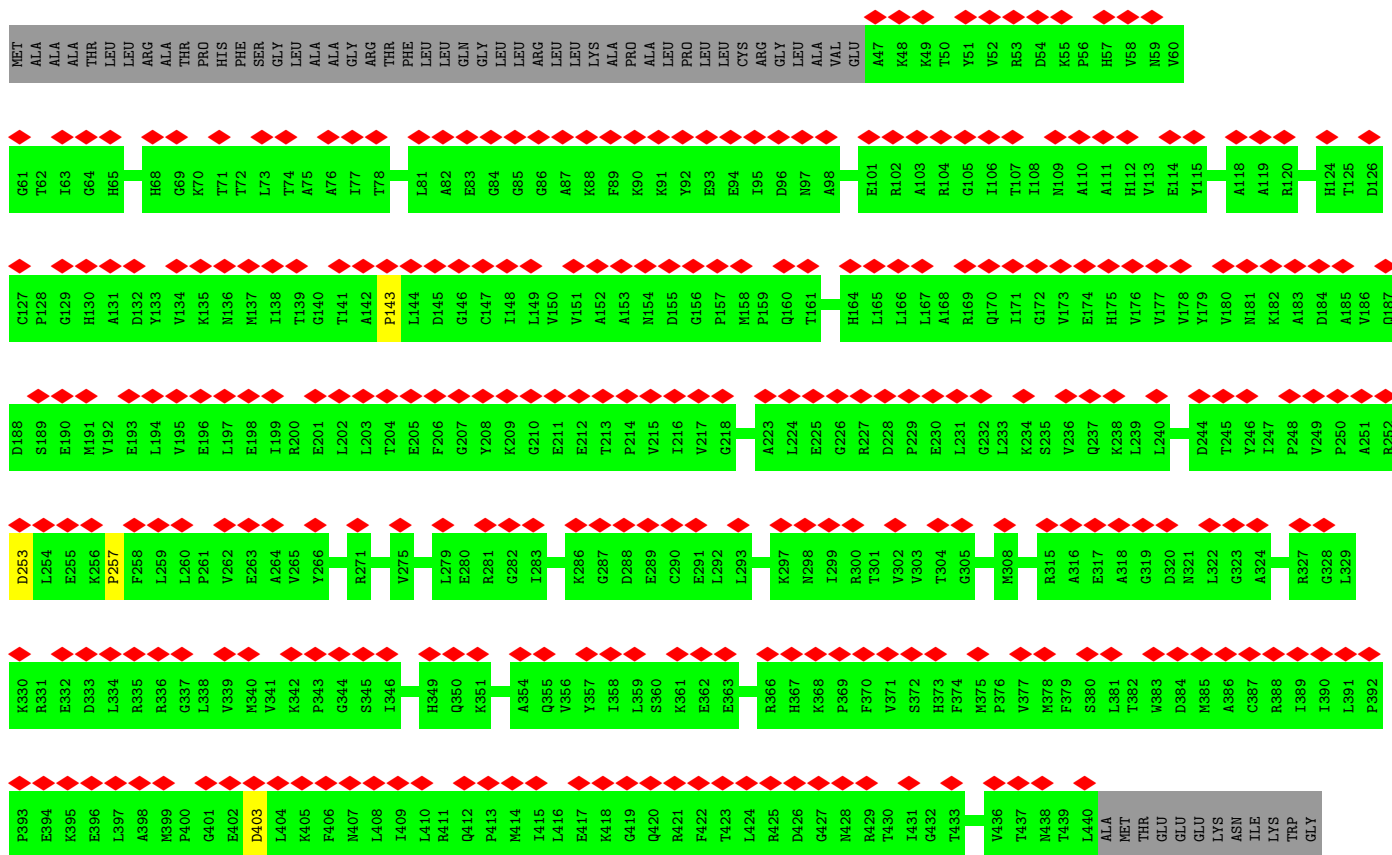
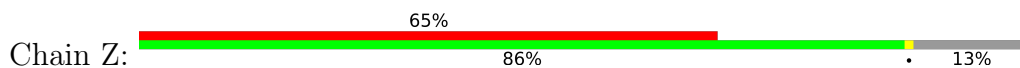


• Molecule 88: 39S ribosomal protein L40, mitochondrial

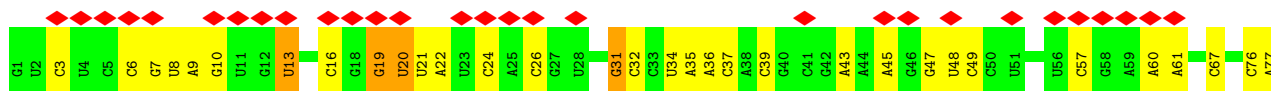




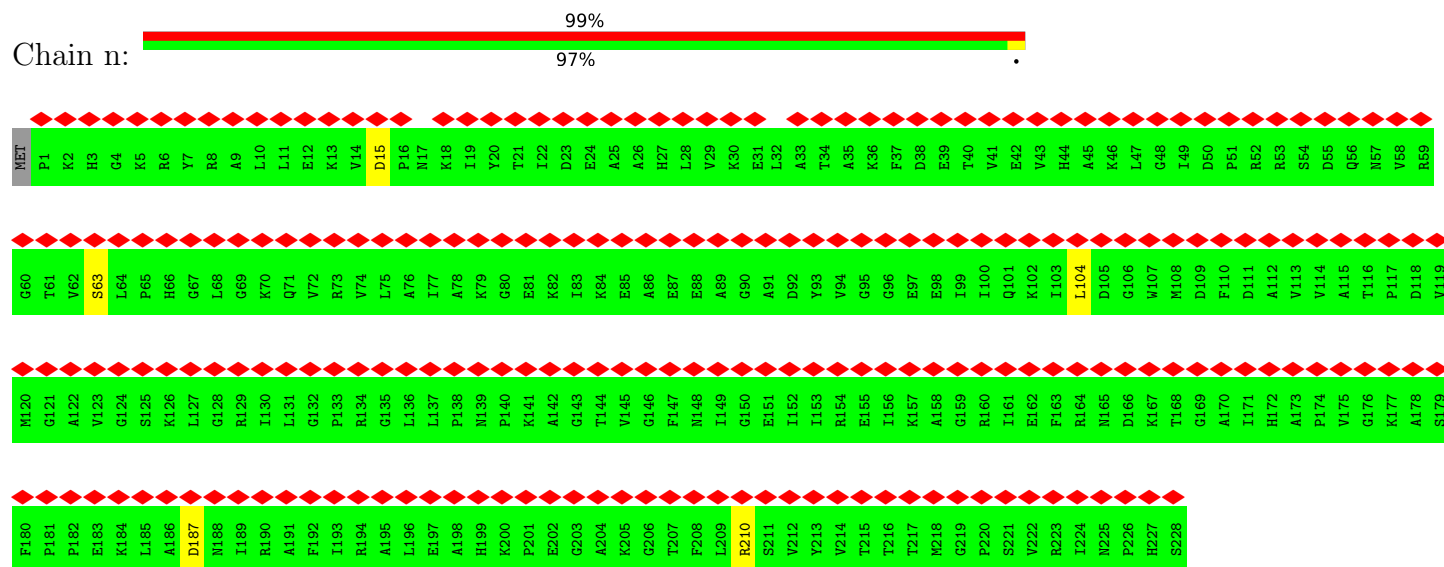
• Molecule 89: Elongation factor Tu, mitochondrial



• Molecule 90: E tRNA



- Molecule 91: 50S ribosomal protein L1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	18188	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.227	Depositor
Minimum map value	-0.130	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	532.48, 532.48, 532.48	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	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: MLI, SO4, SPD, GDP, CL, GCP, ZN, MG, NA

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	Y2	0.31	0/144	0.72	0/200
2	A3	0.95	2/35697 (0.0%)	1.29	424/55544 (0.8%)
3	B3	0.67	0/1328	1.24	12/2056 (0.6%)
4	D3	0.48	0/1879	0.64	2/2527 (0.1%)
5	E3	0.50	0/2433	0.62	0/3299
6	F3	0.48	0/2071	0.65	1/2817 (0.0%)
7	D	0.38	0/665	0.70	0/905
7	H3	0.42	0/798	0.64	0/1073
8	I3	0.37	0/1308	0.58	0/1761
9	J3	0.35	0/1077	0.60	0/1452
10	K3	0.48	0/1495	0.61	0/2029
11	L3	0.44	0/904	0.64	0/1218
12	M3	0.49	0/2359	0.67	0/3185
13	N3	0.48	0/1697	0.60	0/2281
14	O3	0.48	0/1269	0.65	0/1708
15	P3	0.46	0/1103	0.60	0/1491
16	Q3	0.43	0/1863	0.61	1/2509 (0.0%)
17	R3	0.51	0/1174	0.60	0/1572
18	S3	0.52	1/1276 (0.1%)	0.65	0/1729
19	T3	0.50	0/1402	0.58	0/1886
20	U3	0.52	0/946	0.65	0/1283
21	V3	0.45	0/1590	0.68	1/2151 (0.0%)
22	W3	0.54	0/893	0.64	1/1204 (0.1%)
23	X3	0.48	0/2081	0.71	3/2812 (0.1%)
24	Y3	0.45	0/1552	0.57	0/2079
25	Z3	0.46	0/1003	0.62	0/1354
26	03	0.44	0/895	0.62	0/1201
27	13	0.40	0/438	0.68	0/583
28	23	0.46	0/382	0.60	0/507
29	33	0.50	0/852	0.61	0/1136
30	43	0.51	0/329	0.56	0/435
31	53	0.46	0/3154	0.66	1/4295 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	63	0.44	0/2722	0.61	2/3709 (0.1%)
33	73	0.44	0/2207	0.60	0/2978
34	93	0.45	0/896	0.60	0/1205
35	a3	0.43	0/709	0.57	0/963
36	b3	0.46	0/1202	0.61	0/1626
37	c3	0.42	0/2264	0.57	0/3059
38	d3	0.41	0/1385	0.70	1/1877 (0.1%)
39	e3	0.36	0/1797	0.66	1/2422 (0.0%)
40	f3	0.50	0/1055	0.78	1/1427 (0.1%)
41	g3	0.49	0/1102	0.62	0/1503
42	h3	0.44	0/847	0.74	3/1150 (0.3%)
43	i3	0.49	0/849	0.66	1/1135 (0.1%)
44	j3	0.44	0/698	0.57	0/940
45	k3	0.35	0/665	0.66	0/897
46	l3	0.38	0/226	0.47	0/299
47	m3	0.38	0/379	0.60	0/510
48	o3	0.47	0/818	0.57	0/1097
49	p3	0.34	0/1071	0.56	0/1433
50	q3	0.41	0/1107	0.57	1/1498 (0.1%)
51	r3	0.46	0/1238	0.56	0/1676
52	s3	0.47	0/3114	0.62	1/4225 (0.0%)
53	u3	0.58	0/46	1.07	0/69
55	B6	0.48	0/1811	0.62	0/2451
56	C6	0.50	0/1112	0.60	0/1505
57	D6	0.44	0/2607	0.64	0/3498
58	E6	0.41	0/989	0.63	1/1335 (0.1%)
59	F6	0.44	0/1708	0.62	0/2291
60	G6	0.43	0/2570	0.59	0/3443
61	H6	0.54	0/1019	0.74	1/1379 (0.1%)
62	I6	0.40	0/1031	0.60	1/1390 (0.1%)
63	J6	0.44	0/854	0.67	1/1148 (0.1%)
64	K6	0.47	0/879	0.59	0/1182
65	L6	0.42	0/1406	0.55	0/1878
66	M6	0.38	0/941	0.61	0/1265
67	N6	0.45	0/864	0.66	1/1169 (0.1%)
68	O6	0.40	0/1580	0.61	2/2150 (0.1%)
69	P6	0.47	0/791	0.63	0/1062
70	Q6	0.47	0/752	0.58	0/1001
71	R6	0.39	0/2050	0.62	0/2770
72	S6	0.43	0/1069	0.59	0/1441
73	T6	0.43	0/1361	0.64	0/1829
74	U6	0.37	0/1482	0.56	0/1987
75	V6	0.36	0/2758	0.64	2/3724 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	W6	0.43	0/778	0.67	0/1048
77	X6	0.41	0/2596	0.69	2/3519 (0.1%)
78	Y6	0.42	0/943	0.60	0/1274
79	Z6	0.41	0/757	0.60	0/1011
80	a6	0.37	0/1727	0.61	1/2338 (0.0%)
81	b6	0.39	0/2121	0.63	0/2873
82	c6	0.43	1/939 (0.1%)	0.59	0/1256
83	d6	0.41	0/621	0.65	0/820
84	e6	0.37	0/2859	0.60	3/3864 (0.1%)
85	A6	0.89	0/22053	1.27	237/34324 (0.7%)
86	24	0.61	0/1731	1.55	47/2693 (1.7%)
86	C	0.60	0/1731	1.55	48/2693 (1.8%)
87	i4	0.84	0/242	1.33	4/375 (1.1%)
88	A	0.40	0/1403	0.68	0/1880
89	Z	0.40	0/3097	0.67	1/4190 (0.0%)
90	j	0.60	0/1805	1.36	29/2809 (1.0%)
91	n	0.34	0/1813	0.65	3/2443 (0.1%)
All	All	0.65	4/179304 (0.0%)	0.95	841/255288 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	Y2	0	2
4	D3	0	1
5	E3	0	7
6	F3	0	1
9	J3	0	1
10	K3	0	1
12	M3	0	2
13	N3	0	1
15	P3	0	2
16	Q3	0	2
17	R3	0	1
19	T3	0	1
21	V3	0	3
23	X3	0	6
24	Y3	0	1
25	Z3	0	1
26	03	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
27	13	0	1
31	53	0	4
38	d3	0	3
40	f3	0	6
42	h3	0	2
45	k3	0	2
50	q3	0	1
52	s3	0	2
57	D6	0	2
63	J6	0	1
64	K6	0	1
67	N6	0	1
68	O6	0	1
69	P6	0	1
71	R6	0	3
75	V6	0	1
82	c6	0	2
84	e6	0	1
88	A	0	6
89	Z	0	1
All	All	0	76

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A3	2688	C	C2-O2	-5.81	1.19	1.24
18	S3	57	SER	C-N	-5.78	1.20	1.34
2	A3	1984	A	N7-C5	-5.30	1.36	1.39
82	c6	55	CYS	CB-SG	-5.11	1.73	1.81

All (841) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	24	73	A	N7-C8-N9	15.03	121.31	113.80
86	C	73	A	N7-C8-N9	14.98	121.29	113.80
86	24	73	A	C8-N9-C4	-14.45	100.02	105.80
86	C	73	A	C8-N9-C4	-14.35	100.06	105.80
2	A3	1732	C	N1-C2-O2	13.99	127.30	118.90
85	A6	1373	U	C2-N1-C1'	12.03	132.13	117.70
85	A6	1193	U	N1-C2-O2	11.93	131.15	122.80
2	A3	2900	C	C2-N1-C1'	11.79	131.77	118.80
2	A3	1732	C	N3-C2-O2	-11.75	113.67	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	A6	1193	U	C2-N1-C1'	11.59	131.61	117.70
2	A3	1732	C	C2-N1-C1'	11.58	131.54	118.80
2	A3	2522	U	C2-N1-C1'	11.36	131.34	117.70
2	A3	2523	C	C2-N1-C1'	11.35	131.28	118.80
85	A6	1373	U	N1-C2-O2	11.08	130.55	122.80
2	A3	2523	C	N1-C2-O2	10.94	125.46	118.90
2	A3	3204	C	N1-C2-O2	10.92	125.45	118.90
85	A6	1193	U	N3-C2-O2	-10.62	114.77	122.20
2	A3	2900	C	N1-C2-O2	10.61	125.27	118.90
2	A3	2522	U	N1-C2-O2	10.44	130.11	122.80
4	D3	251	ASP	CB-CG-OD1	10.38	127.64	118.30
2	A3	2960	U	N1-C2-O2	10.19	129.93	122.80
2	A3	2386	C	N1-C2-O2	10.13	124.98	118.90
2	A3	1959	C	N1-C2-O2	9.99	124.89	118.90
2	A3	2282	C	N1-C2-O2	9.98	124.89	118.90
85	A6	1392	C	N1-C2-O2	9.94	124.86	118.90
2	A3	2901	A	O5'-P-OP1	-9.92	96.77	105.70
85	A6	1373	U	N3-C2-O2	-9.90	115.27	122.20
2	A3	2493	C	N1-C2-O2	9.79	124.77	118.90
90	j	20	U	N1-C2-O2	9.71	129.60	122.80
2	A3	1732	C	C6-N1-C2	-9.69	116.42	120.30
2	A3	3212	C	N1-C2-O2	9.64	124.68	118.90
90	j	20	U	C2-N1-C1'	9.64	129.27	117.70
85	A6	717	C	N1-C2-O2	9.57	124.64	118.90
85	A6	1252	C	N1-C2-O2	9.57	124.64	118.90
85	A6	797	C	N1-C2-O2	9.55	124.63	118.90
2	A3	1813	C	N1-C2-O2	9.53	124.61	118.90
86	24	60	C	N1-C2-O2	9.52	124.61	118.90
2	A3	1813	C	C2-N1-C1'	9.48	129.23	118.80
86	C	60	C	N1-C2-O2	9.45	124.57	118.90
2	A3	3204	C	N3-C2-O2	-9.44	115.29	121.90
2	A3	2688	C	C6-N1-C2	-9.37	116.55	120.30
2	A3	2900	C	OP1-P-O3'	9.34	125.74	105.20
85	A6	716	C	N1-C2-O2	9.33	124.50	118.90
85	A6	769	C	C2-N1-C1'	9.31	129.04	118.80
2	A3	2960	U	N3-C2-O2	-9.28	115.71	122.20
86	C	62	C	N1-C2-O2	9.26	124.45	118.90
86	24	62	C	N1-C2-O2	9.22	124.43	118.90
2	A3	2386	C	N3-C2-O2	-9.22	115.45	121.90
2	A3	1902	C	N1-C2-O2	9.19	124.41	118.90
2	A3	2523	C	N3-C2-O2	-9.18	115.48	121.90
85	A6	1392	C	N3-C2-O2	-9.15	115.49	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	h3	65	ASP	CB-CG-OD1	9.15	126.53	118.30
2	A3	1901	C	N1-C2-O2	9.11	124.36	118.90
2	A3	2079	C	C2-N1-C1'	9.07	128.78	118.80
2	A3	1699	C	N1-C2-O2	9.01	124.31	118.90
2	A3	3204	C	C2-N1-C1'	9.01	128.71	118.80
2	A3	2960	U	C2-N1-C1'	9.00	128.50	117.70
2	A3	3212	C	C2-N1-C1'	8.96	128.66	118.80
2	A3	2900	C	C6-N1-C1'	-8.92	110.10	120.80
85	A6	1252	C	N3-C2-O2	-8.91	115.66	121.90
2	A3	1693	C	C2-N1-C1'	8.85	128.54	118.80
2	A3	2079	C	N3-C2-O2	-8.82	115.72	121.90
2	A3	2079	C	N1-C2-O2	8.81	124.19	118.90
2	A3	2282	C	N3-C2-O2	-8.80	115.74	121.90
85	A6	1530	U	N1-C2-O2	8.79	128.95	122.80
2	A3	3228	U	N3-C2-O2	-8.78	116.05	122.20
85	A6	1252	C	C6-N1-C2	-8.78	116.79	120.30
85	A6	1373	U	C6-N1-C1'	-8.78	108.91	121.20
2	A3	2025	C	C6-N1-C2	-8.74	116.81	120.30
85	A6	1237	C	N3-C2-O2	-8.72	115.80	121.90
2	A3	2493	C	C2-N1-C1'	8.71	128.38	118.80
2	A3	2490	C	C6-N1-C2	-8.70	116.82	120.30
2	A3	2493	C	N3-C2-O2	-8.67	115.83	121.90
2	A3	1837	C	C2-N1-C1'	8.63	128.29	118.80
67	N6	110	LEU	CA-CB-CG	8.61	135.11	115.30
2	A3	1837	C	N1-C2-O2	8.61	124.06	118.90
2	A3	3228	U	N1-C2-O2	8.60	128.82	122.80
2	A3	3134	C	N3-C2-O2	-8.59	115.89	121.90
86	24	31	C	C5-C6-N1	8.55	125.28	121.00
85	A6	1456	U	N3-C2-O2	-8.53	116.23	122.20
2	A3	2522	U	N3-C2-O2	-8.49	116.26	122.20
85	A6	1237	C	N1-C2-O2	8.48	123.99	118.90
90	j	26	C	C6-N1-C2	-8.46	116.92	120.30
2	A3	3134	C	N1-C2-O2	8.43	123.96	118.90
86	C	31	C	C5-C6-N1	8.40	125.20	121.00
86	C	62	C	C2-N1-C1'	8.39	128.03	118.80
86	24	62	C	C2-N1-C1'	8.38	128.02	118.80
85	A6	1451	G	C4-N9-C1'	8.36	137.37	126.50
2	A3	2898	U	N3-C2-O2	-8.34	116.36	122.20
2	A3	1902	C	C2-N1-C1'	8.33	127.97	118.80
85	A6	1088	C	N1-C2-O2	8.32	123.89	118.90
2	A3	3077	C	C6-N1-C2	-8.30	116.98	120.30
2	A3	3077	C	N1-C2-O2	8.30	123.88	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A3	2489	C	N3-C2-O2	-8.26	116.12	121.90
2	A3	1901	C	N3-C2-O2	-8.22	116.14	121.90
85	A6	1133	U	C2-N1-C1'	8.20	127.54	117.70
2	A3	1959	C	N3-C2-O2	-8.18	116.17	121.90
2	A3	1813	C	N3-C2-O2	-8.17	116.18	121.90
2	A3	2750	U	N1-C2-O2	8.14	128.50	122.80
85	A6	1541	C	N1-C2-O2	8.12	123.77	118.90
2	A3	3170	C	N1-C2-O2	8.12	123.77	118.90
85	A6	797	C	N3-C2-O2	-8.12	116.22	121.90
85	A6	714	U	C2-N1-C1'	8.11	127.44	117.70
85	A6	1088	C	N3-C2-O2	-8.09	116.24	121.90
90	j	24	C	C5-C6-N1	8.07	125.04	121.00
2	A3	2061	C	N1-C2-O2	8.05	123.73	118.90
2	A3	2061	C	C2-N1-C1'	8.05	127.66	118.80
86	24	73	A	C5-N7-C8	-8.04	99.88	103.90
86	C	73	A	C5-N7-C8	-8.04	99.88	103.90
2	A3	2080	U	N1-C2-O2	8.03	128.42	122.80
2	A3	2386	C	C2-N1-C1'	8.03	127.64	118.80
2	A3	2523	C	C6-N1-C1'	-7.98	111.22	120.80
2	A3	2332	C	N1-C2-O2	7.97	123.68	118.90
2	A3	2282	C	C2-N1-C1'	7.96	127.56	118.80
2	A3	2126	U	N3-C2-O2	-7.96	116.63	122.20
90	j	20	U	N3-C2-O2	-7.91	116.66	122.20
2	A3	2522	U	C6-N1-C1'	-7.89	110.15	121.20
2	A3	2494	C	N3-C2-O2	-7.87	116.39	121.90
86	C	3	U	C2-N1-C1'	7.85	127.12	117.70
86	24	3	U	C2-N1-C1'	7.84	127.11	117.70
85	A6	1433	C	N1-C2-O2	7.81	123.58	118.90
85	A6	1530	U	N3-C2-O2	-7.80	116.74	122.20
86	24	60	C	N3-C2-O2	-7.79	116.45	121.90
85	A6	1252	C	C2-N1-C1'	7.79	127.37	118.80
85	A6	1074	C	N1-C2-O2	7.77	123.56	118.90
86	C	60	C	N3-C2-O2	-7.76	116.46	121.90
2	A3	1947	C	N3-C2-O2	-7.75	116.47	121.90
85	A6	711	C	N1-C2-O2	7.75	123.55	118.90
86	24	30	G	P-O3'-C3'	7.73	128.98	119.70
90	j	26	C	C5-C6-N1	7.73	124.87	121.00
85	A6	1219	U	N3-C2-O2	-7.72	116.80	122.20
2	A3	2080	U	N3-C2-O2	-7.71	116.80	122.20
86	C	30	G	P-O3'-C3'	7.71	128.95	119.70
85	A6	1193	U	C6-N1-C1'	-7.70	110.42	121.20
2	A3	1699	C	N3-C2-O2	-7.69	116.52	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A3	2684	C	N1-C2-O2	7.69	123.51	118.90
85	A6	717	C	N3-C2-O2	-7.68	116.53	121.90
2	A3	2126	U	N1-C2-O2	7.67	128.16	122.80
2	A3	2653	C	C6-N1-C2	-7.66	117.24	120.30
85	A6	906	G	N7-C8-N9	7.66	116.93	113.10
2	A3	2061	C	N3-C2-O2	-7.61	116.57	121.90
85	A6	1451	G	C8-N9-C1'	-7.61	117.10	127.00
2	A3	3134	C	C6-N1-C2	-7.60	117.26	120.30
2	A3	2961	C	N1-C2-O2	7.59	123.46	118.90
85	A6	1433	C	C2-N1-C1'	7.58	127.14	118.80
85	A6	797	C	C2-N1-C1'	7.55	127.11	118.80
85	A6	678	U	C2-N1-C1'	7.54	126.75	117.70
2	A3	2583	C	C6-N1-C2	-7.53	117.29	120.30
2	A3	2066	C	N1-C2-O2	7.53	123.42	118.90
2	A3	2899	C	N1-C2-O2	7.53	123.42	118.90
85	A6	717	C	C2-N1-C1'	7.51	127.06	118.80
2	A3	1715	C	N1-C2-O2	7.48	123.39	118.90
85	A6	951	U	N1-C2-O2	7.47	128.03	122.80
2	A3	2898	U	C2-N1-C1'	7.46	126.66	117.70
85	A6	906	G	C4-N9-C1'	7.46	136.20	126.50
2	A3	2557	C	N1-C2-O2	7.46	123.38	118.90
2	A3	2750	U	N3-C2-O2	-7.45	116.99	122.20
2	A3	1878	U	N3-C2-O2	-7.45	116.99	122.20
2	A3	1902	C	N3-C2-O2	-7.43	116.70	121.90
2	A3	1947	C	C6-N1-C2	-7.40	117.34	120.30
2	A3	2900	C	N3-C2-O2	-7.39	116.72	121.90
2	A3	3077	C	N3-C2-O2	-7.39	116.73	121.90
2	A3	2952	U	N3-C2-O2	-7.39	117.03	122.20
90	j	57	C	C5-C6-N1	7.38	124.69	121.00
2	A3	2490	C	N3-C2-O2	-7.37	116.74	121.90
2	A3	2727	C	C2-N1-C1'	7.36	126.90	118.80
2	A3	1732	C	C6-N1-C1'	-7.35	111.97	120.80
2	A3	3228	U	C2-N1-C1'	7.35	126.53	117.70
2	A3	3077	C	C2-N1-C1'	7.34	126.88	118.80
2	A3	2187	C	N1-C2-O2	7.34	123.31	118.90
2	A3	1693	C	N1-C2-O2	7.32	123.29	118.90
2	A3	2523	C	C6-N1-C2	-7.31	117.38	120.30
2	A3	2379	C	N1-C2-O2	7.30	123.28	118.90
2	A3	2688	C	N3-C2-O2	-7.29	116.80	121.90
85	A6	714	U	N3-C2-O2	-7.27	117.11	122.20
2	A3	2080	U	C2-N1-C1'	7.24	126.39	117.70
2	A3	2357	C	N1-C2-O2	7.23	123.24	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A3	1707	C	N1-C2-O2	7.23	123.24	118.90
85	A6	1451	G	N3-C4-N9	7.22	130.33	126.00
85	A6	716	C	C2-N1-C1'	7.21	126.73	118.80
2	A3	2952	U	N1-C2-O2	7.21	127.84	122.80
63	J6	49	LEU	CA-CB-CG	7.20	131.87	115.30
85	A6	1395	U	C2-N1-C1'	7.19	126.33	117.70
85	A6	1595	C	C6-N1-C2	-7.19	117.42	120.30
2	A3	3212	C	N3-C2-O2	-7.19	116.87	121.90
85	A6	1237	C	C6-N1-C2	-7.18	117.43	120.30
2	A3	2898	U	N1-C2-O2	7.15	127.80	122.80
85	A6	1133	U	C5-C6-N1	7.14	126.27	122.70
85	A6	1433	C	N3-C2-O2	-7.14	116.90	121.90
2	A3	3093	C	C5-C6-N1	7.13	124.57	121.00
85	A6	1139	C	N3-C2-O2	-7.12	116.92	121.90
2	A3	1901	C	C2-N1-C1'	7.11	126.62	118.80
2	A3	2627	G	N3-C4-N9	-7.11	121.74	126.00
2	A3	2646	G	N3-C2-N2	-7.08	114.95	119.90
2	A3	1732	C	C5-C6-N1	7.06	124.53	121.00
2	A3	2961	C	N3-C2-O2	-7.04	116.97	121.90
2	A3	1699	C	C2-N1-C1'	7.02	126.52	118.80
2	A3	2854	U	C2-N1-C1'	7.01	126.11	117.70
2	A3	1770	G	N3-C2-N2	-7.01	115.00	119.90
85	A6	890	C	C2-N1-C1'	6.98	126.48	118.80
85	A6	1451	G	C6-C5-N7	-6.96	126.22	130.40
2	A3	2522	U	C5-C6-N1	6.96	126.18	122.70
2	A3	2372	U	N3-C2-O2	-6.96	117.33	122.20
85	A6	1237	C	C2-N1-C1'	6.95	126.45	118.80
2	A3	1807	U	P-O3'-C3'	6.95	128.04	119.70
85	A6	769	C	C6-N1-C2	-6.95	117.52	120.30
85	A6	1541	C	N3-C2-O2	-6.95	117.04	121.90
2	A3	2494	C	N1-C2-O2	6.94	123.06	118.90
2	A3	2284	C	N1-C2-O2	6.93	123.06	118.90
85	A6	1429	U	N1-C2-O2	6.93	127.65	122.80
90	j	24	C	C6-N1-C2	-6.91	117.54	120.30
85	A6	1074	C	N3-C2-O2	-6.91	117.06	121.90
2	A3	2372	U	C2-N1-C1'	6.89	125.97	117.70
2	A3	2530	A	P-O3'-C3'	6.89	127.97	119.70
2	A3	1806	U	P-O3'-C3'	6.88	127.96	119.70
2	A3	2684	C	C2-N1-C1'	6.88	126.37	118.80
85	A6	1025	U	N1-C2-O2	6.88	127.62	122.80
85	A6	709	C	N1-C2-O2	6.87	123.02	118.90
85	A6	710	C	C2-N1-C1'	6.87	126.36	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A3	2364	C	N1-C2-O2	6.87	123.02	118.90
2	A3	3169	C	C2-N1-C1'	6.86	126.35	118.80
2	A3	2728	C	C5-C6-N1	6.84	124.42	121.00
2	A3	1944	C	N1-C2-O2	6.84	123.00	118.90
2	A3	2066	C	C2-N1-C1'	6.83	126.31	118.80
86	C	53	C	C6-N1-C2	-6.82	117.57	120.30
2	A3	1715	C	N3-C2-O2	-6.80	117.14	121.90
85	A6	714	U	N1-C2-O2	6.80	127.56	122.80
2	A3	2066	C	N3-C2-O2	-6.78	117.15	121.90
85	A6	791	C	C2-N1-C1'	6.78	126.26	118.80
2	A3	2171	U	C2-N1-C1'	6.77	125.83	117.70
85	A6	1392	C	C6-N1-C2	-6.77	117.59	120.30
85	A6	936	C	N1-C2-O2	6.77	122.96	118.90
86	24	53	C	C6-N1-C2	-6.75	117.60	120.30
2	A3	1837	C	N3-C2-O2	-6.75	117.17	121.90
2	A3	1878	U	N1-C2-O2	6.75	127.53	122.80
85	A6	678	U	C5-C6-N1	6.75	126.07	122.70
90	j	16	C	C6-N1-C2	-6.75	117.60	120.30
2	A3	2583	C	C2-N1-C1'	6.75	126.22	118.80
84	e6	66	ASP	CB-CG-OD1	6.75	124.37	118.30
85	A6	1429	U	C2-N1-C1'	6.74	125.79	117.70
2	A3	2900	C	C5-C6-N1	6.73	124.36	121.00
2	A3	3077	C	C5-C6-N1	6.72	124.36	121.00
86	C	60	C	C2-N1-C1'	6.72	126.19	118.80
2	A3	2710	C	N1-C2-O2	6.71	122.93	118.90
2	A3	1813	C	C6-N1-C1'	-6.71	112.75	120.80
2	A3	2295	C	N1-C2-O2	6.71	122.93	118.90
2	A3	2961	C	C6-N1-C2	-6.70	117.62	120.30
2	A3	1984	A	N7-C8-N9	6.69	117.14	113.80
85	A6	1025	U	N3-C2-O2	-6.68	117.52	122.20
86	24	60	C	C2-N1-C1'	6.68	126.15	118.80
90	j	39	C	N1-C2-O2	6.67	122.91	118.90
2	A3	2757	A	O4'-C1'-N9	6.67	113.54	108.20
2	A3	3170	C	C2-N1-C1'	6.66	126.13	118.80
85	A6	906	G	C6-C5-N7	-6.66	126.41	130.40
86	24	52	C	N1-C2-O2	6.66	122.89	118.90
2	A3	2530	A	OP2-P-O3'	6.66	119.84	105.20
23	X3	92	ALA	N-CA-C	6.65	128.97	111.00
2	A3	2079	C	C6-N1-C2	-6.65	117.64	120.30
86	24	2	U	C2-N1-C1'	6.64	125.67	117.70
85	A6	1193	U	C5-C6-N1	6.64	126.02	122.70
86	C	2	U	C2-N1-C1'	6.63	125.66	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	A6	1288	U	N3-C2-O2	-6.63	117.56	122.20
86	C	52	C	N1-C2-O2	6.63	122.88	118.90
2	A3	2870	G	C4-N9-C1'	6.61	135.10	126.50
85	A6	906	G	C8-N9-C4	-6.61	103.75	106.40
2	A3	2332	C	N3-C2-O2	-6.61	117.28	121.90
2	A3	2865	C	N1-C2-O2	6.60	122.86	118.90
2	A3	3116	C	C6-N1-C2	-6.58	117.67	120.30
2	A3	2627	G	C4-N9-C1'	-6.57	117.96	126.50
85	A6	1499	C	N1-C2-O2	6.54	122.82	118.90
85	A6	675	U	C2-N1-C1'	6.53	125.53	117.70
86	24	34	U	N1-C2-O2	6.52	127.37	122.80
90	j	20	U	C6-N1-C1'	-6.51	112.08	121.20
2	A3	2357	C	N3-C2-O2	-6.51	117.34	121.90
2	A3	2750	U	C2-N1-C1'	6.51	125.51	117.70
2	A3	2215	C	N1-C2-O2	6.50	122.80	118.90
87	i4	24	U	N3-C2-O2	-6.49	117.66	122.20
86	C	34	U	N1-C2-O2	6.49	127.34	122.80
85	A6	1595	C	C2-N1-C1'	6.47	125.91	118.80
85	A6	1025	U	C2-N1-C1'	6.45	125.44	117.70
85	A6	1433	C	C6-N1-C2	-6.45	117.72	120.30
86	24	34	U	C2-N1-C1'	6.45	125.44	117.70
85	A6	951	U	N3-C2-O2	-6.45	117.69	122.20
2	A3	1689	C	C2-N1-C1'	6.45	125.89	118.80
2	A3	2870	G	C8-N9-C1'	-6.45	118.62	127.00
85	A6	1397	G	C4-N9-C1'	6.44	134.88	126.50
85	A6	802	C	C6-N1-C2	-6.44	117.72	120.30
85	A6	1426	G	C8-N9-C4	-6.44	103.82	106.40
2	A3	2150	U	N1-C2-O2	6.44	127.31	122.80
85	A6	1433	C	P-O3'-C3'	6.43	127.42	119.70
2	A3	3043	C	N1-C2-O2	6.43	122.76	118.90
2	A3	2295	C	C2-N1-C1'	6.42	125.86	118.80
2	A3	2789	C	P-O3'-C3'	6.42	127.41	119.70
85	A6	887	U	O5'-P-OP1	6.42	118.40	110.70
2	A3	2847	C	C6-N1-C2	-6.42	117.73	120.30
2	A3	2627	G	C8-N9-C1'	6.41	135.34	127.00
2	A3	1919	C	N1-C2-O2	6.41	122.75	118.90
86	C	34	U	C2-N1-C1'	6.41	125.39	117.70
2	A3	3134	C	C2-N1-C1'	6.40	125.84	118.80
2	A3	1809	U	P-O3'-C3'	6.40	127.38	119.70
2	A3	2211	U	N3-C2-O2	-6.40	117.72	122.20
86	24	73	A	C4-N9-C1'	6.40	137.82	126.30
85	A6	1429	U	N3-C2-O2	-6.39	117.73	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A3	2928	C	N1-C2-O2	6.39	122.73	118.90
2	A3	2379	C	C2-N1-C1'	6.38	125.82	118.80
2	A3	2727	C	C5-C6-N1	6.38	124.19	121.00
2	A3	2168	U	N3-C2-O2	-6.38	117.73	122.20
2	A3	2211	U	N1-C2-O2	6.38	127.27	122.80
2	A3	3170	C	N3-C2-O2	-6.38	117.43	121.90
85	A6	1536	C	N1-C2-O2	6.38	122.73	118.90
3	B3	1624	C	C2-N1-C1'	6.37	125.81	118.80
86	C	73	A	C4-N9-C1'	6.37	137.76	126.30
2	A3	1839	C	C6-N1-C2	-6.36	117.75	120.30
2	A3	1902	C	C6-N1-C1'	-6.36	113.17	120.80
2	A3	3212	C	C6-N1-C1'	-6.35	113.18	120.80
85	A6	1374	U	N3-C2-O2	-6.35	117.75	122.20
2	A3	2061	C	C6-N1-C2	-6.32	117.77	120.30
2	A3	3079	G	C4-C5-N7	6.32	113.33	110.80
85	A6	1133	U	N1-C2-O2	6.32	127.22	122.80
85	A6	1346	C	C6-N1-C2	-6.32	117.77	120.30
87	i4	24	U	N1-C2-O2	6.32	127.22	122.80
2	A3	2057	C	C6-N1-C2	-6.31	117.78	120.30
90	j	16	C	C5-C6-N1	6.31	124.15	121.00
2	A3	1993	A	N7-C8-N9	6.30	116.95	113.80
2	A3	1693	C	C6-N1-C1'	-6.29	113.25	120.80
85	A6	716	C	N3-C2-O2	-6.29	117.49	121.90
2	A3	2942	C	N1-C2-O2	6.29	122.67	118.90
2	A3	2443	C	N1-C2-O2	6.28	122.67	118.90
2	A3	2150	U	N3-C2-O2	-6.28	117.81	122.20
2	A3	1783	U	N3-C2-O2	-6.27	117.81	122.20
85	A6	1522	C	N1-C2-O2	6.26	122.66	118.90
2	A3	2493	C	C6-N1-C1'	-6.26	113.29	120.80
2	A3	1837	C	C6-N1-C1'	-6.25	113.30	120.80
2	A3	3009	C	C2-N1-C1'	6.25	125.67	118.80
2	A3	2269	G	N1-C6-O6	-6.24	116.15	119.90
42	h3	64	GLU	C-N-CA	6.24	137.29	121.70
2	A3	2150	U	C2-N1-C1'	6.23	125.18	117.70
86	C	62	C	C5-C6-N1	6.23	124.11	121.00
2	A3	3169	C	N1-C2-O2	6.23	122.64	118.90
2	A3	2168	U	N1-C2-O2	6.23	127.16	122.80
2	A3	2899	C	N3-C2-O2	-6.22	117.54	121.90
2	A3	3204	C	C6-N1-C1'	-6.22	113.33	120.80
2	A3	2243	A	P-O3'-C3'	6.21	127.16	119.70
85	A6	1456	U	N1-C2-O2	6.21	127.15	122.80
2	A3	2075	U	C5-C6-N1	6.20	125.80	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	A6	1133	U	N3-C2-O2	-6.19	117.86	122.20
3	B3	1665	C	C5-C6-N1	6.19	124.09	121.00
85	A6	1335	A	P-O3'-C3'	6.18	127.12	119.70
2	A3	2909	G	C4-C5-N7	6.18	113.27	110.80
2	A3	2688	C	N1-C2-N3	6.17	123.52	119.20
86	24	62	C	C5-C6-N1	6.17	124.09	121.00
2	A3	2445	U	N1-C2-O2	6.17	127.12	122.80
2	A3	2947	U	N3-C2-O2	-6.17	117.88	122.20
2	A3	2269	G	N3-C4-N9	-6.16	122.30	126.00
87	i4	24	U	C2-N1-C1'	6.16	125.09	117.70
2	A3	2047	U	N3-C2-O2	-6.16	117.89	122.20
2	A3	1959	C	C2-N1-C1'	6.15	125.57	118.80
75	V6	129	LEU	CA-CB-CG	6.15	129.44	115.30
2	A3	2909	G	C6-C5-N7	-6.14	126.72	130.40
3	B3	1633	U	N1-C2-O2	6.14	127.10	122.80
85	A6	769	C	C6-N1-C1'	-6.13	113.44	120.80
85	A6	1170	A	P-O3'-C3'	6.13	127.06	119.70
85	A6	809	C	C2-N1-C1'	6.13	125.54	118.80
85	A6	1219	U	N1-C2-O2	6.12	127.09	122.80
2	A3	2746	U	N1-C2-O2	6.11	127.08	122.80
2	A3	3008	C	N1-C2-N3	6.11	123.48	119.20
2	A3	2057	C	N3-C2-O2	-6.10	117.63	121.90
86	24	72	C	O4'-C1'-N1	6.10	113.08	108.20
2	A3	2684	C	N3-C2-O2	-6.09	117.63	121.90
52	s3	229	LEU	CA-CB-CG	6.09	129.32	115.30
2	A3	2557	C	N3-C2-O2	-6.09	117.64	121.90
2	A3	2961	C	C2-N1-C1'	6.09	125.50	118.80
2	A3	3122	U	C2-N1-C1'	6.09	125.00	117.70
90	j	57	C	C6-N1-C2	-6.09	117.87	120.30
86	C	72	C	O4'-C1'-N1	6.08	113.06	108.20
85	A6	1436	U	N3-C2-O2	-6.08	117.95	122.20
85	A6	1139	C	C6-N1-C2	-6.07	117.87	120.30
2	A3	2075	U	N1-C2-O2	6.07	127.05	122.80
2	A3	1984	A	C5-N7-C8	-6.07	100.87	103.90
2	A3	2235	C	C2-N1-C1'	6.06	125.47	118.80
86	24	62	C	C2-N3-C4	6.06	122.93	119.90
2	A3	2386	C	C6-N1-C2	-6.06	117.88	120.30
2	A3	3009	C	N1-C2-O2	6.05	122.53	118.90
85	A6	1394	A	C8-N9-C4	-6.05	103.38	105.80
2	A3	1919	C	N3-C2-O2	-6.05	117.66	121.90
86	C	62	C	C2-N3-C4	6.04	122.92	119.90
85	A6	677	U	N3-C2-O2	-6.04	117.97	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	A6	1250	U	P-O3'-C3'	6.04	126.95	119.70
85	A6	1401	U	N1-C2-O2	6.04	127.03	122.80
85	A6	774	C	N3-C2-O2	-6.04	117.67	121.90
85	A6	1025	U	P-O3'-C3'	6.04	126.94	119.70
90	j	57	C	N1-C2-O2	6.04	122.52	118.90
85	A6	709	C	C2-N1-C1'	6.03	125.44	118.80
2	A3	2952	U	C2-N1-C1'	6.03	124.93	117.70
2	A3	2079	C	C6-N1-C1'	-6.02	113.58	120.80
2	A3	2171	U	N3-C2-O2	-6.02	117.99	122.20
85	A6	1133	U	C6-N1-C2	-6.01	117.39	121.00
2	A3	2928	C	N3-C2-O2	-6.01	117.69	121.90
85	A6	1000	A	N7-C8-N9	6.00	116.80	113.80
2	A3	2854	U	C6-N1-C1'	-6.00	112.80	121.20
2	A3	2710	C	N3-C2-O2	-6.00	117.70	121.90
85	A6	1305	G	C5-C6-O6	-5.99	125.01	128.60
23	X3	92	ALA	N-CA-CB	-5.98	101.72	110.10
90	j	20	U	C5-C6-N1	5.98	125.69	122.70
2	A3	3079	G	C6-C5-N7	-5.98	126.81	130.40
2	A3	2746	U	N3-C2-O2	-5.98	118.02	122.20
2	A3	2854	U	N1-C2-O2	5.97	126.98	122.80
80	a6	68	LEU	CA-CB-CG	5.97	129.03	115.30
85	A6	1059	U	N3-C2-O2	-5.97	118.02	122.20
86	C	62	C	N3-C2-O2	-5.96	117.73	121.90
2	A3	1693	C	C5-C6-N1	5.95	123.97	121.00
85	A6	1212	U	N3-C2-O2	-5.95	118.03	122.20
85	A6	1512	C	N1-C2-O2	5.95	122.47	118.90
2	A3	2025	C	N3-C2-O2	-5.94	117.74	121.90
2	A3	2511	C	N3-C2-O2	-5.94	117.74	121.90
2	A3	1823	A	P-O3'-C3'	5.94	126.83	119.70
85	A6	721	G	P-O3'-C3'	5.94	126.83	119.70
85	A6	1392	C	C2-N1-C1'	5.93	125.32	118.80
85	A6	677	U	C2-N1-C1'	5.92	124.81	117.70
85	A6	1471	C	N1-C2-O2	5.92	122.45	118.90
86	24	62	C	N3-C2-O2	-5.92	117.75	121.90
2	A3	2407	U	N1-C2-O2	5.92	126.94	122.80
2	A3	2096	U	C2-N1-C1'	5.91	124.79	117.70
2	A3	2909	G	N9-C4-C5	-5.91	103.04	105.40
2	A3	2628	U	P-O3'-C3'	5.90	126.78	119.70
85	A6	774	C	N1-C2-O2	5.90	122.44	118.90
86	C	48	U	N1-C2-O2	5.90	126.93	122.80
2	A3	1840	C	C5-C6-N1	5.90	123.95	121.00
2	A3	2646	G	N3-C4-N9	-5.90	122.46	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A3	2650	C	C5-C6-N1	5.90	123.95	121.00
3	B3	1633	U	N3-C2-O2	-5.89	118.07	122.20
2	A3	1975	U	C2-N1-C1'	5.89	124.77	117.70
2	A3	2766	C	C6-N1-C2	-5.88	117.95	120.30
85	A6	1541	C	C6-N1-C2	-5.88	117.95	120.30
2	A3	3008	C	C2-N3-C4	-5.88	116.96	119.90
85	A6	1056	C	C2-N1-C1'	5.88	125.26	118.80
2	A3	2295	C	N3-C2-O2	-5.87	117.79	121.90
2	A3	2375	C	C2-N1-C1'	5.87	125.26	118.80
85	A6	1259	U	N1-C2-O2	5.87	126.91	122.80
86	24	62	C	C6-N1-C1'	-5.87	113.76	120.80
86	24	48	U	N1-C2-O2	5.87	126.91	122.80
85	A6	801	C	C6-N1-C2	-5.86	117.95	120.30
85	A6	904	C	N1-C2-O2	5.86	122.42	118.90
2	A3	2728	C	C6-N1-C2	-5.86	117.96	120.30
2	A3	2947	U	N1-C2-O2	5.86	126.90	122.80
2	A3	3204	C	C6-N1-C2	-5.86	117.96	120.30
86	C	62	C	C6-N1-C1'	-5.86	113.77	120.80
85	A6	1000	A	C8-N9-C4	-5.86	103.46	105.80
86	C	53	C	C5-C6-N1	5.85	123.93	121.00
2	A3	2559	U	P-O3'-C3'	5.85	126.72	119.70
2	A3	3201	A	P-O3'-C3'	5.85	126.72	119.70
85	A6	936	C	C2-N1-C1'	5.85	125.24	118.80
2	A3	1783	U	N1-C2-O2	5.85	126.89	122.80
90	j	39	C	N3-C2-O2	-5.85	117.81	121.90
2	A3	2075	U	N3-C2-O2	-5.84	118.11	122.20
2	A3	3009	C	N3-C2-O2	-5.84	117.81	121.90
86	C	48	U	N3-C2-O2	-5.84	118.11	122.20
86	24	48	U	N3-C2-O2	-5.83	118.12	122.20
90	j	67	C	C6-N1-C2	-5.83	117.97	120.30
2	A3	3116	C	C5-C6-N1	5.83	123.92	121.00
86	24	53	C	C5-C6-N1	5.83	123.91	121.00
84	e6	147	PRO	N-CA-CB	5.82	110.28	103.30
85	A6	1451	G	N3-C4-C5	-5.82	125.69	128.60
85	A6	747	C	N1-C2-O2	5.82	122.39	118.90
85	A6	1579	U	C5-C6-N1	5.82	125.61	122.70
2	A3	1813	C	C6-N1-C2	-5.81	117.97	120.30
2	A3	1993	A	C4-N9-C1'	5.81	136.76	126.30
23	X3	101	LEU	CA-CB-CG	5.81	128.66	115.30
2	A3	1964	U	C5-C6-N1	5.80	125.60	122.70
2	A3	2627	G	C6-C5-N7	5.80	133.88	130.40
39	e3	279	LEU	CA-CB-CG	5.80	128.64	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	A6	709	C	C6-N1-C1'	-5.80	113.84	120.80
85	A6	809	C	N1-C2-O2	5.79	122.38	118.90
85	A6	1070	C	C6-N1-C2	-5.79	117.98	120.30
2	A3	2235	C	N3-C2-O2	-5.79	117.85	121.90
85	A6	1447	U	C2-N1-C1'	5.79	124.64	117.70
2	A3	3201	A	C4-N9-C1'	5.78	136.70	126.30
2	A3	2254	C	C5-C6-N1	5.77	123.89	121.00
86	C	73	A	N1-C2-N3	5.77	132.18	129.30
2	A3	2016	C	C6-N1-C2	-5.77	117.99	120.30
2	A3	2215	C	N3-C2-O2	-5.76	117.87	121.90
2	A3	1839	C	C5-C6-N1	5.76	123.88	121.00
2	A3	1947	C	N1-C2-N3	5.76	123.23	119.20
2	A3	2087	U	C5-C6-N1	5.76	125.58	122.70
2	A3	2777	G	C5-C6-O6	5.76	132.05	128.60
2	A3	2900	C	C6-N1-C2	-5.76	118.00	120.30
85	A6	711	C	N3-C2-O2	-5.75	117.87	121.90
85	A6	1193	U	P-O3'-C3'	5.75	126.59	119.70
2	A3	2960	U	C6-N1-C1'	-5.74	113.16	121.20
2	A3	1984	A	C4-C5-N7	5.74	113.57	110.70
2	A3	2667	U	N1-C2-O2	5.74	126.82	122.80
85	A6	677	U	N1-C2-O2	5.74	126.82	122.80
85	A6	1541	C	P-O3'-C3'	5.74	126.59	119.70
86	C	62	C	C6-N1-C2	-5.74	118.00	120.30
85	A6	802	C	C5-C6-N1	5.74	123.87	121.00
2	A3	2942	C	N3-C2-O2	-5.73	117.89	121.90
2	A3	3093	C	C6-N1-C2	-5.72	118.01	120.30
85	A6	1247	U	N1-C2-O2	5.72	126.80	122.80
2	A3	2667	U	N3-C2-O2	-5.71	118.21	122.20
85	A6	1074	C	C2-N1-C1'	5.70	125.07	118.80
85	A6	1436	U	N1-C2-O2	5.70	126.79	122.80
86	24	62	C	C6-N1-C2	-5.70	118.02	120.30
85	A6	1394	A	N7-C8-N9	5.70	116.65	113.80
2	A3	2364	C	N3-C2-O2	-5.70	117.91	121.90
85	A6	797	C	C6-N1-C1'	-5.70	113.96	120.80
85	A6	1419	G	P-O3'-C3'	5.70	126.53	119.70
2	A3	2479	C	N1-C2-O2	5.69	122.32	118.90
2	A3	1880	C	N3-C2-O2	-5.69	117.92	121.90
86	24	73	A	N1-C2-N3	5.69	132.15	129.30
2	A3	2445	U	C2-N1-C1'	5.69	124.53	117.70
42	h3	66	LEU	CA-CB-CG	5.68	128.37	115.30
2	A3	2186	C	N1-C2-O2	5.68	122.31	118.90
91	n	15	ASP	CB-CG-OD1	5.68	123.41	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	A6	791	C	C5-C6-N1	5.68	123.84	121.00
77	X6	323	TYR	C-N-CA	5.67	135.89	121.70
85	A6	678	U	N1-C2-O2	5.67	126.77	122.80
85	A6	1504	C	C6-N1-C2	-5.67	118.03	120.30
2	A3	2252	C	C2-N1-C1'	5.66	125.03	118.80
2	A3	2780	C	N1-C2-O2	5.66	122.30	118.90
3	B3	1627	C	C2-N1-C1'	5.66	125.03	118.80
2	A3	2790	A	C2-N3-C4	5.65	113.43	110.60
2	A3	2374	A	P-O3'-C3'	5.65	126.48	119.70
85	A6	1374	U	N1-C2-O2	5.65	126.76	122.80
85	A6	1252	C	C5-C6-N1	5.65	123.82	121.00
85	A6	1401	U	N3-C2-O2	-5.65	118.25	122.20
43	i3	63	LEU	CA-CB-CG	5.64	128.28	115.30
2	A3	2245	A	P-O3'-C3'	5.64	126.47	119.70
2	A3	2372	U	N1-C2-O2	5.64	126.75	122.80
85	A6	912	C	C2-N1-C1'	5.64	125.00	118.80
2	A3	1715	C	C6-N1-C2	-5.64	118.05	120.30
2	A3	1984	A	C6-C5-N7	-5.63	128.36	132.30
85	A6	710	C	N1-C2-O2	5.63	122.28	118.90
2	A3	2280	C	N1-C2-O2	5.62	122.28	118.90
2	A3	1689	C	N1-C2-O2	5.62	122.27	118.90
2	A3	2379	C	N3-C2-O2	-5.62	117.97	121.90
91	n	187	ASP	CB-CG-OD1	5.62	123.36	118.30
86	24	2	U	C5-C6-N1	5.61	125.51	122.70
2	A3	2311	U	N3-C2-O2	-5.61	118.27	122.20
86	C	2	U	C5-C6-N1	5.61	125.50	122.70
86	24	56	A	C2-N3-C4	5.60	113.40	110.60
2	A3	1743	U	N1-C2-O2	5.60	126.72	122.80
85	A6	1227	C	C6-N1-C2	-5.60	118.06	120.30
2	A3	2375	C	N3-C4-N4	5.59	121.91	118.00
3	B3	1665	C	C2-N1-C1'	5.59	124.95	118.80
87	i4	23	U	N3-C2-O2	-5.59	118.29	122.20
2	A3	1984	A	C4-N9-C1'	5.58	136.35	126.30
2	A3	2396	C	N1-C2-O2	5.58	122.25	118.90
2	A3	2282	C	C6-N1-C1'	-5.58	114.10	120.80
3	B3	1612	C	C5-C6-N1	5.58	123.79	121.00
2	A3	1993	A	C8-N9-C4	-5.58	103.57	105.80
86	24	34	U	N3-C2-O2	-5.58	118.30	122.20
2	A3	1713	A	P-O3'-C3'	5.58	126.39	119.70
2	A3	2508	C	C5-C6-N1	5.58	123.79	121.00
85	A6	1247	U	C2-N1-C1'	5.58	124.39	117.70
85	A6	1282	C	C2-N1-C1'	5.58	124.93	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	C	3	U	N1-C2-O2	5.57	126.70	122.80
86	24	3	U	N1-C2-O2	5.56	126.69	122.80
85	A6	1156	A	C2-N3-C4	5.56	113.38	110.60
85	A6	936	C	N3-C2-O2	-5.55	118.01	121.90
2	A3	2057	C	C2-N1-C1'	5.55	124.90	118.80
86	C	30	G	N3-C4-C5	-5.55	125.83	128.60
85	A6	1560	C	OP2-P-O3'	5.54	117.39	105.20
2	A3	2235	C	N1-C2-O2	5.54	122.22	118.90
2	A3	2823	U	N3-C2-O2	-5.53	118.33	122.20
90	j	6	C	C6-N1-C2	-5.53	118.09	120.30
2	A3	2024	C	N1-C2-O2	5.53	122.22	118.90
86	C	56	A	C2-N3-C4	5.53	113.36	110.60
2	A3	1714	C	N1-C2-O2	5.52	122.21	118.90
2	A3	2699	C	C2-N1-C1'	5.52	124.87	118.80
2	A3	2375	C	C5-C4-N4	-5.52	116.34	120.20
85	A6	1056	C	C6-N1-C2	-5.52	118.09	120.30
2	A3	1707	C	N3-C2-O2	-5.51	118.04	121.90
2	A3	2832	A	C4-C5-N7	5.51	113.45	110.70
85	A6	738	C	C6-N1-C2	-5.50	118.10	120.30
2	A3	2507	A	P-O3'-C3'	5.50	126.30	119.70
2	A3	2775	A	C2-N3-C4	5.50	113.35	110.60
85	A6	717	C	C6-N1-C2	-5.50	118.10	120.30
2	A3	1699	C	C6-N1-C1'	-5.50	114.21	120.80
2	A3	2852	C	N1-C2-O2	5.49	122.19	118.90
85	A6	1397	G	C8-N9-C1'	-5.49	119.86	127.00
2	A3	2047	U	N1-C2-O2	5.49	126.64	122.80
86	C	72	C	P-O3'-C3'	5.49	126.29	119.70
2	A3	2215	C	C2-N1-C1'	5.48	124.83	118.80
86	24	72	C	P-O3'-C3'	5.48	126.28	119.70
2	A3	2926	A	N9-C4-C5	-5.47	103.61	105.80
2	A3	3117	C	C6-N1-C2	-5.47	118.11	120.30
86	24	11	C	N1-C2-O2	5.47	122.18	118.90
85	A6	1250	U	OP2-P-O3'	5.47	117.24	105.20
2	A3	1807	U	N3-C2-O2	-5.47	118.37	122.20
85	A6	935	C	C6-N1-C2	-5.46	118.11	120.30
40	f3	51	LYS	CB-CA-C	5.46	121.32	110.40
90	j	31	G	C4-N9-C1'	5.46	133.60	126.50
2	A3	1758	U	N3-C2-O2	-5.46	118.38	122.20
85	A6	1305	G	N3-C2-N2	-5.46	116.08	119.90
2	A3	2427	C	C5-C6-N1	5.46	123.73	121.00
85	A6	1308	C	C6-N1-C2	-5.46	118.12	120.30
86	24	30	G	N3-C4-C5	-5.46	125.87	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A3	2750	U	C5-C6-N1	5.45	125.43	122.70
2	A3	3201	A	C2-N3-C4	5.45	113.33	110.60
86	C	34	U	N3-C2-O2	-5.45	118.39	122.20
2	A3	1919	C	C6-N1-C2	-5.44	118.12	120.30
85	A6	1046	U	N1-C2-O2	5.44	126.61	122.80
2	A3	1919	C	C2-N1-C1'	5.43	124.78	118.80
2	A3	2862	C	N1-C2-O2	5.43	122.16	118.90
68	O6	105	CYS	CA-CB-SG	-5.43	104.22	114.00
2	A3	2386	C	C6-N1-C1'	-5.43	114.28	120.80
2	A3	3212	C	C6-N1-C2	-5.43	118.13	120.30
2	A3	2005	C	C6-N1-C2	-5.42	118.13	120.30
2	A3	2870	G	C6-C5-N7	-5.42	127.15	130.40
2	A3	2057	C	N1-C2-O2	5.42	122.15	118.90
2	A3	3043	C	N3-C2-O2	-5.42	118.11	121.90
4	D3	251	ASP	CB-CG-OD2	-5.42	113.42	118.30
85	A6	1545	U	N3-C2-O2	-5.42	118.41	122.20
90	j	3	C	N3-C2-O2	-5.41	118.11	121.90
85	A6	1156	A	C4-N9-C1'	5.41	136.04	126.30
90	j	24	C	C2-N1-C1'	5.41	124.75	118.80
2	A3	2210	C	O5'-P-OP2	-5.41	100.83	105.70
85	A6	1492	C	C6-N1-C2	-5.41	118.14	120.30
2	A3	2865	C	N3-C2-O2	-5.41	118.12	121.90
85	A6	921	C	C5-C6-N1	5.41	123.70	121.00
85	A6	682	U	N3-C2-O2	-5.40	118.42	122.20
85	A6	1247	U	N3-C2-O2	-5.40	118.42	122.20
2	A3	2479	C	N3-C2-O2	-5.40	118.12	121.90
2	A3	2295	C	C6-N1-C1'	-5.39	114.33	120.80
2	A3	2960	U	C5-C6-N1	5.39	125.39	122.70
86	C	2	U	N1-C2-O2	5.38	126.57	122.80
2	A3	2646	G	N9-C4-C5	5.38	107.55	105.40
86	24	2	U	N1-C2-O2	5.38	126.56	122.80
86	C	11	C	N1-C2-O2	5.38	122.13	118.90
85	A6	818	A	C4-N9-C1'	5.37	135.97	126.30
2	A3	2284	C	N3-C2-O2	-5.37	118.14	121.90
2	A3	3008	C	N3-C2-O2	-5.37	118.14	121.90
85	A6	906	G	C8-N9-C1'	-5.37	120.02	127.00
2	A3	2473	A	C4-N9-C1'	5.36	135.95	126.30
85	A6	890	C	C5-C6-N1	5.36	123.68	121.00
2	A3	2989	G	P-O3'-C3'	5.36	126.13	119.70
85	A6	1561	A	O5'-P-OP2	-5.35	100.88	105.70
2	A3	2046	C	C6-N1-C2	-5.35	118.16	120.30
91	n	104	LEU	CA-CB-CG	5.35	127.61	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F3	218	LEU	CA-CB-CG	5.35	127.60	115.30
86	C	2	U	N3-C2-O2	-5.34	118.46	122.20
2	A3	2075	U	C2-N1-C1'	5.33	124.10	117.70
85	A6	1381	C	N1-C2-O2	5.33	122.10	118.90
2	A3	2417	C	N3-C2-O2	-5.33	118.17	121.90
2	A3	2126	U	C2-N1-C1'	5.33	124.09	117.70
85	A6	1233	U	N3-C2-O2	-5.33	118.47	122.20
2	A3	2834	C	N1-C2-O2	5.32	122.09	118.90
2	A3	2851	A	O4'-C1'-N9	5.32	112.45	108.20
2	A3	2523	C	C5-C6-N1	5.31	123.66	121.00
85	A6	890	C	C6-N1-C2	-5.31	118.17	120.30
85	A6	951	U	C2-N1-C1'	5.31	124.08	117.70
85	A6	1429	U	C5-C6-N1	5.31	125.36	122.70
85	A6	716	C	C6-N1-C1'	-5.31	114.43	120.80
2	A3	2558	A	P-O3'-C3'	5.31	126.07	119.70
86	24	12	U	N1-C2-O2	5.31	126.52	122.80
2	A3	2407	U	N3-C2-O2	-5.30	118.49	122.20
85	A6	1230	C	C6-N1-C2	-5.30	118.18	120.30
2	A3	1944	C	N3-C2-O2	-5.30	118.19	121.90
2	A3	2275	U	N3-C2-O2	-5.30	118.49	122.20
85	A6	1499	C	C2-N1-C1'	5.30	124.63	118.80
2	A3	3088	C	OP1-P-OP2	-5.30	111.66	119.60
16	Q3	247	LEU	CA-CB-CG	5.29	127.47	115.30
85	A6	1102	C	C2-N1-C1'	5.29	124.62	118.80
86	C	30	G	OP1-P-O3'	5.29	116.83	105.20
86	24	2	U	N3-C2-O2	-5.28	118.50	122.20
2	A3	1970	G	N1-C2-N3	5.27	127.06	123.90
2	A3	2770	C	C6-N1-C2	-5.27	118.19	120.30
86	24	30	G	OP1-P-O3'	5.27	116.80	105.20
2	A3	1693	C	C6-N1-C2	-5.27	118.19	120.30
85	A6	1259	U	N3-C2-O2	-5.27	118.51	122.20
86	C	12	U	N1-C2-O2	5.26	126.48	122.80
2	A3	3041	U	P-O3'-C3'	5.26	126.01	119.70
85	A6	680	G	C4-N9-C1'	5.26	133.33	126.50
85	A6	1059	U	N1-C2-O2	5.26	126.48	122.80
85	A6	1132	C	N3-C2-O2	-5.25	118.22	121.90
90	j	39	C	C2-N1-C1'	5.25	124.58	118.80
2	A3	2508	C	C6-N1-C2	-5.25	118.20	120.30
2	A3	2727	C	C6-N1-C1'	-5.25	114.50	120.80
38	d3	267	PRO	C-N-CD	-5.25	109.06	120.60
2	A3	1934	U	N3-C2-O2	-5.24	118.53	122.20
2	A3	2427	C	C6-N1-C2	-5.24	118.20	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A3	3012	U	C5-C6-N1	5.24	125.32	122.70
2	A3	2252	C	C6-N1-C2	-5.24	118.20	120.30
2	A3	2007	U	C5-C6-N1	5.24	125.32	122.70
85	A6	1545	U	C2-N1-C1'	5.24	123.98	117.70
3	B3	1627	C	C6-N1-C2	-5.23	118.21	120.30
86	C	42	C	N1-C2-O2	5.23	122.04	118.90
2	A3	1715	C	C2-N1-C1'	5.23	124.56	118.80
2	A3	2284	C	C2-N1-C1'	5.23	124.56	118.80
85	A6	789	C	C6-N1-C2	-5.23	118.21	120.30
86	C	3	U	N3-C2-O2	-5.23	118.54	122.20
2	A3	2726	C	N3-C2-O2	-5.22	118.24	121.90
2	A3	2135	A	C4-N9-C1'	5.22	135.69	126.30
2	A3	2499	U	C2-N1-C1'	5.22	123.96	117.70
85	A6	1324	G	O4'-C1'-N9	5.22	112.38	108.20
2	A3	2171	U	N1-C2-O2	5.22	126.45	122.80
85	A6	1074	C	C6-N1-C2	-5.22	118.21	120.30
86	24	3	U	N3-C2-O2	-5.22	118.55	122.20
2	A3	2646	G	C6-N1-C2	-5.22	121.97	125.10
32	63	226	LEU	CA-CB-CG	5.22	127.30	115.30
86	24	42	C	N1-C2-O2	5.22	122.03	118.90
2	A3	2546	G	N3-C4-N9	5.21	129.13	126.00
85	A6	791	C	C6-N1-C2	-5.21	118.22	120.30
90	j	6	C	C2-N1-C1'	5.21	124.53	118.80
2	A3	2344	C	N1-C2-O2	5.21	122.03	118.90
3	B3	1607	U	P-O3'-C3'	5.21	125.95	119.70
62	I6	159	LEU	CB-CG-CD2	-5.21	102.14	111.00
85	A6	1050	A	OP2-P-O3'	5.21	116.66	105.20
85	A6	1297	C	C2-N1-C1'	5.21	124.53	118.80
2	A3	2650	C	C6-N1-C2	-5.21	118.22	120.30
85	A6	1308	C	N1-C2-O2	5.21	122.02	118.90
85	A6	952	U	N1-C2-O2	5.20	126.44	122.80
2	A3	1693	C	N3-C2-O2	-5.20	118.26	121.90
2	A3	2546	G	C4-N9-C1'	5.20	133.26	126.50
90	j	57	C	C2-N1-C1'	5.20	124.52	118.80
2	A3	2493	C	C6-N1-C2	-5.20	118.22	120.30
85	A6	710	C	O4'-C1'-N1	5.20	112.36	108.20
2	A3	2061	C	C6-N1-C1'	-5.19	114.57	120.80
85	A6	1395	U	N3-C2-O2	-5.19	118.57	122.20
2	A3	1839	C	C2-N1-C1'	5.19	124.51	118.80
85	A6	1181	C	C6-N1-C2	-5.18	118.23	120.30
90	j	19	G	C4-N9-C1'	5.18	133.23	126.50
2	A3	2186	C	C2-N1-C1'	5.18	124.50	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	A6	987	C	N1-C2-O2	5.18	122.01	118.90
2	A3	2269	G	C5-C6-O6	5.17	131.70	128.60
68	O6	122	LEU	CA-CB-CG	5.17	127.20	115.30
2	A3	2131	A	O4'-C1'-N9	-5.17	104.06	108.20
2	A3	2583	C	C5-C6-N1	5.17	123.58	121.00
2	A3	2880	A	O4'-C1'-N9	5.17	112.33	108.20
85	A6	836	U	N1-C2-O2	5.17	126.42	122.80
85	A6	1219	U	C2-N1-C1'	5.17	123.90	117.70
2	A3	2187	C	N3-C2-O2	-5.17	118.28	121.90
22	W3	116	LEU	CA-CB-CG	5.16	127.17	115.30
85	A6	1471	C	C6-N1-C2	-5.16	118.23	120.30
85	A6	1470	C	C5-C6-N1	5.16	123.58	121.00
85	A6	669	C	C5-C6-N1	5.16	123.58	121.00
2	A3	3206	C	N1-C2-O2	5.15	121.99	118.90
85	A6	1282	C	C5-C6-N1	5.15	123.58	121.00
2	A3	2421	G	N9-C4-C5	-5.15	103.34	105.40
21	V3	191	LEU	CA-CB-CG	5.15	127.14	115.30
2	A3	3214	C	N1-C2-O2	5.15	121.99	118.90
2	A3	2726	C	C6-N1-C2	-5.15	118.24	120.30
85	A6	1392	C	C5-C6-N1	5.14	123.57	121.00
2	A3	1933	C	C6-N1-C2	-5.14	118.24	120.30
2	A3	3201	A	OP1-P-O3'	5.14	116.51	105.20
2	A3	2743	U	N3-C2-O2	-5.14	118.61	122.20
77	X6	381	LEU	CA-CB-CG	5.14	127.11	115.30
86	24	73	A	O4'-C1'-N9	5.14	112.31	108.20
2	A3	2744	U	N3-C2-O2	-5.13	118.61	122.20
85	A6	714	U	C6-N1-C1'	-5.13	114.01	121.20
3	B3	1650	A	N9-C4-C5	-5.13	103.75	105.80
85	A6	774	C	C6-N1-C2	-5.13	118.25	120.30
90	j	26	C	C2-N1-C1'	5.13	124.44	118.80
85	A6	988	C	C6-N1-C2	-5.13	118.25	120.30
85	A6	1193	U	OP1-P-O3'	5.13	116.48	105.20
2	A3	3092	U	P-O3'-C3'	5.13	125.85	119.70
3	B3	1665	C	C6-N1-C2	-5.13	118.25	120.30
86	C	52	C	C2-N1-C1'	5.13	124.44	118.80
86	C	73	A	O4'-C1'-N9	5.13	112.30	108.20
90	j	13	U	N1-C2-O2	5.12	126.39	122.80
2	A3	2205	U	N1-C2-O2	5.12	126.38	122.80
2	A3	3043	C	C2-N1-C1'	5.12	124.43	118.80
85	A6	702	C	C6-N1-C2	-5.12	118.25	120.30
2	A3	3043	C	C6-N1-C2	-5.12	118.25	120.30
85	A6	1346	C	C5-C6-N1	5.12	123.56	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B3	1635	C	N3-C2-O2	-5.12	118.32	121.90
86	C	11	C	N3-C2-O2	-5.11	118.32	121.90
2	A3	2443	C	N3-C2-O2	-5.11	118.32	121.90
61	H6	180	LEU	CA-CB-CG	5.11	127.06	115.30
85	A6	1005	C	C6-N1-C2	-5.11	118.26	120.30
2	A3	2269	G	N9-C4-C5	5.11	107.44	105.40
85	A6	1522	C	N3-C2-O2	-5.11	118.32	121.90
85	A6	1137	C	C6-N1-C2	-5.10	118.26	120.30
31	53	270	ILE	CG1-CB-CG2	-5.10	100.17	111.40
86	24	31	C	C6-N1-C2	-5.10	118.26	120.30
2	A3	1788	C	N1-C2-O2	5.10	121.96	118.90
84	e6	91	ASP	C-N-CA	5.10	134.45	121.70
2	A3	1837	C	O4'-C1'-N1	5.10	112.28	108.20
2	A3	3169	C	C6-N1-C1'	-5.10	114.68	120.80
86	24	52	C	C2-N1-C1'	5.10	124.41	118.80
2	A3	2271	C	N1-C2-O2	5.10	121.96	118.90
2	A3	2252	C	C5-C6-N1	5.09	123.55	121.00
85	A6	983	C	C5-C6-N1	5.09	123.55	121.00
2	A3	1685	C	C6-N1-C2	-5.09	118.26	120.30
85	A6	1401	U	C2-N1-C1'	5.09	123.81	117.70
2	A3	1743	U	N3-C2-O2	-5.09	118.64	122.20
2	A3	2484	C	C2-N1-C1'	5.09	124.40	118.80
2	A3	2653	C	C5-C6-N1	5.09	123.54	121.00
2	A3	2870	G	N3-C4-N9	5.08	129.05	126.00
2	A3	2793	C	C6-N1-C2	-5.08	118.27	120.30
32	63	233	LEU	CA-CB-CG	5.08	126.98	115.30
2	A3	1970	G	C6-N1-C2	-5.07	122.06	125.10
85	A6	1426	G	N3-C4-C5	-5.07	126.06	128.60
50	q3	103	LEU	CB-CG-CD1	-5.07	102.38	111.00
2	A3	3171	C	C6-N1-C2	-5.07	118.27	120.30
75	V6	195	ASP	C-N-CA	5.07	134.37	121.70
85	A6	1160	C	C6-N1-C2	-5.07	118.27	120.30
86	24	11	C	N3-C2-O2	-5.07	118.35	121.90
85	A6	921	C	C2-N1-C1'	5.06	124.37	118.80
85	A6	1220	C	C6-N1-C2	-5.06	118.28	120.30
85	A6	1595	C	C5-C6-N1	5.06	123.53	121.00
2	A3	2489	C	C6-N1-C2	-5.06	118.28	120.30
85	A6	1193	U	C6-N1-C2	-5.06	117.97	121.00
2	A3	2329	C	N1-C2-O2	5.05	121.93	118.90
2	A3	2484	C	N1-C2-O2	5.05	121.93	118.90
89	Z	403	ASP	CB-CG-OD1	5.05	122.85	118.30
2	A3	2814	G	N3-C4-C5	-5.05	126.07	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	A6	1562	A	C8-N9-C4	-5.05	103.78	105.80
2	A3	2788	C	P-O3'-C3'	5.05	125.76	119.70
86	C	69	C	N3-C2-O2	-5.04	118.37	121.90
2	A3	1809	U	OP1-P-O3'	5.04	116.30	105.20
86	24	52	C	N3-C2-O2	-5.04	118.37	121.90
86	C	3	U	C6-N1-C1'	-5.04	114.14	121.20
85	A6	717	C	C6-N1-C1'	-5.04	114.75	120.80
85	A6	1046	U	N3-C2-O2	-5.04	118.67	122.20
85	A6	1068	C	N1-C2-O2	5.04	121.92	118.90
2	A3	2427	C	C2-N1-C1'	5.04	124.34	118.80
2	A3	2441	C	N1-C2-O2	5.04	121.92	118.90
2	A3	2375	C	C5-C6-N1	5.03	123.52	121.00
2	A3	2508	C	N1-C2-O2	5.03	121.92	118.90
2	A3	2496	G	N3-C4-N9	5.03	129.01	126.00
90	j	3	C	N1-C2-O2	5.02	121.91	118.90
86	C	52	C	N3-C2-O2	-5.02	118.38	121.90
2	A3	2871	U	C5-C6-N1	5.02	125.21	122.70
86	C	31	C	C6-N1-C2	-5.02	118.29	120.30
86	24	3	U	C6-N1-C1'	-5.02	114.18	121.20
90	j	7	G	P-O3'-C3'	5.02	125.72	119.70
85	A6	987	C	N3-C2-O2	-5.02	118.39	121.90
86	24	69	C	N3-C2-O2	-5.02	118.39	121.90
2	A3	2080	U	C6-N1-C1'	-5.01	114.18	121.20
85	A6	802	C	C2-N1-C1'	5.01	124.32	118.80
85	A6	1462	A	C2-N3-C4	5.01	113.11	110.60
2	A3	1946	C	C6-N1-C2	-5.01	118.30	120.30
2	A3	2173	G	C6-C5-N7	-5.01	127.39	130.40
58	E6	14	GLN	C-N-CA	5.01	134.23	121.70
85	A6	988	C	C5-C6-N1	5.01	123.51	121.00
85	A6	1545	U	N1-C2-O2	5.01	126.31	122.80
85	A6	782	C	N1-C2-O2	5.01	121.91	118.90
2	A3	2511	C	N1-C2-O2	5.00	121.90	118.90
86	C	52	C	C6-N1-C2	-5.00	118.30	120.30
85	A6	912	C	C5-C6-N1	5.00	123.50	121.00

There are no chirality outliers.

All (76) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	03	177	ARG	Peptide
27	13	62	ILE	Peptide
31	53	269	ASN	Peptide

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Mol	Chain	Res	Type	Group
31	53	305	GLN	Peptide
31	53	347	THR	Peptide
31	53	71	ALA	Peptide
88	A	184	ASN	Peptide
88	A	185	TYR	Peptide
88	A	187	PRO	Peptide
88	A	192	TYR	Peptide
88	A	197	LYS	Peptide
88	A	57	ASP	Peptide
4	D3	206	TYR	Peptide
57	D6	285	TYR	Peptide
57	D6	286	GLU	Peptide
5	E3	126	ASP	Peptide
5	E3	169	GLY	Peptide
5	E3	203	TYR	Peptide
5	E3	244	ALA	Peptide
5	E3	250	ARG	Peptide
5	E3	315	PRO	Peptide
5	E3	85	TRP	Peptide
6	F3	129	PRO	Peptide
9	J3	33	PRO	Peptide
63	J6	129	LYS	Peptide
10	K3	3	SER	Peptide
64	K6	64	PRO	Peptide
12	M3	18	GLY	Peptide
12	M3	264	GLN	Peptide
13	N3	237	HIS	Peptide
67	N6	109	PRO	Peptide
68	O6	55	PRO	Peptide
15	P3	174	PRO	Peptide
15	P3	176	ARG	Peptide
69	P6	65	CYS	Peptide
16	Q3	182	ARG	Peptide
16	Q3	226	PRO	Peptide
17	R3	137	GLU	Peptide
71	R6	132	LEU	Peptide
71	R6	154	THR	Peptide
71	R6	291	ARG	Peptide
19	T3	94	ILE	Peptide
21	V3	100	LYS	Peptide
21	V3	170	TRP	Peptide
21	V3	192	LYS	Peptide

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Mol	Chain	Res	Type	Group
75	V6	173	PHE	Peptide
23	X3	51	LYS	Peptide
23	X3	90	ILE	Peptide
23	X3	93	ASN	Peptide
23	X3	95	ASP	Peptide
23	X3	98	SER	Peptide
23	X3	99	LYS	Peptide
1	Y2	21	ALA	Peptide
1	Y2	22	ALA	Peptide
24	Y3	202	LEU	Peptide
89	Z	143	PRO	Peptide
25	Z3	141	SER	Peptide
82	c6	38	ARG	Peptide
82	c6	60	GLU	Peptide
38	d3	163	LEU	Peptide
38	d3	230	ARG	Peptide
38	d3	268	PRO	Peptide
84	e6	67	LYS	Peptide
40	f3	189	HIS	Peptide
40	f3	48	TYR	Peptide
40	f3	49	LYS	Peptide
40	f3	50	THR	Peptide
40	f3	84	THR	Peptide
40	f3	87	GLU	Peptide
42	h3	138	SER	Peptide
42	h3	63	PRO	Peptide
45	k3	14	LYS	Peptide
45	k3	55	VAL	Peptide
50	q3	78	SER	Peptide
52	s3	259	ILE	Peptide
52	s3	270	LYS	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Y2	27/29 (93%)	20 (74%)	6 (22%)	1 (4%)	3	28
4	D3	234/305 (77%)	215 (92%)	18 (8%)	1 (0%)	34	72
5	E3	296/348 (85%)	262 (88%)	32 (11%)	2 (1%)	22	62
6	F3	248/311 (80%)	228 (92%)	20 (8%)	0	100	100
7	D	78/267 (29%)	66 (85%)	11 (14%)	1 (1%)	12	48
7	H3	93/267 (35%)	83 (89%)	9 (10%)	1 (1%)	14	52
8	I3	154/261 (59%)	147 (96%)	7 (4%)	0	100	100
9	J3	138/192 (72%)	127 (92%)	11 (8%)	0	100	100
10	K3	175/178 (98%)	151 (86%)	22 (13%)	2 (1%)	14	52
11	L3	113/145 (78%)	101 (89%)	12 (11%)	0	100	100
12	M3	285/296 (96%)	255 (90%)	27 (10%)	3 (1%)	14	52
13	N3	203/251 (81%)	186 (92%)	16 (8%)	1 (0%)	29	68
14	O3	150/175 (86%)	131 (87%)	18 (12%)	1 (1%)	22	62
15	P3	129/180 (72%)	117 (91%)	11 (8%)	1 (1%)	19	60
16	Q3	217/292 (74%)	193 (89%)	23 (11%)	1 (0%)	29	68
17	R3	138/149 (93%)	133 (96%)	5 (4%)	0	100	100
18	S3	154/205 (75%)	138 (90%)	16 (10%)	0	100	100
19	T3	164/206 (80%)	154 (94%)	10 (6%)	0	100	100
20	U3	109/153 (71%)	97 (89%)	12 (11%)	0	100	100
21	V3	183/216 (85%)	156 (85%)	24 (13%)	3 (2%)	9	45
22	W3	109/148 (74%)	103 (94%)	6 (6%)	0	100	100
23	X3	241/256 (94%)	210 (87%)	29 (12%)	2 (1%)	19	60
24	Y3	174/250 (70%)	162 (93%)	12 (7%)	0	100	100
25	Z3	118/161 (73%)	109 (92%)	9 (8%)	0	100	100
26	03	106/188 (56%)	91 (86%)	14 (13%)	1 (1%)	17	56
27	13	50/65 (77%)	46 (92%)	3 (6%)	1 (2%)	7	40
28	23	44/92 (48%)	42 (96%)	2 (4%)	0	100	100
29	33	93/188 (50%)	88 (95%)	5 (5%)	0	100	100
30	43	34/103 (33%)	32 (94%)	2 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	53	368/423 (87%)	324 (88%)	42 (11%)	2 (0%)	29	68
32	63	313/380 (82%)	273 (87%)	40 (13%)	0	100	100
33	73	258/338 (76%)	234 (91%)	24 (9%)	0	100	100
34	93	105/137 (77%)	90 (86%)	15 (14%)	0	100	100
35	a3	78/142 (55%)	72 (92%)	6 (8%)	0	100	100
36	b3	146/215 (68%)	131 (90%)	15 (10%)	0	100	100
37	c3	271/332 (82%)	249 (92%)	21 (8%)	1 (0%)	34	72
38	d3	156/306 (51%)	142 (91%)	13 (8%)	1 (1%)	25	65
39	e3	211/279 (76%)	191 (90%)	20 (10%)	0	100	100
40	f3	125/212 (59%)	103 (82%)	21 (17%)	1 (1%)	19	60
41	g3	127/166 (76%)	114 (90%)	13 (10%)	0	100	100
42	h3	96/158 (61%)	86 (90%)	8 (8%)	2 (2%)	7	39
43	i3	95/128 (74%)	85 (90%)	10 (10%)	0	100	100
44	j3	83/123 (68%)	78 (94%)	4 (5%)	1 (1%)	13	50
45	k3	82/112 (73%)	67 (82%)	15 (18%)	0	100	100
46	l3	21/138 (15%)	21 (100%)	0	0	100	100
47	m3	43/128 (34%)	37 (86%)	6 (14%)	0	100	100
48	o3	92/102 (90%)	85 (92%)	7 (8%)	0	100	100
49	p3	119/206 (58%)	109 (92%)	10 (8%)	0	100	100
50	q3	126/222 (57%)	117 (93%)	6 (5%)	3 (2%)	6	36
51	r3	140/196 (71%)	126 (90%)	14 (10%)	0	100	100
52	s3	366/467 (78%)	334 (91%)	32 (9%)	0	100	100
55	B6	215/296 (73%)	198 (92%)	17 (8%)	0	100	100
56	C6	130/167 (78%)	119 (92%)	11 (8%)	0	100	100
57	D6	316/430 (74%)	282 (89%)	33 (10%)	1 (0%)	41	76
58	E6	120/125 (96%)	113 (94%)	6 (5%)	1 (1%)	19	60
59	F6	197/242 (81%)	184 (93%)	13 (7%)	0	100	100
60	G6	301/396 (76%)	281 (93%)	20 (7%)	0	100	100
61	H6	120/201 (60%)	105 (88%)	14 (12%)	1 (1%)	19	60
62	I6	134/194 (69%)	123 (92%)	11 (8%)	0	100	100
63	J6	106/138 (77%)	95 (90%)	11 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
64	K6	99/128 (77%)	97 (98%)	2 (2%)	0	100	100
65	L6	162/257 (63%)	154 (95%)	8 (5%)	0	100	100
66	M6	114/137 (83%)	103 (90%)	11 (10%)	0	100	100
67	N6	105/130 (81%)	98 (93%)	7 (7%)	0	100	100
68	O6	183/258 (71%)	163 (89%)	20 (11%)	0	100	100
69	P6	94/142 (66%)	84 (89%)	10 (11%)	0	100	100
70	Q6	84/87 (97%)	77 (92%)	7 (8%)	0	100	100
71	R6	240/360 (67%)	211 (88%)	29 (12%)	0	100	100
72	S6	124/190 (65%)	115 (93%)	9 (7%)	0	100	100
73	T6	160/173 (92%)	144 (90%)	16 (10%)	0	100	100
74	U6	171/205 (83%)	164 (96%)	7 (4%)	0	100	100
75	V6	320/414 (77%)	283 (88%)	36 (11%)	1 (0%)	41	76
76	W6	95/187 (51%)	85 (90%)	10 (10%)	0	100	100
77	X6	310/398 (78%)	265 (86%)	43 (14%)	2 (1%)	25	65
78	Y6	106/395 (27%)	97 (92%)	9 (8%)	0	100	100
79	Z6	85/106 (80%)	81 (95%)	4 (5%)	0	100	100
80	a6	197/218 (90%)	182 (92%)	15 (8%)	0	100	100
81	b6	252/323 (78%)	224 (89%)	28 (11%)	0	100	100
82	c6	114/118 (97%)	97 (85%)	17 (15%)	0	100	100
83	d6	67/199 (34%)	63 (94%)	4 (6%)	0	100	100
84	e6	362/689 (52%)	328 (91%)	30 (8%)	4 (1%)	14	52
88	A	158/206 (77%)	142 (90%)	16 (10%)	0	100	100
89	Z	392/452 (87%)	352 (90%)	39 (10%)	1 (0%)	41	76
91	n	230/229 (100%)	209 (91%)	21 (9%)	0	100	100
All	All	13541/18977 (71%)	12229 (90%)	1268 (9%)	44 (0%)	44	76

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
40	f3	51	LYS
50	q3	43	GLU
84	e6	68	VAL
10	K3	160	GLN
12	M3	288	GLU

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Mol	Chain	Res	Type
23	X3	52	ILE
31	53	349	GLY
57	D6	287	ASP
77	X6	342	PRO
13	N3	238	LYS
16	Q3	183	LEU
21	V3	194	LEU
23	X3	94	ASN
38	d3	231	LEU
42	h3	66	LEU
21	V3	52	GLU
21	V3	101	THR
31	53	270	ILE
50	q3	42	PRO
50	q3	79	PRO
61	H6	126	ILE
75	V6	197	SER
84	e6	66	ASP
1	Y2	22	ALA
7	H3	104	ASN
10	K3	4	PHE
12	M3	265	ILE
14	O3	111	PRO
42	h3	138	SER
84	e6	317	LEU
7	D	212	PRO
12	M3	109	ARG
26	03	178	ASP
27	13	63	ARG
37	c3	313	PRO
44	j3	35	ALA
77	X6	120	PRO
58	E6	15	ARG
4	D3	207	ILE
84	e6	316	ILE
5	E3	79	PRO
5	E3	246	GLY
15	P3	177	ILE
89	Z	257	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D3	190/245 (78%)	189 (100%)	1 (0%)	88	93
5	E3	255/290 (88%)	252 (99%)	3 (1%)	71	84
6	F3	217/262 (83%)	216 (100%)	1 (0%)	88	93
7	D	73/228 (32%)	71 (97%)	2 (3%)	44	66
7	H3	86/228 (38%)	85 (99%)	1 (1%)	71	84
8	I3	145/232 (62%)	145 (100%)	0	100	100
9	J3	113/150 (75%)	113 (100%)	0	100	100
10	K3	155/156 (99%)	155 (100%)	0	100	100
11	L3	98/124 (79%)	98 (100%)	0	100	100
12	M3	245/249 (98%)	240 (98%)	5 (2%)	55	74
13	N3	172/211 (82%)	172 (100%)	0	100	100
14	O3	133/150 (89%)	132 (99%)	1 (1%)	81	89
15	P3	115/155 (74%)	114 (99%)	1 (1%)	78	88
16	Q3	201/256 (78%)	199 (99%)	2 (1%)	76	86
17	R3	118/126 (94%)	117 (99%)	1 (1%)	81	89
18	S3	141/180 (78%)	141 (100%)	0	100	100
19	T3	146/176 (83%)	145 (99%)	1 (1%)	84	90
20	U3	99/135 (73%)	99 (100%)	0	100	100
21	V3	169/191 (88%)	166 (98%)	3 (2%)	59	77
22	W3	91/119 (76%)	91 (100%)	0	100	100
23	X3	217/227 (96%)	215 (99%)	2 (1%)	78	88
24	Y3	159/223 (71%)	158 (99%)	1 (1%)	86	92
25	Z3	111/147 (76%)	111 (100%)	0	100	100
26	03	97/164 (59%)	96 (99%)	1 (1%)	76	86
27	13	49/60 (82%)	48 (98%)	1 (2%)	55	74
28	23	40/72 (56%)	40 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	33	88/166 (53%)	88 (100%)	0	100	100
30	43	35/89 (39%)	35 (100%)	0	100	100
31	53	337/368 (92%)	333 (99%)	4 (1%)	71	84
32	63	266/332 (80%)	264 (99%)	2 (1%)	81	89
33	73	242/303 (80%)	240 (99%)	2 (1%)	81	89
34	93	91/112 (81%)	91 (100%)	0	100	100
35	a3	78/133 (59%)	78 (100%)	0	100	100
36	b3	130/186 (70%)	129 (99%)	1 (1%)	81	89
37	c3	241/288 (84%)	241 (100%)	0	100	100
38	d3	151/274 (55%)	149 (99%)	2 (1%)	69	82
39	e3	188/236 (80%)	188 (100%)	0	100	100
40	f3	117/188 (62%)	117 (100%)	0	100	100
41	g3	119/148 (80%)	119 (100%)	0	100	100
42	h3	95/148 (64%)	95 (100%)	0	100	100
43	i3	86/110 (78%)	86 (100%)	0	100	100
44	j3	68/97 (70%)	68 (100%)	0	100	100
45	k3	74/90 (82%)	73 (99%)	1 (1%)	67	81
46	l3	23/116 (20%)	23 (100%)	0	100	100
47	m3	40/113 (35%)	39 (98%)	1 (2%)	47	68
48	o3	80/87 (92%)	79 (99%)	1 (1%)	69	82
49	p3	117/181 (65%)	117 (100%)	0	100	100
50	q3	110/178 (62%)	109 (99%)	1 (1%)	78	88
51	r3	133/169 (79%)	133 (100%)	0	100	100
52	s3	326/381 (86%)	322 (99%)	4 (1%)	71	84
55	B6	191/249 (77%)	190 (100%)	1 (0%)	88	93
56	C6	115/143 (80%)	113 (98%)	2 (2%)	60	78
57	D6	269/357 (75%)	266 (99%)	3 (1%)	73	85
58	E6	104/107 (97%)	104 (100%)	0	100	100
59	F6	178/209 (85%)	177 (99%)	1 (1%)	86	92
60	G6	265/342 (78%)	264 (100%)	1 (0%)	91	94
61	H6	112/180 (62%)	110 (98%)	2 (2%)	59	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
62	I6	104/147 (71%)	103 (99%)	1 (1%)	76	86
63	J6	93/118 (79%)	92 (99%)	1 (1%)	73	85
64	K6	91/113 (80%)	91 (100%)	0	100	100
65	L6	152/226 (67%)	149 (98%)	3 (2%)	55	74
66	M6	95/113 (84%)	94 (99%)	1 (1%)	73	85
67	N6	93/115 (81%)	93 (100%)	0	100	100
68	O6	166/230 (72%)	166 (100%)	0	100	100
69	P6	87/123 (71%)	87 (100%)	0	100	100
70	Q6	78/79 (99%)	77 (99%)	1 (1%)	69	82
71	R6	224/318 (70%)	223 (100%)	1 (0%)	91	94
72	S6	109/164 (66%)	109 (100%)	0	100	100
73	T6	150/157 (96%)	150 (100%)	0	100	100
74	U6	149/174 (86%)	148 (99%)	1 (1%)	84	90
75	V6	295/364 (81%)	292 (99%)	3 (1%)	76	86
76	W6	84/158 (53%)	83 (99%)	1 (1%)	71	84
77	X6	275/351 (78%)	273 (99%)	2 (1%)	84	90
78	Y6	99/357 (28%)	98 (99%)	1 (1%)	76	86
79	Z6	80/95 (84%)	80 (100%)	0	100	100
80	a6	176/190 (93%)	174 (99%)	2 (1%)	73	85
81	b6	237/291 (81%)	234 (99%)	3 (1%)	69	82
82	c6	99/101 (98%)	97 (98%)	2 (2%)	55	74
83	d6	63/166 (38%)	63 (100%)	0	100	100
84	e6	226/609 (37%)	225 (100%)	1 (0%)	91	94
88	A	151/190 (80%)	150 (99%)	1 (1%)	84	90
89	Z	328/371 (88%)	327 (100%)	1 (0%)	92	95
91	n	184/181 (102%)	181 (98%)	3 (2%)	62	79
All	All	11992/16337 (73%)	11907 (99%)	85 (1%)	84	90

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D3	239	THR
5	E3	47	THR

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Mol	Chain	Res	Type
5	E3	151	THR
5	E3	236	THR
6	F3	76	ARG
7	H3	108	ARG
12	M3	41	ARG
12	M3	84	ASN
12	M3	134	ARG
12	M3	149	THR
12	M3	254	LYS
14	O3	125	TYR
15	P3	48	THR
16	Q3	83	ARG
16	Q3	284	LYS
17	R3	144	ARG
19	T3	100	ASP
21	V3	87	VAL
21	V3	93	THR
21	V3	104	TYR
23	X3	44	ARG
23	X3	131	THR
24	Y3	162	ARG
26	03	113	CYS
27	13	62	ILE
31	53	214	ASN
31	53	239	ILE
31	53	264	ASP
31	53	310	ARG
32	63	44	ASN
32	63	379	ILE
33	73	77	THR
33	73	167	VAL
36	b3	15	LEU
38	d3	218	THR
38	d3	263	THR
45	k3	64	VAL
47	m3	72	ARG
48	o3	82	PHE
50	q3	41	ASP
52	s3	159	ARG
52	s3	230	ARG
52	s3	234	ASP
52	s3	251	VAL

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Mol	Chain	Res	Type
55	B6	169	ARG
56	C6	52	THR
56	C6	153	LEU
57	D6	331	ASP
57	D6	418	LYS
57	D6	419	ARG
59	F6	228	LYS
60	G6	389	ARG
61	H6	126	ILE
61	H6	175	THR
62	I6	179	THR
63	J6	44	ARG
65	L6	137	ARG
65	L6	146	HIS
65	L6	156	LEU
66	M6	13	ARG
70	Q6	80	ARG
71	R6	281	ILE
74	U6	41	ARG
75	V6	116	CYS
75	V6	194	THR
75	V6	337	LEU
76	W6	157	THR
77	X6	290	VAL
77	X6	393	ARG
78	Y6	284	LYS
80	a6	27	ARG
80	a6	121	LYS
81	b6	65	ASP
81	b6	145	LYS
81	b6	322	VAL
82	c6	37	ARG
82	c6	114	LYS
84	e6	369	LEU
88	A	46	ARG
89	Z	253	ASP
7	D	164	VAL
7	D	213	ILE
91	n	63[A]	SER
91	n	63[B]	SER
91	n	210	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (151)

such sidechains are listed below:

Mol	Chain	Res	Type
4	D3	165	ASN
4	D3	233	GLN
4	D3	263	ASN
4	D3	276	HIS
5	E3	57	ASN
5	E3	88	HIS
5	E3	184	ASN
5	E3	233	GLN
5	E3	339	GLN
6	F3	223	HIS
6	F3	249	ASN
7	H3	88	HIS
7	H3	121	ASN
9	J3	103	GLN
10	K3	48	HIS
10	K3	56	HIS
11	L3	43	ASN
12	M3	26	ASN
12	M3	114	GLN
12	M3	276	ASN
14	O3	91	GLN
15	P3	78	HIS
16	Q3	139	GLN
17	R3	30	HIS
17	R3	70	ASN
17	R3	125	HIS
18	S3	91	GLN
18	S3	118	ASN
19	T3	62	GLN
19	T3	109	ASN
19	T3	132	HIS
20	U3	41	GLN
24	Y3	88	GLN
24	Y3	147	GLN
24	Y3	157	GLN
26	03	170	GLN
27	13	31	ASN
28	23	54	GLN
28	23	92	HIS
30	43	95	HIS
30	43	98	HIS
30	43	100	GLN

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Mol	Chain	Res	Type
31	53	65	HIS
31	53	96	HIS
31	53	102	GLN
31	53	119	GLN
31	53	221	GLN
31	53	353	HIS
31	53	358	GLN
32	63	66	GLN
32	63	149	GLN
32	63	163	HIS
33	73	165	ASN
33	73	198	ASN
33	73	309	HIS
37	c3	80	GLN
37	c3	123	GLN
37	c3	168	HIS
37	c3	193	GLN
38	d3	119	GLN
39	e3	75	GLN
39	e3	207	ASN
39	e3	212	HIS
39	e3	252	HIS
41	g3	102	HIS
42	h3	67	GLN
43	i3	48	ASN
43	i3	89	GLN
43	i3	122	ASN
45	k3	72	HIS
48	o3	21	HIS
50	q3	81	GLN
50	q3	107	GLN
50	q3	130	GLN
51	r3	69	GLN
52	s3	164	HIS
52	s3	427	ASN
55	B6	99	HIS
55	B6	178	ASN
55	B6	197	HIS
55	B6	201	ASN
56	C6	75	ASN
56	C6	81	HIS
56	C6	130	HIS

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Mol	Chain	Res	Type
57	D6	175	GLN
57	D6	308	GLN
57	D6	317	HIS
57	D6	347	GLN
57	D6	356	GLN
57	D6	415	GLN
58	E6	96	HIS
59	F6	127	HIS
60	G6	77	GLN
60	G6	90	ASN
60	G6	156	GLN
60	G6	312	GLN
61	H6	83	HIS
61	H6	125	HIS
61	H6	130	HIS
61	H6	147	HIS
63	J6	35	GLN
64	K6	60	ASN
67	N6	79	HIS
68	O6	80	ASN
68	O6	166	HIS
68	O6	181	HIS
68	O6	207	GLN
69	P6	115	GLN
70	Q6	18	ASN
70	Q6	79	ASN
71	R6	277	ASN
72	S6	61	GLN
72	S6	97	GLN
73	T6	18	GLN
73	T6	56	GLN
73	T6	128	ASN
74	U6	117	HIS
74	U6	133	GLN
74	U6	135	GLN
74	U6	186	ASN
75	V6	115	GLN
75	V6	122	GLN
75	V6	170	GLN
75	V6	179	GLN
75	V6	217	ASN
75	V6	342	GLN

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Mol	Chain	Res	Type
75	V6	388	GLN
75	V6	396	GLN
76	W6	91	GLN
77	X6	81	HIS
77	X6	90	GLN
77	X6	140	HIS
77	X6	143	HIS
77	X6	367	GLN
78	Y6	290	ASN
78	Y6	331	HIS
80	a6	66	GLN
81	b6	261	ASN
81	b6	301	ASN
82	c6	15	ASN
83	d6	141	HIS
83	d6	158	GLN
84	e6	115	ASN
84	e6	122	ASN
84	e6	455	ASN
88	A	143	GLN
89	Z	412	GLN
7	D	196	ASN
91	n	172	HIS
91	n	188	ASN
91	n	225	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	A3	1490/1559 (95%)	437 (29%)	31 (2%)
3	B3	51/69 (73%)	15 (29%)	1 (1%)
53	u3	1/2 (50%)	1 (100%)	0
85	A6	921/954 (96%)	232 (25%)	14 (1%)
86	24	73/73 (100%)	41 (56%)	5 (6%)
86	C	73/73 (100%)	42 (57%)	5 (6%)
87	i4	9/10 (90%)	2 (22%)	0
90	j	74/76 (97%)	23 (31%)	0
All	All	2692/2816 (95%)	793 (29%)	56 (2%)

All (793) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	A3	1674	A
2	A3	1676	A
2	A3	1677	C
2	A3	1678	C
2	A3	1679	U
2	A3	1680	A
2	A3	1681	G
2	A3	1685	C
2	A3	1689	C
2	A3	1692	A
2	A3	1693	C
2	A3	1694	U
2	A3	1696	C
2	A3	1700	U
2	A3	1702	A
2	A3	1704	U
2	A3	1705	A
2	A3	1708	A
2	A3	1709	G
2	A3	1712	A
2	A3	1713	A
2	A3	1714	C
2	A3	1715	C
2	A3	1716	U
2	A3	1717	U
2	A3	1724	A
2	A3	1727	A
2	A3	1728	U
2	A3	1741	A
2	A3	1743	U
2	A3	1748	G
2	A3	1750	G
2	A3	1751	A
2	A3	1770	G
2	A3	1774	U
2	A3	1777	A
2	A3	1781	A
2	A3	1782	G
2	A3	1788	C
2	A3	1794	A
2	A3	1797	G
2	A3	1804	A
2	A3	1805	A

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Mol	Chain	Res	Type
2	A3	1806	U
2	A3	1807	U
2	A3	1808	A
2	A3	1809	U
2	A3	1810	A
2	A3	1812	C
2	A3	1813	C
2	A3	1823	A
2	A3	1824	U
2	A3	1827	C
2	A3	1828	A
2	A3	1829	A
2	A3	1832	A
2	A3	1836	A
2	A3	1844	A
2	A3	1850	U
2	A3	1852	C
2	A3	1853	A
2	A3	1854	U
2	A3	1856	A
2	A3	1867	A
2	A3	1869	A
2	A3	1870	A
2	A3	1871	A
2	A3	1872	U
2	A3	1873	A
2	A3	1874	A
2	A3	1878	U
2	A3	1882	A
2	A3	1883	G
2	A3	1887	A
2	A3	1888	G
2	A3	1893	A
2	A3	1901	C
2	A3	1902	C
2	A3	1903	C
2	A3	1909	A
2	A3	1918	G
2	A3	1927	G
2	A3	1935	A
2	A3	1939	G
2	A3	1940	A

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Mol	Chain	Res	Type
2	A3	1944	C
2	A3	1958	G
2	A3	1966	G
2	A3	1975	U
2	A3	1985	G
2	A3	1986	A
2	A3	1987	G
2	A3	1992	C
2	A3	1993	A
2	A3	1994	A
2	A3	1995	A
2	A3	2000	C
2	A3	2001	C
2	A3	2015	G
2	A3	2021	U
2	A3	2022	G
2	A3	2029	A
2	A3	2032	G
2	A3	2036	C
2	A3	2037	U
2	A3	2039	A
2	A3	2059	C
2	A3	2060	A
2	A3	2065	A
2	A3	2066	C
2	A3	2074	A
2	A3	2079	C
2	A3	2083	U
2	A3	2085	A
2	A3	2093	U
2	A3	2097	A
2	A3	2098	G
2	A3	2105	G
2	A3	2111	C
2	A3	2113	G
2	A3	2117	U
2	A3	2124	A
2	A3	2132	A
2	A3	2135	A
2	A3	2142	A
2	A3	2143	G
2	A3	2147	G

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Mol	Chain	Res	Type
2	A3	2154	A
2	A3	2157	U
2	A3	2159	U
2	A3	2163	A
2	A3	2165	C
2	A3	2166	C
2	A3	2167	A
2	A3	2168	U
2	A3	2169	A
2	A3	2171	U
2	A3	2172	A
2	A3	2173	G
2	A3	2174	G
2	A3	2180	A
2	A3	2182	G
2	A3	2183	C
2	A3	2187	C
2	A3	2189	C
2	A3	2190	C
2	A3	2193	U
2	A3	2194	U
2	A3	2195	A
2	A3	2197	G
2	A3	2198	A
2	A3	2200	A
2	A3	2201	G
2	A3	2204	U
2	A3	2207	A
2	A3	2210	C
2	A3	2211	U
2	A3	2216	A
2	A3	2230	A
2	A3	2233	U
2	A3	2237	A
2	A3	2239	A
2	A3	2241	A
2	A3	2243	A
2	A3	2244	U
2	A3	2245	A
2	A3	2246	A
2	A3	2262	C
2	A3	2263	C

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Mol	Chain	Res	Type
2	A3	2283	C
2	A3	2284	C
2	A3	2285	U
2	A3	2297	A
2	A3	2299	U
2	A3	2300	G
2	A3	2309	A
2	A3	2315	A
2	A3	2322	C
2	A3	2324	U
2	A3	2332	C
2	A3	2342	U
2	A3	2345	G
2	A3	2364	C
2	A3	2369	A
2	A3	2370	A
2	A3	2371	U
2	A3	2372	U
2	A3	2373	A
2	A3	2374	A
2	A3	2375	C
2	A3	2379	C
2	A3	2380	C
2	A3	2381	A
2	A3	2383	U
2	A3	2387	U
2	A3	2390	A
2	A3	2393	C
2	A3	2396	C
2	A3	2397	C
2	A3	2398	A
2	A3	2399	A
2	A3	2401	A
2	A3	2404	U
2	A3	2405	C
2	A3	2407	U
2	A3	2410	U
2	A3	2414	C
2	A3	2415	C
2	A3	2416	U
2	A3	2417	C
2	A3	2418	A

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Mol	Chain	Res	Type
2	A3	2426	C
2	A3	2432	A
2	A3	2434	A
2	A3	2435	G
2	A3	2443	C
2	A3	2444	A
2	A3	2447	A
2	A3	2451	A
2	A3	2464	G
2	A3	2476	C
2	A3	2478	G
2	A3	2493	C
2	A3	2498	U
2	A3	2500	A
2	A3	2504	A
2	A3	2508	C
2	A3	2511	C
2	A3	2520	C
2	A3	2521	A
2	A3	2522	U
2	A3	2523	C
2	A3	2524	A
2	A3	2527	A
2	A3	2530	A
2	A3	2531	U
2	A3	2532	U
2	A3	2536	G
2	A3	2539	A
2	A3	2540	C
2	A3	2557	C
2	A3	2558	A
2	A3	2559	U
2	A3	2560	G
2	A3	2563	U
2	A3	2570	C
2	A3	2587	G
2	A3	2590	A
2	A3	2592	G
2	A3	2593	G
2	A3	2594	U
2	A3	2596	G
2	A3	2601	A

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Mol	Chain	Res	Type
2	A3	2603	C
2	A3	2608	G
2	A3	2618	U
2	A3	2625	C
2	A3	2626	U
2	A3	2627	G
2	A3	2628	U
2	A3	2629	A
2	A3	2630	U
2	A3	2632	A
2	A3	2633	A
2	A3	2634	U
2	A3	2635	G
2	A3	2638	U
2	A3	2641	A
2	A3	2645	G
2	A3	2652	G
2	A3	2654	U
2	A3	2655	G
2	A3	2656	U
2	A3	2660	U
2	A3	2683	C
2	A3	2686	G
2	A3	2694	A
2	A3	2695	G
2	A3	2696	A
2	A3	2706	A
2	A3	2708	C
2	A3	2709	A
2	A3	2718	C
2	A3	2719	G
2	A3	2723	A
2	A3	2724	G
2	A3	2725	A
2	A3	2726	C
2	A3	2727	C
2	A3	2732	G
2	A3	2733	G
2	A3	2739	U
2	A3	2740	A
2	A3	2745	A
2	A3	2750	U

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Mol	Chain	Res	Type
2	A3	2755	A
2	A3	2757	A
2	A3	2758	G
2	A3	2762	C
2	A3	2763	U
2	A3	2764	A
2	A3	2765	A
2	A3	2767	A
2	A3	2768	A
2	A3	2769	A
2	A3	2770	C
2	A3	2773	A
2	A3	2774	C
2	A3	2775	A
2	A3	2776	G
2	A3	2777	G
2	A3	2779	C
2	A3	2780	C
2	A3	2782	A
2	A3	2784	A
2	A3	2785	C
2	A3	2786	U
2	A3	2789	C
2	A3	2790	A
2	A3	2791	A
2	A3	2792	A
2	A3	2793	C
2	A3	2804	A
2	A3	2810	G
2	A3	2814	G
2	A3	2831	G
2	A3	2832	A
2	A3	2833	A
2	A3	2842	C
2	A3	2844	G
2	A3	2847	C
2	A3	2852	C
2	A3	2853	A
2	A3	2854	U
2	A3	2861	A
2	A3	2864	U
2	A3	2865	C

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Mol	Chain	Res	Type
2	A3	2870	G
2	A3	2871	U
2	A3	2880	A
2	A3	2892	A
2	A3	2893	A
2	A3	2900	C
2	A3	2901	A
2	A3	2906	C
2	A3	2909	G
2	A3	2910	A
2	A3	2913	A
2	A3	2915	C
2	A3	2916	G
2	A3	2917	G
2	A3	2922	A
2	A3	2926	A
2	A3	2927	C
2	A3	2928	C
2	A3	2932	G
2	A3	2935	A
2	A3	2936	U
2	A3	2938	A
2	A3	2939	C
2	A3	2955	U
2	A3	2956	A
2	A3	2962	C
2	A3	2963	A
2	A3	2965	A
2	A3	2989	G
2	A3	2990	A
2	A3	2991	U
2	A3	2992	G
2	A3	2994	U
2	A3	3005	A
2	A3	3007	C
2	A3	3012	U
2	A3	3016	G
2	A3	3017	C
2	A3	3022	G
2	A3	3029	A
2	A3	3041	U
2	A3	3042	U

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Mol	Chain	Res	Type
2	A3	3043	C
2	A3	3049	U
2	A3	3053	A
2	A3	3054	G
2	A3	3056	C
2	A3	3060	C
2	A3	3061	G
2	A3	3063	G
2	A3	3069	A
2	A3	3070	G
2	A3	3072	U
2	A3	3077	C
2	A3	3078	C
2	A3	3086	U
2	A3	3088	C
2	A3	3089	A
2	A3	3090	G
2	A3	3093	C
2	A3	3096	U
2	A3	3098	U
2	A3	3099	C
2	A3	3100	U
2	A3	3108	U
2	A3	3109	U
2	A3	3114	U
2	A3	3122	U
2	A3	3123	G
2	A3	3124	U
2	A3	3128	A
2	A3	3129	A
2	A3	3134	C
2	A3	3135	A
2	A3	3141	A
2	A3	3150	U
2	A3	3151	A
2	A3	3155	C
2	A3	3157	C
2	A3	3158	A
2	A3	3160	A
2	A3	3162	C
2	A3	3168	C
2	A3	3169	C

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Mol	Chain	Res	Type
2	A3	3172	C
2	A3	3173	G
2	A3	3176	A
2	A3	3180	A
2	A3	3184	C
2	A3	3189	C
2	A3	3190	A
2	A3	3196	G
2	A3	3202	U
2	A3	3204	C
2	A3	3207	A
2	A3	3217	A
2	A3	3218	A
2	A3	3220	A
2	A3	3223	A
2	A3	3228	U
3	B3	1607	U
3	B3	1608	G
3	B3	1609	U
3	B3	1611	G
3	B3	1614	U
3	B3	1615	A
3	B3	1625	A
3	B3	1631	C
3	B3	1632	U
3	B3	1634	A
3	B3	1641	G
3	B3	1644	G
3	B3	1645	A
3	B3	1649	C
3	B3	1665	C
53	u3	2	A
85	A6	654	U
85	A6	655	A
85	A6	660	U
85	A6	678	U
85	A6	684	U
85	A6	686	A
85	A6	687	G
85	A6	692	A
85	A6	693	U
85	A6	694	U

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Mol	Chain	Res	Type
85	A6	695	A
85	A6	698	C
85	A6	708	U
85	A6	715	U
85	A6	716	C
85	A6	717	C
85	A6	722	A
85	A6	725	U
85	A6	726	C
85	A6	749	A
85	A6	755	A
85	A6	757	A
85	A6	761	A
85	A6	765	A
85	A6	768	A
85	A6	769	C
85	A6	770	G
85	A6	777	U
85	A6	781	G
85	A6	785	A
85	A6	787	A
85	A6	795	G
85	A6	797	C
85	A6	798	U
85	A6	799	A
85	A6	800	G
85	A6	811	A
85	A6	812	C
85	A6	813	G
85	A6	818	A
85	A6	819	C
85	A6	831	A
85	A6	833	C
85	A6	834	U
85	A6	836	U
85	A6	839	C
85	A6	840	A
85	A6	850	A
85	A6	851	G
85	A6	872	C
85	A6	873	C
85	A6	874	C

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Mol	Chain	Res	Type
85	A6	884	C
85	A6	886	A
85	A6	887	U
85	A6	888	U
85	A6	890	C
85	A6	894	C
85	A6	895	C
85	A6	897	G
85	A6	901	C
85	A6	903	G
85	A6	906	G
85	A6	907	U
85	A6	908	C
85	A6	916	U
85	A6	923	A
85	A6	926	C
85	A6	931	G
85	A6	932	A
85	A6	937	G
85	A6	942	A
85	A6	943	A
85	A6	945	G
85	A6	946	A
85	A6	947	G
85	A6	951	U
85	A6	952	U
85	A6	954	A
85	A6	957	U
85	A6	959	A
85	A6	970	A
85	A6	971	A
85	A6	981	A
85	A6	982	A
85	A6	992	G
85	A6	996	U
85	A6	997	A
85	A6	1005	C
85	A6	1006	C
85	A6	1014	A
85	A6	1015	C
85	A6	1018	A
85	A6	1019	A

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Mol	Chain	Res	Type
85	A6	1026	A
85	A6	1032	G
85	A6	1034	G
85	A6	1046	U
85	A6	1050	A
85	A6	1051	A
85	A6	1052	C
85	A6	1056	C
85	A6	1069	C
85	A6	1082	A
85	A6	1084	A
85	A6	1085	U
85	A6	1086	A
85	A6	1101	G
85	A6	1102	C
85	A6	1107	A
85	A6	1109	C
85	A6	1110	C
85	A6	1113	A
85	A6	1125	A
85	A6	1127	C
85	A6	1129	A
85	A6	1130	A
85	A6	1133	U
85	A6	1142	G
85	A6	1147	C
85	A6	1148	U
85	A6	1155	C
85	A6	1157	C
85	A6	1158	A
85	A6	1159	G
85	A6	1171	A
85	A6	1176	C
85	A6	1183	G
85	A6	1184	U
85	A6	1189	C
85	A6	1191	U
85	A6	1192	A
85	A6	1193	U
85	A6	1194	C
85	A6	1196	C
85	A6	1197	U

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Mol	Chain	Res	Type
85	A6	1201	G
85	A6	1210	G
85	A6	1218	A
85	A6	1219	U
85	A6	1224	A
85	A6	1226	A
85	A6	1227	C
85	A6	1229	C
85	A6	1233	U
85	A6	1234	C
85	A6	1235	A
85	A6	1249	U
85	A6	1250	U
85	A6	1251	G
85	A6	1252	C
85	A6	1255	A
85	A6	1258	C
85	A6	1265	C
85	A6	1269	C
85	A6	1273	U
85	A6	1274	U
85	A6	1275	C
85	A6	1276	A
85	A6	1287	A
85	A6	1288	U
85	A6	1294	C
85	A6	1296	A
85	A6	1297	C
85	A6	1299	A
85	A6	1300	A
85	A6	1304	A
85	A6	1330	A
85	A6	1331	G
85	A6	1334	C
85	A6	1335	A
85	A6	1336	A
85	A6	1346	C
85	A6	1347	A
85	A6	1348	U
85	A6	1357	A
85	A6	1359	G
85	A6	1360	A

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Mol	Chain	Res	Type
85	A6	1369	A
85	A6	1371	A
85	A6	1372	U
85	A6	1373	U
85	A6	1380	C
85	A6	1381	C
85	A6	1382	C
85	A6	1394	A
85	A6	1401	U
85	A6	1406	A
85	A6	1420	A
85	A6	1424	U
85	A6	1426	G
85	A6	1428	U
85	A6	1434	A
85	A6	1441	U
85	A6	1447	U
85	A6	1451	G
85	A6	1452	U
85	A6	1458	G
85	A6	1466	G
85	A6	1469	C
85	A6	1470	C
85	A6	1478	G
85	A6	1485	C
85	A6	1486	A
85	A6	1492	C
85	A6	1516	A
85	A6	1521	A
85	A6	1522	C
85	A6	1528	A
85	A6	1529	C
85	A6	1531	A
85	A6	1536	C
85	A6	1537	C
85	A6	1539	U
85	A6	1540	A
85	A6	1541	C
85	A6	1542	G
85	A6	1543	C
85	A6	1544	A
85	A6	1551	U

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Mol	Chain	Res	Type
85	A6	1559	A
85	A6	1561	A
85	A6	1563	G
85	A6	1572	U
85	A6	1575	U
85	A6	1586	G
85	A6	1588	A
85	A6	1598	G
85	A6	1599	G
85	A6	1602	G
85	A6	1603	A
85	A6	1604	A
86	24	2	U
86	24	3	U
86	24	7	G
86	24	8	U
86	24	9	A
86	24	11	C
86	24	12	U
86	24	13	U
86	24	14	A
86	24	16	A
86	24	17	U
86	24	18	U
86	24	19	A
86	24	20	U
86	24	21	C
86	24	22	A
86	24	28	A
86	24	29	G
86	24	30	G
86	24	31	C
86	24	33	C
86	24	34	U
86	24	35	G
86	24	40	U
86	24	41	G
86	24	44	U
86	24	45	A
86	24	46	G
86	24	50	A
86	24	51	G

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Mol	Chain	Res	Type
86	24	52	C
86	24	55	C
86	24	56	A
86	24	58	A
86	24	59	G
86	24	62	C
86	24	63	C
86	24	67	A
86	24	71	C
86	24	72	C
86	24	73	A
87	i4	18	A
87	i4	24	U
90	j	8	U
90	j	9	A
90	j	10	G
90	j	13	U
90	j	19	G
90	j	20	U
90	j	21	U
90	j	22	A
90	j	31	G
90	j	32	C
90	j	34	U
90	j	35	A
90	j	36	A
90	j	37	C
90	j	43	A
90	j	45	A
90	j	47	G
90	j	48	U
90	j	49	C
90	j	60	A
90	j	61	A
90	j	76	C
90	j	77	A
86	C	2	U
86	C	3	U
86	C	7	G
86	C	8	U
86	C	9	A
86	C	11	C

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Mol	Chain	Res	Type
86	C	12	U
86	C	13	U
86	C	14	A
86	C	16	A
86	C	17	U
86	C	18	U
86	C	19	A
86	C	20	U
86	C	21	C
86	C	22	A
86	C	28	A
86	C	29	G
86	C	30	G
86	C	31	C
86	C	33	C
86	C	34	U
86	C	35	G
86	C	40	U
86	C	41	G
86	C	44	U
86	C	45	A
86	C	46	G
86	C	49	G
86	C	50	A
86	C	51	G
86	C	52	C
86	C	55	C
86	C	56	A
86	C	58	A
86	C	59	G
86	C	62	C
86	C	63	C
86	C	67	A
86	C	71	C
86	C	72	C
86	C	73	A

All (56) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	A3	1703	C
2	A3	1713	A

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Mol	Chain	Res	Type
2	A3	1805	A
2	A3	1806	U
2	A3	1807	U
2	A3	1809	U
2	A3	1823	A
2	A3	1871	A
2	A3	1901	C
2	A3	2165	C
2	A3	2172	A
2	A3	2186	C
2	A3	2243	A
2	A3	2245	A
2	A3	2374	A
2	A3	2507	A
2	A3	2530	A
2	A3	2531	U
2	A3	2558	A
2	A3	2559	U
2	A3	2628	U
2	A3	2653	C
2	A3	2744	U
2	A3	2788	C
2	A3	2789	C
2	A3	2900	C
2	A3	2905	A
2	A3	2989	G
2	A3	3041	U
2	A3	3092	U
2	A3	3201	A
3	B3	1607	U
85	A6	721	G
85	A6	797	C
85	A6	886	A
85	A6	1025	U
85	A6	1045	A
85	A6	1170	A
85	A6	1193	U
85	A6	1250	U
85	A6	1335	A
85	A6	1419	G
85	A6	1433	C
85	A6	1538	C

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Mol	Chain	Res	Type
85	A6	1541	C
85	A6	1560	C
86	24	1	G
86	24	30	G
86	24	49	G
86	24	70	A
86	24	71	C
86	C	1	G
86	C	30	G
86	C	49	G
86	C	70	A
86	C	71	C

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 148 ligands modelled in this entry, 141 are monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
96	GCP	Z	501	-	27,34,34	3.44	13 (48%)	34,54,54	1.86	7 (20%)
99	MLI	n	303	-	6,6,6	1.33	0	7,7,7	1.34	0
98	SO4	n	301	-	4,4,4	0.17	0	6,6,6	0.10	0
99	MLI	n	302	-	6,6,6	1.36	0	7,7,7	1.30	0
93	SPD	A3	3396	-	9,9,9	0.34	0	8,8,8	0.59	0
99	MLI	n	304	-	6,6,6	1.48	0	7,7,7	1.45	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
95	GDP	X6	500	-	24,30,30	1.05	1 (4%)	30,47,47	1.58	6 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
96	GCP	Z	501	-	-	4/15/38/38	0/3/3/3
99	MLI	n	303	-	-	4/4/4/4	-
99	MLI	n	302	-	-	2/4/4/4	-
93	SPD	A3	3396	-	-	4/7/7/7	-
99	MLI	n	304	-	-	2/4/4/4	-
95	GDP	X6	500	-	-	4/12/32/32	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
96	Z	501	GCP	O4'-C4'	8.82	1.64	1.45
96	Z	501	GCP	C3'-C4'	-7.75	1.33	1.53
96	Z	501	GCP	O4'-C1'	-6.89	1.31	1.41
96	Z	501	GCP	O6-C6	5.61	1.38	1.24
96	Z	501	GCP	C2-N2	4.97	1.43	1.33
96	Z	501	GCP	O2'-C2'	-4.66	1.32	1.43
95	X6	500	GDP	C6-N1	-3.34	1.32	1.37
96	Z	501	GCP	PB-O2B	-2.94	1.49	1.56
96	Z	501	GCP	PB-O3A	2.85	1.61	1.58
96	Z	501	GCP	C2-N1	-2.74	1.30	1.35
96	Z	501	GCP	C2'-C1'	2.63	1.57	1.53
96	Z	501	GCP	C8-N7	-2.39	1.30	1.34
96	Z	501	GCP	PG-O3G	-2.35	1.49	1.54
96	Z	501	GCP	O3'-C3'	2.10	1.47	1.43

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
96	Z	501	GCP	C2-N3-C4	4.79	120.83	115.36
95	X6	500	GDP	PA-O3A-PB	-4.57	117.16	132.83
96	Z	501	GCP	N3-C2-N1	-4.57	121.13	127.22
96	Z	501	GCP	C4-C5-C6	-4.05	116.93	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
95	X6	500	GDP	C3'-C2'-C1'	3.93	106.90	100.98
96	Z	501	GCP	C2-N1-C6	3.38	121.30	115.93
96	Z	501	GCP	C3'-C2'-C1'	3.20	105.80	100.98
95	X6	500	GDP	C5-C6-N1	2.98	119.22	113.95
95	X6	500	GDP	O6-C6-C5	-2.73	119.05	124.37
96	Z	501	GCP	C5-C6-N1	-2.55	119.94	123.43
96	Z	501	GCP	C4-C5-N7	-2.44	106.85	109.40
95	X6	500	GDP	C2-N1-C6	-2.28	120.90	125.10
95	X6	500	GDP	C8-N7-C5	2.22	107.22	102.99
99	n	304	MLI	O9-C3-C1	2.20	121.58	114.54

There are no chirality outliers.

All (20) torsion outliers are listed below:

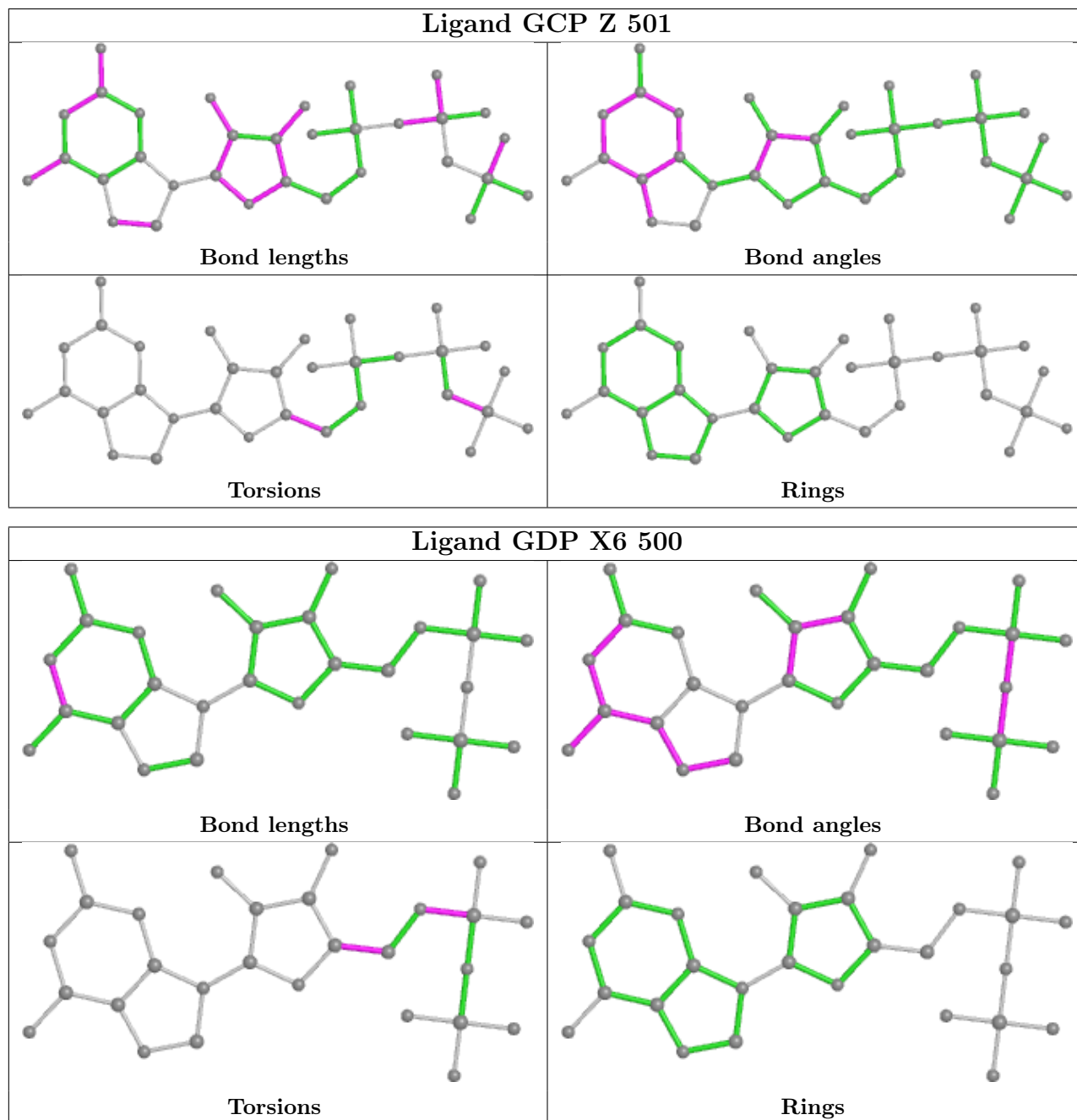
Mol	Chain	Res	Type	Atoms
95	X6	500	GDP	C5'-O5'-PA-O1A
96	Z	501	GCP	PB-C3B-PG-O1G
96	Z	501	GCP	PB-C3B-PG-O2G
96	Z	501	GCP	PB-C3B-PG-O3G
95	X6	500	GDP	C3'-C4'-C5'-O5'
93	A3	3396	SPD	C3-C4-C5-N6
93	A3	3396	SPD	C2-C3-C4-C5
93	A3	3396	SPD	C4-C5-N6-C7
93	A3	3396	SPD	N6-C7-C8-C9
95	X6	500	GDP	O4'-C4'-C5'-O5'
99	n	304	MLI	C2-C1-C3-O8
99	n	303	MLI	C3-C1-C2-O6
99	n	304	MLI	C2-C1-C3-O9
99	n	303	MLI	C3-C1-C2-O7
99	n	303	MLI	C2-C1-C3-O8
99	n	303	MLI	C2-C1-C3-O9
95	X6	500	GDP	C5'-O5'-PA-O3A
96	Z	501	GCP	O4'-C4'-C5'-O5'
99	n	302	MLI	C3-C1-C2-O6
99	n	302	MLI	C3-C1-C2-O7

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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
90	j	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	j	16:C	O3'	18:G	P	5.97

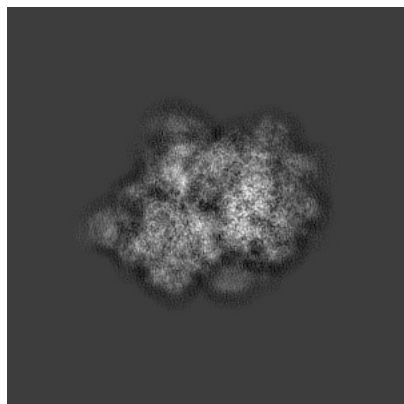
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11642. These allow visual inspection of the internal detail of the map and identification of artifacts.

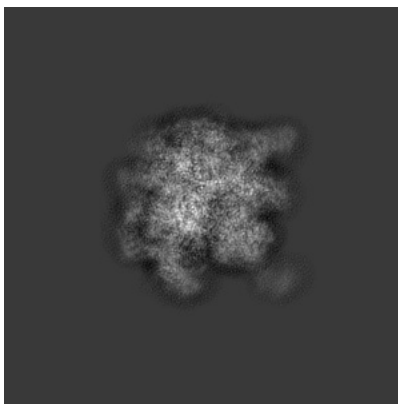
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

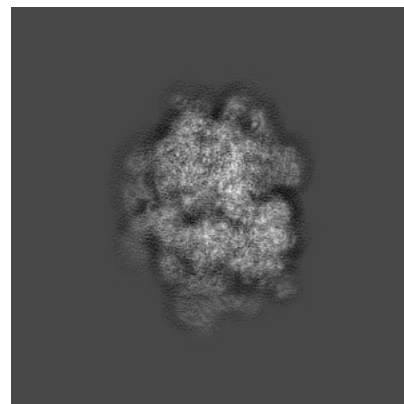
6.1.1 Primary map



X

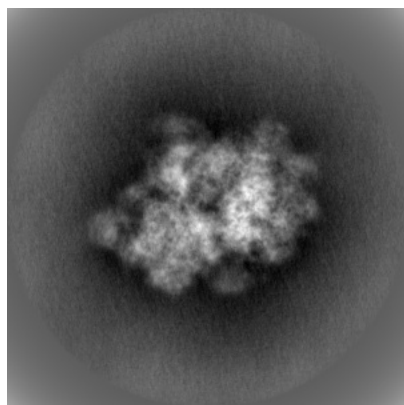


Y

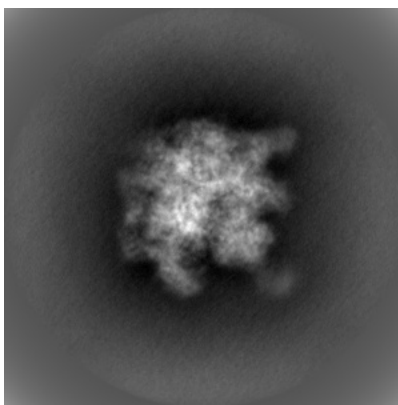


Z

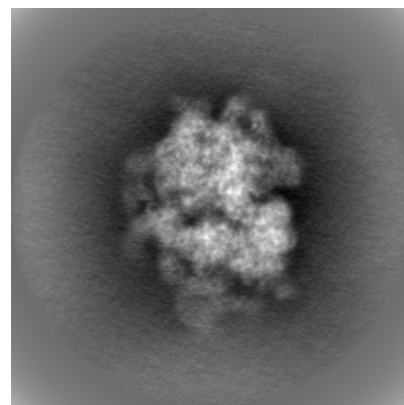
6.1.2 Raw map



X



Y

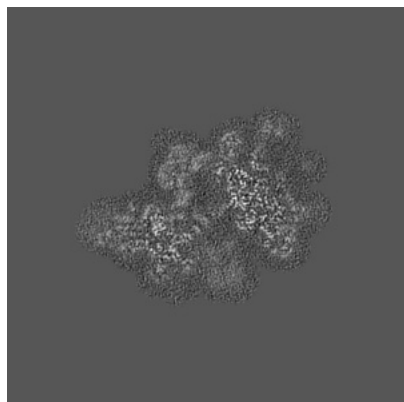


Z

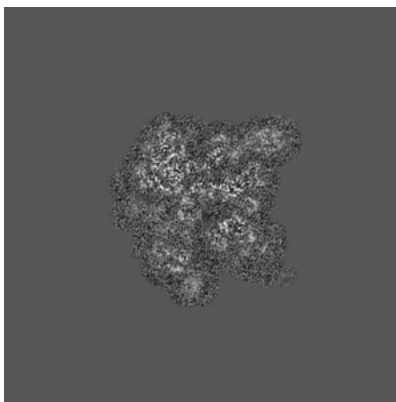
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

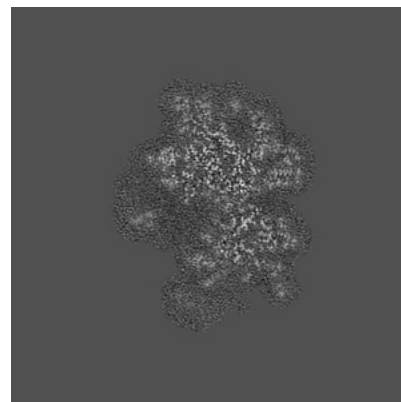
6.2.1 Primary map



X Index: 256

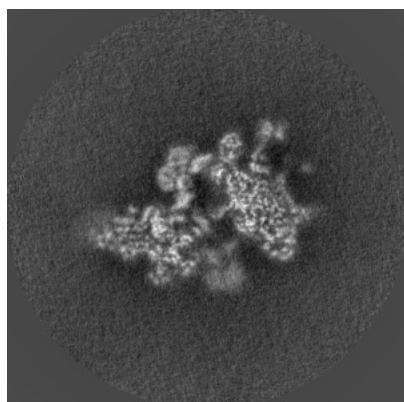


Y Index: 256

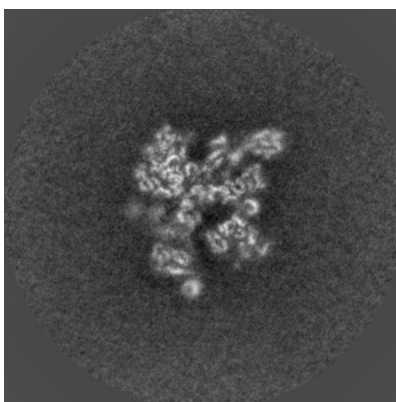


Z Index: 256

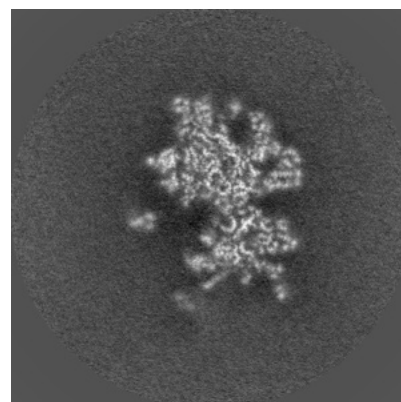
6.2.2 Raw map



X Index: 256



Y Index: 256

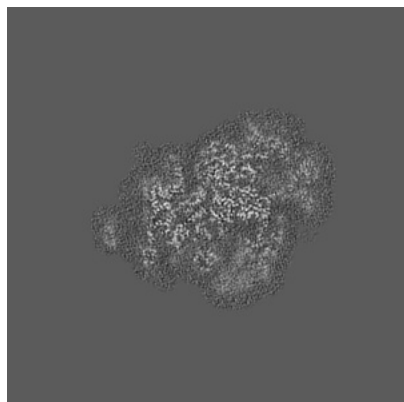


Z Index: 256

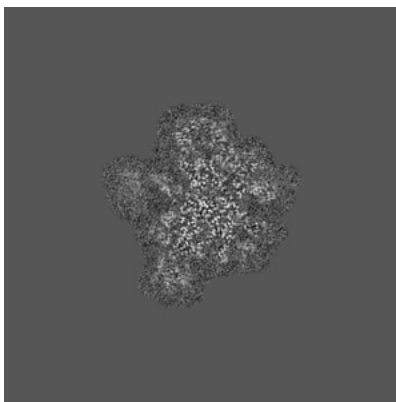
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

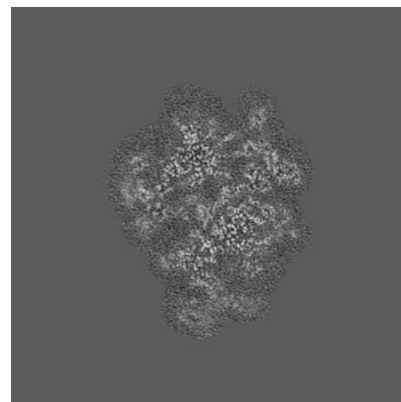
6.3.1 Primary map



X Index: 288

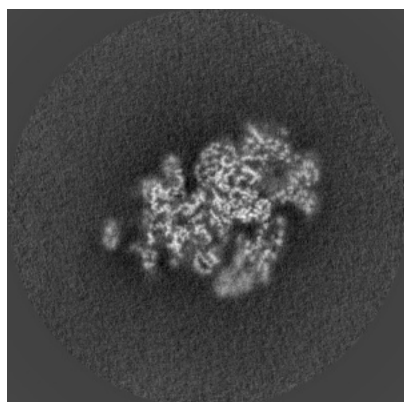


Y Index: 304

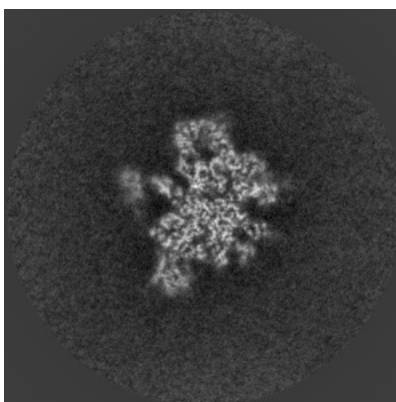


Z Index: 228

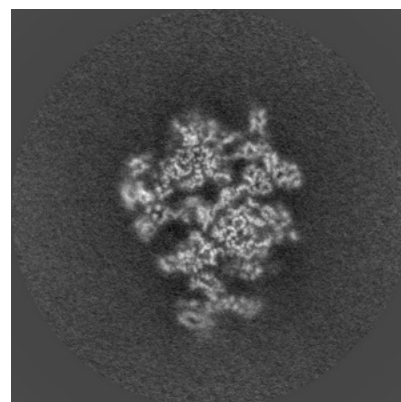
6.3.2 Raw map



X Index: 287



Y Index: 305

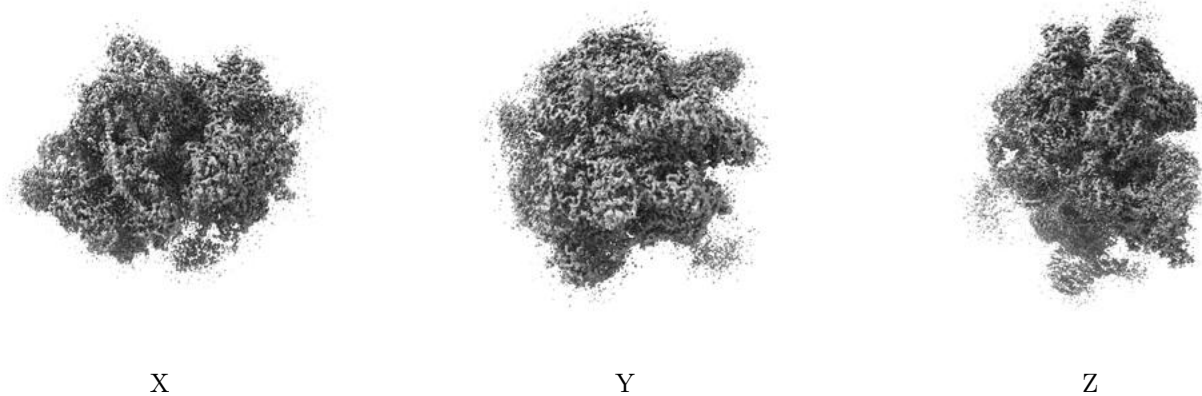


Z Index: 228

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

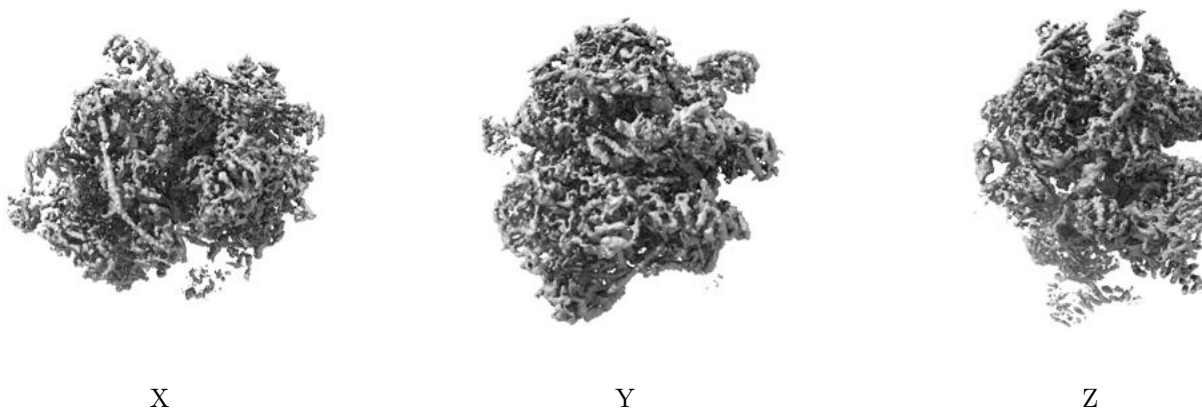
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

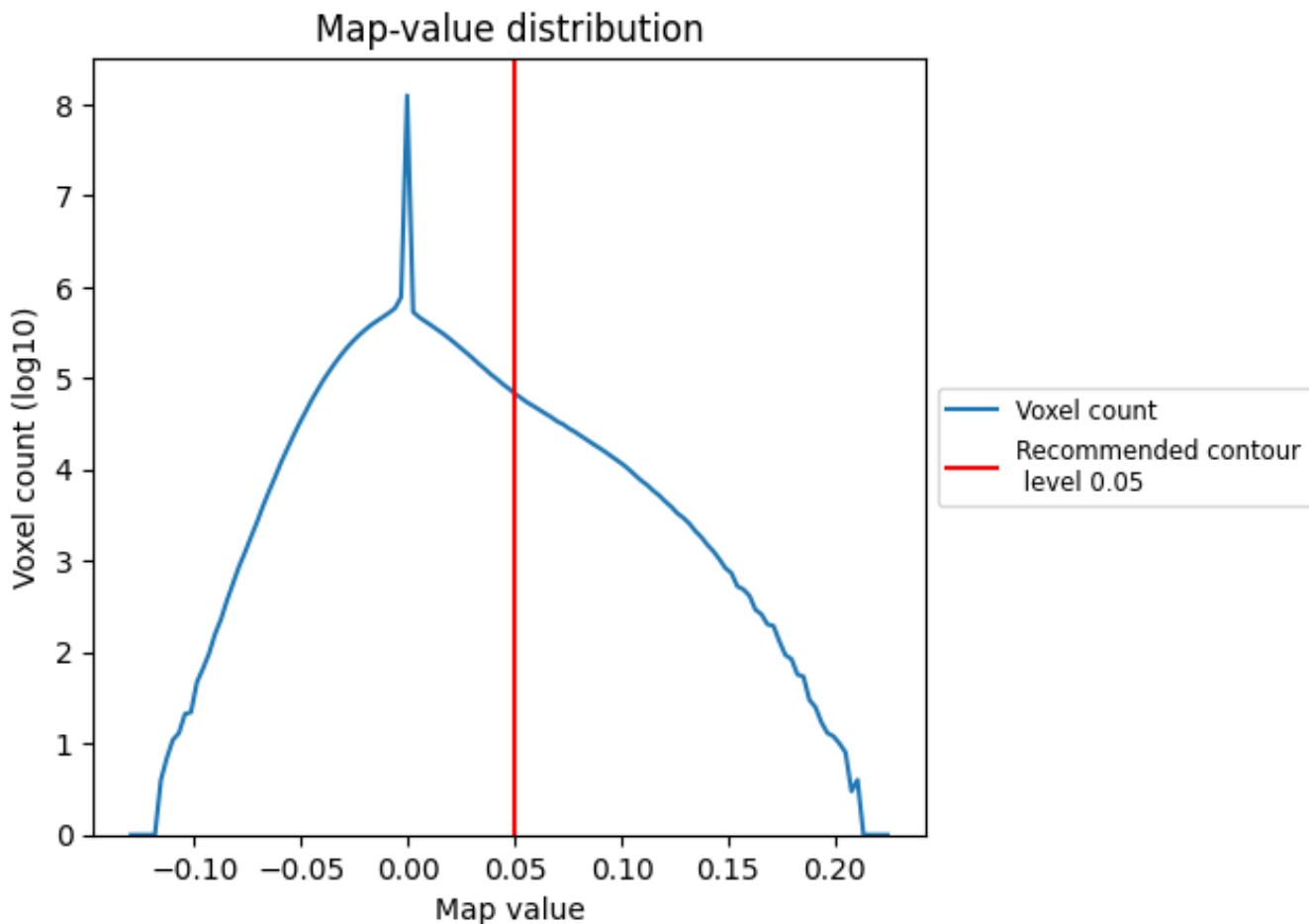
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

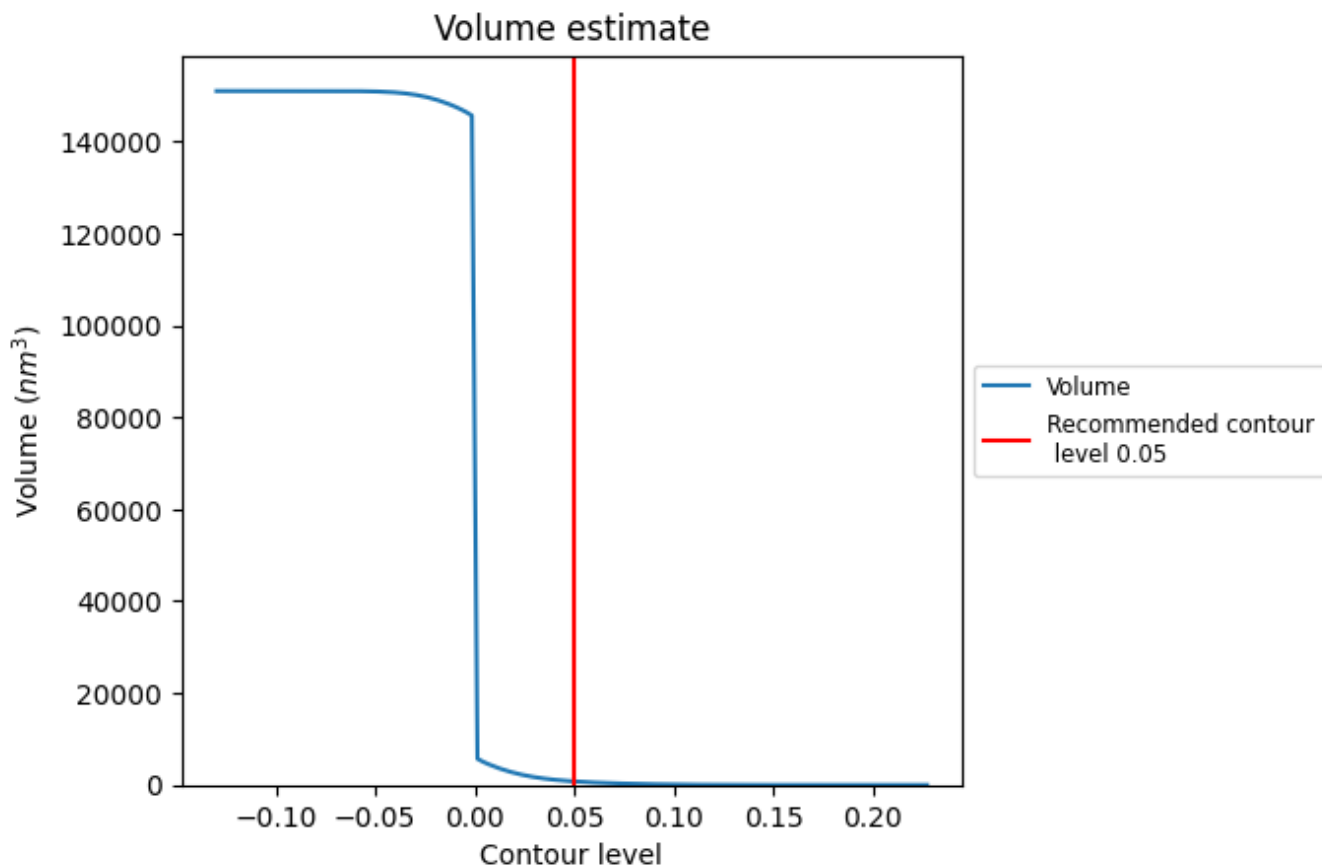
This section contains the results of statistical analysis of the map.

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.

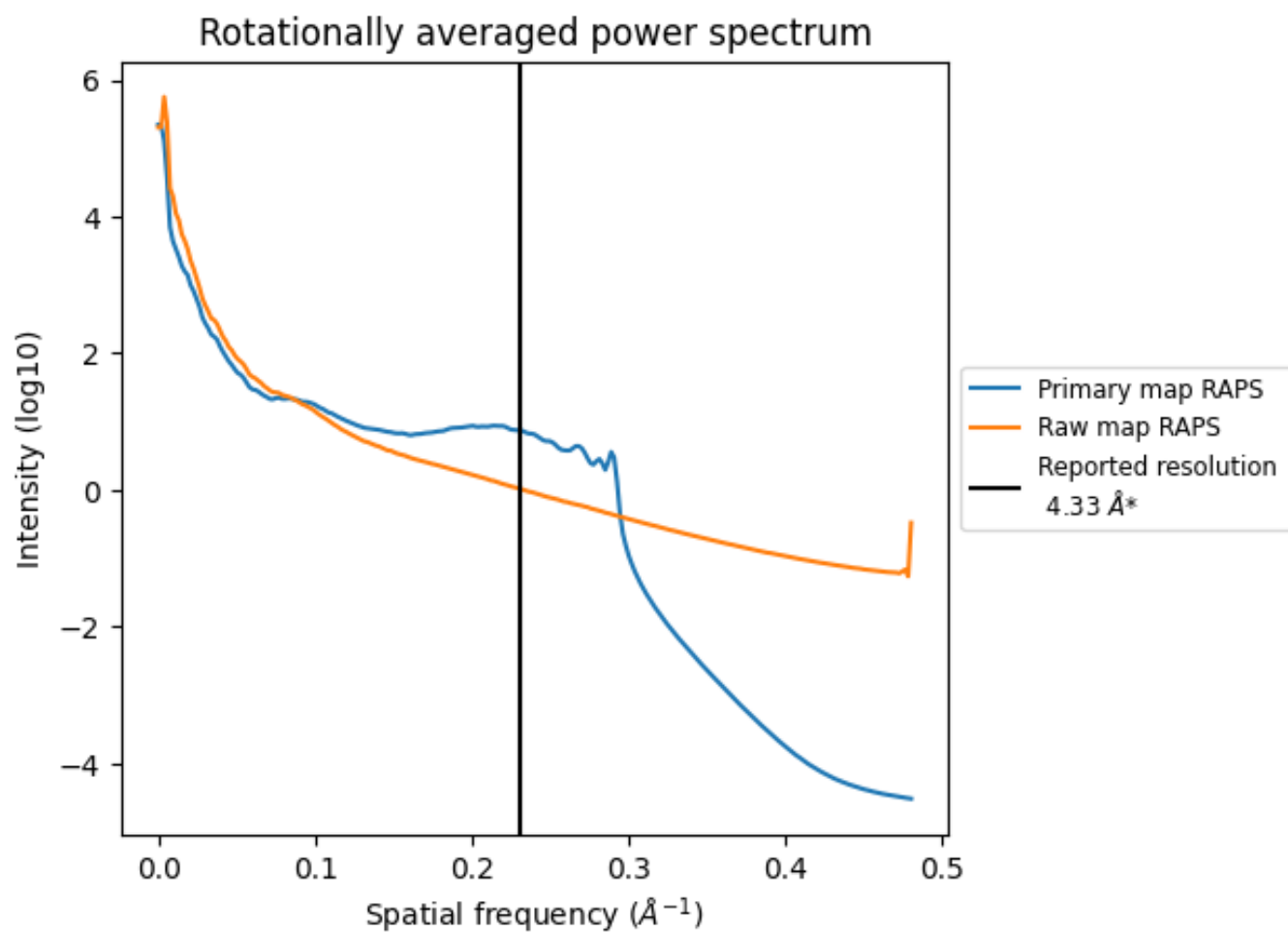
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 775 nm^3 ; this corresponds to an approximate mass of 700 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 [\(i\)](#)

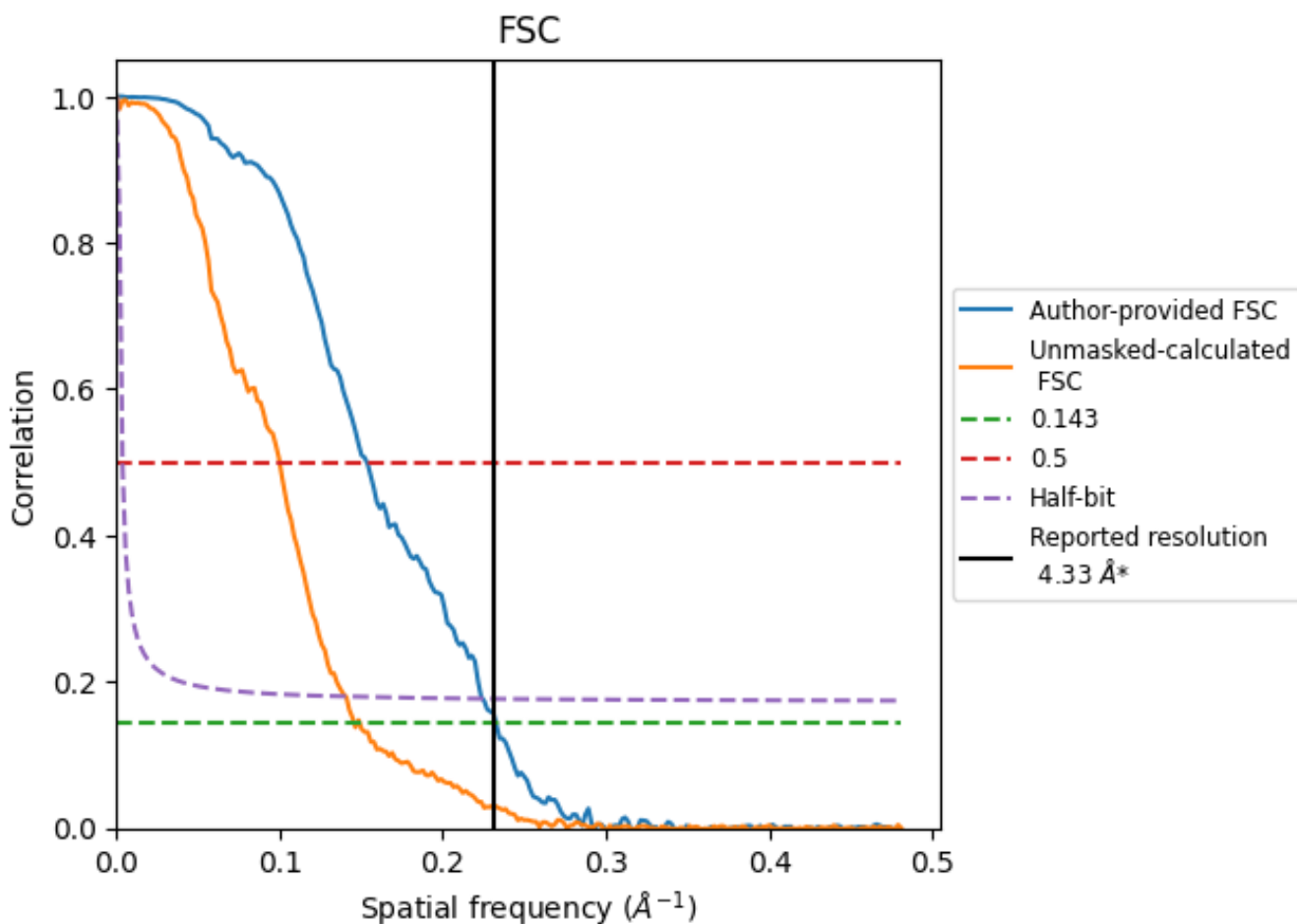


*Reported resolution corresponds to spatial frequency of 0.231 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.231 Å⁻¹

8.2 Resolution estimates [i](#)

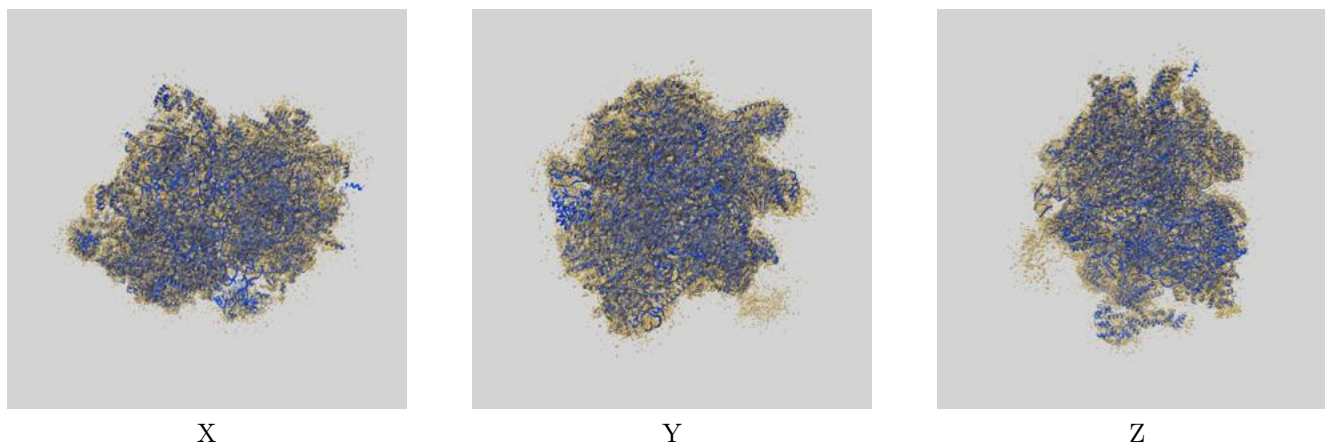
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.33	-	-
Author-provided FSC curve	4.30	6.52	4.46
Unmasked-calculated*	6.86	10.00	7.11

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.86 differs from the reported value 4.33 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11642 and PDB model 7A5G. Per-residue inclusion information can be found in section 3 on page 25.

9.1 Map-model overlay [i](#)

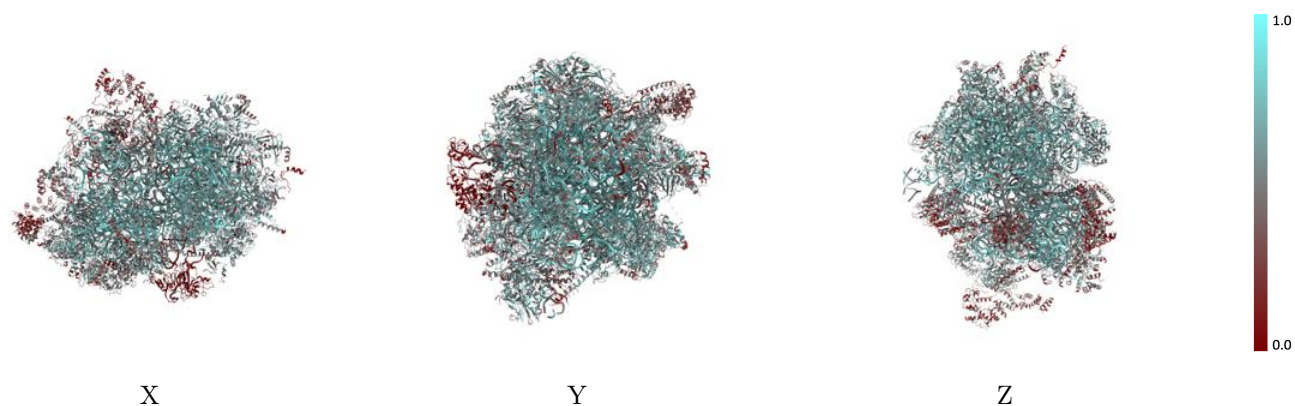


The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

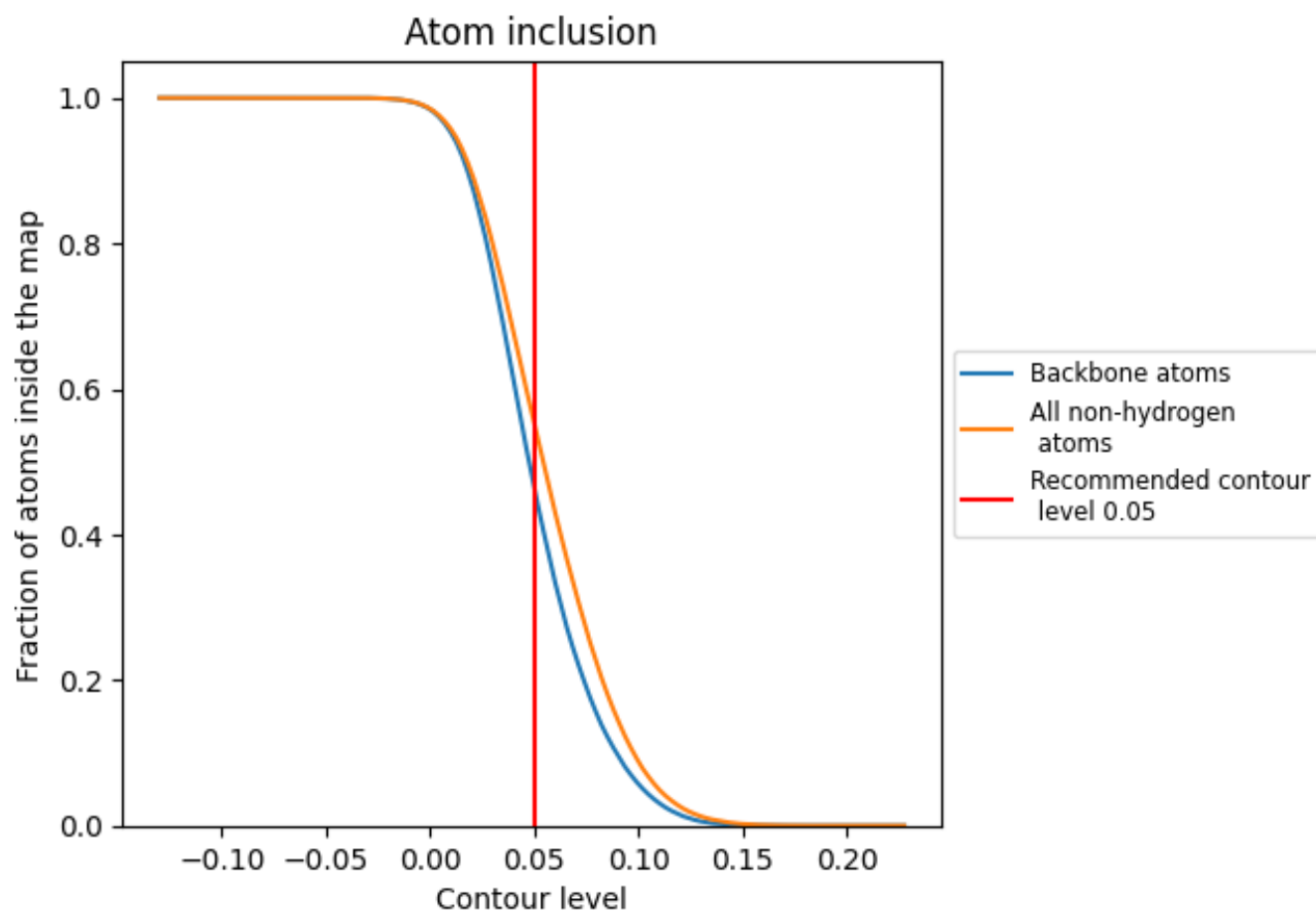
This section was not generated.

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 (0.05).

9.4 Atom inclusion [i](#)



At the recommended contour level, 46% of all backbone atoms, 55% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion
All	0.5527
03	0.5487
13	0.4952
23	0.6639
24	0.4215
33	0.6316
43	0.6678
53	0.5785
63	0.5605
73	0.5005
93	0.5612
A	0.2905
A3	0.7372
A5	0.0000
A6	0.7376
B3	0.6541
B6	0.6168
C	0.0407
C6	0.5480
D	0.1034
D3	0.6269
D6	0.5016
E3	0.6030
E6	0.5291
F3	0.5864
F6	0.4726
G6	0.5027
H3	0.4604
H6	0.5138
I3	0.3612
I6	0.5337
J3	0.2252
J6	0.4908
K3	0.6192
K6	0.5968





















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Chain	Atom inclusion
L3	0.5081
L6	0.5529
M3	0.5748
M6	0.4787
N3	0.5644
N6	0.5369
O3	0.5875
O6	0.4858
P3	0.5929
P6	0.5598
Q3	0.5099
Q6	0.5497
R3	0.6200
R6	0.4356
S3	0.6211
S6	0.4822
T3	0.5787
T6	0.5498
U3	0.6002
U6	0.4533
V3	0.5023
V6	0.2740
W3	0.6357
W6	0.5441
X3	0.5289
X6	0.4636
Y2	0.1655
Y3	0.6020
Y6	0.4292
Z	0.2599
Z3	0.6354
Z6	0.4680
a3	0.5910
a6	0.3910
b3	0.6019
b6	0.4347
c3	0.5343
c6	0.4145
d3	0.4947
d6	0.5447
e3	0.3235
e6	0.2885

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Chain	Atom inclusion
f3	 0.4556
g3	 0.5768
h3	 0.4745
i3	 0.6101
i4	 0.6713
j	 0.4653
j3	 0.5779
k3	 0.3261
l3	 0.5388
m3	 0.4901
n	 0.0512
o3	 0.6435
p3	 0.4579
q3	 0.4913
r3	 0.6454
s3	 0.5801
t3	 0.2071
u3	 0.1905