Full wwPDB EM Validation Report ⓘ

Oct 13, 2024 – 07:33 am BST

PDB ID	:	7A5F
EMDB ID	:	EMD-11641
Title	:	Structure of the stalled human mitoribosome with P- and E-site mt-tRNAs
Authors	:	Desai, N.; Yang, H.; Chandrasekaran, V.; Kazi, R.; Minczuk, M.; Ramakrishnan, V.
Deposited on	:	2020-08-21
Resolution	:	4.40 Å(reported)

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

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

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

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

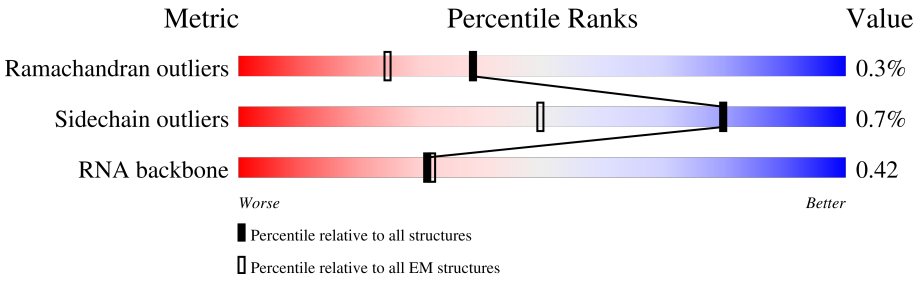
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	93% 97% ·
2	A3	1559	6% 64% 29% · ·
3	B3	69	12% 52% 28% · 19%
4	D3	305	12% 77% · 23%
5	E3	348	12% 84% · 14%
6	F3	311	15% 79% · 20%
7	D	267	26% 30% 70%
7	H3	267	18% 34% · 64%

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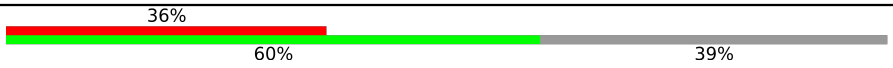
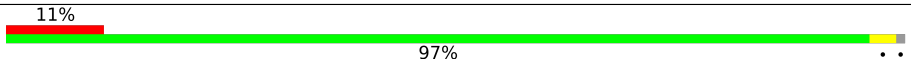
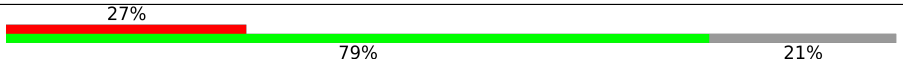
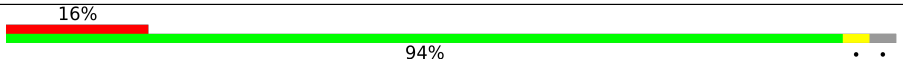
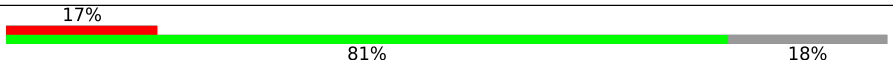
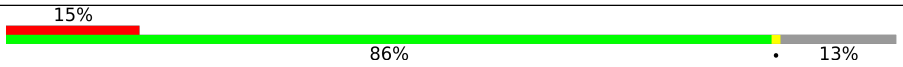
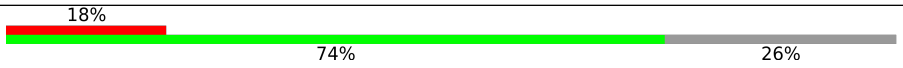
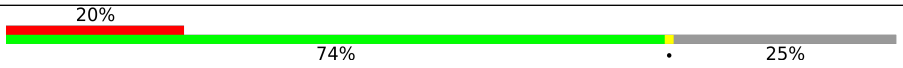
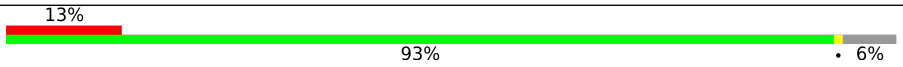
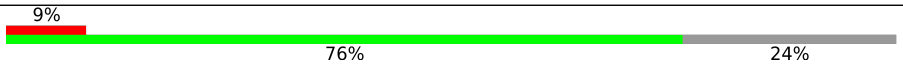
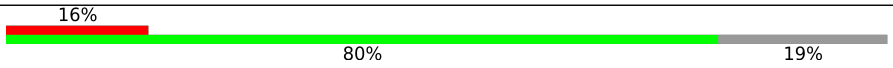
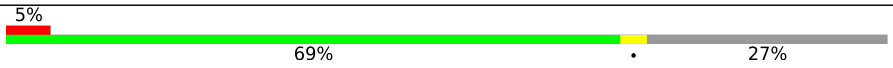
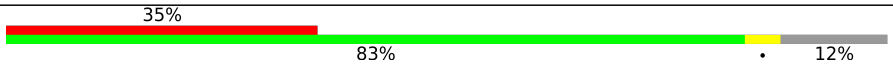
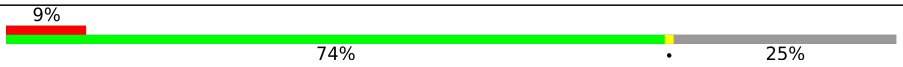
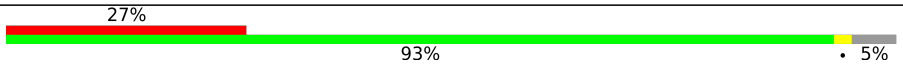
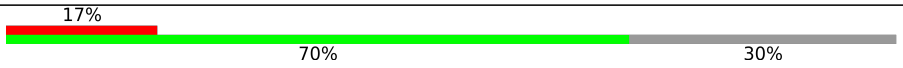
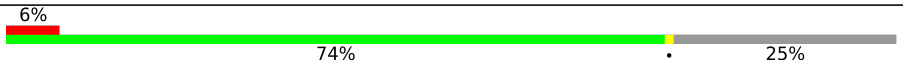
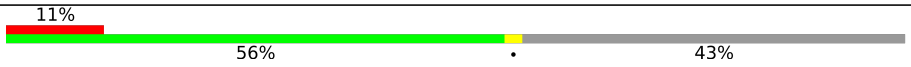
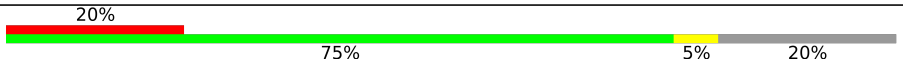
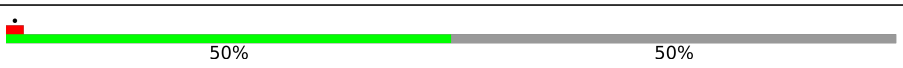
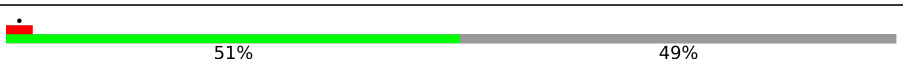
Mol	Chain	Length	Quality of chain
8	I3	261	
9	J3	192	
10	K3	178	
11	L3	145	
12	M3	296	
13	N3	251	
14	O3	175	
15	P3	180	
16	Q3	292	
17	R3	149	
18	S3	205	
19	T3	206	
20	U3	153	
21	V3	216	
22	W3	148	
23	X3	256	
24	Y3	250	
25	Z3	161	
26	03	188	
27	13	65	
28	23	92	
29	33	188	
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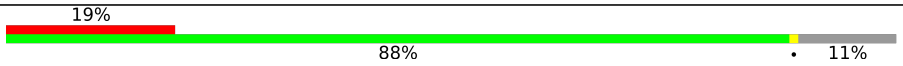
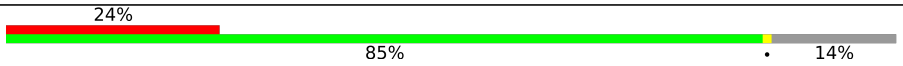
31	53	423	
32	63	380	

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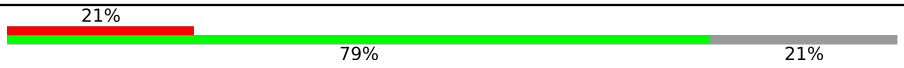
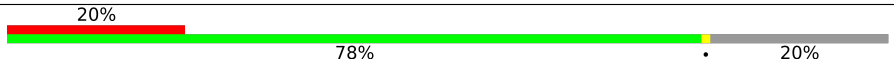
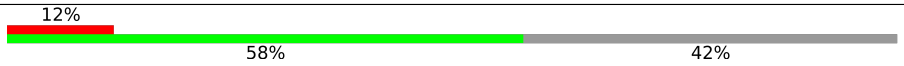
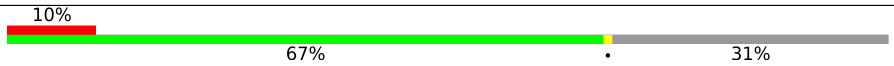
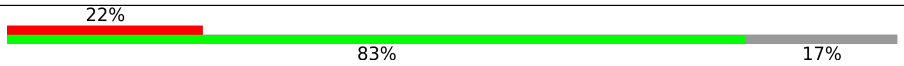
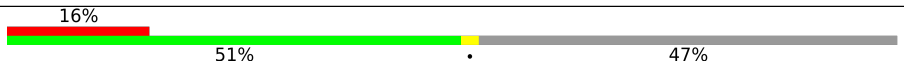
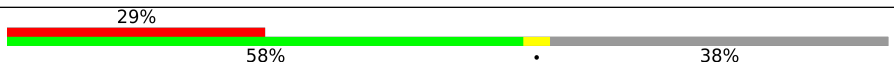
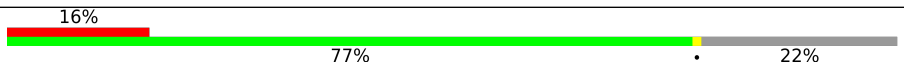
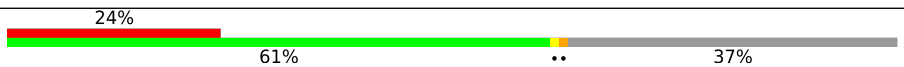
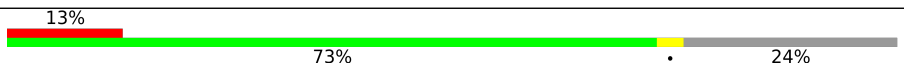
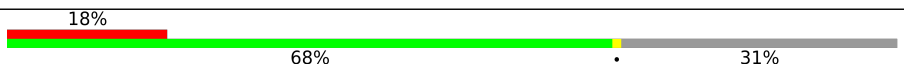
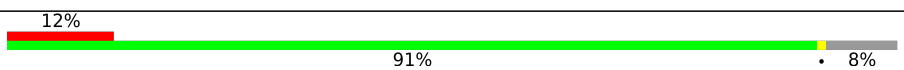
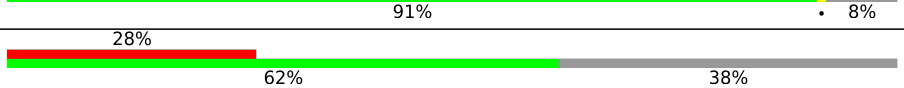
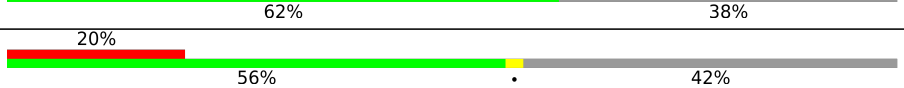
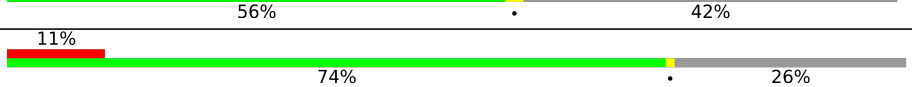
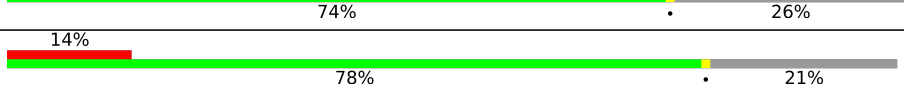
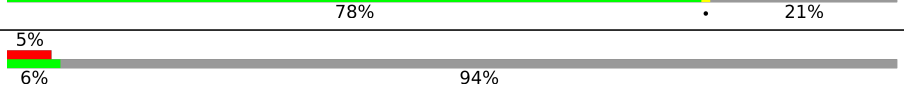
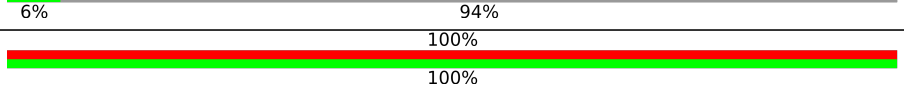
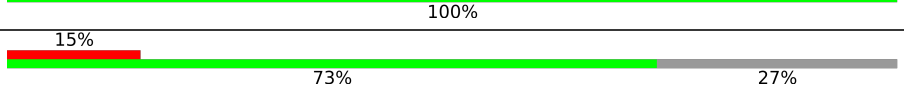
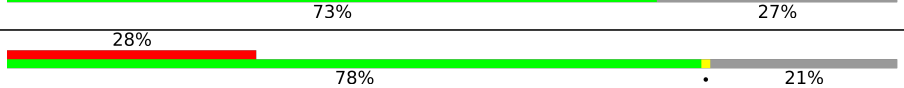
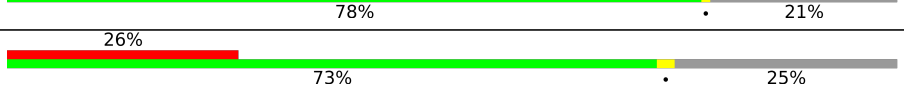
Mol	Chain	Length	Quality of chain
33	73	338	
34	93	137	
35	a3	142	
36	b3	215	
37	c3	332	
38	d3	306	
39	e3	279	
40	f3	212	
41	g3	166	
42	h3	158	
43	i3	128	
44	j3	123	
45	k3	112	
46	l3	138	
47	m3	128	
48	o3	102	
49	p3	206	
50	q3	222	
51	r3	196	
52	s3	467	
52	t3	467	
53	A5	28	
54	B6	296	
55	C6	167	
56	D6	430	

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Mol	Chain	Length	Quality of chain
57	E6	125	33% 96%
58	F6	242	37% 82% 17%
59	G6	396	26% 76% 23%
60	H6	201	27% 60% 39%
61	I6	194	22% 69% 30%
62	J6	138	25% 77% 22%
63	K6	128	26% 78% 21%
64	L6	257	18% 64% 36%
65	M6	137	32% 84% 15%
66	N6	130	25% 82% 18%
67	O6	258	28% 71% 28%
68	P6	142	15% 68% 32%
69	Q6	87	24% 99%
70	R6	360	31% 66% 33%
71	S6	190	27% 66% 34%
72	T6	173	29% 94% 6%
73	U6	205	36% 84% 16%
74	V6	414	60% 78% 21%
75	W6	187	17% 51% 48%
76	X6	398	39% 78% 21%
77	Y6	395	16% 27% 73%
78	Z6	106	34% 82% 18%
79	a6	218	52% 91% 8%
80	b6	323	42% 79% 21%
81	c6	118	39% 95%

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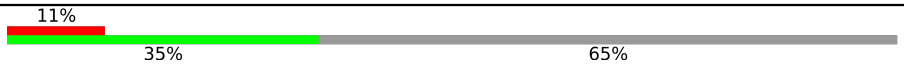
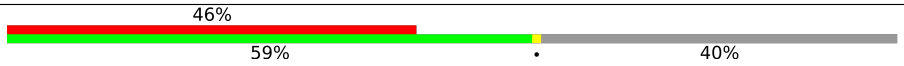
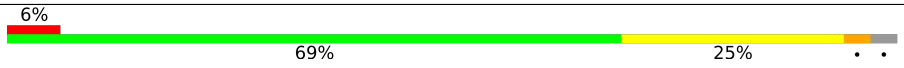
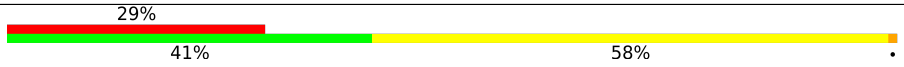
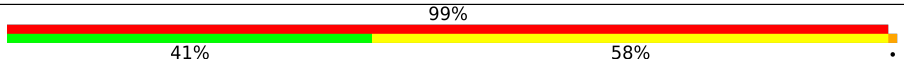
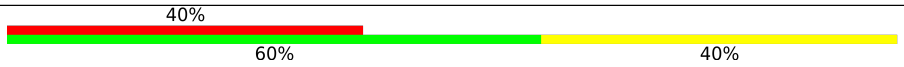
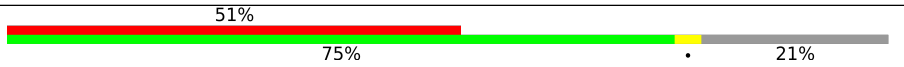
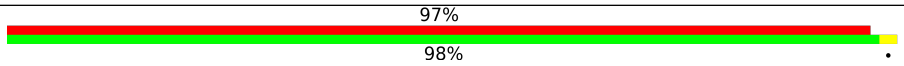
Mol	Chain	Length	Quality of chain
82	d6	199	
83	e6	689	
84	A6	954	
85	24	73	
85	C	73	
86	i4	10	
87	A	206	
88	n	229	

2 Entry composition

There are 96 unique types of molecules in this entry. The entry contains 165767 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-tRNA Val.

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
13	N3	205	Total	C	N	O	S	0	0
			1654	1056	308	280	10		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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
24	Y3	176	Total	C	N	O	S	0	0
			1517	970	291	252	4		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 53 is a protein called Oxa1L.

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

- Molecule 54 is a protein called 28S ribosomal protein S2, mitochondrial.

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

- Molecule 55 is a protein called 28S ribosomal protein S24, mitochondrial.

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

- Molecule 56 is a protein called 28S ribosomal protein S5, mitochondrial.

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

- Molecule 57 is a protein called 28S ribosomal protein S6, mitochondrial.

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

- Molecule 58 is a protein called 28S ribosomal protein S7, mitochondrial.

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

- Molecule 59 is a protein called 28S ribosomal protein S9, mitochondrial.

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

- Molecule 60 is a protein called 28S ribosomal protein S10, mitochondrial.

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

- Molecule 61 is a protein called 28S ribosomal protein S11, mitochondrial.

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

- Molecule 62 is a protein called 28S ribosomal protein S12, mitochondrial.

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

- Molecule 63 is a protein called 28S ribosomal protein S14, mitochondrial.

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

- Molecule 64 is a protein called 28S ribosomal protein S15, mitochondrial.

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

- Molecule 65 is a protein called 28S ribosomal protein S16, mitochondrial.

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

- Molecule 66 is a protein called 28S ribosomal protein S17, mitochondrial.

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

- Molecule 67 is a protein called 28S ribosomal protein S18b, mitochondrial.

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

- Molecule 68 is a protein called 28S ribosomal protein S18c, mitochondrial.

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

- Molecule 69 is a protein called 28S ribosomal protein S21, mitochondrial.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 70 is a protein called 28S ribosomal protein S22, mitochondrial.

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

- Molecule 71 is a protein called 28S ribosomal protein S23, mitochondrial.

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

- Molecule 72 is a protein called 28S ribosomal protein S25, mitochondrial.

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

- Molecule 73 is a protein called 28S ribosomal protein S26, mitochondrial.

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

- Molecule 74 is a protein called 28S ribosomal protein S27, mitochondrial.

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

- Molecule 75 is a protein called 28S ribosomal protein S28, mitochondrial.

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

- Molecule 76 is a protein called 28S ribosomal protein S29, mitochondrial.

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

- Molecule 77 is a protein called 28S ribosomal protein S31, mitochondrial.

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

- Molecule 78 is a protein called 28S ribosomal protein S33, mitochondrial.

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

- Molecule 79 is a protein called 28S ribosomal protein S34, mitochondrial.

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

- Molecule 80 is a protein called 28S ribosomal protein S35, mitochondrial.

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

- Molecule 81 is a protein called Coiled-coil-helix-coiled-coil-helix domain-containing protein 1.

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

- Molecule 82 is a protein called Aurora kinase A-interacting protein.

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

- Molecule 83 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

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

- Molecule 84 is a RNA chain called 12S rRNA.

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

- Molecule 85 is a RNA chain called mt-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	24	73	Total	C	N	O	P	0	0
			1547	696	280	499	72		
85	C	73	Total	C	N	O	P	0	0
			1547	696	280	499	72		

- Molecule 86 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	i4	10	Total	C	N	O	P	0	0
			219	99	47	63	10		

- Molecule 87 is a protein called 39S ribosomal protein L40, mitochondrial.

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

- Molecule 88 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
88	n	228	Total 1766	C 1121	N 321	O 321	S 3	4	0

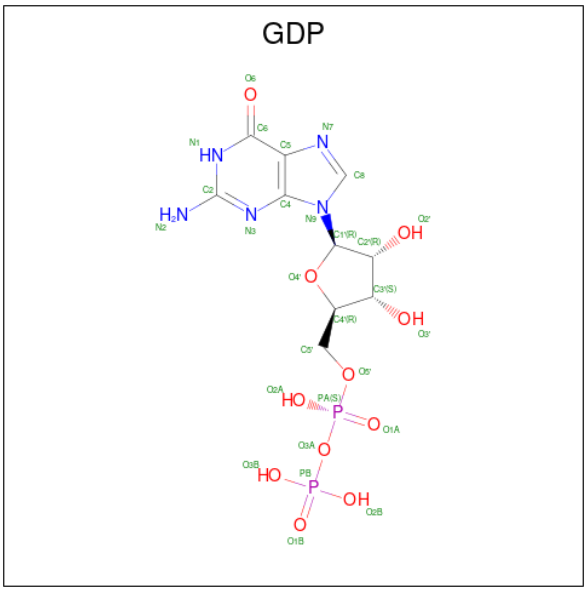
- Molecule 89 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
89	A3	97	Total 97	Mg 97	0
89	D3	1	Total 1	Mg 1	0
89	g3	1	Total 1	Mg 1	0
89	A6	28	Total 28	Mg 28	0
89	n	1	Total 1	Mg 1	0

- Molecule 90 is ZINC ION (three-letter code: ZN) (formula: Zn).

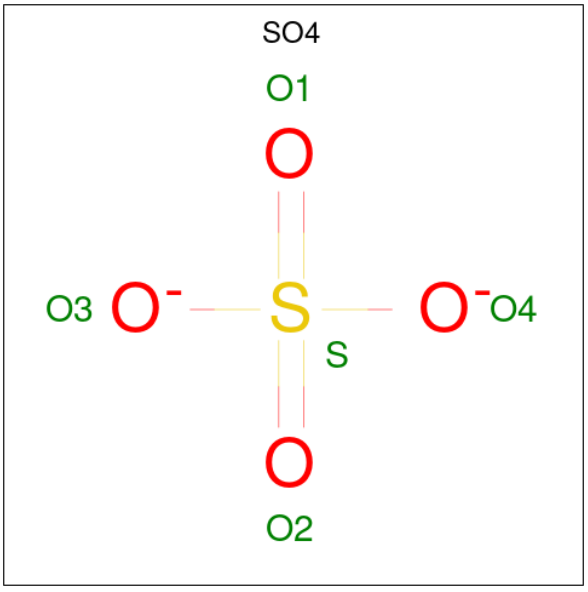
Mol	Chain	Residues	Atoms		AltConf
90	03	1	Total 1	Zn 1	0
90	43	1	Total 1	Zn 1	0
90	r3	1	Total 1	Zn 1	0
90	B6	1	Total 1	Zn 1	0
90	O6	1	Total 1	Zn 1	0
90	P6	1	Total 1	Zn 1	0
90	T6	1	Total 1	Zn 1	0

- Molecule 91 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



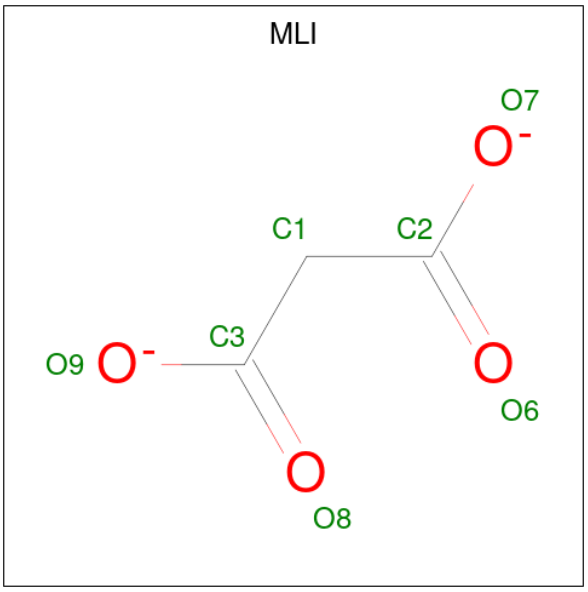
Mol	Chain	Residues	Atoms					AltConf
91	X6	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 92 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 93 is MALONATE ION (three-letter code: MLI) (formula: $C_3H_2O_4$).



Mol	Chain	Residues	Atoms	AltConf
93	n	1	Total C O 7 3 4	0
93	n	1	Total C O 7 3 4	0
93	n	1	Total C O 7 3 4	0

- Molecule 94 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 95 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 96 is water.

Mol	Chain	Residues	Atoms	AltConf
96	A3	4	Total O 4 4	0

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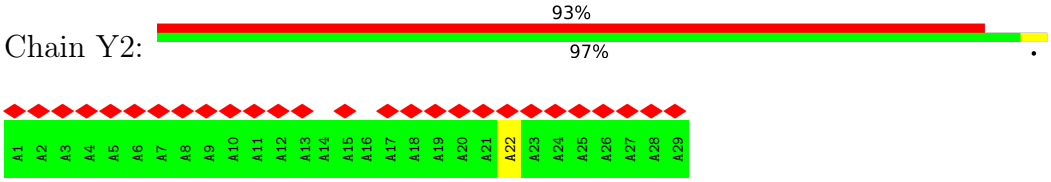
Mol	Chain	Residues	Atoms	AltConf
96	n	67	Total O 67 67	0
96	D	8	Total O 8 8	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

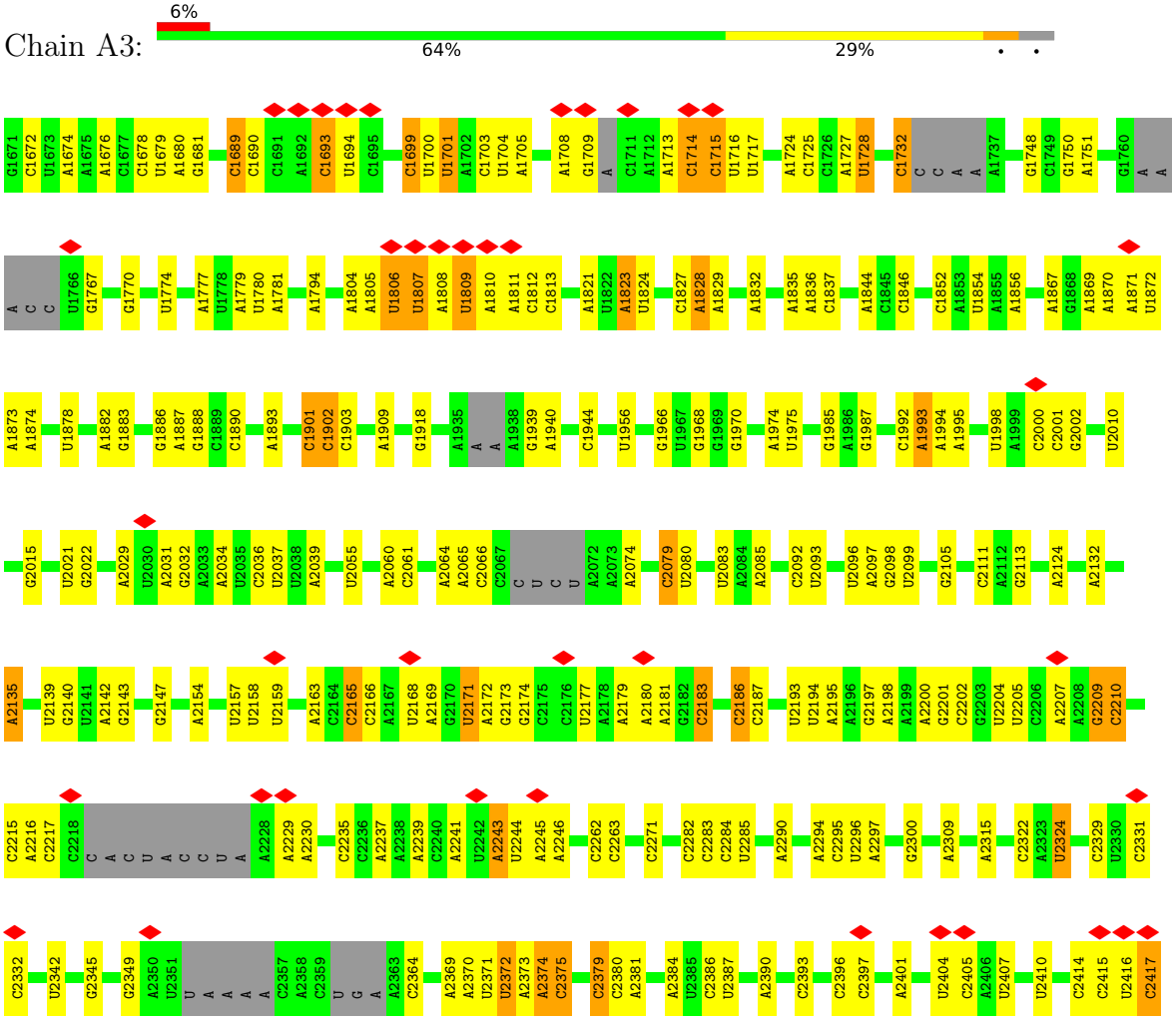
• Molecule 1: nascent chain

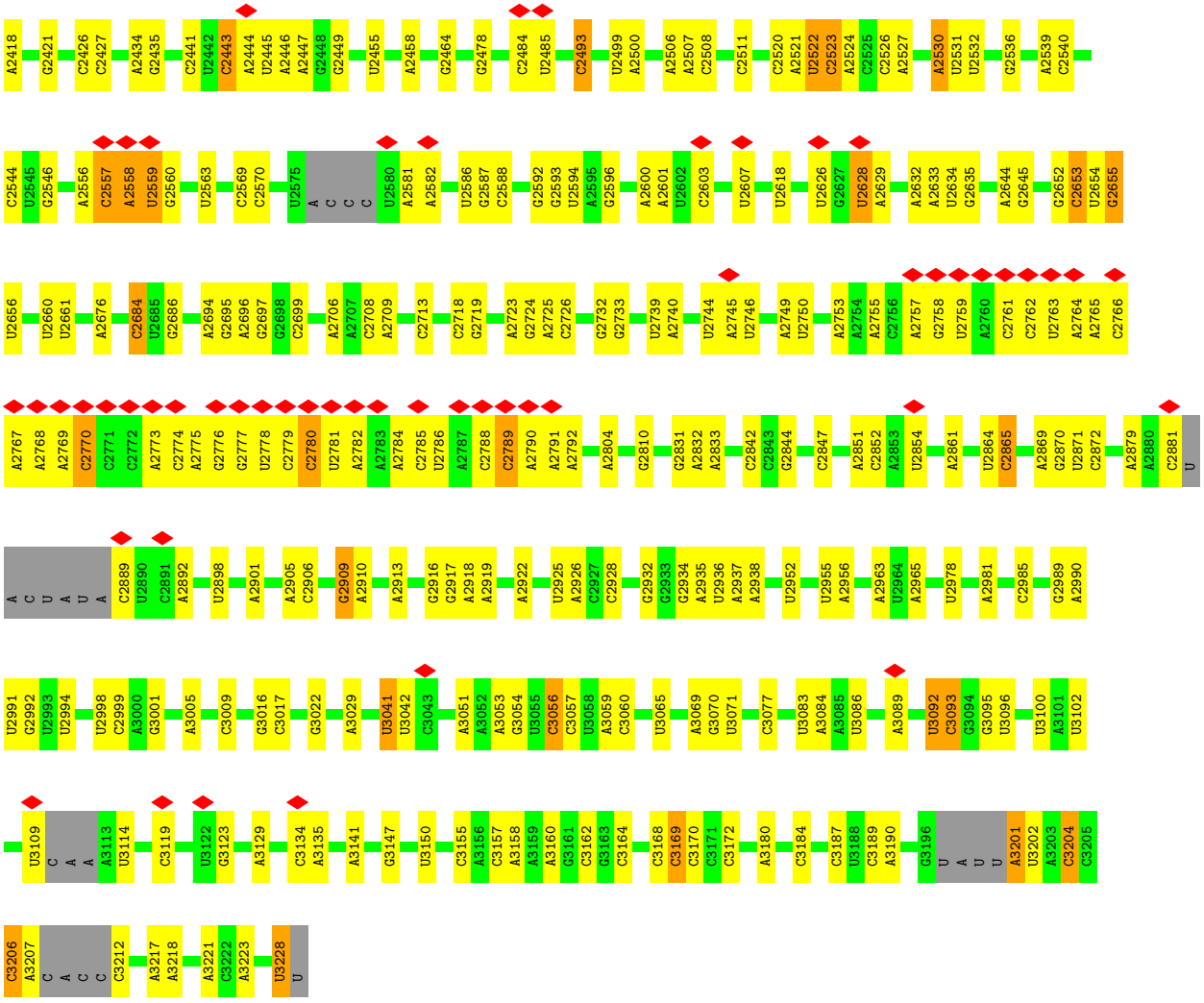
Chain Y2:



• Molecule 2: 16S rRNA

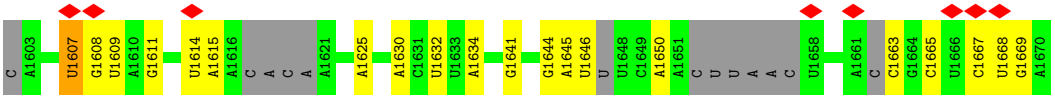
Chain A3:





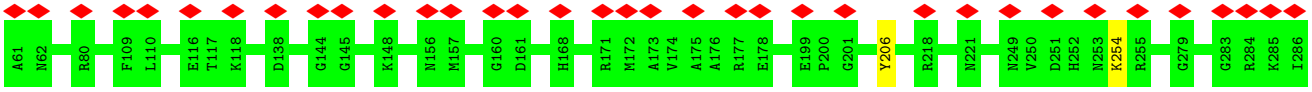
• Molecule 3: mt-tRNA Val

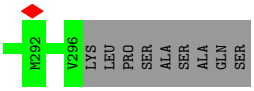
Chain B3:



• Molecule 4: 39S ribosomal protein L2, mitochondrial

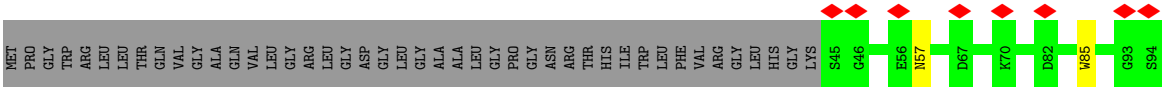
Chain D3:

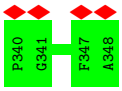




• Molecule 5: 39S ribosomal protein L3, mitochondrial

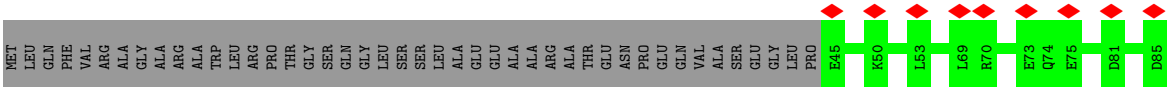
Chain E3:

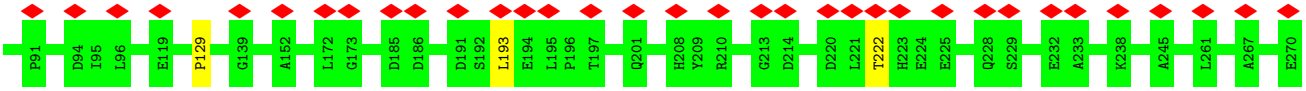


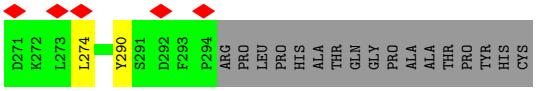


• Molecule 6: 39S ribosomal protein L4, mitochondrial

Chain F3:

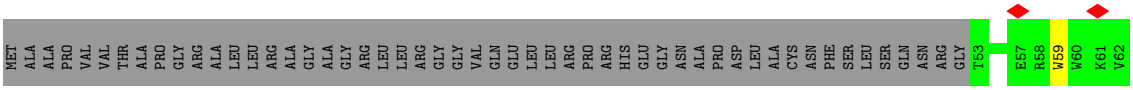


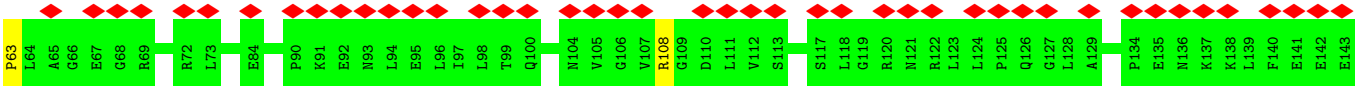


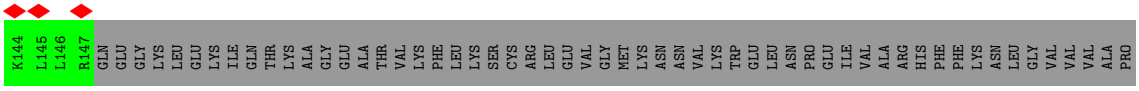


• Molecule 7: 39S ribosomal protein L9, mitochondrial

Chain H3:

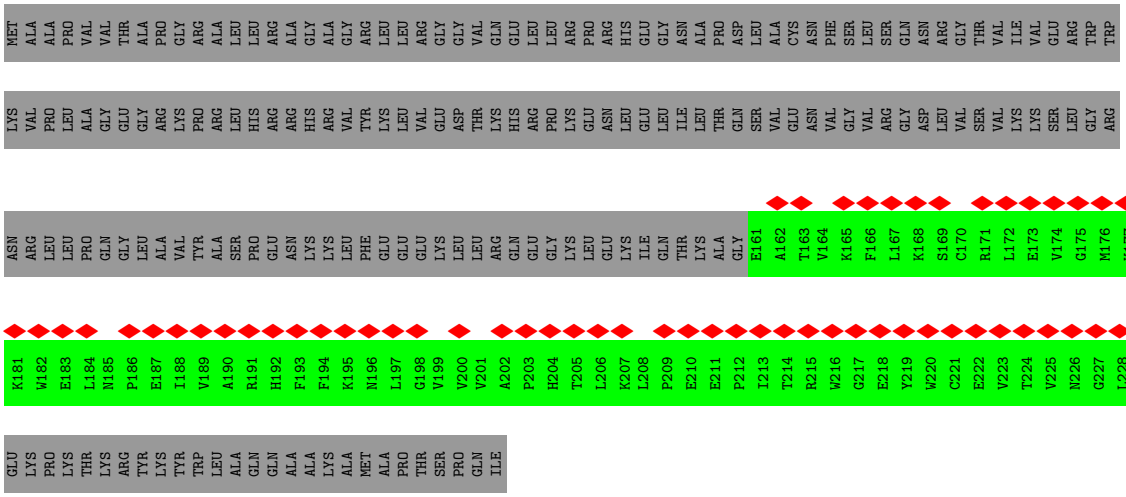






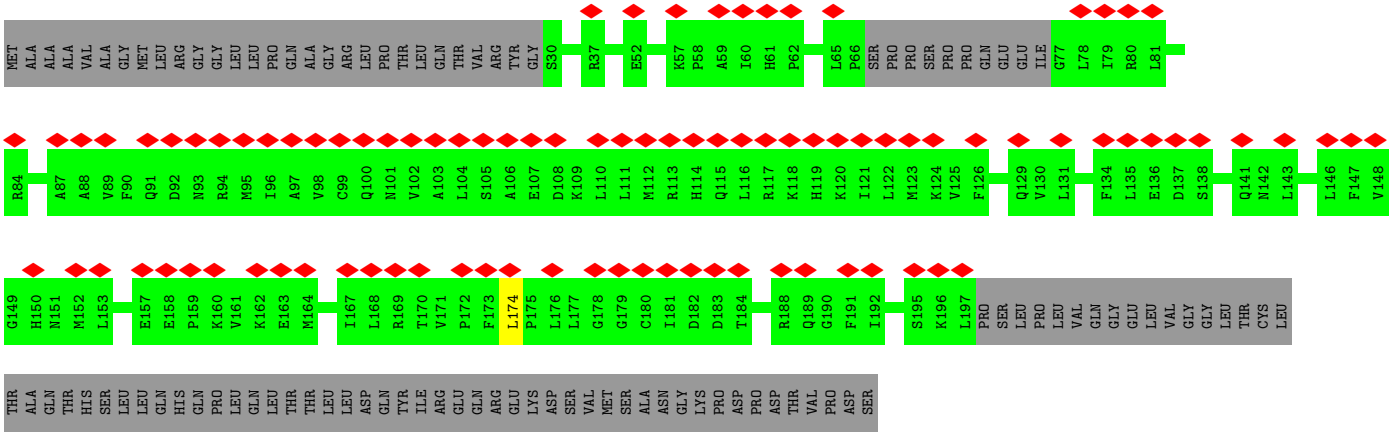
• Molecule 7: 39S ribosomal protein L9, mitochondrial

Chain D:



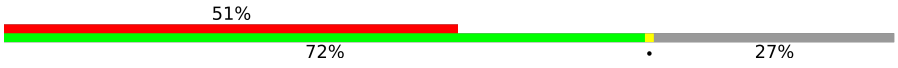
• Molecule 8: 39S ribosomal protein L10, mitochondrial

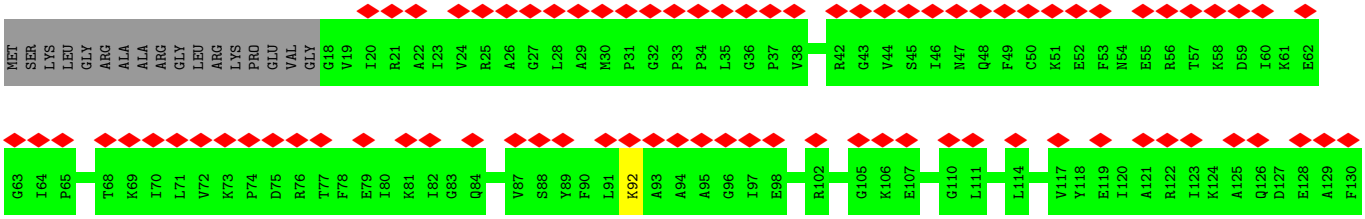
Chain I3:

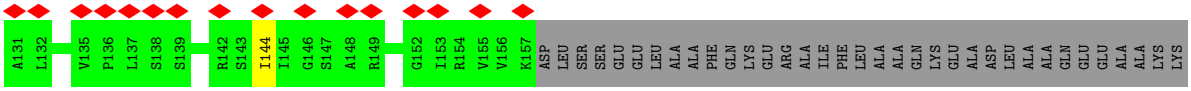


• Molecule 9: 39S ribosomal protein L11, mitochondrial

Chain J3:

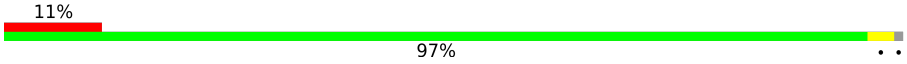


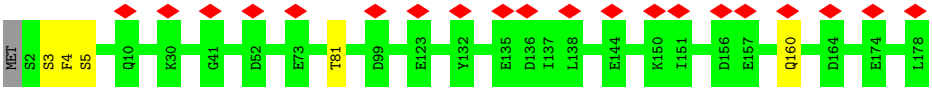




• Molecule 10: 39S ribosomal protein L13, mitochondrial

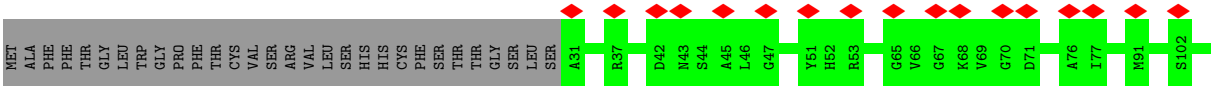
Chain K3:

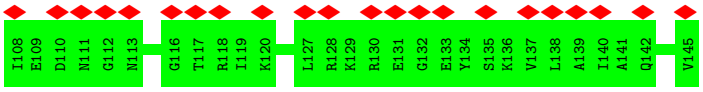




• Molecule 11: 39S ribosomal protein L14, mitochondrial

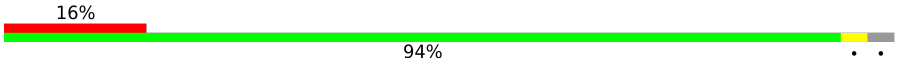
Chain L3:

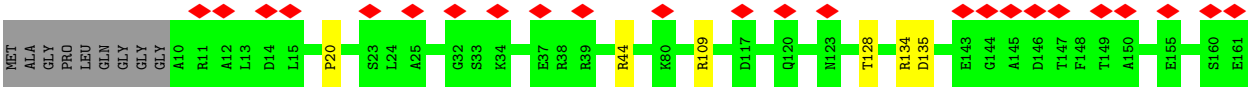


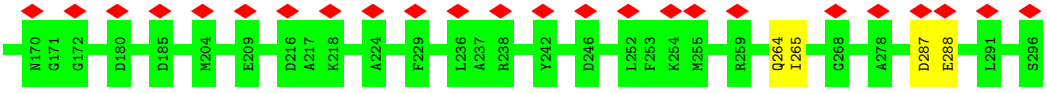


• Molecule 12: 39S ribosomal protein L15, mitochondrial

Chain M3:

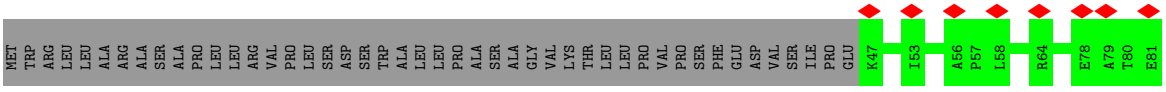


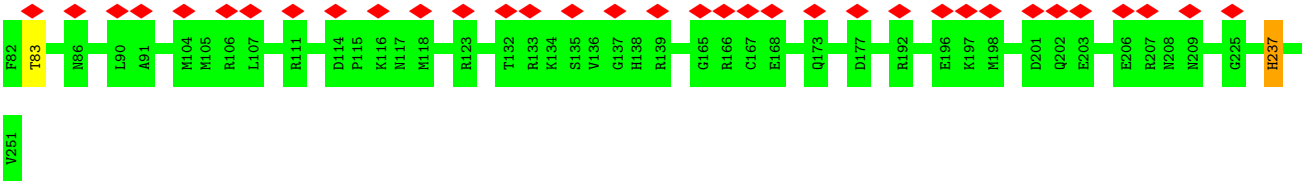




• Molecule 13: 39S ribosomal protein L16, mitochondrial

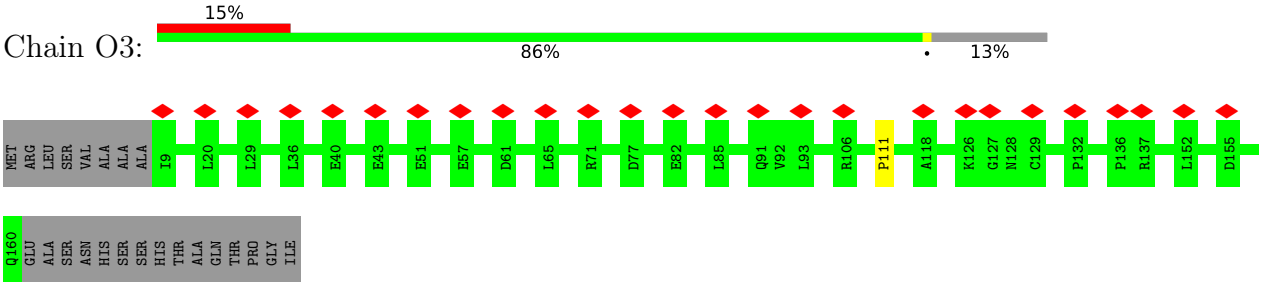
Chain N3:





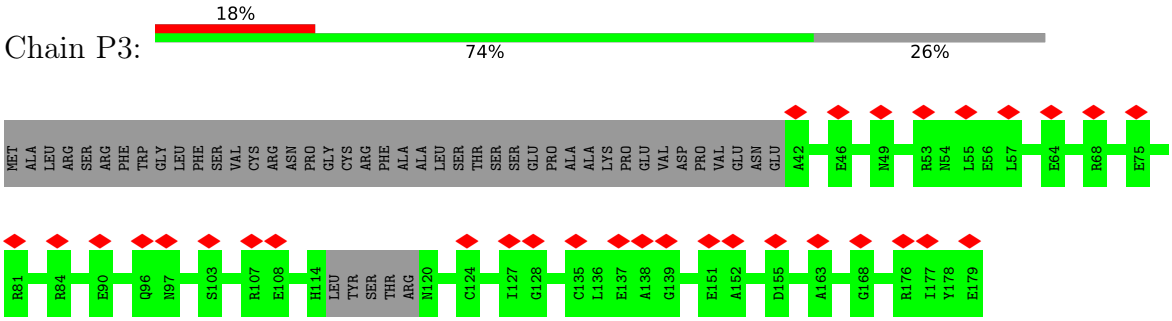
• Molecule 14: 39S ribosomal protein L17, mitochondrial

Chain O3:



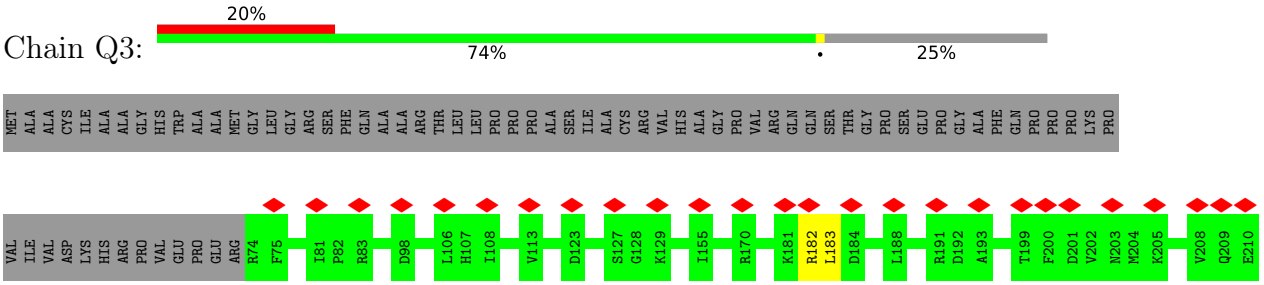
• Molecule 15: 39S ribosomal protein L18, mitochondrial

Chain P3:



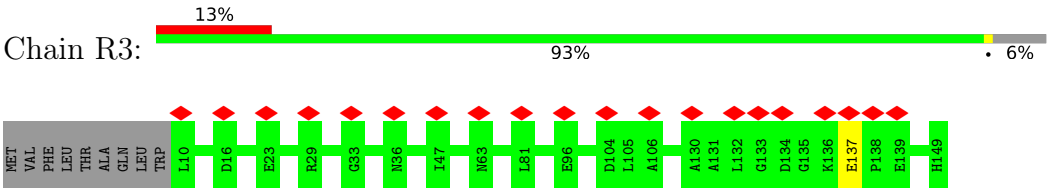
• Molecule 16: 39S ribosomal protein L19, mitochondrial

Chain Q3:



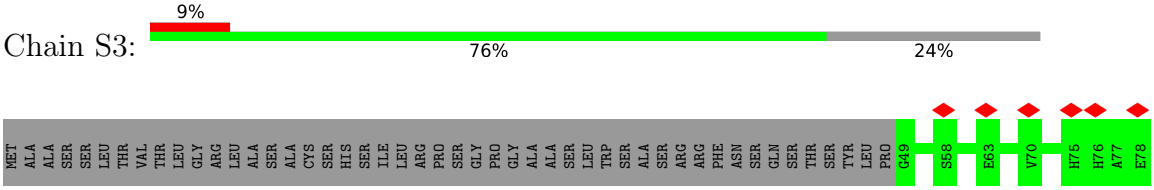
• Molecule 17: 39S ribosomal protein L20, mitochondrial

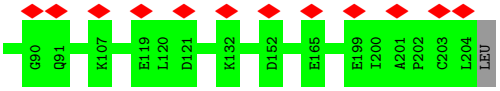
Chain R3:



• Molecule 18: 39S ribosomal protein L21, mitochondrial

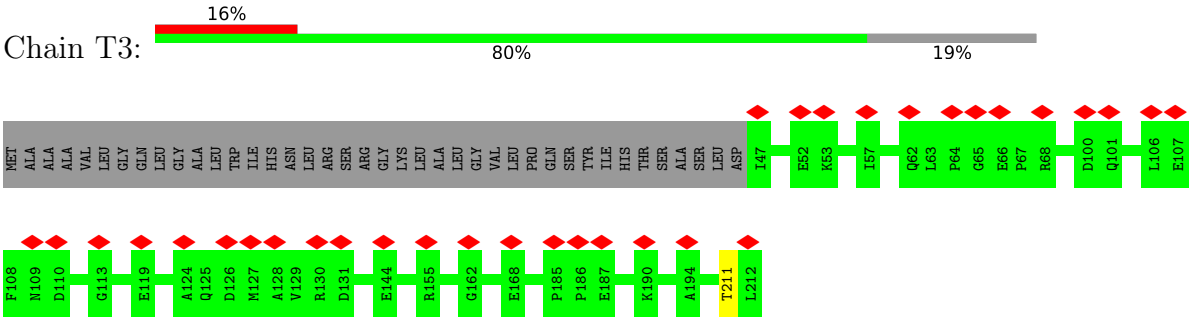
Chain S3:





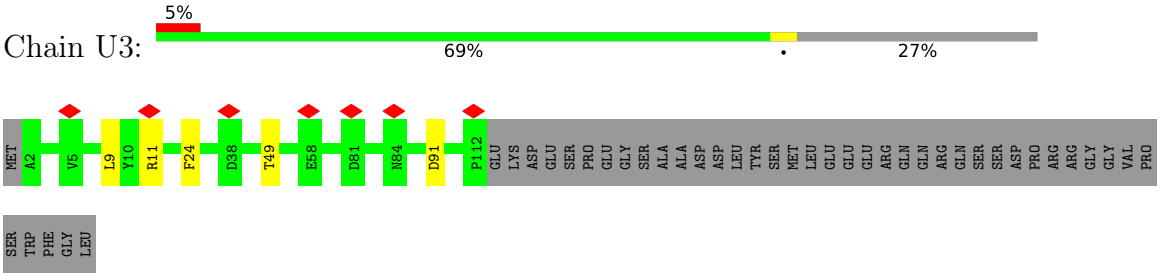
• Molecule 19: 39S ribosomal protein L22, mitochondrial

Chain T3:



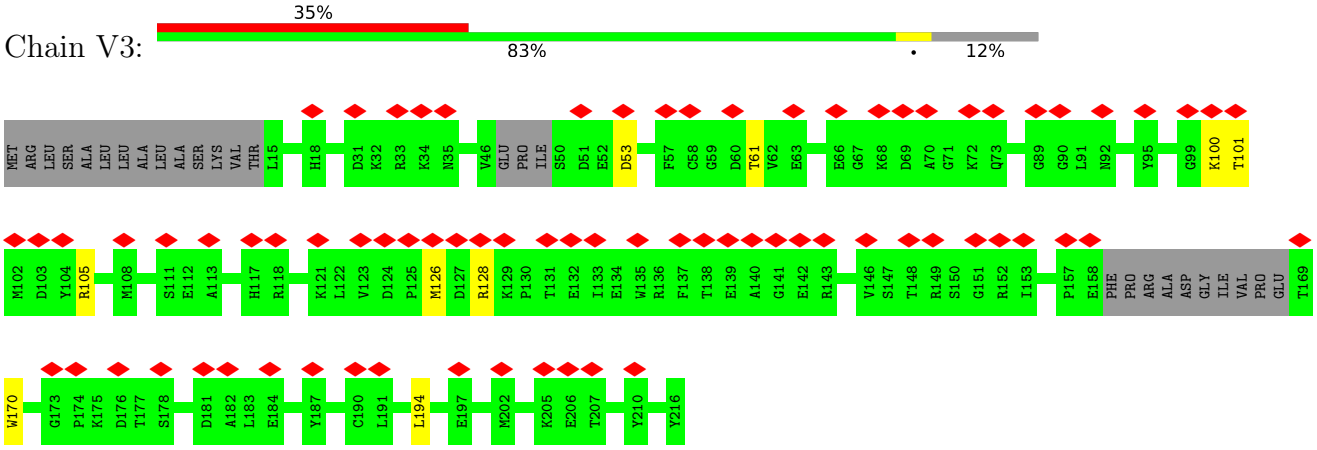
• Molecule 20: 39S ribosomal protein L23, mitochondrial

Chain U3:



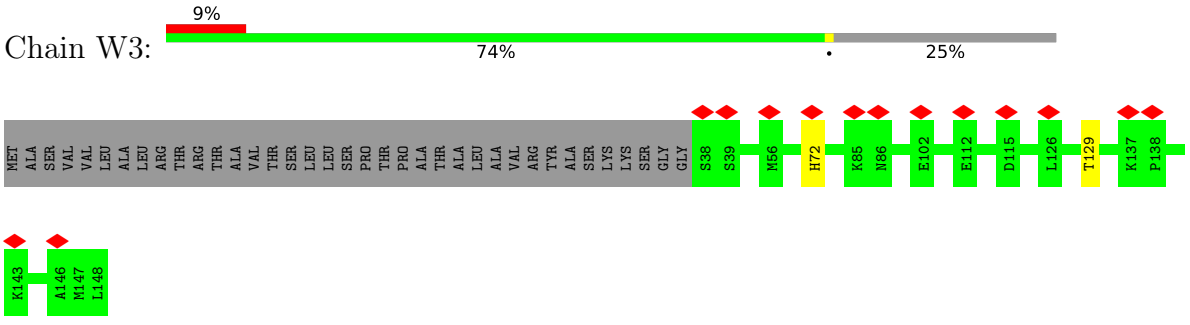
• Molecule 21: 39S ribosomal protein L24, mitochondrial

Chain V3:



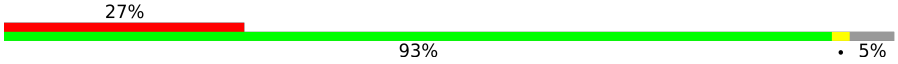
• Molecule 22: 39S ribosomal protein L27, mitochondrial

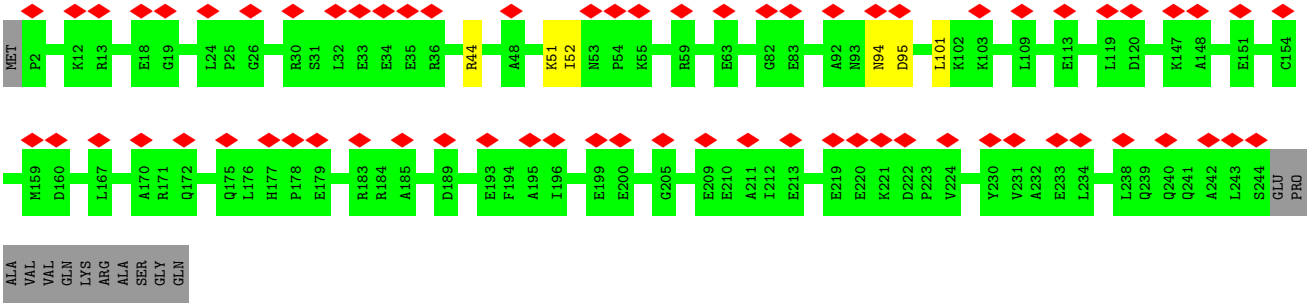
Chain W3:



• Molecule 23: 39S ribosomal protein L28, mitochondrial

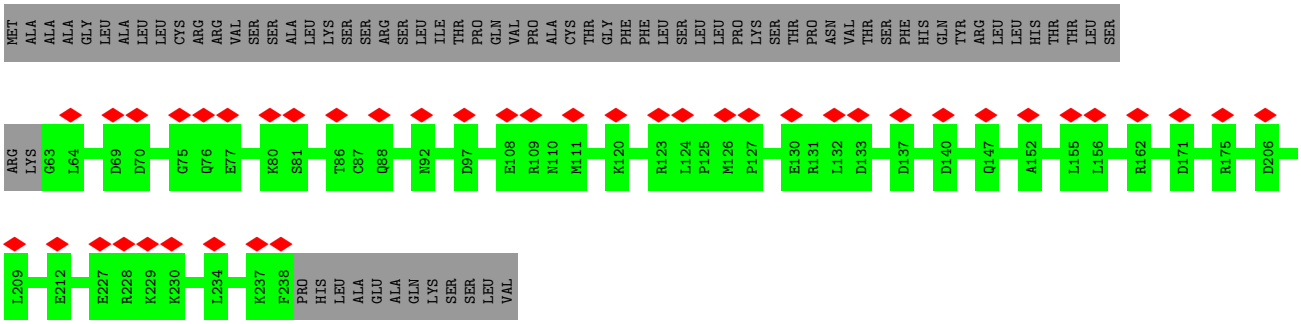
Chain X3:





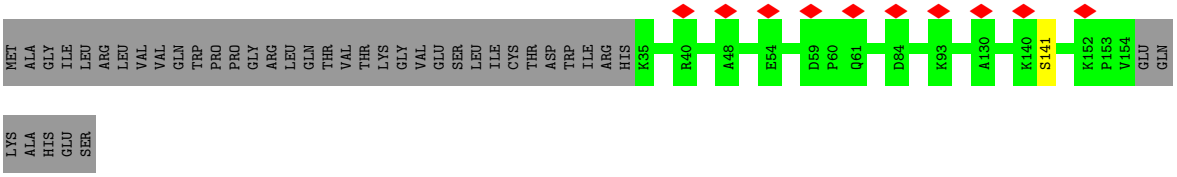
• Molecule 24: 39S ribosomal protein L47, mitochondrial

Chain Y3:



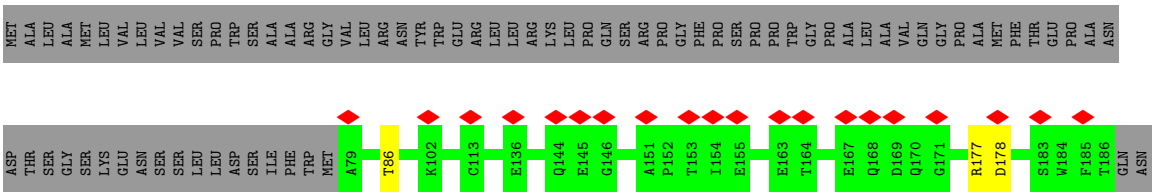
• Molecule 25: 39S ribosomal protein L30, mitochondrial

Chain Z3:



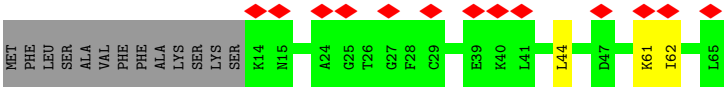
• Molecule 26: 39S ribosomal protein L32, mitochondrial

Chain 03:



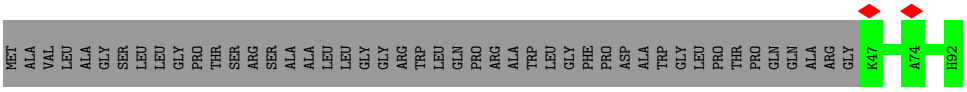
• Molecule 27: 39S ribosomal protein L33, mitochondrial

Chain 13:



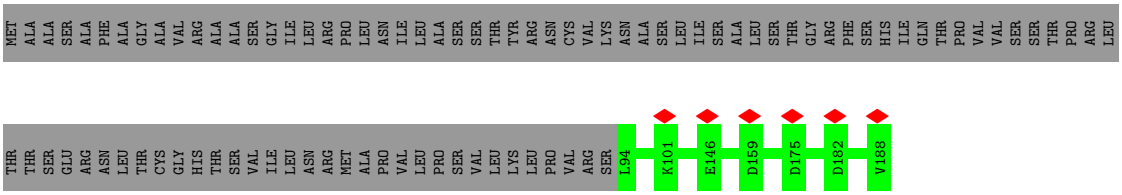
• Molecule 28: 39S ribosomal protein L34, mitochondrial

Chain 23:



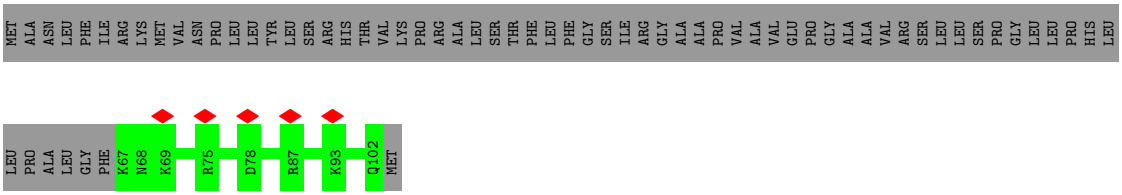
• Molecule 29: 39S ribosomal protein L35, mitochondrial

Chain 33:



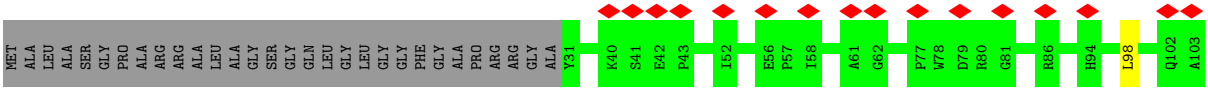
• Molecule 30: 39S ribosomal protein L36, mitochondrial

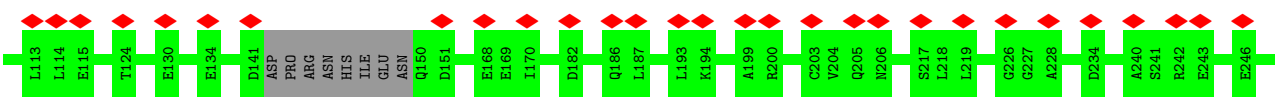
Chain 43:

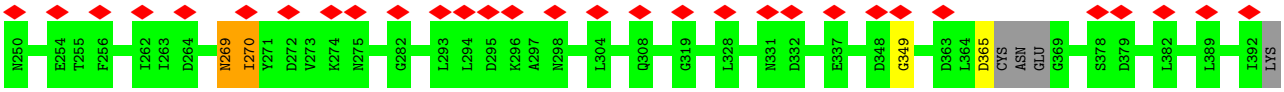


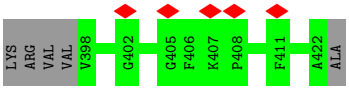
• Molecule 31: 39S ribosomal protein L37, mitochondrial

Chain 53:



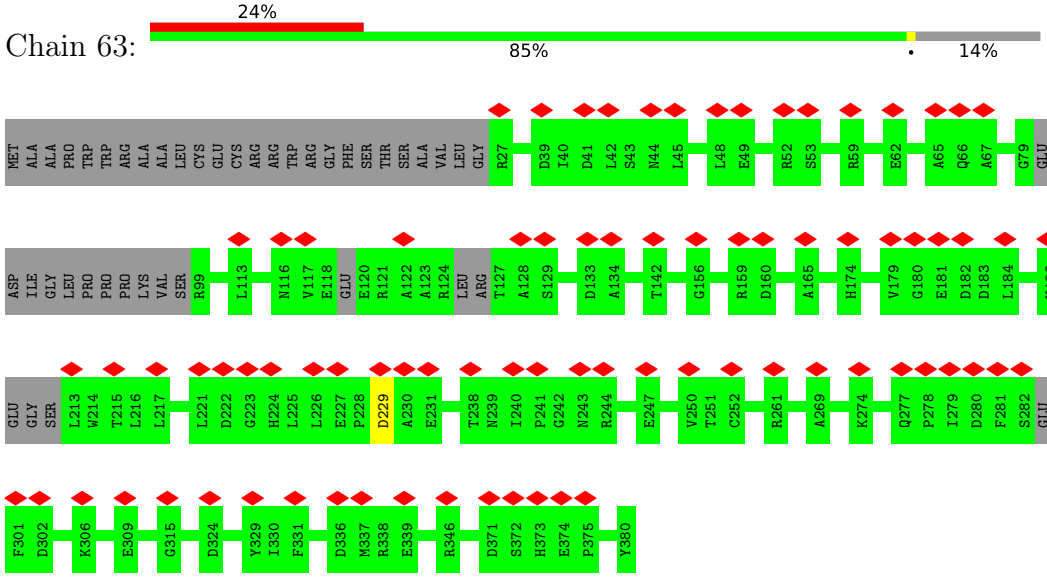






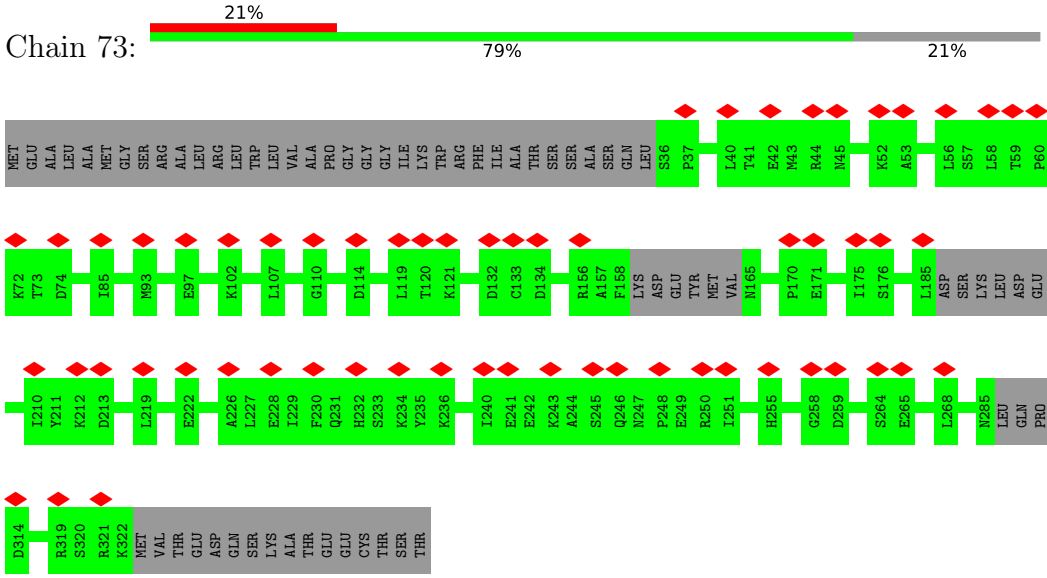
• Molecule 32: 39S ribosomal protein L38, mitochondrial

Chain 63:



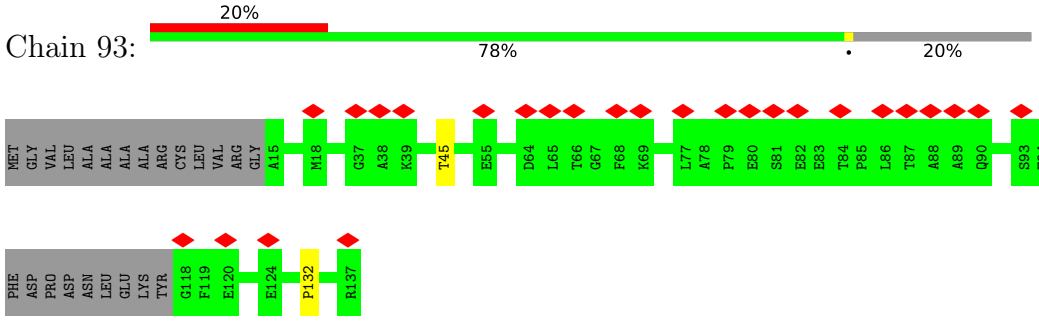
• Molecule 33: 39S ribosomal protein L39, mitochondrial

Chain 73:



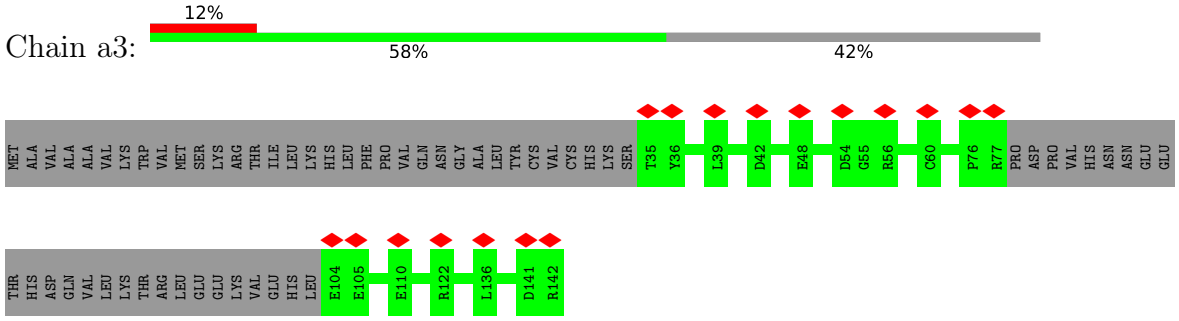
• Molecule 34: 39S ribosomal protein L41, mitochondrial

Chain 93:



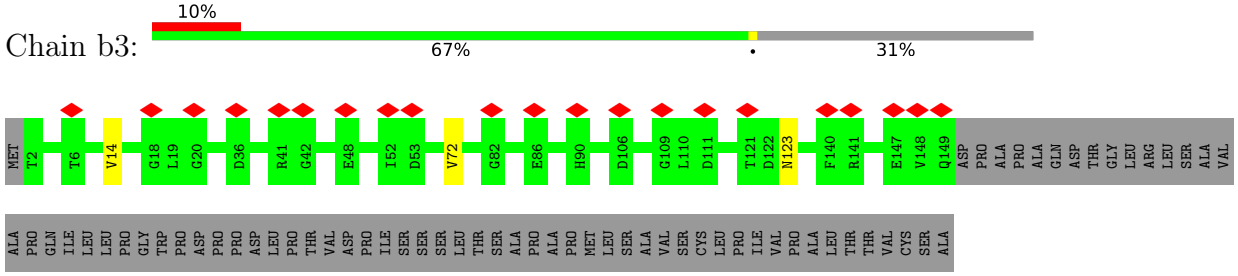
• Molecule 35: 39S ribosomal protein L42, mitochondrial

Chain a3:



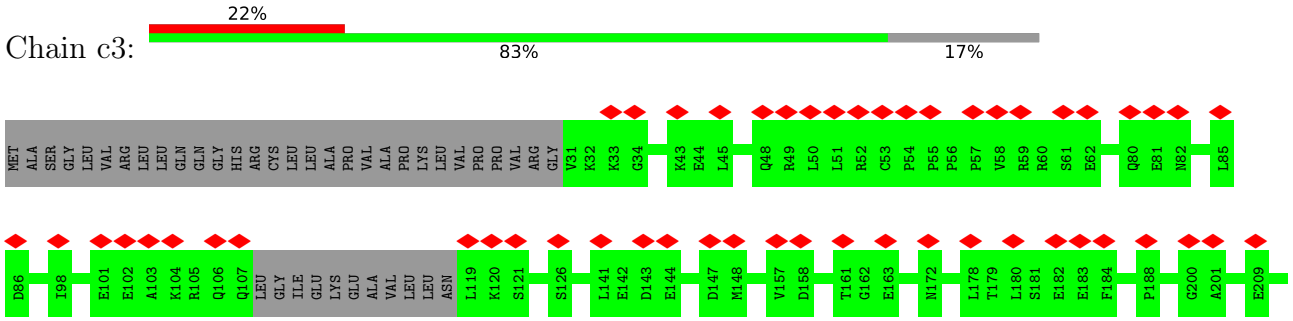
• Molecule 36: 39S ribosomal protein L43, mitochondrial

Chain b3:



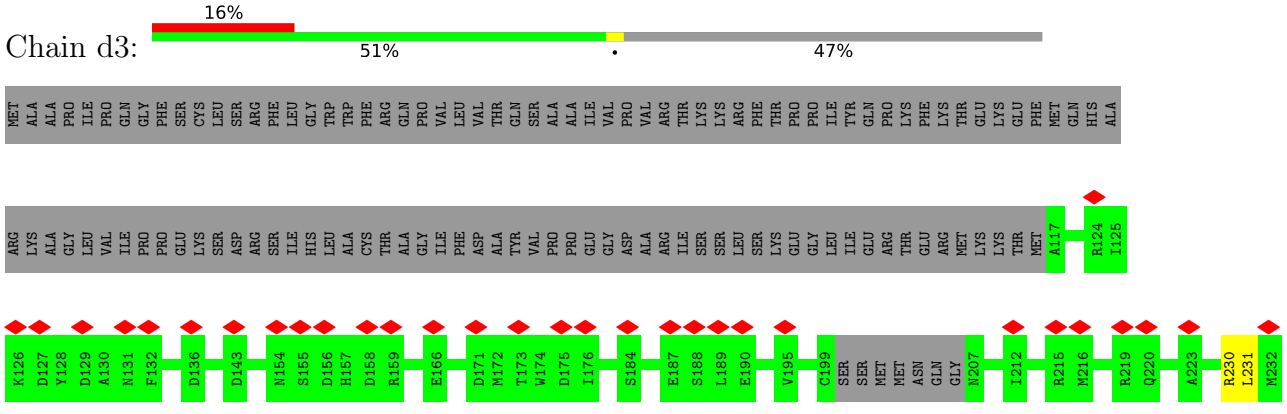
• Molecule 37: 39S ribosomal protein L44, mitochondrial

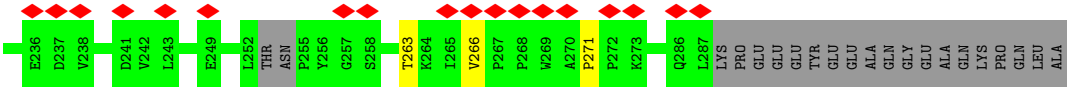
Chain c3:



• Molecule 38: 39S ribosomal protein L45, mitochondrial

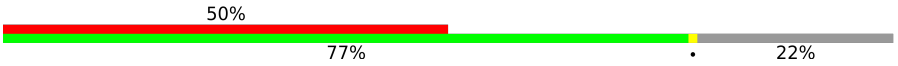
Chain d3:

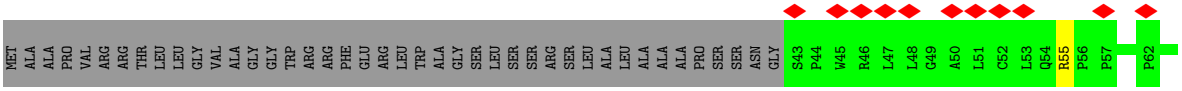


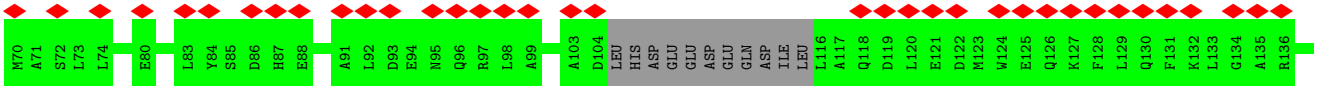


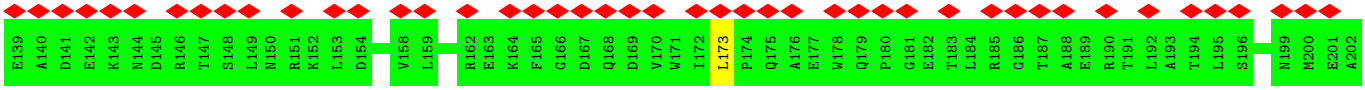
• Molecule 39: 39S ribosomal protein L46, mitochondrial

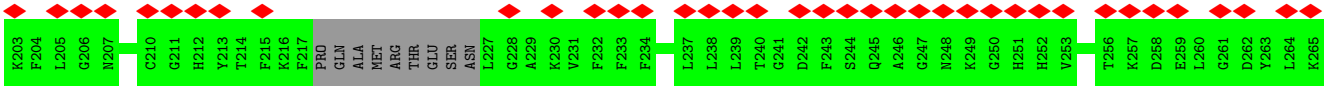
Chain e3:





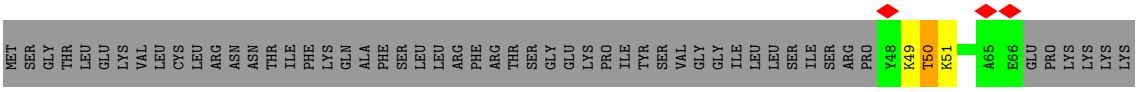


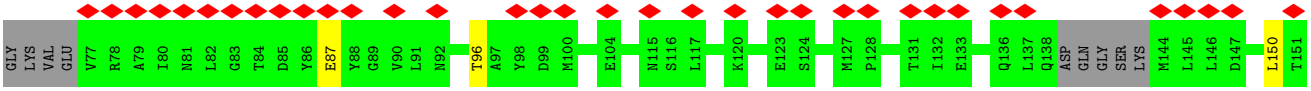


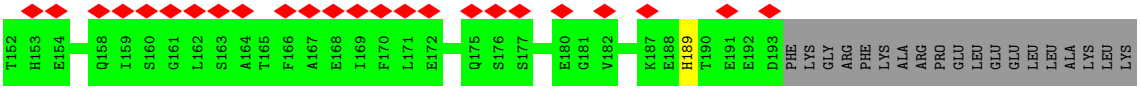


• Molecule 40: 39S ribosomal protein L48, mitochondrial

Chain f3:

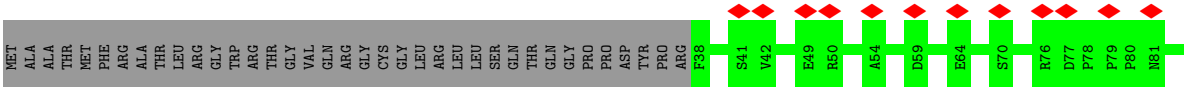


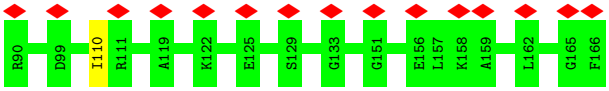




• Molecule 41: 39S ribosomal protein L49, mitochondrial

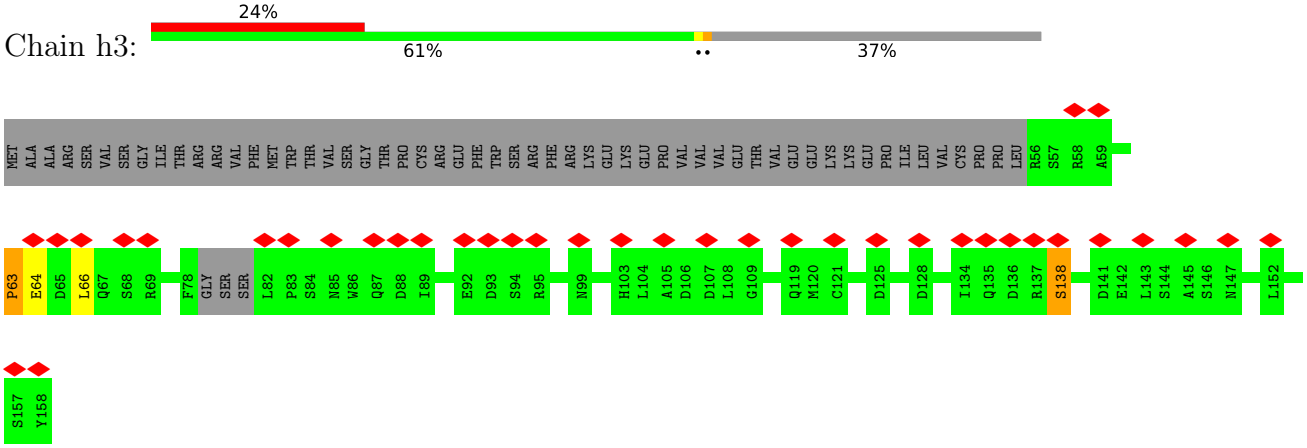
Chain g3:





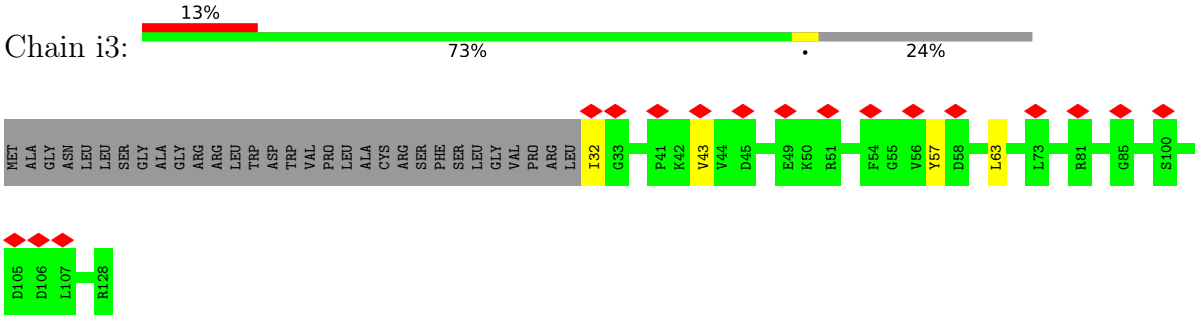
• Molecule 42: 39S ribosomal protein L50, mitochondrial

Chain h3:



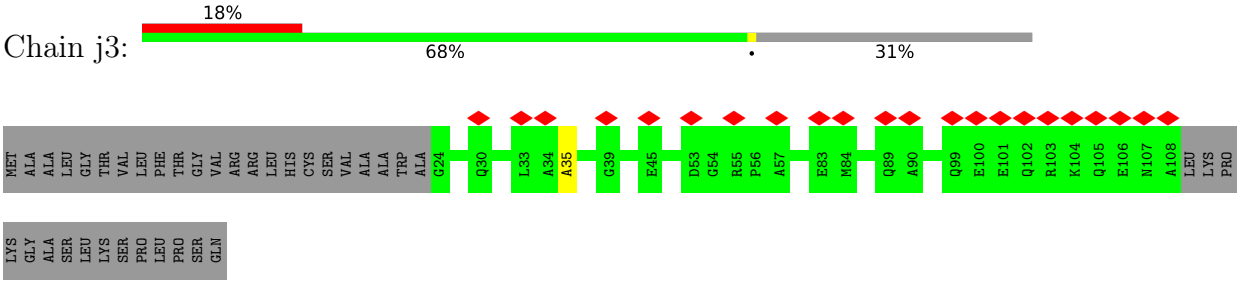
• Molecule 43: 39S ribosomal protein L51, mitochondrial

Chain i3:



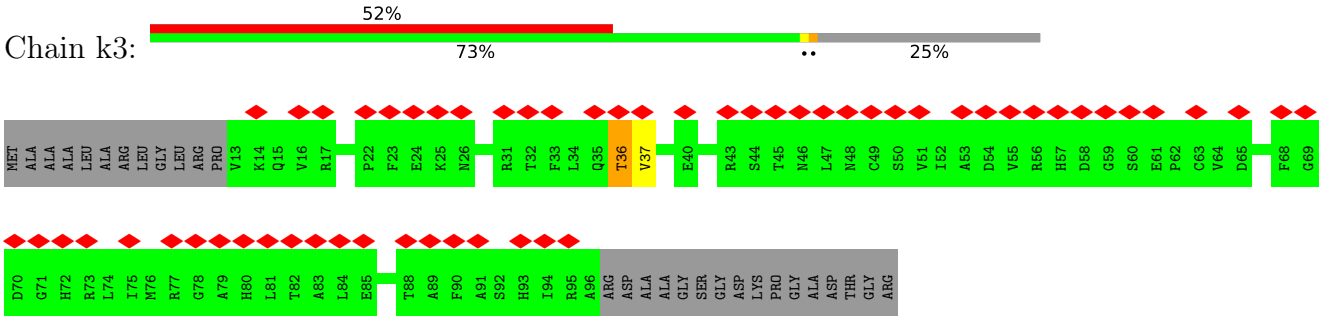
• Molecule 44: 39S ribosomal protein L52, mitochondrial

Chain j3:



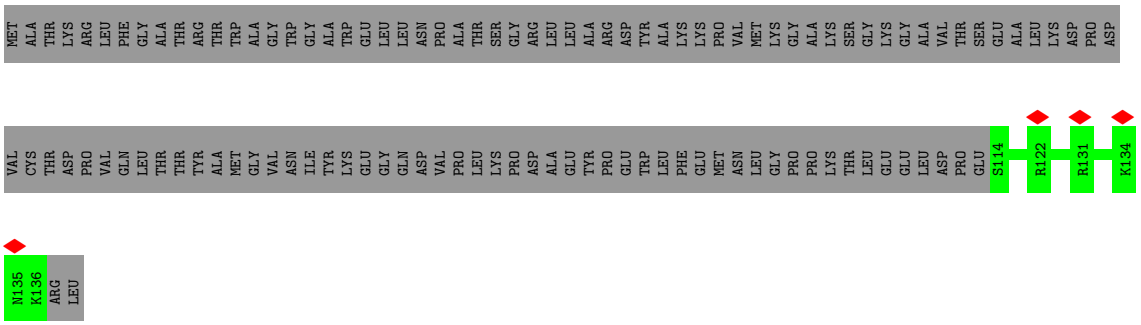
• Molecule 45: 39S ribosomal protein L53, mitochondrial

Chain k3:



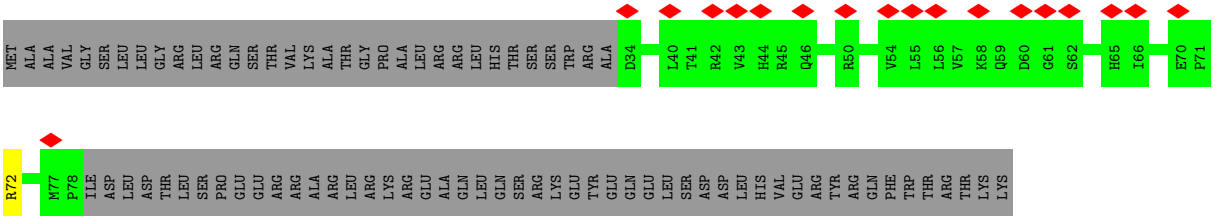
• Molecule 46: 39S ribosomal protein L54, mitochondrial

Chain l3:



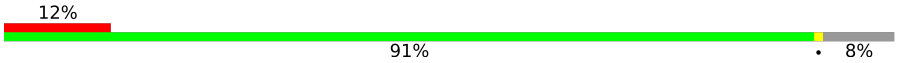
• Molecule 47: 39S ribosomal protein L55, mitochondrial

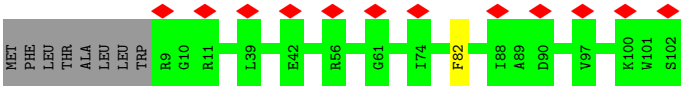
Chain m3:



• Molecule 48: Ribosomal protein 63, mitochondrial

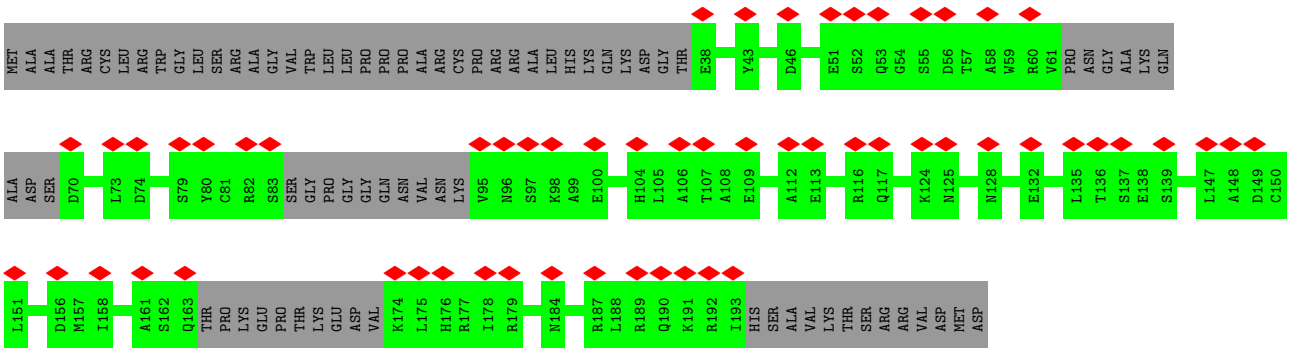
Chain o3:





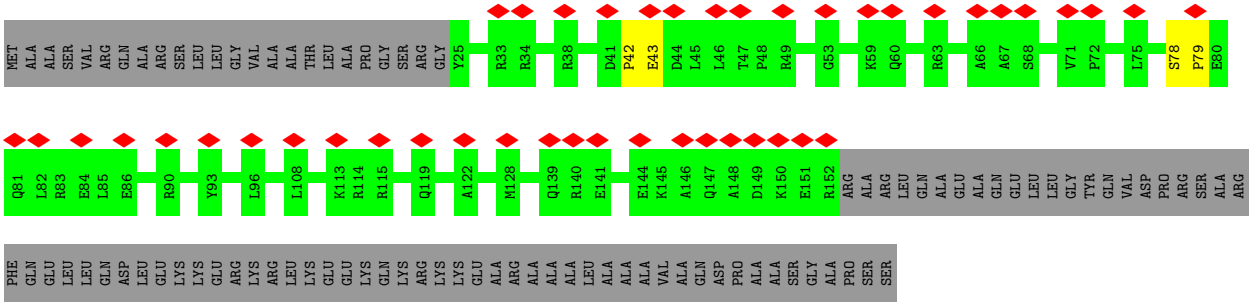
• Molecule 49: Peptidyl-tRNA hydrolase ICT1, mitochondrial

Chain p3:



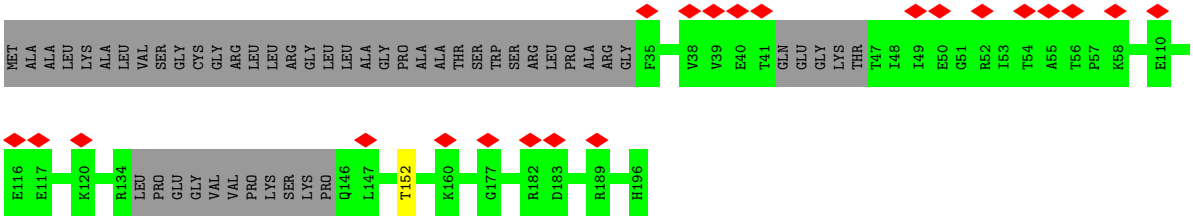
• Molecule 50: Growth arrest and DNA damage-inducible proteins-interacting protein 1

Chain q3:



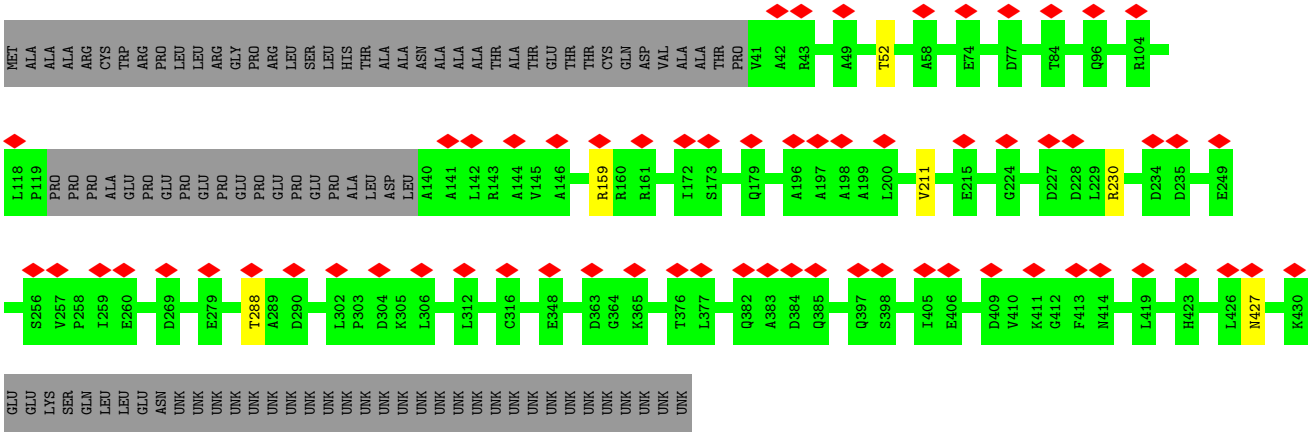
• Molecule 51: 39S ribosomal protein S18a, mitochondrial

Chain r3:



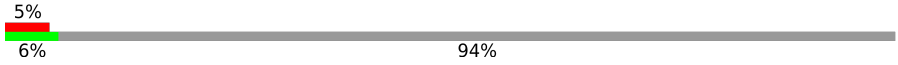
• Molecule 52: 39S ribosomal protein S30, mitochondrial,39S ribosomal protein S30, mitochondrial,39S ribosomal protein S30, mitochondrial,mL65

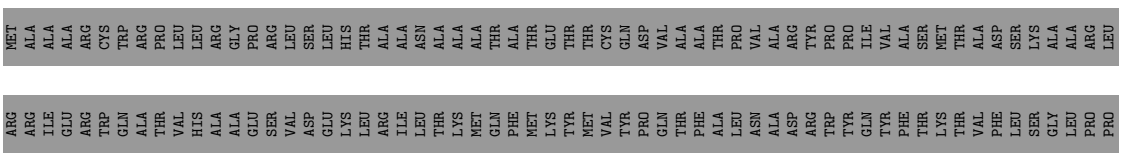
Chain s3:

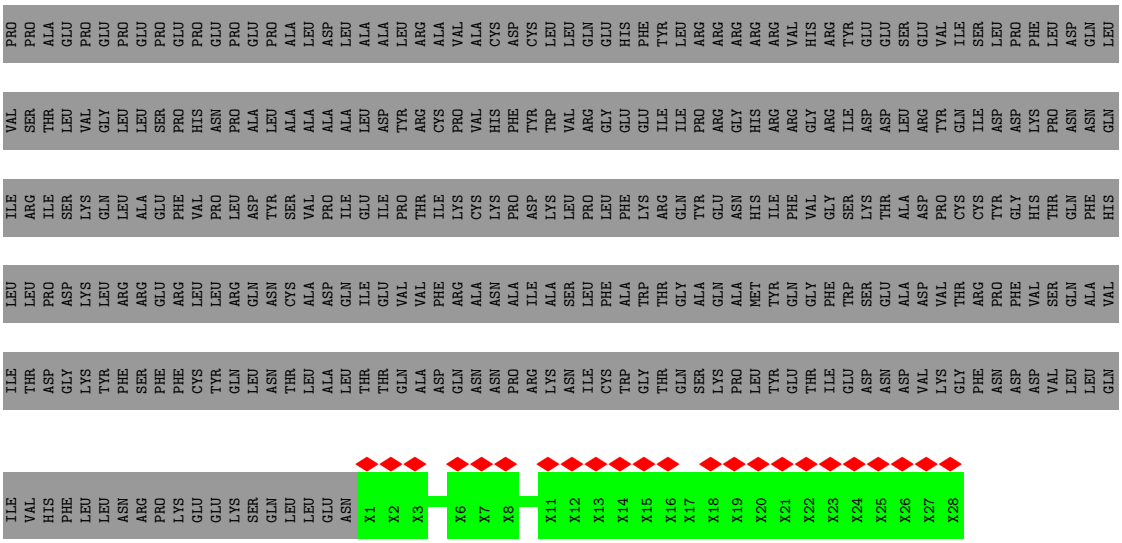


• Molecule 52: 39S ribosomal protein S30, mitochondrial,39S ribosomal protein S30, mitochondrial,39S ribosomal protein S30, mitochondrial,mL65

Chain t3:

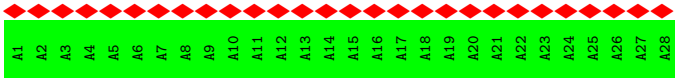






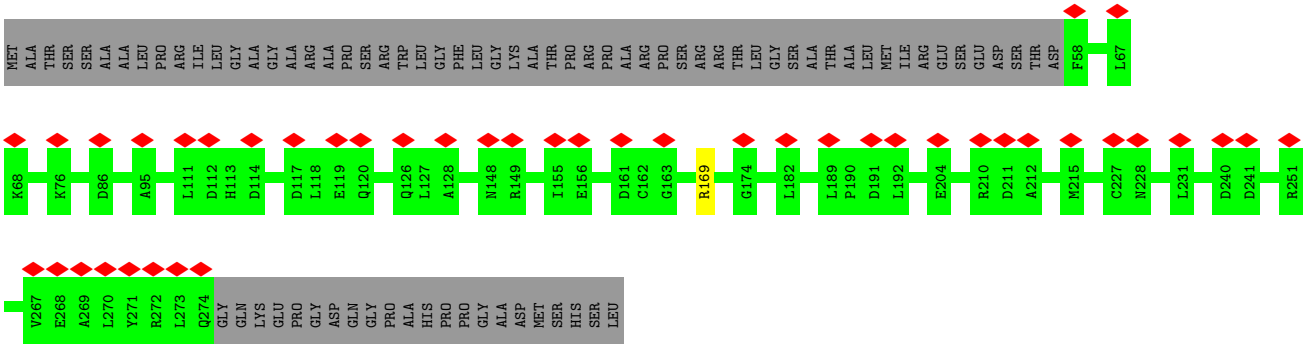
• Molecule 53: Oxa1L

Chain A5:



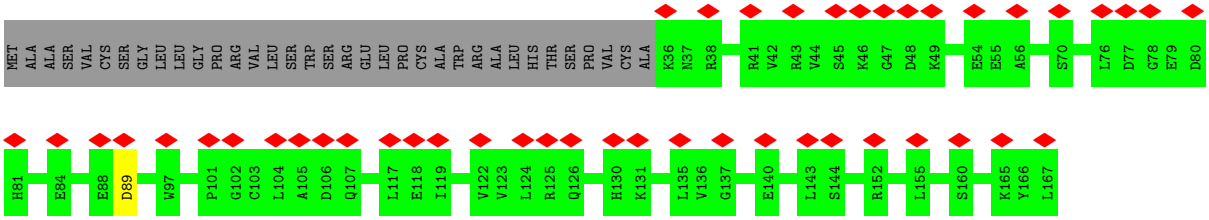
• Molecule 54: 28S ribosomal protein S2, mitochondrial

Chain B6:



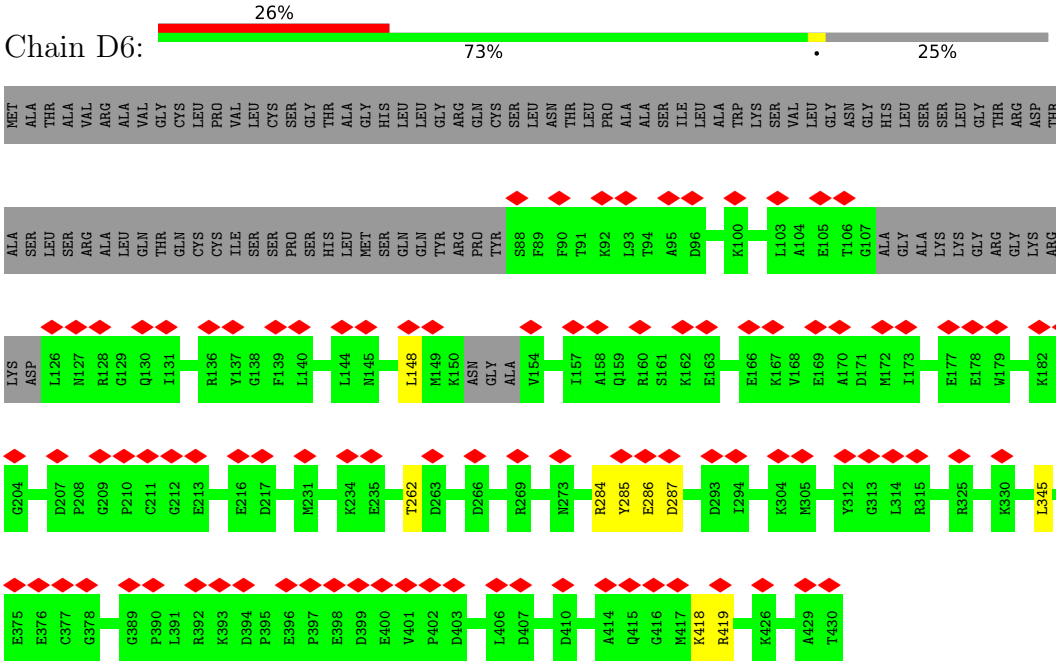
• Molecule 55: 28S ribosomal protein S24, mitochondrial

Chain C6:



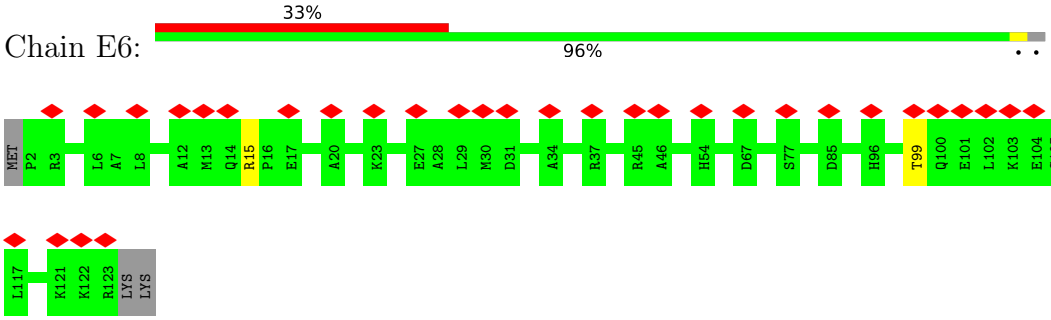
• Molecule 56: 28S ribosomal protein S5, mitochondrial

Chain D6:



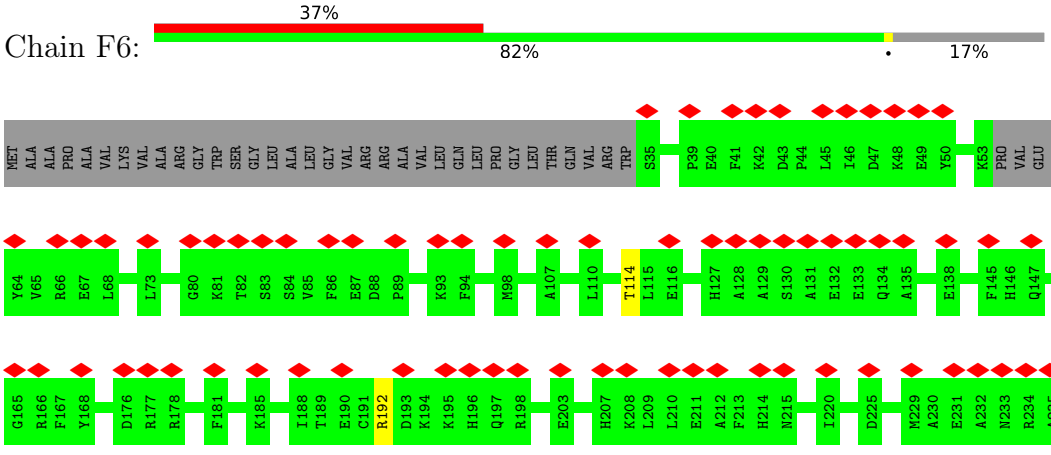
• Molecule 57: 28S ribosomal protein S6, mitochondrial

Chain E6:



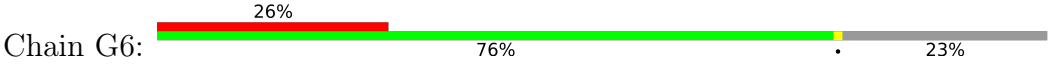
• Molecule 58: 28S ribosomal protein S7, mitochondrial

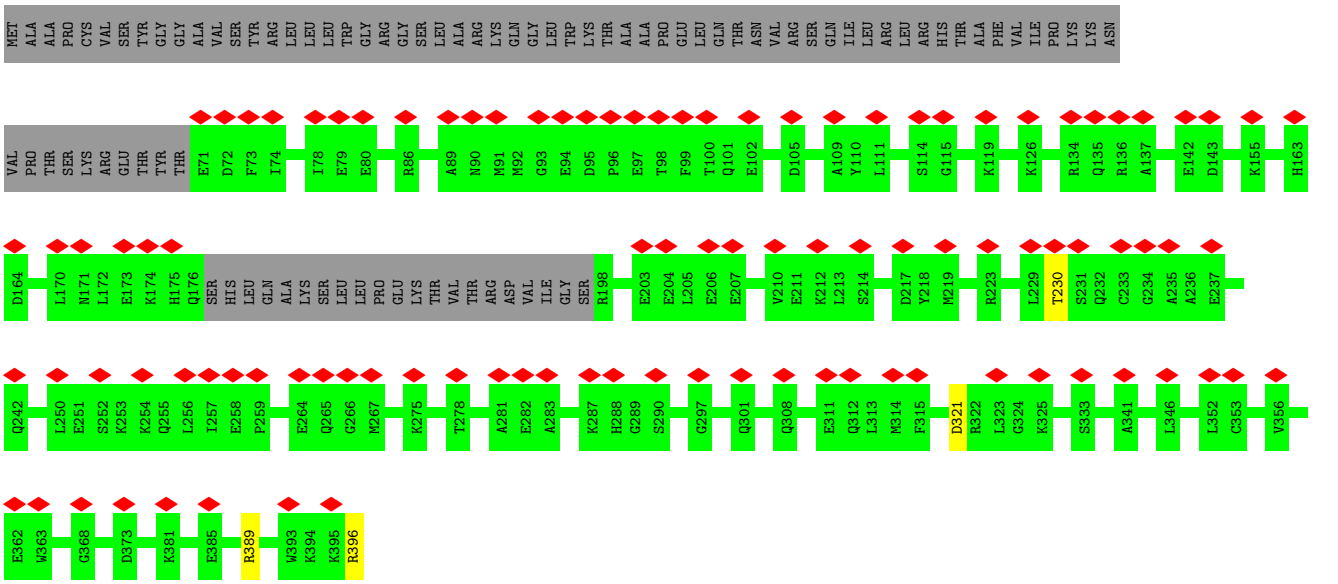
Chain F6:



• Molecule 59: 28S ribosomal protein S9, mitochondrial

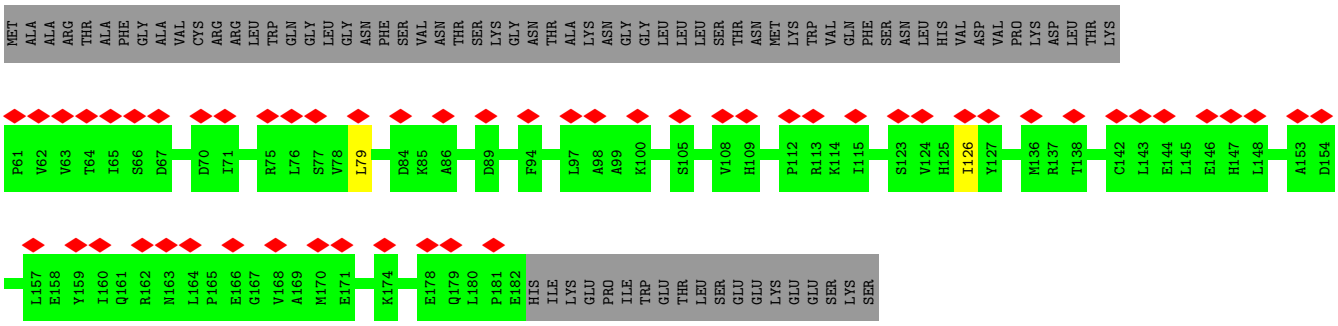
Chain G6:





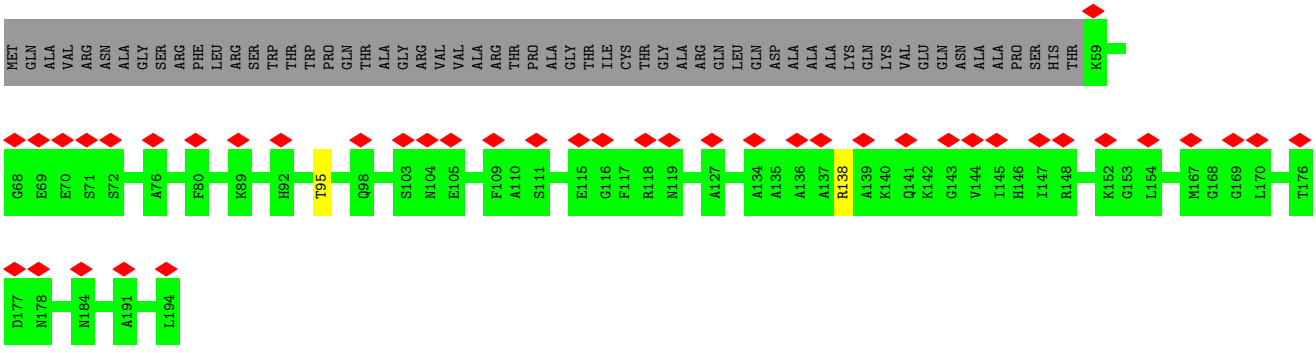
• Molecule 60: 28S ribosomal protein S10, mitochondrial

Chain H6:



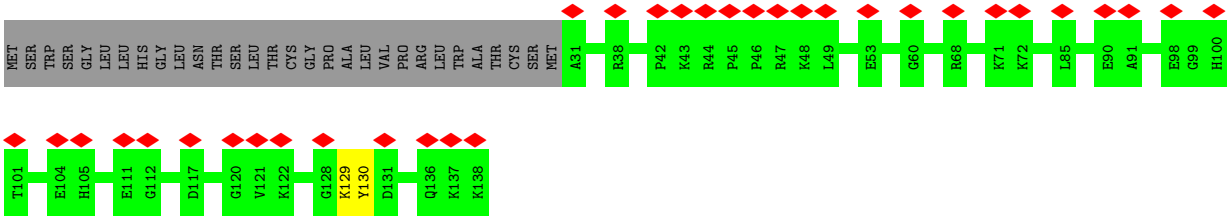
• Molecule 61: 28S ribosomal protein S11, mitochondrial

Chain I6:



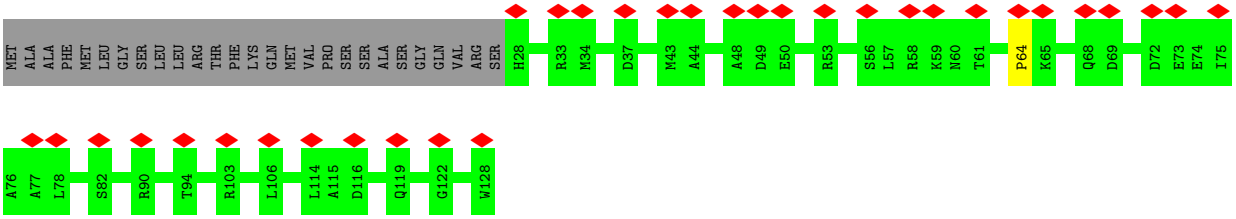
• Molecule 62: 28S ribosomal protein S12, mitochondrial

Chain J6:



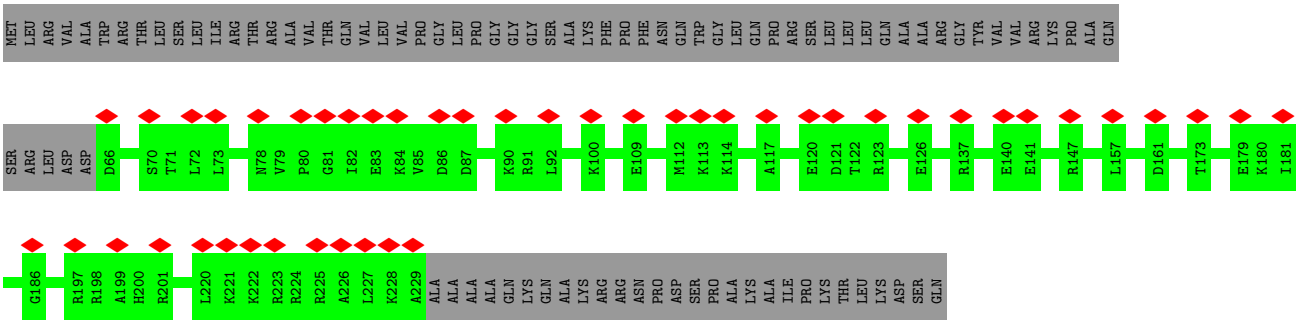
• Molecule 63: 28S ribosomal protein S14, mitochondrial

Chain K6:



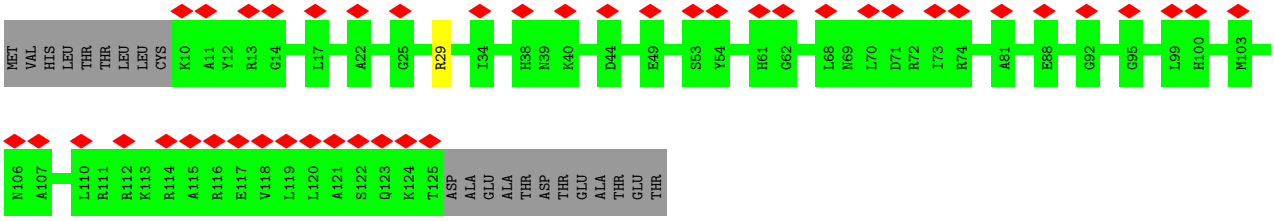
• Molecule 64: 28S ribosomal protein S15, mitochondrial

Chain L6:



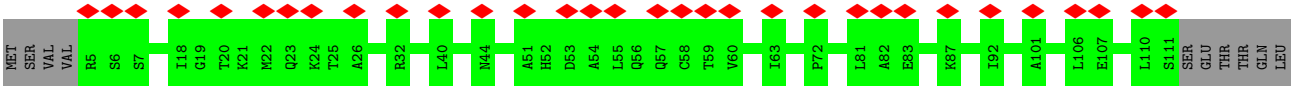
• Molecule 65: 28S ribosomal protein S16, mitochondrial

Chain M6:



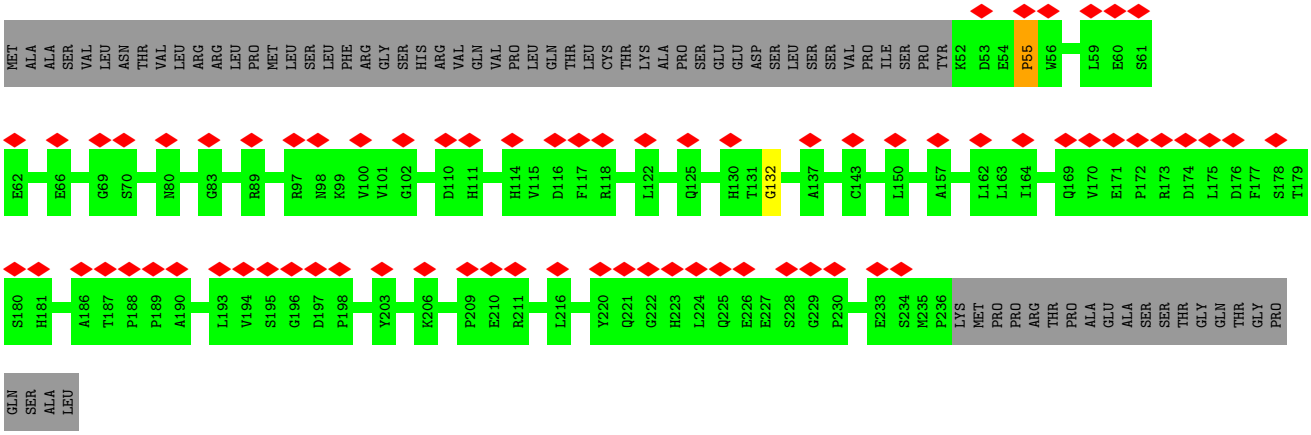
• Molecule 66: 28S ribosomal protein S17, mitochondrial

Chain N6:



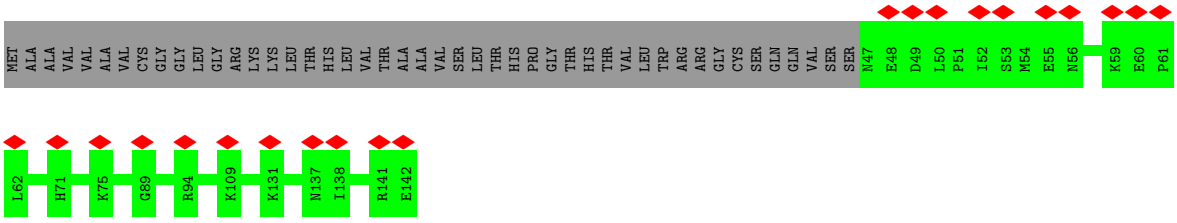
• Molecule 67: 28S ribosomal protein S18b, mitochondrial

Chain O6:



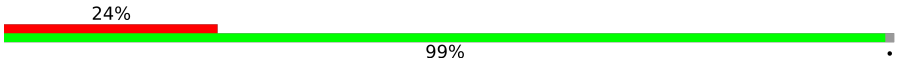
• Molecule 68: 28S ribosomal protein S18c, mitochondrial

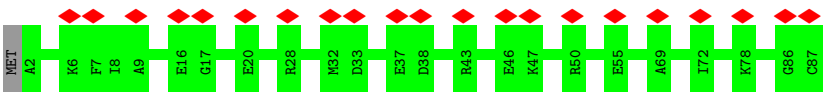
Chain P6:



• Molecule 69: 28S ribosomal protein S21, mitochondrial

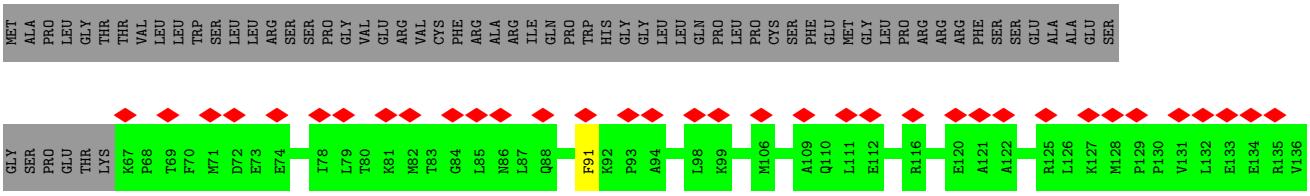
Chain Q6:

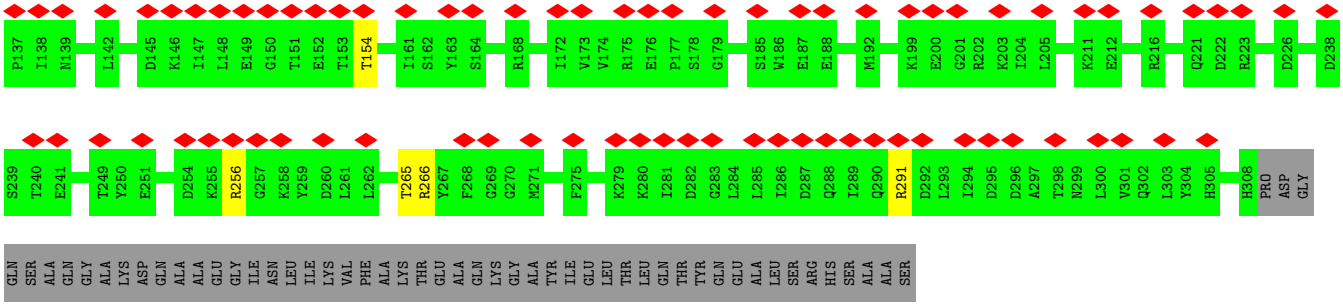




• Molecule 70: 28S ribosomal protein S22, mitochondrial

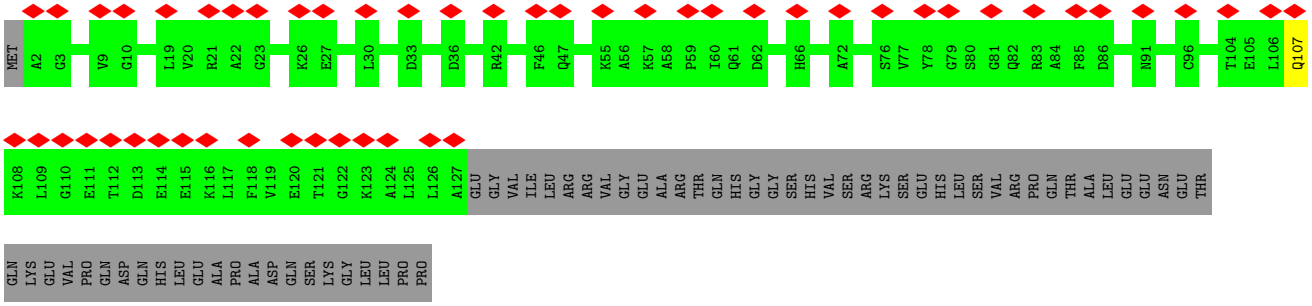
Chain R6:





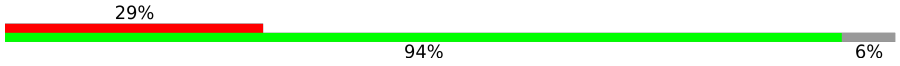
• Molecule 71: 28S ribosomal protein S23, mitochondrial

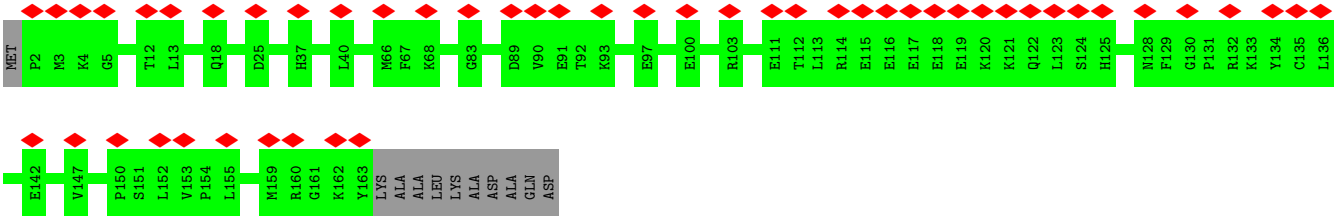
Chain S6:



• Molecule 72: 28S ribosomal protein S25, mitochondrial

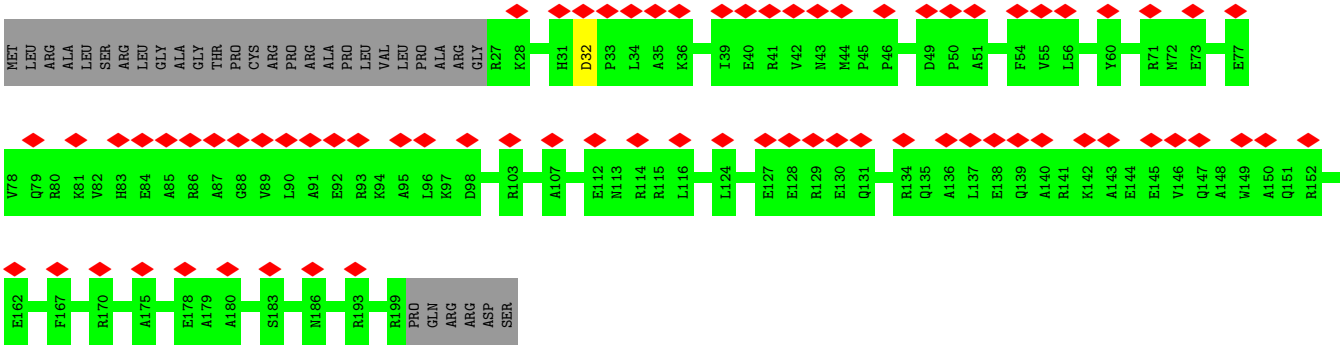
Chain T6:





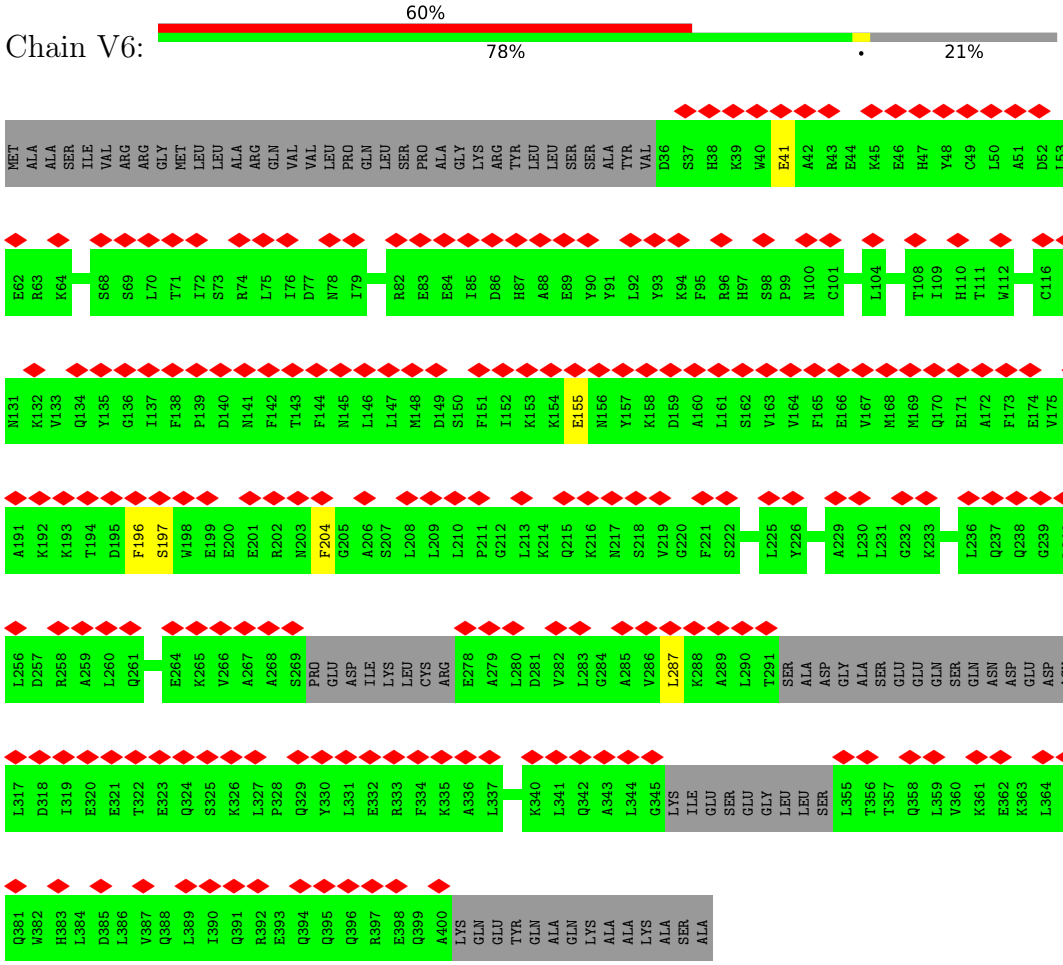
• Molecule 73: 28S ribosomal protein S26, mitochondrial

Chain U6:



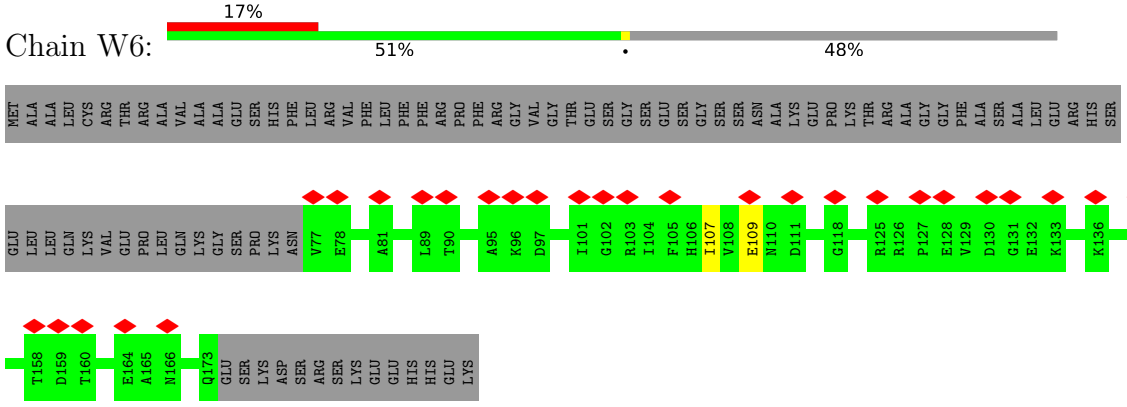
• Molecule 74: 28S ribosomal protein S27, mitochondrial

Chain V6:



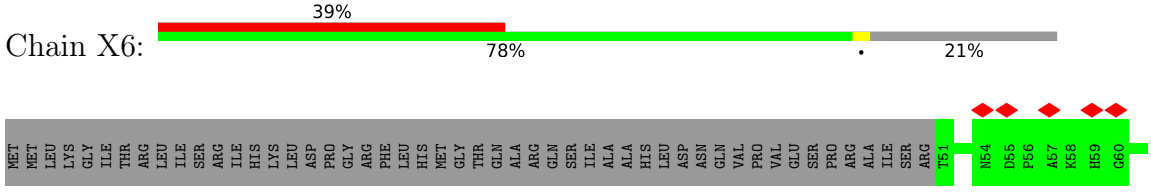
• Molecule 75: 28S ribosomal protein S28, mitochondrial

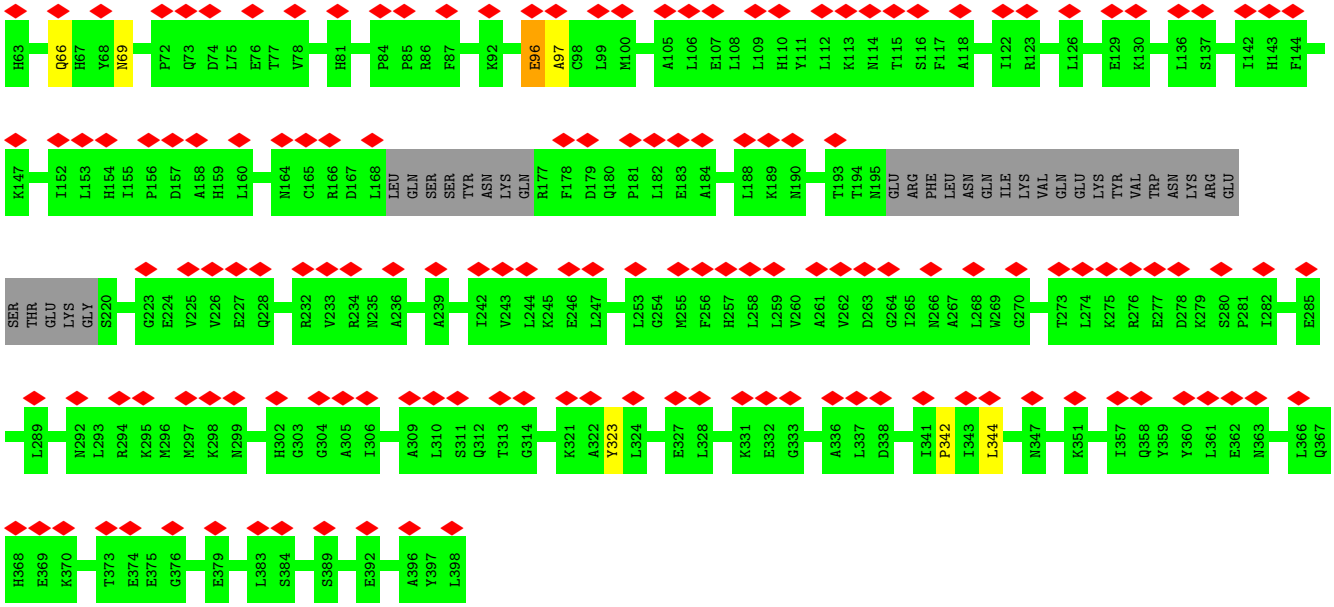
Chain W6:



• Molecule 76: 28S ribosomal protein S29, mitochondrial

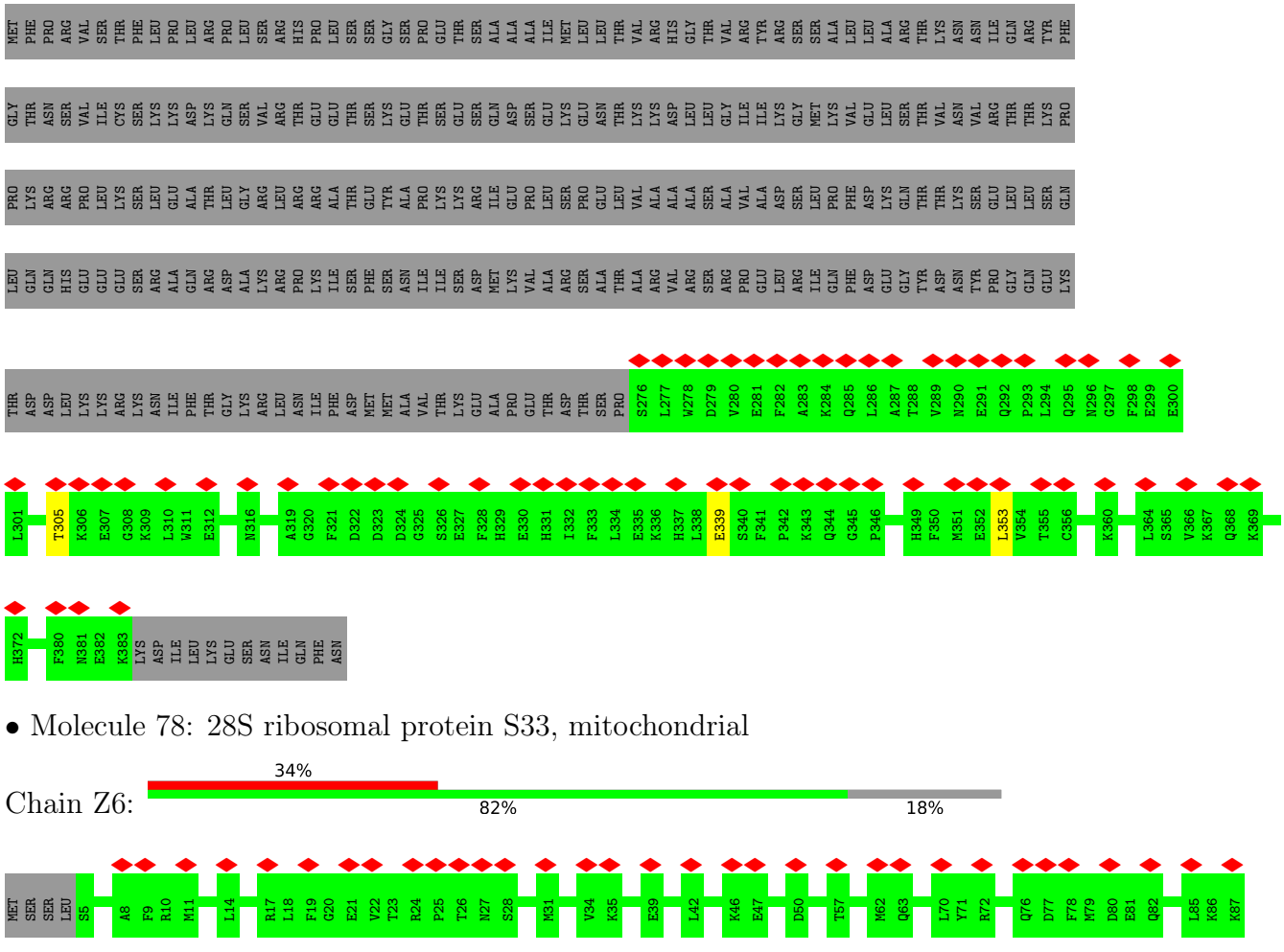
Chain X6:





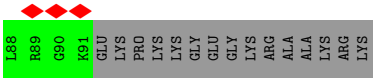
• Molecule 77: 28S ribosomal protein S31, mitochondrial

Chain Y6:



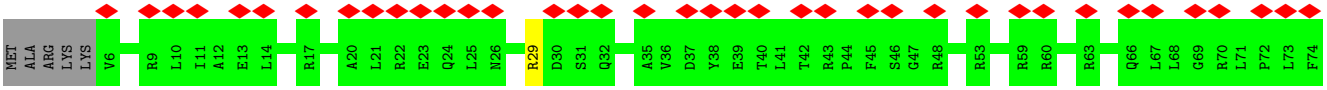
• Molecule 78: 28S ribosomal protein S33, mitochondrial

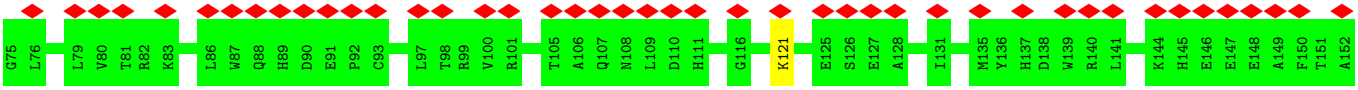
Chain Z6:

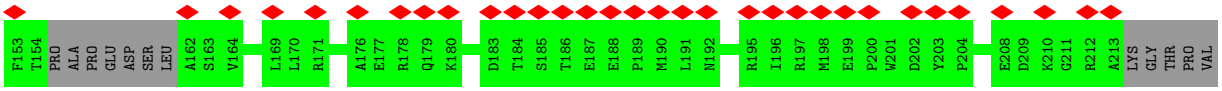


• Molecule 79: 28S ribosomal protein S34, mitochondrial

Chain a6:

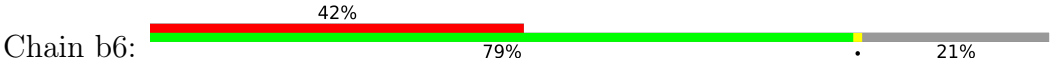


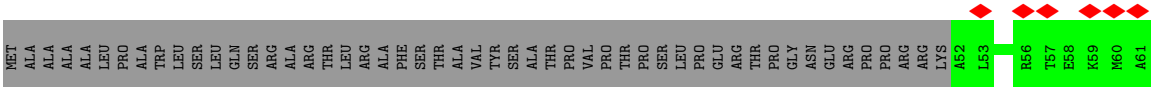


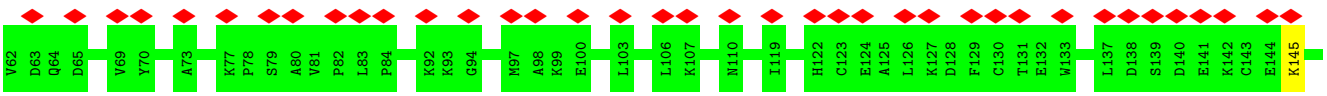


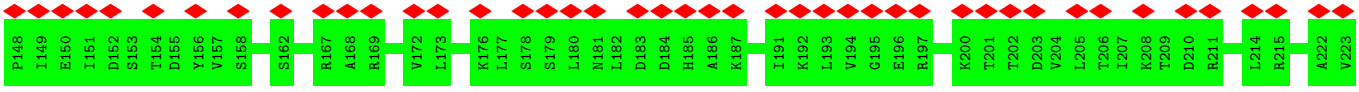
• Molecule 80: 28S ribosomal protein S35, mitochondrial

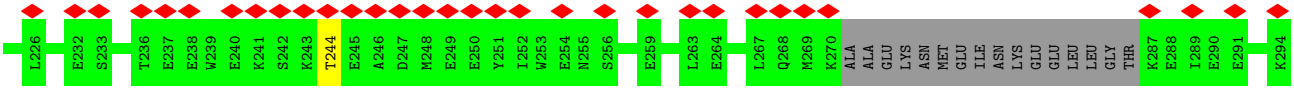
Chain b6:

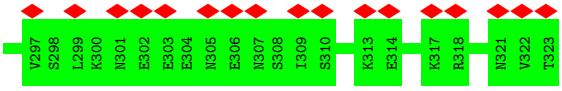






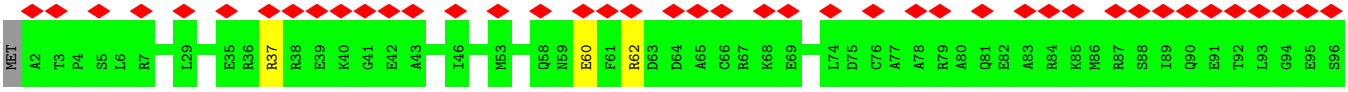


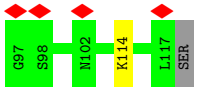




• Molecule 81: Coiled-coil-helix-coiled-coil-helix domain-containing protein 1

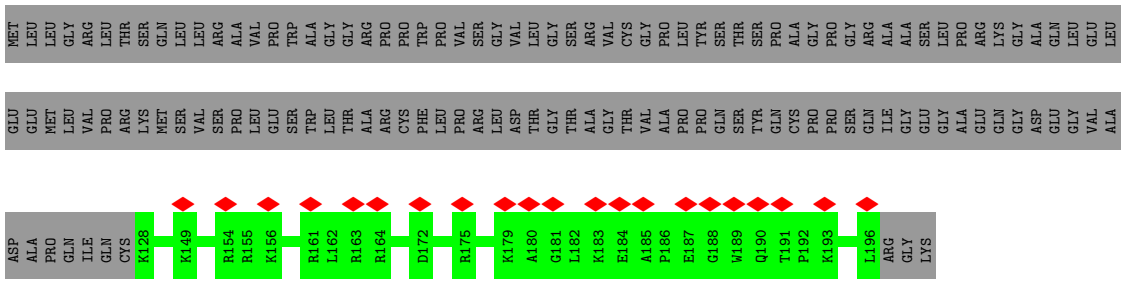
Chain c6:





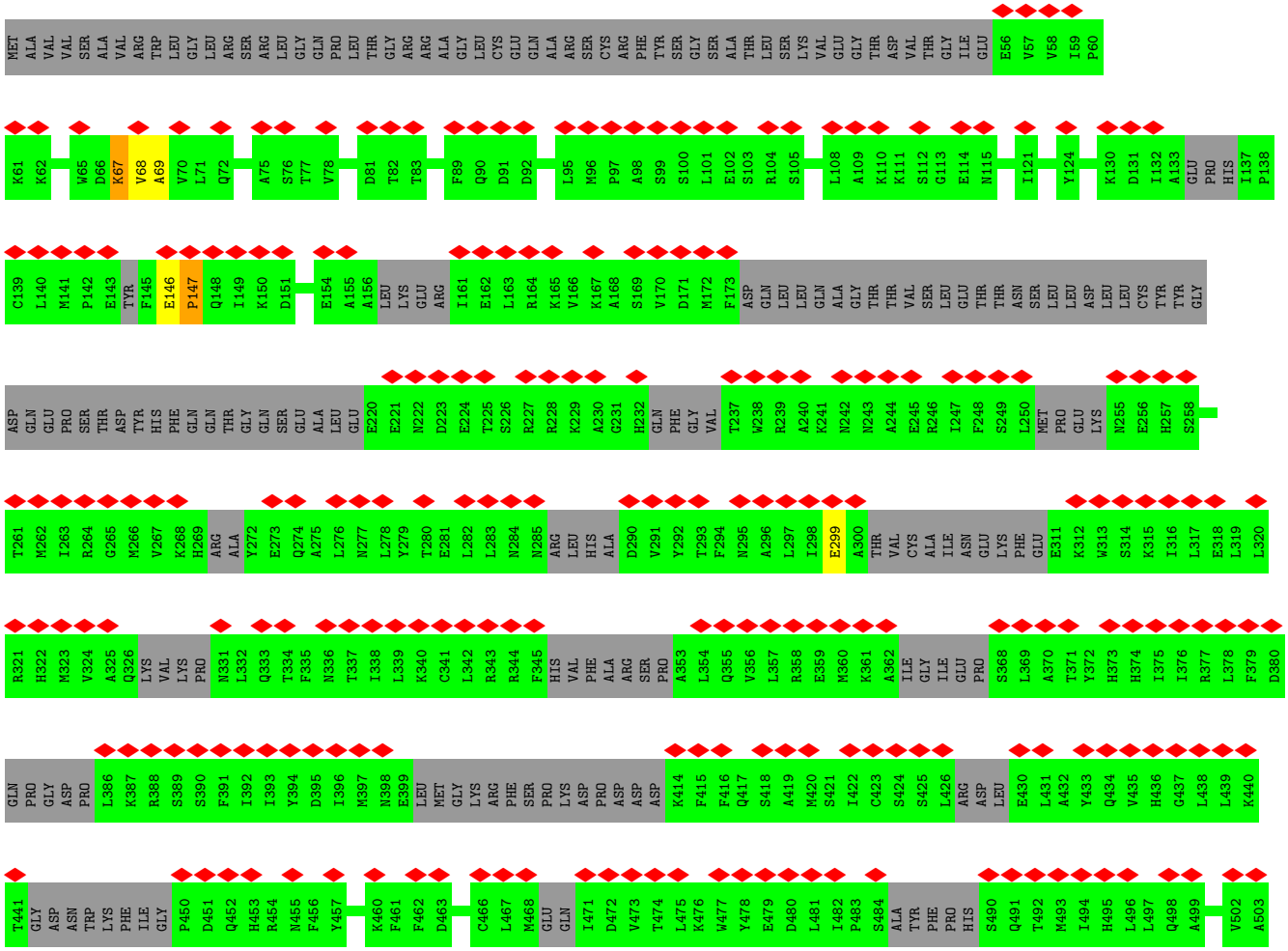
• Molecule 82: Aurora kinase A-interacting protein

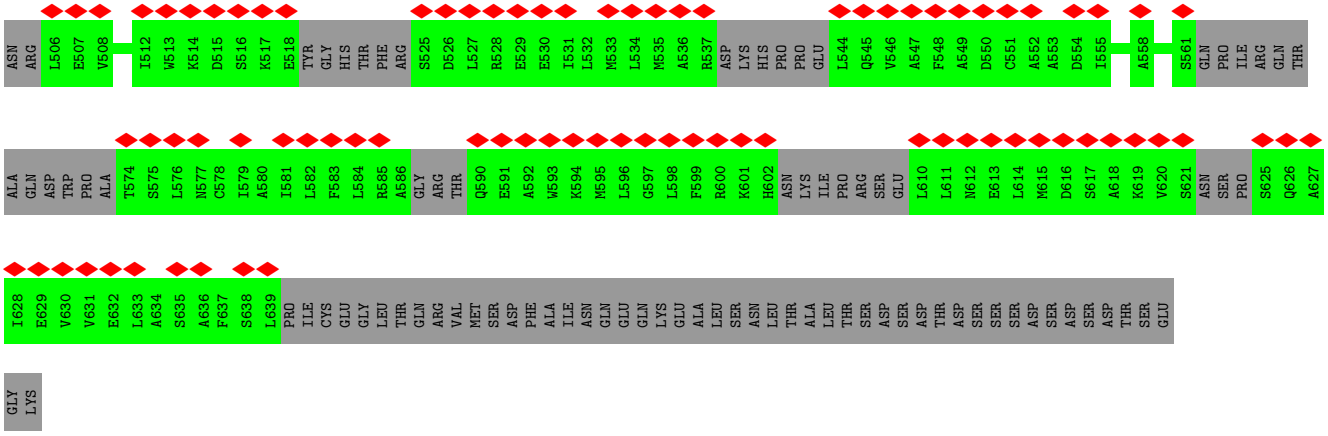
Chain d6:



• Molecule 83: Pentatricopeptide repeat domain-containing protein 3, mitochondrial

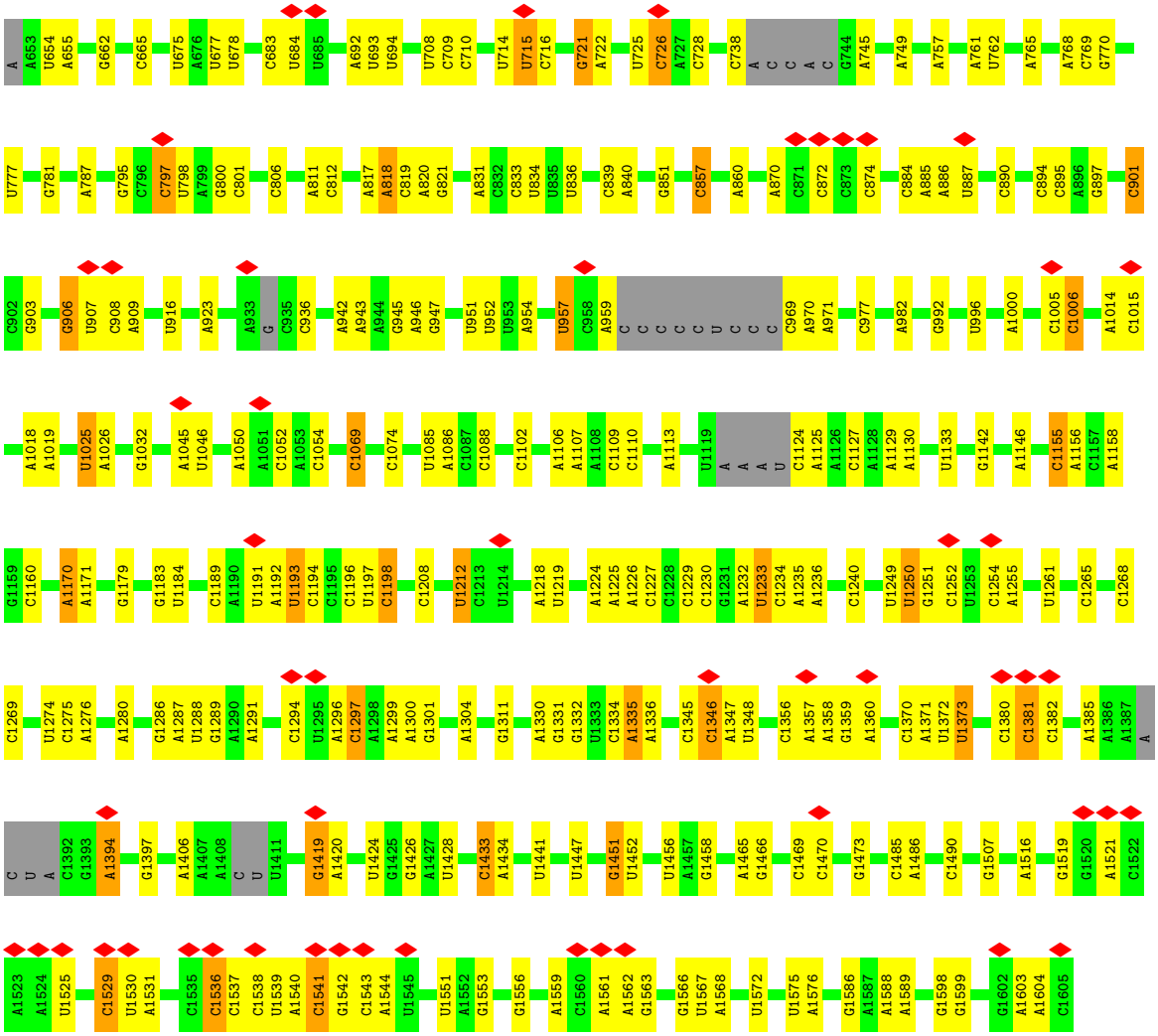
Chain e6:





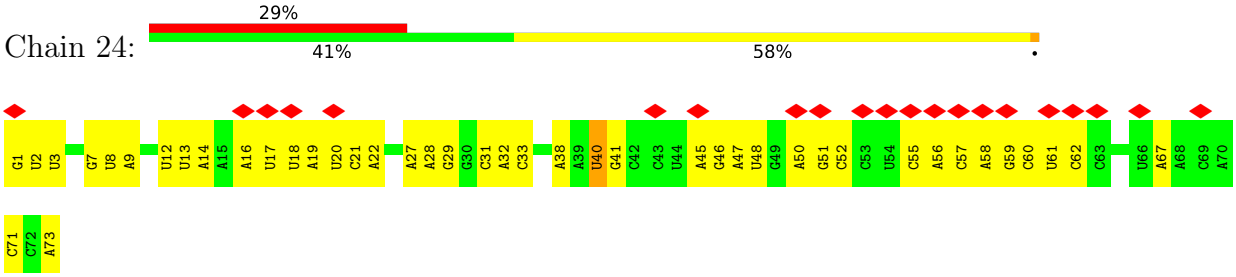
• Molecule 84: 12S rRNA

Chain A6:



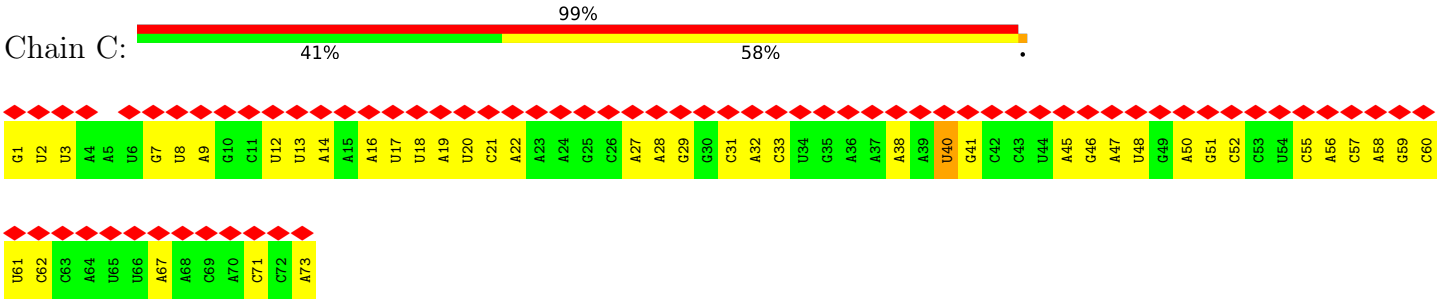
• Molecule 85: mt-tRNA

Chain 24:



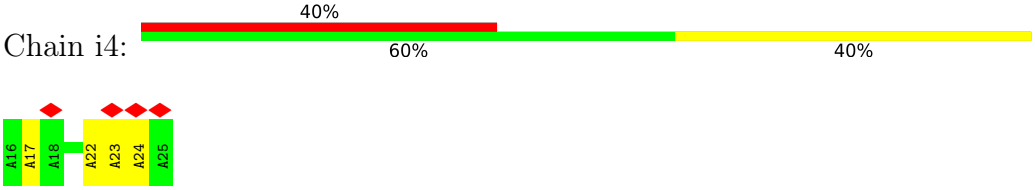
• Molecule 85: mt-tRNA

Chain C:



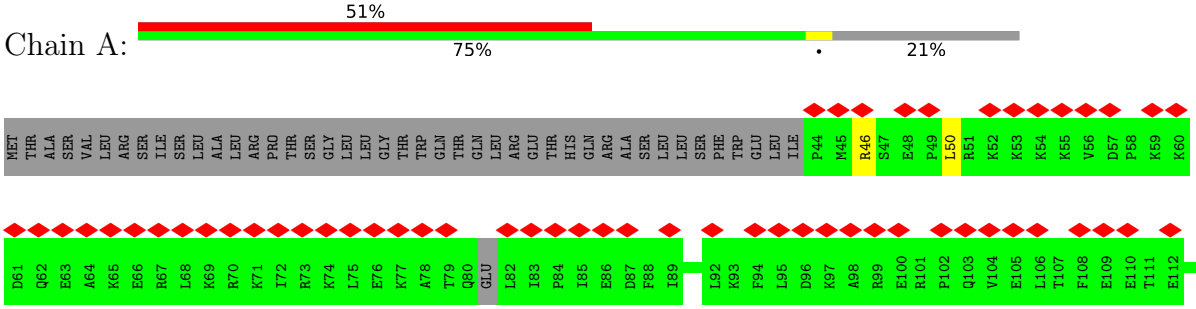
• Molecule 86: mRNA

Chain i4:



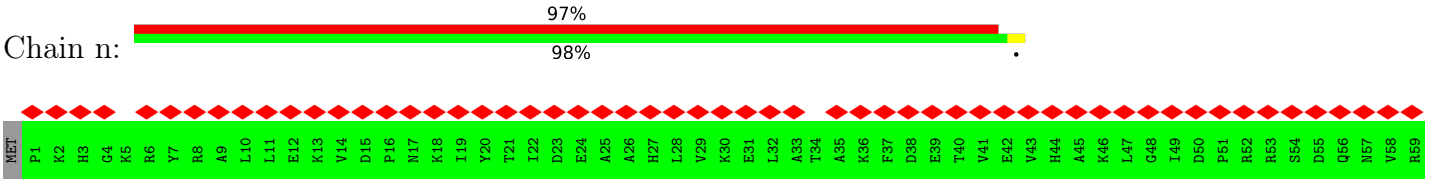
• Molecule 87: 39S ribosomal protein L40, mitochondrial

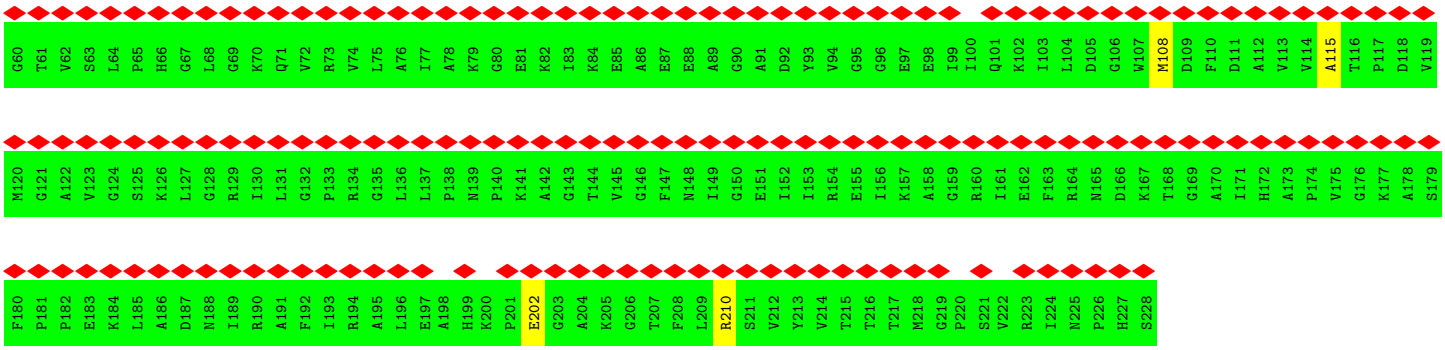
Chain A:



• Molecule 88: 50S ribosomal protein L1

Chain n:




G60 T61 V62 S63 L64 P65 H66 G67 L68 G69 K70 Q71 V72 R73 V74 L75 A76 I77 A78 K79 G80 E81 K82 I83 K84 E85 A86 E87 E88 A89 G90 A91 D92 Y93 V94 G95 G96 E97 E98 I99 I100 Q101 K102 I103 L104 D105 G106 W107 M108 D109 F110 D111 A112 V113 V114 A115 T116 P117 D118 V119
M120 G121 A122 V123 G124 S125 K126 L127 G128 R129 I130 L131 G132 P133 R134 G135 L136 L137 P138 N139 P140 K141 A142 G143 T144 V145 G146 F147 N148 I149 G150 E151 I152 I153 R154 E155 I156 K157 A158 G159 R160 I161 E162 F163 R164 N165 D166 K167 T168 G169 A170 I171 H172 A173 P174 V175 G176 K177 A178 S179
F180 P181 P182 E183 K184 L185 A186 D187 N188 I189 R190 A191 F192 I193 R194 A195 L196 E197 A198 H199 K200 P201 E202 G203 A204 K205 G206 T207 F208 L209 R210 S211 V212 Y213 V214 T215 T216 T217 M218 G219 P220 S221 V222 R223 I224 N225 P226 H227 S228

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	16588	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 ($e^-/Å^2$)	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	0.252	Depositor
Minimum map value	-0.143	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: ZN, MLI, CL, MG, GDP, SO4, 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	0.33	0/144	0.75	0/200
2	A3	0.75	1/35697 (0.0%)	1.11	233/55544 (0.4%)
3	B3	0.50	0/1328	1.06	3/2056 (0.1%)
4	D3	0.40	0/1879	0.58	0/2527
5	E3	0.41	0/2433	0.60	0/3299
6	F3	0.41	0/2071	0.63	0/2817
7	D	0.31	0/665	0.62	0/905
7	H3	0.38	0/798	0.61	0/1073
8	I3	0.34	0/1308	0.61	1/1761 (0.1%)
9	J3	0.32	0/1077	0.62	0/1452
10	K3	0.39	0/1495	0.57	0/2029
11	L3	0.39	0/904	0.62	0/1218
12	M3	0.40	0/2359	0.64	0/3185
13	N3	0.39	0/1697	0.57	1/2281 (0.0%)
14	O3	0.41	0/1269	0.62	0/1708
15	P3	0.41	0/1103	0.59	0/1491
16	Q3	0.38	0/1863	0.57	0/2509
17	R3	0.42	0/1174	0.55	0/1572
18	S3	0.44	0/1276	0.65	0/1729
19	T3	0.42	0/1402	0.54	0/1886
20	U3	0.45	0/946	0.60	1/1283 (0.1%)
21	V3	0.38	0/1590	0.61	0/2151
22	W3	0.49	0/893	0.59	0/1204
23	X3	0.38	0/2081	0.61	1/2812 (0.0%)
24	Y3	0.40	0/1552	0.54	0/2079
25	Z3	0.40	0/1003	0.57	0/1354
26	03	0.38	0/895	0.60	0/1201
27	13	0.37	0/438	0.74	1/583 (0.2%)
28	23	0.38	0/382	0.52	0/507
29	33	0.42	0/852	0.54	0/1136
30	43	0.43	0/329	0.53	0/435
31	53	0.40	0/3154	0.63	1/4295 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	63	0.40	0/2722	0.63	1/3709 (0.0%)
33	73	0.38	0/2207	0.56	0/2978
34	93	0.39	0/896	0.60	0/1205
35	a3	0.38	0/709	0.56	0/963
36	b3	0.40	0/1202	0.58	0/1626
37	c3	0.37	0/2264	0.57	0/3059
38	d3	0.36	0/1385	0.63	0/1877
39	e3	0.33	0/1797	0.62	0/2422
40	f3	0.36	0/1055	0.71	1/1427 (0.1%)
41	g3	0.41	0/1102	0.59	0/1503
42	h3	0.35	0/847	0.67	3/1150 (0.3%)
43	i3	0.41	0/849	0.65	1/1135 (0.1%)
44	j3	0.38	0/698	0.51	0/940
45	k3	0.33	0/665	0.62	0/897
46	l3	0.29	0/226	0.50	0/299
47	m3	0.35	0/379	0.65	0/510
48	o3	0.44	0/818	0.53	0/1097
49	p3	0.31	0/1071	0.53	0/1433
50	q3	0.35	0/1107	0.54	0/1498
51	r3	0.39	0/1238	0.54	0/1676
52	s3	0.41	1/3114 (0.0%)	0.62	0/4225
53	A5	0.30	0/139	0.59	0/193
54	B6	0.39	0/1811	0.59	0/2451
55	C6	0.40	0/1112	0.57	0/1505
56	D6	0.37	0/2607	0.63	1/3498 (0.0%)
57	E6	0.36	0/989	0.59	0/1335
58	F6	0.35	0/1708	0.58	1/2291 (0.0%)
59	G6	0.37	0/2570	0.60	1/3443 (0.0%)
60	H6	0.40	0/1019	0.68	0/1379
61	I6	0.35	0/1031	0.57	0/1390
62	J6	0.38	0/854	0.57	0/1148
63	K6	0.37	0/879	0.52	0/1182
64	L6	0.37	0/1406	0.55	0/1878
65	M6	0.37	0/941	0.61	0/1265
66	N6	0.38	0/864	0.63	0/1169
67	O6	0.37	0/1580	0.60	1/2150 (0.0%)
68	P6	0.42	0/791	0.56	0/1062
69	Q6	0.38	0/752	0.56	0/1001
70	R6	0.38	1/2050 (0.0%)	0.64	0/2770
71	S6	0.37	0/1069	0.58	0/1441
72	T6	0.36	0/1361	0.58	0/1829
73	U6	0.32	0/1482	0.53	0/1987
74	V6	0.33	0/2758	0.60	0/3724

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
75	W6	0.36	0/778	0.64	0/1048
76	X6	0.39	1/2596 (0.0%)	0.69	2/3519 (0.1%)
77	Y6	0.36	0/943	0.55	0/1274
78	Z6	0.33	0/757	0.55	0/1011
79	a6	0.38	0/1727	0.59	0/2338
80	b6	0.36	0/2121	0.63	0/2873
81	c6	0.38	0/939	0.58	0/1256
82	d6	0.36	0/621	0.51	0/820
83	e6	0.32	0/2859	0.54	1/3864 (0.0%)
84	A6	0.67	0/22053	1.08	117/34324 (0.3%)
85	24	0.47	0/1731	1.08	6/2693 (0.2%)
85	C	0.47	0/1731	1.08	6/2693 (0.2%)
86	i4	0.54	0/247	0.98	0/383
87	A	0.36	0/1403	0.67	1/1880 (0.1%)
88	n	0.33	0/1812	0.63	2/2443 (0.1%)
All	All	0.52	4/174499 (0.0%)	0.83	387/248421 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	Y2	0	1
4	D3	0	1
5	E3	0	6
6	F3	0	1
7	H3	0	1
9	J3	0	1
10	K3	0	2
12	M3	0	4
16	Q3	0	1
17	R3	0	1
21	V3	0	2
22	W3	0	1
23	X3	0	3
25	Z3	0	1
26	03	0	1
27	13	0	1
31	53	0	1
34	93	0	2
38	d3	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
39	e3	0	1
40	f3	0	4
41	g3	0	1
42	h3	0	2
43	i3	0	1
45	k3	0	1
48	o3	0	1
50	q3	0	1
56	D6	0	3
62	J6	0	2
63	K6	0	1
67	O6	0	1
70	R6	0	3
71	S6	0	1
74	V6	0	3
75	W6	0	1
76	X6	0	2
77	Y6	0	1
81	c6	0	1
83	e6	0	1
87	A	0	4
All	All	0	69

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
76	X6	323	TYR	C-N	-6.35	1.19	1.34
70	R6	91	PHE	C-N	-5.39	1.21	1.34
52	s3	427	ASN	C-N	-5.34	1.21	1.34
2	A3	1828	A	N9-C4	-5.10	1.34	1.37

All (387) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A3	1732	C	N1-C2-O2	13.12	126.77	118.90
2	A3	3169	C	N1-C2-O2	12.73	126.54	118.90
2	A3	3169	C	C2-N1-C1'	12.37	132.41	118.80
84	A6	1433	C	N1-C2-O2	11.71	125.93	118.90
2	A3	2522	U	N1-C2-O2	11.09	130.56	122.80
2	A3	2522	U	C2-N1-C1'	11.01	130.91	117.70
2	A3	1732	C	N3-C2-O2	-10.75	114.38	121.90
84	A6	1433	C	C2-N1-C1'	10.22	130.05	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A3	3204	C	N1-C2-O2	10.20	125.02	118.90
2	A3	1732	C	C2-N1-C1'	10.08	129.89	118.80
59	G6	321	ASP	CB-CG-OD1	9.63	126.97	118.30
2	A3	3169	C	N3-C2-O2	-9.56	115.20	121.90
84	A6	1433	C	N3-C2-O2	-9.51	115.25	121.90
2	A3	2079	C	N1-C2-O2	9.43	124.56	118.90
2	A3	3212	C	N1-C2-O2	9.36	124.52	118.90
2	A3	1902	C	N1-C2-O2	9.32	124.50	118.90
84	A6	709	C	N1-C2-O2	9.32	124.49	118.90
2	A3	2557	C	N1-C2-O2	9.24	124.45	118.90
2	A3	2079	C	C2-N1-C1'	9.21	128.93	118.80
2	A3	3204	C	N3-C2-O2	-9.18	115.47	121.90
84	A6	1381	C	N1-C2-O2	9.16	124.39	118.90
2	A3	2066	C	C2-N1-C1'	9.01	128.71	118.80
2	A3	3134	C	N1-C2-O2	9.01	124.31	118.90
2	A3	3169	C	C6-N1-C1'	-8.99	110.01	120.80
2	A3	2066	C	N1-C2-O2	8.98	124.29	118.90
2	A3	3212	C	C2-N1-C1'	8.80	128.48	118.80
2	A3	3204	C	C2-N1-C1'	8.75	128.42	118.80
2	A3	2158	U	N1-C2-O2	8.72	128.90	122.80
2	A3	1837	C	C2-N1-C1'	8.70	128.37	118.80
2	A3	2523	C	N1-C2-O2	8.55	124.03	118.90
84	A6	709	C	N3-C2-O2	-8.51	115.94	121.90
2	A3	2522	U	N3-C2-O2	-8.48	116.26	122.20
84	A6	1451	G	N3-C4-N9	8.41	131.05	126.00
2	A3	2158	U	N3-C2-O2	-8.37	116.34	122.20
84	A6	769	C	C2-N1-C1'	8.35	127.99	118.80
84	A6	714	U	C2-N1-C1'	8.31	127.67	117.70
2	A3	2079	C	N3-C2-O2	-8.26	116.12	121.90
2	A3	1715	C	N1-C2-O2	8.25	123.85	118.90
84	A6	709	C	C2-N1-C1'	8.24	127.86	118.80
84	A6	769	C	N1-C2-O2	8.20	123.82	118.90
2	A3	2080	U	C2-N1-C1'	8.14	127.47	117.70
2	A3	1732	C	C6-N1-C2	-8.13	117.05	120.30
2	A3	2522	U	C6-N1-C1'	-8.01	109.99	121.20
2	A3	2186	C	N1-C2-O2	7.86	123.62	118.90
2	A3	2066	C	N3-C2-O2	-7.84	116.41	121.90
2	A3	2080	U	N1-C2-O2	7.84	128.29	122.80
2	A3	2493	C	C2-N1-C1'	7.81	127.39	118.80
84	A6	1381	C	C2-N1-C1'	7.78	127.36	118.80
84	A6	1451	G	C4-N9-C1'	7.75	136.57	126.50
2	A3	2523	C	C2-N1-C1'	7.70	127.27	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A3	3134	C	C2-N1-C1'	7.70	127.27	118.80
2	A3	1902	C	C2-N1-C1'	7.69	127.26	118.80
84	A6	1346	C	N1-C2-O2	7.68	123.51	118.90
2	A3	1813	C	N3-C2-O2	-7.67	116.53	121.90
84	A6	797	C	C2-N1-C1'	7.66	127.23	118.80
2	A3	2158	U	C2-N1-C1'	7.62	126.85	117.70
2	A3	2386	C	N1-C2-O2	7.59	123.45	118.90
84	A6	1451	G	C8-N9-C1'	-7.58	117.15	127.00
84	A6	1529	C	N1-C2-O2	7.54	123.42	118.90
2	A3	1701	U	C2-N1-C1'	7.44	126.63	117.70
2	A3	1813	C	C2-N1-C1'	7.42	126.96	118.80
2	A3	1728	U	N1-C2-O2	7.41	127.99	122.80
84	A6	1433	C	C6-N1-C2	-7.41	117.34	120.30
2	A3	2557	C	C2-N1-C1'	7.32	126.85	118.80
2	A3	3009	C	N1-C2-O2	7.31	123.29	118.90
2	A3	3212	C	N3-C2-O2	-7.31	116.78	121.90
2	A3	3134	C	N3-C2-O2	-7.28	116.80	121.90
2	A3	2759	U	N1-C2-O2	7.26	127.88	122.80
2	A3	2865	C	N1-C2-O2	7.23	123.24	118.90
2	A3	3170	C	N1-C2-O2	7.22	123.23	118.90
2	A3	2445	U	C2-N1-C1'	7.21	126.36	117.70
84	A6	957	U	C2-N1-C1'	7.21	126.35	117.70
2	A3	3228	U	N1-C2-O2	7.19	127.83	122.80
84	A6	714	U	N1-C2-O2	7.17	127.82	122.80
2	A3	1728	U	N3-C2-O2	-7.16	117.19	122.20
2	A3	2865	C	C2-N1-C1'	7.14	126.66	118.80
2	A3	3009	C	C2-N1-C1'	7.13	126.64	118.80
2	A3	1806	U	P-O3'-C3'	7.13	128.25	119.70
2	A3	2484	C	C2-N1-C1'	7.12	126.63	118.80
2	A3	2557	C	N3-C2-O2	-7.11	116.93	121.90
2	A3	2898	U	C2-N1-C1'	7.10	126.22	117.70
2	A3	3201	A	P-O3'-C3'	7.09	128.21	119.70
2	A3	2445	U	N1-C2-O2	7.06	127.74	122.80
2	A3	1835	A	O4'-C1'-N9	7.06	113.85	108.20
84	A6	1536	C	N1-C2-O2	7.05	123.13	118.90
2	A3	1837	C	N1-C2-O2	7.02	123.11	118.90
27	13	44	LEU	CA-CB-CG	7.01	131.44	115.30
84	A6	709	C	C6-N1-C2	-7.00	117.50	120.30
2	A3	2386	C	C2-N1-C1'	6.97	126.47	118.80
2	A3	2205	U	C2-N1-C1'	6.94	126.02	117.70
84	A6	1346	C	C6-N1-C2	-6.91	117.54	120.30
84	A6	710	C	C2-N1-C1'	6.91	126.40	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A3	2080	U	N3-C2-O2	-6.86	117.39	122.20
2	A3	2205	U	N1-C2-O2	6.84	127.59	122.80
84	A6	1433	C	C6-N1-C1'	-6.84	112.59	120.80
2	A3	1902	C	N3-C2-O2	-6.82	117.12	121.90
2	A3	1714	C	N1-C2-O2	6.82	122.99	118.90
2	A3	2271	C	N1-C2-O2	6.81	122.99	118.90
2	A3	3169	C	C6-N1-C2	-6.79	117.58	120.30
2	A3	2235	C	N3-C2-O2	-6.79	117.15	121.90
2	A3	3228	U	C2-N1-C1'	6.78	125.83	117.70
84	A6	769	C	C6-N1-C1'	-6.75	112.70	120.80
2	A3	2386	C	N3-C2-O2	-6.74	117.18	121.90
2	A3	2493	C	N1-C2-O2	6.73	122.94	118.90
2	A3	2235	C	N1-C2-O2	6.72	122.94	118.90
84	A6	1447	U	N3-C2-O2	-6.72	117.50	122.20
2	A3	1807	U	P-O3'-C3'	6.72	127.76	119.70
2	A3	2235	C	C2-N1-C1'	6.72	126.19	118.80
84	A6	801	C	C6-N1-C2	-6.71	117.62	120.30
2	A3	2898	U	N3-C2-O2	-6.69	117.52	122.20
84	A6	1451	G	C6-C5-N7	-6.68	126.39	130.40
2	A3	2295	C	N3-C2-O2	-6.66	117.24	121.90
2	A3	3009	C	N3-C2-O2	-6.66	117.24	121.90
84	A6	1529	C	N3-C2-O2	-6.66	117.24	121.90
84	A6	714	U	N3-C2-O2	-6.61	117.57	122.20
2	A3	3228	U	N3-C2-O2	-6.60	117.58	122.20
2	A3	2066	C	C6-N1-C1'	-6.57	112.92	120.80
2	A3	2759	U	N3-C2-O2	-6.56	117.61	122.20
84	A6	797	C	N1-C2-O2	6.55	122.83	118.90
2	A3	1901	C	N1-C2-O2	6.51	122.80	118.90
2	A3	1693	C	C2-N1-C1'	6.50	125.95	118.80
2	A3	2183	C	C6-N1-C2	-6.50	117.70	120.30
2	A3	1813	C	N1-C2-O2	6.50	122.80	118.90
2	A3	1732	C	C6-N1-C1'	-6.47	113.03	120.80
2	A3	3134	C	C6-N1-C2	-6.47	117.71	120.30
2	A3	2909	G	N3-C4-N9	6.47	129.88	126.00
84	A6	1335	A	P-O3'-C3'	6.47	127.46	119.70
88	n	115	ALA	C-N-CA	6.46	137.84	121.70
84	A6	1381	C	N3-C2-O2	-6.45	117.38	121.90
2	A3	3212	C	C6-N1-C2	-6.44	117.72	120.30
2	A3	1701	U	N1-C2-O2	6.43	127.30	122.80
2	A3	2061	C	C2-N1-C1'	6.43	125.87	118.80
40	f3	150	LEU	CA-CB-CG	6.41	130.04	115.30
2	A3	1993	A	C8-N9-C4	-6.39	103.24	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A3	2079	C	C6-N1-C1'	-6.38	113.14	120.80
83	e6	147	PRO	N-CA-CB	6.38	110.96	103.30
84	A6	901	C	C6-N1-C2	-6.38	117.75	120.30
2	A3	2295	C	N1-C2-O2	6.37	122.72	118.90
2	A3	1693	C	N1-C2-O2	6.37	122.72	118.90
2	A3	2417	C	N1-C2-O2	6.36	122.72	118.90
2	A3	2499	U	N1-C2-O2	6.33	127.23	122.80
2	A3	1715	C	C2-N1-C1'	6.33	125.77	118.80
84	A6	1250	U	OP2-P-O3'	6.33	119.12	105.20
2	A3	2235	C	C6-N1-C2	-6.30	117.78	120.30
84	A6	1193	U	N1-C2-O2	6.28	127.19	122.80
2	A3	2530	A	P-O3'-C3'	6.27	127.23	119.70
2	A3	3169	C	C5-C6-N1	6.27	124.14	121.00
84	A6	1346	C	N3-C2-O2	-6.26	117.52	121.90
2	A3	2493	C	N3-C2-O2	-6.25	117.52	121.90
85	C	48	U	C2-N1-C1'	6.25	125.20	117.70
85	24	48	U	N1-C2-O2	6.25	127.17	122.80
85	C	48	U	N1-C2-O2	6.25	127.17	122.80
2	A3	2522	U	C5-C6-N1	6.25	125.82	122.70
2	A3	1993	A	N7-C8-N9	6.24	116.92	113.80
85	24	48	U	C2-N1-C1'	6.24	125.19	117.70
87	A	50	LEU	CA-CB-CG	6.24	129.66	115.30
84	A6	1250	U	P-O3'-C3'	6.22	127.17	119.70
84	A6	936	C	C2-N1-C1'	6.19	125.61	118.80
2	A3	2135	A	C2-N3-C4	6.19	113.69	110.60
84	A6	769	C	N3-C2-O2	-6.18	117.57	121.90
2	A3	2205	U	N3-C2-O2	-6.17	117.88	122.20
2	A3	2499	U	C2-N1-C1'	6.17	125.10	117.70
2	A3	1732	C	C5-C6-N1	6.16	124.08	121.00
2	A3	2375	C	C5-C6-N1	6.16	124.08	121.00
84	A6	1006	C	N1-C2-O2	6.15	122.59	118.90
2	A3	2909	G	C4-N9-C1'	6.14	134.48	126.50
84	A6	1394	A	C8-N9-C4	-6.13	103.35	105.80
84	A6	1451	G	N3-C4-C5	-6.11	125.55	128.60
2	A3	2386	C	C6-N1-C2	-6.10	117.86	120.30
84	A6	1170	A	P-O3'-C3'	6.10	127.02	119.70
2	A3	3204	C	C6-N1-C2	-6.10	117.86	120.30
2	A3	2898	U	N1-C2-O2	6.10	127.07	122.80
3	B3	1668	U	C5-C6-N1	6.10	125.75	122.70
2	A3	2324	U	N1-C2-O2	6.08	127.06	122.80
2	A3	2096	U	C2-N1-C1'	6.08	124.99	117.70
84	A6	1447	U	N1-C2-O2	6.06	127.04	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A3	2523	C	N3-C2-O2	-6.05	117.67	121.90
2	A3	1699	C	N1-C2-O2	6.05	122.53	118.90
2	A3	1837	C	N3-C2-O2	-6.05	117.67	121.90
84	A6	1447	U	C2-N1-C1'	6.05	124.96	117.70
2	A3	3093	C	N1-C2-O2	6.03	122.52	118.90
84	A6	1433	C	P-O3'-C3'	6.03	126.94	119.70
85	C	48	U	N3-C2-O2	-6.02	117.99	122.20
2	A3	2165	C	C6-N1-C2	-6.01	117.89	120.30
85	24	48	U	N3-C2-O2	-6.01	117.99	122.20
84	A6	1193	U	N3-C2-O2	-6.01	118.00	122.20
2	A3	2789	C	P-O3'-C3'	6.00	126.90	119.70
84	A6	1193	U	P-O3'-C3'	5.99	126.89	119.70
84	A6	1025	U	P-O3'-C3'	5.99	126.89	119.70
2	A3	2484	C	N1-C2-O2	5.98	122.49	118.90
84	A6	1346	C	C5-C6-N1	5.98	123.99	121.00
2	A3	2852	C	N1-C2-O2	5.97	122.48	118.90
2	A3	1837	C	C6-N1-C2	-5.96	117.92	120.30
2	A3	2530	A	OP2-P-O3'	5.96	118.30	105.20
2	A3	3204	C	C6-N1-C1'	-5.96	113.65	120.80
2	A3	1715	C	N3-C2-O2	-5.95	117.73	121.90
42	h3	64	GLU	CA-CB-CG	5.95	126.49	113.40
84	A6	857	C	N1-C2-O2	5.93	122.46	118.90
2	A3	3056	C	C6-N1-C2	-5.93	117.93	120.30
2	A3	2079	C	C6-N1-C2	-5.93	117.93	120.30
2	A3	1699	C	C2-N1-C1'	5.93	125.32	118.80
2	A3	1837	C	C6-N1-C1'	-5.92	113.69	120.80
2	A3	1993	A	C2-N3-C4	5.92	113.56	110.60
84	A6	710	C	N1-C2-O2	5.92	122.45	118.90
2	A3	2852	C	C2-N1-C1'	5.92	125.31	118.80
2	A3	1813	C	C6-N1-C2	-5.91	117.94	120.30
2	A3	2759	U	C2-N1-C1'	5.89	124.77	117.70
2	A3	1901	C	C2-N1-C1'	5.89	125.28	118.80
2	A3	3212	C	C6-N1-C1'	-5.87	113.76	120.80
84	A6	957	U	N3-C2-O2	-5.86	118.10	122.20
2	A3	2372	U	C2-N1-C1'	5.86	124.73	117.70
2	A3	2186	C	N3-C2-O2	-5.85	117.80	121.90
31	53	270	ILE	CG1-CB-CG2	-5.85	98.53	111.40
84	A6	1373	U	N3-C2-O2	-5.85	118.11	122.20
2	A3	3170	C	C2-N1-C1'	5.85	125.23	118.80
2	A3	1902	C	C6-N1-C1'	-5.84	113.79	120.80
2	A3	1807	U	C2-N1-C1'	5.84	124.70	117.70
2	A3	2770	C	C6-N1-C2	-5.83	117.97	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	A6	1160	C	N1-C2-O2	5.82	122.39	118.90
2	A3	1689	C	C2-N1-C1'	5.82	125.20	118.80
85	C	40	U	N3-C2-O2	-5.82	118.13	122.20
23	X3	101	LEU	CA-CB-CG	5.81	128.67	115.30
88	n	108	MET	CA-CB-CG	5.80	123.17	113.30
2	A3	1809	U	P-O3'-C3'	5.80	126.66	119.70
2	A3	2282	C	N3-C2-O2	-5.80	117.84	121.90
84	A6	1373	U	C2-N1-C1'	5.80	124.66	117.70
2	A3	1689	C	N1-C2-O2	5.79	122.38	118.90
84	A6	1250	U	N3-C2-O2	-5.79	118.15	122.20
2	A3	2061	C	N1-C2-O2	5.78	122.37	118.90
85	24	40	U	N3-C2-O2	-5.78	118.16	122.20
84	A6	1541	C	P-O3'-C3'	5.77	126.63	119.70
84	A6	1370	C	C5-C6-N1	5.77	123.88	121.00
2	A3	2493	C	C6-N1-C1'	-5.76	113.89	120.80
84	A6	1069	C	N1-C2-O2	5.76	122.35	118.90
2	A3	2909	G	C8-N9-C1'	-5.75	119.53	127.00
84	A6	1373	U	N1-C2-O2	5.75	126.83	122.80
2	A3	2523	C	C5-C6-N1	5.74	123.87	121.00
84	A6	1156	A	C4-N9-C1'	5.73	136.62	126.30
84	A6	797	C	C6-N1-C1'	-5.73	113.92	120.80
84	A6	1381	C	C6-N1-C1'	-5.73	113.92	120.80
2	A3	2445	U	N3-C2-O2	-5.73	118.19	122.20
2	A3	2628	U	P-O3'-C3'	5.73	126.58	119.70
2	A3	1714	C	N3-C2-O2	-5.73	117.89	121.90
84	A6	1193	U	OP1-P-O3'	5.72	117.79	105.20
84	A6	728	C	C6-N1-C2	-5.71	118.01	120.30
84	A6	1370	C	C6-N1-C2	-5.71	118.01	120.30
84	A6	1419	G	P-O3'-C3'	5.71	126.55	119.70
84	A6	818	A	C4-N9-C1'	5.70	136.57	126.30
2	A3	2559	U	P-O3'-C3'	5.70	126.53	119.70
84	A6	1006	C	C6-N1-C2	-5.69	118.02	120.30
84	A6	1230	C	C6-N1-C2	-5.69	118.03	120.30
84	A6	1074	C	N3-C2-O2	-5.68	117.92	121.90
2	A3	2653	C	C6-N1-C2	-5.68	118.03	120.30
2	A3	2215	C	C6-N1-C2	-5.68	118.03	120.30
2	A3	3164	C	N1-C2-O2	5.66	122.30	118.90
84	A6	1193	U	C2-N1-C1'	5.66	124.49	117.70
2	A3	2952	U	N3-C2-O2	-5.62	118.27	122.20
2	A3	2499	U	N3-C2-O2	-5.62	118.27	122.20
3	B3	1663	C	C6-N1-C2	-5.61	118.06	120.30
84	A6	1155	C	N1-C2-O2	5.61	122.27	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A3	2282	C	N1-C2-O2	5.61	122.27	118.90
2	A3	3170	C	N3-C2-O2	-5.61	117.97	121.90
2	A3	1993	A	C4-N9-C1'	5.61	136.39	126.30
8	I3	174	LEU	CA-CB-CG	5.60	128.19	115.30
84	A6	1433	C	C5-C6-N1	5.60	123.80	121.00
2	A3	2699	C	C6-N1-C2	-5.60	118.06	120.30
84	A6	906	G	N3-C4-C5	-5.59	125.80	128.60
84	A6	1155	C	N3-C2-O2	-5.59	117.99	121.90
84	A6	1074	C	N1-C2-O2	5.58	122.25	118.90
32	63	229	ASP	CB-CG-OD1	5.57	123.32	118.30
84	A6	683	C	N1-C2-O2	5.57	122.24	118.90
84	A6	721	G	P-O3'-C3'	5.56	126.37	119.70
2	A3	3119	C	N1-C2-O2	5.55	122.23	118.90
2	A3	3187	C	C6-N1-C2	-5.55	118.08	120.30
2	A3	2080	U	C6-N1-C1'	-5.55	113.43	121.20
84	A6	1297	C	N1-C2-O2	5.53	122.22	118.90
84	A6	1025	U	OP2-P-O3'	5.52	117.35	105.20
2	A3	2889	C	C5-C6-N1	5.52	123.76	121.00
2	A3	2243	A	P-O3'-C3'	5.51	126.31	119.70
42	h3	63	PRO	C-N-CA	5.50	135.45	121.70
2	A3	2209	G	P-O3'-C3'	5.49	126.29	119.70
84	A6	1233	U	N3-C2-O2	-5.48	118.36	122.20
2	A3	3057	C	N1-C2-O2	5.48	122.19	118.90
84	A6	957	U	N1-C2-O2	5.46	126.62	122.80
2	A3	1701	U	N3-C2-O2	-5.46	118.38	122.20
2	A3	2324	U	N3-C2-O2	-5.46	118.38	122.20
2	A3	1823	A	P-O3'-C3'	5.45	126.25	119.70
84	A6	1208	C	N1-C2-O2	5.45	122.17	118.90
2	A3	2865	C	C6-N1-C1'	-5.43	114.28	120.80
84	A6	1451	G	C5-C6-O6	-5.42	125.35	128.60
2	A3	2889	C	C6-N1-C2	-5.41	118.14	120.30
2	A3	2417	C	N3-C2-O2	-5.41	118.11	121.90
84	A6	714	U	C6-N1-C1'	-5.41	113.62	121.20
2	A3	2952	U	N1-C2-O2	5.41	126.58	122.80
84	A6	1198	C	C6-N1-C2	-5.40	118.14	120.30
2	A3	2684	C	N1-C2-O2	5.39	122.14	118.90
84	A6	710	C	N3-C2-O2	-5.39	118.12	121.90
84	A6	1451	G	C4-C5-N7	5.39	112.96	110.80
43	i3	63	LEU	CA-CB-CG	5.39	127.69	115.30
84	A6	906	G	N3-C4-N9	5.39	129.23	126.00
2	A3	2210	C	O5'-P-OP1	5.38	117.16	110.70
2	A3	2271	C	N3-C2-O2	-5.38	118.14	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A3	2557	C	C6-N1-C1'	-5.38	114.35	120.80
2	A3	2909	G	C6-C5-N7	-5.37	127.18	130.40
84	A6	797	C	N3-C2-O2	-5.37	118.14	121.90
2	A3	2441	C	N1-C2-O2	5.36	122.12	118.90
2	A3	2655	G	O4'-C1'-N9	-5.36	103.91	108.20
2	A3	3065	U	N1-C2-O2	5.36	126.55	122.80
85	C	40	U	N1-C2-O2	5.35	126.54	122.80
2	A3	2215	C	C2-N1-C1'	5.34	124.67	118.80
85	C	61	U	C5-C6-N1	5.34	125.37	122.70
2	A3	3041	U	P-O3'-C3'	5.33	126.10	119.70
2	A3	1807	U	N1-C2-O2	5.33	126.53	122.80
2	A3	2282	C	C2-N1-C1'	5.32	124.65	118.80
2	A3	3212	C	C5-C6-N1	5.31	123.66	121.00
2	A3	2523	C	C6-N1-C1'	-5.31	114.43	120.80
84	A6	715	U	N1-C2-O2	5.31	126.52	122.80
2	A3	2780	C	N1-C2-O2	5.30	122.08	118.90
84	A6	801	C	C5-C6-N1	5.30	123.65	121.00
85	24	61	U	C5-C6-N1	5.30	125.35	122.70
2	A3	2374	A	P-O3'-C3'	5.29	126.05	119.70
2	A3	3083	U	N1-C2-O2	5.29	126.50	122.80
2	A3	2558	A	P-O3'-C3'	5.28	126.04	119.70
85	24	40	U	N1-C2-O2	5.28	126.50	122.80
84	A6	806	C	C6-N1-C2	-5.28	118.19	120.30
42	h3	64	GLU	C-N-CA	5.25	134.81	121.70
84	A6	1006	C	N3-C2-O2	-5.25	118.23	121.90
2	A3	3119	C	N3-C2-O2	-5.24	118.23	121.90
84	A6	857	C	N3-C2-O2	-5.24	118.23	121.90
2	A3	1699	C	N3-C2-O2	-5.23	118.24	121.90
2	A3	2523	C	C6-N1-C2	-5.23	118.21	120.30
20	U3	9	LEU	CB-CG-CD2	-5.23	102.11	111.00
2	A3	2135	A	C4-N9-C1'	5.22	135.70	126.30
2	A3	2445	U	C6-N1-C1'	-5.20	113.92	121.20
2	A3	3164	C	N3-C2-O2	-5.19	118.27	121.90
84	A6	916	U	C2-N1-C1'	5.18	123.92	117.70
2	A3	1837	C	O4'-C1'-N1	5.18	112.35	108.20
58	F6	162	LEU	CA-CB-CG	5.18	127.22	115.30
2	A3	2443	C	N1-C2-O2	5.18	122.01	118.90
2	A3	1837	C	C5-C6-N1	5.18	123.59	121.00
13	N3	237	HIS	C-N-CA	5.17	134.63	121.70
67	O6	55	PRO	C-N-CA	5.17	134.61	121.70
2	A3	1689	C	N3-C2-O2	-5.16	118.29	121.90
2	A3	2061	C	C6-N1-C1'	-5.16	114.61	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A3	3206	C	C2-N1-C1'	5.16	124.47	118.80
2	A3	2183	C	C5-C6-N1	5.15	123.57	121.00
84	A6	1541	C	N3-C2-O2	-5.15	118.30	121.90
84	A6	1541	C	C6-N1-C2	-5.14	118.24	120.30
2	A3	3057	C	N3-C2-O2	-5.14	118.30	121.90
2	A3	1701	U	C6-N1-C1'	-5.14	114.00	121.20
84	A6	709	C	C6-N1-C1'	-5.14	114.63	120.80
2	A3	2064	A	N1-C6-N6	-5.14	115.52	118.60
2	A3	2421	G	C6-C5-N7	-5.13	127.32	130.40
2	A3	3065	U	N3-C2-O2	-5.13	118.61	122.20
84	A6	1297	C	C2-N1-C1'	5.13	124.44	118.80
2	A3	1725	C	N1-C2-O2	5.12	121.97	118.90
84	A6	906	G	C4-N9-C1'	5.12	133.16	126.50
84	A6	969	C	N1-C2-O2	5.12	121.97	118.90
2	A3	3041	U	OP1-P-O3'	5.12	116.46	105.20
76	X6	344	LEU	CA-CB-CG	5.12	127.07	115.30
84	A6	1156	A	C2-N3-C4	5.12	113.16	110.60
2	A3	3134	C	C5-C6-N1	5.11	123.56	121.00
2	A3	2789	C	OP1-P-O3'	5.11	116.43	105.20
2	A3	3092	U	P-O3'-C3'	5.11	125.83	119.70
2	A3	2295	C	C2-N1-C1'	5.10	124.41	118.80
2	A3	2999	C	C6-N1-C2	-5.10	118.26	120.30
2	A3	3206	C	N1-C2-O2	5.09	121.96	118.90
2	A3	2484	C	N3-C2-O2	-5.09	118.34	121.90
84	A6	936	C	N1-C2-O2	5.08	121.95	118.90
84	A6	977	C	C6-N1-C2	-5.08	118.27	120.30
2	A3	3201	A	C4-N9-C1'	5.07	135.42	126.30
84	A6	1088	C	N1-C2-O2	5.07	121.94	118.90
84	A6	1124	C	N1-C2-O2	5.05	121.93	118.90
2	A3	2379	C	C2-N1-C1'	5.05	124.35	118.80
84	A6	726	C	N1-C2-O2	5.05	121.93	118.90
3	B3	1607	U	P-O3'-C3'	5.04	125.75	119.70
84	A6	1006	C	C5-C6-N1	5.04	123.52	121.00
84	A6	1529	C	C6-N1-C2	-5.03	118.29	120.30
2	A3	2171	U	N1-C2-O2	5.03	126.32	122.80
2	A3	2952	U	C2-N1-C1'	5.03	123.73	117.70
2	A3	2329	C	N1-C2-O2	5.02	121.91	118.90
76	X6	96	GLU	C-N-CA	5.02	134.26	121.70
56	D6	148	LEU	CA-CB-CG	5.02	126.84	115.30
2	A3	2889	C	N1-C2-O2	5.02	121.91	118.90
84	A6	728	C	C5-C6-N1	5.02	123.51	121.00
84	A6	1233	U	C2-N1-C1'	5.01	123.71	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	A6	1212	U	N3-C2-O2	-5.01	118.69	122.20

There are no chirality outliers.

All (69) 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
34	93	132	PRO	Peptide
34	93	45	THR	Peptide
87	A	184	ASN	Peptide
87	A	185	TYR	Peptide
87	A	196	THR	Peptide
87	A	197	LYS	Peptide
4	D3	206	TYR	Peptide
56	D6	284	ARG	Peptide
56	D6	285	TYR	Peptide
56	D6	286	GLU	Peptide
5	E3	126	ASP	Peptide
5	E3	169	GLY	Peptide
5	E3	244	ALA	Peptide
5	E3	315	PRO	Peptide
5	E3	326	GLU	Peptide
5	E3	85	TRP	Peptide
6	F3	129	PRO	Peptide
7	H3	63	PRO	Peptide
9	J3	144	ILE	Peptide
62	J6	129	LYS	Peptide
62	J6	130	TYR	Peptide
10	K3	3	SER	Peptide
10	K3	5	SER	Peptide
63	K6	64	PRO	Peptide
12	M3	109	ARG	Peptide
12	M3	20	PRO	Peptide
12	M3	264	GLN	Peptide
12	M3	287	ASP	Peptide
67	O6	55	PRO	Peptide
16	Q3	182	ARG	Peptide
17	R3	137	GLU	Peptide
70	R6	154	THR	Peptide
70	R6	265	THR	Peptide

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Mol	Chain	Res	Type	Group
70	R6	291	ARG	Peptide
71	S6	107	GLN	Peptide
21	V3	100	LYS	Peptide
21	V3	170	TRP	Peptide
74	V6	155	GLU	Peptide
74	V6	196	PHE	Peptide
74	V6	41	GLU	Peptide
22	W3	72	HIS	Peptide
75	W6	107	ILE	Peptide
23	X3	51	LYS	Peptide
23	X3	94	ASN	Peptide
23	X3	95	ASP	Peptide
76	X6	66	GLN	Peptide
76	X6	96	GLU	Peptide
1	Y2	22	ALA	Peptide
77	Y6	339	GLU	Peptide
25	Z3	141	SER	Peptide
81	c6	60	GLU	Peptide
38	d3	230	ARG	Peptide
38	d3	271	PRO	Peptide
39	e3	173	LEU	Peptide
83	e6	67	LYS	Peptide
40	f3	189	HIS	Peptide
40	f3	49	LYS	Peptide
40	f3	50	THR	Peptide
40	f3	87	GLU	Peptide
41	g3	110	ILE	Peptide
42	h3	138	SER	Peptide
42	h3	63	PRO	Peptide
43	i3	57	TYR	Peptide
45	k3	36	THR	Peptide
48	o3	82	PHE	Peptide
50	q3	78	SER	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%)	18 (67%)	9 (33%)	0	100	100
4	D3	234/305 (77%)	213 (91%)	21 (9%)	0	100	100
5	E3	296/348 (85%)	263 (89%)	32 (11%)	1 (0%)	37	72
6	F3	248/311 (80%)	228 (92%)	20 (8%)	0	100	100
7	D	78/267 (29%)	66 (85%)	12 (15%)	0	100	100
7	H3	93/267 (35%)	86 (92%)	7 (8%)	0	100	100
8	I3	154/261 (59%)	148 (96%)	6 (4%)	0	100	100
9	J3	138/192 (72%)	125 (91%)	13 (9%)	0	100	100
10	K3	175/178 (98%)	149 (85%)	24 (14%)	2 (1%)	12	46
11	L3	113/145 (78%)	103 (91%)	10 (9%)	0	100	100
12	M3	285/296 (96%)	264 (93%)	19 (7%)	2 (1%)	19	56
13	N3	203/251 (81%)	189 (93%)	13 (6%)	1 (0%)	25	63
14	O3	150/175 (86%)	134 (89%)	15 (10%)	1 (1%)	19	56
15	P3	129/180 (72%)	118 (92%)	11 (8%)	0	100	100
16	Q3	217/292 (74%)	188 (87%)	28 (13%)	1 (0%)	25	63
17	R3	138/149 (93%)	129 (94%)	9 (6%)	0	100	100
18	S3	154/205 (75%)	138 (90%)	16 (10%)	0	100	100
19	T3	164/206 (80%)	152 (93%)	12 (7%)	0	100	100
20	U3	109/153 (71%)	97 (89%)	12 (11%)	0	100	100
21	V3	183/216 (85%)	158 (86%)	23 (13%)	2 (1%)	12	46
22	W3	109/148 (74%)	100 (92%)	9 (8%)	0	100	100
23	X3	241/256 (94%)	214 (89%)	26 (11%)	1 (0%)	30	67
24	Y3	174/250 (70%)	164 (94%)	10 (6%)	0	100	100
25	Z3	118/161 (73%)	106 (90%)	12 (10%)	0	100	100
26	03	106/188 (56%)	88 (83%)	17 (16%)	1 (1%)	14	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	13	50/65 (77%)	46 (92%)	4 (8%)	0	100	100
28	23	44/92 (48%)	41 (93%)	3 (7%)	0	100	100
29	33	93/188 (50%)	90 (97%)	3 (3%)	0	100	100
30	43	34/103 (33%)	33 (97%)	1 (3%)	0	100	100
31	53	368/423 (87%)	322 (88%)	43 (12%)	3 (1%)	16	53
32	63	313/380 (82%)	267 (85%)	46 (15%)	0	100	100
33	73	258/338 (76%)	232 (90%)	26 (10%)	0	100	100
34	93	105/137 (77%)	93 (89%)	12 (11%)	0	100	100
35	a3	78/142 (55%)	75 (96%)	3 (4%)	0	100	100
36	b3	146/215 (68%)	130 (89%)	16 (11%)	0	100	100
37	c3	271/332 (82%)	251 (93%)	19 (7%)	1 (0%)	30	67
38	d3	156/306 (51%)	141 (90%)	14 (9%)	1 (1%)	22	59
39	e3	211/279 (76%)	193 (92%)	18 (8%)	0	100	100
40	f3	125/212 (59%)	104 (83%)	20 (16%)	1 (1%)	16	53
41	g3	127/166 (76%)	117 (92%)	10 (8%)	0	100	100
42	h3	96/158 (61%)	81 (84%)	13 (14%)	2 (2%)	5	30
43	i3	95/128 (74%)	83 (87%)	12 (13%)	0	100	100
44	j3	83/123 (68%)	75 (90%)	7 (8%)	1 (1%)	11	43
45	k3	82/112 (73%)	66 (80%)	15 (18%)	1 (1%)	11	43
46	l3	21/138 (15%)	19 (90%)	2 (10%)	0	100	100
47	m3	43/128 (34%)	38 (88%)	5 (12%)	0	100	100
48	o3	92/102 (90%)	86 (94%)	6 (6%)	0	100	100
49	p3	119/206 (58%)	115 (97%)	4 (3%)	0	100	100
50	q3	126/222 (57%)	115 (91%)	8 (6%)	3 (2%)	5	28
51	r3	140/196 (71%)	122 (87%)	18 (13%)	0	100	100
52	s3	366/467 (78%)	341 (93%)	25 (7%)	0	100	100
53	A5	26/28 (93%)	19 (73%)	7 (27%)	0	100	100
54	B6	215/296 (73%)	197 (92%)	18 (8%)	0	100	100
55	C6	130/167 (78%)	120 (92%)	10 (8%)	0	100	100
56	D6	316/430 (74%)	293 (93%)	22 (7%)	1 (0%)	37	72
57	E6	120/125 (96%)	110 (92%)	9 (8%)	1 (1%)	16	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
58	F6	197/242 (81%)	187 (95%)	10 (5%)	0	100	100
59	G6	301/396 (76%)	276 (92%)	25 (8%)	0	100	100
60	H6	120/201 (60%)	104 (87%)	15 (12%)	1 (1%)	16	53
61	I6	134/194 (69%)	122 (91%)	12 (9%)	0	100	100
62	J6	106/138 (77%)	95 (90%)	11 (10%)	0	100	100
63	K6	99/128 (77%)	95 (96%)	4 (4%)	0	100	100
64	L6	162/257 (63%)	151 (93%)	11 (7%)	0	100	100
65	M6	114/137 (83%)	106 (93%)	8 (7%)	0	100	100
66	N6	105/130 (81%)	92 (88%)	13 (12%)	0	100	100
67	O6	183/258 (71%)	164 (90%)	18 (10%)	1 (0%)	25	63
68	P6	94/142 (66%)	85 (90%)	9 (10%)	0	100	100
69	Q6	84/87 (97%)	74 (88%)	10 (12%)	0	100	100
70	R6	240/360 (67%)	207 (86%)	32 (13%)	1 (0%)	30	67
71	S6	124/190 (65%)	114 (92%)	10 (8%)	0	100	100
72	T6	160/173 (92%)	149 (93%)	11 (7%)	0	100	100
73	U6	171/205 (83%)	159 (93%)	12 (7%)	0	100	100
74	V6	320/414 (77%)	284 (89%)	35 (11%)	1 (0%)	37	72
75	W6	95/187 (51%)	82 (86%)	12 (13%)	1 (1%)	12	46
76	X6	310/398 (78%)	268 (86%)	40 (13%)	2 (1%)	22	59
77	Y6	106/395 (27%)	94 (89%)	12 (11%)	0	100	100
78	Z6	85/106 (80%)	80 (94%)	5 (6%)	0	100	100
79	a6	197/218 (90%)	176 (89%)	21 (11%)	0	100	100
80	b6	252/323 (78%)	217 (86%)	35 (14%)	0	100	100
81	c6	114/118 (97%)	100 (88%)	14 (12%)	0	100	100
82	d6	67/199 (34%)	63 (94%)	4 (6%)	0	100	100
83	e6	362/689 (52%)	334 (92%)	22 (6%)	6 (2%)	7	36
87	A	158/206 (77%)	140 (89%)	18 (11%)	0	100	100
88	n	230/229 (100%)	211 (92%)	19 (8%)	0	100	100
All	All	13175/18553 (71%)	11882 (90%)	1253 (10%)	40 (0%)	38	72

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
83	e6	68	VAL
12	M3	265	ILE
21	V3	101	THR
23	X3	52	ILE
31	53	270	ILE
50	q3	43	GLU
70	R6	266	ARG
83	e6	67	LYS
83	e6	147	PRO
16	Q3	183	LEU
44	j3	35	ALA
60	H6	126	ILE
74	V6	197	SER
75	W6	109	GLU
76	X6	97	ALA
76	X6	342	PRO
12	M3	288	GLU
21	V3	194	LEU
26	03	178	ASP
38	d3	231	LEU
42	h3	66	LEU
42	h3	138	SER
56	D6	287	ASP
83	e6	69	ALA
10	K3	4	PHE
10	K3	160	GLN
13	N3	237	HIS
31	53	269	ASN
50	q3	42	PRO
31	53	349	GLY
37	c3	313	PRO
83	e6	299	GLU
5	E3	246	GLY
45	k3	37	VAL
57	E6	15	ARG
67	O6	132	GLY
40	f3	51	LYS
50	q3	79	PRO
83	e6	146	GLU
14	O3	111	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%)	86 90
5	E3	255/290 (88%)	254 (100%)	1 (0%)	89 91
6	F3	217/262 (83%)	213 (98%)	4 (2%)	54 71
7	D	73/228 (32%)	73 (100%)	0	100 100
7	H3	86/228 (38%)	84 (98%)	2 (2%)	45 65
8	I3	145/232 (62%)	145 (100%)	0	100 100
9	J3	113/150 (75%)	112 (99%)	1 (1%)	75 83
10	K3	155/156 (99%)	154 (99%)	1 (1%)	84 88
11	L3	98/124 (79%)	98 (100%)	0	100 100
12	M3	245/249 (98%)	241 (98%)	4 (2%)	58 74
13	N3	172/211 (82%)	171 (99%)	1 (1%)	84 88
14	O3	133/150 (89%)	133 (100%)	0	100 100
15	P3	115/155 (74%)	115 (100%)	0	100 100
16	Q3	201/256 (78%)	201 (100%)	0	100 100
17	R3	118/126 (94%)	118 (100%)	0	100 100
18	S3	141/180 (78%)	141 (100%)	0	100 100
19	T3	146/176 (83%)	145 (99%)	1 (1%)	81 87
20	U3	99/135 (73%)	95 (96%)	4 (4%)	27 48
21	V3	169/191 (88%)	164 (97%)	5 (3%)	36 57
22	W3	91/119 (76%)	90 (99%)	1 (1%)	70 80
23	X3	217/227 (96%)	216 (100%)	1 (0%)	86 90
24	Y3	159/223 (71%)	159 (100%)	0	100 100
25	Z3	111/147 (76%)	111 (100%)	0	100 100
26	03	97/164 (59%)	96 (99%)	1 (1%)	73 81
27	13	49/60 (82%)	48 (98%)	1 (2%)	50 69
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%)	335 (99%)	2 (1%)	84 88
32	63	266/332 (80%)	265 (100%)	1 (0%)	89 91
33	73	242/303 (80%)	242 (100%)	0	100 100
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%)	127 (98%)	3 (2%)	45 65
37	c3	241/288 (84%)	241 (100%)	0	100 100
38	d3	151/274 (55%)	149 (99%)	2 (1%)	65 77
39	e3	188/236 (80%)	187 (100%)	1 (0%)	86 90
40	f3	117/188 (62%)	115 (98%)	2 (2%)	56 72
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%)	84 (98%)	2 (2%)	45 65
44	j3	68/97 (70%)	68 (100%)	0	100 100
45	k3	74/90 (82%)	73 (99%)	1 (1%)	62 76
46	l3	23/116 (20%)	23 (100%)	0	100 100
47	m3	40/113 (35%)	39 (98%)	1 (2%)	42 62
48	o3	80/87 (92%)	80 (100%)	0	100 100
49	p3	117/181 (65%)	117 (100%)	0	100 100
50	q3	110/178 (62%)	110 (100%)	0	100 100
51	r3	133/169 (79%)	132 (99%)	1 (1%)	79 85
52	s3	326/381 (86%)	321 (98%)	5 (2%)	60 75
54	B6	191/249 (77%)	190 (100%)	1 (0%)	86 90
55	C6	115/143 (80%)	114 (99%)	1 (1%)	75 83
56	D6	269/357 (75%)	264 (98%)	5 (2%)	52 70
57	E6	104/107 (97%)	103 (99%)	1 (1%)	73 81
58	F6	178/209 (85%)	176 (99%)	2 (1%)	70 80
59	G6	265/342 (78%)	262 (99%)	3 (1%)	70 80
60	H6	112/180 (62%)	111 (99%)	1 (1%)	75 83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
61	I6	104/147 (71%)	102 (98%)	2 (2%)	52 70
62	J6	93/118 (79%)	93 (100%)	0	100 100
63	K6	91/113 (80%)	91 (100%)	0	100 100
64	L6	152/226 (67%)	152 (100%)	0	100 100
65	M6	95/113 (84%)	94 (99%)	1 (1%)	70 80
66	N6	93/115 (81%)	93 (100%)	0	100 100
67	O6	166/230 (72%)	166 (100%)	0	100 100
68	P6	87/123 (71%)	87 (100%)	0	100 100
69	Q6	78/79 (99%)	78 (100%)	0	100 100
70	R6	224/318 (70%)	223 (100%)	1 (0%)	89 91
71	S6	109/164 (66%)	109 (100%)	0	100 100
72	T6	150/157 (96%)	150 (100%)	0	100 100
73	U6	149/174 (86%)	148 (99%)	1 (1%)	81 87
74	V6	295/364 (81%)	292 (99%)	3 (1%)	73 81
75	W6	84/158 (53%)	84 (100%)	0	100 100
76	X6	275/351 (78%)	274 (100%)	1 (0%)	89 91
77	Y6	99/357 (28%)	97 (98%)	2 (2%)	50 69
78	Z6	80/95 (84%)	80 (100%)	0	100 100
79	a6	176/190 (93%)	174 (99%)	2 (1%)	70 80
80	b6	237/291 (81%)	235 (99%)	2 (1%)	79 85
81	c6	99/101 (98%)	96 (97%)	3 (3%)	36 57
82	d6	63/166 (38%)	63 (100%)	0	100 100
83	e6	226/609 (37%)	226 (100%)	0	100 100
87	A	151/190 (80%)	149 (99%)	2 (1%)	65 77
88	n	184/181 (102%)	181 (98%)	3 (2%)	58 74
All	All	11664/15966 (73%)	11577 (99%)	87 (1%)	80 87

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D3	254	LYS
5	E3	57	ASN
6	F3	193	LEU

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Mol	Chain	Res	Type
6	F3	222	THR
6	F3	274	LEU
6	F3	290	TYR
7	H3	59	TRP
7	H3	108	ARG
9	J3	92	LYS
10	K3	81	THR
12	M3	44	ARG
12	M3	128	THR
12	M3	134	ARG
12	M3	135	ASP
13	N3	83	THR
19	T3	211	THR
20	U3	11	ARG
20	U3	24	PHE
20	U3	49	THR
20	U3	91	ASP
21	V3	53	ASP
21	V3	61	THR
21	V3	105	ARG
21	V3	126	MET
21	V3	128	ARG
22	W3	129	THR
23	X3	44	ARG
26	03	86	THR
27	13	61	LYS
31	53	98	LEU
31	53	365	ASP
32	63	297	THR
36	b3	14	VAL
36	b3	72	VAL
36	b3	123	ASN
38	d3	263	THR
38	d3	266	VAL
39	e3	55	ARG
40	f3	50	THR
40	f3	96	THR
43	i3	32	ILE
43	i3	43	VAL
45	k3	36	THR
47	m3	72	ARG
51	r3	152	THR

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Mol	Chain	Res	Type
52	s3	52	THR
52	s3	159	ARG
52	s3	211	VAL
52	s3	230	ARG
52	s3	288	THR
54	B6	169	ARG
55	C6	89	ASP
56	D6	262	THR
56	D6	345	LEU
56	D6	372	GLU
56	D6	418	LYS
56	D6	419	ARG
57	E6	99	THR
58	F6	114	THR
58	F6	192	ARG
59	G6	230	THR
59	G6	389	ARG
59	G6	396	ARG
60	H6	79	LEU
61	I6	95	THR
61	I6	138	ARG
65	M6	29	ARG
70	R6	256	ARG
73	U6	32	ASP
74	V6	204	PHE
74	V6	250	ILE
74	V6	287	LEU
76	X6	69	ASN
77	Y6	305	THR
77	Y6	353	LEU
79	a6	29	ARG
79	a6	121	LYS
80	b6	145	LYS
80	b6	244	THR
81	c6	37	ARG
81	c6	62	ARG
81	c6	114	LYS
87	A	46	ARG
87	A	129	ARG
88	n	202[A]	GLU
88	n	202[B]	GLU
88	n	210	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (157) such sidechains are listed below:

Mol	Chain	Res	Type
4	D3	165	ASN
4	D3	233	GLN
4	D3	276	HIS
5	E3	52	HIS
5	E3	57	ASN
5	E3	115	GLN
6	F3	58	HIS
6	F3	98	GLN
6	F3	130	GLN
6	F3	153	HIS
6	F3	184	GLN
6	F3	249	ASN
7	H3	88	HIS
8	I3	189	GLN
9	J3	47	ASN
9	J3	126	GLN
10	K3	61	ASN
10	K3	64	HIS
12	M3	157	GLN
13	N3	138	HIS
13	N3	178	GLN
14	O3	128	ASN
15	P3	96	GLN
16	Q3	262	GLN
17	R3	89	ASN
18	S3	118	ASN
18	S3	140	ASN
19	T3	62	GLN
19	T3	125	GLN
20	U3	4	ASN
20	U3	41	GLN
20	U3	55	ASN
21	V3	73	GLN
21	V3	92	ASN
21	V3	117	HIS
22	W3	72	HIS
22	W3	80	HIS
22	W3	86	ASN
23	X3	76	GLN
23	X3	215	GLN
24	Y3	179	HIS

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Mol	Chain	Res	Type
24	Y3	225	ASN
25	Z3	95	HIS
25	Z3	126	GLN
26	03	118	GLN
26	03	170	GLN
28	23	57	ASN
28	23	77	GLN
30	43	100	GLN
31	53	65	HIS
31	53	338	GLN
31	53	384	GLN
31	53	420	HIS
32	63	351	HIS
32	63	354	GLN
34	93	123	GLN
34	93	134	ASN
35	a3	71	HIS
37	c3	168	HIS
37	c3	172	ASN
37	c3	192	GLN
38	d3	274	GLN
39	e3	199	ASN
40	f3	108	GLN
40	f3	115	ASN
40	f3	136	GLN
40	f3	153	HIS
40	f3	175	GLN
41	g3	102	HIS
41	g3	104	ASN
42	h3	119	GLN
42	h3	135	GLN
43	i3	86	ASN
43	i3	89	GLN
43	i3	124	HIS
45	k3	15	GLN
45	k3	57	HIS
48	o3	58	GLN
48	o3	85	HIS
48	o3	91	GLN
49	p3	104	HIS
49	p3	143	GLN
50	q3	81	GLN

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Mol	Chain	Res	Type
50	q3	137	GLN
51	r3	130	ASN
52	s3	152	GLN
52	s3	240	GLN
52	s3	315	ASN
54	B6	64	ASN
54	B6	69	HIS
54	B6	99	HIS
54	B6	120	GLN
54	B6	130	ASN
54	B6	134	HIS
54	B6	197	HIS
54	B6	201	ASN
54	B6	226	ASN
56	D6	155	GLN
56	D6	302	HIS
56	D6	415	GLN
58	F6	122	GLN
59	G6	127	HIS
59	G6	308	GLN
59	G6	366	GLN
60	H6	130	HIS
60	H6	179	GLN
61	I6	141	GLN
61	I6	146	HIS
62	J6	74	ASN
67	O6	181	HIS
68	P6	71	HIS
69	Q6	4	HIS
69	Q6	27	ASN
70	R6	139	ASN
70	R6	214	ASN
70	R6	221	GLN
70	R6	277	ASN
71	S6	97	GLN
73	U6	43	ASN
73	U6	61	GLN
73	U6	117	HIS
74	V6	97	HIS
74	V6	131	ASN
74	V6	170	GLN
74	V6	203	ASN

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Mol	Chain	Res	Type
75	W6	86	HIS
75	W6	166	ASN
76	X6	81	HIS
76	X6	266	ASN
76	X6	299	ASN
76	X6	312	GLN
76	X6	387	ASN
77	Y6	290	ASN
77	Y6	296	ASN
77	Y6	303	GLN
77	Y6	331	HIS
78	Z6	54	ASN
78	Z6	82	GLN
79	a6	66	GLN
80	b6	165	ASN
80	b6	268	GLN
80	b6	301	ASN
81	c6	24	ASN
81	c6	71	GLN
81	c6	81	GLN
82	d6	129	ASN
82	d6	158	GLN
82	d6	166	GLN
83	e6	79	ASN
83	e6	129	GLN
83	e6	455	ASN
87	A	143	GLN
87	A	158	HIS
88	n	56	GLN
88	n	66	HIS
88	n	101	GLN
7	D	185	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	A3	1490/1559 (95%)	452 (30%)	29 (1%)
3	B3	51/69 (73%)	18 (35%)	1 (1%)
84	A6	921/954 (96%)	243 (26%)	16 (1%)
85	24	73/73 (100%)	40 (54%)	1 (1%)
85	C	73/73 (100%)	40 (54%)	1 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
86	i4	9/10 (90%)	4 (44%)	0
All	All	2617/2738 (95%)	797 (30%)	48 (1%)

All (797) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	A3	1672	C
2	A3	1674	A
2	A3	1676	A
2	A3	1678	C
2	A3	1679	U
2	A3	1680	A
2	A3	1681	G
2	A3	1689	C
2	A3	1690	C
2	A3	1693	C
2	A3	1694	U
2	A3	1699	C
2	A3	1700	U
2	A3	1701	U
2	A3	1704	U
2	A3	1705	A
2	A3	1708	A
2	A3	1709	G
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	1732	C
2	A3	1748	G
2	A3	1750	G
2	A3	1751	A
2	A3	1767	G
2	A3	1770	G
2	A3	1774	U
2	A3	1777	A
2	A3	1779	A
2	A3	1780	U

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Mol	Chain	Res	Type
2	A3	1781	A
2	A3	1794	A
2	A3	1804	A
2	A3	1805	A
2	A3	1806	U
2	A3	1807	U
2	A3	1808	A
2	A3	1809	U
2	A3	1810	A
2	A3	1811	A
2	A3	1812	C
2	A3	1821	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	1846	C
2	A3	1852	C
2	A3	1854	U
2	A3	1856	A
2	A3	1867	A
2	A3	1869	A
2	A3	1870	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	1886	G
2	A3	1887	A
2	A3	1888	G
2	A3	1890	C
2	A3	1893	A
2	A3	1901	C
2	A3	1902	C
2	A3	1903	C
2	A3	1909	A
2	A3	1918	G

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Mol	Chain	Res	Type
2	A3	1939	G
2	A3	1940	A
2	A3	1944	C
2	A3	1956	U
2	A3	1966	G
2	A3	1968	G
2	A3	1970	G
2	A3	1974	A
2	A3	1975	U
2	A3	1985	G
2	A3	1987	G
2	A3	1992	C
2	A3	1993	A
2	A3	1994	A
2	A3	1995	A
2	A3	1998	U
2	A3	2000	C
2	A3	2001	C
2	A3	2002	G
2	A3	2010	U
2	A3	2015	G
2	A3	2021	U
2	A3	2022	G
2	A3	2029	A
2	A3	2031	A
2	A3	2032	G
2	A3	2034	A
2	A3	2036	C
2	A3	2037	U
2	A3	2039	A
2	A3	2055	U
2	A3	2060	A
2	A3	2065	A
2	A3	2074	A
2	A3	2079	C
2	A3	2083	U
2	A3	2085	A
2	A3	2092	C
2	A3	2093	U
2	A3	2097	A
2	A3	2098	G
2	A3	2099	U

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Mol	Chain	Res	Type
2	A3	2105	G
2	A3	2111	C
2	A3	2113	G
2	A3	2124	A
2	A3	2132	A
2	A3	2135	A
2	A3	2139	U
2	A3	2140	G
2	A3	2142	A
2	A3	2143	G
2	A3	2147	G
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	2168	U
2	A3	2169	A
2	A3	2171	U
2	A3	2172	A
2	A3	2173	G
2	A3	2174	G
2	A3	2177	U
2	A3	2179	A
2	A3	2180	A
2	A3	2181	A
2	A3	2183	C
2	A3	2187	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	2202	C
2	A3	2204	U
2	A3	2207	A
2	A3	2209	G
2	A3	2210	C
2	A3	2216	A

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Mol	Chain	Res	Type
2	A3	2217	C
2	A3	2229	A
2	A3	2230	A
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
2	A3	2283	C
2	A3	2284	C
2	A3	2285	U
2	A3	2290	A
2	A3	2294	A
2	A3	2296	U
2	A3	2297	A
2	A3	2300	G
2	A3	2309	A
2	A3	2315	A
2	A3	2322	C
2	A3	2324	U
2	A3	2331	C
2	A3	2332	C
2	A3	2342	U
2	A3	2345	G
2	A3	2349	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	2384	A
2	A3	2387	U

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Mol	Chain	Res	Type
2	A3	2390	A
2	A3	2393	C
2	A3	2396	C
2	A3	2397	C
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
2	A3	2426	C
2	A3	2427	C
2	A3	2434	A
2	A3	2435	G
2	A3	2443	C
2	A3	2444	A
2	A3	2446	A
2	A3	2447	A
2	A3	2449	G
2	A3	2455	U
2	A3	2458	A
2	A3	2464	G
2	A3	2478	G
2	A3	2485	U
2	A3	2493	C
2	A3	2500	A
2	A3	2506	A
2	A3	2507	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	2526	C
2	A3	2527	A
2	A3	2530	A

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Mol	Chain	Res	Type
2	A3	2531	U
2	A3	2532	U
2	A3	2536	G
2	A3	2539	A
2	A3	2540	C
2	A3	2544	C
2	A3	2546	G
2	A3	2556	A
2	A3	2557	C
2	A3	2558	A
2	A3	2559	U
2	A3	2560	G
2	A3	2563	U
2	A3	2569	C
2	A3	2570	C
2	A3	2581	A
2	A3	2582	A
2	A3	2586	U
2	A3	2587	G
2	A3	2588	C
2	A3	2592	G
2	A3	2593	G
2	A3	2594	U
2	A3	2596	G
2	A3	2600	A
2	A3	2601	A
2	A3	2603	C
2	A3	2607	U
2	A3	2618	U
2	A3	2626	U
2	A3	2629	A
2	A3	2632	A
2	A3	2633	A
2	A3	2634	U
2	A3	2635	G
2	A3	2644	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

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Mol	Chain	Res	Type
2	A3	2661	U
2	A3	2676	A
2	A3	2684	C
2	A3	2686	G
2	A3	2694	A
2	A3	2695	G
2	A3	2696	A
2	A3	2697	G
2	A3	2706	A
2	A3	2708	C
2	A3	2709	A
2	A3	2713	C
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	2732	G
2	A3	2733	G
2	A3	2739	U
2	A3	2740	A
2	A3	2745	A
2	A3	2746	U
2	A3	2749	A
2	A3	2750	U
2	A3	2753	A
2	A3	2755	A
2	A3	2757	A
2	A3	2758	G
2	A3	2761	C
2	A3	2762	C
2	A3	2763	U
2	A3	2764	A
2	A3	2765	A
2	A3	2766	C
2	A3	2767	A
2	A3	2768	A
2	A3	2769	A
2	A3	2770	C
2	A3	2773	A
2	A3	2774	C

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Mol	Chain	Res	Type
2	A3	2775	A
2	A3	2776	G
2	A3	2777	G
2	A3	2778	U
2	A3	2779	C
2	A3	2780	C
2	A3	2781	U
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	2804	A
2	A3	2810	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	2851	A
2	A3	2854	U
2	A3	2861	A
2	A3	2864	U
2	A3	2865	C
2	A3	2869	A
2	A3	2870	G
2	A3	2871	U
2	A3	2872	C
2	A3	2879	A
2	A3	2881	C
2	A3	2892	A
2	A3	2901	A
2	A3	2906	C
2	A3	2909	G
2	A3	2910	A
2	A3	2913	A
2	A3	2916	G
2	A3	2917	G

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Mol	Chain	Res	Type
2	A3	2918	A
2	A3	2919	A
2	A3	2922	A
2	A3	2925	U
2	A3	2926	A
2	A3	2928	C
2	A3	2932	G
2	A3	2934	G
2	A3	2935	A
2	A3	2936	U
2	A3	2937	A
2	A3	2938	A
2	A3	2955	U
2	A3	2956	A
2	A3	2963	A
2	A3	2965	A
2	A3	2978	U
2	A3	2981	A
2	A3	2985	C
2	A3	2989	G
2	A3	2990	A
2	A3	2991	U
2	A3	2992	G
2	A3	2994	U
2	A3	2998	U
2	A3	3001	G
2	A3	3005	A
2	A3	3016	G
2	A3	3017	C
2	A3	3022	G
2	A3	3029	A
2	A3	3041	U
2	A3	3042	U
2	A3	3051	A
2	A3	3053	A
2	A3	3054	G
2	A3	3056	C
2	A3	3059	A
2	A3	3060	C
2	A3	3069	A
2	A3	3070	G
2	A3	3071	U

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Mol	Chain	Res	Type
2	A3	3077	C
2	A3	3084	A
2	A3	3086	U
2	A3	3089	A
2	A3	3093	C
2	A3	3095	G
2	A3	3096	U
2	A3	3100	U
2	A3	3102	U
2	A3	3109	U
2	A3	3114	U
2	A3	3123	G
2	A3	3129	A
2	A3	3135	A
2	A3	3141	A
2	A3	3147	G
2	A3	3150	U
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
2	A3	3172	C
2	A3	3180	A
2	A3	3184	C
2	A3	3189	C
2	A3	3190	A
2	A3	3202	U
2	A3	3204	C
2	A3	3206	C
2	A3	3207	A
2	A3	3217	A
2	A3	3218	A
2	A3	3221	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

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Mol	Chain	Res	Type
3	B3	1614	U
3	B3	1615	A
3	B3	1625	A
3	B3	1630	A
3	B3	1632	U
3	B3	1634	A
3	B3	1641	G
3	B3	1644	G
3	B3	1645	A
3	B3	1646	U
3	B3	1650	A
3	B3	1665	C
3	B3	1667	C
3	B3	1669	G
84	A6	654	U
84	A6	655	A
84	A6	662	G
84	A6	665	C
84	A6	675	U
84	A6	677	U
84	A6	678	U
84	A6	684	U
84	A6	692	A
84	A6	693	U
84	A6	694	U
84	A6	708	U
84	A6	715	U
84	A6	716	C
84	A6	722	A
84	A6	725	U
84	A6	726	C
84	A6	738	C
84	A6	745	A
84	A6	749	A
84	A6	757	A
84	A6	761	A
84	A6	762	U
84	A6	765	A
84	A6	768	A
84	A6	770	G
84	A6	777	U
84	A6	781	G

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Mol	Chain	Res	Type
84	A6	787	A
84	A6	795	G
84	A6	797	C
84	A6	798	U
84	A6	800	G
84	A6	811	A
84	A6	812	C
84	A6	817	A
84	A6	818	A
84	A6	819	C
84	A6	820	A
84	A6	821	G
84	A6	831	A
84	A6	833	C
84	A6	834	U
84	A6	836	U
84	A6	839	C
84	A6	840	A
84	A6	851	G
84	A6	857	C
84	A6	860	A
84	A6	870	A
84	A6	872	C
84	A6	874	C
84	A6	884	C
84	A6	885	A
84	A6	887	U
84	A6	890	C
84	A6	894	C
84	A6	895	C
84	A6	897	G
84	A6	901	C
84	A6	903	G
84	A6	907	U
84	A6	908	C
84	A6	909	A
84	A6	923	A
84	A6	942	A
84	A6	943	A
84	A6	945	G
84	A6	946	A
84	A6	947	G

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Mol	Chain	Res	Type
84	A6	951	U
84	A6	952	U
84	A6	954	A
84	A6	957	U
84	A6	959	A
84	A6	970	A
84	A6	971	A
84	A6	982	A
84	A6	992	G
84	A6	996	U
84	A6	1000	A
84	A6	1005	C
84	A6	1006	C
84	A6	1014	A
84	A6	1015	C
84	A6	1018	A
84	A6	1019	A
84	A6	1026	A
84	A6	1032	G
84	A6	1045	A
84	A6	1046	U
84	A6	1050	A
84	A6	1052	C
84	A6	1054	C
84	A6	1069	C
84	A6	1085	U
84	A6	1086	A
84	A6	1102	C
84	A6	1106	A
84	A6	1107	A
84	A6	1109	C
84	A6	1110	C
84	A6	1113	A
84	A6	1125	A
84	A6	1127	C
84	A6	1129	A
84	A6	1130	A
84	A6	1133	U
84	A6	1142	G
84	A6	1146	A
84	A6	1155	C
84	A6	1158	A

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Mol	Chain	Res	Type
84	A6	1171	A
84	A6	1179	G
84	A6	1183	G
84	A6	1184	U
84	A6	1189	C
84	A6	1191	U
84	A6	1192	A
84	A6	1193	U
84	A6	1194	C
84	A6	1196	C
84	A6	1197	U
84	A6	1198	C
84	A6	1212	U
84	A6	1218	A
84	A6	1219	U
84	A6	1224	A
84	A6	1225	A
84	A6	1226	A
84	A6	1227	C
84	A6	1229	C
84	A6	1232	A
84	A6	1233	U
84	A6	1234	C
84	A6	1235	A
84	A6	1236	A
84	A6	1240	C
84	A6	1249	U
84	A6	1250	U
84	A6	1251	G
84	A6	1252	C
84	A6	1254	C
84	A6	1255	A
84	A6	1261	U
84	A6	1265	C
84	A6	1268	C
84	A6	1269	C
84	A6	1274	U
84	A6	1275	C
84	A6	1276	A
84	A6	1280	A
84	A6	1286	G
84	A6	1287	A

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Mol	Chain	Res	Type
84	A6	1288	U
84	A6	1289	G
84	A6	1291	A
84	A6	1294	C
84	A6	1296	A
84	A6	1297	C
84	A6	1299	A
84	A6	1300	A
84	A6	1301	G
84	A6	1304	A
84	A6	1311	G
84	A6	1330	A
84	A6	1331	G
84	A6	1332	G
84	A6	1334	C
84	A6	1336	A
84	A6	1345	C
84	A6	1346	C
84	A6	1347	A
84	A6	1348	U
84	A6	1356	C
84	A6	1357	A
84	A6	1358	A
84	A6	1359	G
84	A6	1360	A
84	A6	1371	A
84	A6	1372	U
84	A6	1373	U
84	A6	1380	C
84	A6	1381	C
84	A6	1382	C
84	A6	1385	A
84	A6	1394	A
84	A6	1397	G
84	A6	1406	A
84	A6	1420	A
84	A6	1424	U
84	A6	1426	G
84	A6	1428	U
84	A6	1434	A
84	A6	1441	U
84	A6	1451	G

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Mol	Chain	Res	Type
84	A6	1452	U
84	A6	1456	U
84	A6	1458	G
84	A6	1465	A
84	A6	1466	G
84	A6	1469	C
84	A6	1470	C
84	A6	1473	G
84	A6	1485	C
84	A6	1486	A
84	A6	1490	C
84	A6	1507	G
84	A6	1516	A
84	A6	1519	G
84	A6	1521	A
84	A6	1525	U
84	A6	1529	C
84	A6	1530	U
84	A6	1531	A
84	A6	1536	C
84	A6	1537	C
84	A6	1539	U
84	A6	1540	A
84	A6	1541	C
84	A6	1542	G
84	A6	1543	C
84	A6	1544	A
84	A6	1551	U
84	A6	1553	G
84	A6	1556	G
84	A6	1559	A
84	A6	1561	A
84	A6	1562	A
84	A6	1563	G
84	A6	1566	G
84	A6	1567	U
84	A6	1568	A
84	A6	1572	U
84	A6	1575	U
84	A6	1576	A
84	A6	1586	G
84	A6	1588	A

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Mol	Chain	Res	Type
84	A6	1589	A
84	A6	1598	G
84	A6	1599	G
84	A6	1603	A
84	A6	1604	A
85	24	2	U
85	24	3	U
85	24	7	G
85	24	8	U
85	24	9	A
85	24	12	U
85	24	13	U
85	24	14	A
85	24	16	A
85	24	17	U
85	24	18	U
85	24	19	A
85	24	20	U
85	24	21	C
85	24	22	A
85	24	27	A
85	24	28	A
85	24	29	G
85	24	31	C
85	24	32	A
85	24	33	C
85	24	38	A
85	24	40	U
85	24	41	G
85	24	45	A
85	24	46	G
85	24	47	A
85	24	50	A
85	24	51	G
85	24	52	C
85	24	55	C
85	24	56	A
85	24	57	C
85	24	58	A
85	24	59	G
85	24	60	C
85	24	62	C

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Mol	Chain	Res	Type
85	24	67	A
85	24	71	C
85	24	73	A
86	i4	17	A
86	i4	22	A
86	i4	23	A
86	i4	24	A
85	C	2	U
85	C	3	U
85	C	7	G
85	C	8	U
85	C	9	A
85	C	12	U
85	C	13	U
85	C	14	A
85	C	16	A
85	C	17	U
85	C	18	U
85	C	19	A
85	C	20	U
85	C	21	C
85	C	22	A
85	C	27	A
85	C	28	A
85	C	29	G
85	C	31	C
85	C	32	A
85	C	33	C
85	C	38	A
85	C	40	U
85	C	41	G
85	C	45	A
85	C	46	G
85	C	47	A
85	C	50	A
85	C	51	G
85	C	52	C
85	C	55	C
85	C	56	A
85	C	57	C
85	C	58	A
85	C	59	G

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Mol	Chain	Res	Type
85	C	60	C
85	C	62	C
85	C	67	A
85	C	71	C
85	C	73	A

All (48) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	A3	1703	C
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	2523	C
2	A3	2530	A
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	2905	A
2	A3	2989	G
2	A3	3041	U
2	A3	3092	U
2	A3	3201	A
3	B3	1607	U
84	A6	721	G
84	A6	797	C
84	A6	818	A

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Mol	Chain	Res	Type
84	A6	886	A
84	A6	906	G
84	A6	1025	U
84	A6	1045	A
84	A6	1170	A
84	A6	1193	U
84	A6	1249	U
84	A6	1250	U
84	A6	1335	A
84	A6	1419	G
84	A6	1433	C
84	A6	1538	C
84	A6	1541	C
85	24	1	G
85	C	1	G

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 146 ligands modelled in this entry, 141 are monoatomic - leaving 5 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	$\#\|Z\| > 2$
91	GDP	X6	500	-	24,30,30	1.01	1 (4%)	30,47,47	1.46	6 (20%)
92	SO4	n	301	-	4,4,4	0.14	0	6,6,6	0.08	0
93	MLI	n	303	-	6,6,6	1.27	0	7,7,7	1.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
93	MLI	n	302	-	6,6,6	1.22	0	7,7,7	1.19	0
93	MLI	n	304	-	6,6,6	1.39	0	7,7,7	1.22	0

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
91	GDP	X6	500	-	-	6/12/32/32	0/3/3/3
93	MLI	n	302	-	-	2/4/4/4	-
93	MLI	n	304	-	-	2/4/4/4	-
93	MLI	n	303	-	-	4/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
91	X6	500	GDP	C6-N1	-2.97	1.33	1.37

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
91	X6	500	GDP	PA-O3A-PB	-4.16	118.57	132.83
91	X6	500	GDP	C3'-C2'-C1'	3.41	106.11	100.98
91	X6	500	GDP	C5-C6-N1	2.83	118.95	113.95
91	X6	500	GDP	O6-C6-C5	-2.31	119.85	124.37
91	X6	500	GDP	C2-N1-C6	-2.08	121.28	125.10
91	X6	500	GDP	C8-N7-C5	2.02	106.85	102.99

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
91	X6	500	GDP	PA-O3A-PB-O2B
91	X6	500	GDP	PA-O3A-PB-O3B
91	X6	500	GDP	C5'-O5'-PA-O3A
91	X6	500	GDP	C3'-C4'-C5'-O5'
93	n	302	MLI	C2-C1-C3-O8
91	X6	500	GDP	O4'-C4'-C5'-O5'
93	n	302	MLI	C2-C1-C3-O9

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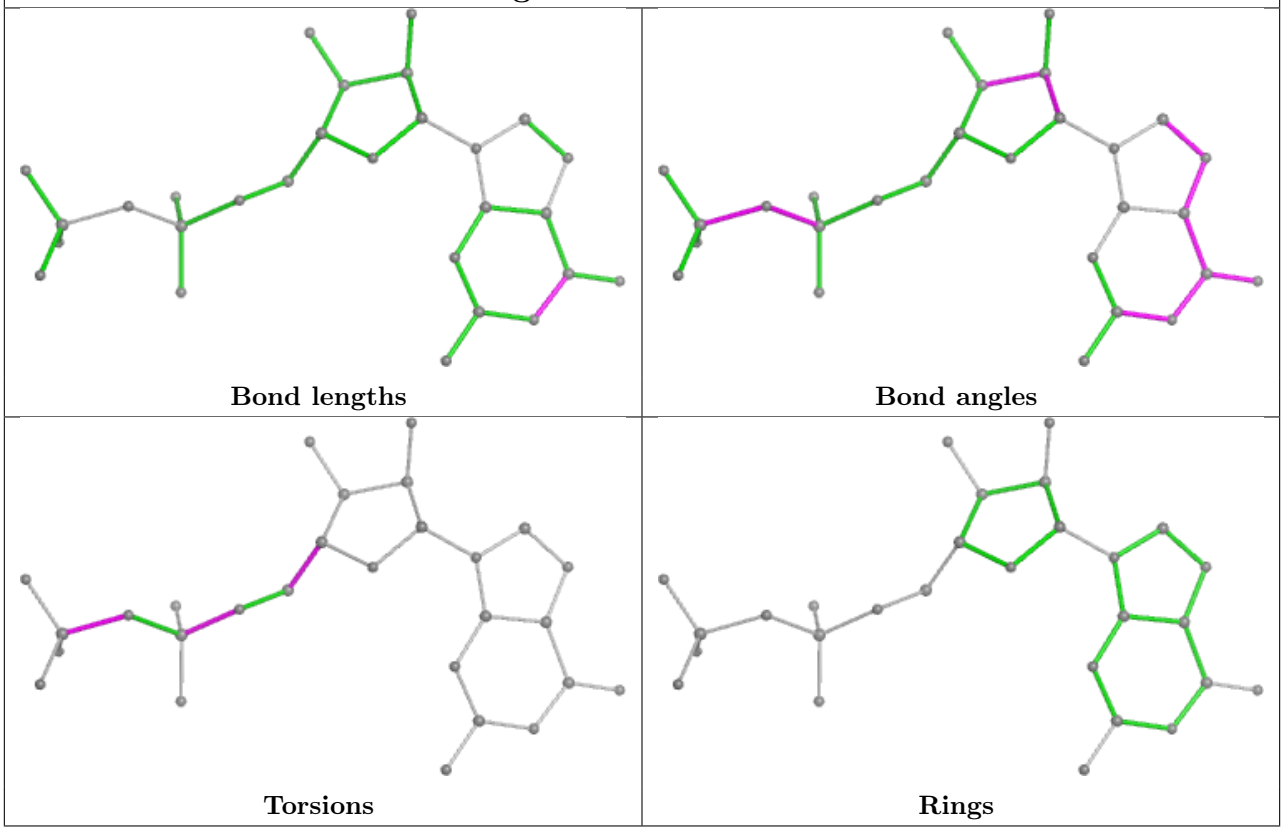
Mol	Chain	Res	Type	Atoms
93	n	304	MLI	C2-C1-C3-O8
91	X6	500	GDP	C5'-O5'-PA-O1A
93	n	303	MLI	C3-C1-C2-O6
93	n	304	MLI	C2-C1-C3-O9
93	n	303	MLI	C3-C1-C2-O7
93	n	303	MLI	C2-C1-C3-O8
93	n	303	MLI	C2-C1-C3-O9

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 then 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.

Ligand GDP X6 500



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
76	X6	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	X6	323:TYR	C	324:LEU	N	1.19

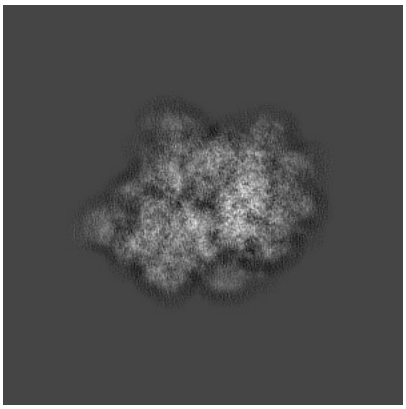
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11641. These allow visual inspection of the internal detail of the map and identification of artifacts.

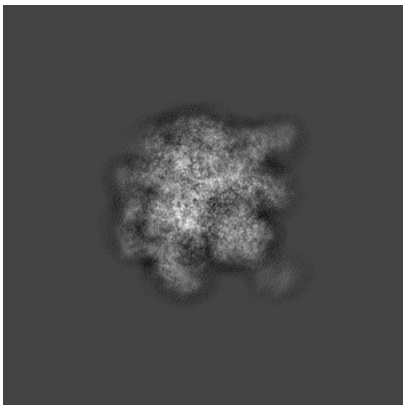
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

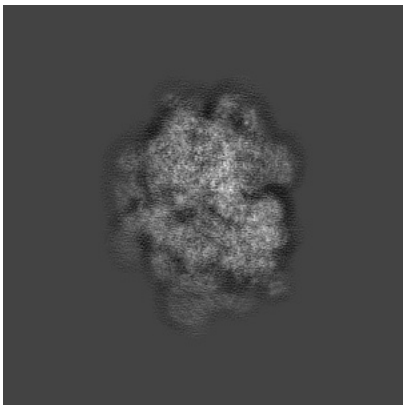
6.1.1 Primary map



X

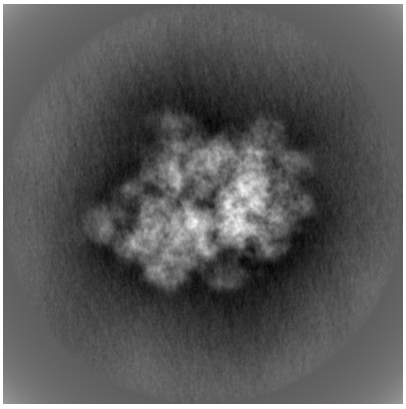


Y

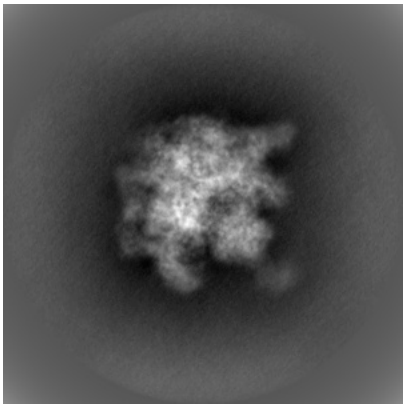


Z

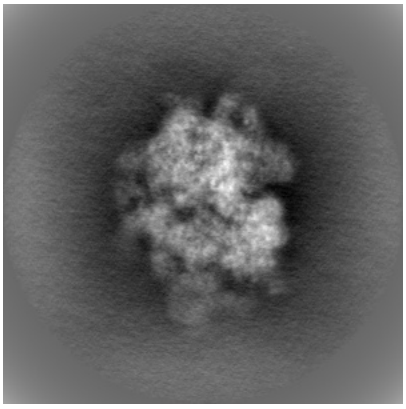
6.1.2 Raw map



X



Y

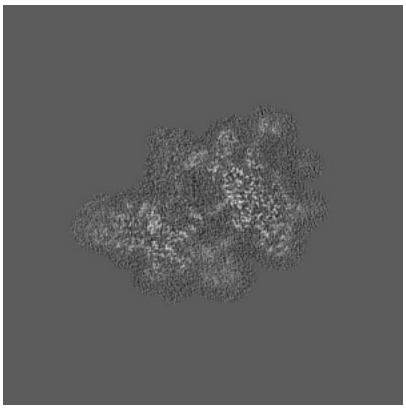


Z

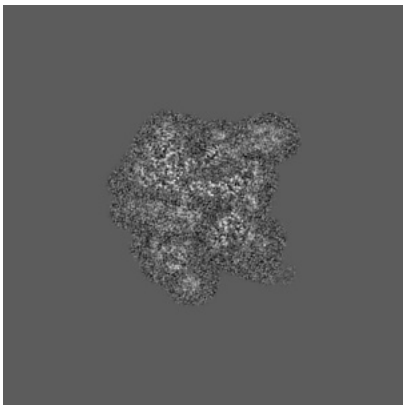
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

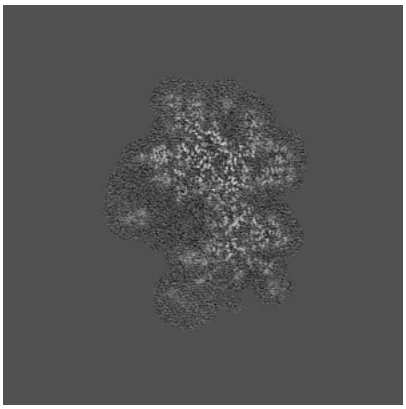
6.2.1 Primary map



X Index: 256

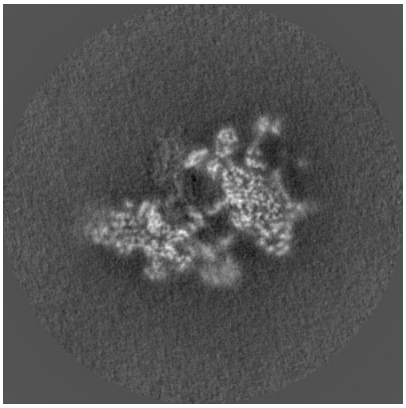


Y Index: 256

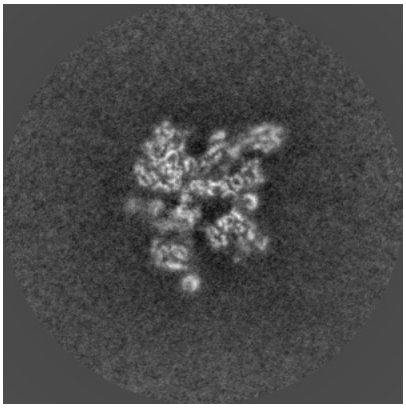


Z Index: 256

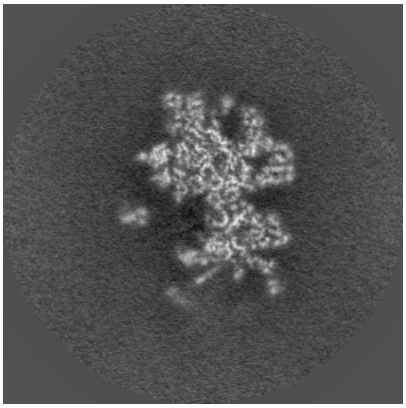
6.2.2 Raw map



X Index: 256



Y Index: 256

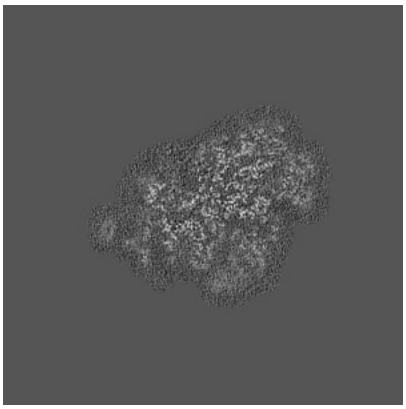


Z Index: 256

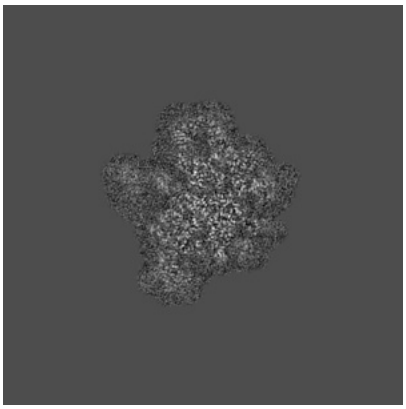
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

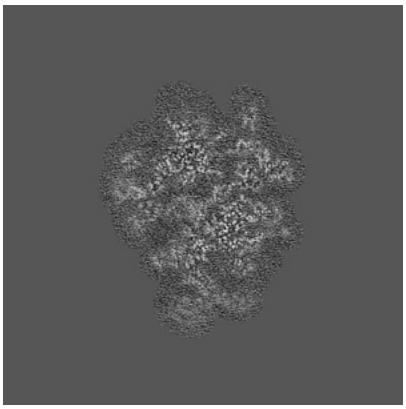
6.3.1 Primary map



X Index: 284

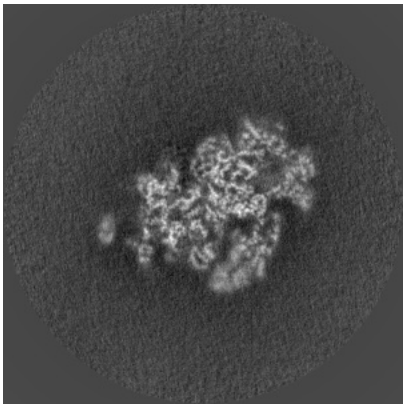


Y Index: 305

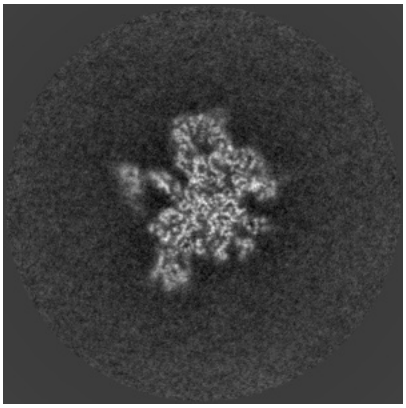


Z Index: 228

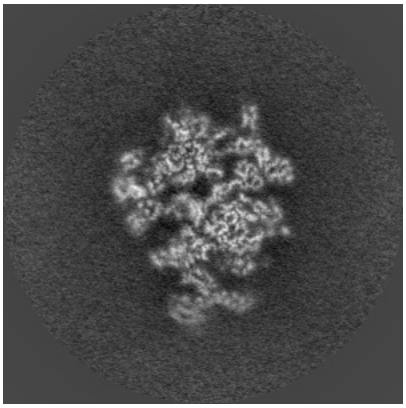
6.3.2 Raw map



X Index: 287



Y Index: 304

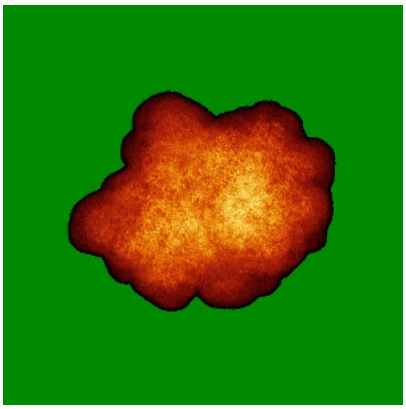


Z Index: 228

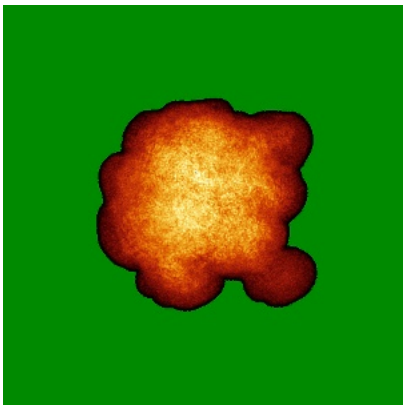
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

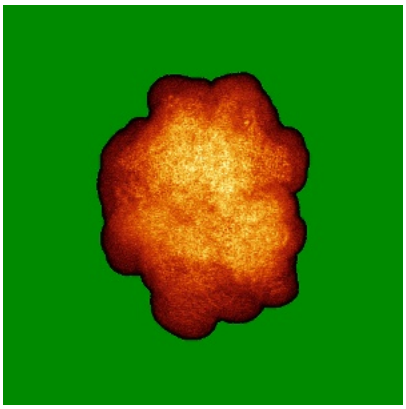
6.4.1 Primary map



X

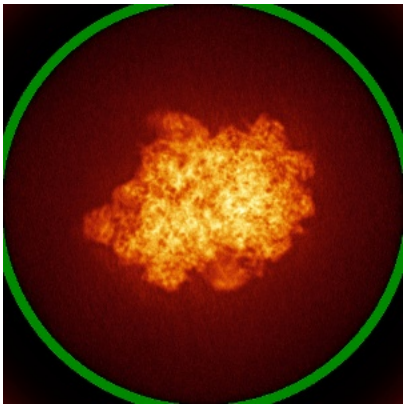


Y

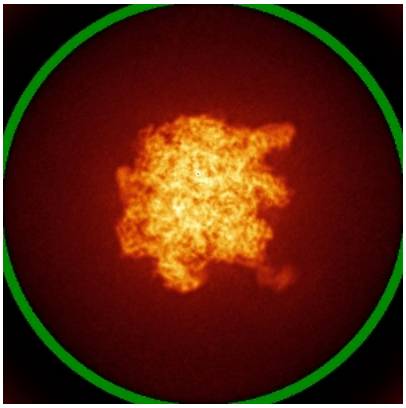


Z

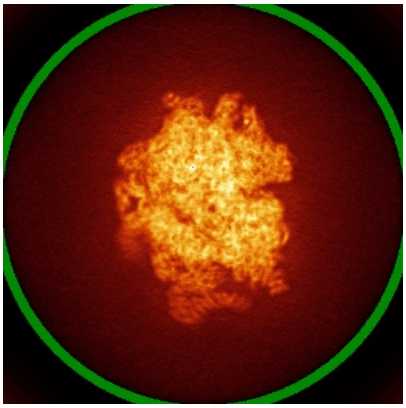
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

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

6.5.2 Raw map

X Y Z

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.

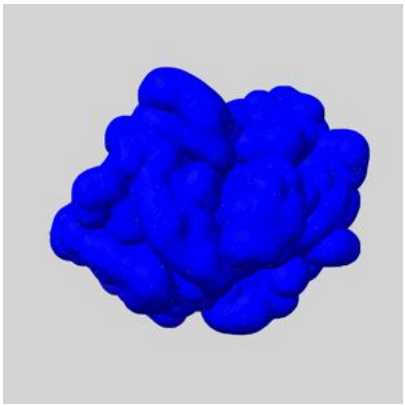
6.6 Mask visualisation

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

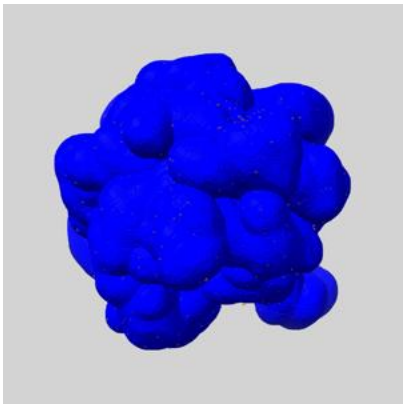
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

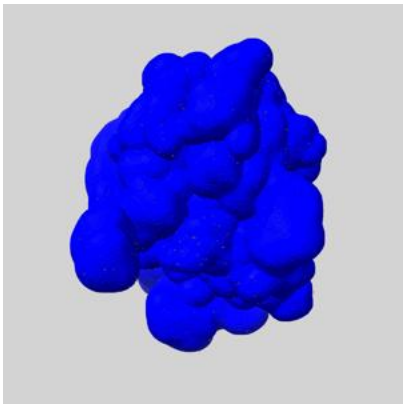
6.6.1 emd_11641_msk_1.map



X



Y

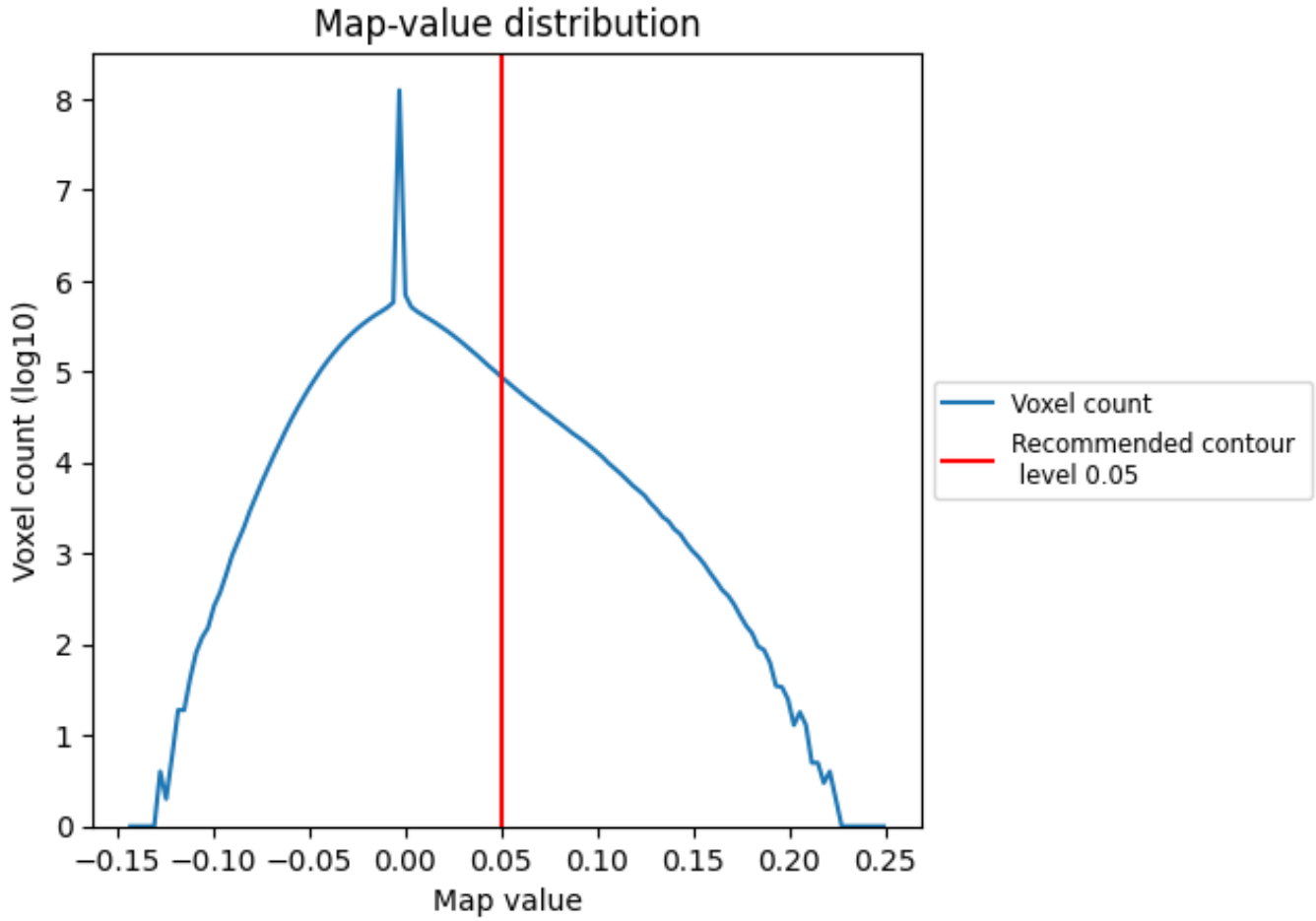


Z

7 Map analysis

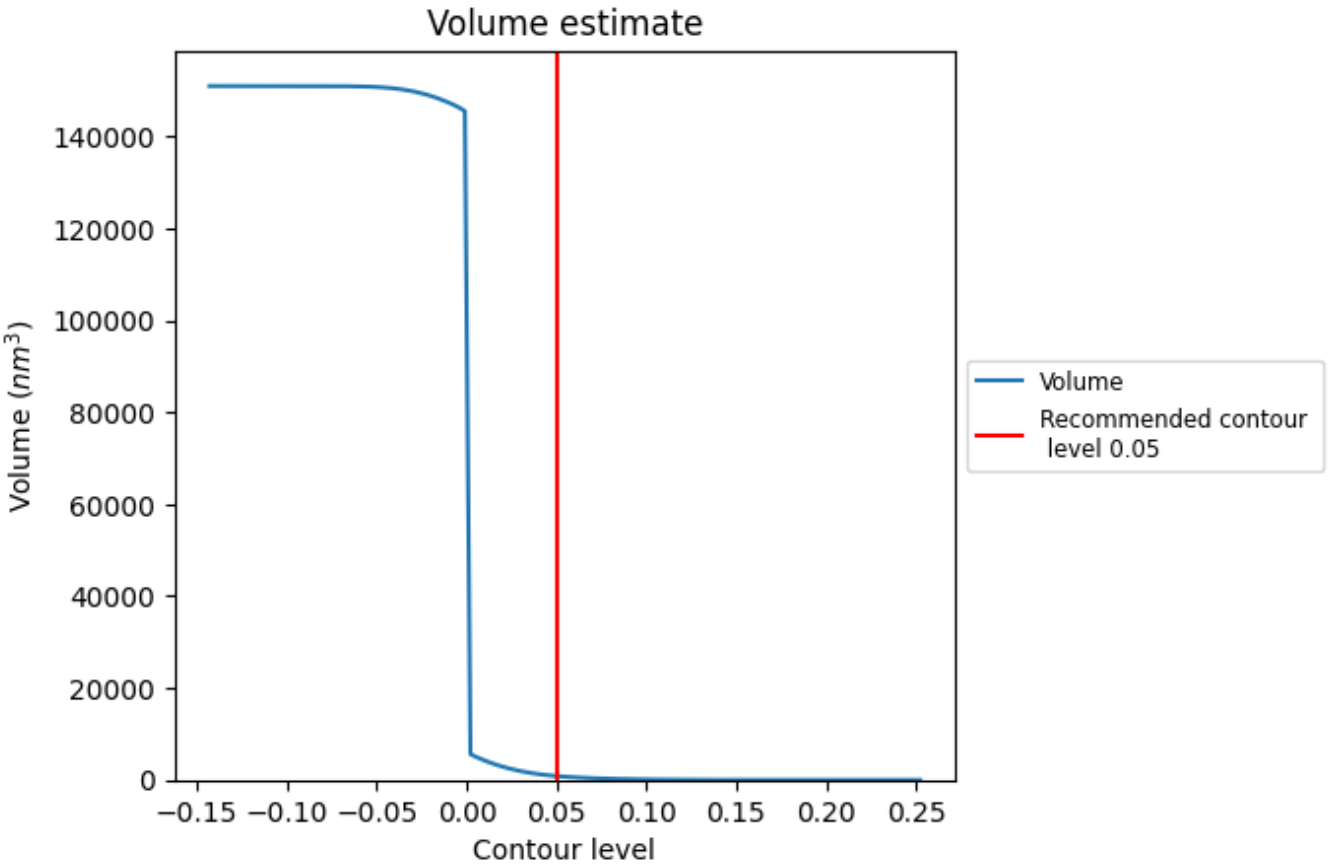
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

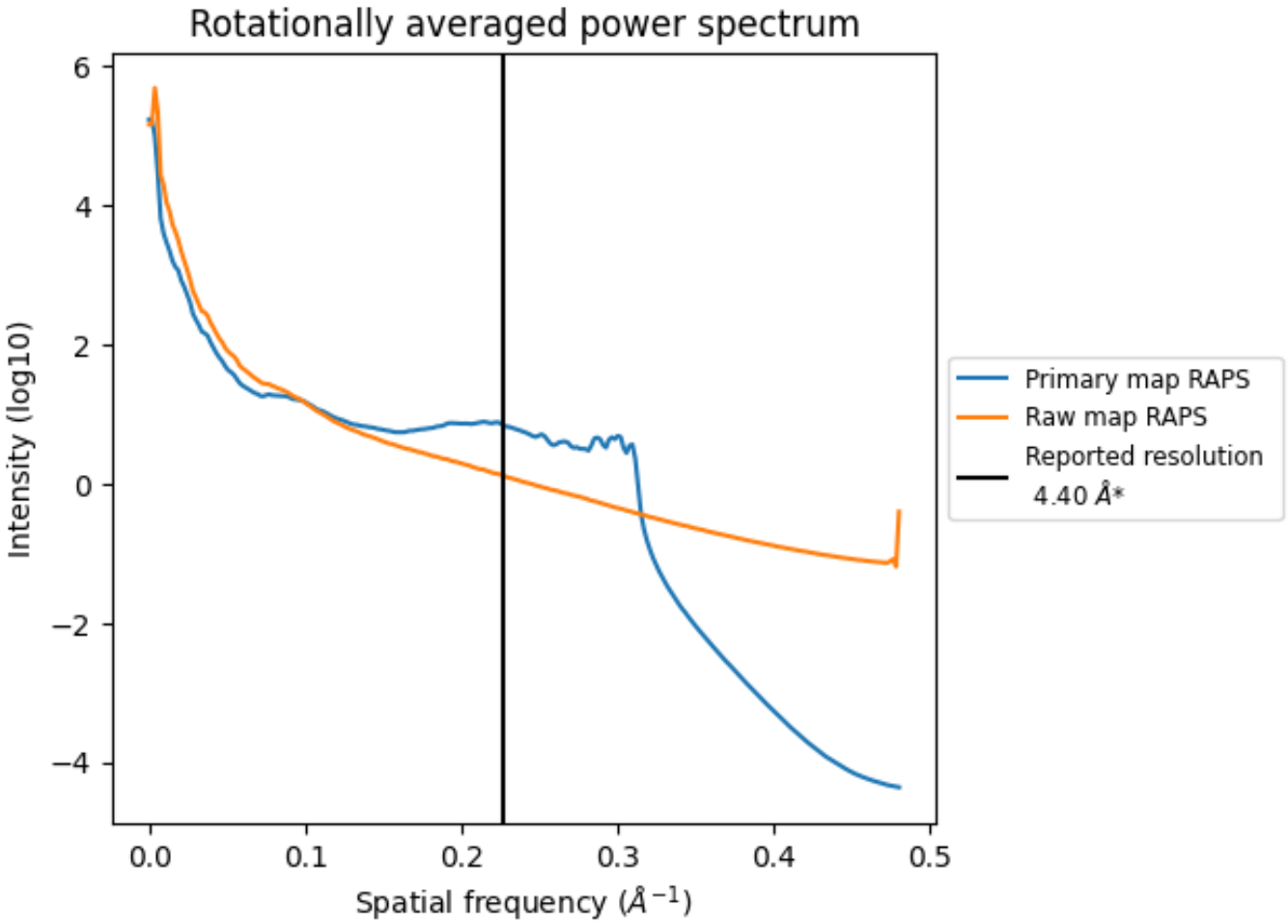
7.2 Volume estimate



The volume at the recommended contour level is 848 nm^3; this corresponds to an approximate mass of 766 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)

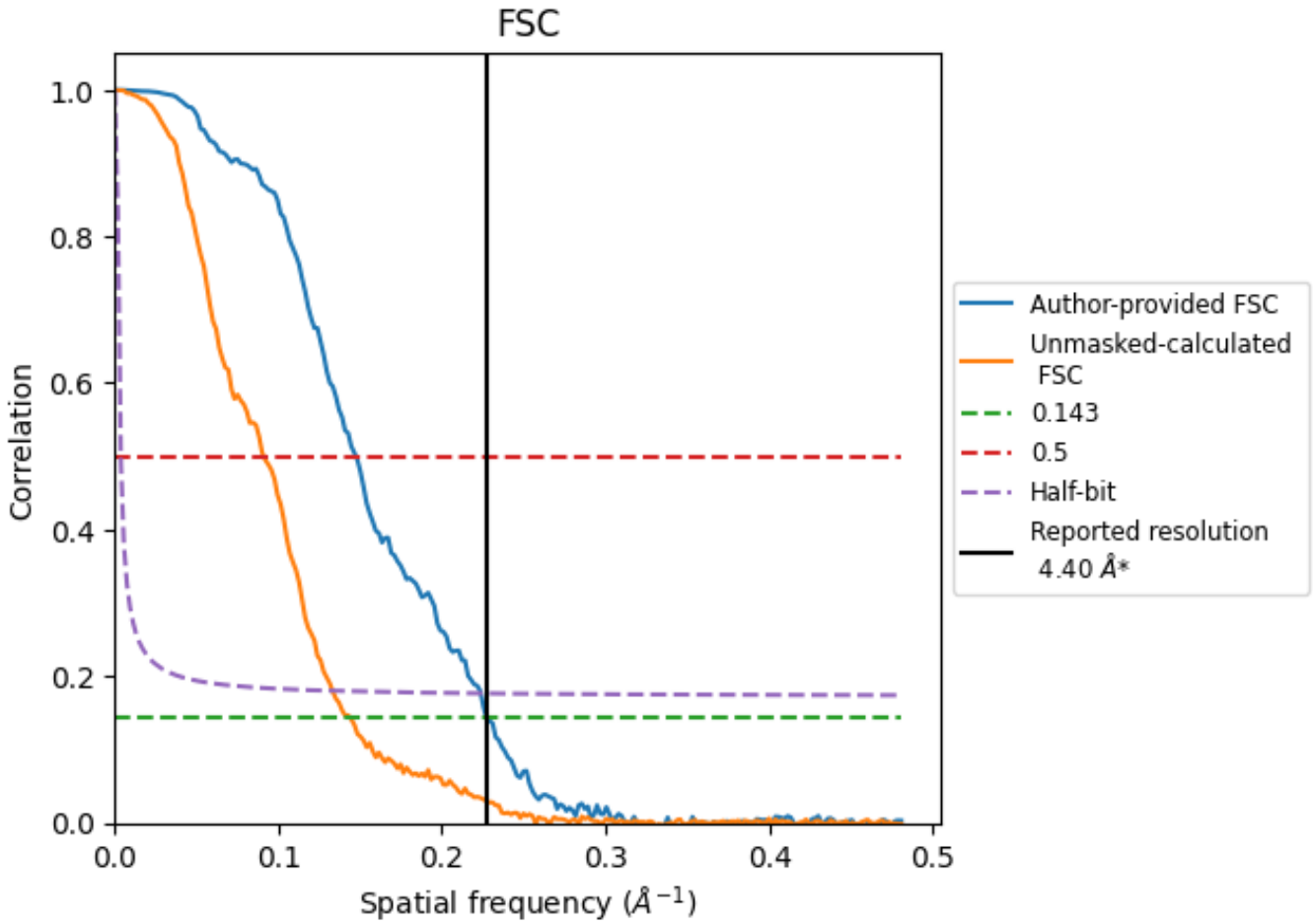


*Reported resolution corresponds to spatial frequency of 0.227 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.227 Å^{-1}

8.2 Resolution estimates (i)

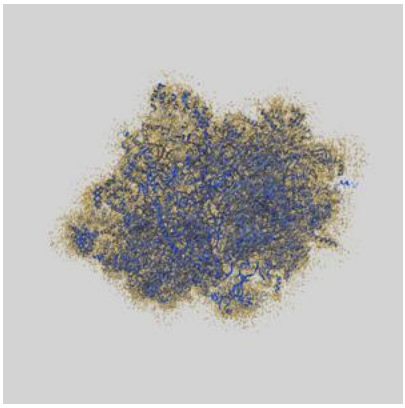
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	4.40	6.79	4.47
Unmasked-calculated*	6.94	10.98	7.51

*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 6.94 differs from the reported value 4.4 by more than 10 %

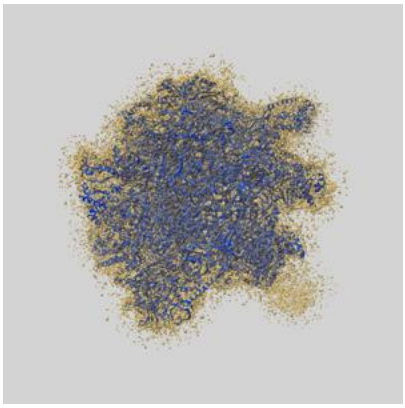
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-11641 and PDB model 7A5F. Per-residue inclusion information can be found in section 3 on page 24.

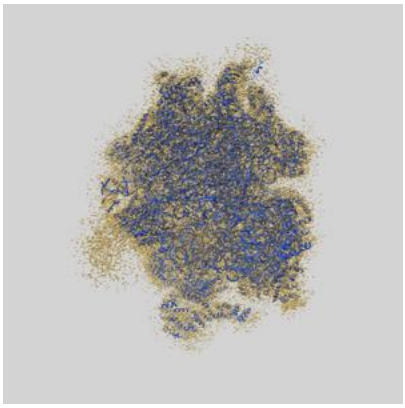
9.1 Map-model overlay



X



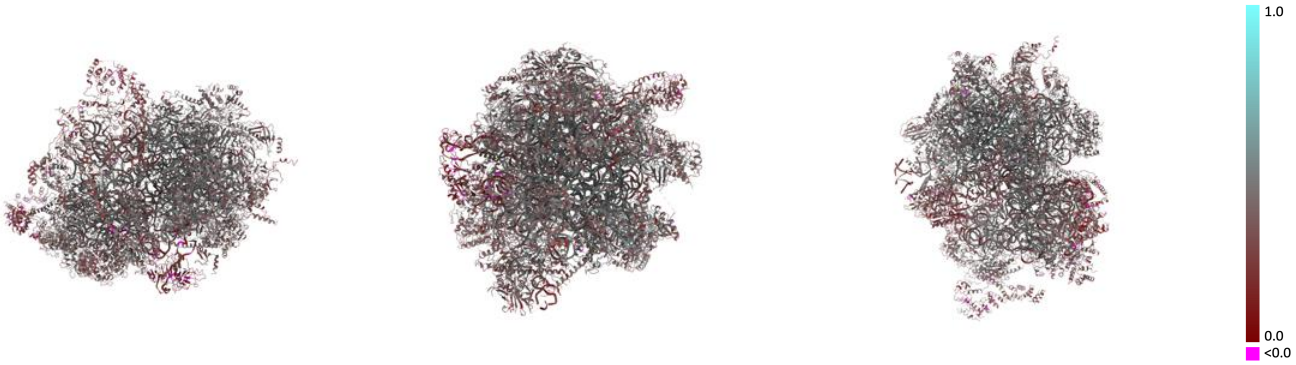
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05 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.

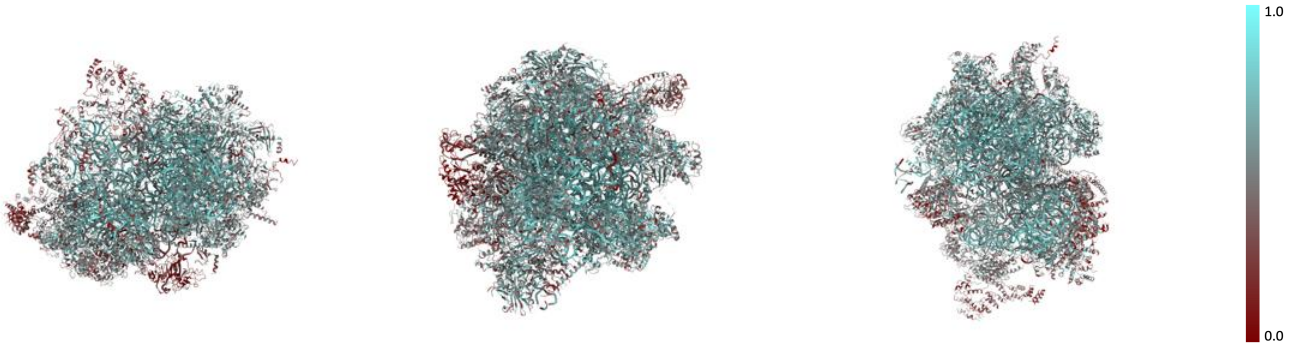
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

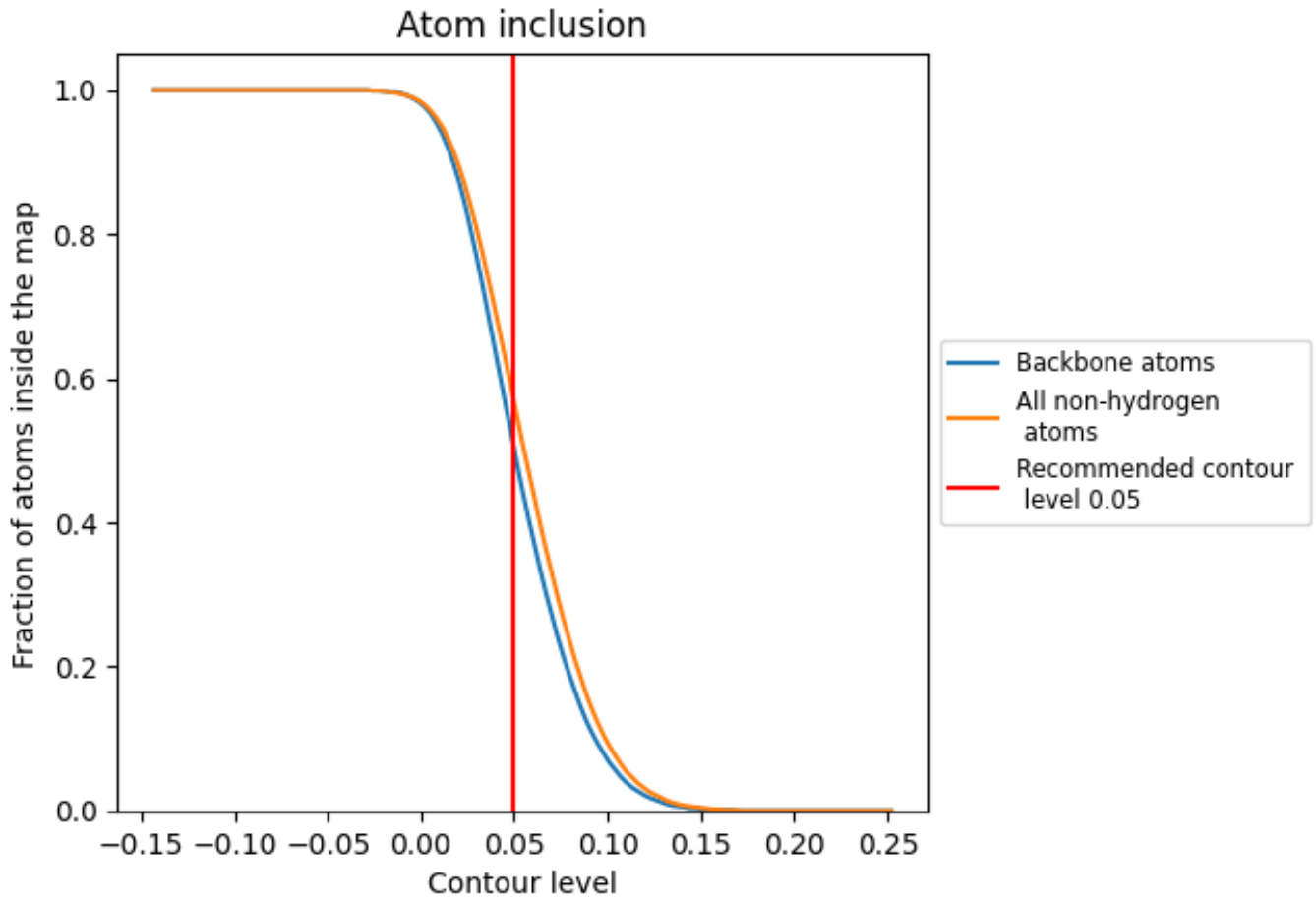
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).

9.4 Atom inclusion (i)



At the recommended contour level, 50% of all backbone atoms, 57% 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	Q-score
All	0.5660	0.3960
03	0.5800	0.4330
13	0.5550	0.4340
23	0.6500	0.4880
24	0.5310	0.2670
33	0.6530	0.4910
43	0.6290	0.4690
53	0.5730	0.4100
63	0.5550	0.3870
73	0.5180	0.3870
93	0.5250	0.4040
A	0.3020	0.2770
A3	0.7460	0.4360
A5	0.0000	0.1490
A6	0.7310	0.4150
B3	0.6420	0.3190
B6	0.5830	0.4280
C	0.1490	0.1190
C6	0.4840	0.4320
D	0.1790	0.1710
D3	0.6190	0.4630
D6	0.4970	0.4170
E3	0.5970	0.4410
E6	0.5130	0.4170
F3	0.5810	0.4360
F6	0.4340	0.3610
G6	0.4810	0.3910
H3	0.4510	0.3800
H6	0.4520	0.3750
I3	0.3960	0.3400
I6	0.4950	0.4050
J3	0.3000	0.2600
J6	0.5150	0.4290
K3	0.6330	0.4580
K6	0.5160	0.3940

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Chain	Atom inclusion	Q-score
L3	0.4920	0.4330
L6	0.5330	0.4060
M3	0.5850	0.4310
M6	0.4770	0.3710
N3	0.5810	0.4420
N6	0.5430	0.4240
O3	0.6030	0.4440
O6	0.4780	0.3580
P3	0.5770	0.4180
P6	0.5520	0.4210
Q3	0.5230	0.4270
Q6	0.5740	0.4310
R3	0.6380	0.4620
R6	0.4430	0.3440
S3	0.6110	0.4470
S6	0.4570	0.3620
T3	0.5830	0.4560
T6	0.5150	0.4150
U3	0.6380	0.4570
U6	0.4560	0.3390
V3	0.4690	0.3680
V6	0.2860	0.2600
W3	0.6290	0.4860
W6	0.4850	0.3990
X3	0.5250	0.4050
X6	0.4180	0.3240
Y2	0.2210	0.2810
Y3	0.5730	0.4160
Y6	0.3670	0.3290
Z3	0.6320	0.4610
Z6	0.4570	0.3840
a3	0.6060	0.4410
a6	0.3840	0.3250
b3	0.6060	0.4380
b6	0.3810	0.3310
c3	0.5480	0.4080
c6	0.4510	0.4040
d3	0.4930	0.3830
d6	0.5450	0.4390
e3	0.3430	0.3000
e6	0.2790	0.2730
f3	0.4370	0.3440

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Chain	Atom inclusion	Q-score
g3	0.5690	0.4180
h3	0.5020	0.3590
i3	0.6230	0.4580
i4	0.4520	0.3320
j3	0.5600	0.4200
k3	0.3350	0.2690
l3	0.5870	0.4110
m3	0.4820	0.3720
n	0.1000	0.2080
o3	0.6670	0.4720
p3	0.4550	0.3770
q3	0.4930	0.3780
r3	0.6370	0.4460
s3	0.6000	0.4270
t3	0.2930	0.2650